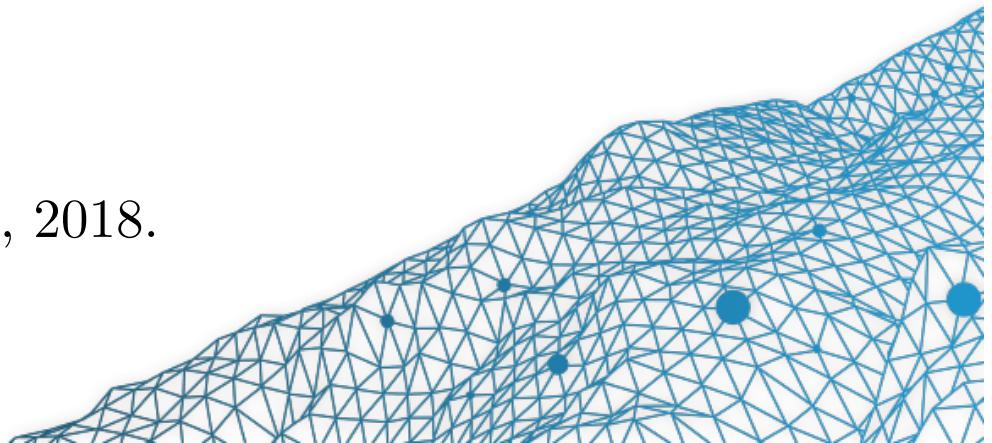


Big Data for Economics # 6

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<https://github.com/freakonometrics/ub>

UB School of Economics Summer School, 2018.



#6 Variable and model selection

References

Motivation

Banerjee, A., Chandrasekhar, A.G., Duflo, E. & Jackson, M.O. (2016). **Gossip: Identifying Central Individuals in a Social Networks.**

References

Belloni, A. & Chernozhukov, V. 2009. **Least squares after model selection in high-dimensional sparse models.**

Hastie, T., Tibshirani, R. & Wainwright, M. 2015 **Statistical Learning with Sparsity: The LASSO and Generalizations.** CRC Press.

Preamble

Consider a parametric model, with true (unkown) parameter θ , then

$$\text{mse}(\hat{\theta}) = \mathbb{E} [(\hat{\theta} - \theta)^2] = \underbrace{\mathbb{E} [(\hat{\theta} - \mathbb{E}[\hat{\theta}])^2]}_{\text{variance}} + \underbrace{\mathbb{E} [(\mathbb{E}[\hat{\theta}] - \theta)^2]}_{\text{bias}^2}$$

One can think of a [shrinkage](#) of an unbiased estimator,

Let $\tilde{\theta}$ denote an unbiased estimator of θ . Then

$$\hat{\theta} = \frac{\theta^2}{\theta^2 + \text{mse}(\tilde{\theta})} \cdot \tilde{\theta} = \tilde{\theta} - \underbrace{\frac{\text{mse}(\tilde{\theta})}{\theta^2 + \text{mse}(\tilde{\theta})} \cdot \tilde{\theta}}_{\text{penalty}}$$

satisfies $\text{mse}(\hat{\theta}) \leq \text{mse}(\tilde{\theta})$.

Bayes vs. Frequentist, inference on heads/tails

Consider some Bernoulli sample $\mathbf{x} = \{x_1, x_2, \dots, x_n\}$, where $x_i \in \{0, 1\}$.

X_i 's are i.i.d. $\mathcal{B}(p)$ variables, $f_X(x) = p^x[1-p]^{1-x}$, $x \in \{0, 1\}$.

Standard frequentist approach

$$\hat{p} = \frac{1}{n} \sum_{i=1}^n x_i = \text{argmax} \left\{ \underbrace{\prod_{i=1}^n f_X(x_i)}_{\mathcal{L}(p; \mathbf{x})} \right\}$$

From the central limit theorem

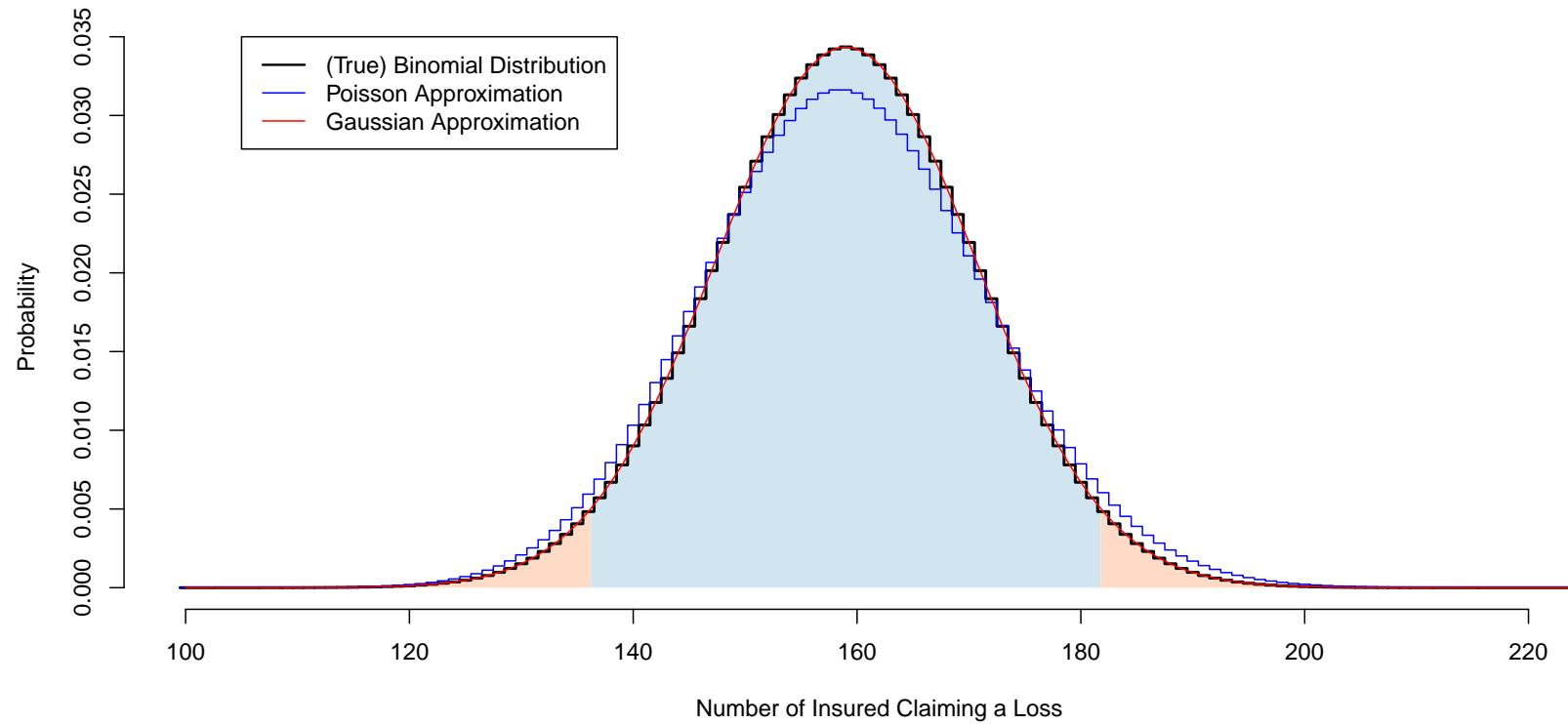
$$\sqrt{n} \frac{\hat{p} - p}{\sqrt{p(1-p)}} \xrightarrow{\mathcal{L}} \mathcal{N}(0, 1) \text{ as } n \rightarrow \infty$$

we can derive an approximated 95% confidence interval

$$\left[\hat{p} \pm \frac{1.96}{\sqrt{n}} \sqrt{\hat{p}(1-\hat{p})} \right]$$

Bayes vs. Frequentist, inference on heads/tails

Example out of 1,047 contracts, 159 claimed a loss



Bayes's theorem

Consider some hypothesis H and some evidence E , then

$$\mathbb{P}_E(H) = \mathbb{P}(H|E) = \frac{\mathbb{P}(H \cap E)}{\mathbb{P}(E)} = \frac{\mathbb{P}(H) \cdot \mathbb{P}(E|H)}{\mathbb{P}(E)}$$

Bayes rule,

$$\left\{ \begin{array}{l} \text{prior probability } \mathbb{P}(H) \\ \text{versus posterior probability after receiving evidence } E, \mathbb{P}_E(H) = \mathbb{P}(H|E). \end{array} \right.$$

In Bayesian (parametric) statistics, $H = \{\theta \in \Theta\}$ and $E = \{\mathbf{X} = \mathbf{x}\}$.

Bayes' Theorem,

$$\pi(\theta|\mathbf{x}) = \frac{\pi(\theta) \cdot f(\mathbf{x}|\theta)}{f(\mathbf{x})} = \frac{\pi(\theta) \cdot f(\mathbf{x}|\theta)}{\int f(\mathbf{x}|\theta)\pi(\theta)d\theta} \propto \pi(\theta) \cdot f(\mathbf{x}|\theta)$$

Small Data and Black Swans

Consider sample $\mathbf{x} = \{0, 0, 0, 0, 0\}$.

Here the likelihood is

$$\begin{cases} f(x_i|\theta) = \theta^{x_i}[1-\theta]^{1-x_i} \\ f(\mathbf{x}|\theta) = \theta^{\mathbf{x}^\top \mathbf{1}}[1-\theta]^{n-\mathbf{x}^\top \mathbf{1}} \end{cases}$$

and we need a priori distribution $\pi(\cdot)$ e.g.
a beta distribution

$$\pi(\theta) = \frac{\theta^\alpha [1-\theta]^\beta}{B(\alpha, \beta)}$$

$$\pi(\theta|\mathbf{x}) = \frac{\theta^{\alpha+\mathbf{x}^\top \mathbf{1}}[1-\theta]^{\beta+n-\mathbf{x}^\top \mathbf{1}}}{B(\alpha + \mathbf{x}^\top \mathbf{1}, \beta + n - \mathbf{x}^\top \mathbf{1})}$$

On Bayesian Philosophy, Confidence vs. Credibility

for frequentists, a probability is a measure of the frequency of repeated events

→ parameters are fixed (but unknown), and data are random

for Bayesians, a probability is a measure of the degree of certainty about values

→ parameters are random and data are fixed

“Bayesians : *Given our observed data, there is a 95% probability that the true value of θ falls within the credible region*

vs. Frequentists : *There is a 95% probability that when I compute a confidence interval from data of this sort, the true value of θ will fall within it.*” in [Vanderplas \(2014\)](#)

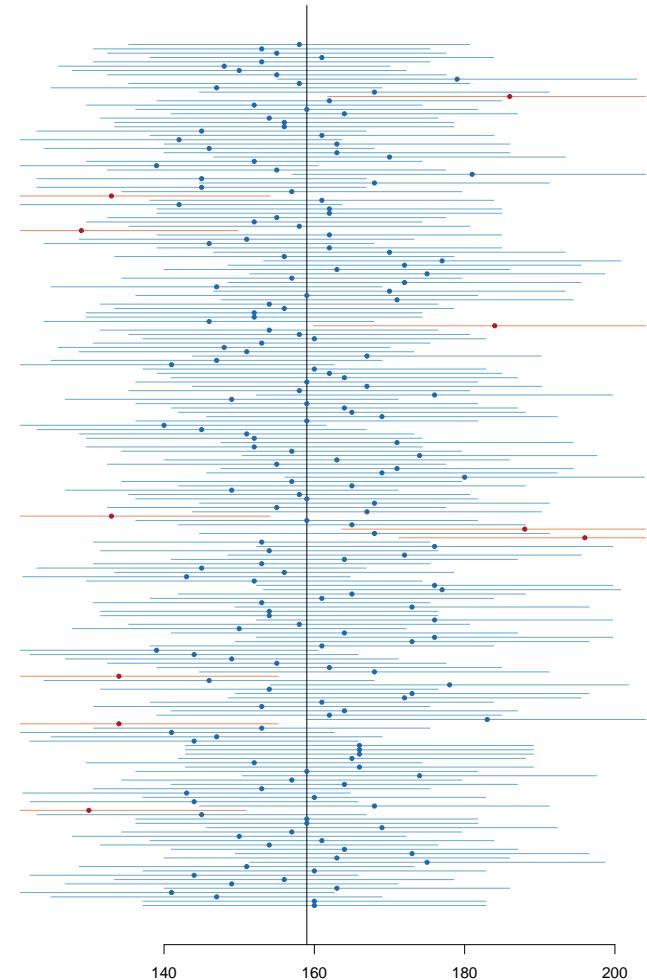
Example see [Jaynes \(1976\)](#), e.g. the truncated exponential

On Bayesian Philosophy, Confidence vs. Credibility

Example What is a 95% confidence interval of a proportion ? Here $\bar{x} = 159$ and $n = 1047$.

1. draw sets $(\tilde{x}_1, \dots, \tilde{x}_n)_k$ with $X_i \sim \mathcal{B}(\bar{x}/n)$
2. compute for each set of values confidence intervals
3. determine the fraction of these confidence interval that contain \bar{x}

→ the parameter is fixed, and we guarantee that 95% of the confidence intervals will contain it.



On Bayesian Philosophy, Confidence vs. Credibility

Example What is 95% credible region of a proportion ? Here $\bar{x} = 159$ and $n = 1047$.

1. draw random parameters p_k with from the posterior distribution, $\pi(\cdot|\boldsymbol{x})$
2. sample sets $(\tilde{x}_1, \dots, \tilde{x}_n)_k$ with $X_{i,k} \sim \mathcal{B}(p_k)$
3. compute for each set of values means \bar{x}_k
4. look at the proportion of those \bar{x}_k that are within this credible region $[\Pi^{-1}(.025|\boldsymbol{x}); \Pi^{-1}(.975|\boldsymbol{x})]$

→ the credible region is fixed, and we guarantee that 95% of possible values of \bar{x} will fall within it.

Occam's Razor

The “law of parsimony”, “*pluralitas non est ponenda sine necessitate*”

CORE PRINCIPLES IN RESEARCH



OCCAM'S RAZOR

"WHEN FACED WITH TWO POSSIBLE EXPLANATIONS, THE SIMPLER OF THE TWO IS THE ONE MOST LIKELY TO BE TRUE."



OCCAM'S PROFESSOR

"WHEN FACED WITH TWO POSSIBLE WAYS OF DOING SOMETHING, THE MORE COMPLICATED ONE IS THE ONE YOUR PROFESSOR WILL MOST LIKELY ASK YOU TO DO."

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Penalize too complex models

JORGE CHAM © 2009

James & Stein Estimator

Let $\boldsymbol{X} \sim \mathcal{N}(\boldsymbol{\mu}, \sigma^2 \mathbb{I})$. We want to estimate $\boldsymbol{\mu}$.

$$\hat{\boldsymbol{\mu}}_{\text{mle}} = \bar{\boldsymbol{X}}_n \sim \mathcal{N}\left(\boldsymbol{\mu}, \frac{\sigma^2}{n} \mathbb{I}\right).$$

From James & Stein (1961) **Estimation with quadratic loss**

$$\hat{\boldsymbol{\mu}}_{\text{JS}} = \left(1 - \frac{(d-2)\sigma^2}{n\|\bar{\boldsymbol{y}}\|^2}\right) \bar{\boldsymbol{y}}$$

where $\|\cdot\|$ is the Euclidean norm.

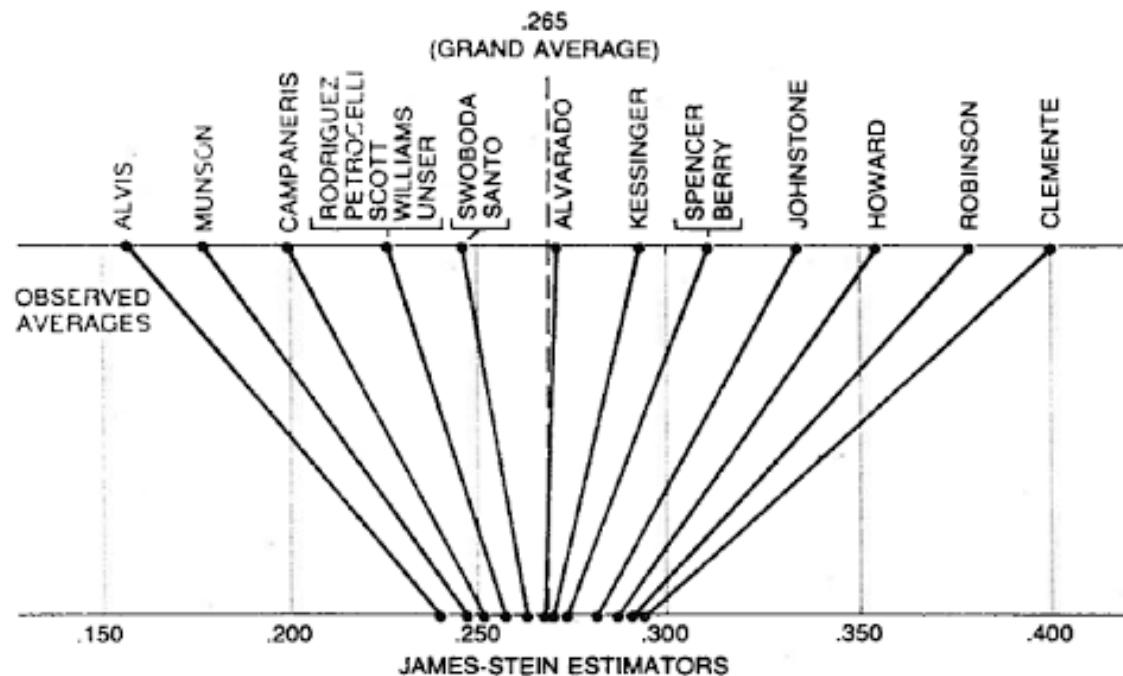
One can prove that if $d \geq 3$,

$$\mathbb{E}[(\hat{\boldsymbol{\mu}}_{\text{JS}} - \hat{\boldsymbol{\mu}})^2] < \mathbb{E}[(\hat{\boldsymbol{\mu}}_{\text{mle}} - \hat{\boldsymbol{\mu}})^2]$$

Samworth (2015) **Stein's paradox**, “*one should use the price of tea in China to obtain a better estimate of the chance of rain in Melbourne*”.

James & Stein Estimator

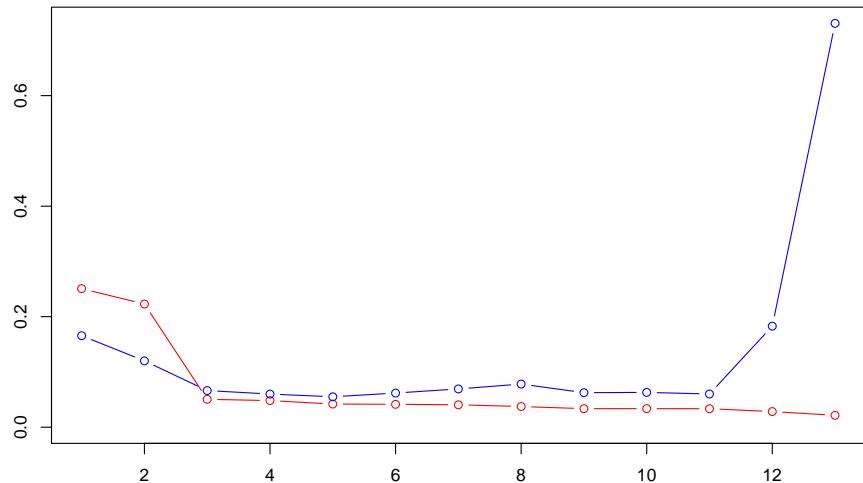
Heuristics : consider a biased estimator, to decrease the variance.



See Efron (2010) Large-Scale Inference

Motivation: Avoiding Overfit

Generalization : the model should perform well on **new** data (and not only on the training ones).



Reducing Dimension with PCA

Use **principal components** to reduce dimension (on centered and scaled variables):
we want d vectors $\mathbf{z}_1, \dots, \mathbf{z}_d$ such that

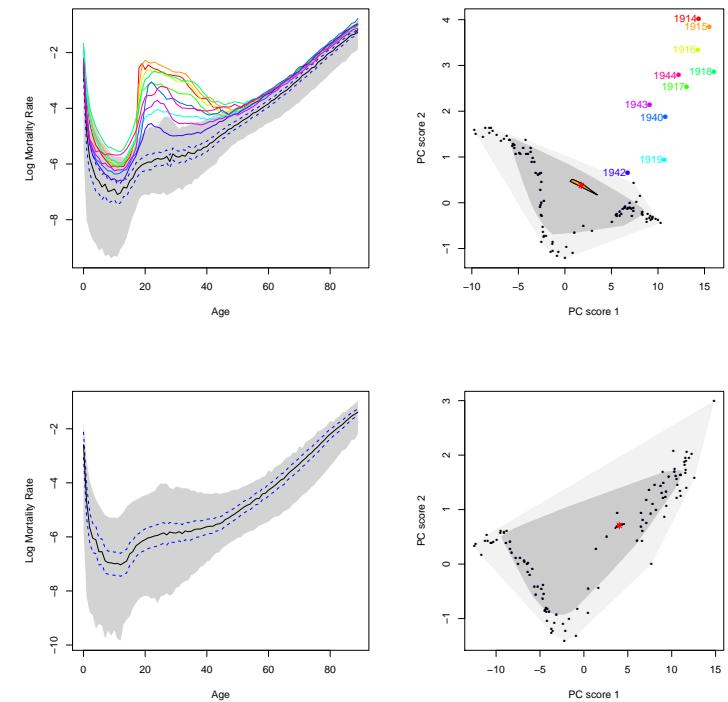
First Component is $\mathbf{z}_1 = \mathbf{X}\boldsymbol{\omega}_1$ where

$$\boldsymbol{\omega}_1 = \underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}} \left\{ \|\mathbf{X} \cdot \boldsymbol{\omega}\|^2 \right\} = \underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}} \left\{ \boldsymbol{\omega}^\top \mathbf{X}^\top \mathbf{X} \boldsymbol{\omega} \right\}$$

Second Component is $\mathbf{z}_2 = \mathbf{X}\boldsymbol{\omega}_2$ where

$$\boldsymbol{\omega}_2 = \underset{\|\boldsymbol{\omega}\|=1}{\operatorname{argmax}} \left\{ \|\widetilde{\mathbf{X}}^{(1)} \cdot \boldsymbol{\omega}\|^2 \right\}$$

with $\widetilde{\mathbf{X}}^{(1)} = \mathbf{X} - \underbrace{\mathbf{X}\boldsymbol{\omega}_1}_{\mathbf{z}_1} \boldsymbol{\omega}_1^\top$.



Reducing Dimension with PCA

A regression on (the d) principal components, $y = z^\top \beta + \eta$ could be an interesting idea, unfortunatley, principal components have no reason to be correlated with y . First compoment was $z_1 = \mathbf{X}\omega_1$ where

$$\omega_1 = \underset{\|\omega\|=1}{\operatorname{argmax}} \left\{ \| \mathbf{X} \cdot \omega \|^2 \right\} = \underset{\|\omega\|=1}{\operatorname{argmax}} \left\{ \omega^\top \mathbf{X}^\top \mathbf{X} \omega \right\}$$

It is a non-supervised technique.

Instead, use **partial least squares**, introduced in Wold (1966) **Estimation of Principal Components and Related Models by Iterative Least squares**. First compoment is $z_1 = \mathbf{X}\omega_1$ where

$$\omega_1 = \underset{\|\omega\|=1}{\operatorname{argmax}} \left\{ \langle \mathbf{y}, \mathbf{X} \cdot \omega \rangle \right\} = \underset{\|\omega\|=1}{\operatorname{argmax}} \left\{ \omega^\top \mathbf{X}^\top \mathbf{y} \mathbf{y}^\top \mathbf{X} \omega \right\}$$

Terminology

Consider a dataset $\{y_i, \mathbf{x}_i\}$, assumed to be generated from Y, \mathbf{X} , from an unknown distribution \mathbb{P} .

Let $m_0(\cdot)$ be the “true” model. Assume that $y_i = m_0(\mathbf{x}_i) + \varepsilon_i$.

In a regression context (**quadratic loss function** function), the **risk** associated to m is

$$\mathcal{R}(m) = \mathbb{E}_{\mathbb{P}}[(Y - m(\mathbf{X}))^2]$$

An optimal model m^* within a class \mathcal{M} satisfies

$$\mathcal{R}(m^*) = \inf_{m \in \mathcal{M}} \{\mathcal{R}(m)\}$$

Such a model m^* is usually called **oracle**.

Observe that $m^*(\mathbf{x}) = \mathbb{E}[Y | \mathbf{X} = \mathbf{x}]$ is the solution of

$\mathcal{R}(m^*) = \inf_{m \in \mathcal{M}} \{\mathcal{R}(m)\}$ where \mathcal{M} is the set of measurable functions

The empirical risk is

$$\mathcal{R}_n(m) = \frac{1}{n} \sum_{i=1}^n (y_i - m(\mathbf{x}_i))^2$$

For instance, m can be a linear predictor, $m(\mathbf{x}) = \beta_0 + \mathbf{x}^\top \boldsymbol{\beta}$, where $\boldsymbol{\theta} = (\beta_0, \boldsymbol{\beta})$ should be estimated (trained).

$\mathbb{E}[R_n(\hat{m})] = \mathbb{E}[(\hat{m}(\mathbf{X}) - Y)^2]$ can be expressed as

$$\begin{aligned} & \mathbb{E}[(\hat{m}(\mathbf{X}) - \mathbb{E}[\hat{m}(\mathbf{X})|\mathbf{X}])^2] \quad \text{variance of } \hat{m} \\ & + \mathbb{E}\left[\left(\mathbb{E}[\hat{m}(\mathbf{X})|\mathbf{X}] - \underbrace{\mathbb{E}[Y|\mathbf{X}]}_{m_0(\mathbf{X})}\right)^2\right] \quad \text{bias of } \hat{m} \\ & + \mathbb{E}\left[\left(Y - \underbrace{\mathbb{E}[Y|\mathbf{X}]}_{m_0(\mathbf{X})}\right)^2\right] \quad \text{variance of the noise} \end{aligned}$$

The third term is the risk of the “optimal” estimator m , that cannot be decreased.

Mallows Penalty and Model Complexity

Consider a linear predictor (see #1), i.e. $\hat{\mathbf{y}} = \hat{m}(\mathbf{x}) = \mathbf{A}\mathbf{y}$.

Assume that $\mathbf{y} = m_0(\mathbf{x}) + \boldsymbol{\varepsilon}$, with $\mathbb{E}[\boldsymbol{\varepsilon}] = \mathbf{0}$ and $\text{Var}[\boldsymbol{\varepsilon}] = \sigma^2\mathbb{I}$.

Let $\|\cdot\|$ denote the Euclidean norm

Empirical risk : $\widehat{\mathcal{R}}_n(m) = \frac{1}{n}\|\mathbf{y} - m(\mathbf{x})\|^2$

Vapnik's risk : $\mathbb{E}[\widehat{\mathcal{R}}_n(m)] = \frac{1}{n}\|m_0(\mathbf{x} - m(\mathbf{x}))\|^2 + \frac{1}{n}\mathbb{E}(\|\mathbf{y} - m_0(\mathbf{x})\|^2)$ with
 $m_0(\mathbf{x}) = \mathbb{E}[Y|\mathbf{X} = \mathbf{x}]$.

Observe that

$$n\mathbb{E}[\widehat{\mathcal{R}}_n(\hat{m})] = \mathbb{E}(\|\mathbf{y} - \hat{m}(\mathbf{x})\|^2) = \|(\mathbb{I} - \mathbf{A})m_0\|^2 + \sigma^2\|\mathbb{I} - \mathbf{A}\|^2$$

while

$$= \mathbb{E}(\|m_0(\mathbf{x}) - \hat{m}(\mathbf{x})\|^2) = \underbrace{\|(\mathbb{I} - \mathbf{A})m_0\|^2}_{\text{bias}} + \underbrace{\sigma^2\|\mathbf{A}\|^2}_{\text{variance}}$$

Mallows Penalty and Model Complexity

One can obtain

$$\mathbb{E}[\mathcal{R}_n(\hat{m})] = \mathbb{E}[\widehat{\mathcal{R}}_n(\hat{m})] + 2\frac{\sigma^2}{n}\text{trace}(\mathbf{A}).$$

If $\text{trace}(\mathbf{A}) \geq 0$ the empirical risk underestimate the true risk of the estimator.

The number of degrees of freedom of the (linear) predictor is related to $\text{trace}(\mathbf{A})$

$2\frac{\sigma^2}{n}\text{trace}(\mathbf{A})$ is called Mallow's penalty C_L .

If \mathbf{A} is a projection matrix, $\text{trace}(\mathbf{A})$ is the dimension of the projection space, p , then we obtain Mallow's C_P , $2\frac{\sigma^2}{n}p$.

Remark : Mallows (1973) [Some Comments on \$C_p\$](#) introduced this penalty while focusing on the R^2 .

Penalty and Likelihood

C_P is associated to a quadratic risk

an alternative is to use a distance on the (conditional) distribution of Y , namely
Kullback-Leibler distance

$$\text{discrete case: } D_{\text{KL}}(P\|Q) = \sum_i P(i) \log \frac{P(i)}{Q(i)}$$

continuous case :

$$D_{\text{KL}}(P\|Q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx \quad D_{\text{KL}}(P\|Q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx$$

Let f denote the true (unknown) density, and f_θ some parametric distribution,

$$D_{\text{KL}}(f\|f_\theta) = \int_{-\infty}^{\infty} f(x) \log \frac{f(x)}{f_\theta(x)} dx = \int f(x) \log[f(x)] dx - \underbrace{\int f(x) \log[f_\theta(x)] dx}_{\text{relative information}}$$

Hence

$$\text{minimize } \{D_{\text{KL}}(f\|f_\theta)\} \iff \text{maximize } \{ \mathbb{E}[\log[f_\theta(X)]] \}$$

Penalty and Likelihood

Akaike (1974) **A new look at the statistical model identification** observe that for n large enough

$$\mathbb{E}[\log[f_\theta(X)]] \sim \log[\mathcal{L}(\hat{\theta})] - \dim(\theta)$$

Thus

$$AIC = -2 \log \mathcal{L}(\hat{\theta}) + 2\dim(\theta)$$

Example : in a (Gaussian) linear model, $y_i = \beta_0 + \mathbf{x}_i^\top \boldsymbol{\beta} + \varepsilon_i$

$$AIC = n \log \left(\frac{1}{n} \sum_{i=1}^n \hat{\varepsilon}_i^2 \right) + 2[\dim(\boldsymbol{\beta}) + 2]$$

Penalty and Likelihood

Remark : this is valid for large sample (rule of thumb $n/\dim(\theta) > 40$), otherwise use a corrected AIC

$$AICc = AIC + \underbrace{\frac{2k(k+1)}{n-k-1}}_{\text{bias correction}} \quad \text{where } k = \dim(\theta)$$

see Sugiura (1978) [Further analysis of the data by Akaike's information criterion and the finite corrections](#) second order AIC.

Using a Bayesian interpretation, Schwarz (1978) [Estimating the dimension of a model](#) obtained

$$BIC = -2 \log \mathcal{L}(\hat{\theta}) + \log(n)\dim(\theta).$$

Observe that the criteria considered is

$$\text{criteria} = -\text{function}(\mathcal{L}(\hat{\theta})) + \text{penalty(complexity)}$$

Estimation of the Risk

Consider a naive bootstrap procedure, based on a bootstrap sample
 $\mathcal{S}_b = \{(y_i^{(b)}, \mathbf{x}_i^{(b)})\}$.

The **plug-in** estimator of the empirical risk is

$$\hat{\mathcal{R}}_n(\hat{m}^{(b)}) = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{m}^{(b)}(\mathbf{x}_i))^2$$

and then

$$\hat{\mathcal{R}}_n = \frac{1}{B} \sum_{b=1}^B \hat{\mathcal{R}}_n(\hat{m}^{(b)}) = \frac{1}{B} \sum_{b=1}^B \frac{1}{n} \sum_{i=1}^n (y_i - \hat{m}^{(b)}(\mathbf{x}_i))^2$$

Estimation of the Risk

One might improve this estimate using a **out-of-bag** procedure

$$\widehat{\mathcal{R}}_n = \frac{1}{n} \sum_{i=1}^n \frac{1}{\#\mathcal{B}_i} \sum_{b \in \mathcal{B}_i} (y_i - \widehat{m}^{(b)}(\boldsymbol{x}_i))^2$$

where \mathcal{B}_i is the set of all bootstrap sample that contain (y_i, \boldsymbol{x}_i) .

Remark: $\mathbb{P}((y_i, \boldsymbol{x}_i) \notin \mathcal{S}_b) = \left(1 - \frac{1}{n}\right)^n \sim e^{-1} = 36,78\%$.

Linear Regression Shortcoming

Least Squares Estimator $\hat{\beta} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$

Unbiased Estimator $\mathbb{E}[\hat{\beta}] = \beta$

$$\text{Variance } \text{Var}[\hat{\beta}] = \sigma^2(\mathbf{X}^\top \mathbf{X})^{-1}$$

which can be (extremely) large when $\det[(\mathbf{X}^\top \mathbf{X})] \sim 0$.

$$X = \begin{bmatrix} 1 & -1 & 2 \\ 1 & 0 & 1 \\ 1 & 2 & -1 \\ 1 & 1 & 0 \end{bmatrix} \text{ then } X^T X = \begin{bmatrix} 4 & 2 & 2 \\ 2 & 6 & -4 \\ 2 & -4 & 6 \end{bmatrix} \text{ while } X^T X + \mathbb{I} = \begin{bmatrix} 5 & 2 & 2 \\ 2 & 7 & -4 \\ 2 & -4 & 7 \end{bmatrix}$$

eigenvalues : $\{10, 6, 0\}$ $\{11, 7, 1\}$

Ad-hoc strategy: use $X^T X + \lambda \mathbb{I}$

Linear Regression Shortcoming

Evolution of $(\beta_1, \beta_2) \mapsto \sum_{i=1}^n [y_i - (\beta_1 x_{1,i} + \beta_2 x_{2,i})]^2$

when $\text{cor}(X_1, X_2) = r \in [0, 1]$, on top.

Below, Ridge regression

$(\beta_1, \beta_2) \mapsto \sum_{i=1}^n [y_i - (\beta_1 x_{1,i} + \beta_2 x_{2,i})]^2 + \lambda(\beta_1^2 + \beta_2^2)$

where $\lambda \in [0, \infty)$, below,

when $\text{cor}(X_1, X_2) \sim 1$ (colinearity).

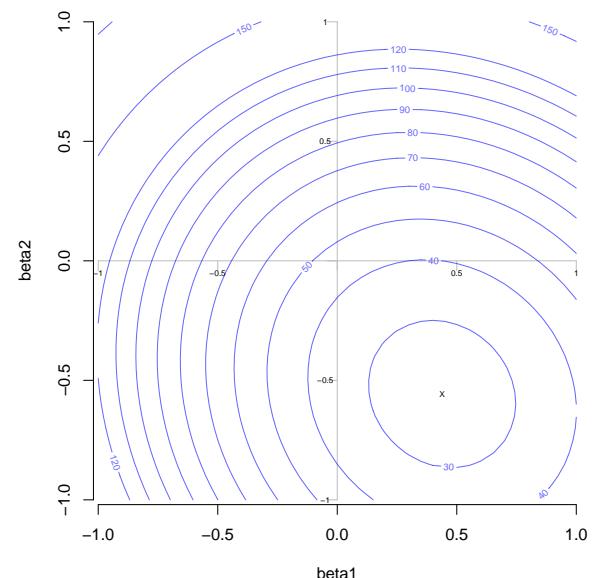
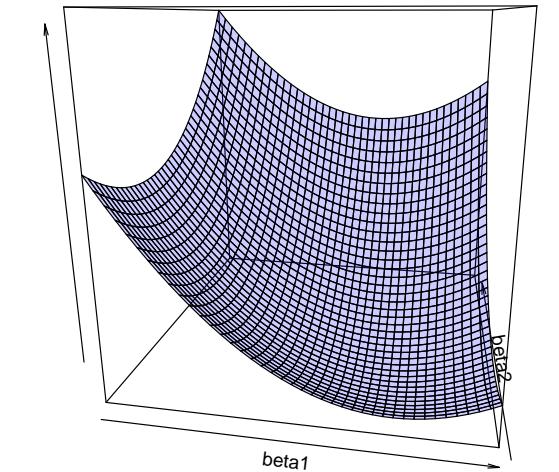
Normalization : Euclidean ℓ_2 vs. Mahalanobis

We want to penalize complicated models :
 if β_k is “too small”, we prefer to have $\beta_k = 0$.



Instead of $d(\mathbf{x}, \mathbf{y}) = (\mathbf{x} - \mathbf{y})^\top (\mathbf{x} - \mathbf{y})$

use $d_{\Sigma}(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^\top \Sigma^{-1} (\mathbf{x} - \mathbf{y})}$



Ridge Regression

... like the least square, but it shrinks estimated coefficients towards 0.

$$\hat{\beta}_\lambda^{\text{ridge}} = \operatorname{argmin} \left\{ \sum_{i=1}^n (y_i - \mathbf{x}_i^\top \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^p \beta_j^2 \right\}$$

$$\hat{\beta}_\lambda^{\text{ridge}} = \operatorname{argmin} \left\{ \underbrace{\|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|_{\ell_2}^2}_{=\text{criteria}} + \underbrace{\lambda \|\boldsymbol{\beta}\|_{\ell_2}^2}_{=\text{penalty}} \right\}$$

$\lambda \geq 0$ is a tuning parameter.

The constant is usually unpenalized. The *true* equation is

$$\hat{\beta}_\lambda^{\text{ridge}} = \operatorname{argmin} \left\{ \underbrace{\|\mathbf{y} - (\beta_0 + \mathbf{X}\boldsymbol{\beta})\|_{\ell_2}^2}_{=\text{criteria}} + \underbrace{\lambda \|\boldsymbol{\beta}\|_{\ell_2}^2}_{=\text{penalty}} \right\}$$

Ridge Regression

$$\hat{\beta}_\lambda^{\text{ridge}} = \underset{\|\beta\|_{\ell_2}^2 \leq h_\lambda}{\operatorname{argmin}} \left\{ \|y - (\beta_0 + X\beta)\|_{\ell_2}^2 + \lambda \|\beta\|_{\ell_2}^2 \right\}$$

can be seen as a constrained optimization problem

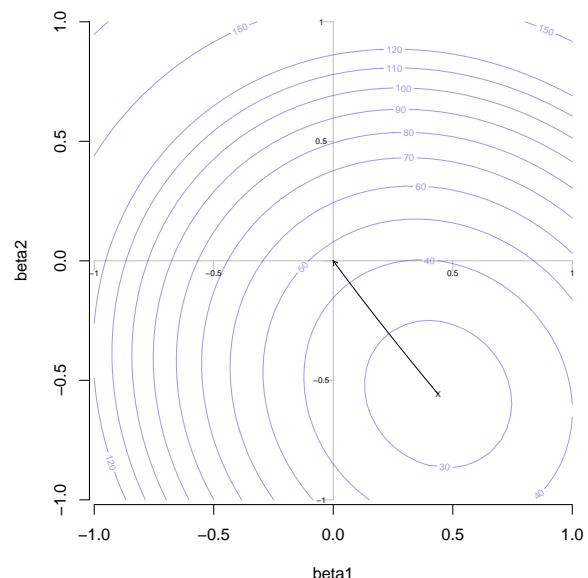
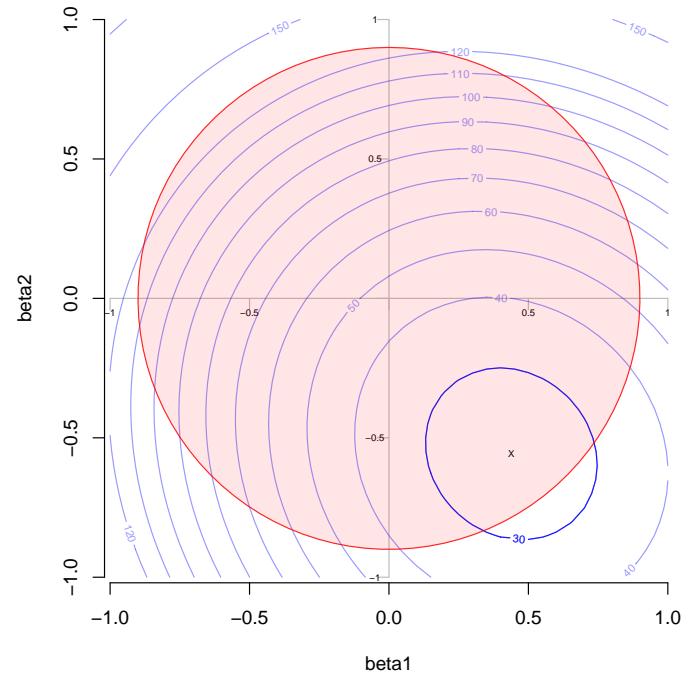
$$\hat{\beta}_\lambda^{\text{ridge}} = \underset{\|\beta\|_{\ell_2}^2 \leq h_\lambda}{\operatorname{argmin}} \left\{ \|y - (\beta_0 + X\beta)\|_{\ell_2}^2 \right\}$$

Explicit solution

$$\hat{\beta}_\lambda = (X^\top X + \lambda \mathbb{I})^{-1} X^\top y$$

If $\lambda \rightarrow 0$, $\hat{\beta}_0^{\text{ridge}} = \hat{\beta}^{\text{ols}}$

If $\lambda \rightarrow \infty$, $\hat{\beta}_\infty^{\text{ridge}} = \mathbf{0}$.



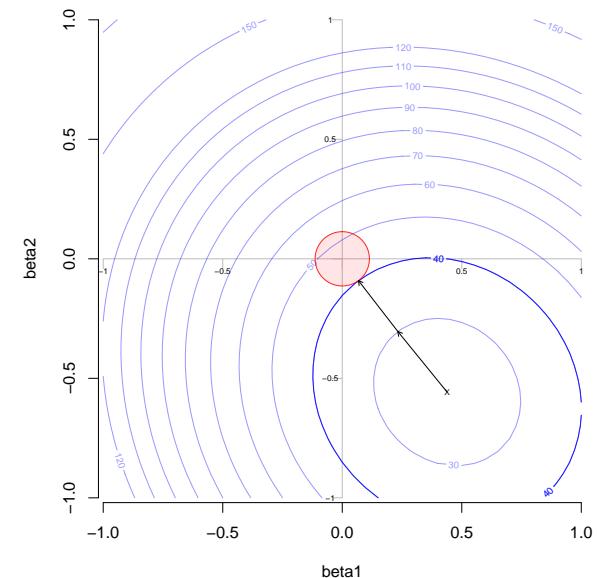
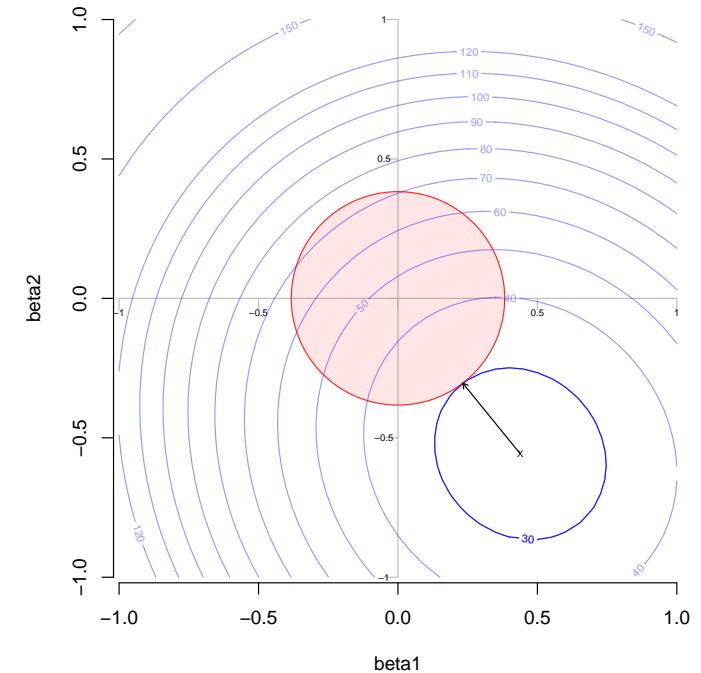
Ridge Regression

This penalty can be seen as rather unfair if components of \boldsymbol{x} are not expressed on the same scale

- center: $\bar{\boldsymbol{x}}_j = 0$, then $\hat{\beta}_0 = \bar{\boldsymbol{y}}$
- scale: $\boldsymbol{x}_j^\top \boldsymbol{x}_j = 1$

Then compute

$$\hat{\boldsymbol{\beta}}_\lambda^{\text{ridge}} = \operatorname{argmin} \left\{ \underbrace{\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|_{\ell_2}^2}_{\text{loss}} + \underbrace{\lambda \|\boldsymbol{\beta}\|_{\ell_2}^2}_{\text{penalty}} \right\}$$



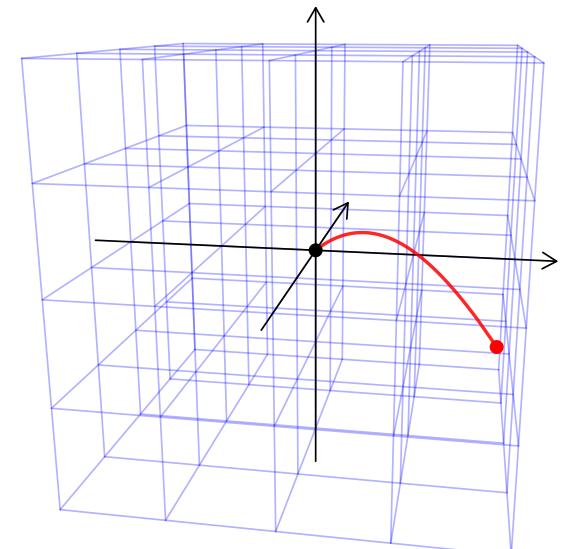
Ridge Regression

Observe that if $\mathbf{x}_{j_1} \perp \mathbf{x}_{j_2}$, then

$$\hat{\boldsymbol{\beta}}_{\lambda}^{\text{ridge}} = [1 + \lambda]^{-1} \hat{\boldsymbol{\beta}}_{\lambda}^{\text{ols}}$$

which explain relationship with shrinkage.

But generally, it is not the case...



Theorem There exists λ such that $\text{mse}[\hat{\boldsymbol{\beta}}_{\lambda}^{\text{ridge}}] \leq \text{mse}[\hat{\boldsymbol{\beta}}_{\lambda}^{\text{ols}}]$

Ridge Regression

$$\mathcal{L}_\lambda(\boldsymbol{\beta}) = \sum_{i=1}^n (y_i - \beta_0 - \mathbf{x}_i^\top \boldsymbol{\beta})^2 + \lambda \sum_{j=1}^p \beta_j^2$$

$$\frac{\partial \mathcal{L}_\lambda(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = -2\mathbf{X}^\top \mathbf{y} + 2(\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})\boldsymbol{\beta}$$

$$\frac{\partial^2 \mathcal{L}_\lambda(\boldsymbol{\beta})}{\partial \boldsymbol{\beta} \partial \boldsymbol{\beta}^\top} = 2(\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})$$

where $\mathbf{X}^\top \mathbf{X}$ is a semi-positive definite matrix, and $\lambda \mathbb{I}$ is a positive definite matrix, and

$$\hat{\boldsymbol{\beta}}_\lambda = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

The Bayesian Interpretation

From a Bayesian perspective,

$$\underbrace{\mathbb{P}[\boldsymbol{\theta}|\mathbf{y}]}_{\text{posterior}} \propto \underbrace{\mathbb{P}[\mathbf{y}|\boldsymbol{\theta}]}_{\text{likelihood}} \cdot \underbrace{\mathbb{P}[\boldsymbol{\theta}]}_{\text{prior}} \quad \text{i.e.} \quad \log \mathbb{P}[\boldsymbol{\theta}|\mathbf{y}] = \underbrace{\log \mathbb{P}[\mathbf{y}|\boldsymbol{\theta}]}_{\text{log likelihood}} + \underbrace{\log \mathbb{P}[\boldsymbol{\theta}]}_{\text{penalty}}$$

If $\boldsymbol{\beta}$ has a prior $\mathcal{N}(\mathbf{0}, \tau^2 \mathbb{I})$ distribution, then its posterior distribution has mean

$$\mathbb{E}[\boldsymbol{\beta}|\mathbf{y}, \mathbf{X}] = \left(\mathbf{X}^\top \mathbf{X} + \frac{\sigma^2}{\tau^2} \mathbb{I} \right)^{-1} \mathbf{X}^\top \mathbf{y}.$$

Properties of the Ridge Estimator

$$\hat{\beta}_\lambda = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} \mathbf{X}^\top \mathbf{y}$$

$$\mathbb{E}[\hat{\beta}_\lambda] = \mathbf{X}^\top \mathbf{X} (\lambda \mathbb{I} + \mathbf{X}^\top \mathbf{X})^{-1} \beta.$$

i.e. $\mathbb{E}[\hat{\beta}_\lambda] \neq \beta$.

Observe that $\mathbb{E}[\hat{\beta}_\lambda] \rightarrow \mathbf{0}$ as $\lambda \rightarrow \infty$.

Assume that \mathbf{X} is an orthogonal design matrix, i.e. $\mathbf{X}^\top \mathbf{X} = \mathbb{I}$, then

$$\hat{\beta}_\lambda = (1 + \lambda)^{-1} \hat{\beta}^{\text{ols}}.$$

Properties of the Ridge Estimator

Set $\mathbf{W}_\lambda = (\mathbb{I} + \lambda[\mathbf{X}^\top \mathbf{X}]^{-1})^{-1}$. One can prove that

$$\mathbf{W}_\lambda \hat{\boldsymbol{\beta}}^{\text{ols}} = \hat{\boldsymbol{\beta}}_\lambda.$$

Thus,

$$\text{Var}[\hat{\boldsymbol{\beta}}_\lambda] = \mathbf{W}_\lambda \text{Var}[\hat{\boldsymbol{\beta}}^{\text{ols}}] \mathbf{W}_\lambda^\top$$

and

$$\text{Var}[\hat{\boldsymbol{\beta}}_\lambda] = \sigma^2 (\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} \mathbf{X}^\top \mathbf{X} [(\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1}]^\top.$$

Observe that

$$\text{Var}[\hat{\boldsymbol{\beta}}^{\text{ols}}] - \text{Var}[\hat{\boldsymbol{\beta}}_\lambda] = \sigma^2 \mathbf{W}_\lambda [2\lambda(\mathbf{X}^\top \mathbf{X})^{-2} + \lambda^2(\mathbf{X}^\top \mathbf{X})^{-3}] \mathbf{W}_\lambda^\top \geq \mathbf{0}.$$

Properties of the Ridge Estimator

Hence, the confidence ellipsoid of ridge estimator is indeed smaller than the OLS,

If \mathbf{X} is an orthogonal design matrix,

$$\text{Var}[\hat{\boldsymbol{\beta}}_\lambda] = \sigma^2(1 + \lambda)^{-2}\mathbb{I}.$$

$$\text{mse}[\hat{\boldsymbol{\beta}}_\lambda] = \sigma^2\text{trace}(\mathbf{W}_\lambda(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{W}_\lambda^\top) + \boldsymbol{\beta}^\top(\mathbf{W}_\lambda - \mathbb{I})^\top(\mathbf{W}_\lambda - \mathbb{I})\boldsymbol{\beta}.$$

If \mathbf{X} is an orthogonal design matrix,

$$\text{mse}[\hat{\boldsymbol{\beta}}_\lambda] = \frac{p\sigma^2}{(1 + \lambda)^2} + \frac{\lambda^2}{(1 + \lambda)^2}\boldsymbol{\beta}^\top\boldsymbol{\beta}$$

Properties of the Ridge Estimator

$$\text{mse}[\hat{\beta}_\lambda] = \frac{p\sigma^2}{(1 + \lambda)^2} + \frac{\lambda^2}{(1 + \lambda)^2} \beta^\top \beta$$

is minimal for

$$\lambda^* = \frac{p\sigma^2}{\beta^\top \beta}$$

Note that there exists $\lambda > 0$ such that $\text{mse}[\hat{\beta}_\lambda] < \text{mse}[\hat{\beta}_0] = \text{mse}[\hat{\beta}^{\text{ols}}]$.

SVD decomposition

For any matrix A , $m \times n$, there are orthogonal matrices U ($m \times m$), V ($n \times n$) and a "diagonal" matrix Σ ($m \times n$) such that $A = U\Sigma V^\top$, or $AV = U\Sigma$.

Hence, there exists a special orthonormal set of vectors (i.e. the columns of V), that is mapped by the matrix A into an orthonormal set of vectors (i.e. the columns of U).

Let $r = \text{rank}(A)$, then $A = \sum_{i=1}^r \sigma_i \mathbf{u}_i \mathbf{v}_i^\top$ (called the dyadic decomposition of A).

Observe that it can be used to compute (e.g.) the Frobenius norm of A ,

$$\|A\| = \sqrt{\sum a_{i,j}^2} = \sqrt{\sigma_1^2 + \dots + \sigma_{\min\{m,n\}}^2}.$$

Further $A^\top A = V\Sigma^\top \Sigma V^\top$ while $AA^\top = U\Sigma\Sigma^\top U^\top$.

Hence, σ_i^2 's are related to eigenvalues of $A^\top A$ and AA^\top , and $\mathbf{u}_i, \mathbf{v}_i$ are associated eigenvectors.

Golub & Reinsch (1970) **Singular Value Decomposition and Least Squares Solutions**

SVD decomposition

Consider the singular value decomposition of \mathbf{X} , $\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\top$.

Then

$$\hat{\boldsymbol{\beta}}^{\text{ols}} = \mathbf{V} \underbrace{\mathbf{D}^{-2} \mathbf{D}}_{\mathbf{D}^2} \mathbf{U}^\top \mathbf{y}$$

$$\hat{\boldsymbol{\beta}}_\lambda = \mathbf{V} \underbrace{(\mathbf{D}^2 + \lambda \mathbb{I})^{-1} \mathbf{D}}_{(\mathbf{R}^\top \mathbf{R} + \lambda \mathbb{I})^{-1}} \mathbf{U}^\top \mathbf{y}$$

Observe that

$$\mathbf{D}_{i,i}^{-1} \geq \frac{\mathbf{D}_{i,i}}{\mathbf{D}_{i,i}^2 + \lambda}$$

hence, the ridge penalty shrinks singular values.

Set now $\mathbf{R} = \mathbf{U}\mathbf{D}$ ($n \times n$ matrix), so that $\mathbf{X} = \mathbf{R}\mathbf{V}^\top$,

$$\hat{\boldsymbol{\beta}}_\lambda = \mathbf{V} (\mathbf{R}^\top \mathbf{R} + \lambda \mathbb{I})^{-1} \mathbf{R}^\top \mathbf{y}$$

Hat matrix and Degrees of Freedom

Recall that $\hat{\mathbf{Y}} = \mathbf{H}\mathbf{Y}$ with

$$\mathbf{H} = \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top$$

Similarly

$$\mathbf{H}_\lambda = \mathbf{X}(\mathbf{X}^\top \mathbf{X} + \lambda \mathbb{I})^{-1} \mathbf{X}^\top$$

$$\text{trace}[\mathbf{H}_\lambda] = \sum_{j=1}^p \frac{d_{j,j}^2}{d_{j,j}^2 + \lambda} \rightarrow 0, \text{ as } \lambda \rightarrow \infty.$$

Sparsity Issues

In several applications, k can be (very) large, but a lot of features are just noise: $\beta_j = 0$ for many j 's. Let s denote the number of relevant features, with $s \ll k$, cf Hastie, Tibshirani & Wainwright (2015) **Statistical Learning with Sparsity**,

$$s = \text{card}\{\mathcal{S}\} \text{ where } \mathcal{S} = \{j; \beta_j \neq 0\}$$

The model is now $y = \mathbf{X}_{\mathcal{S}}^\top \boldsymbol{\beta}_{\mathcal{S}} + \varepsilon$, where $\mathbf{X}_{\mathcal{S}}^\top \mathbf{X}_{\mathcal{S}}$ is a full rank matrix.

Going further on sparsity issues

The Ridge regression problem was to solve

$$\hat{\beta} = \underset{\beta \in \{\|\beta\|_{\ell_2} \leq s\}}{\operatorname{argmin}} \{\|Y - X^\top \beta\|_{\ell_2}^2\}$$

Define $\|a\|_{\ell_0} = \sum \mathbf{1}(|a_i| > 0)$.

Here $\dim(\beta) = k$ but $\|\beta\|_{\ell_0} = s$.

We wish we could solve

$$\hat{\beta} = \underset{\beta \in \{\|\beta\|_{\ell_0} = s\}}{\operatorname{argmin}} \{\|Y - X^\top \beta\|_{\ell_2}^2\}$$

Problem: it is usually not possible to describe all possible constraints, since $\binom{s}{k}$ coefficients should be chosen here (with k (very) large).

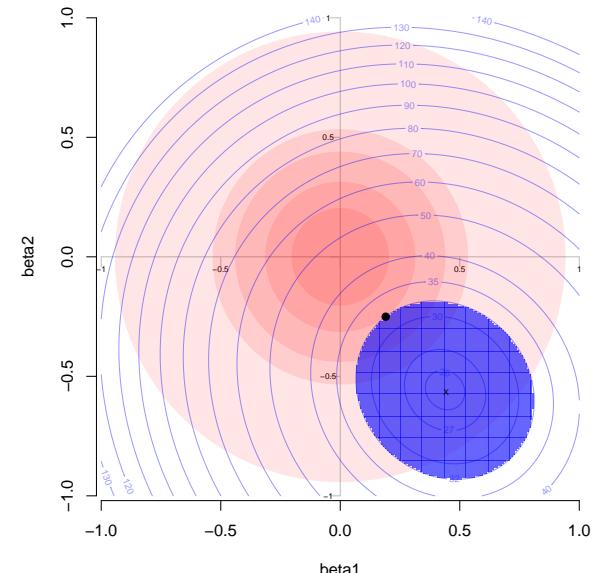
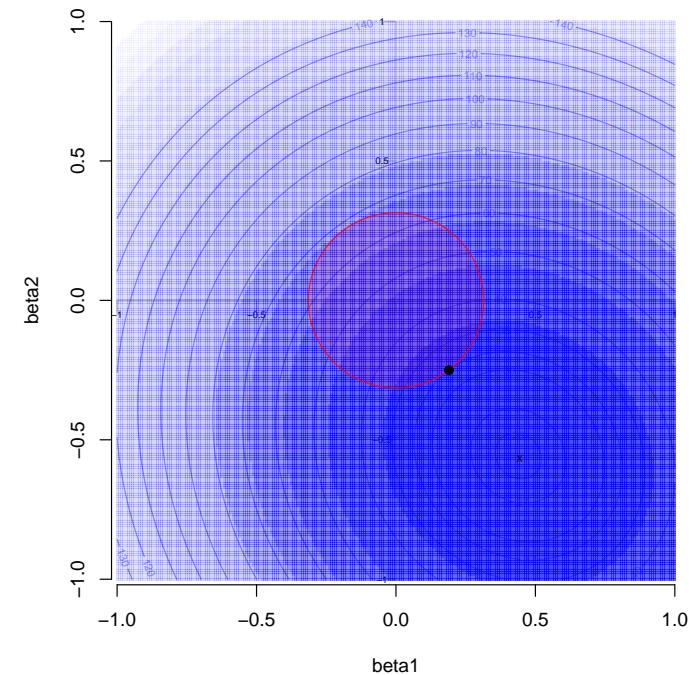
Going further on sparsity issues

In a convex problem, solve the **dual problem**,
e.g. in the Ridge regression : primal problem

$$\min_{\beta \in \{\|\beta\|_{\ell_2} \leq s\}} \{\|Y - X^\top \beta\|_{\ell_2}^2\}$$

and the dual problem

$$\min_{\beta \in \{\|Y - X^\top \beta\|_{\ell_2} \leq t\}} \{\|\beta\|_{\ell_2}^2\}$$

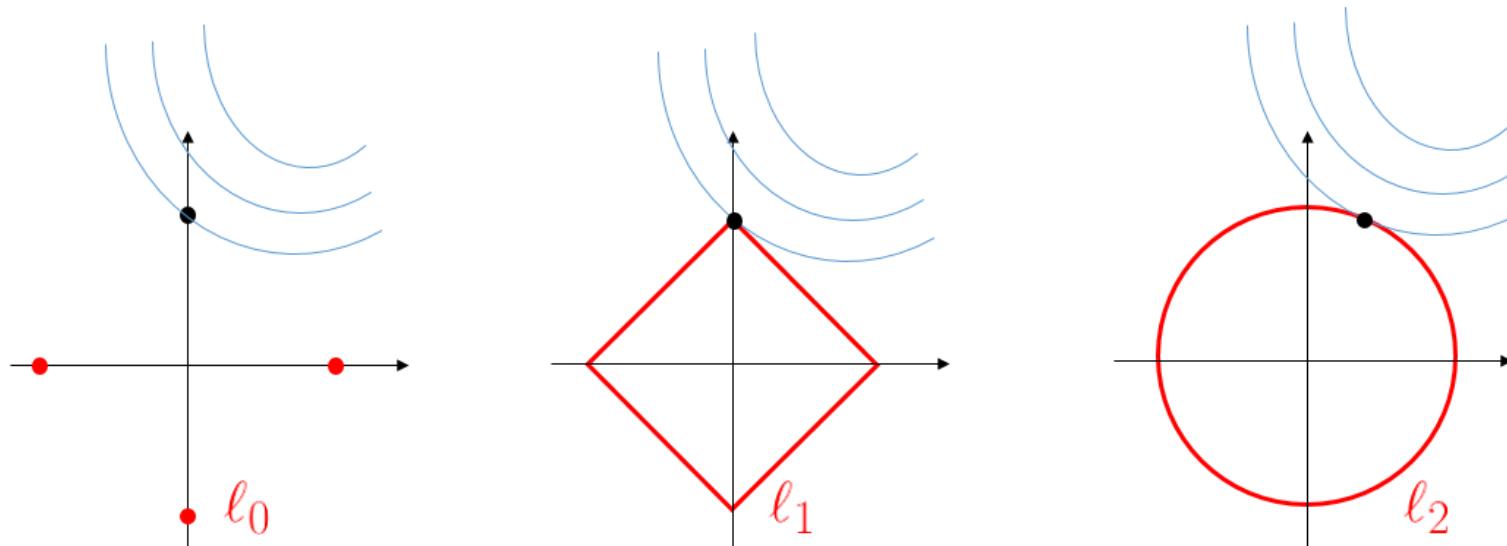


Going further on sparsity issues

Idea: solve the dual problem

$$\hat{\beta} = \operatorname{argmin}_{\beta \in \{\|\mathbf{Y} - \mathbf{X}^\top \beta\|_{\ell_2} \leq h\}} \{\|\beta\|_{\ell_0}\}$$

where we might convexify the ℓ_0 norm, $\|\cdot\|_{\ell_0}$.



Going further on sparsity issues

On $[-1, +1]^k$, the convex hull of $\|\beta\|_{\ell_0}$ is $\|\beta\|_{\ell_1}$

On $[-a, +a]^k$, the convex hull of $\|\beta\|_{\ell_0}$ is $a^{-1}\|\beta\|_{\ell_1}$

Hence, why not solve

$$\hat{\beta} = \underset{\beta: \|\beta\|_{\ell_1} \leq \tilde{s}}{\operatorname{argmin}} \{ \|Y - X^\top \beta\|_{\ell_2} \}$$

which is equivalent (Kuhn-Tucker theorem) to the Lagragian optimization problem

$$\hat{\beta} = \operatorname{argmin} \{ \|Y - X^\top \beta\|_{\ell_2}^2 + \lambda \|\beta\|_{\ell_1} \}$$

LASSO *Least Absolute Shrinkage and Selection Operator*

$$\hat{\boldsymbol{\beta}} \in \operatorname{argmin}\{\|\mathbf{Y} - \mathbf{X}^\top \boldsymbol{\beta}\|_{\ell_2}^2 + \lambda \|\boldsymbol{\beta}\|_{\ell_1}\}$$

is a convex problem (several algorithms^{*}), but not strictly convex (no unicity of the minimum). Nevertheless, predictions $\hat{\mathbf{y}} = \mathbf{x}^\top \hat{\boldsymbol{\beta}}$ are unique.

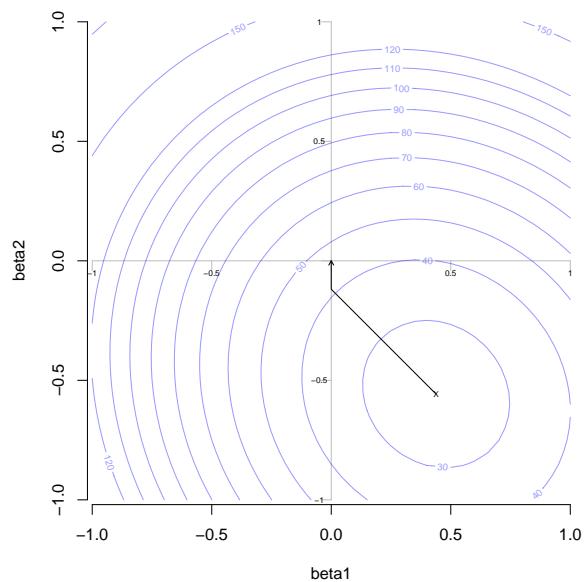
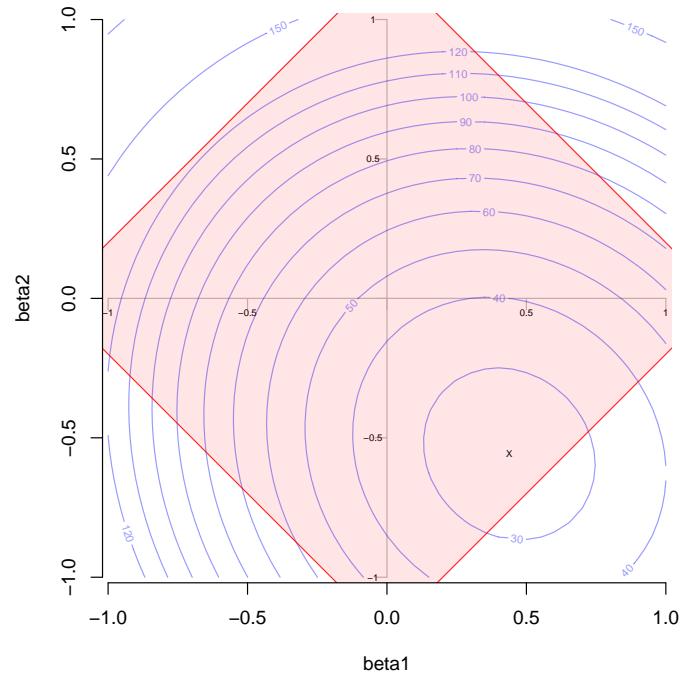
* MM, minimize majorization, coordinate descent Hunter & Lange (2003) [A Tutorial on MM Algorithms](#).

LASSO Regression

No explicit solution...

If $\lambda \rightarrow 0$, $\hat{\beta}_0^{\text{lasso}} = \hat{\beta}^{\text{ols}}$

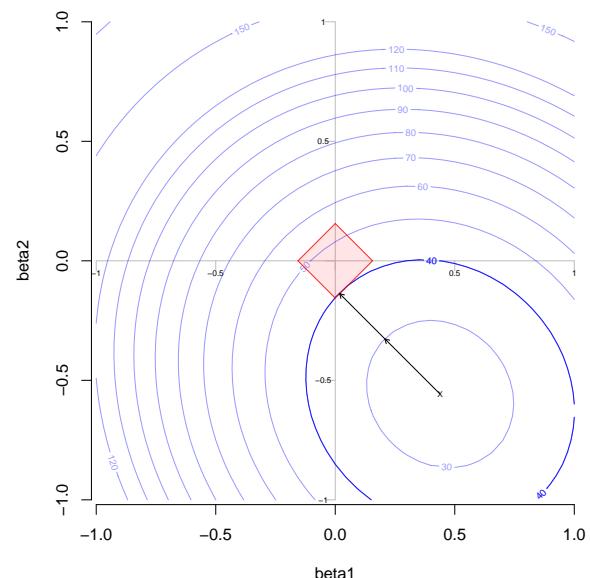
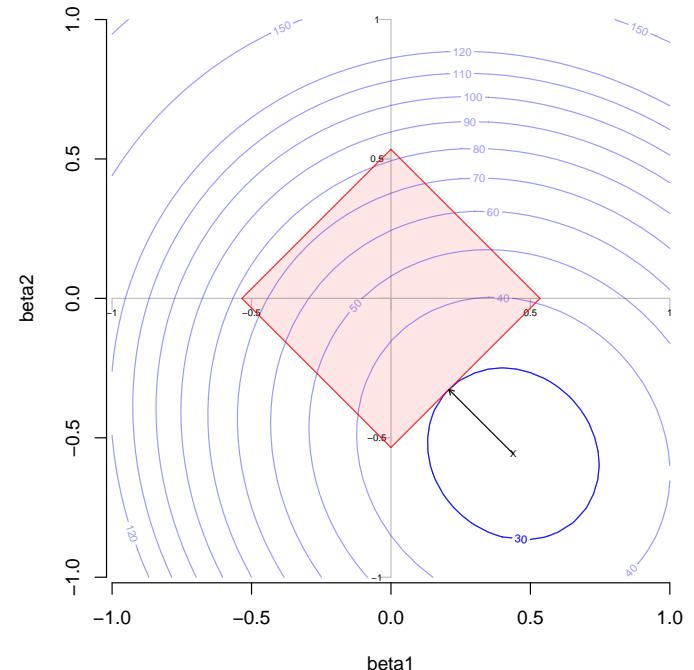
If $\lambda \rightarrow \infty$, $\hat{\beta}_{\infty}^{\text{lasso}} = \mathbf{0}$.



LASSO Regression

For some λ , there are k 's such that $\hat{\beta}_{k,\lambda}^{\text{lasso}} = 0$.

Further, $\lambda \mapsto \hat{\beta}_{k,\lambda}^{\text{lasso}}$ is piecewise linear

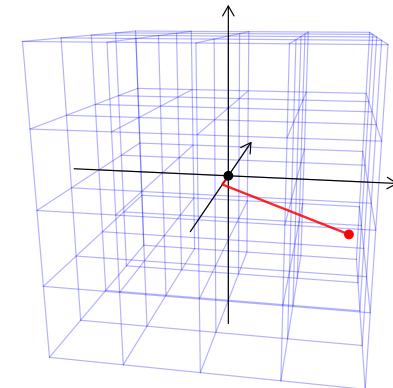


LASSO Regression

In the orthogonal case, $\mathbf{X}^\top \mathbf{X} = \mathbb{I}$,

$$\hat{\boldsymbol{\beta}}_{k,\lambda}^{\text{lasso}} = \text{sign}(\hat{\boldsymbol{\beta}}_k^{\text{ols}}) \left(|\hat{\boldsymbol{\beta}}_k^{\text{ols}}| - \frac{\lambda}{2} \right)$$

i.e. the LASSO estimate is related to the soft threshold function...



Optimal LASSO Penalty

Use cross validation, e.g. k -fold,

$$\widehat{\boldsymbol{\beta}}_{(-k)}(\lambda) = \operatorname{argmin} \left\{ \sum_{i \notin \mathcal{I}_k} [y_i - \mathbf{x}_i^\top \boldsymbol{\beta}]^2 + \lambda \|\boldsymbol{\beta}\|_{\ell_1} \right\}$$

then compute the sum of the squared errors,

$$Q_k(\lambda) = \sum_{i \in \mathcal{I}_k} [y_i - \mathbf{x}_i^\top \widehat{\boldsymbol{\beta}}_{(-k)}(\lambda)]^2$$

and finally solve

$$\lambda^* = \operatorname{argmin} \left\{ \overline{Q}(\lambda) = \frac{1}{K} \sum_k Q_k(\lambda) \right\}$$

Optimal LASSO Penalty

Note that this might overfit, so Hastie, Tibshirani & Friedman (2009) [Elements of Statistical Learning](#) suggest the largest λ such that

$$\bar{Q}(\lambda) \leq \bar{Q}(\lambda^*) + \text{se}[\lambda^*] \text{ with } \text{se}[\lambda]^2 = \frac{1}{K^2} \sum_{k=1}^K [Q_k(\lambda) - \bar{Q}(\lambda)]^2$$

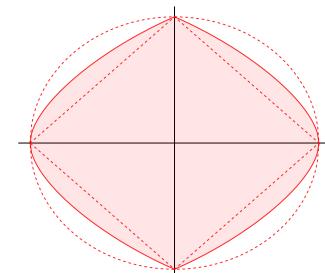
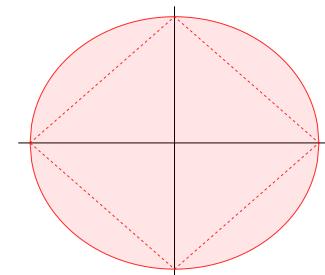
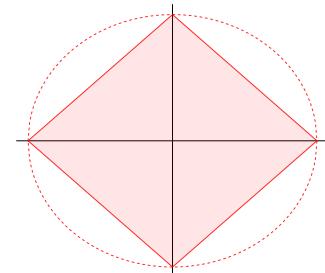
LASSO and Ridge, with R

```

1 > library(glmnet)
2 > chicago=read.table("http://freakonometrics.free.fr/
  chicago.txt",header=TRUE,sep=";")
3 > standardize <- function(x) {(x-mean(x))/sd(x)}
4 > z0 <- standardize(chicago[, 1])
5 > z1 <- standardize(chicago[, 3])
6 > z2 <- standardize(chicago[, 4])
7 > ridge <-glmnet(cbind(z1, z2), z0, alpha=0, intercept=
  FALSE, lambda=1)
8 > lasso <-glmnet(cbind(z1, z2), z0, alpha=1, intercept=
  FALSE, lambda=1)
9 > elastic <-glmnet(cbind(z1, z2), z0, alpha=.5,
  intercept=FALSE, lambda=1)

```

Elastic net, $\lambda_1 \|\beta\|_{\ell_1} + \lambda_2 \|\beta\|_{\ell_2}^2$



Going further, ℓ_0 , ℓ_1 and ℓ_2 penalty

Define

$$\|\mathbf{a}\|_{\ell_0} = \sum_{i=1}^d \mathbf{1}(a_i \neq 0), \quad \|\mathbf{a}\|_{\ell_1} = \sum_{i=1}^d |a_i| \quad \text{and} \quad \|\mathbf{a}\|_{\ell_2} = \left(\sum_{i=1}^d a_i^2 \right)^{1/2}, \quad \text{for } \mathbf{a} \in \mathbb{R}^d.$$

constrained
optimization

penalized
optimization

$\underset{\beta; \ \beta\ _{\ell_0} \leq s}{\operatorname{argmin}} \left\{ \sum_{i=1}^n \ell(y_i, \beta_0 + \mathbf{x}^\top \beta) \right\}$	$\underset{\beta, \lambda}{\operatorname{argmin}} \left\{ \sum_{i=1}^n \ell(y_i, \beta_0 + \mathbf{x}^\top \beta) + \lambda \ \beta\ _{\ell_0} \right\}$	($\ell 0$)
$\underset{\beta; \ \beta\ _{\ell_1} \leq s}{\operatorname{argmin}} \left\{ \sum_{i=1}^n \ell(y_i, \beta_0 + \mathbf{x}^\top \beta) \right\}$	$\underset{\beta, \lambda}{\operatorname{argmin}} \left\{ \sum_{i=1}^n \ell(y_i, \beta_0 + \mathbf{x}^\top \beta) + \lambda \ \beta\ _{\ell_1} \right\}$	($\ell 1$)
$\underset{\beta; \ \beta\ _{\ell_2} \leq s}{\operatorname{argmin}} \left\{ \sum_{i=1}^n \ell(y_i, \beta_0 + \mathbf{x}^\top \beta) \right\}$	$\underset{\beta, \lambda}{\operatorname{argmin}} \left\{ \sum_{i=1}^n \ell(y_i, \beta_0 + \mathbf{x}^\top \beta) + \lambda \ \beta\ _{\ell_2} \right\}$	($\ell 2$)

Assume that ℓ is the quadratic norm.

Going further, ℓ_0 , ℓ_1 and ℓ_2 penalty

The two problems (ℓ_2) are equivalent : $\forall(\beta^*, s^*)$ solution of the left problem, $\exists\lambda^*$ such that (β^*, λ^*) is solution of the right problem. And conversely.

The two problems (ℓ_1) are equivalent : $\forall(\beta^*, s^*)$ solution of the left problem, $\exists\lambda^*$ such that (β^*, λ^*) is solution of the right problem. And conversely. Nevertheless, if there is a theoretical equivalence, there might be numerical issues since there is not necessarily unicity of the solution.

The two problems (ℓ_0) are **not** equivalent : if (β^*, λ^*) is solution of the right problem, $\exists s^*$ such that β^* is a solution of the left problem. But the converse is not true.

More generally, consider a ℓ_p norm,

- **sparsity** is obtained when $p \leq 1$
- **convexity** is obtained when $p \geq 1$

Going further, ℓ_0 , ℓ_1 and ℓ_2 penalty

Foster & George (1994) **the risk inflation criterion for multiple regression** tried to solve directly the penalized problem of (ℓ_0) .

But it is a complex combinatorial problem in high dimension (Natarajan (1995) **sparse approximate solutions to linear systems** proved that it was a NP-hard problem)

One can prove that if $\lambda \sim \sigma^2 \log(p)$, alors

$$\mathbb{E}([x^\top \hat{\beta} - x^\top \beta_0]^2) \leq \underbrace{\mathbb{E}([x_{\mathcal{S}}^\top \hat{\beta}_{\mathcal{S}} - x^\top \beta_0]^2)}_{=\sigma^2 \#\mathcal{S}} \cdot (4 \log p + 2 + o(1)).$$

In that case

$$\hat{\beta}_{\lambda,j}^{\text{sub}} = \begin{cases} 0 & \text{si } j \notin \mathcal{S}_\lambda(\beta) \\ \hat{\beta}_j^{\text{ols}} & \text{si } j \in \mathcal{S}_\lambda(\beta), \end{cases}$$

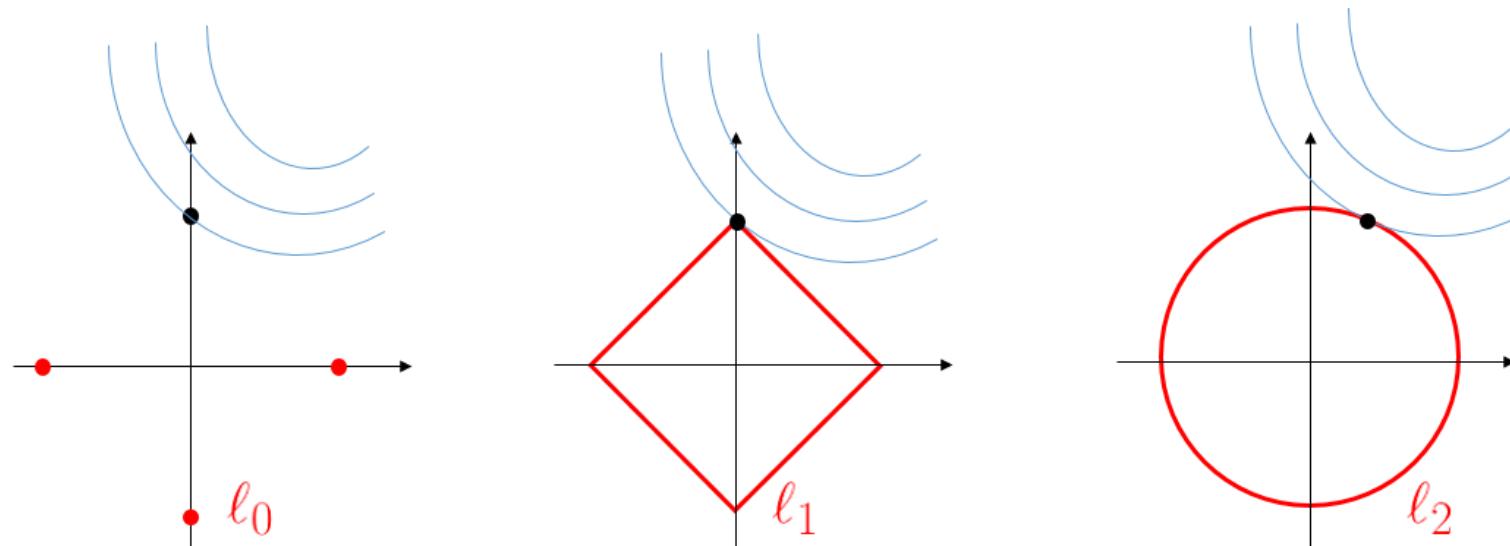
where $\mathcal{S}_\lambda(\beta)$ is the set of non-null values in solutions of (ℓ_0) .

If ℓ is no longer the quadratic norm but ℓ_1 , problem (ℓ_1) is not always strictly convex, and optimum is not always unique (e.g. if $\mathbf{X}^\top \mathbf{X}$ is singular).

But in the quadratic case, ℓ is strictly convex, and at least $\widehat{\mathbf{X}}\widehat{\beta}$ is unique.

Further, note that solutions are necessarily coherent (signs of coefficients) : it is not possible to have $\widehat{\beta}_j < 0$ for one solution and $\widehat{\beta}_j > 0$ for another one.

In many cases, problem (ℓ_1) yields a corner-type solution, which can be seen as a "best subset" solution - like in (ℓ_0) .



Going further, ℓ_0 , ℓ_1 and ℓ_2 penalty

Consider a simple regression $y_i = x_i\beta + \varepsilon$, with ℓ_1 -penalty and a ℓ_2 -loss function. (l1) becomes

$$\min \left\{ \mathbf{y}^\top \mathbf{y} - 2\mathbf{y}^\top \mathbf{x}\beta + \beta \mathbf{x}^\top \mathbf{x}\beta + 2\lambda |\beta| \right\}$$

First order condition can be written

$$-2\mathbf{y}^\top \mathbf{x} + 2\mathbf{x}^\top \mathbf{x}\hat{\beta} \pm 2\lambda = 0.$$

(the sign in \pm being the sign of $\hat{\beta}$). Assume that least-square estimate ($\lambda = 0$) is (strictly) positive, i.e. $\mathbf{y}^\top \mathbf{x} > 0$. If λ is not too large $\hat{\beta}$ and $\hat{\beta}^{\text{ols}}$ have the same sign, and

$$-2\mathbf{y}^\top \mathbf{x} + 2\mathbf{x}^\top \mathbf{x}\hat{\beta} + 2\lambda = 0.$$

with solution $\hat{\beta}_\lambda^{\text{lasso}} = \frac{\mathbf{y}^\top \mathbf{x} - \lambda}{\mathbf{x}^\top \mathbf{x}}$.

Going further, ℓ_0 , ℓ_1 and ℓ_2 penalty

Increase λ so that $\hat{\beta}_\lambda = 0$.

Increase slightly more, $\hat{\beta}_\lambda$ cannot become negative, because the sign of the first order condition will change, and we should solve

$$-2\mathbf{y}^\top \mathbf{x} + 2\mathbf{x}^\top \mathbf{x}\hat{\beta} - 2\lambda = 0.$$

and solution would be $\hat{\beta}_\lambda^{\text{lasso}} = \frac{\mathbf{y}^\top \mathbf{x} + \lambda}{\mathbf{x}^\top \mathbf{x}}$. But that solution is positive (we assumed that $\mathbf{y}^\top \mathbf{x} > 0$), so we should have $\hat{\beta}_\lambda < 0$.

Thus, at some point $\hat{\beta}_\lambda = 0$, which is a corner solution.

In higher dimension, see Tibshirani & Wasserman (2016) [a closer look at sparse regression](#) or Candès & Plan (2009) [Near-ideal model selection by \$\ell_1\$ minimization.](#),

With some additional technical assumption, that LASSO estimator is "sparsistent" in the sense that the support of $\hat{\beta}_\lambda^{\text{lasso}}$ is the same as β ,

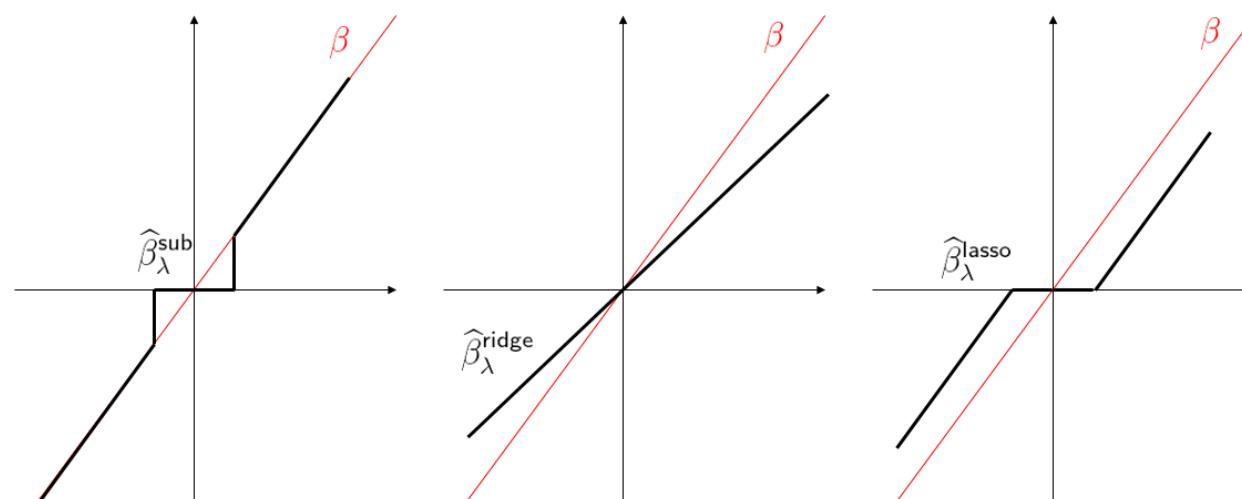
Going further, ℓ_0 , ℓ_1 and ℓ_2 penalty

Thus, LASSO can be used for variable selection (see Hastie *et al.* (2001) **The Elements of Statistical Learning**).

Generally, $\hat{\beta}_\lambda^{\text{lasso}}$ is a biased estimator but its variance can be small enough to have a smaller least squared error than the OLS estimate.

With orthonormal covariance, one can prove that

$$\hat{\beta}_{\lambda,j}^{\text{sub}} = \hat{\beta}_j^{\text{ols}} \mathbf{1}_{|\hat{\beta}_{\lambda,j}^{\text{sub}}| > b}, \quad \hat{\beta}_{\lambda,j}^{\text{ridge}} = \frac{\hat{\beta}_j^{\text{ols}}}{1 + \lambda} \quad \text{and} \quad \hat{\beta}_{\lambda,j}^{\text{lasso}} = \text{signe}[\hat{\beta}_j^{\text{ols}}] \cdot (|\hat{\beta}_j^{\text{ols}}| - \lambda)_+.$$



Optimization Heuristics

First idea: given some initial guess $\beta_{(0)}$, $|\beta| \sim |\beta_{(0)}| + \frac{1}{2|\beta_{(0)}|}(\beta^2 - \beta_{(0)}^2)$

LASSO estimate can probably be derived from iterated Ridge estimates

$$\|\mathbf{y} - \mathbf{X}\beta_{(k+1)}\|_{\ell_2}^2 + \lambda\|\beta_{(k+1)}\|_{\ell_1} \sim \mathbf{X}\beta_{(k+1)}\|_{\ell_2}^2 + \frac{\lambda}{2} \sum_j \frac{1}{|\beta_{j,(k)}|} [\beta_{j,(k+1)}]^2$$

which is a **weighted ridge penalty function**

Thus,

$$\beta_{(k+1)} = (\mathbf{X}^\top \mathbf{X} + \lambda \Delta_{(k)})^{-1} \mathbf{X}^\top \mathbf{y}$$

where $\Delta_{(k)} = \text{diag}[|\beta_{j,(k)}|^{-1}]$. Then $\beta_{(k)} \rightarrow \hat{\beta}^{\text{lasso}}$, as $k \rightarrow \infty$.

Properties of LASSO Estimate

From this iterative technique

$$\hat{\beta}_\lambda^{\text{lasso}} \sim (\mathbf{X}^\top \mathbf{X} + \lambda \Delta)^{-1} \mathbf{X}^\top \mathbf{y}$$

where $\Delta = \text{diag}[|\hat{\beta}_{j,\lambda}^{\text{lasso}}|^{-1}]$ if $\hat{\beta}_{j,\lambda}^{\text{lasso}} \neq 0$, 0 otherwise.

Thus,

$$\mathbb{E}[\hat{\beta}_\lambda^{\text{lasso}}] \sim (\mathbf{X}^\top \mathbf{X} + \lambda \Delta)^{-1} \mathbf{X}^\top \mathbf{X} \beta$$

and

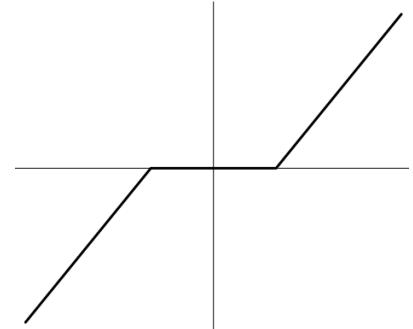
$$\text{Var}[\hat{\beta}_\lambda^{\text{lasso}}] \sim \sigma^2 (\mathbf{X}^\top \mathbf{X} + \lambda \Delta)^{-1} \mathbf{X}^\top \mathbf{X}^\top \mathbf{X} (\mathbf{X}^\top \mathbf{X} + \lambda \Delta)^{-1} \mathbf{X}^\top$$

Optimization Heuristics

Consider here a simplified problem, $\min_{a \in \mathbb{R}} \left\{ \underbrace{\frac{1}{2}(a - b)^2 + \lambda|a|}_{g(a)} \right\}$ with $\lambda > 0$.

Observe that $g'(0) = -b \pm \lambda$. Then

- if $|b| \leq \lambda$, then $a^* = 0$
- if $b \geq \lambda$, then $a^* = b - \lambda$
- if $b \leq -\lambda$, then $a^* = b + \lambda$



$$a^* = \operatorname{argmin}_{a \in \mathbb{R}} \left\{ \frac{1}{2}(a - b)^2 + \lambda|a| \right\} = S_\lambda(b) = \operatorname{sign}(b) \cdot (|b| - \lambda)_+,$$

also called **soft-thresholding** operator.

Optimization Heuristics

Definition for any convex function h , define the **proximal operator** operator of h ,

$$\text{proximal}_h(\mathbf{y}) = \underset{\mathbf{x} \in \mathbb{R}^d}{\operatorname{argmin}} \left\{ \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_{\ell_2}^2 + h(\mathbf{x}) \right\}$$

Note that

$$\text{proximal}_{\lambda \|\cdot\|_{\ell_2}^2}(\mathbf{y}) = \frac{1}{1 + \lambda} \mathbf{x} \quad \text{shrinkage operator}$$

$$\text{proximal}_{\lambda \|\cdot\|_{\ell_1}}(\mathbf{y}) = S_\lambda(\mathbf{y}) = \text{sign}(\mathbf{y}) \cdot (|\mathbf{y}| - \lambda)_+$$

Optimization Heuristics

We want to solve here

$$\hat{\boldsymbol{\theta}} \in \operatorname{argmin}_{\boldsymbol{\theta} \in \mathbb{R}^d} \left\{ \underbrace{\frac{1}{n} \|\mathbf{y} - m_{\boldsymbol{\theta}}(\mathbf{x})\|_{\ell_2}^2}_{f(\boldsymbol{\theta})} + \underbrace{\lambda \cdot \text{penalty}(\boldsymbol{\theta})}_{g(\boldsymbol{\theta})} \right\}.$$

where f is convex and smooth, and g is convex, but not smooth...

1. Focus on f : descent lemma, $\forall \boldsymbol{\theta}, \boldsymbol{\theta}'$

$$f(\boldsymbol{\theta}) \leq f(\boldsymbol{\theta}') + \langle \nabla f(\boldsymbol{\theta}'), \boldsymbol{\theta} - \boldsymbol{\theta}' \rangle + \frac{t}{2} \|\boldsymbol{\theta} - \boldsymbol{\theta}'\|_{\ell_2}^2$$

Consider a gradient descent sequence $\boldsymbol{\theta}_k$, i.e. $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - t^{-1} \nabla f(\boldsymbol{\theta}_k)$, then

$$f(\boldsymbol{\theta}) \leq \underbrace{f(\boldsymbol{\theta}_k) + \langle \nabla f(\boldsymbol{\theta}_k), \boldsymbol{\theta} - \boldsymbol{\theta}_k \rangle + \frac{t}{2} \|\boldsymbol{\theta} - \boldsymbol{\theta}_k\|_{\ell_2}^2}_{\varphi(\boldsymbol{\theta}): \boldsymbol{\theta}_{k+1} = \operatorname{argmin}\{\varphi(\boldsymbol{\theta})\}}$$

Optimization Heuristics

2. Add function g

$$f(\boldsymbol{\theta}) + g(\boldsymbol{\theta}) \leq f(\boldsymbol{\theta}_k) + \langle \nabla f(\boldsymbol{\theta}_k), \boldsymbol{\theta} - \boldsymbol{\theta}_k \rangle + \underbrace{\frac{t}{2} \|\boldsymbol{\theta} - \boldsymbol{\theta}_k\|_{\ell_2}^2}_{\psi(\boldsymbol{\theta})} + g(\boldsymbol{\theta})$$

And one can proof that

$$\boldsymbol{\theta}_{k+1} = \operatorname{argmin}_{\boldsymbol{\theta} \in \mathbb{R}^d} \left\{ \psi(\boldsymbol{\theta}) \right\} = \operatorname{proximal}_{g/t} (\boldsymbol{\theta}_k - t^{-1} \nabla f(\boldsymbol{\theta}_k))$$

so called proximal gradient descent algorithm, since

$$\operatorname{argmin} \left\{ \psi(\boldsymbol{\theta}) \right\} = \operatorname{argmin} \left\{ \frac{t}{2} \left\| \boldsymbol{\theta} - (\boldsymbol{\theta}_k - t^{-1} \nabla f(\boldsymbol{\theta}_k)) \right\|_{\ell_2}^2 + g(\boldsymbol{\theta}) \right\}$$

Coordinate-wise minimization

Consider some convex differentiable $f : \mathbb{R}^k \rightarrow \mathbb{R}$ function.

Consider $\mathbf{x}^* \in \mathbb{R}^k$ obtained by minimizing along each coordinate axis, i.e.

$$f(x_1^*, x_{i-1}^*, \mathbf{x}_i, x_{i+1}^*, \dots, x_k^*) \geq f(x_1^*, x_{i-1}^*, \mathbf{x}_i^*, x_{i+1}^*, \dots, x_k^*)$$

for all i . Is \mathbf{x}^* a global minimizer? i.e.

$$f(\mathbf{x}) \geq f(\mathbf{x}^*), \quad \forall \mathbf{x} \in \mathbb{R}^k.$$

Yes. If f is convex and differentiable.

$$\nabla f(\mathbf{x})|_{\mathbf{x}=\mathbf{x}^*} = \left(\frac{\partial f(\mathbf{x})}{\partial x_1}, \dots, \frac{\partial f(\mathbf{x})}{\partial x_k} \right) = \mathbf{0}$$

There might be problem if f is not differentiable (except in each axis direction).

If $f(\mathbf{x}) = g(\mathbf{x}) + \sum_{i=1}^k h_i(x_i)$ with g convex and differentiable, yes, since

$$f(\mathbf{x}) - f(\mathbf{x}^*) \geq \nabla g(\mathbf{x}^*)^\top (\mathbf{x} - \mathbf{x}^*) + \sum_i [h_i(x_i) - h_i(x_i^*)]$$

Coordinate-wise minimization

$$f(\mathbf{x}) - f(\mathbf{x}^*) \geq \sum_i \underbrace{[\nabla_i g(\mathbf{x}^*)^\top (x_i - x_i^*) h_i(x_i) - h_i(x_i^*)]}_{\geq 0} \geq 0$$

Thus, for functions $f(\mathbf{x}) = g(\mathbf{x}) + \sum_{i=1}^k h_i(x_i)$ we can use coordinate descent to find a minimizer, i.e. at step j

$$x_1^{(j)} \in \operatorname{argmin}_{x_1} f(x_1, x_2^{(j-1)}, x_3^{(j-1)}, \dots, x_k^{(j-1)})$$

$$x_2^{(j)} \in \operatorname{argmin}_{x_2} f(x_1^{(j)}, x_2, x_3^{(j-1)}, \dots, x_k^{(j-1)})$$

$$x_3^{(j)} \in \operatorname{argmin}_{x_3} f(x_1^{(j)}, x_2^{(j)}, x_3, \dots, x_k^{(j-1)})$$

Tseng (2001) **Convergence of Block Coordinate Descent Method**: if f is continuous, then \mathbf{x}^∞ is a minimizer of f .

Application in Linear Regression

Let $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{y} - \mathbf{Ax}\|^2$, with $\mathbf{y} \in \mathbb{R}^n$ and $\mathbf{A} \in \mathcal{M}_{n \times k}$. Let $\mathbf{A} = [\mathbf{A}_1, \dots, \mathbf{A}_k]$.

Let us minimize in direction i . Let \mathbf{x}_{-i} denote the vector in \mathbb{R}^{k-1} without x_i .

Here

$$0 = \frac{\partial f(\mathbf{x})}{\partial x_i} = \mathbf{A}_i^\top [\mathbf{Ax} - \mathbf{y}] = \mathbf{A}_i^\top [\mathbf{A}_i x_i + \mathbf{A}_{-i} \mathbf{x}_{-i} - \mathbf{y}]$$

thus, the optimal value is here

$$x_i^* = \frac{\mathbf{A}_i^\top [\mathbf{A}_{-i} \mathbf{x}_{-i} - \mathbf{y}]}{\mathbf{A}_i^\top \mathbf{A}_i}$$

Application to LASSO

Let $f(\mathbf{x}) = \frac{1}{2}\|\mathbf{y} - \mathbf{Ax}\|^2 + \lambda\|\mathbf{x}\|_{\ell_1}$, so that the non-differentiable part is separable, since $\|\mathbf{x}\|_{\ell_1} = \sum_{i=1}^k |x_i|$.

Let us minimize in direction i . Let \mathbf{x}_{-i} denote the vector in \mathbb{R}^{k-1} without x_i .
Here

$$0 = \frac{\partial f(\mathbf{x})}{\partial x_i} = \mathbf{A}_i^\top [\mathbf{A}_i x_i + \mathbf{A}_{-i} \mathbf{x}_{-i} - \mathbf{y}] + \lambda s_i$$

where $s_i \in \partial|x_i|$. Thus, solution is obtained by soft-thresholding

$$x_i^* = S_{\lambda/\|\mathbf{A}_i\|^2} \left(\frac{\mathbf{A}_i^\top [\mathbf{A}_{-i} \mathbf{x}_{-i} - \mathbf{y}]}{\mathbf{A}_i^\top \mathbf{A}_i} \right)$$

Convergence rate for LASSO

Let $f(\mathbf{x}) = g(\mathbf{x}) + \lambda \|\mathbf{x}\|_{\ell_1}$ with

- g convex, ∇g Lipschitz with constant $L > 0$, and $Id - \nabla g/L$ monotone increasing in each component
- there exists \mathbf{z} such that, componentwise, either $\mathbf{z} \geq S_\lambda(\mathbf{z} - \nabla g(\mathbf{z}))$ or $\mathbf{z} \leq S_\lambda(\mathbf{z} - \nabla g(\mathbf{z}))$

Saka & Tewari (2010), [On the finite time convergence of cyclic coordinate descent methods](#) proved that a coordinate descent starting from \mathbf{z} satisfies

$$f(\mathbf{x}^{(j)}) - f(\mathbf{x}^*) \leq \frac{L \|\mathbf{z} - \mathbf{x}^*\|^2}{2j}$$

LASSO for Autoregressive Time Series

Consider some $\text{AR}(p)$ autoregressive time series,

$$X_t = \phi_1 X_{t-1} + \phi_2 X_{t-2} + \cdots + \phi_{p-1} X_{t-p+1} + \phi_p X_{t-p} + \varepsilon_t,$$

for some white noise (ε_t), with a causal type representation. Write $y = \mathbf{x}^\top \boldsymbol{\phi} + \varepsilon$.

The LASSO estimator $\hat{\boldsymbol{\phi}}$ is a minimizer of

$$\frac{1}{2T} \|y - \mathbf{x}^\top \boldsymbol{\phi}\|^2 + \lambda \sum_{i=1}^p \lambda_i |\phi_i|,$$

for some tuning parameters $(\lambda, \lambda_1, \dots, \lambda_p)$.

See [Nardi & Rinaldo \(2011\)](#).

LASSO and Non-Linearities

Consider knots k_1, \dots, k_m , we want a function m which is a cubic polynomial between every pair of knots, continuous at each knot, and with continuous first and second derivatives at each knot.

We can write m as

$$m(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3 + \beta_4 (x - k_1)_+^3 + \dots + \beta_{m+3} (x - k_m)_+^3$$

One strategy is the following

- fix the number of knots m ($m < n$)
- find the natural cubic spline \hat{m} which minimizes $\sum_{i=1}^n (y_i - m(x_i))^2$
- then choose m by cross validation

and alternative is to use a penalty based approach (Ridge type) to avoid overfit (since with $m = n$, the residual sum of square is null).

GAM, splines and Ridge regression

Consider a univariate nonlinear regression problem, so that $\mathbb{E}[Y|X = x] = m(x)$.

Given a sample $\{(y_1, x_1), \dots, (y_n, x_n)\}$, consider the following penalized problem

$$m^* = \operatorname{argmin}_{m \in \mathcal{C}^2} \left\{ \sum_{i=1}^n (y_i - m(x_i))^2 + \lambda \int_{\mathbb{R}} m''(x) dx \right\}$$

with the Residual sum of squares on the left, and a penalty for the roughness of the function.

The solution is a natural cubic spline with knots at unique values of x (see [Eubank \(1999\)](#))

Consider some spline basis $\{h_1, \dots, h_n\}$, and let $m(x) = \sum_{i=1}^n \beta_i h_i(x)$.

Let \mathbf{H} and $\boldsymbol{\Omega}$ be the $n \times n$ matrices $H_{i,j} = h_j(x_i)$, and $\Omega_{i,j} = \int_{\mathbb{R}} h_i''(x) h_j''(x) dx$.

GAM, splines and Ridge regression

Then the objective function can be written

$$(\mathbf{y} - \mathbf{H}\boldsymbol{\beta})^\top (\mathbf{y} - \mathbf{H}\boldsymbol{\beta}) + \lambda \boldsymbol{\beta}^\top \boldsymbol{\Omega} \boldsymbol{\beta}$$

Recognize here a generalized Ridge regression, with solution

$$\hat{\boldsymbol{\beta}}_\lambda = (\mathbf{H}^\top \mathbf{H} + \lambda \boldsymbol{\Omega})^{-1} \mathbf{H}^\top \mathbf{y}.$$

Note that predicted values are linear functions of the observed value since

$$\hat{\mathbf{y}} = \mathbf{H}(\mathbf{H}^\top \mathbf{H} + \lambda \boldsymbol{\Omega})^{-1} \mathbf{H}^\top \mathbf{y} = \mathbf{S}_\lambda \mathbf{y},$$

with degrees of freedom $\text{trace}(\mathbf{S}_\lambda)$.

One can obtain the so-called [Reinsch form](#) by considering the singular value decomposition of $\mathbf{H} = \mathbf{U} \mathbf{D} \mathbf{V}^\top$.

GAM, splines and Ridge regression

Here \mathbf{U} is orthogonal since \mathbf{H} is square ($n \times n$), and \mathbf{D} is here invertible. Then

$$\mathbf{S}_\lambda = (\mathbb{I} + \lambda \mathbf{U}^\top \mathbf{D}^{-1} \mathbf{V}^\top \boldsymbol{\Omega} \mathbf{V} \mathbf{D}^{-1} \mathbf{U})^{-1} = (\mathbb{I} + \lambda \mathbf{K})^{-1}$$

where \mathbf{K} is a positive semidefinite matrix, $\mathbf{K} = \mathbf{B} \boldsymbol{\Delta} \mathbf{B}^\top$, where columns of \mathbf{B} are known as the Demmler-Reinsch basis.

In that (orthonormal) basis, \mathbf{S}_λ is a diagonal matrix,

$$\mathbf{S}_\lambda = \mathbf{B} (\mathbb{I} + \lambda \boldsymbol{\Delta})^{-1} \mathbf{B}^\top$$

Observe that $\mathbf{S}_\lambda \mathbf{B}_k = \frac{1}{1 + \lambda \Delta_{k,k}} \mathbf{B}_k$.

Here again, eigenvalues are shrinkage coefficients of basis vectors.

With more covariates, consider an **additive** problem

$$(h_1, \dots, h_p)^* = \underset{h_1, \dots, h_p \in \mathcal{C}^2}{\operatorname{argmin}} \left\{ \sum_{i=1}^n \left(y_i - \sum_{j=1}^p m(x_{i,j}) \right)^2 + \lambda \sum_{j=1}^p \int_{\mathbb{R}} m_j''(x) dx \right\}$$

GAM, splines and Ridge regression

which can be written

$$\min \left\{ (\mathbf{y} - \sum_{j=1}^p \mathbf{H}_j \boldsymbol{\beta}_j)^\top (\mathbf{y} - \sum_{j=1}^p \mathbf{H}_j \boldsymbol{\beta}_j) + \lambda (\boldsymbol{\beta}_1^\top \sum_{j=1}^p \boldsymbol{\Omega}_j \boldsymbol{\beta}_j) \right\}$$

where each matrix \mathbf{H}_j is a Demmler-Reinsch basis for variable x_j .

Chouldechova & Hastie (2015) **Generalized Additive Model Selection**

Assume that the mean function for the j th variable is $m_j(x) = \alpha_j x + \mathbf{m}_j(x)^\top \boldsymbol{\beta}_j$.

One can write

$$\begin{aligned} \min \left\{ (\mathbf{y} - \alpha_0 - \sum_{j=1}^p \alpha_j x_j - \sum_{j=1}^p \mathbf{H}_j \boldsymbol{\beta}_j)^\top (\mathbf{y} - \alpha_0 - \sum_{j=1}^p \alpha_j x_j - \sum_{j=1}^p \mathbf{H}_j \boldsymbol{\beta}_j) \right. \\ \left. + \lambda (\gamma |\alpha_1| + (1 - \gamma) \|\boldsymbol{\beta}_j\|_{\Omega_j}) + (\psi_1 \boldsymbol{\beta}_1^\top \boldsymbol{\Omega}_1 \boldsymbol{\beta}_1 + \cdots + \psi_p \boldsymbol{\beta}_p^\top \boldsymbol{\Omega}_p \boldsymbol{\beta}_p) \right\} \end{aligned}$$

where $\|\boldsymbol{\beta}_j\|_{\Omega_j} = \sqrt{\boldsymbol{\beta}_j^\top \boldsymbol{\Omega}_j \boldsymbol{\beta}_j}$.

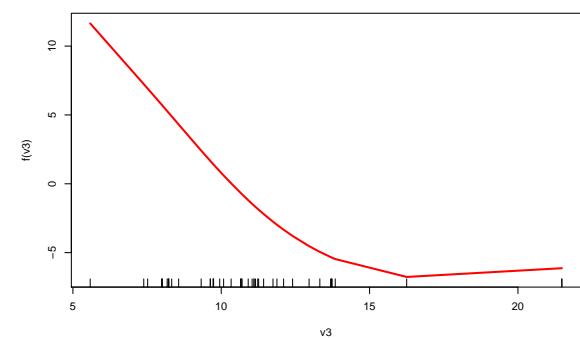
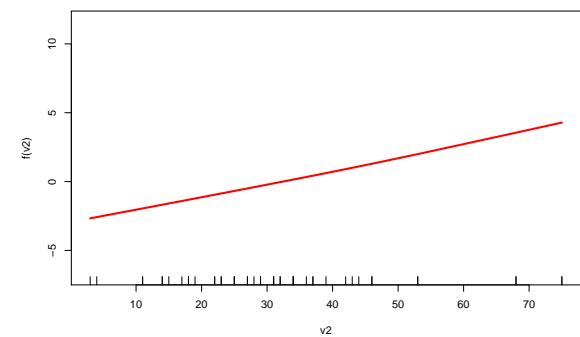
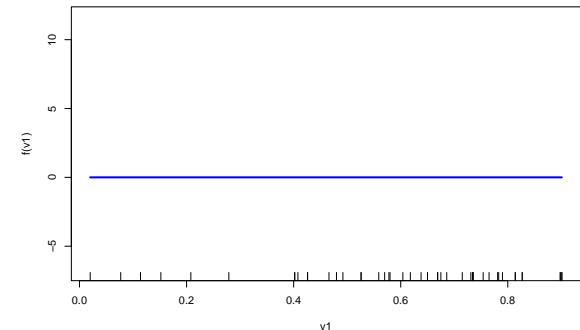
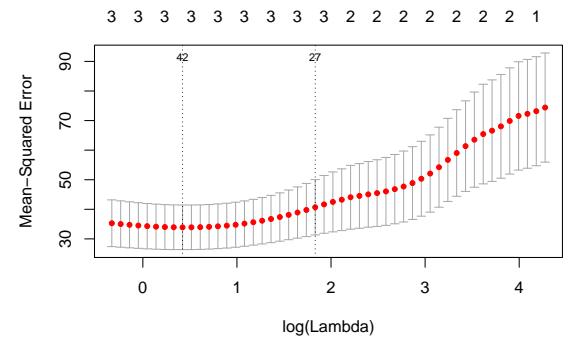
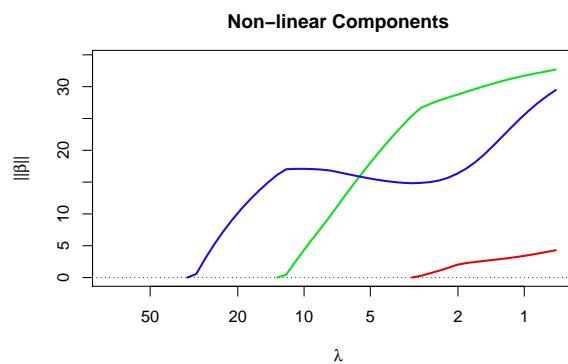
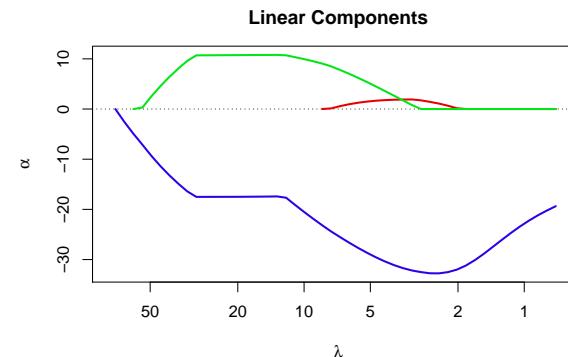
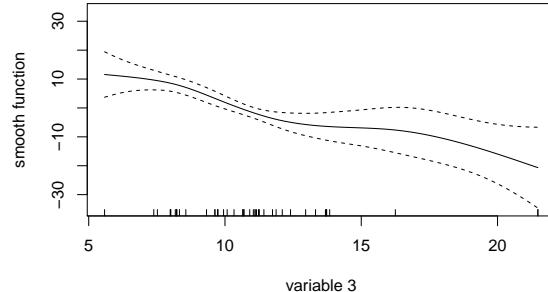
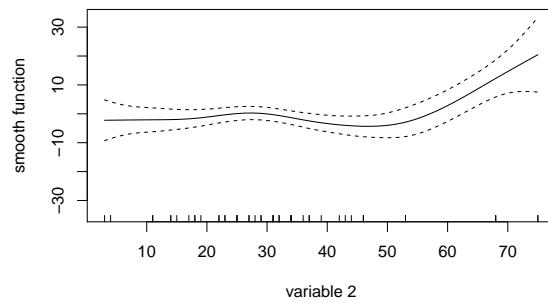
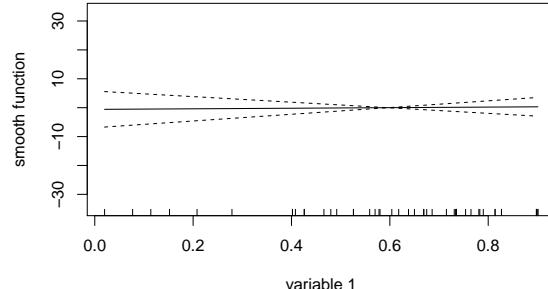
GAM, splines and Ridge regression

The **second term** is the selection penalty, with a mixture of ℓ_1 and ℓ_2 (type) norm-based penalty

The **third term** is the end-to-path penalty (GAM type when $\lambda = 0$).

For each predictor x_j , there are three possibilities

- zero, $\alpha_j = 0$ and $\beta_j = \mathbf{0}$
- linear, $\alpha_j \neq 0$ and $\beta_j = \mathbf{0}$
- nonlinear, $\beta_j \neq \mathbf{0}$



Graphical LASSO and Covariance Estimation

We want to estimate an (unknown) covariance matrix Σ , or Σ^{-1} .

An estimate for Σ^{-1} is Θ^* solution of

$$\Theta \in \underset{\Theta \in \mathcal{M}_{k \times k}}{\operatorname{argmin}} \left\{ -\log[\det(\Theta)] + \operatorname{trace}[S\Theta] + \lambda \|\Theta\|_{\ell_1} \right\} \text{ where } S = \frac{X^\top X}{n}$$

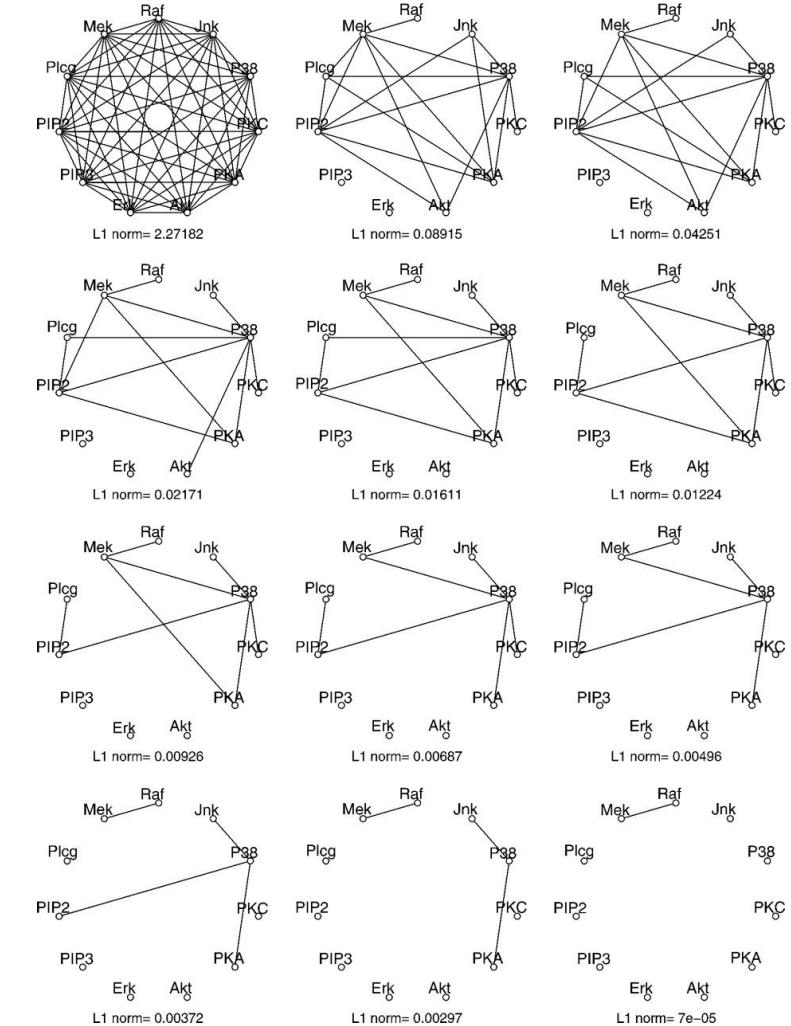
and where $\|\Theta\|_{\ell_1} = \sum |\Theta_{i,j}|$.

See van Wieringen (2016) [Undirected network reconstruction from high-dimensional data](#) and <https://github.com/kaizhang/glasso>

Application to Network Simplification

Can be applied on networks, to spot ‘significant’ connexions...

Source: <http://khughitt.github.io/graphical-lasso/>



Extention of Penalization Techniques

In a more general context, we want to solve

$$\hat{\boldsymbol{\theta}} \in \operatorname{argmin}_{\boldsymbol{\theta} \in \mathbb{R}^d} \left\{ \frac{1}{n} \sum_{i=1}^n \ell(y_i, m_{\boldsymbol{\theta}}(\mathbf{x}_i)) + \lambda \cdot \text{penalty}(\boldsymbol{\theta}) \right\}.$$

The quadratic loss function was related to the Gaussian case, but much more alternatives can be considered...

Linear models, nonlinear modes and GLMs

linear model

- $(Y|\boldsymbol{X} = \boldsymbol{x}) \sim \mathcal{N}(\theta_{\boldsymbol{x}}, \sigma^2)$
- $\mathbb{E}[Y|\boldsymbol{X} = \boldsymbol{x}] = \theta_{\boldsymbol{x}} = \boldsymbol{x}^\top \boldsymbol{\beta}$

```
1 > fit <- lm(y ~ x, data = df)
```

Linear models, nonlinear modes and GLMs

Nonlinear models

- $(Y|\boldsymbol{X} = \boldsymbol{x}) \sim \mathcal{N}(\theta_{\boldsymbol{x}}, \sigma^2)$
- $\mathbb{E}[Y|\boldsymbol{X} = \boldsymbol{x}] = \theta_{\boldsymbol{x}} = m(\boldsymbol{x})$

```
1 > fit <- lm(y ~ poly(x, k), data = df)
2 > fit <- lm(y ~ bs(x), data = df)
```

Linear models, nonlinear modes and GLMs

Generalized Linear Models

- $(Y|\boldsymbol{X} = \boldsymbol{x}) \sim \mathcal{L}(\theta_{\boldsymbol{x}}, \varphi)$
- $\mathbb{E}[Y|\boldsymbol{X} = \boldsymbol{x}] = h^{-1}(\theta_{\boldsymbol{x}}) = \tilde{h}^{-1}(\boldsymbol{x}^\top \boldsymbol{\beta})$

```
1 > fit <- glm(y ~ x, data = df,
2 + family = poisson(link = "log")
```

The Exponential Family

Consider distributions with parameter θ (and φ) with density (with respect to the appropriate measure, on \mathbb{N} or on \mathbb{R})

$$f(y|\theta, \varphi) = \exp\left(\frac{y\theta - b(\theta)}{a(\varphi)} + c(y, \varphi)\right),$$

where $a(\cdot)$, $b(\cdot)$ and $c(\cdot)$ are functions, where θ is called **canonical parameter**.

θ is the quantity of interest, while φ is a **nuisance parameter**.

The Exponential Family

Example The **Gaussian** distribution with mean μ and variance σ^2 , $\mathcal{N}(\mu, \sigma^2)$ belongs to that family $\theta = \mu$, $\varphi = \sigma^2$, $a(\varphi) = \varphi$, $b(\theta) = \theta^2/2$ and

$$c(y, \varphi) = -\frac{1}{2} \left(\frac{y^2}{\sigma^2} + \log(2\pi\sigma^2) \right), \quad y \in \mathbb{R},$$

Example **Bernoulli** distribution, with mean π , $\mathcal{B}(\pi)$ is obtained with $\theta = \log\{p/(1-p)\}$, $a(\varphi) = 1$, $b(\theta) = \log(1 + \exp(\theta))$, $\varphi = 1$ and $c(y, \varphi) = 0$.

Example The **binomiale** distribution with mean $n\pi$, $\mathcal{B}(n, \pi)$ is obtained with $\theta = \log\{p/(1-p)\}$, $a(\varphi) = 1$, $b(\theta) = n \log(1 + \exp(\theta))$, $\varphi = 1$ and $c(y, \varphi) = \log \binom{n}{y}$.

Example The **Poisson** distribution with mean λ , $\mathcal{P}(\lambda)$ belongs to that family

$$f(y|\lambda) = \exp(-\lambda) \frac{\lambda^y}{y!} = \exp \left(y \log \lambda - \lambda - \log y! \right), \quad y \in \mathbb{N},$$

with $\theta = \log \lambda$, $\varphi = 1$, $a(\varphi) = 1$, $b(\theta) = \exp \theta = \lambda$ and $c(y, \varphi) = -\log y!$.

The Exponential Family

Example The Negative Binomiale distribution with parameters r and p ,

$$f(k|r,p) = \binom{y+r-1}{y} (1-p)^r p^y, \quad y \in \mathbb{N}.$$

can be written, equivalently

$$f(k|r,p) = \exp \left(y \log p + r \log(1-p) + \log \binom{y+r-1}{y} \right)$$

i.e. $\theta = \log p$, $b(\theta) = -r \log p$ and $a(\varphi) = 1$

The Exponential Family

Example The **Gamma** distribution, with mean μ and variance ν^{-1} ,

$$f(y|\mu, \nu) = \frac{1}{\Gamma(\nu)} \left(\frac{\nu}{\mu} \right)^\nu y^{\nu-1} \exp \left(-\frac{\nu}{\mu} y \right), \quad y \in \mathbb{R}_+,$$

is also in the Exponential family $\theta = -\frac{1}{\mu}$, $a(\varphi) = \varphi$, $b(\theta) = -\log(-\theta)$, $\varphi = \nu^{-1}$

and

$$c(y, \varphi) = \left(\frac{1}{\varphi} - 1 \right) \log(y) - \log \left(\Gamma \left(\frac{1}{\varphi} \right) \right)$$

Mean and Variance

Let Y be a random variable in the Exponential family

$$\mathbb{E}(Y) = b'(\theta) \text{ and } \text{Var}(Y) = b''(\theta)\varphi,$$

i.e. the variance of Y is the product of two quantities

- $b''(\theta)$ is a function θ (only) and is called the variance function,
- a function of φ .

Observe that $\mu = \mathbb{E}(Y)$, hence parameter θ is related to mean μ . Hence, the variance function is function of μ , and can be denote

$$V(\mu) = b''([b']^{-1}(\mu))\varphi.$$

Example In the Gaussian case, $V(\mu) = 1$, while for the Poisson distribution, $V(\mu) = \mu$ and for the Gamma one $V(\mu) = \mu^2$.

From the Exponential Family to GLMs

Consider independent random variables Y_1, Y_2, \dots, Y_n such that

$$f(y_i|\theta_i, \varphi) = \exp \left\{ \frac{y_i\theta_i - b(\theta_i)}{a(\varphi)} + c(y_i, \varphi) \right\}$$

so that the likelihood can be written

$$\mathcal{L}(\boldsymbol{\theta}, \varphi | \mathbf{y}) = \prod_{i=1}^n f(y_i|\theta_i, \varphi) = \exp \left\{ \frac{\sum_{i=1}^n y_i\theta_i - \sum_{i=1}^n b(\theta_i)}{a(\varphi)} + \sum_{i=1}^n c(y_i, \varphi) \right\}.$$

or

$$\log \mathcal{L}(\boldsymbol{\beta}) = \sum_{i=1}^n \frac{y_i\theta_i - b(\theta_i)}{a(\varphi)}$$

(up to an additive constant...)

Penalized Generalized Linear Models

The Maximum Likelihood Estimator is $\hat{\boldsymbol{\beta}}^{\text{MLE}} = \operatorname{argmax}\{\log \mathcal{L}(\boldsymbol{\beta})\}$

One can consider a penalized estimator

$$\hat{\boldsymbol{\beta}}^{\text{LASSO}} = \operatorname{argmin}\left\{-\log \mathcal{L}(\boldsymbol{\beta}) + \sum_{j=1}^p J_\lambda(|\beta_j|)\right\}$$

for some penalty $J_\lambda(|\beta_j|)$.

Consider the logistic regression, with $y_i \in \{0, 1\}$, so that

$$\mathbb{P}[Y = 1 | \mathbf{X} = \mathbf{x}] = \frac{\exp[\mathbf{x}^\top \boldsymbol{\beta}]}{1 + \exp[\mathbf{x}^\top \boldsymbol{\beta}]}$$

Set $p_i = \mathbb{P}[Y_i = 1 | \mathbf{X} = \mathbf{x}_i]$ so that the log-likelihood becomes

$$\log \mathcal{L}(\boldsymbol{\beta}) = \sum_{i=1}^n (y_i \log[p_i] + (1 - y_i) \log[1 - p_i])$$

Penalized Generalized Linear Models

Consider the Cox regression, with obsevations $\{(t_i, \mathbf{x}_i, \delta_i)\}$, where $\delta_i \in \{0, 1\}$ is the censoring indicator ($\delta = 1$ means complete observation here).

Let $t_1 < t_2 < \dots < t_n$ denote the times when events are observed. In Cox regression model (from Cox (1972) [Regression Models and Life-Tables](#)) the hazard rate at time t is assumed to be

$$h(t|\mathbf{x}) = h_0(t) \exp[\mathbf{x}^\top \boldsymbol{\beta}]$$

where $h_0(t)$ is some baseline hazard. Consider then partial log-likelihood

$$\log \mathcal{L}(\boldsymbol{\beta}) = \sum_{i=1}^n \delta_i \left(\mathbf{x}_i^\top \boldsymbol{\beta} - \log \left[\sum_{j:t_j \geq t_i} \exp[\mathbf{x}_j^\top \boldsymbol{\beta}] \right] \right)$$