Data Analysis: Statistical Modeling and Computation in Applications

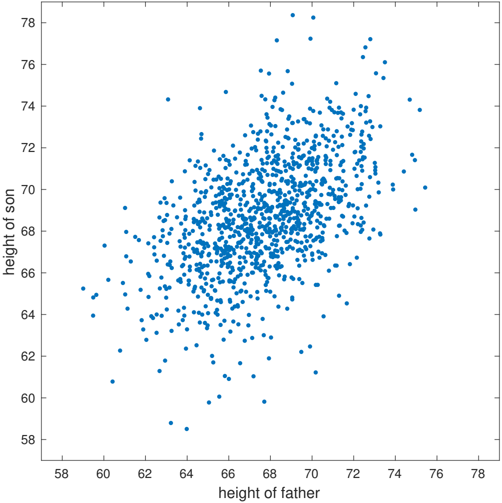
Correlation and Least Squares Regression

Outline

- Correlation
- Regression line
- Evaluation
- Multiple regression
- Computing the estimator
- Variable selection and regularization

Scatter diagram: height of 1078 fathers and their sons

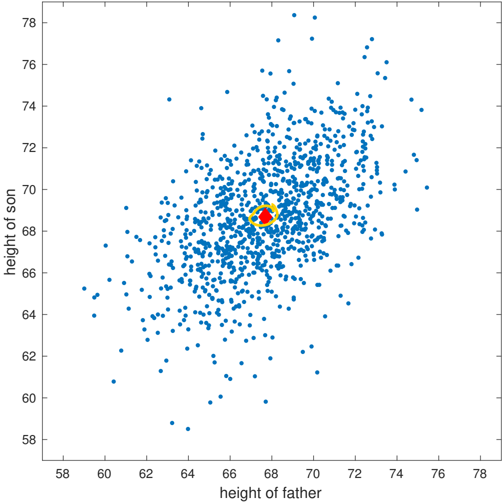
Is there an association?
What kind?



Data: Pearson K and Lee A. (1903). On the laws of inheritance in man. Biometrika, 2:357-462.
Downloaded from `https://myweb.uiowa.edu/pbreheny/data/pearson.html`

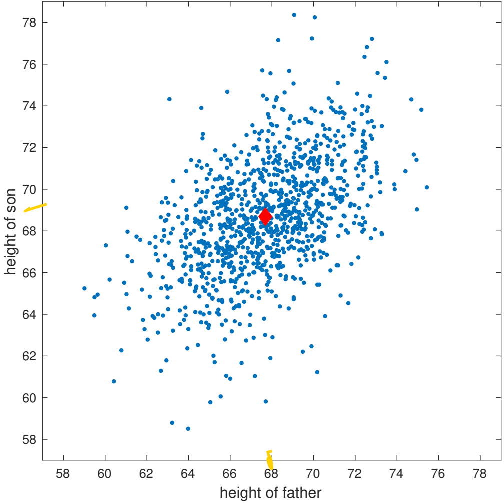
Summarizing the Plot

- average $\bar{x}$, $\bar{y}$



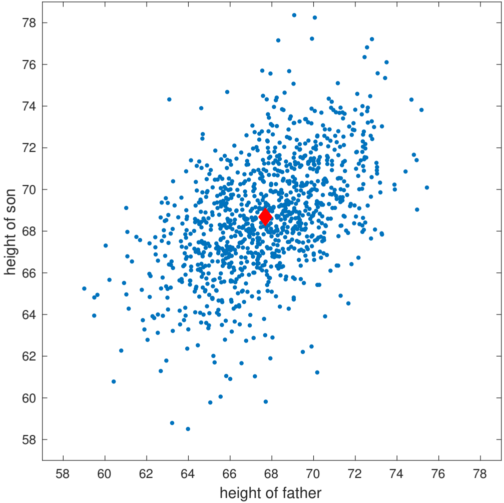
Summarizing the Plot

- average $\bar{x}$, $\bar{y}$
  fathers: $\bar{x} \approx 68$,
  sons: $\bar{y} \approx 69$



Summarizing the Plot

- average $\bar{x}$, $\bar{y}$
  fathers: $\bar{x} \approx 68$,
  sons: $\bar{y} \approx 69$
- standard deviation
  $s_x = \frac{1}{N}\sqrt{\sum_{i=1}^{N}(x_i - \bar{x})^2}$
  here: $s_x \approx s_y \approx 2.7$



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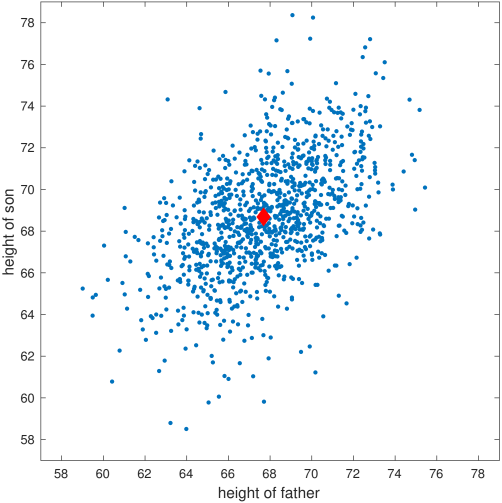
  $s_x = \frac{1}{N}\sqrt{\sum_{i=1}^{N}(x_i - \bar{x})^2}$
  here: $s_x \approx s_y \approx 2.7$
- correlation coefficient
  $r \approx 0.5$



Correlation Coefficient

$$r = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{x_i - \bar{x}}{s_x}\right)\left(\frac{y_i - \bar{y}}{s_y}\right) = \frac{\mathrm{cov}(x, y)}{s_x s_y}$$

(convert to standard units and take average product)

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1. symmetric

Correlation Coefficient

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(convert to standard units and take average product)

1. symmetric
2. Why standard units?

Correlation Coefficient

$$r = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{x_i - \bar{x}}{s_x}\right)\left(\frac{y_i - \bar{y}}{s_y}\right) = \frac{\mathrm{cov}(x, y)}{s_x s_y}$$

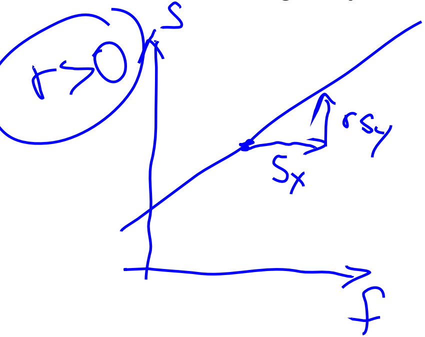
(convert to standard units and take average product)

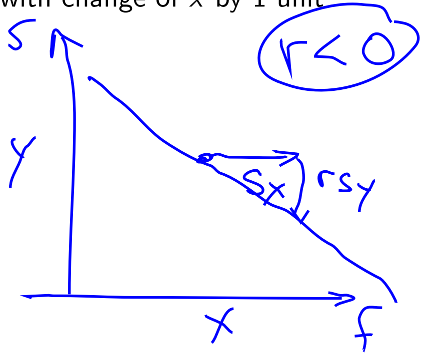
1. symmetric
2. Why standard units?
   adding or multiplying constants to all x_i or y_i does not change r
3. What does $r \approx 0.5$ mean?

What does the Correlation coefficient mean? (1)

$$r = \frac{1}{N}\sum_{i=1}^{N}\left(\frac{x_i-\bar{x}}{s_x}\right)\left(\frac{y_i-\bar{y}}{s_y}\right)$$

- measures *linear* association between variables:
  how much change of y is associated with change of x by 1 unit





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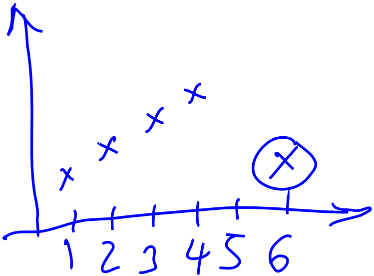
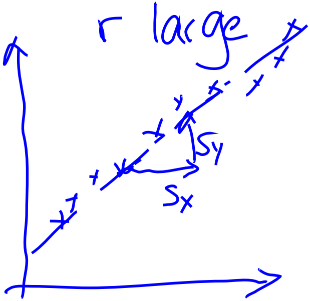
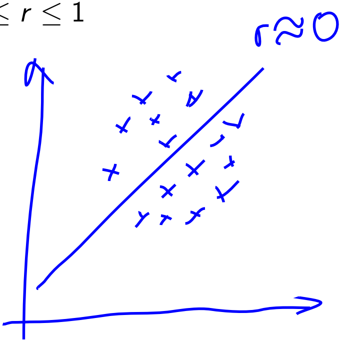


$$r = \frac{1}{N} \sum_{i=1}^{N} \left(\frac{x_i - \bar{x}}{s_x} \right) \left(\frac{y_i - \bar{y}}{s_y} \right)$$

- measures *clusteredness* along a line: $-1 \leq r \leq 1$
  sign?



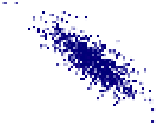


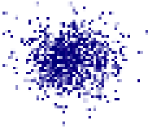
Examples

1.

2.

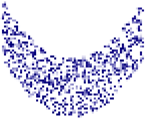
3.





4.

5.



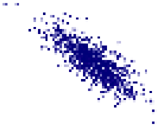
6.

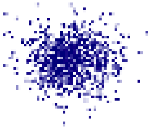
Examples

1. $r = 1$

2.

3.





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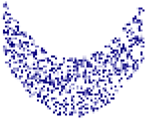
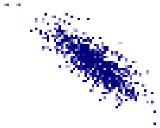


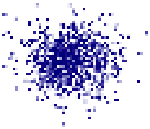
6.

1. $r = 1$

2. $r = -1$

3.





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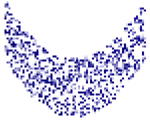

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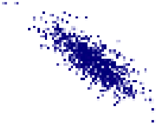
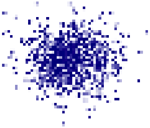
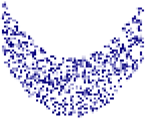




4. $r = 0$

5.



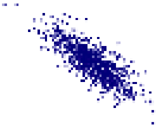
6.

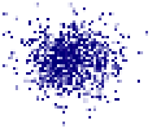
Examples

1. $r = 1$

2. $r = -1$

3. $r = -0.8$





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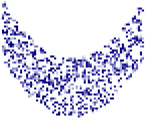
5.



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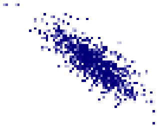
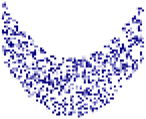


5. $r = 0$



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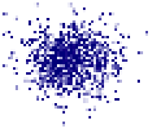

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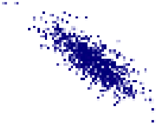

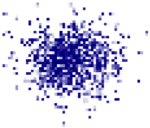

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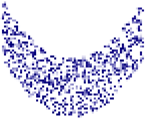

6. $r = 0$

Careful with nonlinearities and outliers!

Correlation coefficient: summary

$$r = \frac{1}{N} \sum_{i=1}^{N} \left(\frac{x_i - \bar{x}}{s_x} \right) \left(\frac{y_i - \bar{y}}{s_y} \right)$$

- measures *linear* association between variables:
- measures clusteredness along a line
- symmetric (swapping x and y)
- between -1 and 1, and invariant to
  - adding a constant to all x_i or all y_i
  - multiplying to all x_i (all y_i) by a positive constant

Data Analysis:
Statistical Modeling and Computation in Applications

Correlation and Least Squares Regression
Part 4

Outline

- Correlation
- Regression line
- Evaluation
- Multiple regression
- Computing the estimator
- Variable selection and regularization

Multiple regression

- Model: $y_i = \beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \underline{\epsilon_i}$

ozone	radiation	temp
41	190	67
36	118	72
12	149	74
18	313	62
y_i	x_{i1}	x_{i2}

Multiple regression

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12	149	74
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- Model: $y_i = \beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \epsilon_i$
- vector form: $y_i = \mathbf{x}_i \boldsymbol{\beta} + \epsilon_i$

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- Matrix-vector form: $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \epsilon$

$$41 = \beta_0 + 190\beta_1 + 67\beta_2 + \epsilon_1$$

$$\underbrace{\begin{pmatrix} \boxed{41} \\ 36 \\ 12 \\ 18 \end{pmatrix}}_{y} = \underbrace{\begin{pmatrix} 1 & 190 & 67 \\ 1 & 118 & 72 \\ 1 & 149 & 74 \\ 1 & 313 & 62 \end{pmatrix}}_{X} \underbrace{\begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}}_{\beta} + \underbrace{\begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \end{pmatrix}}_{\epsilon}$$

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- Matrix-vector form: $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \epsilon$
  - $\mathbf{y}$ dependent / response variable: $N \times 1$

$$N \quad \underbrace{\begin{pmatrix} 41 \\ 36 \\ 12 \\ 18 \end{pmatrix}}_{Y} = \begin{pmatrix} 1 & 190 & 67 \\ 1 & 118 & 72 \\ 1 & 149 & 74 \\ 1 & 313 & 62 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \end{pmatrix}$$

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  - $\mathbf{X}$ design matrix: $N \times p$

$$\begin{pmatrix} 41 \\ 36 \\ 12 \\ 18 \end{pmatrix} = N \overbrace{\begin{pmatrix} 1 & 190 & 67 \\ 1 & 118 & 72 \\ 1 & 149 & 74 \\ 1 & 313 & 62 \end{pmatrix}}^{p} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \end{pmatrix}$$

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  - $\mathbf{X}$ design matrix: $N \times p$
  - $\boldsymbol{\beta}$ parameters: $p \times 1$
  - ϵ: random error / disturbances
    ϵ_i are iid, $\mathbb{E}[\epsilon_i] = 0$, $Var(\epsilon_i) = \sigma^2$

$$\begin{pmatrix} 41 \\ 36 \\ 12 \\ 18 \end{pmatrix} = \begin{pmatrix} 1 & 190 & 67 \\ 1 & 118 & 72 \\ 1 & 149 & 74 \\ 1 & 313 & 62 \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \end{pmatrix}$$

Examples of multiple regression

- **Simple linear regression**:

$$p = 2,\ X = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_N \end{pmatrix},\ \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix},\ \ y_i = \beta_0 + \beta_1 x_1$$

Examples of multiple regression

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- **Quadratic (polynomial) regression**:

$$p = 3,\ X = \begin{pmatrix} 1 & x_1 & x_1^2 \\ \vdots & \vdots & \vdots \\ 1 & x_N & X_N^2 \end{pmatrix},\ \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix},\ \ y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i1}^2$$

Examples of multiple regression

- **Effect on groups**. Consider an example where we have data obtained on different days. The effect of the days can be modeled as
  $y_i = \underbrace{\beta_0}_{\text{day 1}} + \underbrace{\beta_1}_{\text{day 2}} + \underbrace{\beta_2}_{\text{day 3}} + \epsilon_i$

Examples of multiple regression

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$y_i = \underbrace{\beta_0}_{\text{day 1}} + \underbrace{\beta_1}_{\text{day 2}} + \underbrace{\beta_2}_{\text{day 3}} + \epsilon_i$

$$p = 3, \quad X = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 1 \\ \vdots & \vdots & \vdots \end{pmatrix}, \ \beta = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}$$

Multiple regression

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$$\underbrace{\begin{pmatrix} 41 \\ 36 \\ 12 \\ 18 \end{pmatrix}}_{Y} \underbrace{=}_{=} \underbrace{\begin{pmatrix} 1 & 190 & 67 \\ 1 & 118 & 72 \\ 1 & 149 & 74 \\ 1 & 313 & 62 \end{pmatrix}}_{X} \underbrace{\begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}}_{\beta} \underbrace{+}_{+} \underbrace{\begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \end{pmatrix}}_{\epsilon}$$

Ordinary Least Squares estimator (OLS)

- model: $y_i = \beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \epsilon_i$
- fitted values: $\hat{y}_i = \hat{\beta}_0 + x_{i1}\hat{\beta}_1 + x_{i2}\hat{\beta}_2$
  or $\hat{y}_i = \mathbf{x}_i\hat{\boldsymbol{\beta}}$

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  or $\hat{y}_i = \mathbf{x}_i\hat{\boldsymbol{\beta}}$
- least squares:

$$\|a\|^2 = a^T a = \sum_{j=1}^{N} a_j^2$$

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{N} (y_i - \underbrace{\mathbf{x}_i\boldsymbol{\beta}}_{\hat{y}_i})^2 = \arg\min_{\beta} \underbrace{\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2}$$

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- fitted values: $\hat{y}_i = \hat{\beta}_0 + x_{i1}\hat{\beta}_1 + x_{i2}\hat{\beta}_2$
  or $\hat{y}_i = \mathbf{x}_i\hat{\boldsymbol{\beta}}$
- least squares:

$$\hat{\beta} = \arg\min_{\beta} \sum_{i=1}^{N} (y_i - \mathbf{x}_i\boldsymbol{\beta})^2 = \arg\min_{\beta} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2$$

- setting derivative to zero gives *normal equations*

$$(X^\top X)^{-1} \quad \underbrace{\mathbf{X}^\top\mathbf{X}}\hat{\beta} = \mathbf{X}^\top\mathbf{y}$$

Ordinary Least Squares estimator (OLS)

- model: $y_i = \beta_0 + x_{i1}\beta_1 + x_{i2}\beta_2 + \epsilon_i$
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- setting derivative to zero gives *normal equations*

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$$\nabla_{\boldsymbol{\beta}} f(\boldsymbol{\beta}) = \begin{pmatrix} \frac{\partial f}{\partial \beta_0} \\ \frac{\partial f}{\partial \beta_1} \\ \vdots \\ \frac{\partial f}{\partial \beta_{p-1}} \end{pmatrix} = 0$$

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$$\vdots$$

If $\boldsymbol{\beta}$ is $p \times 1$, then $\nabla_{\boldsymbol{\beta}} f(\boldsymbol{\beta})$ is $p \times 1$.

Partial derivative

- example: 1 data point, $p = 2$:

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- similarly:

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$$X\beta = X^T X y$$

Data Analysis: Statistical Modeling and Computation in Applications

Correlation and Least Squares Regression
Part 5

Outline

- Correlation
- Regression line
- Evaluation
- Multiple regression
- Computing the estimator
- Variable selection and regularization

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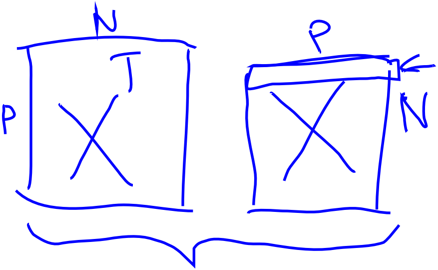
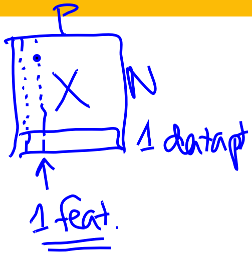


1 datapoint

$p \times p$ matrix

- $N \geq P$
- all cols linearly independent

When is $\mathbf{X}^\top\mathbf{X}$ invertible?



- if $\mathbf{X}^\top\mathbf{X}$ has *full rank*:
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$$\beta_0 + 2\beta_1 = 5$$

$N = 1$
$p = 2$

$\beta_1 \quad \beta_2$

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penalizes large values of β_j
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- ℓ_1 **penalty (Lasso)**: minimize

$$\sum_{i=1}^{N}(y_i - \hat{y}_i)^2 + \lambda \underbrace{\|\boldsymbol{\beta}\|_1}_{\sum_{j=0}^{p-1} |\beta_j|}$$

  prefers *sparse* β (few nonzero coordinates)

Model selection: Which variables to include in the model?

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- *t-test to test $\beta_j = 0$ vs. $\beta_j \neq 0$*: estimate σ^2 as $\hat{\sigma}^2 = \frac{1}{N-p-1} \sum_{i-1}^{N} (y_i - \hat{y}_i)^2$, then $(N-p-1)\hat{\sigma}^2 \sim \sigma^2 \chi^2_{N-p}$.

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- Use the t-test to determine variables that are not significant. Of those, remove the one with the largest p-value. Re-fit and repeat until all variables have significant p-values.

References

- D. Freedman, R. Pisani, R. Purves. *Statistics*. 2007.
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- D. Freedman. *Statistical Models – Theory and Practice*. 2009.
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