Applied Data Science

Machine Learning
Lecture 1

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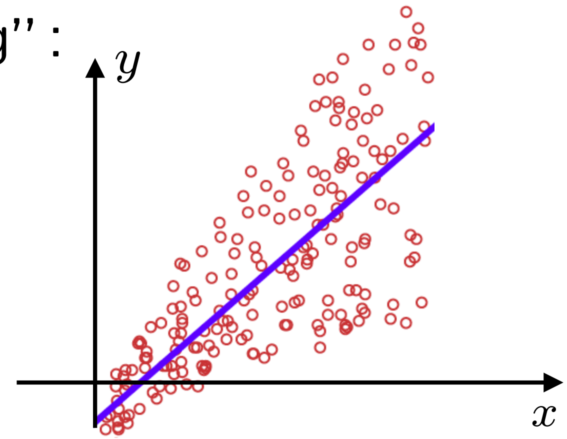
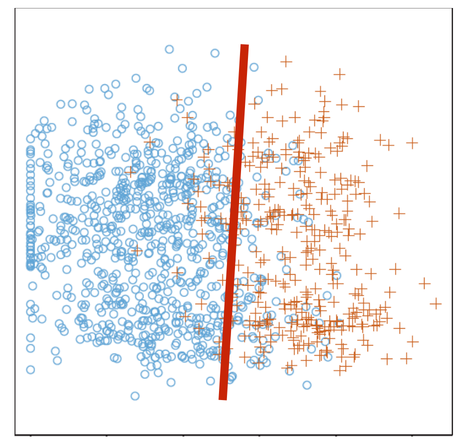
Overview of this week/module

- Central methods in Machine Learning
  - we will only discuss "supervised learning": learn from labeled examples



- Predict the value of an unobserved y

  Regression (linear)



- Predict the type/color of a new individual

  Classification

- Assessment

  How good is our method, our model, and our prediction?

  Testing, validation

Today's agenda

- Regression
  - formulation
  - solution
  - interpretation
  - (classical) performance assessment

- Further topics (next session)
  - what can go wrong
  - using nonlinear features of the data
  - overfitting and regularization

    ridge regression

    sparse regression and lasso

  - more on performance assessment

    cross-validation

    bootstrap

MACHINE LEARNING AND STATISTICS

A conceptual big picture

Model?

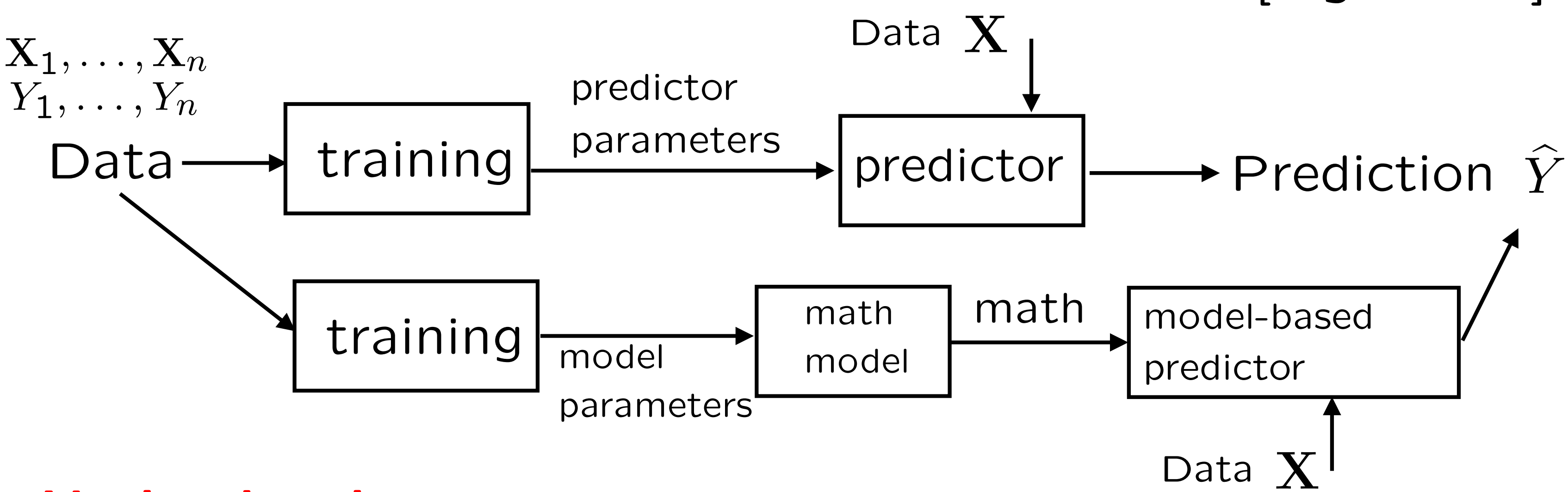
$\mathbf{X}_1$	Y_1
$\vdots$	$\vdots$
$\vdots$	$\vdots$
$\mathbf{X}_n$	Y_n
$\mathbf{X}$	Y?

$\mathbf{X}$: symptoms, test results, etc.
Y: state of health

- **"Predict"** Y based on $\mathbf{X}$

Y: sick or not (binary) [classification]

Y: life expectancy (any real number) [regression]



- **Understand**
  - build a model, a theory, a narrative, a mechanism

"All models are wrong, some are useful" (George E.P. Box)

Some language

- predict Y from $\mathbf{X} = (X_1, \ldots, X_m)$

- X_i: covariates, independent variables, features

- Y: response, dependent variable, target

Notation key

- vectors: boldface
  scalars: normal font
  - $\mathbf{X}_2$: second data record
  - X_2: second component of a vector $\mathbf{X}$

$$\mathbf{X} = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix}$$

$$\mathbf{X}^T = [X_1 \ X_2 \ X_3]$$

$$\mathbf{X}^T\mathbf{Y} = X_1Y_1 + X_2Y_2 + X_3Y_3$$

- "star" for true quantity, e.g., θ^*

- "hat" for estimates, e.g., $\widehat{\Theta}$

The overall field

Statistics

Machine learning

- Data Science: Extracting useful information from data

- Need a language: probability

- Build on two centuries of statistical knowledge

(LINEAR) REGRESSION

formulation

solution

interpretation

An example: Advertising and Sales

- Data across 200 Markets
  - Spending for TV, Radio, NewsPaper
  - Sales

	TV	Radio	Newspaper	Sales
0	230.1	37.8	69.2	22.1
1	44.5	39.3	45.1	10.4
2	17.2	45.9	69.3	9.3
3	151.5	41.3	58.5	18.5
4	180.8	10.8	58.4	12.9
...	...	...	...	...
195	38.2	3.7	13.8	7.6
196	94.2	4.9	8.1	9.7
197	177.0	9.3	6.4	12.8
198	283.6	42.0	66.2	25.5
199	232.1	8.6	8.7	13.4

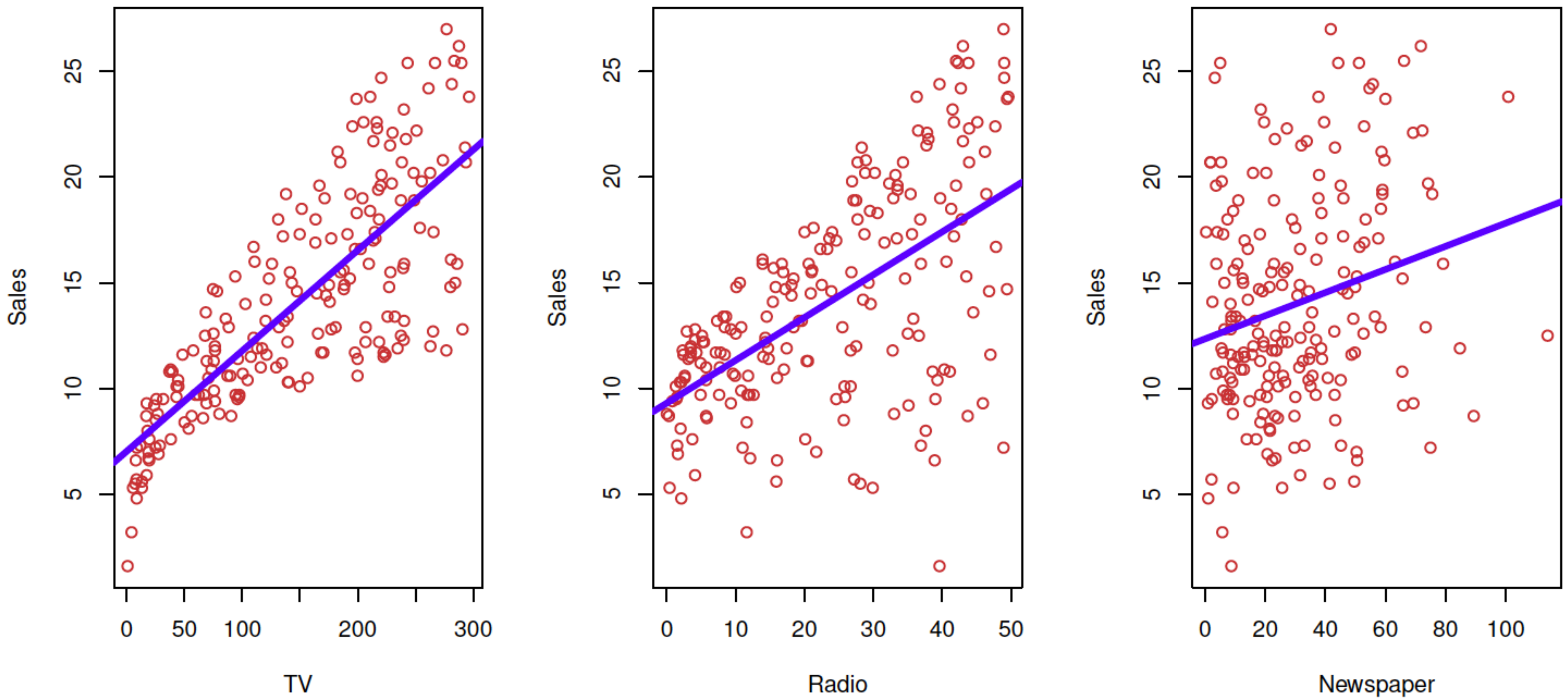
200 rows × 4 columns

- Questions

– Is there a relation between Advertising Channel Budgets and Sales?

– If yes, can we “predict” Sales given the Channel Budgets?

Visualize!



Sales
25
20
15
10
5
0
50
100
200
300
TV
Sales
25
20
15
10
5
0
10
20
30
40
50
Radio
Sales
25
20
15
10
5
0
20
40
60
80
100
Newspaper

Regression

data

$$\begin{array}{c|c} \mathbf{X}_1 & Y_1 \\ \vdots & \vdots \\ \vdots & \vdots \\ \mathbf{X}_n & Y_n \\ \hline \mathbf{X} & Y? \end{array}$$

vector $\rightarrow$ $\mathbf{X}_n$, dimension m

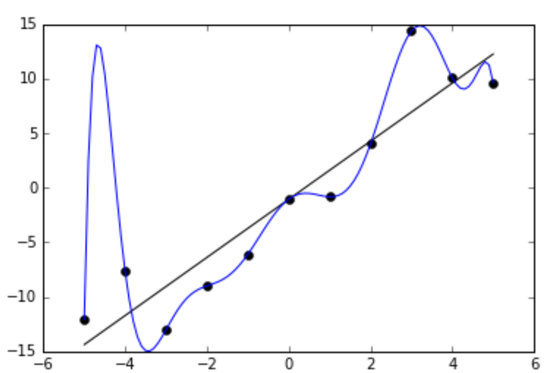
Y_n $\leftarrow$ scalar

- **Regressor/predictor:** $\widehat{Y} = g(\mathbf{X})$

- "Learn" a "good" g from the data

objective: (risk) $\mathbb{E}\left[\left(g(\mathbf{X}) - Y\right)^2\right]$

proxy: $\frac{1}{n}\sum_{i=1}^{n}\left(g(\mathbf{X}_i) - Y_i\right)^2$ "empirical risk minimization"



https://en.wikipedia.org/wiki/Overfitting

- Restrict to limited class of predictors

Linear regression

	$\mathbf{X}_1$	Y_1
data	$\vdots$	$\vdots$
vector dimension m →	$\mathbf{X}_n$	Y_n
	$\mathbf{X}$	$Y?$

- Restrict to limited class of predictors:

$$\widehat{Y} = \theta_0 + \theta_1 X_1 + \cdots + \theta_m X_m$$

let $\mathbf{X} = (1, X_1, \ldots, X_m)$

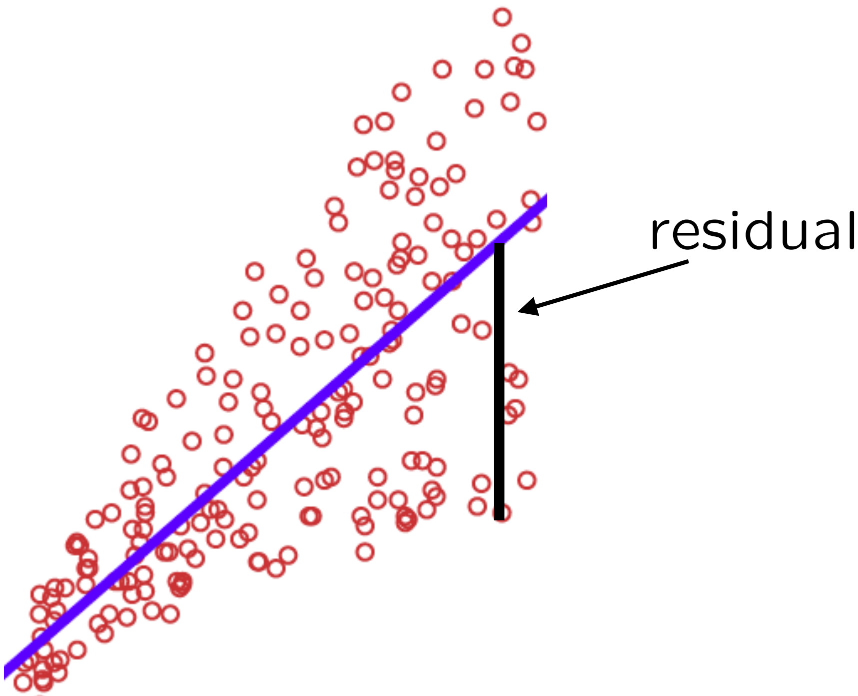
$$\boldsymbol{\theta} = (\theta_0, \theta_1, \ldots, \theta_m)$$

$$\widehat{Y} = g(\mathbf{X}) = \boldsymbol{\theta}^T \mathbf{X}$$

$$\frac{1}{n}\sum_{i=1}^{n}\Big(g(\mathbf{X}_i) - Y_i\Big)^2$$

sum of over data points

$$\min_{\boldsymbol{\theta}} \sum_{i=1}^{n}(\boldsymbol{\theta}^T \mathbf{X}_i - Y_i)^2$$



- ordinary least squares (OLS)

Solution to the regression problem

$$\min_{\boldsymbol{\theta}} \sum_{i=1}^{n} (\boldsymbol{\theta}^T \mathbf{X}_i - Y_i)^2$$

n data points

$\mathbf{X}_i$ and $\boldsymbol{\theta}$ have dimension $m+1$

$$\begin{array}{cc} n & \begin{bmatrix} \cdots \mathbf{X}_1^T \cdots \\ \vdots \\ \vdots \\ \cdots \mathbf{X}_n^T \cdots \end{bmatrix} \\ & m+1 \end{array} \begin{bmatrix} Y_1 \\ \vdots \\ \vdots \\ Y_n \end{bmatrix} = \left[\mathbb{X} \mid \mathbf{Y}\right]$$

- Formulas: $\boxed{\widehat{\boldsymbol{\theta}} = (\mathbb{X}^T \mathbb{X})^{-1} \mathbb{X}^T \mathbf{Y}}$

Math details:

$\min_{\boldsymbol{\theta}} H(\boldsymbol{\theta})$ quadratic in $\boldsymbol{\theta}$

optimality conditions: $\nabla H(\boldsymbol{\theta}) = 0$ $\quad \dfrac{\partial H}{\partial \theta_j} = 0, \quad j = 0, 1, \ldots, m$

linear system of $m+1$ equations

Results for our example

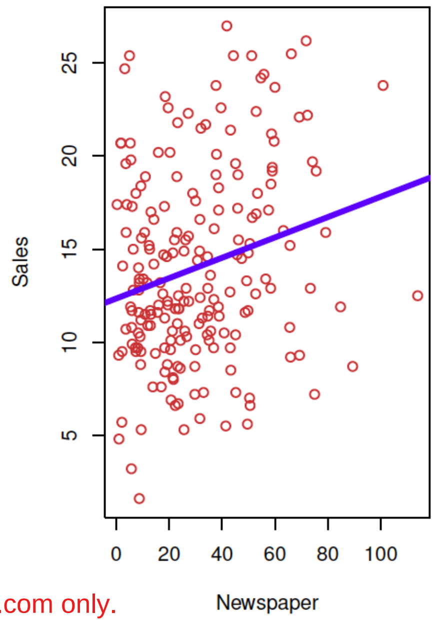
$n = 200 \qquad m + 1 = 4$

$$\hat{\boldsymbol{\theta}} = \begin{bmatrix} 2.94 \\ 0.046 \\ 0.19 \\ -0.001 \end{bmatrix}$$

$$\widehat{\text{Sales}} = 2.94 + 0.046 \cdot (\text{TV}) + 0.19 \cdot (\text{Radio}) - 0.001 \cdot (\text{NewsP})$$

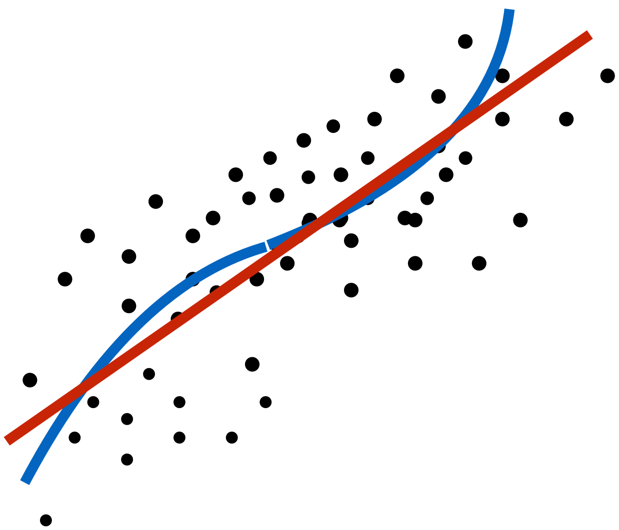
- Compare with simple linear regression

$$\widehat{\text{Sales}} = 12.35 + 0.055 \cdot (\text{NewsP})$$



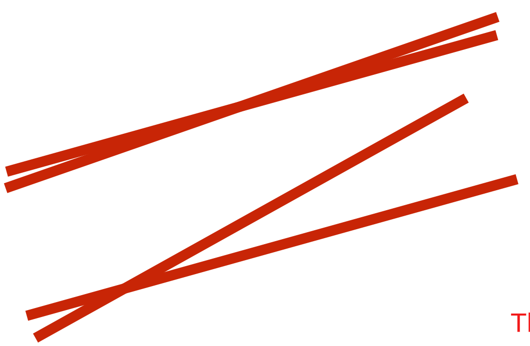
Interpretation and justification: empirical risk minimization

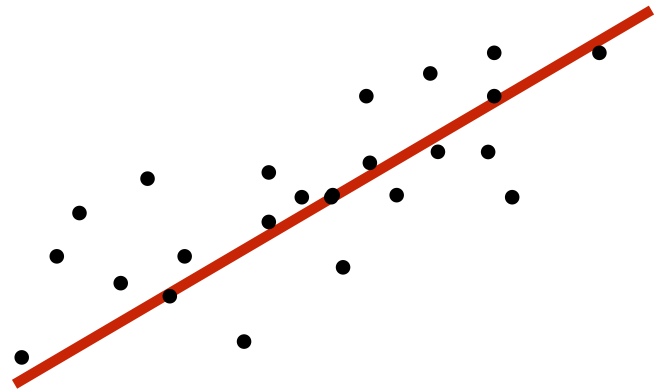
- Large true population



– true relation may be complex

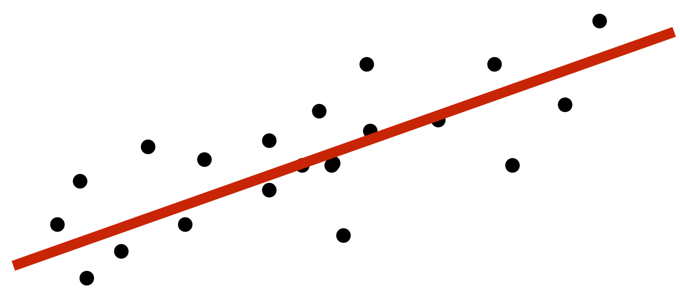
– interested in best linear predictor





- Finite sample: find best linear fit

$n \to \infty$: recover "population best"
(as long as samples are
drawn representatively)



- Another finite sample: different results

how much variation do we expect?

Interpretation and justification: maximum likelihood

- independent variables $\mathbb{X}$ are somehow fixed; then $\mathbf{Y}$ is observed
  - For any candidate $\boldsymbol{\theta}$, how probable would it be to observe the Ys that were actually observed?

    Likelihood: $\mathbb{P}(\mathbf{Y} \mid \mathbb{X}; \boldsymbol{\theta})$
  - **Maximum likelihood method:** $\max_{\boldsymbol{\theta}} \mathbb{P}(\mathbf{Y} \mid \mathbb{X}; \boldsymbol{\theta})$

- Illustrate for $m = 1$. Assume:
  - structural model: $Y_i = \theta_0^* + \theta_1^* X_i + W_i$
  - conditioned on all the X_i: all the W_i are independent and Normal$(0, \sigma^2)$

Maximizing the likelihood function = minimizing the empirical risk

Y_i : Normal$(\theta_0^* + \theta_1^* X_i,\ \sigma^2)$

$$\mathbb{P}(\mathbf{Y} \mid \mathbb{X}; \boldsymbol{\theta}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(Y_i - \theta_0 - \theta_1 X_i)^2}{2\sigma^2}\right\}$$

$$\log \mathbb{P}(\mathbf{Y} \mid \mathbb{X}; \boldsymbol{\theta}) = (\text{constant}) - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (Y_i - \theta_0 - \theta_1 X_i)^2$$

Summary of the two interpretations

- $(\mathbf{X}, Y)$ (data, and new examples) come from some distribution
  - we learn best **linear predictor**

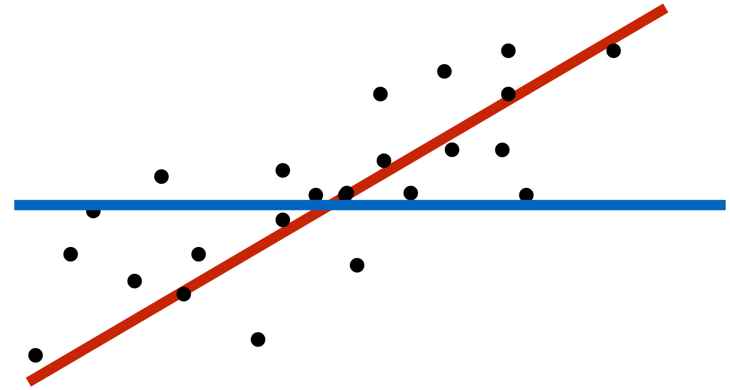
versus

- The world is linear; we know the structure of the relation
  - we learn the **coefficients of the structural relation**

PERFORMANCE ASSESSMENT

R^2 (R-squared)

- Prediction if no regression: $\overline{Y} = \frac{1}{n} Y_i$



- Total sum of squares:

$$\text{TSS} = \sum_{i=1}^{n} (Y_i - \overline{Y})^2$$

"initial" variation in Y

- Residual sum of squares: $\text{RSS} = \sum_{i=1}^{n} (Y_i - \widehat{\boldsymbol{\theta}}^T \mathbf{X}_i)^2$

unexplained variation in Y, after taking into account X

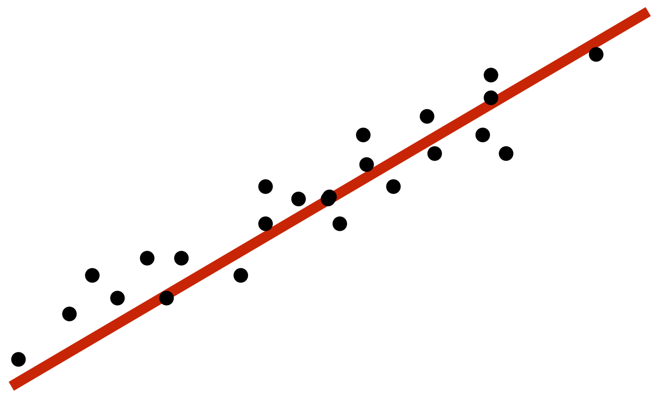
- $R^2 = 1 - \frac{\text{RSS}}{\text{TSS}}$ fraction of variation in Y that has been explained

$0 \leq R^2 \leq 1$ high R^2 is preferred

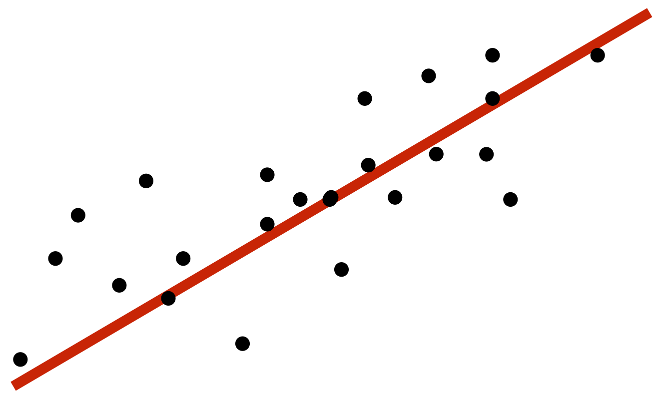
in simple regression R^2 is an estimate of
the squared correlation coefficient between X and Y

R^2 illustration

- Higher R^2



- Lower R^2



R^2 for our example

- $\widehat{\text{Sales}} = 2.94 + 0.046 \cdot (\text{TV}) + 0.19 \cdot (\text{Radio}) - 0.001 \cdot (\text{NewsP})$

  $R^2 = 0.897$ All the budgets together explain a lot

- $\widehat{\text{Sales}} = 12.35 + 0.055 \cdot (\text{NewsP})$

  $R^2 = 0.05$ Newspaper budget explains little

  For TV alone: $R^2 = 0.61$

  For Radio alone: $R^2 = 0.33$

- More variables: R^2 can only go up (or stay the same)

  - but this may be a mirage
  - adjusted R^2: $1 - \dfrac{\text{RSS}/(n-m-1)}{\text{TSS}/(n-1)}$ $0.897 \to 0.896$

How noisy/reliable are my estimates of θ^*

- Assume structural model

$$\boxed{\begin{aligned} &Y_i = (\boldsymbol{\theta}^*)^T \mathbf{X}_i + W_i \\ &\quad W_i\text{: independent,} \\ &\quad\quad \text{zero mean, variance } \sigma^2 \end{aligned}}$$

(If not, need to resort to simulation/bootstrap methods)

next session

$\widehat{\boldsymbol{\Theta}}$ is a random variable
(depends on random data)

$$\boxed{\widehat{\boldsymbol{\Theta}} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbf{Y}}$$

$$\mathbb{E}\Big[(\widehat{\Theta}_j - \theta_j^*)^2\Big] = \Big(\mathbb{E}[\widehat{\Theta}_j] - \theta_j^*\Big)^2 + \text{var}(\widehat{\Theta}_j)$$

$\mathbb{E}[X^2] = \big(\mathbb{E}[X]\big)^2 + \text{var}(X)$

bias

variance

$$\boxed{\mathbb{E}[\widehat{\Theta}_j] = \theta_j^*}$$

(OLS is unbiased)

- Hence focus on the variance of $\widehat{\Theta}_j$

The distribution of $\widehat{\boldsymbol{\Theta}}$ (given, deterministic, $\mathbb{X}$)

$$Y_i = (\boldsymbol{\theta}^*)^T \mathbf{X}_i + W_i$$

W_i: independent, zero mean, variance σ^2

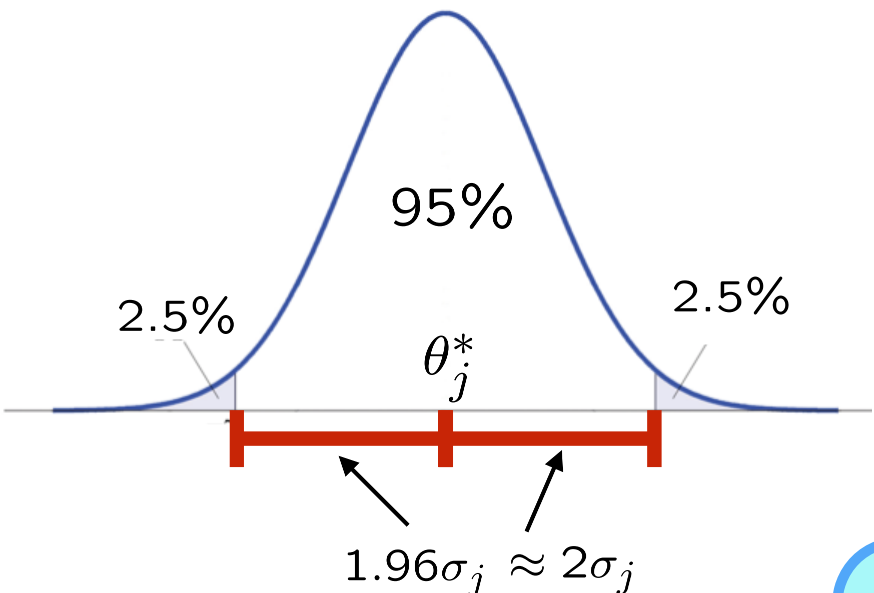
$$\widehat{\boldsymbol{\Theta}} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbf{Y}$$

- Each $\widehat{\Theta}_j$ is normal

$$\widehat{\Theta}_j \sim \mathcal{N}(\theta_j^*, \sigma_j^2)$$

– approximately: large n, central limit theorem

– exactly: if W_i are normal



$$\sigma_j = \sqrt{\text{var}(\widehat{\Theta}_j)} = \text{se}(\widehat{\Theta}_j)$$

standard error

- Agenda:

calculate/approximate standard error

use it (confidence intervals, hypothesis testing)

Standard error calculation

- There is a formula
- Software implements it (approximately)

The covariance matrix of $\widehat{\Theta}$ (given, deterministic, $\mathbb{X}$)

$$Y_i = (\boldsymbol{\theta}^*)^T \mathbf{X}_i + W_i$$

W_i: independent, zero mean, variance σ^2

$$\widehat{\boldsymbol{\Theta}} = (\mathbb{X}^T\mathbb{X})^{-1}\mathbb{X}^T\mathbf{Y}$$

diagonal entries: Var$(\widehat{\boldsymbol{\Theta}}_j)$

off-diagonal entries: Cov$(\widehat{\boldsymbol{\Theta}}_i, \widehat{\boldsymbol{\Theta}}_j)$

	const	TV	Radio	Newspaper
const	**9.72867479E-02**	-2.65727337E-04	-1.11548946E-03	-5.91021239E-04
TV	-2.65727337E-04	**1.9457371E-06**	-4.47039463E-07	-3.26595026E-07
Radio	-1.11548946E-03	-4.47039463E-07	**7.41533504E-05**	-1.78006245E-05
News paper	-5.91021239E-04	-3.26595026E-07	-1.78006245E-05	**3.44687543E-05**

dimensions $(m+1) \times (m+1)$

formula: $\sigma^2(\mathbb{X}^T\mathbb{X})^{-1}$

use $\hat{\sigma}^2$

- Estimate σ^2 by $$\boxed{\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \hat{\boldsymbol{\theta}}^T\mathbf{X}_i\right)^2}$$

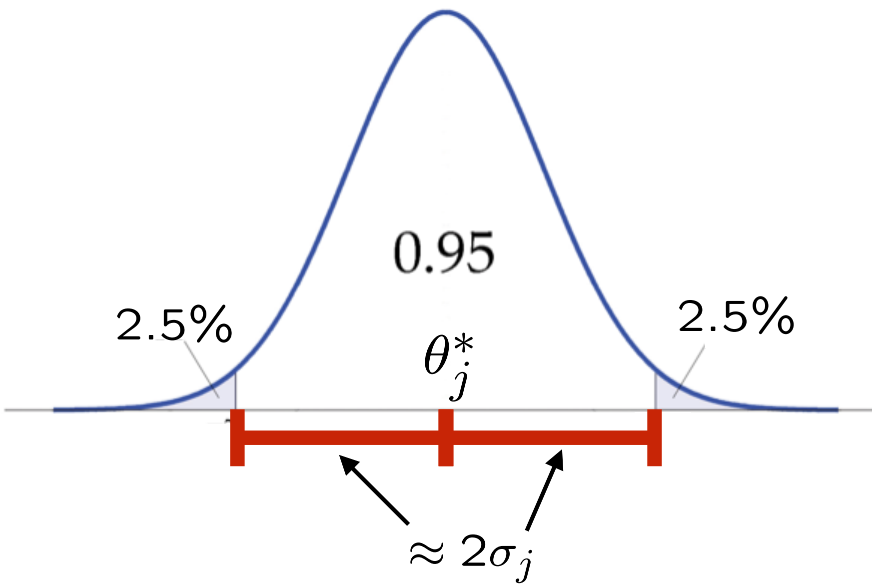
slight downwards bias

negligible bias if $m \ll n$

Why? For large samples, $\widehat{\boldsymbol{\Theta}} \approx \boldsymbol{\theta}^*$, and

$$\sigma^2 = \mathbb{E}[W_i^2] \approx \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - (\boldsymbol{\theta}^*)^T\mathbf{X}_i\right)^2 \approx \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \widehat{\boldsymbol{\Theta}}^T\mathbf{X}_i\right)^2$$

Confidence Interval (CI)



$\widehat{\Theta}_j \sim \mathcal{N}(\theta_j^*, \sigma_j^2)$

- With probability 95%: $\quad |\text{error}| = |\widehat{\Theta}_j - \theta_j^*| \leq 2\sigma_j$

$$\boxed{\theta_j^* \in \left[\widehat{\Theta}_j - 2\hat{\sigma}_j, \quad \widehat{\Theta}_j + 2\hat{\sigma}_j\right]}$$ 95%-CI

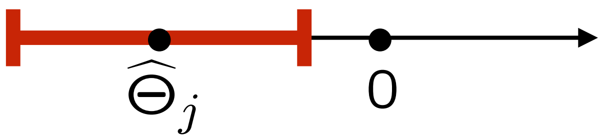
$$\boxed{\mathbb{P}(\theta_j^* \in \mathrm{CI}) \approx 0.95}$$

- Needs careful (“frequentist”) interpretation

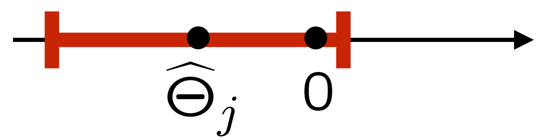
Testing the hypothesis $\theta_j^* = 0$

- Are the data compatible with the null hypothesis $\theta_j^* = 0$?
  (jth feature has "no effect")

Wald test:



reject the null



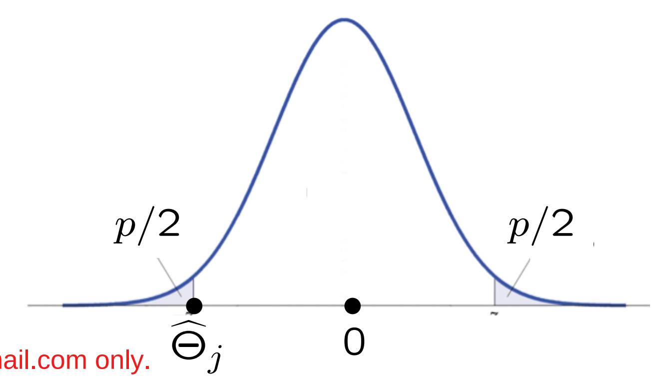
do not reject the null
(data compatible with $\theta_j^* = 0$)

$\mathbb{P}(\text{reject} \mid \theta_j^* = 0)$ (false discovery rate)

$= \mathbb{P}(\text{the CI "misses" } 0 \mid \theta_j^* = 0) \approx 5\%$

- how much of an outlier (under the null) do I see?

p-value: probability of seeing something at least as extreme as the observed $\widehat{\Theta}_j$, under $\theta_j^* = 0$



- reject if p-value < 0.05

Back to our example

	coef	std err	[0.025	0.975]
Intercept	2.9389	0.312	2.324	3.554
TV	0.0458	0.001	0.043	0.049
Radio	0.1885	0.009	0.172	0.206
Newspaper	-0.0010	0.006	-0.013	0.011

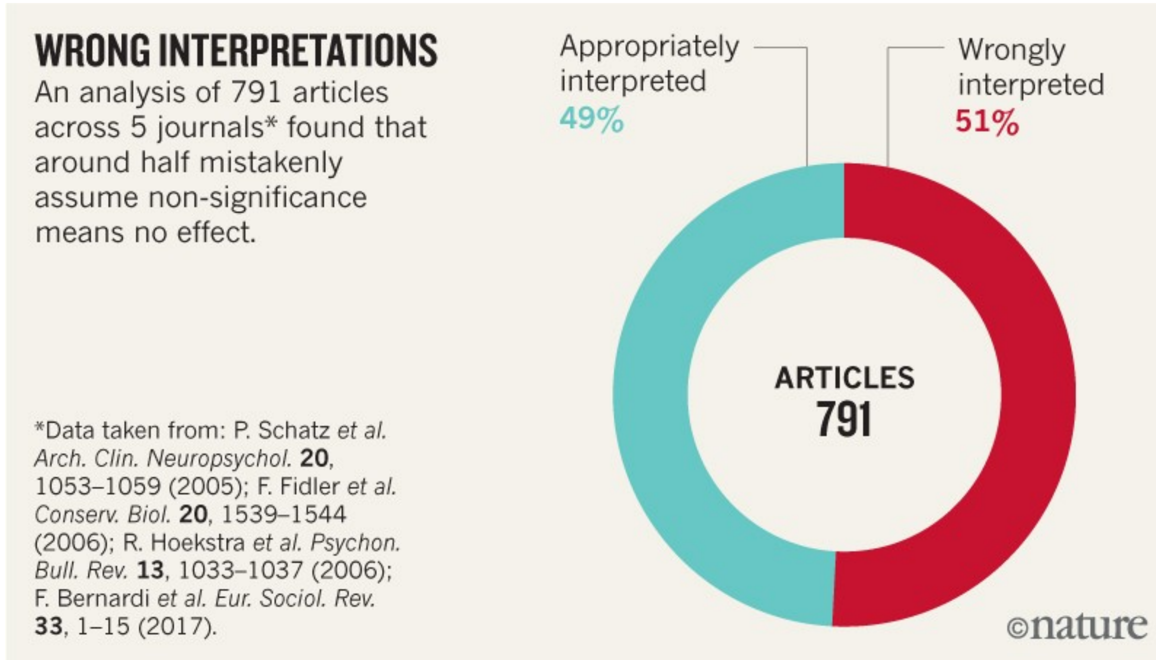
Confidence intervals: [0.025, 0.975]

- Wald test: intercept, TV, Radio are "significant" (reject the hypothesis that they are zero)

  Newspaper: the hypothesis that $\theta^*_{\text{NewsP}} = 0$ "survives" (not rejected)

Interpretation needs care

Scientists rise up against statistical significance, *Nature*, 20 March 2019



- Reject the null $\theta_j^* = 0$ (decide "there is an effect"):
  what we see is unlikely to have been generated by a model with $\theta_j^* = 0$
  – but also could be due to noise in the data; 5% "false discovery" prob.

- Do not reject the null $\theta_j^* = 0$ ("see no effect"):
  data do not provide compelling evidence that $\theta_j^* \neq 0$
  - no effect: θ_j^* is zero
  - small effect: θ_j^* is so close to zero that data cannot detect it
  - too few data: θ_j^* may be nonzero, but need more data to "see it"

Making new predictions

- After running the regression

  given some new $\mathbf{X}$, predict Y $\qquad \widehat{Y} = \widehat{\boldsymbol{\theta}}^T \mathbf{X}$

$\mathbf{X}_1$	Y_1
$\vdots$	$\vdots$
$\vdots$	$\vdots$
$\mathbf{X}_n$	Y_n
$\mathbf{X}$	$Y?$

- Keep assuming structural model: $Y = (\boldsymbol{\theta}^*)^T \mathbf{X} + W$
- $\widehat{\boldsymbol{\theta}}$ is unbiased estimate of $\boldsymbol{\theta}^*$

  $\Rightarrow \widehat{\boldsymbol{\theta}}^T \mathbf{X}$ is unbiased estimate of $(\boldsymbol{\theta}^*)^T \mathbf{X}$ (and of Y)

- Two sources of error:
  - unavoidable, from W; variance σ^2
  - variance of $(\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}^*)^T \mathbf{X}$ $\qquad \sigma^2 \mathbf{X}^T (\mathbb{X}^T \mathbb{X})^{-1} \mathbf{X}$
  - Total prediction error variance: $\qquad \sigma^2 + \sigma^2 \mathbf{X}^T (\mathbb{X}^T \mathbb{X})^{-1} \mathbf{X}$

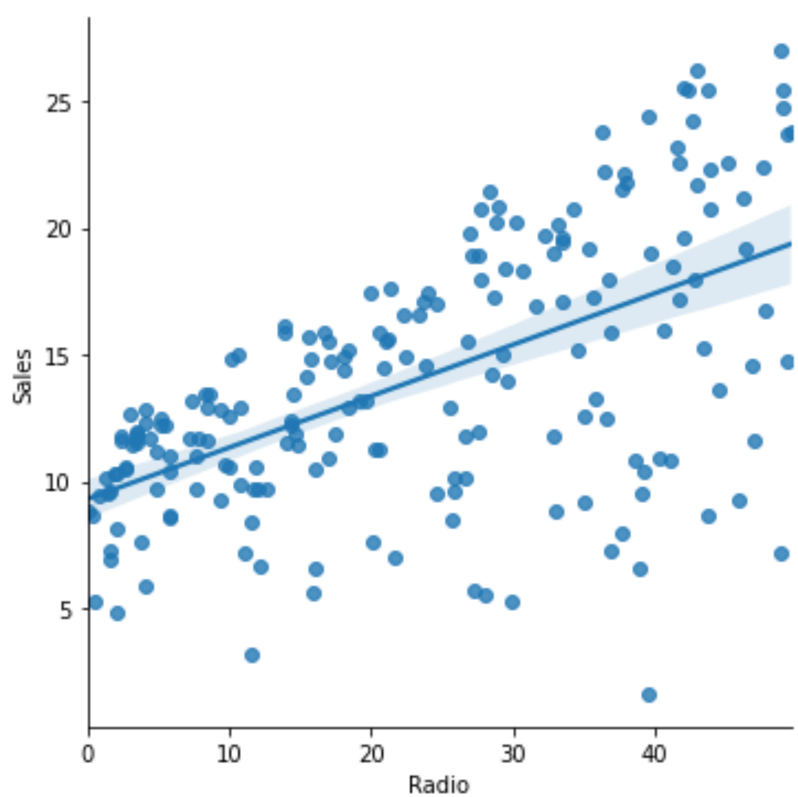
Confidence bands

- 95% confidence interval about the value of $(\boldsymbol{\theta}^*)^T \mathbf{X}$:

  $(\widehat{\boldsymbol{\theta}})^T \mathbf{X}$ plus or minus $\quad 2 \cdot \widehat{\sigma} \sqrt{\mathbf{X}^T (\mathbb{X}^T \mathbb{X})^{-1} \mathbf{X}}$

  – confidence interval width changes with $\mathbf{X}$

  – in simple regression, this gives a confidence band



Summary

- Linear regression
  - formulation
  - underlying assumptions
  - formulas
  - results: their interpretation and usage

- Two types of questions:

  $\widehat{\Theta} \approx \theta^*$? (modeling) $\hat{Y} \approx Y$? (prediction)

- Still, many things can go wrong or be misinterpreted

- New issues when $\boldsymbol{\theta}$ has high dimension

- Next session...

Some references

- James et al., An Introduction to Statistical Learning: with Applications in R (accessible)

- Hastie et al., The Elements of Statistical Learning: Data Mining, Inference, and Prediction (more comprehensive, and more advanced version of above)

- Wasserman, All of Statistics (short, elegant, and more mathematical)