CentraleSupélec

Statistics and Learning

Lecturers (alphabetic order):

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† Course coordinator

Lecture 8/9

Regularization and model selection

Course objectives

- Introduction to regularization for regression and classification.
- Estimation of generalization error.
- Selection of hyperparameter values and model selection.

Lecture outline

1 – Regularized regression (or classification): penalization

2 – Estimation of the risk (generalization error)

3 – Hyper-parameters, model selection

4 – Exercises and solutions

5 – Appendices

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1 – Regularized regression (or classification): penalization
- 1.1 – Limitations of "ordinary least squares"
- 1.2 – Ridge regression
- 1.3 – LASSO regression

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Limitations of "ordinary least squares"

Recall that $\underline{X}$ has size #individuals $\times$ #variables ($n \times (p+1)$).

Critical situations for (ordinary) linear regression:

- when $\underline{X}^\top \underline{X}$ is singular
- or poorly conditioned

Typical cases

1. when the number of variables is large
2. when there are strong correlations between explanatory variables

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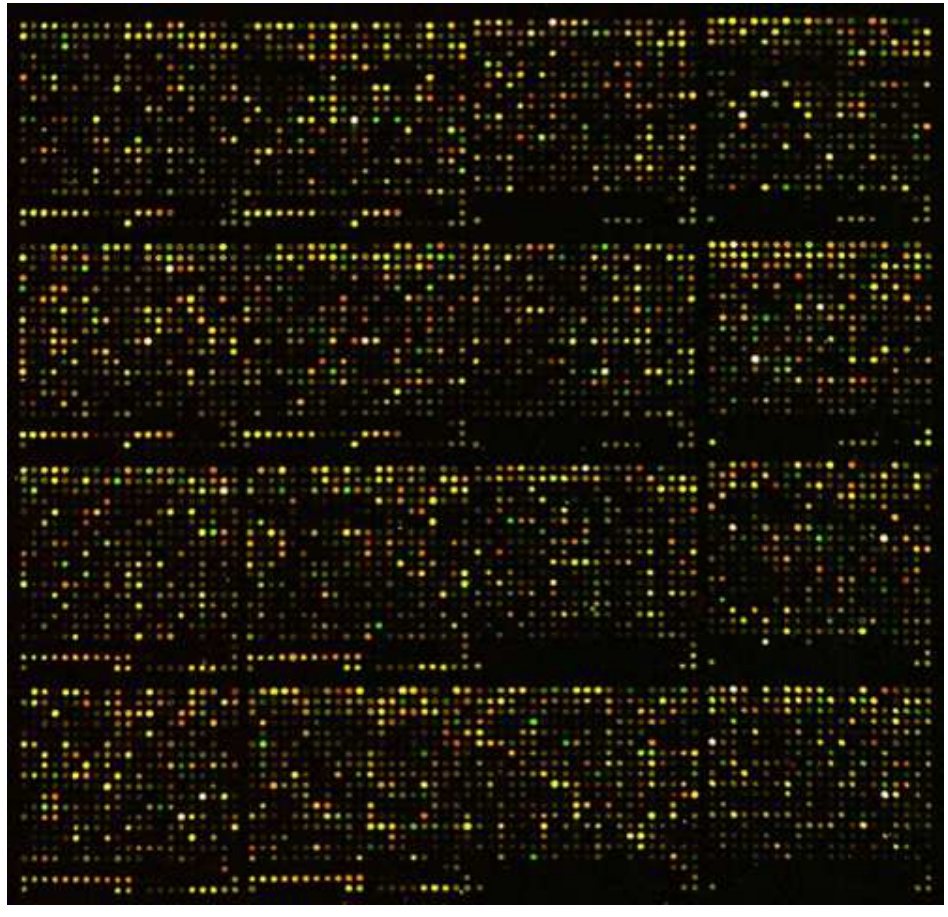
Example: $p \gg n$



Subset of a microarray for transcriptome analysis,
$p \approx 25000$ *for one patient*

Typically, $n \approx 10$ or 100!

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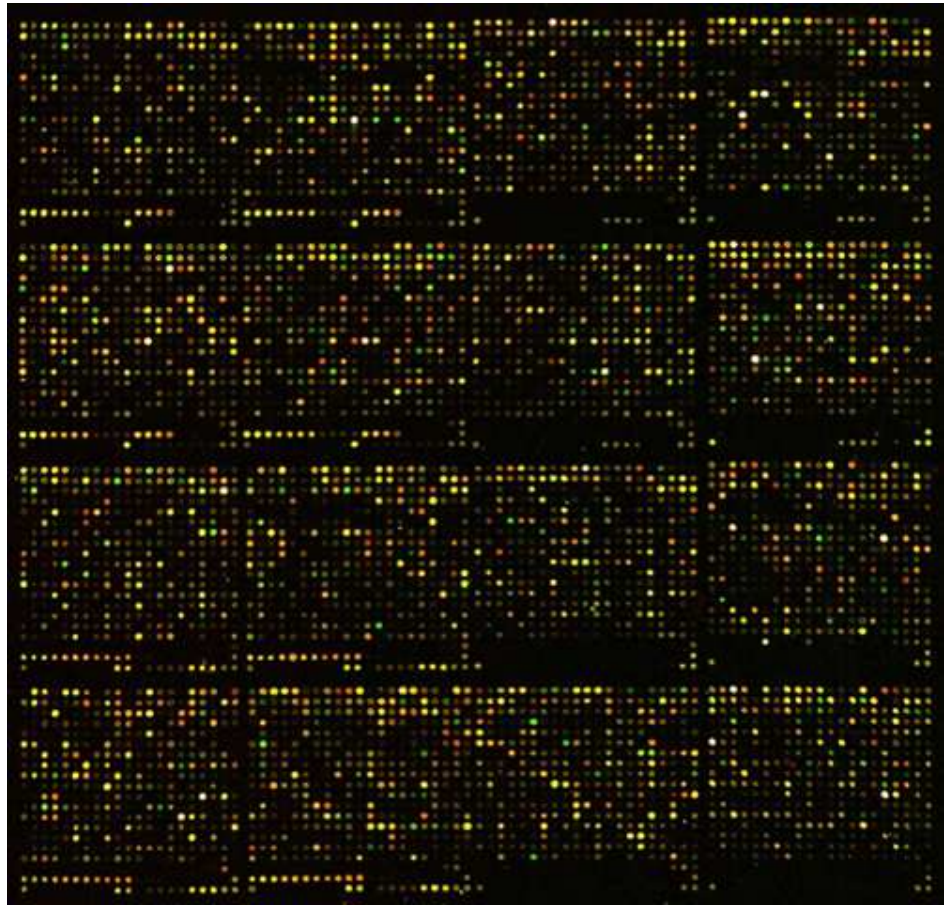

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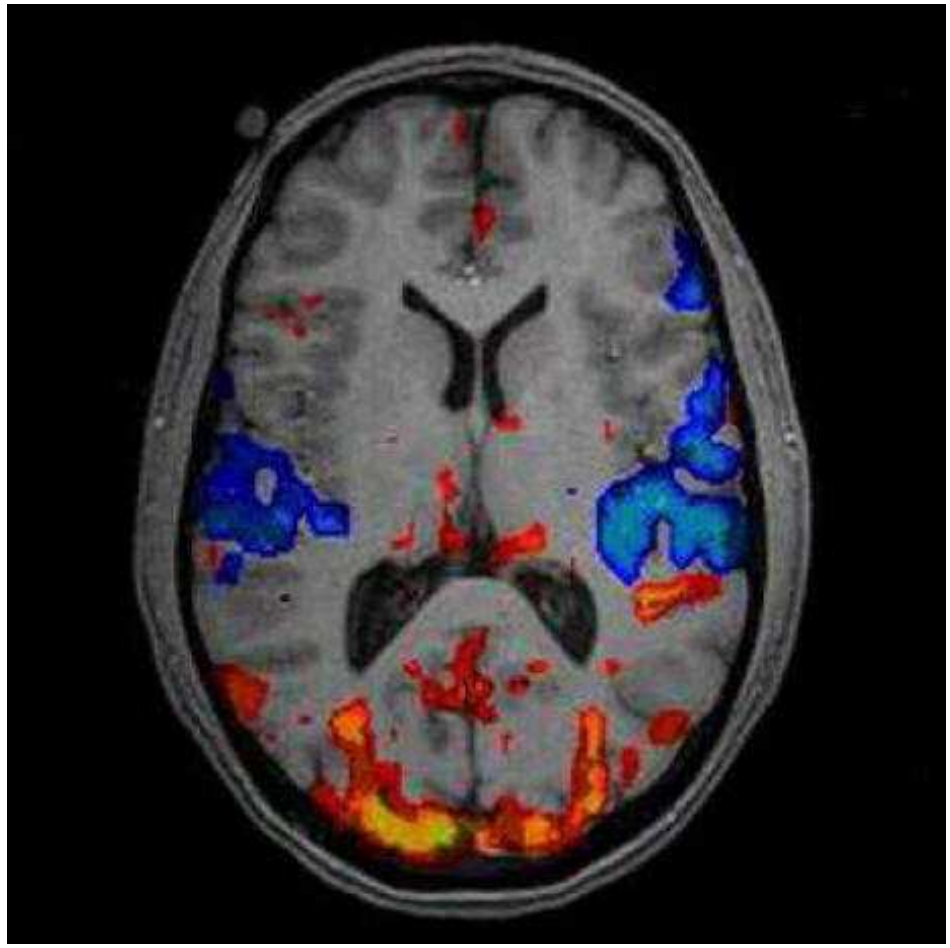
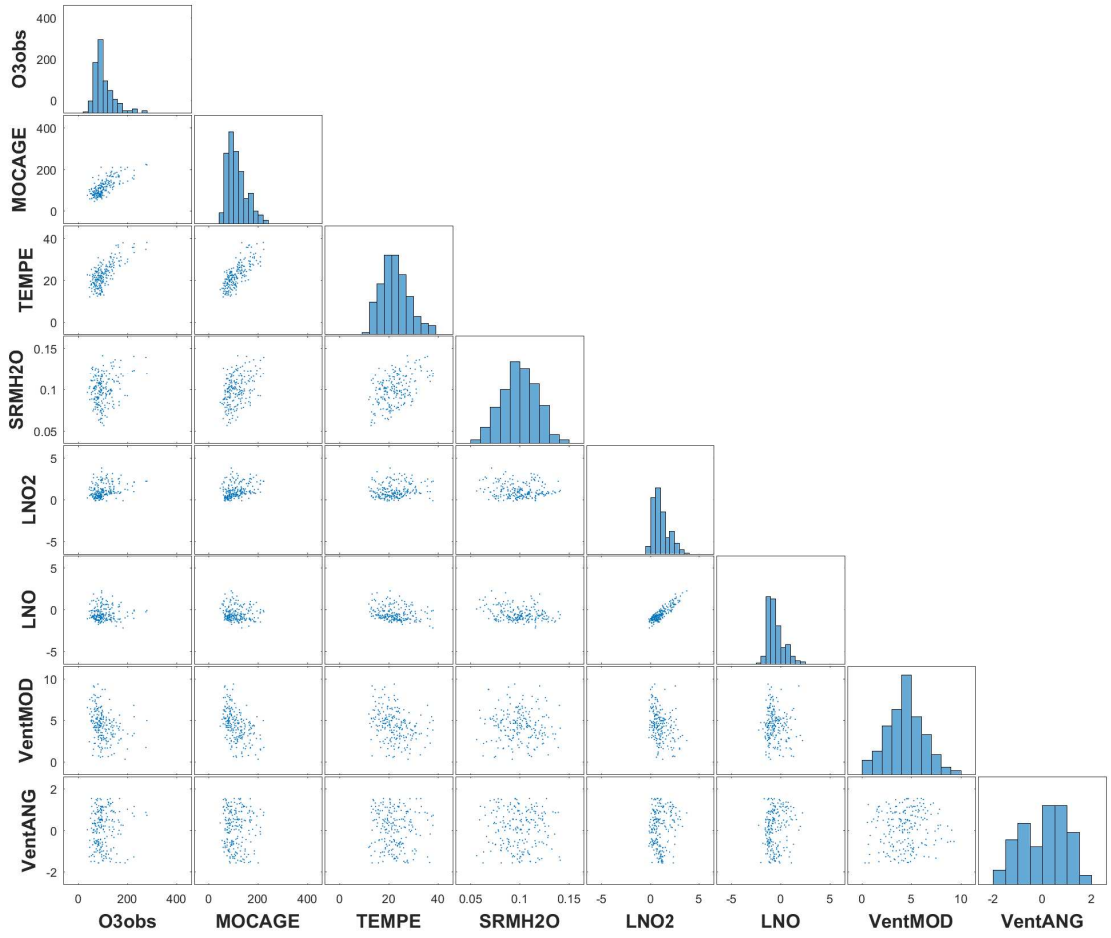


Functional Magnetic Resonance Imaging (fMRI), with approximately, $p \approx 300000$ *voxels*

Typically, $n \approx 10$ or 100!

Example: strong correlation between explanatory variables



"Ozone" example $\longrightarrow$ correlation between variables NO and NO2

Example: strong correlation. . . (cont'd)

Vector $\hat{\beta}$ obtained by OLS regression:

β_0	MOCAGE	TEMPE	RMH2O	NO2	NO	VentMOD	VentANG
103.4	28.9	22.5	-3.2	-34.4	37.9	1.4	2.6

Observations:

- The negative coefficient associated to NO2 is surprising
  ➠ hazardous interpretation of the coefficients
- The least influential variables (small coefficients) could perhaps be removed from the model?

One possible solution: penalized regression

A penalty term is added to the empirical risk:

$$\hat{\beta} = \arg\min_{\beta} \underbrace{\|\underline{Y} - \underline{X}\beta\|^2}_{\text{data "fidelity"}} + \underbrace{\lambda}_{\text{hyperparameter}} \underbrace{\Omega(\beta)}_{\text{penalty}} . \qquad (\star)$$

Expected benefits of penalization:

- make the solution of $(\star)$ unique,
- take prior information into account (this is related to the Bayesian approach),
- avoid over-fitting when the family of predictor functions is "large" (for linear models: $p \gg n$),
- make it easier to interpret the resulting model.

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Ridge regression

Penalty

$\Omega(\beta) = \|\beta\|^2$

$$\hat{\beta}^{\text{RIDGE}} = \arg\min_{\beta} \|\underline{Y} - \underline{X}\beta\|^2 + \lambda\|\beta\|^2$$

It can be proved that (➠ see PC) :

$$\hat{\beta}^{\text{RIDGE}} = \left(\underline{X}^\top \underline{X} + \lambda I_{p+1}\right)^{-1} \underline{X}^\top \underline{Y}.$$

➠ When $\lambda \nearrow$, the conditioning of $\left(\underline{X}^\top \underline{X} + \lambda I_{p+1}\right)$ improves.

Remark: $\hat{\beta}^{\text{RIDGE}}$ has a Bayesian interpretation (➠ see PC).

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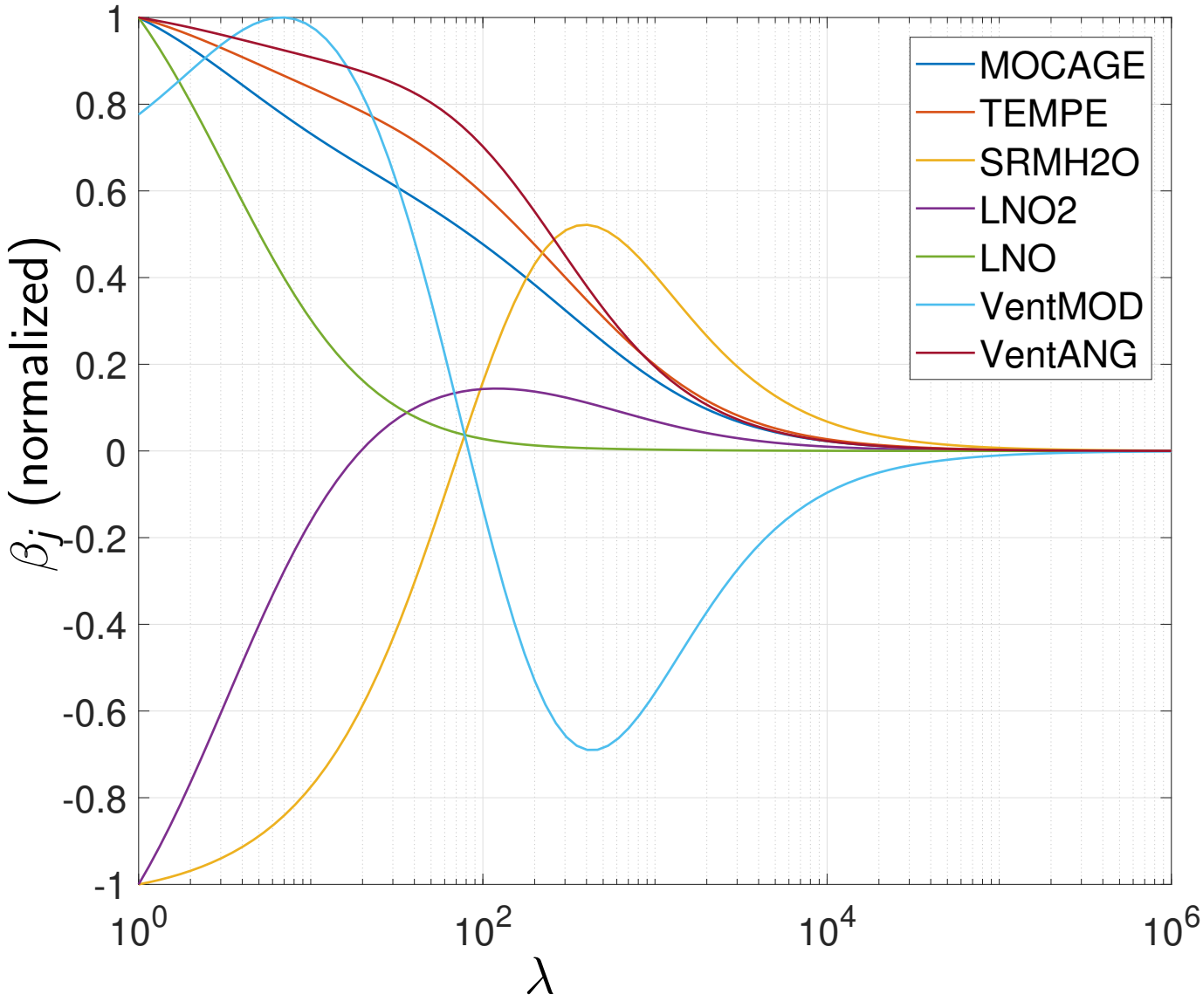
"Ozone" example: Evolution of $\hat{\beta}^{RIDGE}$ as a function of λ



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LASSO regression

Penalty

$\Omega(\beta) = \|\beta\|_1 = \sum_{j=1}^{n} |\beta_j|$

$$\hat{\beta}^{\text{LASSO}} = \arg\min_{\beta} \|\underline{Y} - \underline{X}\beta\|^2 + \lambda\|\beta\|_1 \qquad (\star)$$

Minimization of the criterion

- no explicit solution for $\hat{\beta}^{\text{LASSO}}$ (except in some cases, exercice 1)
- dedicated algorithms

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LASSO regression: reformulation

$$\hat{\beta}^{\text{LASSO}} = \arg\min_{\beta} \|\underline{Y} - \underline{X}\beta\|^2 + \lambda\|\beta\|_1 \qquad (\star)$$

- Let $\hat{\beta}^{\text{OLS}}$ denote the OLS estimator of β:

$$\hat{\beta}^{\text{LASSO}} = \hat{\beta}^{\text{OLS}} \qquad \text{for} \lambda = 0$$

- Since $\|\underline{Y} - \underline{X}\beta\|^2 = \|\underline{X}(\beta - \hat{\beta}^{\text{OLS}})\|^2 + c$, we have:

$$\hat{\beta}^{\text{LASSO}} = \arg\min_{\beta} \|\underline{X}(\beta - \hat{\beta}^{\text{OLS}})\|^2 + \lambda\|\beta\|_1$$

- Reformulation with a contraint: it can be proved that there exists $c_\lambda \in \mathbb{R}^+$ such that

$$\hat{\beta}^{\text{LASSO}} = \arg\min_{\beta} \|\underline{X}(\beta - \hat{\beta}^{\text{OLS}})\|^2 \text{ such that} \|\beta\|_1 \leq c_\lambda$$

(and similarly for $\hat{\beta}^{\text{RIDGE}}$)

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LASSO regression: intuitive interpretation

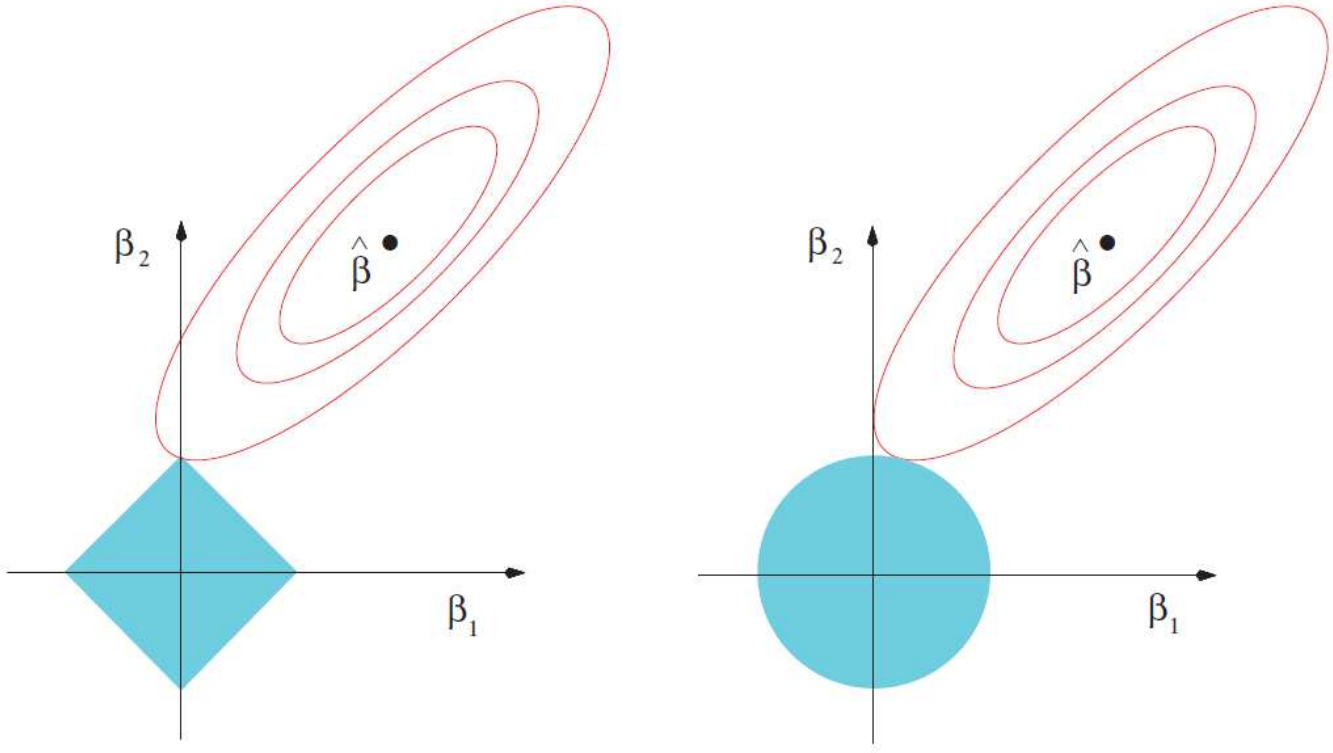
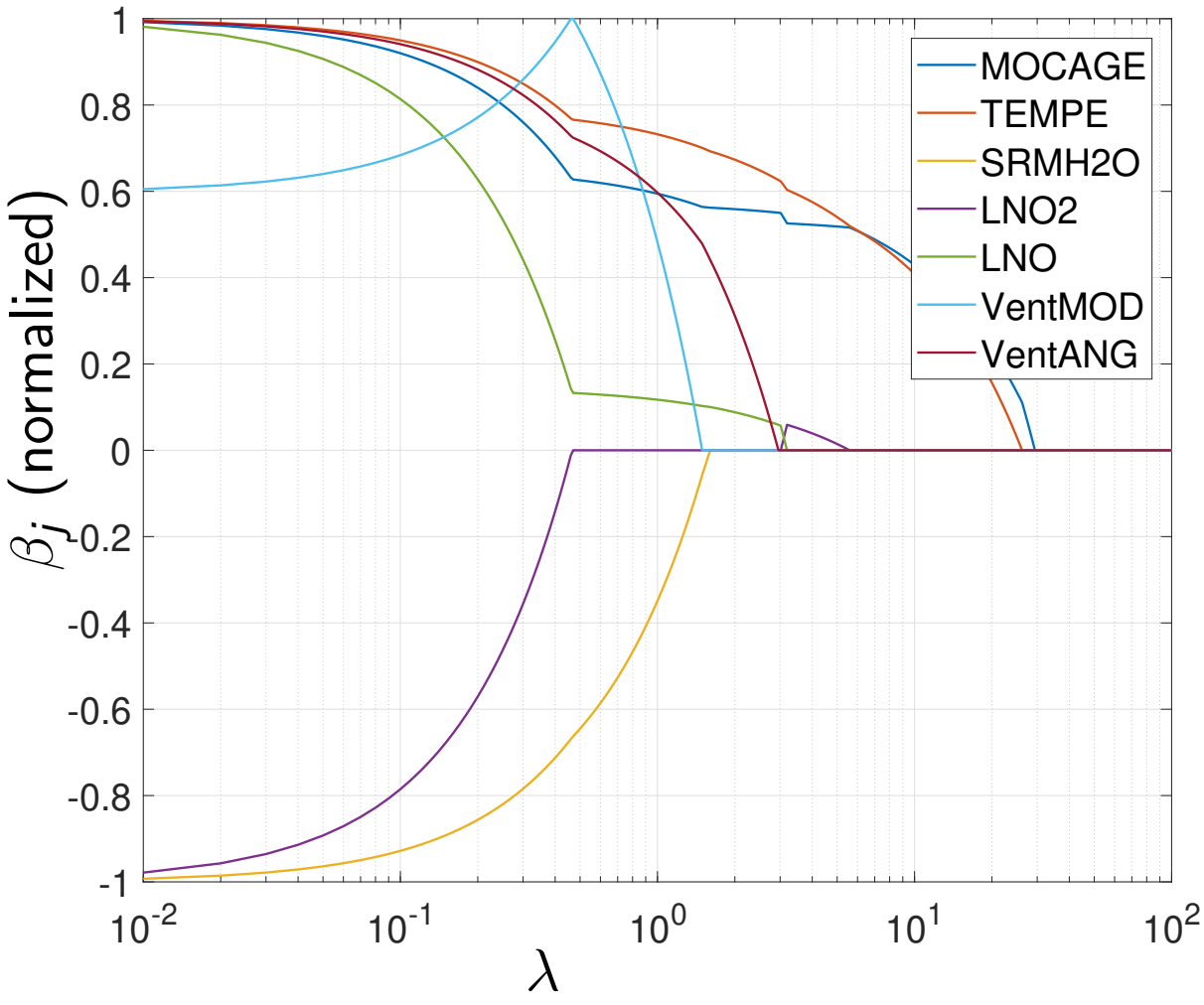


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$, *respectively, while the red ellipses are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

"Ozone" example: $\hat{\beta}^{\mathrm{LASSO}}$ versus λ



When $\lambda \nearrow$, the number of coefficients equal to zero $\nearrow$

"Ozone" example: $\hat{\beta}^{\text{LASSO}}$ for several λ

With $\lambda = 0$ (OLS)

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➠ The coefficient for NO2 may seem surprising

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➠ One of the two correlated variables is discarded,
makes it easier to interpret the coefficients

With $\lambda = 3$

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➠ The remaining variables are progressively discarded

Choice of the hyper-parameter λ ?

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Problem

Back to the general setting (regression/classification).

Let $\hat{h}$ be a predictor $\mathcal{X} \to \mathcal{Y}$ learned from data:

$$\hat{h}(x) \;=\; \hat{h}(x; (X_1, Y_1), \ldots, (X_n, Y_n)) \;=\; \hat{h}(x; \underline{X}, \underline{Y}).$$

Recall that, given a loss function L, we define the risk, or generalization error :

$$\begin{aligned} \mathscr{R}(\hat{h}) \;&=\; \mathbb{E}\left(L(Y, \hat{h}(X)) \;\middle|\; \underline{X}, \underline{Y} \right) \\ &= \iint_{\mathcal{X}\times\mathcal{Y}} L(y, \hat{h}(x)) \, \mathrm{P}^{X,Y}(\mathrm{d}x, \mathrm{d}y). \end{aligned}$$

Examples. $L(y, \tilde{y}) = (y - \tilde{y})^2$, $L(y, \tilde{y}) = |y - \tilde{y}|$, $L(y, \tilde{y}) = \mathbb{1}_{y \neq \tilde{y}}$, ...

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How can we estimate this risk (which depends on $\mathrm{P}^{X,Y}$) ?

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Refresher: empirical risk

We call empirical risk the risk

$$\widehat{\mathscr{R}}_n = \iint_{\mathcal{X}\times\mathcal{Y}} L(y, \hat{h}(x))\, \hat{\mathrm{P}}_n(\mathrm{d}x, \mathrm{d}y) = \frac{1}{n}\sum_{i=1}^{n} L(Y_i, \hat{h}(X_i))$$

computed with $\mathrm{P}^{X,Y}$ equal to $\hat{\mathrm{P}}_n = \frac{1}{n}\sum_{i=1}^{n} \delta_{X_i,Y_i}$.

Question

Is this empirical risk $\widehat{\mathscr{R}}_n$, in general, a "good" estimator of the true risk $\mathscr{R}(\hat{h})$?

the data is used twice !

Intuition: It is "risky" to estimate the risk from the error observed on the same data already used to construct $\hat{h}$...

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Zoom in on an illuminating special case

Consider the case of "ordinary" linear regression:

- $h(x) = \beta_0 + \beta_1 x^{(1)} + \ldots + \beta_p x^{(p)}$,
- quadratic loss: $L(y, \tilde{y}) = (y - \tilde{y})^2$,
- $p+1 \leq n$ and $\underline{X}^\top \underline{X}$ an a.s. invertible $(p+1) \times (p+1)$ matrix.

Empirical risk minimization : $\hat{\beta} = \left(\underline{X}^\top \underline{X}\right)^{-1} \underline{X}^\top \underline{Y}$.

Remark: link between $\hat{\mathscr{R}}_n$ and the coefficient R^2 of determination:

$$R^2 = 1 - \frac{\mathrm{RSS}(\hat{\beta})}{\mathrm{TSS}} = 1 - \frac{\sum_{i=1}^n \left(Y_i - \hat{\beta}^\top X_i\right)^2}{\sum_{i=1}^n \left(Y_i - \bar{Y}\right)^2}$$

$$= 1 - \frac{\hat{\mathscr{R}}_n}{\widehat{\mathrm{var}}_n(Y)} \qquad \text{with } \widehat{\mathrm{var}}_n(Y) = \frac{1}{n} \sum_{i=1}^n \left(Y_i - \bar{Y}\right)^2.$$

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$$= 1 - \frac{\widehat{\mathscr{R}}_n}{\widehat{\mathrm{var}}_n(Y)} \qquad \text{with } \widehat{\mathrm{var}}_n(Y) = \frac{1}{n} \sum_{i=1}^n \left(Y_i - \bar{Y}\right)^2.$$

Zoom in on an illuminating special case

Consider the case of "ordinary" linear regression:

- $h(x) = \beta_0 + \beta_1 x^{(1)} + \ldots + \beta_p x^{(p)}$,
- quadratic loss: $L(y, \tilde{y}) = (y - \tilde{y})^2$,
- $p+1 \leq n$ and $\underline{X}^\top \underline{X}$ an a.s. invertible $(p+1) \times (p+1)$ matrix.

Empirical risk minimization : $\hat{\beta} = \left(\underline{X}^\top \underline{X}\right)^{-1} \underline{X}^\top \underline{Y}$.

Remark: link between $\hat{\mathscr{R}}_n$ and the coefficient R^2 of determination:

$$R^2 = 1 - \frac{\mathrm{RSS}(\hat{\beta})}{\mathrm{TSS}} = 1 - \frac{\sum_{i=1}^n \left(Y_i - \hat{\beta}^\top X_i\right)^2}{\sum_{i=1}^n \left(Y_i - \bar{Y}\right)^2}$$

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Zoom on an illuminating special case (cont'd)

Consider the generalization error wrt responses only:

$$\widetilde{\mathscr{R}}_n \;=\; \mathbb{E}\left(\frac{1}{n}\sum_{i=1}^{n}\left(\widetilde{Y}_i - \hat{\beta}^\top X_i\right)^2 \;\middle|\; \underline{X}, \underline{Y}\right),$$

with, for all i, $\widetilde{Y}_i$ and Y_i iid conditionally to $\underline{X}$.

Proposition

Assume that the unknown distribution $\mathrm{P}^{X,Y}$ is such that $Y_i = \beta^\top X_i + \varepsilon_i$, with $\varepsilon_i \sim \mathscr{N}(0, \sigma^2)$, independent of X_i. Then

$$\mathbb{E}\left(\widetilde{\mathscr{R}}_n\right) \;=\; \sigma^2\left(1 + \frac{p+1}{n}\right),$$

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Zoom on an illuminating special case (cont'd)

Interpretation. On average, the empirical risk under-estimates the generalization error:

$$\mathbb{E}\left(\widetilde{\mathscr{R}}_n - \widehat{\mathscr{R}}_n\right) \;=\; 2\,\frac{p+1}{n}\,\sigma^2 \;>\; 0.$$

Another way of looking at this result. Set

$$\eta \;=\; \frac{p+1}{n} \;=\; \frac{\text{number of coefficients}}{\text{sample size}}.$$

Then

$$\frac{\mathbb{E}\left(\widetilde{\mathscr{R}}_n\right)}{\mathbb{E}\left(\widehat{\mathscr{R}}_n\right)} \;=\; \frac{1+\eta}{1-\eta} \;\xrightarrow[\eta\to 1]{}\; +\infty.$$

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Proof. Let us compute first $\mathbb{E}\left(\widetilde{\mathscr{R}}_n \mid \underline{X}\right)$ with (reminder)

$$\widetilde{\mathscr{R}}_n \;=\; \mathbb{E}\left(\frac{1}{n}\sum_{i=1}^{n}\left(\widetilde{Y}_i - \hat{\beta}^\top X_i\right)^2 \;\middle|\; \underline{X}, \underline{Y}\right).$$

We have $\mathbb{E}\left(\widetilde{Y}_i \mid \underline{X}\right) = \mathbb{E}\left(\hat{\beta}^\top X_i \mid \underline{X}\right) = \beta^\top X_i$, therefore

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Zoom on an illuminating special case (cont'd)

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$$\begin{aligned} \circledast &= \text{var}\left(\hat{\beta}^\top X_i \mid \underline{X}\right) \\ &= X_i^\top \text{var}\left(\hat{\beta} \mid \underline{X}\right) X_i \\ &= \sigma^2 X_i^\top \left(\underline{X}^\top \underline{X}\right)^{-1} X_i \\ &= \sigma^2 \, \text{tr}\left(\left(\underline{X}^\top \underline{X}\right)^{-1} X_i X_i^\top\right). \end{aligned}$$

By noting that $\underline{X}^\top \underline{X} = \sum_i X_i X_i^\top$, we get:

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$$\mathbb{E}\left(\widetilde{\mathscr{R}}_n \mid \underline{X}\right) = \frac{1}{n}\sum_{i=1}^{n}\left(\underbrace{\mathsf{var}\left(\widetilde{Y}_i \mid \underline{X}\right)}_{=\sigma^2} + \underbrace{\mathsf{var}\left(\hat{\beta}^\top X_i \mid \underline{X}\right)}_{=\circledast}\right)$$
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Hence the result: $\mathbb{E}\left(\widetilde{\mathscr{R}}_n\right) = \sigma^2\left(1+\frac{p+1}{n}\right)$.

Exercise: prove the second inequality, i.e.,

$$\mathbb{E}\left(\widehat{\mathscr{R}}_n\right) = \sigma^2\left(1-\frac{p+1}{n}\right).$$

➠ see PC

Zoom on an illuminating special case (cont'd)

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Lecture outline

1 – Regularized regression (or classification): penalization

2 – Estimation of the risk (generalization error)
- 2.1 – Problem
- 2.2 – Zoom in on an illuminating special case
- 2.3 – Training set and test set

3 – Hyper-parameters, model selection

4 – Exercises and solutions

5 – Appendices

Training set and test set

Conclusion/extrapolation. The empirical risk is in general

- a negatively biased estimator of the risk,
- with a bias that is increasing when $p \nearrow$.

Solution: split the data in two sets

- training data: used to construct $\hat{h}$,
- test data: used to estimate the generalization error.

Example:

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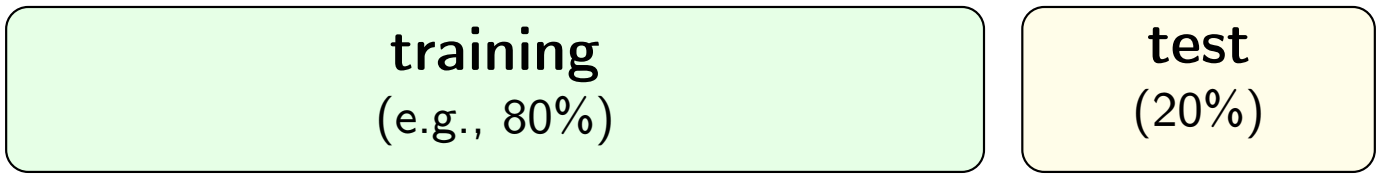
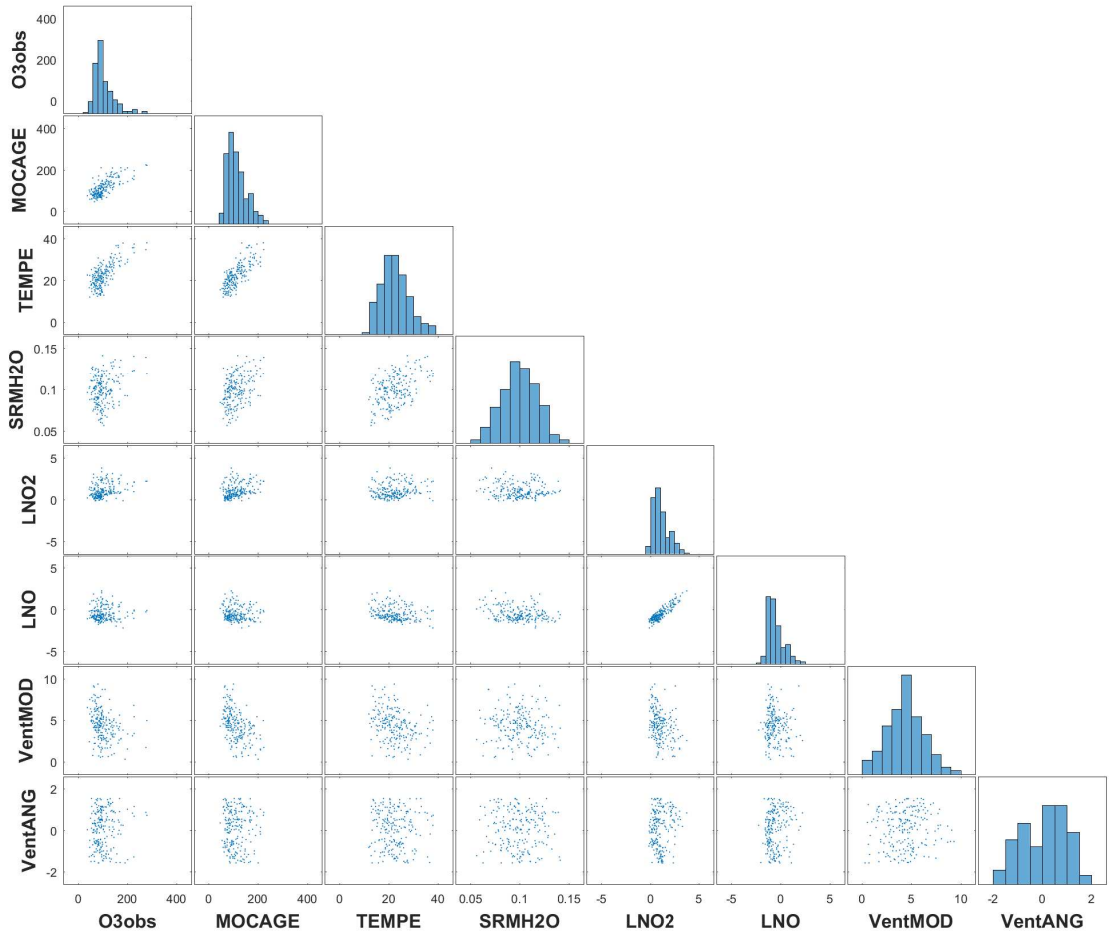


Exemple "Ozone" (cont'd from lecture #6)



Goal: predict the ozone concentation on day $t+1$ from data available on day t

"Ozone" example: 70/30

All 7 explanatory variables and their 21 interactions are used.

Results from 10 random splits, 70% / 30%:

R^2	$\hat{\mathscr{R}}_n$	$\hat{\mathscr{R}}_n^{\text{test}}$
0.77185	345.1	573.32
0.76831	371.41	496.03
0.77292	343.96	608.62
0.76093	350.53	606.14
0.78584	345.45	669.66
0.75459	399.9	476.61
0.71367	343.72	643.72
0.77689	377.32	524.74
0.8176	317.83	695.86
0.79784	373.18	554.25

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Problem #1: choosing a "good" family $\mathscr{H}$

Example. Selection of k variables among p. Let $J \subset \{1, \dots p\}$:

$$h(x) = \beta_0 + \sum_{j \in J} \beta_j x^{(j)}.$$

➠ Defines a family $\mathscr{H}_J$ with $k_J = \text{card}(J) + 1$ parameters.

Example. Expansion in a basis, truncated at order J :

$$h(x) = \sum_{k=0}^{J} \beta_j \psi_j(x).$$

➠ Defines a family $\mathscr{H}_J$ with $k_J = J + 1$ parameters. ➠ complement

Problem: model selection

How to choose the family $\mathscr{H}_J$ (and, in particular, its "size" k_J) ?

Remark: replace $h(x)$ with $\ln \frac{h(x)}{1-h(x)}$ for logistic regression.

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Problem #2: choosing a regularization hyper-parameter

Most methods require some "tuning"...

- Ridge/LASSO regression: $\hat{\beta} = \text{argmin}\, \hat{\mathscr{R}}^{\text{pen}}_{n,\lambda}$, with

$$\hat{\mathscr{R}}^{\text{pen}}_{n,\lambda}(\beta) \;=\; \hat{\mathscr{R}}_n(\beta) + \lambda \sum_j |\beta_j|^q, \quad q \in \{1, 2\},$$

- Choosing the number k of neighbors in a k-NN model:

$$h(x) = \frac{1}{k} \sum_{i \in \mathcal{V}_{n,k}(x)} y_i,$$

with $\mathcal{V}_{n,k}(x)$ the indices of the k nearest neighboors of x.

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Over-fitting: beware!

Idea

Choose the family $\mathscr{H}_J$, or the hyperparameter λ, in order to minimize (an estimation of) the generalization error.

⚠ again, the empirical risk $\hat{\mathscr{R}}_n$, estimated on the training data, is not appropriate !

Example. Polynomial regression with $x \in \mathbb{R}$, degree $\leq J$:

$$h(x) = \beta_0 + \beta_1 x + \ldots + \beta_J x^J,$$

with $J = 2, 5, 8, 11$.

Recall that, in linear regression, the empirical risk has a downward bias proportional to the number of parameters in the model.

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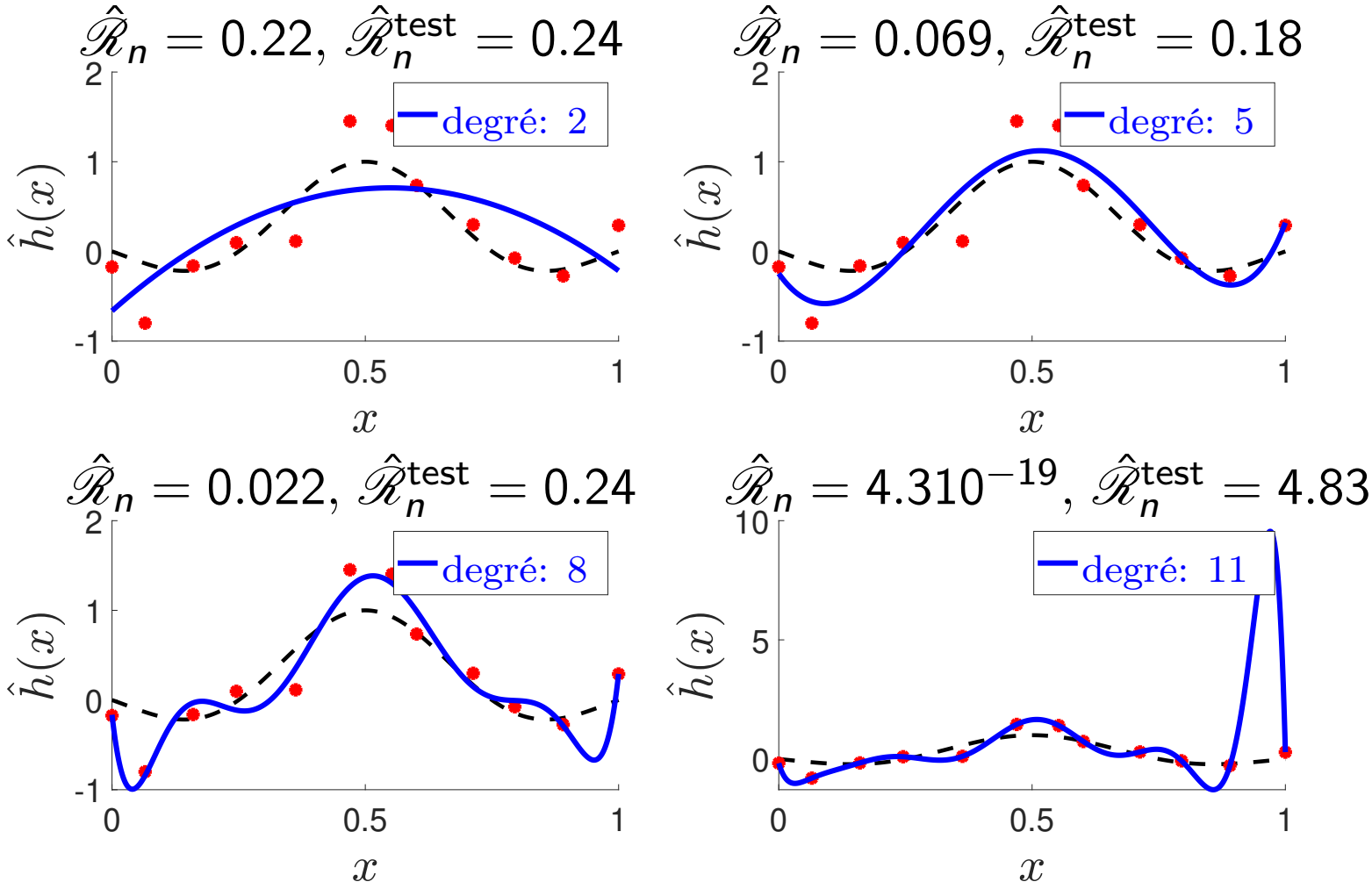
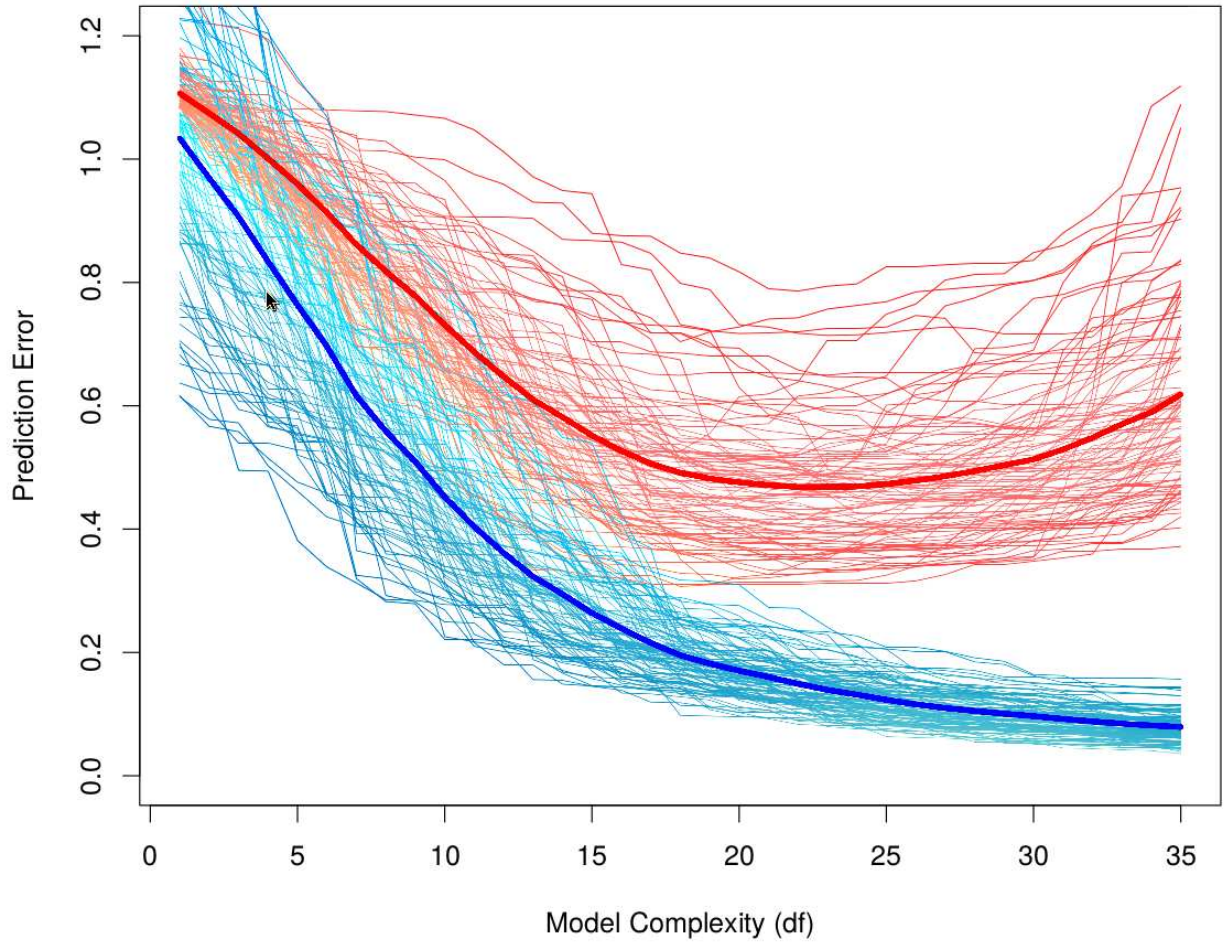


Understanding over-fitting: simulations



Blue: empirical risk $\hat{\mathscr{R}}_n$ / Red: error on the test set

Figure from Hastie, Tibshirani & Friedman (2017).
The Elements of Statistical Learning (12th edition), Springer.

Let's recapitulate...

Problem. We want to estimate the error to choose $\mathscr{H}$ or λ but...

- it should be done neither on the training data
  (➠ over-fitting problem),
- nor on the test data
  (➠ bias in the final estimation of the generalization error).

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Solution: validation set

Idea: split the data in three sets

- training data: construct $\hat{h}$ with given $\mathscr{H}$ / λ,
- validation set: choose $\mathscr{H}$, λ, etc.
- test data: estimate the generalization error.

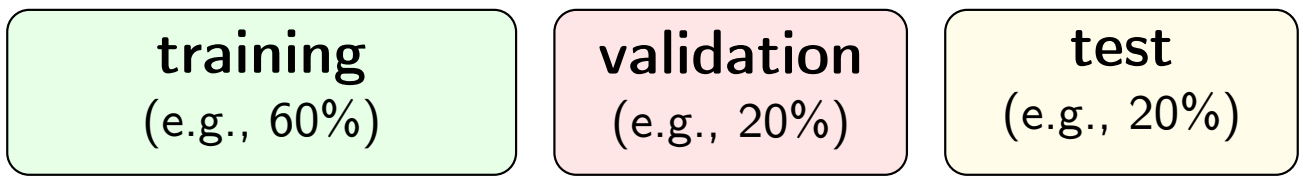
Simple validation (hold-out)

Solution: validation set

Idea: split the data in three sets

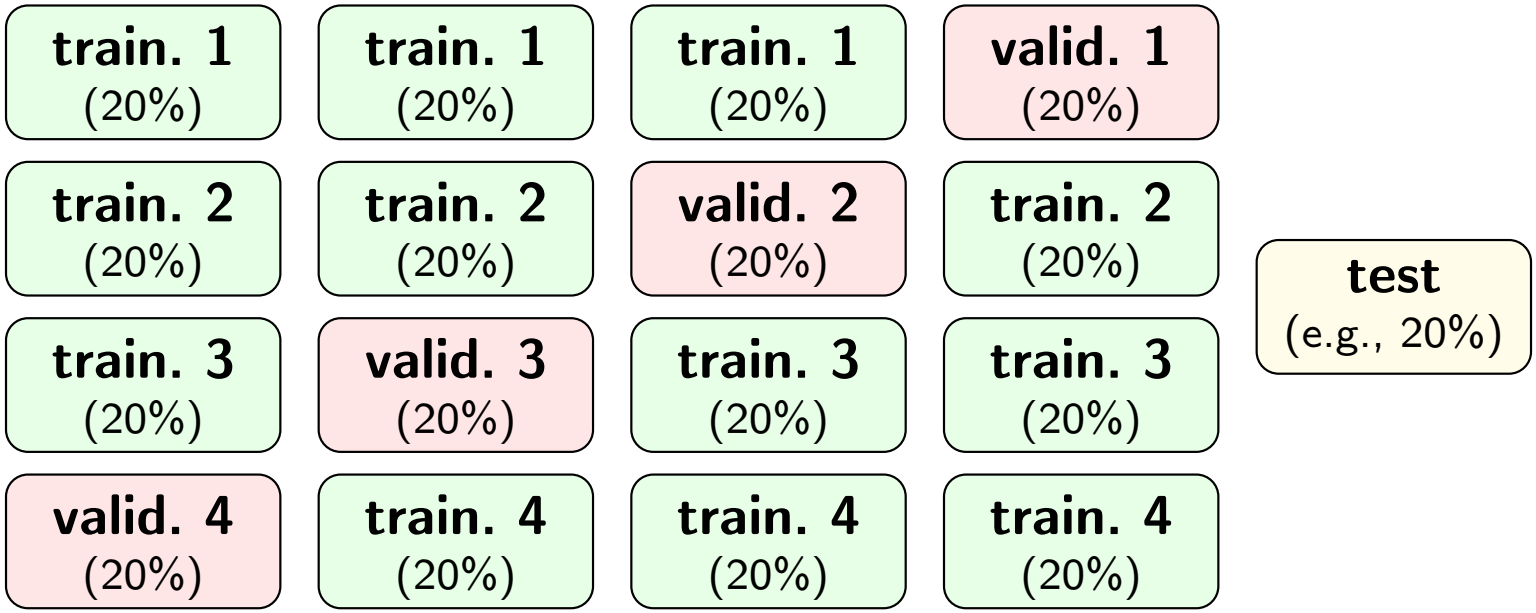
- training data: construct $\hat{h}$ with given $\mathscr{H}/\lambda$,
- validation set: choose $\mathscr{H}$, λ, etc.
- test data: estimate the generalization error.

Simple validation (hold-out)



Better validation: the cross validation method

k-fold cross-validation, here with $k = 4$:



➠ the error is averaged over the k validation sets.

Special case: leave-one-out cross validation

- $k = n$ blocks (of size $n/k = 1$).

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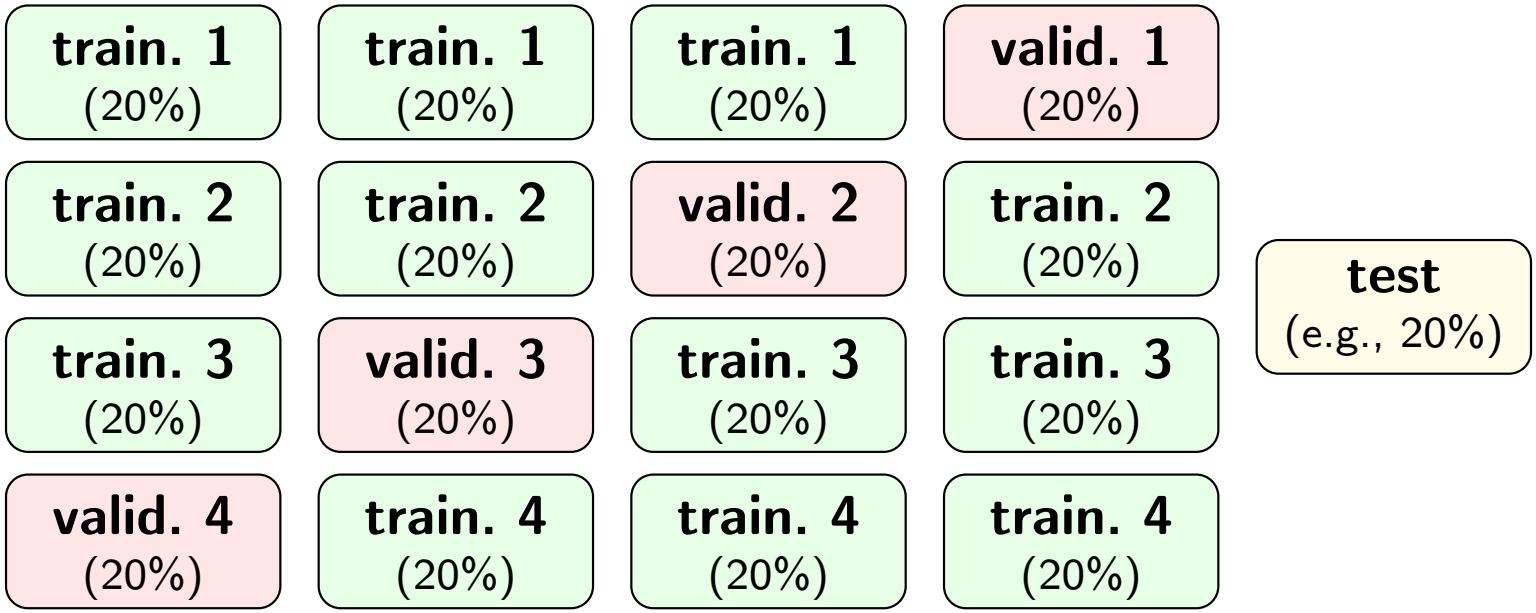

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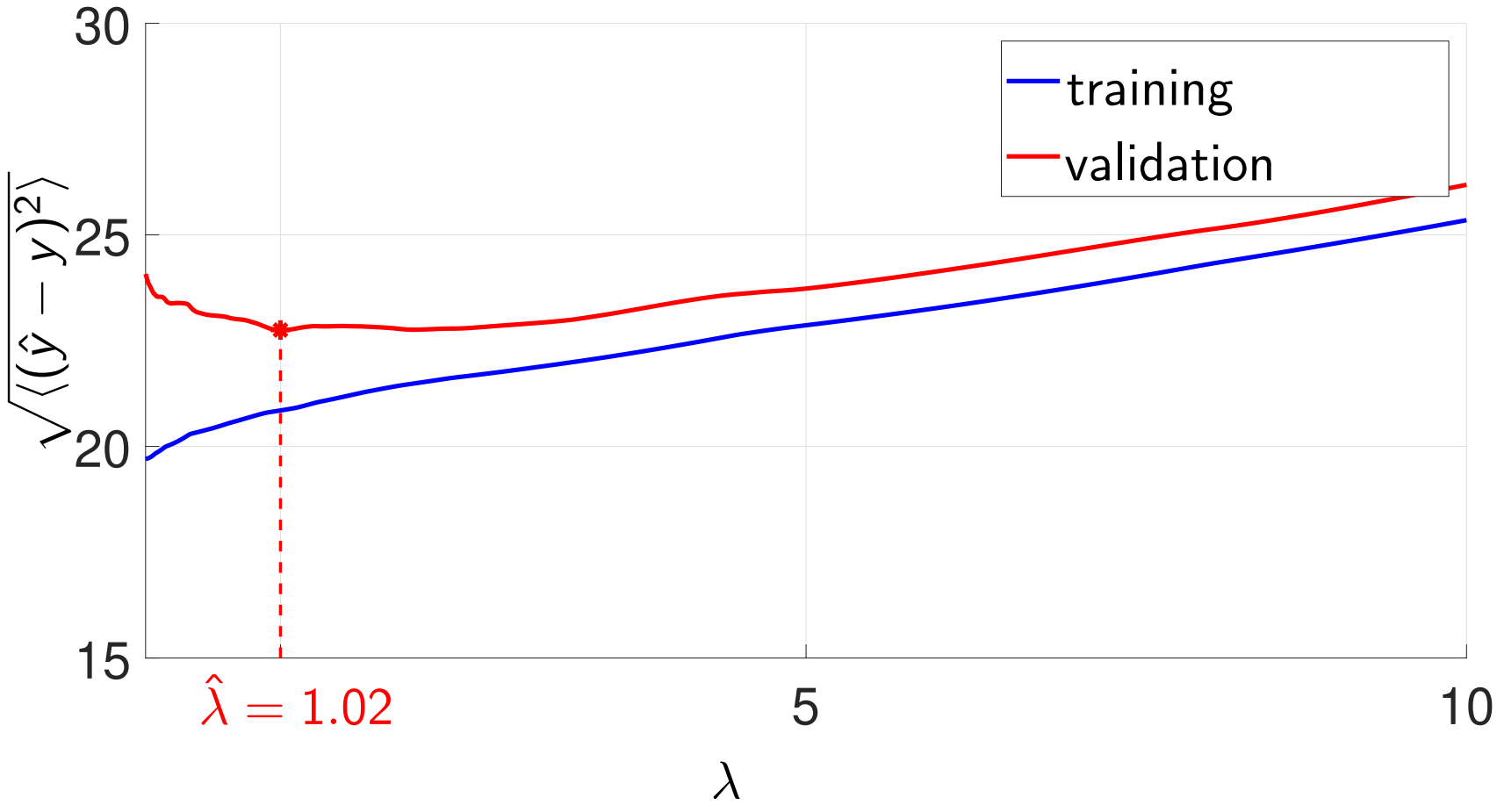
Special case: leave-one-out cross validation

- $k = n$ blocks (of size $n/k = 1$).

"Ozone" example: LASSO / choice of λ

- Predictor: LASSO regression using all variables and their interactions
- $\hat{\lambda}$ obtained by CV (LOO)



"Ozone" example: interactions

- We add variables of the form $X^{(j)}X^{(j')}$ and $X^{(j)}X^{(j')}X^{(j'')}$.
- LASSO regression (L^1 penalty).
- Hyper-parameter λ estimated through 10-fold CV.

model	$X^{(j)}$	$X^{(j)}\,X^{(j')}$	$X^{(j)}\,X^{(j')}\,X^{(j'')}$
total number of variables	7	35	119
number of selected variables ($\beta_j \neq 0$)	4	9	8
$\sqrt{MSE}$ CV (10-fold)	49.1	41.5	33.0
selected variables	MOCAGE TEMPE NO VentANG	MOCAGE TEMPE NO2 MOCAGE · TEMPE TEMPE^2 TEMPE · MH2O TEMPE · NO2 NO2 · VentANG VentANG · VentANG	MOCAGE TEMPE NO2 MOCAGE · TEMPE TEMPE^2 TEMPE · RMH2O TEMPE^2 · MOCAGE VentANG^2 · TEMPE

Lecture outline

1 – Regularized regression (or classification): penalization

2 – Estimation of the risk (generalization error)

3 – Hyper-parameters, model selection
- 3.1 – Problem
- 3.2 – Cross validation
- 3.3 – AIC criterion

4 – Exercises and solutions

5 – Appendices

Another approach to model selection: the AIC criterion

Assumption: parametric statistical models $\mathscr{M}_j$ for $\mathrm{P}^{Y|X}$.

Denote by $\hat{\theta}_j^{\mathrm{MLE}}$ the MLE of θ in model $\mathscr{M}_j$.

Then the AIC criterion can also be used for model selection:

$$\hat{j} = \operatorname{argmin} \mathrm{AIC}(j), \qquad \mathrm{AIC}(j) = -2 \ln \mathcal{L}\left(\hat{\theta}_j^{\mathrm{MLE}}; \underline{X}, \underline{Y}\right) + 2k_j,$$

with k_j the number of parameters in model $\mathscr{M}_j$.

➠ see PC for a partial justification (OLS linear regression)

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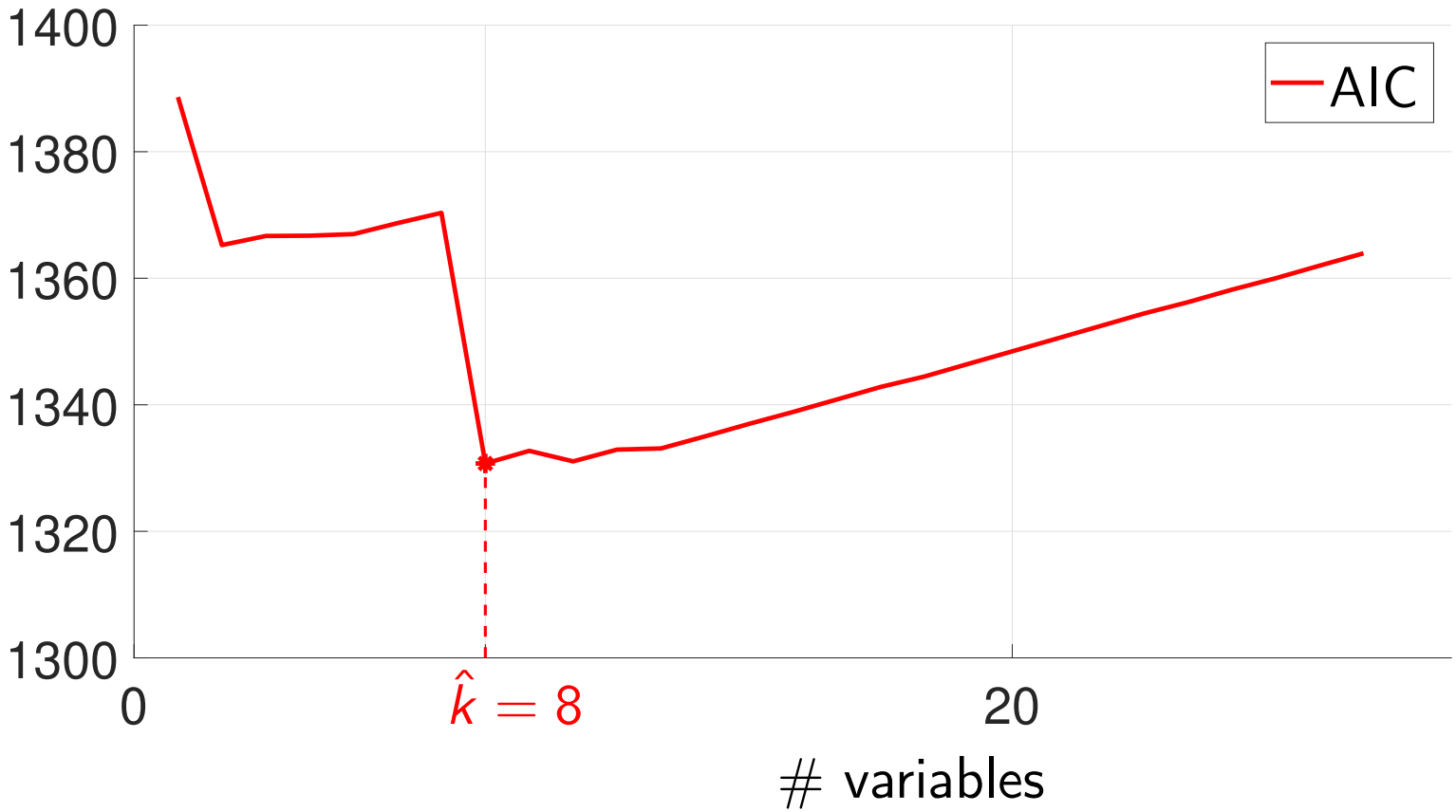
"Ozone" example: AIC

- Predictor obtained by the ordinary least squares method, on an increasing number of variables

  (linear terms first, then interactions)



Lecture outline

1 – Regularized regression (or classification): penalization

2 – Estimation of the risk (generalization error)

3 – Hyper-parameters, model selection

4 – Exercises and solutions
- 4.1 – Questions
- 4.2 – Solutions

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Exercise 1 (Penalized regression)

solution

Let $X_1, \ldots, X_n$ represent the examples, taking values in $\mathbb{R}^p$, and $Y_1, \ldots, Y_n$ be the labels, taking values in $\mathbb{R}$ The relationship between Y_i and X_i is given by:

$$Y_i = \beta_1 X_i^{(1)} + \ldots + \beta_p X_i^{(p)} + \varepsilon_i,$$

where β is the parameter vector to be estimated, and ε_i is a random variable following $\mathcal{N}(0, \sigma^2)$, independent of X_i.
We aim to estimate β by minimizing a criterion of the form

$$\frac{1}{2} \sum_{i=1}^{n} \left(Y_i - \beta^\top X_i \right)^2 + \lambda \mathcal{P}(\beta) \tag{1}$$

where $\mathcal{P}$ is a penalty term, and $\lambda \geq 0$ is a hyper-parameter.

Exercise 1 (Penalized regression)

solution

slide 12

We denote $X = [X_1 \dots X_n]^\top$, the $n \times p$ matrix containing the observations. **We are considering the case where $X^\top X = I_p$.**

Question

1. Give the expression of the estimator when $\lambda = 0$. Denote this estimator $\hat{\beta}$.
2. We consider a penalty of the form $\mathcal{P}(\beta) = \|\beta\|_2^2$. Give the expression of this estimator, denoted $\hat{\beta}^R$, and deduce that there exists a constant $c_{1,\lambda}$ (to be specified) such that $\hat{\beta}_j^R = c_{1,\lambda}\hat{\beta}_j$, $j = 1, \dots, p$.

Exercise 1 (Penalized regression)

solution

slide 12

Question

3. We consider a penalty of the form $\mathcal{P}(\beta) = \|\beta\|_1$.
   To begin with, demonstrate that the minimum on $\mathbb{R}$ of the function
   $$f : \alpha \mapsto \frac{1}{2}(x-\alpha)^2 + \lambda|\alpha|$$
   is achieved at$\alpha^* = \text{sign}(x)\max(0, |x| - \lambda)$.
4. Deduce the solution of the optimization problem (1) for $\mathcal{P}(\beta) = \|\beta\|_1$, which will be expressed in terms of $\hat{\beta}$. Denote this estimator $\hat{\beta}^L$.

Lecture outline

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Solution of exercise 1

back to questions

1. We recognize the least squares criterion, and we have:

$$\hat{\beta} = (X^\top X)^{-1} X^\top Y = X^\top Y$$

2. This corresponds to ridge regression..

$$\begin{aligned} \hat{\beta}^R &= (X^\top X + 2\lambda I)^{-1} X^\top Y \\ &= (1 + 2\lambda)^{-1} \hat{\beta} \end{aligned}$$

Therefore $\hat{\beta}_j^R = (1 + 2\lambda)^{-1} \hat{\beta}_j$.

Solution of exercise 1

back to questions

3. The function f is not differentiable, but it is differentiable at every point $\alpha \neq 0$ *and continuous at* $\alpha = 0$. Thus, we can determine its minimum by analyzing its variations using the sign of the derivative, as if it were differentiable everywhere. The derivative at every $\alpha \neq 0$ is given by

$$f'(\alpha) = \begin{cases} \alpha - x + \lambda & \text{si } \alpha > 0, \\ \alpha - x - \lambda & \text{si } \alpha < 0, \end{cases}$$

hence

$$f'(\alpha) > 0 \quad \Leftrightarrow \quad (\alpha > x - \lambda \text{ et } \alpha > 0) \text{ ou } (\alpha > x + \lambda \text{ et } \alpha < 0)\,. \tag{2}$$

Solution of exercise 1

back to questions

3. Let's consider, for example, $x > 0$. Then, the second case in the right-hand side of (2) is impossible, and we're left with:

$$f'(\alpha) > 0 \quad \Leftrightarrow \quad \alpha > x - \lambda \text{ et } \alpha > 0 \quad \Leftrightarrow \quad \alpha > \max(0, x - \lambda)\,. \tag{3}$$

Similarly, still assuming $x > 0$,

$$\begin{aligned} f'(\alpha) < 0 \quad &\Leftrightarrow \quad (\alpha < x - \lambda \text{ et } \alpha > 0) \text{ ou } (\alpha < x + \lambda \text{ et } \alpha < 0) \\ &\Leftrightarrow \quad (0 < \alpha < \max(0, x - \lambda)) \text{ ou } (\alpha < 0) \\ &\Leftrightarrow \quad (\alpha < \max(0, x - \lambda)) \text{ et } (\alpha \neq 0)\,. \end{aligned}$$

Thus, f strictly decreases to the left of $\max(0, x - \lambda)$, and strictly increases to the right, which concludes the case $x > 0$. The case $x < 0$ follows similarly.

Solution of exercise 1

back to questions

4. Here, we'll manipulate the initial optimization problem to reduce it to the optimization problem from the previous question.:

$$\begin{aligned}\hat{\beta}^L &= \underset{\beta}{\operatorname{argmin}} \frac{1}{2}\|Y - X\beta\|^2 + \lambda\|\beta\|_1 \\ &= \underset{\beta}{\operatorname{argmin}} \frac{1}{2}\|Y - X\hat{\beta} + X\hat{\beta} - X\beta\|^2 + \lambda\|\beta\|_1 \\ &= \underset{\beta}{\operatorname{argmin}} \frac{1}{2}\left\{\|Y - X\hat{\beta}\|^2 + \|X\hat{\beta} - X\beta\|^2\right\} + \lambda\|\beta\|_1\end{aligned}$$

The cross product vanishes because the residual $(Y - X\hat{\beta})$ is, by construction, orthogonal to any linear combination of columns of X, thus $(Y - X\hat{\beta})^\top (X\hat{\beta} - X\beta) = 0$.

Solution of exercise 1

back to questions

4. Since the first term is independent of β, we have:

$$\begin{aligned}\hat{\beta}^L &= \underset{\beta}{\operatorname{argmin}} \frac{1}{2}\|X\hat{\beta} - X\beta\|^2 + \lambda\|\beta\|_1 \\ &= \underset{\beta}{\operatorname{argmin}} \frac{1}{2}(\hat{\beta} - \beta)^\top X^\top X(\hat{\beta} - \beta) + \lambda\|\beta\|_1 \\ &= \underset{\beta}{\operatorname{argmin}} \frac{1}{2}(\hat{\beta} - \beta)^\top (\hat{\beta} - \beta) + \lambda\|\beta\|_1 \\ &= \underset{\beta}{\operatorname{argmin}} \frac{1}{2}\sum_{j=1}^{p}(\hat{\beta}_j - \beta_j)^2 + \lambda|\beta_j|\end{aligned}$$

The problem is separable and, from the previous question, we have:

$$\hat{\beta}_j^L = \operatorname{sign}(\hat{\beta}_j)\max(0, |\hat{\beta}_j| - \lambda)$$

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5.1 – Model building: feature engineering

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5.1 – Model building: feature engineering

Non-linearities in linear models...

If the empirical risk $\hat{\mathscr{R}}(\hat{h})$ is high, several possible causes:

- noise: intrinsic difficulty in predicting Y
  - ➠ irreducible statistical error.
- non-linearity of the optimal predictor wrt the $X^{(j)}$'s
  - ➠ reducible approximation error.

Possible workaround: $x^{(1)}, \ldots, x^{(p)} \mapsto \tilde{x}^{(1)}, \ldots, \tilde{x}^{(q)}$

- with $\tilde{x}^{(j)}$ function of $x^{(1)}, \ldots, x^{(p)}$.
- The model is still linear with respect to β.

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Examples

A few examples:

- scalar transformations: $\ln(x^{(j)})$, $\sqrt{x^{(j)}}$, $(x^{(j)})^k \ldots$
- interactions (here, of order two): $x^{(j)}x^{(k)}$, $j \neq k$,
- higher-order interactions,
- (truncated) expansion in a basis...

 if $q \gg p$, risk of over-fitting.

Remarks: *feature engineering*

- Proposing new relevant variables
  - ➠ domain expertise (or model selection...?)
- The same principle can be used to *reduce* dimension
  - ➠ features extraction.

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Expansion in a basis

Principle

Let $\{\psi_m\}_{m>0}$ be a function basis of $L^2(\mathcal{X})^\dagger$.

Consider $\tilde{X}^{(m)} = \psi_m(X)$, $m = 1, \ldots, M$

➠ truncated expansion in the basis $\{\psi_m\}$.

Examples of bases (preferably orthogonal):

- polynomial bases,
- wavelet bases,
- Fourier bases...

† or any other function space assumed to contain the optimal predictor h^*.

➠ back to slide 28

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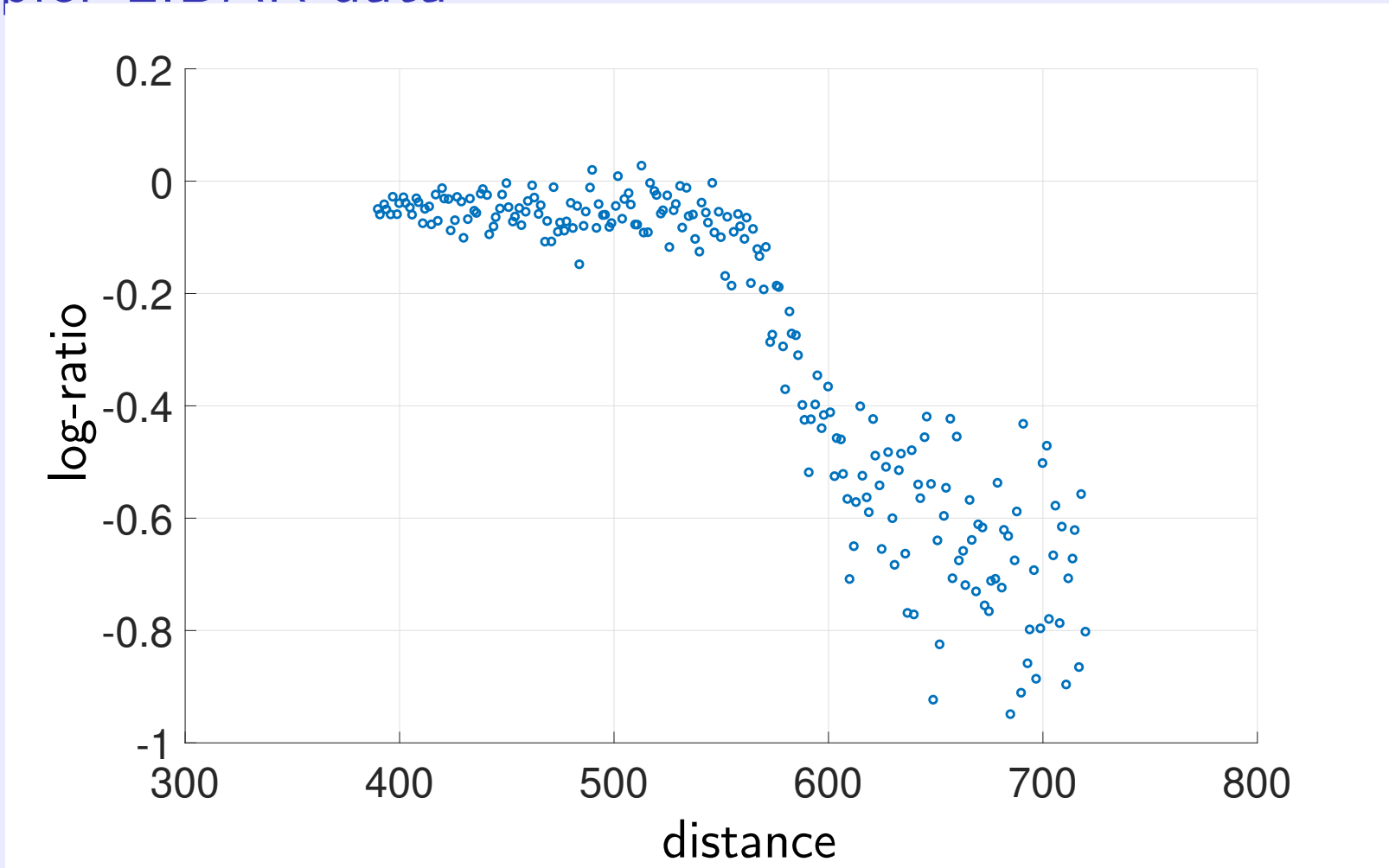
➠ back to slide 28

Example: LIDAR data



x-axis: distance travelled before the light is reflected back to its source

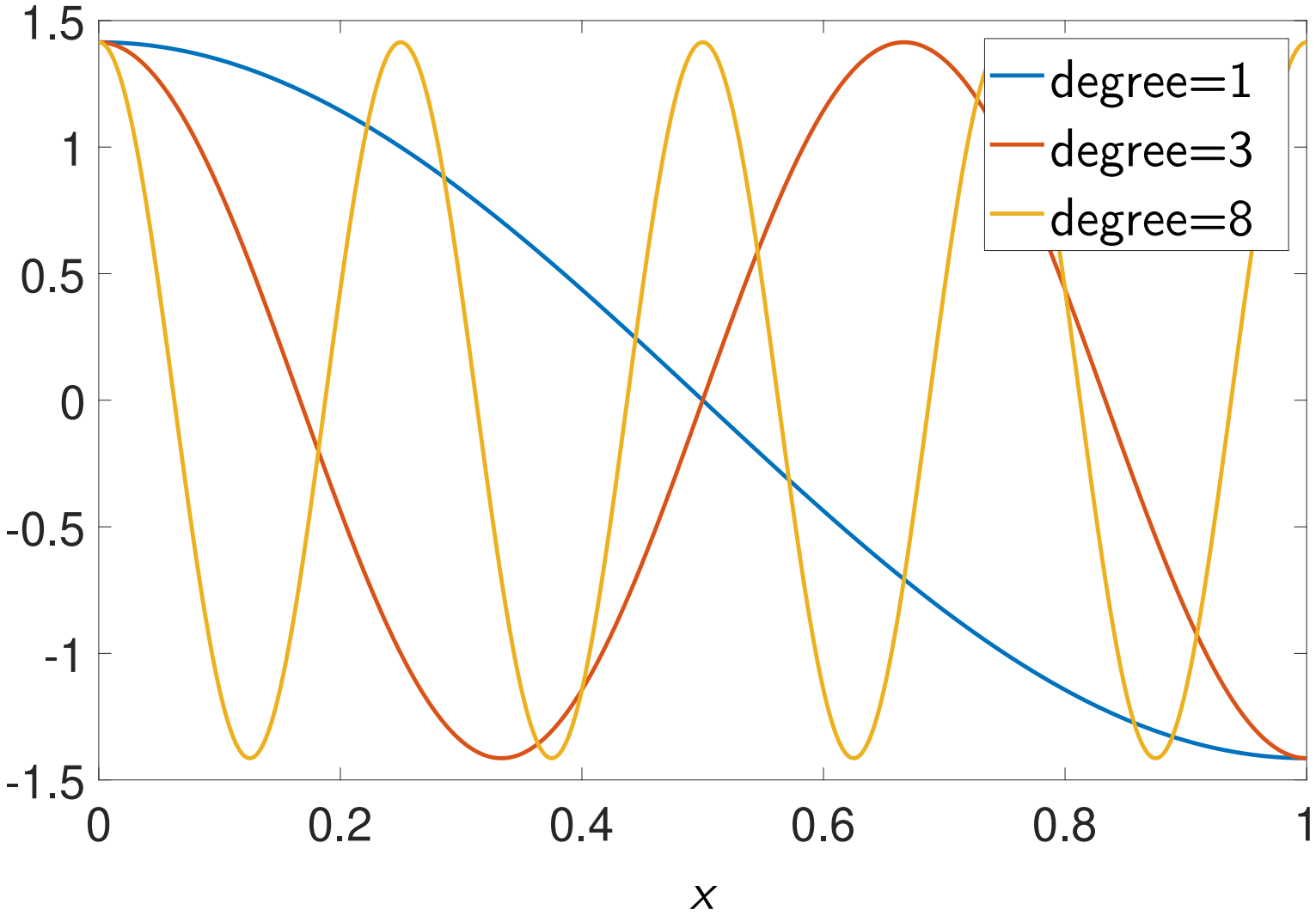
y-axis: logarithm of the ratio of received light from two laser sources

Data obtained from `http://matt-wand.utsacademics.info/webspr/lidar.html`

LIDAR: LIght Detection And Ranging

back to slide 28

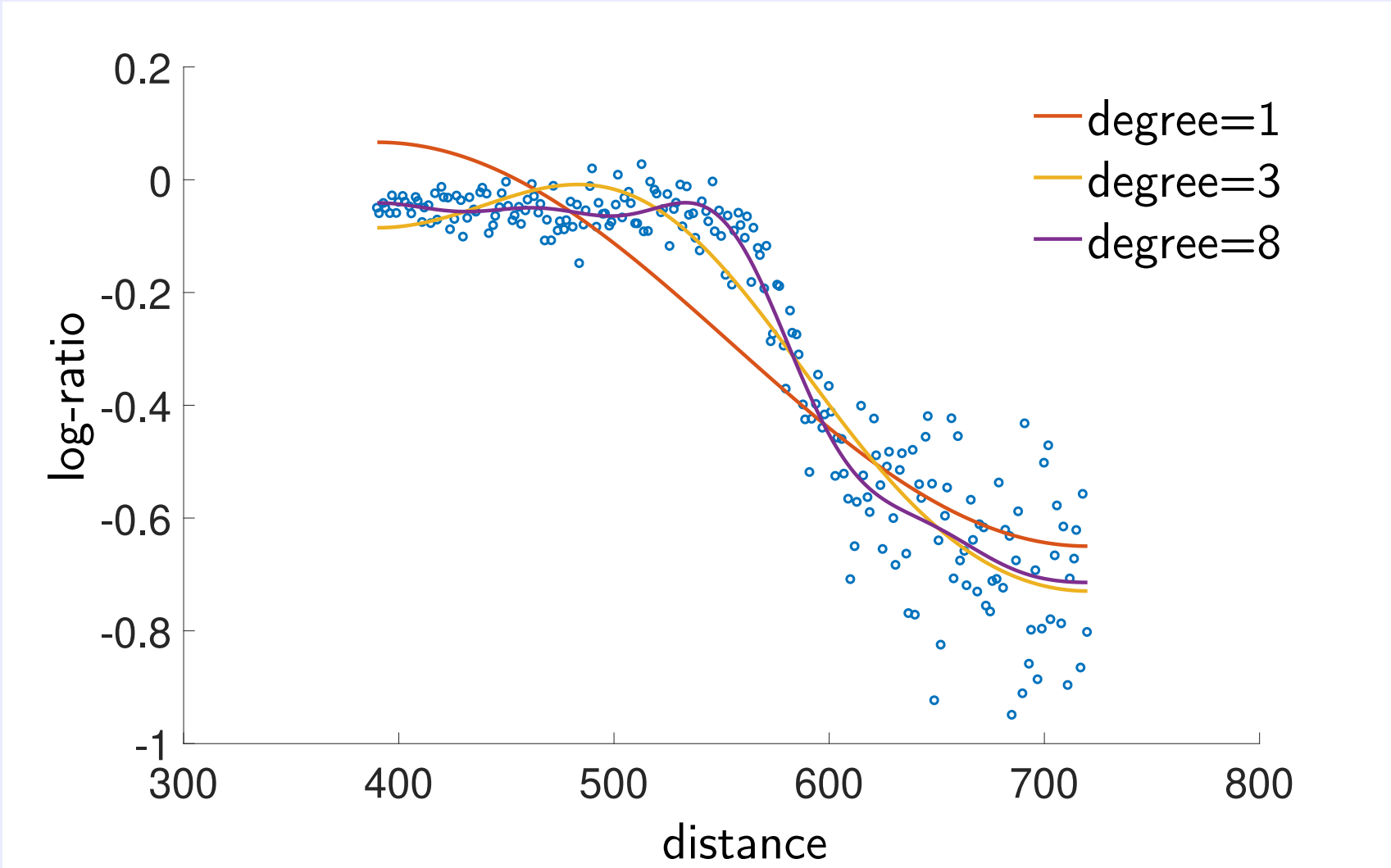
Basis of orthogonal cosines (basis of $L^2([0,1])$



back to slide 28

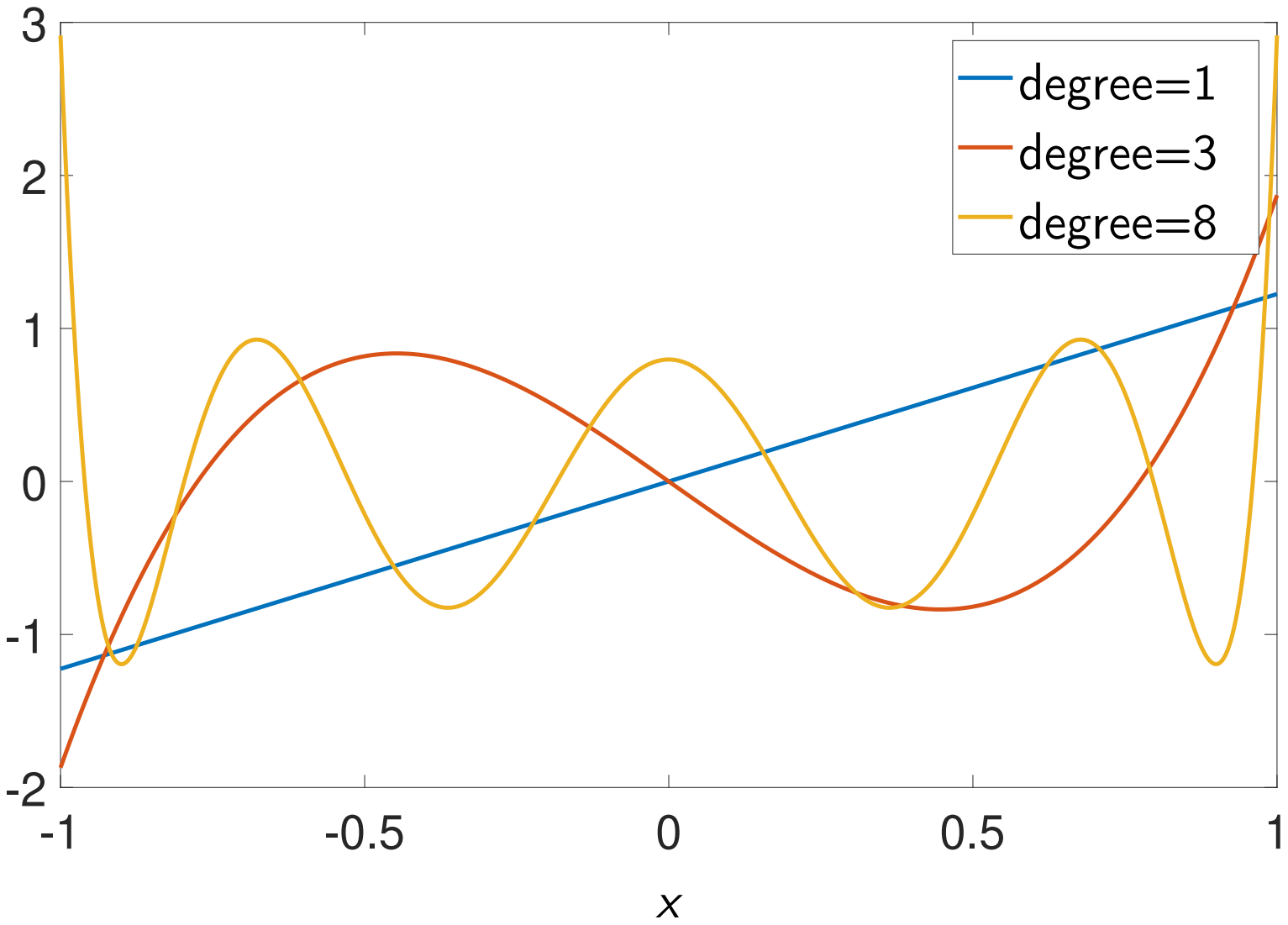
Example: LIDAR data (cont'd)

Quadratic loss + basis of cosines



back to slide 28

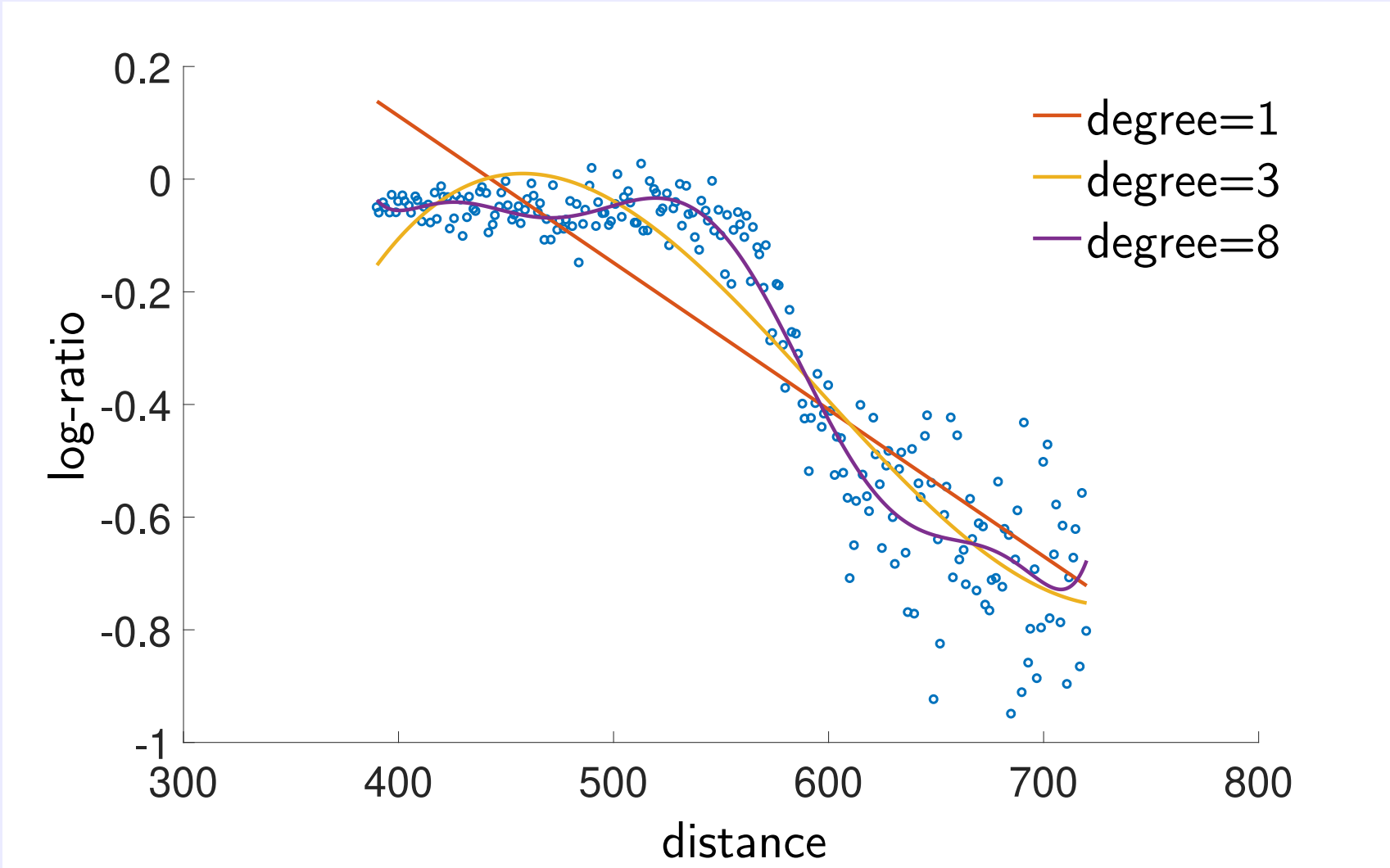
Legendre polynomials (orthonormal basis of $L^2([-1,1])$)



back to slide 28

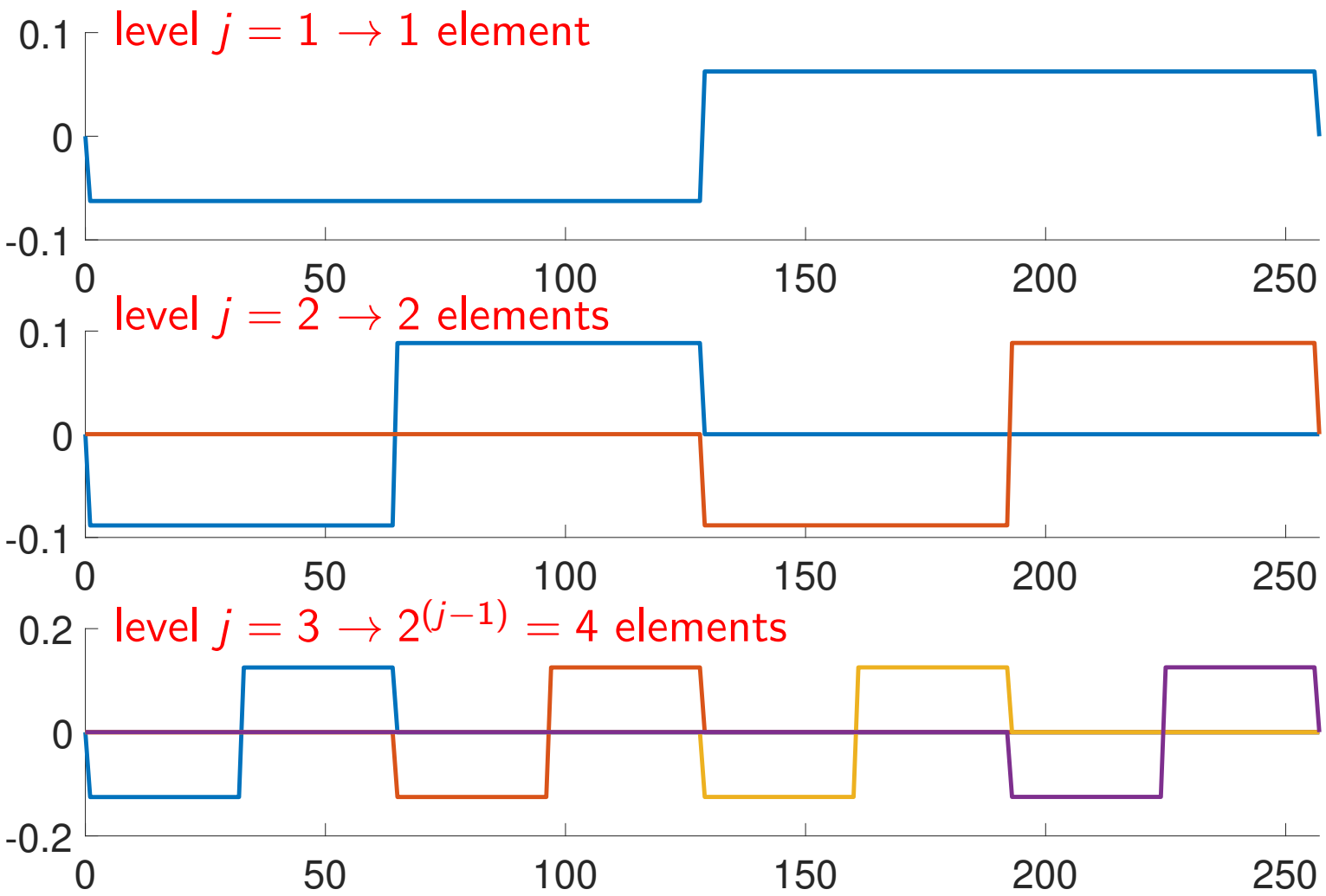
Example: LIDAR data (cont'd)

Quadratic loss + Legendre polynomials



back to slide 28

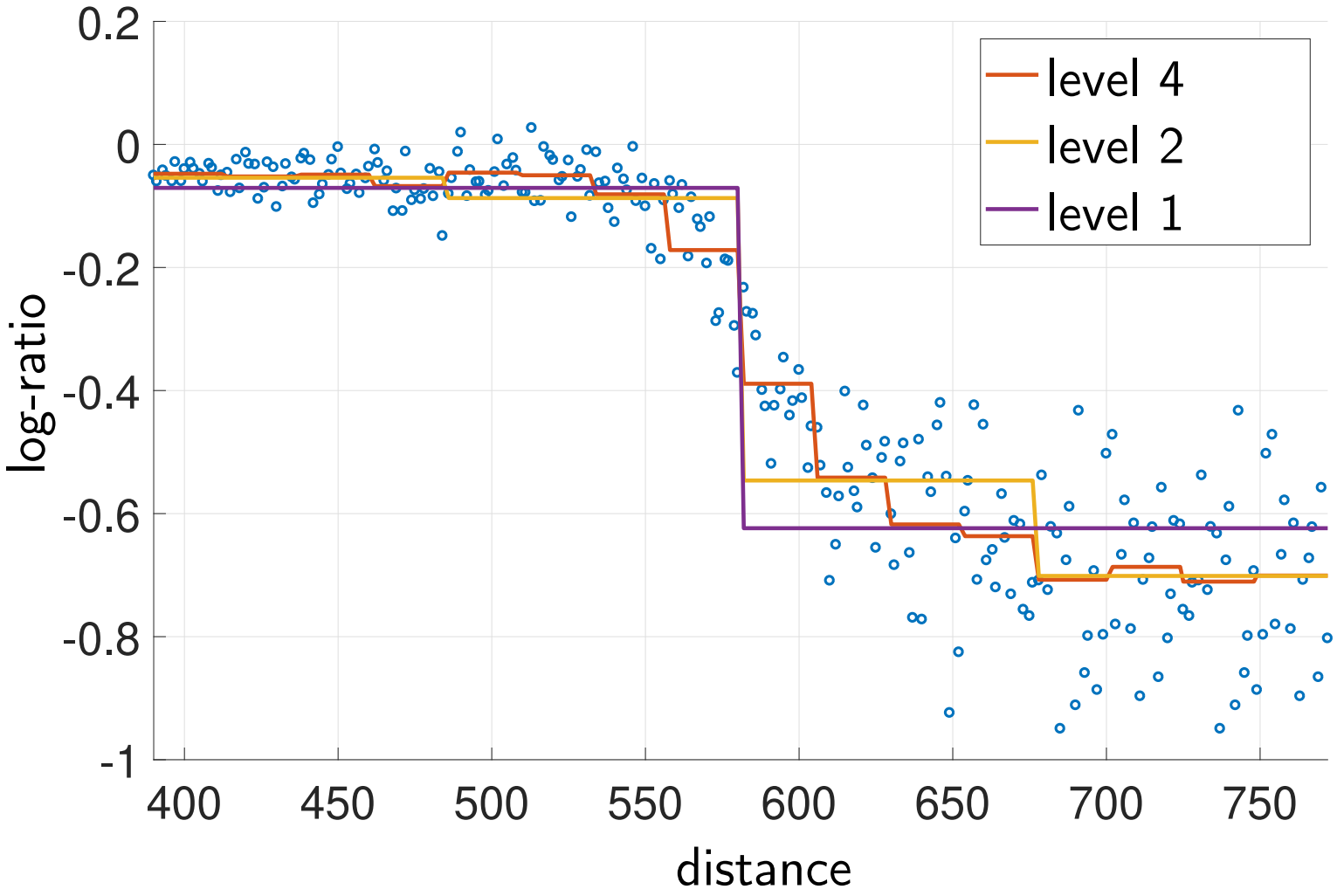
Haar wavelet basis



back to slide 28

Example: LIDAR data (cont'd)

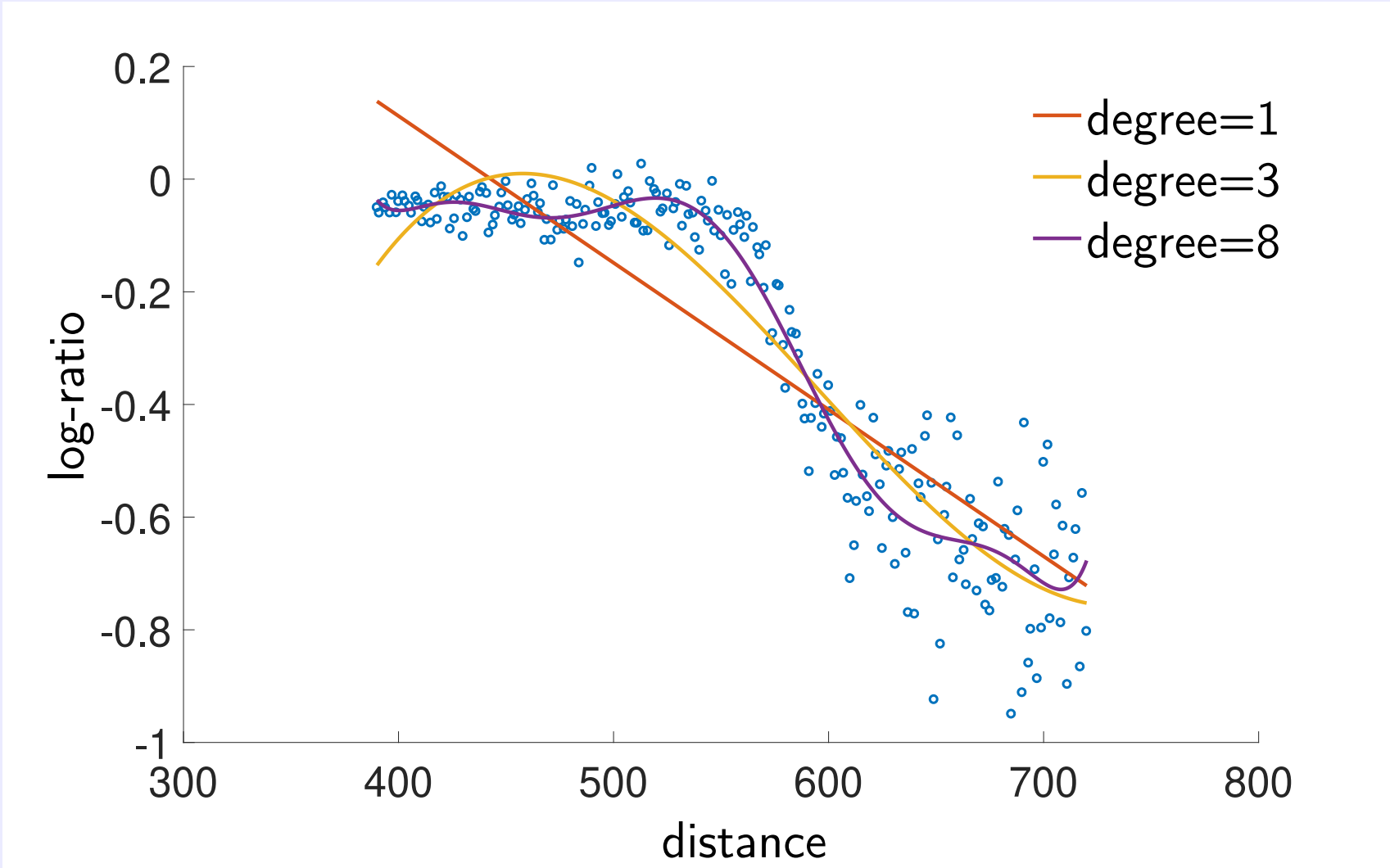
Quadratic loss + Haar wavelets



back to slide 28

Example: LIDAR data (cont'd)

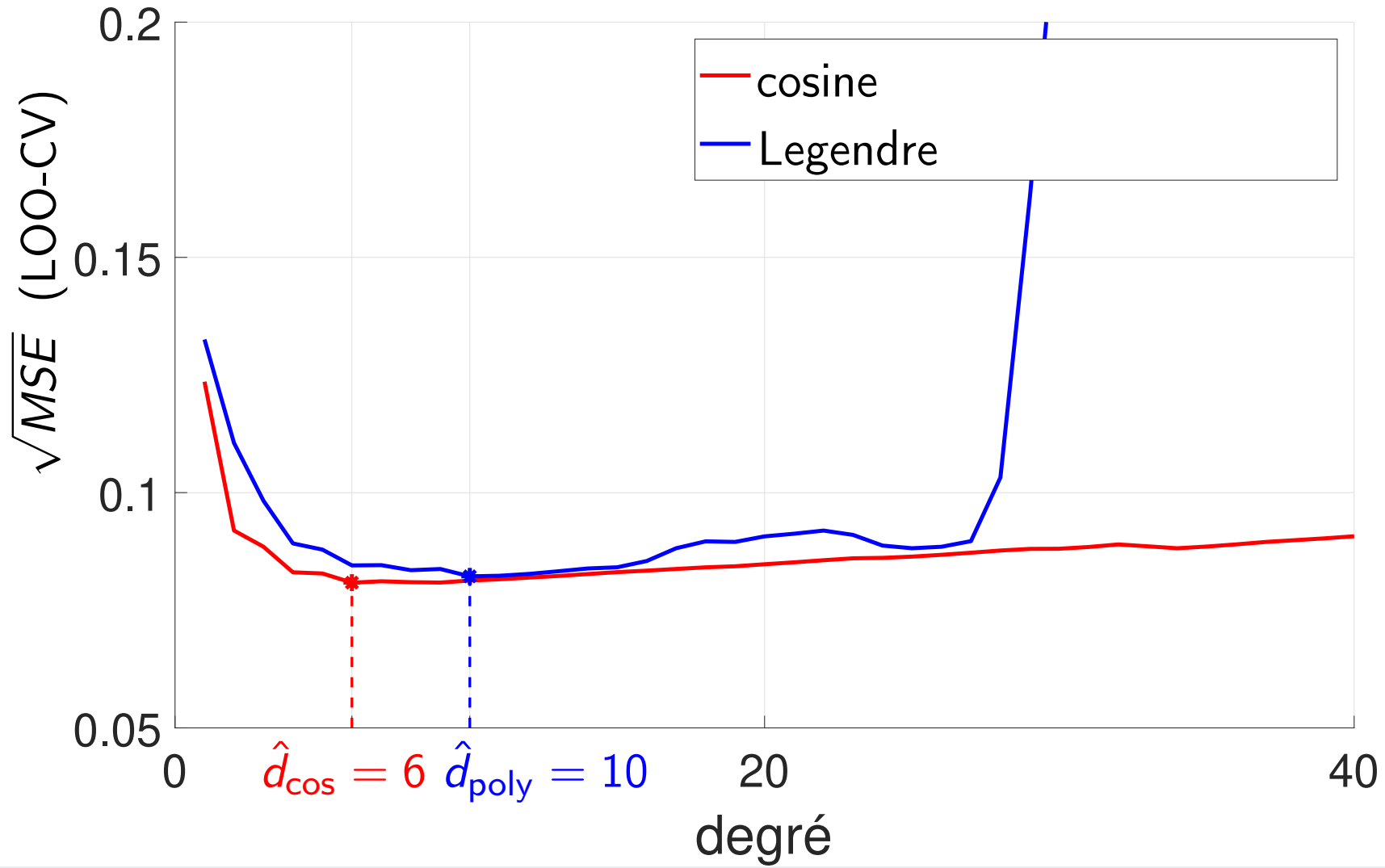
Quadratic loss + Legendre polynomials



back to slide 28

Example: LIDAR data (cont'd)

Model selection



back to slide 28