Machine Learning

moodle https://dl1.cuni.cz/course/view.php?id=5765

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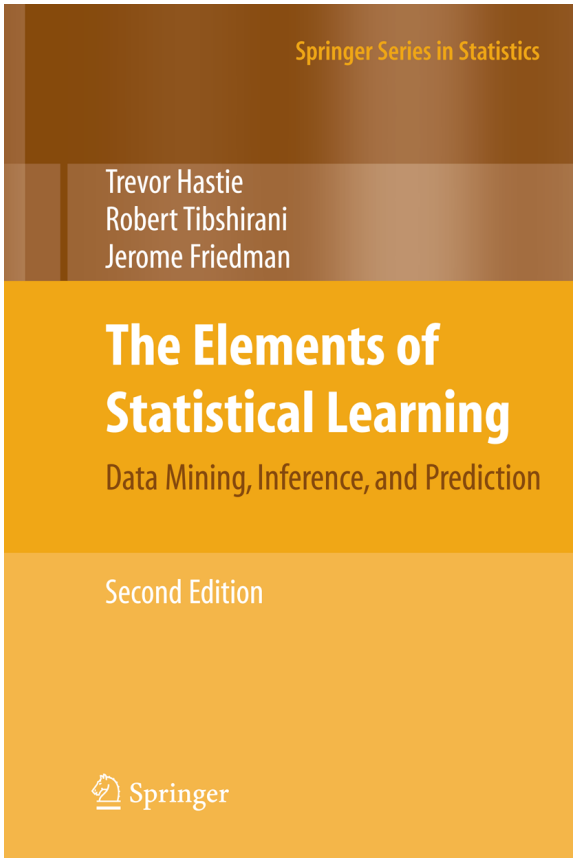
Literature



- T. Hastie, R. Tishirani, and J. Friedman. *The Elements of Statistical Learning, Data Mining, Inference and Prediction.* Springer Series in Statistics. Corrected 12th printing 2017 https://web.stanford.edu/ hastie/ElemStatLearn/printings/ESLII_print12_toc.pdf
- C. E. Rasmussen & C. K. I. Williams, Gaussian Processes for Machine Learning, the MIT Press, 2006
- Peter I. Frazier: A Tutorial on Bayesian Optimization, 2018
- Højsgaard, Søren, Edwards, David, Lauritzen, Steffen: Graphical Models with R, Springer 2012
- Gareth James, Daniela Witten, Trevor Hastie and Robert Tibshirani: *An Introduction to Statistical Learning with Applications in R* (2013)
- S. Russel and P. Norwig. Artificial Intelligence: A Modern Approach. Prentice Hall, 2003.

Exam

- Oral exam on topics covered by lectures.
- Most of it is covered by T. Hastie, R. Tishirani, and J. Friedman. *The Elements of Statistical Learning, Data Mining, Inference and Prediction.* Springer Series in Statistics. Corrected 12th printing 2017 https://web.stanford.edu/ hastie/ElemStatLearn/printings/ESLII_print12_toc.pdf

Table of Contens

Statistical Decision Theory (for Regression)

- Let $X \in \mathbb{R}^p$ denote a real valued random input vector, and $Y \in \mathbb{R}$ a real valued random output variable, with joint distribution $P(X, Y)$.
- We seek a function $f(X)$ for prediction Y given values of the input X.
- The theory requires a **loss function (chybovou funkci)** $L(Y, f(X))$ for penalizing errors in predictions.
- The far most common and convenient is **squared error loss (kvadratická chybová funkce)** $L(Y, f(X)) = (Y - f(X))^2$
- this leads us to a criterion for choosing f, the **expected (squared) prediction error (očekávanou chybu)** (EPE),

$$\begin{aligned} EPE(f) &= \mathbb{E}(Y - f(X))^2 \\ &= \int (y - f(x))^2 P(dx, dy) \end{aligned}$$

- by conditioning on X we get

$$EPE(f) = \mathbb{E}_X \mathbb{E}_{Y|X}([Y - f(X)]^2 | X)$$

- and we see that it suffices to minimize EPE poinwise:

$$f(x) = \text{argmin}_c \mathbb{E}_{Y|X}([Y - c]^2 | X = x).$$

- the solution is the conditional expectation also known as the **regression**

k-NN and Conditional Expectation

- We seek the conditional expectation:

$$f(x) \quad = \quad \mathbb{E}(Y|X = x).$$

- Thus the best prediction of Y at any point $X = x$ is the conditional mean, when the best is measured by the average squared error.
- Assume we have **a training set of data** $\mathcal{T} = \{(\mathbf{x}_i, y_i)\}_{i=1}^{N}$.
- The nearest neighbor methods attempt to directly implement this.
  - Since there are typically at most one observation at any point x, we settle for

$$\hat{f}(x) \quad = \quad mean(y_i|x \in N_k(x)),$$

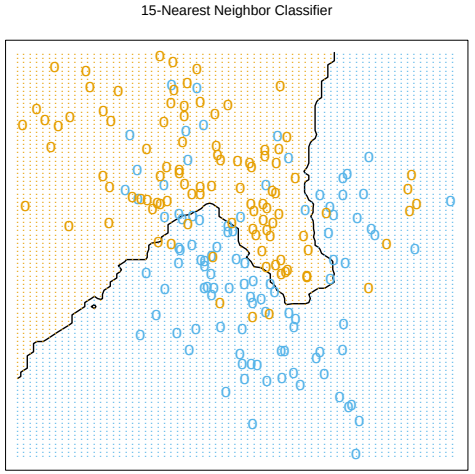
  - where *mean* denotes average, and $N_k(x)$ is the neighborhood containing k points in $\mathcal{T}$ closest to x.
- Under mild regularity conditions on $P(X, Y)$ one can show as $k, N \to \infty$, such that $\frac{k}{N} \to 0$ then $\hat{f}(x) \to \mathbb{E}(Y|X = x)$.
- **The rate of convergence decreases as the dimension increases**. The problem is the speed of the convergence.

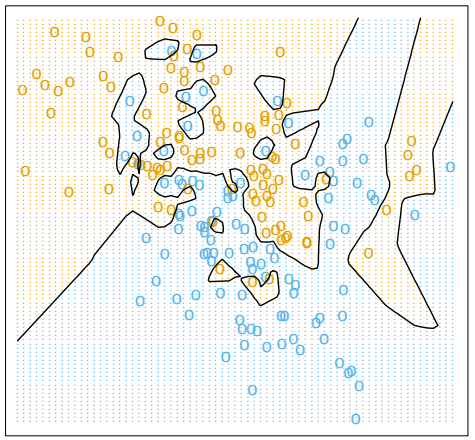
Nearest-Neighbor Methods

- The **nearest-neighbor methods** use those observations in the training set $\mathcal{T}$ closest in the input space to x to form $\hat{f}$.

$$\hat{f}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i$$

- In classification, majority vote is used.
- Figures correspond to 15 nearest neighbor and 1 nearest neighbor respectively.
- Training error (usually) increases with increasing k.





Effective number of parameters

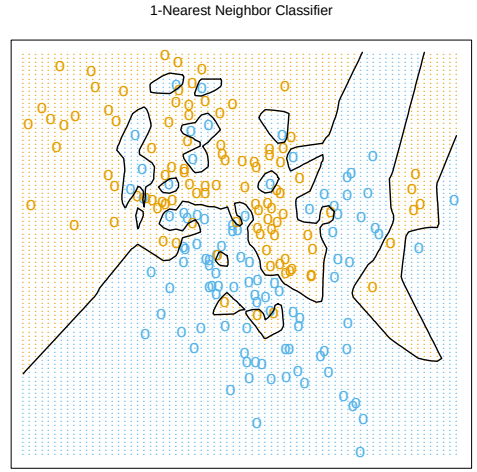
The effective number of parameters of k nearest neighbors is N/k and is generally bigger than p of the linear regression.

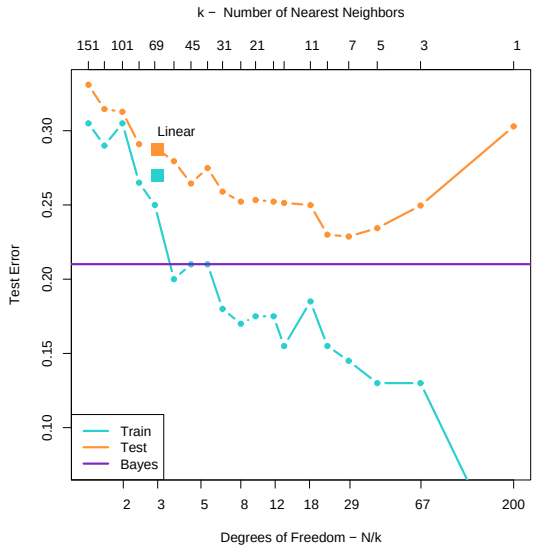
Prediction complexity

'Naive' $O(Np)$.

Overfitting

- Our goal is the minimal expected prediction error usually estimated by the error on the **test data** (orange).
- Usually, **overfitting** appears for complex models - an increase of the test error despite the decrease of the training error.
- This is the reason for other models then nearest neighbor model.
- Possible improvements:
  - Kernel methods
  - different weights for dimensions
  - local regression fits
  - linear models fit to a basis expansion
  - sums of non-linearly transformed linear models.

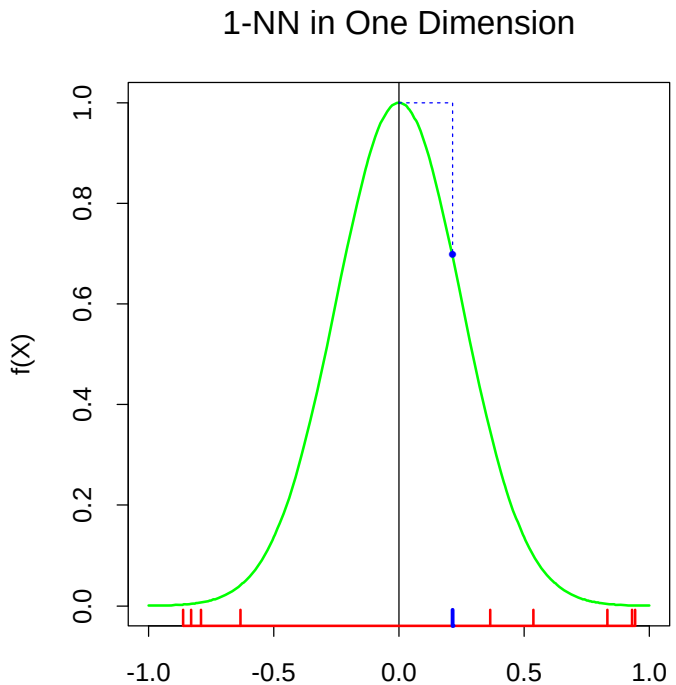


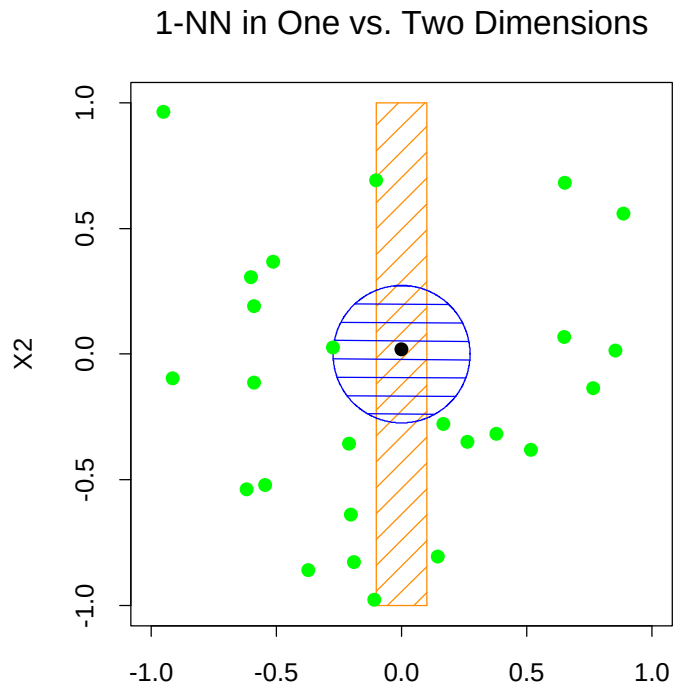


Curse of Dimensionality demonstration

Prediction

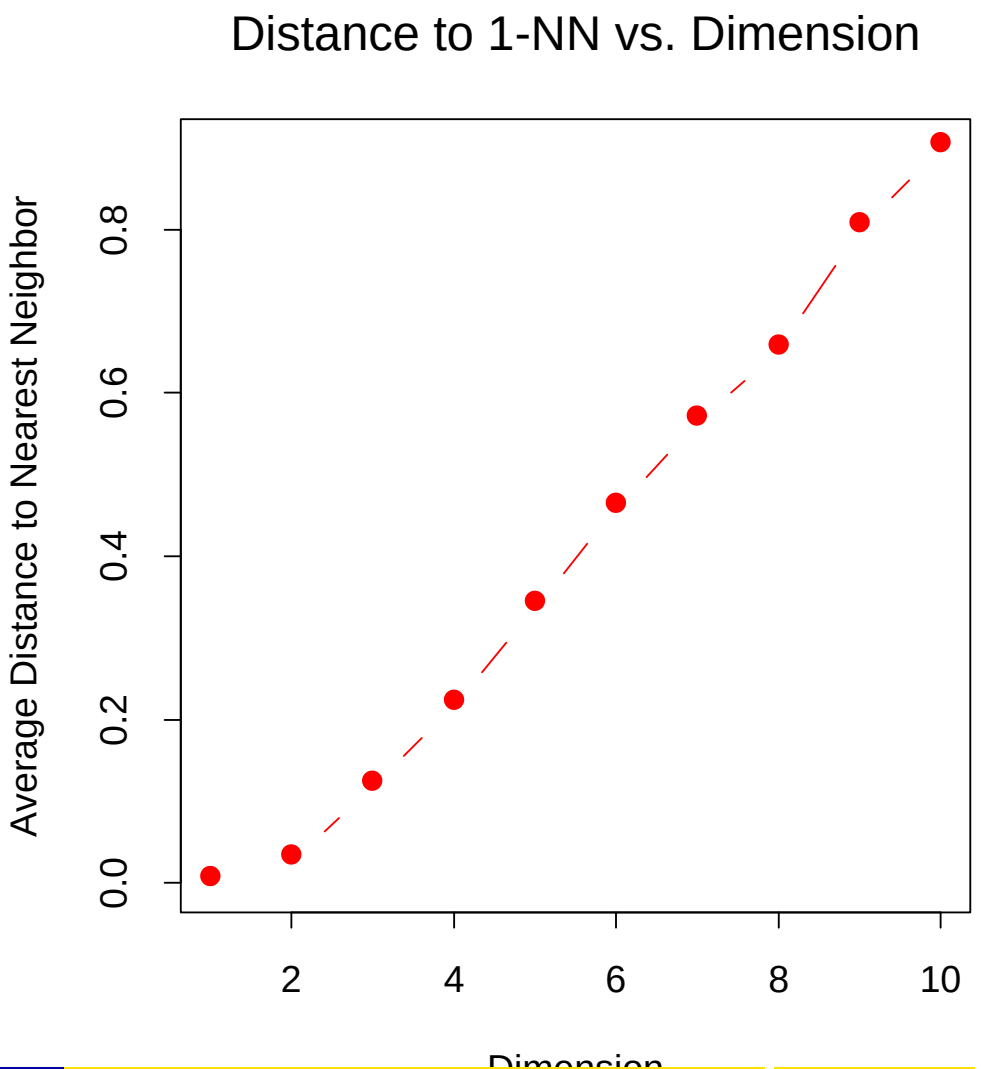
- Assume x_i uniformly generated form the interval $\langle -1, 1 \rangle^p$
- We have $Y = f(X) = e^{-8\|X\|^2}$, without any noise, for x_i we know exactly $f(x_i)$.
- We use 1–NN to estimate $f(0)$ based on 1000 data sample.
- Predicted value for $x = \langle 0, \ldots, 0 \rangle$ is lower that 1 and in high dimensions p it goes to 0.
- Increasing k in k–NN does not help here.





Empirical Nearest Neighbor Distance

- Assume x_i uniformly generated form the interval $\langle -1, 1 \rangle^p$
- We use 1–NN to estimate $f(0)$ based on 1000 data sample.



Curse of dimensionality

Most points are close to the border

- Consider N instances uniformly distributed in a p–dimensional unit ball.
- Median distance of the nearest neighbor from the center is:

$$d(p, N) = \left(1 - \frac{1}{2}^{\frac{1}{N}}\right)^{\frac{1}{p}}$$

- The formula: 1 point inside: $\frac{d^p}{1^p}$, outside: $(1 - d^p)$, N outside $(1 - d^p)^N = \frac{1}{2}$.
- For $N = 500$, $p = 10$, we get $d(p, N) \approx 0.52$, that is more than a half way to the border.
- For $N = 10^6$, $p = 200$, we get $d(p, N) \approx 0.93$.
- Close to the border, we must **extrapolate**, what is more difficult than interpolation.

Training data (and their notation)

We have

- a set of random variables (features) $X_1, \ldots, X_p$
- numerical goal variable Y (for regression)
- training data $\mathcal{T} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$

		Goal attribute
X^T = vector	$\langle X_1 \quad X_j \quad X_p \rangle$	Y or G
$\mathbf{x}_1^T$		
$\mathbf{x}_i^T$ = vector	$\langle x_1 \quad x_j \quad x_p \rangle$	y or g
$\mathbf{x}_N^T$		

  - x and $\mathbf{x}_i$ are p-dimensional column vectors
  - $\mathbf{X}$ is the $N \times p$ matrix
  - $\mathbf{x}_j$ is the N vector consisting of all observations on variable X_j.
- $\mathbf{y} = (y_1, \ldots, y_N)^T$ denotes the vector of training goal data.

Linear regression

- Given a vector of inputs $X^T = (X_1, \ldots, X_p)$ we predict the output Y via the model f_β, $\beta \in \mathbb{R}^{p+1}$

$$\hat{Y} = \hat{f}_\beta(X) = \hat{\beta}_0 + \sum_{j=1}^{p} X_j \hat{\beta}_j$$

- $\hat{\beta}_0$ is the **intercept, bias, (průsečík)**.
- We include the constant variable 1 to X, include $\hat{\beta}_0$ in $\hat{\beta}$ to get the model in vector form as an inner product

$$\hat{Y} = \sum_{j=0}^{p} X_j \hat{\beta}_j = \mathbf{X^T} \widehat{\beta}$$

- The sum $\sum_{j=0}^{p} X_j \hat{\beta}_j$ can be written as $\mathbf{X^T} \widehat{\beta}$.

Linear regression from the data

- Let i range over the data samples, $\mathbf{X}$ be an $N \times p$ data matrix, $\mathbf{y}$ is a column vector of the goal variable. We can write:

$$\hat{\mathbf{y}} = \mathbf{X}\beta$$

- We search optimal $\hat{\beta}$ to minimize the residual sum squares RSS:

$$RSS(\beta) = \sum_{i=1}^{N}(y_i - \mathbf{x}_i^T\beta)^2 = (\mathbf{y} - \mathbf{X}\beta)^{\mathbf{T}}(\mathbf{y} - \mathbf{X}\beta) \tag{1}$$

- Differentiating w.r.t. β we get *normal equations*

$$\mathbf{X}^{\mathbf{T}}(\mathbf{y} - \mathbf{X}\beta) = \mathbf{0}$$

- If $\mathbf{X}^{\mathbf{T}}\mathbf{X}$ is not singular, then the unique solution is given by

$$\hat{\beta} = (\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{y} \tag{2}$$

- For a given x_i the estimate $\hat{y}_i$ is $\hat{y}_i = \hat{y}(x_i) = x_i^T\hat{\beta}$.
- From a singular $\mathbf{X}^{\mathbf{T}}\mathbf{X}$ we should remove dependent features or filter the data to make it invertible.

Linear Regression

- Let us have a data $N = 6, p = 2$ (Fatt11, Meat11), 1 column is for β_0, does not count:

$$\mathbf{X} = \begin{array}{|cc|}\hline 1 & Fat11 & Meat11 \\ \hline 1 & 17 & 51 \\ 1 & 17 & 49 \\ 1 & 14 & 38 \\ 1 & 17 & 58 \\ 1 & 14 & 51 \\ 1 & 20 & 40 \\ \hline \end{array} \qquad \mathbf{y} = \begin{array}{|c|}\hline LeanMeat \\ \hline 56.5 \\ 57.6 \\ 55.9 \\ 61.8 \\ 63.0 \\ 54.6 \\ \hline \end{array}$$

- We are searching parameters $\beta = (\beta_0, \beta_1, \beta_2)^T$ to minimize:

$$\begin{aligned} RSS(\beta, \mathbf{X}, \mathbf{y}) &= \sum_{i=1}^{N} (y_i - \mathbf{x}_i^T \beta)^2 = (\mathbf{y} - \mathbf{X}\beta)^{\mathbf{T}} (\mathbf{y} - \mathbf{X}\beta) \\ &= (56.5 - (1 * \beta_0 + 17 * \beta_1 + 51 * \beta_2))^2 + \dots \\ &\quad \dots + (54.6 - (1 * \beta_0 + 20 * \beta_1 + 40 * \beta_2))^2 \end{aligned}$$

Linear regression from the data

- If $\mathbf{X}^{\mathbf{T}}\mathbf{X}$ is not singular, then the unique solution is given by

$$\hat{\beta} = (\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{y}$$

$$\mathbf{X}^{\mathbf{T}} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 17 & 17 & 14 & 17 & 14 & 20 \\ 51 & 49 & 38 & 58 & 51 & 40 \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} 1 & 17 & 51 \\ 1 & 17 & 49 \\ 1 & 14 & 38 \\ 1 & 17 & 58 \\ 1 & 14 & 51 \\ 1 & 20 & 40 \end{bmatrix}$$

$$\mathbf{X}^{\mathbf{T}}\mathbf{X} = \begin{bmatrix} 6 & 99 & 287 \\ 99 & 1659 & 4732 \\ 287 & 4732 & 14011 \end{bmatrix}$$

$$(\mathbf{X}^{\mathbf{T}}\mathbf{X})(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1} = \begin{bmatrix} 19.7320 & -0.6714120 & -0.1774305 \\ -0.6714 & 0.0392824 & 0.0004861 \\ -0.1774 & 0.0004861 & 0.0035416 \end{bmatrix}$$

Linear regression from the data

$$\hat{\beta} = (\mathbf{X}^\mathbf{T}\mathbf{X})^{-1}\mathbf{X}^\mathbf{T}\mathbf{y}$$

$$\mathbf{X}^\mathbf{T} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 17 & 17 & 14 & 17 & 14 & 20 \\ 51 & 49 & 38 & 58 & 51 & 40 \end{bmatrix} \qquad \mathbf{y} = \begin{bmatrix} 56.5 \\ 57.6 \\ 55.9 \\ 61.8 \\ 63.0 \\ 54.6 \end{bmatrix}$$

$$\mathbf{X}^\mathbf{T}\mathbf{y} = \begin{bmatrix} 349.3498 \\ 5746.1340 \\ 16807.4663 \end{bmatrix}$$

$$\hat{\beta} = \begin{bmatrix} 19.7320 & -0.6714120 & -0.1774305 \\ -0.6714 & 0.0392824 & 0.0004861 \\ -0.1774 & 0.0004861 & 0.0035416 \end{bmatrix} \begin{bmatrix} 349.3498 \\ 5746.1340 \\ 16807.4663 \end{bmatrix} = \begin{bmatrix} 53.2097294 \\ -0.6653895 \\ 0.3343728 \end{bmatrix} \begin{matrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{matrix}$$

Prediction

- Linear regression predicts:

$$\hat{y} = \hat{f}(\mathbf{x}) = \mathbf{x}^{\mathbf{T}}\widehat{\beta}$$

- Prediction for training data:

$$\hat{\mathbf{y}} = \hat{f}(\mathbf{X}) = \mathbf{X}\widehat{\beta} = \mathbf{X}(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}\mathbf{y} = \begin{bmatrix} 58.95112 \\ 58.28237 \\ 56.60044 \\ 61.29173 \\ 60.94729 \\ 53.27685 \end{bmatrix}$$

- **The hat matrix** $H = \mathbf{X}(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}}$ transforms $\mathbf{y}$ to $\hat{\mathbf{y}}$.

$$H = \begin{bmatrix} 0.21 & 0.19 & 0.00 & 0.29 & 0.15 & 0.15 \\ 0.19 & 0.18 & 0.07 & 0.22 & 0.13 & 0.20 \\ 0.00 & 0.07 & 0.78 & -0.25 & 0.31 & 0.09 \\ 0.29 & 0.22 & -0.25 & 0.55 & 0.22 & -0.03 \\ 0.15 & 0.13 & 0.31 & 0.22 & 0.44 & -0.25 \\ 0.15 & 0.20 & 0.09 & -0.03 & -0.25 & 0.84 \end{bmatrix}$$

- You may notice that $trace(H) = sum(diag(H)) = 3$.

Residual Sum of Squares

- Residual Sum of Squares is

$$
\begin{aligned}
RSS(\beta, \mathbf{X}, \mathbf{y}) &= \sum_{i=1}^{N} (y_i - \mathbf{x}_i^T \beta)^2 = (\mathbf{y} - \hat{\mathbf{y}})^T (\mathbf{y} - \hat{\mathbf{y}}) \\
&= \left(\begin{bmatrix} 56.5 \\ 57.6 \\ 55.9 \\ 61.8 \\ 63.0 \\ 54.6 \end{bmatrix} - \begin{bmatrix} 58.95112 \\ 58.28237 \\ 56.60044 \\ 61.29173 \\ 60.94729 \\ 53.27685 \end{bmatrix} \right)^T \left(\begin{bmatrix} 56.5 \\ 57.6 \\ 55.9 \\ 61.8 \\ 63.0 \\ 54.6 \end{bmatrix} - \begin{bmatrix} 58.95112 \\ 58.28237 \\ 56.60044 \\ 61.29173 \\ 60.94729 \\ 53.27685 \end{bmatrix} \right) \\
&= \left(\begin{bmatrix} -2.4263727 \\ -0.7027914 \\ -0.7105023 \\ 0.5254632 \\ 2.0123528 \\ 1.3018505 \end{bmatrix} \right)^T \left(\begin{bmatrix} -2.4263727 \\ -0.7027914 \\ -0.7105023 \\ 0.5254632 \\ 2.0123528 \\ 1.3018505 \end{bmatrix} \right) \\
&= 12.9065
\end{aligned}
$$

Linear regression complexity

$$\hat{\beta} = (\mathbf{X}^\mathbf{T}\mathbf{X})^{-1}\mathbf{X}^\mathbf{T}\mathbf{y}$$

Linear Regression Complexity

Training complexity

- The complexity of the direct approach to linear regression is $O(p^2N + p^3)$.
- $\mathbf{X}^\mathbf{T}\mathbf{X}$ is $O(p^2N)$
- the result is $p \times p$ matrix,
- its inversion takes $O(p^3)$.

Cholevsky decomposition

- $O(p^3 + \frac{p^2}{2}N)$

QR decomposition

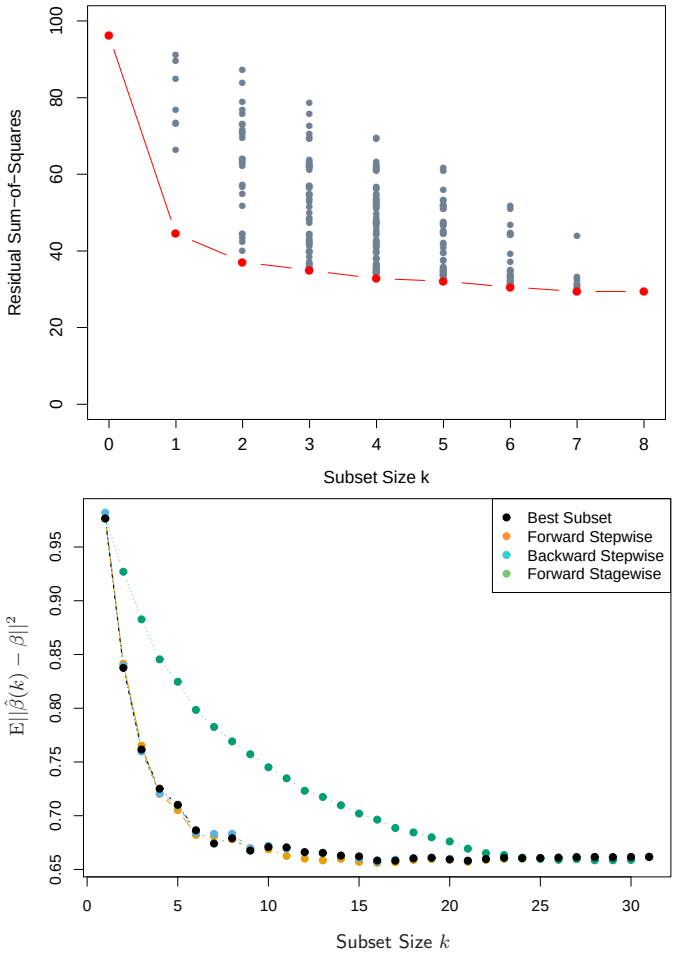
- $O(p^2N)$

Prediction complexity

- To calculate $\beta^T x$ takes $O(p)$.

Improving Least Square Estimate

- Reasons
  - improve prediction accuracy (decrease variance)
  - improve interpret ability
- methods
  - Best Subset selection
  - **Forward**- and Backward-**Stepwise Selection**
  - Forward-Stagewise Regression
    - as Forward-Stepwise
    - do **not** change previous coefficients
    - slow convergence
    - may be useful in high dimension p!
  - Penalized methods.



Centering, Standardization

Definition (Centering, Standardization)

- To **center** the variables replace each feature to have zero mean,

$$\mathbf{x}_j \leftarrow \mathbf{x}_j - \overline{x_j}$$

- The sample **variance** of a variable $\mathbf{x}_j$ is defined,

$$s_j^2 \leftarrow \frac{1}{N}\sum_{i=1}^{N}(x_{ij} - \overline{x}_j)^2$$

Both my sources use N. I know about $N-1$ used in statistics.

- **Standardization** performs the centering and divides features by their standard deviation,

$$\mathbf{x_j} \leftarrow \frac{\mathbf{x}_j - \overline{x_j}}{s_j}.$$

Sample Covariance, Correlation

Definition (Sample Covariance, Correlation)

- The **sample covariance** is a $p \times p$ symmetric matrix

$$S = \frac{1}{N}\sum_{i=1}^{N}(\mathbf{x}_i - \bar{x})(\mathbf{x}_i - \bar{x})^T$$

- with elements

$$s_{j,k} = \frac{1}{N}\sum_{i=1}^{N}(x_{ij} - \overline{x}_j)(x_{ik} - \overline{x}_k)$$

- The **sample correlation** of the columns $\mathbf{x}_j, \mathbf{x}_k$ is

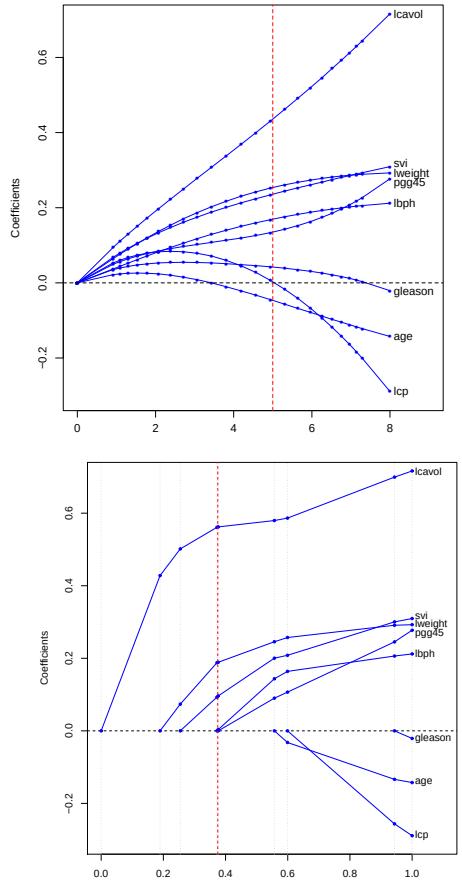
$$\rho_{j,k} \leftarrow corr(\mathbf{x}_j, \mathbf{x}_k) \leftarrow \frac{s_{j,k}}{s_j s_k} = \frac{\frac{1}{N}\sum_{i=1}^{N}(x_{ij} - \overline{x}_j)(x_{ik} - \overline{x}_k)}{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_{ij} - \overline{x}_j)^2}\sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_{ik} - \overline{x}_k)^2}}$$

- For standardized features, the correlation is just $\frac{\mathbf{x}_j^T \mathbf{x}_k}{N}$.

Penalized Methods

$$\hat{\beta} \quad = \quad argmin_{\beta} \left(\sum_{i=1}^{N} (y_i - \beta_0 - \mathbf{x}_i^T \beta)^2 + \lambda \sum_{j=1}^{p} |\beta_j|^q \right)$$

- We add the complexity penalty $\lambda \sum_{j=1}^{p} |\beta_j|^q$ to the RSS.
- **Ridge regression** $q = 2$
- **Lasso regression** $q = 1$
- **Elastic net** penalty $\lambda \sum_{j=1}^{p} (\alpha |\beta_j|^2 + (1 - \alpha)|\beta_j|)$
  - a compromise between ridge and lasso
  - selects variable like the lasso, and shirks together the coefficients of correlated predictors like ridge.
  - It also has considerable computational advantage over the L_q penalties.




```
from sklearn import linear_model
linear_model.BayesianRidge()
```

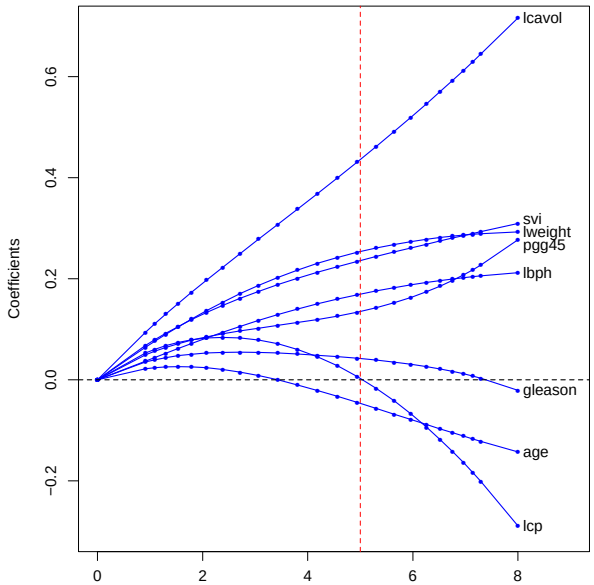
Rigde Regression

$$\hat{\beta}^{ridge} = argmin_{\beta} \left(\sum_{i=1}^{N} (y_i - \beta_0 - \mathbf{x}_i^T \beta)^2 + \lambda \sum_{j=1}^{p} |\beta_j|^2 \right)$$

- The solution is

$$\begin{aligned} \mathbf{X} &\leftarrow \text{centered } (N \times p) \text{ input matrix} \\ \hat{\beta}_0 &= \frac{1}{N} \sum_{i=1}^{N} y_i \\ \hat{\beta} &= (\mathbf{X^T X} - \lambda \mathbf{I})^{-1} \mathbf{X^T y}. \end{aligned}$$

sklearn.linear_model.Ridge



Lasso Regression

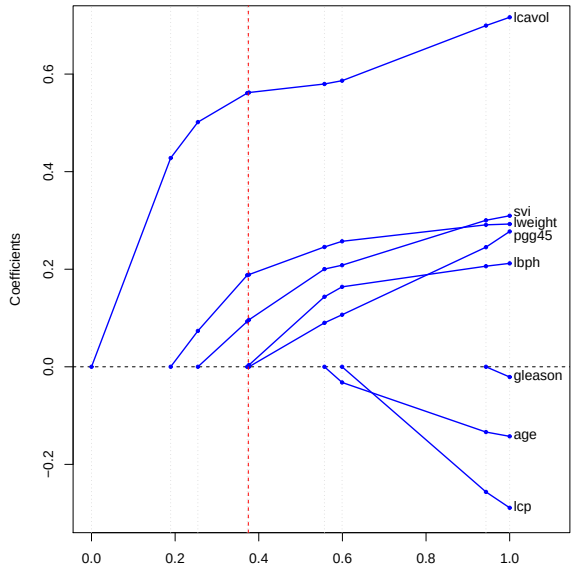
$$\hat{\beta}^{lasso} = argmin_{\beta} \left(\sum_{i=1}^{N} (y_i - \beta_0 - \mathbf{x}_i^T \beta)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right)$$

- Solved by a quadratic programming algorithm

  sklearn.linear_model.Lasso

- or LARS modification, that calculates full Lasso path in in $O(p^2 N + p^3)$.
- we use LARS on standardized data.

  sklearn.linear_model.Lars

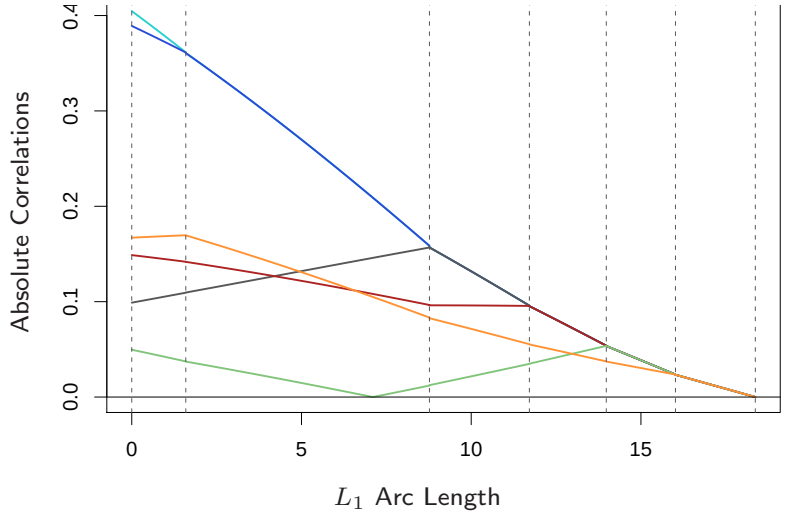


LARS Idea

- For active set of parameters $\mathcal{A}_k$ the parameters $\beta_{\mathcal{A}_k}$
- consider current **residuals** $\mathbf{r}_k = \mathbf{y} - \mathbf{X}_{\mathcal{A}_k}\beta_{\mathcal{A}_k}$
- and the correlation of each predictor with the residuals $\langle \mathbf{x}_j, \mathbf{r}_k \rangle$
- the correlations are equal for the predictors in the active set $\mathcal{A}_k$
- we change $\beta_{\mathcal{A}_k} \leftarrow \beta_{\mathcal{A}_k} + \alpha\delta_k$ in the direction

$$\delta_k = (\mathbf{X}_{\mathcal{A}_k}^{\mathsf{T}}\mathbf{X}_{\mathcal{A}_k})^{-1}\mathbf{X}_{\mathcal{A}_k}^{\mathsf{T}}\mathbf{r}$$

- and the correlation $X_{\mathcal{A}_k}$ with residuals decreases.
- Correlations of other features change linearly and we can calculate next intersection point.

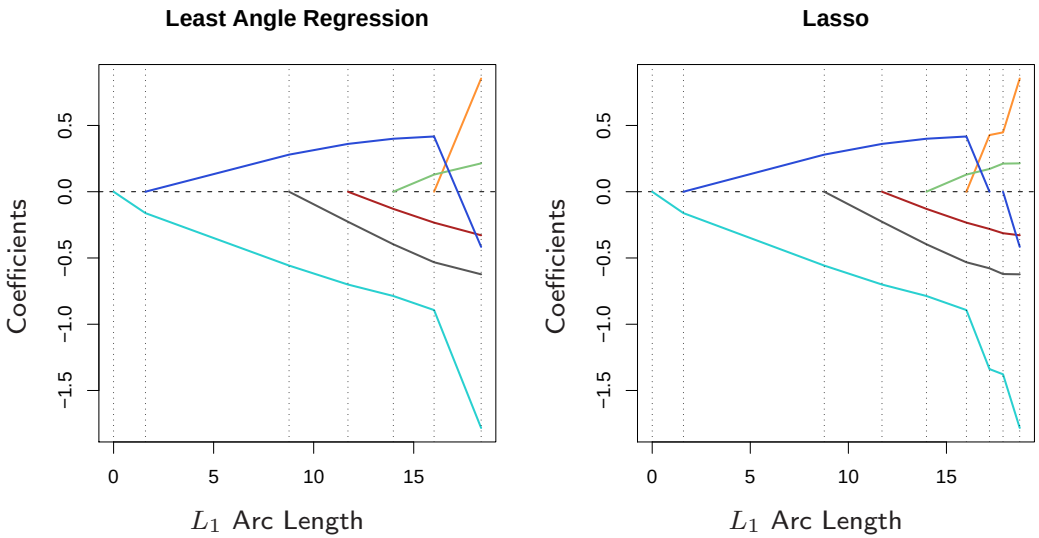


LARS Least Angle Regression

- democratic version of forward stepwise regression
- provides an extremely efficient algorithm for computing the entire lasso path.

Least Angle Regression

procedure LEAST ANGLE REGRESSION:(**X**, **y**)
    $\beta_1, \ldots, \beta_p \leftarrow 0$ initialize
    $r \leftarrow y - \bar{y}$ residuals
    find the predictor x_j most correlated with r
    Move β_j from 0 towards its least-squares coefficient $\langle x_j, r \rangle$ until some other competitor x_k has as much correlation with the current residual as does x_j.
    $\mathcal{A}_1 \leftarrow \{x_j\}$ active coefficients
    for $k = 2, \ldots, min(N-1, p)$ **do**
        move current set of $\beta_{\mathcal{A}_k}$ by their joint least squares coefficient of the current residual until some other competitor x_ℓ catches up.
        $\mathcal{A}_k \leftarrow \mathcal{A}_{k-1} \cup \{x_\ell\}$ active coefficients
    end for
end procedure



Lasso Modification of the Least Angle Regression

8a: If a non-zero coefficient hits zero, drop its variable from the active set of variables and recompute the current joint least squares direction.

Complexity of LARS

- LARS requires the same order of computation as that of a single least squares fit using the p predictors.
- hidden in the p's in $O(p^2N + p^3)$ or Cholevsky decomposition.

Model Complexity

Effective Degrees of Freedom

- Linear regression p
- Ridge regression $df(\hat{y}) = tr(\mathbf{X}(\mathbf{X}^\mathbf{T}\mathbf{X} - \lambda\mathbf{I})^{-1}\mathbf{X}^\mathbf{T})$.
- LARS: after k steps, $df(\hat{y}) = k$.
- LASSO: roughly the number of predictors in the model (may take more than p steps, some predictors drop out).

Summary

- Introduction
  - classification and regression,
  - training data,
  - RSS,
  - expected prediction error,
  - overfitting,
  - effective number of parameters,
  - curse of dimensionality,
- k Nearest neighbor model,
- Linear regression and its modifications
  - Best subset
  - Ridge, BayesianRidge
  - Lasso
  - LARS

Pathwise Coordinate Optimization

- LARS modification, iteratively by the coordinates
- fix the penalty parameter λ
- optimize successively over each parameter, holding the other parameters fixed at their current values.
- Assume the predictors are all standardized to have mean zero and unit norm,
- $\tilde{\beta}_k(\lambda)$ the current estimate for β_k at penalty parameter λ

$$R(\widetilde{\beta}(\lambda), \beta_j) = \frac{1}{2}\sum_{i=1}^{N}\left(y_i - \sum_{k\neq j} x_{ik}\widetilde{\beta}_k(\lambda) - x_{ij}\beta_j\right)^2 + \lambda\sum_{k\neq j}|\tilde{\beta}_k(\lambda)| + \lambda|\beta_j|$$

- this can be viewed as a univariate lasso problem with response variable the partial residual

$$y_i - \tilde{y}_i^{(j)} = y_i - \sum_{k\neq j} x_{ik}\widetilde{\beta}_k(\lambda).$$

Pathwise Coordinate Optimization

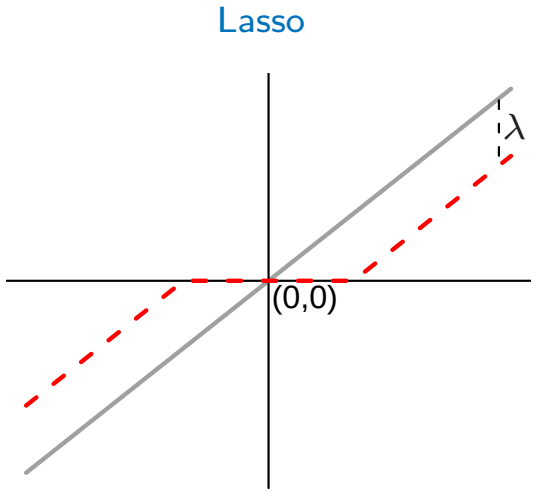
- this has an explicit solution, resulting in the update

$$\widetilde{\beta}_j(\lambda) \leftarrow S\left(\sum_{i=i}^{N} x_{ij}(y_i - \tilde{y}_i^{(j)}), \lambda\right)$$

- where S is the soft-thresholding operator

$$S(t, \lambda) = sign(t)(|t| - \lambda)_+ \tag{3}$$

- Estimators of β_j in case of orthonormal columns of X.



Grouped Lasso - not presented this year

- Dummy variables for representing the levels of a categorical predictor.
- Genes that belong to the same biological pathway.
- Suppose that the p predictors are divided into L groups
  - with p_ℓ the number in group ℓ.
  - a matrix X_ℓ represents the predictors corresponding to the ℓth group
  - with corresponding coefficient vector β_ℓ.
- the grouped-lasso minimizes the convex criterion

$$min_{\beta \in \mathbb{R}^p} \left(||y - \beta_0 1 - \sum_{\ell=1}^{L} X_\ell \beta_\ell||_2^2 + \lambda \sum_{\ell=1}^{L} \sqrt{p_\ell} ||\beta_\ell||_2 \right) \tag{4}$$

- $||\cdot||_2$ is the Euclidean norm (not squared)
- $\sqrt{p_\ell}$ accounts for the varying group sizes.

Example – Storch brings babies in Europa

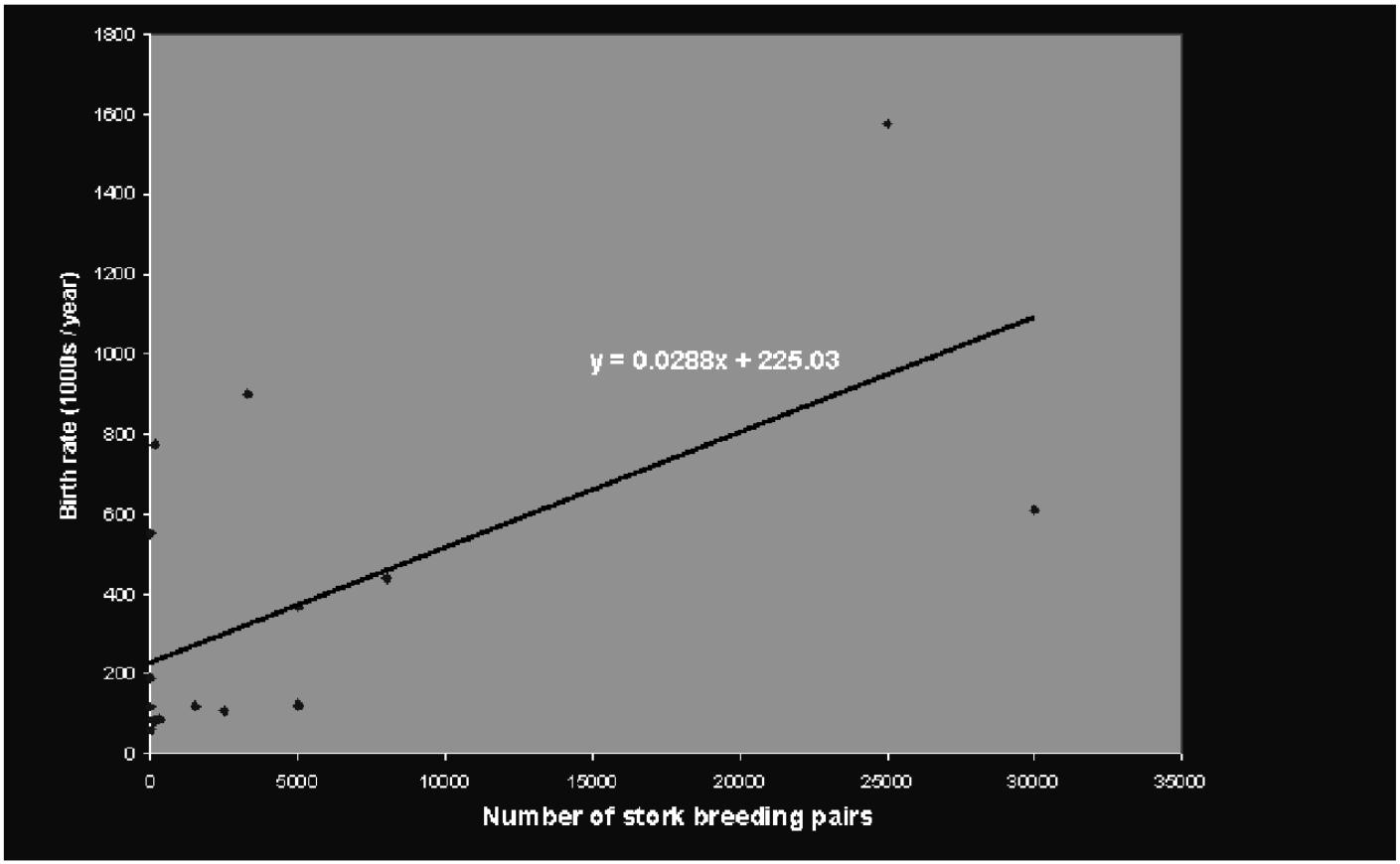


Fig 1. How the number of human births varies with stork populations in 17 European countries.

Linear methods for classification

- We are given two features X_1, X_2 and the goal *BLUE* or *ORANGE*.
- Later, we will see better ways. For now, we encode *BLUE* $= 0$ a *ORANGE* $= 1$, and find a linear regression model.
- The fitted values $\hat{Y}$ are converted to a fitted class variable $\hat{G}$ as follows:
$$\hat{G} = \left\{ \begin{array}{l} \textit{BLUE} \text{ for } Y \leq 0.5 \\ \textit{ORANGE} \text{ for } Y > 0.5 \end{array} \right\}$$
- The hyperplane $\{x : x^T \beta = 0.5\}$ is called the **decision boundary (rozhodovací hranice)**.
- Better to use **logistic regression**, that gives also a linear decision boundary.

FIGURE 2.1. *A classification example in two dimensions. The classes are coded as a binary variable (BLUE = 0, ORANGE = 1), and then fit by linear regression. The line is the decision boundary defined by $x^T \hat{\beta} = 0.5$. The orange shaded region denotes that part of input space classified as ORANGE, while the blue region is classified as BLUE.*

Two Scenarios

- The training data in each class were generated from bivariate Gaussian distribution with uncorrelated components and different means.
- The linear model is (almost) optimal.

FIGURE 2.1. *A classification example in two dimensions. The classes are coded as a binary variable (*BLUE $= 0$, ORANGE $= 1$*), and then fit by linear regression. The line is the decision boundary defined by* $x^T\hat{\beta} = 0.5$*. The orange shaded region denotes that part of input space classified as* ORANGE*, while the blue region is classified as* BLUE*.*

- The training data in each class came from a mixture of 10 low-variance Gaussian distributions, with individual means themselves distributed as Gaussians.
- The linear model is **not** optimal.

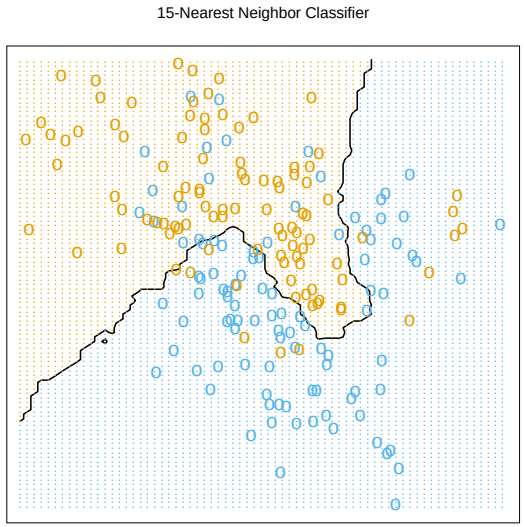


FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable (*BLUE $= 0$, ORANGE $= 1$*) and then fit by* 15*-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the* 15*-nearest neighbors.*

Basis expansion and regularization

Linear and logistic regression assume linear function of X.

- Regression: We estimate $f(X) = \mathbb{E}(Y|X)$
- Classification: We estimate $log \frac{P(Y=1|X)}{P(Y=0|X)}$

Linear basis expansion in X

- we replace the vector of inputs X with additional variables h_m,
- $h_m(X) : \mathbb{R}^p \to \mathbb{R}$, $m = 1, \ldots, M$.

$$f(x) = \sum_{m=1}^{M} \beta_m h_m(X).$$

- 'the only change' is a different matrix of the features X, further fit is the same.

Simple derived features

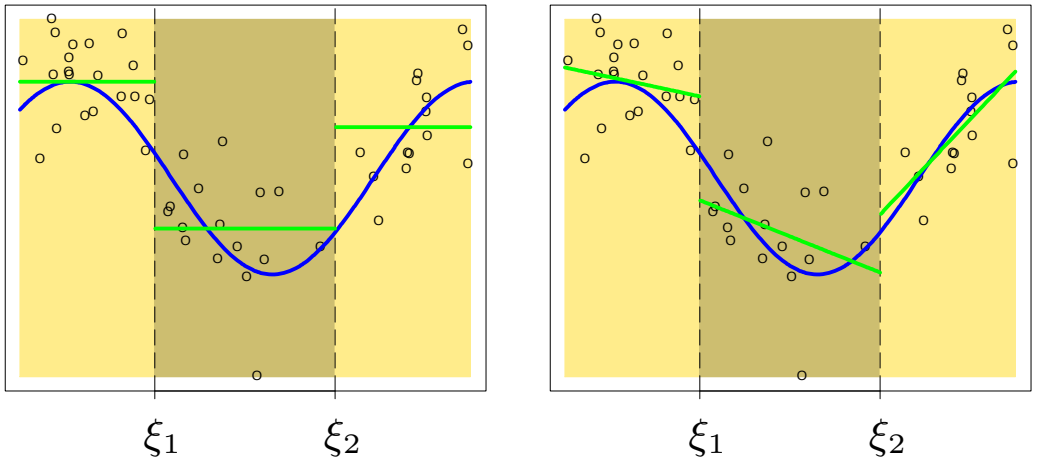
- We fit the model:

$$f(x) = \sum_{m=1}^{M} \beta_m h_m(X).$$

- $h_m(X) = X_m$, $m = 1, \ldots, M$ recovers the original linear model.
- $h_m(X) = X_j^2$ or $h_m(X) = X_j X_k$ polynomial terms to achieve higher-order Taylor expansions.
  - ! The number of variables grows exponentially in the degreee of the polynomial.
- $h_m(X) = log(X_j)$, $\sqrt{X_j}$, $||X||$,..., other nonlinear transformations.
- $h_m(X) = I(L_m \leq X_k < U_m)$, an indicator for a region of X_k.
  - piecewise constant contribution for X_K.
  - With non-overlapping regions used in regression trees.
- $h_m(X) = max((X_j - \xi_k)^3, 0)$ piecewise-polynomial spline basis
- wavelet bases.

Piecewise Polynomials and Splines

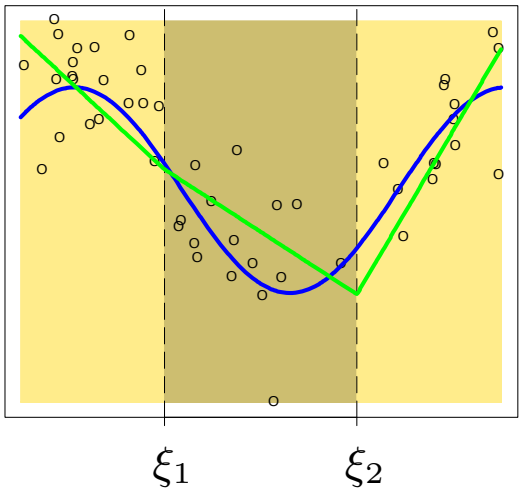
- For most of today we assume one-dimensional feature X.
- A **piecewise polynomial** function $f(X)$ is obtained by
  - division the domain of X into continuous intervals by the knots $\xi_1, \ldots, \xi_{M-1}$
  - and representing f by a separate polynomial in each interval.
  - Examples:
    - Three basis functions:
      $h_1(X) = I(X < \xi_1)$, $h_2(X) = I(\xi_1 \leq X < \xi_2)$, $h_3(X) = I(\xi_2 \leq X)$.
    - Additional linear functions:
      $h_{m+3} = h_m(X) \cdot X$, $m = 1, \ldots, 3$.
    - Additional cubic functions:
      $h_{m+6} = h_m(X) \cdot X^2$, $h_{m+9} = h_m(X) \cdot X^3$, $m = 1, \ldots, 3$.



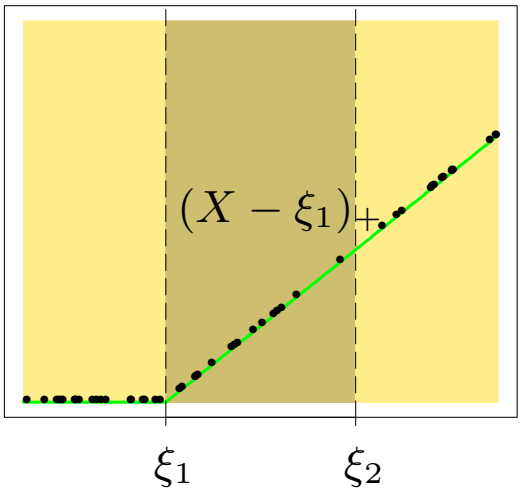
Continuous functions

- We add the continuity restriction: the value in ξ_j is the unique.
- Continuous piecewise linear basis:
  $h_1(X) = 1$, $h_2(X) = X$, $h_3(X) = (X - \xi_1)_+$, $h_4(X) = (X - \xi_2)_+$.
- We have spared two parameters for two continuity conditions.

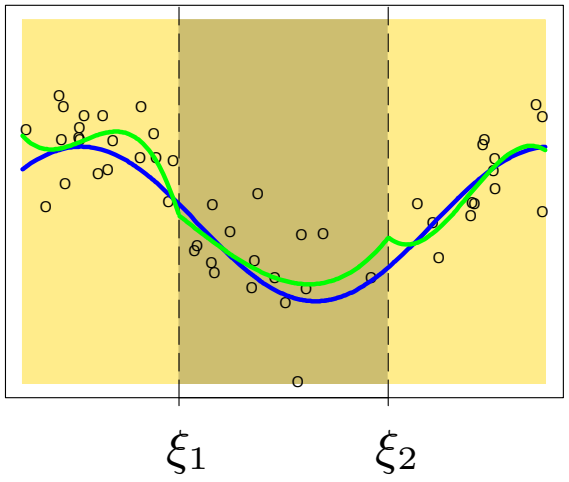
Continuous Piecewise Linear



Piecewise-linear Basis Function



Continuous

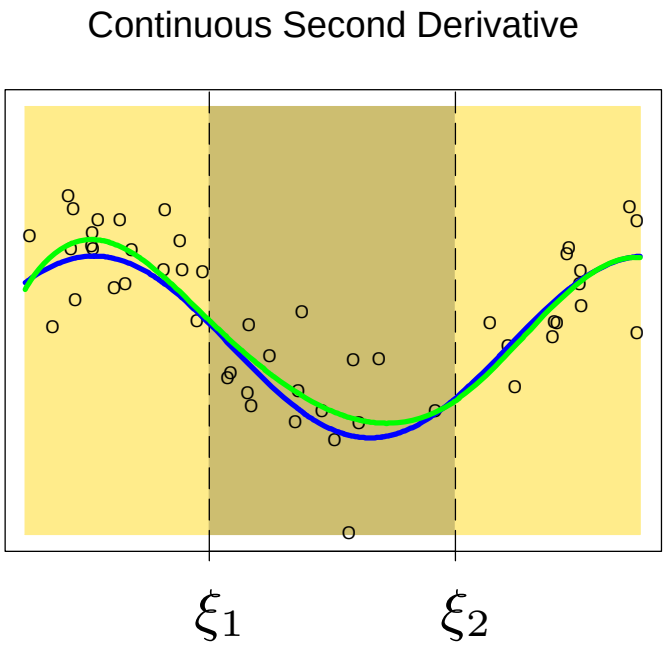


- For the cubic fit, the figure looks ugly, we need continous first and second derivative.

Cubic spline

- **Cubic spline** is a piecewise cubic fit with continuous first and second derivatives at the knots ξ_i.

- The basis functions with knots ξ_1, ξ_2 are:
  $h_1(X) = 1,$
  $h_2(X) = X,$
  $h_3(X) = X^2,$
  $h_4(X) = X^3,$
  $h_5(X) = (X - \xi_1)^3_+,$
  $h_6(X) = (X - \xi_2)^3_+.$



- Parameter count:
  (3 regions)x(4 pars per region)-(2 knots)x(3 constraints per knot)=6.

Order-M splines

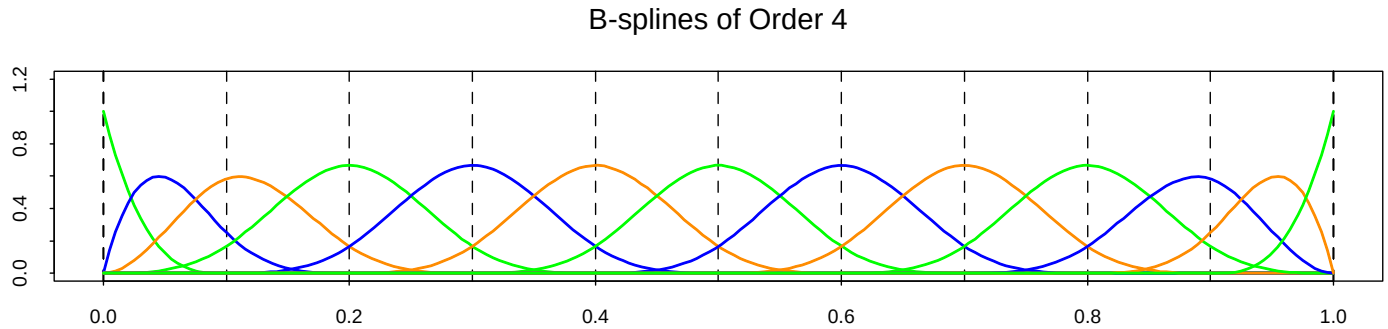
- Cubic spline is an order-4 spline.
- Generally, order-M spline with knots ξ_j, $j = 1, \ldots, K$ is a piecewise-polynomial of order $(M-1)$ and has continuous derivatives to order $(M-2)$.
- General truncated basis functions are:
  - $h_j(X) = X^{j-1}$, $j = 1, \ldots, M$,
  - $h_{M+\ell} = (X - \xi_\ell)_+^{M-1}$, $\ell = 1, \ldots, K$.
- **Regression splines**
  - splines with fixed knots
  - usually at percentiles of the data X.
  - the number of knots is specified by the degree an the degrees of freedom $(df - M)$. h_0 does not count.

B-splines

B-splines use other basis describing the same linear feature space.

- $\{h_i\}$ is a basis of a linear space of functions
- we may choose a different base to cover the same space of functions.
- B-splines are more stable numerically, useful for large number of knots K.
- B-splines have quite difficult recursive formula (not needed for the exam).

$$
\begin{aligned}
B_{i,1}(x) &= \begin{cases} 1 & \text{if } \xi_i \leq x \leq \xi_{i+1} \\ 0 & \text{otherwise} \end{cases} \\
B_{i,k+1}(x) &= \omega_{i,k}(x) B_{i,k}(x) + [1 - \omega_{i+1,k}(x)] B_{i+1,k}(x) \\
\omega_{i,k}(x) &= \begin{cases} \frac{x - \xi_i}{\xi_{i+k} - \xi_i} & \text{if } \xi_{i+k} \neq \xi_i \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}
$$



Computational complexity

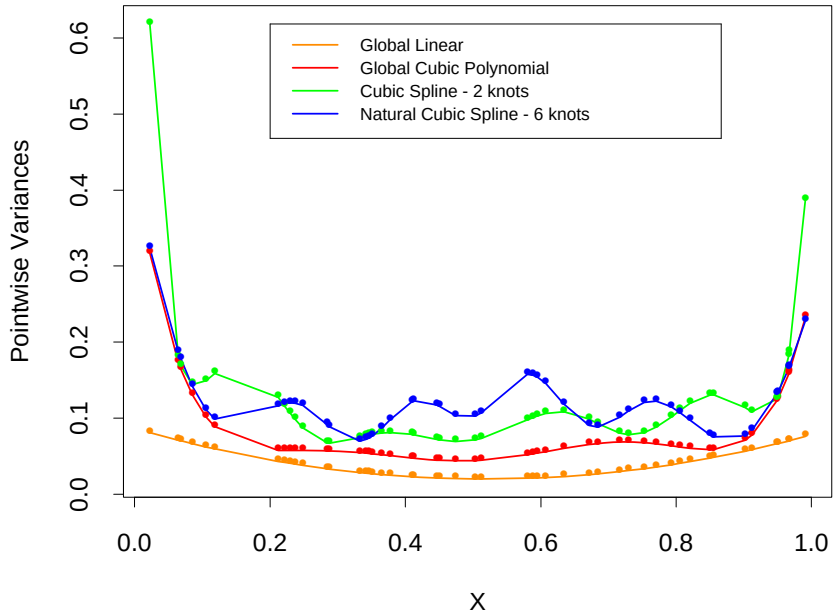
Spline fit time complexity

- (Standard) regression splines
  - N observations, $K + M$ variables (basis functions) take $O(N(K + M)^2 + (K + M)^3)$.
- B-splines
  - sort values of X
  - Cubic B splines have local support, B is lower 4-banded.
  - order $(M + 1)$ B splines have local support, B is lower $(M + 1)$-banded.
  - Cholesky decomposition $B = LL^T$ can be computed easily.
  - Solution of $\hat{f}$ is in $O(N(M + 1))$ operations.

B-splines implemented in scipy

Natural Cubic Spline

- Polynomial fit tends to be erratic near the boundaries.



- **Natural cubic spline** is a spline that the function is linear beyond the boundary knots.
- Basis functions N_i, $i = 1, \ldots, K$:
  $N_1(X) = 1, N_2(X) = X, N_{k+2}(X) = d_k(X) - d_{K-1}(X)$ for

$$d_k(X) = \frac{(X - \xi_k)_+^3 - (X - \xi_K)_+^3}{\xi_K - \xi_k}.$$

Smoothing Splines

- Maximal number of knots: N, the number of examples.
- But, we need a penalty for model complexity.

$$RSS(f, \lambda) = \sum_{i=1}^{N} (y_i - f(x_i))^2 + \lambda \int (f''(t))^2 dt$$

- λ is **smoothing parameter**
  - $\lambda = 0$: can be any function that interpolates the data.
  - $\lambda = \infty$: the simple least squares line fit, no nonzero second derivative is tolerated.
- Has a unique finite-dimensional minimizer, a natural cubic spline with knots at the unique values of the x_i, $i = 1, \ldots, N$.
- The solution is in the form: $f(x) = \sum_{j=1}^{N} N_j(x)\theta_j$.
- The criterion reduces for:

$$RSS(\theta, \lambda) = (\mathbf{y} - \mathbf{N}\theta)^T (\mathbf{y} - \mathbf{N}\theta) + \lambda \theta^T \Omega_N \theta$$

- where $\{\mathbf{N}\}_{ij} = N_j(x_i)$ and $\{\Omega\}_{jk} = \int N_j''(t) N_k''(t) dt$.

let $a = x_1 = 0$, $b = x_{101} = 1$, and knots $\xi_l = x_{l+1}$ for $l = 1, \ldots, K$ and $K = 99$. Also, the basis functions for a cubic spline $M = 4$ are

$$\begin{aligned} h_j(x) &= x^{j-1} && j = 1, \ldots, M, \\ h_{M+l}(x) &= (x - \xi_l)_+^{M-1} && l = 1, \ldots, K. \end{aligned}$$

Then, $\boldsymbol{H} = (h_j(x_i))_{N,M+K}$ where $h_j(x_i)$ is for the i-th row and the j-th column. Let $\boldsymbol{\Omega} = (\omega_{i,j})_{M+K,M+K}$ be a symmetric matrix and the upper triangular $\omega_{i,j} = \int_a^b h_i''(t) h_j''(t) dt$ is

$$\begin{aligned} \omega_{i,j} &= 0 && \text{for } i < M, \\ \omega_{M,j} &= \tfrac{1}{3}b^3 - \tfrac{1}{2}b^2\xi_j + \tfrac{1}{6}\xi_j^3 && \text{for } j > M, and \\ \omega_{i,j} &= \tfrac{1}{3}(b^3 - \xi_0^3) - \tfrac{1}{2}(b^2 - \xi_0^2)(\xi_{i-M} + \xi_{j-M}) + (b - \xi_0)\xi_{i-M}\xi_{j-M} && \text{for } j \geq i > M, \end{aligned}$$

where $\xi_0 = \max\{\xi_{i-M}, \xi_{j-M}\}$.

https://vardeman.public.iastate.edu/stat602/602x_hw4_sol.pdf

Smoothing Splines solution

- Smoothing spline solution is a generalized ridge regression

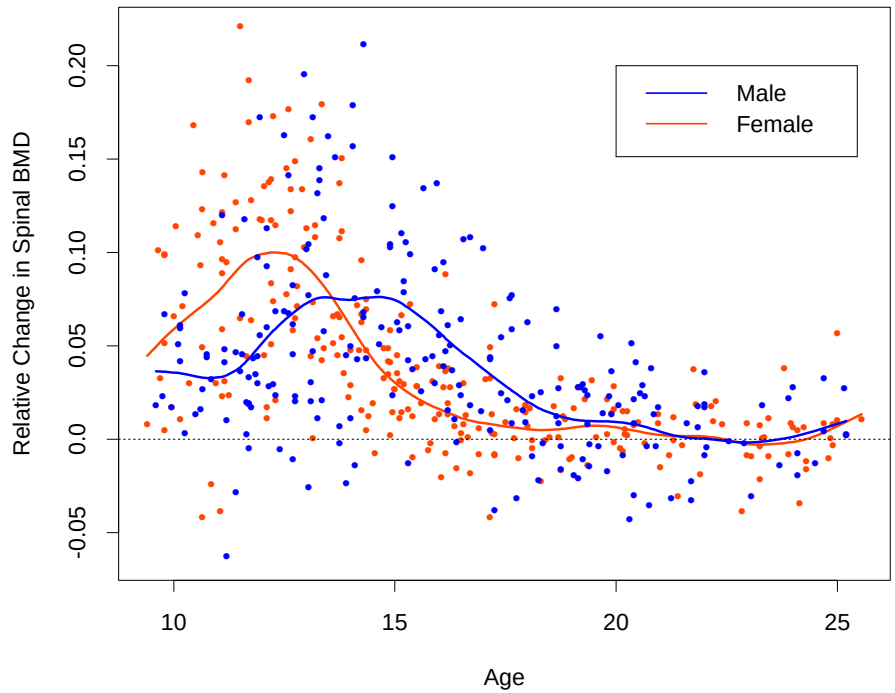
$$\hat{\theta} = (\mathbf{N}^T\mathbf{N} + \lambda\Omega_N)^{-1}\mathbf{N}^T\mathbf{y}$$

- The fitted smoothing spline is given by:

$$\hat{f}(x) = \sum_{j=1}^{N} N_j(x)\hat{\theta}_j$$

Example

- Bone mineral density (BMD) in adolescents.
- Response: the change in BMD over two consecutive visits, typically about one year apart.
- coded by gender, females precedes growth spurt about two years.
- $\lambda \approx 0.00022$, $df_\lambda = 12$.



Degrees of Freedom and Smoother Matrices

- Smoothing spline is a linear smoother:

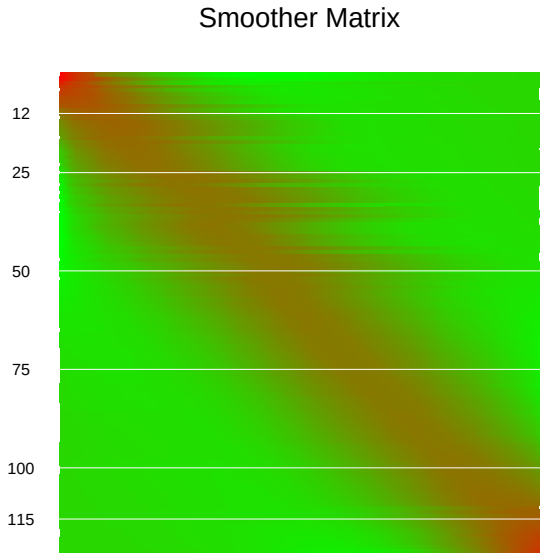
$$\begin{aligned} \hat{f} &= \mathbf{N}(\mathbf{N}^T\mathbf{N} + \lambda\Omega_N)^{-1}\mathbf{N}^T\mathbf{y} \\ &= \mathbf{S}_\lambda \mathbf{y} \end{aligned}$$

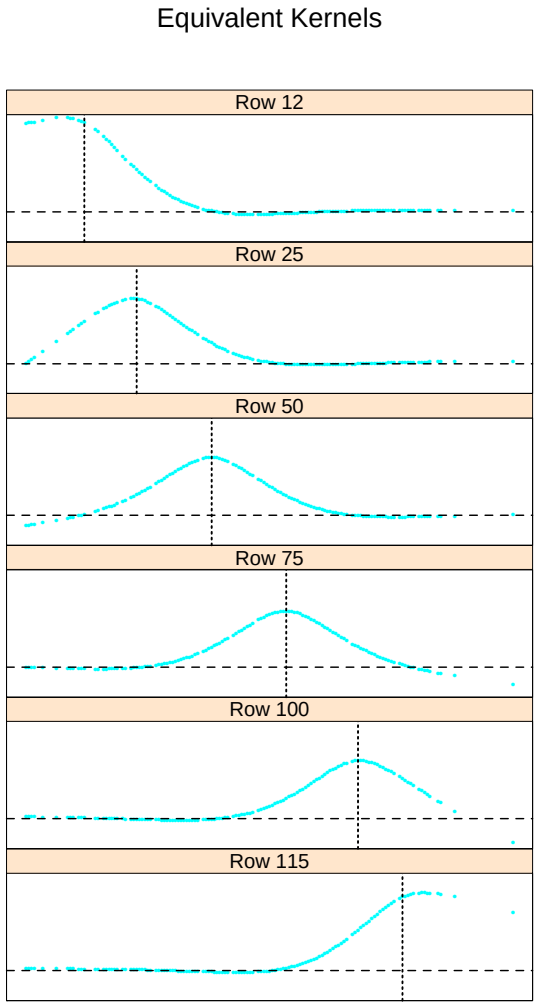
- $\mathbf{S}_\lambda$ is known as smoother matrix.
- $df_\lambda = trace(\mathbf{S}_\lambda)$
  - the sum of the diagonal elements
  - $\lambda \approx 0.00022$ derived numerically by solving $trace(\mathbf{S}_\lambda) = 12$.

smoothing splines only in R

Smoother Matrix

- rows $\mathbf{S}_\lambda$ ordered with x
- right: selected rows
- $\lambda \to 0$ means $df_\lambda \to N$ and $\mathbf{S}_\lambda \to \mathbf{I}$
- $\lambda \to \infty$ means $df_\lambda \to 2$ and $\mathbf{S}_\lambda \to \mathbf{H}$, the hat matrix for linear regression on $\mathbf{x}$.
- $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$ since $(\hat{y} = Hy)$



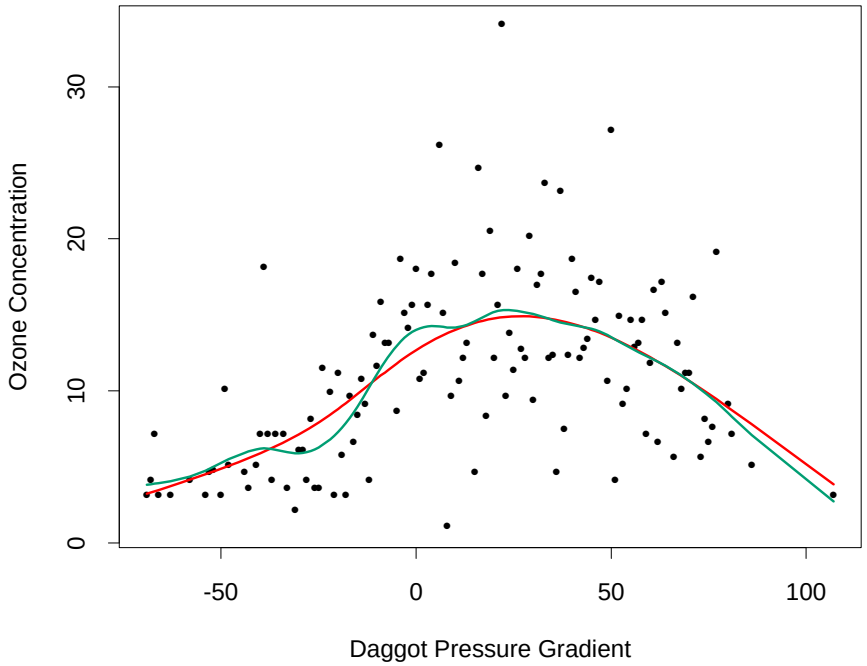


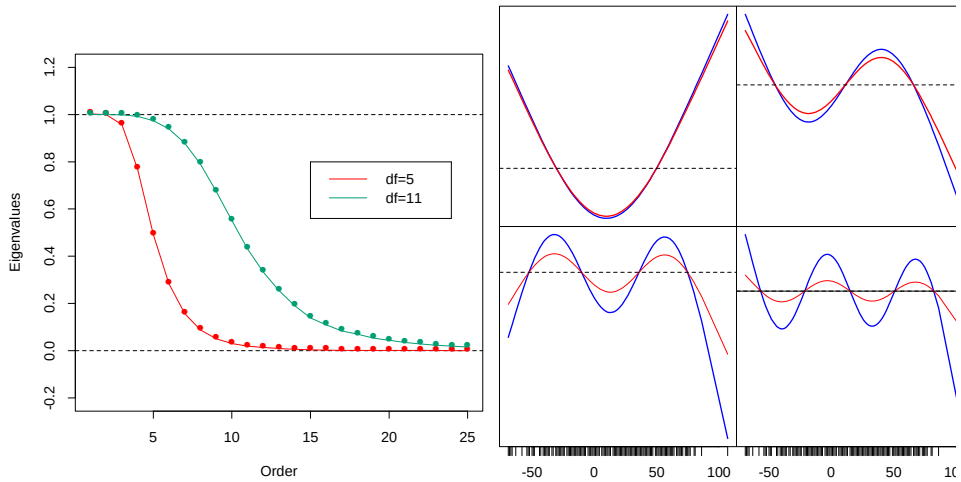
Pollution data example

Example

- 128 observations of pressure and ozone.
- Two fitted smoothing splines.
- third to sixth eigenvectors of the spline smoother matrices u_k against x.
- eigendecomposition of S:

$$\mathbf{S}_\lambda = \sum_{k=1}^{N} \rho_k(\lambda) u_k u_k^T$$



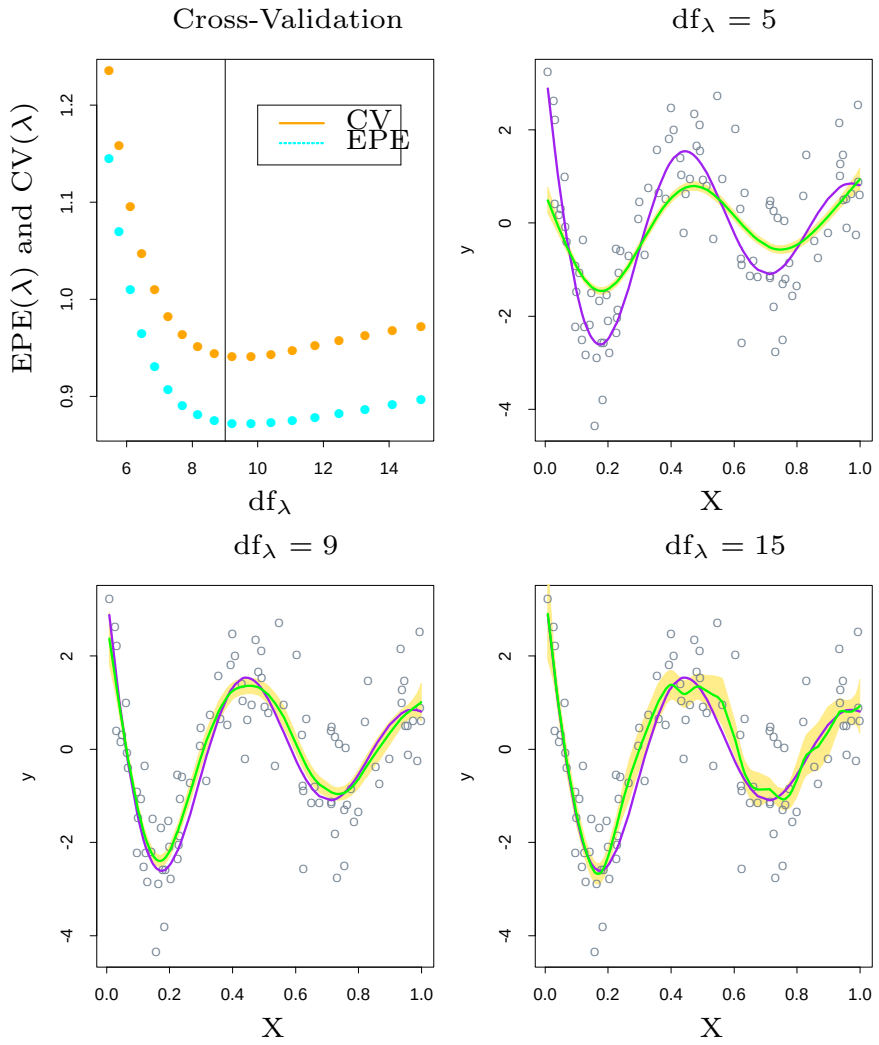


Selection degrees of freedom

- The degrees of freedom *df* (or the complexity penalty λ) are usually selected to minimize the expected prediction error.
- More specifically, the crossvalidation estimate of the error.

Example

- $f(X) = \frac{sin(12(X+0.2))}{X+0.2}$
- $Y = f(X) + \epsilon$
- $X \sim U[0,1]$, $\epsilon \sim N(0,1)$, $N = 100$.
- *df* selected by crossvalidation is 9.



Multidimensional Splines

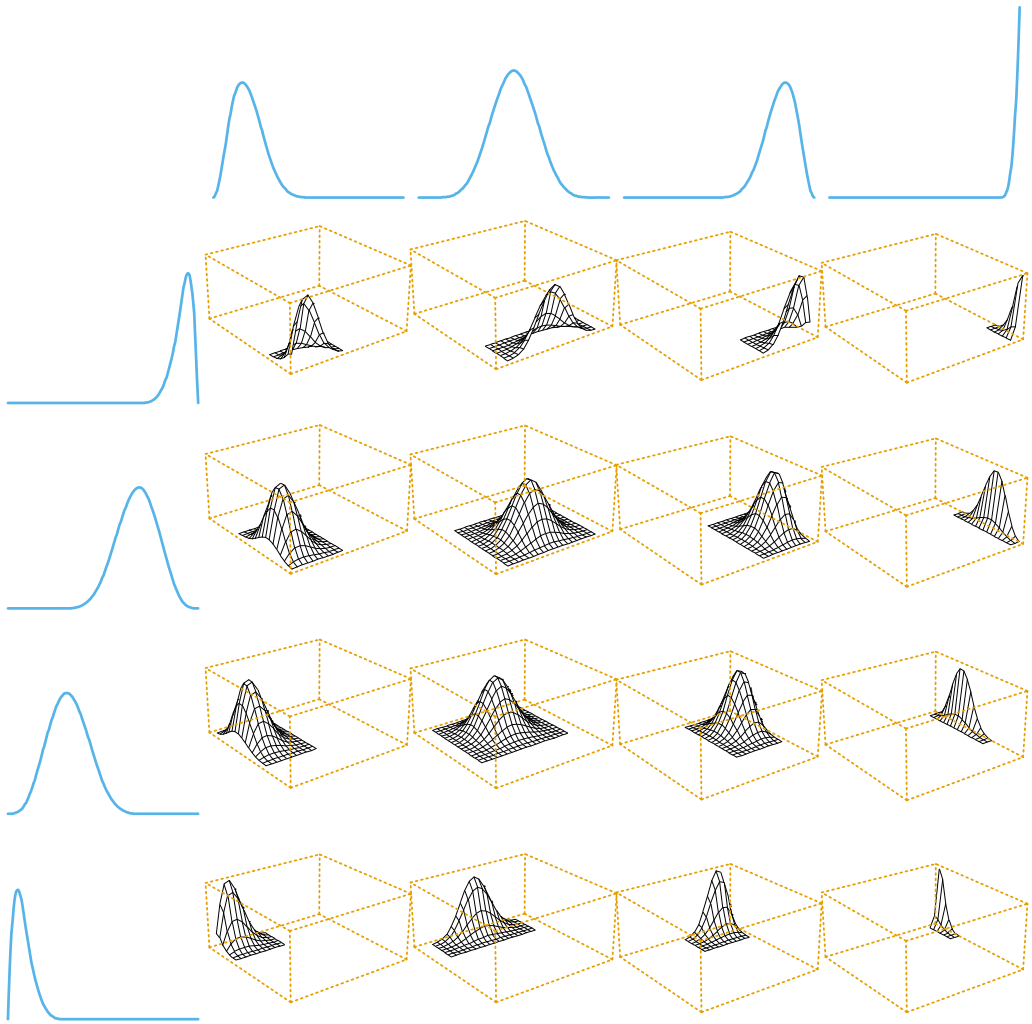
- $X \in \mathbb{R}^2$
- $h_{1k}(X_1),\ k = 1, \ldots, M_1$ in the first coordinate
- $h_{2k}(X_2),\ k = 1, \ldots, M_2$ in the second coordinate.
- $M_1 \times M_2$ dimensional tensor product basis is defined by

$$g_{jk}(X) = h_{1j}(X_1) h_{2k}(X_2)$$

- can be used for representing a two-dimensional function:

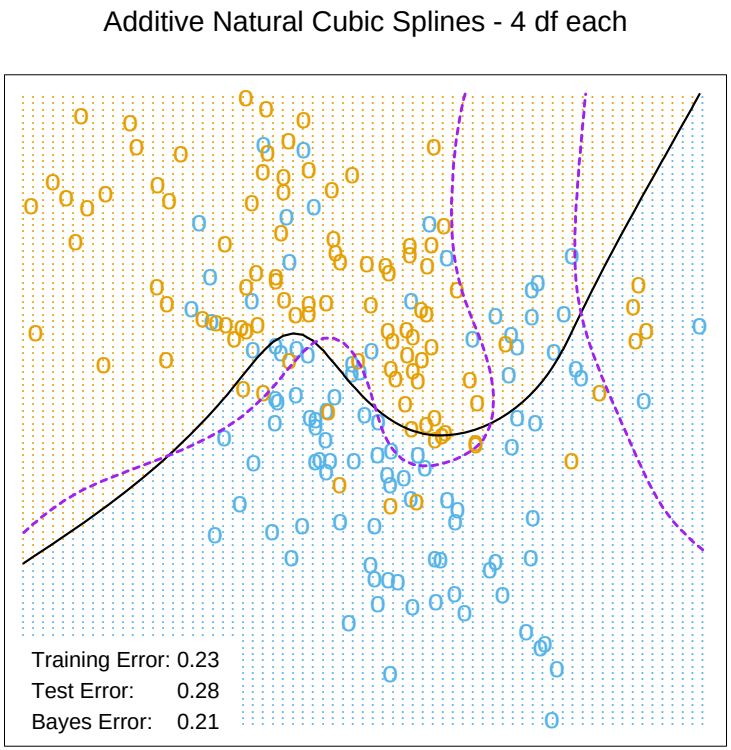
$$g(X) = \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \theta_{jk} g_{jk}(X)$$

- coefficients can be fitted by least squares.



Additive logistic regression vs. tensor product

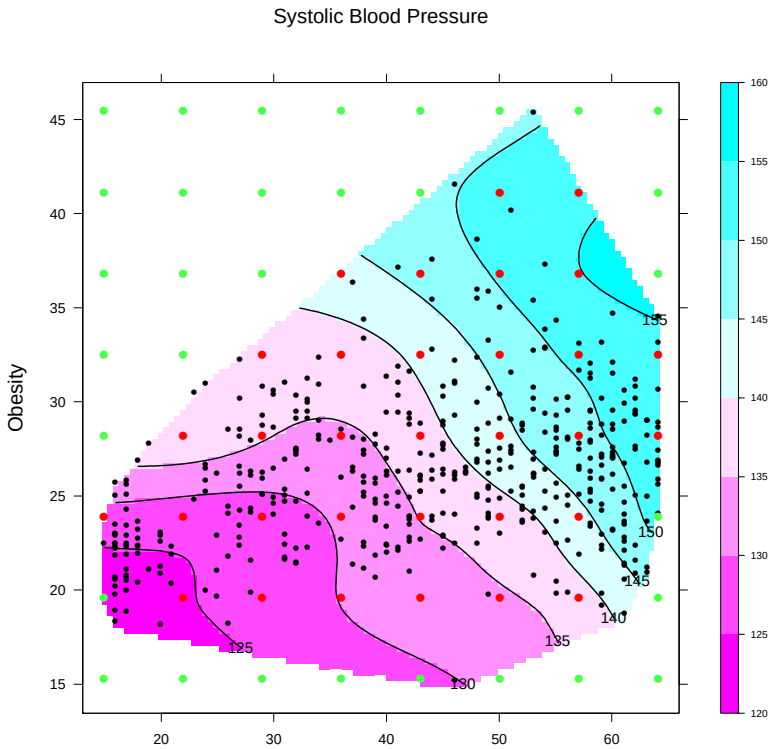
- In higher dimensions, the number of basic functions and parameters grows rapidly.
- Consider to add the basic elements iteratively, as the additive MARS method introduced later.
- left: df=7, right df=16



Multidimensional smoothing splines

- Let us place the knot into each example
- and add a complexity penalty J (below).
- It can be generalized for an arbitrary dimension.
- The solution has the form:
  - $f(x) = \beta_0 + \beta^T x + \sum_{j=1}^{N} \alpha_j h_j(x)$
  - where $h_j(x) = \eta(||x - x_j||)$ and $\eta(z) = z^2 2 \log z^2$.

- complexity $O(N^3)$
- or $O(NK^2 + K^3)$ with K knots.



$$J[f] = \int \int_{\mathbb{R}^2} \left[\left(\frac{\partial^2 f(x)}{\partial x_1^2}\right) + \left(\frac{\partial^2 f(x)}{\partial x_1 \partial x_2}\right) + \left(\frac{\partial^2 f(x)}{\partial x_2^2}\right) \right] dx_1 dx_2$$

implemented in R and OpenCV

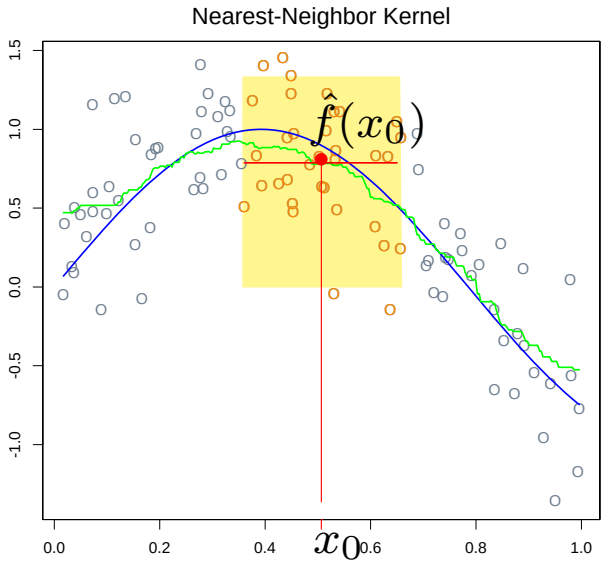
Summary

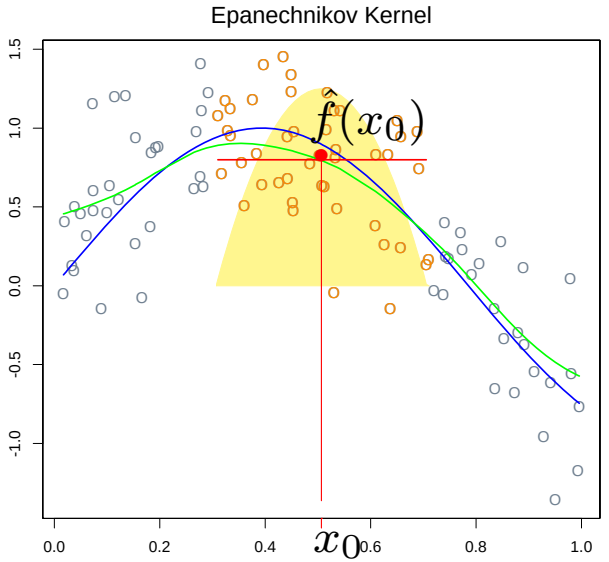
We learned about

- splines (one dimensional)
- B-splines - for faster fit
- natural splines - linear on the borders
- **smoothing splines** - complexity penalty for the second derivative
  - the solution is a natural spline.
- Generalizations to more dimensions
  - thin plate splines
  - multidimensional smoothing splines.

Kernel Methods

- estimate regression function $f(x) \in \mathbb{R}$
- a different but simple model separately at each query point x_0.
- The resulting $\hat{f}(X)$ is smooth in $\mathbb{R}^p$.
- Localization is achieved via a weighting function er **kernel** $k_\lambda(x_0, x_i)$
  - assigns a weight to x_i based on its distance form x_0.
- λ is a parameter that dictates the width of the neighbourhood.
- **memory based methods**
  - little or no training
  - the model is the entire training data set.





k-NN, Epanechnikov Kernel

- **k-Nearest Heighbour** kernel
  - $N_k(x)$ is the set of k points nearest to x in squared distance
  - all have equal weight
  - $\hat{f}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i$.
  - $\hat{f}(x)$ is bumpy, discontinuous.
- **Nadaraya-Watson** kernel-weighted average

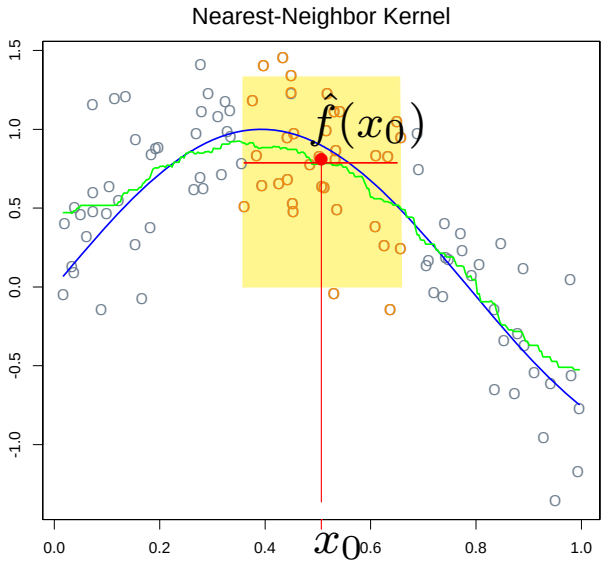
$$\hat{f}(x_0) = \frac{\sum_{i=1}^{N} k_\lambda(x_0, x_i) y_i}{\sum_{i=1}^{N} k_\lambda(x_0, x_i)}$$

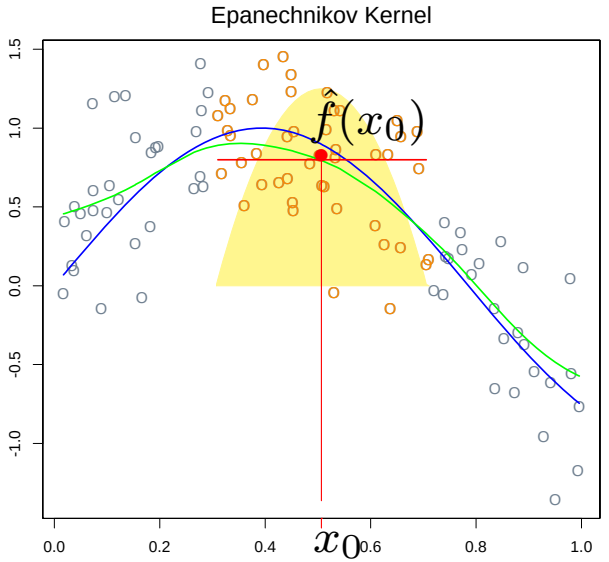
- with the **Epanechnikov** quadratic kernel

$$k_\lambda(x_0, x) = D\left(\frac{|x - x_0|}{\lambda}\right)$$

- with

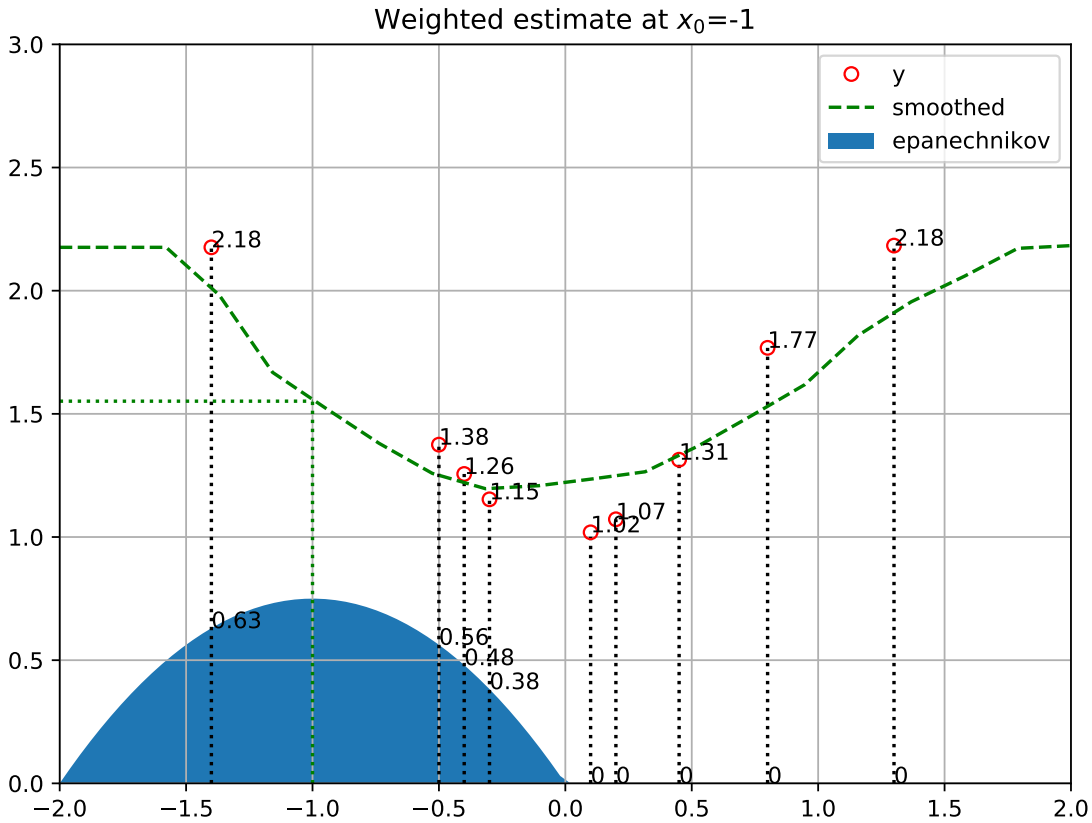
$$D(t) = \begin{cases} \frac{3}{4}(1 - t^2) & \text{if } |t| \leq 1 \\ 0 & \text{otherwise.} \end{cases}$$





Example

- Red circles: data
- Blue: epanechnikov kernel for (-1.0)
- Predicted values: green dashed line
- predicted value $\hat{f}(-1.0) = 1.55$.



$$\frac{(0.63 * 2.18 + 0.56 * 1.38 + 0.48 * 1.26 + 0.38 * 1.15 + 0 * others)}{(0.63 + 0.56 + 0.48 + 0.38)} = 1.55$$

Kernels - variable width, shapes

- The width λ may vary $h_\lambda(x_0)$ with x_0
- mo general formula for he kernel

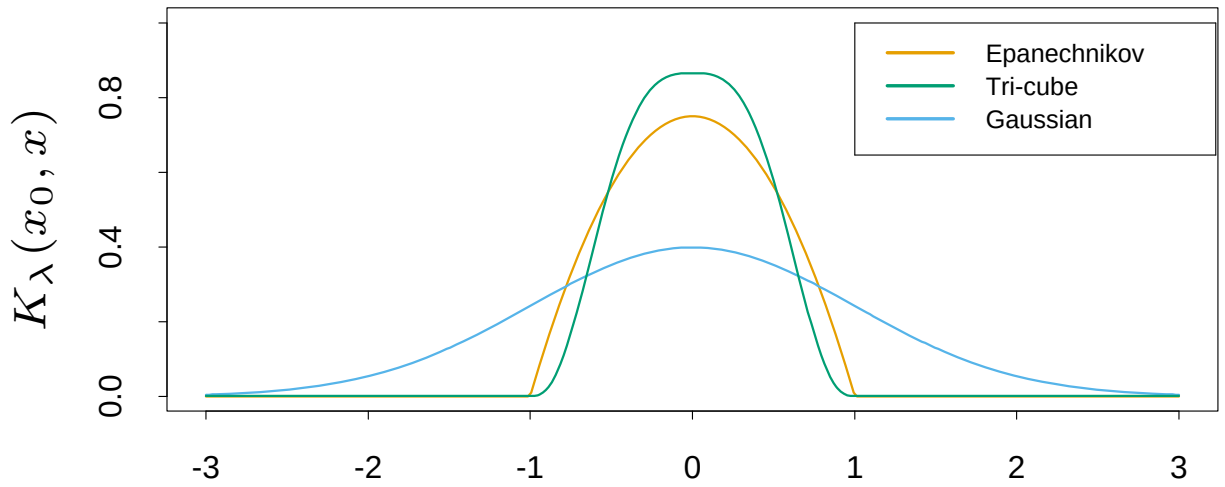
  $k_\lambda(x_0, x) = D\left(\frac{|x-x_0|}{h_\lambda(x_0)}\right)$
- for k-NN, $h_k(x_0) = |x_0 - x_{|k|}|$
- where $x_{|k|}$ is the kth closest x_i to x_0.

- **Tri-cube kernel**

  $$D(t) = \begin{cases} (1-|t|^3)^3 & \text{if } |t| \leq 1 \\ 0 & \text{otherwise.} \end{cases}$$
- **Gaussian kernel**

  $$D(t) = \frac{1}{\lambda} e^{-\frac{\|x-x_0\|^2}{2\lambda}}$$
- **Epanechnikov**

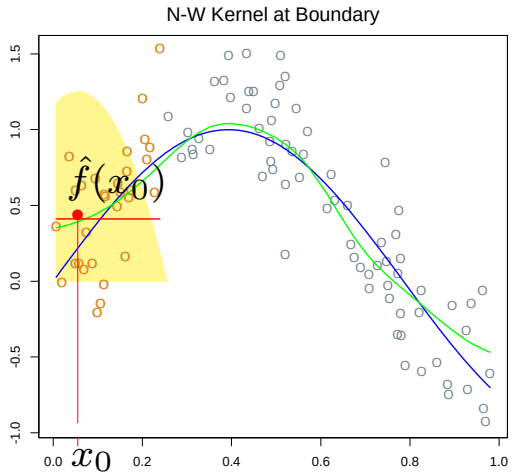
  $$D(t) = \begin{cases} \frac{3}{4}(1-t^2) & \text{if } |t| \leq 1 \\ 0 & \text{otherwise.} \end{cases}$$



Local Linear Regression

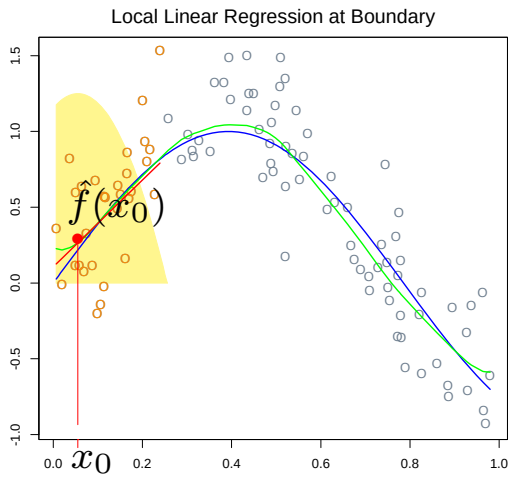
- Locally-weighted averages can be badly biased on the boundaries of the domain
- or whenever X are not equally spaced.
- Fitting straight lines may help (a bit).
- **Locally weighted regression**

$$min_{\alpha(x_0),\beta(x_0)} \sum_{i=1}^{N} k_\lambda(x_0, x_i)[y_i - \alpha(x_0) - \beta(x_0)x_i]^2$$



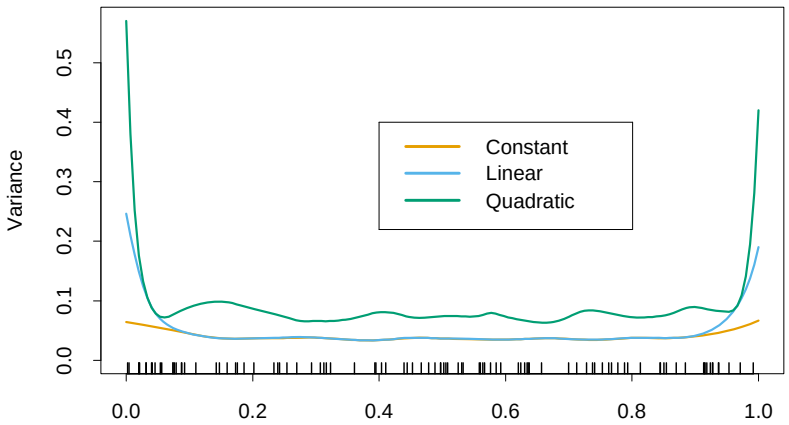
- The estimate is: $\hat{f}(x_0) = \hat{\alpha}(x_0) + \hat{\beta}(x_0)x_0$.
  - For $x^T \to (1, x)$, $\mathbf{X}$ is $N \times (p+1)$ matrix, $\mathbf{W}$ $N \times N$ diagonal matrix $k_\lambda(x_0, x_i)$. Then

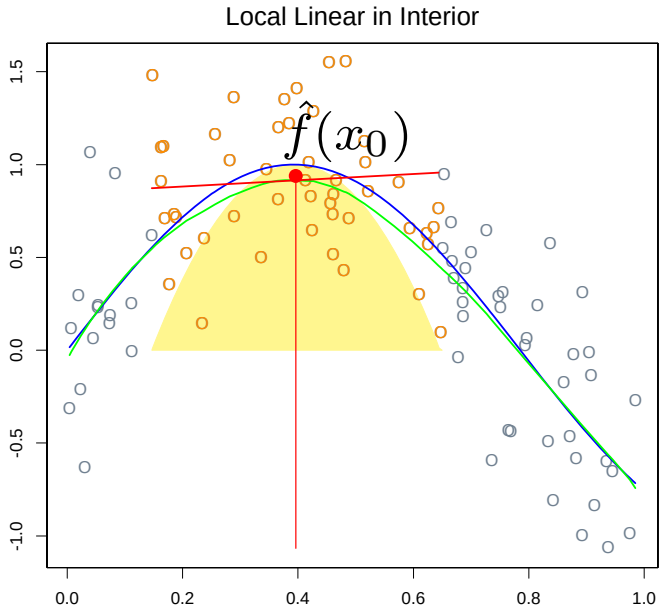
  $\hat{f}(x_0) = x_0^T(X^T W(x_0)X)^{-1}X^T)W(x_0)y$
- what is linear function of y.

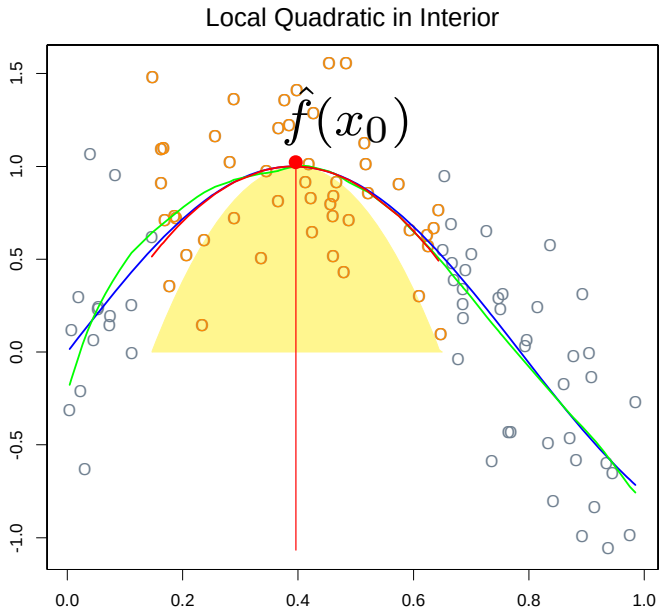


Local Polynomial Regression

- Local linear fits can help bias dramatically at the boundaries.
- local quadratic fits tend to be most helpful in reducing bias due to curvature in the interior of the domain.
- Recommended to select the degree by the application, not to combine linear boundaries and quadratic interior.

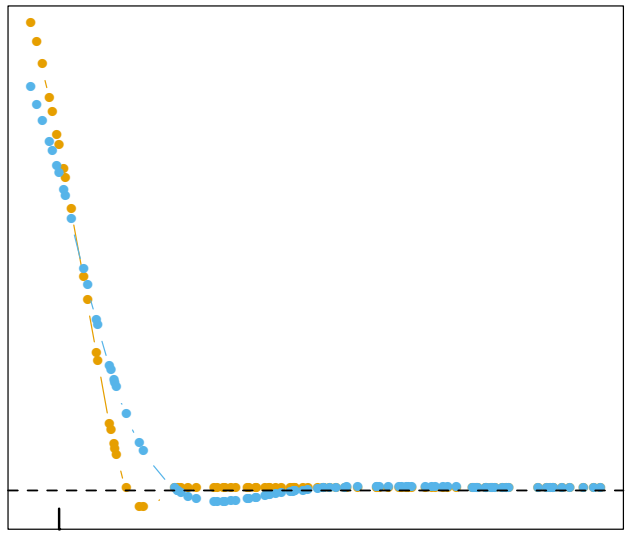


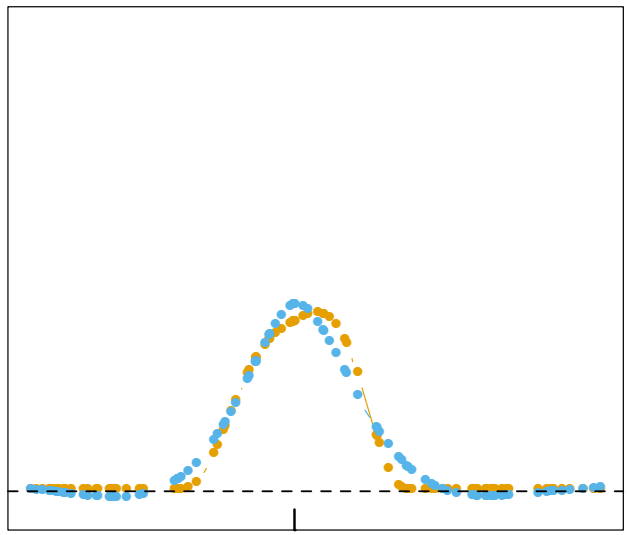




Selecting the Width of the Kernel

- crossvalidation
- $\hat{f} = S_\lambda y$
  - $df = trace(S_\lambda)$
- Right: comparison of the tri-cube local linear regression kernels (orange) and smoothing splines (blue) with matching degrees of freedom 5.86.



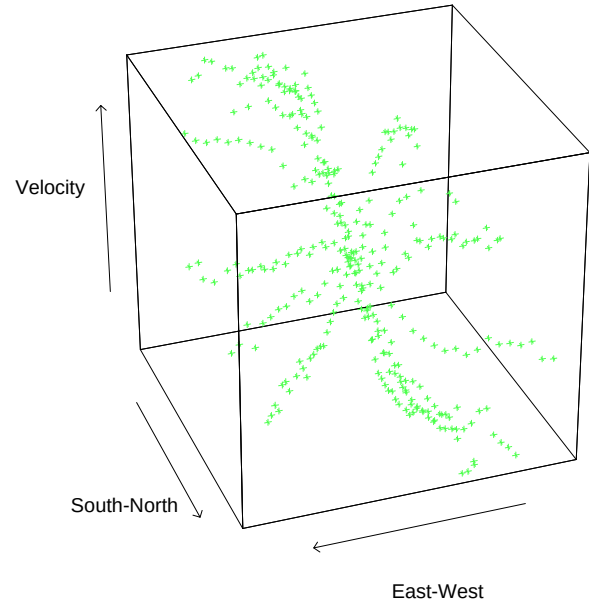


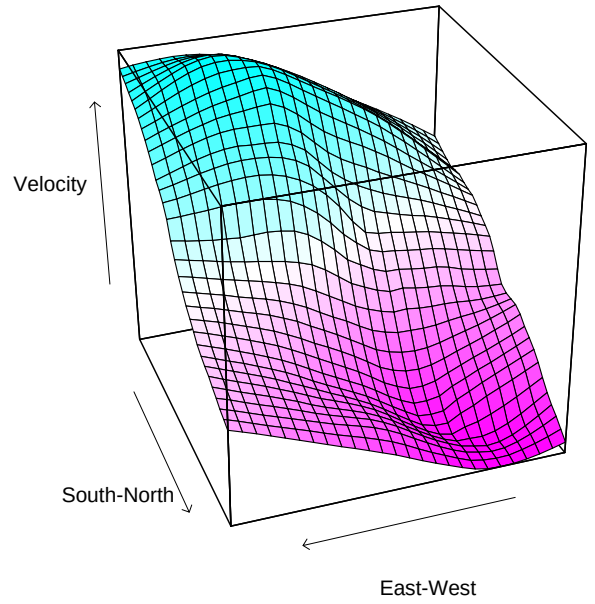
(Structured Local Regression in $\mathbb{R}^p$)

$$k_\lambda(x_0, x) = D\left(\frac{\|x - x_0\|}{h_\lambda(x_0)}\right)$$

- Structured local regression: a positive semidefinite matrix A to weigh the different coordinates:

$$k_\lambda(x_0, x) = D\left(\frac{(x - x_0)^T A(x - x_0)}{h_\lambda(x_0)}\right)$$





Computational Consideration

Kernel smoothing complexity

- Model is the entire training data set.
- The fitting is done at evaluation or prediction.
- Single observation x_0 fit is $O(N)$,
- expansion in M basis functions $O(M)$ for one evaluation, typically $M \sim O(logN)$.
- Basis function method have an initial cost at least $O(NM^2 + M^3)$.
- Smoothing parameter λ usually determined off-line by cross-validation, at cost of $O(N^2)$.
- Popular implementations of local regression *loess* is S-PLUS compute the fit exactly at M locations $O(NM)$ and interpolate to fit elsewhere ($O(M)$ per evaluation).

Linear methods for classification and their extensions

- likelihood example
- logistic regression
  - ext. logistic regression with L_1 penalty
  - ext. local likelihood
    - spline basis extension
- linear and quadratic discriminant analysis
- Local likelihood (local logistic regression)

ext. When p is Much Bigger than N.

- ext. Diagonal linear discriminant analysis
- ext. reduced rank linear discriminant analysis
- ext. Elastic net penalty

? Support Vector Machines

Probability of the data given the model

- Assume we have 15 red balls and 5 blue balls in a bag.
- Repeat 5x:
  - select a ball
  - put it back.
- The probability of the sequence red, blue, blue,red, red is $\frac{3}{4} \cdot \frac{1}{4} \cdot \frac{1}{4} \cdot \frac{3}{4} \cdot \frac{3}{4}$.
- The logarithm log_2 of the probability is $\approx -0.4 - 2 - 2 - 0.4 - 0.4 = -5.2$

Likelihood of the model given the data

- Assume we do not know the probabilities, let θ be the probability of *red*. We have following probabilities of data for different θ.

θ	red	blue	blue	red	red	
$\frac{3}{4}$	$\frac{3}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{3}{4}$	$\frac{3}{4}$	$\frac{3^3}{4^5}$

- Take the log_2 of the probabilities:

θ	red	blue	blue	red	red	
$\frac{1}{2}$	-1	-1	-1	-1	-1	-5
$\frac{3}{5}$	-0.74	-1.32	-1.32	-0.74	-0.74	-4.86
$\frac{3}{4}$	-0.4	-2	-2	-0.4	-0.4	-5.2

- Probability of the data given model is called **likelihood** of the model θ given the data.
- Maximum likelihood θ estimate is in our case $\frac{3}{5}$.
- Predicting probabilities, maximum likelihood estimate is the same as maximum log-likelihood estimate.

(Log)likelihood

train data		prediction			likelihood	loglik
x_i	g_i	$P(green\|x_i)$	$P(blue\|x_i)$	$P(yellow\|x_i)$		
1	green	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	-1
1	yellow	$\frac{1}{2}$	0	$\frac{1}{2}$	$\frac{1}{2}$	-1
2	green	$\frac{2}{3}$	$\frac{1}{3}$	0	$\frac{2}{3}$	$log_2\frac{2}{3}$
2	green	$\frac{2}{3}$	$\frac{1}{3}$	0	$\frac{2}{3}$	$log_2\frac{2}{3}$
2	blue	$\frac{2}{3}$	$\frac{1}{3}$	0	$\frac{1}{3}$	$-log_2 3$
3	blue	0	1	0	1	0
						$-2 - log_2 3$ $+2log_2\frac{2}{3}$

- **loglik** logarithm of likelihood function is defined as:

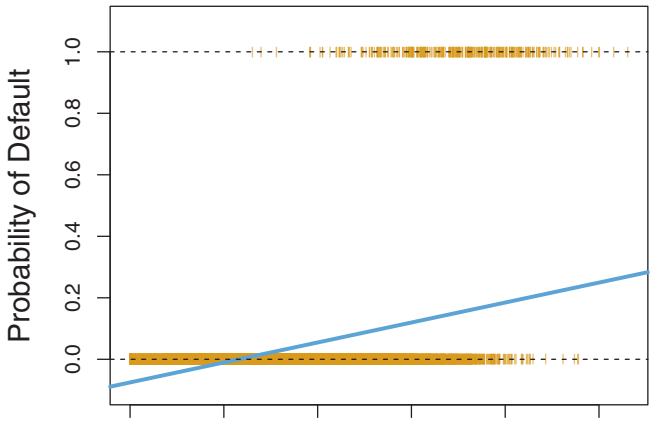
$$\ell(\theta) = \sum_{i=1}^{N} log(P(G = g_i|x_i, \theta))$$

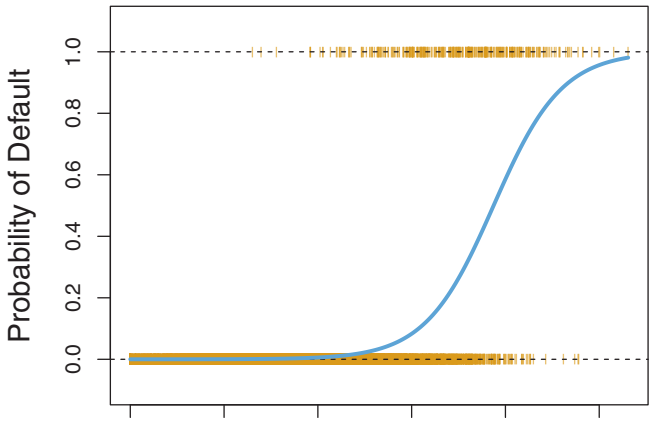
- Logistic regression uses:

$$P(G = g_k|X = x) = \frac{e^{\beta_{k0}+\beta_k^T x}}{1+\sum_{l=1,\ldots,K-1} e^{\beta_{l0}+\beta_l^T x}}.$$

Logistic Function

- Probability should be from the interval $\langle 0, 1 \rangle$.
- Linear prediction is transformed by logistic function (sigmoid) with the maximum L.
- **logistic** $\frac{L}{1+e^{-k(x-x_0)}}$.
- Inverse function is called logit.
- **logit** $\log \frac{p}{1-p}$,





Logistic Regression

- For $K-$ class classification we estimate $(p+1)\times(K-1)$ parameters $\theta = \{\beta_{10}, \beta_1^T, \ldots, \beta_{(K-1)0}, \beta_{K-1}^T\}$.

$$\begin{aligned}
\log \frac{P(G=g_1|X=x)}{P(G=g_K|X=x)} &= \beta_{10} + \beta_1^T x \\
\log \frac{P(G=g_2|X=x)}{P(G=g_K|X=x)} &= \beta_{20} + \beta_2^T x \\
&\vdots \\
\log \frac{P(G=g_{K-1}|X=x)}{P(G=g_K|X=x)} &= \beta_{(K-1)0} + \beta_{K-1}^T x
\end{aligned}$$

that is

$$p_k(x;\theta) \leftarrow P(G=g_k|X=x) = \frac{e^{\beta_{k0}+\beta_k^T x}}{1+\sum_{l=1,\ldots,K-1} e^{\beta_{l0}+\beta_l^T x}}$$

$$p_K(x;\theta) \leftarrow P(G=g_K|X=x) = \frac{1}{1+\sum_{l=1,\ldots,K-1} e^{\beta_{l0}+\beta_l^T x}}.$$

Fitting Logistic Regression Two class

- This model is estimated iteratively maximizing conditional likelihood of G given X.

$$\ell(\theta) = \sum_{i=1}^{N} \log p_{g_i}(x_i; \theta)$$

- Two class model: g_i encoded via a $0/1$ response y_i; $y_i = 1$ iff $g_k = g_1$. Let $p(x;\theta) = p_1(x;\theta)$, $p_2(x;\theta) = 1 - p(x;\theta)$. Then:

$$\begin{aligned} \ell(\theta) &= \sum_{i=1}^{N} (y_i \log p(x_i;\beta) + (1-y_i)\log(1-p(x_i;\beta)) \\ &= \sum_{i=1}^{N} (y_i \beta^T x_i - \log(1+e^{\beta^T x_i})) \end{aligned}$$

- Set derivatives to zero:

$$\frac{\partial \ell(\beta)}{\partial \beta} = \sum_{i=1}^{N} x_i (y_i - p(x_i;\beta)) = 0,$$

- which is $p+1$ nonlinear equations in β.
- First component: $x_i \equiv 1$ specifies $\sum_{i=1}^{N} y_i = \sum_{i=1}^{N} p(x_i;\beta)$ the expected

Newton–Raphson Algorithm

- We use Newton–Raphson Algorithm to solve the system of equations

$$\frac{\partial \ell(\beta)}{\partial \beta} = \sum_{i=1}^{N} x_i (y_i - p(x_i; \beta)) = 0,$$

- we need the second–derivative or Hessian matrix

$$\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} = -\sum_{i=1}^{N} x_i x_i^T p(x_i; \beta)(1 - p(x_i; \beta)).$$

- Starting with β^{old} a single Newton–Raphson update is

$$\beta^{new} = \beta^{old} - \left(\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} \right)^{-1} \frac{\partial \ell(\beta)}{\partial \beta},$$

- where the derivatives are evaluated at β^{old}.

Newton–Raphson Algorithm in Matrix Notation

Let us denote:

$\mathbf{y}$ the vector of y_i

$\mathbf{X}$ $N \times (p+1)$ data matrix x_i

$\mathbf{p}$ the vector of fitted probabilities with ith element $p(x_i; \beta^{old})$

$\mathbf{W}$ diagonal matrix with weights $p(x_i; \beta^{old})(1 - p(x_i; \beta^{old}))$

$$\frac{\partial \ell(\beta)}{\partial \beta} = \mathbf{X}^T(\mathbf{y} - \mathbf{p})$$

$$\frac{\partial^2 \ell(\beta)}{\partial \beta \partial \beta^T} = -\mathbf{X}^T\mathbf{W}\mathbf{X}$$

The Newton–Raphson step is ($\beta^0 \leftarrow 0$)

$$\begin{aligned}
\beta^{new} &= \beta^{old} + (\mathbf{X}^\mathbf{T}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{y} - \mathbf{p}) \\
&= (\mathbf{X}^\mathbf{T}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}(\mathbf{X}\beta^{old} + \mathbf{W}^{-1}(\mathbf{y} - \mathbf{p})) \\
&= (\mathbf{X}^\mathbf{T}\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\mathbf{z} \\
\mathbf{z} &= \mathbf{X}\beta^{old} + \mathbf{W}^{-1}(\mathbf{y} - \mathbf{p}) \quad \textbf{adjusted response}
\end{aligned}$$

- p, W, z change each step

This algorithm is reffered to as **iteratively reweighted least squares IRLS**

$$\beta^{new} \leftarrow \arg\min_{\beta} (\mathbf{z} - \mathbf{X}\beta)^T\mathbf{W}(\mathbf{z} - \mathbf{X}\beta)$$

South African Heart Disease

- Analyzing the risk factors of myocardian infarction MI
- prevalence 5.1%, in the data 160 positive 302 controls

TABLE 4.2. *Results from a logistic regression fit to the South African heart disease data.*

	Coefficient	Std. Error	Z Score
(Intercept)	−4.130	0.964	−4.285
sbp	0.006	0.006	1.023
tobacco	0.080	0.026	3.034
ldl	0.185	0.057	3.219
famhist	0.939	0.225	4.178
obesity	-0.035	0.029	−1.187
alcohol	0.001	0.004	0.136
age	0.043	0.010	4.184

- Wald test: Z score $|Z| > 2$ is significant at at the 5% level.

TABLE 4.3. *Results from stepwise logistic regression fit to South African heart disease data.*

	Coefficient	Std. Error	Z score
(Intercept)	−4.204	0.498	−8.45
tobacco	0.081	0.026	3.16
ldl	0.168	0.054	3.09
famhist	0.924	0.223	4.14
age	0.044	0.010	4.52

South African Heart Disease

- Wald test: Z score $|Z| > 2$ is significant at at the 5% level.

TABLE 4.3. *Results from stepwise logistic regression fit to South African heart disease data.*

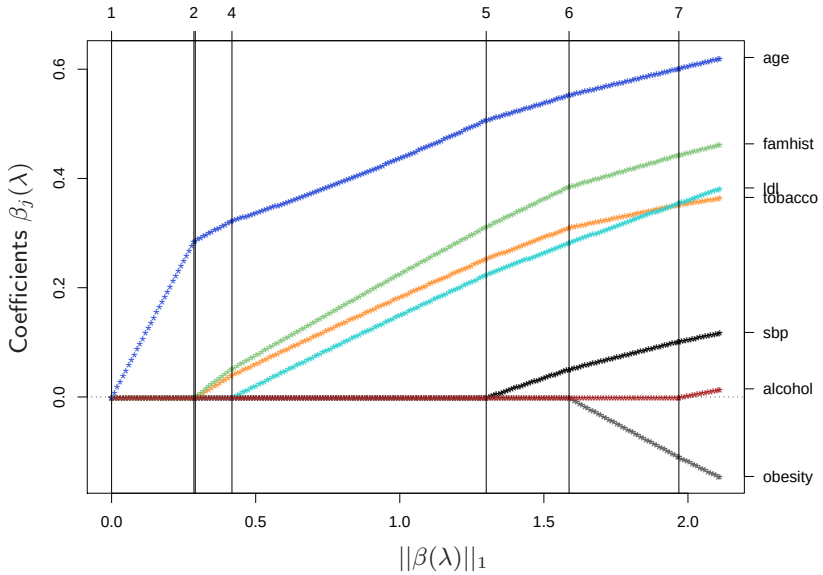
	Coefficient	Std. Error	Z score
`(Intercept)`	−4.204	0.498	−8.45
`tobacco`	0.081	0.026	3.16
`ldl`	0.168	0.054	3.09
`famhist`	0.924	0.223	4.14
`age`	0.044	0.010	4.52

- $P(MI|x_i, \theta) = \frac{e^{-4.204+0.081x_{tobacco}+0.168x_{ldl}+0.924x_{famhist}+0.044x_{age}}}{1+(e^{-4.204+0.081x_{tobacco}+0.168x_{ldl}+0.924x_{famhist}+0.044x_{age}})}$
- Interval estimate $odds_{tobacco} = e^{0.081 \pm 2 \times 0.026} = (1.03, 1.14)$ increase of odds of MI based of the increase of $x_{tobacco}$.

L_1 regularization 'Lasso'-like

$$argmax_{\beta_0,\beta}\left(\sum_{i=1}^{N}(y_i(\beta_0+\beta^T x_i)-\log(1+e^{(\beta_0+\beta^T x_i)}))-\lambda\sum_{j=1}^{p}|\beta_j|\right)$$

- Newton–Raphson Algorithm or nonlinear programming.
- $\lambda = 0$ standard logistic regression.
- $\lambda \to \infty$ moves coefficients towards 0.
- β_0 is not included into the penalty.

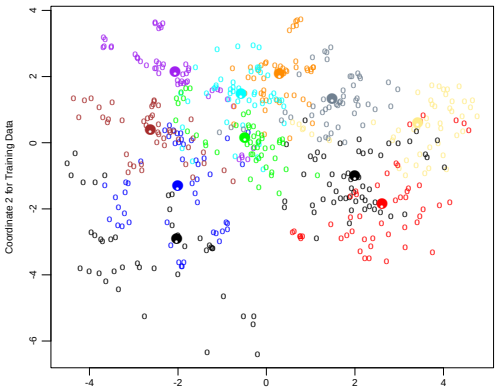


Linear Discriminant Analysis

- LDA assumes multivariate gaussian distribution of each class with a common covariance matrix.

$$\phi(k) = \frac{1}{\sqrt{|2\pi\Sigma|}} e^{-\frac{1}{2}(x-\mu_k)^T\Sigma^{-1}(x-\mu_k)}$$

  - Under this assumptions it provides bayes optimal estimate.
- Different covariance matrix for each class leads to Quadratic Discriminant Analysis.
- Let us denote N_k number of training data in the class G_k.



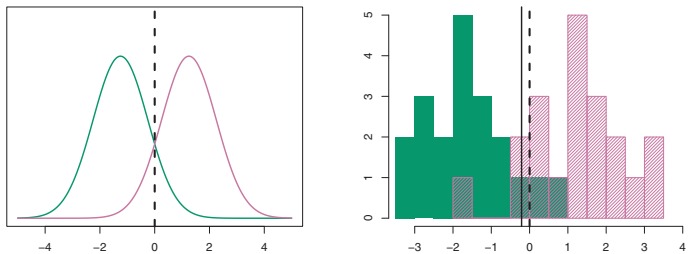


FIGURE 4.4. Left: *Two one-dimensional normal density functions are shown.*

Linear Discriminant Analysis

The LDA model parameters: the mean and probability of each class $\{\mu_i, \pi_i\}_{i=1}^K$ and the common covariance matrix Σ can be evaluated directly.

$$
\begin{aligned}
\hat{\pi}_k &= \frac{N_k}{N} \\
\hat{\mu}_k &= \frac{\sum_{\{x_i : G(x_i) = g_k\}} x_i}{N_k} \\
\hat{\Sigma} &= \sum_{k=1}^{K} \sum_{\{x_i : G(x_i) = g_k\}} \frac{(x_i - \mu_k)(x_i - \mu_k)^T}{(N - K)} \\
\phi_k(x) &= N(\mu_k, \Sigma) \\
P(G = g_k | X = x) &= \frac{\phi_k(x)\pi_k}{\sum_{\ell=1}^{K} \phi_\ell(x)\pi_\ell}
\end{aligned}
$$

To classify new instance x we predict the G_k with maximal δ_k:

$$\delta_k(x) = x^T \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^T \Sigma^{-1} \mu_k + log \pi_k$$

Linear Discriminant Analysis

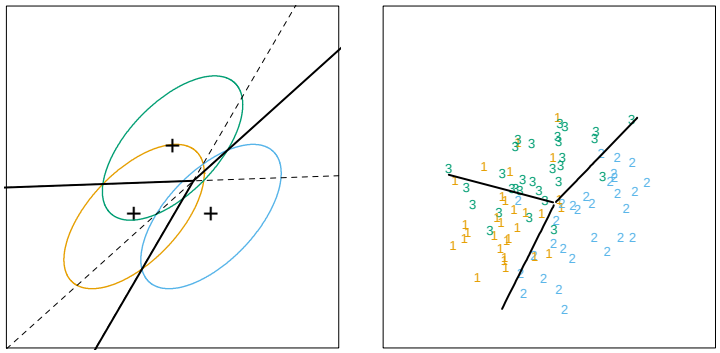


FIGURE 4.5. *The left panel shows three Gaussian distributions, with the same covariance and different means. Included are the contours of constant density*

Example Vovel data ESL $X \in \mathbb{R}^{10}$:

	train	test
Linear regression	0.48	0.67
Linear discriminant analysis	0.32	0.56
Quadratic discriminant analysis	0.01	0.53
Logistic regression	0.22	0.51

Notes: Common covariance matrix, masking.

Quadratic Discriminant Analysis

Quadratic discriminant analysis estimates the covariance matrix for each class independently. The rest is the same as for the LDA.

$$
\begin{aligned}
\hat{\pi}_k &= \frac{N_k}{N} \\
\hat{\mu}_k &= \frac{\sum_{\{x_i : G(x_i) = g_k\}} x_i}{N_k} \\
\hat{\Sigma}_k &= \sum_{\{x_i : G(x_i) = g_k\}} \frac{(x_i - \mu_k)(x_i - \mu_k)^T}{(|G_k| - 1)} \\
f_k(x) &= N(\mu_k, \Sigma_k) \\
P(G = g_k | X = x) &= \frac{f_k(x)\pi_k}{\sum_{\ell=1}^{K} f_\ell(x)\pi_\ell}
\end{aligned}
$$

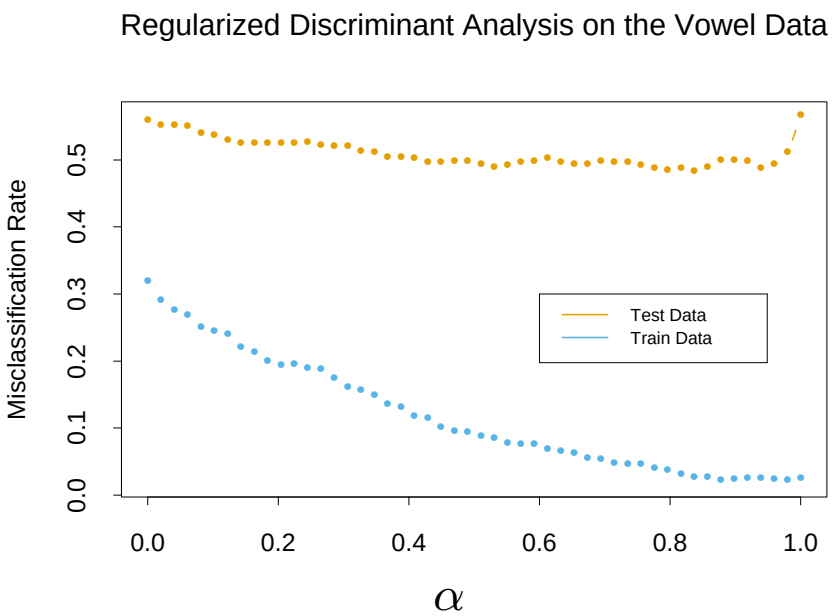
To classify new instance x we predict the G_k with maximal δ_k:

$$
\delta_k(x) = -\frac{1}{2}(x - \mu_k)^T \Sigma_k^{-1}(x - \mu_k) - \frac{1}{2}\log|\Sigma_k| + \log \pi_k
$$

Quadratic and Regularized Discriminant Analysis

- QDA has substantially more parameters. It is questionable whether it is worth to increase the model complexity.
  - LDA parameters: $(K-1) \times (p+1)$
  - QDA parameters: $(K-1) \times (\frac{p(p+3)}{2} + 1)$.
- **Regularized discriminant analysis** takes a weighted average of LDA and QDA to tune the model complexity.

$$\hat{\Sigma}_k(\alpha) = \alpha\hat{\Sigma}_k + (1-\alpha)\hat{\Sigma}$$



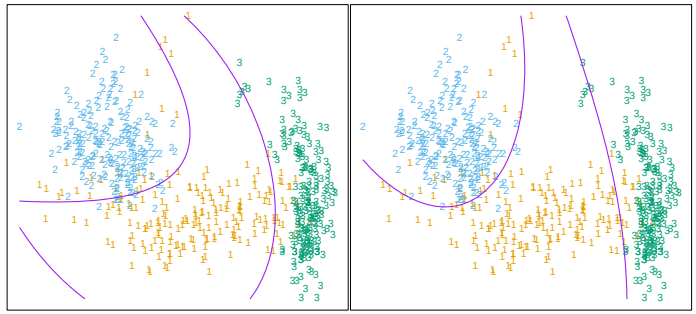


FIGURE 4.6. *Two methods for fitting quadratic boundaries. The left plot shows the quadratic decision boundaries for the data in Figure 4.1 (obtained using LDA in the five-dimensional space $X_1, X_2, X_1X_2, X_1^2, X_2^2$). The right plot shows the*

Computations for LDA

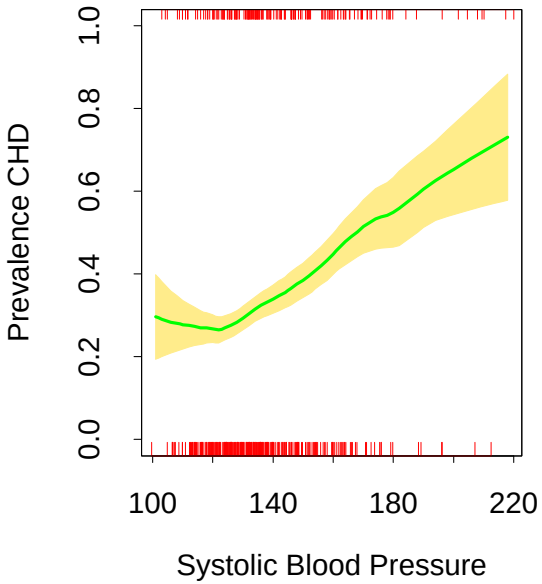
Linear and Quadratic Discriminant Analysis

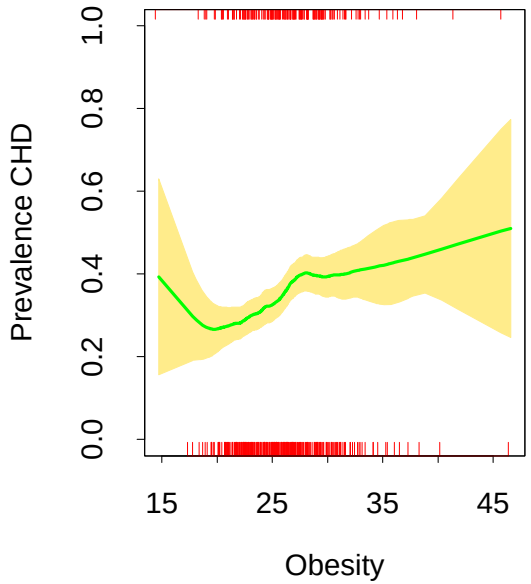
- $O(N^3)$, often $O(N^{2.376})$
- QDA and LDA may be computed using matrix decomposition:
  - Compute the eigendecomposition for each $(x - \hat{\mu}_k)^T \hat{\Sigma}_k^{-1} (x - \hat{\mu}_k) = [\mathbf{U}_k^T (x - \hat{\mu}_k)]^T \mathbf{D}_k^{-1} [\mathbf{U}_k^T (x - \hat{\mu}_k)]$
  - $\log |\hat{\Sigma}_k| = \sum_\ell \log d_{k\ell}$.
- Using this decomposition, LDA classifier can be implemented by the following pair of steps:
  - *Sphere* the data with respect to the common covariance estimate $\hat{\Sigma}$: $X^* \leftarrow \mathbf{D}^{-\frac{1}{2}} \mathbf{U}^T X$, where $\hat{\Sigma} = \mathbf{U}\mathbf{D}\mathbf{U}^T$.
    The common covariance estimate of X^* will now be the identity.
  - Classify to the closest class centroid in the transformed space, modulo the effect of the class prior probabilities π_k.

Local Likelihood and other methods

- Logistic and log-linear models involve the covariates in a linear fashion.
- We fit the model locally at x_0 and weight the loglik by the kernel k_λ
- and center the estimate at x_0.

$$\begin{aligned}\ell(\beta_{x_0}) &= \sum_{i=1}^{N} k_\lambda(x_0, x_i)\ell(y_i, (x - x_0)^T \beta_{x_0}) \\ &= \sum_{i=1}^{N} k_\lambda(x_0, x_i)\left\{y_i \beta_{x_0}^T (x_i - x_0) - \log(1 + e^{\beta_{x_0}^T (x_i - x_0)})\right\}\end{aligned}$$





Note: Increased prevalence for small values due to retrospective data: some people with diagnosed CHD started more healthy life.

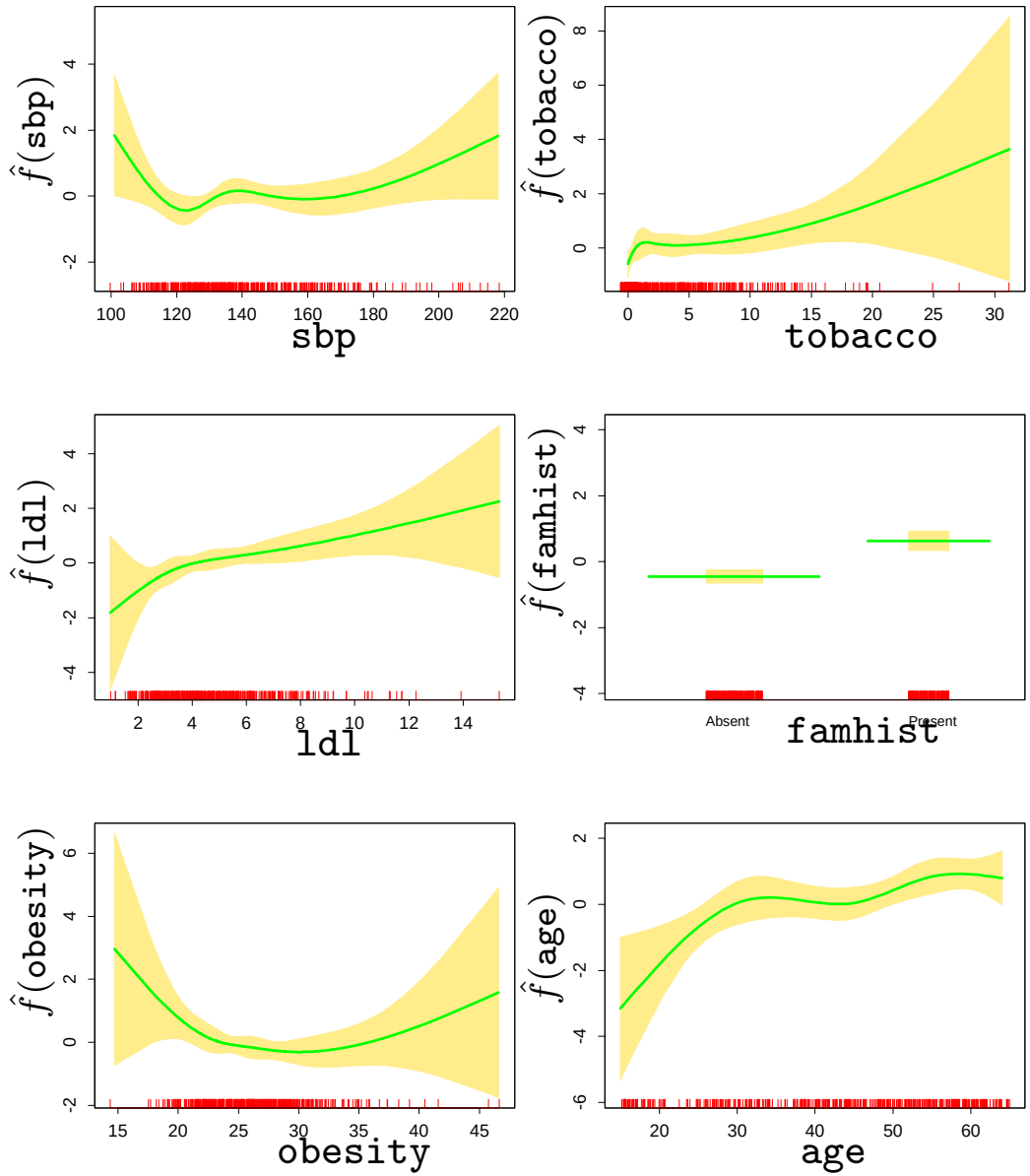
South African Heart Disease continued

- Each feature X_j is approximated by a natural spline.
- The overall model is:

$$logit[P(CHD|X)] = \theta_0 + h_1(X_1)^T\theta_1 + h_2(X_2)^T\theta_2 + \ldots + h_p(X_p)^T\theta_p$$

- θ_j are vectors of coefficients multiplying their associated vector of natural spline basis functions h_j
- four basis functions (three inner knots) per spline in this example.
- binary *familyhist* with a single coefficient.
- Combine all p vectors of basic functions into one big vector $h(X)$, $df = 1 + \sum_{j=1}^{p} df_j$
- each basis function is evaluated at each of the N samples
- resulting in a $N \times df$ basis matrix $\mathbf{H}$.
- and use 'standard' logistic regression.

- Alcohol not significant by AIC test
- covariance $Cov(\hat{\theta})$ is estimated by $\hat{\Sigma} = (\mathbf{H^T W H})^{-1}$
  - W the diagonal weight matrix
- variance of a single variable j is:
  - $v_j(X_j) = Var[f_j(X_j)] = h_j(X_j)^T \hat{\Sigma}_{jj} h_j(X_j)$
- error bounds $\hat{f}_j(X_j) \pm 2\sqrt{v_j(X_j)}$.



Summary

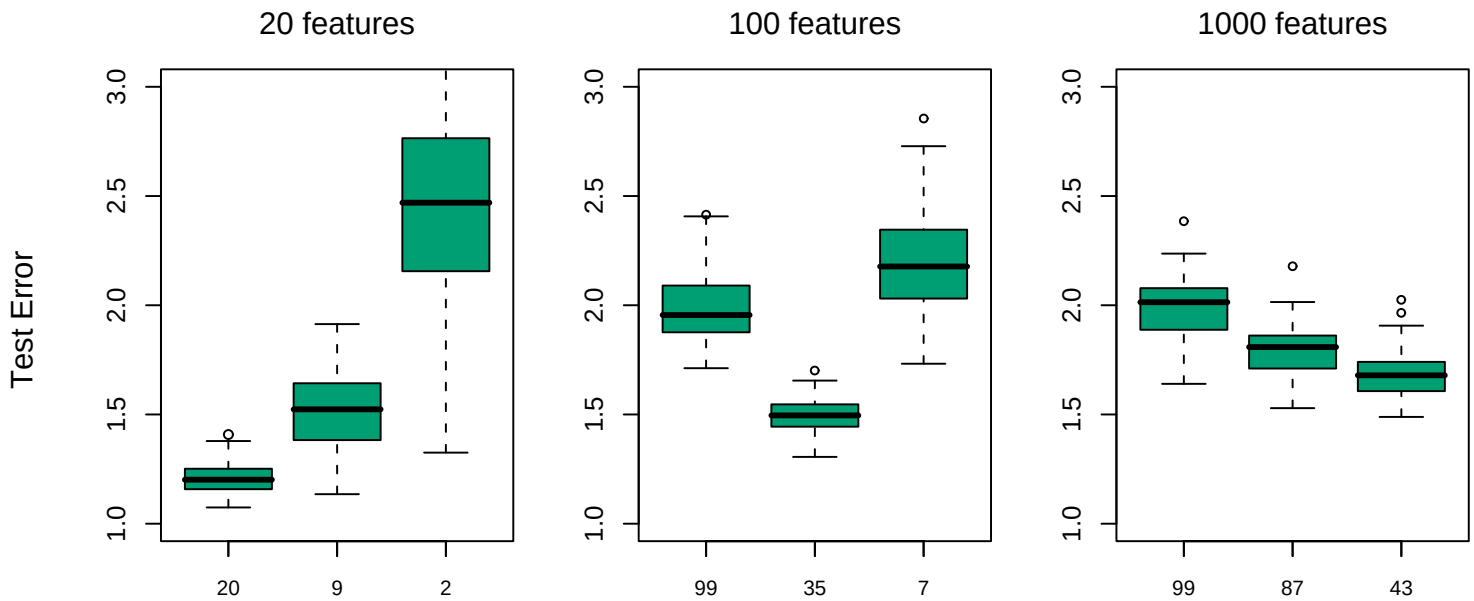
- likelihood example
- logistic regression
- linear and quadratic discriminant analysis
- (logistic regression with L_1 penalty and other advanced methods).

When p is Much Bigger than N

- Simulated experiments (ridge regression models):
  - $N = 100$
  - $p = 20, 100$ and 1000 with standard Gaussian distribution with pairwise correlation 0.2

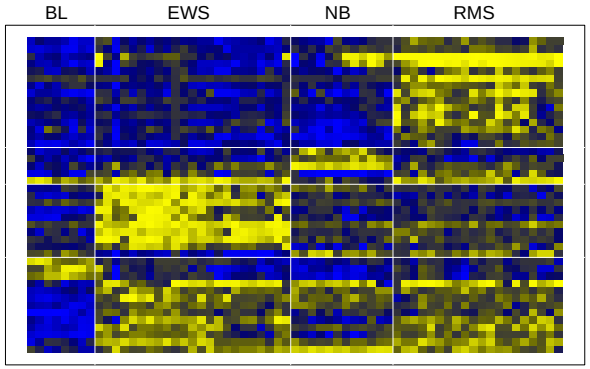
$$Y = \sum_{j=1}^{p} X_j \beta_j + \sigma\varepsilon$$

  - β_j with standard Gaussian distribution
  - σ to make signal-to-noise ratio $Var[\mathbb{E}(Y|X)]/\sigma^2 = 2$.
  - The (average) number of significant coefficients was 9, 33 and 331.



Diagonal Linear Discriminant Analysis

- Gene expression experiment
  - 2308 genes (columns)
  - 63 samples (rows), from a set of microarray experiments.
  - The samples arose from small, round blue-cell tumors (SRBCT) found in children, and are classified into four major types:
    - BL (Burkitt lymphoma),
    - EWS (Ewing's sarcoma),
    - NB (neuroblastoma),
    - and RMS (rhabdomyosarcoma).
  - There is an additional test data set of 20 observations.

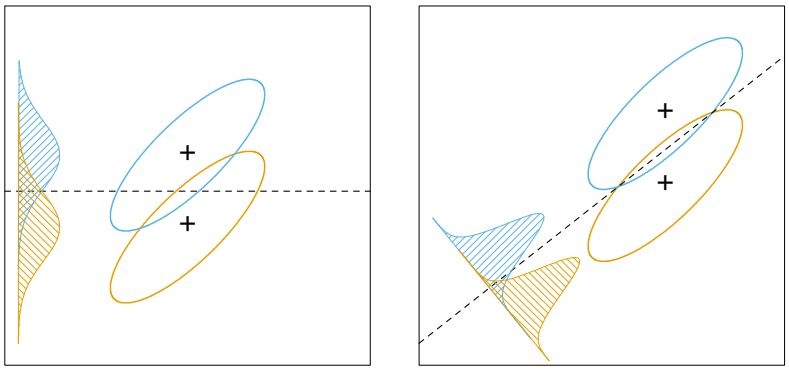


- diagonal-covariance LDA

$$\delta_k(x^*) = -\sum_{j=1}^{p} \frac{(x_j^* - \overline{x}_{jk})^2}{s_j^2} + 2\log(\pi_k)$$

- s_j is the pooled within-class standard deviation of the jth gene
- $\overline{x}_{jk} = \sum_{i \in C_k} \frac{x_{ij}}{N_k}$
- $\tilde{x}_k = (\bar{x}_{1k}, \ldots, \bar{x}_{jk}, \ldots, \overline{x}_{pk})^T$ is the k class centroid.

Reduced–Rank Linear Discriminant Analysis

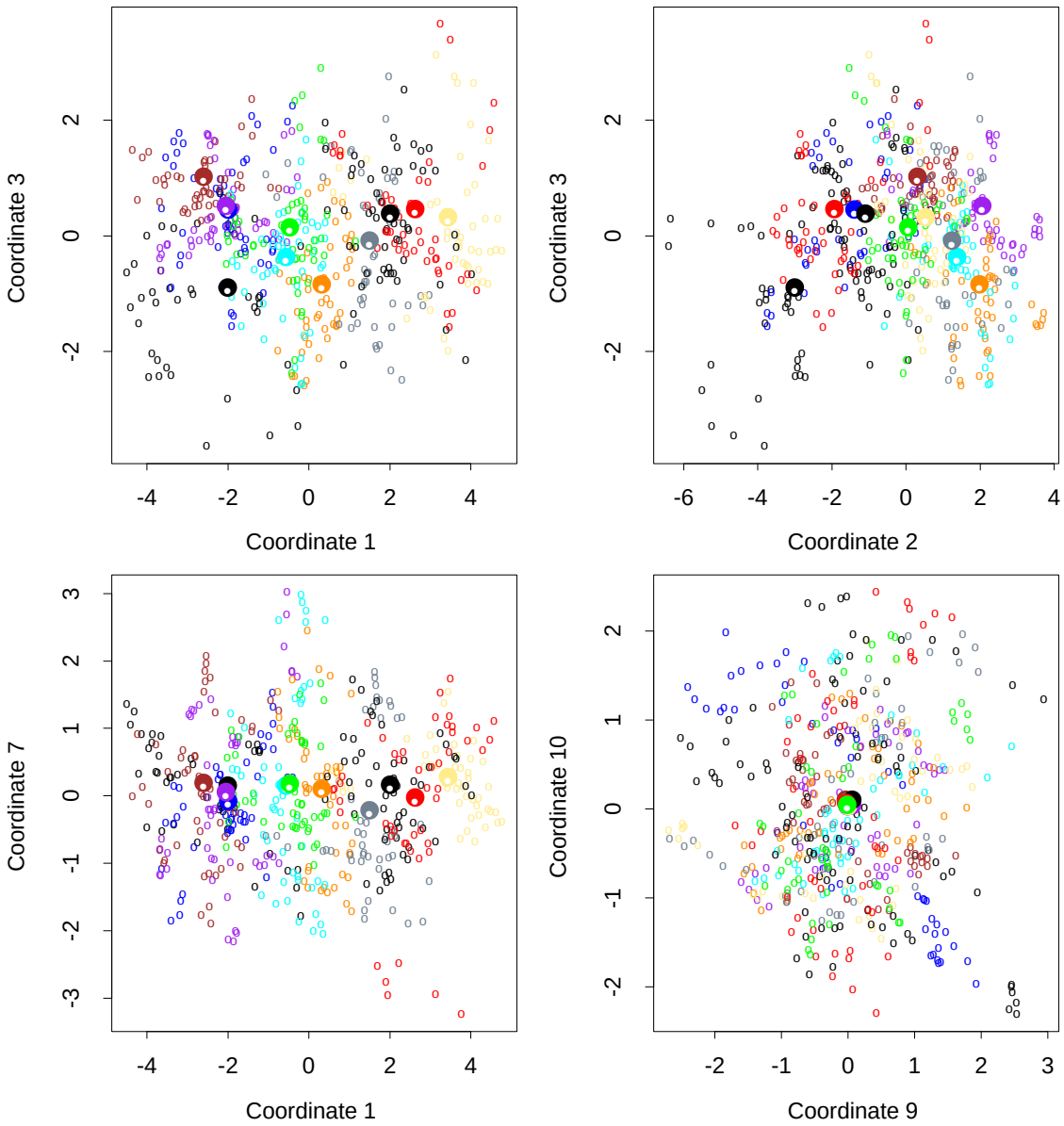


$$max_a \frac{a^T B a}{a^T W a}$$

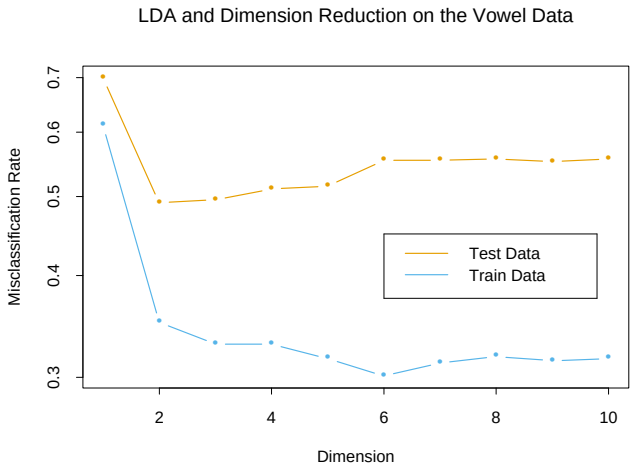
Finding the sequence of optimal subspaces for LDA:

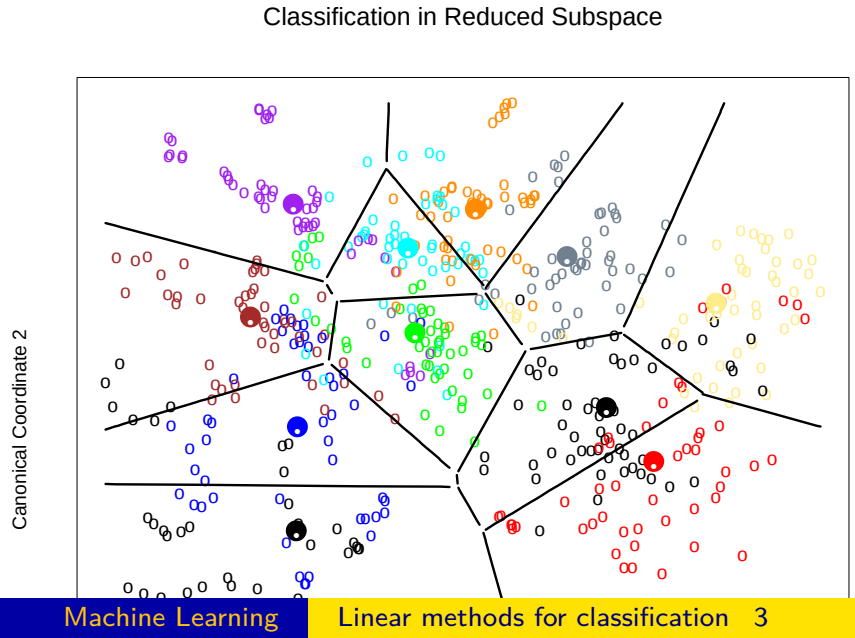
- compute the $K \times p$ matrix of class centroids M and the common covariance matrix W (**within–class** covariance);
- compute $M^* = MW^{-\frac{1}{2}}$ using the eigen–decomposition of W;
- compute B^* **between–class** covariance, the covariance matrix of M^* and its eigen–decomposition $B^* = V^* D_B V^{*T}$.
  - order D_B in the decreasing order
  - v_ℓ^* of V^* in sequence define the coordinates of the optimal subspaces
  - $Z_\ell = v_\ell^T X$ with $v_\ell = W^{-\frac{1}{2}} v_\ell^*$.

Reduced–Rank Linear Discriminant Analysis



Vovel Example

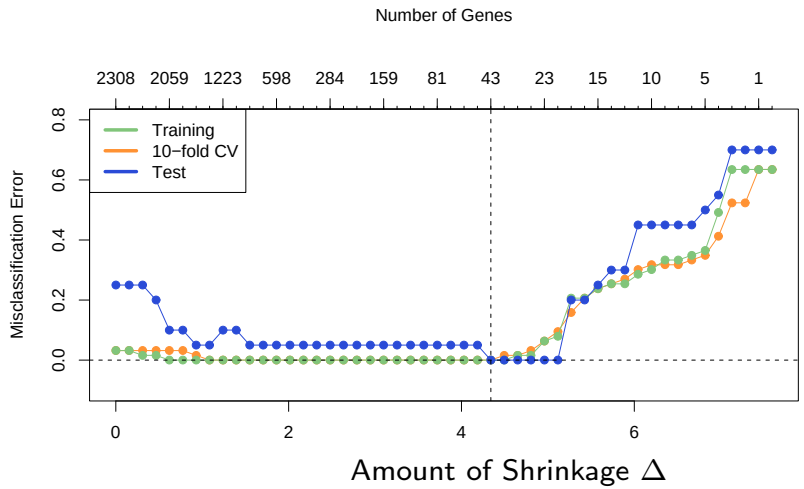


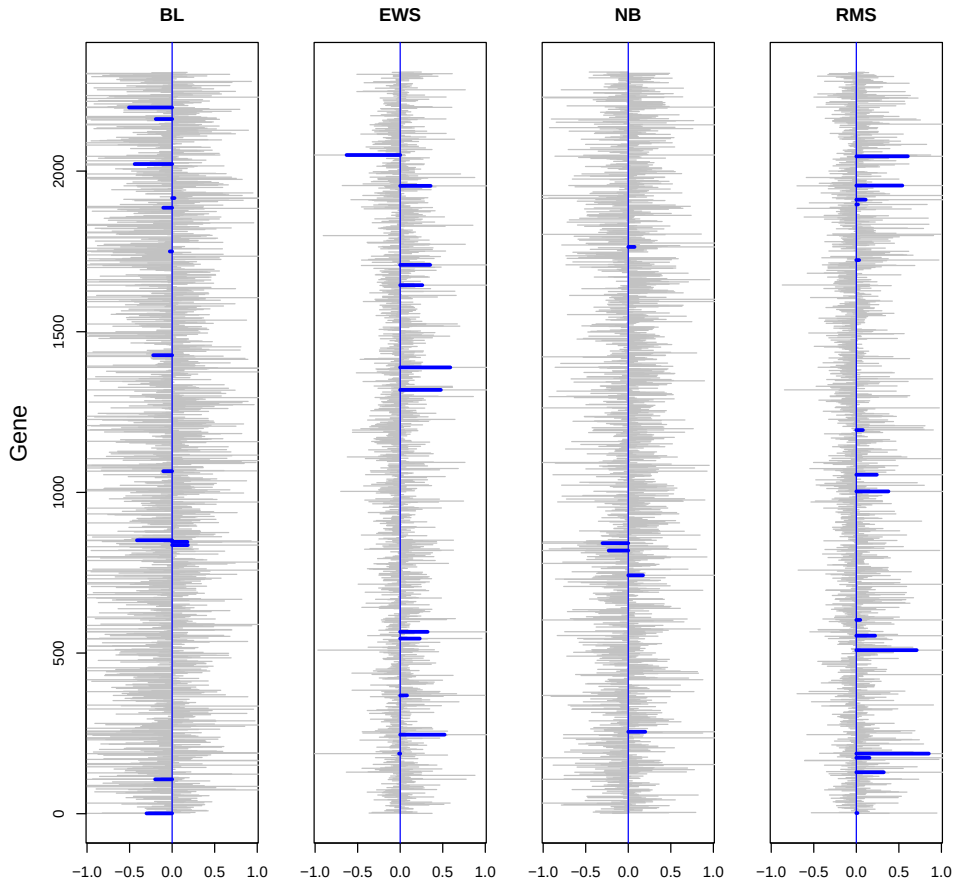


And many other models

- Elastic net penalty

$$max_{\{\beta_{0k},\beta_k\in\mathbb{R}^p\}_1^K}\left[\sum_{i=1}^{N}\log P(g_i|x_i)-\lambda\left(\sum_{k=1}^{K}\sum_{j=1}^{p}(\alpha|\beta_{kj}|+(1-\alpha)\beta_{kj}^2)\right)\right]$$

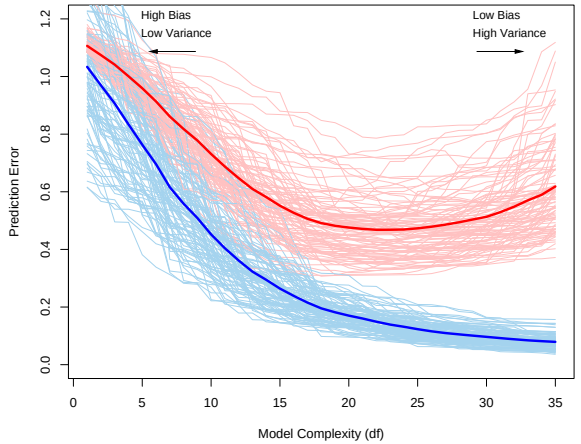




Centroids: Average Expression Centered at Overall Centroid

Model Assessment and Selection

- We assume i.i.d. data
  - independently (independent samples)
  - identically (the same distribution)
  - distributed
- Assume many iid datasets
  - 1 line= train/test curve for 1 set of samples (data)
  - data used to fit the model
    Training error is
    $\overline{err} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$,
  - data not used to fit the model
    Test error is
    $err = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$,
  - Test error is a point estimate of the generalization error.
  - Dark red line is an average of test errors, a more robust estimate.



Definition (Generalization error)

Generalization error is the expected prediction error over an independent test sample

$$Err = \mathbb{E}[L(Y, \hat{f}(X))]$$

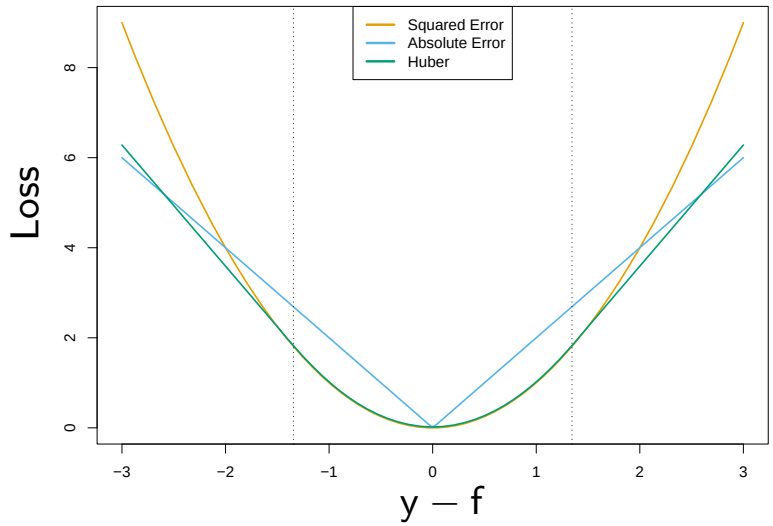
where both X and Y are drawn randomly from their joint distribution (population).

Loss functions for regression

Definition

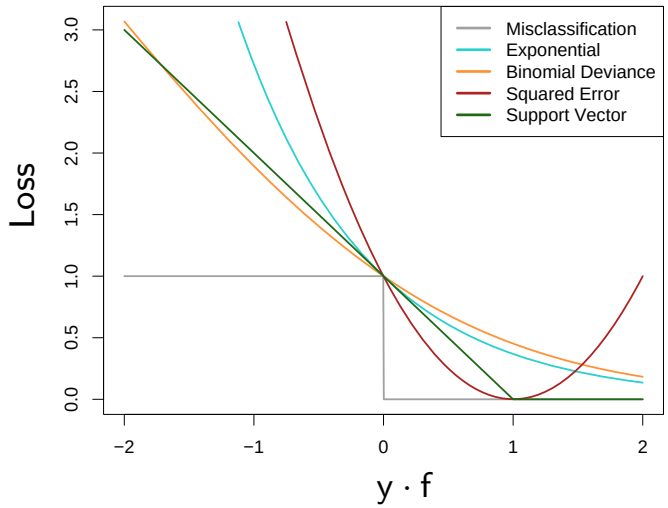
- **Square error loss** $L(y, \hat{y}) = (y - \hat{y})^2$
- **Absolute error loss** $L(y, \hat{y}) = |y - \hat{y}|$
- **Huber error loss**

$$L_\delta(y, \hat{y}) = \begin{cases} \frac{1}{2}(y - \hat{y})^2 & \text{for } |y - \hat{y}| \leq \delta, \\ \delta|y - \hat{y}| - \frac{1}{2}\delta^2, & \text{otherwise.} \end{cases}$$



Classifier Assessment and Selection

- Qualitative response G taking one of K values labeled as $1, \ldots, K$.
- Typically $\hat{G}(X) = \arg\max_k \hat{p}_k(X)$.



Definition (Loss functions for classification)

- **0-1 loss, misclassification**

$$L(G, \hat{G}(X)) = I(G \neq \hat{G}(X))$$

- **log-likelihood, cross-entropy, deviance**

$$L(G, \hat{p}(X)) = -2I(G = k) \log \hat{p}_k(X)$$

- two classes encoded $\{-1, +1\}$
  - **exponential**

$$e^{-yf}$$

  - **support vector**

$$max(0, 1 - yf(x))$$

- Non-negative loss matrix $L \in \mathbb{R}^{K \times K}$ with 0 on the diagonal.

Data Rich Situation

If we have enough data, we split the dataset

- **Train** train the model
- **Validate** select appropriate model parameter α, λ, usually the model complexity, cost penalty
- **Test** estimate the test error on an independent sample.

Recommended ratios:

- $\frac{1}{2} : \frac{1}{4} : \frac{1}{4}$ with the validation set
- $\frac{2}{3} : \frac{1}{3}$ without the validation need.

Stratified Selection

- Assume small disease prevalence.
  - We split the data healthy/sick and split each group separately.
- Consider a model over different branches of your company:
  - to estimate a new branch, all data from some branches should be selected as test ones
  - not a random sample from each branch.

Other methods only since we almost never have enough of the data.

Error Estimation with a few data

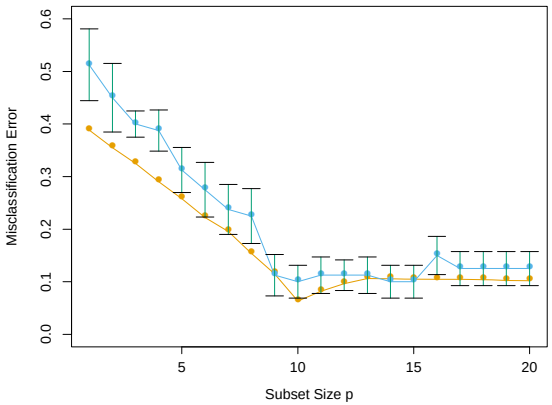
Amount of data needed depends on:

- true function complexity
- the noise ratio.

The estimation method depends on the purpourse:

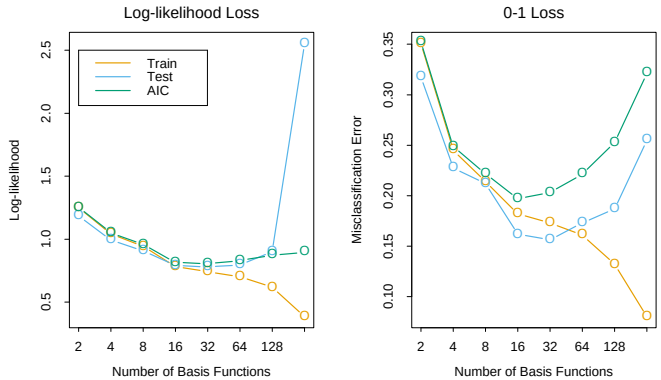
Model selection

- absolute value is not necessary, the difference is crucial
- any method can be used (AIC, BIC, cross-validation,...)



Test error estimation

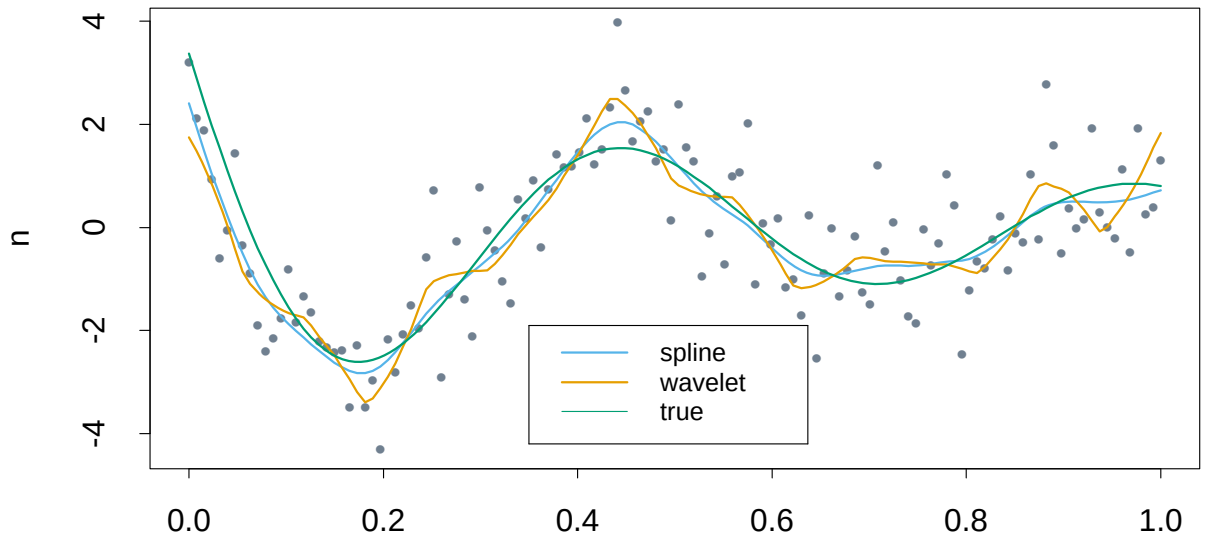
- absolute value is necessary
- direct estimation (cross-validation, one-leave-out) preferred.



Bias Variance Decomposition

- Assume $Y = f(X) + \epsilon$ where $\mathbb{E}(\epsilon) = 0$ and $Var(\epsilon) = \sigma_\epsilon^2$.
- we derive the expected prediction error of the regression fit $\hat{f}(X)$ at an input point $X = x_0$ using squared-error loss:

$$\begin{aligned} Err(x_0) &= \mathbb{E}[(Y - \hat{f}(x_0))^2 | X = x_0] \\ &= \sigma_\epsilon^2 + [\mathbb{E}\hat{f}(x_0) - f(x_0)]^2 + \mathbb{E}[\hat{f}(x_0) - \mathbb{E}\hat{f}(x_0)]^2 \\ &= \sigma_\epsilon^2 + Bias^2(\hat{f}(x_0)) + Var(\hat{f}(x_0)) \\ &= \text{Irreducible Error} + \text{Bias}^2 + \text{Variance}. \end{aligned}$$



Bias Variance Decomposition

K-Nearest neighbour

$$\begin{aligned} Err(x_0) &= \mathbb{E}[(Y - \hat{f}(x_0))^2 | X = x_0] \\ &= \sigma_\epsilon^2 + [\mathbb{E}\hat{f}(x_0) - f(x_0)]^2 + \mathbb{E}[\hat{f}(x_0) - \mathbb{E}\hat{f}(x_0)]^2 \\ &= \sigma_\epsilon^2 + [f(x_0) - \frac{1}{k}\sum_{\ell=1}^{k} f(x_{(\ell)})]^2 + \frac{\sigma_\epsilon^2}{k}. \end{aligned}$$

Linear fit

$$\begin{aligned} Err(x_0) &= \mathbb{E}[(Y - \hat{f}(x_0))^2 | X = x_0] \\ &= \sigma_\epsilon^2 + [\mathbb{E}\hat{f}_p(x_0) - f(x_0)]^2 + \|\mathbf{h}(x_0)\|\sigma_\epsilon^2 \\ \mathbf{h}(x_0)\mathbf{y} &= (x_0^T(\mathbf{X}^\mathbf{T}\mathbf{X})^{-1}\mathbf{X}^\mathbf{T})\mathbf{y} = \hat{f}_p(x_0). \end{aligned}$$

- hence $Var[\hat{f}_p(x_0)] = \|\mathbf{h}(x_0)\|\sigma_\epsilon^2$ and its average is $\frac{p}{N}\sigma_\epsilon^2$, hence

$$\frac{1}{N}\sum_{i=1}^{N} Err(x_i) = \sigma_\epsilon^2 + \frac{1}{N}\sum_{i=1}^{N}[f(x_i) - \mathbb{E}\hat{f}(x_i)]^2 + \frac{p}{N}\sigma_\epsilon^2,$$

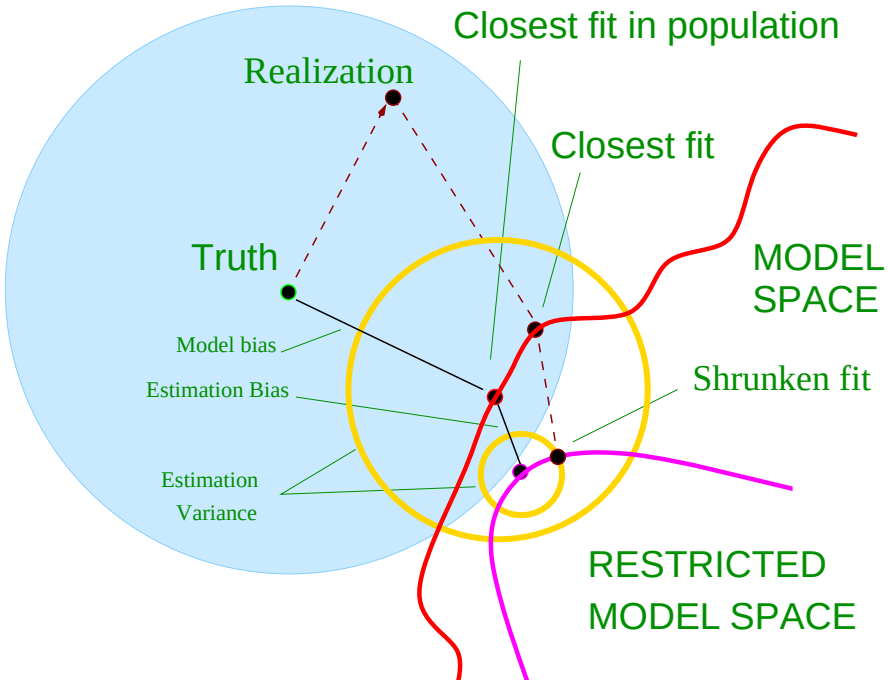
Penalized model complexity

- Consider ridge regression fit $\hat{f}_\alpha(x_0)$ with the fit

$$\mathbf{h}(x_0)\mathbf{y} = x_0^T(\mathbf{X}^\mathbf{T}\mathbf{X} + \alpha I)^{-1}\mathbf{X}^\mathbf{T}\mathbf{y}$$

- we break the bias more finely. Let β_* be the fit with $\alpha = 0$, $\beta_* = \arg\min_\beta \mathbb{E}(f(X) - \beta^T X)^2$.

$$\begin{aligned}\mathbb{E}_{x_0}[f(x_0) - \mathbb{E}\hat{f}_\alpha(x_0)]^2 &= \mathbb{E}_{x_0}[f(x_0) - \beta_*^T x_0]^2 + \mathbb{E}_{x_0}[\beta_*^T x_0 - \mathbb{E}\hat{\beta}_\alpha^T x_0]^2 \\ &= Ave[\text{Model Bias}]^2 + Ave[\text{Estimation Bias}]^2.\end{aligned}$$



Example: Bias-Variance Tradeoff

- 50 observations, 20 predictors, uniformly distributed in the hypercube $[0,1]^{20}$.

Left Y is 0 if $X_1 \leq \frac{1}{2}$ and 1 if $X_1 > \frac{1}{2}$ and we apply k-NN

Right Y is 1 if $\sum_{j=1}^{10} X_j > 5$ and 0 otherwise, and we use best subset linear regression of size p.

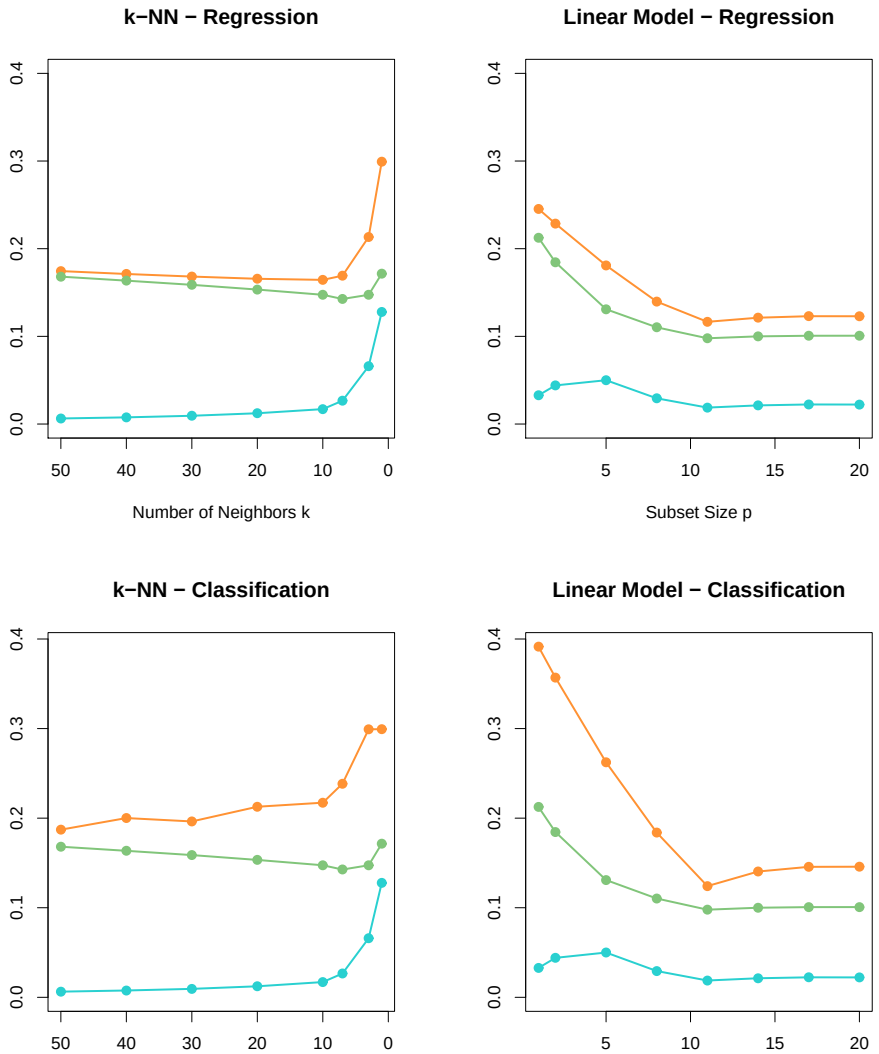


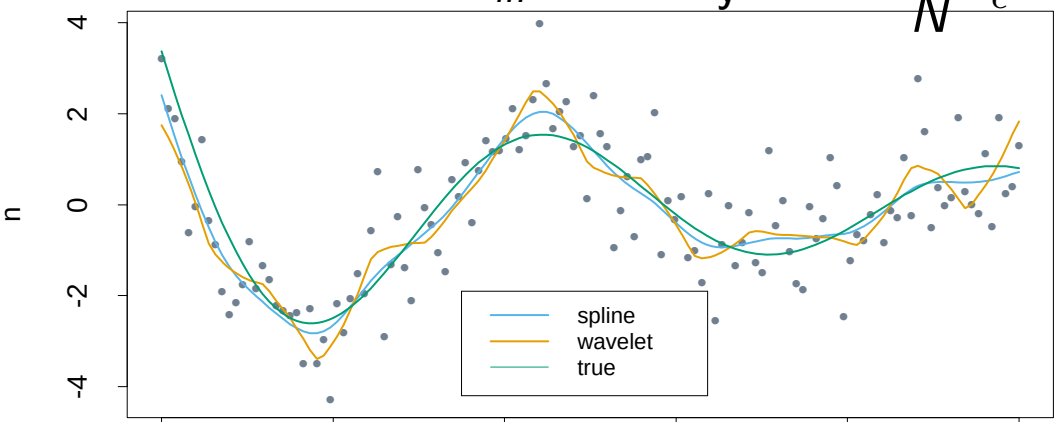
Fig. 7.3.

Optimism of the Training Error Rate

- **training error** $\overline{err} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$
- usually less than the true error $Err = \mathbb{E}[L(Y, \hat{f}(X))]$.
- we keep x_i points fixed, we take new sample of $\mathbf{y}$ at these points.
- **in-sample error** $Err_{in} = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_{\mathbf{y}}\mathbb{E}_{Y^{new}} L(Y_i^{new}, \hat{f}(x_i))$.
- **optimism** $op \leftarrow Err_{in} - \mathbb{E}_{\mathbf{y}}(\overline{err})$.
- for squared error, 0-1, and other loss functions: $op = \frac{2}{N}\sum_{i=1}^{N} cov(\hat{y}_i, y_i)$
- For a linear fit with $d = p$ inputs of basis functions and additive error model $Y = f(X) + \epsilon$ it simplifies

$$\sum_{i=1}^{N} cov(\hat{y}_i, y_i) = d\sigma_\epsilon^2$$

$$Err_{in} = \mathbb{E}_{\mathbf{y}}\overline{err} + 2\frac{d}{N}\sigma_\epsilon^2 = C_p = AIC_{gauss}..$$



The Optimism (Just for fun)

$$y_i - \hat{y}_i = (y_i - f(x_i)) + (f(x_i) - \mathbb{E}\hat{f}(x_i)) + (\mathbb{E}\hat{f}(x_i) - \hat{y}_i).$$

- We get six terms of the sum of squares:

$A_1 = \sum_i (y_i - f(x_i))^2$ $\quad$ $D_1 = 2\sum_i (y_i - f(x_i))(f(x_i) - \mathbb{E}\hat{f}(x_i))$

$B = \sum_i (f(x_i) - \mathbb{E}\hat{f}(x_i))^2$ $\quad$ $E = 2\sum_i (f(x_i) - \mathbb{E}\hat{f}(x_i))(\mathbb{E}\hat{f}(x_i) - \hat{y}_i)$

$C = \sum_i (\mathbb{E}\hat{f}(x_i) - \hat{y}_i)^2$ $\quad$ $F_1 = 2\sum_i (y_i - f(x_i))(\mathbb{E}\hat{f}(x_i) - \hat{y}_i)$

- For the new sample Y, taking the expectation.
- $A_2 = \sum_i \mathbb{E}_{Y^0}(Y_i^0 - f(x_i))^2$
- and similarly D_2, F_2.

$$\begin{aligned} N(Err_{in} - \overline{err}) &= (A_2 + B + C + D_2 + E + F_2) - (A_1 + B + C + D_1 + E + F_1) \\ &= (A_2 - A_1) + (D_2 - D_1) + (F_2 - F_1) \end{aligned}$$

- $\mathbb{E}(A_1) = \mathbb{E}(A_2) = N\sigma_\epsilon^2$,
- $\mathbb{E}(D_1) = 2\sum_i (\mathbb{E}(y_i) - f(x_i))(f(x_i) - \mathbb{E}\hat{f}(x_i)) = 0$ since $\mathbb{E}(y_i) = f(x_i)$
- $\mathbb{E}(D_2) = 0$ as well.
- $F_2 = 2\sum_i (\mathbb{E}_{Y^0}\left[(Y_i^0 - f(x_i))(\mathbb{E}\hat{f}(x_i) - \hat{y}_i)\right] = 0$
  - as $\mathbb{E}(Y^0) = f(x_i)$ and Y_i^0 and $\hat{y}_i$ are independent.
- $\mathbb{E}(F_1) = -2\sum_i^N cov(y_i, \hat{y}_i)$.

The Covariance (Just for fun)

$$\begin{aligned} cov(\hat{\mathbf{y}}, \mathbf{y}) &= cov((\mathbf{X}(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}})\mathbf{y}, \mathbf{y}) = (\mathbf{X}(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathbf{T}})cov(\mathbf{y}, \mathbf{y}) \\ cov(y, y) &= \sigma_\epsilon^2. \end{aligned}$$

- The values $cov(\hat{y}_i, y_i)$ are the diagonal values of the above matrix $cov(\hat{\mathbf{y}}, \mathbf{y})$. Thus

$$\begin{aligned} \sum_{i=1}^{N} cov(\hat{y}_i, y_i) &= trace(\mathbf{X}(\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}(\mathbf{X}^T))\sigma_\epsilon^2 \\ &= trace((\mathbf{X}^{\mathbf{T}}\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{X}))\sigma_\epsilon^2 \\ &= trace(I_d)\sigma_\epsilon^2 = d\sigma_\epsilon^2. \end{aligned}$$

- Similarly,

$$\sum_{i=1}^{N} cov(\mathbf{S}_\lambda y_i, y_i) = trace(\mathbf{S}_\lambda).$$

https://www.waxworksmath.com/Authors/G_M/Hastie/WriteUp/Weatherwax_Epstein_Hastie_Solution_Manual.pdf

AIC Akaike Information Criterion

Definition (AIC)

The **AIC Akaike Information Criterion** is defined

- Logistic regression, binomial log likelihood

$$AIC = -\frac{2}{N} loglik + 2\frac{d}{N}.$$

- Gaussian model with variance σ_ϵ^2

$$AIC(\alpha) = \overline{err(\alpha)} + 2\frac{d(\alpha)}{N}\sigma_\epsilon^2.$$

the sum of the training error $\overline{err(\alpha)}$ and the complexity penalty for $d, d(\alpha)$ model parameters, N samples, *loglik* the logarithm of likelihood.

- The effective number of parameters
  - for a linear fit $\widehat{\mathbf{y}} = \mathbf{Sy}$ is $d(\mathbf{S}) = trace(\mathbf{S})$, the sum of the diagonal elements.
- For 0-1 loss does not hold in general, only as approximation.

BIC Bayesian Information Criterion

$$\begin{aligned} P(\mathcal{M}_m|\mathbf{Z}) &= \frac{P(\mathbf{Z}|\mathcal{M}_m)\cdot P(\mathcal{M}_m)}{P(\mathbf{Z})} \\ &\propto P(\mathbf{Z}|\mathcal{M}_m)\cdot P(\mathcal{M}_m) \\ &\propto P(\mathcal{M}_m)\cdot \int P(\mathbf{Z}|\theta_m,\mathcal{M}_m)P(\theta_m|\mathcal{M}_m)d\theta_m \end{aligned}$$

Laplace approximation to the integral gives with $\hat{\theta}_m$ the ML estimate of θ:

$$\begin{aligned} \log P(\mathbf{Z}|\mathcal{M}_m) &= \log P(\mathbf{Z}|\hat{\theta}_m,\mathcal{M}_m) - \frac{d_m}{2}\cdot \log N + O(1) \\ &= loglik - \frac{d_m}{2}\cdot \log N + O(1) \end{aligned}$$

Definition (Bayesian Information Criterion (BIC))

$$BIC_m = -2loglik_m + (\log N)\cdot d_m$$

BIC may be used to compare the model posterior probabilities $\frac{e^{\frac{1}{2}\cdot BIC_m}}{\sum_{\ell=1}^{M} e^{\frac{1}{2}\cdot BIC_\ell}}$.

Crossvalidation

Crossvalidation

- Split the data into K roughly equal-sized parts. Usually, $K = 5$ or 10 or $K = N$
  - For $K = 10$ it is called **tenfold** crossvalidation.
  - For $K = N$ it is called **one-leave-out** crossvalidation.
  - $\kappa : \{1, \ldots, N\} \to \{1, \ldots, K\}$ is the partition function
  - $\hat{f}^{-k}$ is the fitted function with kth part removed.
- For $k = 1, \ldots, K$
  - For the kth part we fit the model to the other $K - 1$ parts of the data, and calculate the prediction error of the fitted model when predicting the kth part of the data.
- Average the error estimates.

$$CV = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \hat{f}^{-\kappa(i)}(x_i)).$$

10 times 10 Crossvalidation

Parameter Tuning by Crossvalidation

Parameter Tuning by Crossvalidation

- Given a set of models $f(x, \alpha)$ indexed by a tuning parameter α, we define

$$CV(\alpha) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \hat{f}^{-\kappa(i)}(x_i, \alpha)).$$

- The $CV(\alpha)$ provides an estimate of the test error curve and we find the tuning parameter $\hat{\alpha}$ that minimizes it.
- Our final model is $f(x, \hat{\alpha})$.

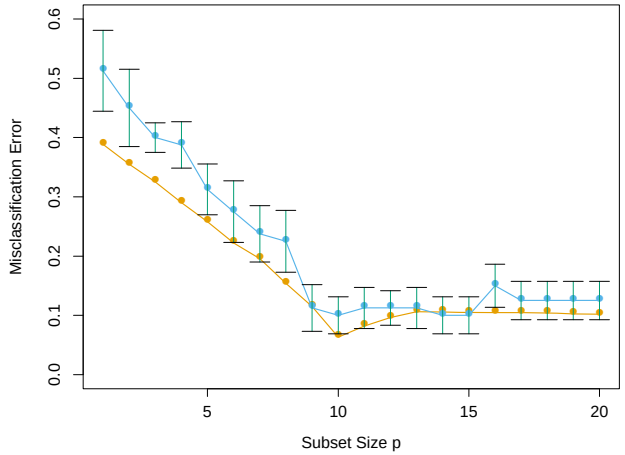


FIGURE 7.9. *Prediction error (orange) and tenfold cross-validation curve (blue) estimated from a single training set, from the scenario in the bottom right panel of Figure 7.3.*

Definition (One standard error rule)

We choose the most parsimonious model whose error is no more than one standard error above the error of the best model.

Here, $p = 9$.

Generalized Crossvalidation

- For a linear fitting method we can write

$$\hat{\mathbf{y}} = \mathbf{S}\mathbf{y}.$$

- For many linear fitting methods,

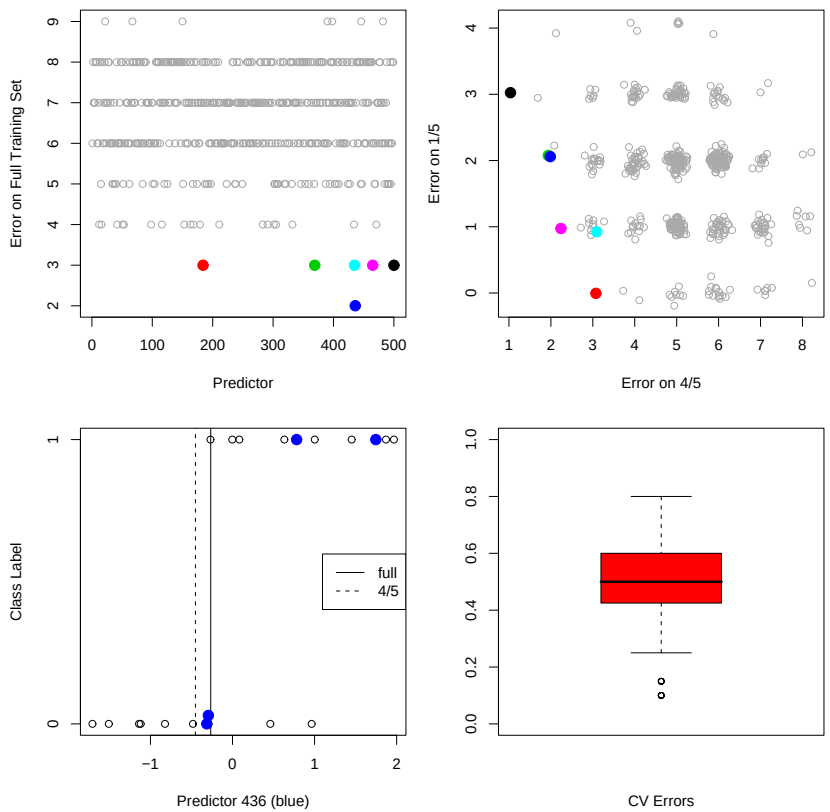
$$\frac{1}{N}\sum_{i=1}^{N}[y_i - \hat{f}^{-i}(x_i)]^2 = \frac{1}{N}\sum_{i=1}^{N}[\frac{y_i - \hat{f}(x_i)}{1 - S_{ii}}]^2,$$

- The **generalized crossvalidation** GCV approximation is

$$GCV = \frac{1}{N}\sum_{i=1}^{N}\left[\frac{y_i - \hat{f}(x_i)}{1 - trace(\mathbf{S})/N}\right]^2.$$

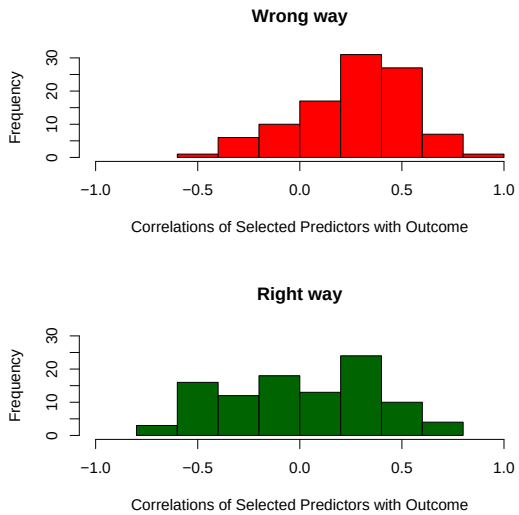
Bad and good Crossvalidation

- $p = 500$ dimensions
- $N = 20$
- random data, y independent of x.
- We search for the best 'decision stump' (decision rule based on one single attribute).



Wrong way

- choose 100 good predictors
- Using just this subset of predictors, build a multivariate classifier, using all of the samples except those in fold k.
- Use the classifier to predict the class labels for the samples in fold k.



One–leave–out

- Use all but one data samples for learning.
- Evaluate the error or the hidden sample.
- Repeat for each sample and calculate the average.

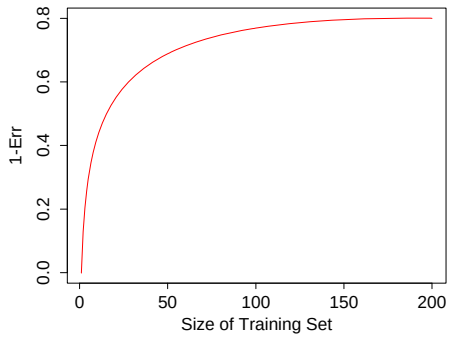
Advantage:

- The largest possible training set.
- Deterministic evaluation (no sense to repeat it).

Disadvantage:

- Time consuming.
- May be misleading – take randomly 50 : 50 generated goal G, the one–leave–out error is 100%.

Learning curve



Bootstrap

- Select elements with replacement.
- We have N data samples, we select with replacement N samples – some are selected more than one, some are not selected at all. *The not selected are used for testing.*
- The probability of not-selecting a sample is $\left(1 - \frac{1}{N}\right)^N \approx e^{-1} = 0.368$.
- The error estimate is pessimistic since we learn a model on N samples that come from only 0.632 samples.
  The usual error estimate is:

$$err = 0.632 \cdot e_{\text{test}} + 0.368 \cdot e_{\text{train}}$$

- Again, may be misled by similar data as one–leave–out.

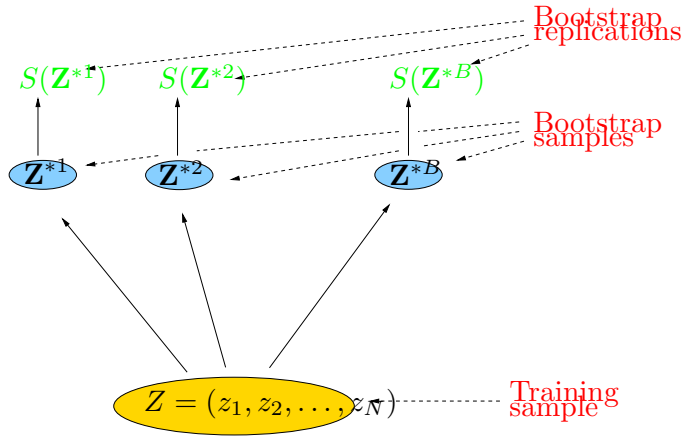


FIGURE 7.12. *Schematic of the bootstrap process. We wish to assess the statistical accuracy of a quantity $S(\mathbf{Z})$ computed from our dataset. B training sets $\mathbf{Z}^{*b}$, $b = 1, \ldots, B$ each of size N are drawn with replacement from the original dataset. The quantity of interest $S(\mathbf{Z})$ is computed from each bootstrap training set, and the values $S(\mathbf{Z}^{*1}), \ldots, S(\mathbf{Z}^{*B})$ are used to assess the statistical accuracy of $S(\mathbf{Z})$.*

Confusion Matrix

true class \ prediction	+	-
+	TP – true positive	FN – false negative
-	FP – false positive	TN true negative

Česky se říká správně/falešně positivní/negativní.

Basic measures:

celková správnost	accurancy	$Acc = \frac{TP+TN}{TP+TN+FP+FN}$
chyba	error	$Err = \frac{FP+FN}{TP+TN+FP+FN}$
přesnost	precision	$Prec = \frac{TP}{TP+FP}$
úplnost, sensitivita	recall, sensitivity	$Rec = \frac{TP}{TP+FN}$
specificita	specificity	$Specificity = \frac{TN}{TN+FP}$
F míra	F measure	$F = \frac{2 \cdot Prec \cdot Rec}{Prec+Rec} = \frac{2 \cdot TP}{2 \cdot TP+FP+FN}$
	TP rate	$\frac{TP}{TP+FN}$
	FP rate (=1–Specificity)	$\frac{FP}{FP+TN}$

Additional Remarks

- ROC - curve
  - Precision recall curve
- Interval estimates
- t-test
  - paired t-test
- ANOVA
- Q-Q plot
- $R^2(y, \hat{y}) = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \overline{y}_i)^2}$, 1 or 0 instead of nan and infinity.
  - explained variance - identical for zero mean residuals.
- Mc Nemar's test (two classifiers, confusion matrix with values <5; i.e. not χ^2 test).
  - statsmodels.stats.contingency_tables.mcnemar()

Additive Models, Trees, and Related Methods

- **Generalized additive models (GAMs)** are automatic flexible statistical methods that may be used to identify and characterize nonlinear regression effects.
- GAM has the form

$$\mathbb{E}(Y|X_1, \ldots, X_p) = \alpha + f_1(X_1) + \ldots + f_p(X_p)$$

  - where f_j's are unspecified smooth functions
  - X_j predictors, Y the outcome.
- Compared to the basis expansion, here we use use a scatterplot smoother
  - use a cubic smoothing spline or kernel smoother
- and simultaneously estimate all p functions.

GAM for non Gaussian distributions

- Denote $\mu(X) = P(Y = 1|X)$ in a two class classification with 0-1 encoding and recall the logistic regression

$$\log\left(\frac{\mu(X)}{1-\mu(X)}\right) = \alpha + \beta_1 X_1 + \ldots + \beta_p X_p,$$

- **Additive logistic regression** model replaces the linear terms by the smoothers

$$\log\left(\frac{\mu(X)}{1-\mu(X)}\right) = \alpha + f_1(X_1) + \ldots + f_p(X_p),$$

- The conditional mean $\mu(X)$ of a response Y is related to an additive function of the predictors via a **link function** g

$$g[\mu(X)] = \alpha + f_1(X_1) + \ldots + f_p(X_p).$$

- Examples of classical link functions are the following
  - $g(\mu) = \mu$ the identity link, used for linear and additive models for Gaussian response data.
  - $g(\mu) = \mathit{logit}(\mu)$ as above
  - $g(\mu) = \mathit{probit}(\mu)$ **probit** link function for modeling binomial probabilities is the inverse of Gaussian cumulative distribution function $\mathit{probit}(\mu) = \Phi^{-1}(\mu)$
  - $g(\mu) = \log(\mu)$ for log-linear or **log-additive models** for Poisson count data.

Models with Feature Interactions

- We may add a function $g_{ZW}(Z, W)$ of two features
$$g(\mu) = f(X) + g_{ZW}(Z, W)$$
- Assume qualitative variables V (factors) and Z one of the predictors and we create an interaction term $g(V, Z) = g_k(Z)$ for each index level k of V,
$$g(\mu) = f(X) + g_k(Z)$$
- a **semiparametric model** keeps the effect of the kth predictor and the effect of the predictor Z additive
$$g(\mu) = X^T\beta + \alpha_k + f(Z).$$
- Note: logit, probit, log, gamma and negative-binomial distributions belong the an exponential family, therefore have some nice properties (fit together).

Fitting Additive Model

The backfitting algorithm for additive models

1: **procedure** GENERALIZED ADDITIVE MODEL FITTING:($\mathbf{X}$, $\mathbf{y}$)
2: $\hat{\alpha} = \frac{1}{N}\sum_1^N y_i$, $\hat{f}_j \equiv 0$ initialize $\forall i, j$.
3: **repeat** for $j = 1, 2, \ldots, p, \ldots, 1, 2, \ldots$
4: $\hat{f}_j \leftarrow \mathcal{S}_j\left[\{y_i - \hat{\alpha} - \sum_{j\neq k}\hat{f}_k(x_{ij})\}_1^N\right]$,
5: $\hat{f}_j \leftarrow \hat{f}_j - \sum_{i=1}^N \hat{f}_j(x_{ij})$.
6: **until** the functions $\hat{f}_j$ change less than a prespecified threshold.
7: **end procedure**

- $\mathcal{S}_j$ denotes the smoother, for example the smoothing spline with predefined degrees of freedom.
- All $\hat{f}_j$ should have zero mean, the constant is fitted by α.
- Re-normalization is recommended because of rounding errors.

Generalized Additive Logistic Regression

1: **procedure** ADDITIVE LOGISTIC REGRESSION:(**X**, **y** in 0-1 encoding)
2: $\hat{y} = \frac{1}{N}\sum_1^N y_i, \hat{\alpha} = \log(\frac{\hat{y}}{1-\hat{y}})$, $\hat{f}_j \equiv 0$ initialize $\forall j$.
3: $\hat{\eta}_i = \hat{\alpha} + \sum_j \hat{f}_j(x_{ij})$ and $\hat{p}_i = \frac{1}{1+\exp(-\hat{\eta}_i)}$
4: **repeat**
5: Construct the working target variable

$$z_i = \hat{\eta}_i + \frac{y_i - \hat{p}_i}{p_i(1-p_i)}.$$

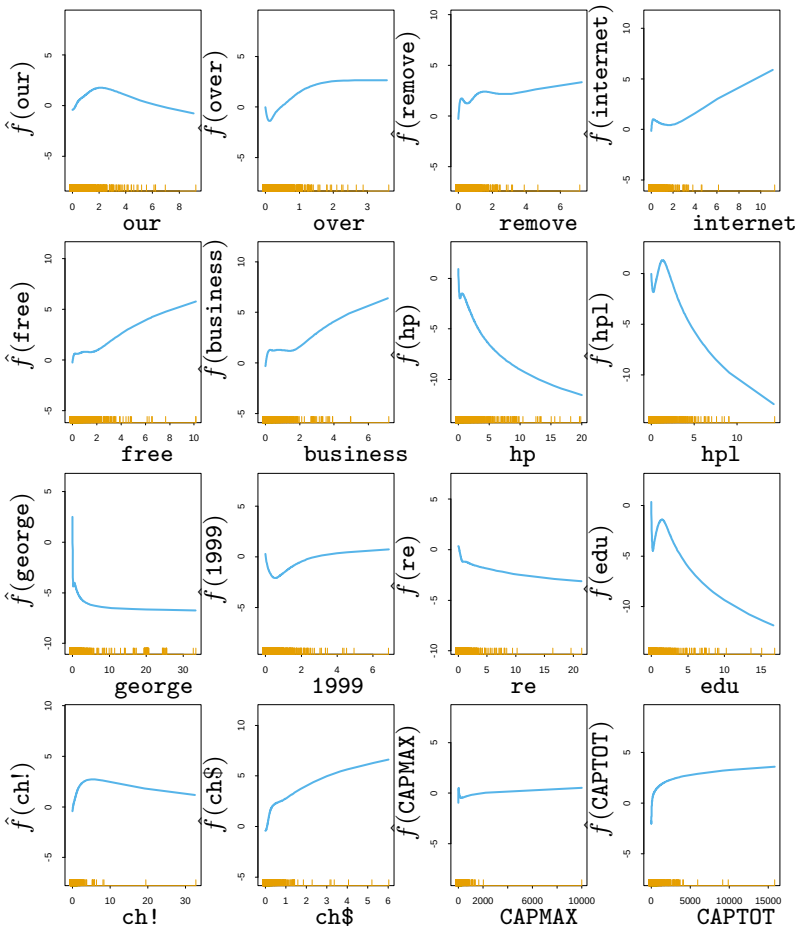
6: Construct the weight $w_i = p_i(1-p_i)$
7: Fit an additive model to the targets z_i with weights w_i, using a weighted backfitting algorithm. This gives new estimates $\hat{\alpha}, \hat{f}_j \ \forall j$
8: **until** the functions change less than a prespecified threshold.
9: **end procedure**

Spam Example

- Email classification as email/spam.
- word frequency as X features.
- Important features:

TABLE 9.2. *Significant predictors from the additive model fit to the spam training data. The coefficients represent the linear part of $\hat{f}_j$, along with their standard errors and Z-score. The nonlinear P-value is for a test of nonlinearity of $\hat{f}_j$.*

Name	Num.	df	Coefficient	Std. Error	Z Score	Nonlinear P-value
Positive effects						
our	5	3.9	0.566	0.114	4.970	0.052
over	6	3.9	0.244	0.195	1.249	0.004
remove	7	4.0	0.949	0.183	5.201	0.093
internet	8	4.0	0.524	0.176	2.974	0.028
free	16	3.9	0.507	0.127	4.010	0.065
business	17	3.8	0.779	0.186	4.179	0.194
hpl	26	3.8	0.045	0.250	0.181	0.002
ch!	52	4.0	0.674	0.128	5.283	0.164
ch$	53	3.9	1.419	0.280	5.062	0.354
CAPMAX	56	3.8	0.247	0.228	1.080	0.000
CAPTOT	57	4.0	0.755	0.165	4.566	0.063
Negative effects						
hp	25	3.9	−1.404	0.224	−6.262	0.140
george	27	3.7	−5.003	0.744	−6.722	0.045
1999	37	3.8	−0.672	0.191	−3.512	0.011
re	45	3.9	−0.620	0.133	−4.649	0.597
edu	46	4.0	−1.183	0.209	−5.647	0.000

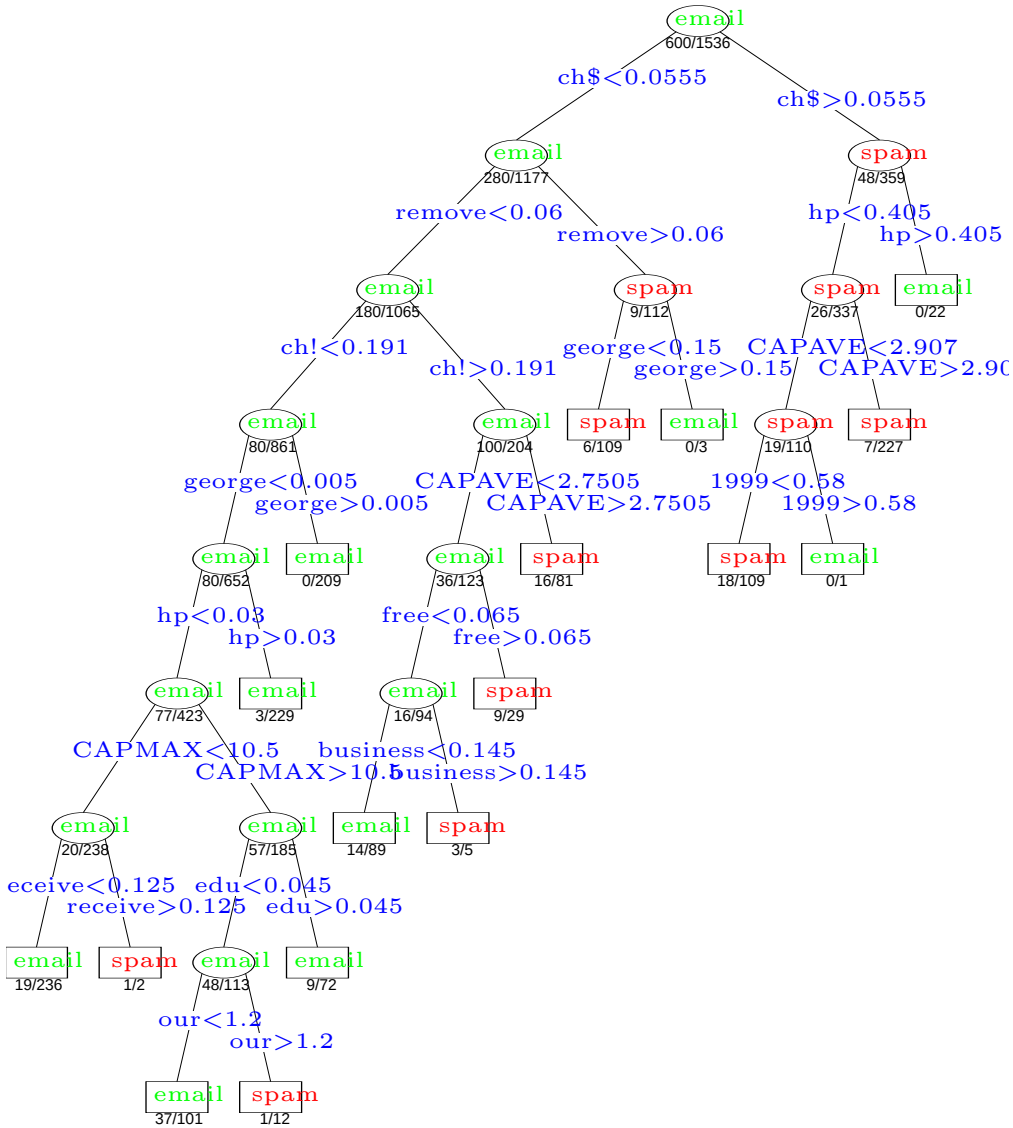


Decision Trees

Decision tree for a given goal attribute G is a rooted tree with

- a root and inner nodes labeled by attributes; for each possible value of the attribute there is an outgoing edge from the node;
- leaves are labeled with predicted goal class $g \in G$ assuming other attributes have values as labeled on the path from the root.

Attributes not present on the path from the root to the leaf are irrelevant.



Construction

Tree construction idea:

- select an attribute; create a node and split the data according the value of the attribute
- for each attribute value construct a subtree based on the appropriate part of the data
- stop if there is a unique value of the goal G in the data or no attributes to split, create a leaf labeled by the most common class $g \in G$.

The criterion to select an attribute follows.

Entropy

The entropy of an attribute A ('uncertainty', negative information) we would like:

- to be zero for the pure data (only one value of the attribute A)
- the highest entropy for uniform distribution on values of A (no information at all)
- two step split leads to the same result as split at once:

$$H([2,3,4]) = H([2,7]) + \frac{7}{9} \cdot H([3,4])$$

Definition

Entropy These properties has the **entropy** $H([p_1, \ldots, p_k]) = -\sum_{i=1}^{k} p_i \log p_i$, the base of the logarithm usually e, sometimes 2.

If we do not normalize we get the entropy multiplied by $\sum_{i=1}^{k} p_i$.

The lower index A denotes the attribute to calculate the entropy H_A, for the goal attribute H_G.

The Entropy for a binary attribute

x axis: p_i, y axis: entropy.
$Gini = 1 - \sum_i (p_i)^2$

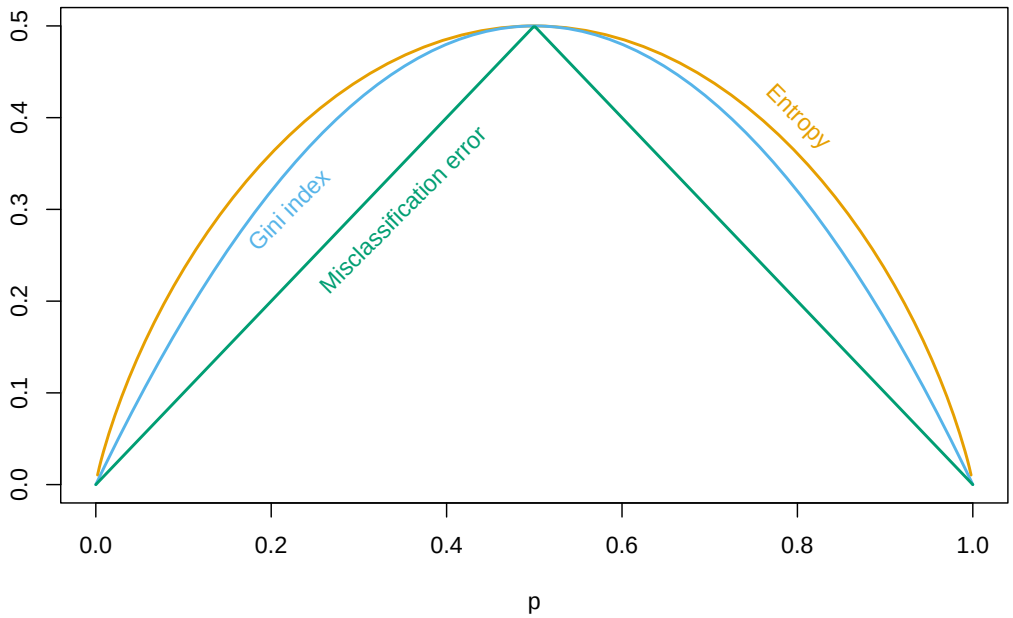


FIGURE 9.3. *Node impurity measures for two-class classification, as a function of the proportion p in class 2. Cross-entropy has been scaled to pass through* $(0.5, 0.5)$.

ID3 algorithm

We select an attribute with the maximal **information gain**, defined for the *data* and an attribute X_j:

$$Gain(data, X_j) = H_G(data) - \sum_{x_j \in X_j} \frac{|data_{X_j=x_j}|}{|data|} H_G(data_{X_j=x_j})$$

where $data_{X_j=x_j}$ is a subset of *data* where $X_j = x_j$, the entropy is defined

$$H_G(data) = \sum_{g \in G} -\frac{|data_{G=g}|}{|data|} \cdot log_2 \frac{|data_{G=g}|}{|data|} = \sum_{i=1}^{|G|} -p_i \cdot log_2 p_i$$

where p_i denotes the ratio of $G = g_i$ in the *data*.

It is equivalent to minimize the weighted entropy after the split, that is

$$\arg\min_{X_i} \sum_{x_j \in X_j} \frac{|data_{X_j=x_j}|}{|data|} \sum_{g \in G} -\frac{|data_{G=g \& X_j=x_j}|}{|data_{X_j=x_j}|} \cdot log_2 \frac{|data_{G=g \& X_j=x_j}|}{|data_{X_j=x_j}|}$$

ID3 algorithm(*data*, *G* goal, *Attributes* attributes)

ID3

Create the root *root*
If all data have the same g, label the root g and return,
If no attributes *Attributes*, label the *root*
by the most frequent g in the *data* and return
otherwise
$X_j \leftarrow$ the attribute from *Attributes* with the maximal $Gain(data, X_j)$
label *root* as X_j
for each possible value x_j of X_j,
add an edge from *root* labeled $X_j = x_j$
$data_{X_j=x_j} \leftarrow$ the subset of the *data* with $X_j = x_j$
If $data_{X_j=x_j}$ is empty, add a leaf labeled by
the most common class g in *data* and return
add a subtree $ID3(data_{X_j=x_j}, G, Attributes \setminus \{X_j\})$
return *root*

Categorical Attribute Notes

- CART in the sklearn DecisionTreeClassifier does not support categorical attributes
  - uses just binary splits.
- It is requires exponential complexity with respect to the number of categories to find optimal binary split.
  - The recommended heuristic is to sort categories according to the goal class probabilities and search the split in a linear time.
- We should avoid the split into too many branches.
  - ID3 used penalization $Gain^*(X_i, data) = \frac{Gain(X_i, data)}{H(X_i)}$
  - so for the identifier with unique values $Gain^*(X_i, data) = \frac{Gain(X_i, data)}{\log N}$.
  - min_samples_split, min_samples_leaf, min_weight_fraction_leaf can do it too.

Prunning Introduction

To avoid overfitting we try to remove unnecessary nodes

- **postprunning** – build a tree, prune afterwards;
  - usuall way
- **preprunning** – prune during the construction
  - This seems nice but we could prune two attributes combined by XOR since both has information gain (close to) zero.

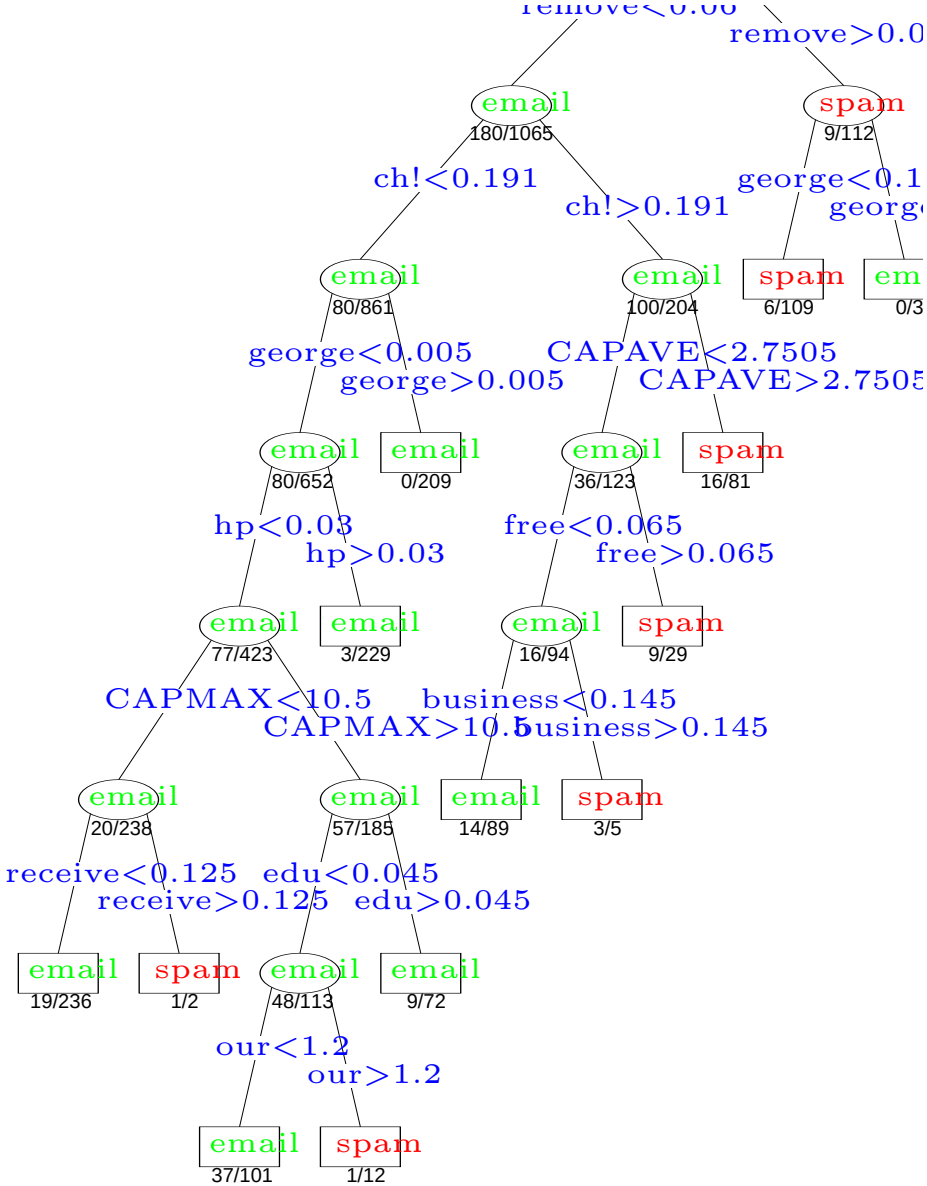
Postprunning

- **subtree replacement** – select a tree and replace it by a leaf;
  - it increases the training error
  - it may decrease the error on validation data
  - step by step, we try to prune each subtree: we prune if we do not increase validation error.
- **subtree raising** – remove an inner node. Used in C4.5. The data samples must be re-send to the remaining branch, it is time consuming.
  - Usually checked only for the most frequent branch in the tree.

Reduced Error Pruning

Reduced Error Pruning

- **reduced error pruning –** we keep part of the data for validation (pruning).
- for each inner node compare
  - validation error with this node as a leaf
  - validation error with the (pruned) subtree of this node
- select whatever gives the lower error.



- there exist also a criterion based on the training data
- **Reduced Cost Pruning** CART - few slides later.

Numerical attributes

64	65	68	69	70	71	72	75	80	81	83	85
yes	no	yes	yes	yes	no	no,yes	yes,yes	no	yes	yes	no

- we require a binary split
- 11 split points
- for each split we calculate the information gain
  - $$H([9,5]) - H([4,2],[5,3]) = H([9,5]) - (\frac{6}{14} \cdot H([4,2]) + \frac{8}{14} \cdot H([5,3]))$$

    $= 0.940 - 0.939$ bits.
- We allow multiple splits based on this attribute.

Regression trees - numerical prediction

- **Model tree** has linear fit in the leaves
  - not so popular as regression trees; increases complexity and discontunuity
- **CART**
  - use the decrease of the square error loss to select an attribute
  - binary splits
  - predict the average value in the leaves.

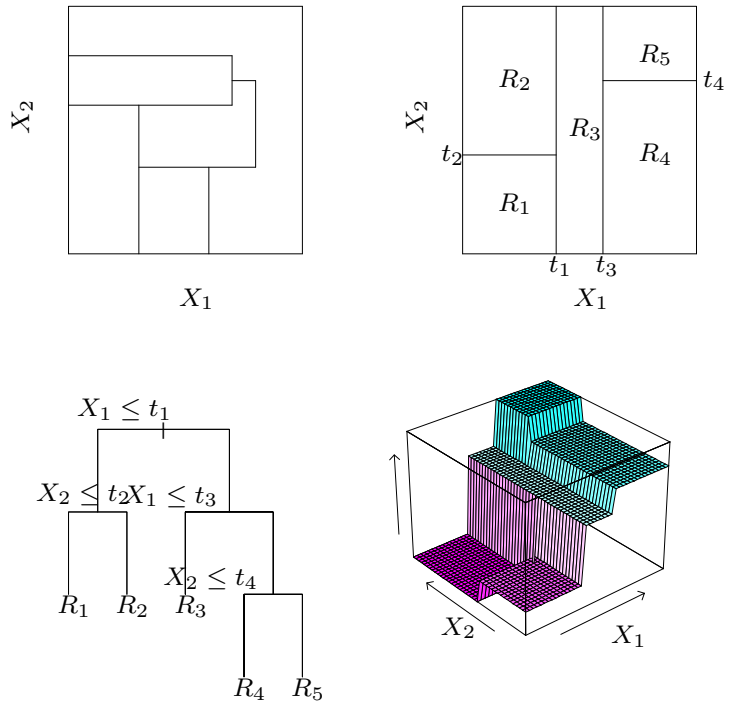


FIGURE 9.2. *Partitions and CART. Top right panel shows a partition of a two-dimensional feature space by recursive binary splitting, as used in CART, applied to some fake data. Top left panel shows a general partition that cannot be obtained from recursive binary splitting. Bottom left panel shows the tree corresponding to the partition in the top right panel, and a perspective plot of the prediction surface appears in the bottom right*

CART (Classification and) Regression Trees

- Regions R_m, we predict a constant c_m inside any region.

$$f(x) = \sum_{m=1}^{M} c_m I(x \in R_m)$$

$$\hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i.$$

Single Regression Tree for CART

- Start with all data in one region R_0
- Select the best attribute j and its value s for the split:

$$\min_{j,s}[min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2]$$

  - Inner minimum is the average $\hat{c}_1 = ave(y_i | \ x_i \in R_1)$.
- iterate until stop (number of samples in the leaf $\leq n_0$).

Reduced Cost Pruning

- Split the data into K folds
- For each fold k:
  - use all except fold k to train the tree T
  - Build a sequence of subtrees $T^k \supset T_1^k \supset T_2^k \ldots \supset T_{|T|}^k$
    - always join two leaves with the minimal increase in the training error
  - use fold k do calculate the crossvalidation error of each tree
  - consider the error function $C_\alpha(T^k)$ as a function of α
- Select the minimum of $\sum_k C_\alpha(T^k)$
- Build a tree on the full training data
- Return the subree corresponding to the optimal α.

- Average error on a leaf m

$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \frac{1}{N_m} \sum_{x_i \in R_m} y_i)^2,$$

- Cost of the tree with α penalty for the number of leaves

$$C_\alpha(T) = \sum^{|T|} N_m Q_m(T) + \alpha|T|.$$

Missing values,Class and Samples Weights

- Trees can handle missing data well.
- Often we cannot **omit** missing data since many samples have missing values.
  - Furthermore, missing values in unused attributes are irrelevant.
- If the value is **not missing at random** then take the missingness as another value of the attribute
  - example: very small and very high wages are more ofter missing
- If the data are **missing at random**
  - **split the instance**
  - according the data ratio following each branch
  - weight and average the predictions on leaves.
- Similarly, we use weighted information gain to select the attribute.
  - by setting setting class_weight
  - fit(X, y, sample_weight=None).

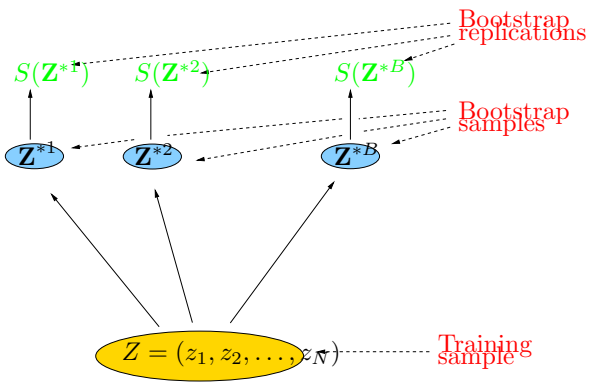
Complexity considerations

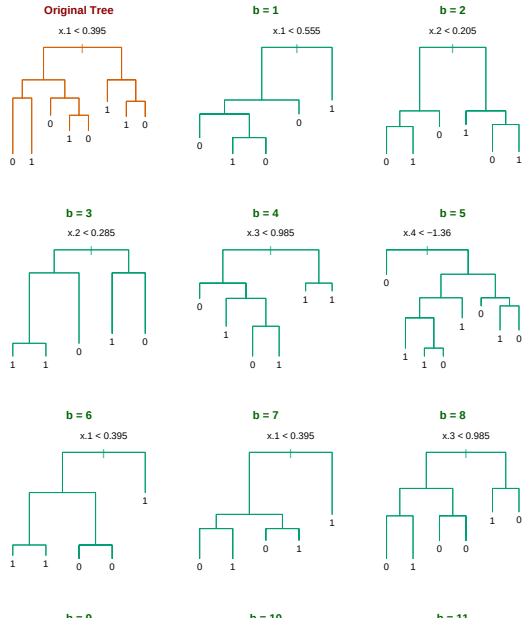
CART

- Let us have N instances with p attributes.
- Assume a reasonably balanced tree with the tree depth $O(logN)$.
- To build the tree we need $O(p \cdot N^2 \cdot logN)$ time.
  - At each depth, each instance occurs exactly ones, $logN$ depth levels, p attributes on each level, the time $O(p \cdot N^2 \cdot \log N)$.
- Subtree replacement $O(N)$, Subtree raising $O(N(logN)^2)$.
- Naive tree construction comlpexity is $O(p \cdot N^2 \cdot logN) + O(N(logN)^2)$.
- With sorted features and clever indexing
  - Overall tree construction comlpexity is $O(p \cdot N \cdot logN) + O(N(logN)^2)$.

Ensemble Methods

- Random forest (+ Bagging)
- Boosting
  - Adaboost - classification
  - Gradient boosting - regression and classification
- Stacking
- MARS (=earth).





Bootstrap

- Select elements with replacement.
- We have N data samples, we select with replacement N samples – some are selected more than one, some are not selected at all. *The not selected are used for testing.*
- The probability of not-selecting a sample is $\left(1 - \frac{1}{N}\right)^N \approx e^{-1} = 0.368$.
- Selected samples used to learn a model (usually a tree).
- These are used for the **OutOfBag** error computation.

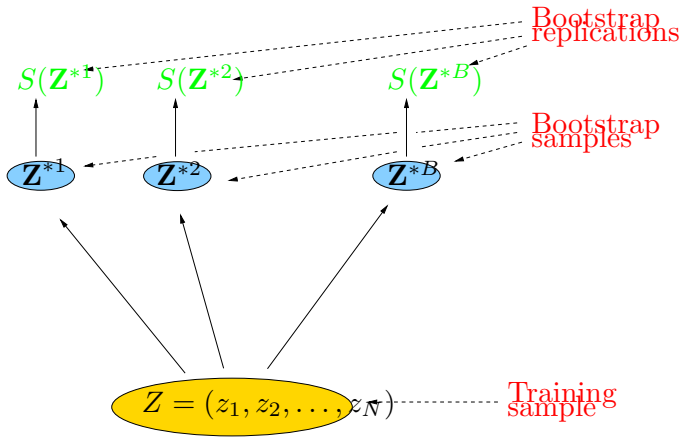


FIGURE 7.12. *Schematic of the bootstrap process. We wish to assess the statistical accuracy of a quantity $S(\mathbf{Z})$ computed from our dataset. B training sets $\mathbf{Z}^{*b}$, $b = 1, \ldots, B$ each of size N are drawn with replacement from the original dataset. The quantity of interest $S(\mathbf{Z})$ is computed from each bootstrap training set, and the values $S(\mathbf{Z}^{*1}), \ldots, S(\mathbf{Z}^{*B})$ are used to assess the statistical accuracy of $S(\mathbf{Z})$.*

Random Forest for Regression or Classification

1: **procedure** RANDOM FOREST:(X, y training data)
2: **for** $b = 1, 2, \ldots, B$ **do**
3: Draw a bootstrap sample $\mathbf{Z}^*$ of size N
4: Grow a random forest tree T_b
5: **repeat**
6: Select m variables at random from p variables.
7: Pick the best variable/split–point among the m
8: Split the node into two daughter nodes.
9: **until** the minimum node size n_{min} is reached.
10: **end for**
11: Output the ensamble of trees $\{T_b\}_1^B$.
12: **end procedure**

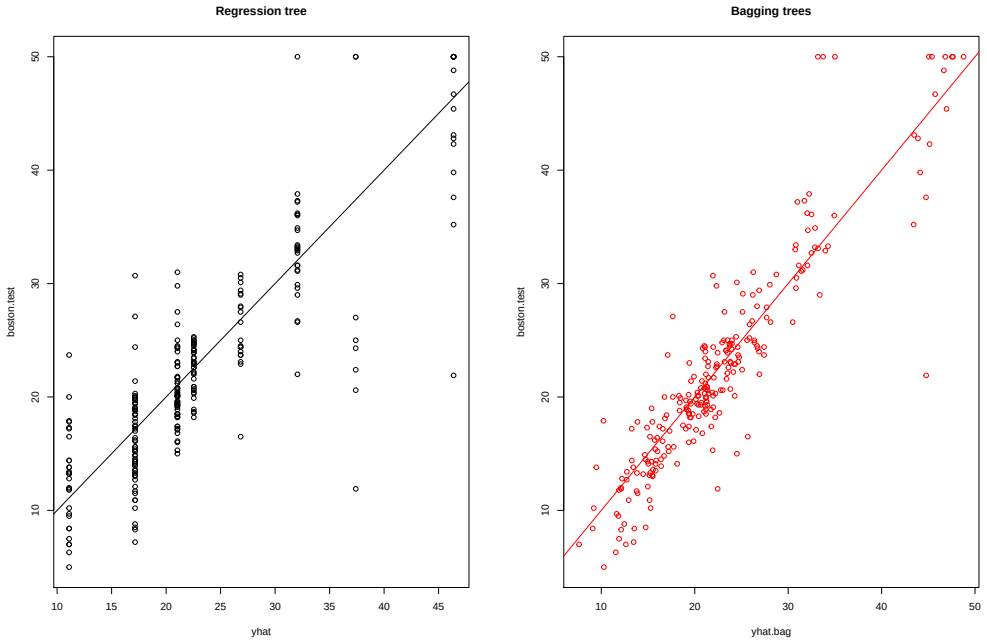
To make a prediction at a new point x:

- Regression: $\hat{f}_{rf}^B(x) = \frac{1}{B}\sum_{b=1}^B T_b(x)$.
- Classification: Let $\widehat{C}_b(x)$ be the class prediction of the bth random–forest tree.
  - Predict $\widehat{C}_{rf}^B(x) = \textit{majority vote}\ \{\widehat{C}_b(x)\}_1^B$.

Bagging (Bootstrap aggregating)

- It is a Random Forest, where we use all predictors, that is $m = p$.
- both regression and classification.
- Training data $\mathbf{Z} = \{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$

$$\hat{f}_{bag}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^{*b}(x).$$



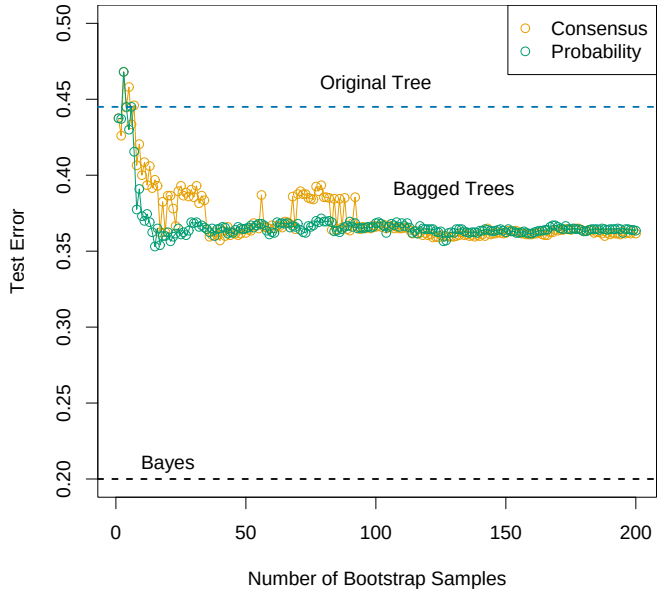
Bagging for Classification

- Training data $\mathbf{Z} = \{(x_1, g_1), (x_2, g_2), \ldots, (x_N, g_N)\}$
- for each bootstrap sample, $b = 1, 2, \ldots, B$, we fit our model, giving prediction $\hat{f}^{*b}(x)$.
- Take either
  - predict probabilities of classes and find the class with the highest predicted probability over the bootstrap samples

$$\hat{G}(x) = \mathit{argmax}_k \sum_{b=1}^{B} \hat{f}^{*b}(x)$$

  - predict class and

$$\hat{G}_{bag}(x) = \mathit{majority\ vote}\ \{\hat{G}^{*b}(x)\}_{b=1}^{B}.$$



Behind Random Forest

The variance of the random forest estimate $Var(\hat{f}_{rf}^{B}(x)) = \mathbb{E}(\hat{f}(x) - \mathbb{E}\hat{f}(x))^2$ is

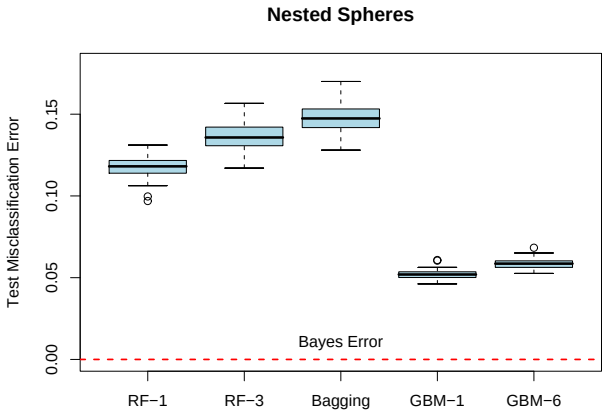
- iid data variables, independent features, each with variance σ^2:
  - $\frac{1}{B}\sigma^2$
- id identically distributed data, each with variance σ^2 with positive pairwise correlation ρ:
  - $\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$.
- The second part is addressed by bagging.
- The idea behind random random forest is to address the first part of the formula.
  - Before each split, select $m \leq p$ variables as candidates for splitting.
  - $m \leftarrow \sqrt{p}$ for regression, even as low as 1. $\frac{p}{3}$ for classification.
- For boot–strapped trees
  - ρ is typically small (0.05 or lower)
  - σ^2 is not much larger than for the original tree.
- Bagging does not change linear estimates, such as the sample mean
  - The pairwise correlation between bootstrapped means is about 50%.

Random Forest Experiments

Spam example misclassification error

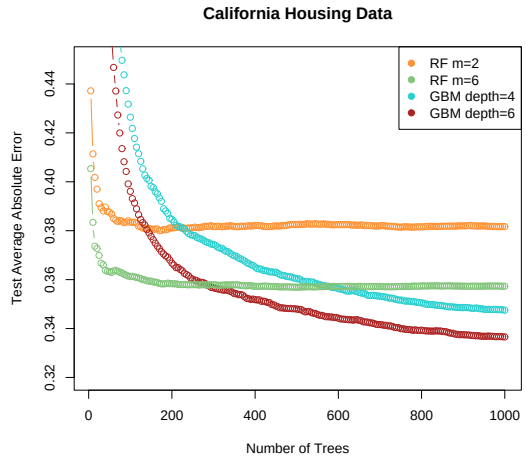
- bagging 5.4%
- random forest 4.88%
- gradient boosting 4.5%

Nested spheres in $\mathbb{R}^{10}$, 2500 trees, the number selected by 10–fold crossvalidation



California housing data

- Random forests stabilize at about 200 trees, while at 1000 trees boosting continues to improve.
  - Boosting is slowed down by the shrinkage
  - the trees are much smaller (decision stumps, interaction depth=1 or 2).
- Boosting outperforms random forests here.

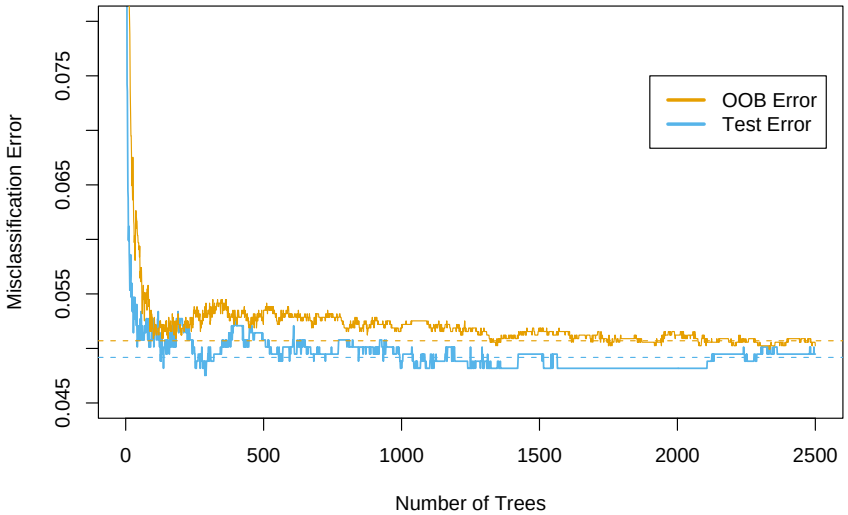


OOB Error

Definition (Out of bag error (OOB))

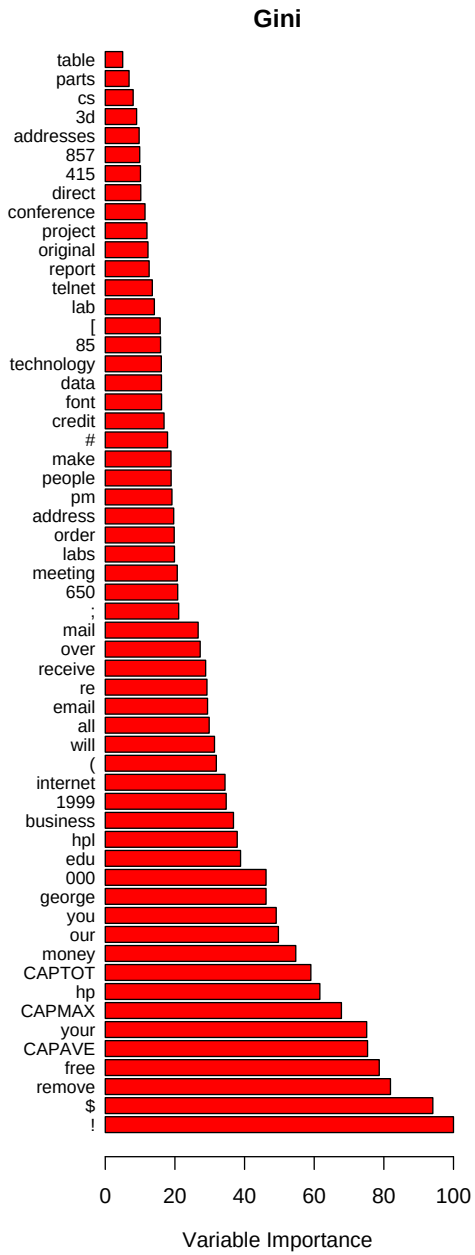
For each observation $z_i = (x_i, y_i)$, construct is random forest predictor by averaging only those trees corresponding to bootstrap samples in which z_i did not appear.

- An OOB error estimate is almost identical to that obtained by N-fold crossvalidation.
- Unlike many other nonlinear estimators, random forests can be fit in one sequence.



Variable Importance (Gini, RSS)

- **Variable Importance** of a predictor X_ℓ in a single tree T is
  $I_\ell^2(T) = \sum_{t=1}^{J} \hat{i}_t^2 \cdot I(v(t) = \ell)$
  - For each internal node t of the tree, we calculate the *Gini* or *RSS* gain
  - where $\hat{i}_t^2$ is the Gini/RSS improvement of the predictor in the inner node t.
    - Gini $\hat{p}_k(t)(1 - \hat{p}_k(t))$ before and after the split
    - for K goal classes, a separate tree for each class against others
    - weighted by the probability of reaching the node t.
- For a set of trees, we average over M all trees
  $I_\ell^2 = \frac{1}{M} \sum_{i=1}^{M} I_\ell^2(T_m)$.
- Usually scaled to the interval $(0, 100)$.



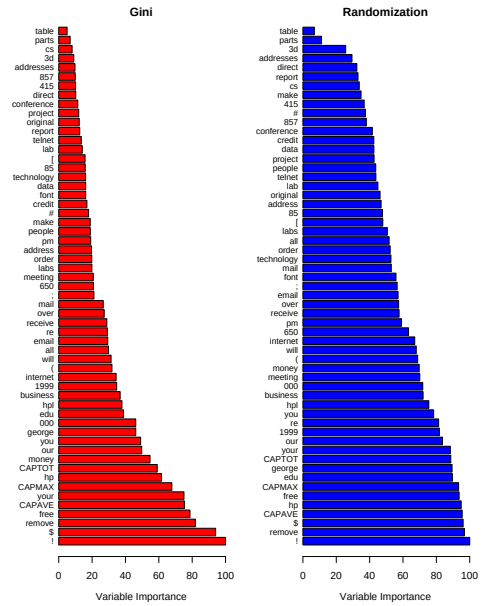
OOB Variable Importance

OOB Variable Importance

procedure OOBN VarImportance:(data)
  for $b = 1, 2, \ldots, B$ **do**
    Draw a bootstrap sample $\mathbf{Z}^*$ of size N
    Grow a random forest tree T_b
    Calculate accuracy on OOB samples
    for $j = 1, 2, \ldots, p$ **do**
      permute the values for the jth variable randomly in the OOB samples
      Calculate the decrease in the accuracy
    end for
  end for
  Output average accuracy gain for each $j = 1, 2, \ldots, p$.
end procedure

Alternative Variable Importance

with quite different results



- The randomization voids the effect of a variable.

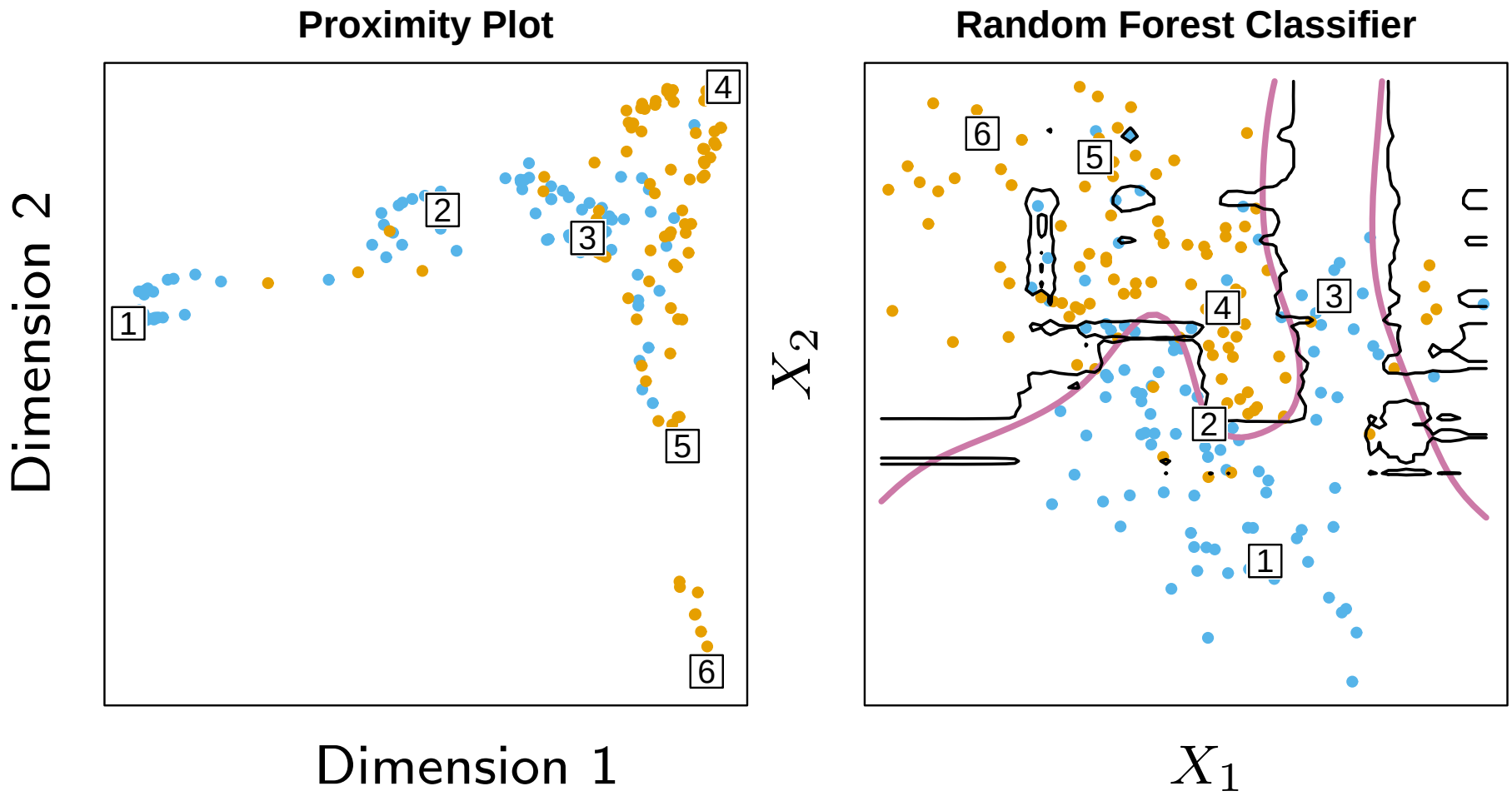
Proximity plot

Proximity plot

1: **procedure** PROXIMITY PLOT(X, y training data)
2: **for** $b = 1, 2, \ldots, B$ **do**
3: Draw a bootstrap sample $\mathbf{Z}^*$ of size N
4: Grow a random forest tree T_b
5: **Calculate prediction accuracy on OOB samples**
6: **for** any pair of OOB samples sharing the same leaf **do**
7: **increase the proximity by one.**
8: **end for**
9: **end for**
10: **end procedure**

Proximity Plot

- Distinct samples usually come from the pure regions
- Samples in the 'star center' are close to the decision boundary.

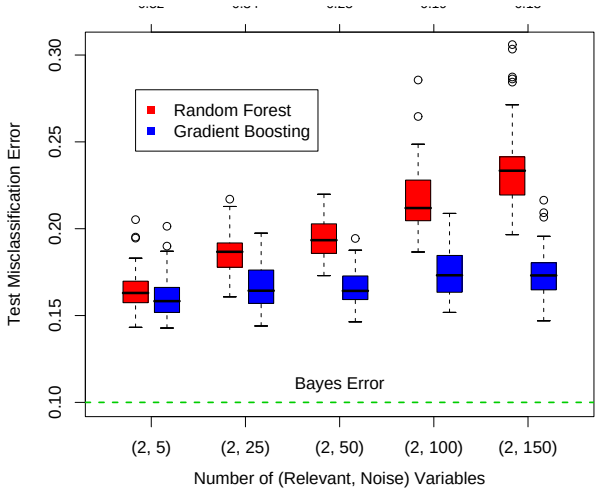


Overfitting

- Though the random forest cannot overfit the limit distribution

$$\hat{f}_{rf}(x) = \mathbb{E}_{\Theta} T(x; \Theta) = \lim_{B \to \infty} \hat{f}_{rf}^{B}(x)$$

- the limit distribution (the average of fully grown trees) may overfit the data.
- Small number of relevant variables with many irrelevant hurts the random forest approach.
- With higher number of relevant variables RF is quite robust.
- 6 relevant and 100 noisy variables, $m = \sqrt{6 + 100} \sim 10$
- probability of a relevant variable being selected at any split is 0.46.



- Seldom the pruning improves the random forest result
- usually, fully grown trees are used.
  - Two additive vars, 10 noisy,
  - plus additive Gaussian noise.

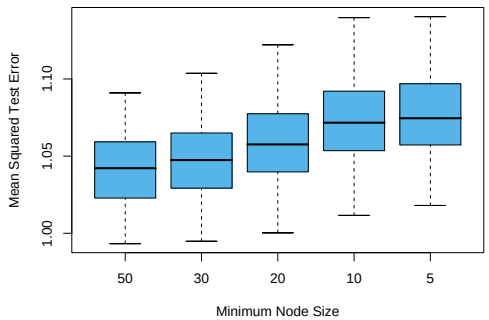


FIGURE 15.8. *The effect of* tree size *on the erro*

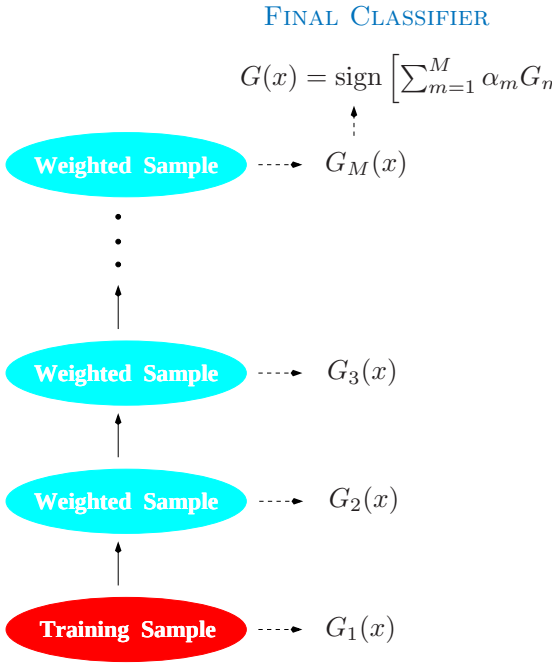
Boosting

! Use a week classifier as a decision stump (a decision tree with the depth= 1).

AdaBoost.M1

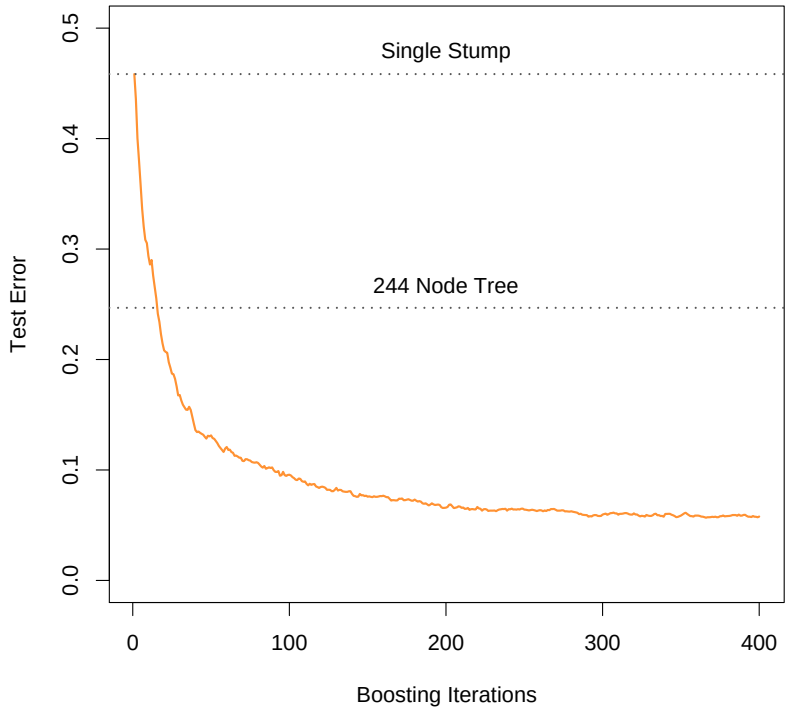
1: **procedure** ADABOOST CLASSIFIER(X, G)
2: Initialize the observation weights $w_i \leftarrow \frac{1}{N}$.
3: **for** $m = 1, 2, \ldots, M$ **do**
4: Fit a classifier $G_m(x)$ to the training data using weights w_i
5: compute $err_m \leftarrow \frac{\sum_{i=1}^{N} w_i I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i}$
6: compute $\alpha_m \leftarrow log\frac{(1-err_m)}{err_m}$
7: Set $w_i \leftarrow w_i \cdot e^{I(y_i \neq G_m(x_i)) \cdot \alpha_m}$
8: (normalize weights)
9: **end for**
10: Output $G(x) = sign[\sum_{m=1}^{M} \alpha_m G_m(x)]$.
11: **end procedure**

- Two class problem with encoding $Y \in \{-1, 1\}$
- $\overline{err} = \frac{1}{N} \sum_{i=1}^{N} I(y_i \neq G(x_i))$.



Nested Spheres Example

- The features $X_1, \ldots, X_{10}$ are standard independent Gaussian
- deterministic target
  - $Y = 1$ iff $\sum_{j=1}^{10} X_j^2 > \chi^2_{10}(0.5) = 9.34$,
  - $Y = -1$ otherwise.
- 2000 training cases
- 10000 test observations.
- Decision stumps.



Additive Model

- We encode the binary goal by $Y \in \{-1, +1\}$.
- Boosting fits an additive model:

$$f(x) = \sum_{m=1}^{M} \beta_m b(x; \gamma_m)$$

- where β_m for $m = 1, \ldots, M$ are the expansion coefficients
- $b(x; \gamma) \in \mathbb{R}$ are usually simple functions of the multivariate argument x
  - characterized by a set of parameters γ.
- For trees, γ parametrizes the split variables and split points at the internal nodes, and the predictions at the terminal nodes.
- Forward stagewise Additive Modeling sequentially adds one new basis function without adjusting the parameters and coefficients of the previously fitted.
- For squared–error loss

$$L(y, f(x)) = (y - f(x))^2,$$

we have

$$\begin{aligned} L(y_i, f_{m-1}(x) + \beta_m b(x_i; \gamma_m)) &= (y_i - f_{m-1}(x) - \beta_m b(x_i; \gamma_m))^2 \\ &= (r_{im} - \beta_m b(x_i; \gamma_m))^2 \end{aligned}$$

Exponential Loss and AdaBoost

- Let us use the $Y \in \{-1, 1\}$ encoding and the **exponential loss**

$$L(y, f(x)) = e^{-yf(x)}.$$

- We have to solve

$$\begin{aligned}
(\beta_m, G_m) &= \arg\min_{\beta, G} \sum_{i=1}^{N} e^{[-y_i(f_{m-1}(x_i)+\beta G(x_i)]} \\
&= \arg\min_{\beta, G} \sum_{i=1}^{N} e^{[-y_i(f_{m-1}(x_i)]} e^{[-y_i \beta G(x_i)]} \\
&= \arg\min_{\beta, G} \sum_{i=1}^{N} w_i^{(m)} e^{[-y_i \beta G(x_i)]}
\end{aligned}$$

- where $w_i^{(m)} = e^{[-y_i f_{m-1}(x_i)]}$ does not depend on β nor $G(x)$.
- this weight depends on $f_{m-1}(x_i)$ and change with each iteration m.

Exponential Loss and AdaBoost

- For any $\beta > 0$ the solution for $G_m(x;\gamma)$ is

$$G_m = \arg\min_{\gamma} \sum_{i=1}^{N} w_i^{(m)} I(y_i \neq G(x_i;\gamma)),$$

$$err_m = \frac{\sum_{i=1}^{N} w_i^{(m)} I(y_i \neq G_m(x_i))}{\sum_{i=1}^{N} w_i^{(m)}}$$

- since

$$\begin{aligned}
(\beta_m, G_m) &= \arg\min_{\beta,G} \sum_{i=1}^{N} w_i^{(m)} e^{[-y_i \beta G(x_i)]} \\
&= \arg\min_{\beta,G} \left[e^{-\beta} \cdot \sum_{y_i = G(x_i)} w_i^{(m)} + e^{\beta} \cdot \sum_{y_i \neq G(x_i)} w_i^{(m)} \right] \\
&= \arg\min_{\beta,G} \left[(e^{\beta} - e^{-\beta}) \cdot \sum_{i=1}^{N} w_i^{(m)} I(y_i \neq G(x_i)) + e^{-\beta} \cdot \sum_{i=1}^{N} w_i^{(m)} \right]
\end{aligned}$$

Adaboost Update

- Solving previous equation for β_m gives:

$$\beta_m = \frac{1}{2} log \frac{1 - err_m}{err_m}$$

- The approximation is updated

$$f_m(x) = f_{m-1}(x) + \beta_m G_m(x)$$

- which causes the weights for the next iteration to be:

$$w_i^{m+1} = w_i^m \cdot e^{-\beta_m y_i G_m(x_i)}.$$

- using the fact $-y_i G_m(x_i) = 2 \cdot I(y_i \neq G_m(x_i)) - 1$ we get

$$w_i^{m+1} = w_i^m \cdot e^{\alpha I(y_i \neq G_m(x_i))} \cdot e^{-\beta_m}.$$

Why exponential loss?

- The population minimizer is

$$f^*(x) = \arg\min_{f(x)} \mathbb{E}_{Y|x}(e^{-Yf(x)}) = \frac{1}{2} log \frac{P(Y=1|x)}{P(Y=-1|x)}.$$

- therefore

$$P(Y=1|x) = \frac{1}{1+e^{-2f^*(x)}}.$$

- The same function $f^*(x)$ minimizes also deviance (cross–entropy, binomial negative log–likelihood)
  - interpreting f^* as the logit transform. Let:

$$p(x) = P(Y=1|x) = \frac{e^{f^*(x)}}{e^{-f^*(x)} + e^{f^*(x)}} = \frac{1}{1+e^{-2f^*(x)}}.$$

  - and define $Y^| = (Y+1)/2 \in \{0,1\}$. Log–likelihood is

$$\ell(Y, p(x)) = Y^| \log p(x) + (1 - Y^|) \log(1 - p(x))$$

  - or equivalently the deviance:

$$-\ell(Y, f(x)) = log\left(1 + e^{-2Yf(x)}\right).$$

- Exponential loss decreases long after missclassification loss is stable at zero.

Partial Dependence Plots

- **Partial Dependence** of f on $S \subset \{1, \ldots, p\}$ is defined as:

$$f_S(X_S) = \mathbb{E}_{X_C} f(X_S, X_C)$$

$$\overline{f}_S(X_S) = \frac{1}{N} \sum_{i=1}^{N} f(X_S, x_{iC})$$

- It estimates the dependence on S averaging other predictors (not ignoring them).

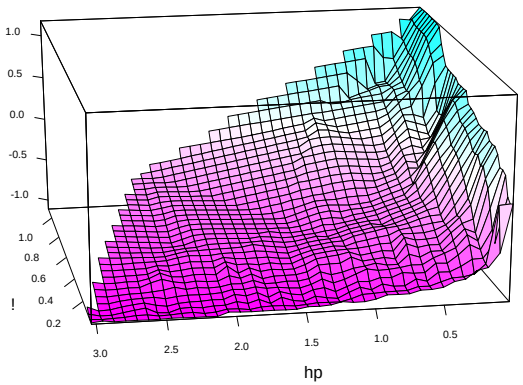


FIGURE 10.8. *Partial dependence of the log-odds o* `spam` *vs.* `email` *as a function of joint frequencies of* `h` *and the character* `!`.

Forward Stagewise Additive Modeling

- A general iterative fitting approach.
- In each step, we select the best function from the dictionary $b(x_i; \gamma)$, fit its parameters γ and the weight of this basis function β_m.
- Stagewise approximation is often faster then iterative fitting of the full model.

Forward Stagewise Additive Modeling

procedure FORWARD STAGEWISE ADDITIVE MODELING(L, X, Y, b)
    Initialize $f_0 \leftarrow 0$.
    for $m = 1, 2, \ldots, M$ **do**
        Compute $(\beta_m, \gamma_m) \leftarrow \arg\min_{\beta,\gamma} \sum_{i=1}^{N} L(y_i, f_{m-1}(x_i) + \beta b(x_i; \gamma))$.
        Set $f_m(x) \leftarrow f_{m-1}(x) + \beta_m b(x_i; \gamma_m)$
    end for
end procedure

- For example, our basis functions are decision trees, γ represents the splits and fitted values $T(*; \gamma)$).
- For square error loss, any new tree $T(*; \gamma)$ is the best tree fitting residuals $r_i = y_i - f_{m-1}(x_i)$.

Gradient Tree Boosting Algorithm

Gradient Tree Boosting Algorithm

procedure GRADIENT TREE BOOSTING ALGORITHM(X, Y, L)
  Initialize $f_0(x) \leftarrow \arg\min_\gamma \sum_{i=1}^{N} L(y_i, \gamma)$.
  for $m = 1, 2, \ldots, M$ **do**
    for $i = 1, 2, \ldots, N$ **do**
      compute $r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f(x_i)=f_{m-1}(x_i)} =^{[*]} y_i - f_{m-1}(x_i)$
    end for
    Fit reg. tree to the target r_{im} giving regions $\{R_{jm}\}_{j=1,\ldots,J_m}$.
    for $j = 1, 2, \ldots, J_m$ **do**
      Compute $\gamma_{jm} \leftarrow \arg\min_\gamma \sum_{i \in R_{jm}} L(y_i, f_{m-1}(x_i) + \gamma)$.
    end for
    Set $f_m(x) \leftarrow f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$.
  end for
  Output $\hat{f}(x) = f_M(x)$.
end procedure

[*] for square error loss.

Stacking

- Over a set of models (possibly different types) learn a simple model (like a linear regression)
- Assume predictions $\hat{f}_1(x), \hat{f}_2(x), \ldots, \hat{f}_M(x)$ under square error loss
- Predictors trained without ith example are denoted
  - $\hat{f}_1^{-i}(x), \hat{f}_2^{-i}(x), \ldots, \hat{f}_M^{-i}(x)$
- we can seek weights $w = (w_1, \ldots, w_m)$ such that

$$\hat{w}^{st} = \arg\min_w \sum_{i=1}^{N} \left[y_i - \sum_{m=1}^{M} w_m \hat{f}_m^{-i}(x) \right]^2 .$$

- The final prediction is

$$\hat{f}^{st}(x) = \sum_{m=1}^{M} w_m^{st} \hat{f}_m(x).$$

  - Using cross–validated predictions $\hat{f}_m^{-i}(x)$ stacking avoids giving unfairly high weight to models with higher complexity
  - Better results can be obtained by restricting the weights to be nonnegative and to sum to 1.

Decision Rules from Decision Trees

- We can represent a tree as a set of rules
  - one rule for each leaf.
- These rules may be improved by testing each attribute in each rule
  - Has the rule without this test a better precision than with the test?
  - Use validation data
  - May be time consuming.
- These rules are sorted by (decreasing) precision.

Loss Matix

The cost of missclassification may be different for each class. The general loss specification is a **loss matrix** $L_{kk'}$, an element represent the cost of classifying k as k'. Must be zero at the diagonal, non-negative everywhere.

- we can modify $Gini(m) = \sum_{k \neq k'} L_{kk'} \hat{p}_{mk} \hat{p}_{mk'}$
- or weight the data samples k $L_{kk'}$ times (only in binary classification)
- we classify according to $k(m) = argmin_k \sum_l L_{lk} \hat{p}_{ml}$ in the leaves.

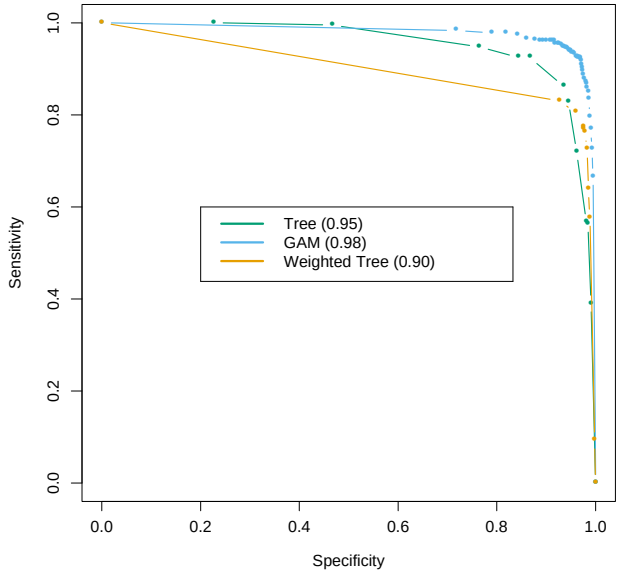


FIGURE 9.6. *ROC curves for the classification rules fit to the* `spam` *data. Curves that are closer to the north-east corner represent better classifiers. In this case the GAM classifier dominates the trees. The weighted tree achieves better sensitivity for higher specificity than the unweighted tree. The numbers in the legend represent the area under the curve.*

CART Weaknesses

- the high variance
  - the tree may be very different for very similar datasets
  - ensemble learning addresses this issue
- the cuts are perpendicular to the axis
- the result is not smooth but stepwise.
  - MARS (Multivariate Adaptive Regression Splines) addresses this issue.
- it is difficult to capture an additive structure

$$Y = c_1 I(X_1 < t_1) + c_2 I(X_2 < t_2) + \ldots + c_k I(X_k < t_k) + \epsilon$$

  - MARS (Multivariate Adaptive Regression Splines) addresses this issue.

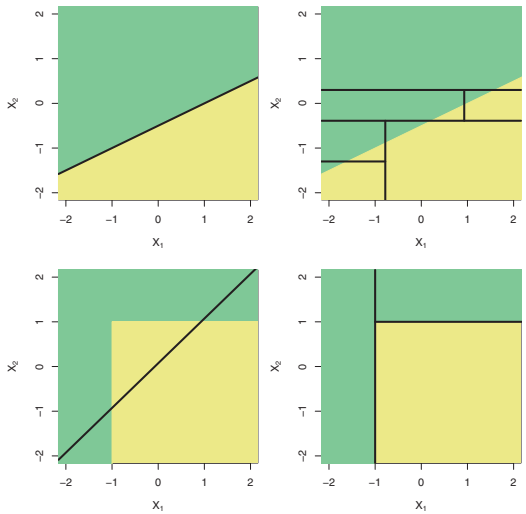


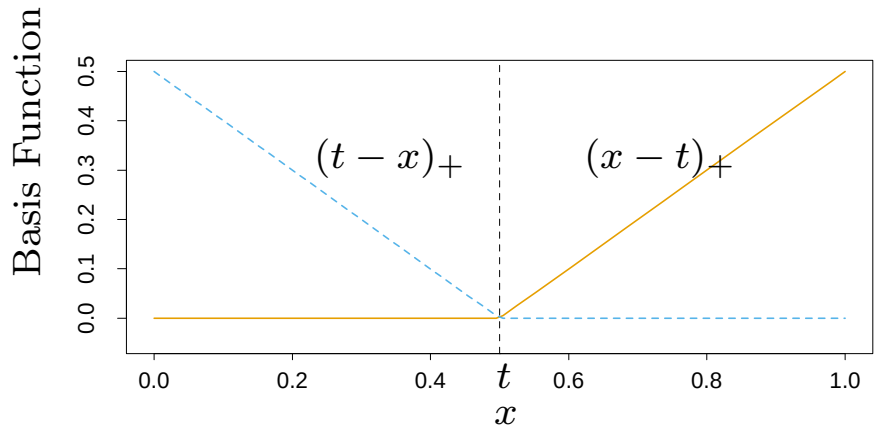
FIGURE 8.7. Top Row: *A two-dimensional classification example in which the true decision boundary is linear, and is indicated by the shaded regions. A classical approach that assumes a linear boundary (left) will outperform a de-*

MARS Multivariate Adaptive Regression Splines

- generalization of linear regression and decision trees CART
- for each feature and each data point we create a **reflected pair** of basis functions
- $(x - t)_+$ and $(t - x)_+$ where $+$ denotes non–negative part, minimum is zero.
- we have the set of functions

$$\mathcal{C} = \{(X_j - t)_+, (t - X_j)_+\}_{t \in \{x_{1,j}, x_{2,j}, \ldots, x_{N,j}\}, j=1,2,\ldots,p}$$

- that is $2Np$ functions for non–duplicated data points.

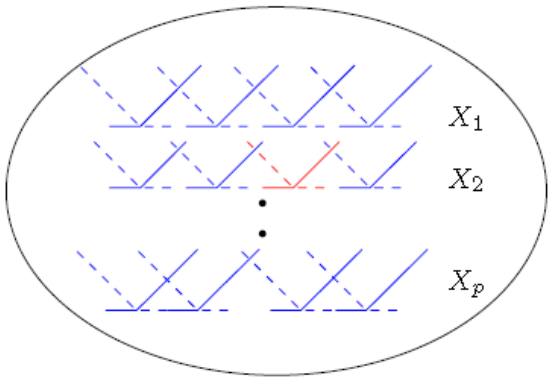


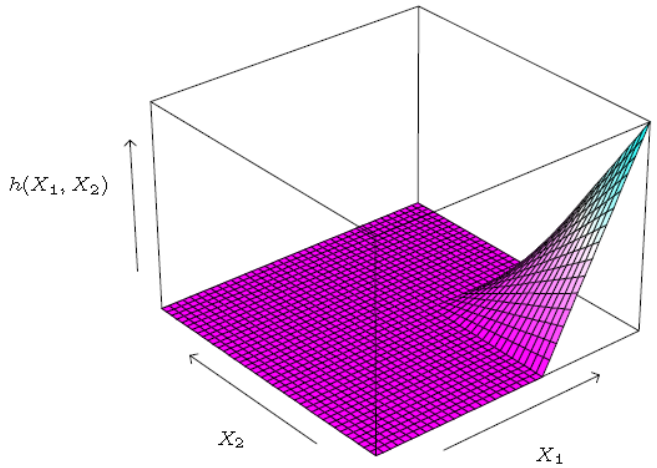
MARS – continuation

- our model is in the form

$$f(X) = \beta_0 + \sum_{m=1}^{M} \beta_m h_m(X)$$

  where $h_m(X)$ is a function from $\mathcal{C}$ or a product of any amount of functions from $\mathcal{C}$
- for a fixed set of h_m's we calculate coefficients β_m by usual linear regression (minimizing RSS)
- the set of functions h_m is selected iteratively.



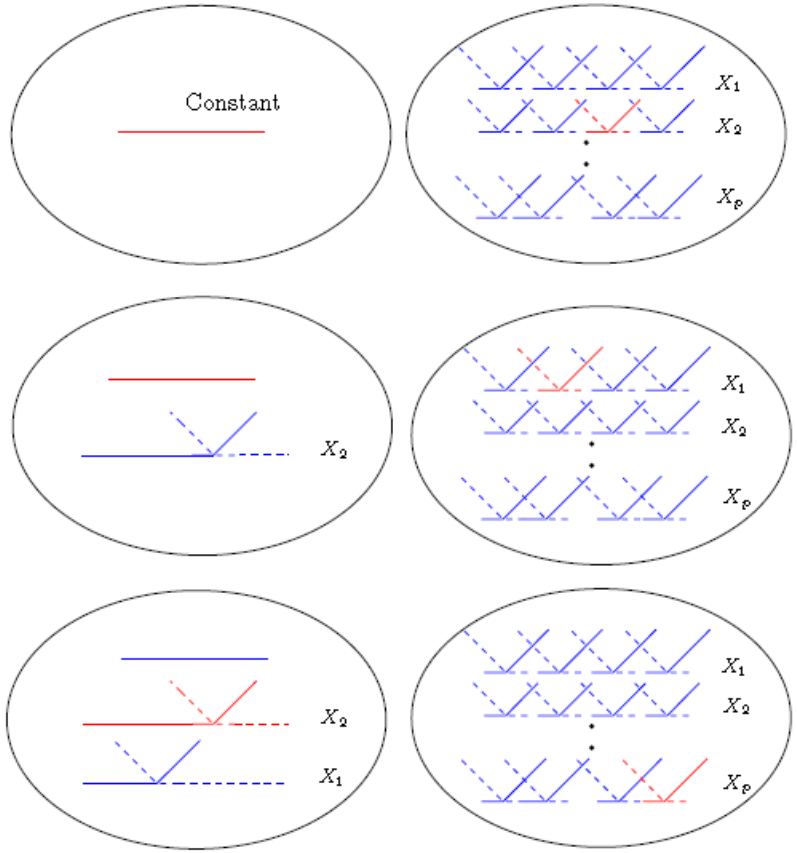


MARS – basis selections

- We start with $h_0 = 1$, we put this function into the model $\mathcal{M} = \{h_0\}$.
- We consider the product of any member $h_\ell \in \mathcal{M}$ with any pair from $\mathcal{C}$,

  $$\hat{\beta}_{M+1} h_\ell(X) \cdot (X_j - t)_+ + \hat{\beta}_{M+2} h_\ell(X) \cdot (t - X_j)_+$$

  we select the one minimizing training error RSS (for any product candidate, we estimate $\hat{\beta}$).
- Repeat until predefined number of functions in $\mathcal{M}$



MARS – model pruning

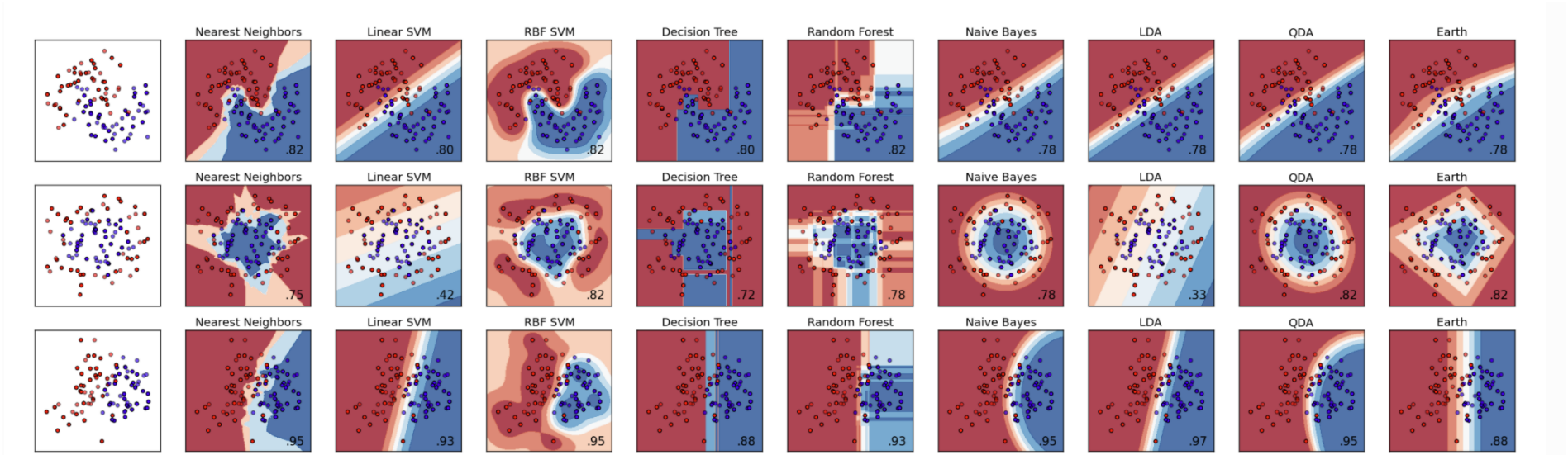
- The model is usually overfitted. We select (remove) iteratively the one minimizing the increase of training RSS. We have a sequence of models $\hat{f}_\lambda$ for different numbers of parameters λ.
- (we want to speed–up cross-validation for computational reasons)
- we select λ (and the model) minimizing **generalized cross-validation**

$$GCV(\lambda) = \frac{\sum_{i=1}^{N}(y_i - \hat{f}_\lambda(x_i))^2}{(1 - M(\lambda)/N)^2}.$$

- where $M(\lambda)$ is the number of effective parameters, the number of function h_m (denoted r) plus the number of knots K, the authors suggest to multiply K by 3: $M(\lambda) = r + 3K$.

MARS is a generalization of CART

- We select piecewise constant functions $I(x - t > 0)$ and $I(x - t \leq 0)$
- If h_m uses multiplication we remove this function from the candidate list. It cannot be used any more.
  - This guarantees binary split.
- Its CART.



https://contrib.scikit-learn.org/py-earth/auto_examples/plot_classifier_comp.html

https://contrib.scikit-learn.org/py-earth/auto_examples/index.html

Patient Rule Induction Method PRIM = Bump Hunting

- Rule induction method
- We iteratively search regions with the high Y values
  - for each region, a rule is created.
- CART runs of data after aproximately $\log_2(N) - 1$ cuts.
- PRIM can affort $-\frac{\log(N)}{\log(1-\alpha)}$.
  For $N = 128$ data samples and $\alpha = 0.1$ it is 6 and 46 respectively 29, since the number of observations must be a whole number.

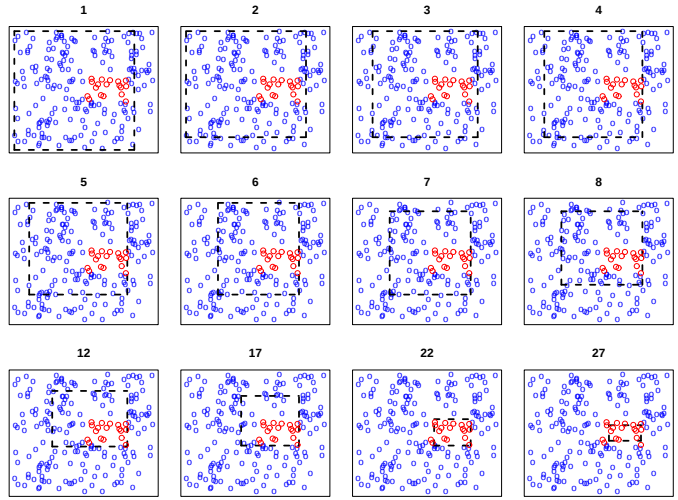
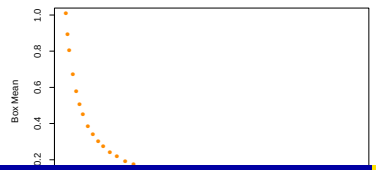


FIGURE 9.7. *Illustration of PRIM algorithm. There are two classes, indicated by the blue (class 0) and red (class 1) points. The procedure starts with a rectangle (broken black lines) surrounding all of the data, and then peels away points along one edge by a prespecified amount in order to maximize the mean of the points remaining in the box. Starting at the top left panel, the sequence of peelings is shown, until a pure red region is isolated in the bottom right panel. The iteration number is indicated at the top of each panel.*

PRIM Patient Rule induction Algorithm

PRIM

- Consider the whole space and all data. Set $\alpha = 0.05$ or 0.10.
- Find X_j and its upper or lower boundary such that the cut of $\alpha \cdot 100\%$ observations leads to the maximal mean of the remaining data.
- Repeat until less then 10 observations left.
- Enlarge the region in any direction that increases the mean value.
- Select the number of regions by the crossvalidation. All regions generated 1-4 are considered.
- Denote the best region B_1.
- Create a rule that describes B_1.
- Remove all data in B_1 from the dataset.
- Repeat 2-5, create B_2 continue until final condition met.



Unsupervised Learning

- No goal class (either Y nor G).
- We are interested in relations in the data:

  Clustering Are the data organized in natural clusters? (Clustering, Segmentation)
  EM algorithm for clustering
  (Dirichlet Process Mixture Models)
  (Spectral Clustering)

  Association Rules Are there some frequent combinations, implication relations? (Market Basket Analysis) *later*

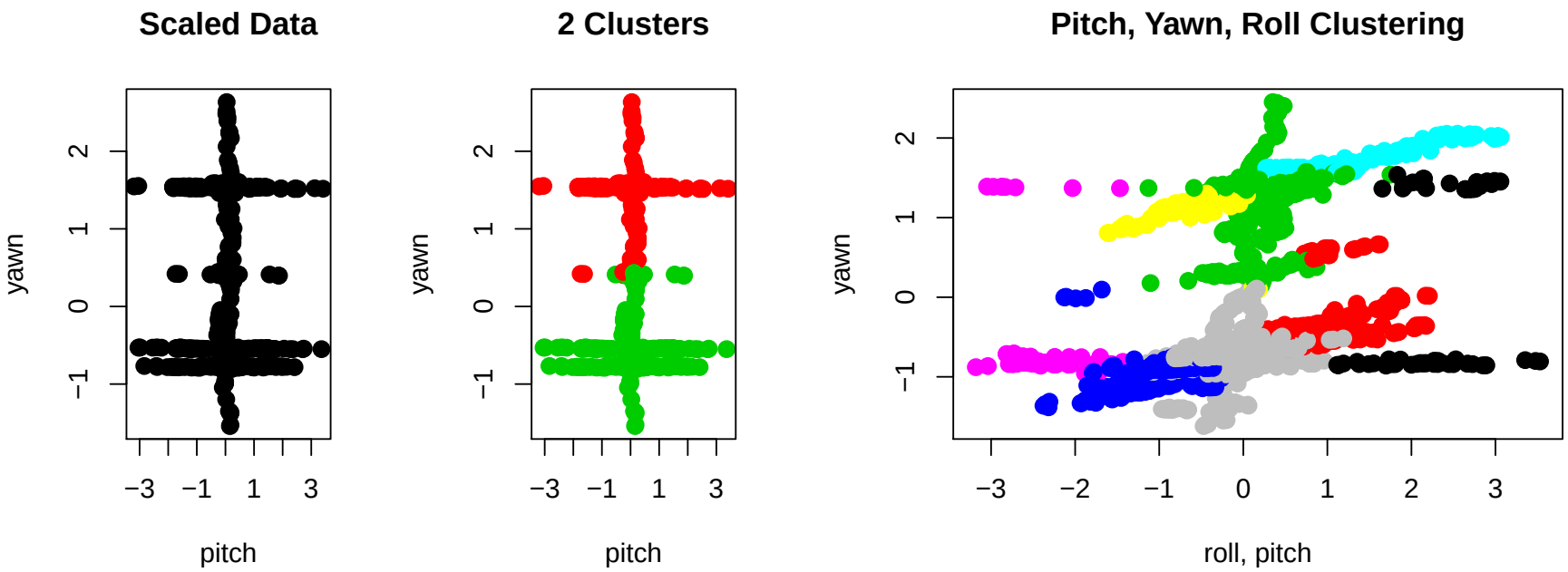
  Other The Elements of Statistical Learning Chapter 14

  SOM Self Organizing Maps

  PCA Principal Component Analysis Linear Algebra; k linear combinations of features minimizing reconstruction error (= first k principal components).
  - Principal Curves and Surfaces, Kernel and Spare Principal Components

  ICA Independent Component Analysis.

Clustering Example



- We set the color of items, no colour in train data.
- We want to assign same color to nearby points.

K – means !

K–means

1: **procedure** $K-\text{MEANS}$:(X data, K the number of clusters)
2: select randomly K centers of clusters μ_k
3: # either random data points or random points in the feature space
4: **repeat**
5: **for** each data record **do**
6: $C(x_i) \leftarrow argmin_{k \in \{1,\ldots,K\}} d(x_i, \mu_k)$
7: **end for**
8: **for** each cluster k **do** # find new centers μ_k
9: $\mu_k = \sum_{x_i : C(x_i)=k} \frac{x_i}{|C(k)|}$.
10: **end for**
11: **until** no chance in assignment
12: **end procedure**

K – means

K–means

The t iterations of K–means algorithm take $O(tkpN)$ time.

- To find global optimum is NP-hard.
- The result depends on initial values.
- May get stuck in local minimum.
- May not be robust to data sampling.
  - We may generate datasets by bootstrap method.
  - The cluster centers found in different dataset may be quite different.

  (for example, different bootstrap samples may give very different clustering results).
- Each record must belong to some cluster. Sensitive to outliers.

Distance measures

the most common distance measures:

Euclidian	$d(x_i, x_j) = \sqrt{\sum_{r=1}^{p}(x_{ir} - x_{jr})^2}$
Hamming (Manhattan)	$d(x_i, x_j) = \sum_{r=1}^{p} \lvert x_{ir} - x_{jr} \rvert$
overlap (překrytí) categorical variables	$d(x_i, x_j) = \sum_{r=1}^{p} I(x_{ir} \neq x_{jr})$
cosine similarity	$s(x_i, x_j) = \frac{\sum_{r=1}^{p}(x_{ir} \cdot x_{jr})}{\sqrt{\sum_{r=1}^{p}(x_{jr} \cdot x_{jr}) \cdot \sum_{r=1}^{p}(x_{ir} \cdot x_{ir})}}$
cosine distance	$d(x_i, x_j) = 1 - \frac{\sum_{r=1}^{p}(x_{ir} \cdot x_{jr})}{\sqrt{\sum_{r=1}^{p}(x_{jr} \cdot x_{jr}) \cdot \sum_{r=1}^{p}(x_{ir} \cdot x_{ir})}}$

Distance – key issue, application dependent

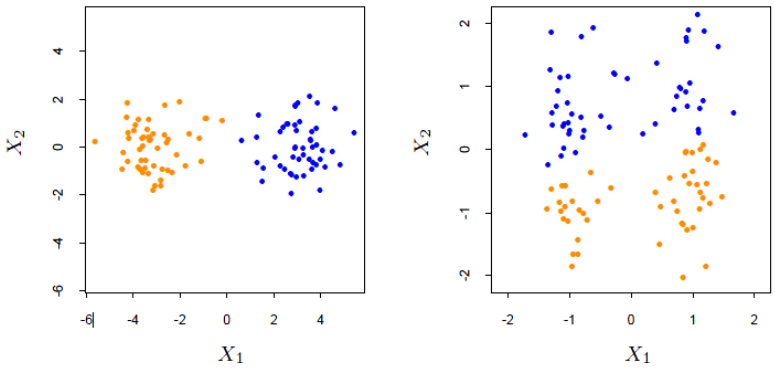
- The result depends on the choice of distance measure $d(x_i, \mu_k)$.
- The choice is application dependent.
- Scaling of the data is recommended.
- Weights for equally important attributes are: $w_j = \frac{1}{\hat{d}j}$ where

$$\hat{d}_j = \frac{1}{N^2} \sum_{i_1=1}^{N} \sum_{i_2=1}^{N} d_j(x_{i_1}, x_{i_2}) = \frac{1}{N^2} \sum_{i_1=1}^{N} \sum_{i_2=1}^{N} (x_{i_1} - x_{i_2})^2$$

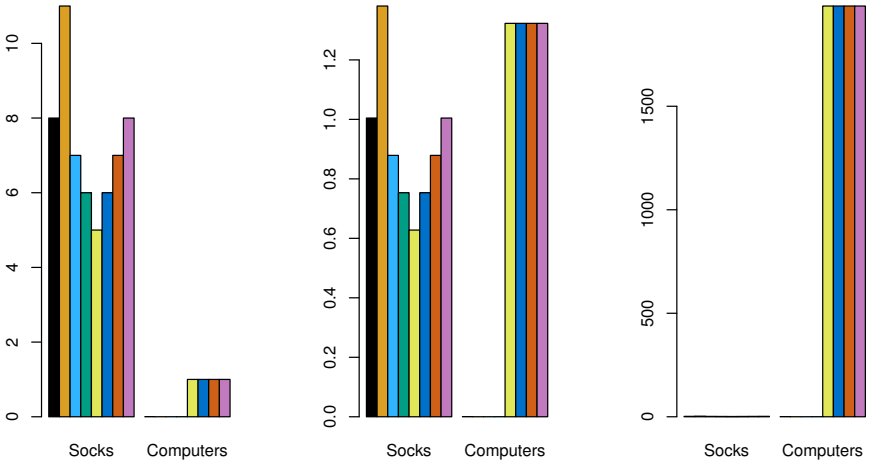
- Total distance as a weighted sum of attribute distances.
- Distance may be specified directly by a symmetric matrix, 0 at the diagonal, should fulfill triangle inequality

$$d(x_i, x_\ell) \leq d(x_i, x_r) + d(x_r, x_\ell).$$

Alternative Ideas



- Scaling may remove natural clusters
- Weighting Attributes
  - Consider internet shop offering socks and computers.
  - Compare: number of sales, standardized data, $



Number of Clusters

- We may focus on the **Within cluster variation** measure:

$$W(C) = \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \sum_{C(i')=k} d(x_i, x_{i'})$$

- Notice that $W(C)$ is decreasing also for uniformly distributed data.
- We look for small drop of $W(C)$ as a function of K or maximal difference between $W(C)$ on our data and on the uniform data.
- **Total** cluster variation is the sum of **between** cluster variation and **within** cluster variation

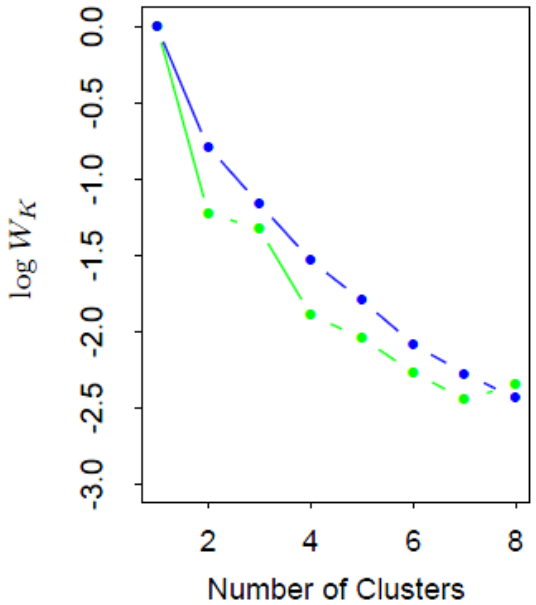
$$\begin{aligned} T(C) &= \frac{1}{2} \sum_{i,i'=1}^{N} d(x_i, x_{i'}) = W(C) + B(C) \\ &= \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \left(\sum_{C(i')=k} d(x_i, x_{i'}) \right) + \frac{1}{2} \sum_{k=1}^{K} \sum_{C(i)=k} \left(\sum_{C(i')\neq k} d(x_i, x_{i'}) \right) \end{aligned}$$

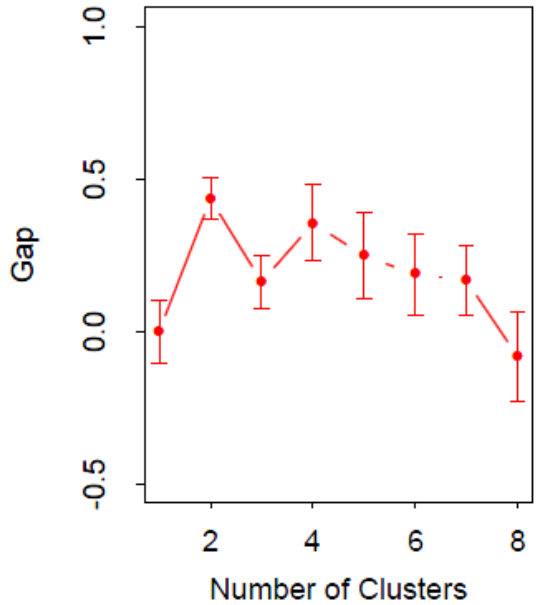
GAP function for Number of Clusters

- denote W_k the expected W for uniformly distributed data and k clusters, the average over 20 runs
- GAP is expected $log(W_k)$ minus observed $log(W(k))$

$$K^* = argmin\{k|G(k) \geq G(k+1) - s'_{k+1}\}$$

$$s'_k = s_k\sqrt{1+\frac{1}{20}} \text{ where } s_k \text{ is the standard deviation of } log(W_k)$$





Silhouette

For each data sample x_i we define

- $a(i) = \frac{1}{|C_i|-1} \sum_{j \in C_i, i \neq j} d(i,j)$ if $|C_i| > 1$
- $b(i) = min_{k \neq i} \frac{1}{|C_k|} \sum_{j \in C_k} d(i,j)$

Definition (Silhouette)

Silhouette s is defined

- $s(i) = \frac{b(i)-a(i)}{max\{a(i),b(i)\}}$ if $|C_i| > 1$
- $s(i) = 0$ for $|C_i| = 1$.

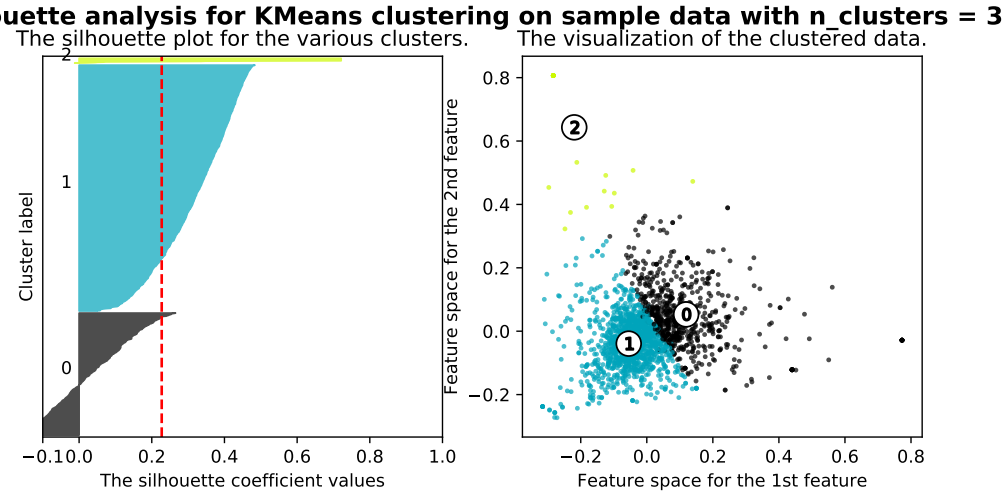
Optimal number of clusters k may be selected by the SC.

Definition (Silhouette Score)

The Silhouette score is $\frac{1}{N} \sum_i^N s(i)$.

Silhouette is always between

- $-1 \leq s(i) \leq 1$.



Note: One cluster $(-1,1),(1,1)$, other cluster $(0,-1.2),(0,-1.1)$, the point $(0,0)$ is assigned to the first cluster but has a negative silhouette. https://stackoverflow.com/a/66751204

Country Similarity Example

- Data from a political science survey: values are average pairwise dissimilarities of countries from a questionnaire given to political science students.

	BEL	BRA	CHI	CUB	EGY	FRA	IND	ISR	USA	USS	YUG
BRA	5.58										
CHI	7.00	6.50									
CUB	7.08	7.00	3.83								
EGY	4.83	5.08	8.17	5.83							
FRA	2.17	5.75	6.67	6.92	4.92						
IND	6.42	5.00	5.58	6.00	4.67	6.42					
ISR	3.42	5.50	6.42	6.42	5.00	3.92	6.17				
USA	2.50	4.92	6.25	7.33	4.50	2.25	6.33	2.75			
USS	6.08	6.67	4.25	2.67	6.00	6.17	6.17	6.92	6.17		
YUG	5.25	6.83	4.50	3.75	5.75	5.42	6.08	5.83	6.67	3.67	
ZAI	4.75	3.00	6.08	6.67	5.00	5.58	4.83	6.17	5.67	6.50	6.92

K–medoids

1: **procedure** $K-$MEDOIDS:(X data, K the number of clusters)
2: select randomly K data samples to be centroids of clusters
3: **repeat**
4: **for** each data record **do**
5: assign to the closest cluster
6: **end for**
7: **for** each cluster k **do** # find new centroids $i_k^* \in C_k$
8: $i_k^* \leftarrow argmin_{\{i:C(i)=k\}} \sum_{C(i')=k} d(x_i, x_{i'})$
9: **end for**
10: **until** no chance in assignment
11: **end procedure**

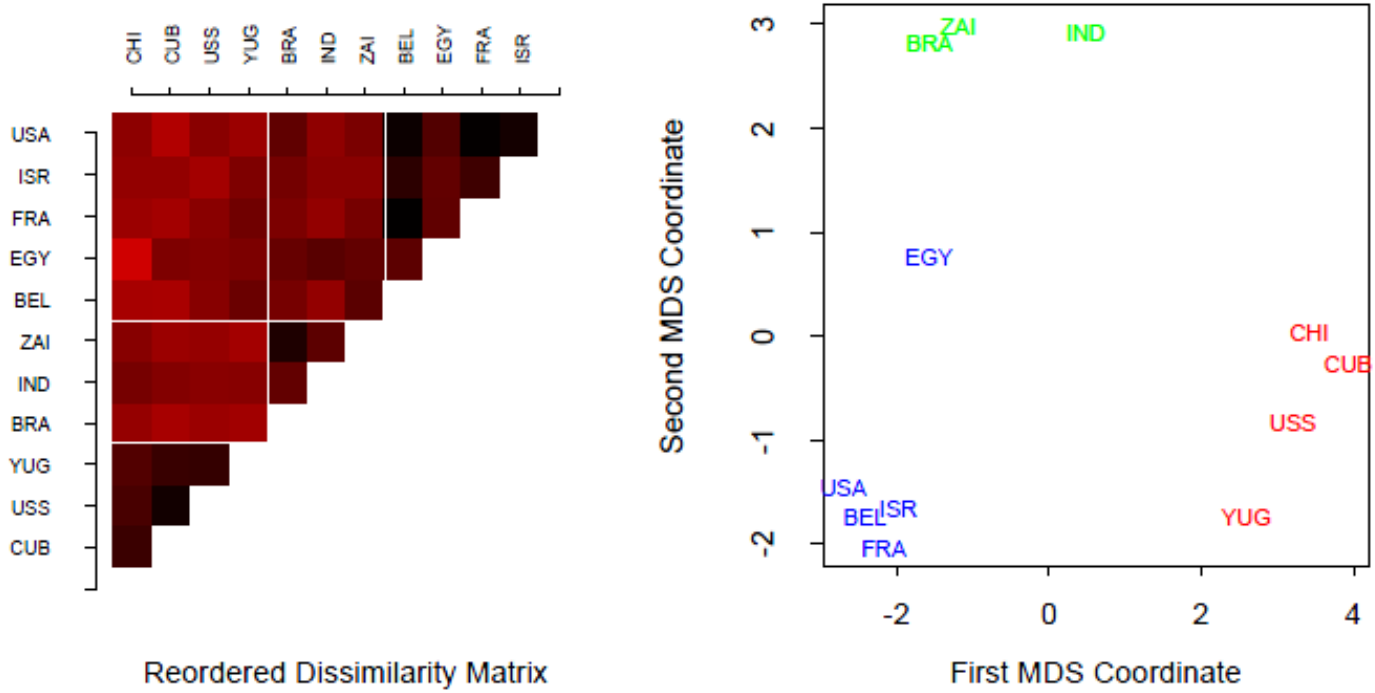
- To find a centroid requires quadratic time compared to linear k–means.
- We may use any distance, for example number of differences in binary attributes.

Complexity

The t iterations of K–medoids take $O(tkpN^2)$.

Clusters of Countries

- Survey of country dissimilarities.
- Left: dissimilarities
  - Reordered and blocked according to 3-medoid clustering.
  - Heat map is coded from most similar (dark red) to least similar (bright red).
- Right: Two-dimensional multidimensional scaling plot
  - with 3-medoid clusters indicated by different colors.



Multidimensional Scaling

- The right figure on previous slide was done by Multidimesional scaling.
- We know only distances of countries, not a metric space.
- We try to keep proximity of countries (*least squares scaling*).
- We choose the number of dimensions p.

Definition (Multidimensional Scaling)

For a given data $x_1, \ldots, x_N$ with their distance matrix d, we search $(z_1, \ldots, z_N) \in \mathbb{R}^p$ projections of data minimizing stress function

$$S_D(z_1, \ldots, z_N) = \left[\sum_{i \neq \ell} (d[x_i, x_\ell] - \|z_i - z_\ell\|)^2 \right]^{\frac{1}{2}}.$$

- It is evaluated gradiently.
- Note: Spectral clustering.

Hierarchical clustering – Bottom Up

Start with each data sample in its own cluster. Iteratively join two nearest clusters. Measures for join

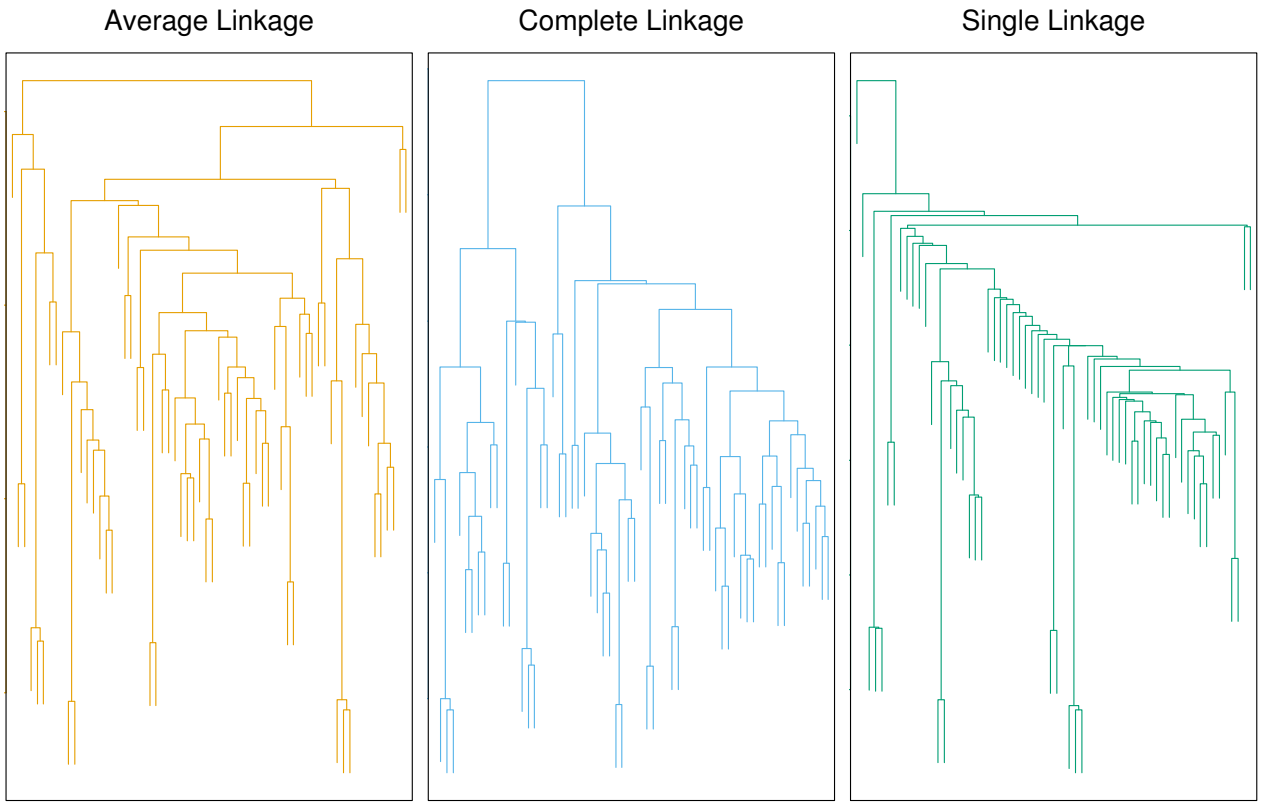
- closest points (**single linkage**)
- maximally distant points (**complete linkage**)
- **average linkage**, $d_{GA}(C_A, C_B) = \frac{1}{|C_A| \cdot |C_B|} \sum_{x_i \in C_A, x_j \in C_B} d(x_i, x_j)$
- **Ward distance** minimizes the sum of squared differences within all clusters.

$$\begin{aligned} Ward(C_A, C_B) &= \sum_{i \in C_A \cup C_B} d(x_i, \mu_{A \cup B})^2 - \sum_{i \in C_A} d(x_i, \mu_A)^2 - \sum_{i \in C_B} d(x_i, \mu_B)^2 \\ &= \frac{|C_A| \cdot |C_B|}{|C_A| + |C_B|} \cdot d(\mu_A, \mu_B)^2 \end{aligned}$$

- where μ are the centers of clusters (A, B and joined cluster).
- It is a variance-minimizing approach and in this sense is similar to the k-means objective function but tackled with an agglomerative hierarchical approach.

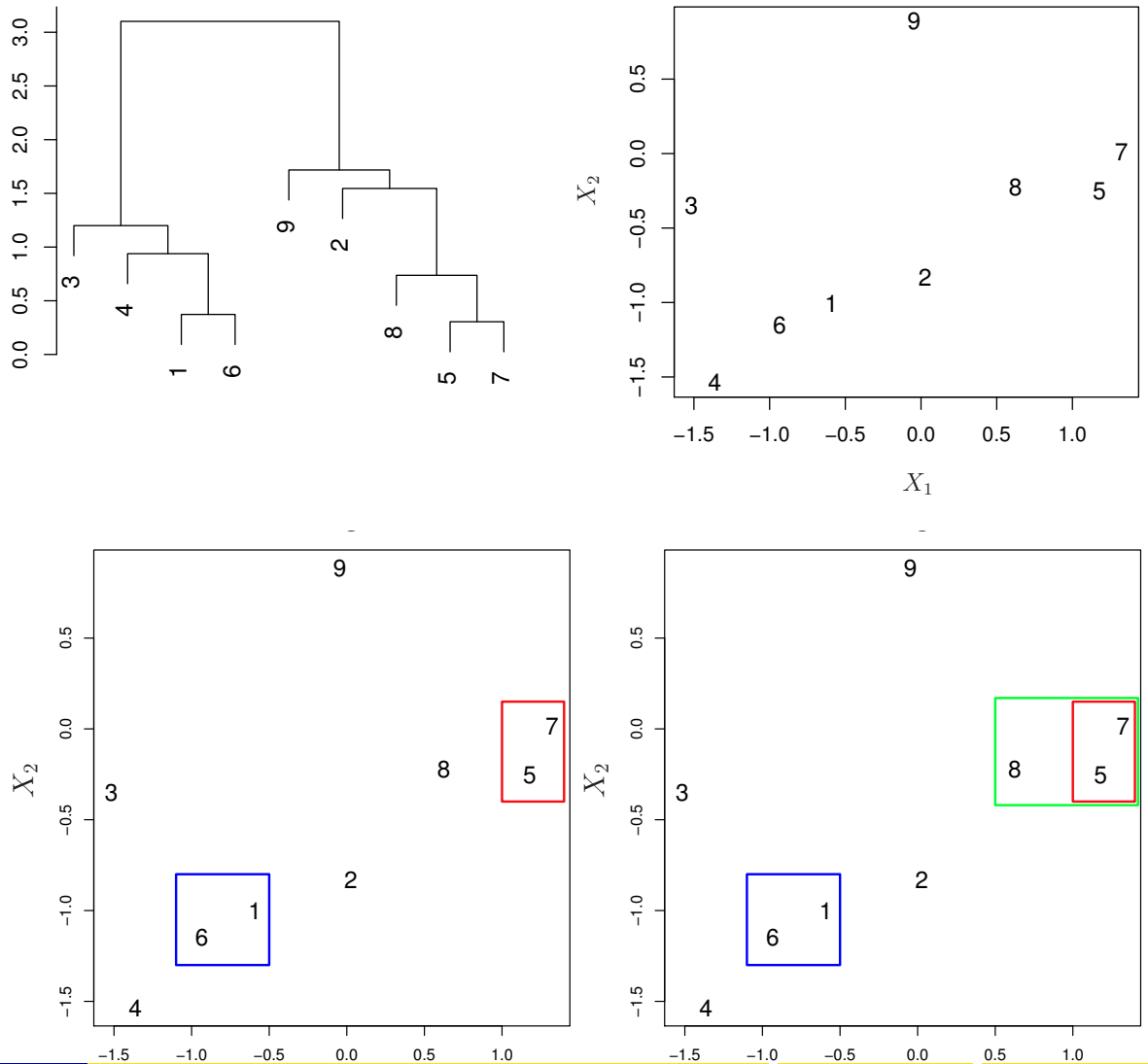
Dendrograms

- Dendrogram is the result plot of a hierarchical clustering.
- Cutting the tree of a fixed high splits samples at leaves into clusters.
  - The length of the two legs of the U-link represents the distance between the child clusters.



Interpretation of Dendrograms – 2 and 9 are NOT close

Samples fused at very bottom are close each other.



Mean Shift Clustering

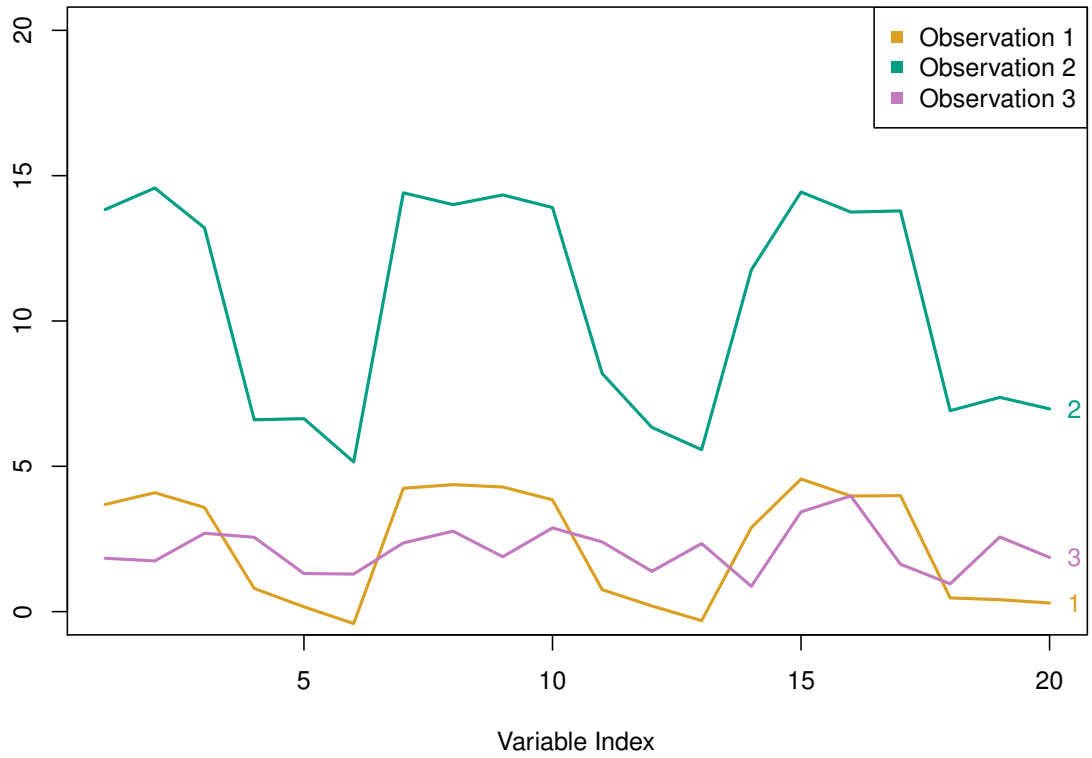
Mean Shift Clustering

1: **procedure** MEAN SHIFT CLUSTERING:(X data, $K(\cdot)$ the kernel, λ the bandwidth)
2: $\mathcal{C} \leftarrow \emptyset$
3: **for** each data record **do**
4: **repeat** # shift each mean x to the weighted average
5: $m(x) \leftarrow \frac{\sum_{i=1}^{N} K(x_i - x) x_i}{\sum_{i=1}^{N} K(x_i - x)}$
6: **until** no chance in assignment
7: add the new $m(x)$ to $\mathcal{C}$
8: **end for**
9: return prunned $\mathcal{C}$
10: **end procedure**

Kernels:

- flat kernel λ ball
- Gaussian kernel $K(x_i - x) = e^{\frac{\|x_i - x\|^2}{\lambda^2}}$

Other Distance Measures



Correlation Proximity

- Euclidian distance: Observations 1 and 3 are close.
- Correlation distance: 1 and 2 look very similar.

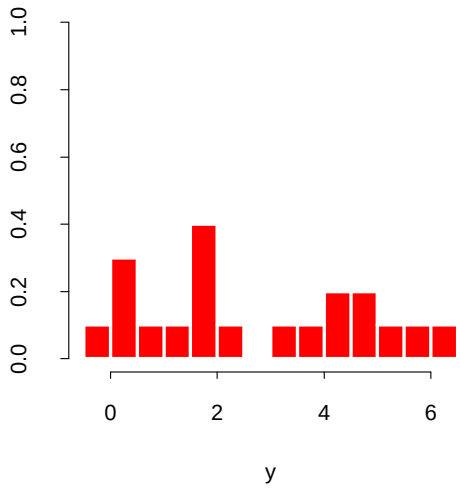
$$\rho_{X,Y} = corr(X, Y) = \frac{cov(X, Y)}{\sigma_X \sigma_Y} = \frac{E[(X - \mu_X)(Y - \mu_Y)]}{\sigma_X \sigma_Y}$$

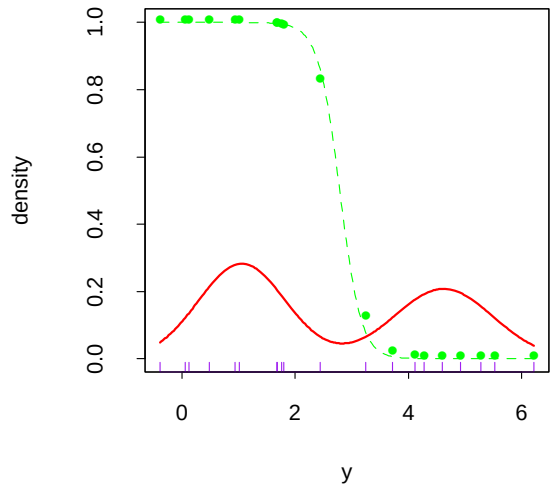
Summary

- K-means clustering - the basic one
  - the number of clusters:
  - GAP
  - Silhouette
- The distance is crucial.
  - Consider standardization or weighting the features.
- K-medoids - does need metric, just a distance
- hierarchical clustering
  - different distance measures
  - dendrogram
- other approaches (mean shift clustering, Self Organizing Maps, Spectral Clustering).

Gaussian Mixture Model

- Assume the data come from a set of k gaussian distributions
- each with
  - prior probability π_k
  - mean μ_k
  - covariance matrix Σ_k
  - $\phi_{\mu_k,\Sigma_k}(x) = \frac{1}{\sqrt{(2\pi)^p|\Sigma_k|}} e^{-\frac{1}{2}(x-\mu_k)^T\Sigma_k^{-1}(x-\mu_k)}$.
- We want to find the maximum likelihood estimate of the model parameters.
- We use (more general) EM algorithm.





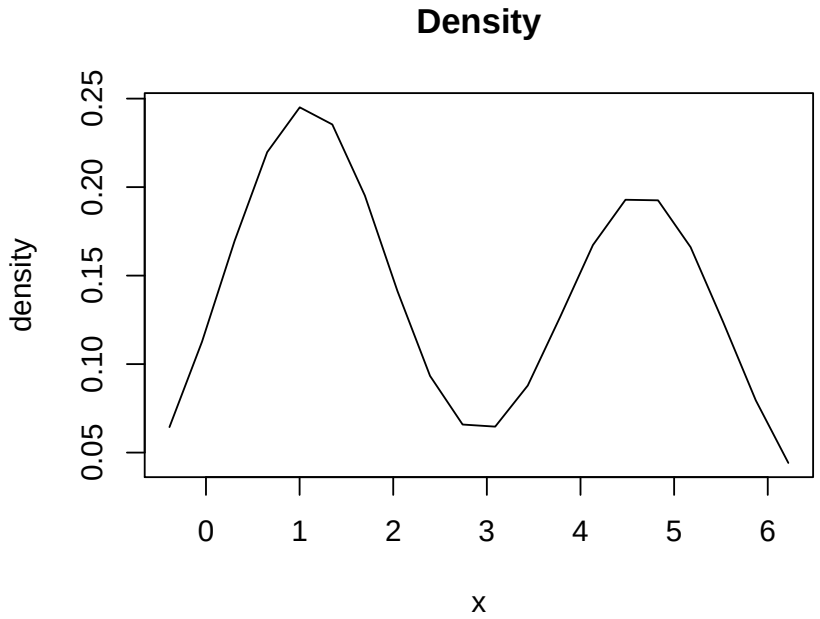
EM learning of Mixture of K Gaussians !

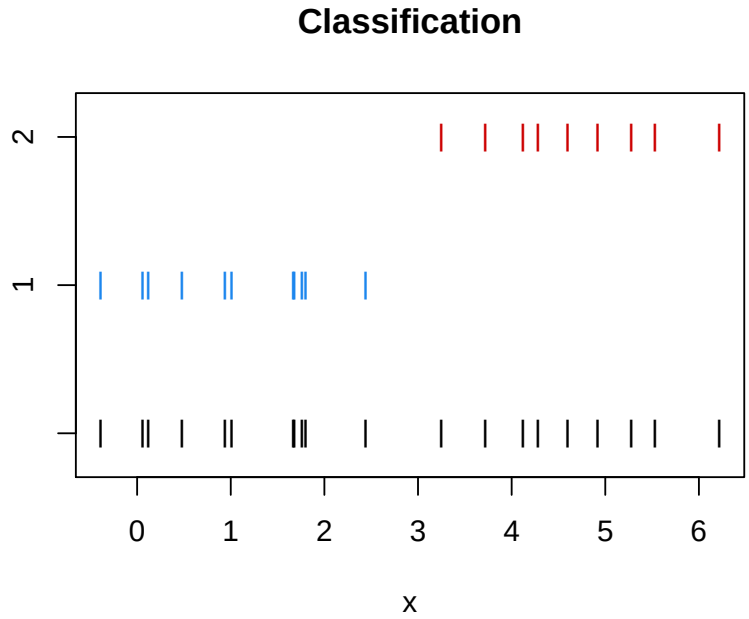
- Model parameters $\pi_1, \ldots, \pi_k, \mu_1, \ldots, \mu_k, \Sigma_1, \ldots, \Sigma_k$ such that $\sum_{k=1}^{K} \pi_k = 1$.
- **E**xpectation: weights of unobserved 'fill–ins' k of variable C:

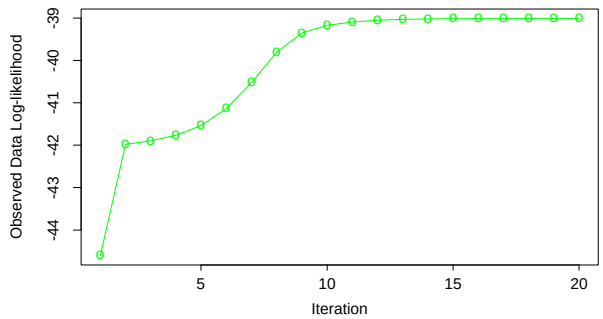
$$\begin{aligned} p_{ik} &= P(C = k|x_i) = \alpha \cdot P(x_i|C_i = k) \cdot P(C_i = k) \\ &= \frac{\pi_k \phi_{\theta_k}(x_i)}{\sum_{l=1}^{K} \pi_l \phi_{\theta_l}(x_i)} \\ p_k &= \sum_{i=1}^{N} p_{ik} \end{aligned}$$

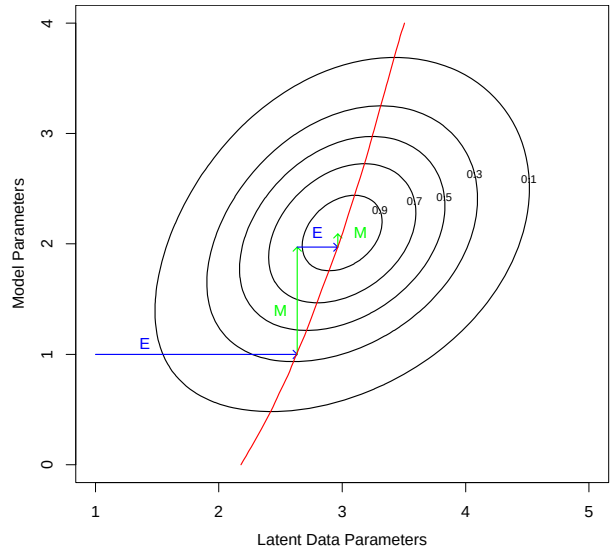
- **M**aximize: mean, variance and cluster 'prior' for each cluster k:

$$\begin{aligned} \mu_k &\leftarrow \sum_i \frac{p_{ik}}{p_k} x_i \\ \Sigma_k &\leftarrow \sum_i \frac{p_{ik}}{p_k} (x_i - \mu_k)(x_i - \mu_k)^T \\ \pi_k &\leftarrow \frac{p_k}{\sum_{l=1}^{K} p_l}. \end{aligned}$$


Density
density
0.05
0.10
0.15
0.20
0.25
0
1
2
3
4
5
6
x


Classification
1
2
0
1
2
3
4
5
6
x


Observed Data Log-likelihood
-39
-40
-41
-42
-43
-44
5
10
15
20
Iteration


Model Parameters
0
1
2
3
4
1
2
3
4
5
Latent Data Parameters
E
M
E
M
0.9
0.7
0.5
0.3
0.1

ML Estimate of Gaussian Distribution Parameters

- Assume x to have Gaussian distribution with unknown parameters μ a σ.
- Our hypotheses are $h_{\mu,\sigma} = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$.
- We have observed $x_1, \ldots, x_n$.
- Log likelihood is:

$$\begin{aligned} LL &= \sum_{j=1}^{N} log \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-(x-\mu)^2}{2\sigma^2}} \\ &= N \cdot (log \frac{1}{\sqrt{2\pi}\sigma}) - \sum_{j=1}^{N} \frac{(x_j - \mu)^2}{2\sigma^2} \end{aligned}$$

- Find the maximum.

Linear Gaussian Distribution

- Assume random variable (feature) X.
- Assume goal variable Y with linear gaussian distribution where $\mu = b \cdot x + b_0$ and fixed variance σ^2 $p(Y|X = x) = N(b \cdot x + b_0; \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{-(y-((b \cdot x + b_0))^2}{2\sigma^2}}$.
- Find maximum likelihood estimate of b, b_0 given a set of observations $data = \{\langle x_1, y_1 \rangle, \ldots, \langle x_N, y_N \rangle\}$.
- (Look for maximum of the logarithm of it; change the max to min with the opostite sign. Do you know this formula?)

$$argmax_{b,b_0}(log_e(\Pi_{i=1}^{N}(e^{-(y_i-(b \cdot x_i+b_0))^2}))) = argmin_{b,b_0}(?)$$

Bayesian Learning

Complicated derivation of known things.

- **Maximum a posteriori probability hypothesis** (MAP) (nejpravděpodobnější hypotéza)
- **Maximum likelihood hypothesis** (ML) (maximálně věrohodná hypotéza)
- **Bayesian optimal prediction** (Bayes Rate)
- Bayesian methods, bayesian smoothing
- **EM algorithm**
- **Naive Bayes model (classifier)**.

Candy Example (Russel, Norvig: Artif. Intell. a MA)

- Our favorite candy comes in two flavors: cherry and lime, both in the same wrapper.
- They are in a bag in one of following rations of cherry candies and prior probability of bags:

hypothesis (bag type)	h_1	h_2	h_3	h_4	h_5
cherry	100%	75%	50%	25%	0%
prior probability h_i	10%	20%	40%	20%	10%

- The first candy is cherry.

  MAP Which of h_i is the most probable given first candy is cherry?

  Bayes estimate What is the probability next candy from the same bag is cherry?

Maximum Aposteriory Probability Hypothesis (MAP)

- We assume large bags of candies, the result of one missing candy in the bag is negligable.
- Recall Bayes formula:

$$P(h_i|B=c) = \frac{P(B=c|h_i)\cdot P(h_i)}{\sum_{j=1,\ldots,5} P(B=c|h_j)\cdot P(h_j)} = \frac{P(B=c|h_i)\cdot P(h_i)}{P(B=c)}$$

- We look for the MAP hypothesis **maximálně aposteriorně pravděpodobná**

$$argmax_i P(h_i|B=c) = argmax_i P(B=c|h_i)\cdot P(h_i).$$

- Aposteriory probabilities of hypotheses are in the following table.

Candy Example: Aposteriory Probability of Hypotheses

index	prior	cherry ratio	cherry AND h_i	aposteriory prob. h_i
i	$P(h_i)$	$P(B = c\|h_i)$	$P(B = c\|h_i) \cdot P(h_i)$	$P(h_i\|B = c)$
1	0.1	1	0.1	0.2
2	0.2	0.75	0.15	0.3
3	0.4	0.5	0.2	**0.4**
4	0.2	0.25	0.05	0.1
5	0.1	0	0	0

- Which hypothesis is most probable?

$$h_{MAP} = argmax_i P(data|h_i) \cdot P(h_i)$$

- What is the prediction of a new candy according the most probable hypothesis h_{MAP}?

Bayesian Learning, Bayesian Optimal Prediction

- **Bayesian optimal prediction** is weigthed average of predictions of all hypotheses:

$$\begin{aligned} P(N = c|data) &= \sum_{j=1,\ldots,5} P(N = c|h_j, data) \cdot P(h_j|data) \\ &= \sum_{j=1,\ldots,5} P(N = c|h_j) \cdot P(h_j|data) \end{aligned}$$

- If our model is correct, no prediction has smaller expected error then Bayesian optimal prediction.
- We always assume i.i.d. data, independently identically distributed.
- We assume the hypothesis fully describes the data behavior. Observations are mutually conditionally independent given the hypothesis. This allows the last equation above.

Candy Example: Bayesian Optimal Prediction

i	$P(h_i \mid B = c)$	$P(N = c \mid h_i)$	$P(N = c \mid h_i) \cdot P(h_i \mid B = c)$
1	0.2	1	0.2
2	0.3	0.75	0.225
3	0.4	0.5	0.2
4	0.1	0.25	0.02
5	0	0	0
$\sum$	1		0.645

Maximum Likelihood Estimate (ML)

- Usually, we do not know prior probabilities of hypotheses.
- Setting all prior probabilities equal leads to **Maximum Likelihood Estimate, maximálně věrohodný odhad**

$$h_{ML} = argmax_i P(data|h_i)$$

- Probability of data given hypothesis = likelihood of hypothesis given data.
- Find the ML estimate:

index	prior	cherry ratio	cherry AND h_i	Aposteriory prob. h_i
i	$P(h_i)$	$P(B = c\|h_i)$	$P(B = c\|h_i) \cdot P(h_i)$	$P(h_i\|B = c)$
1	0.1	1	0.1	0.2
2	0.2	0.75	0.15	0.3
3	0.4	0.5	0.2	0.4
4	0.2	0.25	0.05	0.1
5	0.1	0	0	0

- In this example, do you prefer ML estimate or MAP estimate?
- (Only few data, over-fitting, penalization is useful. AIC, BIC)

MAP and Penalized Methods

- MAP hypothesis maximizes:

$$h_{MAP} = argmax_i P(data|h_i) \cdot P(h_i)$$

- therefore minimizes:

$$\begin{aligned} h_{MAP} &= argmax_h P(data|h)P(h) \\ &= argmin_h[-log_2 P(data|h) - log_2 P(h)] \\ &= argmin_h[-loglik + \text{complexity penalty}] \\ &= argmin_h[RSS + \text{complexity penalty}] \text{ Gaussian models} \\ &= argmax_h[loglik - \text{complexity penalty}] \text{ Categorical models} \end{aligned}$$

Maximum Likelihood: Continuous Parameter θ

- New producer on the market. We do not know the ratios of candies, any h_θ, kde $\theta \in \langle 0; 1 \rangle$ is possible, any prior probabilities h_θ are possible.
- We look for maximum likelihood estimate.
- For a given hypothesis h_θ, the probability of a cherry candy is θ, of a lime candy $1 - \theta$.
- Probability of a sequence of c cherry and l lime candies is:

$$P(data|h_\theta) = \theta^c \cdot (1 - \theta)^l.$$

ML Estimate of Parameter θ

- Probability of a sequence of c cherry and l lime candies is:

$$P(data|h_\theta) = \theta^c \cdot (1-\theta)^l$$

- Usual trick is to take logarithm:

$$\ell(h_\theta; data) = c \cdot \log_2 \theta + l \cdot \log_2(1-\theta)$$

- To find the maximum of ℓ (log likelihood of the hypothesis) with respect to θ we set the derivative equal to 0:

$$\begin{aligned} \frac{\partial \ell(h_\theta; data)}{\partial \theta} &= \frac{c}{\theta} - \frac{l}{1-\theta} \\ \frac{c}{\theta} &= \frac{l}{1-\theta} \\ \theta &= \frac{c}{c+l}. \end{aligned}$$

ML Estimate of Multiple Parameters

- Producer introduced two colors of wrappers - red r and green g.
- Both flavors are wrapped in both wrappers, but with different probability of the red/green wrapper.
- We need three parameters to model this situation:

$P(B = c)$	$P(W = r \mid B = c)$	$P(W = r \mid B = l)$
θ_0	θ_1	θ_2

- Following table denotes observed frequences:

wrapper\ flavor	cherry	lime
red	r_c	r_l
green	g_c	g_l

ML Estimate of Multiple Parameters

Parameters are:

$P(B=c)$	$P(W=r\|B=c)$	$P(W=r\|B=l)$
θ_0	θ_1	θ_2

Probability of data given the hypothesis $h_{\theta_0,\theta_1,\theta_2}$ is:

$$\begin{aligned} P(data|h_{\theta_0,\theta_1,\theta_2}) &= \theta_1^{r_c}\cdot(1-\theta_1)^{g_c}\cdot\theta_0^{r_c+g_c}\cdot\theta_2^{r_l}\cdot(1-\theta_2)^{g_l}\cdot(1-\theta_0)^{r_l+g_l} \\ \ell(h_{\theta_0,\theta_1,\theta_2};data) &= r_c\log_2\theta_1 + g_c\log_2(1-\theta_1) + (r_c+g_c)\log_2\theta_0 \\ &\quad + r_l\log_2\theta_2 + g_l\log_2(1-\theta_2) + (r_l+g_l)\log_2(1-\theta_0) \end{aligned}$$

We look for maximum:

$$\begin{aligned} \frac{\partial\ell(h_{\theta_0,\theta_1,\theta_2};data)}{\partial\theta_0} &= \frac{r_c+g_c}{\theta_0} - \frac{r_l+g_l}{1-\theta_0} \\ \theta_0 &= \frac{(r_c+g_c)}{r_c+g_c+r_l+g_l} \\ \frac{\partial\ell(h_{\theta_0,\theta_1,\theta_2};data)}{\partial\theta_2} &= \frac{r_l}{\theta_2} - \frac{g_l}{1-\theta_2} \\ \theta_2 &= \frac{r_l}{r_l+g_l}. \end{aligned}$$

Naive Bayes Model, Bayes Classifier

- Maximum Likelihood estimate is the ratio of frequences.
- **Naive Bayes Model, Bayes Classifier** assumes independent features given the class variable.
  - Calculate prior probability of classes $P(c_i)$
  - For each feature f, calculate for each class the probability of this feature $P(f|c_i)$
  - For a new observation of features f predict the most probable class $argmax_{c_i} P(f|c_i) \cdot P(c_i)$.

  Bayes factor
  - We can start with a comparison ratio of two classes $\frac{P(c_i)}{P(c_j)}$
  - after each observation x_p multiply it by the **bayes factor** $\frac{P(x_p|c_i)}{P(x_p|c_j)}$
  - that is:

$$\frac{P(c_i|x_1,\ldots,x_p)}{P(c_j|x_1,\ldots,x_p)} = \frac{P(c_i)}{P(c_j)} \cdot \frac{P(x_1|c_i)}{P(x_1|c_j)} \cdot \ldots \cdot \frac{P(x_p|c_i)}{P(x_p|c_j)}.$$

- Bayesian Networks learn more complex (in)dependencies between features.

Bayesian Methods

- We specify a sampling model $P(\mathbf{Z}|\theta)$
- and a prior distribution for parameters $P(\theta)$
- then we compute

$$P(\theta|\mathbf{Z}) = \frac{P(\mathbf{Z}|\theta) \cdot P(\theta)}{\int P(\mathbf{Z}|\theta) \cdot P(\theta) d\theta},$$

  - we may draw samples
  - or summarize by the mean or mode.
  - it provides the **Bayesian optimal predictive distribution**:

$$P(z^{new}|\mathbf{Z}) = \int P(z^{new}|\theta) \cdot P(\theta|\mathbf{Z}) d\theta.$$

Example

Tossing a biased coin

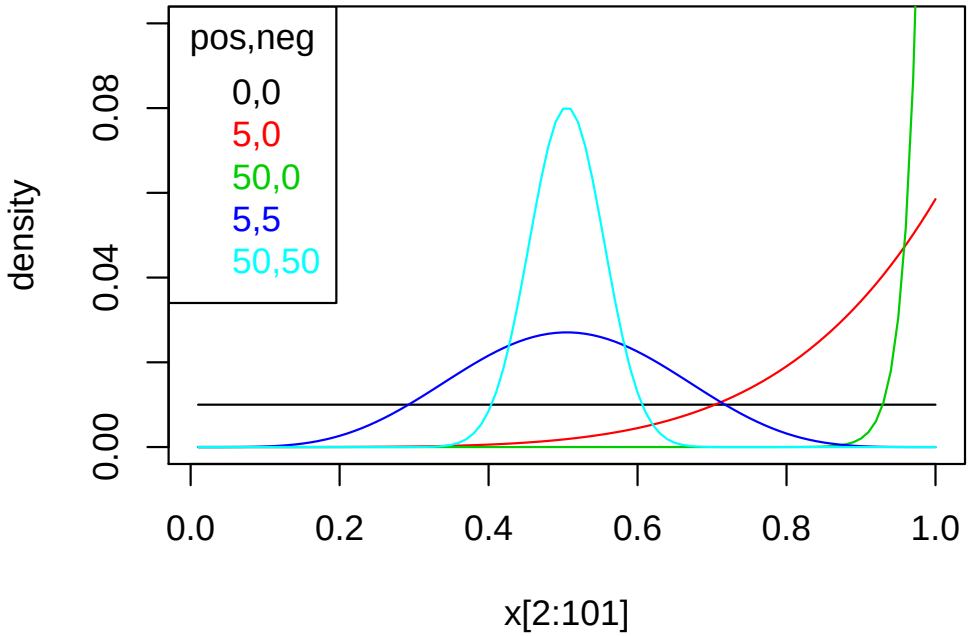
- $P(Z = head|\theta) = \theta$
- $p(\theta)$ =uniform
- $P(\theta|\mathbf{Z})$ follows the Beta distribution.

Discrete Model Parameter Learning

- For binary features, Beta function is used, a is the number of positive examples, b the number of negative examples.

$$beta[a, b](\theta) = \alpha\theta^{a-1}(1-\theta)^{b-1}$$

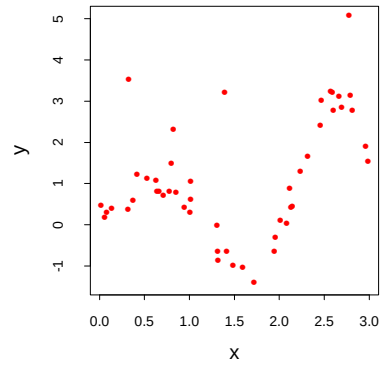
- Beta Function:

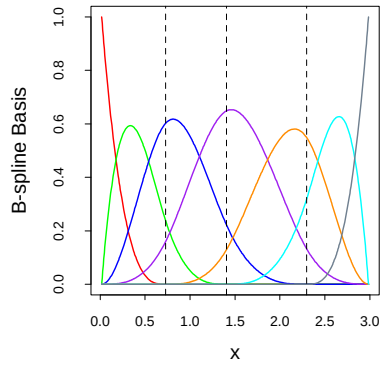


- For categorical features, Dirichlet priors and multinomial distribution is used. (Dirichlet-multinomial distribution).
- For Gaussian, μ has Gaussian prior, $\frac{1}{\sigma}$ has gamma prior (to stay in exponential family).

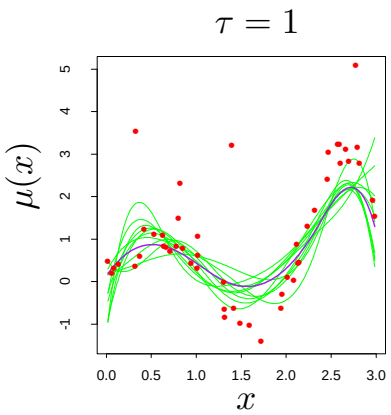
Bayesian smoothing example

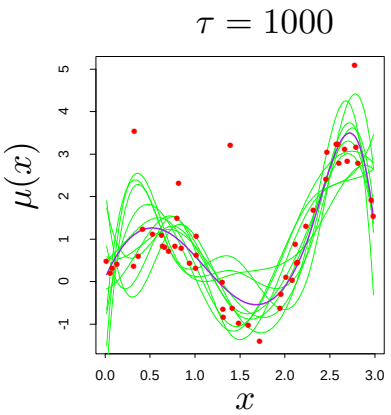
- Training data $\mathbf{Z} = \{z_i, \ldots, z_N\}$, $z_i = (x_i, y_i)$, $i = 1, \ldots, N$.
- We look for a cubic spline with three knots in quartiles of the X values. It corresponds to B-spline basis $h_j(x)$, $j = 1, \ldots, 7$.





- We estimate the conditional mean $\mathbb{E}(Y|X = x)$: $\mu(x) = \sum_{j=1}^{7} \beta_j h_j(x)$
- Let $\mathbf{H}$ be the $N \times 7$ matrix $h_j(x_i)$.
- RSS β estimate is $\hat{\beta} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$.





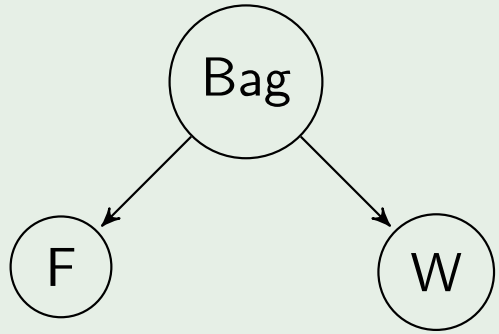
We assume to know σ^2, fixed x_i, we specifying prior on $\beta \sim N(0, \tau\Sigma)$.

$$\mathbb{E}(\beta|\mathbf{Z}) = (\mathbf{H}^T\mathbf{H} + \frac{\sigma^2}{\tau}\Sigma^{-1})^{-1}\mathbf{H}^T\mathbf{y}$$

$$\mathbb{E}(\mu(x)|\mathbf{Z}) = h(x)^T(\mathbf{H}^T\mathbf{H} + \frac{\sigma^2}{\tau}\Sigma^{-1})^{-1}\mathbf{H}^T\mathbf{y}.$$

Example (EM Algorithm for Missing Data)

- Two bags of bonbons mixed together. Each bonbon has a *Wrapper* and flavor *Flavor* and may have *Holes*. Each bag had another ratio of *Wrapper* color and *Flavor*.



Bag	F	W
?	c	r
1	l	r
1	c	?
1	c	g
?	l	?

- Initialize all parameters randomly close to uniform distribution, $\theta_* \approx 0.5$.

$\mathbb{E}$ step

$w = \hat{P}(\mathbf{Z}^m \mid \theta, \mathbf{Z})$	Bag	F	W
$P_\theta(Bag = 1 \mid F = c, W = r)$	1	c	r
$P_\theta(Bag = 2 \mid F = c, W = r)$	2	c	r
1	1	l	r
$P_\theta(W = r \mid Bag = 1, F = c)$	1	c	r
$P_\theta(W = g \mid Bag = 1, F = c)$	1	c	g
1	1	c	g
$P_\theta(Bag = 1, W = r \mid F = l)$	1	l	r
$P_\theta(Bag = 1, W = g \mid F = l)$	1	l	g
$P_\theta(Bag = 0, W = r \mid F = l)$	2	l	r
$P_\theta(Bag = 0, W = g \mid F = l)$	2	l	g

M step – update θs

$$\theta_{Bag=1} \leftarrow \frac{\sum_{Bag=1} w}{\sum w}$$

$$\theta_{F=c|Bag=1} \leftarrow \frac{\sum_{Bag=1,F=c} w}{\sum_{Bag=1} w}$$

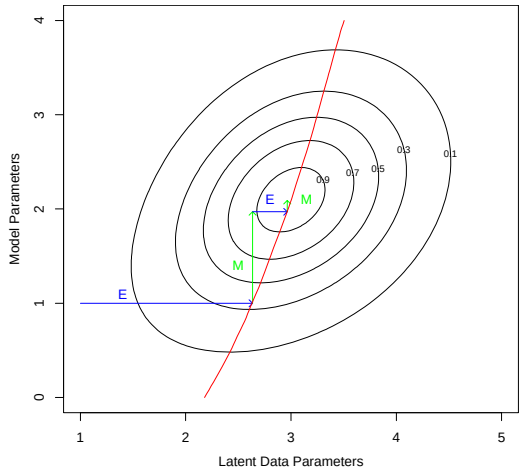
$$\theta_{F=c|Bag=2} \leftarrow \frac{\sum_{Bag=2,F=c} w}{\sum_{Bag=2} w}$$

$$\theta_{W=r|Bag=1} \leftarrow \frac{\sum_{Bag=1,W=r} w}{\sum_{Bag=1} w}$$

$$\theta_{W=r|Bag=2} \leftarrow \frac{\sum_{Bag=2,W=r} w}{\sum_{Bag=2} w}$$

EM as a Maximization-Maximization Procedure

- $\mathbf{Z}$ the observed data (the usual X with missing values)
- $\ell(\theta; \mathbf{Z})$ the log–likelihood of the model θ
- $\mathbf{Z}^m$ the latent or missing data
- $T = (\mathbf{Z}, \mathbf{Z}^m)$ the complete data with the log–likelihood $\ell_0(\theta; \mathbf{T})$.
- $\hat{P}(\mathbf{Z}^m)$,$\hat{P}(\mathbf{Z}^m|\theta, \mathbf{Z})$ any distribution over the latent data $\mathbf{Z}^m$.



- Consider the function F

$$F(\theta', \hat{P}) = \mathbb{E}_{\hat{P}}[\ell_0(\theta'; \mathbf{T})] - \mathbb{E}_{\hat{P}}[log\hat{P}(\mathbf{Z}^m)]$$

- for $\hat{P} = \hat{P}(\mathbf{Z}^m|\theta', \mathbf{Z})$ is F the log–likelihood of the observed data
  - $F(\theta', \hat{P}(\mathbf{Z}^m|\theta', \mathbf{Z})) = \mathbb{E}[\ell_0(\theta'; \mathbf{T})|\theta', \mathbf{Z}] - \mathbb{E}[\ell_1(\theta'; \mathbf{Z}^m|\mathbf{Z})|\theta', \mathbf{Z}]$

The EM Algorithm in General

$$
\begin{aligned}
P(\mathbf{Z}^m|\mathbf{Z},\theta') &= \frac{P(\mathbf{Z}^m,\mathbf{Z}|\theta')}{P(\mathbf{Z}|\theta')},\\
P(\mathbf{Z}|\theta') &= \frac{P(\mathbf{Z}^m,\mathbf{Z}|\theta')}{P(\mathbf{Z}^m|\mathbf{Z},\theta')},
\end{aligned}
$$

- In the log–likelihoods

$$\ell(\theta';\mathbf{Z}) = \ell_0(\theta';\mathbf{T}) - \ell_1(\theta';\mathbf{Z}^m|\mathbf{Z})$$

- where ℓ_1 is based on the conditional density $P(\mathbf{Z}^m|\mathbf{Z})$.
- Taking the expectation w.r.t. $\mathbf{T}|\mathbf{Z}$ governed by parameter θ gives

$$
\begin{aligned}
\ell(\theta';\mathbf{Z}) &= \mathbb{E}[\ell_0(\theta';\mathbf{T})|\theta,\mathbf{Z}] - \mathbb{E}[\ell_1(\theta';\mathbf{Z}^m|\mathbf{Z})|\theta,\mathbf{Z}]\\
&\equiv Q(\theta',\theta) - R(\theta',\theta)
\end{aligned}
$$

- $R()$ is the expectation of a density with respect the same density
  - it is maximized when $\theta' = \theta$.
- Therefore:

$$
\begin{aligned}
\ell(\theta';\mathbf{Z}) - \ell(\theta;\mathbf{Z}) &= [Q(\theta',\theta) - Q(\theta,\theta)] - [R(\theta',\theta) - R(\theta,\theta)]\\
&\geq 0
\end{aligned}
$$

The EM Algorithm

procedure THE EM ALGORITHM:(**Z** observed data, the model(θ))
  $\hat{\theta}^{(0)} \leftarrow$ an initial guess (usually close to the uniform distribution)
  repeat
    Expectation step: at the jth step, compute

$$Q(\theta', \hat{\theta}^{(j)}) = \mathbb{E}(\ell_0(\theta'; \mathbf{T})|Z, \hat{\theta}^{(j)})$$

      as a function of the dummy argument θ'.
    Maximization step: determine the new estimate $\hat{\theta}^{(j+1)}$
      as the maximizer of $Q(\theta', \hat{\theta}^{(j)})$ over θ'.
  until convergence
  return $\hat{\theta}$
end procedure

- Full maximization is not necessary.
- We need to find a value $\hat{\theta}^{(j+1)}$ so that $Q(\hat{\theta}^{(j+1)}, \hat{\theta}^{(j)}) > Q(\hat{\theta}^{(j)}, \hat{\theta}^{(j)})$.
- Such prodecures are called **generalized EM algorithms (GEM)**.

BN example of EM algorithm (Russel, Norvig) - can be omitted

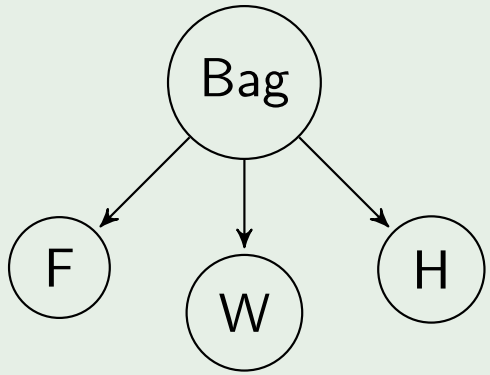
- Two bags of bonbons mixed together. Each bonbon has a *Wrapper* and flavor *Flavor* and may have *Holes*. Each bag had another ratio of *Wrapper* color, *Flavor* and *Holes*.

We can model the situation by a naive bayes model, *Bag* as the class variable.

Example

Example We have tested 1000 bonbones and observed:

	W=red		W=green	
	H=1	H=0	H=1	H=0
F=cherry	273	93	104	90
F=lime	79	100	94	167



We choose the initial parameters

$$\theta^{(0)} = 0.6,\ \theta^{(0)}_{F1} = \theta^{(0)}_{W1} = \theta^{(0)}_{H1} = 0.6,\ \theta^{(0)}_{F2} = \theta^{(0)}_{W2} = \theta^{(0)}_{H2} = 0.4$$

EM example - can be omitted

- Expectation of θ is the ratio of the expected counts

$$\theta^{(1)} = \frac{1}{N}\sum_{j=1}^{N} \frac{P(flavor_j|Bag=1)P(wrapper_j|Bag=1)P(holes_j|Bag=1)P(Bag=1)}{\sum_{i=1}^{2} P(flavor_j|Bag=i)P(wrapper_j|Bag=i)P(holes_j|Bag=i)P(Bag=i)}$$

(normalization constant **depends** on parameter values).

For the type *red*, *cherry*, *holes* we get:

$$\frac{\theta_{F1}^{(0)}\theta_{W1}^{(0)}\theta_{H1}^{(0)}\theta^{(0)}}{\theta_{F1}^{(0)}\theta_{W1}^{(0)}\theta_{H1}^{(0)}\theta^{(0)} + \theta_{F2}^{(0)}\theta_{W2}^{(0)}\theta_{H2}^{(0)}\theta^{(0)}} \approx 0.835055$$

we have 273 bonbons of this type, therefore we add $\frac{273}{N} \cdot 0.835055$.
Similarly for all seven other types and we get

$$\theta^{(1)} = 0.6124$$

EM example continued - can be omitted

- The estimate of θ_{F1} for fully observed data is $\frac{\#(Bag{=}1, Flavor{=}cherry)}{\#(Flavor{=}cherry)}$
- We have to use expected counts $Bag = 1 \& F = cherry$ and $Bag = 1$,

$$\theta_{F1}^{(1)} = \frac{\sum_{j;Flavor_j=cherry} P(Bag = 1 | Flavor_j = cherry, wrapper_j, holes_j)}{\sum_j P(Bag = 1 | cherry_j, wrapper_j, holes_j)}$$

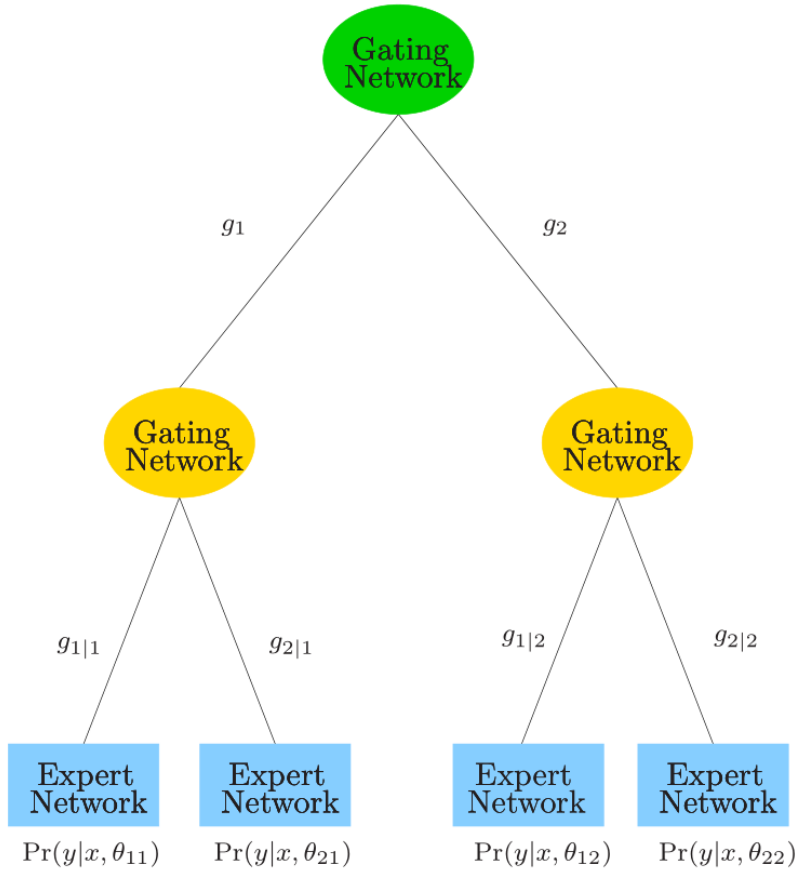
- Similarly we get:

$$\theta^{(1)} = 0.6124,\ \theta_{F1}^{(1)} = 0.6684, \theta_{W1}^{(1)} = 0.6483, \theta_{H1}^{(1)} = 0.6558,$$

$$\theta_{F2}^{(1)} = 0.3887, \theta_{W2}^{(1)} = 0.3817, \theta_{H2}^{(1)} = 0.3827.$$

Hierarchical Mixture of Experts

- a hierarchical extension of naive Bayes (latent class model)
- a decision tree with 'soft splits'
- splits are probabilistic functions of a linear combination of inputs (not a single input as in CART)
- terminal nodes called 'experts'
- non–terminal nodes are called gating network
- may be extended to multilevel.

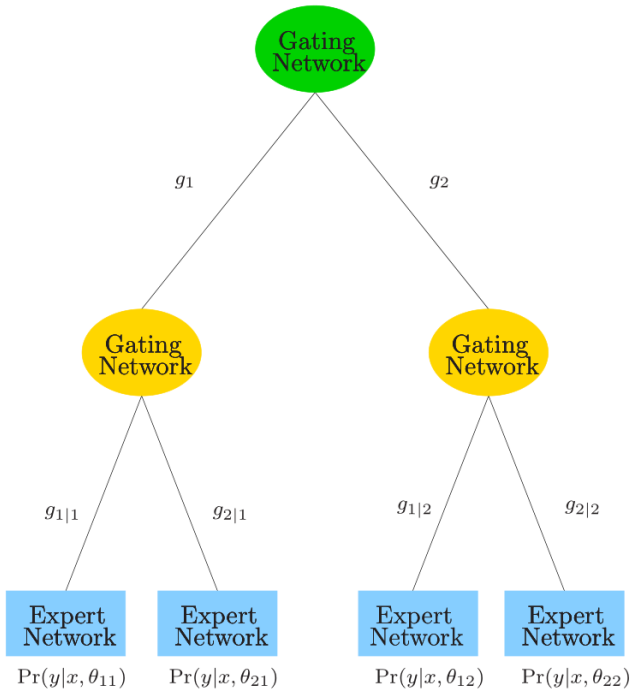


Hierarchical Mixture of Experts

- data (x_i, y_i), $i = 1, \ldots, N$, y_i continuous or categorical, first $x_i \equiv 1$ for intercepts.
- $g_i(x, \gamma_j) = \frac{e^{\gamma_j^T x}}{\sum_{k=1}^{K} e^{\gamma_k^T x}}$, $j = 1, \ldots, K$ children of the root,
- $g_{\ell|j}(x, \gamma_{j\ell}) = \frac{e^{\gamma_{j\ell}^T x}}{\sum_{k=1}^{K} e^{\gamma_{jk}^T x}}$, $\ell = 1, \ldots, K$ children of the root,
- Terminals (Experts)

Regression Gaussian linear reg. model,
$\theta_{j\ell} = (\beta_{j\ell}, \sigma^2_{j\ell})$, $Y = \beta^T_{j\ell} + \epsilon$

Classification The linear logistic reg. model:
$Pr(Y = 1|x, \theta_{j\ell}) = \frac{1}{1+e^{-\theta^T_{j\ell} x}}$



- EM algorithm
- Δ_i, $\Delta_{\ell|j}$ 0–1 latent variables – branching

E step expectations for Δ's

M step estimate parameters HME by a version of multiple logistic

Missing data (T.D. Nielsen)

Die tossed N times. Result reported via noisy telephone line. When transmission not clearly audible, record missing value:

$$4, 2, ?, 6, 5, 4, ?, 3, 4, 1, \ldots$$

"2" and "3" sound similar, therefore:

$$P(Y_i = ?|X_i = k) = P(M_i = 1|X_i = k) = \begin{cases} 1/4 & \text{k} = 2,3 \\ 1/8 & \text{k} = 1,4,5,6 \end{cases}$$

Distribution of the Y is (for fair die):

?	$\frac{1}{3}\frac{1}{4} + \frac{2}{3}\frac{1}{8} = \frac{1}{6}$
2,3	$\frac{1}{6}\frac{3}{4} = \frac{1}{8}$
1,4,5,6	$\frac{1}{6}\frac{7}{8} = \frac{7}{48}$

If we simply ignore the missing data items, we obtain as the maximum likelihood estimate for the parameters of the die:

$$\theta^* = (\frac{7}{48}, \frac{1}{8}, \frac{1}{8}, \frac{7}{48}, \frac{7}{48}, \frac{7}{48}) * \frac{6}{5} = (0.175, 0.15, 0.15, 0.175, 0.175, 0.175)$$

Incomplete data

How do we handle cases with missing values:

- Faulty sensor readings.
- Values have been intentionally removed.
- Some variables may be unobservable.

How is the data missing?
We need to take into account how the data is missing:

- **Missing completely at random** The probability that a value is missing is independent of both the observed and unobserved values (a monitoring system that is not completely stable and where some sensor values are not stored properly).
- **Missing at random** The probability that a value is missing depends only on the observed values (a database containing the results of two tests, where the second test has only performed (as a "backup test") when the result of the first test was negative).
- **Non-ignorable** Neither MAR nor MCAR (an exit poll, where an extreme right-wing party is running for parlament).

Frequent itemsets, Association Rules

Unsupervised learning

- No goal class (either Y nor G).
- Usually binary data $X_{ij} \in \{0,1\}^{N \times p}$
- Value $= 1$ is our interest; for example purchase.
- p may be very large; for example the size of the range of goods in an market.
- Popular application: Market basket analysis.
- Generally: We look for L prototypes $v_1, \ldots, v_L \in X^p$ such that $P(v_\ell)$ is relatively large.
- With large p, we do not have enough data to estimate $P(v_\ell)$ since number of observations with $P(X = v_\ell)$ is too small.
- We seek for regions where $P(x)$ is large, that can be written as conjunctive rule on dimension conditions $\bigcap_{j=1}^{p}(X_j \in s_j)$ where s_j are selected values of the feature X_j.

Hypothesis space for Apriori

ESL book Figure:

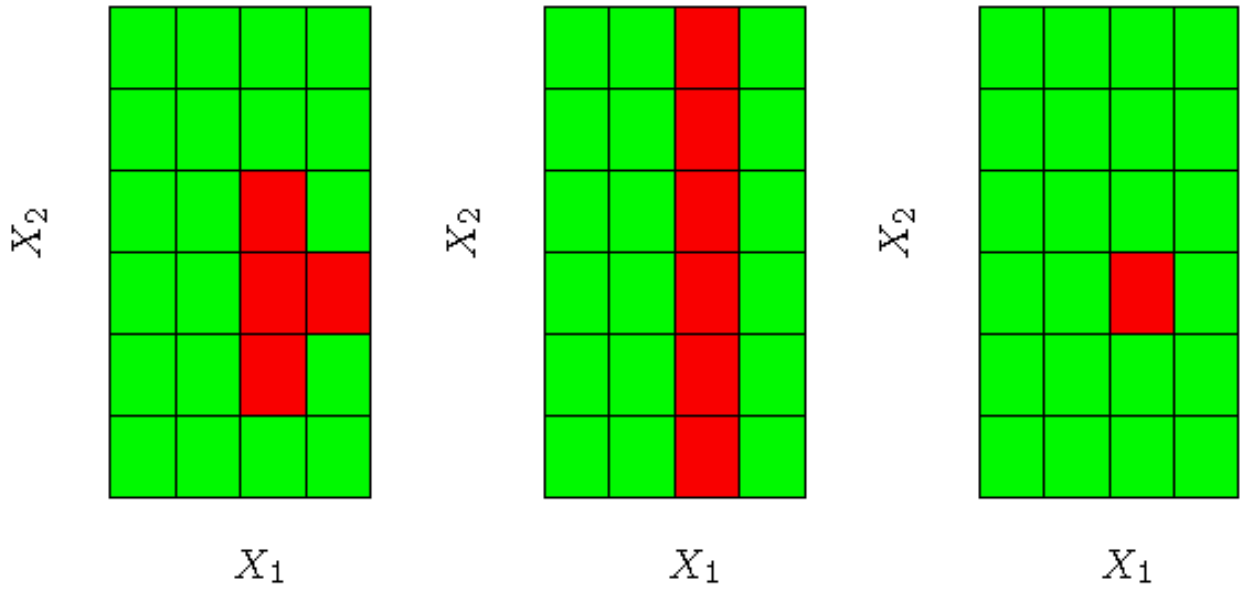


FIGURE 14.1. *Simplifications for association rules. Here there are two inputs X_1 and X_2, taking four and six distinct values, respectively. The red squares indicate areas of high density. To simplify the computations, we assume that the derived subset corresponds to either a single value of an input or all values. With this assumption we could find either the middle or right pattern, but not the left one.*

Market Basket Analysis

- For very large datasets, $p \approx 10^4, N \approx 10^8$; in unit ball is the distance to the nearest neighbour ≈ 0.9981.
- Simplifications: Test on feature X_j either equal to a specific value or no restriction at all,
- I select combinations of items with higher number of occurences (**support**) than predefined threshold t.
- I select all combinations fulfilling conditions above.
- Categorical variables may be codded by dummy variables in advance (if not too many).
  - **OneHotEncoder** for each class g, a new variable $X_g = [X == g]$.

Apriori Algorithm!

```
1: procedure APRIORI:(X dataset, t threshold for support )
2:     i ← 0
3:     Generate list of candidates of the length i
4:     while Candidate set not empty do
5:         for each data sample do
6:             for each candidate do
7:                 if all items of candidate appear in the data sample then
8:                     increase the candidate counter by 1
9:                 end if
10:            end for
11:        end for
12:        i ← i + 1
13:        Discard candidates with support less than t.
14:        Generate list of candidates of the length i
15:            Join any two candidates from previous step having i − 2
   elements common. (More pruning possible.)
16:    end while
17: end procedure
```

Example: Apriori Algorithm

- $t = 0.2$
- $t * N = 2 = 0.20 * 10$
- Data

a b c e f o
a c g
e i
a c d e g
a c e g l
e j
a b c e f p
a c d
a c e g m
a c e g n

i=1
a=8
b=2
c=8
d=2
e=8
f=2
g=5
i=j=l=o=1
p=m=n=1

i=2
ab=2
ac=8
ad=2
ae=6
af=2
ag=5
bc=2
bd=0
be=2
bf=2
bg=0
cd=2
ce=6
cf=2
cg=5
de=1
df=0
dg=1
ef=2

i=3
abc=2
abd=0
abe=2
abf=2
abg=0
acd=2
ace=6
acf=2
acg=5
ade=1
adf=0
adg=1
aeg=4
...

i=4 ...
abce=2
abcf=2
abef=2
abeg=0
acef=2
aceg=4
adeg=1
aefg=0
...

Properties of the Apriori Algorithm

- Applicable for very large data (with high threshold t).
- The key idea:
  - Only few of 2^K combinations have high support $> t$,
  - **subset of high–support combination has also high support**.
- The number of passes through the data is equal to the size of the longest supported combination. The data does not to be in memory simultaneously.
- *FPgrowth* algorithm needs only two passes through the data.

Association Rules !

- From each supported itemset $\mathcal{K}$ found by Apriori algorithm we create a list of **association rules**, implications of the form $A \Rightarrow B$ where:
  - A, B are disjoint and $A \cup B = \mathcal{K}$
  - A is called **antecedent**
  - B is called **consequent**.
- Support of the rule $T(A \Rightarrow B)$ is defined as normalized support of the itemset $\mathcal{K}$, that is normalized support of the conjunction $A\&B$.

$$T(\mathcal{K}) = \frac{|data_{\mathcal{K}}|}{|data|}$$

$$T(A \Rightarrow B) = \frac{|data_{A\&B}|}{|data|}$$

Rule Confidence and Lift

There are two important measures for a rule $A \Rightarrow B$:

- **Confidence** (predictability, přesnost)

$$C(A \Rightarrow B) = \frac{T(A \Rightarrow B)}{T(A)}$$

  that is an estimate of $P(B|A)$,
- Support $T(B)$ is an estimate of $P(B)$,
- **Lift** is the ration of confidence and expected precision:

$$L(A \Rightarrow B) = \frac{C(A \Rightarrow B)}{T(B)}$$

  that is an estimate of $\frac{P(A\&B)}{P(A) \cdot P(B)}$.
- **Leverage** is the difference of supports:

$$\mathit{leverage}(A \Rightarrow B) = T(A \Rightarrow B) - T(A) \cdot T(B)$$

- **Conviction** is the ratio:

$$\mathit{conviction}(A \Rightarrow B) = \frac{1 - T(B)}{1 - C(A \Rightarrow B)}.$$

Association Rule Example

ESL book example:

Association rule 2: Support 13.4%, confidence 80.8%, and lift 2.13.

$$\left[\begin{array}{rcl} \text{language in home} & = & \textit{English} \\ \text{householder status} & = & \textit{own} \\ \text{occupation} & = & \{\textit{professional/managerial}\} \end{array}\right] \Downarrow \text{income} \geq \textit{\$40,000}$$

- $\mathcal{K} = \{$English, own, prof/man, income>\$40000$\}$,
- 13.4% people has all four properties,
- 80.8% of people with {English, own, prof/man} have income> \$40000,
- $T(\text{income} > \$40000) = 37.94\%$, therefore $\mathit{Lift} = 2.13$.

The Goal of Apriori Algorithm !

- Apriori finds all rules with high support.
- Frequently, it finds many of rules.
- We usually select lower threshold c on confidence, that is we select rules with $T(A \Rightarrow B) > t$ and $C(A \Rightarrow B) > c$.
- Conversion of itemsets to rules is usually relatively fast compared to search of itemsets.
- See lispMiner for user interface and a lot of more.
- Python Apriori library:

```
from mlxtend.preprocessing import TransactionEncoder

from mlxtend.frequent_patterns import apriori, association_rules
from mlxtend.frequent_patterns import fpgrowth,fpmax

from mlxtend.frequent_patterns import hmine
```

Demographical Data ESL Example

Feature	Demographic	# Values	Type
1	Sex	2	Categorical
2	Marital status	5	Categorical
3	Age	7	Ordinal
4	Education	6	Ordinal
5	Occupation	9	Categorical
6	Income	9	Ordinal
7	Years in Bay Area	5	Ordinal
8	Dual incomes	3	Categorical
9	Number in household	9	Ordinal
10	Number of children	9	Ordinal
11	Householder status	3	Categorical
12	Type of home	5	Categorical
13	Ethnic classification	8	Categorical
14	Language in home	3	Categorical

Demographical Example – Continuing

- $N = 9409$ questionnaires, the ESL authors selected 14 questions.
- Preprocessing:
  - `na.omit() remove records with missing values,`
  - `ordinal features cut by median to binary,`
  - `for categorical create dummy variable for each category.`
- Apriori input was matrix 6876×50.
- Output: 6288 association rules
  - with max. 5 elements
  - with support at least 10%.

Negated Literals – Useful, Problematic

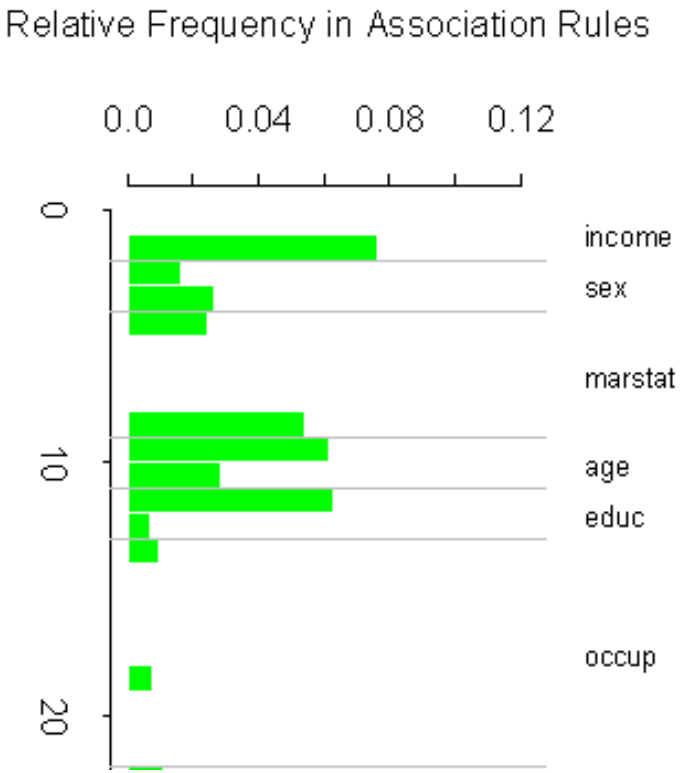
Association rule 3: Support 26.5%, confidence 82.8% and lift 2.15.

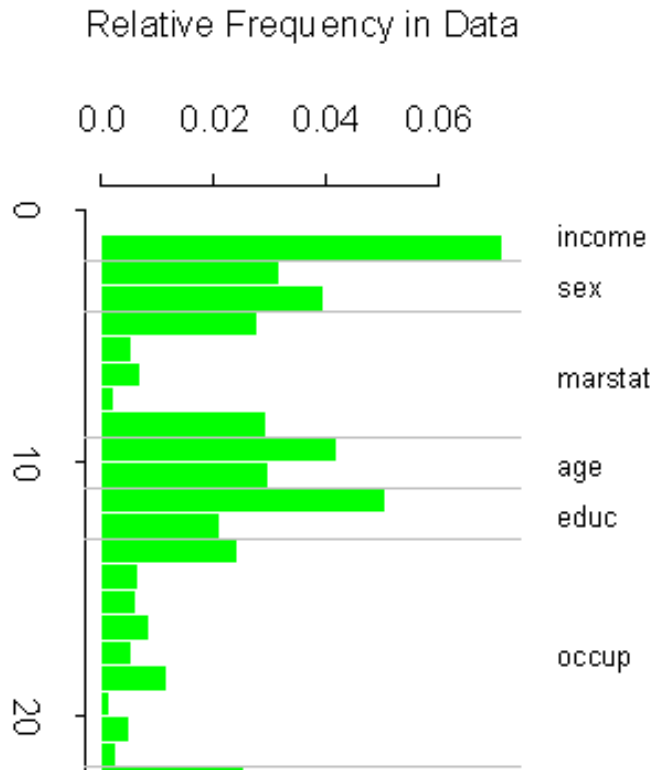
$$\left[\begin{array}{rcl} \text{language in home} & = & \textit{English} \\ \text{income} & < & \textit{\$40,000} \\ \text{marital status} & = & \textit{not married} \\ \text{number of children} & = & \textit{0} \end{array}\right]$$

$$\Downarrow$$

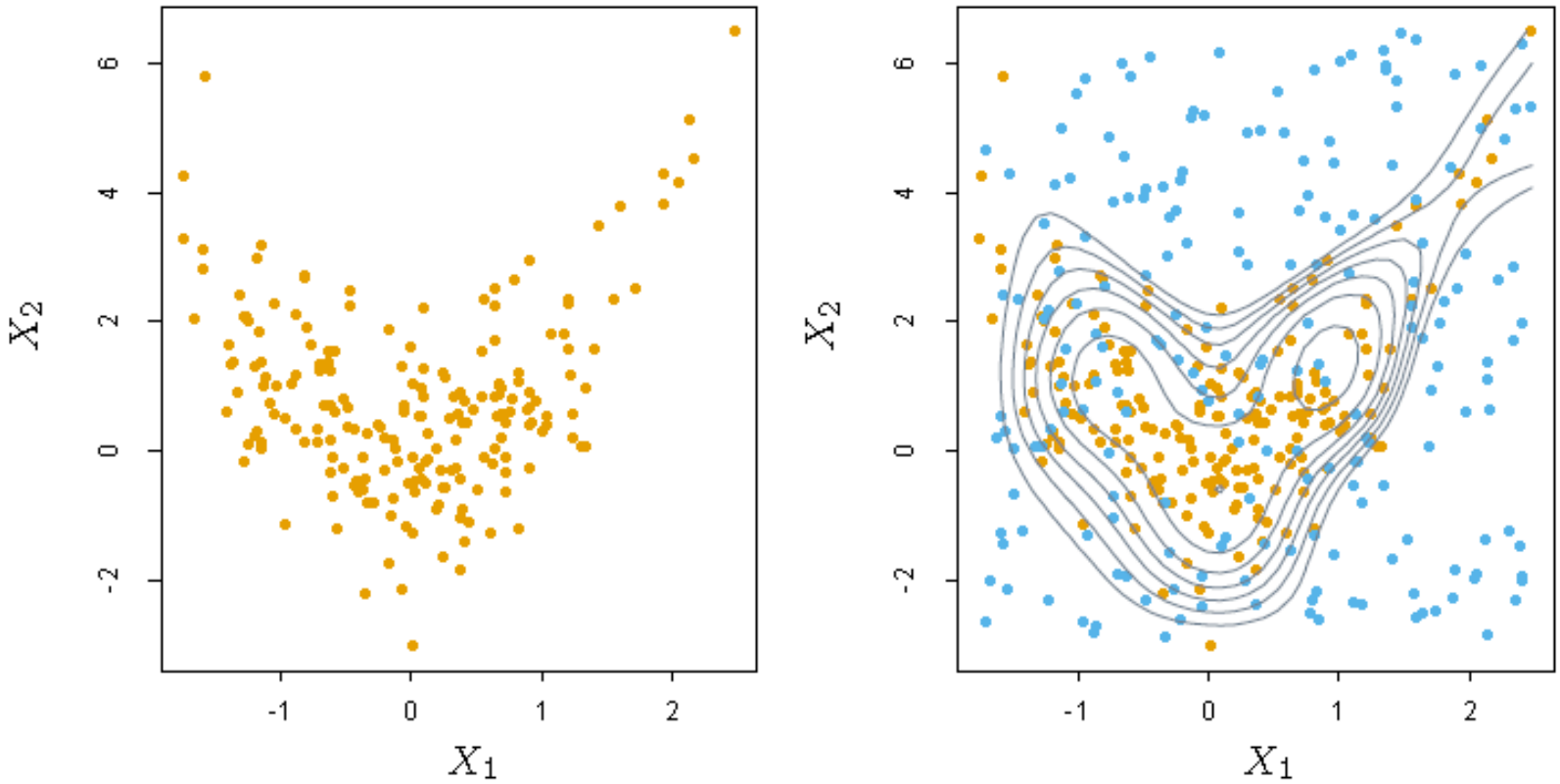
$$\text{education} \notin \{\textit{college graduate}, \textit{graduate study}\}$$

Non–frequent Values Dissapear





Unsupervised Learning as Supervised Learning



- We add additional attribute Y_G.
- $Y_G = 1$ for all our data.
- We generate randomly a dataset of similar size with uniform distribution, set $Y_G = 0$ for this artificial data.
- The task is to separate $Y_G = 1$ and $Y_G = 0$.

Generalize Association Rules

- We search for high lift, where probability of conjunction is greater than expected.
- Hypothesis is specified by column indexes j and subsets of values s_j corresponding features X_j. We aim:

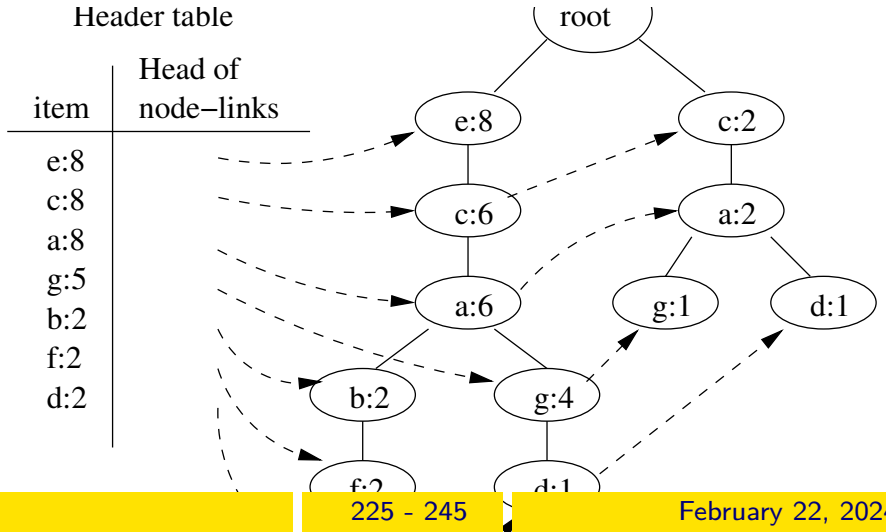
$$\hat{P}\left(\bigcap_{j\in\mathcal{J}}(X_j \in s_j)\right) = \frac{1}{N}\sum_{1}^{N} I\left(\bigcap_{j\in\mathcal{J}}(x_{ij} \in s_j)\right) >> \Pi_{j\in\mathcal{J}}\hat{P}(X_j \in s_j)$$

- On the data from previous slide, CART (decision tree alg.) or PRIM ('bump hunting') may be used.
- Figure on previous slide: Logistic regression on tensor product of natural splines.
- Other methods may be used. All are heuristics compared to full evaluation by Apriori.

FP–tree

```
1: procedure FP–TREE:(Data )
2:     Calculate counts of items (singletons)
3:     Create table header ordered by decreasing item count
4:     for each data sample do
5:         order items according to header
6:         insert branch into the tree
7:         increase all counters on the inserted branch
8:     end for
9:     return the tree
10: end procedure
```

Data	ordered
a b c e f o	e c a b f
a c g	c a g
e i	e
a c d e g	e c a g d
a c e g l	e c a g
e j	
a b c e f p	
a c d	

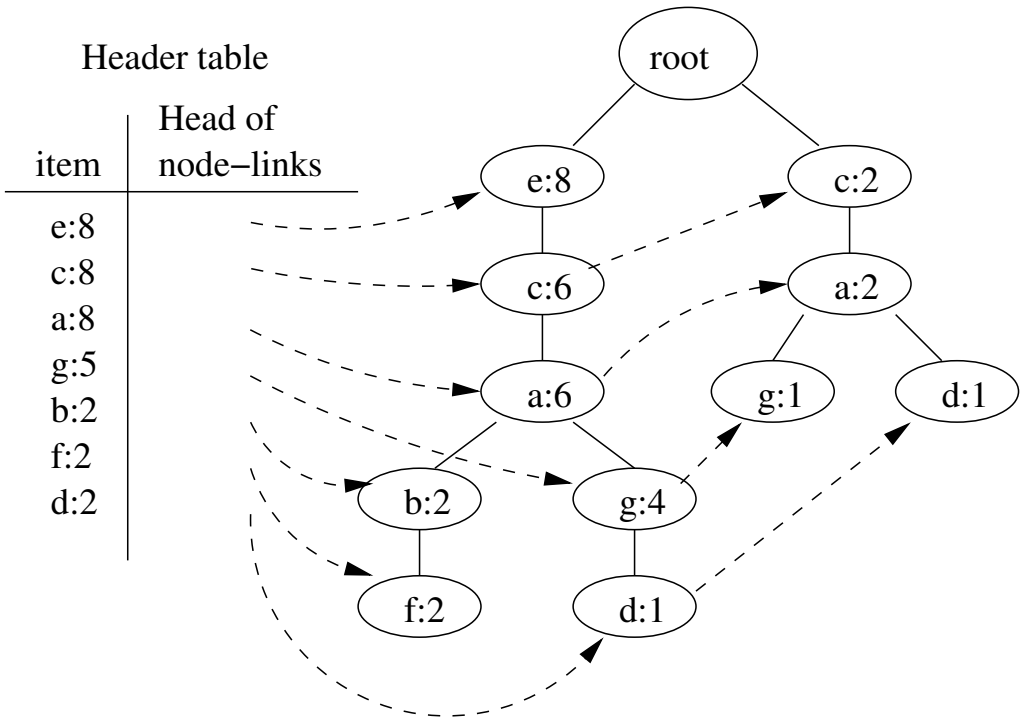


Frequent Itemsets with only 2 pass through data

- Build an internal structure called FP-tree
- Call FP-growth to generate frequent itemsets
  - Each construction of a conditional tree needs 2 pass through the parent tree
  - an optimized version with only 1 pass is presented. (It needs an additional data structure array.)
- FP-max to find maximal itemsets
  - non of immediate supersets is frequent
- FP-close to find close itemsets
  - non of immediate supersets has the same support.

FP-tree

- **FP-tree** contains all frequency information of the database.
- Principle: If X and Y are two itemsets, the count of itemsets $X \cup Y$ in the database is exactly that of Y in the restriction of the database to those transactions containing X.



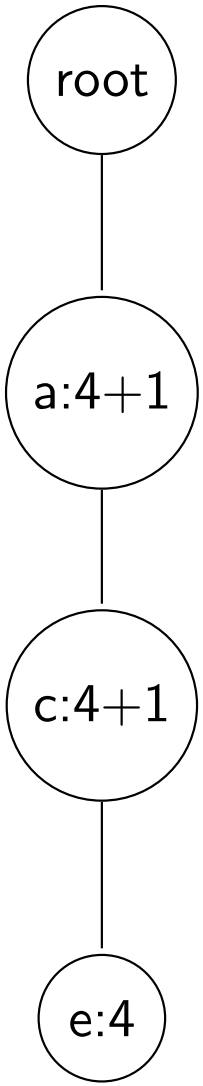
i=3
abc=2
abd=0
abe=2
abf=2
abg=0
acd=2
ace=6
acf=2
acg=5
ade=1
adf=0
adg=1
aeg=4
...

FPgrowth*

```
1: procedure FPgrowth*:(T a conditional FP-tree )
2:     if T only contains a single path P then
3:         for each subpath Y of P do
4:             output pattern Y ∪ T.base with
5:                 count = smallest count of nodes in Y
6:         end for
7:     else
8:         for each i in T.header do
9:             Y ← T.base ∪ {i} with i.count
10:            if T.array is not NULL then
11:                construct a new header table for Y's FP-tree from T.array
12:            else
13:                construct a new header table for Y's from T
14:            end if
15:            construct Y's conditional FP-tree T_Y and its array A_Y;
16:            if T_Y ≠ ∅ then
17:                call FPgrowth*(T_Y)
18:            end if
19:        end for
20:    end if
```

$$t = 2$$

$$T_{\{g\}} = [a:5, c:5, e:4]$$

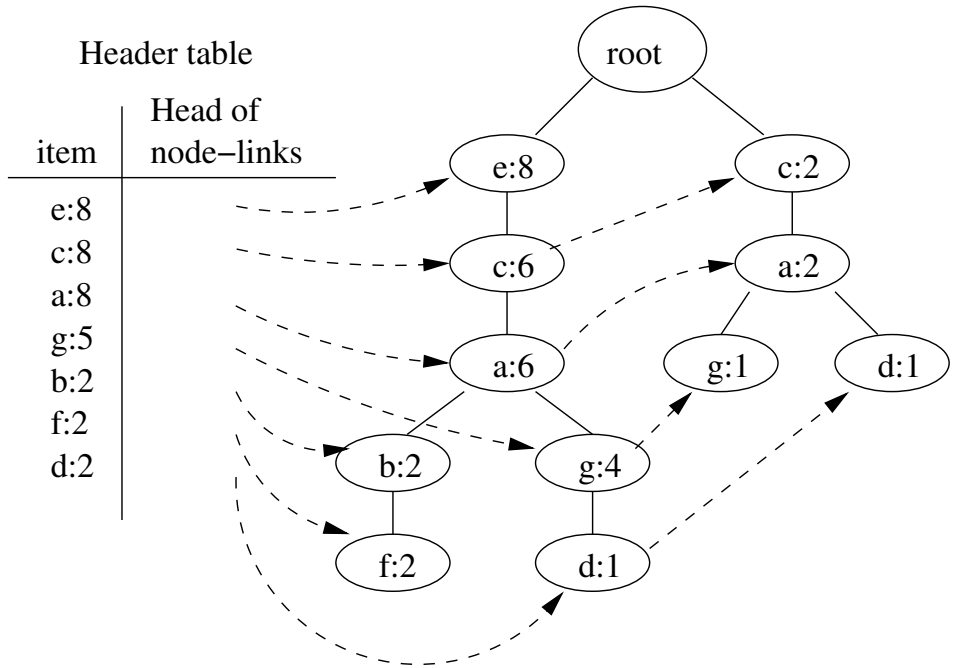


	e	c	a	g	b	f
c	6					
a	6	8				
g	4	5	5			
b	2	2	2	0		
f	2	2	2	0	2	
d	1	2	2	1	0	0

(a) $A_{\emptyset}$

	a	c
c	5	
e	4	4

(b) $A_{\{g\}}$



Version Space Search

Example (Tennis Dataset)

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Overcast	Mild	High	Weak	Yes
D5	Overcast	Mild	High	Strong	Yes
D6	Overcast	Hot	Normal	Weak	Yes
D7	Rain	Mild	High	Strong	No

Version Space Search

- Our **hypothesis** is a conjunction of attritute tests that imply $PlayTennis = yes$.
  - $h = \langle ?, Cold, High, ?, ?, ? \rangle$ represents the hypothesis $Temperature = cold \ \& \ Humidity = high \Rightarrow PlayTennis = yes$.
    - ? is satisfied by any value
    - $\emptyset$ cannot be satisfied
  - For binary attributes, we have $3^{|\#attributes|} + 1$ hypotheses
    - hypotheses with $\emptyset$ are not satisfiable, therefore they are equivalent.
    - We perform a systematic search.
    - The hypothesis space is partially ordered by the subsumption.

Definition (More general, more specific)

- The hypothesis h_g is **more general** than the hypothesis $h_g \succeq h_s$ iff any sample that satisfies h_s satisfies also h_g.
- In the above case, the hypothesis $h_s, h_g \succeq h_s$ is called **more specific that** h_g.

  - $\langle ?, ?, ?, ? \rangle$ is more general than $\langle Sunny, \ldots, Same \rangle$.
  - The most general hypothesis $\langle ?, ?, ?, ? \rangle$ is satisfied by all data.
  - The most specific hypothesis $\langle \emptyset, \ldots \rangle$ is not satisfied by any data.
  - The hypothesis space for a **lattice** partially ordered by the 'more general' relation.

Find–S

- We search for a hypothesis satisfied by all positive examples and no negative example.

Find–S (to be improved)

```
1: procedure FIND-S:(X dataset with the goal attritute yes/no )
2:     h ← ⟨∅, ∅, ∅, ∅⟩ # the most specific hypothesis
3:     for each positive data sample x_i do
4:         for each attribute condition X_j = x_{i,j} in h do
5:             if x_i does not satisfy X_j = x_{i,j} then
6:                 replace the condition by
7:                         a closest more general condition satisfied by x_i
8:             end if
9:         end for
10:    end for
11:    return h
12: end procedure
```

Version Space

- Now we look for all hypotheses consistent with the data.

Definition (Version Space)

- **The version space** for the hypothesis space H and the data X is a subset of H that is consistent with X

$$VS(H, X) = \{h \in H | Consistent(h, X)\}.$$

- The version space is characterized by the most general and the most specific boundary.
- Any hypothesis between these boundaries is consistent with the data.

Definition (General Boundary)

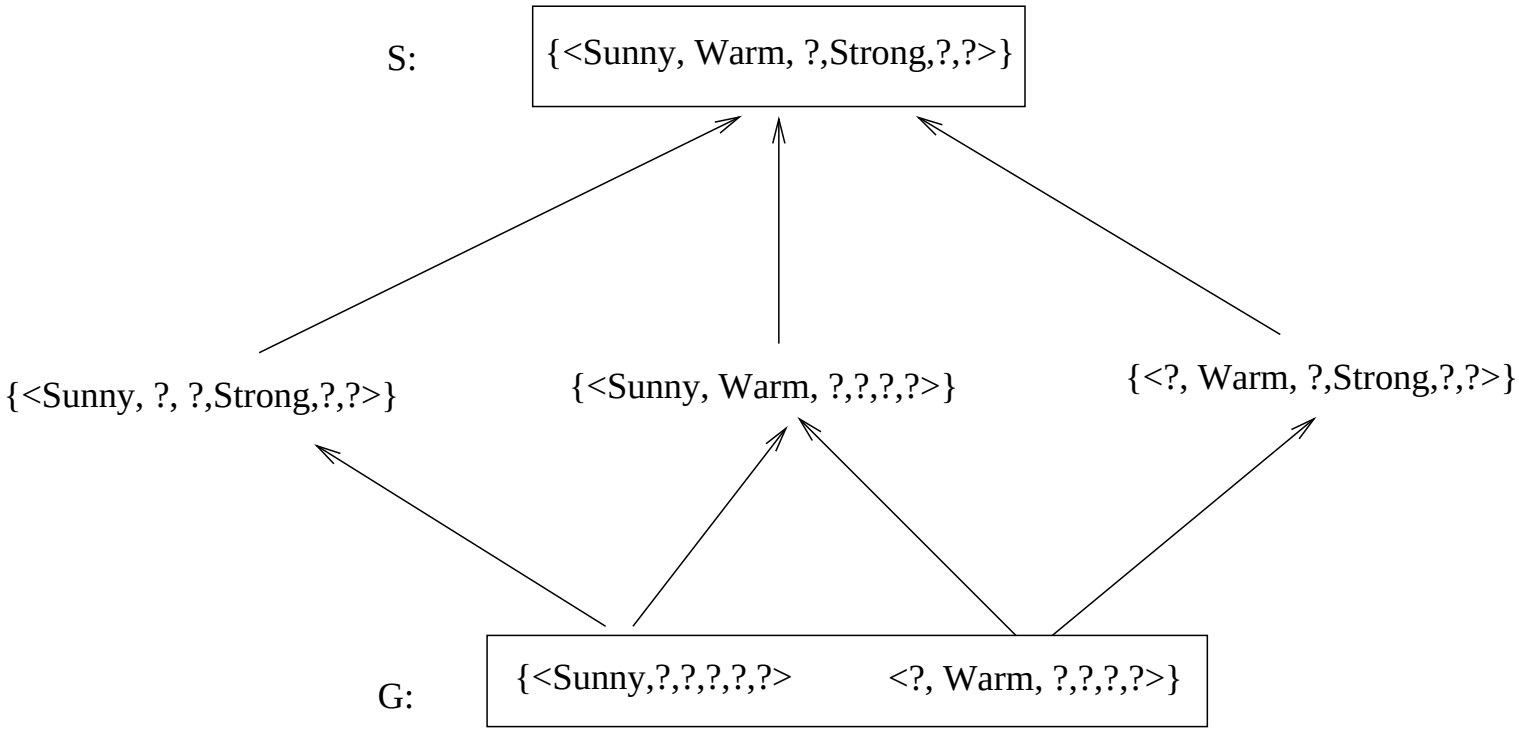
- **The general boundary** for the hypothesis space H and the data X is a set of most general hypothesis from H that are consistent with X

$$G(H, X) = \{g \in H | Consistent(g, X) \& (\nexists g_1 \in H)[g_1 \succ g \& Consistent(g_1, X)]\}.$$

Definition (Specific Boundary)

- **The specific boundary** for the hypothesis space H and the data X is a set of most specific hypothesis from H that are consistent with X

$$S(H,X) = \{s \in H | Consistent(s,X) \& (\nexists s_1 \in H)[s \succ s_1 \& Consistent(s_1,X)]\}.$$



- We search for a hypothesis satisfied by all positive examples and no negative example.

1: **procedure** CANDIDATE–ELIMINATION:(X data,the goal att. yes/no)
2: $G \leftarrow \{\langle ?, ?, ?, ? \rangle\}, S \leftarrow \{\langle \emptyset, \emptyset, \emptyset, \emptyset \rangle\}$ # general,specific
3: **for** each data sample x_i **do**
4: **if** x_i is positive **then**
5: remove from G all h inconsistent with x_i
6: **for** each $s \in S$ inconsistent with x_i **do**
7: add to S all minimal generalizations h
8: $Consistent(h, x_i) \& (\exists g \in G)(g \succeq h)$
9: remove from S $\{s | (\exists s_1 \in S)(s \succ s_1)\}$ # not most specific
10: **end for**
11: **else**x_i is negative
12: remove from S all h inconsistent with x_i
13: **for** each $g \in G$ inconsistent with x_i **do**
14: add to G all minimal specifications h
15: $Consistent(h, X) \& (\exists s \in S)(h \succeq s)$
16: remove from G $\{g | (\exists g_1 \in G)(g_1 \succ g)\}$ # not most gen.
17: **end for**
18: **end if**
19: **end for**
20: return G, S
21: **end procedure**

Literature

- A. Cropper and S. Dumancic. Inductive logic programming at 30: a new introduction. CoRR, abs/2008.07912, 2020.
- S. Muggleton & all.: Meta-interpretive learning: application to grammatical inference, http://www.doc.ic.ac.uk/~shm/FLOC_ILP/Paper03.pdf

Predicate Logic

- Recall predicate logic.
- CNF, DNF the conjunctive and disjunctive normal form
- **clause**: a disjunction of literals $father(X, Y) \vee \neg parent(X, Y) \vee \neg male(X)$
- **Horn clauses** with at most one positive literal, written as a rule
  - **definite clause** $father(X, Y) :- male(X), parent(X, Y).$
  - **fact** - no negative literal $male(adam).$
  - **goal clause** - no positive literal $false :- father(X, bob).$
- **Ground term, clause** - a term, a clause without variables.
- We have our data in the form of a set of clauses B, E^+, E^-,
  - the background knowledge B is a set of (Horn) clauses,
  - the positive and examples E^+, E^- are sets of ground literals (facts).

Example

$$B = \left\{ \begin{array}{c} lego\_builder(alice). \\ enjoys\_lego(A) := lego\_builder(A). \\ estate\_agent(dave). \\ enjoys\_lego(alice). \\ enjoys\_lego(claire). \end{array} \right\}$$

$$E^+ = \{happy(alice).\}$$

$$E^- = \left\{ \begin{array}{c} happy(bob). \\ happy(claire). \\ happy(dave). \end{array} \right\}$$

Substitution, Subsumption

- Clauses ale implicitly generally quantified.
- They should not have a variable with the same name.

Definition (Substitution, Subsumption)

- Given a **substitution** $\theta = \{v_i/t_i\}$ and formula F. $F\theta$ is formed by replacing every variable v_i in F by t_i.
- Substitution θ **unifies** atom A and B in the case $A\theta = B\theta$.
- Atom A subsumes atom B, $A \succeq B$, iff there exists a substitution θ such that $A\theta = B$.
- **Clause C subsumes clause D**, $C \succeq D$, iff there exists a substitution θ such that $C\theta \subseteq D$.

Example

- $C_1 = f(A, B) :- head(A, B)$.
- $C_2 = f(X, Y) :- head(X, Y), empty(Y)$.
- C_1 subsumes C_2 since $C_1\theta \subseteq C_2$ with $\theta = \{A/X, B/Y\}$.

Definition (Generalisation)

- Clause C **is more general than** clause D, iff $C \models D$.
- Clause C is more general than clause D with respect to B, iff $B, C \models D$.
  - B is the **background knowledge**.

Example

- Statement A: Daffy Duck can fly. $can\_fly(daffy)$
- Statement B: All ducks can fly. $can\_fly(X) \succeq can\_fly(daffy)$.

Example

- Statement C: Marek lives in London.
- Statement D: Marek lives in England.

- $lives(marek, london)$
- $lives(marek, england)$
- Background knowledge $lives(x, england) : -lives(x, london)$.
- $B, C \models D$, 'C is more general than D with respect to B'.
- $C \succeq D$ with respect to B.
- `http://www.doc.ic.ac.uk/~shm/FLOC_ILP/Lecture1.1.pdf`

ILP general logical setting

Definition (Hypothesis Properies)

The background knowledge B and the hypothesis H should entail E, that is:

Necessity	B	$\not\models$	E^+	we need H
Sufficiency (úplnost)	$B \& H$	$\models$	E^+	H explains positive examples
Weak consistency	$B \& H$	$\not\models$	$\bot$	H does not contradict B
(Strong) **consistency**	$B \& H \& E^-$	$\not\models$	$\bot$	... neither negative examples

ILP task

- Given
  - B background knowledge (logic program)
  - E^+, E^- examples – sets of ground unit clauses
- Given B, E find a logic program H such that is necessary, sufficient and consistent.
- Often, we assume noisy data and accept some errors, but we try to minimize them.

Example

$$B = \left\{ \begin{array}{c} lego\_builder(alice). \\ lego\_builder(bob). \\ estate\_agent(claire). \\ estate\_agent(dave). \\ enjoys\_lego(alice). \\ enjoys\_lego(claire). \end{array} \right\}$$

$$E^+ = \{happy(alice).\}$$

$$E^- = \left\{ \begin{array}{c} happy(bob). \\ happy(claire). \\ happy(dave). \end{array} \right\}$$

Our hypothesis space:

$$\mathcal{H} = \left\{ \begin{array}{c} h_1 : happy(A) :- lego\_builder(A). \\ h_2 : happy(A) :- estate\_agent(A). \\ h_3 : happy(A) :- enjoys\_lego(A). \\ h_4 : happy(A) :- lego\_builder(A), estate\_agent(A). \\ h_5 : happy(A) :- lego\_builder(A), enjoys\_lego(A). \\ h_6 : happy(A) :- estate\_agent(A), enjoys\_lego(A). \end{array} \right\}$$

- $B \cup h_1 \models happy(bob)$ therefore h_1 is inconsistent.
- $B \cup h_2 \not\models happy(alice)$ therefore h_2 is incomplete.
- $B \cup h_3 \models happy(claire)$ therefore h_3 is inconsistent.
- $B \cup h_4 \not\models happy(alice)$ therefore h_4 is incomplete.
- h_5 is both complete and consistent.
- $B \cup h_6 \not\models happy(alice)$ therefore h_1 in incomplete.

Hypothesis Space

- To specify (restrict) the hypothesis space usually mode declarations are used.

Definition (Mode declarations)

Mode declarations denote which literals may appear in the head/body of a rule. A mode declaration is of the form:

$$mode(recall, pred(m_1, m_2, \ldots, m_a))$$

where *recall* is the maximum number of occurrences of the predicate
m_i are the argument types and they may be assigned as input $+$, output $-$, constant $\#$.

Example

```
modeb(2,parent(+person,-person)).
modeh(1,happy(+person)).
modeb(*,member(+list,-element)).
modeb(1,head(+list,-element)).
```

A. Cropper and S. Dumancic. Inductive logic programming at 30: a new introduction.

Non-monotonic reasoning

- In Prolog, there is negation as a failure.

Example

$$Program = \left\{ \begin{array}{c} sunny. \\ happy :- sunny, not\ weekday. \end{array} \right\}$$

- Prolog tries to prove *weekday*.
- It does not prove it, therefore it concludes *happy*.
- With additional knowledge *weekday* some of entailments are not true any more.

Definition (Normal logic program)

Normal logic programs may include negated literals in the body of a clause, e.g.

$$h :- b_1, \ldots, b_n, not\ b_{n+1}, \ldots, not\ b_m.$$

Aleph ILP system (based on Progol)

- Given
  - A set of mode declaration M
  - Background knowledge B in the form of a normal program allows negation, with the semantics negation as a failure
  - Positive E^+ and negative E^- examples as a set of ground facts
- Return: A normal program hypothesis H that:
  - H is consistent with M
  - $\forall e \in E^+$, $H \cup B \models e$ (H is complete)
  - $\forall e \in E^-$, $H \cup B \not\models e$ (H is consistent).

Aleph

1. Select a positive example to generalize.
2. Construct the most specific clause consistent with M that entails the example (the bottom clause).
3. Search for a clause more general than the bottom clause.
   - Add the clause to the hypothesis and remove all examples covered.
   - If a positive example left, return to step 1.

Bottom Clause Construction

- The purpose is to bound the search in the step in 3.
- Without mode declarations, the bottom clause may have infinite cardinality.

Definition (Bottom clause)

Let H be a clausal hypothesis and C be a clause. The bottom clause $\bot(C)$ is the most specific clause such that:

$$H \cup \bot(C) \models C.$$

Example (Bottom clause)

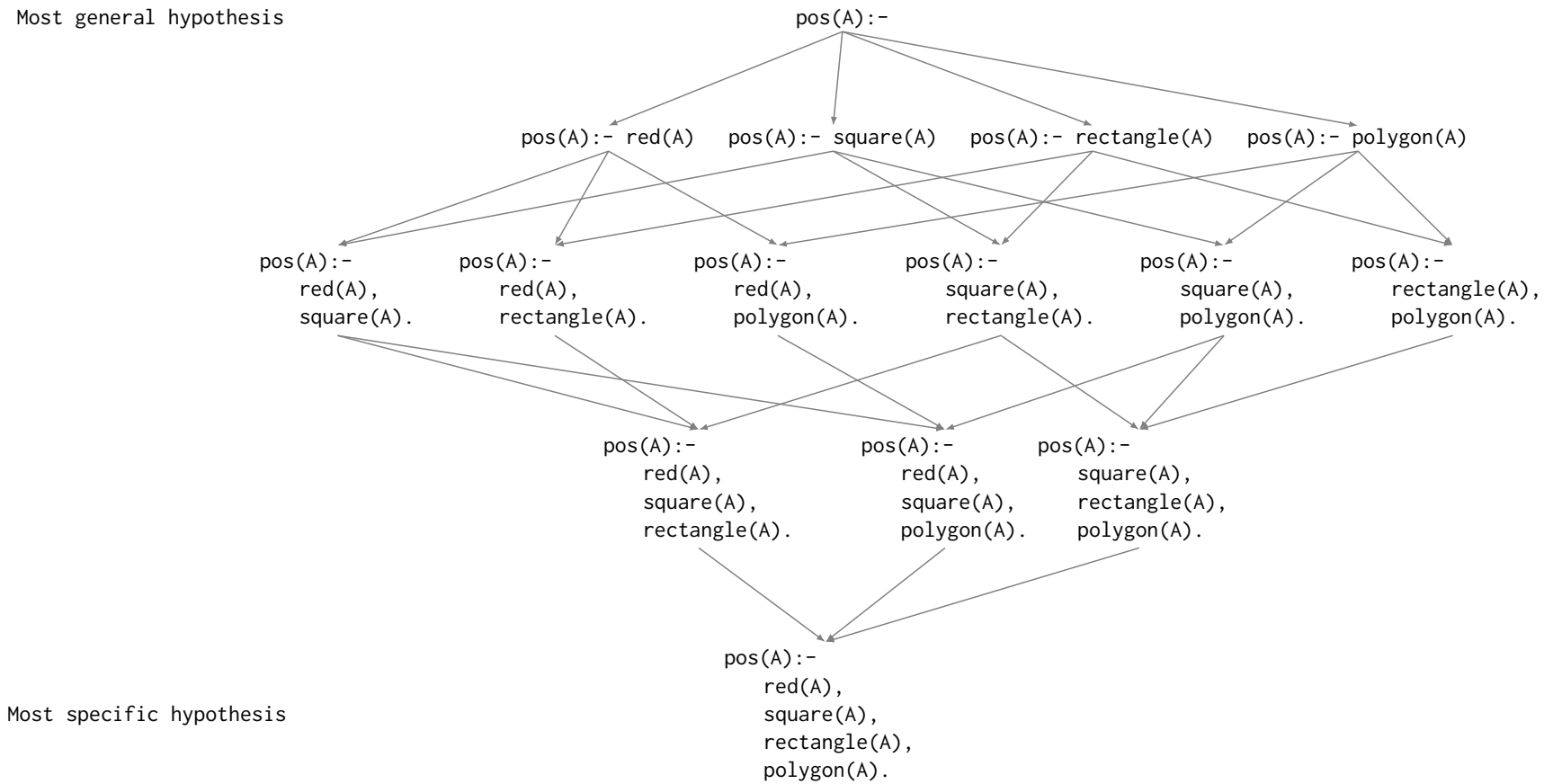
$$M = \left\{ \begin{array}{c} :-modeh(*, pos(+shape)). \\ :-modeb(*, red(+shape)). \\ :-modeb(*, square(+shape)). \\ :-modeb(*, triangle(+shape)). \\ :-modeb(*, polygon(+shape)). \end{array} \right\} \quad B = \left\{ \begin{array}{c} red(s1). \\ blue(s2). \\ square(s1). \\ triange(s2). \\ polygon(A) :- rectangle(A). \\ rectangle(A) :- square(A). \end{array} \right\}$$

Let e be the positive example $pos(s1)$. Then:

$$\bot(e) = pos(A) :- red(A), square(A), rectangle(A), polygon(A).$$

Clause Search

- Aleph performs a bounded breadth-first search to enumerate the shorter clauses before longer ones.
- The search is bounded by several parameters (max. clause size, max. proof depth).



Aleph 2, Popper

- Aleph default evaluation function is **coverage** defined as $P - N$,
  - P is the number of positive examples covered
  - N is the number of positive examples covered by the clause
  - that means it accepts some noise.
- It starts from the most general one $pos(A) :-$.
- It tries to specialize the clause
  - by adding literals to the body of it, which it selects from the bottom clause
- or by instantiating variables.
- Each specialization is called **refinement**.
- Aleph Advantages
  - one Prolog file, easy to download and use.
    - https://www.cs.ox.ac.uk/activities/programinduction/Aleph/aleph.html
  - It has good empirical performance.
  - Allows numerical reasoning, user defined cost functions, handles noisy data.
- Aleph Disadvantages
  - It has many parameters to tune.
  - It struggles to learn recursive programs and optimal programs
    - since it learns only a single clause a time.

Metagol

- Given
  - A set of metarules M
  - Background knowledge B in the form of a normal program
  - Positive E^+ and negative E^- examples as a set of facts (atoms).
- Return: A definite program hypothesis H that:
  - H is consistent with M
  - $\forall e \in E^+, H \cup B \models e$ (H is complete)
  - $\forall e \in E^-, H \cup B \not\models e$ (H is consistent)
  - $\forall h \in H, \exists m \in M$ such that $h = m\theta$
    - where θ is a substitution that grounds all the existentially quantified variables in m.

Example (Metarule)

- An example is the **chain** metarule $P(A, B) \leftarrow Q(A, C), R(C, B)$
- that allows Metagol to induce programs such as

$$f(A, B) \quad :- \quad tail(A, C), tail(C, B).$$
$$grandparent(A, B) \quad :- \quad parent(A, C), parent(C, B).$$

Metagol

- Metagol is a form of ILP besed on a Prolog meta-interpreter.

Metagol

1. Select a positive example to generalize.
   - If none exists, test the hypothesis on the negative examples.
     - If the hypothesis does not entail any negative example stop and return the hypothesis.
     - otherwise backtrack to a choice point at step 2 and continue.
2. Try to prove the atom by:
   - using given BK or an already induced clauses
   - unifying the atom with the head of a metarule
   - binding the variables in a metarule to symbols in the predicate and constant signatures
   - save the substitution
   - try to prove the body of the metarule by treating the body atoms as examples and applying step 2 to them.

Recursion

- Metagol can learn recursive programs.

Example (Reachability)

Consider learning the concept of *reachability* in a graph. Without recursion, with the maximal depth 4 we could learn:

$$
\begin{aligned}
reachable(A,B) &:- edge(A,B).\\
reachable(A,B) &:- edge(A,C), edge(C,B).\\
reachable(A,B) &:- edge(A,C), edge(C,D), edge(D,B).\\
reachable(A,B) &:- edge(A,C), edge(C,D), edge(D,E), edge(E,B).
\end{aligned}
$$

With recursion, we can learn:

$$
\begin{aligned}
reachable(A,B) &:- edge(A,B).\\
reachable(A,B) &:- edge(A,C), reachable(C,B).
\end{aligned}
$$

Iterative deepening

iterative deepening

- Metagol uses iterative deepening to search for hypotheses.
  - at depth $d = 1$, at least one metasub.
  - at iteration d, it introduces $d - 1$ new predicate symbols and is allowed to use d clauses.

Metagol Example

Example (Kinship example)

$$B = \left\{ \begin{array}{c} mother(ann, amy).mother(ann, andy). \\ mother(amy, amelia), mother(amy, bob). \\ mother(linda, gavin). \\ father(steve, amy).father(steve, andy). \\ father(andy, sponegebob).father(gavin, amelia). \end{array} \right\}$$

$$metarule(ident, [P, Q], [P, A, B], [[Q, A, B]]).$$
$$metarule(chain, [P, Q, R], [P, A, B], [[Q, A, C], [R, C, B]]).$$

$$E^+ = \left\{ \begin{array}{c} grandparent(ann, amelia). \\ grandparent(steve, amelia). \\ grandparent(ann, spongebob). \\ grandparent(linda, amelia). \end{array} \right\}$$
$$E^- = \{grandparent(amy, amelia).\}$$

Tracing Metagol

- It select the first example to generalize $grandparent(ann, amelia)$.
- It tries to prove it from BK and induced clauses. It fails.
- Metagol tries to use the first metarule:

$$grandparent(ann, amelia) : -Q(ann, amelia).$$

  stores $sub(ident, [grandparent, Q])$
- and tries to unify Q, but fails.
- Metagol tries to use the second metarule:

$$grandparent(ann, amelia) : -Q(ann, C), R(C, amelia).$$

  stores $sub(chain, [grandparent, Q, R])$
- and recursively tries to prove $Q(ann, C)$ and $R(C, amelia)$.
- It succeedes with the metasum $sub(chain, [grandparent, mother, mother])$
- and induces the first clause;

$$grandparent(A, B) : -mother(A, C), mother(C, B).$$

Metagol Trace 2

- Then, it select the second example to generalize $grandparent(steve, amelia)$.
- It tries to prove it from BK and induced clauses. It fails.
- Metagol can again use the second metarule with another substitution: stores $sub(chain, [grandparent, father, mother])$
- and induces the second clause;

$$grandparent(A, B) :- father(A, C), mother(C, B).$$

- Given no bound on the program size, the Metagol would prove the other two examples the same way and form the program:

$$\begin{aligned}
grandparent(A, B) &:- mother(A, C), mother(C, B).\\
grandparent(A, B) &:- father(A, C), mother(C, B).\\
grandparent(A, B) &:- father(A, C), father(C, B).\\
grandparent(A, B) &:- mother(A, C), father(C, B).
\end{aligned}$$

In praxis, it learns:

$$\begin{aligned}
grandparent(A, B) &:- grandparent_1(A, C), grandparent_1(C, B).\\
grandparent_1(A, B) &:- father(A, B).
\end{aligned}$$

Tail Recursive Metarule

Example (Tail Recursive Metarule)

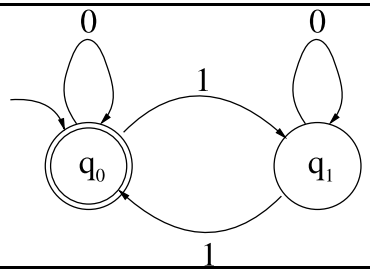
- An example is the **tail recursive** metarule $P(A, B) \leftarrow Q(A, C), P(C, B)$
- Metagol can also learn mutually recursive programs, such:

$$
\begin{aligned}
&even(0).\\
even(A) \quad &:- \quad successor(A, B), even\_1(B).\\
even\_1(A) \quad &:- \quad successor(A, B), even(B).
\end{aligned}
$$

We even do not have to provide the concept of an odd number. We can let the Metagol to invent such predicate (*even_1*).

Automata Example

(a)

Finite acceptor	Production rules	Definite Clause Grammar (DCG)
	$q_0 \rightarrow$	$q_0([], []) \leftarrow$
	$q_0 \rightarrow 0\ q_0$	$q_0([0\|A], B) \leftarrow q_0(A, B)$
	$q_0 \rightarrow 1\ q_1$	$q_0([1\|A], B) \leftarrow q_1(A, B)$
	$q_1 \rightarrow 0\ q_1$	$q_1([0\|A], B) \leftarrow q_1(A, B)$
	$q_1 \rightarrow 1\ q_0$	$q_1([1\|A], B) \leftarrow q_0(A, B)$

(b)

E^+	E^-	Meta-interpreter	Ground facts
λ	1	$parse(S) \leftarrow parse(q0, S, []).$	$acceptor(q0) \leftarrow$
0	01		$delta1(q0, 0, q0) \leftarrow$
00	10	$parse(Q, [], []) \leftarrow acceptor(Q).$	$delta1(q0, 1, q1) \leftarrow$
11	001	$parse(Q, [C\|X], Y) \leftarrow$	$delta1(q1, 0, q1) \leftarrow$
000	010	$delta1(Q, C, P),$	$delta1(q1, 1, q0) \leftarrow$
011	100	$parse(P, X, Y).$	
101	111		

Fig. 1 (**a**) Parity acceptor with associated production rules, DCG; (**b**) positive examples (E^+) and negative examples (E^-), Meta-interpreter and ground facts representing the Parity grammar

Hypothesis in Meta-interpretive learning

E^+	$\neg E^+$	E^-
$parse([]) \leftarrow$	$\leftarrow parse([]),$	$\leftarrow parse([1])$
$parse([1,1]) \leftarrow$	$parse([1,1]),$	$\leftarrow parse([0,1])$
$parse([0,1,1]) \leftarrow$	$parse([0,1,1]),$	$\leftarrow parse([1,0])$
$parse([1,0,1]) \leftarrow$	$parse([1,0,1]),$	$\leftarrow parse([0,0,1])$
$parse([1,1,0]) \leftarrow$	$parse([1,1,0]).$	$\leftarrow parse([1,1,1])$

H	$\neg H$
$acceptor(\$0) \leftarrow$	$\leftarrow acceptor(Q0),$
$delta1(\$0, 0, \$0) \leftarrow$	$delta1(Q0, 0, Q0),$
$delta1(\$0, 1, \$1) \leftarrow$	$delta1(Q0, 1, Q1),$
$delta1(\$1, 0, \$1) \leftarrow$	$delta1(Q1, 0, Q1),$
$delta1(\$1, 1, \$0) \leftarrow$	$delta1(Q1, 1, Q0).$

Fig. 2 Parity example where B_M is the Meta-interpreter shown in Fig. 1b, $B_A = \emptyset$ and E^+, $\neg E^+$, E^-, H, $\neg H$, are as shown above. '$0' and '$1' in H are Skolem constants replacing existentially quantified variables

- The background knowledge is the meta-interpreter from the previous figure.

Metagol

```
:-   parse([],[],G1), parse([0],G1,G2), parse([0,0],G2,G3), parse([1,1],G3,G4),    % Pos
     parse([0,0,0],G4,G5), parse([0,1,1],G5,G6), parse([1,0,1],G6,G),
     not(parse([1],G,G)), not(parse([0,1],G,G)).                                  % Neg

parse(S,G1,G2,S1,S2,K1,K2) :- parse(s(0),S,[],G1,G2,S1,S2,K1,K2).

parse(Q,X,X,G1,G2,S,S,K1,K2) :- abduce(acceptor(Q),G1,G2,K1,K2).
parse(Q,[C|X],Y,G1,G2,S1,S2,K1,K2) :- Skolem(P,S1,S3),
        abduce(delta1(Q,C,P),G1,G3,K3,K2), parse(P,X,Y,G3,G2,S3,S2,K3,K2).

abduce(X,G,G,K,K) :- member(X,G).
abduce(X,G,[X|G],s(K),K) :- not(member(X,G)).

Skolem(s(N),[s(Pre)|SkolemConsts],[s(N),s(Pre)|SkolemConsts]):- N is Pre+1.
Skolem(S,SkolemConsts,SkolemConsts):-member(S,SkolemConsts).
```

Fig. 5 Metagol$_R$

- Hypothesis found by Prolog

$$G = [delta1(s(1), 0, s(1)), delta1(s(1), 1, s(0)), delta1(s(0), 1, s(1)), delta1(s(0), 0, s(0)), acceptor(s(0))]$$

http://www.doc.ic.ac.uk/~shm/FLOC_ILP/Paper03.pdf

ASPAL algorithm

- ASPAL uses Answer Set Programming.
- ASP program can have one, many, or none models (answer sets).
- Computation in ASP is the process of finding models.
- We may specify the range of the number of clauses from a set beeing true. $0\{sunny., weekday., happy(A) : -lego\_builder(A)\}3$
- We may specify an evaluation function to optimize (like to minimize the number of 'true' clauses, e.g. the size of the hypothesis.

ASPAL

- Generate all possible rules consistent with the given mode declarations.

  Assign each rule a unique identifier and add an guessable atom in each rule.
- Use an ASP solver to find a minimal subset of the rules

  by formulating the problem as an ASP optimization problem.

ASPAL Example

Example (ASPAL)

$$B = \left\{ \begin{array}{c} bird(alice). \\ bird(betty). \\ can(alice, fly). \\ can(betty, swim). \\ ability(fly). \\ ability(swim). \end{array} \right\}$$

$$M = \left\{ \begin{array}{c} modeh(1, penguin(+bird)). \\ modeb(1, bird(+bird)). \\ modeb(*, not\ can(+bird, \#ability)). \end{array} \right\}$$

$$\begin{array}{lcl} E^+ & = & \{penguin(betty).\} \\ E^- & = & \{penguin(alice).\} \end{array}$$

Given the modes, the possible rules are:

$$\begin{array}{lcl} penguin(X) & :- & bird(X). \\ penguin(X) & :- & bird(X), not\ can(X, swim). \\ penguin(X) & :- & bird(X), not\ can(X, fly). \\ penguin(X) & :- & bird(X), not\ can(X, swim), not\ can(X, fly). \end{array}$$

ASPAL replaces constants and adds extra literal:

$$\begin{array}{lcl} penguin(X) & :- & bird(X), rule(r1). \\ penguin(X) & :- & bird(X), not\ can(X, C1), rule(r2, C1). \end{array}$$

ASPAL passes to an ASP solver:

$bird(alice).$

$bird(betty).$

$can(alice, fly).$

$can(betty, swim).$

$ability(fly).$

$ability(swim).$

$penguin(X) :- bird(X), rule(r1).$

$penguin(X) :- bird(X), not\ can(X, C1), rule(r2, C1).$

$penguin(X) :- bird(X), not\ can(X, C1), not\ can(X, C2), rule(r3, C1, C2).$

$0\{rule(r1), rule(r2, fly), rule(r2, swim), rule(r3, fly, swim)\}4$

$goal :- penguin(betty), not\ penguin(alice).$

$:- not\ goal.$

- The answer is: $rule(r2, c(fly))$
- Which is translated to a program:

$$penguin(A) :- bird(A), not\ can(A, fly).$$

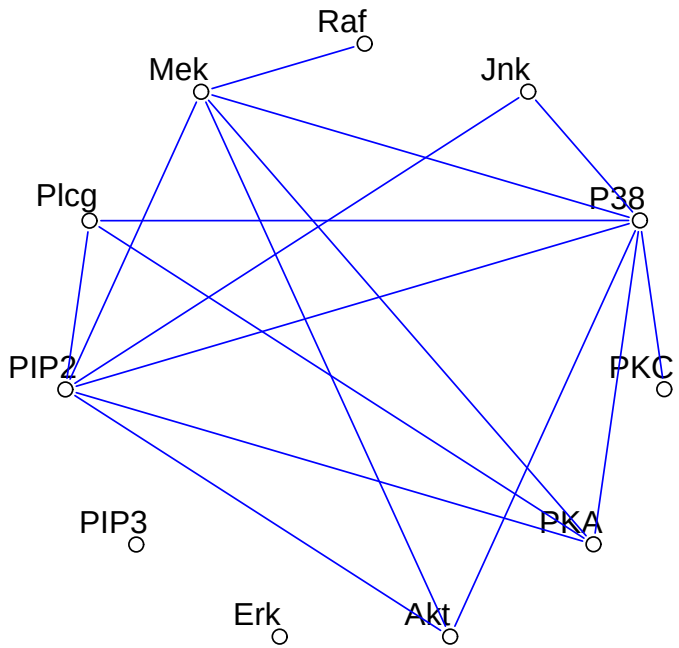
ILP aplications

- Bioinformatics
  - ILP can make predictions based on the (sub)structured biological data.
  - Predict mutagenic activity of molecules and alert the causes of chemical cancers
  - learning protein folding signatures.
- Robot scientist.
  - BK knowledge represents the relationship between protein-coding sequences, enzymes, and metbolites in pathway.
  - Automatically generates hypotheses, run experiments, iterprets results.
- Games
  - Sokoban
  - Bridge
  - Checkers.

Undirected (Pairwise, Continuous) Graphical Models

- The **generative model** represents the full probability distribution $P(X)$.
- Missing edges represent conditional independence of the variables.

- Cytometry dataset (ESLII)
- $N = 7466$ cells
- $p = 11$ proteins
- We ame to model protein co-occurence probability.



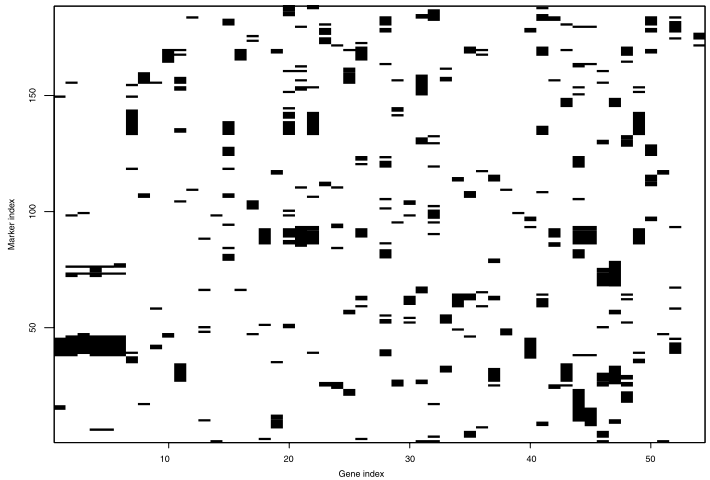
sklearn.covariance.GraphicalLasso # basics

gRbase # the recommended R package

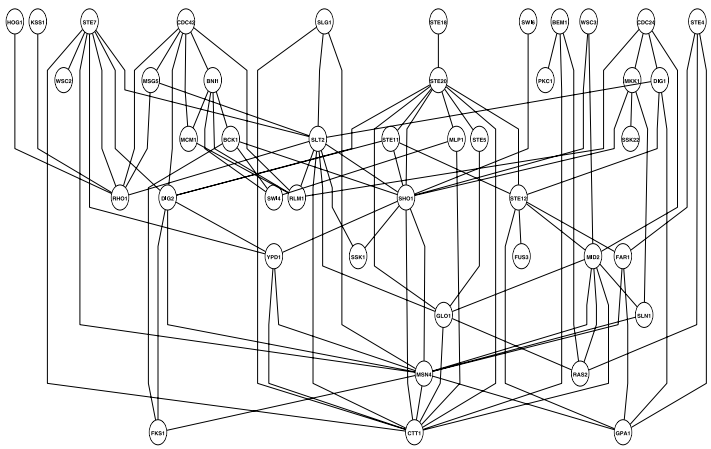
Other Application

Yin, Jianxin & Li, Hongzhe. (2011). *A sparse conditional Gaussian graphical model for analysis of genetical genomics data.* The annals of applied statistics. 5. 2630-2650.

- Cytometry dataset (ESLII)
- $p_Y = 54$ gene level expressions
- $p_X = 188$ markers (discrete)
- $Y^{p_Y} | X^{p_X} \sim \mathcal{N}(M^{p_Y \times p_X} X^{p_X}, \Sigma^{p_Y \times p_Y})$ conditional Gaussian distribution
- Top: Black color indicates significant association $p - value < 0.01$ in the linear regression.
- Bottom: The undirected graph of 43 genes constructed on the cGGM.



(a)



Data: carcass

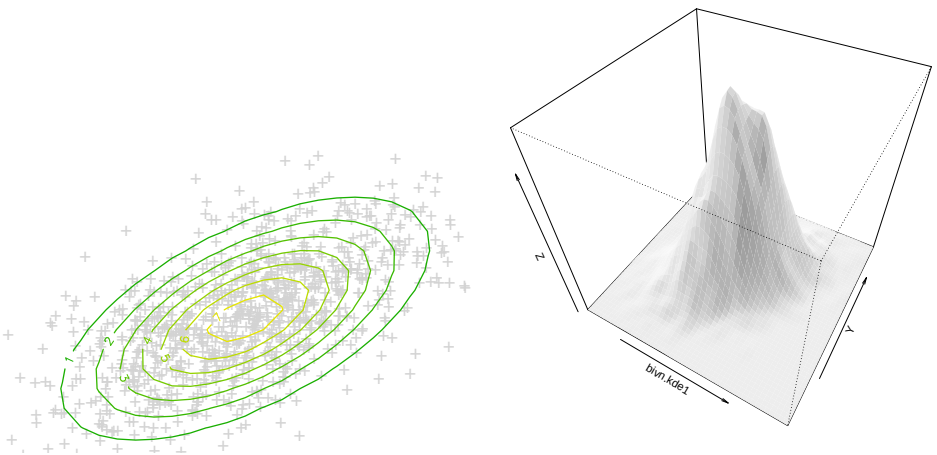
Data: carcass #Source: Soren Hojsgaard, David Edwards, Steffen Lauritzen: *Graphical Models with R*, Springer.

	mean.
Fat11	16.00
Meat11	52.00
Fat12	14.00
Meat12	52.00
Fat13	13.00
Meat13	56.00
LeanMeat	59.00

Σ	Fat11	Meat11	Fat12	Meat12	Fat13	Meat13	LeanMeat
Fat11	11.34	0.74	8.42	2.06	7.66	-0.76	-9.08
Meat11	0.74	32.97	0.67	35.94	2.01	31.97	5.33
Fat12	8.42	0.67	8.91	0.31	6.84	-0.60	-7.95
Meat12	2.06	35.94	0.31	51.79	2.18	41.47	6.03
Fat13	7.66	2.01	6.84	2.18	7.62	0.38	-6.93
Meat13	-0.76	31.97	-0.60	41.47	0.38	41.44	7.23
LeanMeat	-9.08	5.33	-7.95	6.03	-6.93	7.23	12.90

Gaussian Graphical Models (Undirected Graphs)

- **Multivariate Gaussian Distribution** on variables $X = (X_1, \ldots, X_p)$
- $\phi(\mathbf{x}) = \frac{1}{\sqrt{|2\pi\Sigma|}} e^{-\frac{1}{2}(\mathbf{x}-\mu)\Sigma^{-1}(\mathbf{x}-\mu)}$
  - $|.|$ is the determinant. we denote p the number of components in $\mathbf{x}$. Then $|2\pi\Sigma| = (2\pi)^p|\Sigma|$.
- If Σ is not invertible it has dependent columns. It means that the variables $\mathbf{x}_j$ are lineary dependent.
  - If the **rank** of Σ is ℓ then there exists a matrix A and a vector ν so:
  - $x = Az + \nu$ for new coordinates z with ℓ dimensions
  - We just consider the new coordinates and assume Σ has a full rank.



Concentration matrix

- **Concentration (Precision, koncentrační) matrix**

$$K = \Sigma^{-1}$$

Lemma

For $u \neq v$, $k_{uv} = 0$ if and only if y_u and y_v are conditionally independent given all other variables.

k*100	Fat11	Meat11	Fat12	Meat12	Fat13	Meat13	LeanMeat
Fat11	44	3	-20	-7	-16	4	10
Meat11	3	16	-3	-6	-6	-6	-3
Fat12	-20	-3	54	6	-21	-5	9
Meat12	-7	-6	6	14	-1	-9	-0
Fat13	-16	-6	-21	-1	56	3	7
Meat13	4	-6	-5	-9	3	16	-1
LeanMeat	10	-3	9	-0	7	-1	26

- If looking for small values better to 'scale' the entries into Partial Correlation matrix.

Partial correlation matrix

Definition (Partial correlation matrix)

Partial correlation matrix is defined from K by

$$\rho_{uv|V\setminus\{uv\}} = \frac{-k_{uv}}{\sqrt{k_{uu}k_{vv}}}.$$

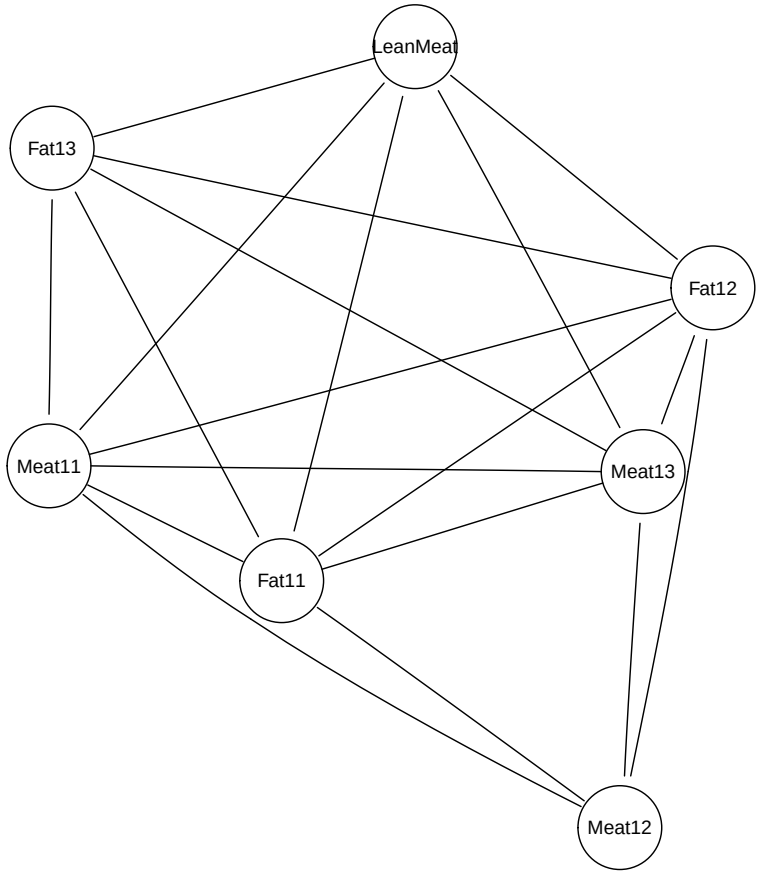
Lemma

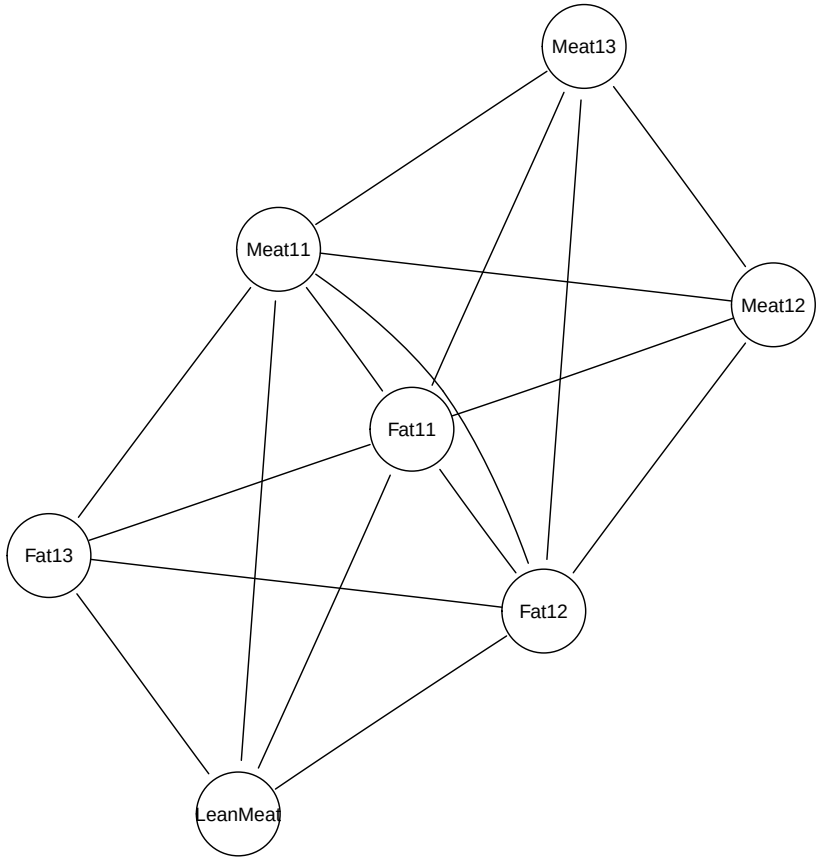
In contrast to concentrations, the partial correlations are invariant under a change of scale and origin in the sense that if $X_j^* = a_j X_j + b_j$, $j = 1, \ldots, p$ *then* $a_v a_u k_{uv}^* = k_{uv}$ *and* $\rho^*_{uv|V\setminus\{uv\}} = \rho_{uv|V\setminus\{uv\}}$.

$\rho * 100$	Fat11	Meat11	Fat12	Meat12	Fat13	Meat13	LeanMeat
Fat11	-	-11	41	30	32	-16	-29
Meat11	-11	-	9	41	19	35	16
Fat12	41	9	-	-24	38	18	-24
Meat12	30	41	-24	-	2	61	2
Fat13	32	19	38	2	-	-9	-18
Meat13	-16	35	18	61	-9	-	7
LeanMeat	-29	16	-24	2	-18	7	-

Models

- The simplest model just removes edges with small $|\rho_{uv|V\setminus\{uv\}}|$. Penalized criteria will be introduced later.





Undirected Gaussian graphical model

Definition (Undirected Gaussian graphical model)

An **undirected Gaussian graphical model** is represented by an undirected graph $\mathcal{G} = (X, E)$, $X = \{X_1, \ldots, X_p\}$ represent the set of variables and E is a set of undirected edges.
When a random vector $\mathbf{x}$ follows a Gaussian distribution $N_p(\mu, \Sigma)$, the graph G represents the model where $K = \Sigma^{-1}$ is a positive definite matrix with $k_{u,v} = 0$ whenever there is no edge between vertices u, v in G.
This graph is called the **dependence graph** of the model.

Lemma

For any non adjacent vertices $u, v \in \mathcal{G}$ it holds: $u \perp\!\!\!\perp v | \mathbf{X} \setminus \{u, v\}$.

Definition (Generating class)

Let $\mathcal{C} = \{C_1, \ldots, C_k\}$ be the set of cliques of the dependence graph $\mathcal{G}$. A set of functions $g_1(), g_2(), \ldots, g_k()$ defined on $g_i(\mathbf{x}_{C_i})$ is called a **generating class** for the distribution

$$f(\mathbf{x}) = \prod_{i=1,\ldots,k} g_i(\mathbf{x}_{C_i}).$$

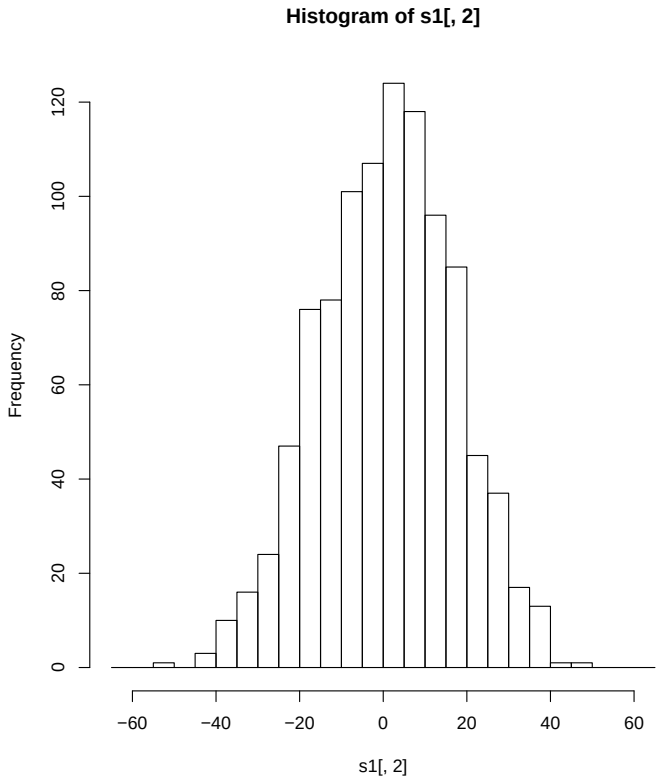
Marginalization

- We have $\frac{1}{\sqrt{|2\pi\Sigma|}} e^{-\frac{1}{2}(\mathbf{x}-\mu)\Sigma^{-1}(\mathbf{x}-\mu)}$
- We want the distribution over variables $\{x_3, x_5, x_7\} \subset \{x_1, \ldots, x_p\}$

Marginal of a Gaussian Distribution

The marginal of a Gaussian distribution is calculated by removing appropriate dimensions from the mean and covariance matrix.

- $\mu_{3,5,7} = (\mu_3, \mu_5, \mu_7)$ and $\Sigma_{3,5,7} = \begin{bmatrix} \Sigma_{33} & \Sigma_{35} & \Sigma_{37} \\ \Sigma_{53} & \Sigma_{55} & \Sigma_{57} \\ \Sigma_{73} & \Sigma_{75} & \Sigma_{77} \end{bmatrix}$
- $\phi_{x_3,x_5,x_7} = \frac{1}{\sqrt{|2\pi\Sigma_{3,5,7}|}} e^{-\frac{1}{2}(x_{3,5,7}-\mu_{3,5,7})\Sigma^{-1}_{3,5,7}(x_{3,5,7}-\mu_{3,5,7})}$



Conditioning

- We ame for $\phi(A|B)$ where
  - $A \subset \{x_1, \ldots, x_p\}$ having q elements,
  - the rest $B = \{x_1, \ldots, x_p\} \setminus A$ has $(p - q)$ elements.
- We rearrange the rows and columns to have A together. Then we get

$$x = \begin{bmatrix} x_A \\ x_B \end{bmatrix} \text{ (one column)}, \ \mu = \begin{bmatrix} \mu_A \\ \mu_B \end{bmatrix} \text{ (one column)},$$

$$\Sigma = \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix} \text{ with dimensions } \begin{bmatrix} q \times q & q \times (p-q) \\ (p-q) \times q & (p-q) \times (p-q) \end{bmatrix}.$$

Conditional Gaussian

The parameters of the conditional Gaussian distribution $\phi(A|B = b) = N(\mu_{A|B=b}, \Sigma_{A|B=b})$ are:

$$\begin{aligned} \mu_{A|B=b} &= \mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(b - \mu_B) \\ \Sigma_{A|B=b} &= \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}. \end{aligned}$$

Covariance matrix differs but does not depend on the observation b. It depends on the fact B was observed.

Conditional Gaussian Example

- $\mu^T = (1, 2, 3, 4)$
- $\Sigma = \begin{bmatrix} 10 & 1 & 5 & 4 \\ 1 & 10 & 2 & 6 \\ 5 & 2 & 10 & 3 \\ 4 & 6 & 3 & 10 \end{bmatrix}$
- We observed (X_3, X_4) to be $(2.8, 4.1)$
- We ask for $\phi(A|B) = \phi(\{X_1, X_2\}|\{X_3, X_4\})$
- $\Sigma_{AB} = \begin{bmatrix} 5 & 4 \\ 2 & 6 \end{bmatrix}$
- $\Sigma_{BB} = \begin{bmatrix} 10 & 3 \\ 3 & 10 \end{bmatrix}$
- $\Sigma_{BB}^{-1} \doteq \begin{bmatrix} 0.11 & -0.033 \\ -0.033 & 0.11 \end{bmatrix}$
- $\Sigma_{AB}\Sigma_{BB}^{-1} \doteq \begin{bmatrix} 0.418 & 0.275 \\ 0.0220 & 0.593 \end{bmatrix}$
- $\mu_{A|B=b} = \mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(b - \mu_B)$
- $\mu_{A|B} \doteq \begin{bmatrix} 1 \\ 2 \end{bmatrix} + \begin{bmatrix} 0.418 & 0.275 \\ 0.0220 & 0.593 \end{bmatrix} \begin{bmatrix} (2.8 - 3) \\ (4.1 - 4) \end{bmatrix}$
- $\mu_{A|B} \doteq \begin{bmatrix} 1 \\ 2 \end{bmatrix} + \begin{bmatrix} -0.056 \\ 0.055 \end{bmatrix} = \begin{bmatrix} 0.944 \\ 2.055 \end{bmatrix}$
- $\Sigma_{A|B=b} = \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}$
- $\Sigma_{A|B=b} \doteq \begin{bmatrix} 10 & 1 \\ 1 & 10 \end{bmatrix} - \begin{bmatrix} 2.53 & 2.26 \\ 2.26 & 4.13 \end{bmatrix}$
- $\Sigma_{A|B=b} \doteq \begin{bmatrix} 7.47 & -1.26 \\ -1.26 & 3.65 \end{bmatrix}$

Partition Matrix Inverse Properties

- The concentration matrix $K = \Sigma^{-1}$ is the inverse of the correlation matrix, therefore:

$$\begin{pmatrix} K_{AA} & K_{AB} \\ K_{BA} & K_{BB} \end{pmatrix} \begin{pmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{pmatrix} = \begin{pmatrix} I_{AA} & \mathbf{0} \\ \mathbf{0} & I_{BB} \end{pmatrix}$$

- From the top right part we get:

$$\begin{aligned} K_{AA}\Sigma_{AB} &+ K_{AB}\Sigma_{BB} = \mathbf{0} \\ -K_{AA}\Sigma_{AB}\Sigma_{BB}^{-1} &= K_{AB}(1) \qquad (5) \\ \Sigma_{AB}\Sigma_{BB}^{-1} &= -K_{AA}^{-1}K_{AB}(2). \qquad (6) \end{aligned}$$

- Take the top left part and substitute (1):

$$\begin{aligned} K_{AA}\Sigma_{AA} &+ K_{AB}\Sigma_{BA} = I_{AA} \\ K_{AA}\Sigma_{AA} &+ (-K_{AA}\Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}) = I_{AA} \\ K_{AA}^{-1} &= \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}. \end{aligned}$$

Regression Coefficients

$$\begin{aligned}\mu_{A|B=b} &= \mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(b - \mu_B) \\ \Sigma_{A|B=b} &= \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA}\end{aligned}$$

- Consider x_1 to be a linear function of others with the noise $\epsilon_1 \sim N(0, \sigma_1^2)$:

$$x_{1|2\ldots p} = \beta_1 + \beta_{12}x_2 + \beta_{13}x_3 + \ldots + \beta_{1p}x_p + \epsilon_1$$

- Set A the first dimension, B the remaining $(p-1) \times (p-1)$ matrix:

$$x_{1|B=(x_2,\ldots,x_p)^T} = \mu_{A|B} + \Sigma_{AB}\Sigma_{BB}^{-1}\left(\begin{bmatrix} x_2 \\ \ldots \\ x_p \end{bmatrix} - \mu_B\right) + \epsilon$$

- Recall (2): $\Sigma_{AB}\Sigma_{BB}^{-1} = -K_{AA}^{-1}K_{AB}$
- then $\sigma_1^2 = \frac{1}{k_{11}}$ with coefficients β

$$(\beta_{12}, \ldots, \beta_{1p}) = -\frac{(k_{12}, \ldots, k_{1p})}{k_{11}}.$$

Fit Linear Gaussian CPD

- To fit ML model of a linear gaussian CPD,
  - you fit the linear regression.

$$
\begin{aligned}
y &= \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_p x_p + \epsilon_1 \\
\hat{\beta} &= (\mathbf{X^T X})^{-1} \mathbf{X^T y} \\
\hat{\sigma}_Y &= Cov(Y, Y) - \sum_i \sum_j \beta_i \beta_j Cov[X_i; X_j] \\
Cov(X_i; X_j) &= \mathbb{E}[X_i \cdot X_j] - \mathbb{E}[X_i] \cdot \mathbb{E}[X_j] \\
\mathbb{E}[X_j] &= \frac{1}{N_{rows}} \sum_{i \in rows} x_{ij}
\end{aligned}
$$

```
from pgmpy.factors.continuous import LinearGaussianCPD
ml=maximum_likelihood_estimator(data, states)
cpdY.fit(data, states, estimator=ml, complete_samples_only=True)
```

https://cedar.buffalo.edu/~srihari/CSE674/Chap7/7.2-GaussBNs.pdf

Parameter Learning for a Gaussian Graphical Model

- Let us have the data $\mathbf{x}_1^T, \ldots, \mathbf{x}_N^T$ over variables $\mathbf{x} \sim N_p(\mu, \Sigma)$.
- $S = \frac{1}{N} \sum_{i=1}^{N} (\mathbf{x}_i - \bar{x})(\mathbf{x}_i - \bar{x})^T$ is the empirical covariance matrix.
- Our model is represented by the concentration matrix $\Theta = \Sigma^{-1}$ and mean μ.
- Log-likelihood of the data is

$$loglik(\Theta, \mu) = \frac{N}{2} \log |\Theta| - \frac{N}{2} tr(\Theta S) - \frac{N}{2} (\bar{x} - \mu)^T \Theta (\bar{x} - \mu).$$

- for a fixed Θ is the maximum for μ: $\mu = \bar{x}$ and the last term is 0. We get
- $loglik(\Theta, \mu) \propto log|\Theta| - tr(\Theta S)$
- where $tr(\Theta S) = \sum_u \sum_v \theta_{uv} s_{uv}$, therefore only s_{uv} corresponding to non-zero θ_{uv} are considered by the sum.
- We replace the equality conditions by Lagrange multiplyers: $\ell_C(\Theta) = log|\Theta| - tr(\Theta S) - \sum_{(j,k) \notin E} \gamma_{jk} \theta_{jk}$
- We maximize. The derivative Θ should be zero (Γ is a matrix with non-zero for missing edges):

$$\Theta^{-1} - S - \Gamma = 0$$

Towards the Algorithm

- We iterate one row/column after another.
- We start with the sample covariance matrix

$$W_0 \leftarrow S$$

- We derive the formula for the last row/column: the derivative

$$\begin{pmatrix} W_{11} & w_{12} \\ w_{12}^T & w_{22} \end{pmatrix} - \begin{pmatrix} S_{11} & s_{12} \\ s_{12}^T & s_{22} \end{pmatrix} - \begin{pmatrix} \Gamma_{11} & \gamma_{12} \\ \gamma_{12}^T & \gamma_{22} \end{pmatrix} = 0$$

- The upper right block can be written as $w_{12} - s_{12} - \gamma_{12} = 0$.
- W is inverse of Θ

$$\begin{pmatrix} W_{11} & w_{12} \\ w_{12}^T & w_{22} \end{pmatrix} \begin{pmatrix} \Theta_{11} & \theta_{12} \\ \theta_{12}^T & \theta_{22} \end{pmatrix} = \begin{pmatrix} I & 0 \\ 0^T & 1 \end{pmatrix}$$

- therefore the last column without last row is:

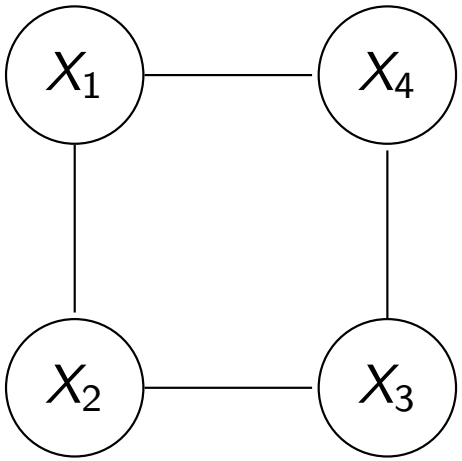
$$w_{12} = -W_{11}\theta_{12}/\theta_{22} = W_{11}\beta$$

- Substitute into the derivative $W_{11}\beta - s_{12} - \gamma_{12} = 0$
- we solve for the rows with zero γ: $\hat{\beta}^* = (W_{11}^*)^{-1} s_{12}^*$.
- The diagonal θ_{22} is (1 bottom right): $\frac{1}{\theta_{22}} = w_{22} - w_{12}^T \beta$.

Estimation of an Undirected Graphical Model Parameters

1: **procedure** GRAPHICAL REGRESSION:(S sample covariance)
2: $W \leftarrow S$ initialize
3: **repeat**
4: **for** $j = 1, 2, \ldots, p$ **do**
5: Partition W; jth row and column, W_{11} the rest
6: solve $W_{11}^{*}\beta^{*} - s_{12}^{*} = 0$ for reduced system
7: $\hat{\beta} \leftarrow \hat{\beta}^{*}$ by padding with zeros
8: update $w_{12} \leftarrow W_{11}\hat{\beta}$
9: **end for**
10: **until** convergence
11: **for** $j = 1, 2, \ldots, p$ **do**
12: lines 5:-8: above and set
13: $\hat{\theta}_{22} \leftarrow \frac{1}{w_{22} - w_{12}^{T}\hat{\beta}}$
14: $\hat{\theta}_{12} \leftarrow -\hat{\beta} \cdot \hat{\theta}_{22}$
15: **end for**
16: **end procedure**

Example (ESLII)



$$W_0 = S = \begin{bmatrix} 10.00 & 1.00 & 5.00 & 4.00 \\ 1.00 & 10.00 & 2.00 & 6.00 \\ 5.00 & 2.00 & 10.00 & 3.00 \\ 4.00 & 6.00 & 3.00 & 10.00 \end{bmatrix}$$

$$W_{11} = \begin{bmatrix} 10.00 & 2.00 & 6.00 \\ 2.00 & 10.00 & 3.00 \\ 6.00 & 3.00 & 10.00 \end{bmatrix} \qquad W_{22} = \begin{bmatrix} 10.00 & 1.16 & 4.00 \\ 1.16 & 10.00 & 3.00 \\ 4.00 & 3.00 & 10.00 \end{bmatrix}$$

$$W_{11}^* = \begin{bmatrix} 10.00 & 6.00 \\ 6.00 & 10.00 \end{bmatrix} \qquad W_{22}^* = \begin{bmatrix} 10.00 & 1.16 \\ 1.16 & 10.00 \end{bmatrix}$$

$$W_{11}^{*,-1} = \begin{bmatrix} 0.156 & -0.094 \\ -0.094 & 0.156 \end{bmatrix} \qquad W_{22}^{*,-1} = \begin{bmatrix} 0.101 & -0.012 \\ -0.012 & 0.101 \end{bmatrix}$$

$$\beta^* = [-0.22, 0.53]^T \qquad \beta 2^* = [0.08, 0.19]^T$$

$$\beta = [-0.22, 0, 0.53]^T \qquad \beta 2 = [0.08, 0.19, 0]^T$$

$$w_{12} \leftarrow [1.00, 1.16, 4.00]^T \qquad w_{2r} \leftarrow [1.00, 2, 0.88]^T$$

Structure Learning

- We add a lasso penalty $||\Theta||_1$ which denotes the L_1 norm
  - the sum of the absolute values of the elements of Θ and we ignore the diagonal.
  - The negative penalized log-likelihood is a convex function of Θ.
- we maximize penalized log-likelihood

$$log|\Theta| - tr(\Theta S) - \lambda||\Theta||_1 \tag{7}$$

- the gradient equation is now

$$\Theta^{-1} - S - \lambda Sign(\Theta) = 0 \tag{8}$$

  - sub-gradient notation
  - $Sign(\theta_{jk}) = sign(\theta_{jk})$ for $\theta_{jk} \neq 0$
  - $Sign(\theta_{jk}) \in [-1, 1]$ for $\theta_{jk} = 0$
- the update for the first row and column will be

$$W_{11}\beta - s_{12} + \lambda Sign(\beta) = 0 \tag{9}$$

  - since β and θ_{12} have opposite signs.

procedure GRAPHICAL LASSO:(S sample covariance,λ penalty)
  $W \leftarrow S + \lambda I$ initialize
  repeat
    for $j = 1, 2, \ldots, p$ **do**
      Partition W; jth row and column, W_{11} the rest
      solve $W_{11}\beta - s_{12} + \lambda Sign(\beta) = 0$ using the cyclical
      ...coordinate-descent algorithm for the modified lasso
      update w_{12} by $W_{11}\hat{\beta}$
    end for
  until convergence
  for $j = 1, 2, \ldots, p$ **do**
    solve $\hat{\theta}_{22} \leftarrow \frac{1}{s_{22} - w_{12}^T \hat{\beta}}$
    solve $\hat{\theta}_{12} \leftarrow -\hat{\beta} \cdot \hat{\theta}_{22}$
  end for
end procedure
procedure COORDINATEDESCENT:($V \leftarrow W_{11}$)
  repeat $j = 1, 2, \ldots, p-1$
    $\hat{\beta}_j \leftarrow S(s_{12j} - \sum_{k \neq j} V_{kj}\hat{\beta}_k, \lambda)/V_{jj}$
  until convergence
end procedure

$$\#S(x,t) = sign(x)(|x| - t)_+$$

Example (glasso)

- $\lambda \leftarrow 1$

$$W_0 = S + \lambda I = \begin{bmatrix} 11.00 & 1.00 & 5.00 & 4.00 \\ 1.00 & 11.00 & 2.00 & 6.00 \\ 5.00 & 2.00 & 11.00 & 3.00 \\ 4.00 & 6.00 & 3.00 & 11.00 \end{bmatrix}$$

$$\begin{aligned} W_{11} &= \begin{bmatrix} 11.00 & 2.00 & 6.00 \\ 2.00 & 11.00 & 3.00 \\ 6.00 & 3.00 & 11.00 \end{bmatrix} \\ s_{12}^T &= \begin{bmatrix} 1.00 & 5.00 & 4.00 \end{bmatrix} \\ \beta^{T,(0)} &= \begin{bmatrix} 0 & 0 & 0 \end{bmatrix} \\ V &\leftarrow W_{11} \\ \beta_2^{(1)} &= S(1-0,1)/11 = 0 \\ \beta_3^{(1)} &= S(5-0,1)/11 = \frac{4}{11} \\ \beta_4^{(1)} &= S(4-\frac{3 \cdot 4}{11},1)/11 = \frac{21}{121} \end{aligned}$$

$$\beta_2^{(2)} = S(1 - \frac{2 \cdot 4}{11} - \frac{6 \cdot 21}{121}, 1)/11 \approx -0.16$$

$$\beta_3^{(2)} = S(5 + 0.32 - \frac{3 \cdot 21}{121}, 1)/11 \approx 0.35$$

$$\beta_4^{(2)} = \dots$$

$$\dots$$

$$\hat{\beta}_1 \approx [-0.22; 0.32; 0.30]$$

$$W_1 \approx \begin{bmatrix} 11.00 & 0.05 & 4.03 & 3.01 \\ 0.05 & 11.00 & 2.00 & 6.00 \\ 4.03 & 2.00 & 11.00 & 3.00 \\ 3.01 & 6.00 & 3.00 & 11.00 \end{bmatrix}$$

Graphical Lasso Properties

- Computational speed
  - The graphical lasso algorithm is extremely fast
  - can solve a moderately sparse problem with 1000 nodes in less than a minute.
  - It can be modified to have edge–specific penalty parameters λ_{jk}
  - setting $\lambda_{jk} = \infty$ will force $\hat{\theta}_{jk}$ to be zero
  - graphical lasso subsumes the parameter learning algorithm.
- Missing data
  - some missing observations may be imputed by EM algorithm from the model
  - latent – fully unobserved variables – do not bring more power in Gaussian graphical model
  - latent variables are very important in discrete distributions.

sklearn.covariance.graphical_lasso

Model Quality (Model Selection)

Definition (Saturated model, GGM Deviance, iDeviance, Likelihood Ratio Test)

- **saturated model** - full model with all edges, it has maximal loglikelihood
- **Deviance**

$$D = dev = 2 \cdot (\hat{\ell}_{sat} - \hat{\ell}) = N \log \frac{|S^{-1}|}{|\hat{K}|} = -N \log |S\hat{K}|$$

- **independent model** - no edges, it has minimal likelihood
- **iDeviance**

$$iD = idev = 2 \cdot (\hat{\ell} - \hat{\ell}_{ind}) = N \left(\log |\hat{K}| + \sum_{i=1}^{p} \log s_{ii} \right)$$

- **lrt likelihood ratio test** for models $\mathcal{M}_1 \subseteq \mathcal{M}_0$

$$lrt = 2 \cdot (\hat{\ell}_0 - \hat{\ell}_1) = N \log \frac{|\hat{K}_0|}{|\hat{K}_1|}.$$

Undirected Graphical Models and Their Properties

Definition (Undirected Graphical Model, Markov Graph)

An **Undirected Graphical Model** (Markov graph, Markov network) is a graph $\mathcal{G} = (V, E)$, where nodes V represent random variables and the absence of an edge (A, B) denoted $A \perp\!\!\!\perp_{\mathcal{G}} B$ implies that the corresponding random variables are conditionally independent given the rest in the probability distribution $P(V)$.

$$A \perp\!\!\!\perp_{\mathcal{G}} B \Longrightarrow A \perp\!\!\!\perp_{P} B | V \setminus \{A, B\}. \tag{10}$$

is known as the **pairwise Markov independencies** of $\mathcal{G}$.

Definition (Separators)

- If A, B and C are subgraphs, then C **is said to separate** A **and** B if every path between A and B intersects a node in C.
- C is called a **separator**.

- Separators break the graph into conditionally independent pieces.

Markov Properties

Definition (Global Markov Property)

A probability measure P over V is **(globally) Markov** with respect to an undirected graph $\mathcal{G}$ iff for any subgraphs A, B and C holds:

- if C separates A and B then the conditional independence $A \perp\!\!\!\perp_P B|C$ holds, that is

$$A \perp\!\!\!\perp_{\mathcal{G}} B|C \Longrightarrow P(A|C) \cdot P(B|C) = P(A, B|C). \tag{11}$$

Theorem

The pairwise and global Markov properties of a graph are equivalent for graphs with strictly positive distributions.

- Gaussian distribution is always positive.
- We may infer global independence relations from simple pairwise properties.
- The global Markov property allows us to decompose graphs into smaller more manageable pieces.

Markov Random Fields (Markovská náhodná pole)

- A probability density function f over a Markov graph $\mathcal{G}$ with the set of maximal cliques $\{C_1, \ldots, C_k\}$ can be represented as

$$f(x) = \prod_{i=1,\ldots,k} \psi_i(x_{C_i}) = \psi_1(x_{C_1}) \cdot \ldots \cdot \psi_k(x_{C_k}) \tag{12}$$

- where ψ_i are positive functions called **clique potentials**.
- they capture the dependence in X_{C_i} by scoring certain instances x_{C_i} higher than others.
- with the **normalizing constant** (partition function) Z

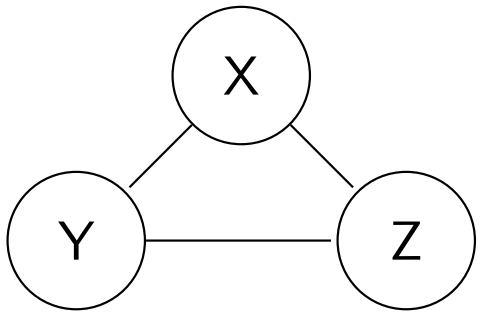
$$Z = \int_X exp\left(\sum_{i=1,\ldots,k} \log g_i(x_{C_i})\right).$$

- For Markov networks with positive distributions the probability density function (12) implies a graph with independence properties defined by the cliques in the product.

Pairwise Markov Graphs

- A graphical model does not always uniquely specify the higher–order dependence structure of ta joint probability distribution.

$$f^{(2)}(x,y,z) = \frac{1}{Z}\psi_1(x,y)\psi_2(x,z)\psi_3(y,z)$$
$$f^{(3)}(x,y,z) = \frac{1}{Z}\psi(x,y,z)$$



- For Gaussian distribution, parwise interactions fully specify the model.
- We focus on **pairwise Markov Graphs**
  - where at most second order interactions are represented (like $f^{(2)}$).

Undirected models with discrete variables

- **Boltzmann machine** (=**Ising models**; a special case of Markov random field)
  - visible and hidden nodes
  - only pairwise interactions
  - binary valued nodes
  - constant node $X_0 \equiv 1$.

$$p(X, \Theta) = exp\left[\sum_{(j,k)\in E} \theta_{jk} X_j X_k - \Phi(\Theta)\right]$$

$$\Phi(\Theta) = log \sum_{x\in\mathcal{X}} \left[exp(\sum_{(j,k)\in E} \theta_{jk} X_j X_k)\right]$$

- Issing model implies a logistic form for each node conditional on the others

$$P(X_j = 1 | X_{-j} = x_{-j}) = \frac{1}{1 + exp(-\theta_{j0} - \sum_{(j,k)\in E} \theta_{jk} x_k)}$$

- Restricted Boltzmann machines
  - two layers, the visible and the hidden layer, no edges inside a layer - it is easier

Boltzmann machine learning

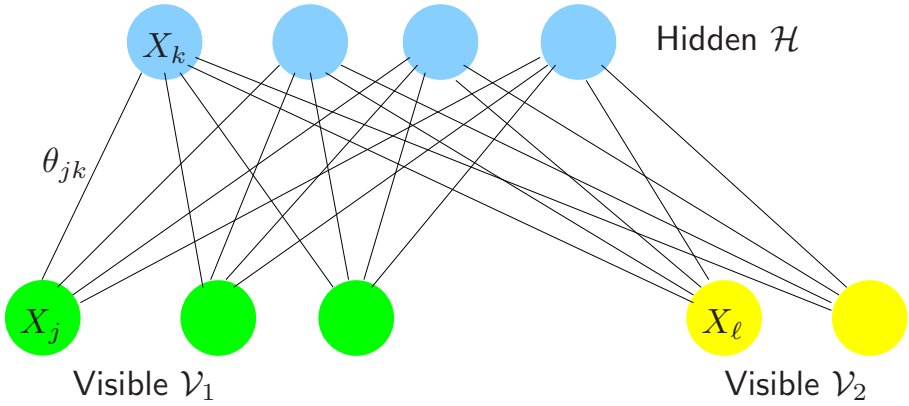
- Parameter learning
  - iteratively
  - for example Iterative proportional fitting IPF Jiroušek and Přeučil.
- Structure learning
  - for example Hoefling and Tibshirany: glasso extension to discrete Markov Networks.
  - still slow and not very precise.
- Restricted Boltzmann machine
  - fitting the model is faster due to the conditional independence.

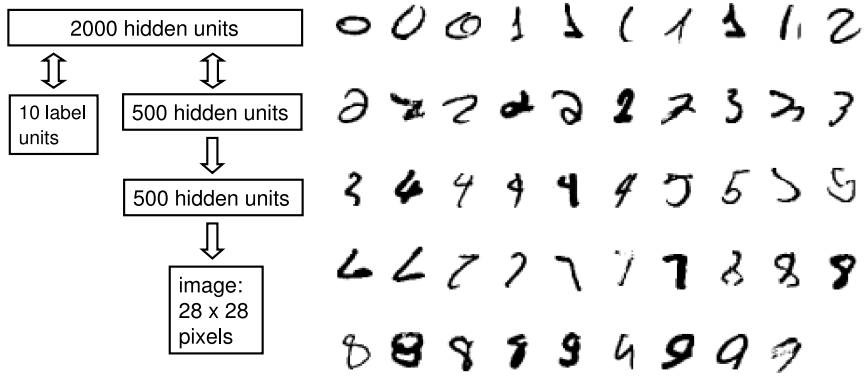
Restricted Boltzmann Machine Example (ESLII)

- Two layers:
- $\mathcal{V}$ a visible layer
- $\mathcal{H}$ a hidden layer
- no links inside a layer.

Example:

- $\mathcal{V}_1$ binary pixels of an image of a handwritten digit
- $\mathcal{V}_2$ 10 units for observed class labels 0-9
- more hidden layers in the lower figure.
- Fitted by **contrastive divergence** (not part of this lecture)
- or Gibbs sampling, but it is slow.





Markov Properties (Zeros are dangerous)

Definition (Markov properties: Global, Local, Pairwise)

Let G be an undirected graph over V, let P be a probability measure P over V.

(GM) P is **(globally) Markov** with respect to $\mathcal{G}$ iff

$$\forall(\mathcal{A},\mathcal{B}\in V,\mathcal{C}\subseteq V)\ \mathcal{A}\perp\!\!\!\perp_{\mathcal{G}}\mathcal{B}|\mathcal{C}\Rightarrow\mathcal{A}\perp\!\!\!\perp_{P}\mathcal{B}|\mathcal{C}\text{ in P.}$$

(LM) A probability measure has the **local Markov property** iff
$(\forall A\in V):\ A\perp\!\!\!\perp_{P} V\setminus Fa_A|N_A$

(PM) P has the **pairwise Markov property** iff $\forall A,B\in V, A\neq B$ not connected by an edge holds $A\perp\!\!\!\perp_{P} B|V\setminus\{A,B\}$.

Theorem

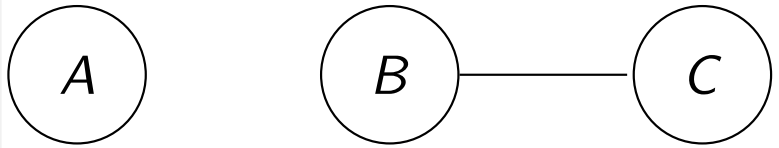
These properties are equivalent for strictly positive measures.

Counterexamples for measures with zero probability everywhere except $(0,0,0)$ and $(1,1,1)$.
See [Milan Studený:*Struktury podmíněné nezávislosti, Matfyzpress 2014*].

Examples

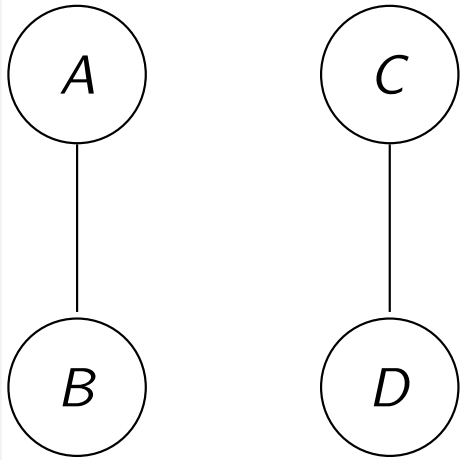
Example (P has the pairvise but not the local property)

$V = \{A, B, C\}, E = \{(b, c)\}$. Let us have a binary probability measure V nonzero at points $(0, 0, 0)$ and $(1, 1, 1)$ [Studený p.101].
$A \perp\!\!\!\perp B|\{C\}$
$A \perp\!\!\!\perp C|\{B\}$ & does not imply $A \perp\!\!\!\perp BC|\{\}$.



Example (P has the local but not the global property)

$V = \{A, B, C, D\}, E = \{(a, b), (c, d)\}$. Let $P(V)$ be nonzero only at points $(0, 0, 0, 0)$ and $(1, 1, 1, 1)$ [Studený p.101].
$A \perp\!\!\!\perp CD|\{B\}$
$B \perp\!\!\!\perp CD|\{A\}$
$C \perp\!\!\!\perp AB|\{D\}$ & does not imply $A \perp\!\!\!\perp C|\{\}$.
$D \perp\!\!\!\perp AB|\{C\}$



Linear Gaussian CPD

Definition (Linear Gaussian CPD)

For a variable Y with parents $X = X_1, \ldots, X_k$ the **Linear Gaussian model** is defined by the mean of Y and a linear function of X and the variance of Y does not depend on X.

```
from pgmpy.factors.continuous import LinearGaussianCPD
cpdY = LinearGaussianCPD('Y', [0.2, -2, 3, 7], 9.6, ['X1', 'X2', 'X3'])
cpdX1 = LinearGaussianCPD('X1', [0.2], 1, [])
```

- We may define **Gaussian Bayesian Networks**.
  - Usually, undirected models are used.
- **Mixed interactions models** Bayesian network with discrete and conditional Gaussian nodes; no descrete child of a gaussian parent
  - (generally, not a clear semantics).

Canonical Form of a Gaussian Distribution

Definition (Canonical Form of a Gaussian Distribution)

For a Gaussian Distribution $\phi(\mathbf{x}) = \frac{1}{\sqrt{|2\pi\Sigma|}} e^{-\frac{1}{2}(\mathbf{x}-\mu)\Sigma^{-1}(\mathbf{x}-\mu)}$ we define its **canonical form** $C(\mathbf{X}; K, h, g)$ where

- concentration matrix $K = \Sigma^{-1}$
- $h = K\mu$
- $g = -\frac{p}{2}\log(2\pi) + \frac{1}{2}log(|K|) - \frac{1}{2}\mu^T K\mu.$

- We can rewrite the join probability density to

$$\begin{aligned}
\phi(\mathbf{x}) &= (2\pi)^{-\frac{p}{2}}|K|^{\frac{1}{2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mu)K(\mathbf{x}-\mu)\right\} \\
&= (2\pi)^{-\frac{p}{2}}|K|^{\frac{1}{2}} \exp\left\{-\frac{1}{2}\mu^T K\mu + h^T\mathbf{x} - \frac{1}{2}\mathbf{x}^T K\mathbf{x}\right\} \\
&= \exp\left\{g + h^T\mathbf{x} - \frac{1}{2}\mathbf{x}^T K\mathbf{x}\right\} \\
&= \exp\left\{g + \Sigma_u h_u \mathbf{x}_u - \frac{1}{2}\Sigma_{u,v} K_{u,v}\mathbf{x}_u\mathbf{x}_v\right\}.
\end{aligned}$$

Gaussian Distribution Decomposition

Lemma

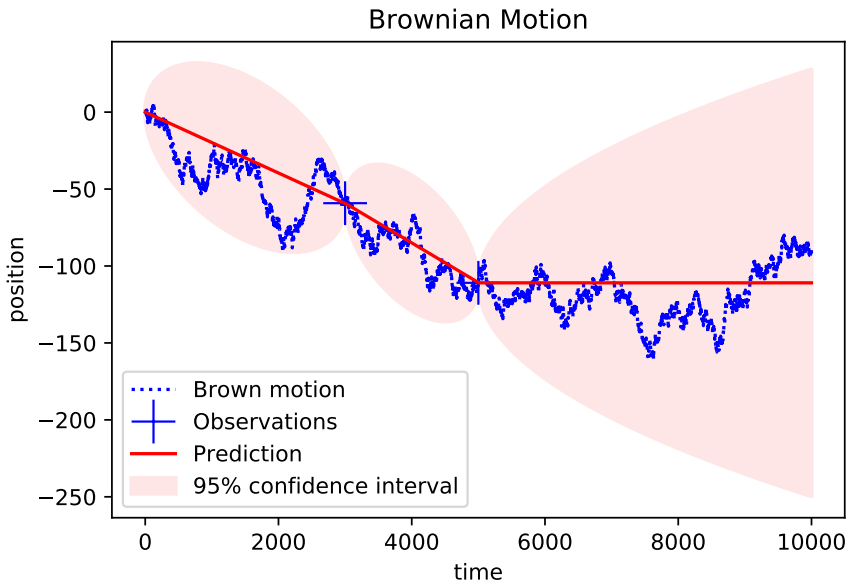
If the concentration matrix of a multivariate Gaussian distribution fulfills condition of a graph model then the distribution can be written as a product of distributions on cliques of the graph.

- $\phi(x) = \exp\left\{g + \Sigma_{u\in U} h_u \mathbf{x}_u - \frac{1}{2}\Sigma_{u,v} K_{u,v}\mathbf{x}_u\mathbf{x}_v\right\}$
- Let us have two sets of vertices A, B separated by the set C. Then $\forall u \in A, v \in B\ k_{uv} = 0$.
- We split the summation in the formula: $\phi(x) = \exp\left\{\begin{array}{c} g + \Sigma_{u\in A\cup C} h_u\mathbf{x}_u + \Sigma_{v\in B\cup C} h_v\mathbf{x}_v - \Sigma_{v\in C} h_v\mathbf{x}_v \\ -\frac{1}{2}(\Sigma_{u,v\in A\cup C} K_{u,v}\mathbf{x}_u\mathbf{x}_v + \Sigma_{u,v\in B\cup C} K_{u,v}\mathbf{x}_u\mathbf{x}_v - \Sigma_{u,v\in C} K_{u,v}\mathbf{x}_u\mathbf{x}_v)\end{array}\right\}$
- therefore $\phi(x) = g(A, C)h(C, B)$.

$$\begin{array}{c|ccc|} & A & C & B \\ A & K_{AA} & K_{AC} & \\ C & K_{AC} & K_{CC} & K_{CB} \\ B & & K_{BC} & K_{BB} \end{array}$$

Gaussian Processes

- An infinite (continuous) number of Gaussian variables
- to any value x a new variable $N(\mu = f(x), \Sigma_{x|rest})$
- we have only a finite number of observations which means a finite number of variables
  - we can marginalize unobserved variables out (the integral is 1, we multiply by 1, we just remove),
- we can predict at any x, continuously.



Gaussian Processes

C. E. Rasmussen & C. K. I. Williams, Gaussian Processes for Machine Learning, the MIT Press, 2006

Definition (Gaussian Process)

A Gaussian process is a set of random variables where any finite subset follows multivariate Gaussian distribution.

We define the mean $m(x)$ and the symmetric positive semidefinite covariance function $k(x, x^{|})$:

$$\begin{aligned} m(\mathbf{x}) &= \mathbb{E}[f(\mathbf{x})] \\ k(\mathbf{x}, \mathbf{x}^{|}) &= \mathbb{E}[(f(\mathbf{x}) - m(\mathbf{x}))(f(\mathbf{x}^{|}) - m(\mathbf{x}^{|}))] \end{aligned}$$

a Gaussian process is

$$f(\mathbf{x}) = \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}^{|})).$$

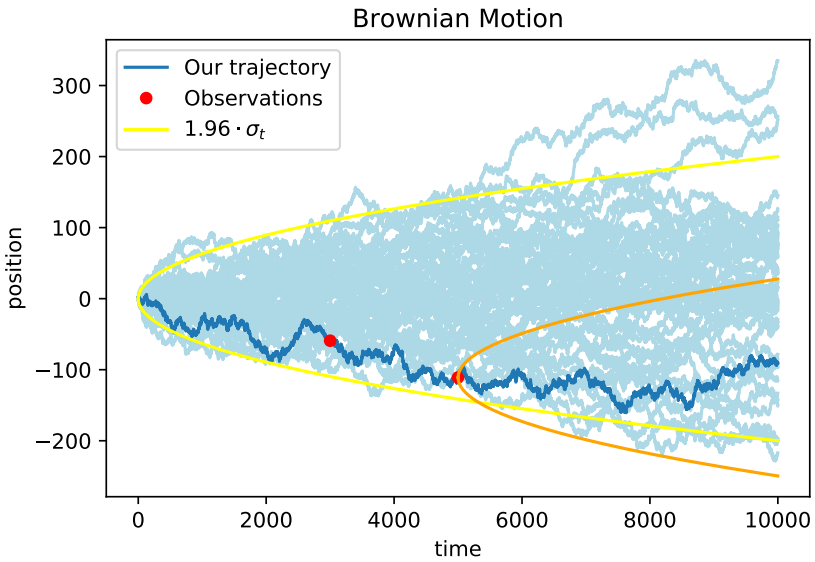
We assume $m(\mathbf{x}) = \mathbf{0}$ it simplifies the formulas.

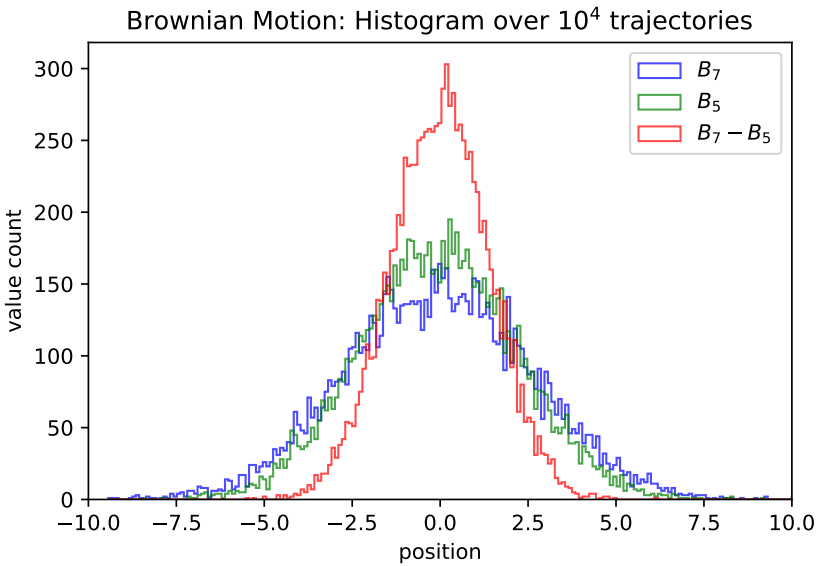
Brownian Motion (Wiener Process)

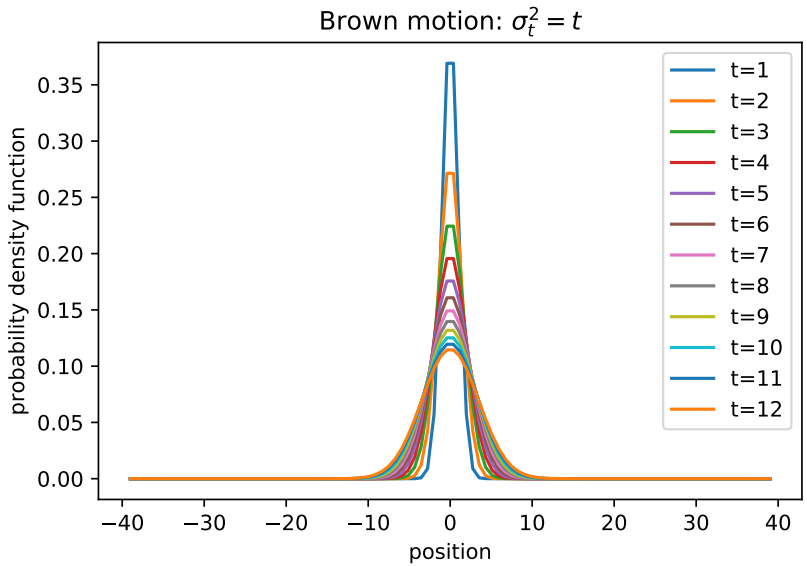
https://www.coursera.org/lecture/stochasticprocesses/week-4-6-two-definitions-of-a-brownian-motion-THRqL

Definition (Brownian motion 1)

- $B_0 = 0$ for sure
- stationary and independent increments
- $B_s - B_t \sim N(0, s - t)$







Definition (Brownian motion 1)

- $B_0 = 0$ almost surely
- B_t stationary and independent increments
- $B_s - B_t \sim N(0, s-t)$

Definition (Brownian motion 2)

Gaussian process with

- $m = 0$ and
- $k(x, x') = min(x, x')$.

Positive semidefinite:

- $min(t, s) = \int_0^\infty f_t(x) f_s(x) dx$
- $f_t(x) f_s(x) = 1$ iff $x \in [0, t] \& x \in [0, s]$

Lemma (2⇒1)

- $K(0,0) = min(0,0) = 0$
- *The process has variance 0 at* $t = 0$ *and* $m(0) = 0$.
- *covariance is linear in both arguments,* $s \geq t$

$$\begin{aligned} cov(B_s - B_t, B_s - B_t) &= cov(B_s, B_s) - cov(B_t, B_s) - cov(B_s, B_t) + cov(B_t, \\ &= s - 2t + t = s - t \end{aligned}$$

- *increments,* $s \geq t \geq b \geq a$ *# independence skipped, from Gaussian vectors*

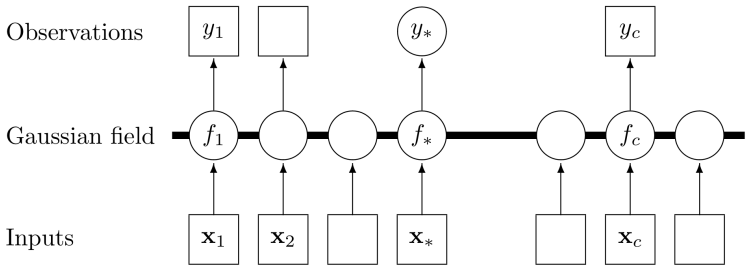
$$\begin{aligned} cov(B_b - B_a, B_s - B_t) &= cov(B_b, B_s) - cov(B_a, B_s) - cov(B_b, B_t) + cov(B_a, B_t) \\ &= b - a - b + a = 0. \end{aligned}$$

Normal Distribution

Definition (Brownian motion 2)

Gaussian process with

- $m = 0$ and
- $k(x, x') = min(x, x')$.



- The covariance on $\mathbf{y}$ is defined by the covariance on the inputs $\mathbf{x}$.
- the covariance defines also the distribution on functions f:

$$\mathbf{f}_* \sim N(\mathbf{0}, K(X_*, X_*)).$$

- Without noise, we observe $\mathbf{y}$ and we want to predict $\mathbf{f}_*$:

$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_* \end{bmatrix} \sim N\left(\mathbf{0}, \begin{bmatrix} K(X, X) & K(X, X_*) \\ K(X_*, X) & K(X_*, X_*) \end{bmatrix}\right)$$

X=[3,7]
y^T=[0.5, 1.11]
K(xs,X)=[min(xs,a) for a in X]

$$K(X, X) = \begin{bmatrix} min(3,3) & min(3,7) \\ min(3,7) & min(7,7) \end{bmatrix} = \begin{bmatrix} 3 & 3 \\ 3 & 7 \end{bmatrix}$$

Prediction

- noisy-free observations $y = f(\mathbf{x})$

$$cov(y_p, y_q) = k(\mathbf{x}_p, \mathbf{x}_q)$$

- noisy observations $y = f(\mathbf{x}) + \epsilon$, $\epsilon \sim N(0, \sigma_n^2)$

$$\begin{aligned} cov(y_p, y_q) &= k(\mathbf{x}_p, \mathbf{x}_q) + \sigma_n^2 \delta_{pq} \\ cov(\mathbf{y}) &= K(X, X) + \sigma_n^2 I \end{aligned}$$

- We observe $\mathbf{y}$ and we want to predict $\mathbf{f}_*$:

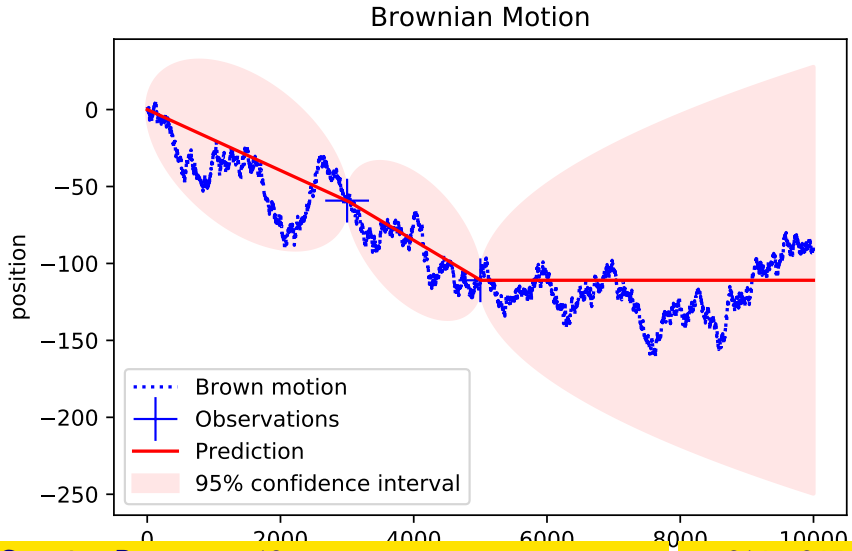
$$\begin{bmatrix} \mathbf{y} \\ \mathbf{f}_* \end{bmatrix} \sim N\left(\mathbf{0}, \begin{bmatrix} K(X, X) + \sigma_n^2 I & K(X, X_*) \\ K(X_*, X) & K(X_*, X_*) \end{bmatrix}\right)$$

- Predictive distribution

$$\begin{aligned} \mathbf{f}_* | X, \mathbf{y}, X_* &\sim N(\bar{\mathbf{f}}_*, cov(\bar{\mathbf{f}}_*)) \\ \bar{\mathbf{f}}_* &\triangleq \mathbb{E}[\mathbf{f}_* | X, \mathbf{y}, X_*] = K(X_*, X)[K(X, X) + \sigma_n^2 I]^{-1} \mathbf{y} \\ cov(\mathbf{f}_*) &= K(X_*, X_*) - K(X_*, X)[K(X_*, X) + \sigma_n^2 I]^{-1} K(X, X_*) \end{aligned}$$

$$
\begin{aligned}
\mathbf{f}_*|X,\mathbf{y},X_* &\sim N(\bar{\mathbf{f}}_*, cov(\bar{\mathbf{f}}_*)) \\
\bar{\mathbf{f}}_* &\triangleq \mathbb{E}[\mathbf{f}_*|X,\mathbf{y},X_*] = K(X_*,X)[K(X,X)+\sigma_n^2 I]^{-1}\mathbf{y} \\
cov(\mathbf{f}_*) &= K(X_*,X_*) - K(X_*,X)[K(X_*,X)+\sigma_n^2 I]^{-1}K(X,X_*)
\end{aligned}
$$

$$
\begin{aligned}
\bar{\mathbf{f}}_* &\triangleq \mathbb{E}\left[\mathbf{f}_*|\begin{bmatrix}3\\7\end{bmatrix},\begin{bmatrix}0.5\\11\end{bmatrix},[4]\right] = [3,4]\begin{bmatrix}3+\sigma_n^2 & 3\\ 3 & 7+\sigma_n^2\end{bmatrix}^{-1}\begin{bmatrix}0.5\\11\end{bmatrix} \\
cov(\mathbf{f}_*) &= min(4,4) - [3,4]\begin{bmatrix}3+\sigma_n^2 & 3\\ 3 & 7+\sigma_n^2\end{bmatrix}^{-1}\begin{bmatrix}3\\4\end{bmatrix}
\end{aligned}
$$

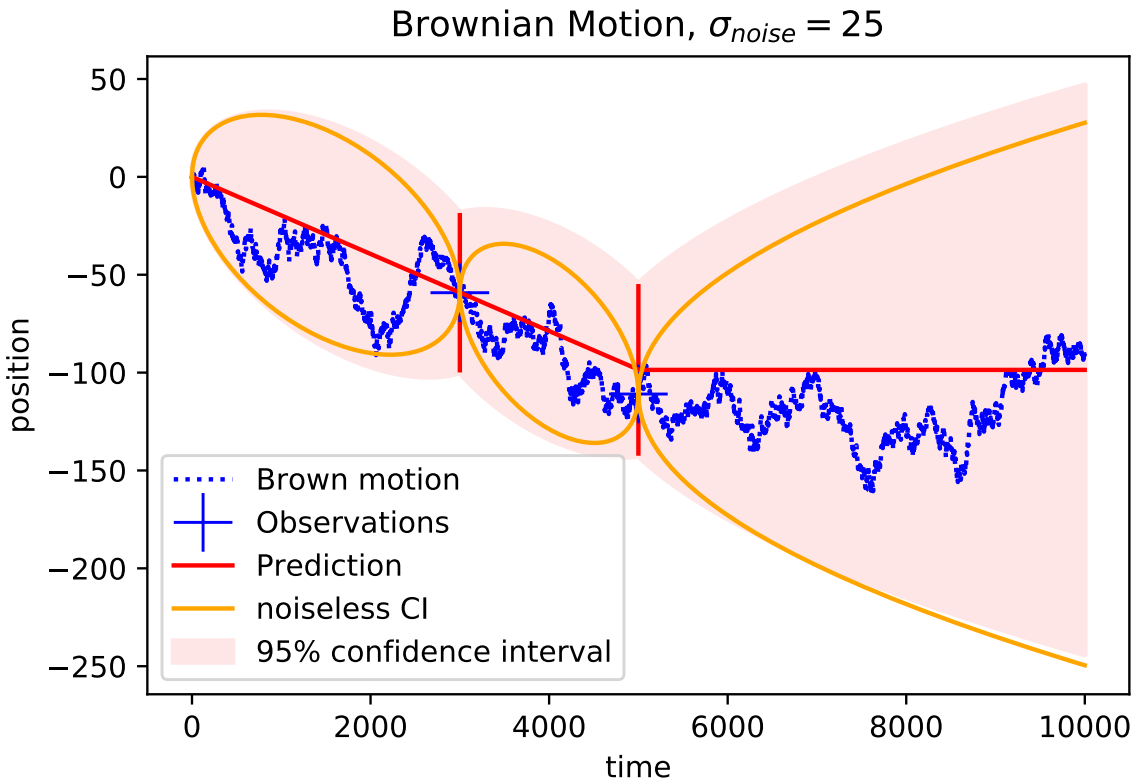


Predictive distribution

Prediction

- is a linear function of observations $\mathbf{y}$
  - for $\alpha \Leftarrow (K + \sigma_n^2 I)^{-1}\mathbf{y}$
  - we predict $\overline{f}(\mathbf{x}_*) \Leftarrow \sum_{i=1}^{N} \alpha_i k(\mathbf{x}_i, \mathbf{x}_*)$

- The red vertical bars show the variance due to the observation noise.



Definition (First Set of Kernel Functions)

- **Radial Basis Function (RBF)** covariance function with the **length scale** parameter ℓ is defined

$$cov(f(\mathbf{x}_p), f(\mathbf{x}_q)) = RBF(\mathbf{x}_p, \mathbf{x}_q) = \exp\left(-\frac{1}{2}\frac{|\mathbf{x}_p - \mathbf{x}_q|^2}{\ell^2}\right).$$

- **Constant** covariance function with the **constant** parameter is defined

$$cov(f(\mathbf{x}_p), f(\mathbf{x}_q)) = Constant(\mathbf{x}_p, \mathbf{x}_q) = constant.$$

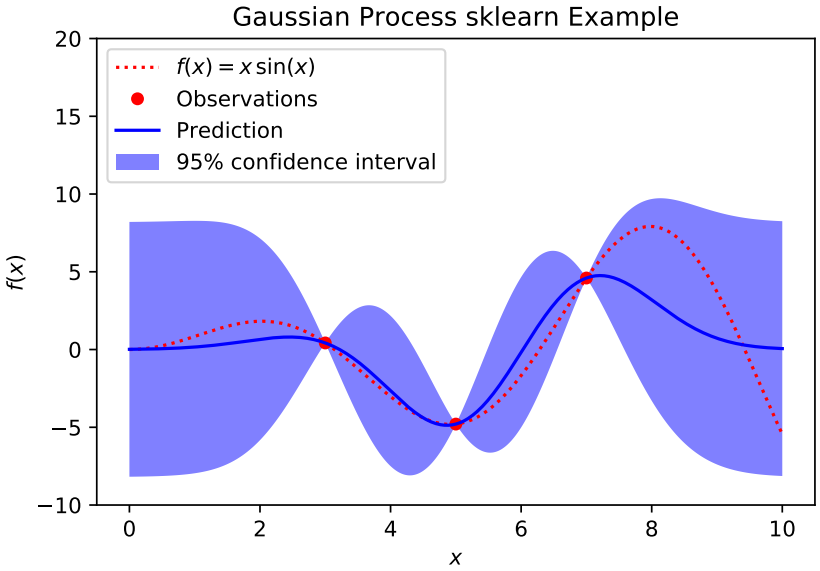
- **Squared exponential (SE)** covariance function with hyperparameters ℓ^2 lenghtscale and σ_f^2 signal variance

$$\begin{aligned} k(\mathbf{x}_p, \mathbf{x}_q) &= \sigma_f^2 \exp\left(-\frac{1}{2}\frac{|\mathbf{x}_p - \mathbf{x}_q|^2}{\ell^2}\right) \\ &= Constant(\mathbf{x}_p, \mathbf{x}_q) * RBF(\mathbf{x}_p, \mathbf{x}_q) \end{aligned}$$

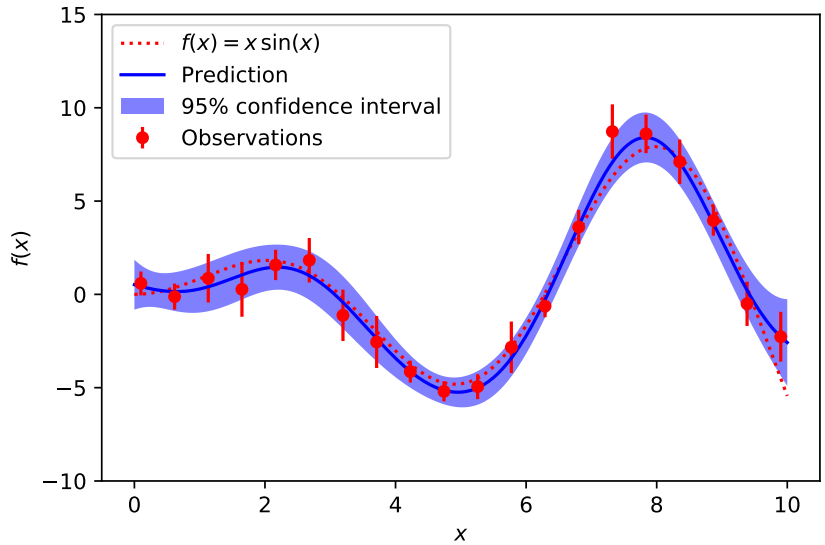
- can be defined as a **product kernel** of the Constant and RBF kernels.
- There is also a **sum kernel** kernel function $+$.

Scikitlearn Examples

- Noiseless observations.



- The red vertical bars show the variance due to the observation noise.



- The parameters may be fitted by the gradient update.
- The observation noise *alpha* may be specific for each observation (right), identically 0 (left) or constant.

```
kernel = C(1.0, (1e-3, 1e3)) * RBF(10, (100e-2, 100e2))
gp = GaussianProcessRegressor(kernel=kernel, alpha=dy ** 2)
gp.fit(X, y)
```

Marginal likelihood

- The parameters may be automatically tuned by gradiently maximize the marginal likelihood.
- 'In sample' prediction $\mathbf{f}$ follows: $\mathbf{f} \sim N(\mathbf{0}, K(X, X))$.

Lemma

The marginal log likelihood is

- *for noisy-free observations* $\mathbf{y} = \mathbf{f}$*:*

$$\log p(\mathbf{y}|X) = \log p(\mathbf{f}|X) = -\frac{1}{2}\mathbf{f}^T K^{-1}\mathbf{f} - \frac{1}{2}\log|K| - \frac{N}{2}\log 2\pi$$

- *For noisy observations* $\mathbf{y}|\mathbf{f} \sim N(\mathbf{f}, \sigma_n^2 I)$, $\mathbf{y} \sim N(0, K + \sigma_n^2 I)$

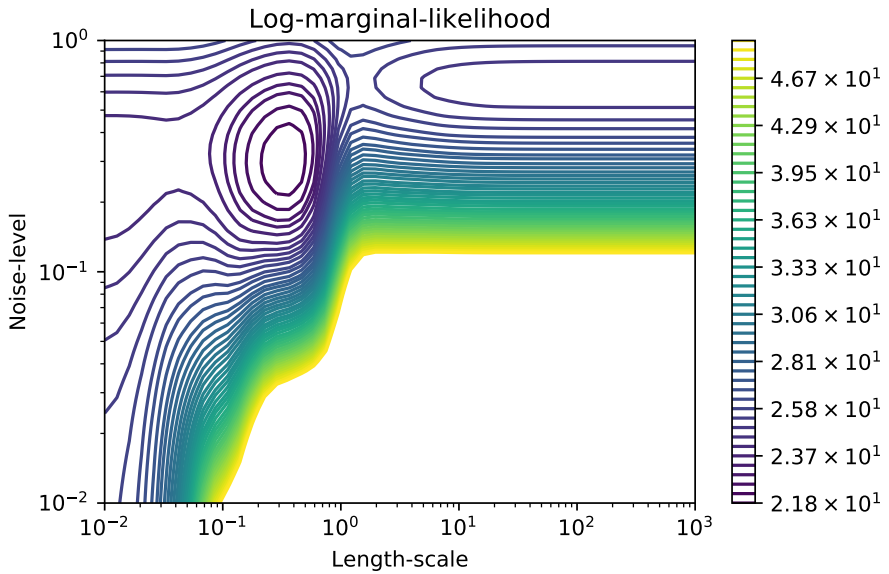
$$\log p(\mathbf{y}|X) = -\frac{1}{2}\mathbf{y}^T(K + \sigma_n^2 I)^{-1}\mathbf{y} - \frac{1}{2}\log|K + \sigma_n^2 I| - \frac{N}{2}\log 2\pi.$$

The noise level may be tuned as well by (sum)adding the **WhiteKernel**. **WhiteKernel**= *noise_level* iff we address the same variable $(\mathbf{x}_p, \mathbf{x}_p)$, otherwise *WhiteKernel* $= 0$.

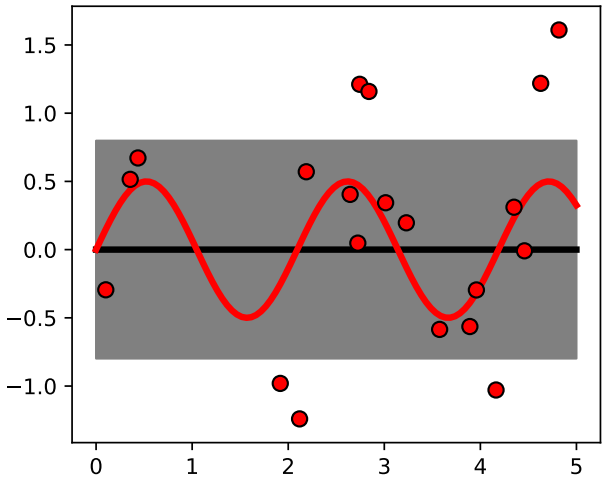
Hyperparameter Fit

Scikitlearn example:

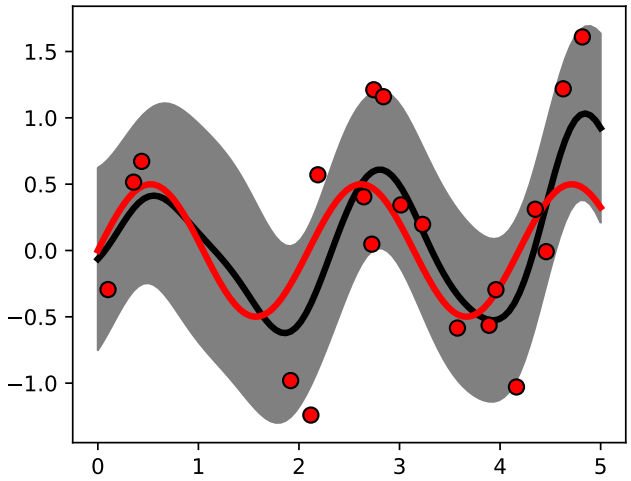
- The log-marginal function has two local maxima.
- The log-marginal maxima corresponds to the two models.



Initial: 1**2 * RBF(length_scale=100) + WhiteKernel(noise_level=1)
ıum: 0.00316**2 * RBF(length_scale=109) + WhiteKernel(noise_level=0
Log-Marginal-Likelihood: -23.87233736198489



Initial: 1**2 * RBF(length_scale=1) + WhiteKernel(noise_level=1e-05)
mum: 0.64**2 * RBF(length_scale=0.365) + WhiteKernel(noise_level=0.
Log-Marginal-Likelihood: -21.80509089016203



Definition (Further Kernel Functions)

- **ExpSineSquared** kernel function with the parameters **length scale** ℓ and the **periodicity** $p > 0$ (d is the distance) is defined

$$cov(f(\mathbf{x}_q), f(\mathbf{x}_r)) = \exp\left(-\frac{2\sin^2(\pi d(\mathbf{x}_q, \mathbf{x}_r)/p)}{\ell^2}\right).$$

  Usefull for periodic functions.

- **Dot product** kernel function with the **inhomogenicity** parameter σ_0 is defined

$$cov(f(\mathbf{x}_p), f(\mathbf{x}_q)) = \sigma_0 + \mathbf{x}_p \cdot \mathbf{x}_q.$$

  Useful to capture the trend, often combined with exponential kernel.

- **Rational Quadratic** kernel function with hyperparameters ℓ^2 lenghtscale and mixture α

$$k(\mathbf{x}_p, \mathbf{x}_q) = \left(1 + \frac{d(\mathbf{x}_p, \mathbf{x}_q)^2}{2\alpha\ell^2}\right)^{-\alpha}$$

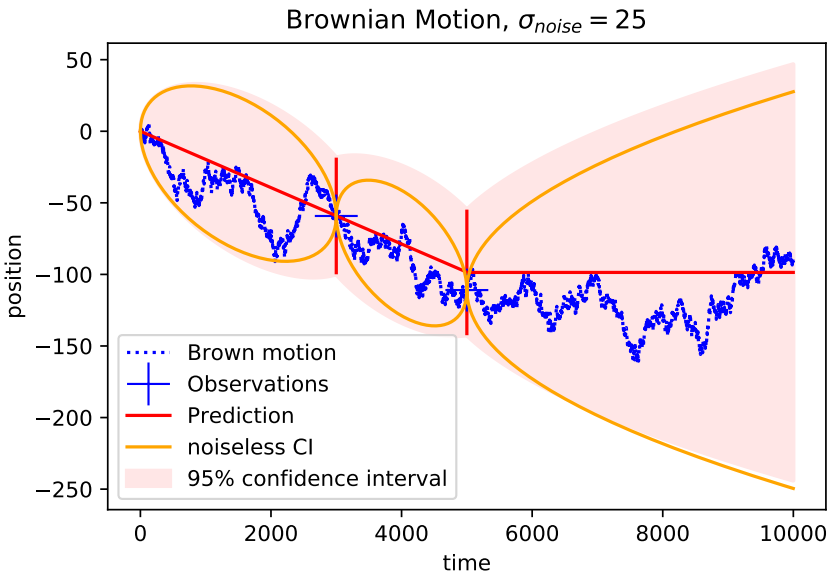
  The mixure of many RBF kernel lengthscales.

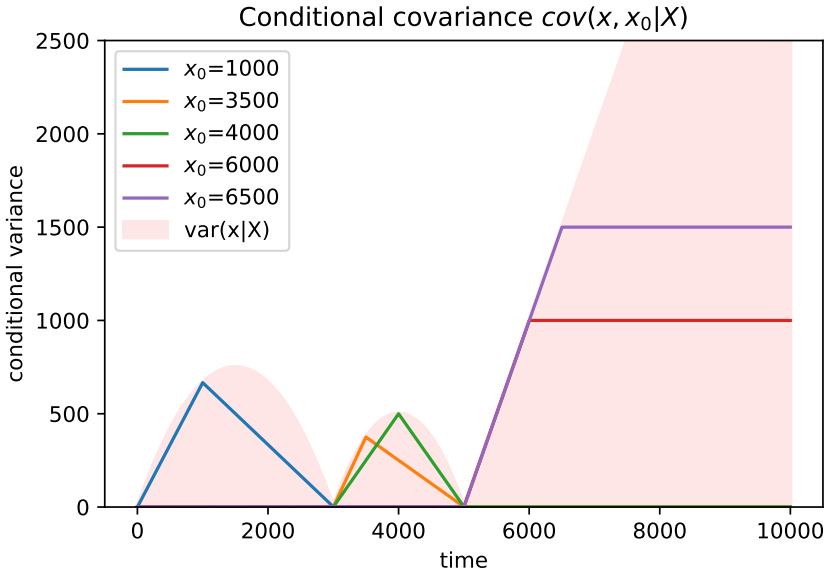
Conditional Covariance

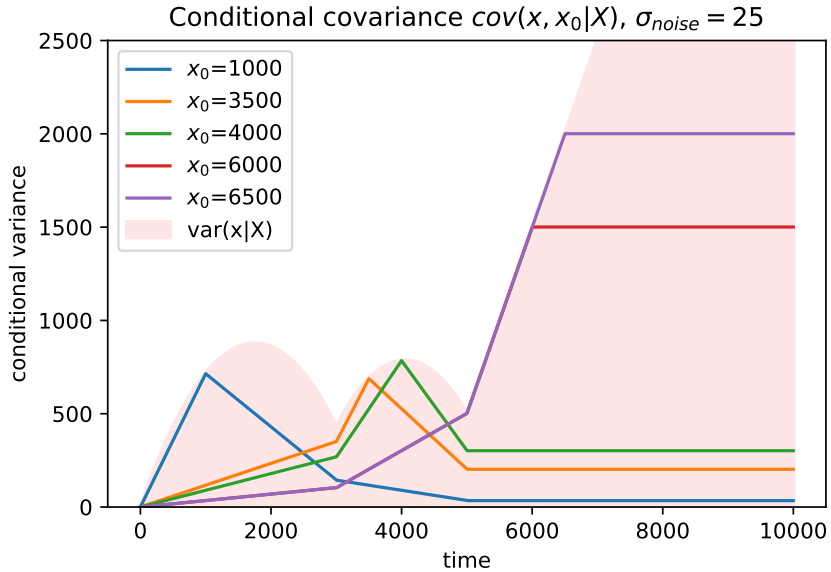
- Consider the conditional covariance, the relation of two unobserved points x and x_0.

left Noiseless Brown motion example. The covariance is zero outside the x_0 closest observations interval.

right Brown motion with a high noise level.

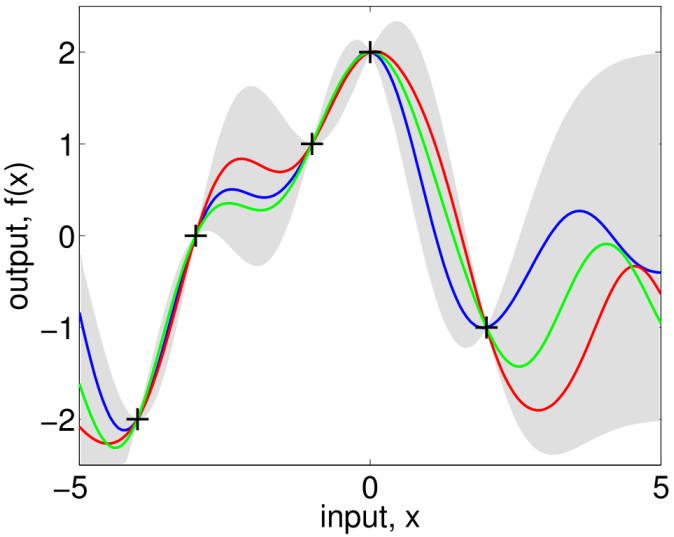




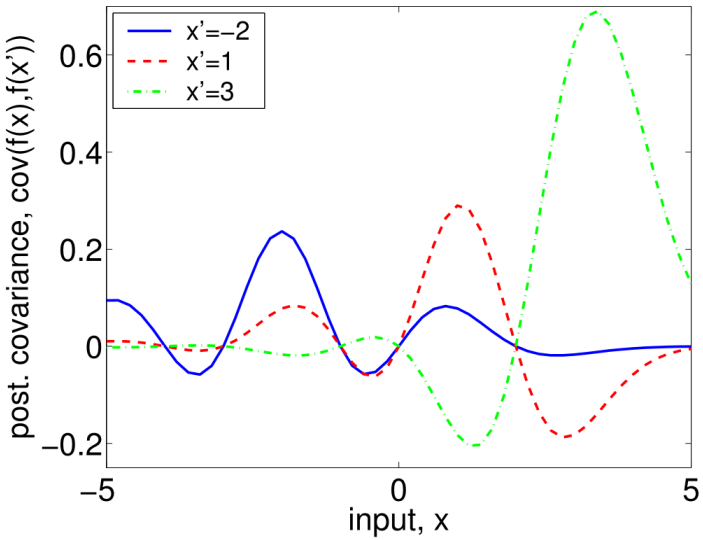


Conditional Covariance Rassmussen Example

- The conditional covariance may be also negative.
- Most kernels have a continuous first derivative. This makes the conditional covariance negative with points on the other side of the closest observation.



(a), posterior



(b), posterior covariance

Matérn

- Most kernel function have many derivatives.
- The Matérn kernel $\nu = 1.5$ ('nu') has only the first derivative. It is able to model less smooth functions.
- As $\nu \to \infty$, it becomes a RBF kernel.

Definition (Matérn kernel)

The **Matérn** kernel with parameters $\nu = k + \frac{1}{2}$ and ℓ is defined

$$k(\mathbf{x}_p, \mathbf{x}_q) = \frac{1}{2^{\nu-1}\Gamma(\nu)} \left(\frac{\sqrt{2\nu}}{\ell} d(\mathbf{x}_p, \mathbf{x}_q) \right)^{\nu} K_\nu \left(\frac{\sqrt{2\nu}}{\ell} d(\mathbf{x}_p, \mathbf{x}_q) \right)$$

The **Modified Bessel functions** (for α not integer, the limit otherwise) are defined

- $I_\alpha(x) = \sum_{m=0}^{\infty} \frac{1}{m!\Gamma(m+\alpha+1)} \left(\frac{x}{2}\right)^{2m+\alpha}$
- $K_\alpha(x) = \frac{\pi}{2} \frac{I_{-\alpha}(x) - I_\alpha(x)}{sin\alpha\pi}$.

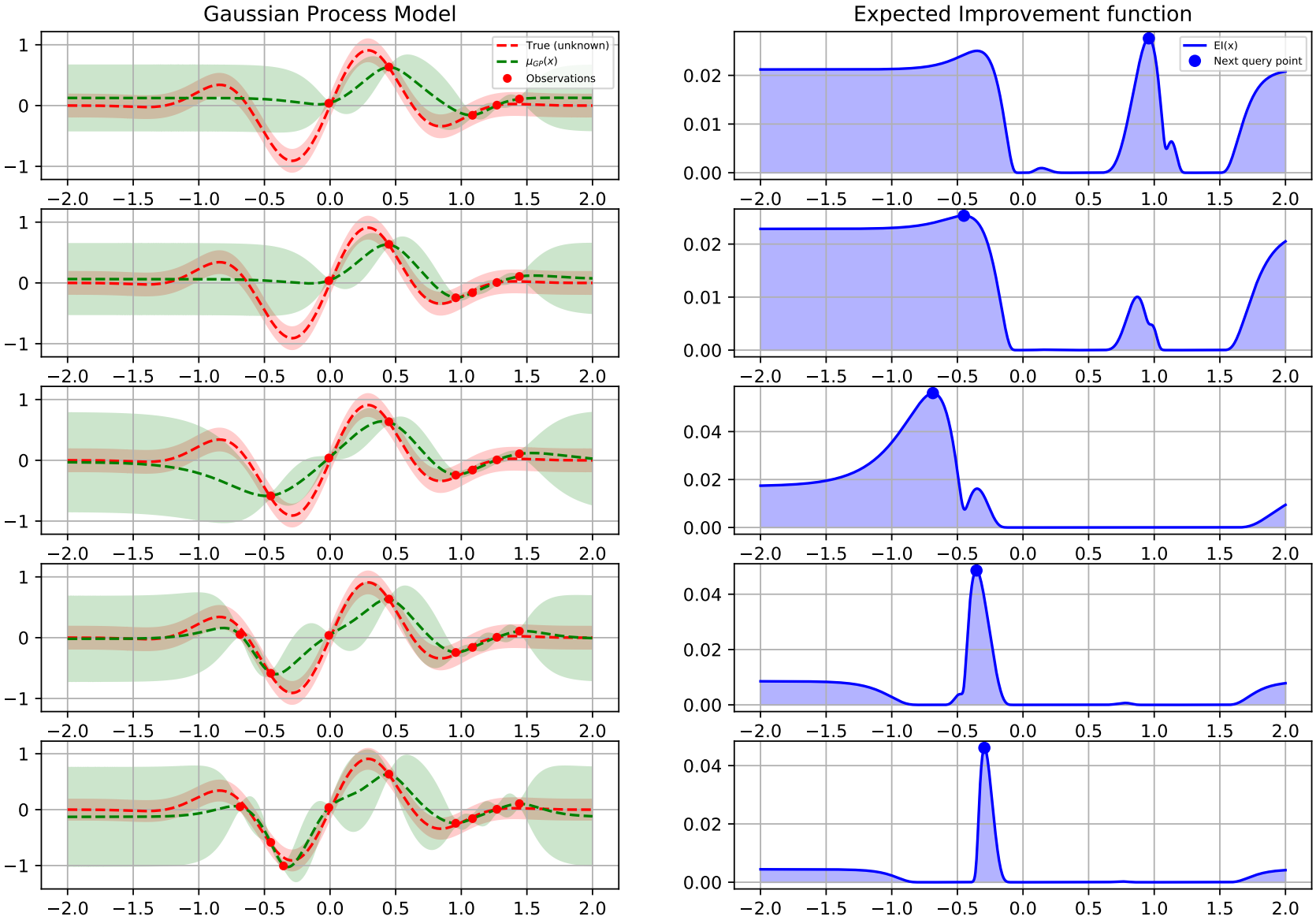
Bayesian Optimization

- Bayesian Optimization is used when
  - We are solving: $x^* = \arg\min_x f(x)$
  - $f(x)$ is a black box function
  - f is expensive to evaluate
  - the evaluations may be noisy.
- If any condition is not true, a better algorithm exists.
- We search the point **x** to observe.
- scikit-optimize = skopt Python package
- we minimize **y** and search the maximal probability of improvement
- 'the chance to improve' is expressed by the **Expected improvement** (EI)

Bayesian Optimization Algorithm

- Evaluate **y** on X, let $\mathbf{y} = y(X)$ and calculate conditional means and covariances
- repeat forever
  - $x^{new} = argmax_x EI(x)$ add x into X
  - Evaluate $\mathbf{y} = y(x)$ and add y to **y**.
  - re–estimate the Gaussian process (the parameters of the covariance).

Bayesian Optimization Example [Skopt]



Expected Improvement Aquisition Function

- we search the point **x** to observe
- we minimize y, we already have the training data X,**y**
- the search the maximal probability of improvement is expressed by the **Expected improvement** (EI)

$$\begin{aligned} EI(x) &= \mathbb{E}[(min(Y(X)) - Y(x))^+ | Y(X) = \mathbf{y}] \\ &= \mathbb{E}[(min(\mathbf{y}) - Y(x))^+ | Y(X) = \mathbf{y}] \end{aligned}$$

this can be solved analytically (Φ cummulative df, ϕ pdf Gaussian distribution):

$$EI(x) = (min(\mathbf{y}) - \mu(x))\Phi\left(\frac{min(\mathbf{y}) - \mu(x)}{\sigma(x)}\right) + \sigma(x)\phi\left(\frac{min(\mathbf{y}) - \mu(x)}{\sigma(x)}\right)$$

to maximize **y**:

$$EI(x) = (\mu(x) - max(\mathbf{y}))\Phi\left(\frac{\mu(x) - max(\mathbf{y}) - \xi}{\sigma(x)}\right) + \sigma(x)\phi\left(\frac{\mu(x) - max(\mathbf{y}) - \xi}{\sigma(x)}\right).$$

- if 'xi' $\xi > 0$ we ignore small improvements.

Paralelization: The Constant Liar

$$\begin{aligned} EI(x) &= \mathbb{E}[(min(Y(X)) - min(Y(x^{(n+1)}), Y(x^{(n+2)}), \ldots, Y(x^{(n+k)})))^+ | Y(X) = \mathbf{y} \\ &= \mathbb{E}[(min(\mathbf{y}) - Y(x))^+ | Y(X) = \mathbf{y}] \end{aligned}$$

it does not have direct formula. It is solved by Markov Chain simulation.

- We estimate the observations y by an estimate (min, max, mean)
- and run the evaluation in parallel.

That means the covariance is correctly estimated, the mean must be corrected later.

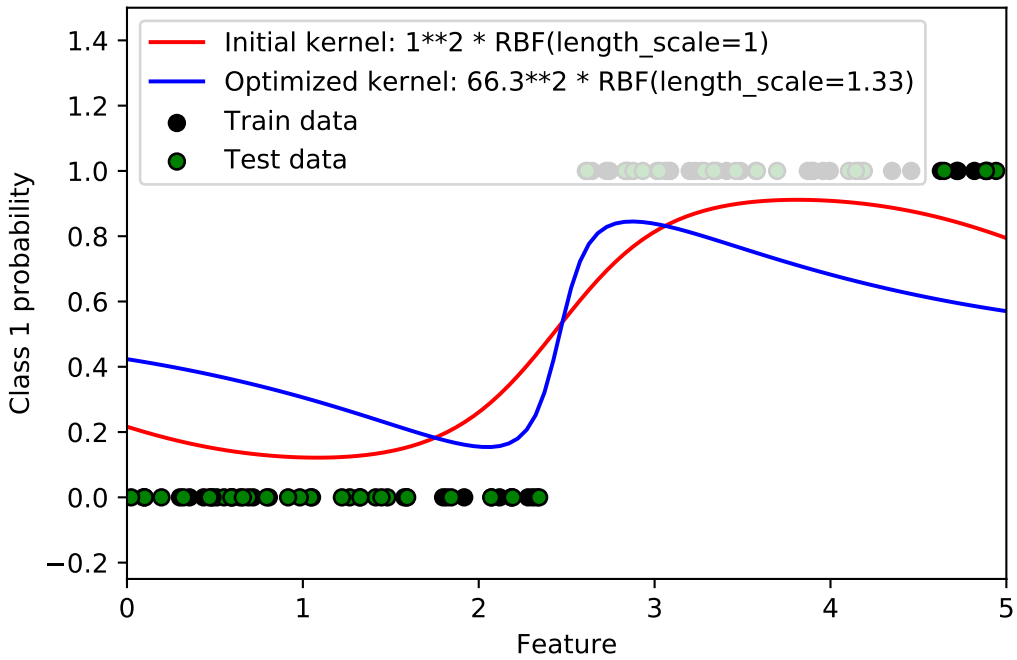
ParBayesianOptimization R package

Definition (Other Aquisition Functions)

- Probability of Improvement: $PI(f(x_*) < min(\mathbf{y})) = \Phi\left(\frac{min(\mathbf{y}) - \mu(x_*)}{\sigma(x_*)}\right)$
- Lower Confidence Bound: $LCB(x) = \mu(x) - \kappa \cdot \sigma(x)$.

GP for Classification

- GP for classification are more complex and 'only an approximation'
- still, it is worth to try the `sklearn.gaussian_process.GaussianProcessClassifier` .
- We estimate a latent function f as before
- we link it to $\langle 0, 1 \rangle$ interval by the sigmoid function (or Φ).
- The log-marginal-likelihood does not have a closed analytical form anymore.
- can be approximated by Hessian matrix, the algorithm works in $O(N^3)$, not too bad.

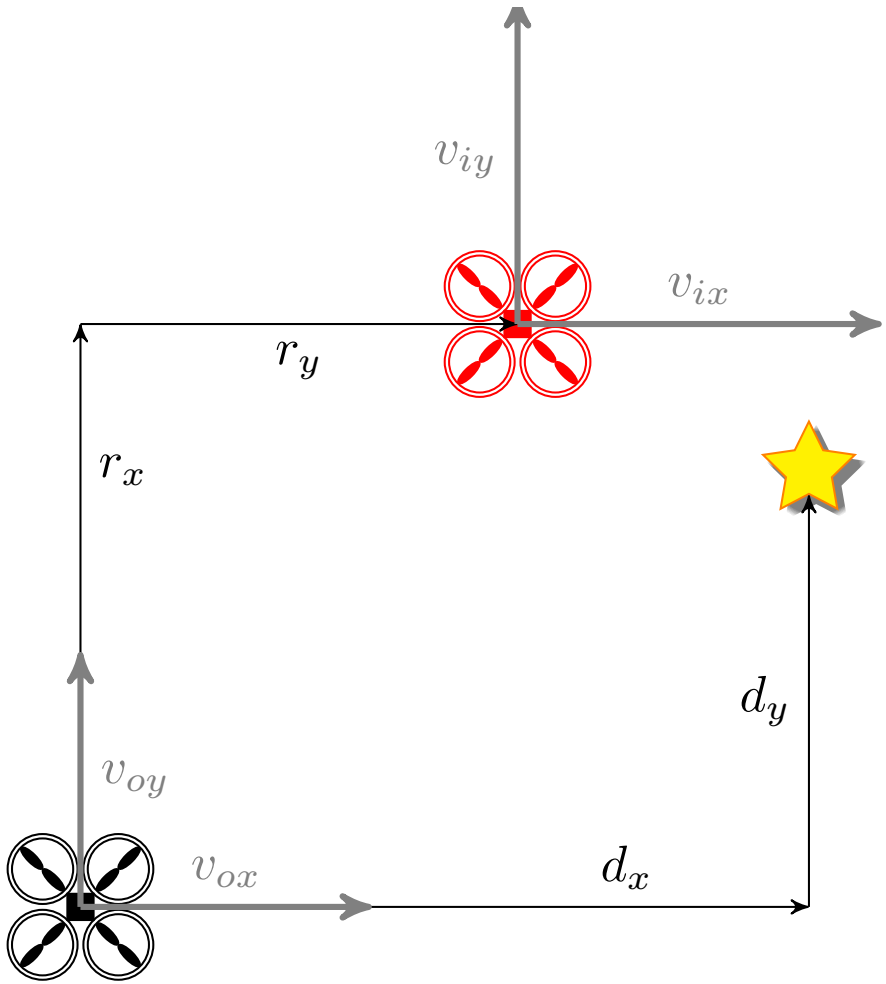


POMDP Applications

- Karkus, Hsu, Lee: **QMDP-Net: Deep Learning for Planning under Partial Observability**
  https://proceedings.neurips.cc/paper/2017/file/e9412ee564384b987d086df32d4Paper.pdf
- Eric Mueller and Mykel J. Kochenderfer :**Multi-Rotor Aircraft Collision Avoidance using Partially Observable Markov Decision Processes**, American Institute of Aeronautics and Astronautics
  https://aviationsystemsdivision.arc.nasa.gov/publications/2016/AIAA-2016-3673.pdf

POMDP Aircraft Collision Avoidance

- the algorithms designed for fixed-wing aircraft analyze
  - turns
  - vertical meneuvers
- multirotor aircraft (drones) and helicopters can also
  - horizontal plane accelerations
- state 2D, (3D)
  - relative range states r_x, r_y, (r_z)
  - velocities for the ownship v_{ox}, v_{oy}, (v_{oz})
  - velocities for the intruder v_{ix}, v_{iy}, (v_{iz})
  - absolute displacement from the desired trajectory d_x, d_y, (d_z)
  - the desired trajectory is normalized to unit velocity in the $x$axis and zero velocity in the y axis.



MDP Transitions

- the prediction horizon is very short
- updates done every 0.1 to 1 seconds
- simple update equation are sufficient
- not a benefit to using more complex dynamic equations.
- a_x, a_y acceleration by the ownship
- N_* noise to the ownship, intruder, x and y axis
  - $N_o(\mu = 0, 0.30s^{-2})$, $N_i(\mu = 0, 0.45s^{-2})$,
- Bellman update

  transition from s with acceleration a to $s^|$

$$Q[s,a] \leftarrow R(s,a) + \gamma \sum_{s^|} T(s^||s,a) max_{a^|} Q[s^|, a^|].$$

$$\begin{aligned}
\dot{r}_x &= v_{ix} - v_{ox} \\
\dot{r}_y &= v_{iy} - v_{oy} \\
\dot{v}_{ox} &= a_x + N_{ox} \\
\dot{v}_{oy} &= a_y + N_{oy} \\
\dot{v}_{ix} &= N_{ix} \\
\dot{v}_{iy} &= N_{iy} \\
\dot{d}_x &= v_{tx} - v_{ox} \\
\dot{d}_y &= v_{ty} - v_{oy}
\end{aligned}$$

Reward

- Minimum reward R_{min}
  - collision
  - physically impossible states
  - keeps the sum finite
- we prefer no acceleration
- we prefer long distance to the intruder
- we prefer short distance to the desired trajectory
- K_s, K_T, R_{min} weights was learned, k weights was $= 1$.

$$R(s,a) = max\left[R_{min}, -(k_{ax}|a_x| + k_{ay}|a_y|) - K_s\frac{1}{k_{rx}r_x^2 + k_{ry}r_y^2} - K_T(k_{dx}d_x^2 + k_{dy}d_y^2)\right]$$

QMDP Approximation

- offline optimization
  - a few hours for coarse discretization, 1 PC
  - initially stationary intruders
  - intruders moving at uniform velocity with a variety of relative headings angles
  - intruders state and dynamic uncertainty were added to the encounters.
- all values normalized
  - the coarse set contained a total of 765,625 discrete states
  - the finely discretized version contained 9,529,569 states.

State variable	State Description	Discretization
r_x, r_y	Intruder range components	$-15, [-7, -3], -1, 0, 1, [3, 7], 15$
v_{ox}, v_{oy}	ownship velocity components	$-5, -3, -1, 0, 1, 3, 5\ s^{-1}$
v_{ix}, v_{iy}	intruder velocity components	$-5, [-3], -1, 0, 1, [3], 5\ s^{-1}$
d_x, d_y	desired trajectory distance	$-10, [-3], -1, 0, 1, [3], 10$

Evaluation Function

- The primary goal is to remain safely separated from the intruder aircraft.
  - $r_{5\%CPA}$ 'the closest point of approach', we allow 5% trajectories a little bit closer.
- Figure: required 1.5 units, never closer than 1.1 units.
- Mean deviation distance from the desired trajectory μ_{dev}.

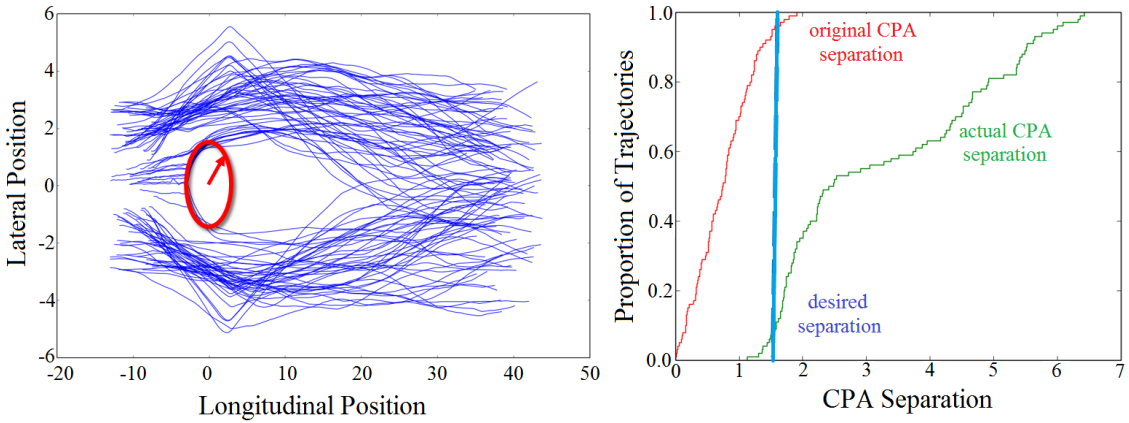
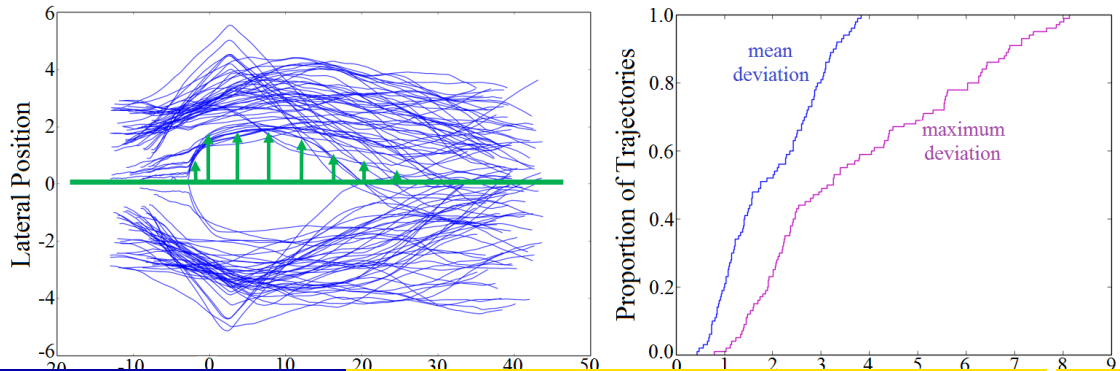


Figure 3: Separation metric used to evaluate the collision avoidance algorithm



Reward Tuning – Bayesian Optimization

- We tune $R_P = (K_T, K_s, R_{min})$
- β weights the two objective functions

$$F(R_P) = (\beta \times (r_{5\%CPA})^{-1} + (1-\beta) \times \mu_{dev}).$$

- Gaussian process models $F(R_P)$.
- We determine the point at which the objective function is expected to have the largest improvement, $E[I(F(R_P))]$ over that of the current minimum.
- This set of R_P is passed to QMDP to evaluate.
- until convergence.

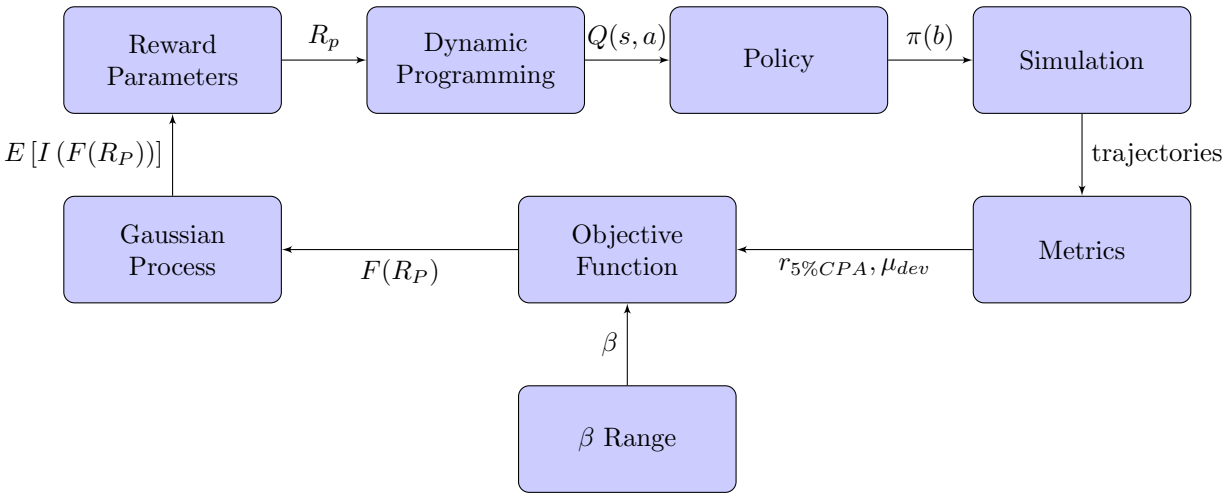
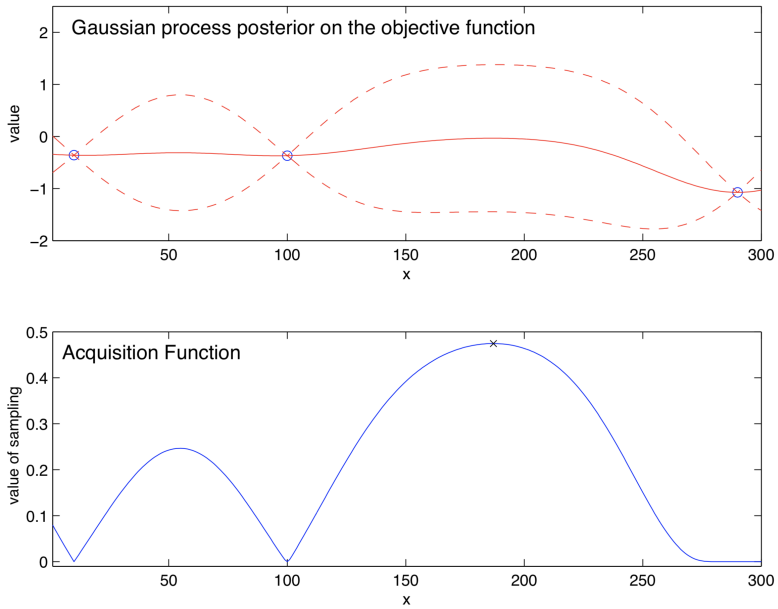


Figure 5: Process for tuning POMDP reward parameters

Bayesian Optimization

- we know QMDP and F values for one or more $\mathbf{x} = R_P$ points
- we search the point $x = R_P^*$ to observe
- we minimize $y = F(R_P^*)$ and search the maximal probability of improvement
- 'the chance to improve' is expressed by the **Expected improvement** (EI)

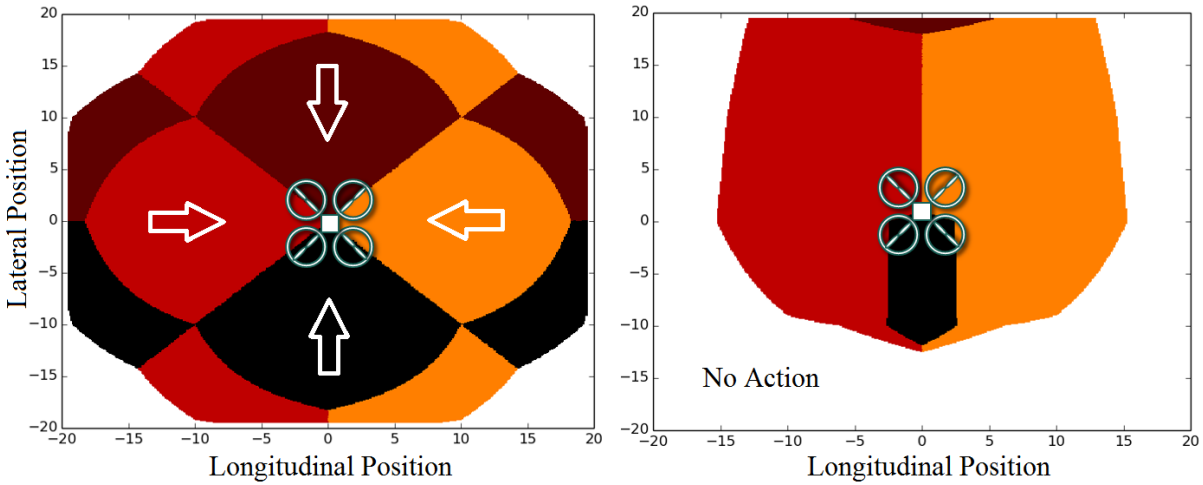


Peter I. Frazier: A Tutorial on Bayesian Optimization, rXiv:1807.02811v1 [stat.ML] 8 Jul 2018

Value Iteration, QMDP Policies

- considerable improvement in convergence speed by initializing by the value of previously evaluated policy
- the value of maximum negative reward influenced the convergence speed
- $\gamma \leftarrow 0.99$ taking hundred iterations to converge.
- smaller γ did not ensure the return to the desired path.

- Figures: Owhship at the origin
- different intruder positions
- policies indicated by color: black=up, red=right
- left: both own and intruder velocities are zero, $d = 0$
- right: owhship is moving in the positive y–axis direction at 1 s^{-1} with zero trajectory error and nominal trajectory matches the velocity.
- The intruder is stationary.



Beliefs

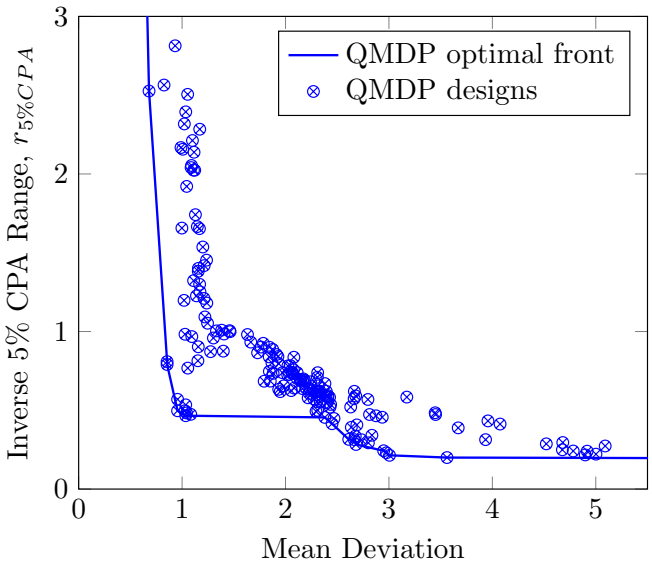
- Uncertainty does not increase with time
- State uncertainty is incorporated only when actions are selected
- a set of potential states is calculated from the observations received at each step.
- the potential states become the beliefs used to select an action.

$$\pi(b) = max_a \left[\sum_k Q(s^{(k)}, a) b^{(k)} \right]$$

- The value $Q(s^{(k)}, a)b^{(k)}$ approximated from QMDP solutions
  - rectangular interpolation between 2^n nearest neighbor
  - simplex interpolation between $n + 1$ nearest neighbor
  - prior work has found little benefit to using more sophisticated approaches.

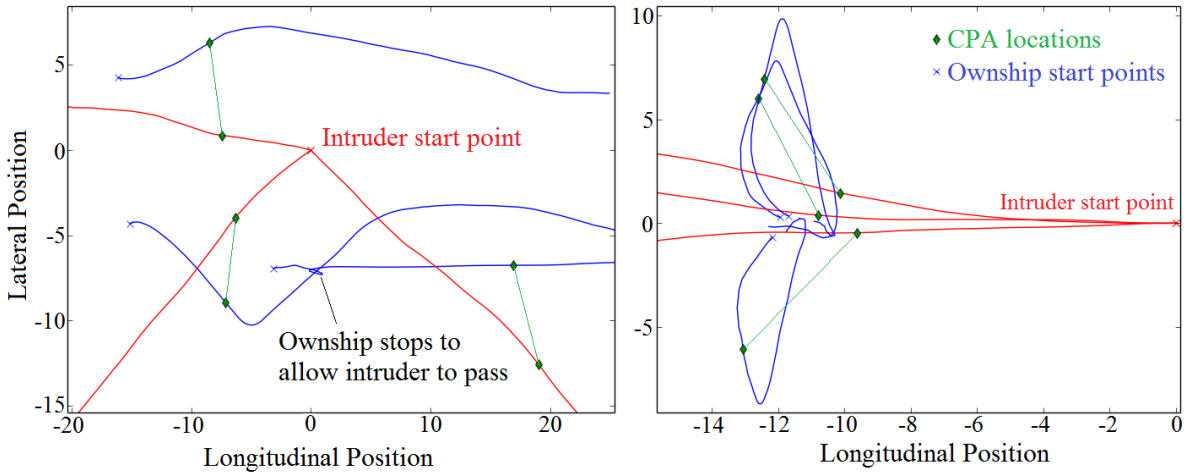
Pareto Optimal frontier

- 194 parameter sets evaluated
- β between 0.01 and 0.99 .
- resulting in nine non-dominated, Pareto–optimal designs.



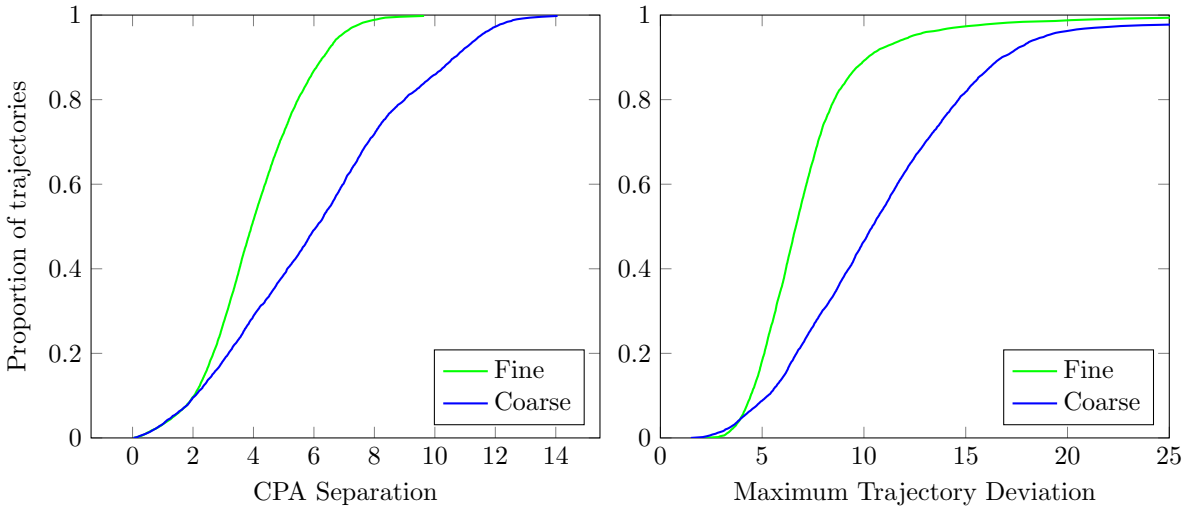
Human Expert Check

- Left: intruder starts at $(0, 0)$,
- random heading, fixed velocity of the intruder
- the ownship starts at the blue cross
- Right: The goal is hovering
- the intruder comes from the right with the unknown behaviour.



State Discretization

The fine discretization improves the results.



(a) CPA separations

(b) Maximum trajectory deviations

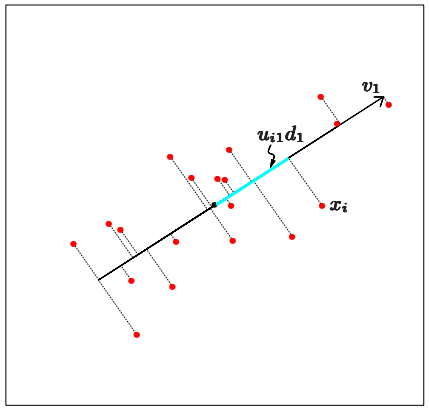
Figure 10: Cumulative distributions of encounter model metrics as a function of state discretization

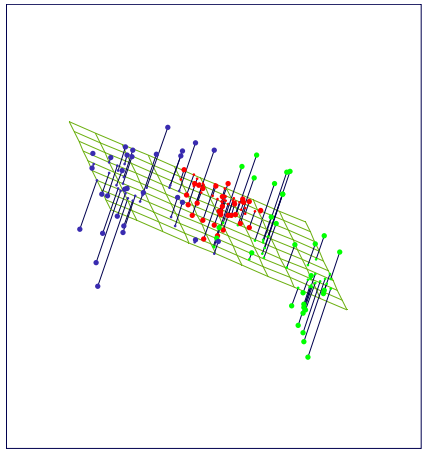
Further ML Methods

- Linear Projections
  - **Principal Component Analysis (PCA)**: 'the most spread variance' directions
    - **Sparse PCA**. (sklearn)
  - **Partial Least Squares**: not mentioned here. (sklearn)
  - **Archetypal analysis**: extremes, instead of 'centers' from clustering; data=lin. comb. of archetypes (archetypes)
  - **NMF Nonnegative Matrix Factorization**: 'linear r-dimensional autoencoder' (sklearn)
  - **Factor analysis**: A view on 'independent factors' observed via a linear combination mixture with a gaussian noise (sklearn)
  - **Independent Component Analysis**: splits the signal according to non-gaussian features (max. divergence from gaussian) (sklearn)
  - **Procrustes transformation** - curve fitting.
- **Principal curves and surfaces** (predefined $f_j(\lambda)$, curve paramater λ) (prinPy),
- **Kernel PCA**. (sklearn)
- **Spectral Clustering**. (sklearn)

PCA Principal Components, Curves and Surfaces

- The **principal components** of a set of data in $\mathbb{R}^p$ provide a sequence of best linear approximations to that data, of all ranks $q \leq p$.
- let μ be a location vector in $\mathbb{R}^p$, V_q is a $p \times q$ matrix with q orthogonal unit vectors as columns, λ is a q vector of parameters.
- $f(\lambda) = \mu + V_q\lambda$ represents an affine hyperplane of rank q.
- We minimize the **reconstruction error** (by least squares)
  - $min_{\mu,\{\lambda_i\}} \sum_{i=1}^{N} \|x_i - \mu - V_q\lambda_i\|^2$.
- We can partially optimize
  - $\hat{\mu} = \overline{x}$
  - $\hat{\lambda}_i = V_q^T(x_i - \overline{x})$.
- This leaves us to find the **orthogonal matrix** V_q $min_{V_q} \sum_{i=1}^{N} \left\|(x_i - \overline{x}) - V_q V_q^T(x_i - \overline{x})\right\|^2$.
- We center the data $\overline{x} = 0$ to simplify the formulas.

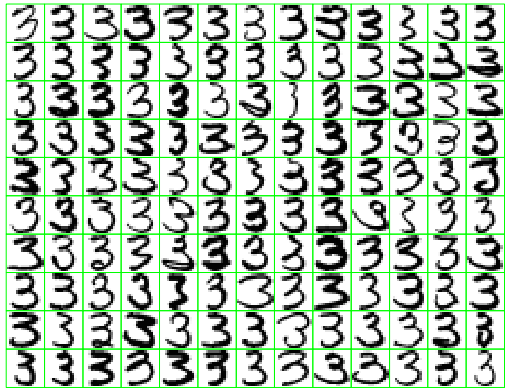


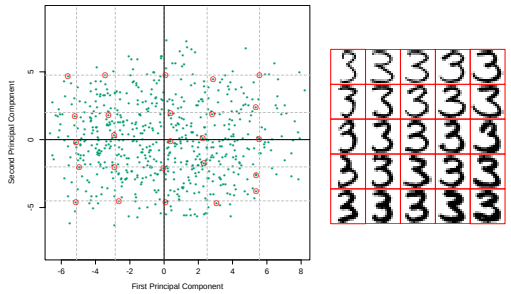


Handwritten 3 Example

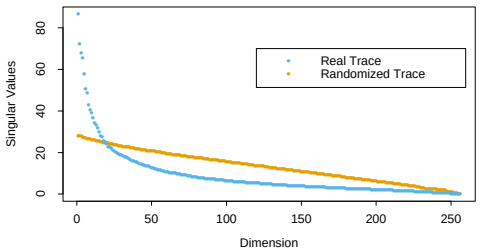
- 130 handwritten digits 3, each 16×16 grayscale image.
  - $x \in \mathbb{R}^{256}$
- First two principal component plot
  - For the first two principal components quantiles 5,25,50,75,95 percent.
  - First component - x axis: mainly the length of 3
  - Second component - the thickness.
- The projection on the first two components is:

$$\begin{aligned} \hat{f}(\lambda) &= \bar{x} + \lambda_1 v_1 + \lambda_2 v_2 \\ &= \bar{x} + \lambda_1 \cdot v_1 + \lambda_2 \cdot v_2. \end{aligned}$$





- First 12 components account for 63% data variations.
- Explained variance by PCA (blue) and randomized directions (orange).



Sparse Principal Components

- We often interpret PCA by examining **loadings**: direction vectors v_j.
- This interpretation is easier if the loadings are sparse.

Definition (Sparse PCA)

Sparse principal component technique solves for a single component:

$$min_{\theta,v} \sum_{i=1}^{N} \|x_i - \theta v^T x_i\|_2^2 + \lambda \|v\|_2^2 + \lambda_1 \|v\|_1$$

$$\text{subject to } \|\theta\|_2 = 1.$$

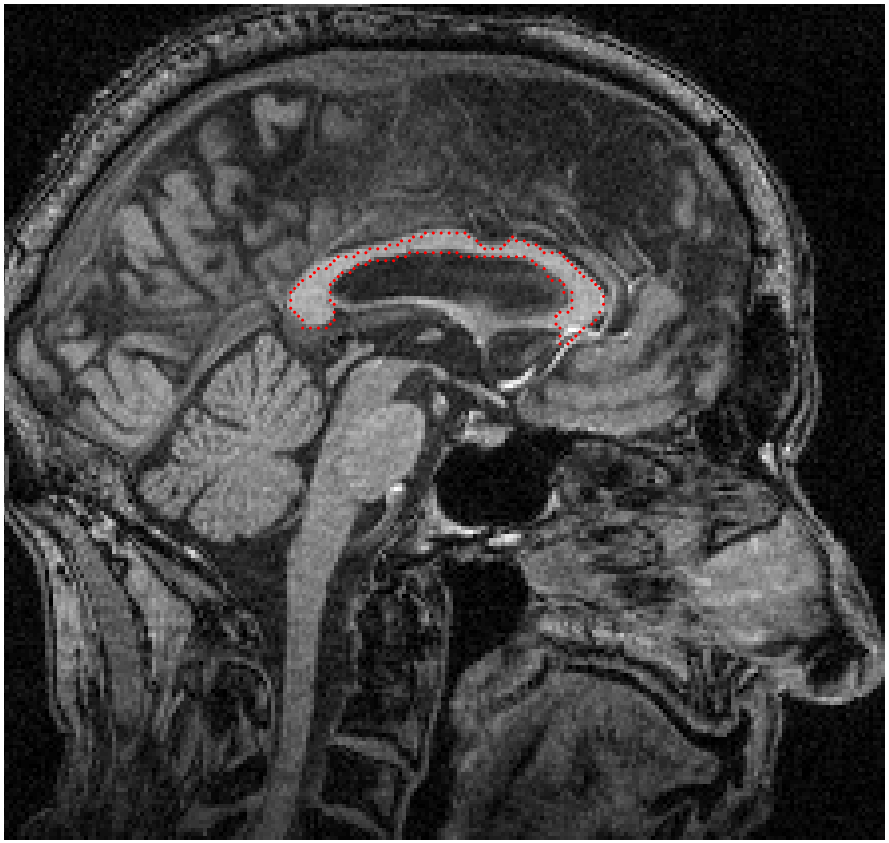
- If both $\lambda = \lambda_1 = 0$ and $N > p$, than $v = \theta$ is the largest principal component direction.
- When $p \gg N$ the solution may not be unique unless $\lambda > 0$. For $\lambda > 0$ and $\lambda_1 = 0$ is the solution proportional to the largest principal component direction.

Sparse principal component for multiple components minimizes Θ and V $p \times K$ matrices

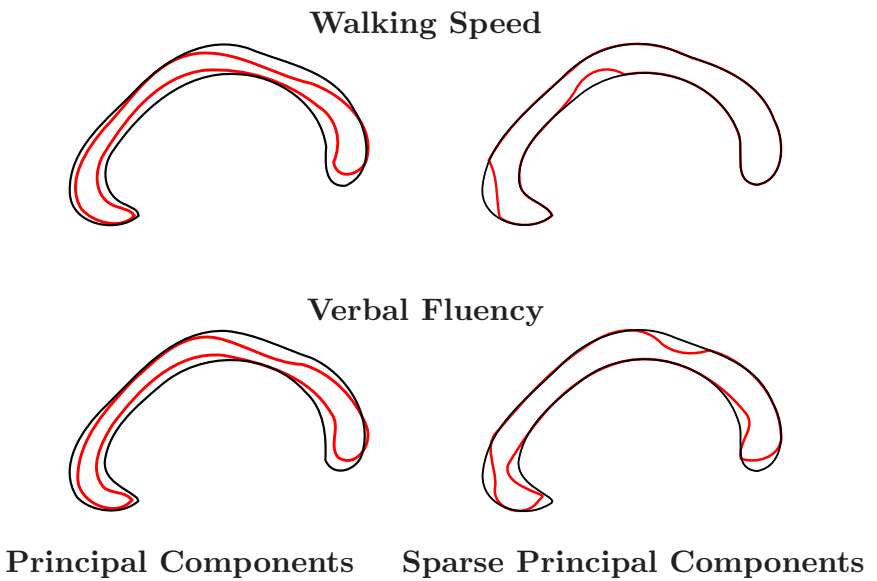
$$min_{\Theta,V} \sum_{i=1}^{N} \|x_i - \Theta V^T x_i\|_2^2 + \lambda \sum_{k=1}^{K} \|v_k\|_2^2 + \sum_{k=1}^{K} \lambda_{1k} \|v_k\|_1$$

$$\text{subject to } \Theta^T \Theta = I_K.$$

Corpus Callosum (CC) Sparse PCA Example



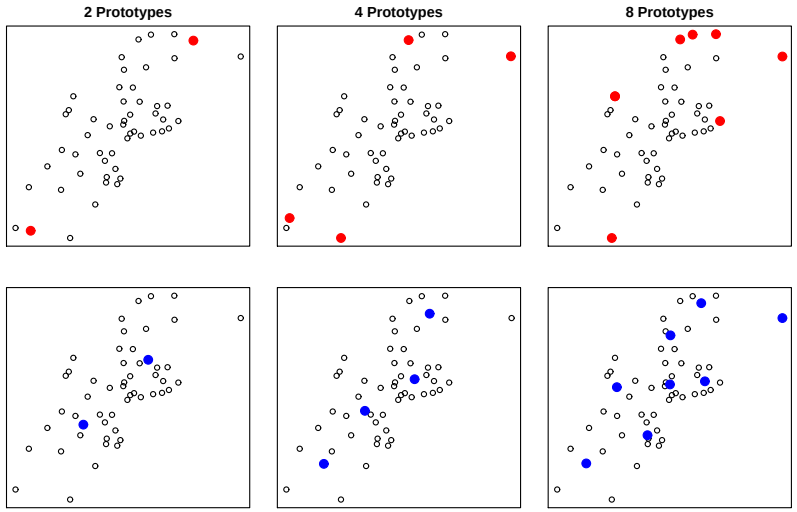
- The Corpus Callosum scan.
- The area represented by a number of points aligned by Procrustes analysis,
- a set of 2d points for now.



Archetypal Analysis

- **Archetypal Analysis** approximates data points by a linear combination of prototypes
  - that are themselves linear combinations of data points.
  - Each data point is approximated by a convex combination of prototypes.
  - This forces the prototypes to lie on the convex hull of the data cloud.
  - In this sense, they are 'archetypal'.

- K-means clustering
  - approximates any point by one prototype
  - each prototype is a linear combination of samples (the mean of a cluster).



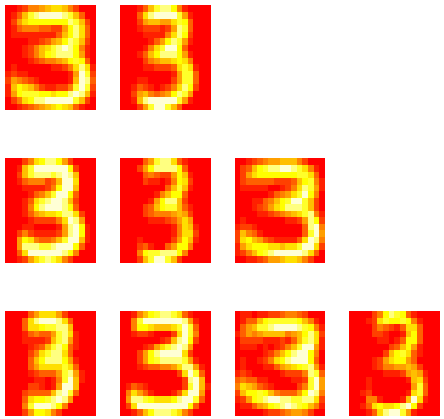
Archetypal Analysis

- "linear autoencoder" of the dimension r

Definition (Archetypal Analysis)

- A non-negative $N \times p$ data matrix X is modeled $X \sim WH$,
  - $H = BX$ is $r \times p$ matrix of r **archetypes** (rows of H),
  - B is $r \times N$ matrix where $b_{ki} \geq 0$ and $(\forall k)$ $(\sum_{i=1}^{N} b_{ki} = 1)$.
  - W is $N \times r$ matrix where $w_{ik} \geq 0$ and $(\forall i)$ $(\sum_{k=1}^{r} w_{ik} = 1)$.
  - We minimize over W and B: $J(W, B) = \|X - WH\|^2 = \|X - WBX\|^2$.

- Its minimized in an alternating fashion, with each separate minimization involving a convex optimization.
- Converges to a local minimum.
- Figure: 2,3, and 4 prototypes for the Handwritten 3 example.
- Extreme 3's both in size and shape.

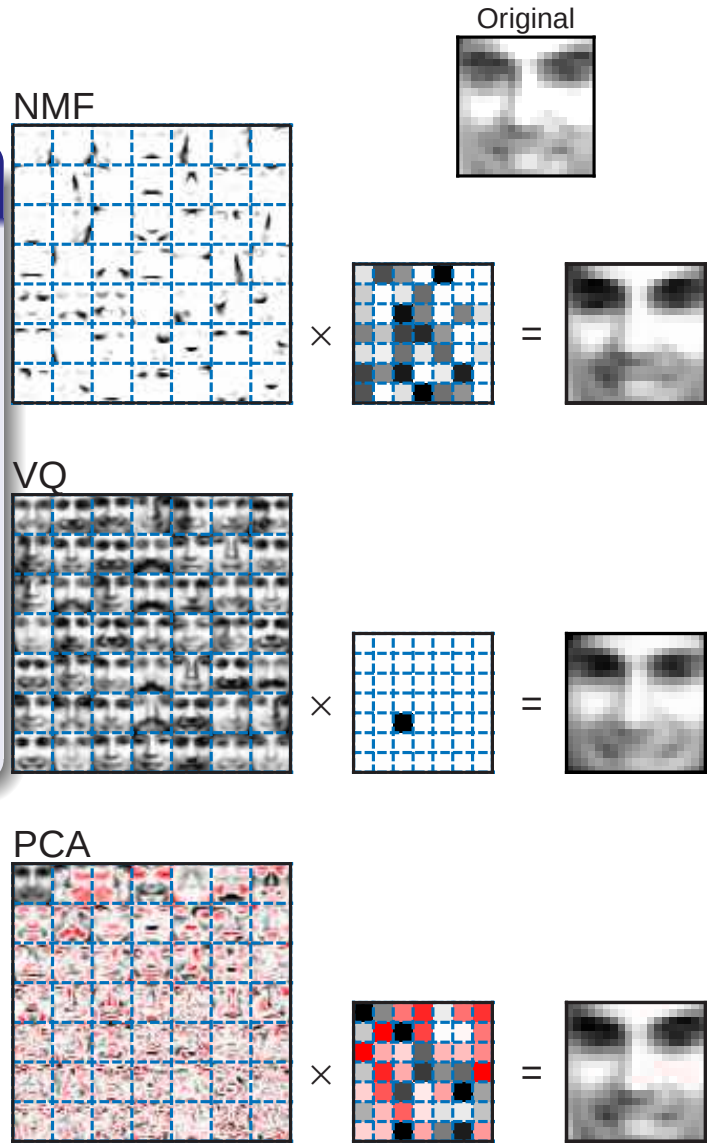


Non-negative Matrix Factorization

Definition (Non-negative Matrix Factorization)

- A centered $N \times p$ data matrix X is modeled $X \sim WH$,
- W is $N \times r$ matrix, H is $r \times p$, $r \leq \max(N, p)$.
- We assume $x_{ij}, w_{ik}, h_{kj} \geq 0$.
- We maximize over W and H: $L(W, H) = \sum_{i=1}^{N} \sum_{j=1}^{p} [x_{ij} \log(WH)_{ij} - (WH)_{ij}]$.

- NMF assumes x_{ij} has a Poisson distribution with mean $(WH)_{ij}$
- we maximize the loglikelihood.



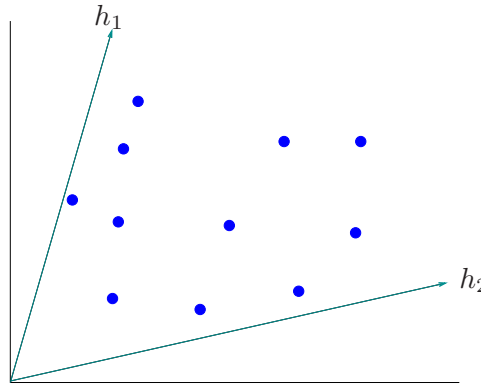
NMF

NMF

1: **procedure** NMF:(X centered data)
2: **repeat**
3: $$w_{ik} \leftarrow w_{ik} \frac{\sum_{j=1}^{p} h_{kj} x_{ij} / (WH)_{ij}}{\sum_{j=1}^{p} h_{kj}},$$
4: $$h_{kj} \leftarrow h_{kj} \frac{\sum_{i=1}^{N} w_{ik} x_{ij} / (WH)_{ij}}{\sum_{i=1}^{N} b_{ik}}$$
5: **until** convergence
6: return W, H
7: **end procedure**

- The NMF solution is not unique.

Any h_1, h_2 basis vectors in the open space between the coordinate axes and data work (given an exact reconstruction of the data).



sklearn.decomposition.NMF has the objective function:

$$0.5\|X - WH\|_{loss}^2 + \alpha_W \cdot l1_{ratio} p \|vec(W)\|_1 + 0.5\alpha_W \cdot (1 - l1_{ratio}) p \|W\|_{Fro}^2 + \alpha_H \cdot l1_{ratio} N \|vec(H)\|_1 + 0.5\alpha_H \cdot (1 - l1_{ratio}) N \|H\|_{Fro}^2$$

- $\|vec(W)\|_1 = \sum_{i,j} abs(W_{i,j})$ elementwise L1 norm
- $\|W\|_{Fro}^2 = \sum_{i,j} W_{i,j}^2$ Frobenius norm
- *loss* is Frobenius norm or another beta-divergence loss, $l1_{ratio} = 0$.

Independent Component Analysis

- Multivariate data as multiple indirect measurements from an underlying source.
- Examples: EEG brain scans, 'body fat', trading prices.
- **Factor analysis**
  - typically wed to Gaussian distributions
  - which has hindered their usefulness
  - and has no unique solution
    - any linear transformation is a solution.

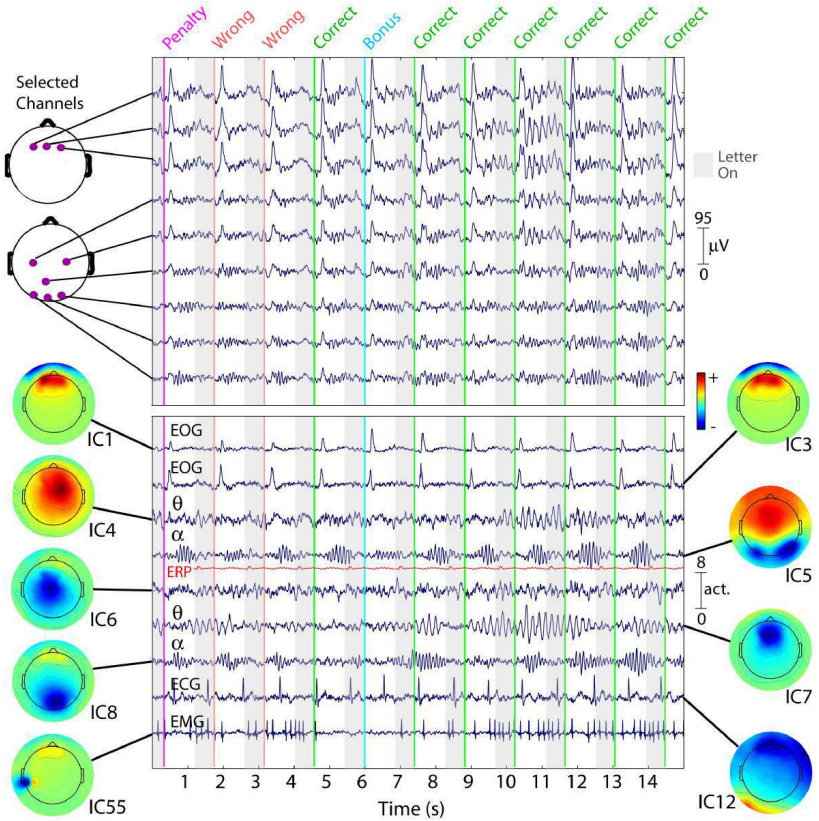


FIGURE 14.41. *Fifteen seconds of EEG data (of 1917 seconds) at nine (of 100) scalp channels (top panel), as well as nine ICA components (lower panel). While nearby electrodes record nearly identical mixtures of brain and non-brain activity, ICA components are temporally distinct. The colored scalps represent the ICA unmixing coefficients $\hat{a}_j$ as a heatmap, showing brain or scalp location of the source.*

Latent Variables and Factor Analysis

- Take the singular value decomposition $X = UDV^T$
  - we assume that the columns of X have zero mean
  - where D is a diagonal matrix
  - U is orthogonal.
- X has a **latent variable decomposition** $X = SA^T$
  - where $S = \sqrt{N}U$, $A^T = \frac{1}{\sqrt{N}}DV^T$
  - each of the columns of X is a linear combination of the columns of S
  - columns of S have zero mean, are uncorrelated and have unit variance, $Cov(S) = I$.
  - we can interpret the SVD, or the corresponding PCA as an estimate of a latent variable model $X = AS$

$$
\begin{aligned}
X_1 &= a_{11}S_1 + a_{12}S_2 + \ldots + a_{1p}S_p \\
X_2 &= a_{21}S_1 + a_{22}S_2 + \ldots + a_{2p}S_p \\
&\ldots \\
X_p &= a_{p1}S_1 + a_{p2}S_2 + \ldots + a_{pp}S_p
\end{aligned}
$$

- Notice that for any orthogonal $p \times p$ matrix R is $X = AS = AR^TRS = A^*S^*$.

Factor Analysis

- In the SVD decomposition any rank $q < p$ truncated decomposition approximates X in an optimal way.
- **Factor analysis model** (popular in psychometrics)
  - with $q < p$, a factor analysis model has the form $X = AS + \epsilon$

$$\begin{aligned} X_1 &= a_{11}S_1 + a_{12}S_2 + \ldots + a_{1q}S_q + \epsilon_1 \\ X_2 &= a_{21}S_1 + a_{22}S_2 + \ldots + a_{2q}S_q + \epsilon_2 \\ &\ldots \\ X_p &= a_{p1}S_1 + a_{p2}S_2 + \ldots + a_{pq}S_q + \epsilon_p \end{aligned}$$

  - S is a vector of $q < p$ underlying latent variables or factors
  - A is a $p \times q$ matrix of factor **loadings**
    - used to name and interpret the factors
  - ϵ_j are uncorrelated zero–mean disturbances.
  - Typically, S_ℓ and ϵ_j are modeled as Gaussian random variables, and the model is fit by maximum likelihood.
  - The parameters all reside in the covariance matrix

$$\Sigma = AA^T + D_\epsilon$$

  - where $D_\epsilon = diag[Var(\epsilon_1), Var(\epsilon_2), \ldots, Var(\epsilon_p)]$
  - S independent factors like intelligence, drive in a battery of educational tests.

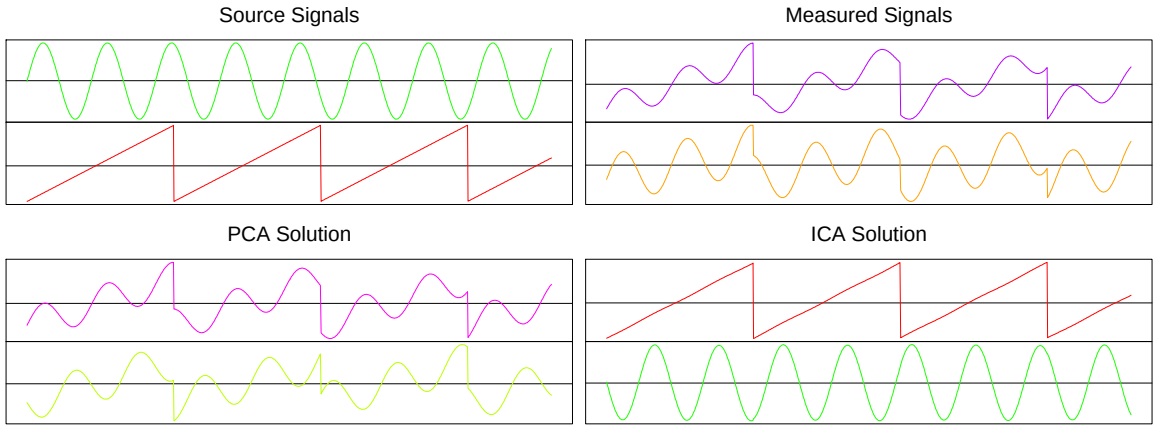
Independent Component Analysis

$$
\begin{aligned}
X_1 &= a_{11}S_1 + a_{12}S_2 + \ldots + a_{1p}S_p \\
X_2 &= a_{21}S_1 + a_{22}S_2 + \ldots + a_{2p}S_p \\
&\ldots \\
X_p &= a_{p1}S_1 + a_{p2}S_2 + \ldots + a_{pp}S_p
\end{aligned}
$$

- S are assumed **statistically independent** rather than uncorrelated
  - correlation: second order interaction
  - independence: all orders of interactions.
  - Multivariate Gaussian is determined by its second moments alone (up to rotation).
  - Otherwise, the extra moments allow to identify the elements of A uniquely.
- We assume X has been **whitened** to have $Cov(X) = I$; Simplest: multiply by $W = \Sigma^{-\frac{1}{2}}$, typically achieved via the SVD to $D^{-\frac{1}{2}}V^T$.
  - $Var(S) = I$, therefore is A orthogonal.
  - ICA searches an orthogonal S such that $S = A^T X$ are independent (not-Gaussian) components.

Example

- **Cocktail party problem** Different microphones X_j pick up mixtures of different independent sources S_ℓ (music, speech from different speakers).
- ICA is able to perform blind source separation
  - by exploiting the independence and non–Gaussianity of the original sources.



Entropy

$$
\begin{aligned}
\text{entropy } H(Y) &= -\int g(y) \log g(y) dy \\
\text{mutual information } I(Y) &= \sum_{j=1}^{p} H(Y_j) - H(Y) \\
I(Y) &= \sum_{j=1}^{p} H(Y_j) - H(X) - \log |\det(A)| \\
&= \sum_{j=1}^{p} H(Y_j) - H(X)
\end{aligned}
$$

- since $Cov(X) = I$, $Y = A^T X$ and A is orthogonal.
- We search A to minimize $I(Y) = I(A^T X)$
  - looks for the orthogonal transformation that leads to the most independence between its components
  - minimizes the sum of the entropies of the separate components of Y
  - this amounts to maximizing their departures from Gaussianity.

Negentropy, FastICA

- For each Y_j, let Z_j be a Gaussian random variable with the same variance as Y_j.
- The **negentropy** $J(Y_j)$ is defined

$$J(Y_j) = H(Z_j) - H(Y_j)$$

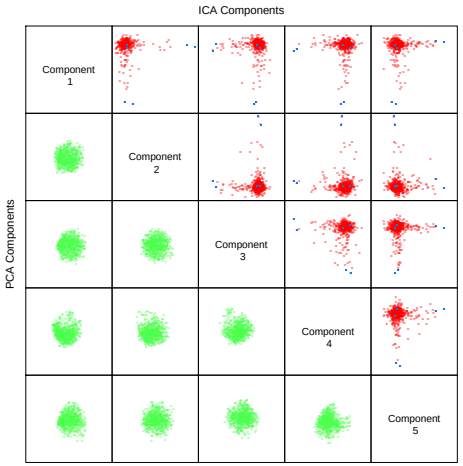
- It is non–negative, and measures the departure of Y_j from Gaussianity.
- Can be approximated by

$$J(Y_j) \sim [\mathbb{E}G(Y_j) - \mathbb{E}G(Z_j)]^2$$

  - $G(u) = \frac{1}{a} \log \cosh(au)$ for $1 \leq a \leq 2$.

FastICA

- ICA starts from essentially a factor analysis solution
- and looks for rotations that lead to independent components.



- Above diagonal: first five ICA components
- Below diagonal: first five PCA components
- all standardized to unit variance.

FastICA

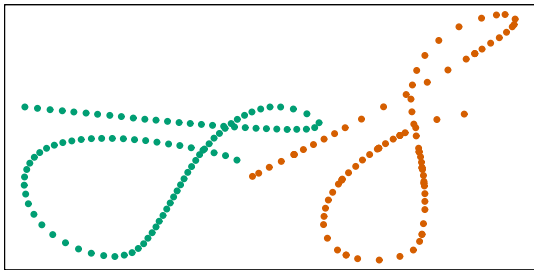
- X are centered and whitened data with $Cov(X) = I$
  - typically achieved via the SVD, $X \leftarrow \sqrt{D}U$ from $X = UDV^T$.
- q the number of components
  - Only one is allowed to follow Gaussian distribution.
- a a parameter.

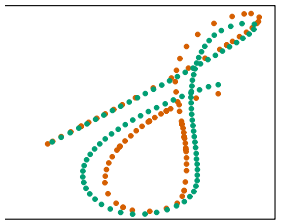
FastICA

procedure FastICA:(**X**, $a \in \langle 1, 2 \rangle$, $q \leq p$)
  $w_1, \ldots, w_q \leftarrow$ randomly initialize N-dimensional weight vectors
  for $\ell = 1, \ldots, q$ **do**
    repeat
      $w_\ell^+ \leftarrow \sum_{i=1}^N x \tanh(a w_\ell^T x) - \left(\sum_{i=1}^N \frac{1}{cosh^2(w_\ell^T x)} \right) w$
      $w_\ell \leftarrow w_\ell^+ - \sum_{j=1}^{\ell-1} w_\ell^T w_j w_j$ # orthogonal to previous
      $w_\ell \leftarrow \frac{w_\ell}{\sqrt{w_\ell^T w_\ell}}$ # normalize
    until convergence
  end for
end procedure

Procrustes Transformations

- Assume each handwritten S is represented as $N = 96$ points.
- Both X_1 and X_2 are $N \times 2$ matrices (green, orange curve).
  - with column means $\overline{x}_1, \overline{x}_2$, centered to $\tilde{X}_1, \tilde{X}_2$.
  - To find landmarks (points) are difficult and subject specific.
  - In this example, dynamic time wrapping of the speed signal along each signature was used.





- **Procrustes** transformation
  - R is an orthonormal $p \times p$ matrix,
    - $\hat{R} \leftarrow UV^T$ from $\tilde{X}_1^T \tilde{X}_2 = UDV^T$.
  - μ a p vector of location coordinates
    - $\mu \leftarrow \overline{x}_2 - \hat{R}\overline{x}_1$.
  - $\|X\|_F^2 = trace(X^T X) = \sum_{i=1}^{N} \sum_{j=1}^{p} |x_{ij}|^2$ is the squared **Frobenius** matrix norm
  - We minimize the **Procrustes distance**

$$min_{\mu,R} \left\| X_2 - (X_1 R + 1\mu^T) \right\|_F^2 .$$

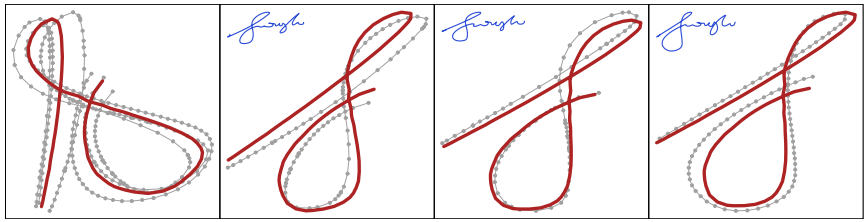
Shape Averaging, Procrustes Average

! From now on, we assume the data are centered.

Definition (Procrustes average)

The **Procrustes average** of a collection of L shapes is M that minimizes

$$min_{\{R_\ell\}_1^L, M} \sum_{\ell=1}^{L} \|X_\ell R_\ell - M\|_F^2 .$$

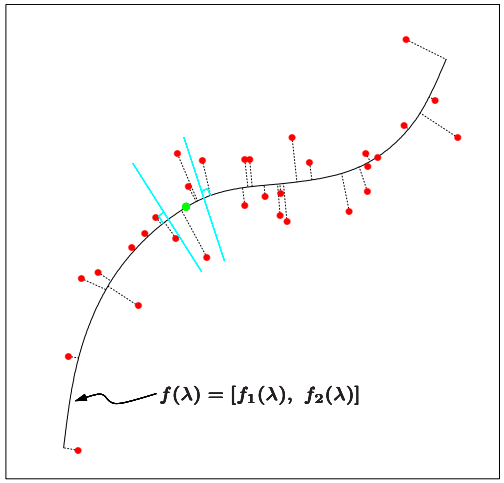


Procrustes Average

1: **procedure** PROCRUSTES AVERAGE:($N \times p$ shapes $\{\mathbf{X}_\ell\}_{\ell=1}^{\mathbf{L}}$)
2: $M \leftarrow X_1$ # init the average
3: **repeat**
4: $X'_\ell \leftarrow X_\ell \hat{R}_\ell$ # M fixed, solve L Procruster rotations $\hat{R}_\ell$
5: $M \leftarrow \frac{1}{L} \sum_{\ell=1}^{L} X'_\ell$ # average
6: **until** convergence
7: **end procedure**

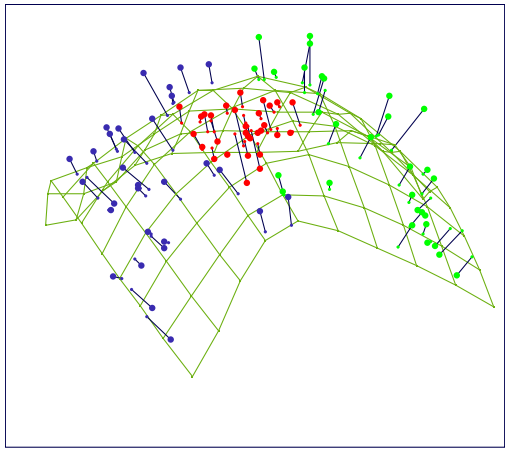
Principal Curves and Surfaces

- To find a principal curve $f(\lambda)$ of a distribution, we consider
- $f(\lambda) = [f_1(\lambda), f_2(\lambda), \ldots, f_p(\lambda)]$ its coordinate functions and let
- $X^T = (X_1, \ldots, X_p)$



Principal Curves and Surfaces

1: **procedure** PRINCIPAL CURVE:$(f(\lambda), X)$
2: **repeat**
3: $\hat{f}_j(\lambda) \leftarrow \mathbb{E}[X_j|\lambda(X) = \lambda]$, $j = 1, \ldots, p$,
4: $\hat{\lambda}_f(x) \leftarrow \arg\min_{\lambda'} \left\|x - \hat{f}(\lambda')\right\|^2$.
5: **until** convergence
6: **end procedure**



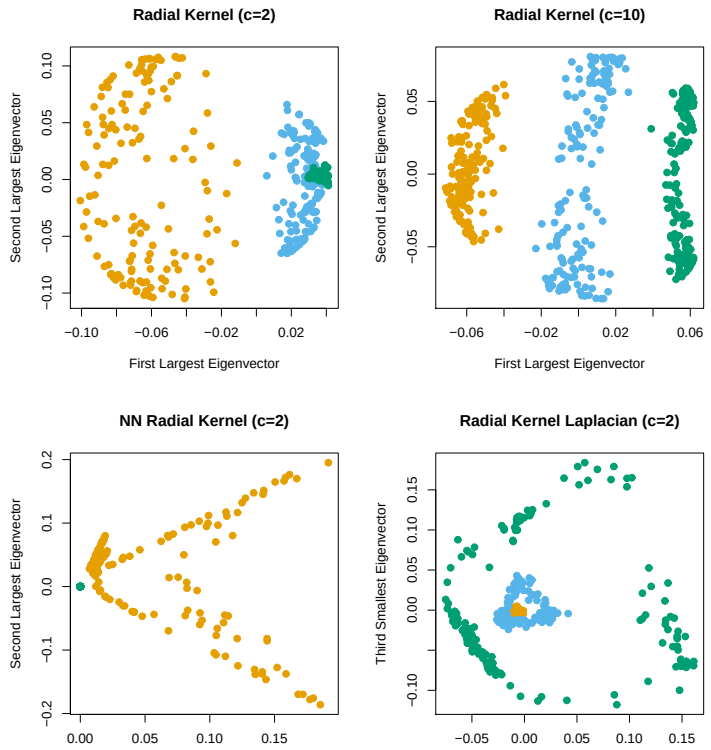
- A scatterplot smoother is used to estimate the conditional expectations in step 3: by smoothing each X_j as a function of the arc-length $\lambda(\hat{X})$.

Kernel Principal Components

- We can select any kernel function, like radial $K(x_i, x_{i'}) = e^{-\frac{\|x-x'\|^2}{c}}$.
- We set $M = 11^T/N$ and calculate double-centered version of K

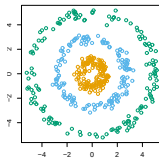
$$\tilde{K} = (I - M)K(I - M) = UD^2U^T$$

- then principal components variables are $Z = UD$.
  - The elements of the mth component z_m (mth column of Z) can be written (up to centering)
  - $z_{im} = \sum_{j=1}^{N} \alpha_{jm} K(x_i, x_j)$, where $\alpha_{jm} = \frac{u_{jm}}{d_m}$.
- Figure: Radial kernel (top) and spectral clustering without NN (bottom right) on the previous 3-'circles' example.



Spectral Clustering

- The idea is to put close points into the same cluster.
- We form a weighted adjacency graph for data samples.



Spectral Clustering

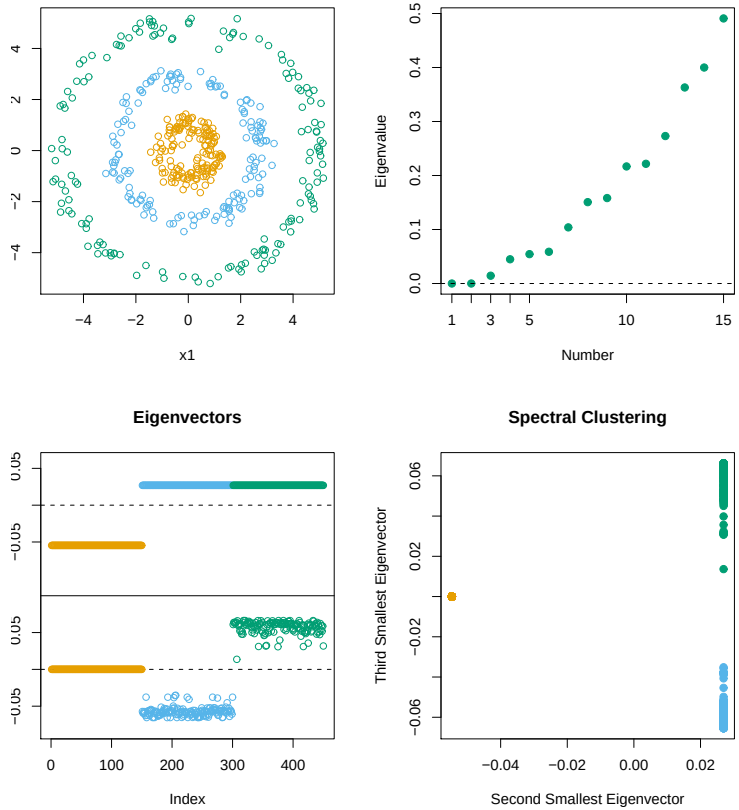
procedure SC:(X as N points in $\mathbb{R}^p$, $c > 0$ scale, $k > 0$)
    $s_{ii'} \leftarrow exp(-d(i,i')^2/c)$ # calculate the similarity matrix
    $W, G \leftarrow$ zero matrix $N \times N$
    for i, i' symmetric nearest neighbors **do**
        $w_{ii'} \leftarrow s_{ii'}$ # connect them
    end for
    for $i \in X$ **do**
        $g_{ii} \leftarrow \sum_{i'} w_{ii'}$ # the degree of vertex i
    end for
    $L \leftarrow G - W$ # the graph Laplacian (unnormalized)
    (or $\tilde{L} \leftarrow I - G^{-1}W$ # (normalized))
    find m eigenvectors $Z_{N \times m}$ with **smalest** eigenvalues of L
    return $Z_{N \times m}$ rows clustered by standard $k - means$
end procedure

Spectral Clustering

- For any vector f

$$
\begin{aligned}
f^T L f &= \sum_{i=1}^{N} g_{ii} f_i^2 - \sum_{i=1}^{N} \sum_{i'=1}^{N} f_i f_{i'} w_{ii'} \\
&= \frac{1}{2} \sum_{i=1}^{N} \sum_{i'=1}^{N} w_{ii'} (f_i - f_{i'})^2.
\end{aligned}
$$

  - $1^T L 1 = 0$ for any graph.
  - For a graph with m connected components,
    - reordered so that L is a block diagonal with a block for each component
  - then L has m eigenvectors of eigenvalue zero.
- In practice zero eigenvalues are approximated by small eigenvalues.



Separating hyperplane, Optimal separating hyperplane

- Classification, we encode the goal class by -1 and 1, respectively.
- separate the space X by a hyperplane
- **Linear Discriminant Analysis** LDA is not necessary optimal.
- **Logistic regression** finds one if it exists.
- **Perceptron** (a neural network with one neuron) finds separating hyperplane if it exists.
  - The exact position depends on initial parameters.

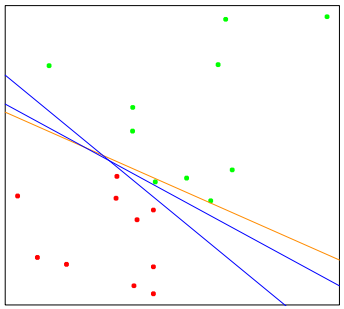


FIGURE 4.14. *A toy example with two classes separable by a hyperplane. The orange line is the least squares solution, which misclassifies one of the training points. Also shown are two blue separating hyperplanes found by the* perceptron learning algorithm *with different random starts.*

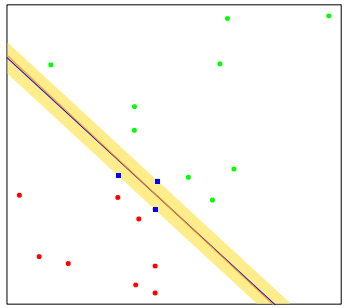


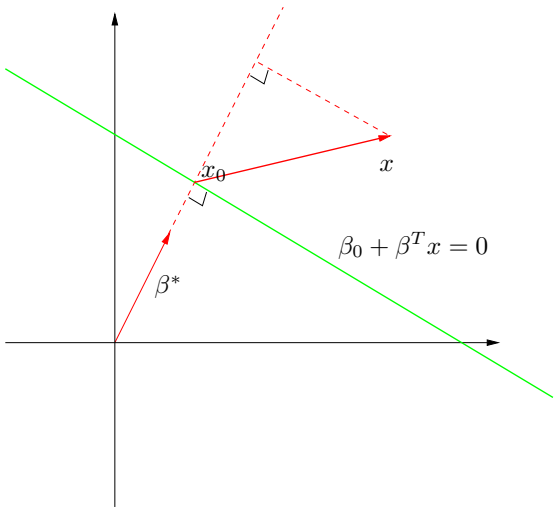
FIGURE 4.16. *The same data as in Figure 4.14. The shaded region delineates the maximum margin separating the two classes. There are three support points indicated, which lie on the boundary of the margin, and the optimal separating hyperplane (blue line) bisects the slab. Included in the figure is the boundary found using logistic regression (red line), which is very close to the optimal separating hyperplane (see Section 12.3.3).*

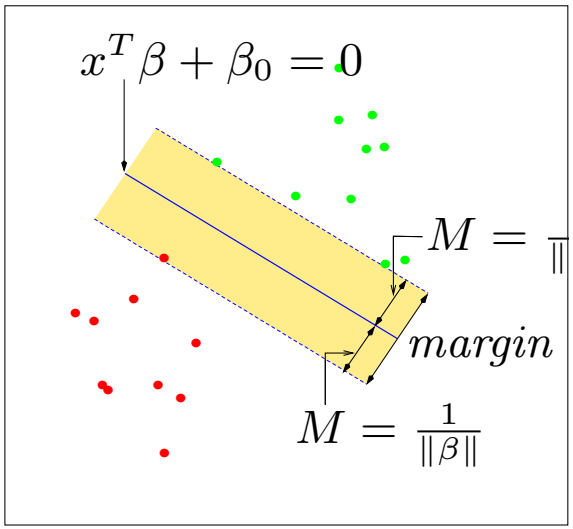
Optimal Separating Hyperplane (separble case)

We define **Optimal Separating Hyperplane** as a separating hyperplane with maximal free space M without any data point around the hyperplane.
Formally:

$$\max_{\beta,\beta_0,\|\beta\|=1} M$$

subject to $y_i(x_i^T\beta + \beta_0) \geq M$ for all $i = 1, \ldots, N$.





Formally:

$$\max_{\beta,\beta_0,\|\beta\|=1} M$$

subject to $y_i(x_i^T\beta + \beta_0) \geq M$ for all $i = 1, \ldots, N$.
We re-define: $\|\beta\| = 1$ can be moved to the condition (and redefine β_0):

$$\frac{1}{\|\beta\|} y_i(x_i^T\beta + \beta_0) \geq M$$

Since for any β and β_0 satisfying these inequalities, any positively scaled multiple satisfies them too, we can set $\|\beta\| = \frac{1}{M}$ and we get:

$$\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2$$

subject to $y_i(x_i^T\beta + \beta_0) \geq 1$ pro $i = 1, \ldots, N$.
This is a convex optimization problem. The Lagrange function, we look for the saddle point w.r.t. β and β_0:

$$L_P = \frac{1}{2}\|\beta\|^2 - \sum_{i=1}^{N} \alpha_i[y_i(x_i^T\beta + \beta_0) - 1].$$

$$L_P = \frac{1}{2}\|\beta\|^2 - \sum_{i=1}^{N} \alpha_i [y_i(x_i^T \beta + \beta_0) - 1].$$

Setting the derivatives to zero, we obtain:

$$\beta = \sum_{i=1}^{N} \alpha_i y_i x_i$$

$$0 = \sum_{i=1}^{N} \alpha_i y_i$$

Substituing these in L_P we obtain the so–called Wolfe dual:

$$L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k x_i^T x_k$$

subject to $\alpha_i \geq 0$
The solution is obtained by maximizing L_D in the positive orthant, for which standard software can be used.

$$L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k x_i^T x_k$$

subject to $\alpha_i \geq 0$.
In addition the solution must satisfy the Karush–Kuhn–Tucker conditions:

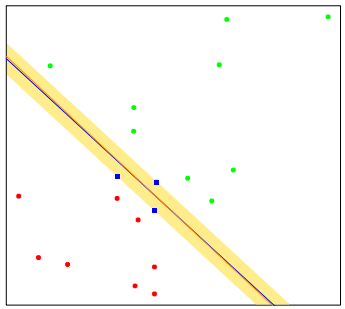
$$\alpha_i [y_i (x_i^T \beta + \beta_0) - 1] = 0$$

for any i, therefore for any $\alpha_i > 0$ must $[y_i (x_i^T \beta + \beta_0) - 1] = 0$, that means x_i is on the boundary and for all x_i outside the boundary is $\alpha_i = 0$.
The boundary is defined by x_i with $\alpha_i > 0$ – so called **support vectors**.

We classify new observations

$$\hat{G}(x) = sign(x^T \beta + \beta_0)$$

- where $\beta = \sum_{i=1}^{N} \alpha_i y_i x_i$,
- $\beta_0 = y_s - x_s^T \beta$ for any support vector $\alpha_s > 0$.



Optimal Separating Hyperplane (nonseparble case)

- We have to accept incorrectly classified instances in a non–separable case.
- We limit the number of incorrectly classified examples.

We define **slack** ξ for each data point $(\xi_1, \ldots, \xi_N) = \xi$ as follows:

- ξ_i is the distance of x_i from the boundary for x_i at the wrong side of the margin
- and $\xi_i = 0$, for x_i at the correct side.

We require $\sum_{i=1}^{N} \xi_i \leq K$.

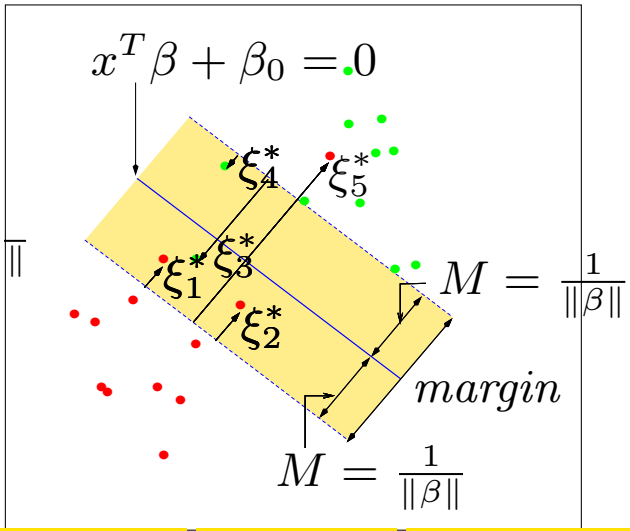
We solve the optimization problem

$$\max_{\beta, \beta_0, \|\beta\|=1} M$$

subject to:

$$y_i(x_i^T \beta + \beta_0) \geq M(1 - \xi_i)$$

where $\forall i$ is $\xi_i \geq 0$ a $\sum_{i=1}^{N} \xi_i \leq K$.



Optimal Separating Hyperplane (nonseparble case)

Again, we omit replace the condition $\|\beta\|$ by defining $M = \frac{1}{\|\beta\|}$ and optimize

$$\min \|\beta\| \text{ subject to } \begin{cases} y_i(x^T\beta + \beta_0) \geq (1 - \xi_i) \forall i \\ \xi_i \geq 0, \sum \xi_i \leq \textit{constant} \end{cases}$$

We replace the constant by a multiplicative parameter γ and solve

$$\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2 + \gamma \sum_{i=1}^{N} \xi_i$$

subject to $\xi_i \geq 0$ and $y_i(x^T\beta + \beta_0) \geq (1 - \xi_i)$.

- We can set $\gamma = \infty$ for the separable case.
- Large γ: a complex boundary, fewer support vectors.
- Small γ: a smooth boundary, a robust model, many support vectors.
- γ usually set by crossvalidation.

We solve

$$\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2 + \gamma \sum_{i=1}^{N} \xi_i$$

subject to $\xi_i \geq 0$ and $y_i(x_i^T\beta + \beta_0) \geq (1 - \xi_i)$.
Lagrange multipliers again for α_i, μ_i:

$$L_P = \frac{1}{2}\|\beta\|^2 + \gamma \sum_{i=1}^{N} \xi_i - \sum_{i=1}^{N} \alpha_i[y_i(x_i^T\beta + \beta_0) - (1 - \xi_i)] - \sum_{i=1}^{N} \mu_i\xi_i$$

Setting the derivative $= 0$ we get:

$$\beta = \sum_{i=1}^{N} \alpha_i y_i x_i$$

$$0 = \sum_{i=1}^{N} \alpha_i y_i$$

$$\alpha_i = \gamma - \mu_i.$$

Substitute to get Wolfe dual:

$$L_D = \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{k=1}^{N} \alpha_i \alpha_k y_i y_k x_i^T x_k$$

and maximize L_D subject to $0 \leq \alpha_i \leq \gamma$ a $\sum_{i=1}^{N} \alpha_i y_i = 0$.
Solution satisfies:

$$\begin{aligned} \alpha_i [y_i (x_i^T \beta + \beta_0) - (1 - \xi_i)] &= 0 \\ \mu_i \xi_i &= 0 \\ \left[y_i (x_i^T \beta + \beta_0) - (1 - \xi_i) \right] &\geq 0 \end{aligned}$$

- The solution is $\hat{\beta} = \sum_{i=1}^{N} \hat{\alpha}_i y_i x_i$.
- **support points** with nonzero coefficients $\widehat{\alpha_i}$ are
  - points at the boundary
    - $\widehat{\xi_i} = 0$ (therefore $0 < \widehat{\alpha_i} < \gamma$),
  - and points on the wrong side of the margin
    - $\widehat{\xi_i} > 0$ (and $\widehat{\alpha_i} = \gamma$).
- Any point with $\widehat{\xi_i} = 0$ can be used to calculate $\widehat{\beta_0}$, typically an average.
  - $\widehat{\beta_0}$ for a boundary point $\alpha_i > 0$, $\xi_i = 0$:

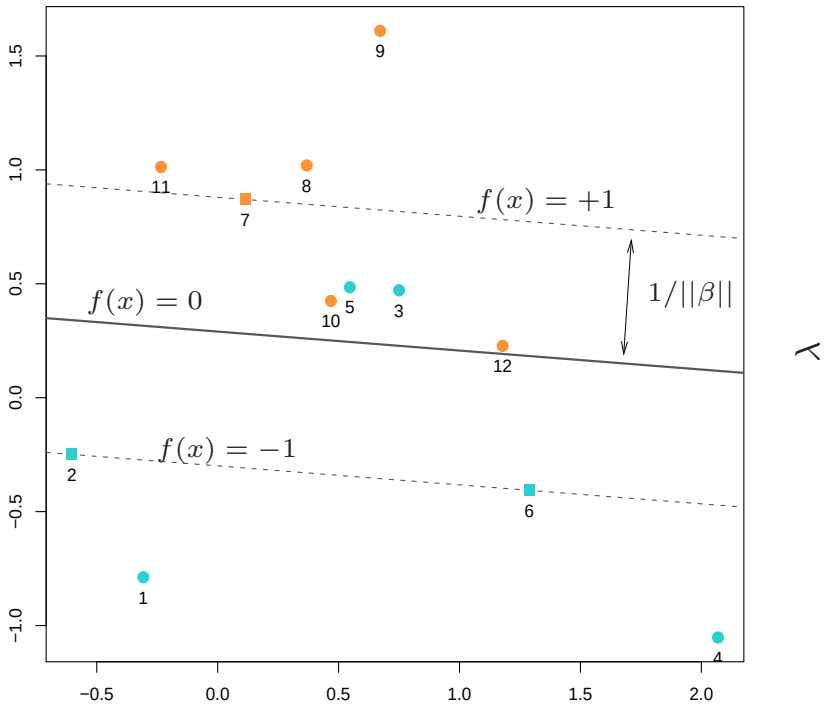
$$\alpha_i \left[y_i (x^T \widehat{\beta} + \widehat{\beta_0}) - (1 - 0) \right] = 0$$

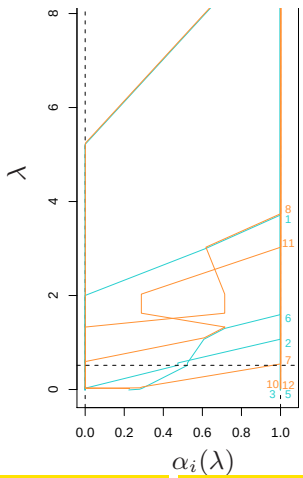
- Parameter γ settled by tuning (crossvalidation)

SVM Solution

- The solution is $\hat{\beta} = \sum_{i=1}^{N} \hat{\alpha}_i y_i x_i$.
- **support points** with nonzero coefficients $\widehat{\alpha}_i$ are
  - points at the boundary
    - $\widehat{\xi}_i = 0$ (therefore $0 < \widehat{\alpha}_i < \gamma$),
  - and points on the wrong side of the margin
    - $\widehat{\xi}_i > 0$ (and $\widehat{\alpha}_i = \gamma$).
- Any point with $\widehat{\xi}_i = 0$ can be used to calculate $\widehat{\beta}_0$, typically an average.
  - $\widehat{\beta}_0$ for a boundary point $\xi_i = 0$:

$$\alpha_i \left[y_i(x^T \widehat{\beta} + \widehat{\beta}_0) - (1 - 0) \right] = 0$$





- $\alpha = \xi = 0$ for points 1,4,8,9,11
- $\alpha > 0, \xi = 0$ for points 2,6,8
- missclassified points 3,5.

Support Vector Machines

Let us have the training data $(x_i, y_i)_{i=1}^N$, $x_i \in \mathbb{R}^p$, y_i in $\{-1, 1\}$. We define a hyperplane

$$\{x : f(x) = x^T \beta + \beta_0 = 0\} \tag{13}$$

where $\|\beta\| = 1$.
We classify according to

$$G(x) = sign\left[x^T \beta + \beta_0\right]$$

where $f(x)$ is a signed distance of x from the hyperplane.
Support vector machines replace the scalar product $\langle x_i, x \rangle$ by a kernel function.

$$\begin{aligned}
\hat{f}(x) &= \beta x + \hat{\beta}_0 \\
\hat{f}(x) &= \sum_{k=1}^{N} \hat{\alpha}_i y_i x_i^T x + \hat{\beta}_0 \\
\hat{f}(x) &= \sum_{k=1}^{N} \hat{\alpha}_i y_i \langle x_i, x \rangle + \hat{\beta}_0 \\
\hat{f}(x) &= \sum_{k=1}^{N} \hat{\alpha}_i y_i K(x_i, x) + \hat{\beta}_0
\end{aligned}$$

SVM Example

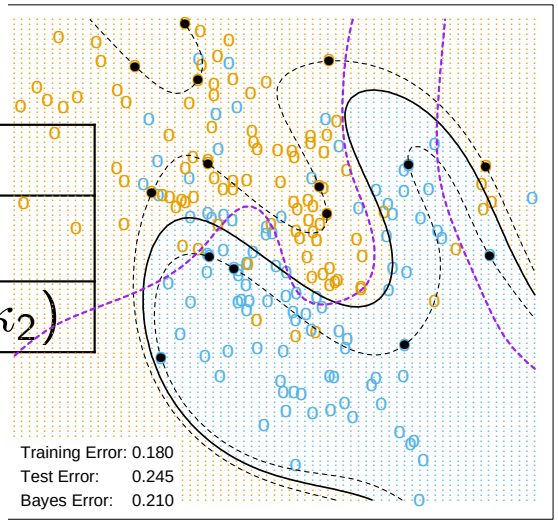
- **kernel functions** are function to replace scalar product with a scalar product in a transformed space.

dth Degree polynomial:	$K(x, x') = (1 + \langle x, x' \rangle)^d$
Radial basis	$K(x, x') = exp(\frac{-\|x-x'\|^2}{\ell})$
Neural network	$K(x, x') = tanh(\kappa_1 \langle x, x' \rangle + \kappa_2)$

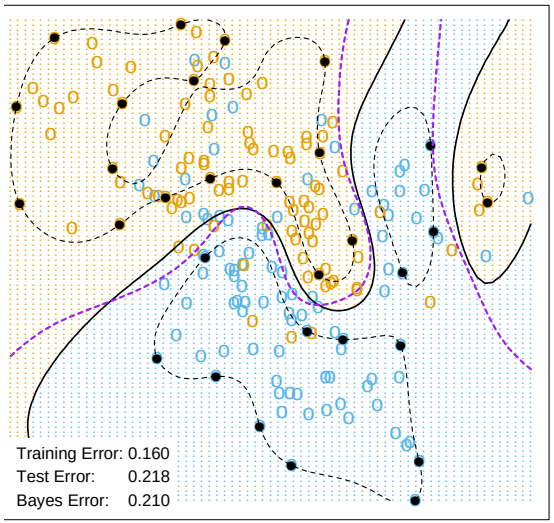
- For example a degree 2 with two dimensional input:
  $K(x, x') = (1 + \langle x, x' \rangle)^2 =$
  $(1 + 2x_1x_1' + 2x_2x_2' + (x_1x_1')^2 + (x_2x_2')^2 + 2x_1x_1'x_2x_2')$
- that is $M = 6$, $h_1(x) = 1$, $h_2(x) = \sqrt{2}x_1$, $h_3(x) = \sqrt{2}x_2$, $h_4(x) = x_1^2$, $h_5(x) = x_2^2$, $h_6(x) = \sqrt{2}x_1x_2$.

The classification function
$\hat{f}(x) = h(x)^T\beta + \beta_0 = \sum_{i=1}^{N} \alpha_i y_i \langle h(x), h(x_i) \rangle + \beta_0$
does not need evaluation of $h(i)$, only the scalar product $\langle h(x), h(x_i) \rangle$.

SVM - Degree-4 Polynomial in Feature Space



SVM - Radial Kernel in Feature Space



String Kernels and Protein Classification

IPTSALVKETLALLSTHRTLLIANETLRIPVPVHKNHQLCTEEIFQGIGTLESQTVQGGTV
ERLFKNLSLIKKYIDGQKKKCGEERRRVNQFLDY**LQE**FLGVMNTEWI

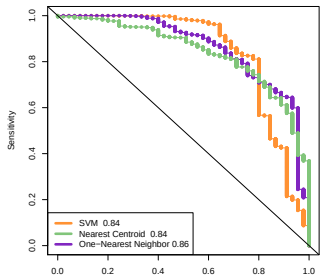
PHRRDLCSRSIWLARKIRSDLTALTESYVKHQGLWSELTEAER**LQE**NLQAYRTFHVLLA
RLLEDQQVHFTPTEGDFHQAIHTLLLQVAAFAYQIEELMILLEYKIPRNEADGMLFEKK

- Consider all possible sequences of length m.
- We define a feature map

$$\Phi_m(x) = \{\phi_a(x)\}_{a \in \mathcal{A}_m}$$

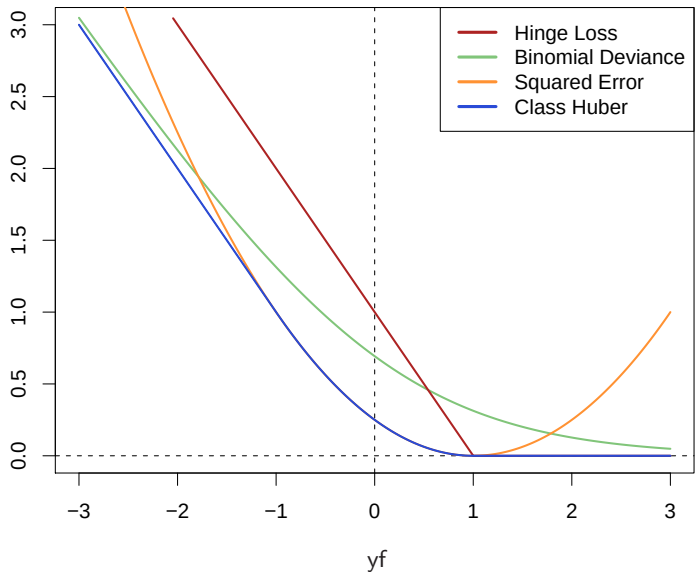
- The kernel function is the inner product:

$$K_m(x_1, x_2) = \langle \Phi_m(x_1), \Phi_m(x_2) \rangle.$$



SVM as a Penalization Method

- We fit a linear function wrt. basis $\{h_i(x)\}$: $f(x) = h^T\beta + \beta_0$.
- Consider the loss function $L(y, f) = [1 - yf]_+$
  - The optimization problem $min_{\beta_0,\beta} \sum_{i=1}^{N}[1 - yf]_+ + \lambda\|\beta\|^2$
- is equivalent to SVM
  - $\min_{\beta,\beta_0} \frac{1}{2}\|\beta\|^2 + \gamma\sum_{i=1}^{N}\xi_i$
  - subject to $\xi_i \geq 0$ and $y_i(x^T\beta + \beta_0) \geq (1 - \xi_i)$.
- is similar to smoothing splines penalty:
  - $\min_{\alpha,\alpha_0} \sum_{i=1}^{N}[1 - yf]_+ + \lambda\alpha^T\mathbf{K}\alpha$
  - where $\alpha^T\mathbf{K}\alpha = J(f)$ is the smoothing penalty.



Loss Function	$L[y, f(x)]$	Minimizing Function
Binomial Deviance	$\log[1 + e^{-yf(x)}]$	$f(x) = \log\frac{\Pr(Y=+1\|x)}{\Pr(Y=-1\|x)}$
SVM Hinge Loss	$[1 - yf(x)]_+$	$f(x) = \text{sign}[\Pr(Y=+1\|x) - \frac{1}{2}]$
Squared Error	$[y - f(x)]^2 = [1 - yf(x)]^2$	$f(x) = 2\Pr(Y=+1\|x) - 1$
"Huberised" Square Hinge Loss	$-4yf(x)$, $yf(x) < -1$ $[1 - yf(x)]_+^2$ otherwise	$f(x) = 2\Pr(Y=+1\|x) - 1$

SVM and Kernel Dimsension

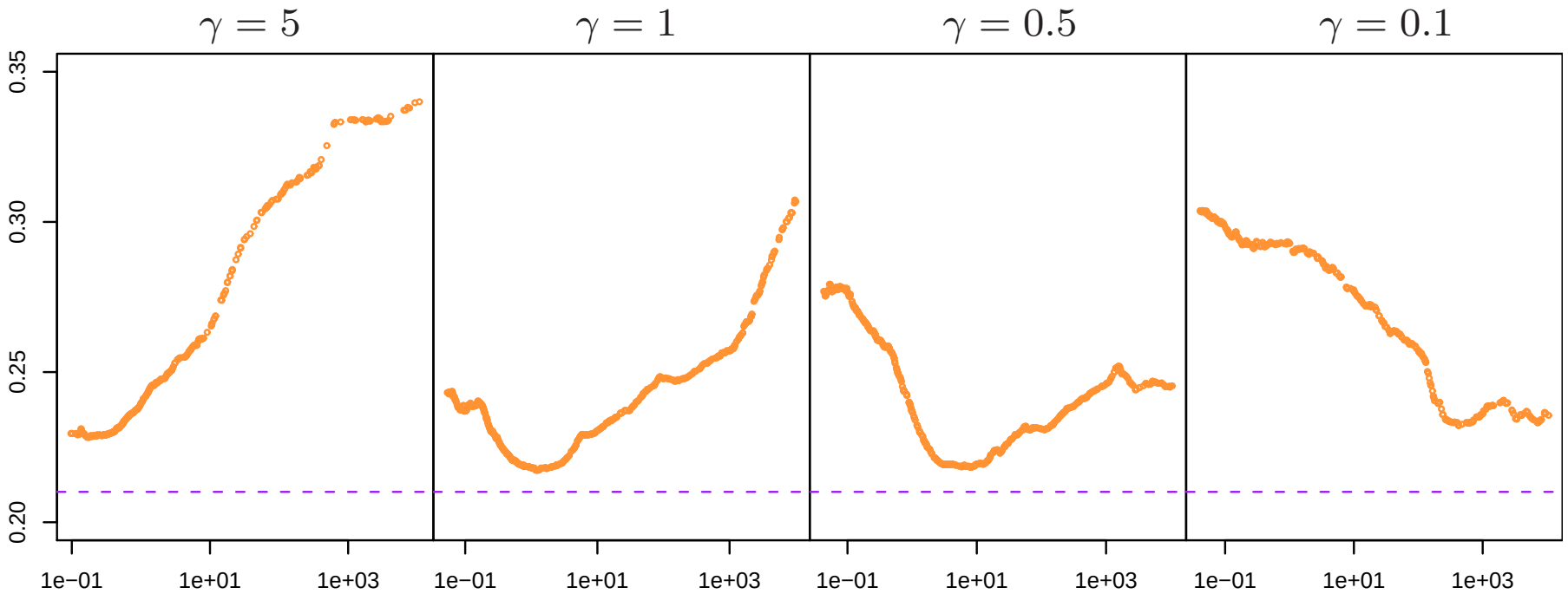
- The first Simulated example
  - 100 observations of each class
  - First class: four standard normal independent features X_1, X_2, X_3, X_4.
  - Second class conditioned on $9 \leq \sum X_j^2 \leq 16$.
- Second example
  - The first one augmented with an additional six standard Gaussian noise features.
- BRUTTO: Additive spline model.
- BRUTTO and MARS has the ability to ignore noisy features.
- We can see the overfitting of SVM. The degree 2 polynomial kernel is the best since the decision boundary is quadratic.

	Test Error (SE)	
Method	No Noise Features	Six Noise Features
SV Classifier	0.450 (0.003)	0.472 (0.003)
SVM/poly 2	0.078 (0.003)	0.152 (0.004)
SVM/poly 5	0.180 (0.004)	0.370 (0.004)
SVM/poly 10	0.230 (0.003)	0.434 (0.002)
BRUTO	0.084 (0.003)	0.090 (0.003)
MARS	0.156 (0.004)	0.173 (0.005)
Bayes	0.029	0.029

SVM Complexity

The SVM complexity is $m^3 + mN + mpN$, where m is the number of support vectors.

Parameter tuning for different radial basis lengthscale γ.



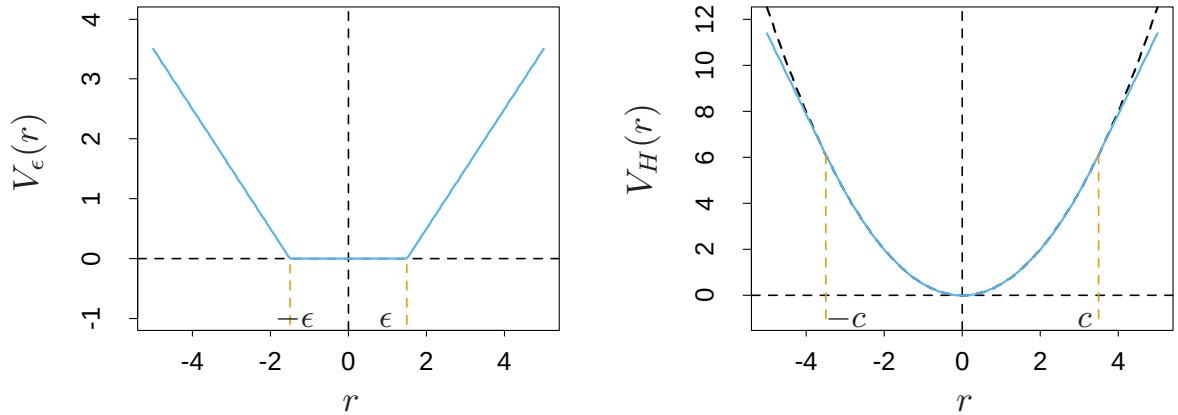
SVM for Regression

- In regression, we fit a function: $f(x) = x^T\beta + \beta_0$
- We consider error function V_ϵ (left figure)

$$V_\epsilon(r) = \begin{cases} 0 & \text{if } |r| < \epsilon, \\ |r| - \epsilon, & \text{otherwise.} \end{cases}$$

- and minimize:

$$H(\beta, \beta_0) = \sum_{i=1}^{N} V_\epsilon(y_i - f(x_i)) + \frac{\lambda}{2}\|\beta\|^2$$



SVM for Regression 2

- The solution has the form: $\hat{\alpha}_i, \hat{\alpha}_i^* \geq 0$

$$\begin{aligned} \hat{\beta} &= \sum_{i=1}^{N} (\hat{\alpha}_i^* - \hat{\alpha}_i) x_i, \\ \hat{f}(x) &= \sum_{i=1}^{N} (\hat{\alpha}_i^* - \hat{\alpha}_i) \langle x, x_i \rangle + \beta_0, \end{aligned}$$

- and solve the quadratic programming problem

$$\min_{\alpha_i, \alpha_i^*} \epsilon \sum_{i=1}^{N} (\alpha_i^* + \alpha_i) - \sum_{i=1}^{N} y_i (\alpha_i^* - \alpha_i) + \frac{1}{2} \sum_{i,i'=1}^{N} (\alpha_i^* - \alpha_i)(\alpha_{i'}^* - \alpha_{i'}) \langle x_i, x_{i'} \rangle$$

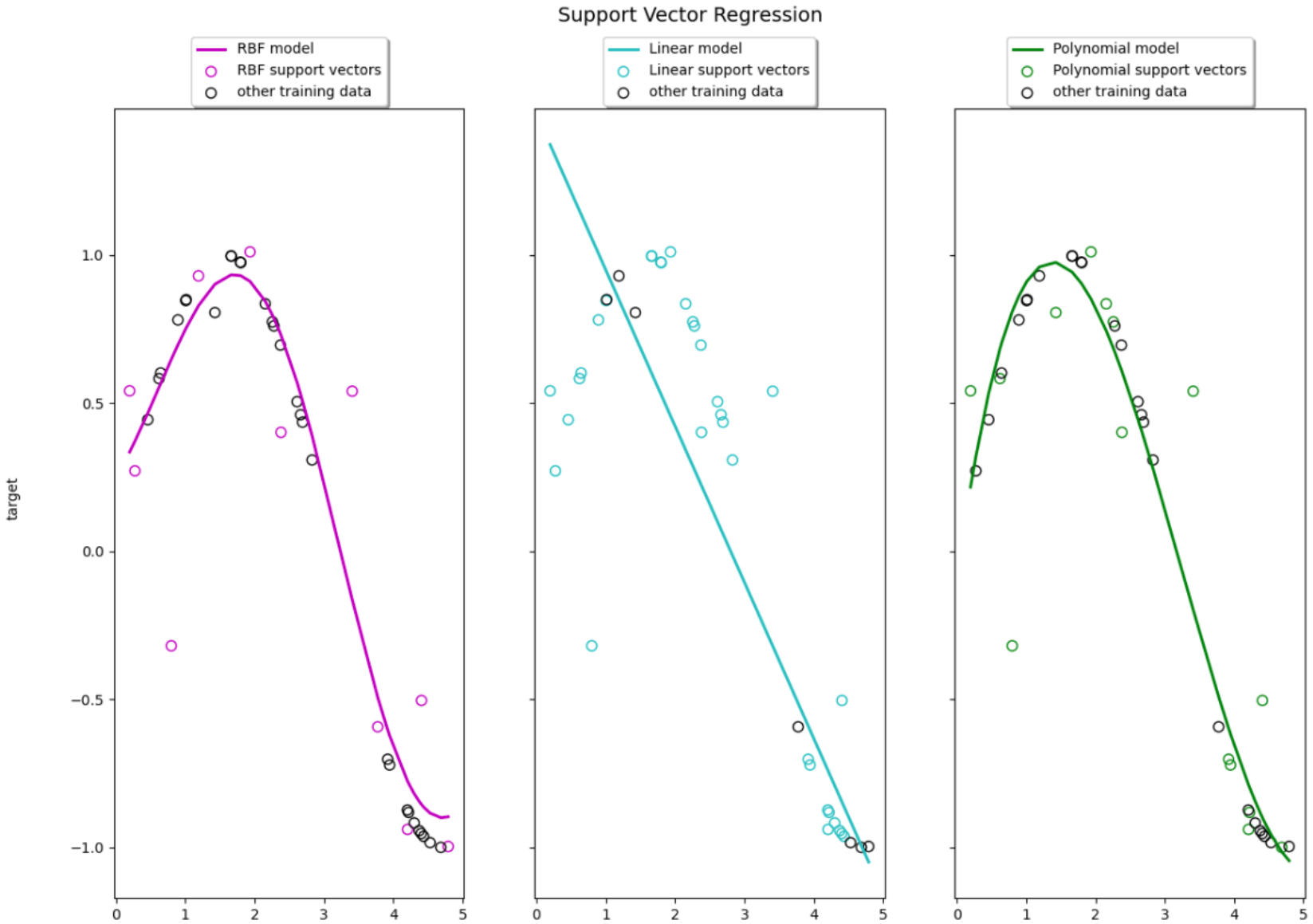
- subject to the constraints

$$\begin{aligned} 0 \leq \alpha_i,\ \alpha_i^* \leq 1/\lambda, \\ \sum_{i=1}^{N} (\alpha_i^* - \alpha_i) = 0, \\ \alpha_i \alpha_i^* = 0. \end{aligned}$$

- Support vectors are those with nonzero $(\hat{\alpha}_i^* - \hat{\alpha}_i)$.
- With scaled response y, you may use the default ϵ.
- λ is tuned by cross-validation.

SVR

sklearn.svm.SVR



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