Advanced Econometrics #3: Model & Variable Selection

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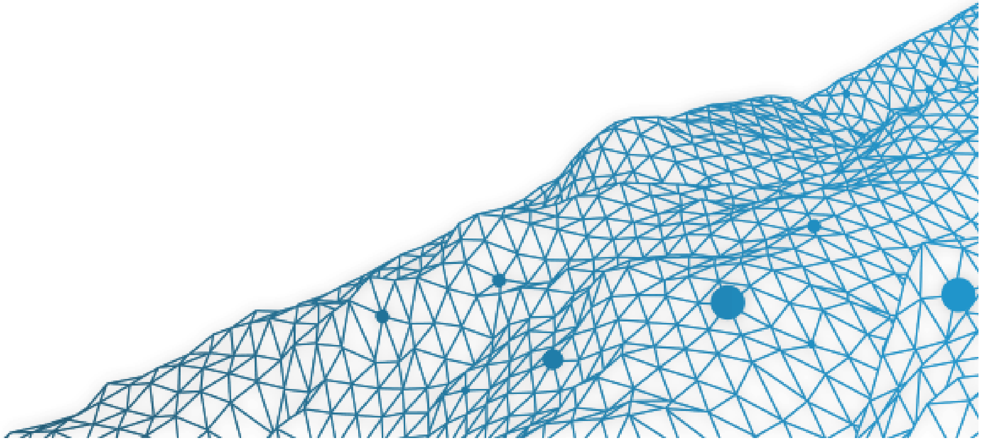
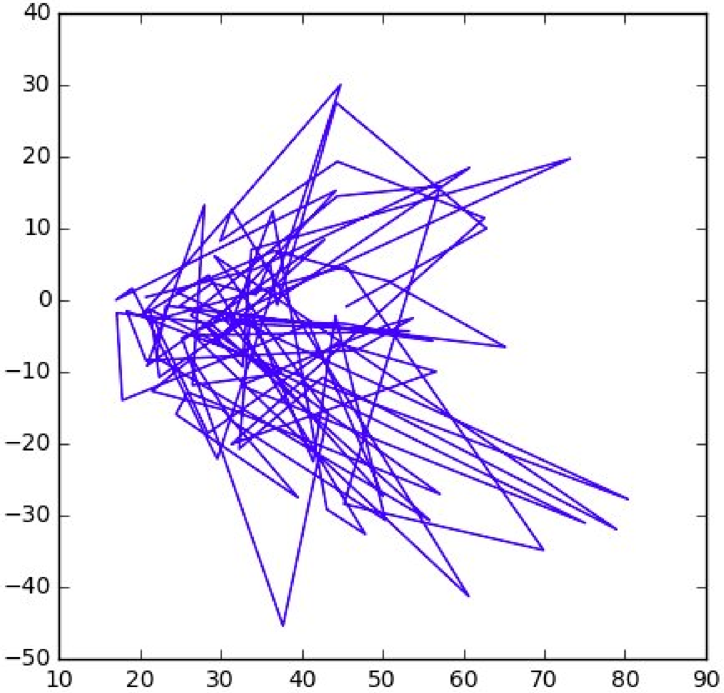


"Great plot.
Now need to find the theory that explains it"
Deville (2017) http://twitter.com



Preliminary Results: Numerical Optimization

Problem : $\boldsymbol{x}^\star \in \text{argmin}\{f(\boldsymbol{x});\ \boldsymbol{x} \in \mathbb{R}^d\}$

Gradient descent : $\boldsymbol{x}_{k+1} = \boldsymbol{x}_k - \eta \nabla f(\boldsymbol{x}_k)$ starting from some $\boldsymbol{x}_0$

Problem : $\boldsymbol{x}^\star \in \text{argmin}\{f(\boldsymbol{x});\ \boldsymbol{x} \in \mathcal{X} \subset \mathbb{R}^d\}$

Projected descent : $\boldsymbol{x}_{k+1} = \Pi_{\mathcal{X}}\big(\boldsymbol{x}_k - \eta \nabla f(\boldsymbol{x}_k)\big)$ starting from some $\boldsymbol{x}_0$

A constrained problem is said to be convex if

$$\begin{cases} \min\{f(\boldsymbol{x})\} & \text{with } f \text{ convex} \\ \text{s.t. } g_i(\boldsymbol{x}) = 0,\ \forall i = 1, \cdots, n & \text{with } g_i \text{ linear} \\ \qquad h_i(\boldsymbol{x}) \leq 0,\ \forall i = 1, \cdots, m & \text{with } h_i \text{ convex} \end{cases}$$

Lagrangian : $\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f(\boldsymbol{x}) + \sum_{i=1}^n \lambda_i g_i(\boldsymbol{x}) + \sum_{i=1}^m \mu_i h_i(\boldsymbol{x})$ where $\boldsymbol{x}$ are primal variables and $(\boldsymbol{\lambda}, \boldsymbol{\mu})$ are dual variables.

Remark $\mathcal{L}$ is an affine function in $(\boldsymbol{\lambda}, \boldsymbol{\mu})$

Preliminary Results: Numerical Optimization

Karush–Kuhn–Tucker conditions : a convex problem has a solution $\boldsymbol{x}^\star$ if and only if there are $(\boldsymbol{\lambda}^\star, \boldsymbol{\mu}^\star)$ such that the following condition hold

- stationarity : $\nabla_{\boldsymbol{x}}\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = \boldsymbol{0}$ at $(\boldsymbol{x}^\star, \boldsymbol{\lambda}^\star, \boldsymbol{\mu}^\star)$
- primal admissibility : $g_i(\boldsymbol{x}^\star) = 0$ and $h_i(\boldsymbol{x}^\star) \leq 0$, $\forall i$
- dual admissibility : $\boldsymbol{\mu}^\star \geq 0$

Let L denote the associated dual function $L(\boldsymbol{\lambda}, \boldsymbol{\mu}) = \min_{\boldsymbol{x}}\{\mathcal{L}(\boldsymbol{x}, \boldsymbol{\lambda}, \boldsymbol{\mu})\}$

L is a convex function in $(\boldsymbol{\lambda}, \boldsymbol{\mu})$ and the dual problem is $\max_{\boldsymbol{\lambda},\boldsymbol{\mu}}\{L(\boldsymbol{\lambda}, \boldsymbol{\mu})\}$.

References

Motivation

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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.

Preambule

Assume that $y = m(\boldsymbol{x}) + \varepsilon$, where ε is some idosyncatic impredictible noise.

The error $\mathbb{E}[(y - m(\boldsymbol{x}))^2]$ is the sum of three terms

- variance of the estimator : $\mathbb{E}[(y - \widehat{m}(\boldsymbol{x}))^2]$
- bias^2 of the estimator : $[m(\boldsymbol{x}) - \widehat{m}(\boldsymbol{x})]^2$
- variance of the noise : $\mathbb{E}[(y - m(\boldsymbol{x}))^2]$

(the latter exists, even with a ‘perfect’ model).

Preambule

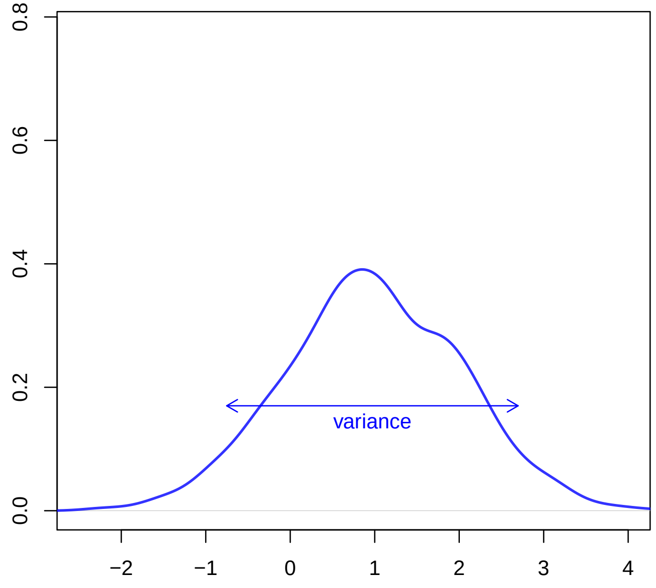
Consider a parametric model, with true (unkown) parameter θ, then

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

Let $\widetilde\theta$ denote an unbiased estimator of θ. Then

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

satisfies $\text{mse}(\hat\theta)\le\text{mse}(\widetilde\theta)$.



Bayes vs. Frequentist, inference on heads/tails

Consider some Bernoulli sample $\boldsymbol{x} = \{x_1, x_2, \cdots, x_n\}$, 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

$$\widehat{p} = \frac{1}{n}\sum_{i=1}^n x_i = \text{argman}\Big\{\underbrace{\prod_{i=1}^n f_X(x_i)}_{\mathcal{L}(p;\boldsymbol{x})}\Big\}$$

From the central limit theorem

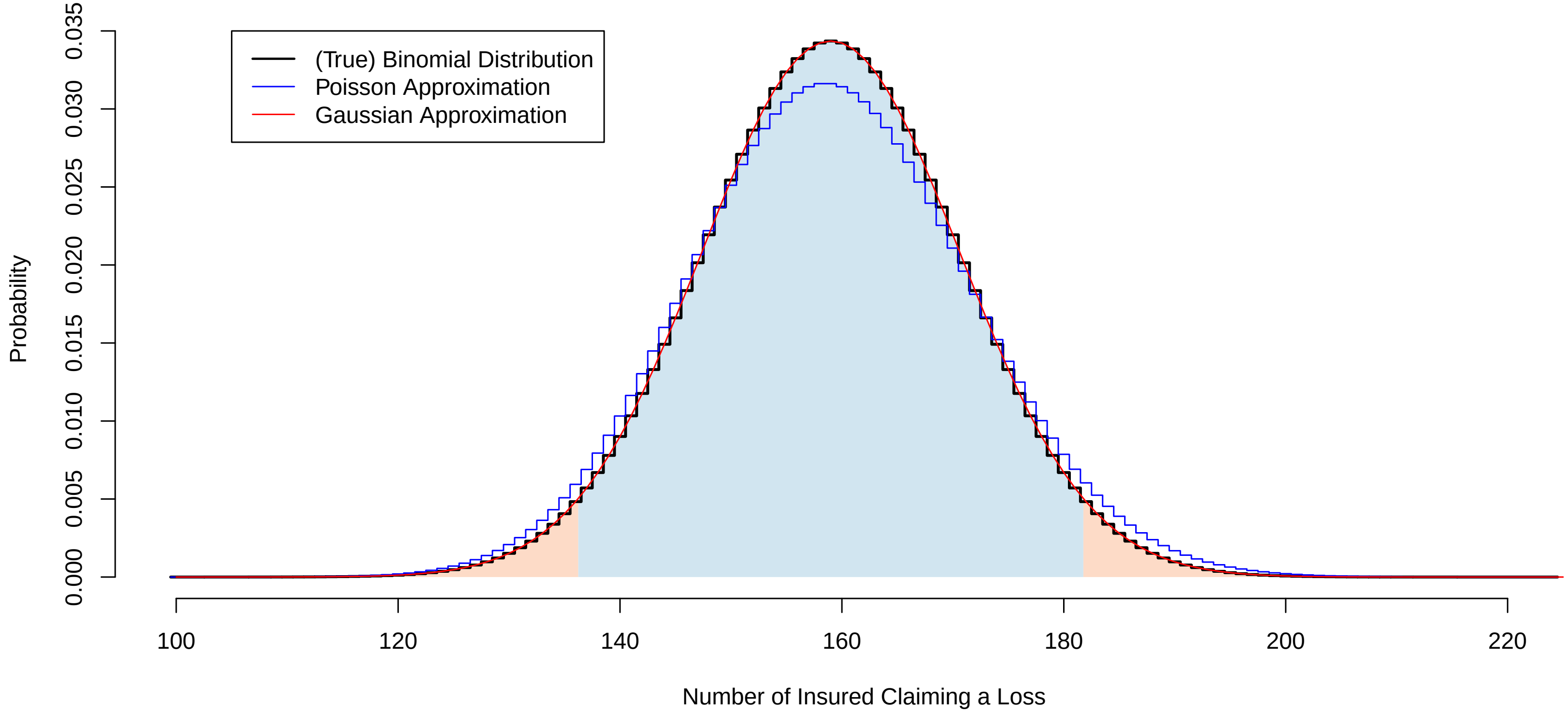
$$\sqrt{n}\frac{\widehat{p}-p}{\sqrt{p(1-p)}} \xrightarrow{\mathcal{L}} \mathcal{N}(0,1) \text{ as } n \to \infty$$

we can derive an approximated 95% confidence interval

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

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,

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

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

Bayes' Theorem,

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

Small Data and Black Swans

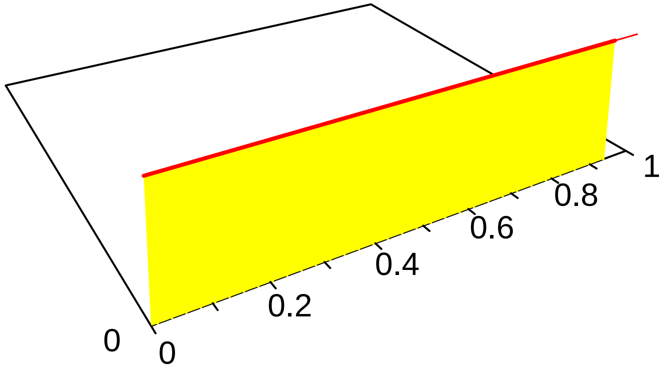
Consider sample $\boldsymbol{x}=\{0,0,0,0,0\}$.
Here the likelihood is

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

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

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

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



On Bayesian Philosophy, Confidence vs. Credibility

for frequentists, a probability is a measure of the 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)

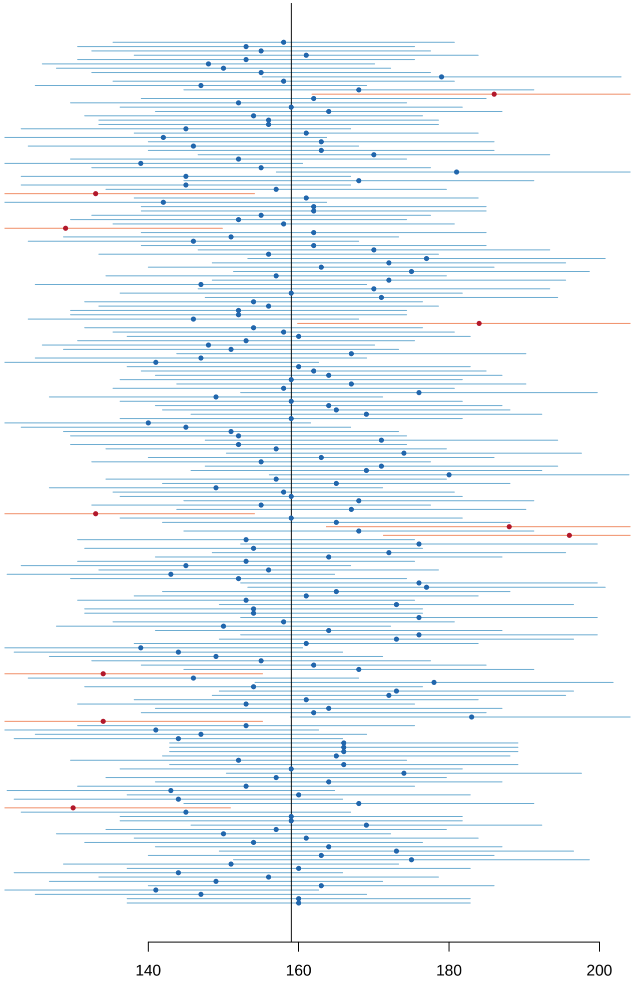
Example see Jaynes (1976), e.g. the truncated exponential

On Bayesian Philosophy, Confidence vs. Credibility

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

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

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

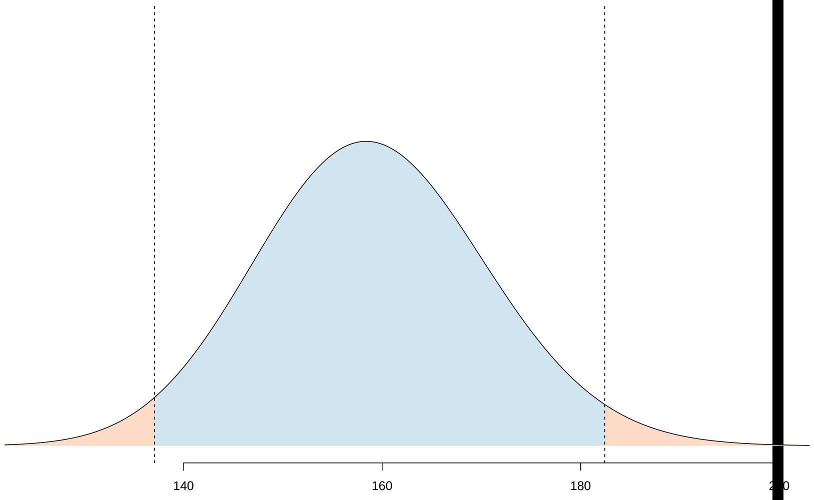


On Bayesian Philosophy, Confidence vs. Credibility

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

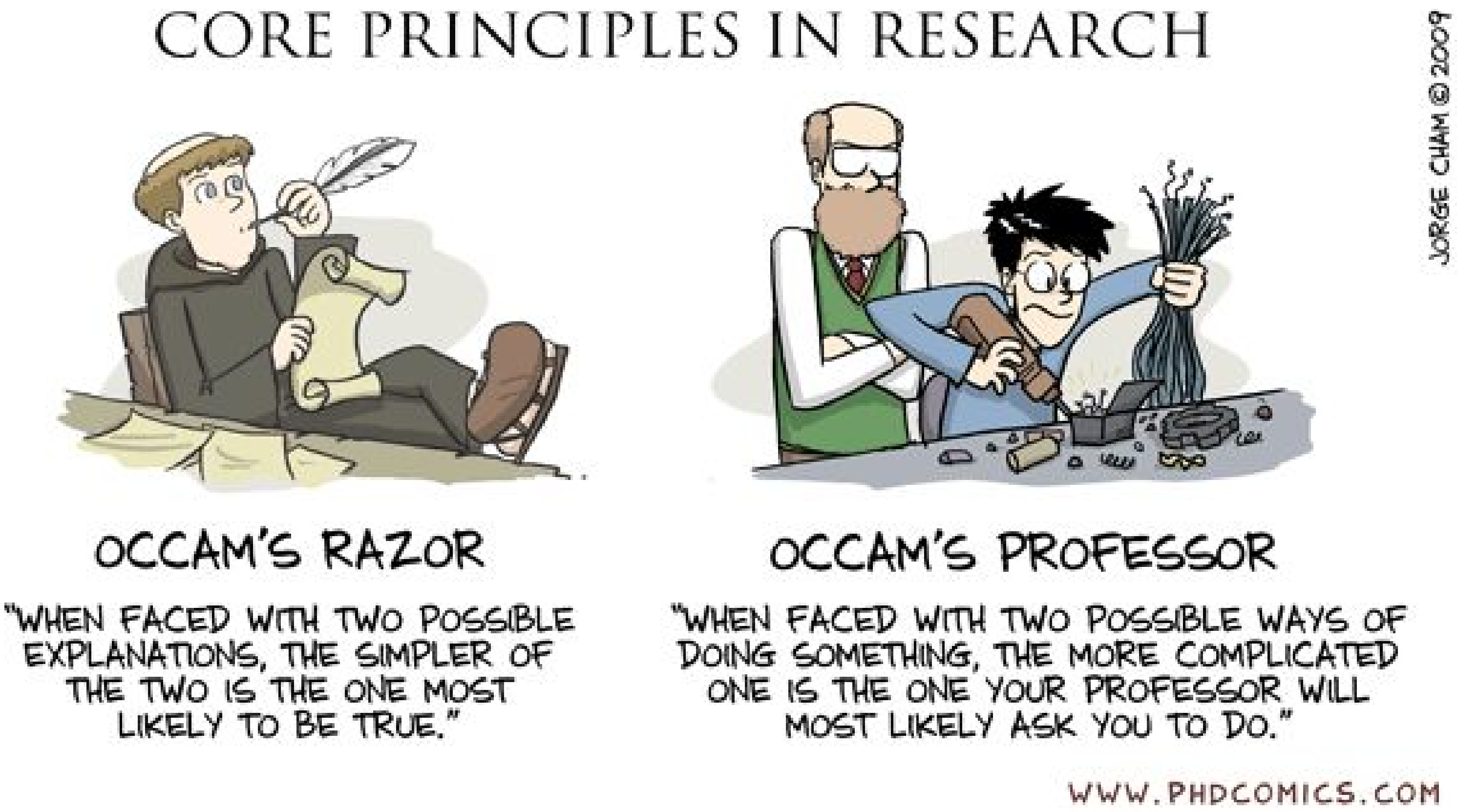
1. draw random parameters p_k with from the posterior distribution, $\pi(\cdot|\boldsymbol{x})$
2. sample sets $(\tilde{x}_1, \cdots, \tilde{x}_n)_k$ with $X_{i,k} \sim \mathcal{B}(p_k)$
3. compute for each set of values means $\overline{x}_k$
4. look at the proportion of those $\overline{x}_k$ that 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 $\overline{x}$ will fall within it it.



Occam's Razor

The “law of parsimony”, “*pluralitas non est ponenda sine necessitate*”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Penalize too complex models

James & Stein Estimator

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

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

From James & Stein (1961) Estimation with quadratic loss

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

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

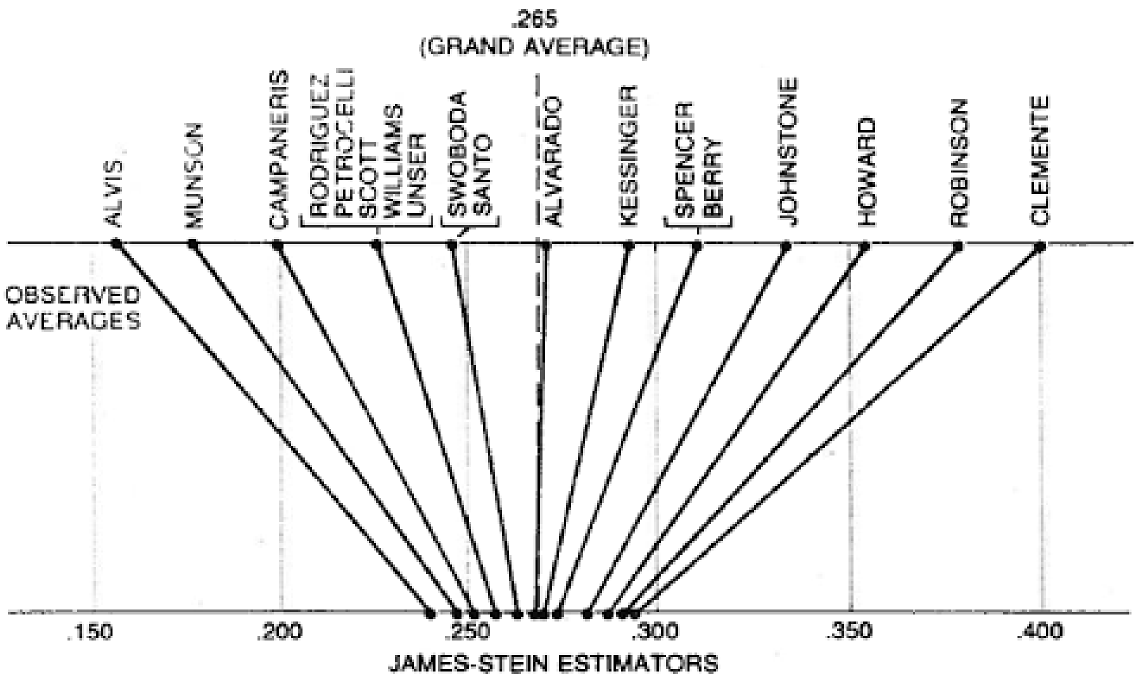
One can prove that if $d \geq 3$,

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

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

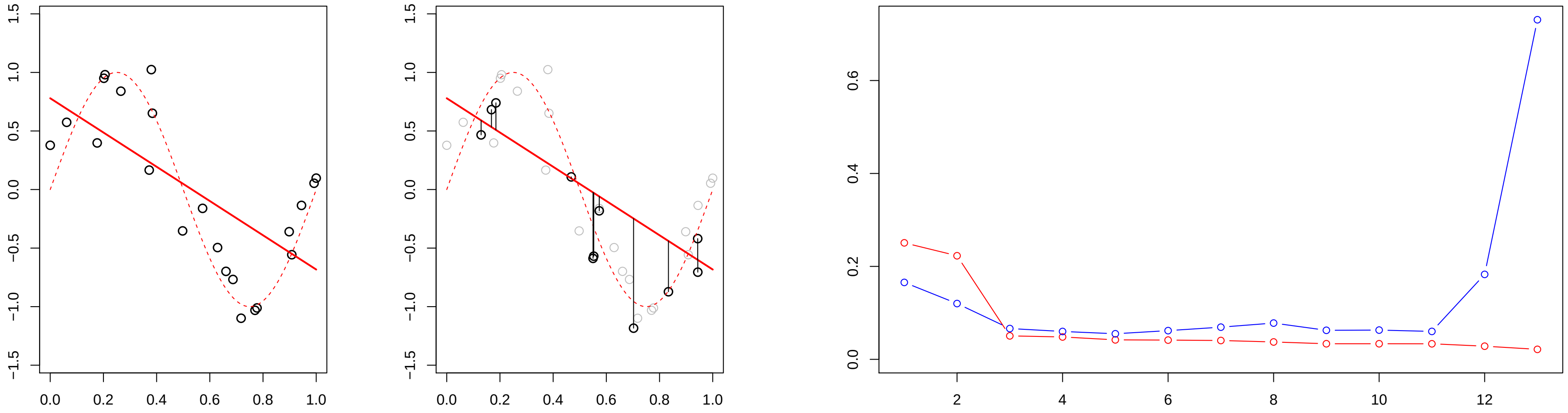
Heuristics : consider a biased estimator, to decrease the variance.



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 $\boldsymbol{z}_1, \cdots, \boldsymbol{z}_d$ such that

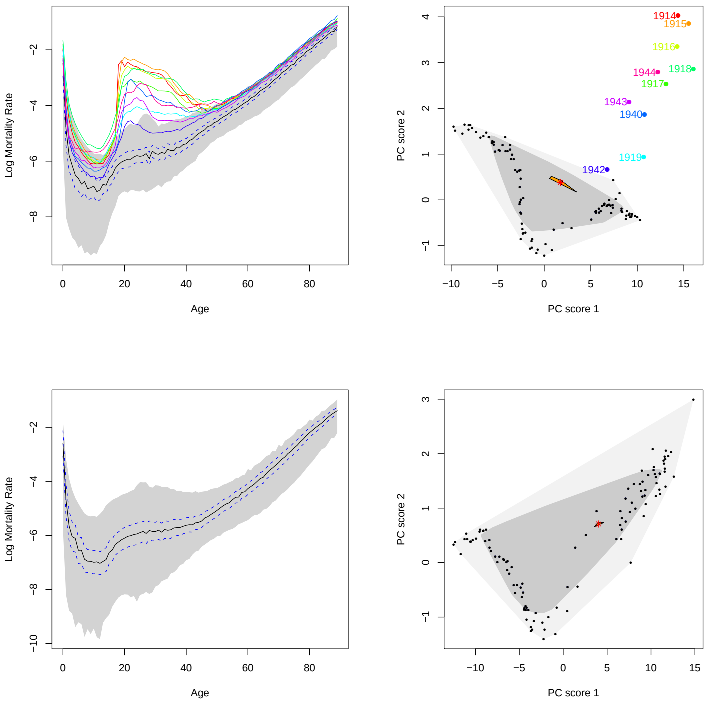
First Compoment is $\boldsymbol{z}_1 = \boldsymbol{X}\boldsymbol{\omega}_1$ where

$$\boldsymbol{\omega}_1 = \underset{\|\boldsymbol{\omega}\|=1}{\text{argmax}}\left\{\|\boldsymbol{X}\cdot\boldsymbol{\omega}\|^2\right\} = \underset{\|\boldsymbol{\omega}\|=1}{\text{argmax}}\left\{\boldsymbol{\omega}^\mathsf{T}\boldsymbol{X}^\mathsf{T}\boldsymbol{X}\boldsymbol{\omega}\right\}$$

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

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

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



Reducing Dimension with PCA

A regression on (the d) principal components, $y = \boldsymbol{z}^\mathsf{T}\boldsymbol{\beta} + \boldsymbol{\eta}$ could be an interesting idea, unfortunatley, principal components have no reason to be correlated with y. First compoment was $\boldsymbol{z}_1 = \boldsymbol{X}\boldsymbol{\omega}_1$ where

$$\boldsymbol{\omega}_1 = \underset{\|\boldsymbol{\omega}\|=1}{\text{argmax}}\left\{\|\boldsymbol{X}\cdot\boldsymbol{\omega}\|^2\right\} = \underset{\|\boldsymbol{\omega}\|=1}{\text{argmax}}\left\{\boldsymbol{\omega}^\mathsf{T}\boldsymbol{X}^\mathsf{T}\boldsymbol{X}\boldsymbol{\omega}\right\}$$

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 $\boldsymbol{z}_1 = \boldsymbol{X}\boldsymbol{\omega}_1$ where

$$\boldsymbol{\omega}_1 = \underset{\|\boldsymbol{\omega}\|=1}{\text{argmax}}\left\{\langle\boldsymbol{y},\boldsymbol{X}\cdot\boldsymbol{\omega}\rangle\right\} = \underset{\|\boldsymbol{\omega}\|=1}{\text{argmax}}\left\{\boldsymbol{\omega}^\mathsf{T}\boldsymbol{X}^\mathsf{T}\boldsymbol{y}\boldsymbol{y}^\mathsf{T}\boldsymbol{X}\boldsymbol{\omega}\right\}$$

Terminology

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

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

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

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

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

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

Such a model $m^\star$ is usually called oracle.

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

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

The empirical risk is

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

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

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

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

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. $\widehat{\boldsymbol{y}} = \widehat{m}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{y}$.

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

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

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

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

Observe that

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

while

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

Mallows Penalty and Model Complexity

One can obtain

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

If trace($\boldsymbol{A}$) ≥ 0 the empirical risk underestimate the true risk of the estimator.

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

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

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

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

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

continuous case :

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

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

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

Penalty and Likelihood

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

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

Thus

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

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

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

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

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

Observe that the criteria considered is

$$\text{criteria} = -\text{function}\big(\mathcal{L}(\widehat{\theta})\big) + \text{penality}\big(\text{complexity}\big)$$

Estimation of the Risk

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

The plug-in estimator of the empirical risk is

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

and then

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

Estimation of the Risk

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

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

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

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

Linear Regression Shortcoming

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

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

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

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

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

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

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

Linear Regression Shortcoming

Evolution of $(\beta_1,\beta_2)\mapsto\displaystyle\sum_{i=1}^n[y_i-(\beta_1x_{1,i}+\beta_2x_{2,i})]^2$

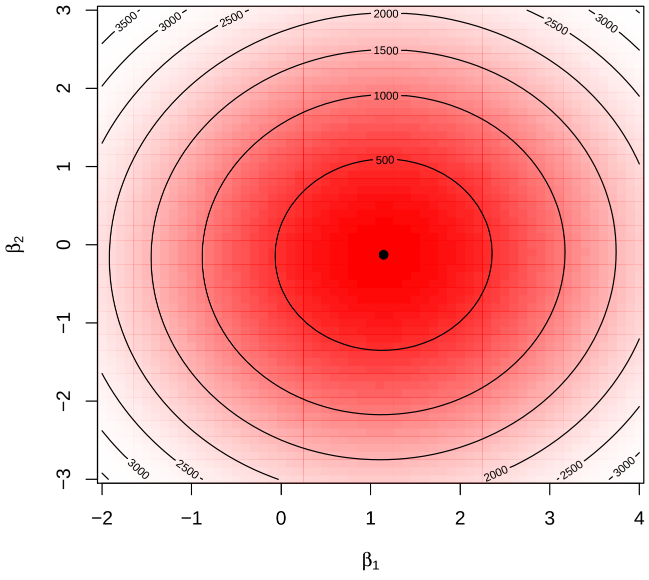
when $\text{cor}(X_1,X_2)=r\in[0,1]$, on top.

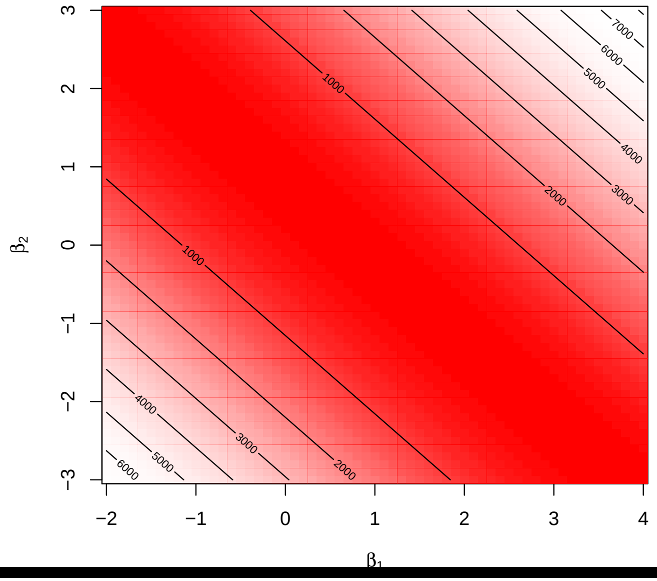
Below, Ridge regression

$$(\beta_1,\beta_2)\mapsto\sum_{i=1}^n[y_i-(\beta_1x_{1,i}+\beta_2x_{2,i})]^2+\lambda(\beta_1^2+\beta_2^2)$$

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

when $\text{cor}(X_1,X_2)\sim1$ (colinearity).

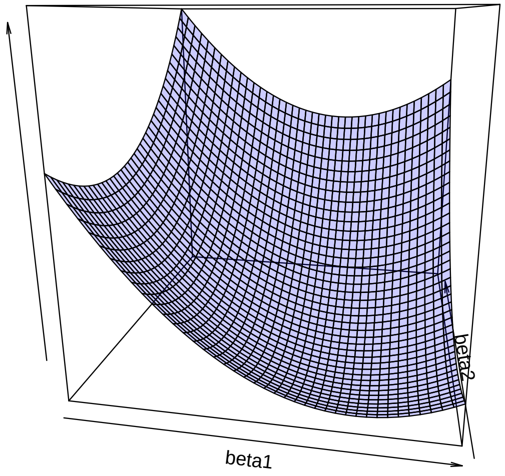


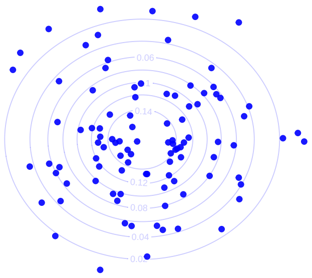


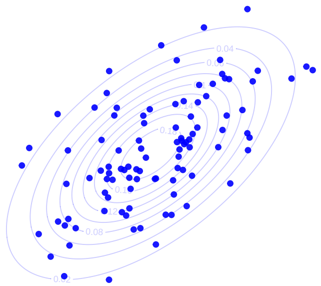
Normalization : Euclidean ℓ_2 vs. Mahalonobis

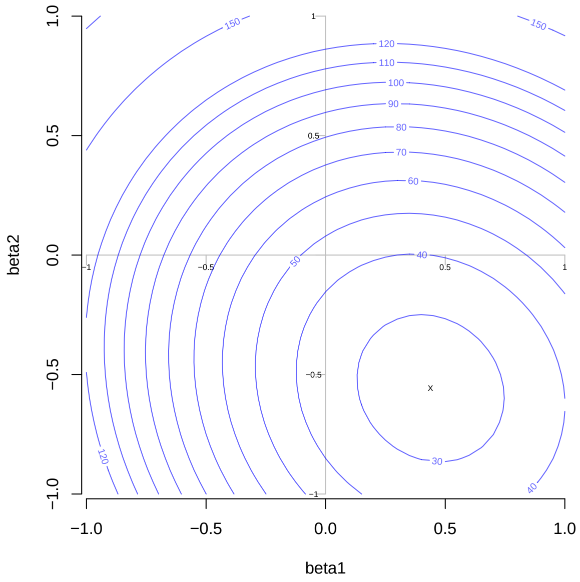
We want to penalize complicated models :

if β_k is "too small", we prefer to have $\beta_k = 0$.









Instead of $d(\boldsymbol{x},\boldsymbol{y}) = (\boldsymbol{x}-\boldsymbol{y})^\mathsf{T}(\boldsymbol{x}-\boldsymbol{y})$

use $d_{\boldsymbol{\Sigma}}(\boldsymbol{x},\boldsymbol{y}) = \sqrt{(\boldsymbol{x}-\boldsymbol{y})^\mathsf{T}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{y})}$

Ridge Regression

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

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

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

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

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

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

Ridge Regression

$$\widehat{\boldsymbol{\beta}}_\lambda^{\text{ridge}} = \text{argmin}\left\{\|\boldsymbol{y}-(\beta_0+\boldsymbol{X}\boldsymbol{\beta})\|_{\ell_2}^2+\lambda\|\boldsymbol{\beta}\|_{\ell_2}^2\right\}$$

can be seen as a constrained optimization problem

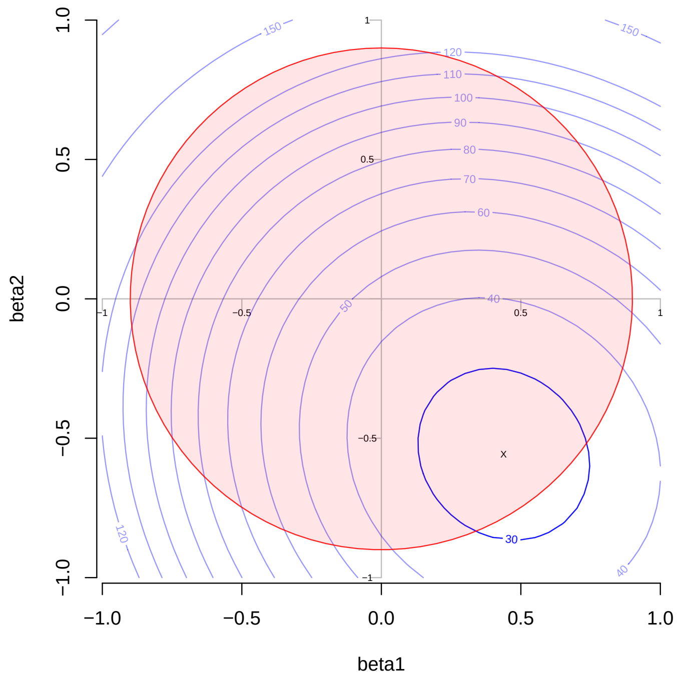
$$\widehat{\boldsymbol{\beta}}_\lambda^{\text{ridge}} = \underset{\|\boldsymbol{\beta}\|_{\ell_2}^2\leq h_\lambda}{\text{argmin}}\left\{\|\boldsymbol{y}-(\beta_0+\boldsymbol{X}\boldsymbol{\beta})\|_{\ell_2}^2\right\}$$

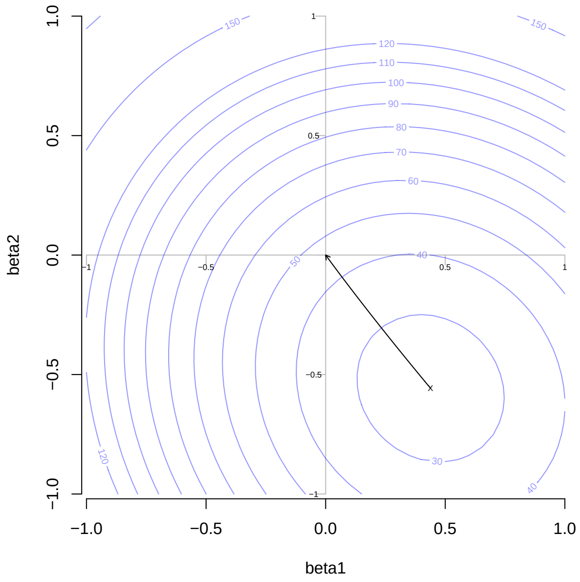
Explicit solution

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

If $\lambda\to 0$, $\widehat{\boldsymbol{\beta}}_0^{\text{ridge}} = \widehat{\boldsymbol{\beta}}^{\text{ols}}$

If $\lambda\to\infty$, $\widehat{\boldsymbol{\beta}}_\infty^{\text{ridge}} = \mathbf{0}$.





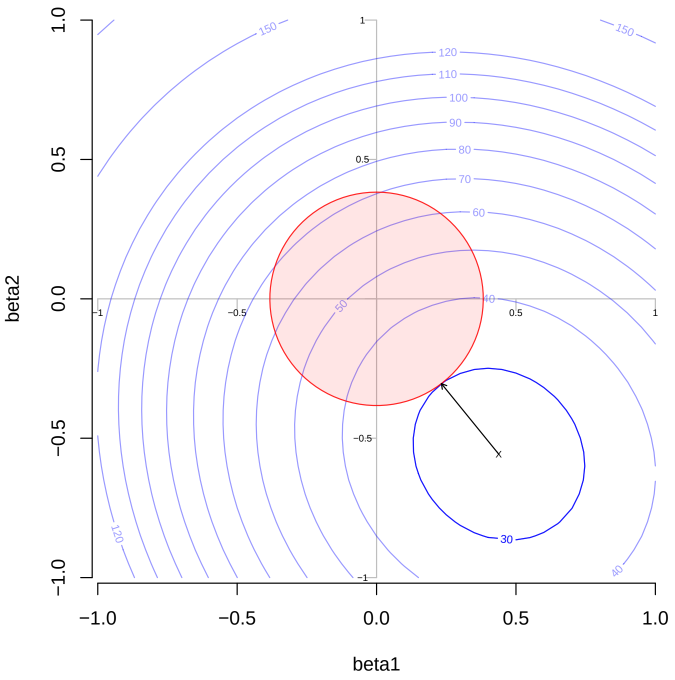
Ridge Regression

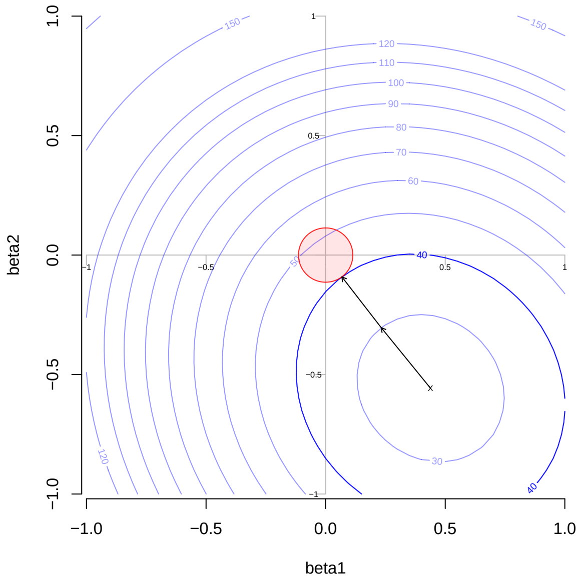
This penalty can be seen as rather unfair if components of $\boldsymbol{x}$ are not expressed on the same scale

- center: $\overline{\boldsymbol{x}}_j = 0$, then $\widehat{\beta}_0 = \overline{\boldsymbol{y}}$
- scale: $\boldsymbol{x}_j^\mathsf{T}\boldsymbol{x}_j = 1$

Then compute

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





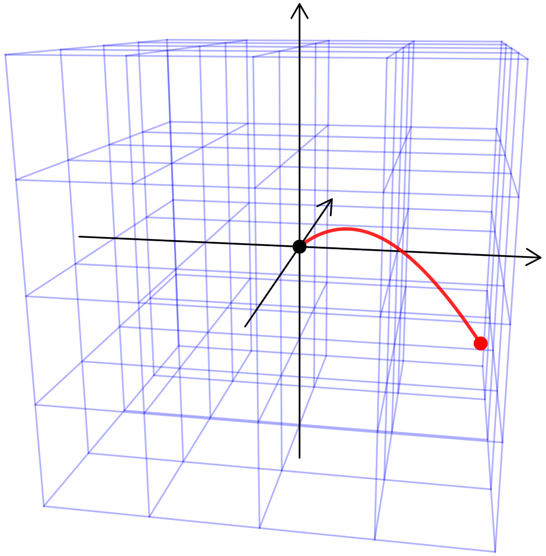
Ridge Regression

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

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

which explain relationship with shrinkage.

But generally, it is not the case...



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

Ridge Regression

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

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

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

where $\boldsymbol{X}^\mathsf{T}\boldsymbol{X}$ is a semi-positive definite matrix, and $\lambda\mathbb{I}$ is a positive definite matrix, and

$$\widehat{\boldsymbol{\beta}}_\lambda = (\boldsymbol{X}^\mathsf{T}\boldsymbol{X} + \lambda\mathbb{I})^{-1}\boldsymbol{X}^\mathsf{T}\boldsymbol{y}$$

The Bayesian Interpretation

From a Bayesian perspective,

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

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

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

Properties of the Ridge Estimator

$$\widehat{\boldsymbol{\beta}}_\lambda = (\boldsymbol{X}^\mathsf{T}\boldsymbol{X} + \lambda\mathbb{I})^{-1}\boldsymbol{X}^\mathsf{T}\boldsymbol{y}$$

$$\mathbb{E}[\widehat{\boldsymbol{\beta}}_\lambda] = \boldsymbol{X}^\mathsf{T}\boldsymbol{X}(\lambda\mathbb{I} + \boldsymbol{X}^\mathsf{T}\boldsymbol{X})^{-1}\boldsymbol{\beta}.$$

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

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

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

$$\widehat{\boldsymbol{\beta}}_\lambda = (1+\lambda)^{-1}\widehat{\boldsymbol{\beta}}^{\mathsf{ols}}.$$

Properties of the Ridge Estimator

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

$$\boldsymbol{W}_\lambda \widehat{\boldsymbol{\beta}}^{\mathsf{ols}} = \widehat{\boldsymbol{\beta}}_\lambda.$$

Thus,

$$\text{Var}[\widehat{\boldsymbol{\beta}}_\lambda] = \boldsymbol{W}_\lambda \text{Var}[\widehat{\boldsymbol{\beta}}^{\mathsf{ols}}]\boldsymbol{W}_\lambda^\mathsf{T}$$

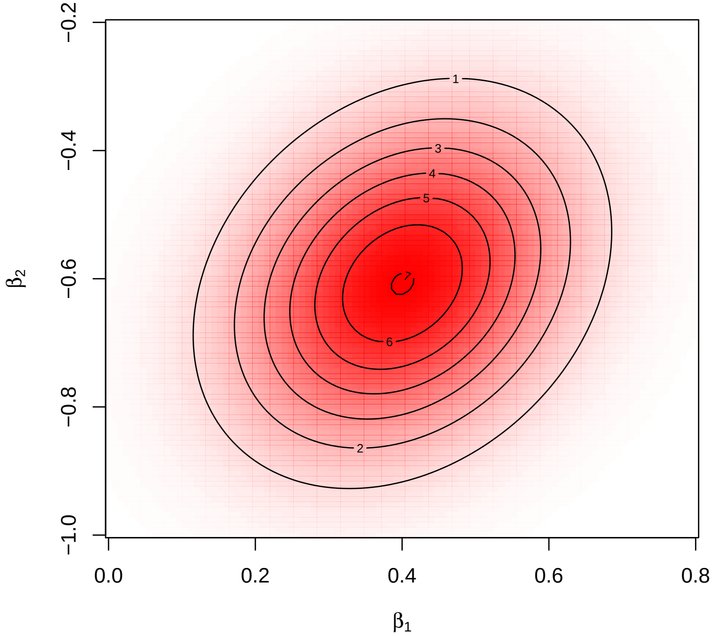
and

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

Observe that

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

Properties of the Ridge Estimator



Hence, the confidence ellipsoid of ridge estimator is indeed smaller than the OLS,
If $\boldsymbol{X}$ is an orthogonal design matrix,

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

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

If $\boldsymbol{X}$ is an orthogonal design matrix,

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

Properties of the Ridge Estimator

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

is minimal for

$$\lambda^\star = \frac{p\sigma^2}{\boldsymbol{\beta}^\mathsf{T}\boldsymbol{\beta}}$$

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

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 $A = \displaystyle\sum_{i=1}^{r} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^\top$ (called the dyadic decomposition of A).

Observe that it can be used to compute (e.g.) the Frobenius norm of A, $\|A\| = \sum a_{i,j}^2 = \sqrt{\sigma_1^2 + \cdots + \sigma_{\min\{m,n\}}^2}$.

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 $\boldsymbol{u}_i, \boldsymbol{v}_i$ are associated eigenvectors.

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

SVD decomposition

Consider the singular value decomposition of $\boldsymbol{X}$, $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^{\mathsf{T}}$.

Then

$$\widehat{\beta}^{\text{ols}} = \boldsymbol{V}\underbrace{\boldsymbol{D}^{-2}\boldsymbol{D}}\boldsymbol{U}^{\mathsf{T}}\boldsymbol{y}$$

$$\widehat{\beta}_{\lambda} = \boldsymbol{V}\underbrace{(\boldsymbol{D}^{2} + \lambda\mathbb{I})^{-1}\boldsymbol{D}}\boldsymbol{U}^{\mathsf{T}}\boldsymbol{y}$$

Observe that

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

hence, the ridge penality shrinks singular values.

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

$$\widehat{\beta}_{\lambda} = \boldsymbol{V}(\boldsymbol{R}^{\mathsf{T}}\boldsymbol{R} + \lambda\mathbb{I})^{-1}\boldsymbol{R}^{\mathsf{T}}\boldsymbol{y}$$

Hat matrix and Degrees of Freedom

Recall that $\widehat{\boldsymbol{Y}}=\boldsymbol{H}\boldsymbol{Y}$ with

$$\boldsymbol{H}=\boldsymbol{X}(\boldsymbol{X}^\mathsf{T}\boldsymbol{X})^{-1}\boldsymbol{X}^\mathsf{T}$$

Similarly

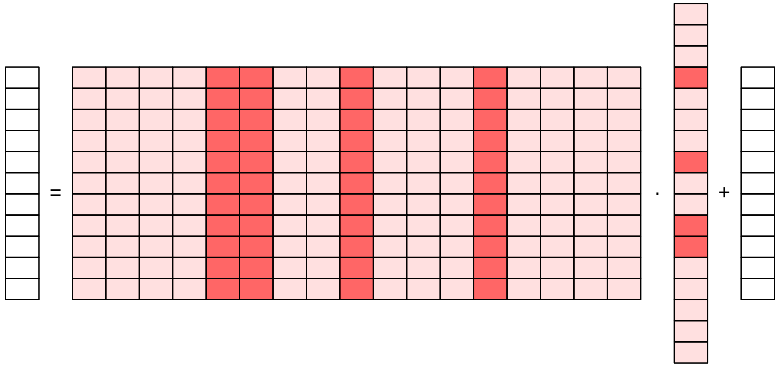
$$\boldsymbol{H}_\lambda=\boldsymbol{X}(\boldsymbol{X}^\mathsf{T}\boldsymbol{X}+\lambda\mathbb{I})^{-1}\boldsymbol{X}^\mathsf{T}$$

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

Sparsity Issues

In severall 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 relevent features, with $s << k$, 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 $y = \boldsymbol{X}_{\mathcal{S}}^{\top}\boldsymbol{\beta}_{\mathcal{S}} + \varepsilon$, where $\boldsymbol{X}_{\mathcal{S}}^{\top}\boldsymbol{X}_{\mathcal{S}}$ is a full rank matrix.

Going further on sparcity issues

The Ridge regression problem was to solve

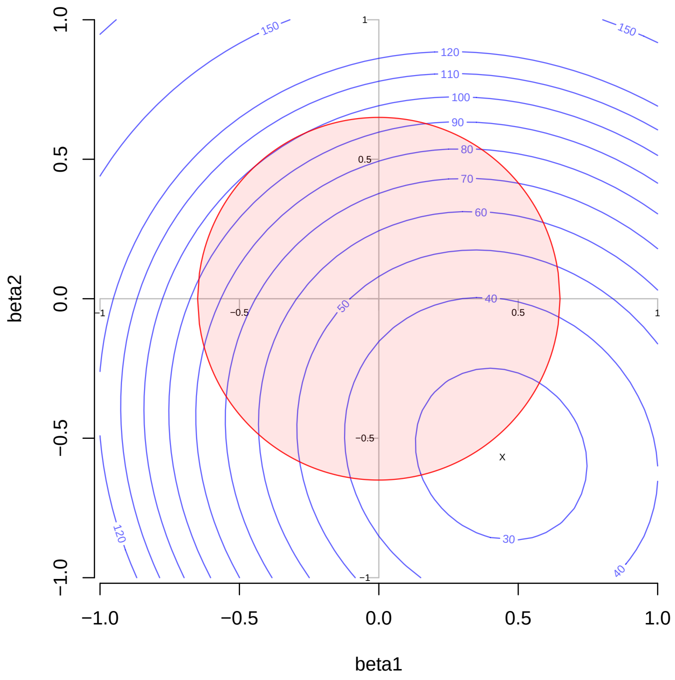
$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}\in\{\|\boldsymbol{\beta}\|_{\ell_2}\leq s\}}{\text{argmin}} \{\|\boldsymbol{Y}-\boldsymbol{X}^{\mathsf{T}}\boldsymbol{\beta}\|_{\ell_2}^2\}$$

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

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

We wish we could solve

$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}\in\{\|\boldsymbol{\beta}\|_{\ell_0}= s\}}{\text{argmin}} \{\|\boldsymbol{Y}-\boldsymbol{X}^{\mathsf{T}}\boldsymbol{\beta}\|_{\ell_2}^2\}$$



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

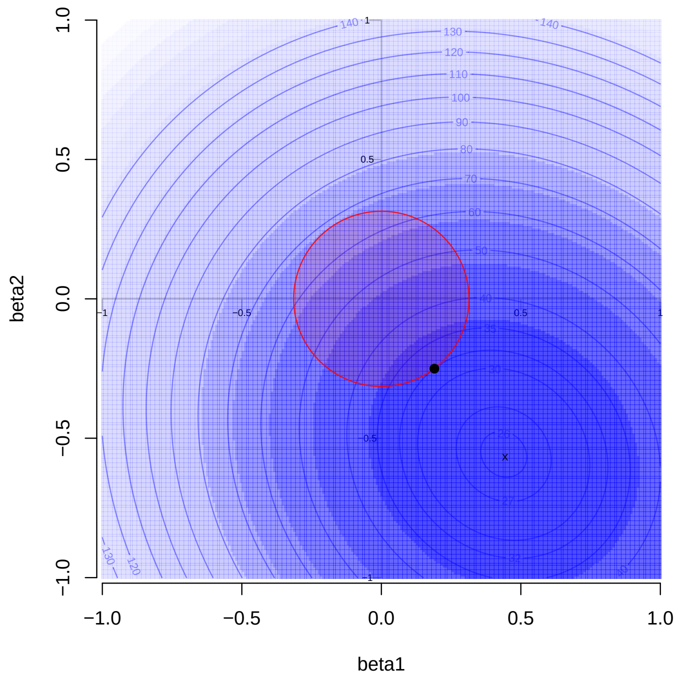
Going further on sparcity issues

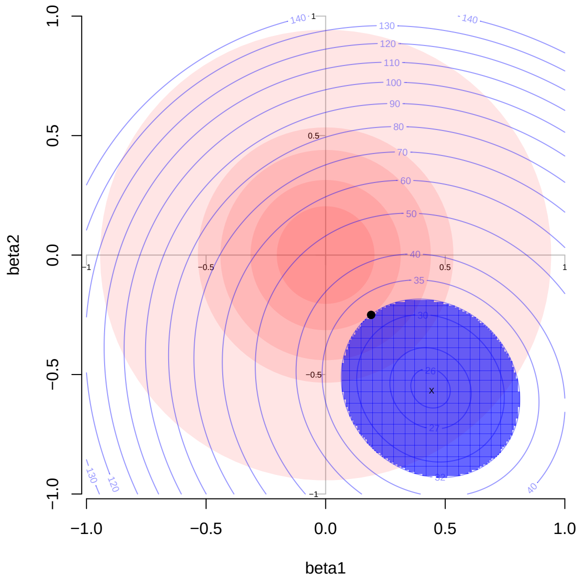
In a convex problem, solve the dual problem, e.g. in the Ridge regression : primal problem

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

and the dual problem

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



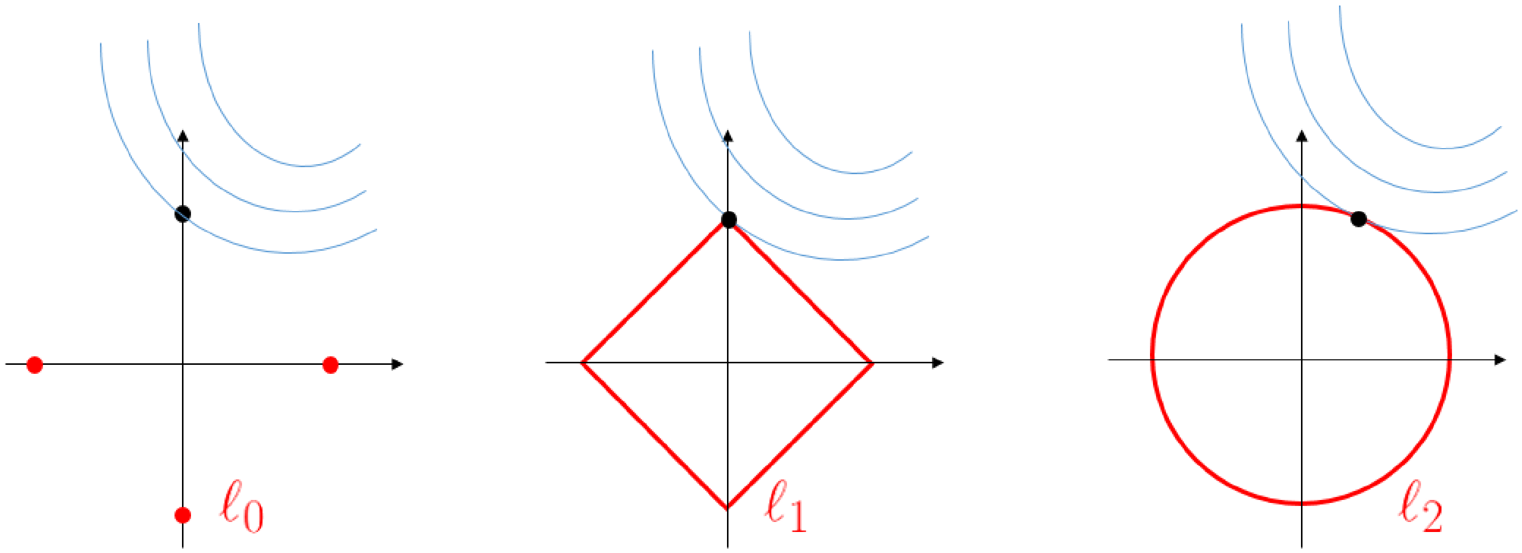


Going further on sparcity issues

Idea: solve the dual problem

$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta}\in\{\|\boldsymbol{Y}-\boldsymbol{X}^\top\boldsymbol{\beta}\|_{\ell_2}\leq h\}}{\text{argmin}} \{\|\boldsymbol{\beta}\|_{\ell_0}\}$$

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



Going further on sparcity issues

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

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

Hence, why not solve

$$\widehat{\boldsymbol{\beta}} = \underset{\boldsymbol{\beta};\|\boldsymbol{\beta}\|_{\ell_1}\leq\tilde{s}}{\text{argmin}}\,\{\|\boldsymbol{Y}-\boldsymbol{X}^{\mathsf{T}}\boldsymbol{\beta}\|_{\ell_2}\}$$

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

$$\widehat{\boldsymbol{\beta}} = \text{argmin}\{\|\boldsymbol{Y}-\boldsymbol{X}^{\mathsf{T}}\boldsymbol{\beta}\|_{\ell_2}^2+\lambda\|\boldsymbol{\beta}\|_{\ell_1}\}$$

LASSO *Least Absolute Shrinkage and Selection Operator*

$$\widehat{\boldsymbol{\beta}} \in \text{argmin}\{\|\boldsymbol{Y} - \boldsymbol{X}^\mathsf{T}\boldsymbol{\beta}\|_{\ell_2}^2 + \lambda\|\boldsymbol{\beta}\|_{\ell_1}\}$$

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

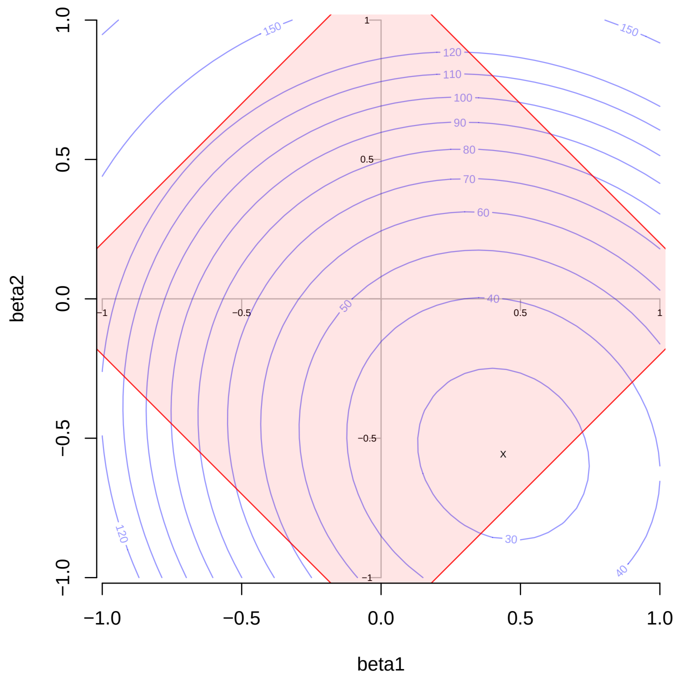
* MM, minimize majorization, coordinate descent Hunter & Lange (2003) A Tutorial on MM Algorithms.

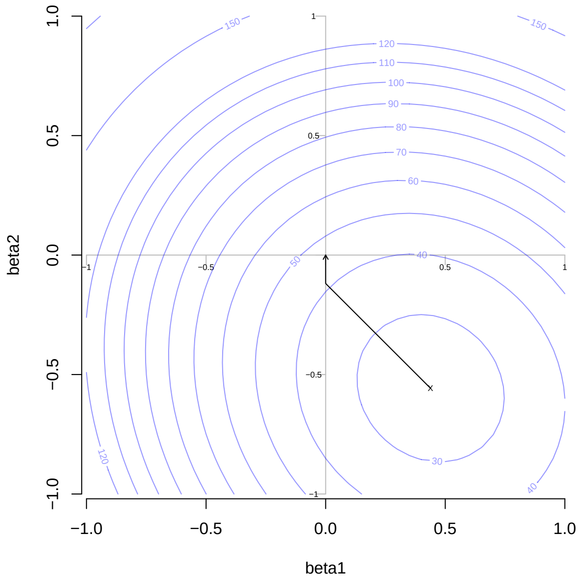
LASSO Regression

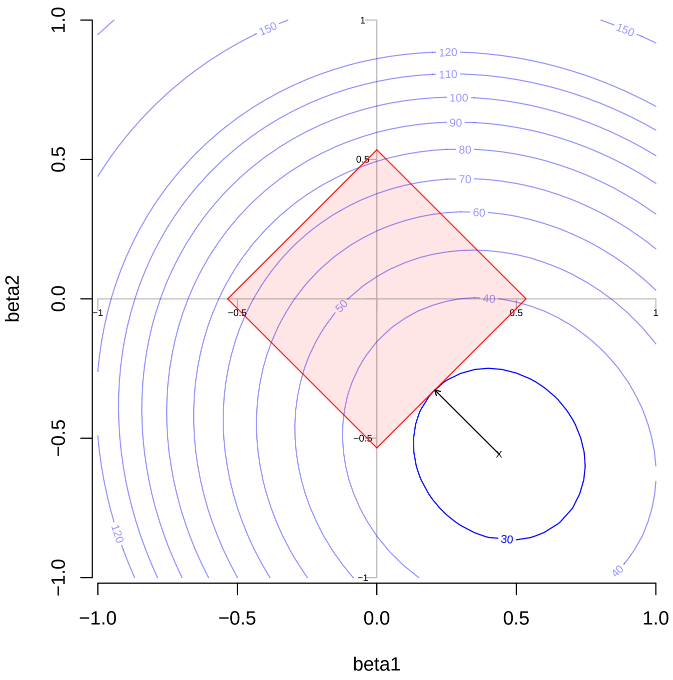
No explicit solution...

If $\lambda \to 0$, $\widehat{\boldsymbol{\beta}}_0^{\text{lasso}} = \widehat{\boldsymbol{\beta}}^{\text{ols}}$

If $\lambda \to \infty$, $\widehat{\boldsymbol{\beta}}_\infty^{\text{lasso}} = \mathbf{0}$.



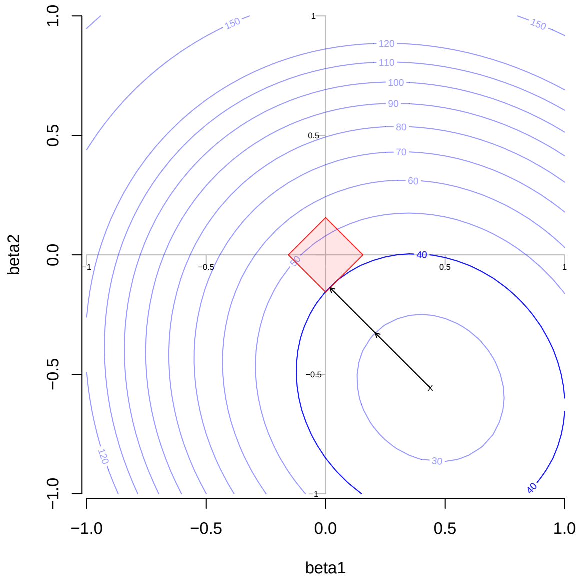




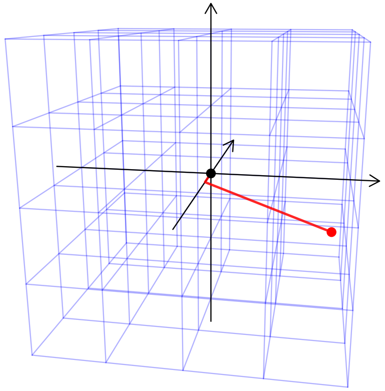
LASSO Regression

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

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



LASSO Regression



In the orthogonal case, $\boldsymbol{X}^\mathsf{T}\boldsymbol{X} = \mathbb{I}$,

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

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

Optimal LASSO Penalty

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

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

then compute the sum of the squared errors,

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

and finally solve

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

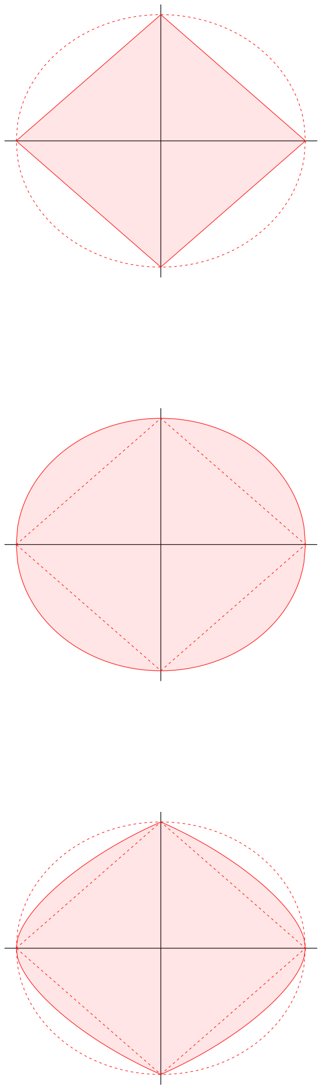
Note that this might overfit, so Hastie, Tibshiriani & Friedman (2009) Elements of Statistical Learning suggest the largest λ such that

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

LASSO and Ridge, with R

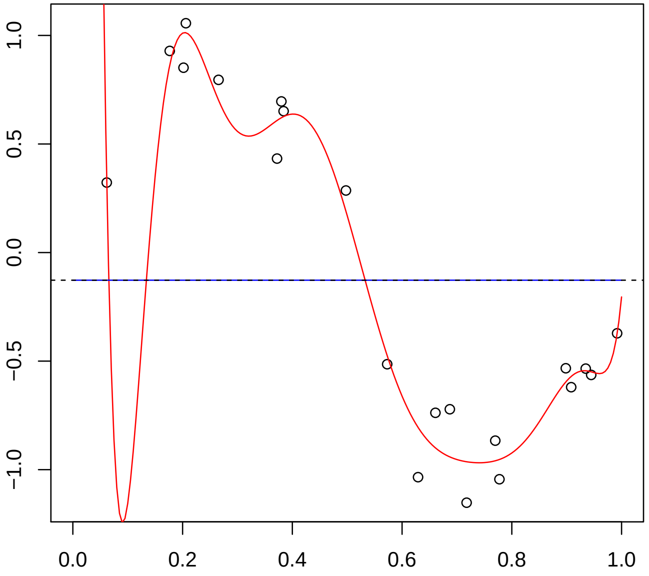
```
> library(glmnet)
> chicago=read.table("http://freakonometrics.free.fr/
    chicago.txt",header=TRUE,sep=";")
> standardize <-  function(x)  {(x-mean(x))/sd(x)}
> z0 <- standardize(chicago[, 1])
> z1 <- standardize(chicago[, 3])
> z2 <- standardize(chicago[, 4])
> ridge <-glmnet(cbind(z1, z2), z0,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

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



LASSO Regression, Smoothing and Overfit

LASSO can be used to avoid overfit.



Going further, ℓ_0, ℓ_1 and ℓ_2 penalty

Define

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

constrained optimization	penalized optimization	
$\underset{\boldsymbol{\beta};\|\boldsymbol{\beta}\|_{\ell_0}\leq s}{\text{argmin}}\left\{\sum_{i=1}^{n}\ell(y_i,\beta_0+\boldsymbol{x}^\mathsf{T}\boldsymbol{\beta})\right\}$	$\underset{\boldsymbol{\beta},\lambda}{\text{argmin}}\left\{\sum_{i=1}^{n}\ell(y_i,\beta_0+\boldsymbol{x}^\mathsf{T}\boldsymbol{\beta})+\lambda\|\boldsymbol{\beta}\|_{\ell_0}\right\}$	$(\ell 0)$
$\underset{\boldsymbol{\beta};\|\boldsymbol{\beta}\|_{\ell_1}\leq s}{\text{argmin}}\left\{\sum_{i=1}^{n}\ell(y_i,\beta_0+\boldsymbol{x}^\mathsf{T}\boldsymbol{\beta})\right\}$	$\underset{\boldsymbol{\beta},\lambda}{\text{argmin}}\left\{\sum_{i=1}^{n}\ell(y_i,\beta_0+\boldsymbol{x}^\mathsf{T}\boldsymbol{\beta})+\lambda\|\boldsymbol{\beta}\|_{\ell_1}\right\}$	$(\ell 1)$
$\underset{\boldsymbol{\beta};\|\boldsymbol{\beta}\|_{\ell_2}\leq s}{\text{argmin}}\left\{\sum_{i=1}^{n}\ell(y_i,\beta_0+\boldsymbol{x}^\mathsf{T}\boldsymbol{\beta})\right\}$	$\underset{\boldsymbol{\beta},\lambda}{\text{argmin}}\left\{\sum_{i=1}^{n}\ell(y_i,\beta_0+\boldsymbol{x}^\mathsf{T}\boldsymbol{\beta})+\lambda\|\boldsymbol{\beta}\|_{\ell_2}\right\}$	$(\ell 2)$

Assume that ℓ is the quadratic norm.

Going further, ℓ_0, ℓ_1 and ℓ_2 penalty

The two problems (ℓ2) are equivalent : $\forall(\boldsymbol{\beta}^\star, s^\star)$ solution of the left problem, $\exists\lambda^\star$ such that $(\boldsymbol{\beta}^\star, \lambda^\star)$ is solution of the right problem. And conversely.

The two problems (ℓ1) are equivalent : $\forall(\boldsymbol{\beta}^\star, s^\star)$ solution of the left problem, $\exists\lambda^\star$ such that $(\boldsymbol{\beta}^\star, \lambda^\star)$ 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 (ℓ0) are not equivalent : if $(\boldsymbol{\beta}^\star, \lambda^\star)$ is solution of the right problem, $\exists s^\star$ such that $\boldsymbol{\beta}^\star$ 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 (ℓ0).

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

$$\mathbb{E}\big([\boldsymbol{x}^\mathsf{T}\widehat{\boldsymbol{\beta}} - \boldsymbol{x}^\mathsf{T}\boldsymbol{\beta}_0]^2\big) \leq \underbrace{\mathbb{E}\big([\boldsymbol{x}_{\mathcal{S}}{}^\mathsf{T}\widehat{\boldsymbol{\beta}}_{\mathcal{S}} - \boldsymbol{x}^\mathsf{T}\boldsymbol{\beta}_0]^2\big)}_{=\sigma^2\#\mathcal{S}} \cdot \big(4\log p + 2 + o(1)\big).$$

In that case

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

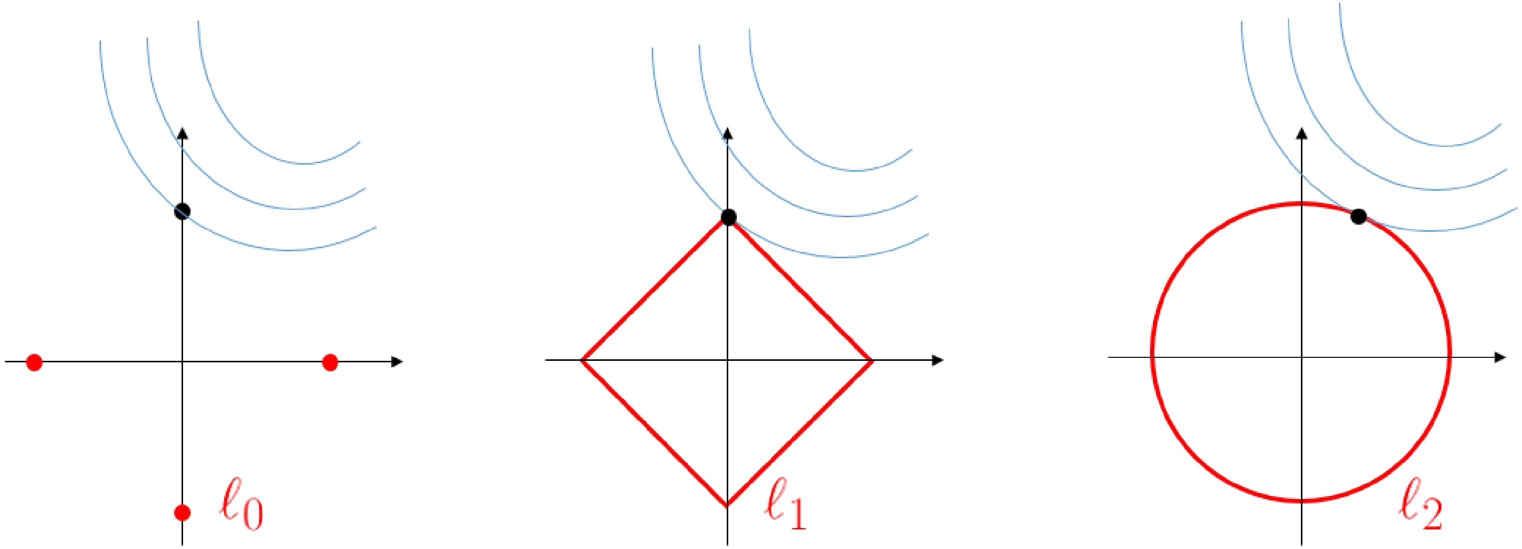
where $\mathcal{S}_\lambda(\boldsymbol{\beta})$ is the set of non-null values in solutions of (ℓ0).

If ℓ is no longer the quadratic norm but ℓ_1, problem ($\ell 1$) is not alway strictly convex, and optimum is not always unique (e.g. if $\boldsymbol{X}^\top\boldsymbol{X}$ is singular).

But in the quadratic case, ℓ is strictly convex, and at least $\boldsymbol{X}\widehat{\boldsymbol{\beta}}$ 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 ($\ell 1$) yields a corner-type solution, which can be seen as a "best subset" solution - like in ($\ell 0$).



Going further, ℓ_0, ℓ_1 and ℓ_2 penalty

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

$$\min\left\{\boldsymbol{y}^\mathsf{T}\boldsymbol{y} - 2\boldsymbol{y}^\mathsf{T}\boldsymbol{x}\beta + \beta\boldsymbol{x}^\mathsf{T}\boldsymbol{x}\beta + 2\lambda|\beta|\right\}$$

First order condition can be written

$$-2\boldsymbol{y}^\mathsf{T}\boldsymbol{x} + 2\boldsymbol{x}^\mathsf{T}\boldsymbol{x}\widehat{\beta}\pm 2\lambda = 0.$$

(the sign in ± being the sign of $\widehat{\beta}$). Assume that least-square estimate ($\lambda = 0$) is (strictely) positive, i.e. $\boldsymbol{y}^\mathsf{T}\boldsymbol{x} > 0$. If λ is not too large $\widehat{\beta}$ and $\widehat{\beta}^{\mathsf{ols}}$ have the same sign, and

$$-2\boldsymbol{y}^\mathsf{T}\boldsymbol{x} + 2\boldsymbol{x}^\mathsf{T}\boldsymbol{x}\widehat{\beta} + 2\lambda = 0.$$

with solution $\widehat{\beta}_\lambda^{\mathsf{lasso}} = \dfrac{\boldsymbol{y}^\mathsf{T}\boldsymbol{x} - \lambda}{\boldsymbol{x}^\mathsf{T}\boldsymbol{x}}$.

Going further, ℓ_0, ℓ_1 and ℓ_2 penalty

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

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

$$-2\boldsymbol{y}^\mathsf{T}\boldsymbol{x} + 2\boldsymbol{x}^\mathsf{T}\boldsymbol{x}\widehat{\beta} - 2\lambda = 0.$$

and solution would be $\widehat{\beta}_\lambda^{\mathsf{lasso}} = \dfrac{\boldsymbol{y}^\mathsf{T}\boldsymbol{x} + \lambda}{\boldsymbol{x}^\mathsf{T}\boldsymbol{x}}$. But that solution is positive (we assumed that $\boldsymbol{y}^\mathsf{T}\boldsymbol{x} > 0$), to we should have $\widehat{\beta}_\lambda < 0$.

Thus, at some point $\widehat{\beta}_\lambda = 0$, 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 ℓ_1 minimization.,

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

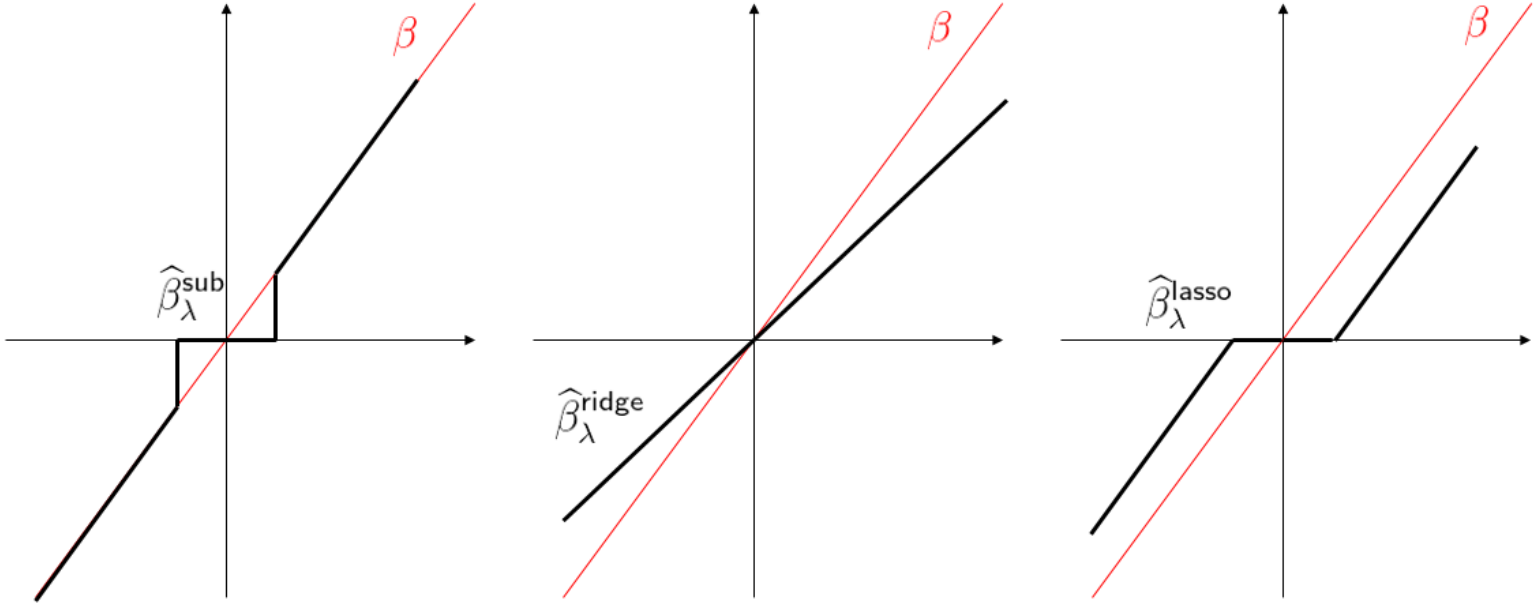
Thus, LASSO can be used for variable selection (see Hastie *et al.* (2001) The

Elements of Statistical Learning).

Generally, $\widehat{\beta}_\lambda^{\text{lasso}}$ 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

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



Optimization Heuristics

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

LASSO estimate can probably be derived from iterated Ridge estimates

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

which is a weighted ridge penalty function

Thus,

$$\boldsymbol{\beta}_{(k+1)} = \left(\boldsymbol{X}^\mathsf{T}\boldsymbol{X} + \lambda\boldsymbol{\Delta}_{(k)}\right)^{-1}\boldsymbol{X}^\mathsf{T}\boldsymbol{y}$$

where $\boldsymbol{\Delta}_{(k)} = \text{diag}[|\boldsymbol{\beta}_{j,(k)}|^{-1}]$. Then $\boldsymbol{\beta}_{(k)} \to \widehat{\boldsymbol{\beta}}^{\text{lasso}}$, as $k \to \infty$.

Properties of LASSO Estimate

From this iterative technique

$$\widehat{\boldsymbol{\beta}}_{\lambda}^{\mathsf{lasso}} \sim \left(\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}+\lambda\boldsymbol{\Delta}\right)^{-1}\boldsymbol{X}^{\mathsf{T}}\boldsymbol{y}$$

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

Thus,

$$\mathbb{E}[\widehat{\boldsymbol{\beta}}_{\lambda}^{\mathsf{lasso}}] \sim \left(\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}+\lambda\boldsymbol{\Delta}\right)^{-1}\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}\beta$$

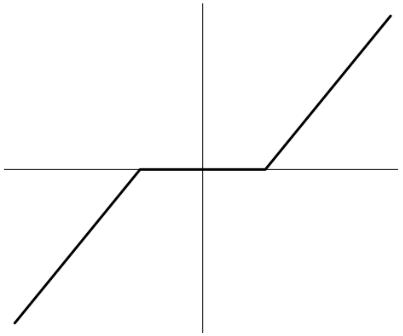
and

$$\text{Var}[\widehat{\boldsymbol{\beta}}_{\lambda}^{\mathsf{lasso}}] \sim \sigma^2\left(\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}+\lambda\boldsymbol{\Delta}\right)^{-1}\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}\left(\boldsymbol{X}^{\mathsf{T}}\boldsymbol{X}+\lambda\boldsymbol{\Delta}\right)^{-1}\boldsymbol{X}^{\mathsf{T}}$$

Optimization Heuristics

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

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



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

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

also called soft-thresholding operator.

Optimization Heuristics

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

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

Note that

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

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

Optimization Heuristics

We want to solve here

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

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

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

Optimization Heuristics

2. Add function g

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

And one can proof that

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

so called proximal gradient descent algorithm, since

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

Coordinate-wise minimization

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

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

$$f(x_1^\star,x_{i-1}^\star,x_i,x_{i+1}^\star,\cdots,x_k^\star)\geq f(x_1^\star,x_{i-1}^\star,x_i^\star,x_{i+1}^\star,\cdots,x_k^\star)$$

for all i. Is $\boldsymbol{x}^\star$ a global minimizer? i.e.

$$f(\boldsymbol{x})\geq f(\boldsymbol{x}^\star),\ \forall\boldsymbol{x}\in\mathbb{R}^k.$$

Yes. If f is convex and differentiable.

$$\nabla f(\boldsymbol{x})|_{\boldsymbol{x}=\boldsymbol{x}^\star}=\left(\frac{\partial f(\boldsymbol{x})}{\partial x_1},\cdots,\frac{\partial f(\boldsymbol{x})}{\partial x_k}\right)=\boldsymbol{0}$$

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

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

$$f(\boldsymbol{x})-f(\boldsymbol{x}^\star)\geq\nabla g(\boldsymbol{x}^\star)^{\mathsf{T}}(\boldsymbol{x}-\boldsymbol{x}^\star)+\sum_i[h_i(x_i)-h_i(x_i^\star)]$$

Coordinate-wise minimization

$$f(\boldsymbol{x}) - f(\boldsymbol{x}^\star) \geq \sum_i \underbrace{[\nabla_i g(\boldsymbol{x}^\star)^\mathsf{T}(x_i - x_i^\star) h_i(x_i) - h_i(x_i^\star)]}_{\geq 0} \geq 0$$

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

$$x_1^{(j)} \in \underset{x_1}{\text{argmin}} f(x_1, x_2^{(j-1)}, x_3^{(j-1)}, \cdots x_k^{(j-1)})$$

$$x_2^{(j)} \in \underset{x_2}{\text{argmin}} f(x_1^{(j)}, x_2, x_3^{(j-1)}, \cdots x_k^{(j-1)})$$

$$x_3^{(j)} \in \underset{x_3}{\text{argmin}} f(x_1^{(j)}, x_2^{(j)}, x_3, \cdots x_k^{(j-1)})$$

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

Application in Linear Regression

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

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

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

thus, the optimal value is here

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

Application to LASSO

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

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

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

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

$$x_i^\star = S_{\lambda/\|\boldsymbol{A}_i\|^2}\left(\frac{\boldsymbol{A}_i^\mathsf{T}[\boldsymbol{A}_{-i}\boldsymbol{x}_{-i} - \boldsymbol{y}]}{\boldsymbol{A}_i^\mathsf{T}\boldsymbol{A}_i}\right)$$

Convergence rate for LASSO

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

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

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

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

Lasso for Autoregressive Time Series

Consider some 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 $y = \boldsymbol{x}^{\mathsf{T}}\boldsymbol{\phi} + \varepsilon$.

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

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

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

See Nardi & Rinaldo (2011).

Graphical Lasso and Covariance Estimation

We want to estimate an (unknown) covariance matrix $\boldsymbol{\Sigma}$, or $\boldsymbol{\Sigma}^{-1}$.

An estimate for $\boldsymbol{\Sigma}^{-1}$ is $\boldsymbol{\Theta}^\star$ solution of

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

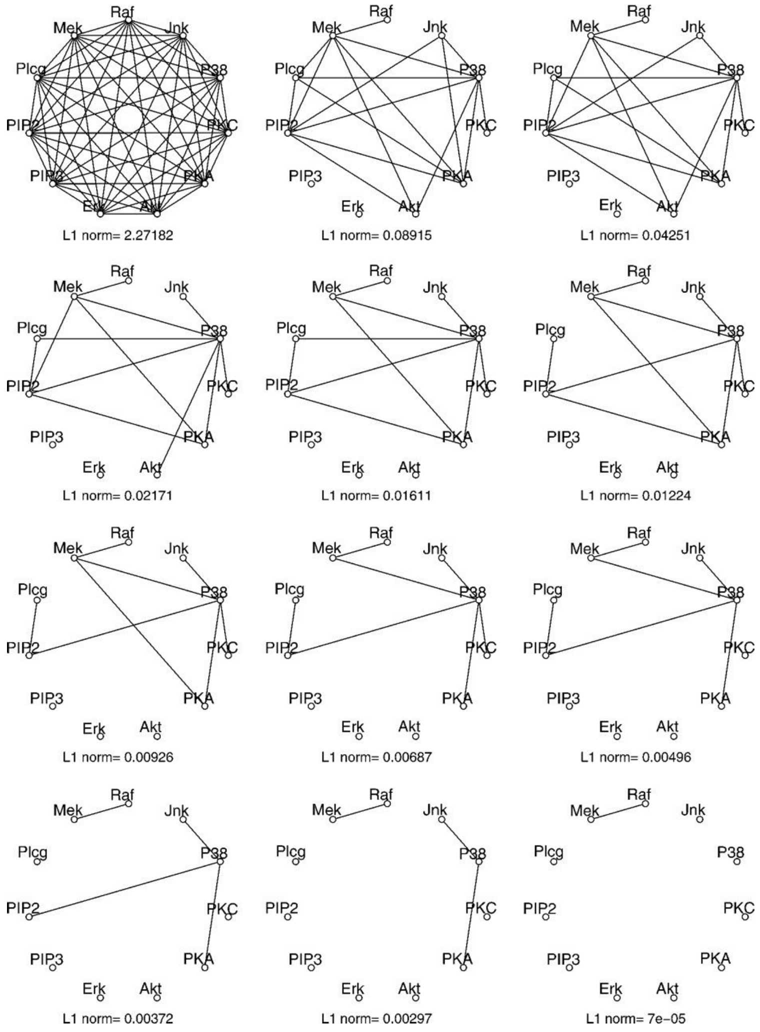
and where $\|\boldsymbol{\Theta}\|_{\ell_1} = \sum|\Theta_{i,j}|$.

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

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

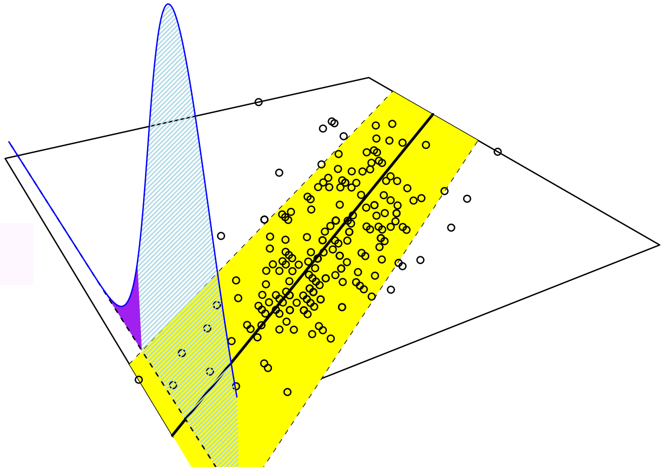
The quadratic loss function was related to the Gaussian case, but much more alternatives can be considered...

Linear models, nonlinear modes and GLMs

linear model

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

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

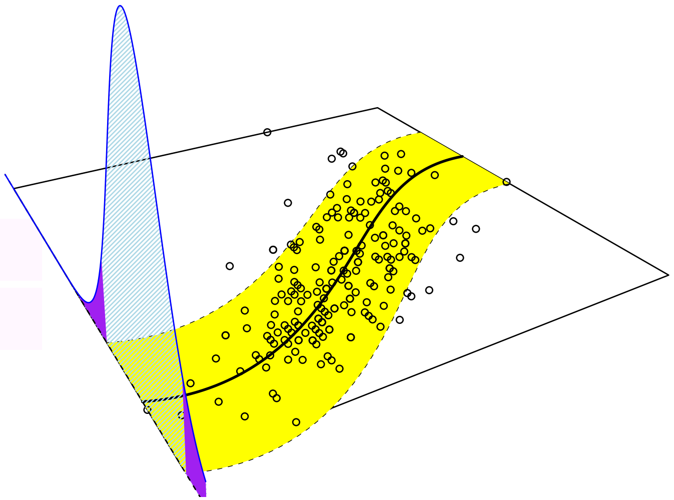


Linear models, nonlinear modes and GLMs

Nonlinear models

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

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

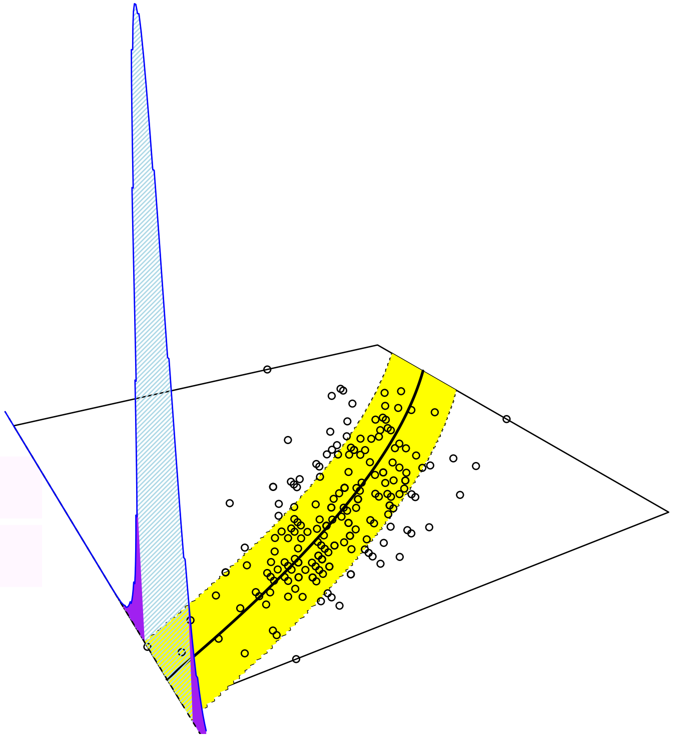


Linear models, nonlinear modes and GLMs

Generalized Linear Models

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

```
> fit <- glm(y ~ x, data = df,
+ 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 paramer.

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 $c(y,\varphi)=\log\begin{pmatrix}n\\y\end{pmatrix}$.

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

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

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

The Exponential Family

Example La loi 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 $\theta=-\dfrac{1}{\mu}$, $a(\varphi)=\varphi$, $b(\theta)=-\log(-\theta)$, $\varphi=\nu^{-1}$

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

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

Example In the Gaussian case, $\text{V}(\mu) = 1$, 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 $Y_1, Y_2, \dots, Y_n$ suchthat

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

so that the likelihood can be written

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

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...)