Méthodes d'optimisation pour le Machine Learning

2 – Le cas de la régression linéaire

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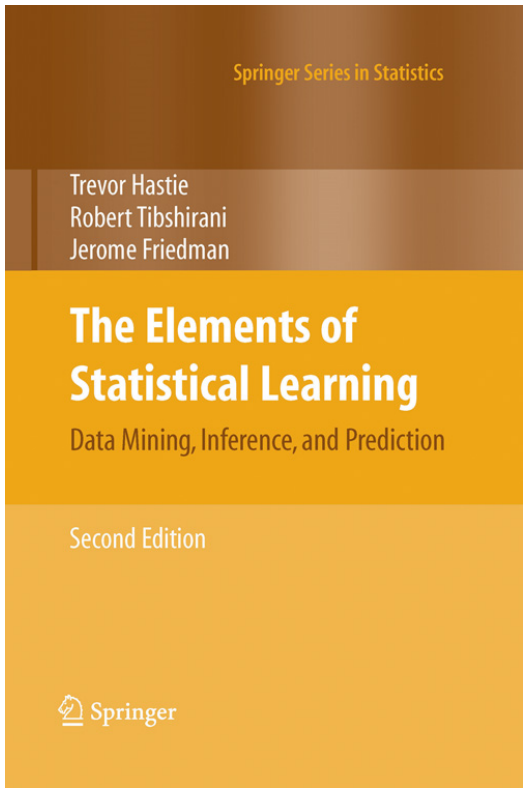

	AGE	SEX	BMI	BP	··· Serum Measurements ···						Response
Patient	x1	x2	x3	x4	x5	x6	x7	x8	x9	x10	y
1	59	2	32.1	101	157	93.2	38	4	4.9	87	151
2	48	1	21.6	87	183	103.2	70	3	3.9	69	75
3	72	2	30.5	93	156	93.6	41	4	4.7	85	141
4	24	1	25.3	84	198	131.4	40	5	4.9	89	206
5	50	1	23.0	101	192	125.4	52	4	4.3	80	135
6	23	1	22.6	89	139	64.8	61	2	4.2	68	97
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
441	36	1	30.0	95	201	125.2	42	5	5.1	85	220
442	36	1	19.6	71	250	133.2	97	3	4.6	92	57

Table 1. Diabetes study. 442 diabetes patients were measured on 10 baseline variables. prediction model was desired for the response variable, a measure of disease progression one yea after baseline.

$$\mathbb{E}(Y|X) = f(X) = \beta_0^\star + \beta_1^\star X_1 + \cdots + \beta_p^\star X_p = \beta_0^\star + \beta^\star X$$

- X the explanatory variables (independent variable or set of predictors)
- Y the response to be predicted (dependent variable)
- $\beta = (\beta_1, \ldots, \beta_p)^\top$ the parameters (unknown)
- β_0 the intercept (also unknown)
- p the number of variables of the model

More notations

$$\mathbb{E}(Y|X) = f(X) = \beta_0^\star + \sum_{j=1}^{p} \beta_j^\star X_j$$

- $\beta^\star$ the true parameters (the good)
- $\widehat{\beta}$ the estimated parameters (the bad)
- β the free parameter (the ugly)

$$\widehat{\beta} = \underset{\beta \in \mathbb{R}^p}{\arg\min}\, J(\beta, data)$$

The parameter estimation error (unknown)

$$\|\beta^\star - \widehat{\beta}\|^2$$

The prediction error (unknown)

$$\|Y - \widehat{\mathbf{y}}\|^2 \text{ with } \widehat{\mathbf{y}} = \widehat{\beta}_0 + \sum_{j=1}^{p} \widehat{\beta}_j X_j$$

Data: $N = 446$ and $p = 10 + 1$ (Diabetes)

$$X = \begin{pmatrix} age & sex & \dots & x_{p=10} \\ 59 & 2 & \dots & 87 \\ \vdots & \vdots & \dots & \vdots \\ 36 & 1 & \dots & 92 \end{pmatrix}; \mathbf{y} = \begin{pmatrix} diab. \\ 151 \\ \vdots \\ 57 \end{pmatrix}$$

	AGE	SEX	BMI	BP	··· Serum Measurements ···						Response
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Table 1. Diabetes study. 442 diabetes patients were measured on 10 baseline variables. prediction model was desired for the response variable, a measure of disease progression one yea after baseline.

The least squares estimation principle

Linear model

$$f(x) = \beta_0 + \sum_{j=1}^{p} \beta_j x_j$$

Minimize the residual sum-of-squares (RSS)

$$\widehat{\beta}^{\text{ls}} = \underset{\beta \in \mathbb{R}^p}{\arg\min}\, RSS(\beta, data)$$

$$\begin{aligned} RSS(\beta, data) &= \sum_{i=1}^{n} \big(y_i - f(x_i)\big)^2 \\ &= \sum_{i=1}^{n} \big(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\big)^2 \\ &= \|\mathbf{y} - \widehat{\mathbf{y}}\|^2 \qquad \text{with} \quad \hat{y}_i = f(x_i), i = 1, n \end{aligned}$$

The intercept as a parameter

X_1	X_2	X_3	...	X_10	Y
-0.6416	-0.3934	-0.7313	...	0.9820	0.5524
0.8415	2.1730	0.3442	...	1.6411	0.7336
0.6521	0.5006	3.4307	...	-0.5842	-1.6001
0.1848	-0.2535	0.3812	...	-0.8544	-0.3328
0.3635	0.5542	1.9298	...	0.6564	0.6291
0.5890	-0.2903	1.5685	...	-1.6603	-0.5648
0.5153	-0.4606	0.2263	...	1.6934	-1.0449
0.9598	1.2378	-2.0753	...	0.5395	-0.4543
1.9332	2.2013	-0.2789	...	0.2030	-1.4092
-0.0956	-2.0578	-0.9055	...	-2.3387	1.0096
0.5377	2.7694	1.4090	...	-0.3034	0.3252
1.8339	-1.3499	1.4172	...	0.2939	-0.7549
-2.2588	3.0349	0.6715	...	-0.7873	1.3703
0.8622	0.7254	-1.2075	...	0.8884	-1.7115
0.3188	-0.0631	0.7172	...	-1.1471	-0.1022
-1.3077	0.7147	1.6302	...	-1.0689	-0.2414
-0.4336	-0.2050	0.4889	...	-0.8095	0.3192
0.3426	-0.1241	1.0347	...	-2.9443	0.3129
3.5784	1.4897	0.7269	...	1.4384	-0.8649

$$\begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1j} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2j} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{i1} & x_{i2} & \cdots & x_{ij} & \cdots & x_{ip} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nj} & \cdots & x_{np} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_i \\ \vdots \\ y_n \end{pmatrix}$$

$$p = 10, \qquad n = 19$$

beware

$$X = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1j} & \cdots & x_{1p} \\ 1 & x_{21} & x_{22} & \cdots & x_{2j} & \cdots & x_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{i1} & x_{i2} & \cdots & x_{ij} & \cdots & x_{ip} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nj} & \cdots & x_{np} \end{pmatrix}$$

n lines and $p + 1$ columns

$$\widehat{\mathbf{y}} = X\beta$$

Intercept elimination through preprocessing

$$Y = \beta_0 + \sum_{j=1}^{p} \beta_j x_j + \varepsilon$$

The normalized input variable is $\widetilde{x_j} = \frac{x_j - \bar{x_j}}{\sigma_j}$ with $\bar{x_j} = \frac{1}{n}\sum_{i=1}^{n} x_{ij}$

$$\begin{aligned} f(x) &= \beta_0 + \sum_{j=1}^{p} \beta_j(\sigma_j \widetilde{x_j} + \bar{x_j}) \\ &= \widetilde{\beta}_0 + \sum_{j=1}^{p} \widetilde{\beta}_j \widetilde{x_j} \end{aligned}$$

with $\widetilde{\beta}_0 = \beta_0 + \sum_{j=1}^{p} \beta_j \bar{x_j}$ and $\widetilde{\beta}_j = \beta_j \sigma_j$

The least square estimate of $\widetilde{\beta}_0$ is $\widehat{\widetilde{\beta}}_0 = \bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$
so that, with $\widetilde{y} = y - \bar{y}$ the equivalent intercept free model is

$$\widetilde{y} = \sum_{j=1}^{p} \widetilde{\beta}_j \widetilde{x_j} + \varepsilon$$

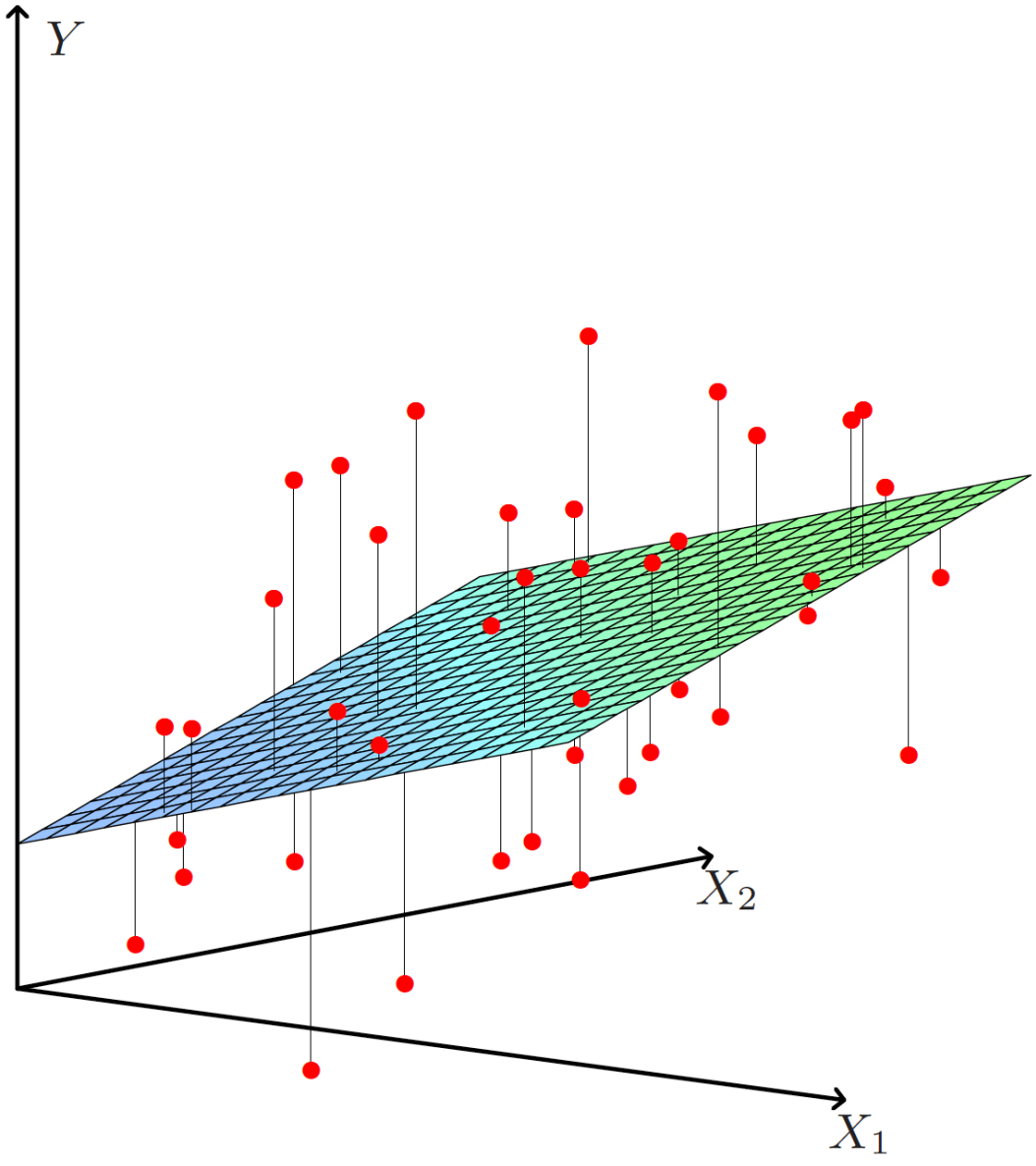


FIGURE 3.1. *Linear least squares fitting with* $X \in \mathbb{R}^2$. *We seek the linear function of* X *that minimizes the sum of squared residuals from* Y.

How do we minimize the residual sum-of-squares

The cost

$$\begin{aligned} RSS(\beta, data) &= \|\mathbf{y} - X\beta\|^2 \\ &= (\mathbf{y} - X\beta)^\top(\mathbf{y} - X\beta) \\ &= \mathbf{y}^\top\mathbf{y} - 2\beta^\top X^\top\mathbf{y} + \beta^\top X^\top X\beta \end{aligned}$$

The gradient

$$\nabla_\beta RSS(\beta, data) = -2X^\top\mathbf{y} + 2X^\top X\beta$$

The Hessian

$$\nabla^2_\beta RSS(\beta, data) = 2X^\top X$$

The Fermat's rule

$$\widehat{\beta}^{\text{ls}} = \underset{\beta\in\mathbb{R}^{p+1}}{\arg\min}\, RSS(\beta, data) \quad \Leftrightarrow \quad \nabla_\beta RSS(\widehat{\beta}^{\text{ls}}, data) = 0$$

The unique solution

$$\widehat{\beta}^{\text{ls}} = (X^\top X)^{-1}X^\top\mathbf{y}$$

The least square estimator

$(X^\top X)^{-1}$ must exist
Optimality as orthogonality

$$\nabla_\beta RSS(\widehat{\beta}^{\text{ls}}, data) = 0 \quad \Leftrightarrow \quad X^\top(\mathbf{y} - X\widehat{\beta}^{\text{ls}}) = 0$$

$$\widehat{\mathbf{y}} = X\widehat{\beta}^{\text{ls}} = X(X^\top X)^{-1}X^\top \mathbf{y} = H\mathbf{y}$$

with H the hat matrix (also called projector of influence matrix)

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

Statistical analysis of $\widehat{\beta}^{\text{ls}}$

the x_j are fixed (non random).

$$Y = \beta_0^\star + \sum_{j=1}^{p} \beta_j^\star x_j + \varepsilon = X\beta^\star + \varepsilon$$

Gaussian and uncorrelated error assumption $\varepsilon \sim \mathcal{N}(0, \sigma^2)$

$$\widehat{\beta}^{\text{ls}} = (X^\top X)^{-1} X^\top Y$$

$$\begin{aligned}
\mathbb{E}(\widehat{\beta}^{\text{ls}}) &= (X^\top X)^{-1} X^\top \mathbb{E}(Y) \\
&= (X^\top X)^{-1} X^\top X\beta^\star + \mathbb{E}(\varepsilon) = \beta^\star \\
V(\widehat{\beta}^{\text{ls}}) &= (X^\top X)^{-1} X^\top V(Y) X (X^\top X)^{-1} \\
&= (X^\top X)^{-1} \sigma^2
\end{aligned}$$

$$\widehat{\beta}^{\text{ls}} \sim \mathcal{N}(\beta^\star, (X^\top X)^{-1}\sigma^2)$$

Variance unbiased estimates

$$\widehat{\sigma}^2 = \frac{1}{n-p-1} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2 \quad \sim \sigma^2 \chi^2_{n-p-1}$$

Z-score: how likely $\beta_j^\star = 0$

$$z_j = \frac{\widehat{\beta}_j^{\text{ls}}}{\widehat{\sigma}\sqrt{v_j}} \sim t_{n-p-1} \qquad \text{with} \qquad v_j \text{ the jth diagonal element of } (X^\top X)^{-1}$$

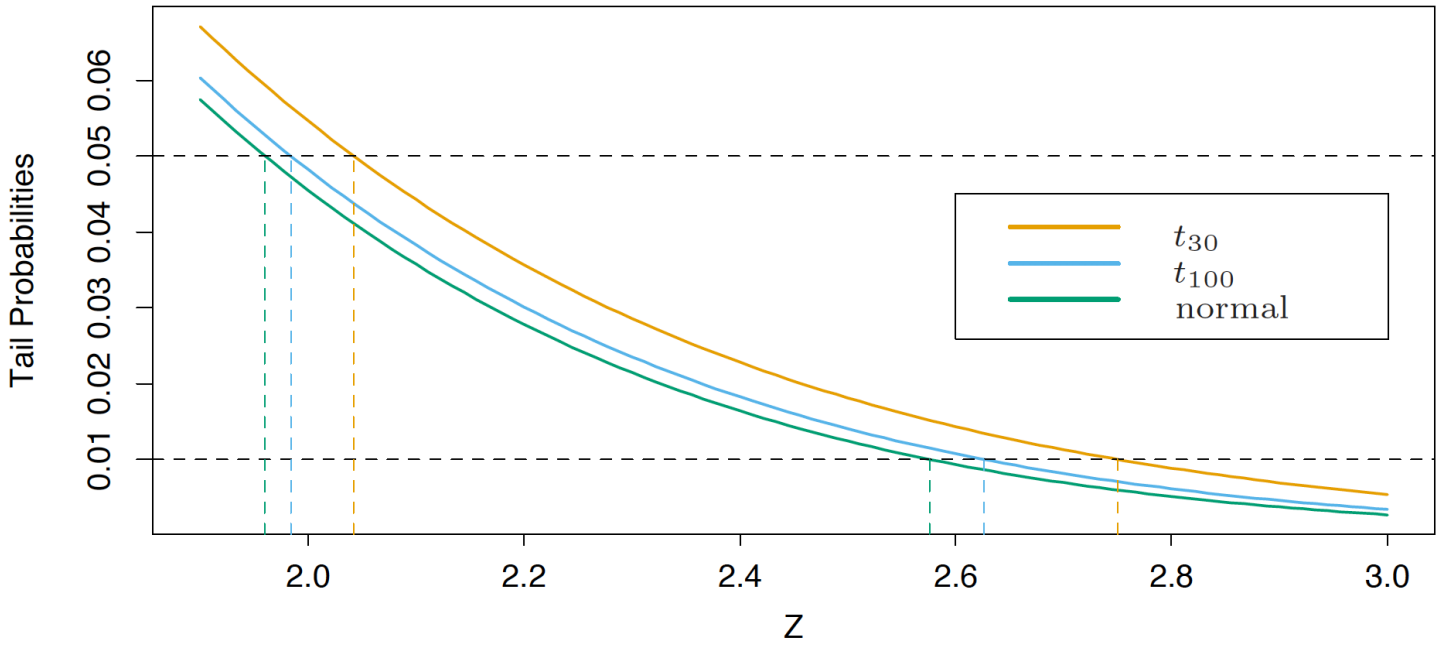


FIGURE 3.3. *The tail probabilities* $\Pr(|Z| > z)$ *for three distributions,* t_{30}, t_{100} *and standard normal. Shown are the appropriate quantiles for testing significance at the* $p = 0.05$ *and* 0.01 *levels. The difference between* t *and the standard normal becomes negligible for* N *bigger than about* 100.

Example: Prostate Cancer

TABLE 3.1. *Correlations of predictors in the prostate cancer data.*

	lcavol	lweight	age	lbph	svi	lcp	gleason
lweight	0.300						
age	0.286	0.317					
lbph	0.063	0.437	0.287				
svi	0.593	0.181	0.129	−0.139			
lcp	0.692	0.157	0.173	−0.089	0.671		
gleason	0.426	0.024	0.366	0.033	0.307	0.476	
pgg45	0.483	0.074	0.276	−0.030	0.481	0.663	0.757

TABLE 3.2. *Linear model fit to the prostate cancer data. The Z score is the coefficient divided by its standard error (3.12). Roughly a Z score larger than two in absolute value is significantly nonzero at the* $p = 0.05$ *level.*

Term	Coefficient	Std. Error	Z Score
Intercept	2.46	0.09	27.60
lcavol	0.68	0.13	5.37
lweight	0.26	0.10	2.75
age	−0.14	0.10	−1.40
lbph	0.21	0.10	2.06
svi	0.31	0.12	2.47
lcp	−0.29	0.15	−1.87
gleason	−0.02	0.15	−0.15
pgg45	0.27	0.15	1.74

Subset selection

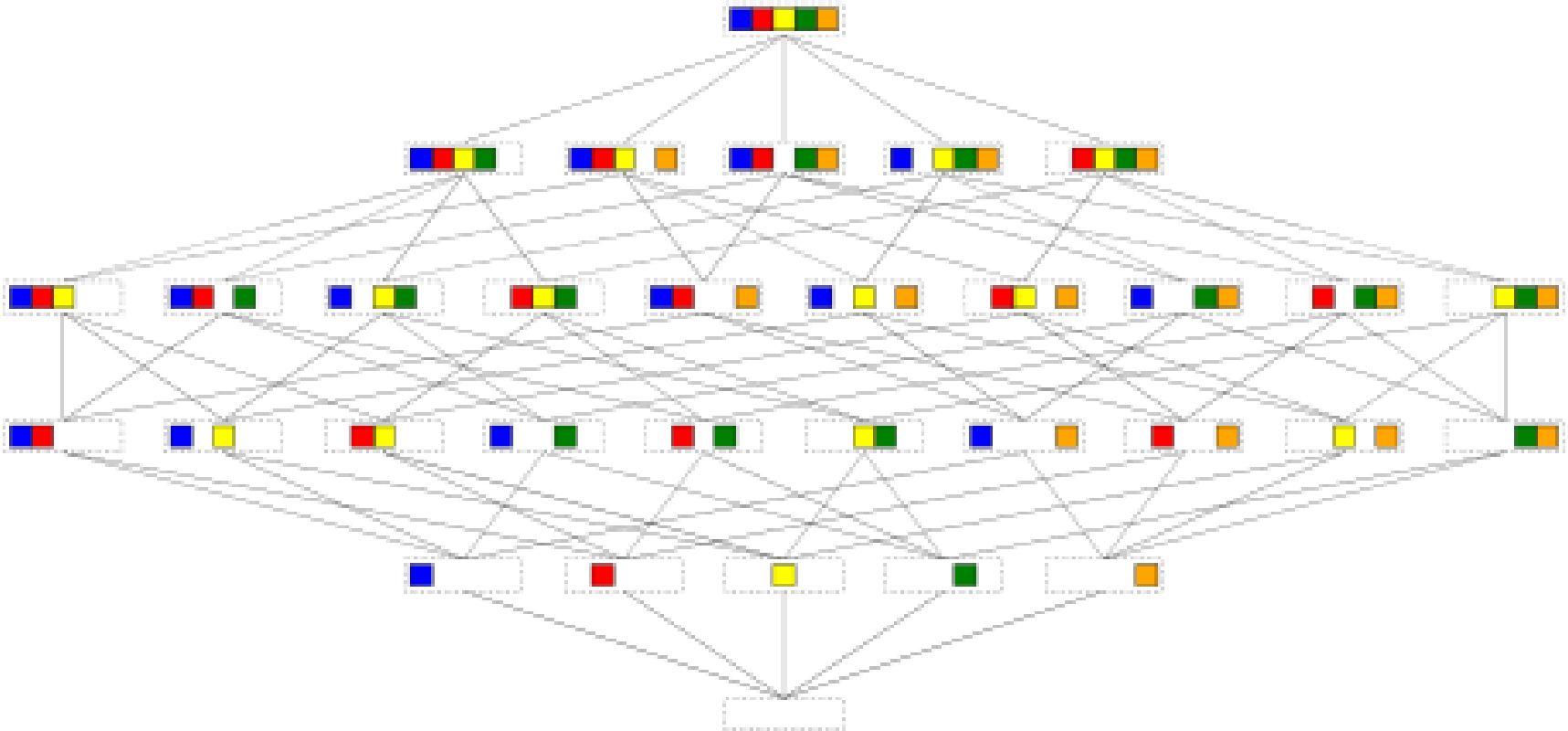
Why subset selection?

- prediction accuracy $\rightarrow$ remove spurious variables
- interpretation $\rightarrow$ reduce the number of variables

Different solutions

- exact solution: best subset minimizing $\|\beta\|_0$ as well
- greedy approaches
  - forward selection (stepwise)
  - backward selection (stepwise)
  - Forward-Stagewise Regression

The variable lattice



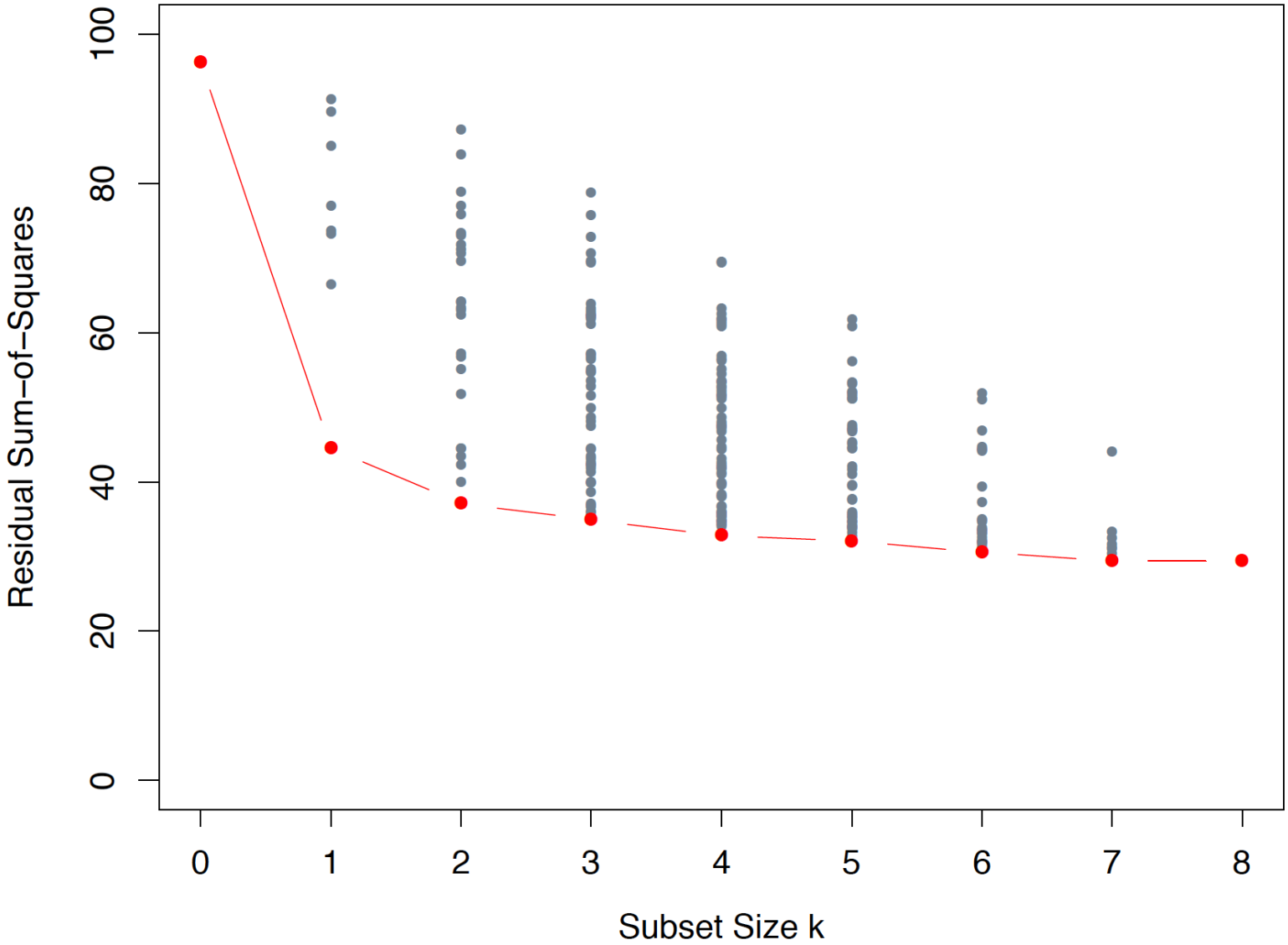


FIGURE 3.5. *All possible subset models for the prostate cancer example. At each subset size is shown the residual sum-of-squares for each model of that size.*

The Shrinkage

Find better estimate - continuous

Shrinkage estimate

$$\widehat{\beta}_j^{\mathsf{S}} = (1-\alpha)\widehat{\beta}_j^{\mathsf{ls}} \qquad 0 \leq \alpha \leq 1$$

Justification from the James-Stein estimator (1960)

$$\widehat{\beta}_j^{\mathsf{JS}} = \left(1 - \frac{(p-2)\sigma^2}{\|\widehat{\beta}_j^{\mathsf{ls}}\|^2}\right)_+ \widehat{\beta}_j^{\mathsf{ls}}$$

the estimator risk and its bias variance decomposition

$$\begin{aligned} \mathbb{E}(\|\beta^\star - \widehat{\beta}\|^2) &= \mathbb{E}(\|\beta^\star - \mathbb{E}(\widehat{\beta}) + \mathbb{E}(\widehat{\beta}) - \widehat{\beta}\|^2) \\ &= \|\beta^\star - \mathbb{E}(\widehat{\beta})\|^2 + \mathbb{E}(\|\widehat{\beta} - \mathbb{E}(\widehat{\beta})\|^2) \end{aligned}$$

improve the estimation

- add some bias
- reduce the variance

The ridge regression: a L^2 penalty

(Hoerl and Kennard, 1970).

given $0 \leq \lambda$, minimize

$$RSSR_\lambda(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2 + \lambda \sum_{j=1}^{p} \beta_j^2.$$

center X and $\beta_0 = \bar{y}$

$$RSSR(\boldsymbol{\beta}) = \|\mathbf{y} - X\boldsymbol{\beta}\|^2 + \lambda\|\boldsymbol{\beta}\|^2.$$

$$\widehat{\beta}^{\mathsf{R}}(\lambda) = \underset{\beta \in \mathbb{R}^p}{\arg\min}\, RSSR_\lambda(\boldsymbol{\beta})$$

$\lambda = 0$ $\widehat{\beta}^{\mathsf{R}}(0) = \widehat{\beta}^{\mathsf{ls}}$

$\lambda \to \infty$ $\widehat{\beta}^{\mathsf{R}}(\lambda) \to 0$

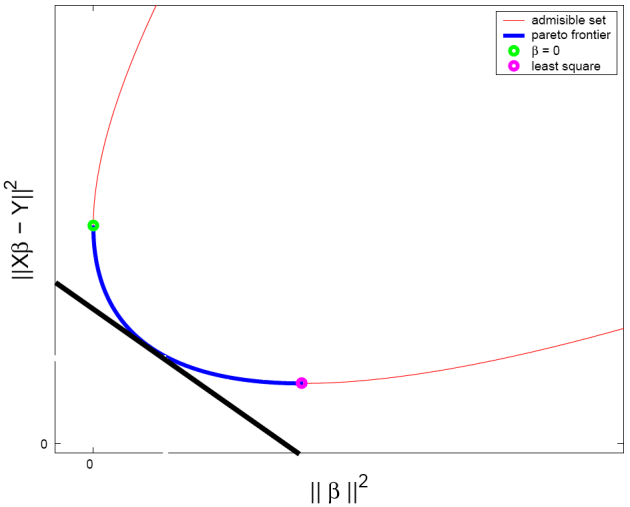
- for a well chosen λ, $\widehat{\beta}^{\mathsf{R}}(0)$ improves on $\widehat{\beta}^{\mathsf{ls}}$

3 equivalent formulations

$$\min_{\beta} \|y - X\beta\|^2 + \lambda \|\beta\|^2$$

$$\begin{cases} \min_{\beta} \|y - X\beta\|^2 \\ \text{s.t. } \|\beta\|^2 \leq t \end{cases}$$

$$\begin{cases} \min_{\beta} \|\beta\|^2 \\ \text{s.t. } \|y - X\beta\|^2 \leq k \end{cases}$$



thanks to convexity

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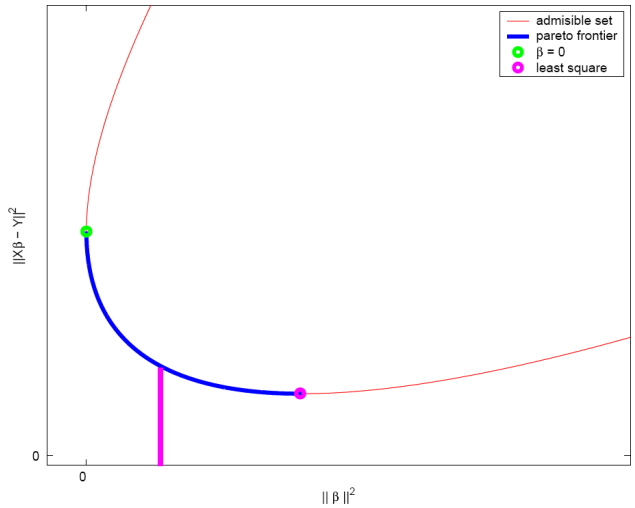

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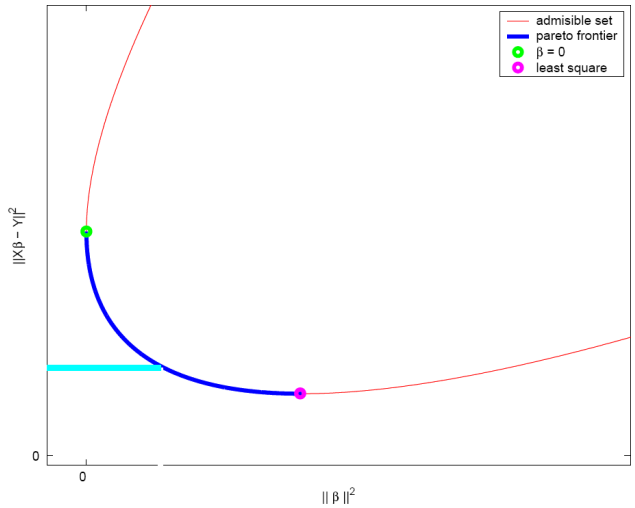


thanks to convexity

How to minimize the ridge loss

The cost

$$\begin{aligned} RSSR(\beta) &= \|\mathbf{y} - X\beta\|^2 + \lambda\|\beta\|^2 \\ &= \mathbf{y}^\top\mathbf{y} - 2\beta^\top X^\top\mathbf{y} + \beta^\top X^\top X\beta + \lambda\beta^\top\beta \\ &= \mathbf{y}^\top\mathbf{y} - 2\beta^\top X^\top\mathbf{y} + \beta^\top(X^\top X + \lambda I)\beta \end{aligned}$$

The gradient

$$\nabla_\beta RSS(\beta, data) = -2X^\top\mathbf{y} + 2(X^\top X + \lambda I)\beta$$

The Hessian

$$\nabla^2_\beta RSS(\beta, data) = 2(X^\top X + \lambda I)$$

The Fermat's rule

$$\widehat{\beta}^{\mathrm{R}} = \underset{\beta\in\mathbb{R}^{p+1}}{\arg\min}\, RSSR(\beta) \quad \Leftrightarrow \quad \nabla_\beta RSSR(\widehat{\beta}^{\mathrm{R}}) = 0$$

The unique solution

$$\widehat{\beta}^{\mathrm{R}} = (X^\top X + \lambda I)^{-1}X^\top\mathbf{y}$$

Least absolute shrinkage and selection operator

(Tibshirani, 1996)

given $0 \leq \lambda$, minimize

$$RSSR_\lambda(\boldsymbol{\beta}) = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j\right)^2 + \lambda \sum_{j=1}^{p} |\beta_j|.$$

center X and $\mathbf{y}$ and set $\beta_0 = \bar{y}$

$$RSSL(\boldsymbol{\beta}) = \|\mathbf{y} - X\boldsymbol{\beta}\|^2 + \lambda\|\boldsymbol{\beta}\|_1.$$

Most often, it is advisable to standardize the data

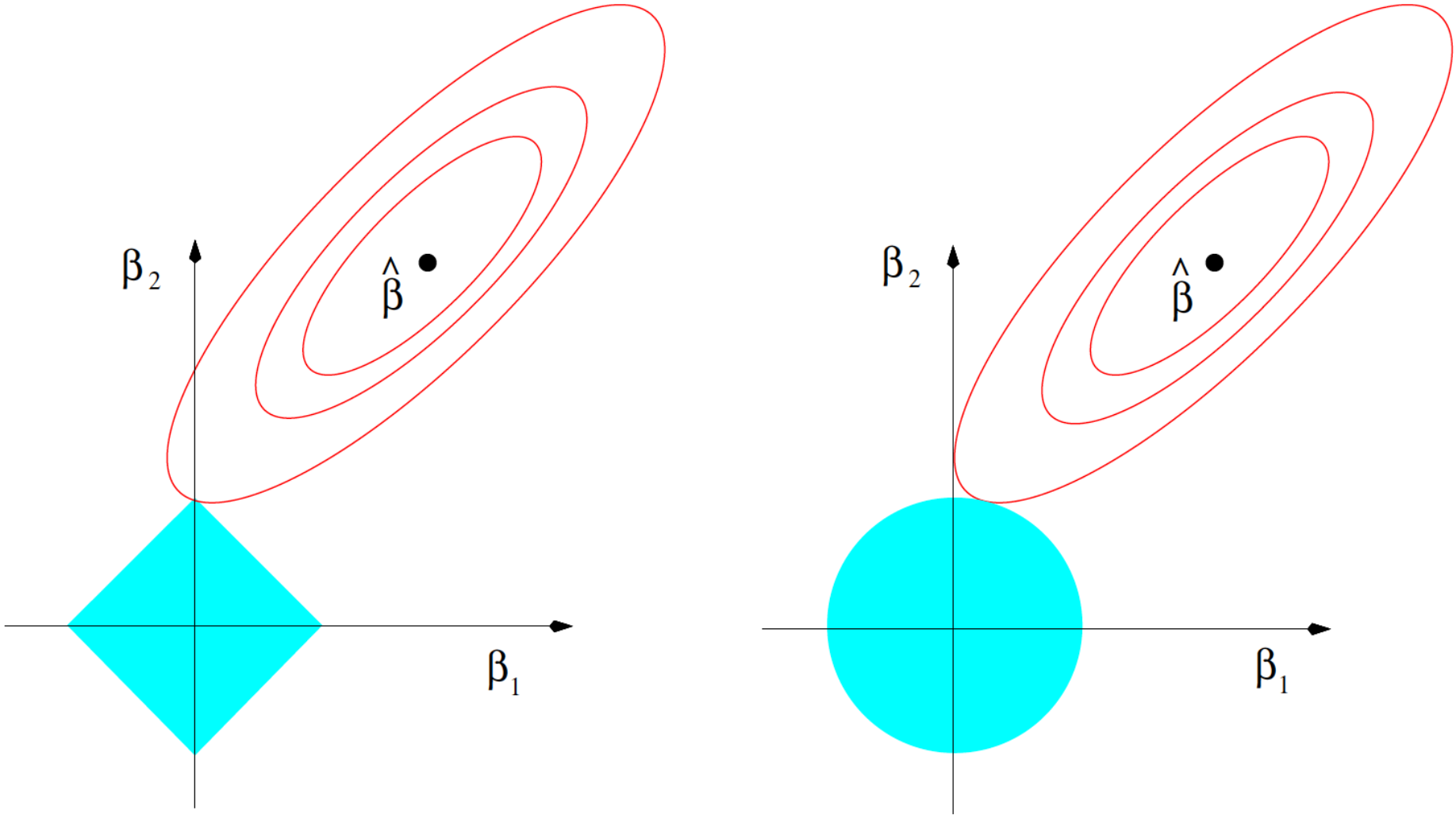


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

3 equivalent formulations

$$\min_{\beta} \ \|y - X\beta\|^2 + \lambda \ \|\beta\|_1$$

$$\begin{cases} \min\limits_{\beta} \ \|y - X\beta\|^2 \\ \text{s.t.} \ \ \|\beta\|_1 \leq t \end{cases}$$

$$\begin{cases} \min\limits_{\beta} \ \|\beta\|_1 \\ \text{s.t.} \ \ \|y - X\beta\|^2 \leq k \end{cases}$$

The Lasso as a pQP

The Lasso is a pQP

$$\begin{cases} \min\limits_{\boldsymbol{\beta}} & \|\mathbf{y} - X\boldsymbol{\beta}\|^2 \\ \text{s.t.} & \|\boldsymbol{\beta}\|_1 \leq t \end{cases}$$

introducing $\alpha_j = |\beta_j|$

$$\begin{cases} \min\limits_{\boldsymbol{\beta},\boldsymbol{\alpha}} & \|\mathbf{y} - X\boldsymbol{\beta}\|^2 \\ \text{s.t.} & \sum\limits_{j=1}^{p} \alpha_j \leq t \\ & -\alpha_j \leq \beta_j \leq \alpha_j \qquad j = 1, \ldots, p \\ & 0 \leq \alpha_j \end{cases}$$

The Lasso as a standard QP

The Lasso

$$\begin{cases} \min\limits_{\boldsymbol{\beta},\boldsymbol{\alpha}} & \|\mathbf{y} - X\boldsymbol{\beta}\|^2 \\ \text{s.t.} & \sum\limits_{j=1}^{p} \alpha_j \le t \\ & -\alpha_j \le \beta_j \le \alpha_j \qquad j = 1, \dots, p \\ & 0 \le \alpha_j \end{cases}$$

A standard QP

$$\begin{cases} \min\limits_{z} & \frac{1}{2} z^\top Q z - c^\top z \\ \text{s.t.} & Az \le b \\ & lb \le z \le ub \end{cases}$$

$z = (\boldsymbol{\beta}^\top, \boldsymbol{\alpha}^\top)^\top$, $Q = (X^\top X, 0_p; (0_p, 0_p))$, $c = (X^\top y, 0_p)^\top$,
$A = ((0_p, 1_p); I_p, -I_p); -I_p - I_p)$, $b = t(1, 0_p, 0_p)^\top$,
$lb = (-\infty, 0_p)^\top$, $ub = (\infty, \infty)^\top$,

The KKT

The Lasso

$$\begin{cases} \min\limits_{\boldsymbol{\beta},\boldsymbol{\alpha}} & \frac{1}{2}\|\mathbf{y} - X\boldsymbol{\beta}\|^2 \\ \text{s.t.} & \sum\limits_{j=1}^{p} \alpha_j \leq t \\ & -\alpha_j \leq \beta_j \leq \alpha_j \qquad j = 1, \ldots, p \\ & 0 \leq \alpha_j \end{cases}$$

The associated lagrangian

$$\begin{aligned} \mathcal{L}(\alpha; \beta,) =& \frac{1}{2}\|\mathbf{y} - X\boldsymbol{\beta}\|^2 - \lambda(\sum_{j=1}^{p} \alpha_j - t) \\ &+ \sum_{j=1}^{p} \mu_j^-(-\alpha_j - \beta_j) + \sum_{j=1}^{p} \mu_j^+(-\alpha_j + \beta_j) - \sum_{j=1}^{p} \gamma_j \alpha_j \end{aligned} \tag{1}$$

The KKT

First order optimality conditions

$$\widehat{\beta}^{\mathsf{L}} = \underset{\beta \in \mathbb{R}^p}{\arg\min}\, RSSL(\boldsymbol{\beta}) \quad \Leftrightarrow \quad \widehat{\beta}^{\mathsf{L}} \text{ has to fulfill the KKT}$$

Karush, Kuhn and Tucker (KKT) conditions

stationarity

$$X^\top(X\boldsymbol{\beta} - \mathbf{y}) - \mu^- + \mu^+ = 0$$
$$\lambda \mathbf{e} - \mu^- + \mu^+ - \gamma = 0$$

primal admissibility

$$\sum_{j=1}^p \alpha_j \leq t$$
$$-\alpha_j \leq \beta_j \leq \alpha_j \qquad j = 1, \ldots, p$$
$$0 \leq \alpha_j \qquad j = 1, \ldots, p$$

dual admissibility

$$\lambda, \mu_j^-, \mu_j^+, \gamma_j \geq 0 \qquad j = 1, \ldots, p$$

complementarity

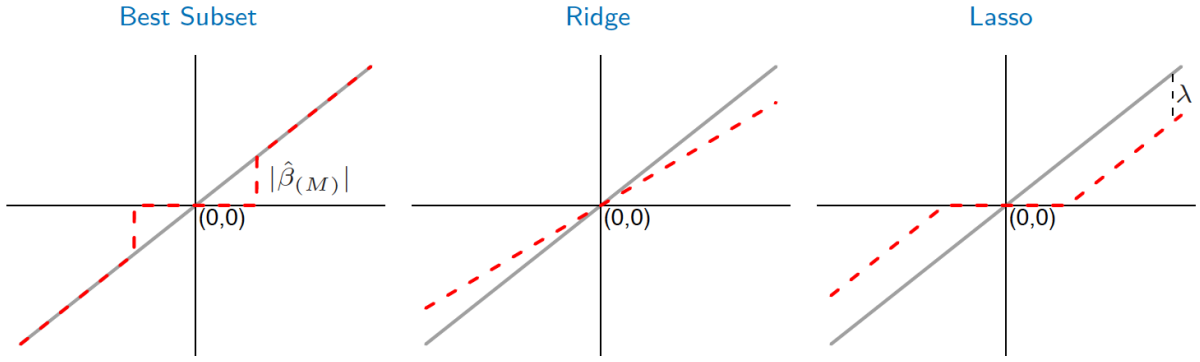
$$\lambda\left(\sum_{j=1}^p \alpha_j - t\right) = 0$$
$$\mu_j^-(-\alpha_j - \beta_j) = 0 \qquad j = 1, \ldots, p$$
$$\mu_j^+(-\alpha_j + \beta_j) = 0 \qquad j = 1, \ldots, p$$
$$\gamma_j \alpha_j = 0 \qquad j = 1, \ldots, p$$

The orthogonal case

$$\widehat{\beta}_j^{\mathsf{L}} = \begin{cases} \widehat{\beta}_j^{\mathsf{ls}} - \lambda \mathit{sign}(\widehat{\beta}_j^{\mathsf{ls}}) & 0 \le \lambda \le \widehat{\beta}_j^{\mathsf{ls}} \\ 0 & \text{else} \end{cases}$$

TABLE 3.4. *Estimators of β_j in the case of orthonormal columns of $\mathbf{X}$. M and λ are constants chosen by the corresponding techniques;* sign *denotes the sign of its argument (± 1), and x_+ denotes "positive part" of x. Below the table, estimators are shown by broken red lines. The 45° line in gray shows the unrestricted estimate for reference.*

Estimator	Formula
Best subset (size M)	$\hat{\beta}_j \cdot I(\lvert\hat{\beta}_j\rvert \ge \lvert\hat{\beta}_{(M)}\rvert)$
Ridge	$\hat{\beta}_j/(1+\lambda)$
Lasso	$\mathrm{sign}(\hat{\beta}_j)(\lvert\hat{\beta}_j\rvert - \lambda)_+$



Lasso implementation as a QP with CVX

$$\begin{cases} \min\limits_{\beta \in \mathbb{R}^p} & \|\mathbf{y} - X\beta\|^2 \\ \text{s.t.} & \|\beta\|_1 \leq t \end{cases}$$

Given X, $\mathbf{y}$ and $0 \leq t$

with R

```
b<-Variable(p)
o<-Minimize(sum((y-X%*%b)^2))
c<-list(sum(abs(b)) <=  t)
problem <- Problem(o, c)
result <- solve(problem)
```

with python

```
import cvxpy as cp

b = cp.Variable(p)
o = cp.Minimize(cp.sum_squares(X@b-y))
c = [cp.norm(b, 1) <= t]
problem = cp.Problem(o, c)
problem.solve()
print("Cost: ", problem.value)
print("Estimation: ", b.value)
```

It works as well with other formulations

http://cvxr.com/cvx/download/

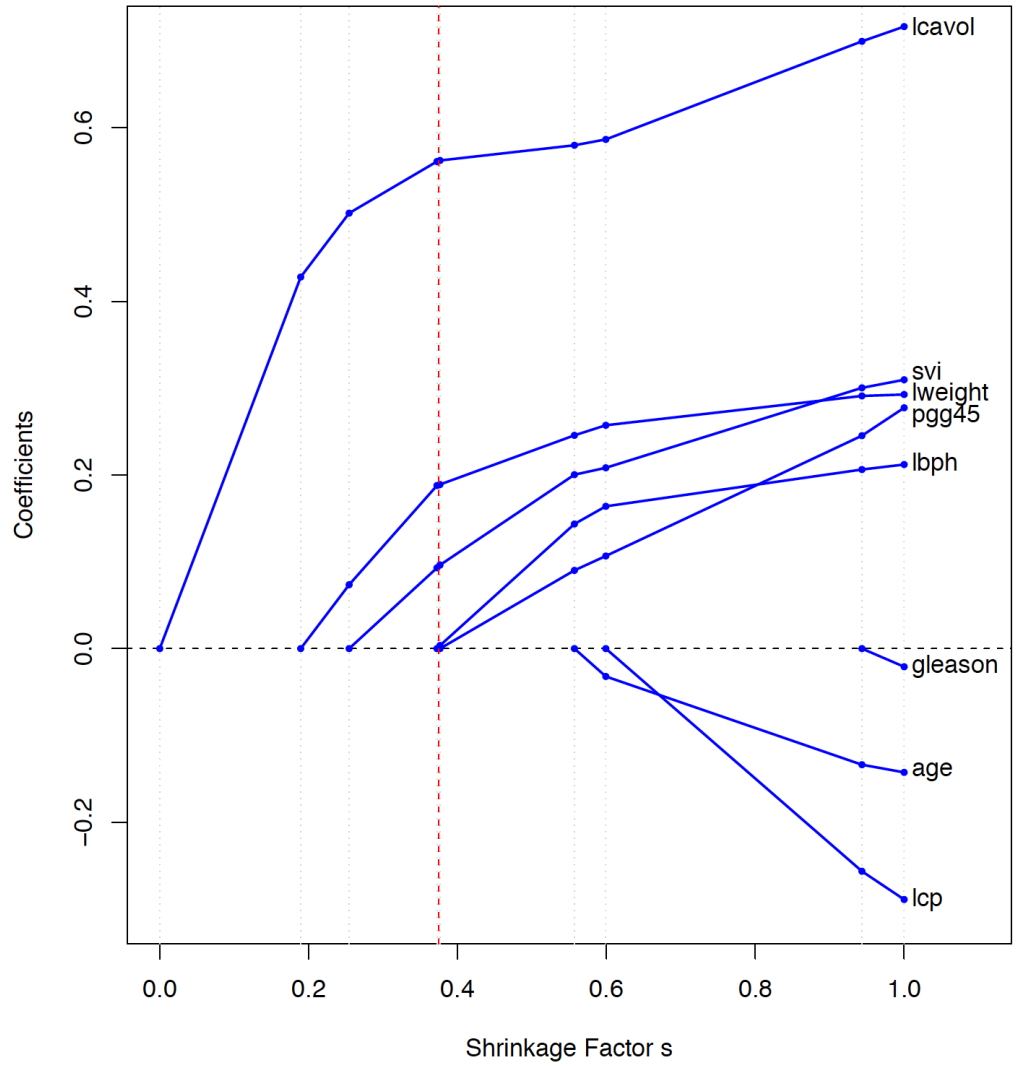
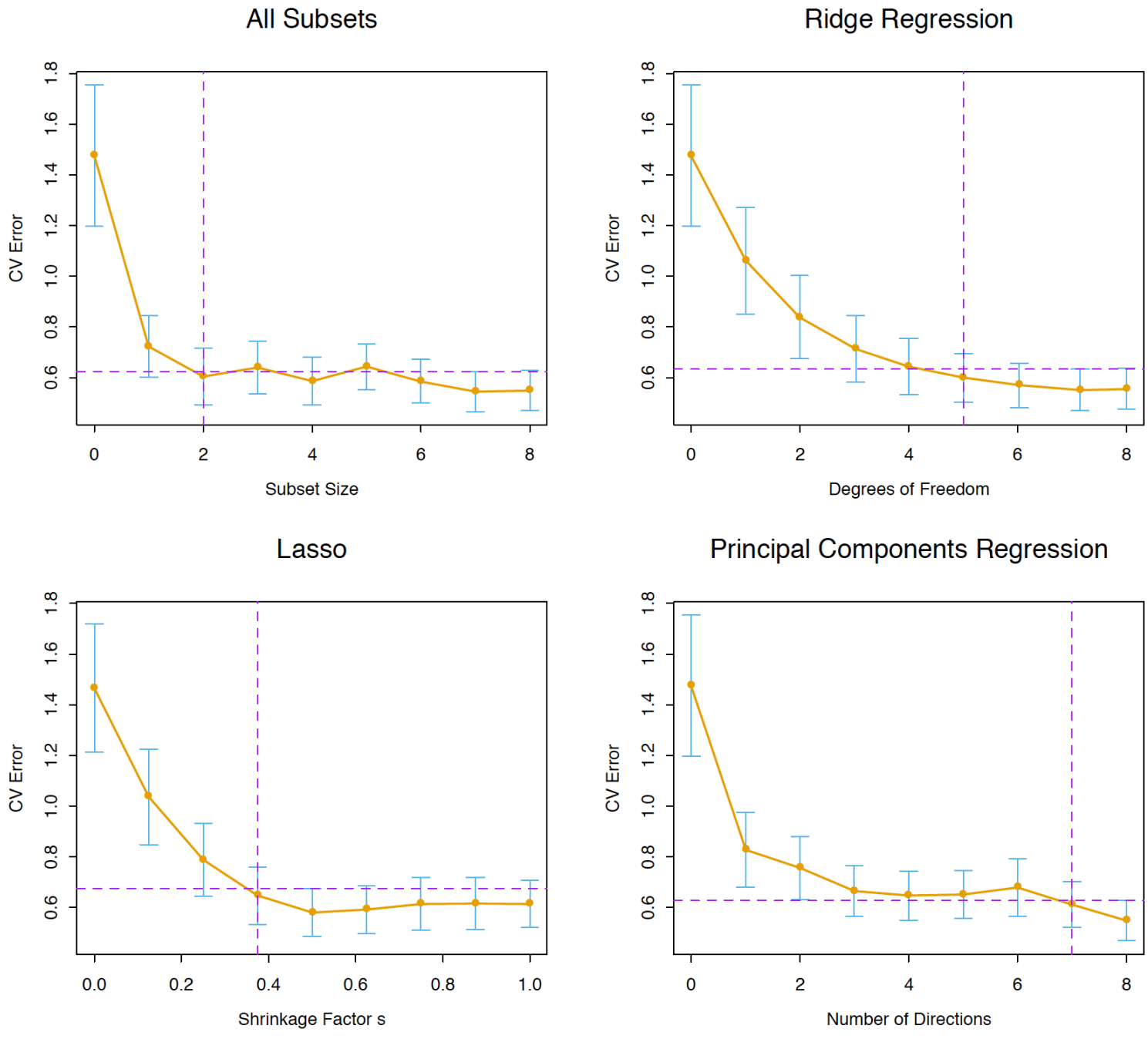


FIGURE 3.10. *Profiles of lasso coefficients, as the tuning parameter t is varied. Coefficients are plotted versus* $s = t/\sum_1^p |\hat{\beta}_j|$. *A vertical line is drawn at* $s = 0.36$, *the value chosen by cross-validation. Compare Figure 3.8 on page 65; the lasso profiles hit zero, while those for ridge do not. The profiles are piece-wise linear, and so are computed only at the points displayed; see Section 3.4.4 for details.*


All Subsets
CV Error
Subset Size
Ridge Regression
Degrees of Freedom
Lasso
Shrinkage Factor s
Principal Components Regression
Number of Directions

Related regression methods

Ridge + Lasso = Elastic Net

$$\min_{\beta} \|\mathbf{y} - X\beta\|^2 + \lambda \left(\alpha\|\beta\|_2^2 + (1-\alpha)\|\beta\|_1\right)$$

The Dantzig Selector

$$\begin{cases} \min\limits_{\beta \in \mathbb{R}^p} \|\beta\|_1 \\ \text{s.t. } \|X^\top(\mathbf{y} - X\beta)\|_\infty \leq t \end{cases}$$

The adaptive Lasso

$$\min_{\beta} \|\mathbf{y} - X\beta\|^2 + \lambda \sum_{j=1}^{p} w_j |\beta_j|$$

The Grouped Lasso
The Fused Lasso
Non convex penalties: MCP and SCAD
. . . just to name a few

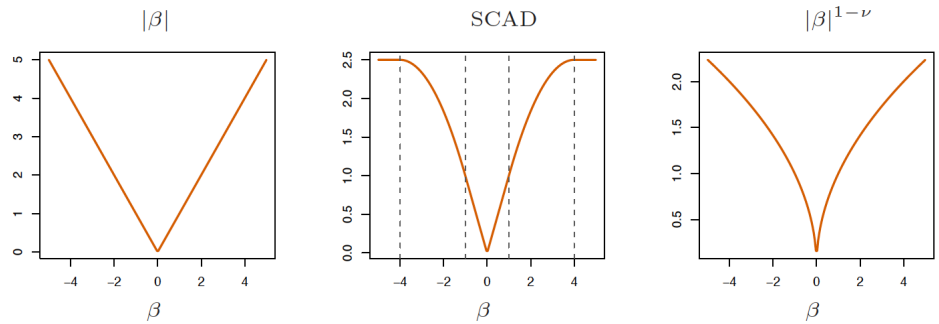


FIGURE 3.20. *The lasso and two alternative non-convex penalties designed to penalize large coefficients less. For SCAD we use $\lambda = 1$ and $a = 4$, and $\nu = \frac{1}{2}$ in*

the L^q penalty

Generalize the Ridge (q=2) and the Lasso (q=1)

$$\min_{\beta} \|\mathbf{y} - X\beta\|^2 + \lambda \sum_{j=1}^{p} |\beta_j|^q$$

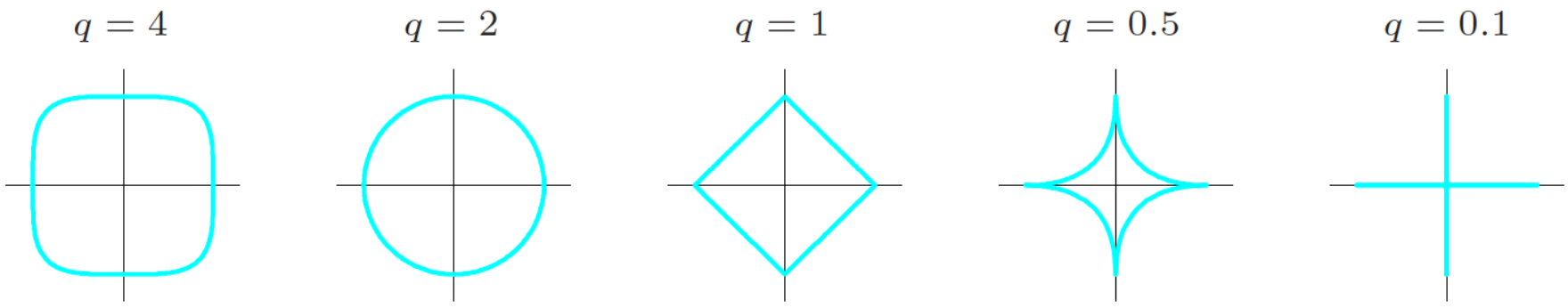
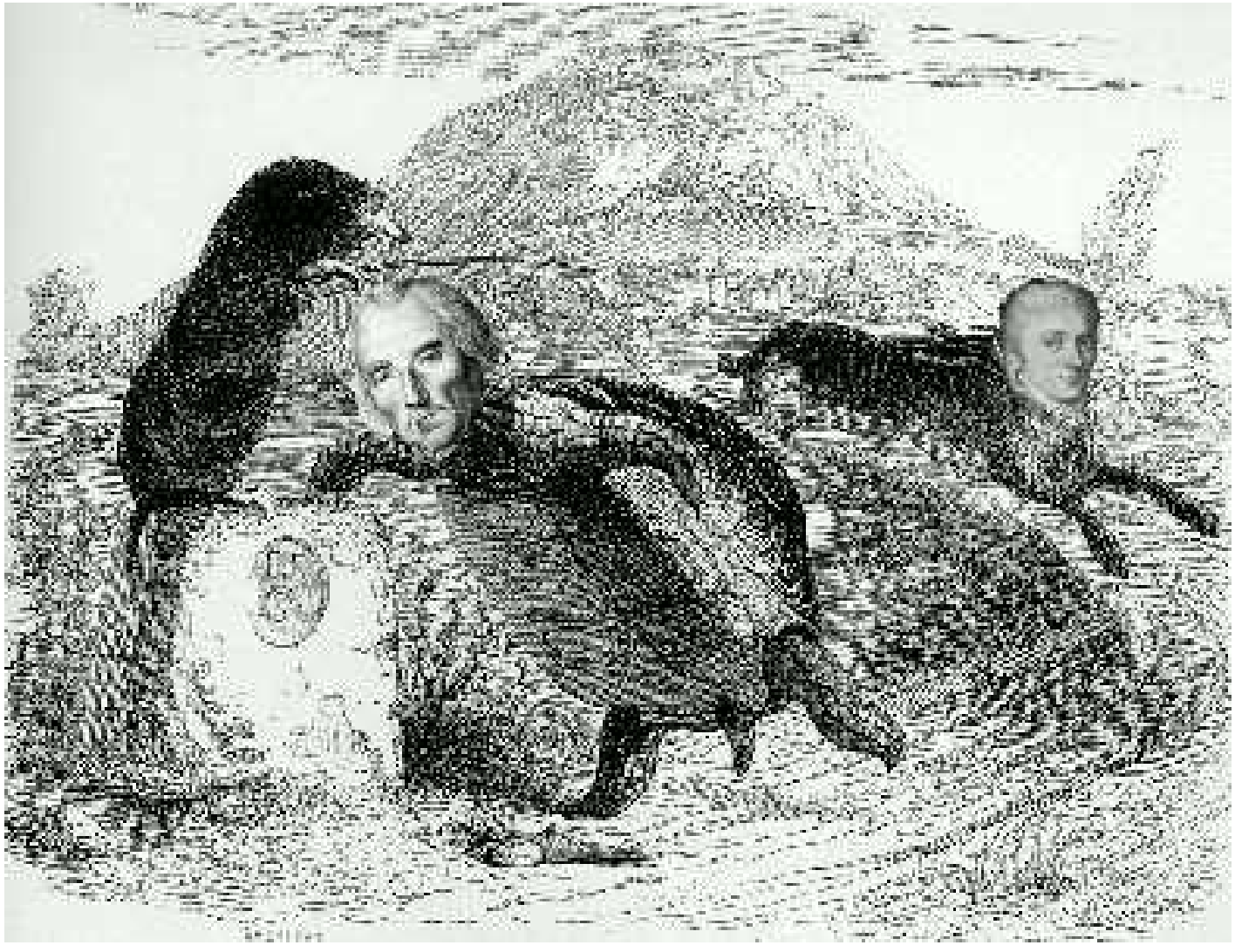


FIGURE 3.12. *Contours of constant value of* $\sum_j |\beta_j|^q$ *for given values of* q.

and the best subset for $q = 0$

The Gaussian Hare and the Laplacian Tortoise



Portnoy , Koenker, Statistical Science, 1997

The linear piecewise regularization path of the Lasso

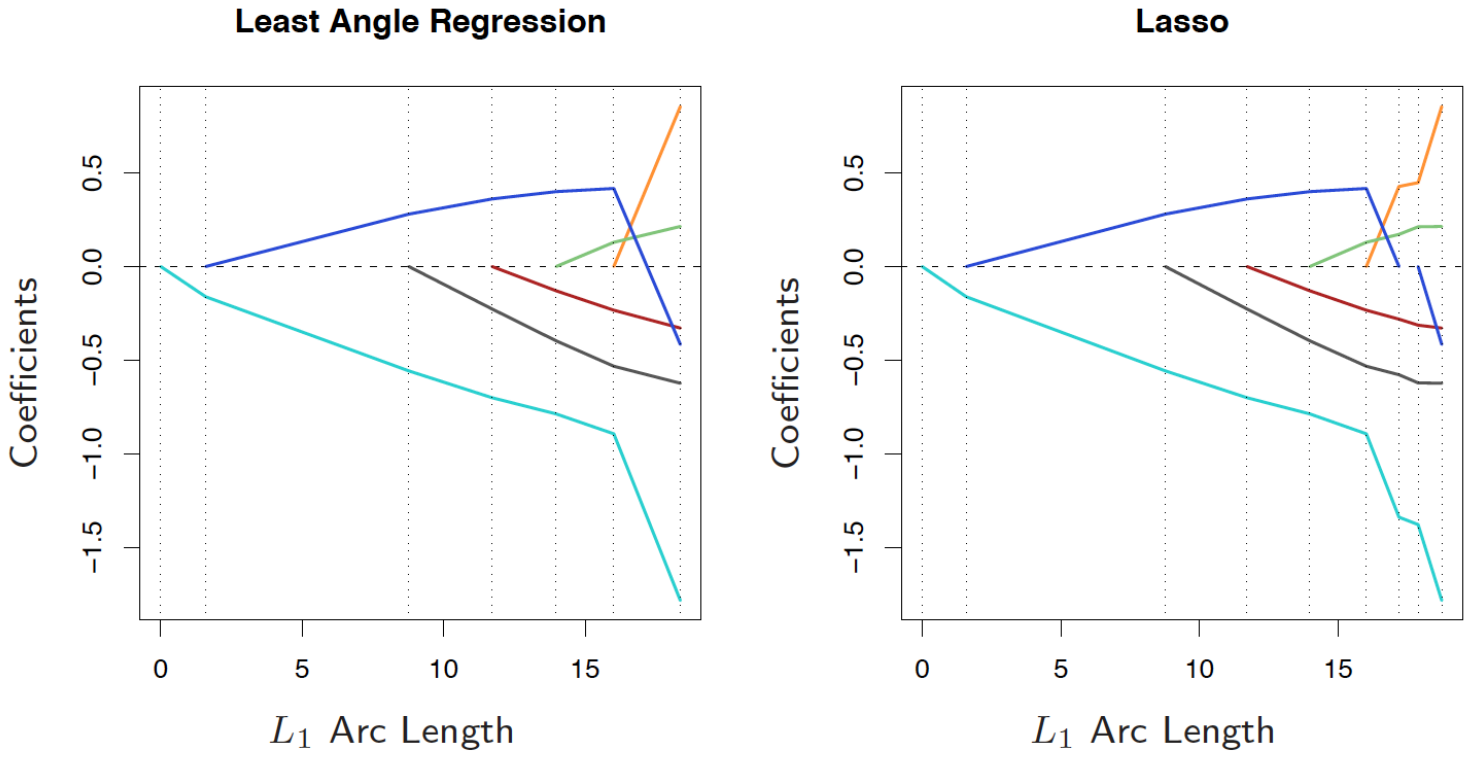


FIGURE 3.15. *Left panel shows the LAR coefficient profiles on the simulated data, as a function of the L_1 arc length. The right panel shows the Lasso profile. They are identical until the dark-blue coefficient crosses zero at an arc length of about* 18.

Principal component regression: PCR

Kendall (1957), Hotelling (1957)

- let $u_1, u_2, \ldots, u_p$ the p singular vectors of matrix X associated with singular values $d_1 \geq d_2 \geq \cdots \geq d_p$ so that $X = UDV^\top$

- perform a least square on the principal components:

$$\min_{\boldsymbol{\beta}} \|\mathbf{y} - X\boldsymbol{\beta}\|^2 = \min_{\boldsymbol{\beta}} \|\mathbf{y} - UDV^\top\boldsymbol{\beta}\|^2 = \min_{\gamma} \|\mathbf{y} - UD\gamma\|^2$$

  with $\gamma = V^\top\beta$. Now consider only $k < p$ components the OLS

$$\hat{\gamma}_k = \arg\min_{\gamma} \|\mathbf{y} - U_k D_k \gamma\|^2$$

- transform this vector back

$$\hat{\boldsymbol{\beta}}_k = V_k \hat{\gamma}_k$$

It is NOT scale invariant

the solution is a sequence (a path) $\beta_k, k = 1, \ldots, p$

Partial least square: PLS

H. Wold (1975) puis S. Wold (1983)

Initially a procedure (an algorithm, NIPALS)

Algorithm 3.3 *Partial Least Squares.*

1. Standardize each $\mathbf{x}_j$ to have mean zero and variance one. Set $\hat{\mathbf{y}}^{(0)} = \bar{y}\mathbf{1}$, and $\mathbf{x}_j^{(0)} = \mathbf{x}_j,\ j = 1, \ldots, p$.
2. For $m = 1, 2, \ldots, p$
   (a) $\mathbf{z}_m = \sum_{j=1}^{p} \hat{\varphi}_{mj}\mathbf{x}_j^{(m-1)}$, where $\hat{\varphi}_{mj} = \langle \mathbf{x}_j^{(m-1)}, \mathbf{y}\rangle$.
   (b) $\hat{\theta}_m = \langle \mathbf{z}_m, \mathbf{y}\rangle / \langle \mathbf{z}_m, \mathbf{z}_m\rangle$.
   (c) $\hat{\mathbf{y}}^{(m)} = \hat{\mathbf{y}}^{(m-1)} + \hat{\theta}_m \mathbf{z}_m$.
   (d) Orthogonalize each $\mathbf{x}_j^{(m-1)}$ with respect to $\mathbf{z}_m$: $\mathbf{x}_j^{(m)} = \mathbf{x}_j^{(m-1)} - [\langle \mathbf{z}_m, \mathbf{x}_j^{(m-1)}\rangle / \langle \mathbf{z}_m, \mathbf{z}_m\rangle]\mathbf{z}_m,\ j = 1, 2, \ldots, p$.
3. Output the sequence of fitted vectors $\{\hat{\mathbf{y}}^{(m)}\}_1^p$. Since the $\{\mathbf{z}_\ell\}_1^m$ are linear in the original $\mathbf{x}_j$, so is $\hat{\mathbf{y}}^{(m)} = \mathbf{X}\hat{\beta}^{\text{pls}}(m)$. These linear coefficients can be recovered from the sequence of PLS transformations.

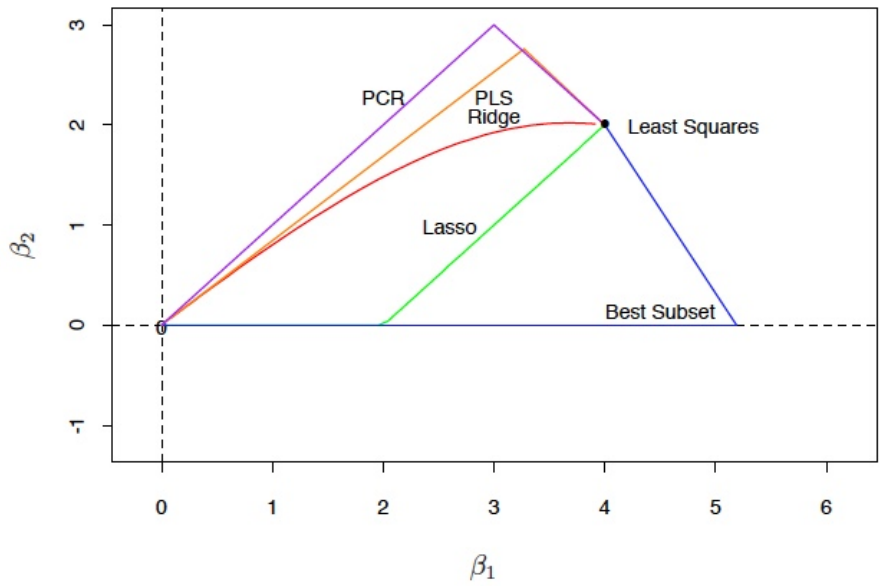
Better regression direction by taking into account the response variable y

PCA direction	PLS direction
$\min_{\mathbf{v}} \quad \|X\mathbf{v}\|^2$	$\min_{\mathbf{v}} \quad cov^2(\mathbf{y}, X\mathbf{v}) = (\mathbf{y}^\top X\mathbf{v})^2$
$\|\mathbf{v}\| = 1,$	$\|\mathbf{v}\| = 1,$

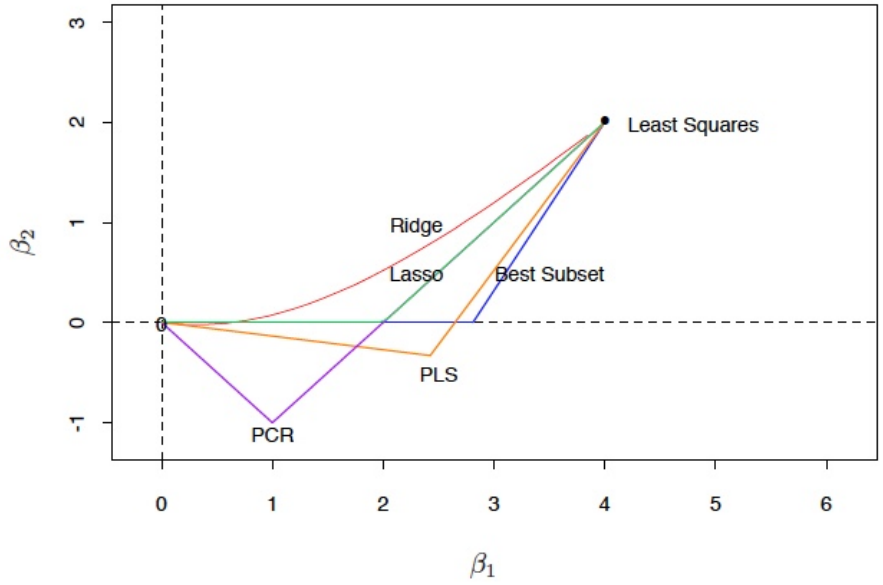
.

Very popular in Chemometrics (analytical chemistry)

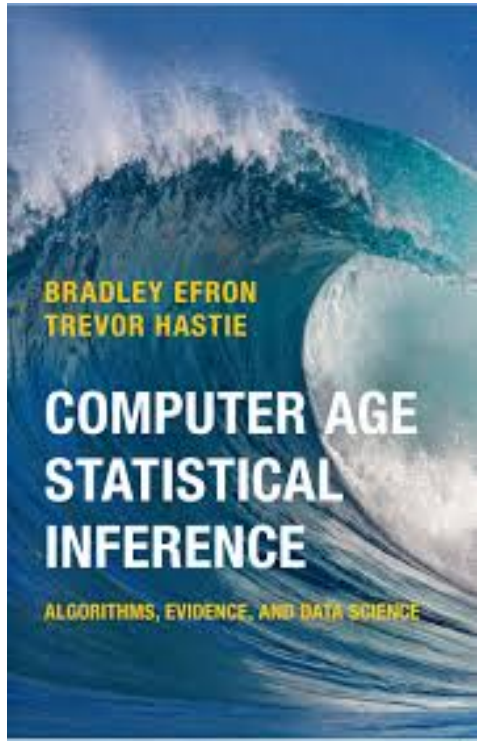
Illustration: Regularization paths in 2d



$\rho = -0.5$



Conclusions



- key issue: Statistics and optimization
- beware: hyperparameter tuning
- focus: details (preprocessing, normalization, intercept. . .)
- my choice: I use the adaptive lasso after variable screening
- my research: non convex and L_0 penalty (MIP optimization)