Machine Learning

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

Marta Vomlelová

marta@ktiml.mff.cuni.cz
http://ktiml.mff.cuni.cz/~marta

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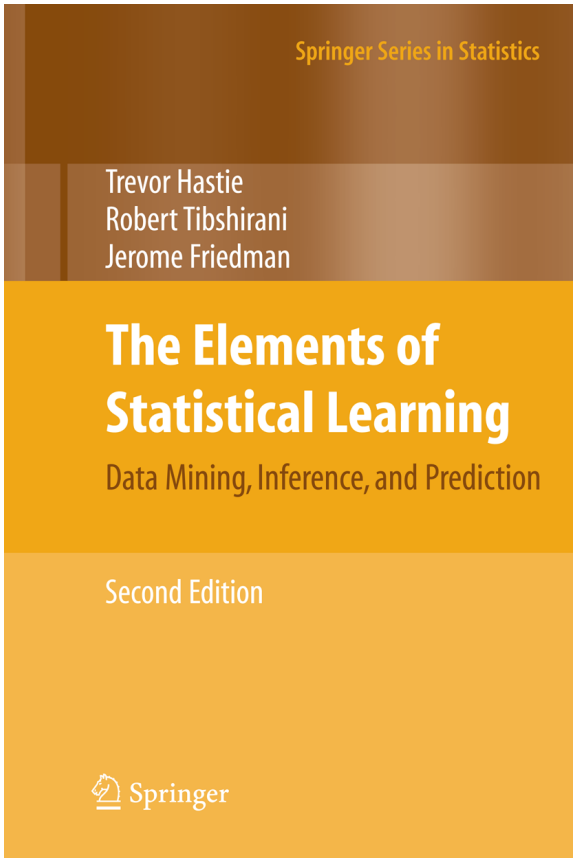
Literature



- 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

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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

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

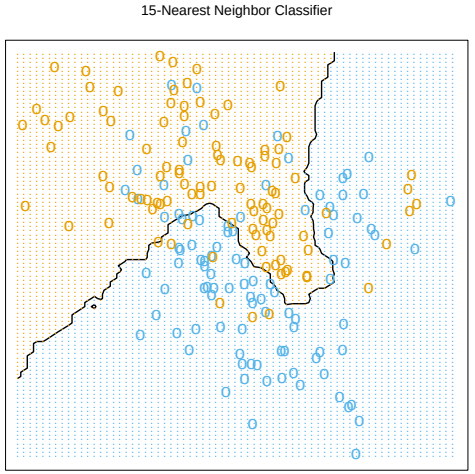
  - where *mean* denotes average, and $N_k(x)$ is the neighborhood containing k points in $\mathcal{T}$ closest to x.
- Under mild regularity conditions on $P(X, Y)$ one can show as $k, N \to \infty$, such that $\frac{k}{N} \to 0$ then $\hat{f}(x) \to \mathbb{E}(Y|X = x)$.
- **The rate of convergence decreases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

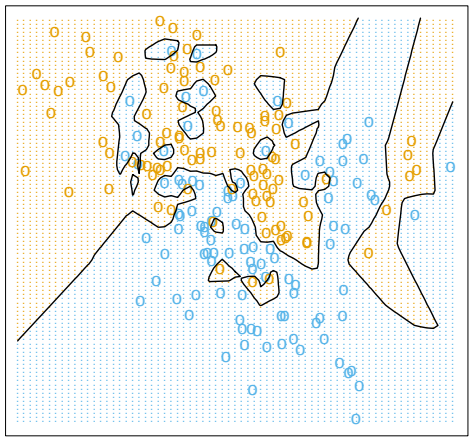
Nearest-Neighbor Methods

- 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

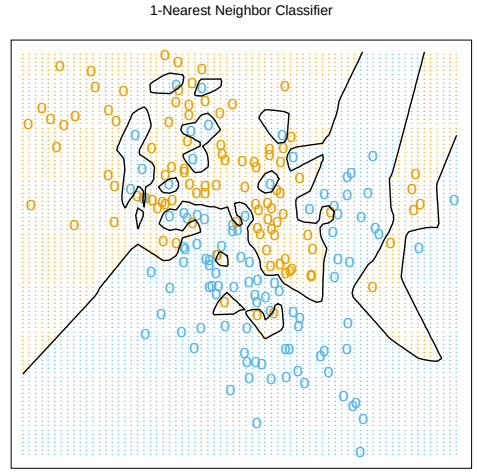
The effective number of parameters of k nearest neighbors is N/k and is generally bigger than p of the linear regression.

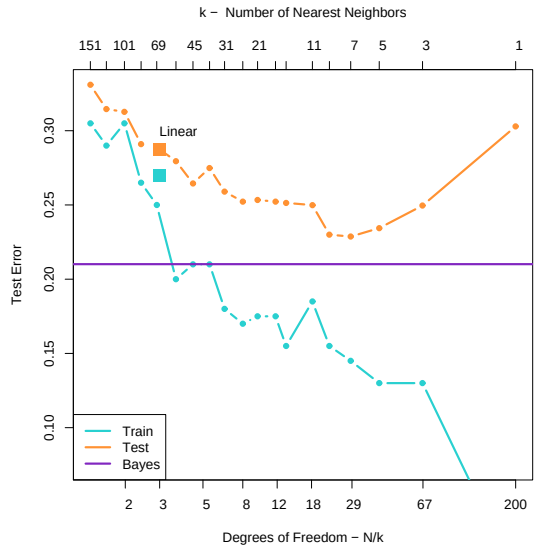
Prediction complexity

'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.

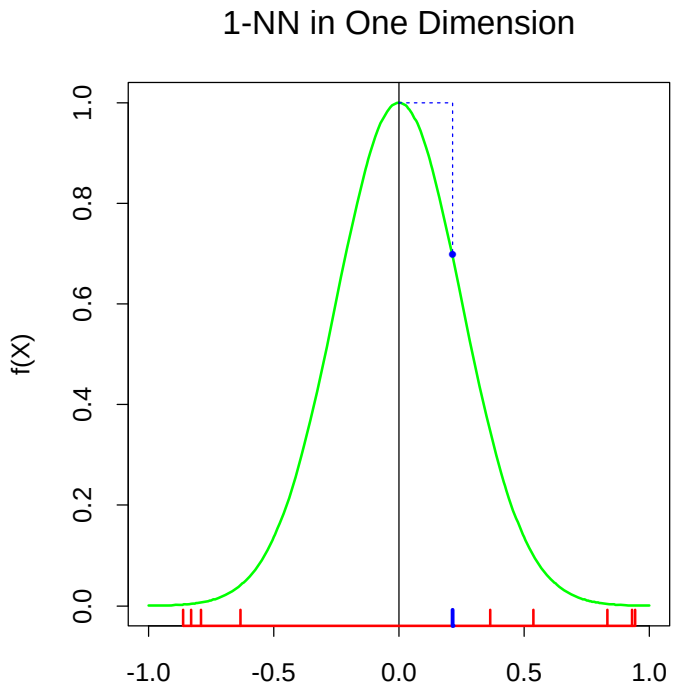


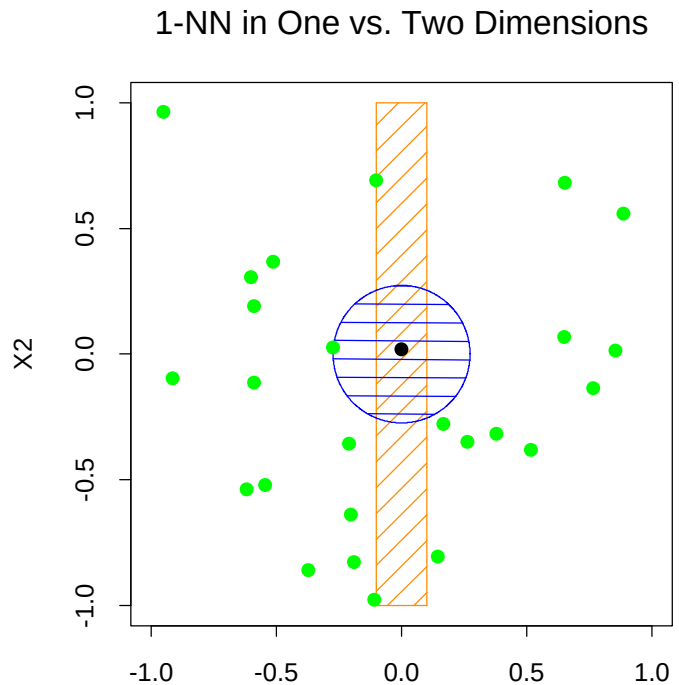


Curse of Dimensionality demonstration

Prediction

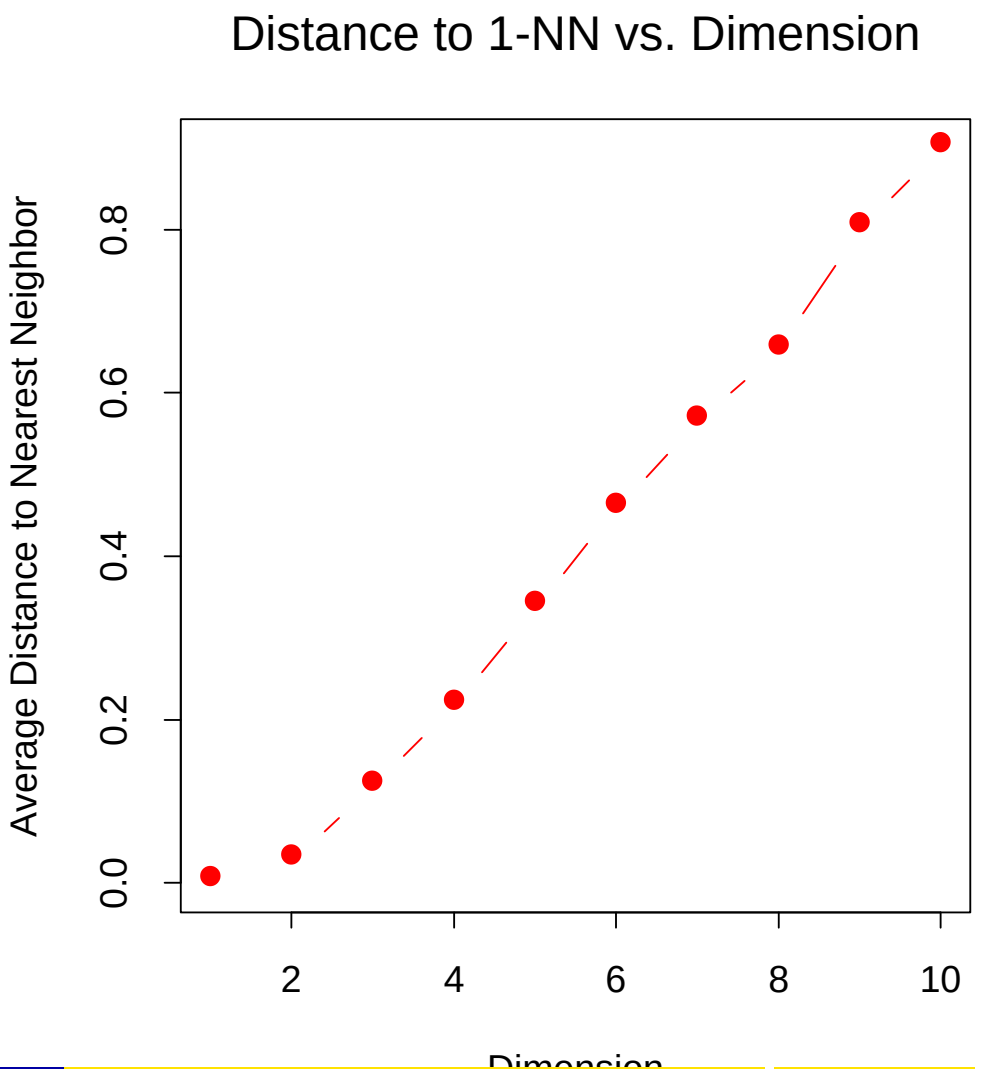
- Assume x_i uniformly generated form the interval $\langle -1, 1 \rangle^p$
- We have $Y = f(X) = e^{-8\|X\|^2}$, without any noise, for x_i we know exactly $f(x_i)$.
- We use 1–NN to estimate $f(0)$ based on 1000 data sample.
- Predicted value for $x = \langle 0, \ldots, 0 \rangle$ is lower that 1 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

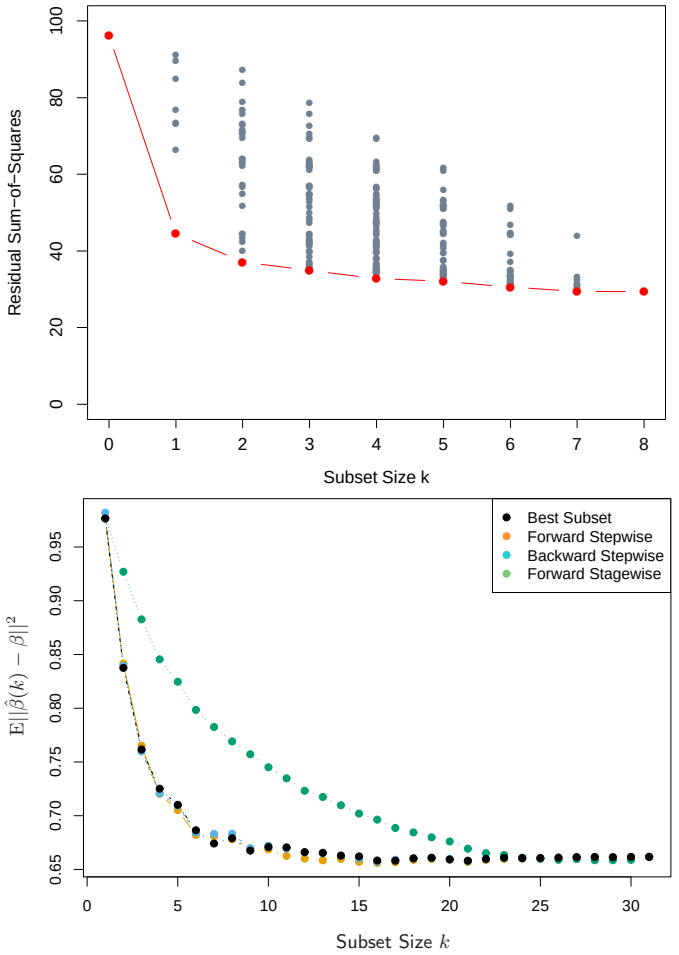
- $O(p^2N)$

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

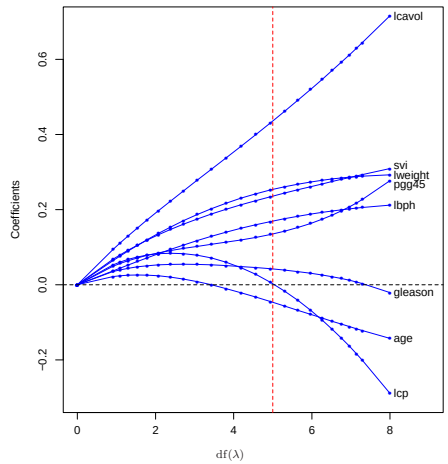
$$\rho_{j,k} \leftarrow corr(\mathbf{x}_j, \mathbf{x}_k) \leftarrow \frac{s_{j,k}}{s_j s_k} = \frac{\frac{1}{N}\sum_{i=1}^{N}(x_{ij} - \overline{x}_j)(x_{ik} - \overline{x}_k)}{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_{ij} - \overline{x}_j)^2}\sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_{ik} - \overline{x}_k)^2}}$$

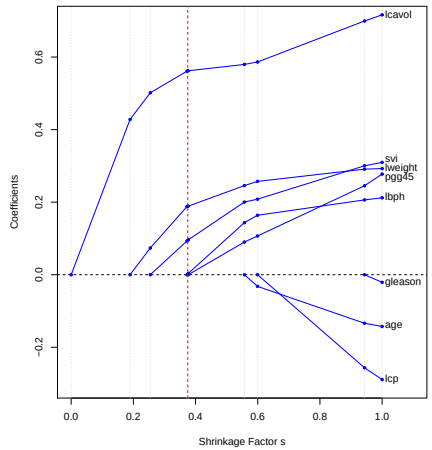
- For standardized features, the correlation is just $\frac{\mathbf{x}_j^T \mathbf{x}_k}{N}$.

Penalized Methods

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

- 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()
```

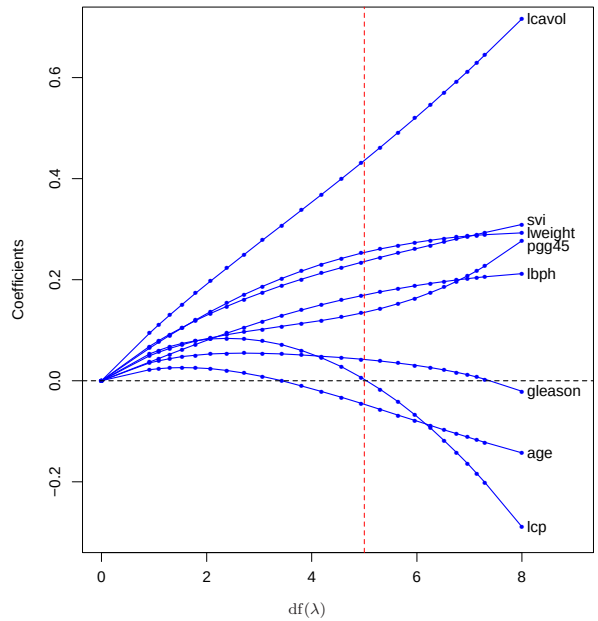
Rigde Regression

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

- 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

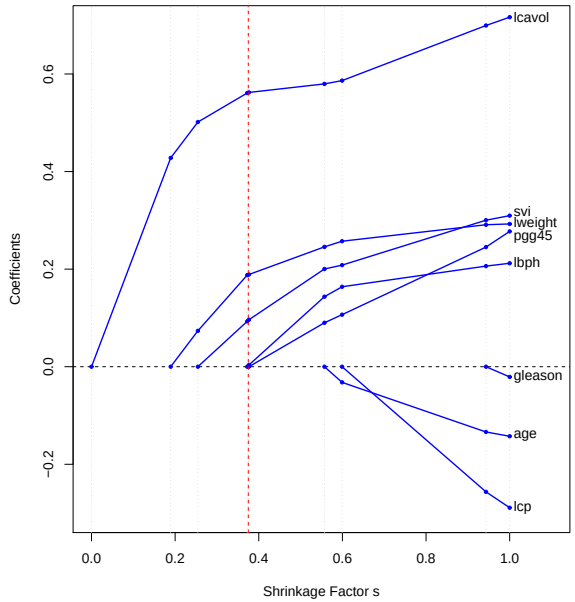
$$\hat{\beta}^{lasso} = argmin_{\beta} \left(\sum_{i=1}^{N} (y_i - \beta_0 - \mathbf{x}_i^T \beta)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right)$$

- Solved by a quadratic programming algorithm

  sklearn.linear_model.Lasso

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

  sklearn.linear_model.Lars

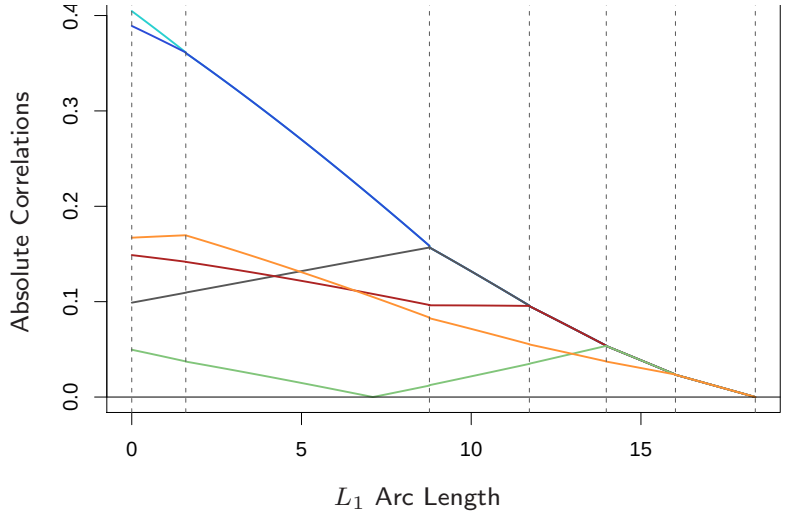


LARS Idea

- 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.

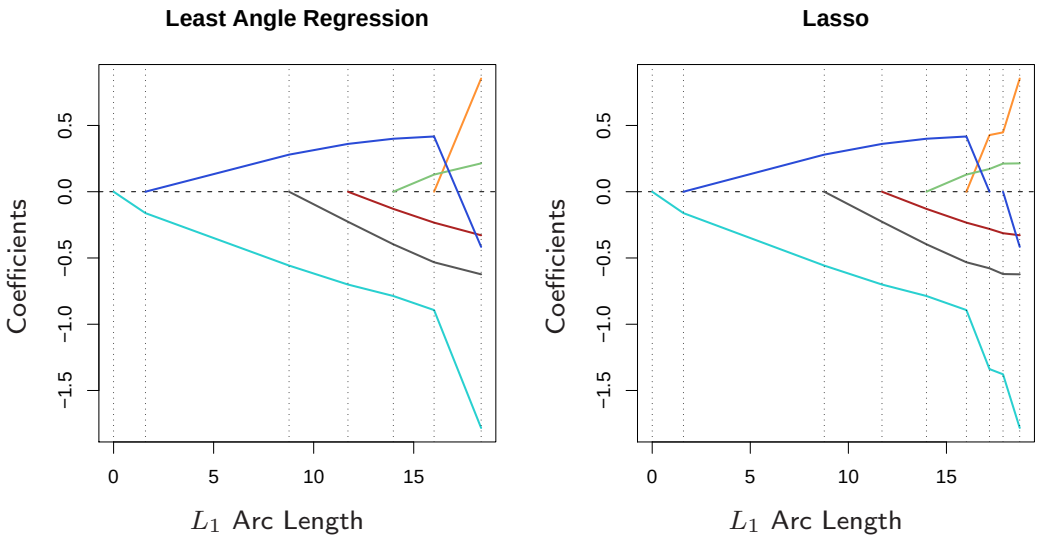


LARS Least Angle Regression

- 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, 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

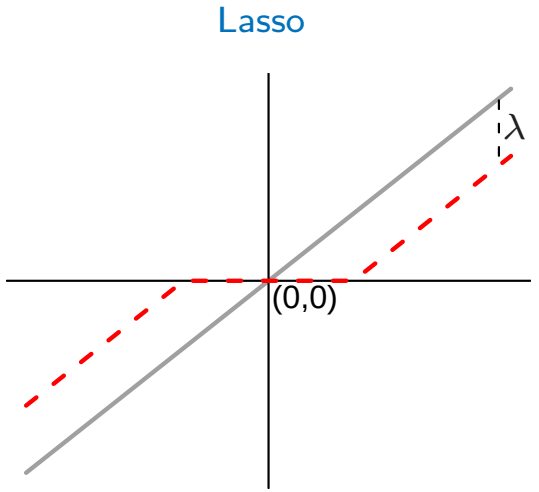
- this has an explicit solution, resulting in the update

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

- 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

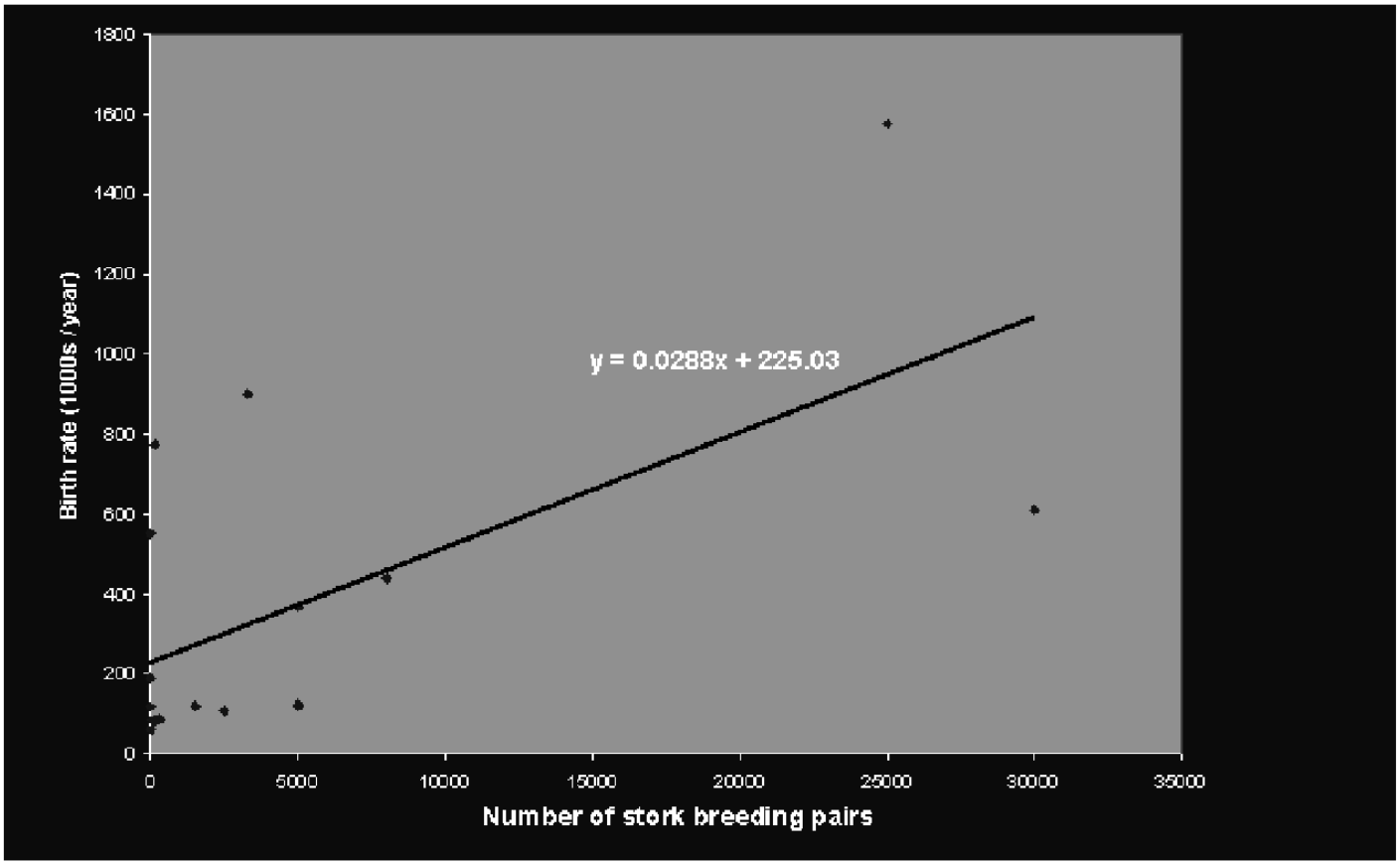


Fig 1. How the number of human births varies with stork populations in 17 European countries.

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.

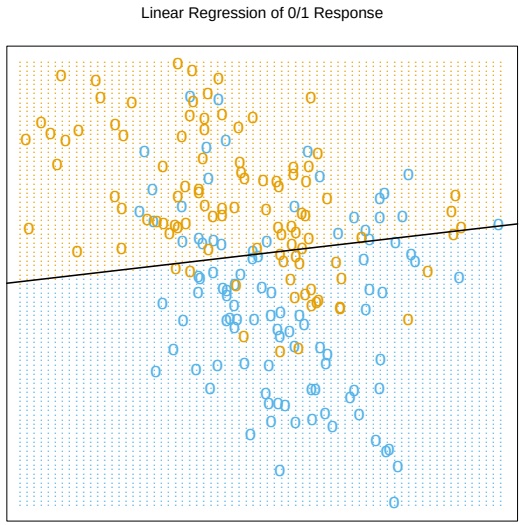


FIGURE 2.1. *A classification example in two dimensions. The classes are coded as a binary variable (*BLUE $= 0$, ORANGE $= 1$*), and then fit by linear regression. The line is the decision boundary defined by* $x^T\hat{\beta} = 0.5$*. The orange shaded region denotes that part of input space classified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

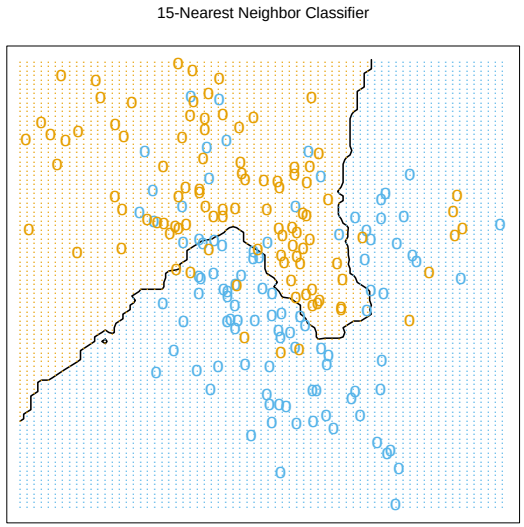


FIGURE 2.2. *The same classification example in two dimensions as in Figure 2.1. The classes are coded as a binary variable (*BLUE $= 0$, ORANGE $= 1$*) and then fit by* 15*-nearest-neighbor averaging as in (2.8). The predicted class is hence chosen by majority vote amongst the* 15*-nearest neighbors.*

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