Machine Learning

A. Supervised Learning: Linear Models & Fundamentals

A.4. High-Dimensional Data

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Syllabus

Fri. 25.10.	(1)	0. Introduction
		A. Supervised Learning: Linear Models & Fundamentals
Fri. 1.11.	(2)	A.1 Linear Regression
Fri. 8.11.	(3)	A.2 Linear Classification
Fri. 15.11.	(4)	A.3 Regularization
Fri. 22.11.	(5)	A.4 High-dimensional Data
		B. Supervised Learning: Nonlinear Models
Fri. 29.11.	(6)	B.1 Nearest-Neighbor Models
Fri. 6.12.	(7)	B.2 Neural Networks
Fri. 13.12.	(8)	B.3 Decision Trees
Fri. 20.12.	(9)	B.4 Support Vector Machines
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Fri. 10.1.	(10)	B.5 A First Look at Bayesian and Markov Networks
		C. Unsupervised Learning
Fri. 17.1.	(11)	C.1 Clustering
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Outline

1. Variable Interactions and Polynomial Models
2. Parameter Variance
3. Variable Selection via Forward and Backward Search
4. Minimizing a Function via Coordinate Descent
5. L1 Regularization / The Lasso

High-Dimensional Data

High-dimensional data occurs in different situations:

1. Data that comes naturally with many predictors.
   - e.g., text classification
     (# predictors = # words in the bag-of-words representation, e.g., 30.000)

2. Models that extract many predictor variables from objects to classify.
   - variable interactions
   - derived variables
   - complex objects such as graphs, texts, etc.
     - Situation 1 often really is a special case of this one.

3. Data with few examples compared to the number of variables ("small n, large p").
   - gene expression / microarray data

Outline

Need for higher orders

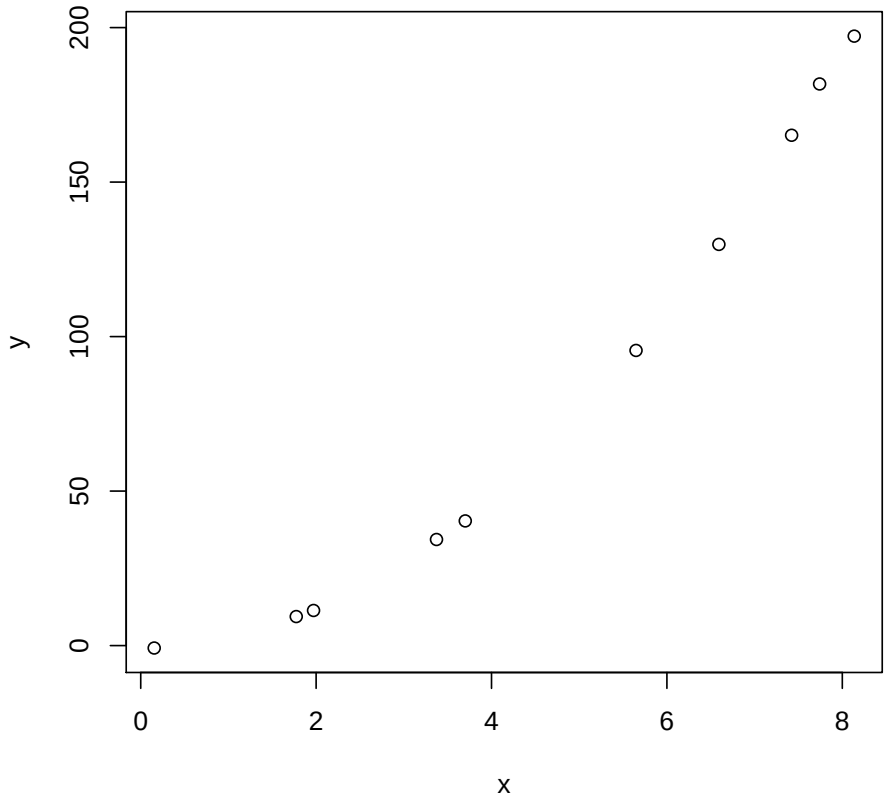
Assume a target variable does not depend linearly on a predictor variable, but say quadratic.

Example: way length vs. duration of a moving object with constant acceleration a.

$$s(t) = \frac{1}{2}at^2 + \epsilon$$

Can we catch such a dependency?

Can we catch it with a linear model?



Need for general transformations

To describe many phenomena, even more complex functions of the input variables are needed.

Example: the number of cells n vs. duration of growth t:

$$n = \beta e^{\alpha t} + \epsilon$$

n does not depend on t directly, but on $e^{\alpha t}$ (with a known α).

Need for variable interactions

In a linear model with two predictors

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$$

Y depends on both, X_1 and X_2.

But changes in X_1 will affect Y the same way, regardless of X_2.

There are problems where X_2 mediates or influences the way X_1 affects Y, e.g. : the way length s of a moving object vs. its constant velocity v and duration t:

$$s = vt + \epsilon$$

Then an additional $1s$ duration will increase the way length not in a uniform way (regardless of the velocity), but a little for small velocities and a lot for large velocities.

v and t are said to **interact**: y does not depend only on each predictor separately, but also on their product.

Derived variables

All these cases can be handled by looking at **derived variables**, i.e., instead of

$$Y = \beta_0 + \beta_1 X_1^2 + \epsilon$$
$$Y = \beta_0 + \beta_1 e^{\alpha X_1} + \epsilon$$
$$Y = \beta_0 + \beta_1 X_1 \cdot X_2 + \epsilon$$

one looks at

$$Y = \beta_0 + \beta_1 X_1' + \epsilon$$

with

$$X_1' := X_1^2$$
$$X_1' := e^{\alpha X_1}$$
$$X_1' := X_1 \cdot X_2$$

Derived variables are computed before the fitting process and taken into account either additional to the original variables or instead of.

Polynomial Models

Polynomial models of degree d take into account systematically all interactions of d different variables (including powers up to degree d):

$$\hat{y}(x) := \hat{\theta}_0 + \sum_{m=1}^{M} \hat{\theta}_m x_m \qquad \text{degree 1}$$

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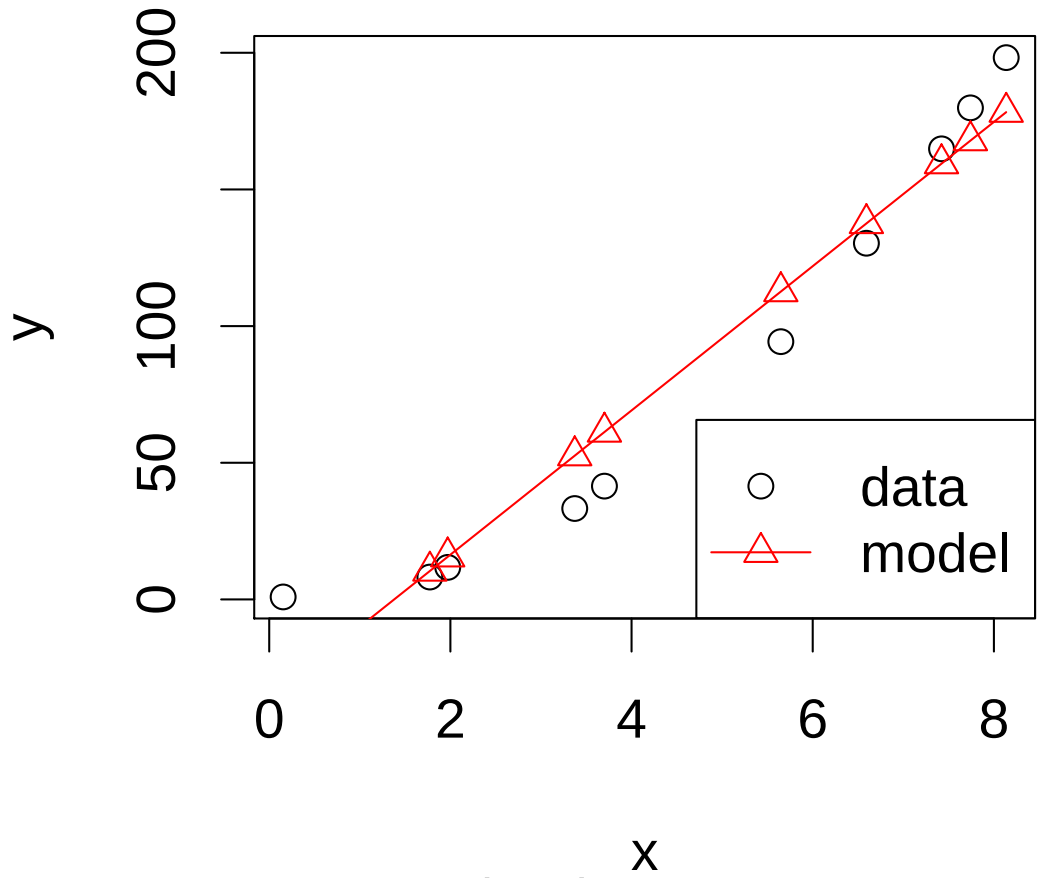
$$\hat{y}(x) := \hat{\theta}_0 + \sum_{m=1}^{M} \hat{\theta}_m x_m + \sum_{m=1}^{M} \sum_{l=m}^{M} \hat{\theta}_{m,l} x_m x_l + \cdots$$

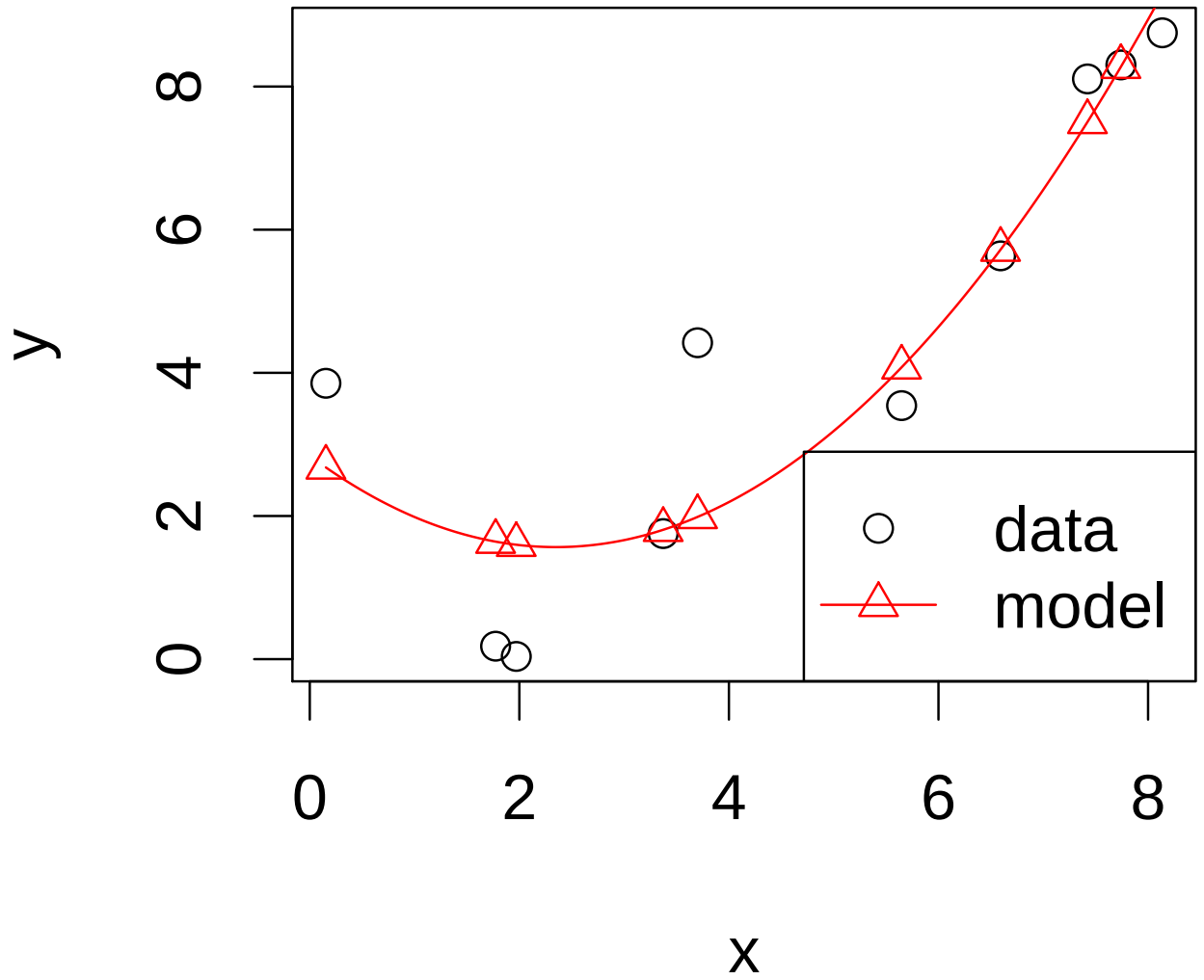
$$+ \sum_{m_1=1}^{M} \sum_{m_2=m_1}^{M} \cdots \sum_{m_d=m_{d-1}}^{M} \hat{\theta}_{m_1,m_2,\ldots,m_d} x_{m_1} x_{m_2} \cdots x_{m_d} \qquad \text{degree } d$$

High Polynomial Degress, High Model Complexity



If a model does not well explain the data,
e.g., if the true model is quadratic, but we try to fit a linear model,
one says, the model **underfits**.

High Polynomial Degress, High Model Complexity



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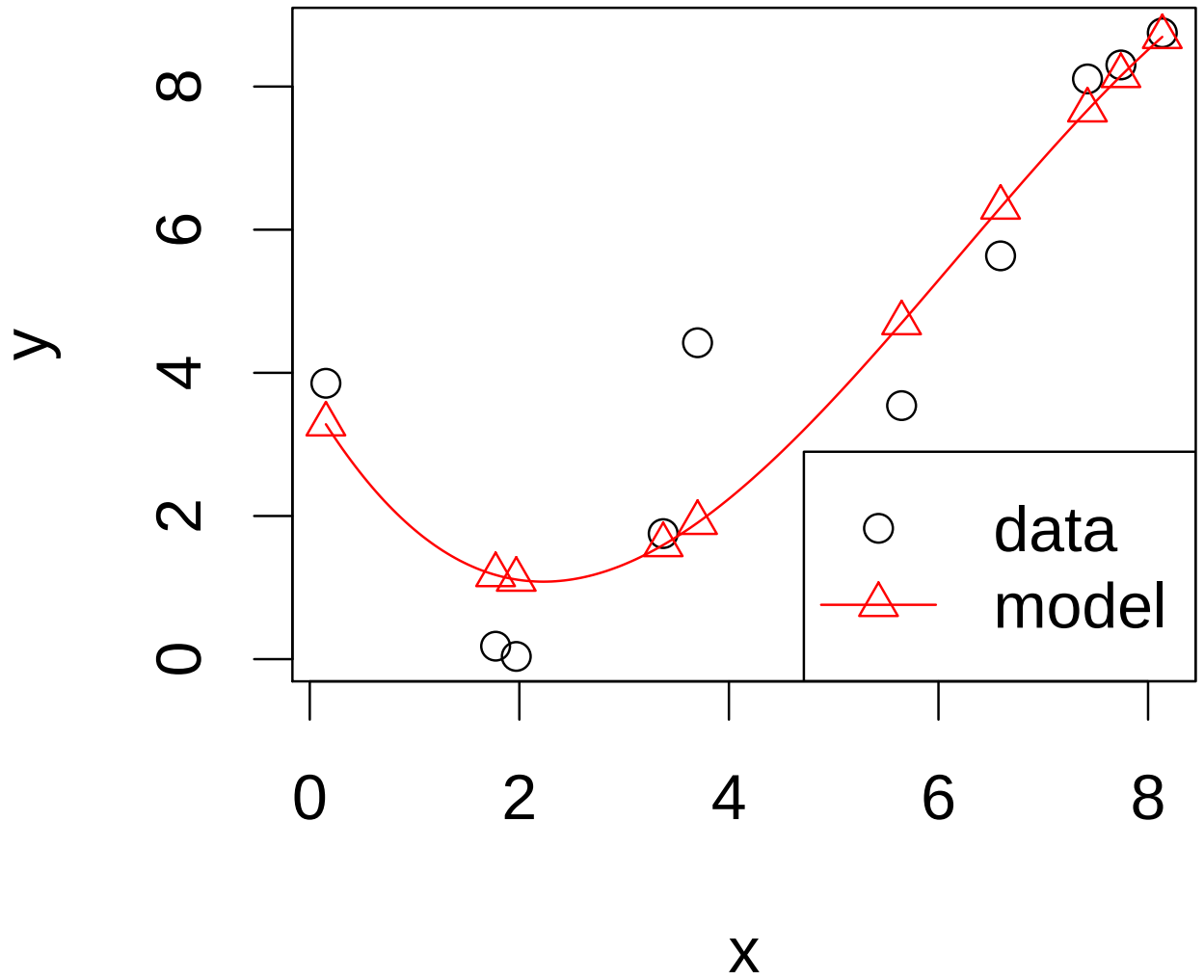

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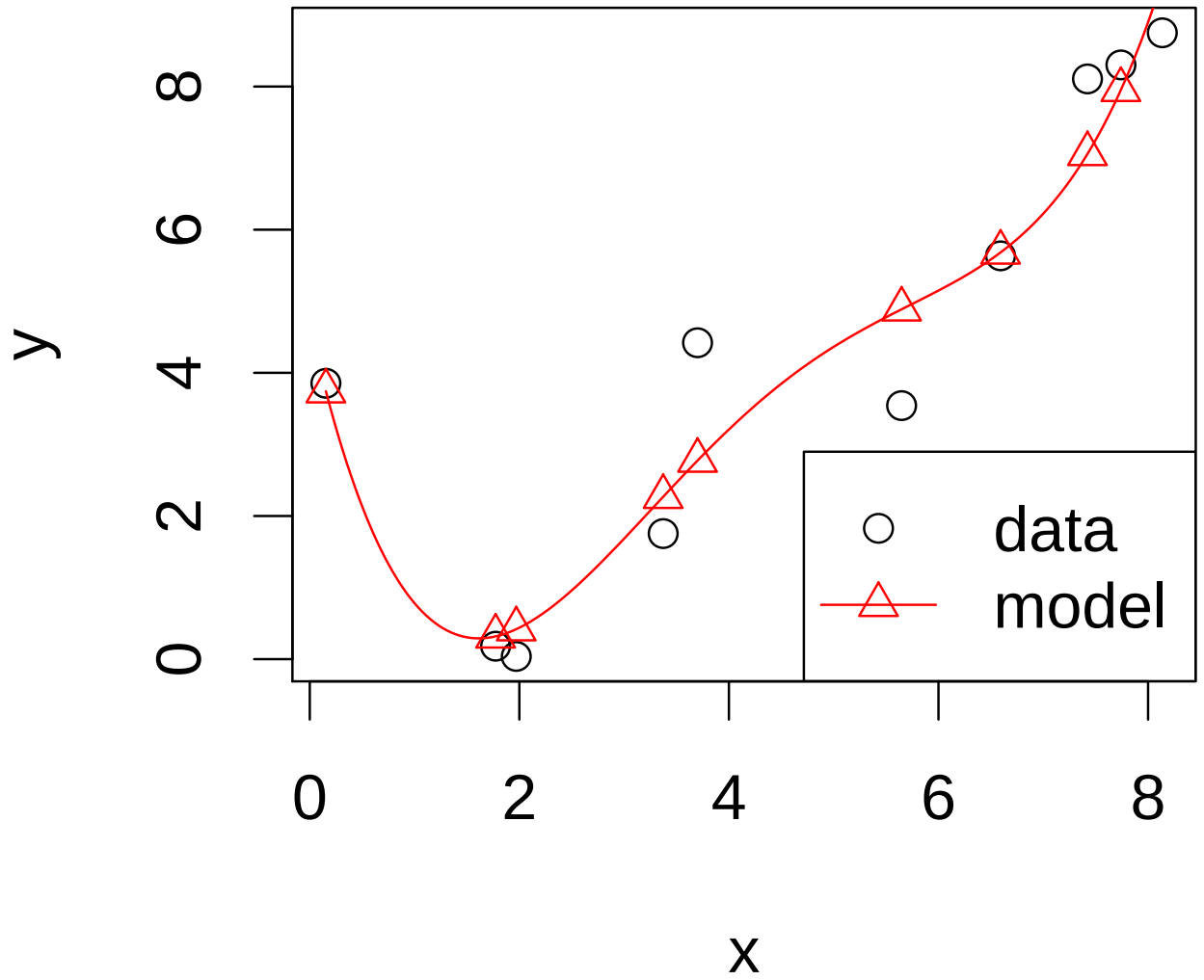
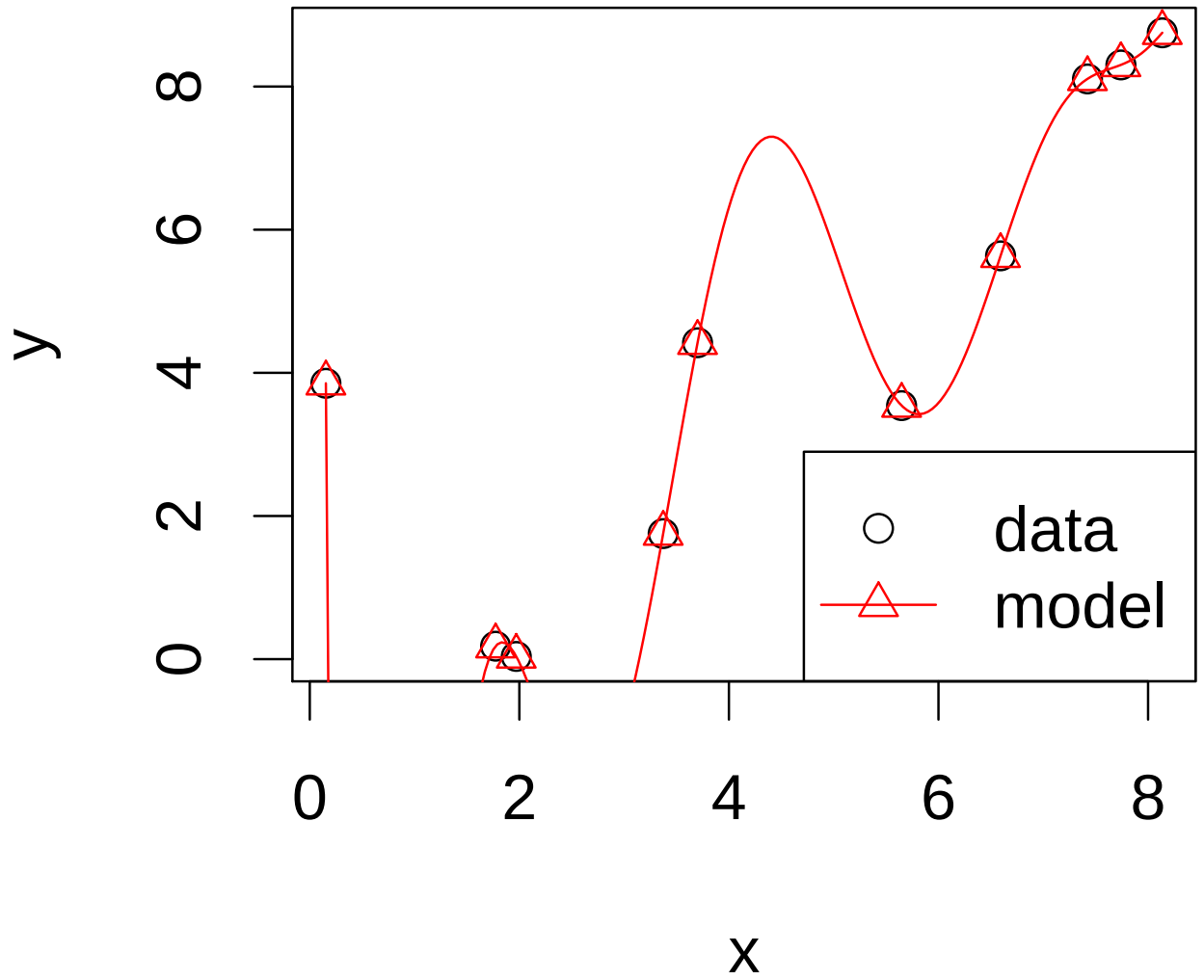


High Polynomial Degress, High Model Complexity



High Polynomial Degress, High Model Complexity

If to data

$$(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)$$

consisting of N points we fit

$$\begin{aligned} X &= \beta_0 + \beta_1 X + \beta_2 X^2 + \cdots + \beta_{N-1} X^{N-1} \\ &= \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_{N-1} X_{N-1}, \quad X_i := X^i \end{aligned}$$

i.e., a polynomial with degree $N - 1$,
then this results in an **interpolation** of the data points
(if there are no repeated measurements, i.e., points with the same X.)

As the polynomial

$$\hat{y}(X) = \sum_{n=1}^{N} y_n \prod_{m \neq n} \frac{X - x_m}{x_n - x_m}$$

is of this type, and has minimal RSS $= 0$.

Variable Types and Coding

The most common variable types:

numerical / **interval-scaled** / **quantitative**

- differences and quotients etc. are meaningful,
- usually with domain $\mathcal{X} := \mathbb{R}$,
- e.g., temperature, size, weight.

nominal / **discrete** / **categorical** / **qualitative** / **factor**

- differences and quotients are **not** defined,
- usually with a finite, enumerated domain,
- e.g., $\mathcal{X} := \{\text{red}, \text{green}, \text{blue}\}$
  or $\mathcal{X} := \{\text{a}, \text{b}, \text{c}, \ldots, \text{y}, \text{z}\}$.

ordinal / **ordered categorical**

- levels are ordered, but differences and quotients are not defined,
- usually with a finite, enumerated domain,

Variable Types and Coding

Nominals are usually encoded as a set of binary **dummy variables** (aka **indicator variables**, **one hot encoding**):

$$\delta_{x_0}(X) := \begin{cases} 1, & \text{if } X = x_0, \\ 0, & \text{else} \end{cases}$$

one for each $x_0 \in \mathcal{X}$ (but one).

Example: $\mathcal{X} := \{\text{red}, \text{green}, \text{blue}\}$

one variable X with 3 levels: red, green, blue

$\downarrow$ replace by

two variables $\delta_{\text{red}}(X)$ and $\delta_{\text{green}}(X)$ with 2 levels each: 0, 1

X	$\delta_{\text{red}}(X)$	$\delta_{\text{green}}(X)$
red	1	0
green	0	1
blue	0	0
—	1	1

Outline

The Normal Distribution (also Gaussian)

written as:

$$X \sim \mathcal{N}(\mu, \sigma^2)$$

with parameters:

- μ mean,
- σ standard deviance.

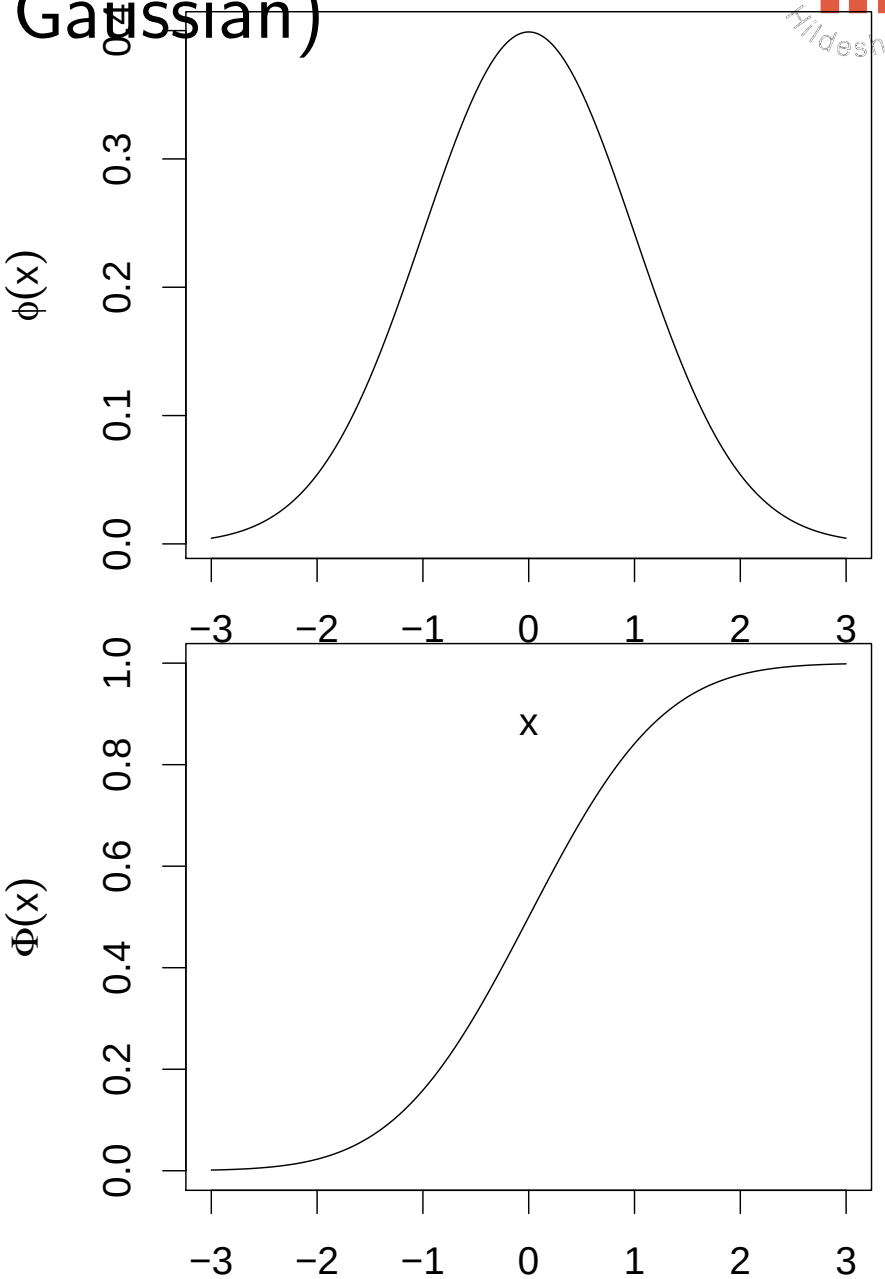
probability density function (pdf):

$$\phi(x) := \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

cumulative distribution function (cdf):

$$\Phi(x) := \int_{-\infty}^{x} \phi(t)dt$$

Φ^{-1} is called **quantile function**.



The t Distribution

written as:

$$X \sim t_p$$

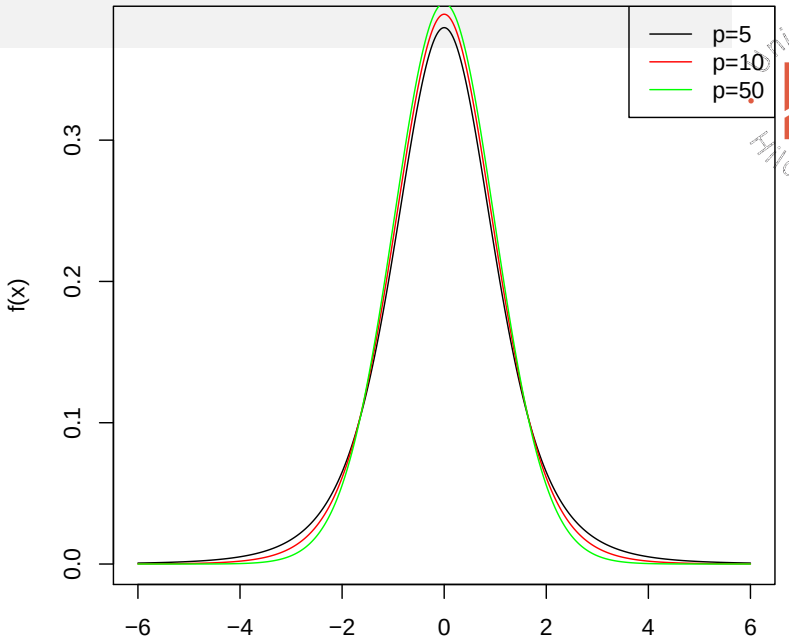
with parameter:

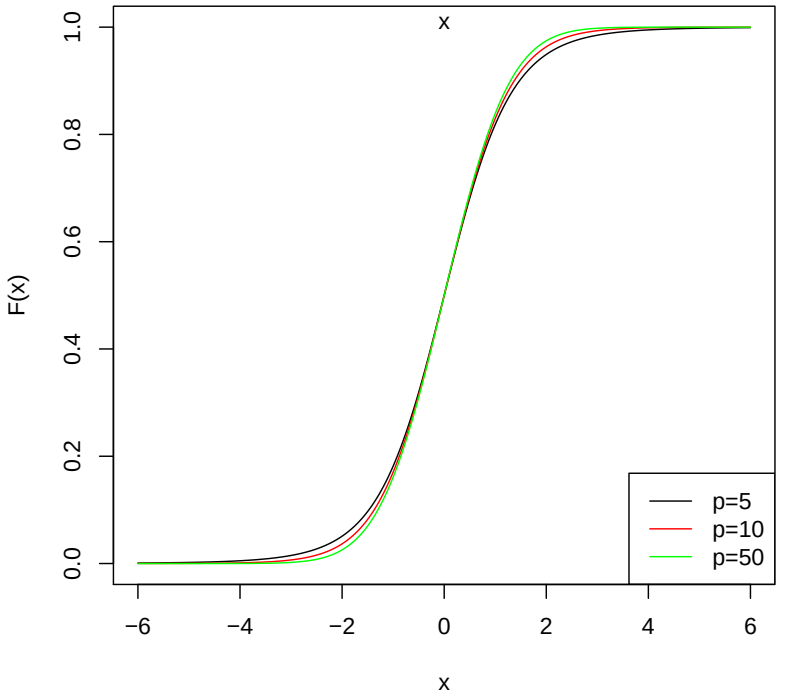
p degrees of freedom.

probability density function (pdf):

$$p(x) := \frac{\Gamma(\frac{p+1}{2})}{\sqrt{p\,\pi}\,\Gamma(\frac{p}{2})}(1 + \frac{x^2}{p})^{-\frac{p+1}{2}}$$

$$t_p \overset{p\to\infty}{\longrightarrow} \mathcal{N}(0,1)$$





The χ^2 Distribution

written as:

$$X \sim \chi^2_p$$

with parameter:

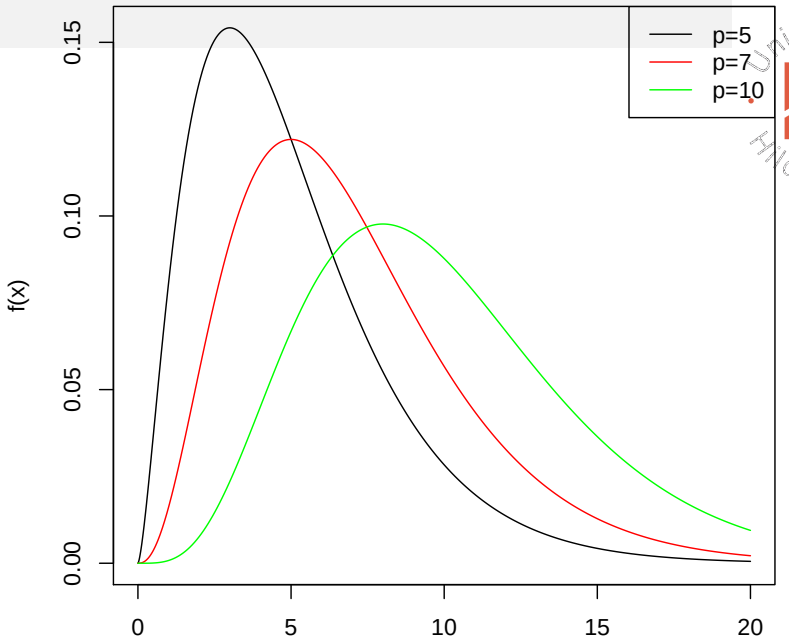
p degrees of freedom.

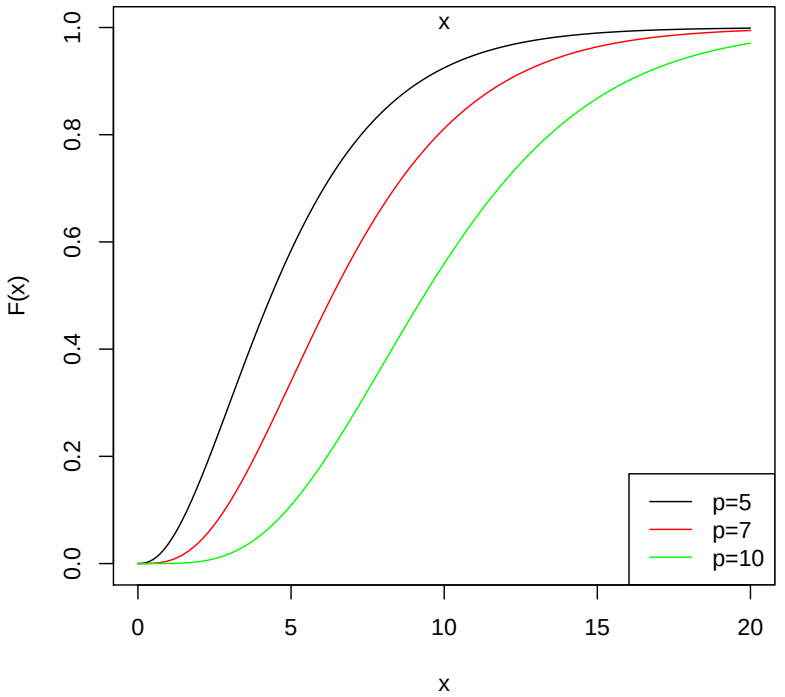
probability density function (pdf):

$$p(x) := \frac{1}{\Gamma(p/2)2^{p/2}} x^{\frac{p}{2}-1} e^{-\frac{x}{2}}, \quad x \geq 0$$

If $X_1, \ldots, X_p \sim \mathcal{N}(0,1)$, then

$$Y := \sum_{i=1}^{p} X_i^2 \sim \chi^2_p$$





Parameter Variance for Linear Regression

$\hat{\beta} = (X^T X)^{-1} X^T y$ is an unbiased estimator for β (i.e., $\mathbb{E}(\hat{\beta}) = \beta$).
Its variance is

$$\mathbb{V}(\hat{\beta}) = (X^T X)^{-1} \sigma^2$$

proof: assume ground truth $Y = X\beta + \epsilon$, $\mathbb{E}(\epsilon) = 0$, $\mathbb{V}(\epsilon) = \sigma^2 I$:

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

$$\rightsquigarrow \quad \mathbb{E}(\hat{\beta}) = \beta + (X^T X)^{-1} X^T \mathbb{E}(\epsilon) = \beta$$

$$\begin{aligned}
\mathbb{V}(\hat{\beta}) &= \mathbb{E}((\hat{\beta} - \mathbb{E}(\hat{\beta}))(\hat{\beta} - \mathbb{E}(\hat{\beta}))^T) \\
&= \mathbb{E}((X^T X)^{-1} X^T \epsilon \epsilon^T X (X^T X)^{-1}) \\
&= (X^T X)^{-1} X^T \mathbb{E}(\epsilon \epsilon^T) X (X^T X)^{-1} \\
&= (X^T X)^{-1} \sigma^2
\end{aligned}$$

Parameter Variance for Linear Regression

An unbiased estimator for σ^2 is

$$\hat{\sigma}^2 = \frac{1}{N-M}\sum_{n=1}^{N}\hat{\epsilon}_n^2 = \frac{1}{N-M}\sum_{n=1}^{N}(y_n - \hat{y}_n)^2$$

For Gaussian errors $\epsilon \sim \mathcal{N}(0, \sigma^2)$:

$$\hat{\beta} \sim \mathcal{N}(\beta, (X^T X)^{-1}\sigma^2)$$

and

$$(N-M)\hat{\sigma}^2 \sim \sigma^2 \chi^2_{N-M}$$

Parameter Variance / Standardized coefficient

standardized coefficient ("z-score"):

$$z_n := \frac{\hat{\beta}_n}{\widehat{\mathrm{se}}(\hat{\beta}_n)}, \quad \text{with } \widehat{\mathrm{se}}^2(\hat{\beta}_n) \text{ the } n\text{-th diagonal element of } (X^T X)^{-1}\hat{\sigma}^2$$

z_n would be $z_n \sim \mathcal{N}(0,1)$ if σ is known (under $H_0 : \beta_n = 0$).
With estimated $\hat{\sigma}$ it is $z_n \sim t_{N-M}$.

The Wald test for $H_0 : \beta_n = 0$ with size α is:

$$\text{reject } H_0 \text{ if } |z_n| = |\frac{\hat{\beta}_n}{\widehat{\mathrm{se}}(\hat{\beta}_n)}| > F^{-1}_{t_{N-M}}(1 - \frac{\alpha}{2})$$

i.e., its p-value is

$$p\text{-value}(H_0 : \beta_n = 0) = 2(1 - F_{t_{N-M}}(|z_n|)) = 2(1 - F_{t_{N-M}}(|\frac{\hat{\beta}_N}{\widehat{\mathrm{se}}(\hat{\beta}_N)}|))$$

and small p-values such as 0.01 and 0.05 are good.

Confidence interval

The $1-\alpha$ confidence interval for β_n:

$$\beta_n \pm F^{-1}_{t_{N-M}}(1-\frac{\alpha}{2})\ \widehat{\mathsf{se}}(\hat{\beta}_n)$$

For large N, $F_{t_{N-M}}$ converges to the standard normal cdf Φ.

As $\Phi^{-1}(1-\frac{0.05}{2}) \approx 1.95996 \approx 2$, the rule-of-thumb for a 5% confidence interval is

$$\beta_n \pm 2\,\widehat{\mathsf{se}}(\hat{\beta}_n)$$

Example

We have already fitted

$$\begin{aligned}\hat{y} =& \hat{\beta}_0 + \hat{\beta}_1 x_1 + \hat{\beta}_2 x_2 \\ =& 5.583 + 0.779 x_1 - 1.699 x_2\end{aligned}$$

to the data:

x_1	x_2	y	$\hat{y}$	$\hat{\epsilon}^2 = (y - \hat{y})^2$
1	2	3	2.965	0.00122
2	3	2	2.045	0.00207
4	1	7	7.003	0.0000122
5	5	1	0.986	0.000196
RSS				0.00350

$$\hat{\sigma}^2 = \frac{1}{N-P}\sum_{n=1}^{N}\hat{\epsilon}_n^2 = \frac{1}{4-3}0.00350 = 0.00350$$

$$(X^T X)^{-1}\hat{\sigma}^2 = \begin{pmatrix} 0.00520 & -0.00075 & -0.00076 \\ -0.00075 & 0.00043 & -0.00020 \\ -0.00076 & -0.00020 & 0.00049 \end{pmatrix}$$

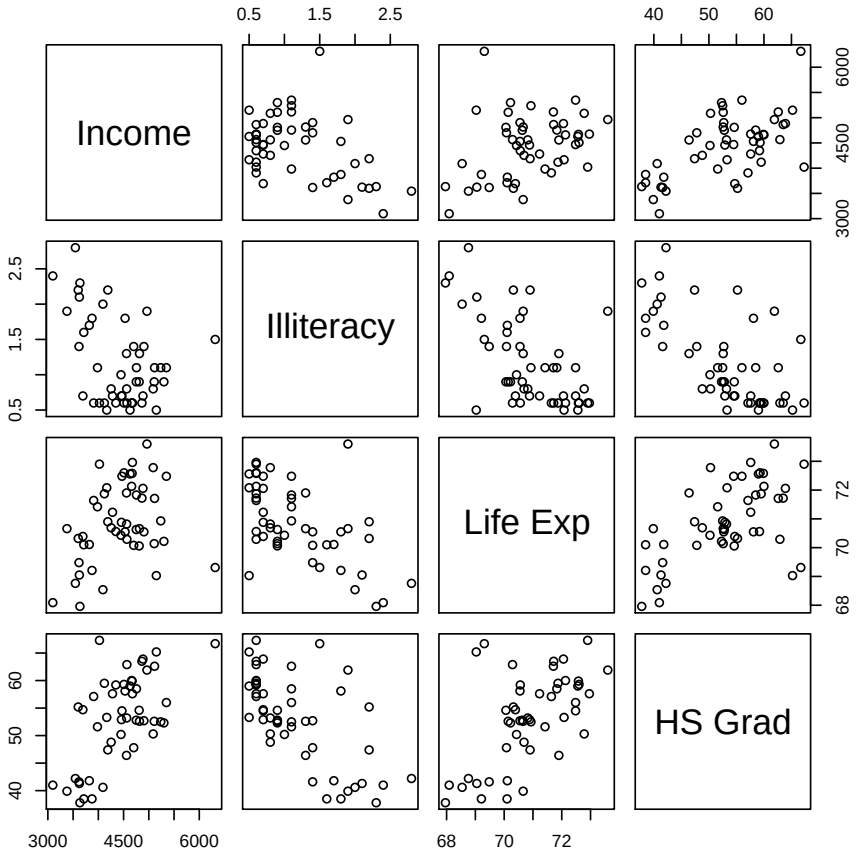
covariate	$\hat{\beta}_n$	$\widehat{\text{se}}(\hat{\beta}_n)$	z-score	p-value
(intercept)	5.583	0.0721	77.5	0.0082
X_1	0.779	0.0207	37.7	0.0169
X_2	−1.699	0.0221	−76.8	0.0083

Example 2

Example: sociographic data of the 50 US states in 1977.

state dataset:

- income (per capita, 1974),
- illiteracy (percent of population, 1970),
- life expectancy (in years, 1969–71),
- percent high-school graduates (1970).
- population (July 1, 1975)
- murder rate per 100,000 population (1976)
- mean number of days with minimum temperature below freezing (1931–1960) in capital or large city
- land area in square miles



Example 2

$$\begin{aligned}\text{Murder} =& \beta_0 + \beta_1 \text{Population} + \beta_2 \text{Income} + \beta_3 \text{Illiteracy} \\ &+ \beta_4 \text{LifeExp} + \beta_5 \text{HSGrad} + \beta_6 \text{Frost} + \beta_7 \text{Area}\end{aligned}$$

$N = 50$ states, $M = 8$ parameters, $N - M = 42$ degrees of freedom.

Least squares estimators:

	Estimate	Std. Error	t value	Pr(>|t|)	
(Intercept)	1.222e+02	1.789e+01	6.831	2.54e-08	***
Population	1.880e-04	6.474e-05	2.905	0.00584	**
Income	-1.592e-04	5.725e-04	-0.278	0.78232	
Illiteracy	1.373e+00	8.322e-01	1.650	0.10641	
‘Life Exp‘	-1.655e+00	2.562e-01	-6.459	8.68e-08	***
‘HS Grad‘	3.234e-02	5.725e-02	0.565	0.57519	
Frost	-1.288e-02	7.392e-03	-1.743	0.08867	.
Area	5.967e-06	3.801e-06	1.570	0.12391	

Outline

The Variable Selection Problem

Given a data set $\mathcal{D}^{\text{train}} \subseteq \mathbb{R}^M \times \mathcal{Y}$,
an error measure err,
a model class with a learning algorithm $\mathcal{A}$,

find the subset $V \subseteq \{1, 2, \ldots, M\}$ of (relevant) variables s.t. the model

$$\hat{y} := \mathcal{A}(\pi_V(\mathcal{D}^{\text{train}}))$$

learned on this subset V is best, i.e., for new test data $\mathcal{D}^{\text{test}}$ its test error

$$\text{err}(\hat{y}, \mathcal{D}^{\text{test}}),$$

is minimal.

Projection onto predictors V:

$$\pi_V(x, y) := (x_{m_1}, x_{m_2}, \ldots, x_{m_{\tilde{M}}}, y), \quad \text{for } V := \{m_1, m_2, \ldots, m_{\tilde{M}}\}$$

Greedy Search

- All 2^M subsets are too many to test (for larger M).
- Use a simple greedy search.
- **forward search:**
  - start with no variables.
  - test adding one more variable not yet in the model.
  - add the one leading to lowest validation error.
- **backward search:**
  - start with all variables.
  - test removing one more variable still in the model.
  - remove the one leading to lowest validation error.
- Does not guarantee to find the best variables subset.
  (But usually finds a useful one.)

Forward Search

selectvars-forward$(\mathcal{D}^{\text{train}\prime} \subseteq \mathbb{R}^M \times \mathcal{Y}, \text{err}, \mathcal{A})$:
  $(\mathcal{D}^{\text{train}}, \mathcal{D}^{\text{val}}) := \text{split}(\mathcal{D}^{\text{train}\prime})$
  $V := \emptyset$
  $e_{\text{allbest}} := \text{err}(\mathcal{A}(\pi_V(\mathcal{D}^{\text{train}})), \pi_V(\mathcal{D}^{\text{val}}))$
  $v_{\text{best}} := 1$
  while $v_{\text{best}} \neq 0$:
    $v_{\text{best}} := 0$
    $e_{\text{best}} := e_{\text{allbest}}$
    for $v \in \{1, 2, \ldots, M\} \setminus V$:
      $V' := V \cup \{v\}$
      $\hat{y} := \mathcal{A}(\pi_{V'}(\mathcal{D}^{\text{train}}))$
      $e := \text{err}(\hat{y}, \pi_{V'}(\mathcal{D}^{\text{val}}))$
        if $e < e_{\text{best}}$:
          $v_{\text{best}} := v$
          $e_{\text{best}} := e$
    if $e_{\text{best}} < e_{\text{allbest}}$:
      $V := V \cup \{v_{\text{best}}\}$
      $e_{\text{allbest}} := e_{\text{best}}$
return V

Backward Search

selectvars-backward$(\mathcal{D}^{\text{train}\prime} \subseteq \mathbb{R}^M \times \mathcal{Y}, \text{err}, \mathcal{A})$:
  $(\mathcal{D}^{\text{train}}, \mathcal{D}^{\text{val}}) := \text{split}(\mathcal{D}^{\text{train}\prime})$
  $V := \{1, 2, \ldots, M\}$
  $e_{\text{allbest}} := \text{err}(\mathcal{A}(\pi_V(\mathcal{D}^{\text{train}})), \pi_V(\mathcal{D}^{\text{val}}))$
  $v_{\text{best}} := 1$
  while $v_{\text{best}} \neq 0$:
    $v_{\text{best}} := 0$
    $e_{\text{best}} := e_{\text{allbest}}$
    for $v \in V$:
      $V' := V \setminus \{v\}$
      $\hat{y} := \mathcal{A}(\pi_{V'}(\mathcal{D}^{\text{train}}))$
      $e := \text{err}(\hat{y}, \pi_{V'}(\mathcal{D}^{\text{val}}))$
        if $e < e_{\text{best}}$:
          $v_{\text{best}} := v$
          $e_{\text{best}} := e$
    if $e_{\text{best}} < e_{\text{allbest}}$:
      $V := V \setminus \{v_{\text{best}}\}$
      $e_{\text{allbest}} := e_{\text{best}}$
return V

Sequential Search with Variable Importance Heuristics

- Forward and backward search has to learn many models.
  - forward search: 1, 2, 3, ...
  - backward search: M, M-1, M-2, ...
- Further simplification: use a sequential search.
- Use a heuristics to assess **variable importance** once (without context)
  - e.g., the error of the single-variable model:

$$\text{imp}(m) := \text{err}(\mathcal{A}(\pi_{\{m\}}(\mathcal{D}^{\text{train}})), \mathcal{D}^{\text{val}})$$

- Add variables in order of increasing heuristics.
- Usually a full sequential sweep through all variables is done.
  - No difference between Forward and Backward Search.
- Faster, but even less reliable than forward/backward search.

Sequential Search

selectvars-seq$(\mathcal{D}^{\text{train}\prime} \subseteq \mathbb{R}^M \times \mathcal{Y}, \text{err}, \mathcal{A}, \text{imp})$:
  $(\mathcal{D}^{\text{train}}, \mathcal{D}^{\text{val}}) := \text{split}(\mathcal{D}^{\text{train}\prime})$
  $\mathcal{V} := \text{sort-increasing}(\{1, 2, \ldots, M\}, \text{imp})$
  $V := \emptyset$
  $e_{\text{best}} := \text{err}(\mathcal{A}(\pi_V(\mathcal{D}^{\text{train}})), \pi_V(\mathcal{D}^{\text{val}}))$
  $m_{\text{best}} := 1$
  for $m = 1, \ldots, M$:
    $v := \mathcal{V}_m$
    $V := V \cup \{v\}$
    $\hat{y} := \mathcal{A}(\pi_V(\mathcal{D}^{\text{train}}))$
    $e := \text{err}(\hat{y}, \pi_V(\mathcal{D}^{\text{val}}))$
    if $e < e_{\text{best}}$:
      $m_{\text{best}} := m$
      $e_{\text{best}} := e$
  $V := \{\mathcal{V}_1, \mathcal{V}_2, \ldots, \mathcal{V}_{m_{\text{best}}}\}$
  return V

Outline

Minimizing a Function via Coordinate Descent (CD)

Given a function $f : \mathbb{R}^N \to \mathbb{R}$, find x with minimal $f(x)$.

- Use the coordinate axes as descent direction
  - first x_1-axis, then x_2-axis, etc. (cyclic)
  - **one-dimensional subproblems**:

$$g_n(x) := \arg\min_{x_n \in \mathbb{R}} f(x_n; x_{-n}) := \arg\min_{x' \in \mathbb{R}} f(x_1, x_2, \ldots, x_{n-1}, x', x_{n+1}, \ldots, x_N)$$

- Coordinate Descent can be fast if solving the one-dimensional subproblems can be done analytically.
  - For smooth f, one needs to solve

$$\frac{\partial f(x_n; x_{-n})}{\partial x_n} \stackrel{!}{=} 0$$

  - Then also no step length is required !

Note: $x_{-n} := (x_1, \ldots, x_2, \ldots, x_{n-1}, x_{n+1}, \ldots, x_N)$ is the vector without element n for a vector $x \in \mathbb{R}^N$.

Coordinate Descent

minimize-CD$(f : \mathbb{R}^N \to \mathbb{R}, g, x^{(0)} \in \mathbb{R}^N, i_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:
  for $i := 1, \ldots, i_{\max}$:
    $x^{(i)} := x^{(i-1)}$
    for $n := 1, \ldots, N$:
      $x_n^{(i)} := g_n(x_{-n}^{(i)})$
    if $f(x^{(i-1)}) - f(x^{(i)}) < \epsilon$:
      return $x^{(i)}$
  raise exception "not converged in $i_{\max}$ iterations"

with

g : solvers g_n for the n-th one-dimensional subproblem

$$g_n(x_1, x_2, \ldots, x_{n-1}, x_{n+1}, \ldots, x_N) := \arg\min_{x' \in \mathbb{R}} f(x_1, \ldots, x_{n-1}, x', x_{n+1}, \ldots, x_N)$$

Example: Simple Quadratic Function

Minimize

$$f(x_1, x_2) := x_1^2 + x_2^2 + x_1 x_2$$

One dimensional problem for x_1:

$$\begin{aligned} f(x_1; x_2) =& x_1^2 + x_2^2 + x_1 x_2 \\ \frac{\partial f}{\partial x_1}(x_1; x_2) =& 2x_1 + x_2 \stackrel{!}{=} 0 \\ \rightsquigarrow\ & x_1 = -\frac{1}{2} x_2 \\ \text{i.e., } & g_1(x_2) := -\frac{1}{2} x_2 \end{aligned}$$

and analogous for x_2:

$$g_2(x_1) := -\frac{1}{2} x_1$$

Example: Simple Quadratic Function

Minimize

$$f(x_1, x_2) := x_1^2 + x_2^2 + x_1 x_2, \quad x^{(0)} := (1, 1)$$

$$g_1(x_2) := -\frac{1}{2} x_2, \quad g_2(x_1) := -\frac{1}{2} x_1$$

i	$x^{(i)}$ before	n	$g_n(x^{(i)})$	$x^{(i)}$ after
1	$(1, 1)$	1	$-1/2$	$(-1/2, 1)$
	$(-1/2, 1)$	2	$1/4$	$(-1/2, 1/4)$
2	$(-1/2, 1/4)$	1	$-1/8$	$(-1/8, 1/4)$
	$(-1/8, 1/4)$	2	$1/16$	$(-1/8, 1/16)$
$\vdots$				

Note: Minimize $f(x_1, x_2) := x_1^2 + x_2^2$ via CD yourself. What is different? Why?

Learn Linear Regression via CD

Minimize

$$f(\hat{\beta}) := ||y - X\hat{\beta}||^2 \propto \hat{\beta}^T X^T X \hat{\beta} - 2y^T X \hat{\beta}$$

$$\begin{aligned} f(\hat{\beta}_m; \hat{\beta}_{-m}) &= x_m^T x_m \hat{\beta}_m^2 + 2\hat{\beta}_{-m}^T X_{-m}^T x_m \hat{\beta}_m + \hat{\beta}_{-m}^T X_{-m}^T X_{-m} \hat{\beta}_{-m} \\ &\quad - 2y^T x_m \hat{\beta}_m - 2y^T X_{-m} \hat{\beta}_{-m} \\ &\propto x_m^T x_m \hat{\beta}_m^2 - 2(y - X_{-m}\hat{\beta}_{-m})^T x_m \hat{\beta}_m \end{aligned}$$

$$\frac{\partial f(\hat{\beta}_m; \hat{\beta}_{-m})}{\partial \hat{\beta}_m} \stackrel{!}{=} 0 \rightsquigarrow \hat{\beta}_m = \frac{(y - X_{-m}\hat{\beta}_{-m})^T x_m}{x_m^T x_m}$$

Note: $x_m := X_{.,m}$ denotes the m-th column of X,
X_{-m} denotes the matrix X without column m.

Learn Linear Regression via CD

learn-linreg-CD$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, i_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$X := (x_1, x_2, \ldots, x_N)^T$

$y := (y_1, y_2, \ldots, y_N)^T$

$\hat{\beta}_0 := (0, \ldots, 0)$

$\hat{\beta} :=$ MINIMIZE-CD($f(\hat{\beta}) := (y - X\hat{\beta})^T(y - X\hat{\beta})$,
$g(\hat{\beta}_m; \hat{\beta}_{-m}) := \frac{(y - X_{-m}\hat{\beta}_{-m})^T x_m}{x_m^T x_m}$
$\hat{\beta}_0, \alpha, i_{\max}, \epsilon)$

return $\hat{\beta}$

Note: $x_m := X_{\cdot,m}$ denotes the m-th column of X,
X_{-m} denotes the matrix X without column m.

Outline

L1 Regularization

Let X the predictor matrix and y the target vector,
$\hat{\theta}$ the model parameters,
$\hat{y}$ the model predictions and
ℓ the loss/error.

L2 regularization:

$$f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X)) + \lambda ||\hat{\theta}||_2^2 = \ldots + \lambda \sum_{p=1}^{P} \hat{\theta}_p^2$$

L1 regularization:

$$f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X)) + \lambda ||\hat{\theta}||_1 = \ldots + \lambda \sum_{p=1}^{P} |\hat{\theta}_p|$$

Why L1 Regularization?

$$\begin{aligned} \text{min.} \quad & f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X)) + \lambda ||\hat{\theta}||_1 \\ & \hat{\theta} \in \mathbb{R}^P \end{aligned}$$

is equivalent to

$$\begin{aligned} \text{min.} \quad & f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X)) \\ & ||\hat{\theta}||_1 \leq B \\ & \hat{\theta} \in \mathbb{R}^P \end{aligned}$$

with

$$B := ||\hat{\theta}^*||_1$$

Note: $\hat{\theta}^*$ denotes the optimal parameters. Thus this equivalence provides insight, but cannot (yet) be used to solve the problem.

Why L1 Regularization?

$$\min_{\hat{\theta} \in \mathbb{R}^P} f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X)) + \lambda ||\hat{\theta}||_1$$

is equivalent to

$$\min_{\hat{\theta} \in \mathbb{R}^P} f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X))$$
$$||\hat{\theta}||_1 \leq B$$

with

$$B := ||\hat{\theta}^*||_1$$

$$\min_{\hat{\theta} \in \mathbb{R}^P} f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X)) + \lambda ||\hat{\theta}||_2^2$$

is equivalent to

$$\min_{\hat{\theta} \in \mathbb{R}^P} f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X))$$
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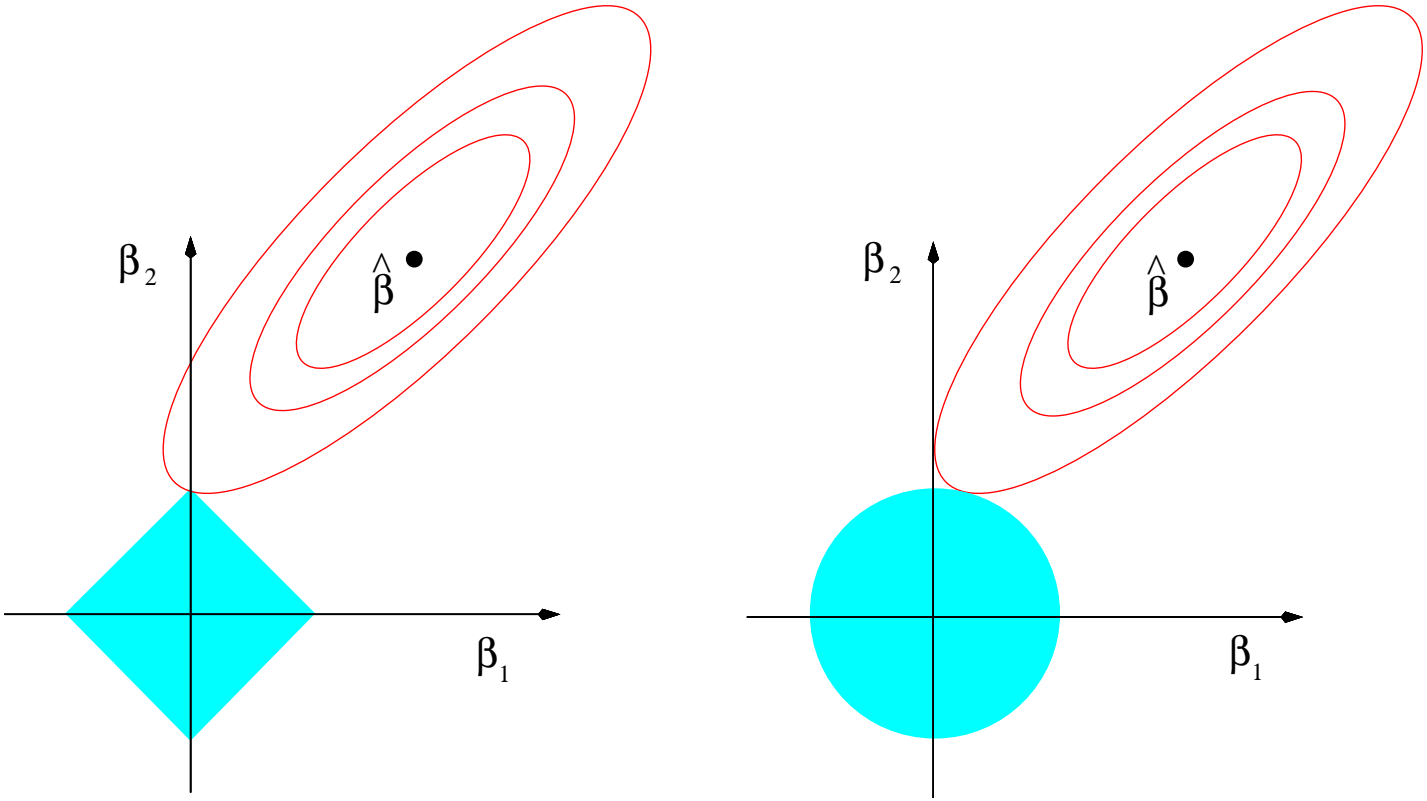
Why L1 Regularization?



source: [Hastie et al., 200

Regularized Linear Regression

Let X the predictor matrix and y the target vector,
$\hat{\beta}$ the linear regression model parameters,
$\hat{y} := X\hat{\beta}$ the linear regression model predictions and
$\ell(y, \hat{y}) := ||y - \hat{y}||_2^2$ the RSS loss/error.

L2 Regularized Linear Regression (**Ridge Regression**):

$$\begin{aligned} f(\hat{\beta}) &:= \ell(y, \hat{y}(\hat{\beta}, X)) + \lambda||\hat{\beta}||_2^2 \\ &\propto \hat{\beta}^T X^T X \hat{\beta} - 2y^T X \hat{\beta} + \lambda \hat{\beta}^T \hat{\beta} \\ &= \hat{\beta}^T (X^T X + \lambda I)\hat{\beta} - 2y^T X \hat{\beta} \end{aligned}$$

- L2 regularized problem has same structure as unregularized one.
- All learning algorithms work seamlessly.

Regularized Linear Regression

Let X the predictor matrix and y the target vector,
$\hat{\beta}$ the linear regression model parameters,
$\hat{y} := X\hat{\beta}$ the linear regression model predictions and
$\ell(y, \hat{y}) := ||y - \hat{y}||_2^2$ the RSS loss/error.

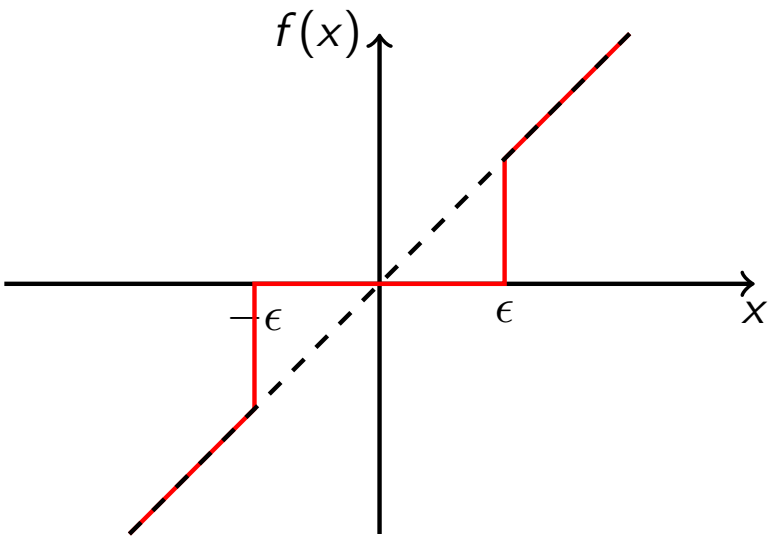
L1 regularized Linear Regression (**Lasso**):

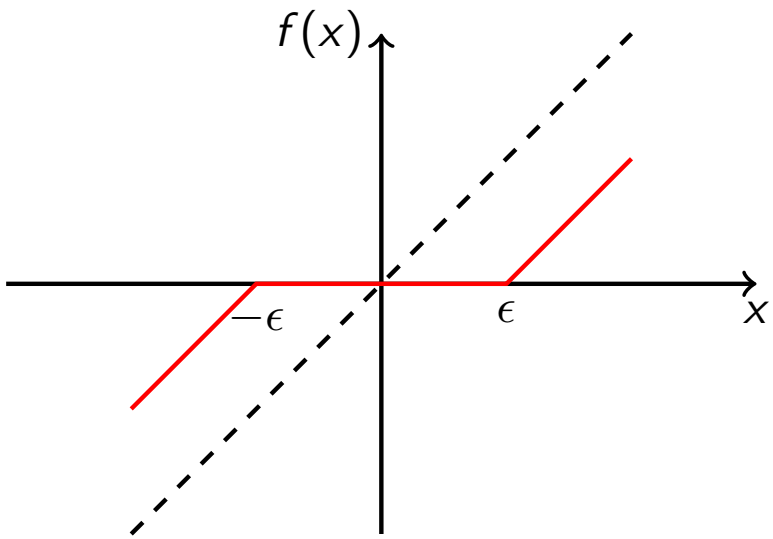
$$f(\beta) := \ell(y, \hat{y}) + \lambda||\beta||_1$$

$$\propto \hat{\beta}^T X^T X\hat{\beta} - 2y^T X\hat{\beta} + \lambda \sum_{m=1}^{M} |\beta_m|$$

- L1 regularized problem has new terms $|\beta_m|$.
  - Esp. non-differentiable at 0.
- All learning algorithms seen so far do not work.
  - Solving SLE is not applicable.
  - Gradient Descent does not work.

Hard & Soft Thresholding





$$\text{hard}(x,\epsilon) := \begin{cases} x, & \text{if } |x| > \epsilon \\ 0, & \text{else} \end{cases}$$

$$\text{soft}(x,\epsilon) := \begin{cases} x-\epsilon, & \text{if } x > \epsilon \\ 0, & \text{if } |x| \leq \epsilon \\ x+\epsilon, & \text{if } x < -\epsilon \end{cases}$$

Coordinate Descent for L1 Regularized Linear Regression

$$f(\hat{\beta}) := \hat{\beta}^T X^T X \hat{\beta} - 2y^T X \hat{\beta} + \lambda \sum_{m=1}^{M} |\beta_m|$$

$$f(\hat{\beta}_m; \hat{\beta}_{-m}) \propto x_m^T x_m \hat{\beta}_m^2 - 2(y - X_{-m}\hat{\beta}_{-m})^T x_m \hat{\beta}_m + \lambda|\beta_m|$$

$$\frac{\partial f(\hat{\beta}_m; \hat{\beta}_{-m})}{\partial \hat{\beta}_m} \stackrel{!}{=} 0 \rightsquigarrow \hat{\beta}_m \stackrel{\text{naive}}{=} \begin{cases} \frac{(y - X_{-m}\hat{\beta}_{-m})^T x_m - \frac{1}{2}\lambda}{x_m^T x_m}, & \hat{\beta}_m > 0 \\ \frac{(y - X_{-m}\hat{\beta}_{-m})^T x_m + \frac{1}{2}\lambda}{x_m^T x_m}, & \hat{\beta}_m < 0 \end{cases}$$

$$\rightsquigarrow \hat{\beta}_m = \text{soft}\left(\frac{(y - X_{-m}\hat{\beta}_{-m})^T x_m}{x_m^T x_m}, \frac{\frac{1}{2}\lambda}{x_m^T x_m}\right)$$

Note: LASSO = Least Absolute Selection and Shrinkage Operator.
naive = without checking that the update might leave the branches $\hat{\beta}_m > 0$ and < 0.

Learn L1-regularized Linear Regression via CD (Shooting Algorithm)

learn-linreg-l1reg-CD$(\mathcal{D}^{\text{train}} := \{(x_1, y_1), \ldots, (x_N, y_N)\}, \lambda \in \mathbb{R}^+, i_{\max} \in \mathbb{N}, \epsilon \in \mathbb{R}^+)$:

$X := (x_1, x_2, \ldots, x_N)^T$

$y := (y_1, y_2, \ldots, y_N)^T$

$\hat{\beta}_0 := (0, \ldots, 0)$

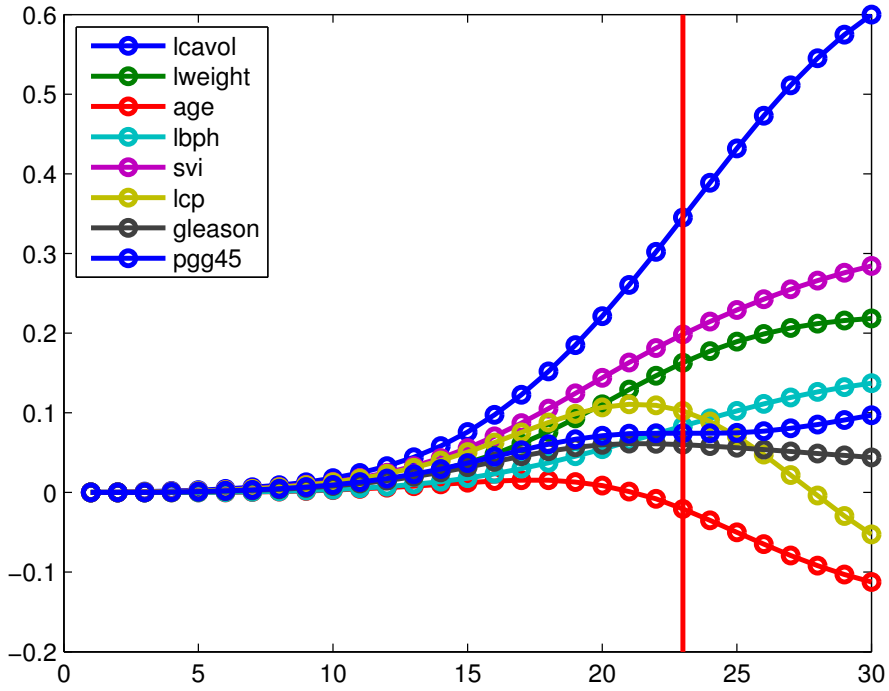
$\hat{\beta} :=$ MINIMIZE-CD($f(\hat{\beta}) := (y - X\hat{\beta})^T(y - X\hat{\beta}) + \lambda||\beta||_1$,
$g(\hat{\beta}_m; \hat{\beta}_{-m}) := \text{soft}(\frac{(y - X_{-m}\hat{\beta}_{-m})^T x_m}{x_m^T x_m}, \frac{\frac{1}{2}\lambda}{x_m^T x_m})$,
$\hat{\beta}_0, \alpha, i_{\max}, \epsilon)$

return $\hat{\beta}$

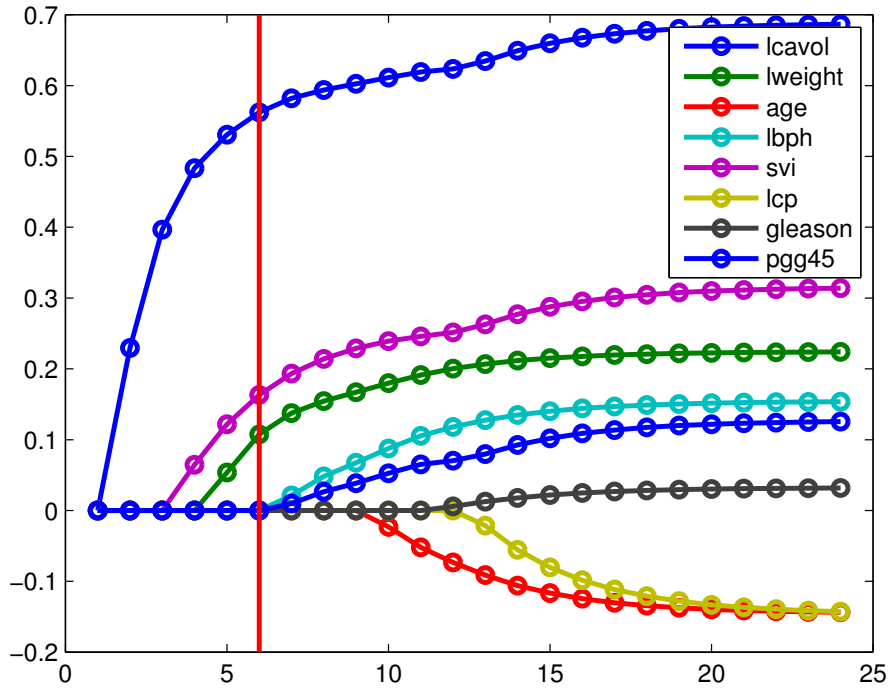
Note: $x_m := X_{\cdot,m}$ denotes the m-th column of X,
X_{-m} denotes the matrix X without column m.

Regularization Paths

L2 regularization



L1 regularization



x-axis: bound B on parameter size.
y-axis: parameter $\hat{\theta}$.

source: [Murphy, 2012, p

Summary

- **High-dimensional data** poses problems as many parameters have to be estimated from comparable few instances.
- Non-linear effects can be captured by **derived predictor variables**.
  - e.g., in **polynomial models**.
  - making even originally low-dimensional data high-dimensional.
- Relevant variables can be searched explicitly through a greedy **forward search** and **backward search**.
- To minimize a function, **coordinate descent** cyclicly chooses the coordinate axes as descent direction.
  - efficient, if the **one-dimensional subproblems** can be solved analytically.
  - does need no step length.

Further Readings

- [James et al., 2013, chapter 6], [Murphy, 2012, chapter 13], [Hastie et al., 2005, chapter 3.3–8].

References

Trevor Hastie, Robert Tibshirani, Jerome Friedman, and James Franklin. *The Elements of Statistical Learning: Data Mining, Inference and Prediction*, volume 27. Springer, 2005.

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Kevin P. Murphy. *Machine Learning: A Probabilistic Perspective*. The MIT Press, 2012.