Foundations of Machine Learning
CentraleSupélec — Fall 2016

6. Regularized linear regression

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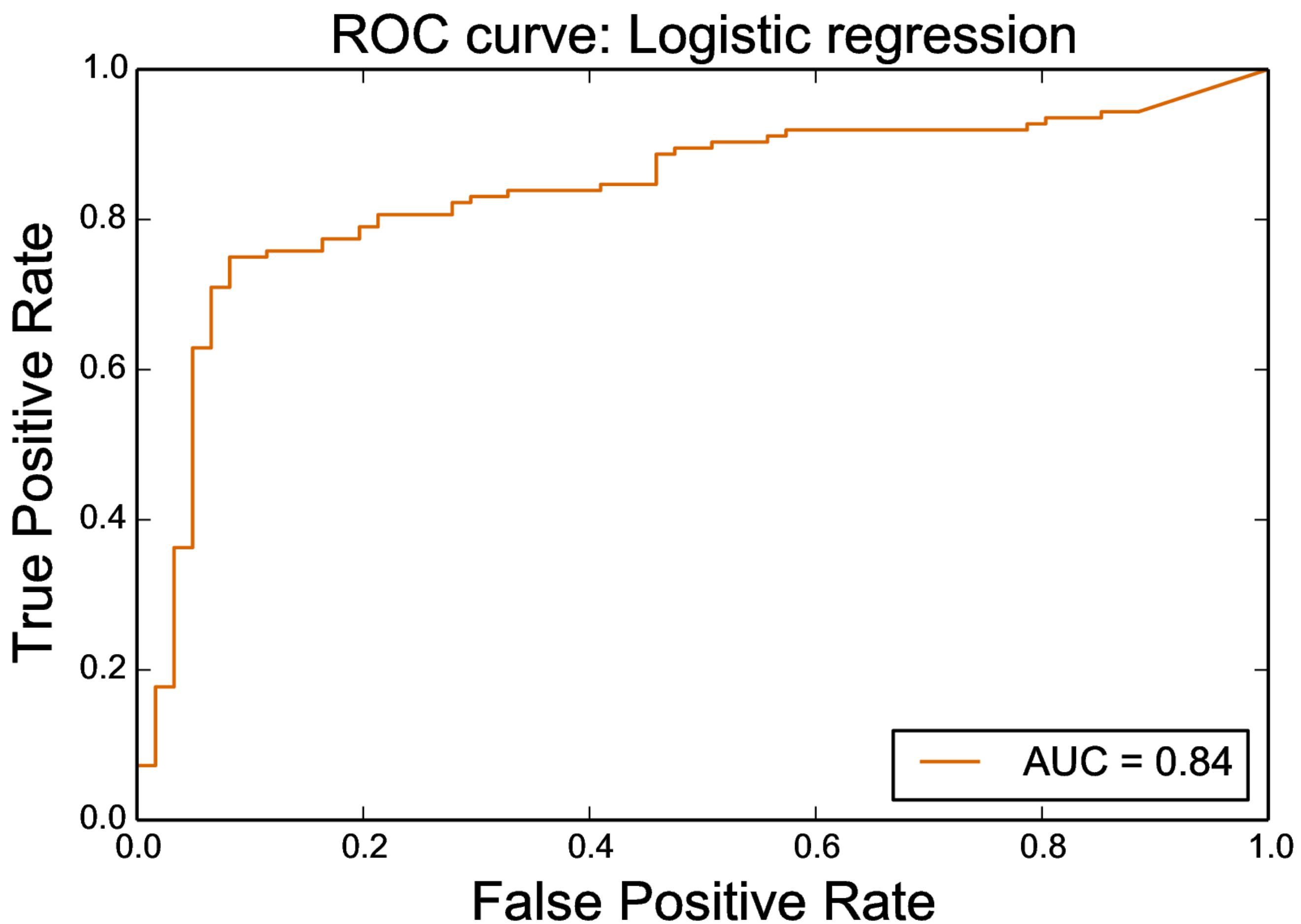
Logistic regression on the Endometrium vs Uterus data



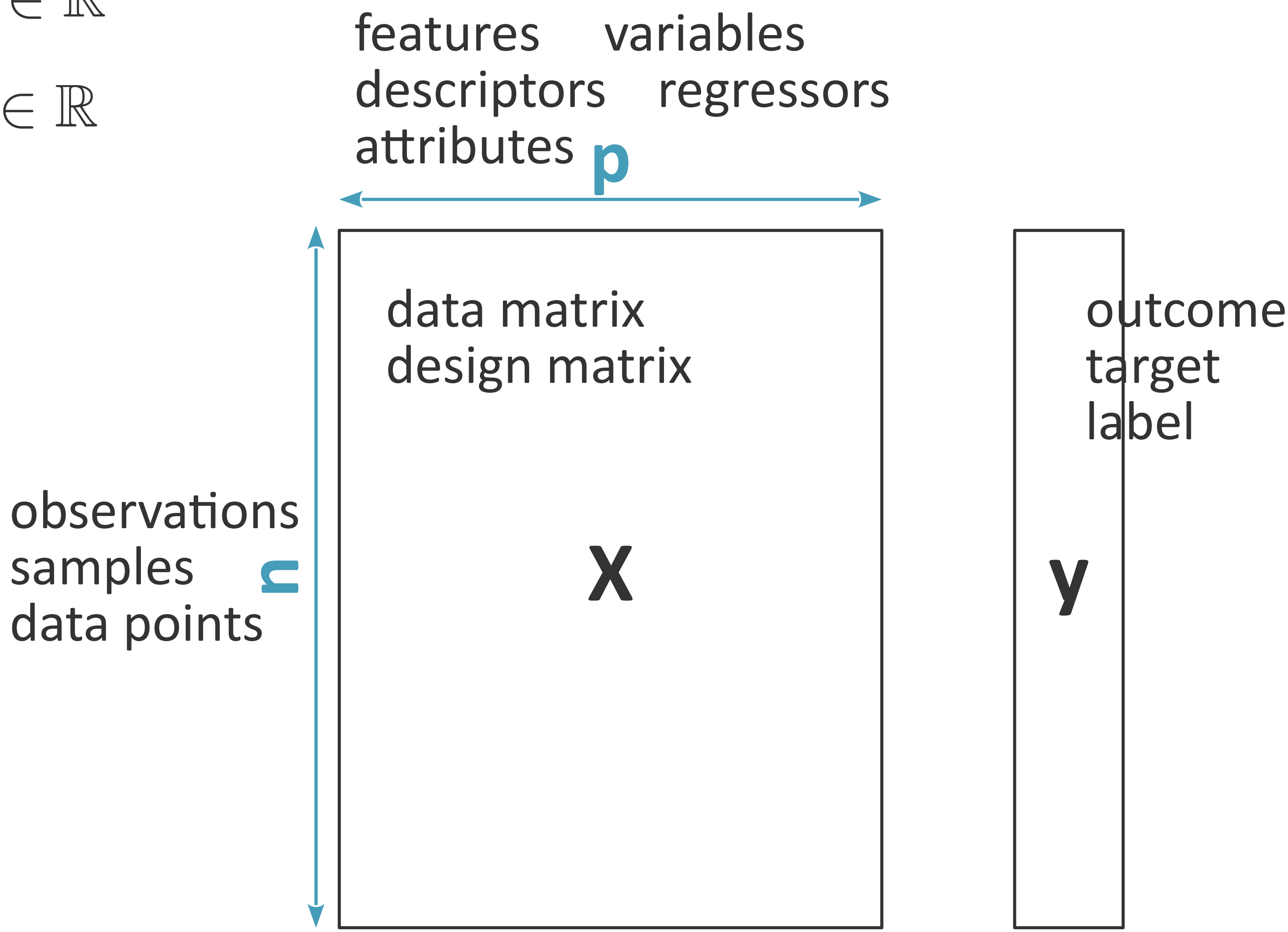
Learning objectives

- Understand **regularization** as a means to control model complexity.
- Define **Lasso**, **ridge regression**, **elastic net.**
- Understand the role of the **l1 and l2 norms** in regularization
- Interpret **solution paths** for Lasso and ridge regression.

Regression setting

$x_j^i \in \mathbb{R}$

$y^i \in \mathbb{R}$



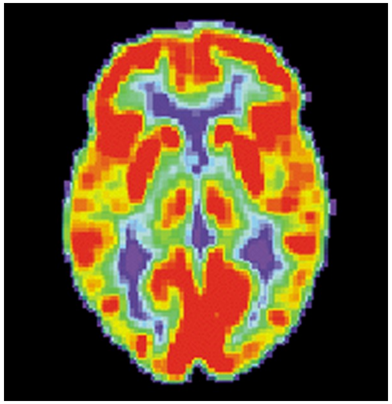
Large p, small n

E.g.

– **neuroimaging**

thousands of brain regions / pixels / voxels

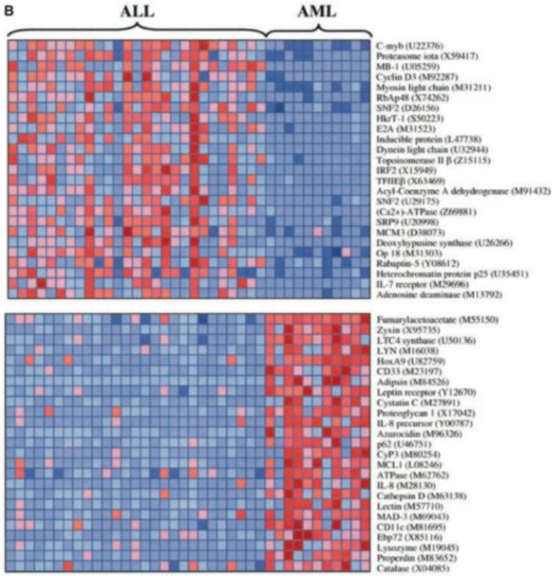
much fewer patients



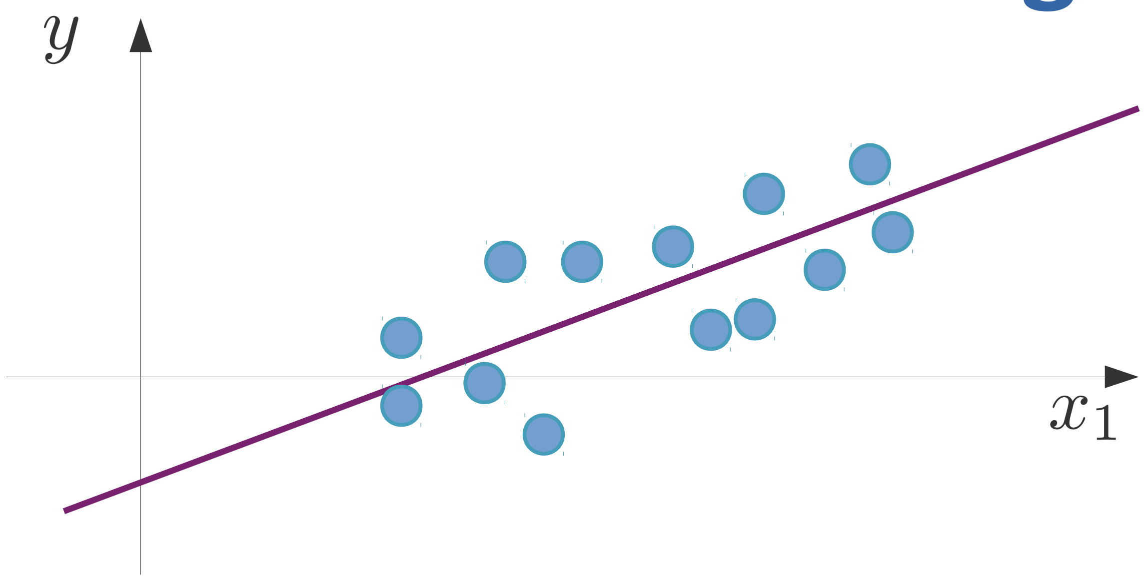
– **genetics and genomics**

thousands of genes, millions of SNPs...

usually, at best thousands of patients



Linear regression



$$\boldsymbol{x} \in \mathbb{R}^p$$

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

Least-squares fit (equivalent to MLE under the assumption of Gaussian noise):

$$\hat{\beta} = \arg\min_{\beta} (y - X\beta)^\top (y - X\beta) = (X^\top X)^{-1} X^\top y$$

The solution is uniquely defined when **$n > p$** and **$X^\top X$ invertible**.

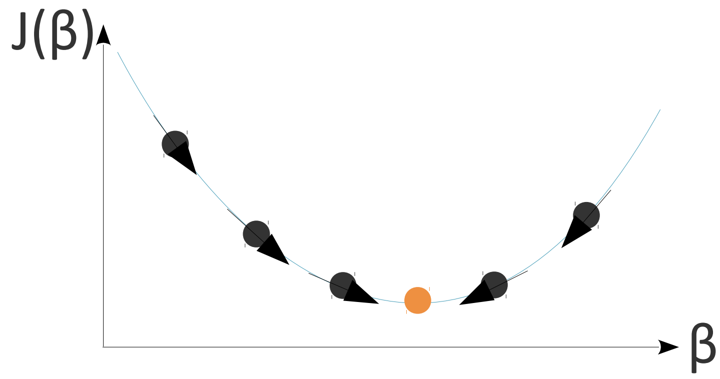
When $X^T X$ not inversible

$$(X^\top X)\hat{\beta} = X^\top y$$

- Pseudo-inverse
- Linear system of p equations:

  Numerical methods

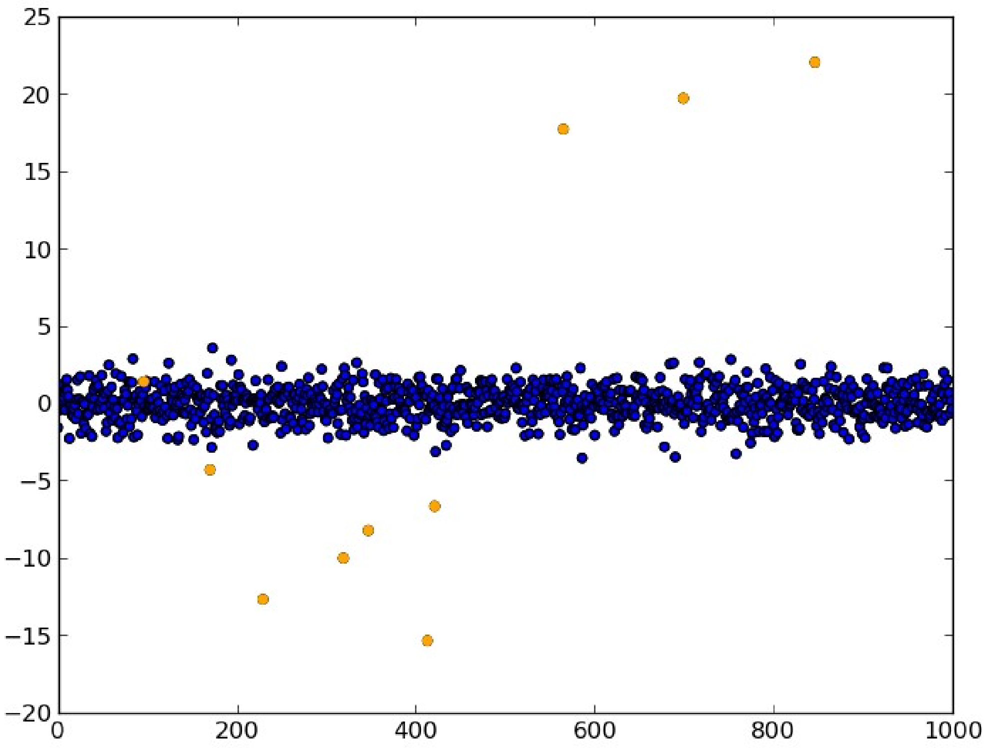
  - **Gaussian elimination**
  - **LU decomposition**
  - **Gradient descent**



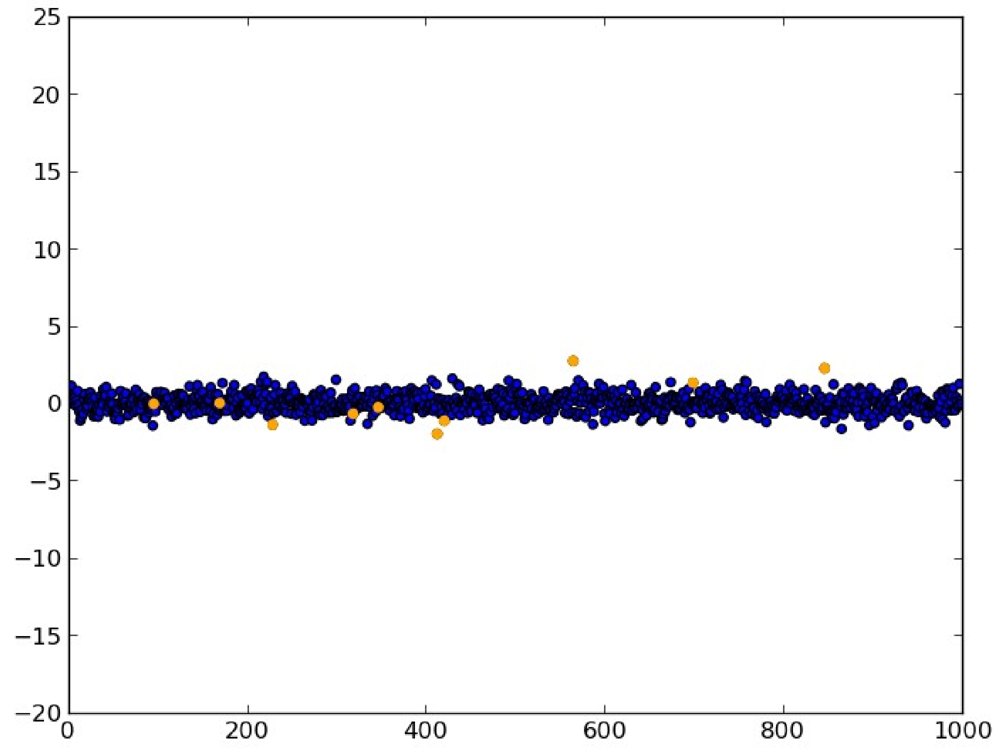
Linear regression when p >> n

Simulated data: p=1000, n=100, 10 causal features

True coefficients



Predicted coefficients



Advantages of least-squares fit

- **Unbiased** $E[\hat{\beta}] = \beta$
- **Explicit form**
- **Computational time?**

Advantages of least-squares fit

- **Unbiased** $E[\hat{\beta}] = \beta$
- **Explicit form**
- **Computational time:** $O(np^2 + p^3)$

compute $X^T X$ invert $X^T X$

computation of $X^T y$: $O(np)$
computation of $(X^T X)^{-1} X^T y$: $O(np)$

Cons of least-squares fit

- **Multicollinearity** leads to high variance of the estimator
- Requires $n > p$
- Prediction error increases linearly as a function of p
- Hard to **interpret** when p is large

Would prefer a small subset with strong effects.

Regularization

Regularization

- Minimize

SSE + **λ** penalty on model complexity

- **Biased estimator** when $\lambda \neq 0$.
- Trade bias for a smaller variance.
- λ can be set by cross-validation.

- Simpler model ≈ fewer parameters

  → **shrinkage:** drive the coefficients of the parameters towards 0.

Ridge regression

Ridge regression

- **Sum-of-squares penalty**

$$\hat{\beta}_{\text{ridge}} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda||\beta||_2^2$$

- **Compute the ridge regression estimator.**

Ridge regression

- **Sum-of-squares penalty**

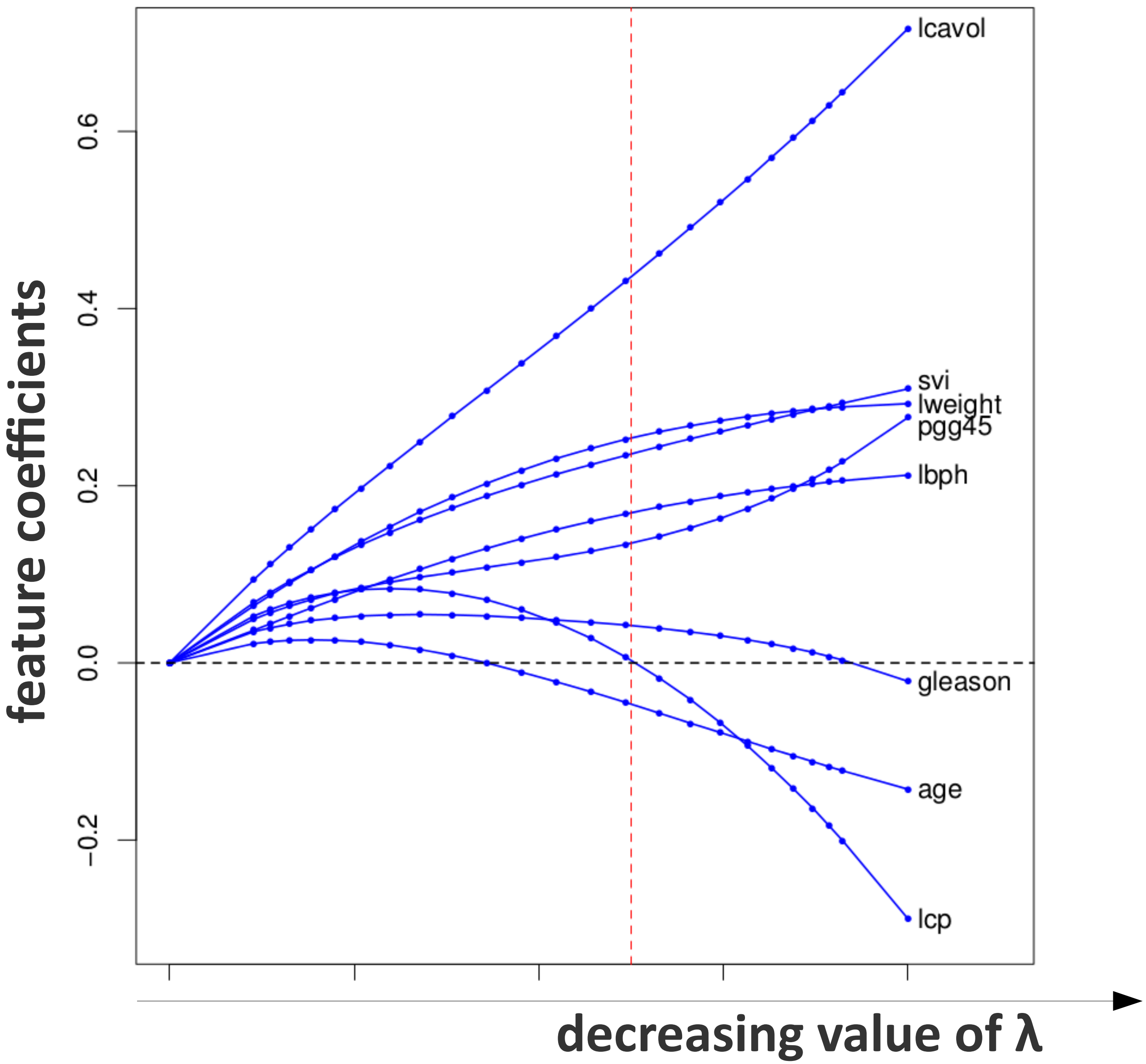
$$\hat{\beta}_{\text{ridge}} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda||\beta||_2^2$$

- **Compute the ridge regression estimator.**

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

$$\text{if } (X^\top X + \lambda I) \text{ invertible.}$$

Ridge regression solution path



Standardization

- **What happens if we multiply x_j by a constant?**
  - For **standard linear regression**
  - For **ridge regression**

Standardization

- What happens if we multiply x_j by a constant?
  - For **standard linear regression:**

$$\hat{\beta}_j \rightarrow \frac{1}{c}\hat{\beta}_j$$

  - For **ridge regression:**

    Not so clear, because of the penalization term $\lambda\beta_j^2$
- Need to **standardize** the features

$$\tilde{x}_j^i = \frac{x_j^i}{\sqrt{\frac{1}{n}\sum_{i=1}^n (x_j^i - \bar{x}_j)^2}}$$

average value of x_j

Ridge regression

- **Grouped selection:**
  - correlated variables get similar weights
  - identical variables get identical weights
- Ridge regression shrinks coefficients towards 0 but does not result in a **sparse model**.
- **Sparsity:**
  - many coefficients get a weight of 0
  - they can be eliminated from the model.

Lasso

Lasso

$$||\beta||_1 = \sum_{j=1}^{p} |\beta_p|$$

- **L1 penalty**

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda||\beta||_{\boxed{1}}$$

- aka **basis pursuit** (signal processing)
- no closed-form solution
- **quadratic programming** problem: equivalent to

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} ||y - X\beta||_2^2 \quad \text{s.t. } ||\beta||_1 \leq t$$

for a unique one-to-one match between t and λ.

QP: maximize a quadratic form under linear constraints.

Equivalence between the formulations

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} ||y - X\beta||_2^2 \quad \text{s.t. } ||\beta||_1 \leq t$$

- **minimize f(β) under the constraint g(β) ≤ 0**

$$f(\beta) = ||y - X\beta||_2^2 \qquad\qquad g(\beta) = ||\beta||_1 - t$$

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$f(\beta) = ||y - X\beta||_2^2$ $\qquad$ $g(\beta) = ||\beta||_1 - t$

Case 1: the unconstrained minimum lies in the **feasible region.** $\{\beta : g(\beta) \leq 0\}$

Equivalence between the formulations

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} ||y - X\beta||_2^2 \quad \text{s.t.} \quad ||\beta||_1 \leq t$$

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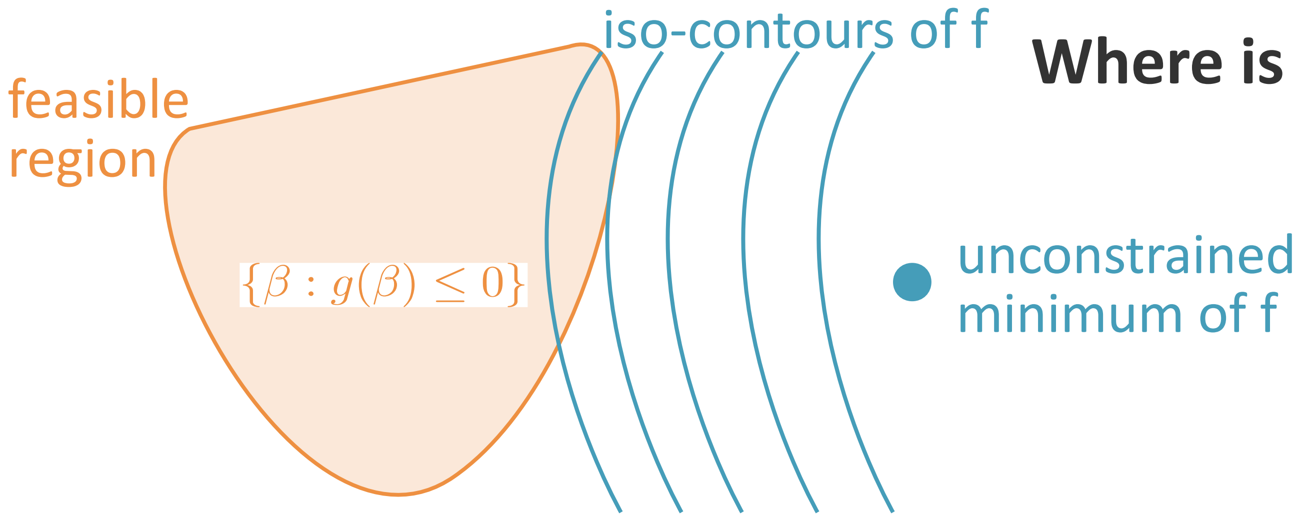
Case 1: the unconstrained minimum lies in the feasible region.

Case 2: it does not.



Where is the solution?

Equivalence between the formulations

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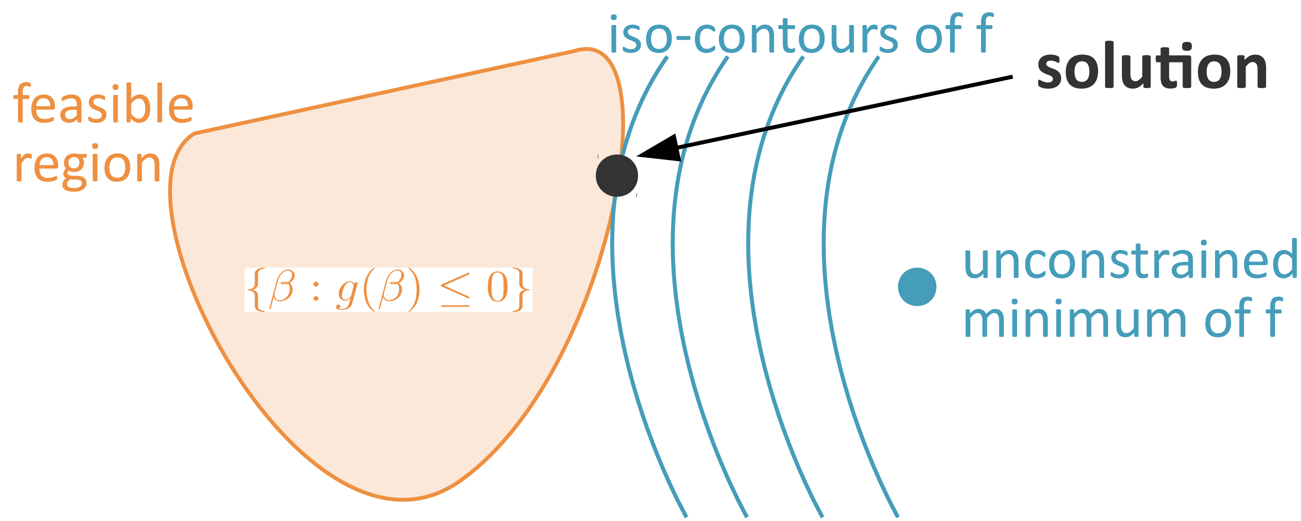

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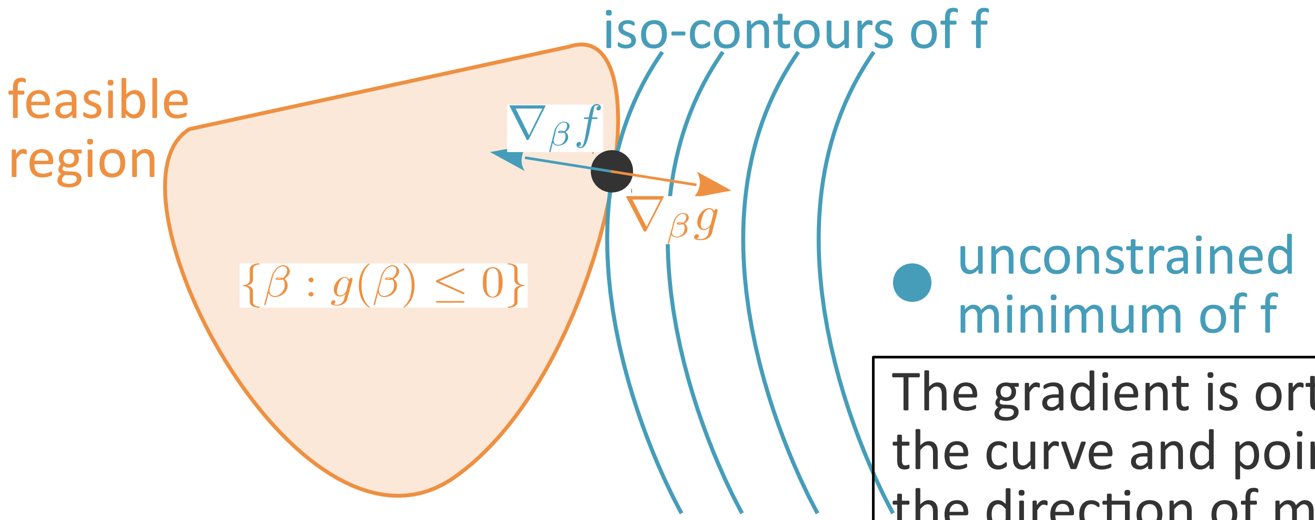


The gradient is orthonormal to the curve and points towards the direction of max increase.

Equivalence between the formulations

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} ||y - X\beta||_2^2 \quad \text{s.t. } ||\beta||_1 \leq t$$

- **minimize f(β) under the constraint g(β) ≤ 0**

$$f(\beta) = ||y - X\beta||_2^2 \qquad\qquad g(\beta) = ||\beta||_1 - t$$

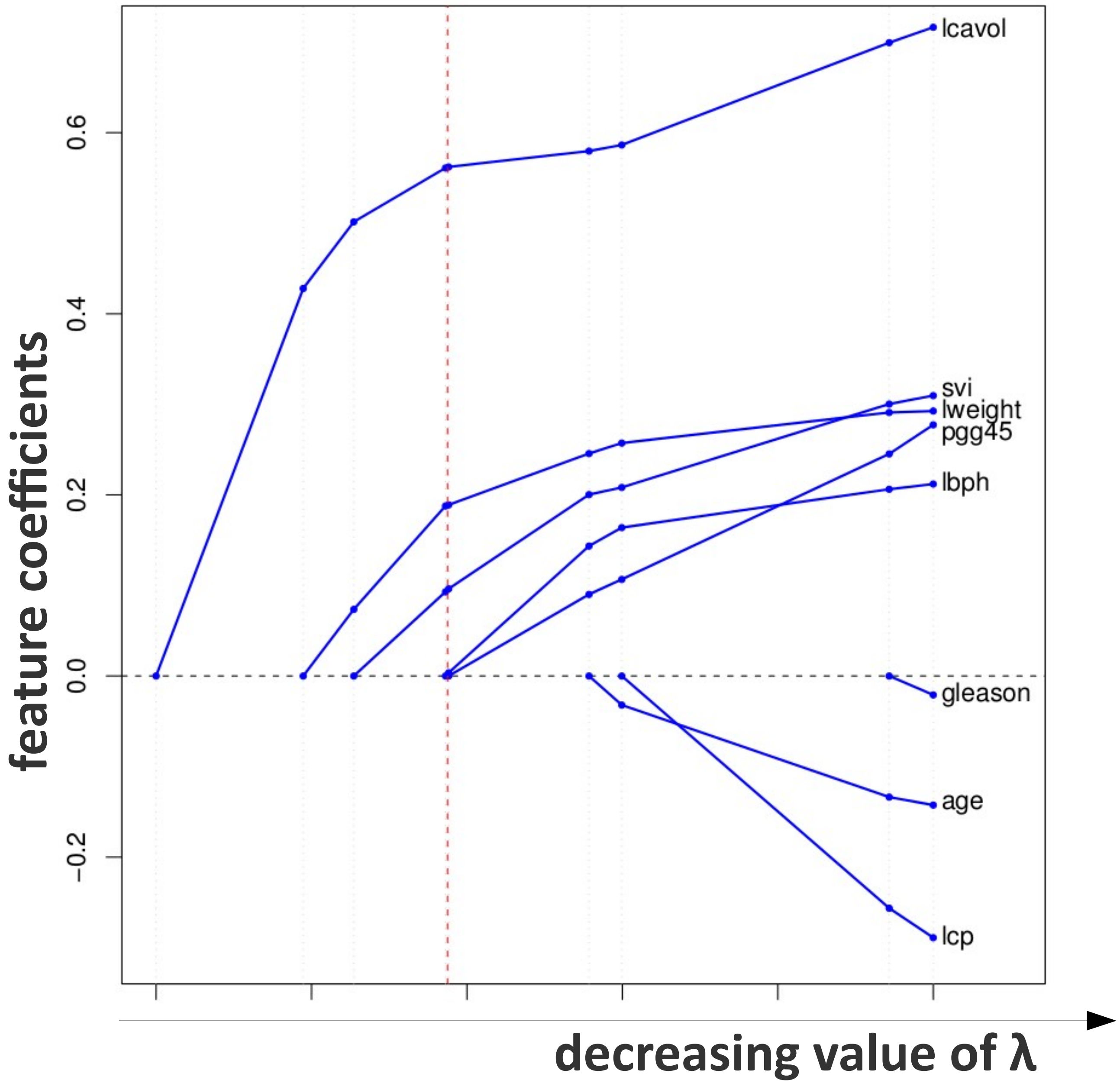
Case 1: the unconstrained minimum lies in the feasible region.

Case 2: it does not. Then it lies at a point where the feasible region and the iso-contours of f are tangent and the gradients are in opposite directions.

The **Lagrangian f(β) + λ g(β) must be minimized (λ ≥ 0)**

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda||\beta||_1$$

Lasso solution path



Forward stepwise regression

- Build model **sequentially**, adding one variable at a time
  - Start with the intercept
  - At each step, add the variable that **most improves the fit**
  - **Stop when** $||\beta||_1 \leq t$
- Greedy solution

Least Angle Regression

At each step, add "only as much of a variable as needed"

1. Standardize the predictors to have mean zero and unit norm. Start with the residual $\mathbf{r} = \mathbf{y} - \bar{\mathbf{y}}$, $\beta_1, \beta_2, \ldots, \beta_p = 0$.

Least Angle Regression

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2. Find the predictor $\mathbf{x}_j$ most correlated with $\mathbf{r}$.
3. Move β_j from 0 towards its least-squares coefficient $\langle \mathbf{x}_j, \mathbf{r} \rangle$, until some other competitor $\mathbf{x}_k$ has as much correlation with the current residual as does $\mathbf{x}_j$.

$$\boxed{\begin{aligned} \beta_j &\leftarrow \beta_j + \alpha \frac{1}{\sum_{i=1}^{n} (x_j^i)^2} \sum_{i=1}^{n} x_j^i r^i \\ &= \beta_j + \alpha (x_j^\top x_j)^{-1} x_j^\top r \\ &= \beta_j + \alpha \langle x_j^\top, x_j \rangle^{-1} \langle x_j, r \rangle \end{aligned}}$$

$$\boxed{r = (y - \bar{y}) - \beta_j x_j}$$

step size

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4. Move β_j and β_k in the direction defined by their joint least squares coefficient of the current residual on $(\mathbf{x}_j, \mathbf{x}_k)$, until some other competitor $\mathbf{x}_l$ has as much correlation with the current residual.

$$\boxed{r = (y - \bar{y}) - \beta_j x_j - \beta_k x_k}$$

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4a. If a non-zero coefficient hits zero, drop its variable from the active set of variables and recompute the current joint least squares direction.

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5. Continue in this way until all p predictors have been entered.

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5. Continue in this way until all p predictors have been entered.

Maximum number of steps: max(n-1, p)

Elastic Net

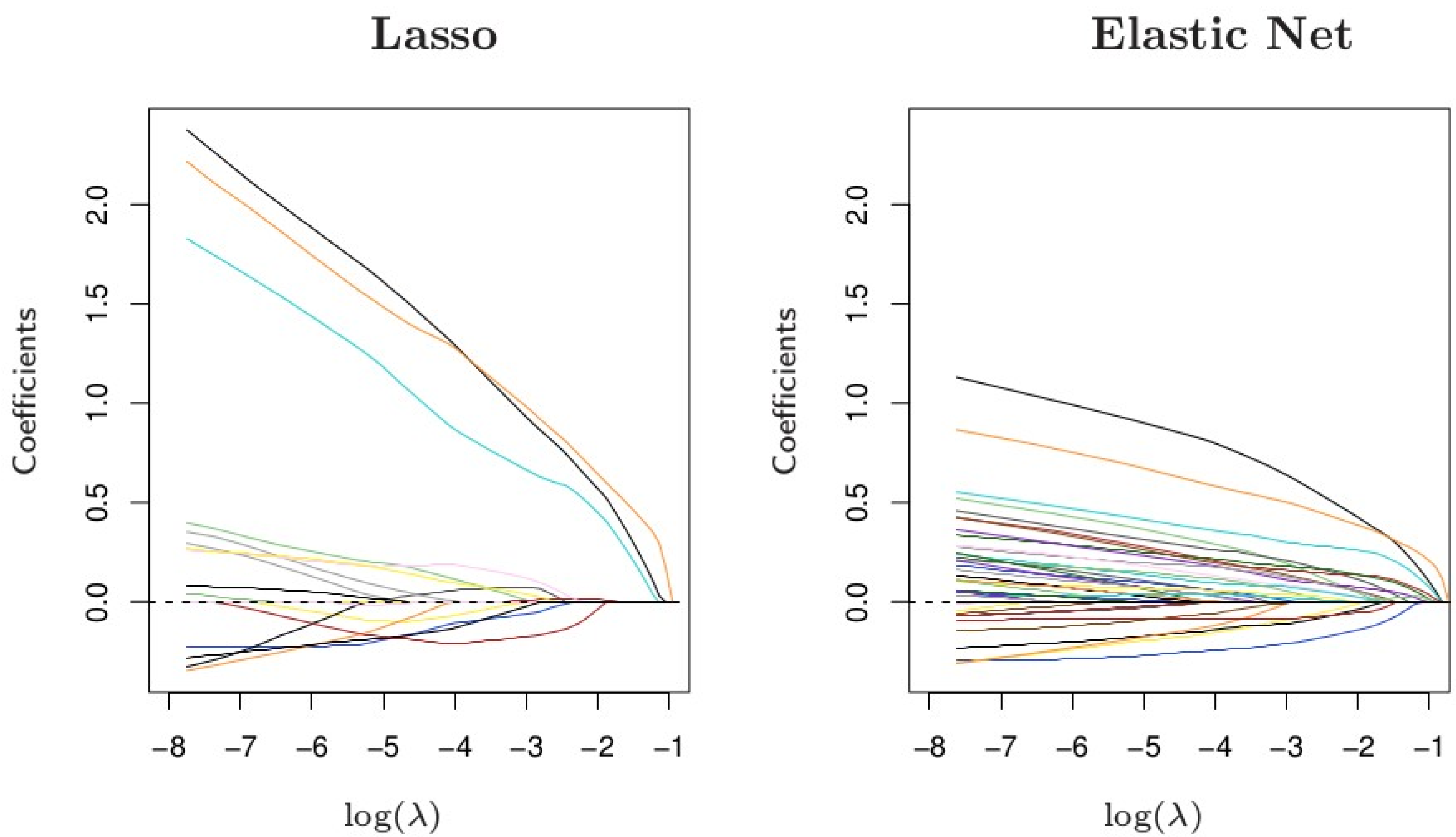
Elastic Net

- **Combine lasso** and **ridge regression**

$$\hat{\beta}_{\text{enet}} = \arg\min_{\beta} ||y - X\beta||_2^2 + \lambda \left(\alpha ||\beta||_2^2 + (1-\alpha)||\beta||_1 \right)$$

  - **Select variables** like the lasso.
  - **Shrinks together coefficients of correlated variables** like the ridge regression.

E.g. Leukemia data



Elastic Net results in more non-zero coefficients than Lasso, but with smaller amplitudes.

Lq-norm regularization

Lq-norm regularization

$$\hat{\beta} = \arg\min_{\beta} ||Y - X\beta||_2^2 + \lambda ||\beta||_q^q \qquad ||\beta||_q = \left(\sum_{j=1}^{p} |\beta_j|^q \right)^{1/q}$$

Equivalently:

$$\hat{\beta} = \arg\min_{\beta} ||Y - X\beta||_2^2 \text{ s. t. } ||\beta||_q^q \leq s$$

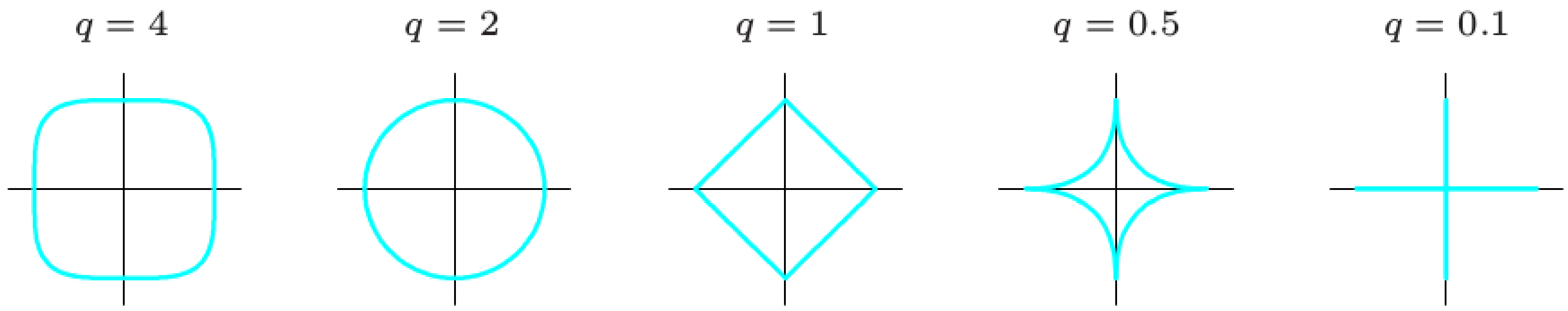
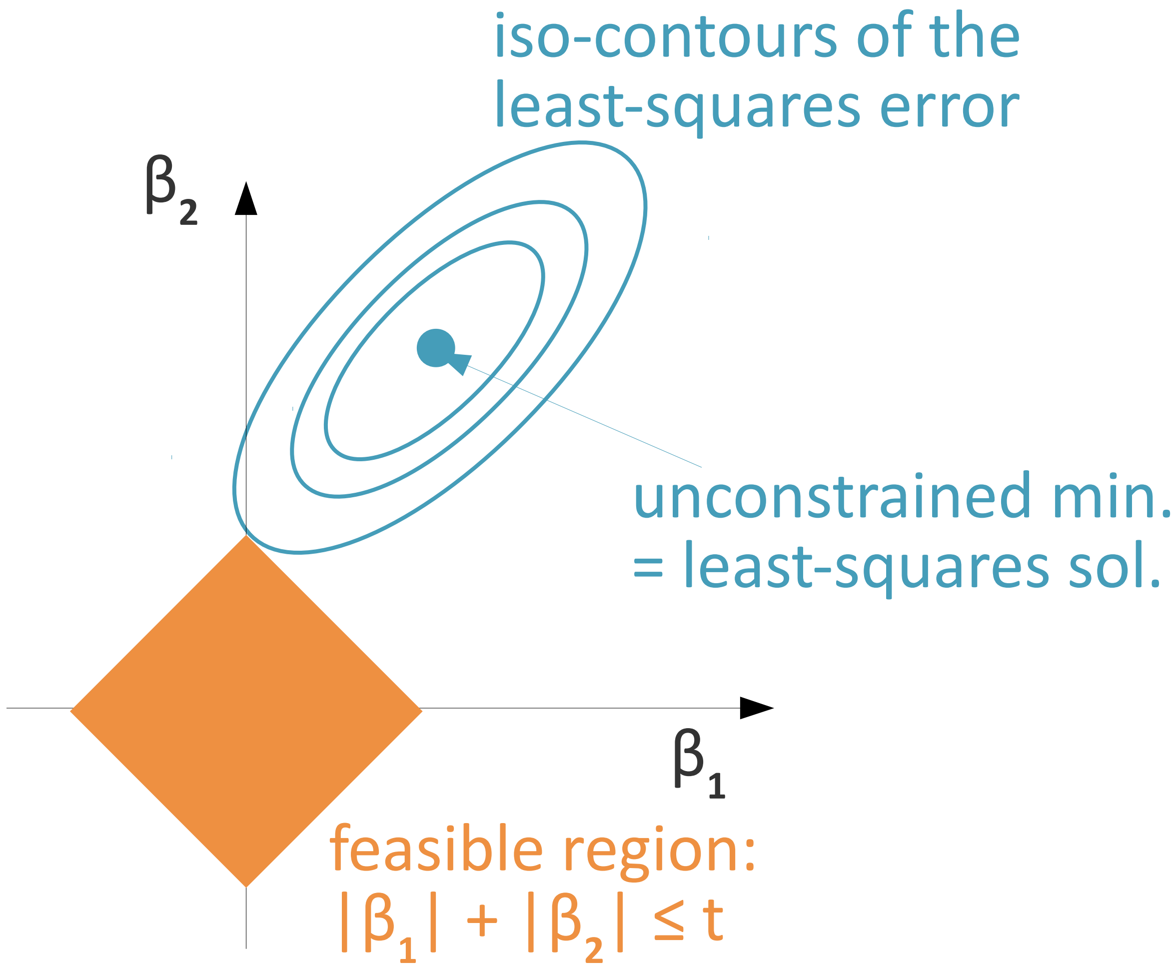


FIGURE 3.12. *Contours of constant value of* $\sum_j |\beta_j|^q$ *for given values of* q.

Lasso vs. ridge

L1 norm



Lasso vs. ridge

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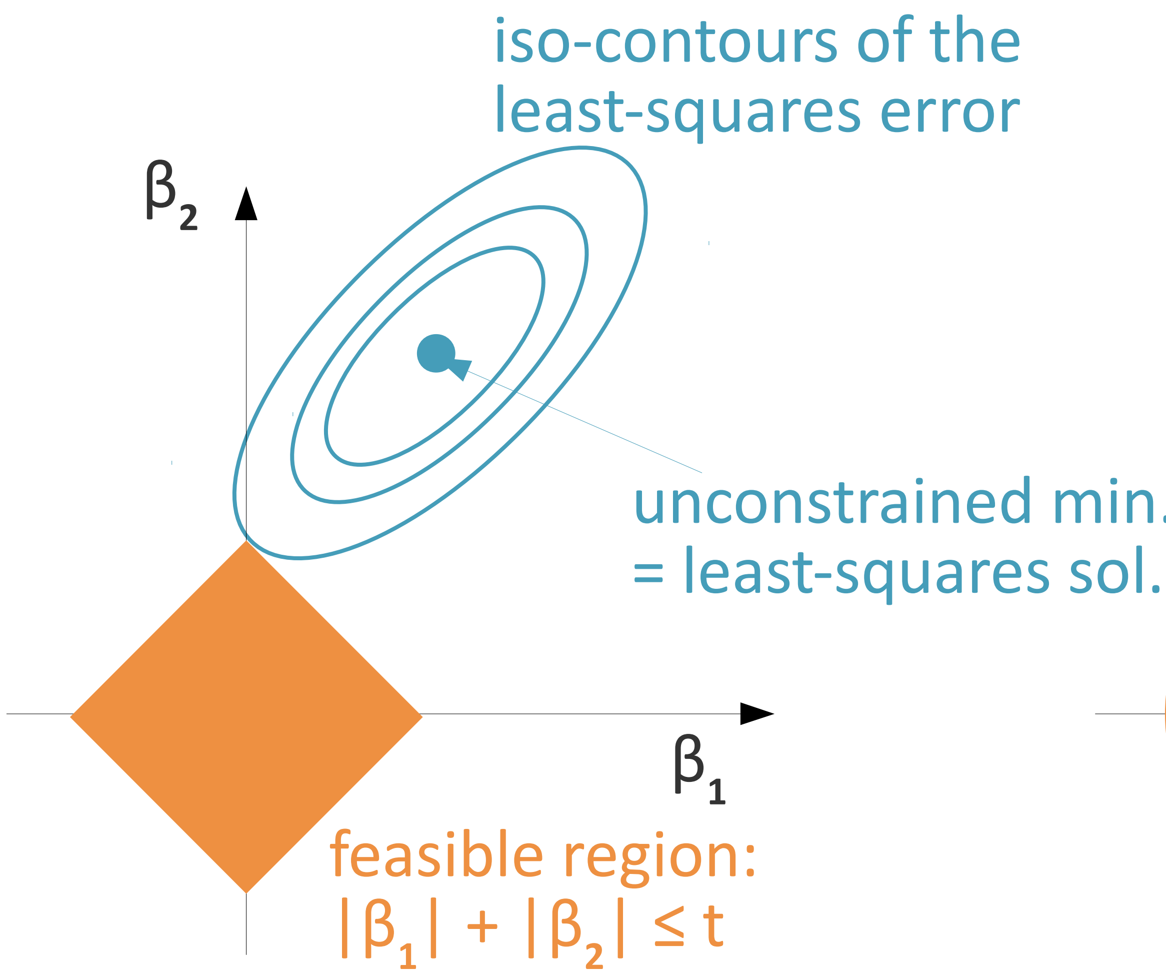
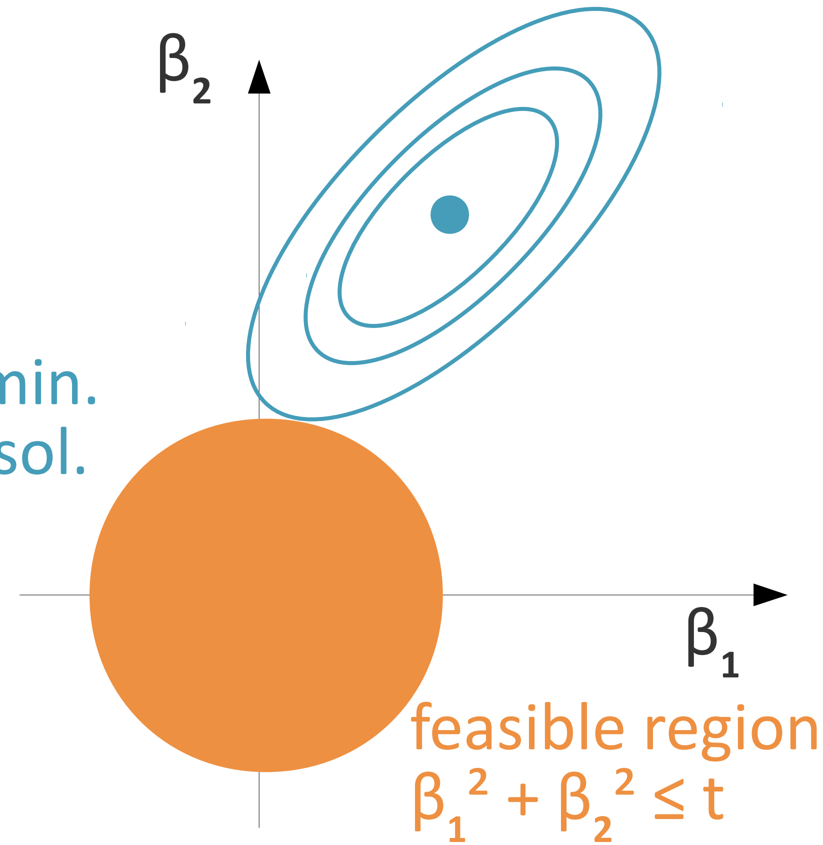


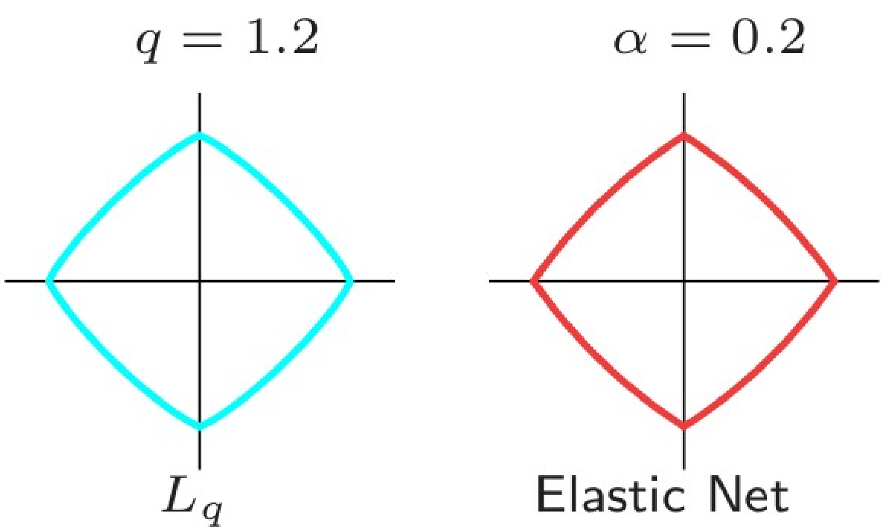
L2 norm



Elastic net

- **Elastic penalty**

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



Structured regularization

Group lasso

Use K predefined groups of variables that are known to "work"together and expected to be either all active or all inactive together.

E.g.

- genes belonging to the same biological pathway.

$$\hat{\beta} = \arg\min_{\beta} ||y - \sum_{k=1}^{K} X_k \beta_k||_2^2 + \lambda \sum_{k=1}^{K} \sqrt{p_k}\, ||\beta_k||_2$$

Size of group k

Features belonging to group k

Other examples of structured penalties

- **Overlapping groups**

  Jacob et al. (2009). Group lasso with overlap and graph lasso. *ICML.*

- **Graphs**

  Li & Li (2010). Variable selection and regression analysis for graph-structured covariates with an application to genomics. *Ann. App. Stats.*

- **Trees**

  Zhao et al. (2006). Grouped and hierarchical model selection through composite absolute penalties. *Ann. Stat.*

- **Multiple related tasks**

  Obozinski et al. (2006). Multitask feature selection. *Technical Report, UC Berkeley.*

Minimize SSE + λ x regularizer

- **Ridge**
  - gives similar weights to similar variables
  - not very sparse
  - analytical solution
- **Lasso**
  - randomly picks one of several correlated variables
  - sparse
  - LAR algorithm
- **Elastic net**
  - selects variables like the lasso
  - shrinks together the coefficients of correlated variables.
- **Many other regularizers** are possible

  Lp norms, groups, graphs, trees...