Machine Learning

A. Supervised Learning
A.4. High-Dimensional Data

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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

Syllabus

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			A. Supervised Learning
Wed.	22.10.	(2)	A.1 Linear Regression
Tue.	28.10.	(3)	A.2 Linear Classification
Wed.	29.10.	(4)	A.3 Regularization
Tue.	4.11.	(5)	A.4 High-dimensional Data
Wed.	5.11.	(6)	A.5 Nearest-Neighbor Models
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Tue.	18.11.	(9)	A.8 A First Look at Bayesian and Markov Networks
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Wed.	19.11.	(10)	B.1 Clustering
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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

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Need for higher orders

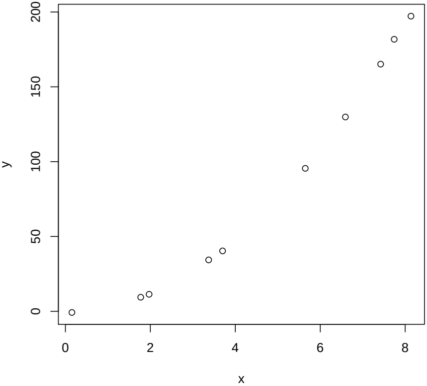
Assume a target variable does not depend linearly on a predictor variable, but say quadratic.

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

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

one looks at

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

with

$$
\begin{aligned}
X_1' :=& X_1^2 \\
X_1' :=& e^{\alpha X_1} \\
X_1' :=& X_1 \cdot X_2
\end{aligned}
$$

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*):

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

Polynomial Models

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

$$\hat{y}(x) := \hat{\theta}_0 + \sum_{m=1}^{M} \hat{\theta}_m x_m + \sum_{m=1}^{M} \sum_{l=m}^{M} \hat{\theta}_{m,l} x_m x_l \qquad \text{degree 2}$$

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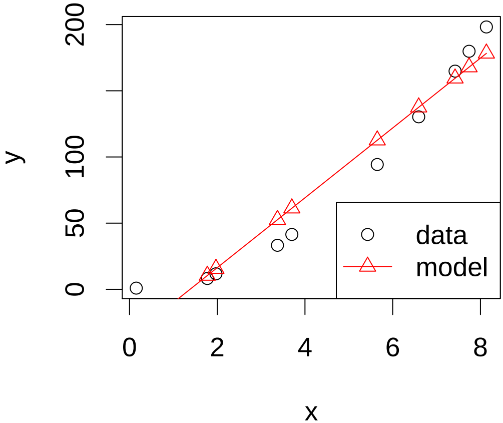
$$\hat{y}(x) := \hat{\theta}_0 + \sum_{m=1}^{M} \hat{\theta}_m x_m + \sum_{m=1}^{M} \sum_{l=m}^{M} \hat{\theta}_{m,l} x_m x_l + \cdots$$

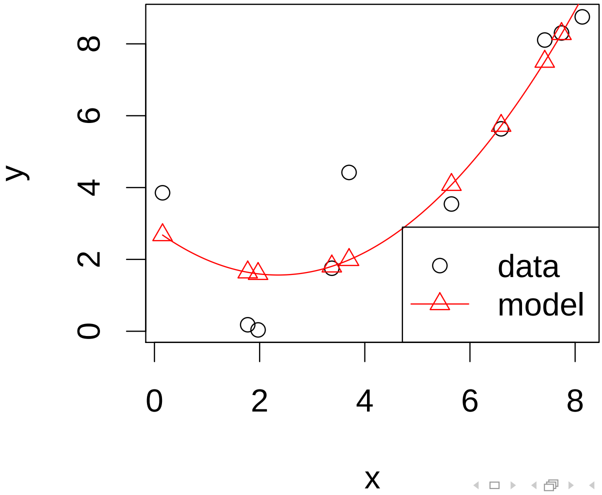
$$+ \sum_{m_1=1}^{M} \sum_{m_2=m_1}^{M} \cdots \sum_{m_d=m_{d-1}}^{M} \hat{\theta}_{m_1,m_2,\ldots,m_d} x_{m_1} x_{m_2} \cdots x_{m_d} \qquad \text{degree } d$$

High Polynomial Degress, High Model Complexity

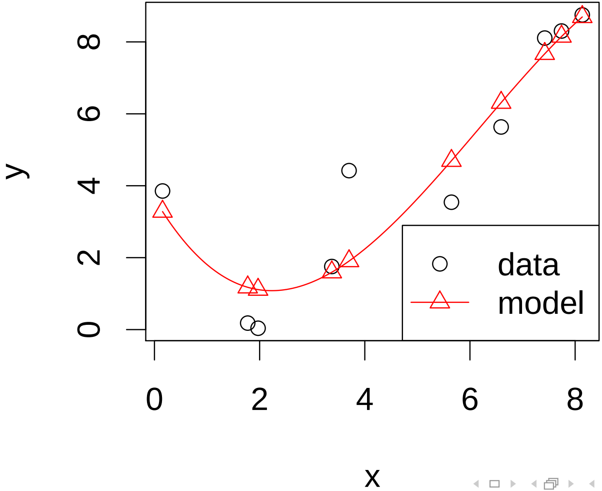


If a model does not well explain the data,
e.g., if the true model is quadratic, but we try to fit a linear model,
one says, the model **underfits**.

High Polynomial Degress, High Model Complexity



High Polynomial Degress, High Model Complexity



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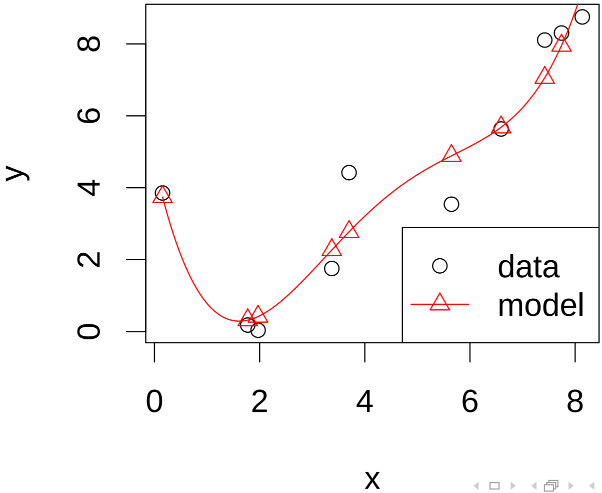
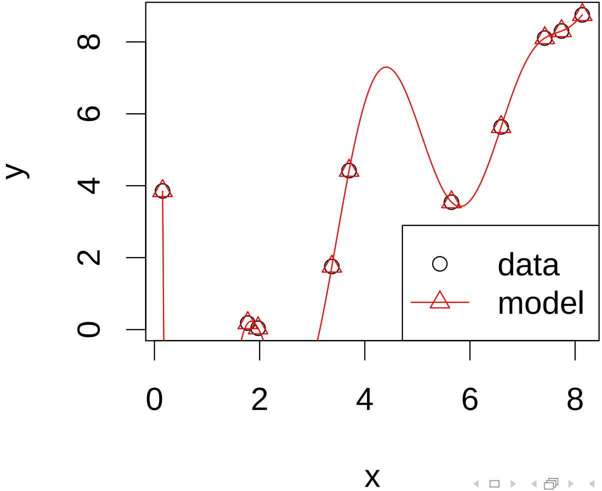


High Polynomial Degress, High Model Complexity



High Polynomial Degress, High Model Complexity

If to data

$$(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$$

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

$$\hat{y}(X) = \sum_{i=1}^{n} y_i \prod_{j \neq i} \frac{X - x_j}{x_i - x_j}$$

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

Variable Types and Coding

The most common variable types:

numerical / interval-scaled / quantitative

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

nominal / discrete / categorical / qualitative / factor

where 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

where levels are ordered, but differences and quotients are not defined,
usually with a finite, enumerated domain,
e.g., $\mathcal{X} := \{\text{small}, \text{medium}, \text{large}\}$

Variable Types and Coding

Nominals are usually encoded as binary **dummy variables**:

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

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

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

Replace

one variable X with 3 levels: $\text{red}, \text{green}, \text{blue}$

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

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The Normal Distribution (also Gaussian)

written as:

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

with parameters:

μ mean,

σ standard deviance.

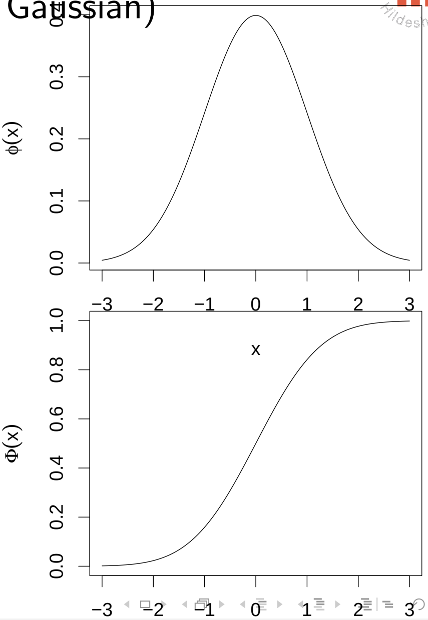
probability density function (pdf):

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

cumulative distribution function (cdf):

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

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



The t Distribution

written as:

$$X \sim t_p$$

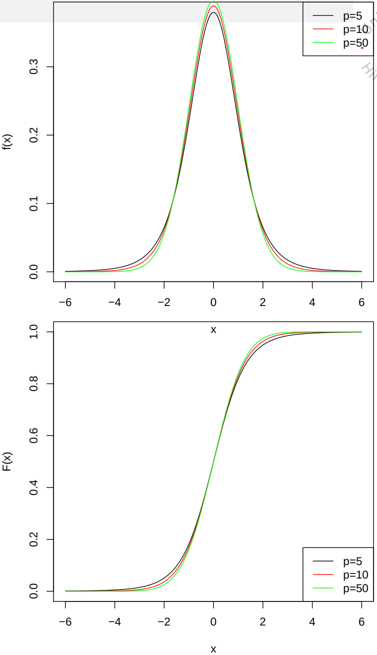
with parameter:

p degrees of freedom.

probability density function (pdf):

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

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



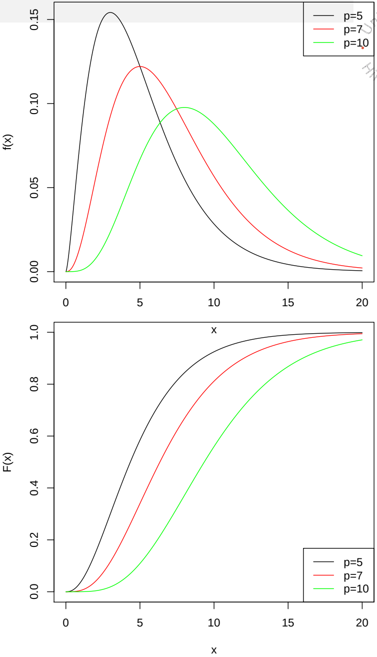
The χ^2 Distribution

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

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

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

proof:

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

As $E(\epsilon) = 0$: $E(\hat{\beta}) = \beta$

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

Parameter Variance

An unbiased estimator for σ^2 is

$$\hat{\sigma}^2 = \frac{1}{n-p}\sum_{i=1}^{n}\hat{\epsilon}_i^2 = \frac{1}{n-p}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

If $\epsilon \sim \mathcal{N}(0, \sigma^2)$, then

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

Furthermore

$$(n-p)\hat{\sigma}^2 \sim \sigma^2\chi^2_{n-p}$$

Parameter Variance / Standardized coefficient

standardized coefficient ("z-score"):

$$z_i := \frac{\hat\beta_i}{\widehat{\text{se}}(\hat\beta_i)}, \quad \text{with } \widehat{\text{se}}^2(\hat\beta_i) \text{ the } i\text{-th diagonal element of } (X^T X)^{-1}\hat\sigma^2$$

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

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

$$\text{reject } H_0 \text{ if } |z_i| = |\frac{\hat\beta_i}{\widehat{\text{se}}(\hat\beta_i)}| > F^{-1}_{t_{n-p}}(1 - \frac{\alpha}{2})$$

i.e., its p-value is

$$p\text{-value}(H_0 : \beta_i = 0) = 2(1 - F_{t_{n-p}}(|z_i|)) = 2(1 - F_{t_{n-p}}(|\frac{\hat\beta_i}{\widehat{\text{se}}(\hat\beta_i)}|))$$

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

Confidence interval

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

$$\beta_i \pm F^{-1}_{t_{n-p}}(1-\frac{\alpha}{2})\widehat{\text{se}}(\hat{\beta}_i)$$

For large n, $F_{t_{n-p}}$ 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

$$\beta_i \pm 2\widehat{\text{se}}(\hat{\beta}_i)$$

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

$$\hat{\sigma}^2 = \frac{1}{n-p} \sum_{i=1}^{n} \hat{\epsilon}_i^2 = \frac{1}{4-3} 0.00350 = 0.00350$$

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

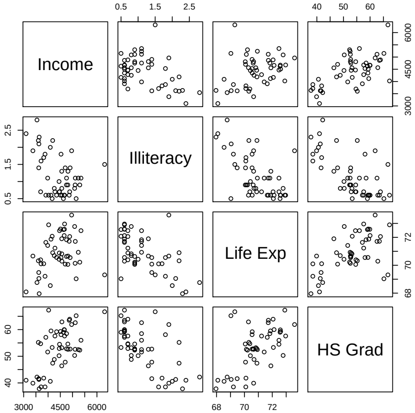
covariate	$\hat{\beta}_i$	$\widehat{\text{se}}(\hat{\beta}_i)$	z-score	p-value
(intercept)	5.583	0.0721	77.5	0.0082
X_1	0.779	0.0207	37.7	0.0169
X_2	−1.699	0.0221	−76.8	0.0083

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, $p = 8$ parameters, $n - p = 42$ 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
```

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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 $\mathcal{D}^{\text{test}}$ it's test error

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

is minimal.

Projection onto predictors V:

$$\pi_V(x, y) := (x_{i_1}, x_{i_2}, \ldots, x_{i_{\tilde{M}}}, y), \quad \text{for } V := \{i_1, i_2, \ldots, i_{\tilde{M}}\}$$

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

```
procedure 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 $v_{\text{best}} \neq 0$ do
        $v_{\text{best}} := 0$
        $e_{\text{best}} := e_{\text{allbest}}$
        for $v \in \{1, 2, \ldots, M\} \setminus V$ do
            $V' := V \cup \{v\}$
            $\hat{y} := \mathcal{A}(\pi_{V'}(\mathcal{D}^{\text{train}}))$
            $e := \text{err}(\hat{y}, \pi_{V'}(\mathcal{D}^{\text{val}}))$
            if $e < e_{\text{best}}$ then
                $v_{\text{best}} := v$
                $e_{\text{best}} := e$
        if $e_{\text{best}} < e_{\text{allbest}}$ then
            $V := V \cup \{v_{\text{best}}\}$
            $e_{\text{allbest}} := e_{\text{best}}$
    return $V$
```

Backward Search

```
procedure 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 $v_{\text{best}} \neq 0$ do
        $v_{\text{best}} := 0$
        $e_{\text{best}} := e_{\text{allbest}}$
        for $v \in V$ do
            $V' := V \setminus \{v\}$
            $\hat{y} := \mathcal{A}(\pi_{V'}(\mathcal{D}^{\text{train}}))$
            $e := \text{err}(\hat{y}, \pi_{V'}(\mathcal{D}^{\text{val}}))$
            if $e < e_{\text{best}}$ then
                $v_{\text{best}} := v$
                $e_{\text{best}} := e$
        if $e_{\text{best}} < e_{\text{allbest}}$ then
            $V := V \setminus \{v_{\text{best}}\}$
            $e_{\text{allbest}} := e_{\text{best}}$
    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 simplication: 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

```
procedure SELECTVARS-SEQ($\mathcal{D}^{\text{train}\prime} \subseteq \mathbb{R}^M \times \mathcal{Y}$, err, $\mathcal{A}$, 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 $m = 1, \ldots, M$ do
        $v := \mathcal{V}_m$
        $V := V \cup \{v\}$
        $\hat{y} := \mathcal{A}(\pi_V(\mathcal{D}^{\text{train}}))$
        $e := \text{err}(\hat{y}, \pi_V(\mathcal{D}^{\text{val}}))$
        if $e < e_{\text{best}}$ then
            $m_{\text{best}} := m$
            $e_{\text{best}} := e$
    $V := \{1, 2, \ldots, m_{\text{best}}\}$
    return $V$
```

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Minimizing a Function via Coordinate Descent (CD)

Given a function $f : \mathbb{R}^N \rightarrow \mathbb{R}$, 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

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

  - 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

```
procedure 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 $i := 1, \ldots, i_{\max}$ do
        $x^{(i)} := x^{(i-1)}$
        for $n := 1, \ldots, N$ do
            $x_n^{(i)} := g_n(x_{-n}^{(i)})$
        if $f(x^{(i-1)}) - f(x^{(i)}) < \epsilon$ then
            return $x^{(i)}$
    error "not converged in $i_{\max}$ iterations"
```

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:

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

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	$g_n(x^{(i)})$	$x^{(i-1)}$ 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

$$\begin{aligned} f(\hat\beta) &:= ||y - X\hat\beta||^2 \propto \hat\beta^T X^T X\hat\beta - 2y^T X\hat\beta \\ f(\hat\beta_m; \hat\beta_{-m}) &= x_m^T x_m \hat\beta_m^2 + 2\hat\beta_{-m}^T X_{-m}^T x_m \hat\beta_m + \hat\beta_{-m}^T X_{-m}^T X_{-m}\hat\beta_{-m} \\ &\quad - 2y^T x_m \hat\beta_m - 2y^T X_{-m}\hat\beta_{-m} \\ &\propto x_m^T x_m \hat\beta_m^2 - 2(y - X_{-m}\hat\beta_{-m})^T x_m \hat\beta_m \end{aligned}$$

$$\frac{\partial f(\hat\beta_m; \hat\beta_{-m})}{\partial \hat\beta_m} \overset{!}{=} 0 \rightsquigarrow \hat\beta_m = \frac{(y - X_{-m}\hat\beta_{-m})^T x_m}{x_m^T x_m}$$

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

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

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

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:

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

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?

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

is equivalent to

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

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?

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

is equivalent to

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

with

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

$$\begin{aligned} \text{min.}\ & f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X)) + \lambda \|\hat{\theta}\|_2^2 \\ & \hat{\theta} \in \mathbb{R}^P \end{aligned}$$

is equivalent to

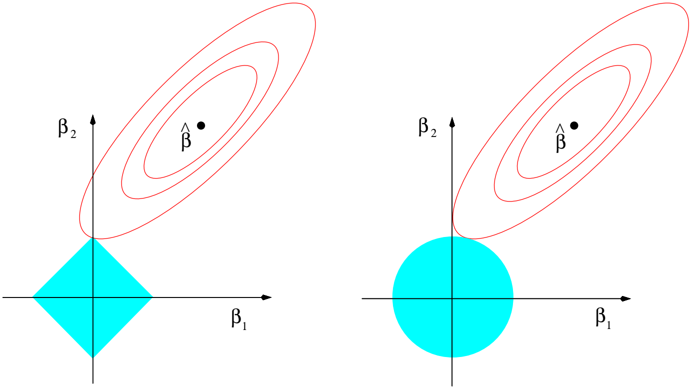
$$\begin{aligned} \text{min.}\ & f(\hat{\theta}) := \ell(y, \hat{y}(\hat{\theta}, X)) \\ & \|\hat{\theta}\|_2^2 \leq B \\ & \hat{\theta} \in \mathbb{R}^P \end{aligned}$$

with

$$B := \|\hat{\theta}^*\|_2^2$$

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

Why L1 Regularization?



source: [HTFF05, p. 90]

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**):

$$\begin{aligned} f(\hat{\beta}) &:= \ell(y, \hat{y}(\hat{\beta}, X)) + \lambda||\hat{\beta}||_2^2 \\ &\propto \hat{\beta}^T X^T X\hat{\beta} - 2y^T X\hat{\beta} + \lambda\hat{\beta}^T\hat{\beta} \\ &= \hat{\beta}^T(X^T + \lambda^{\frac{1}{2}} I)(X + \lambda^{\frac{1}{2}} I)\hat{\beta} - 2y^T X\hat{\beta} \end{aligned}$$

- 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.

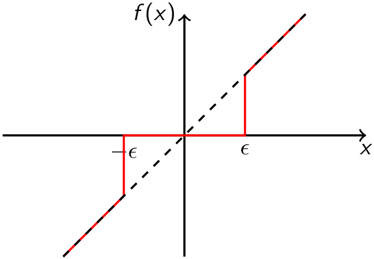
L1 regularized Linear Regression (**Lasso**):

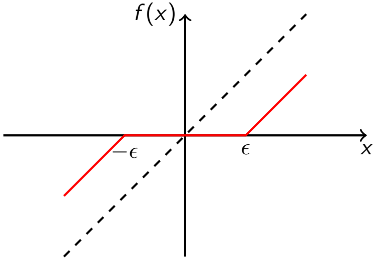
$$f(\beta) := \ell(y, \hat{y}) + \lambda||\beta||_1$$

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

- 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 Gradient for L1 Regularized Linear Regression

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

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

$$\frac{\partial f(\hat{\beta}_m; \hat{\beta}_{-m})}{\partial \hat{\beta}_m} \overset{!}{=} 0 \rightsquigarrow \hat{\beta}_m = \frac{(y - X_{-m}\hat{\beta}_{-m})^T x_m - \frac{1}{2}\lambda}{x_m^T x_m}, \quad \hat{\beta}_m > 0$$

$$\hat{\beta}_m = \frac{(y - X_{-m}\hat{\beta}_{-m})^T x_m + \frac{1}{2}\lambda}{x_m^T x_m}, \quad \hat{\beta}_m < 0$$

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

Note: LASSO = Least Absolute Selection and Shrinkage Operator.

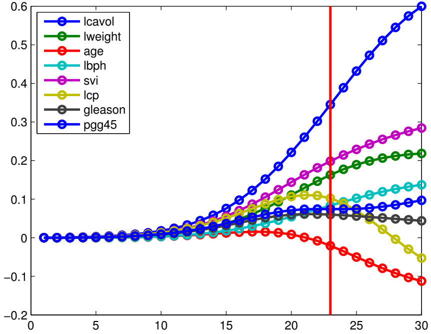
Learn L1-regularized Linear Regression via CD (Shooting Algorithm)

```
procedure 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 $\hat{\beta}$
```

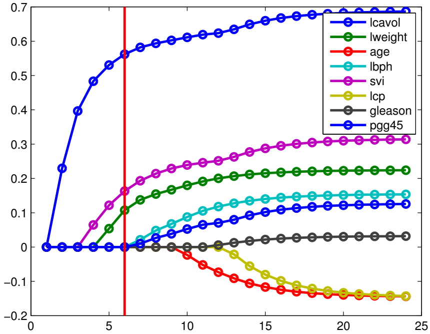
Note: $x_m := X_{.,m}$ denotes the m-th column of X,
X_{-m} denotes the matrix X without column m.

Regularization Paths

L2 regularization



L1 regularization



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

source: [Mur12, p. 437]

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.

- Variable selection also can be accomplished by **L1 regularization**.
  - **L1 regularized linear regression (LASSO)** can be learned by coordinate descent (**shooting algorithm**).

Further Readings

- [JWHT13, chapter 6], [Mur12, chapter 13], [HTFF05, chapter 3.3–8].

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