INSEAD PhD Course

Foundations of Machine Learning and AI

Theodoros Evgeniou - Nicolas Vayatis

Sessions 3-4: From classical statistics to Machine Learning

Summary of sessions 1-2

From previous session
Main messages

1. Machine Learning is about choosing (= estimating = learning) a function from a set of functions (called hypothesis space)

   From information theory: Number of steps to find the unknown function among K functions is of the order $\log K$

2. Estimation-Approximation trade-off

   In the case of Least Square regression with a linear model in dimension d: corresponds to Bias-Variance decomposition where the variance term is proportional to d/n

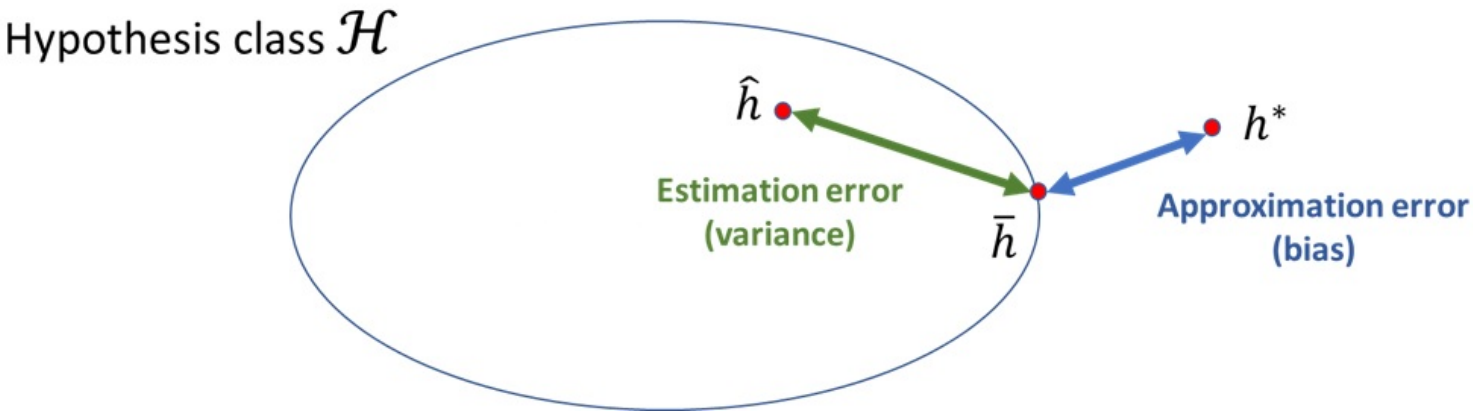
3. Mathematical tool from probability theory

   ERM/Finite case/Nonzero error: deviation inequality of the error of a function on training data from the expected out-of-sample error of the same function (Hoeffding's inequality) - see Exercise set 1

From previous session
Estimation vs. Approximation

- Error measure $L(h)$ for functions $h \in \mathcal{H}$
- Best in the class $\bar{h}$, world-champion h^*
- Key decomposition of error for any estimate $\widehat{h}$:

$$L(\widehat{h}) - L(h^*) = \underbrace{L(\widehat{h}) - L(\bar{h})}_{\text{estimation (stochastic)}} + \underbrace{L(\bar{h}) - L(h^*)}_{\text{approximation (deterministic)}}$$



From previous session
The case of linear models with Gaussian noise

- Linear model in dimension d with vector notations (sample size n):

$$\mathbf{Y} = \mathbf{X}\beta^* + \varepsilon \in \mathbb{R}^n$$

  where $\mathbf{X}$ of size $n \times d$, and ε is a gaussian vector mean zero, variance σ^2

- Least square estimator denoted by $\widehat{\beta}_{\mathbf{n}}$

- error of the LSE (expectation wrt the sample distribution)

$$\frac{1}{n}\mathbb{E}\big(\|\mathbf{X}\beta^* - \mathbf{X}\widehat{\beta}_{\mathbf{n}}\|^2\big) = \mathrm{Bias} + \sigma^2 \frac{d}{n}$$

This session

- Handling models in high dimensions:

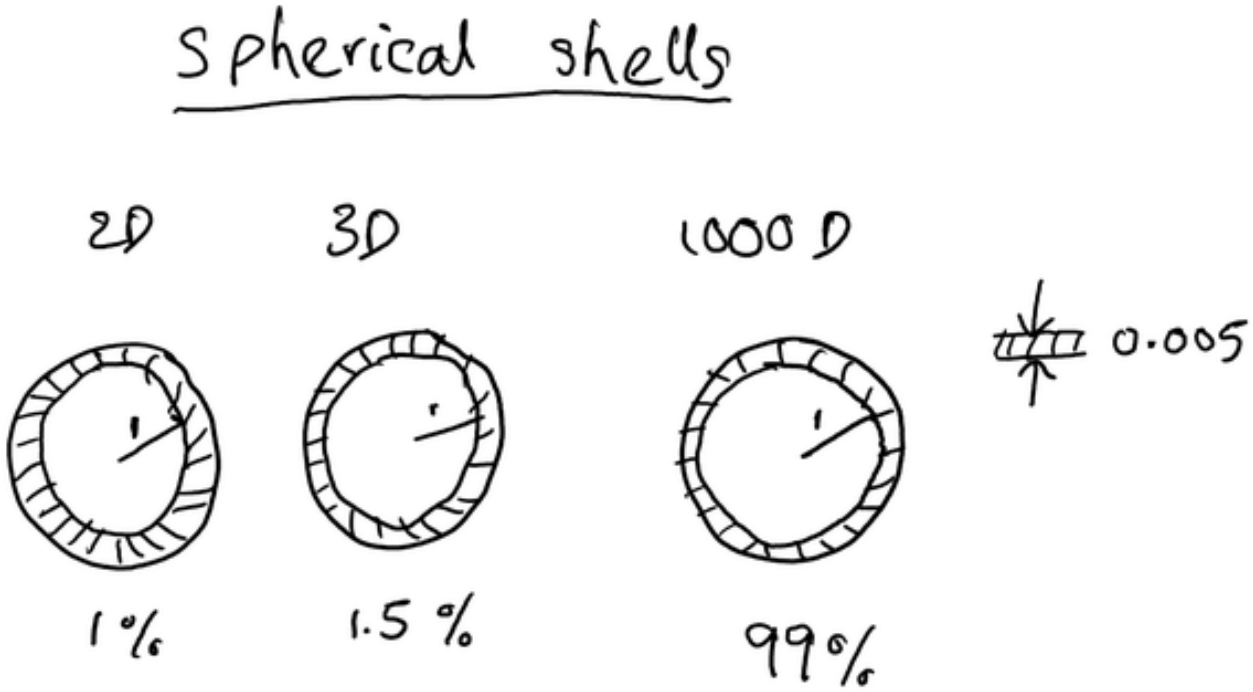
  $d \gg 1$, $d \gg n$

- Questioning dimensionality:

  number of parameters vs. complexity of set of functions

- Key concepts for this session: *sparsity*, *regularization* and *optimization*

High Dimensional Interlude
Some surprising fact



- Ratio shell/volume in Euclidean space of dimension d:

$$\frac{vol(B_d(0,1) - B_d(0,1-\varepsilon))}{vol(B_d(0,1))} = 1-(1-\varepsilon)^d \to 1 \text{ when } d \to \infty$$

High Dimensional Interlude Readings

- High level position paper and talk:

  "High Dimensional Data Analysis : The Curses and Blessings of Dimensionality" by D. Donoho (2000)

- Maths book:

  "High-Dimensional Probability" by Roman Vershynin (2018)

From classical statistics to Machine Learning: Handling high dimensions

A. Sparsity and linear models

B. Generalizations to: other models, other problems, other structural assumptions, other spaces

A. Sparsity and linear models

Tuning the dimension of the model

Linear regression model
Notations

- Vector notations:

  Response vector $\mathbf{Y} \in \mathbb{R}^n$, input data matrix $\mathbf{X}$ (size $n \times d$)

- Linear model with vector notations:

$$\mathbf{Y} = \mathbf{X}\beta^* + \varepsilon$$

  where ε random noise vector (centered, independent of $\mathbf{X}$)

The sparse linear regression model

- Intuition: what if there are uninformative variables in the model but we do not know which they are?
- Sparsity assumption: Let β^* the true parameter which only a subset of variables (called *support*)

$$m^* = \{j : \beta_j^* \neq 0\} \subset \{1, \ldots, d\}$$

- ℓ_0 norm of any β: $\|\beta\|_0 = \sum_{j=1}^{d} \mathbb{I}\{\beta_i \neq 0\}$

Two possible formulations
Constrained vs. Penalized optimization

1. Ivanov formulation: take k between 0 and $\min\{n, d\}$

$$\min_{\beta \in \mathbb{R}^d} \|\mathbf{Y} - \mathbf{X}\beta\|_2^2 \quad \text{subject to } \|\beta\|_0 \leq k$$

2. Tikhonov formulation: take $\lambda > 0$

$$\min_{\beta \in \mathbb{R}^d} \left\{ \|\mathbf{Y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_0 \right\}$$

Comments

- Tikhonov looks as a Lagrange formulation of Ivanov
- But here the two formulations are NOT equivalent due to the lack of smoothness of the ℓ_0 norm
- Ivanov with ℓ_0 constraint is known as the Best Subset Selection problem for which there are algorithms based on heuristics (e.g. Forward Stagewise Regression) which work ok up to $k \simeq 35$. Recent advances: check Mixed Integer Optimization (MIO) formulation by Bertsimas et al. (2016).
- Focus on Tikhonov regularization from now on

Sparsity and linear models

Model selection

Connecting the dots
Tikhonov penalty and variance

Recall:

- Tikhonov formulation with ℓ_0 *penalty*: take $\lambda > 0$

$$\min_{\beta \in \mathbb{R}^d} \left\{ \|\mathbf{Y} - \mathbf{X}\beta\|_2^2 + \lambda \|\beta\|_0 \right\} \tag{1}$$

- Bias-variance decomposition of the error for the LSE $\widehat{\beta}$:

$$\frac{1}{n}\mathbb{E}\left(\|\mathbf{X}\beta^* - \mathbf{X}\widehat{\beta}_{\mathbf{n}}\|^2\right) = \text{Bias} + \sigma^2 \frac{d}{n} \tag{2}$$

  where d is the dimension of the data and σ^2 is the variance of the Gaussian noise

Questions for now: does the bias-variance decomposition (2) explains (1)? Is the penalty correct?

Model selection in linear models

- Model: $\mathbf{Y} = \mathbf{X}\beta^* + \varepsilon$
- Consider a model for β^* that is a subset m of indices of $\{1, \ldots, d\}$
- Example: In dimension $d = 3$, we have:
  - 1 model of size $|m| = 0$: constant model
  - 3 models of size $|m| = 1$: $\{1\}, \{2\}, \{3\}$
  - 3 models of size $|m| = 2$: $\{1, 2\}, \{2, 3\}, \{1, 3\}$
  - 1 model of size $|m| = 3$: $\{1, 2, 3\}$

  We potentially have 8 versions of Least Square Estimator (LSE), we call call constrained LSE (except for the case $|m| = 3$ which is unconstrained).

Model selection in linear models

- Model: $\mathbf{Y} = \mathbf{X}\beta^* + \varepsilon$
- Consider the set $\mathcal{M}$ of subsets m of the variables among indices $\{1, \ldots, d\}$. There are 2^d such sets m.
- For every $m \in \mathcal{M}$, there is a standard linear regression model with dimension $k_m = |m|$. In other words, for those $j \notin m$, we have $\beta_j^* = 0$.
- For each model $m \in \mathcal{M}$, compute the constrained Least Square Estimator $\widehat{\beta}_m$.
- The final estimator is the "best" among $\widehat{\beta}_m$ over all $m \in \mathcal{M}$

What "Best" actually means
The oracle

- Error given by: $r_m = \frac{1}{n}\mathbb{E}\left(\|\mathbf{X}\beta^* - \mathbf{X}\widehat{\beta}_m\|^2\right)$
- Best theoretical estimator (called *oracle*):

$$\widehat{\beta}_{\overline{m}} \quad \text{where} \quad \overline{m} = \arg\min_{m \in \mathcal{M}} r_m$$

- Example of an empirical estimator : Akaike Information Criterion (AIC penalty of Least Squares)

$$\widehat{m} = \arg\min_{m \in \mathcal{M}} \left\{ \|\mathbf{Y} - \mathbf{X}\widehat{\beta}_m\|^2 + 2|m|\sigma^2 \right\}$$

(can be computed from data as long as σ^2 is assumed to be known)

Optional material

Derivation of Akaike Information Criterion

Akaike Information Criterion (1/2)
Derivation

- Recall from last session: error of estimator

$$r_m = \frac{1}{n}\mathbb{E}\left(\|\mathbf{X}\beta^* - \mathbf{X}\widehat{\beta}_m\|^2\right) = \frac{1}{n}\mathbb{E}\left(\|(I_n - \widehat{\Pi}_m)\mathbf{X}\beta^*\|^2\right) + \sigma^2\frac{|m|}{n}$$

- Similarly, we can derive:

$$\frac{1}{n}\mathbb{E}\left(\|\mathbf{Y} - \mathbf{X}\widehat{\beta}_m\|^2\right) = \frac{1}{n}\mathbb{E}\left(\|(I_n - \widehat{\Pi}_m)\mathbf{X}\beta^*\|^2\right) + \sigma^2\frac{(n - |m|)}{n}$$

- Then, we observe:

$$\frac{1}{n}\mathbb{E}\left(\|\mathbf{Y} - \mathbf{X}\widehat{\beta}_m\|^2\right) = r_m + \sigma^2\frac{(n - 2|m|)}{n}$$

Link with last class notations: $\mathbf{h}^* = \mathbf{X}\beta^*$, $\widehat{\mathbf{h}}_\mathbf{m} = \mathbf{X}\widehat{\beta}_m = \widehat{\Pi}_m Y$ where $\widehat{\Pi}_m$ is the orthogonal projection on S_m

Akaike Information Criterion (2/2)
Empirical estimator of the error

- We have obtained that:

$$r_m = \frac{1}{n}\mathbb{E}\left(\|\mathbf{Y} - \mathbf{X}\widehat{\beta}_m\|^2\right) + \sigma^2\frac{(2|m| - n)}{n}$$

- Unbiased estimator of the error (assuming known variance):

$$\widehat{r}_m = \frac{1}{n}\|\mathbf{Y} - \mathbf{X}\widehat{\beta}_m\|^2 + \sigma^2\frac{(2|m| - n)}{n}$$

- Akaike Information Criterion

$$\widehat{m} = \underset{m\in\mathcal{M}}{\arg\min}\left\{\|\mathbf{Y} - \mathbf{X}\widehat{\beta}_m\|^2 + 2|m|\sigma^2\right\}$$

End of optional material

Bottom line on AIC

Is AIC an optimal penalty for model selection in linear models?

- Tikhonov regularization for ℓ_0 norm is equivalent to AIC with $\lambda = 2\sigma^2$ in this case (λ also depends on n if we minimize the average square error on the data)
- In practice, AIC does not pick the right dimension: in high dimensions, $\widehat{r}_m$ fluctuates around r_m due to a large amount of models with same cardinality $|m|$
- The correct penalty should be of the order $2\sigma^2|m|\log(d)$

NB: The number of linear models of given size $|m|$ in dimension d is: $\binom{d}{|m|} \leq \exp\left(|m|(1+\log(d/|m|))\right)$

AIC in large dimensions

- When d is large, is this practical ?
- There are about $e^{d/2}$ models to scan in the worst case where $|m| \simeq d/2$...

A. Sparsity and linear models

From (mathematical) statistics to optimization

Solving the computation burden
The power of convexity

- Practical methods for model selection are essentially greedy heuristics consisting in adding and/or retrieving one variable at the time to explore part of the whole model space which is exponential in the dimension. Examples are: Forward Stagewise Regression, Forward-Backward algorithm...
- Question: would it be possible to solve the optimization wrt the unknown parameter β AND wrt to its support subset of indices jointly?
- Answer is yes at the cost of the so-called relaxation of the non-convex formulation with the ℓ_0 penalty to a convexified problem with an ℓ_1 penalty.

The LASSO for linear models
From ℓ_0 to ℓ_1

- Consider the relaxation of the previous problem replacing the ℓ_0-norm by the ℓ_1-norm:

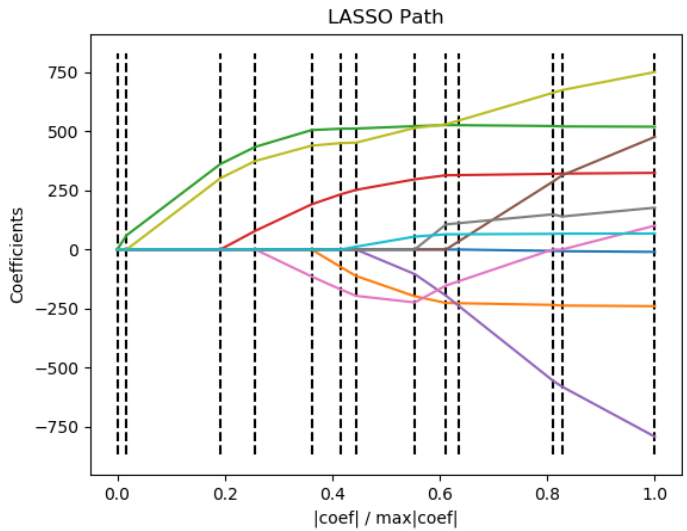
$$\|\beta\|_1 = \sum_{j=1}^{d} |\beta_j|$$

- The new estimator is called the LASSO: for any $\lambda > 0$,

$$\widehat{\beta}_\lambda \in \operatorname*{arg\,min}_{\beta \in \mathbb{R}^d} \left\{ \|\mathbf{Y} - \mathbf{X}\beta\|^2 + \lambda \|\beta\|_1 \right\}$$

Blessings of the LASSO

- Approximate solutions via efficient algorithms building the so-called regularization paths $\lambda \to \widehat{\beta}_\lambda$:



- Theoretical soundness: it can be shown that: as $n, d \to \infty$

$$\frac{1}{n}\mathbb{E}\left(\|\mathbf{X}\beta^* - \mathbf{X}\widehat{\beta}\|^2\right) \leq C\|\beta^*\|_1\sqrt{\frac{\log d}{n}}$$

The "mother" of ML algorithms
Penalized optimization

- Learning process as the optimization of a data-dependent criterion:

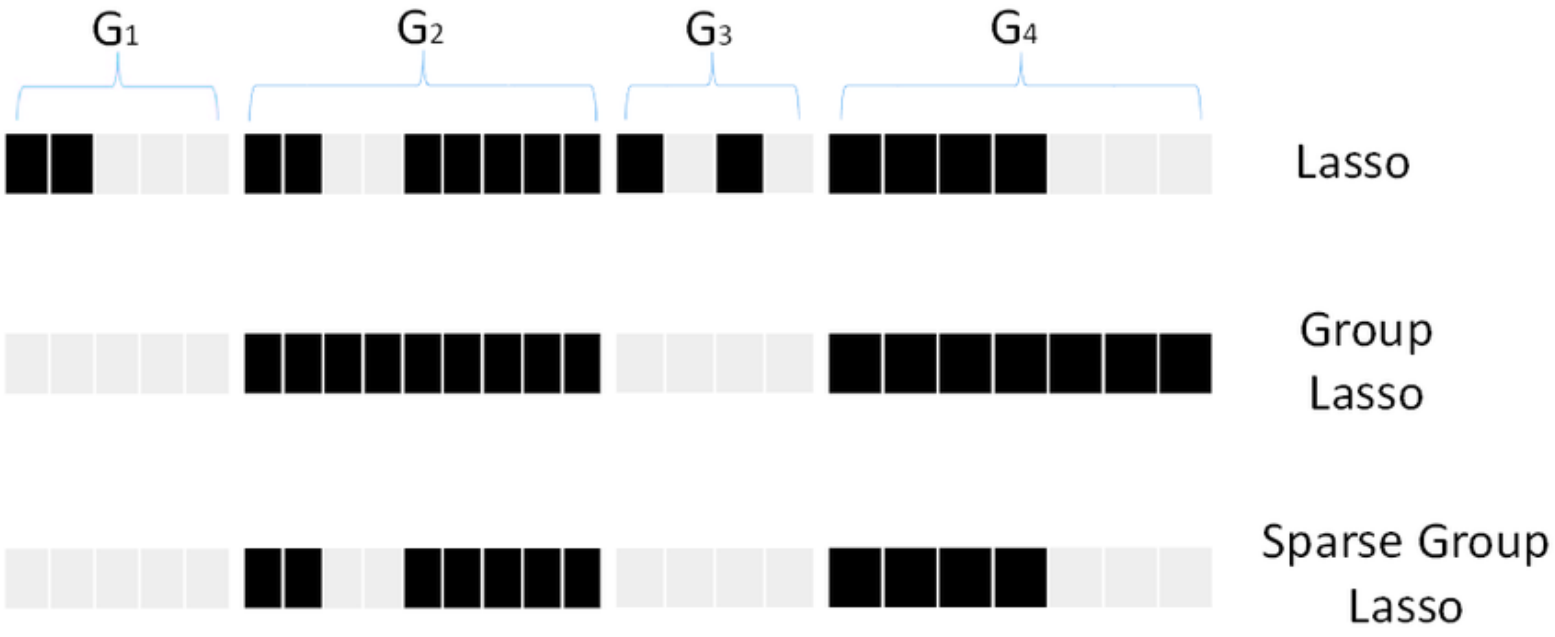
$$\text{Criterion}(h) = \text{Training error}(h) + \lambda \, \text{Penalty}(h)$$

- Training error: data-fitting term related to a loss function
- Penalty: complexity of the decision function
- Constant λ: smoothing parameter tuned through cross-validation procedure

A. Sparsity and linear models

Structured sparsity

Putting human priors in penalties
Sparsity patterns

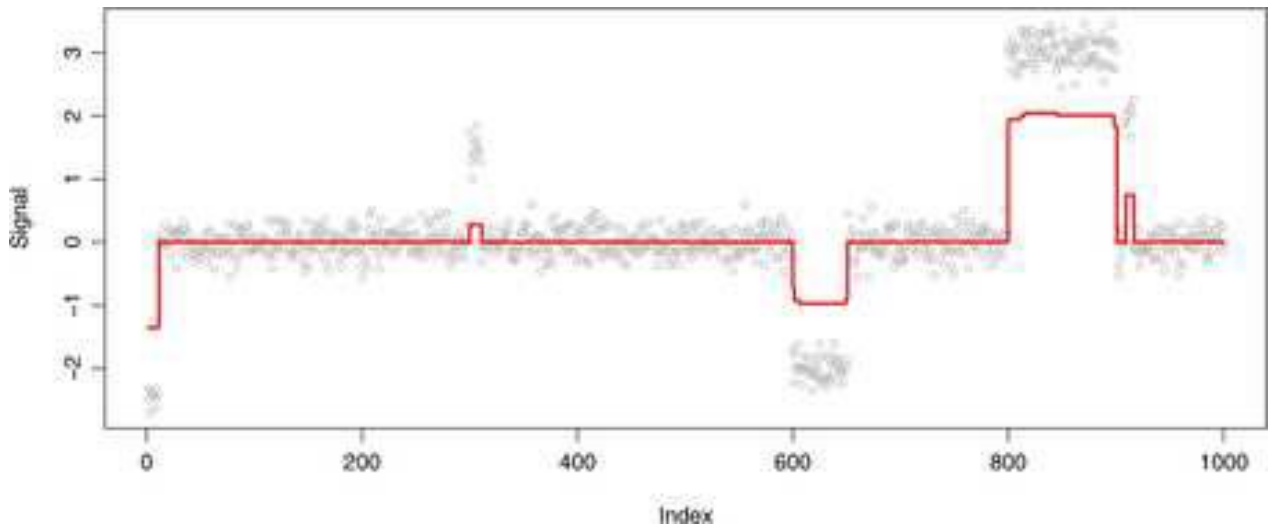


The simplest structured penalty
Group LASSO

- Group structure on the parameter β^*: let G the number of groups of subsets of indices in $\{1, \ldots, d\}$ and, for $g = 1, \ldots, G$, we denote by $\mathbf{X}^{(g)}$ the submatrix of $\mathbf{X}$ with variables in group g and by $\beta^{(g)}$ the coefficient vector applied to variables in group g and d_g is the size of group g.
- Group LASSO formulation:

$$\widehat{\beta}_\lambda \in \operatorname*{arg\,min}_{\beta \in \mathbb{R}^d} \left\{ \|\mathbf{Y} - \mathbf{X}\beta\|^2 + \lambda \sum_{g=1}^{G} \sqrt{d_g} \|\beta^{(g)}\| \right\}$$

Case of temporal patterns
Fused LASSO



- Enforcing temporal coherence leads to adding a penalty term:

$$\widehat{\beta}_\lambda \in \underset{\beta \in \mathbb{R}^d}{\arg\min} \left\{ \|\mathbf{Y} - \mathbf{X}\beta\|^2 + \lambda \|\beta\|_1 + \mu \sum_{j=2}^{d} |\beta_j - \beta_{j-1}| \right\}$$

A. Sparsity and linear models

Ridge regression

Penalized optimization
Other penalties?

- Until now: hypothesis class with linear functions $h \in \mathcal{H}$ and variations on sparsity-inducing penalties

$$\text{Criterion}(h) = \text{Training error}(h) + \lambda \, \text{Penalty}(h)$$

- This idea goes back to the 60s (Ivanov, John, Lavrent'ev, Tikhonov) where the penalty operated as a regularizer of solutions for ill-posed problems.

Ill-posed problem in statistics
High dimensional least square regression

- Assume d larger than n
- Then when solving the least square optimization problem, we observe that we have less equations than variables: this is the case of an *underdetermined* linear system.
- Another way to put this is to observe that $\mathbf{X}^T\mathbf{X}$ is not full rank, hence it is not invertible and there is an infinity of solutions.

The oldest regularizer in statistics
Ridge regression

- The Ridge estimator is the solution of the following penalized optimization problem: for any $\lambda > 0$,

$$\widehat{\beta}_\lambda \in \underset{\beta \in \mathbb{R}^d}{\arg\min} \left\{ \|\mathbf{Y} - \mathbf{X}\beta\|^2 + \lambda \|\beta\|_2^2 \right\}$$

Derivation of ridge regression estimator

- We denote the objective function:

$$F(\beta) = (\mathbf{Y} - \mathbf{X}\beta)^T (\mathbf{Y} - \mathbf{X}\beta) + \lambda \beta^T \beta$$

- Thanks to convexity and differentiability of F, we obtain the solution by solving

$$\nabla F(\beta) = 2\mathbf{X}^T(\mathbf{X}\beta - \mathbf{Y}) + 2\lambda\beta = 0$$

- Solution:

$$\widehat{\beta}_\lambda = \left(\mathbf{X}^T\mathbf{X} + \lambda I_d\right)^{-1} \mathbf{X}^T\mathbf{Y}$$

  because $\mathbf{X}^T\mathbf{X} + \lambda I_d$ always invertible.

- Computation still painful for d very large...

Optional material

Dual formulation of the optimization problem in ridge regression

Dual optimization problem (1/3)
Formulation and KKT conditions

- Equivalent formulation of ridge regression optimization:

$$\min_{\beta \in \mathbb{R}^d, r \in \mathbb{R}^n} \left\{ \frac{1}{2}\|r\|^2 + \frac{\lambda}{2}\|\beta\|^2 \right\} \quad \text{subject to } r = \mathbf{X}\beta - \mathbf{Y}$$

- Lagrange formulation with multiplier vector α

$$\mathcal{L}(\beta, r, \alpha) = \frac{1}{2}\|r\|^2 + \frac{\lambda}{2}\|\beta\|^2 + \alpha^T(r - \mathbf{X}\beta + \mathbf{Y})$$

- Karush-Kuhn-Tucker conditions: zeroing gradient wrt primal variables β, r, leads to:

$$\beta(\alpha) = \frac{1}{\lambda}\mathbf{X}^T\alpha \quad \text{and} \quad r(\alpha) = -\alpha$$

Dual optimization problem (2/3)
Resolution

- Then, an equivalent formulation of ridge regression optimization is given by:

$$\mathcal{L}(\beta(\alpha), r(\alpha), \alpha) = \frac{1}{2}\|\alpha\|^2 + \frac{1}{2\lambda}\|\mathbf{X}^T\alpha\| + \alpha^T\left(-\alpha - \frac{1}{\lambda}\mathbf{X}\mathbf{X}^T\alpha + \mathbf{Y}\right)$$

- Solution:

$$\widehat{\alpha} = \lambda\left(\mathbf{X}\mathbf{X}^T + \lambda I_n\right)^{-1}\mathbf{Y} \quad \text{and} \quad \widehat{\beta} = \frac{1}{\lambda}\mathbf{X}^T\widehat{\alpha}$$

Dual optimization problem (3/3)
Sanity check

- The prediction on $x \in \mathbb{R}^d$ can be expressed in terms of α

$$x^T \widehat{\beta} = \frac{1}{\lambda} x^T \mathbf{X}^T \widehat{\alpha} = \frac{1}{\lambda} \sum_{i=1}^{n} \widehat{\alpha}_i x^T X_i$$

- We can use the identity:
  $\mathbf{X}^T \left(\mathbf{X}\mathbf{X}^T + \lambda I_n\right)^{-1} = \left(\mathbf{X}^T\mathbf{X} + \lambda I_d\right)^{-1} \mathbf{X}^T$ to check the solutions are the same.

End of optional material

Bottom line on dual optimization

- Alternative view on the optimization problem

$$\bar{\mathcal{L}}(\alpha) = \frac{1}{2}\|\alpha\|^2 + \frac{1}{2\lambda}\|\mathbf{X}^T\alpha\| + \alpha^T\left(-\alpha - \frac{1}{\lambda}\mathbf{X}\mathbf{X}^T\alpha + \mathbf{Y}\right)$$

  and solution reconstruction for the optimizer $\widehat{\alpha}$ of $\bar{\mathcal{L}}$:

$$\widehat{\beta}_\lambda = \frac{1}{\lambda}\mathbf{X}^T\widehat{\alpha}$$

- Key observation!
  Optimization and function evaluation only require the scalar products between x's. Pairwise comparisons could be replaced with other metrics and make the dependency nonlinear for free!

B. Examples of generalizations

1. Playing with penalties: combined regularization

Elastic Net
The best of LASSO and Ridge?

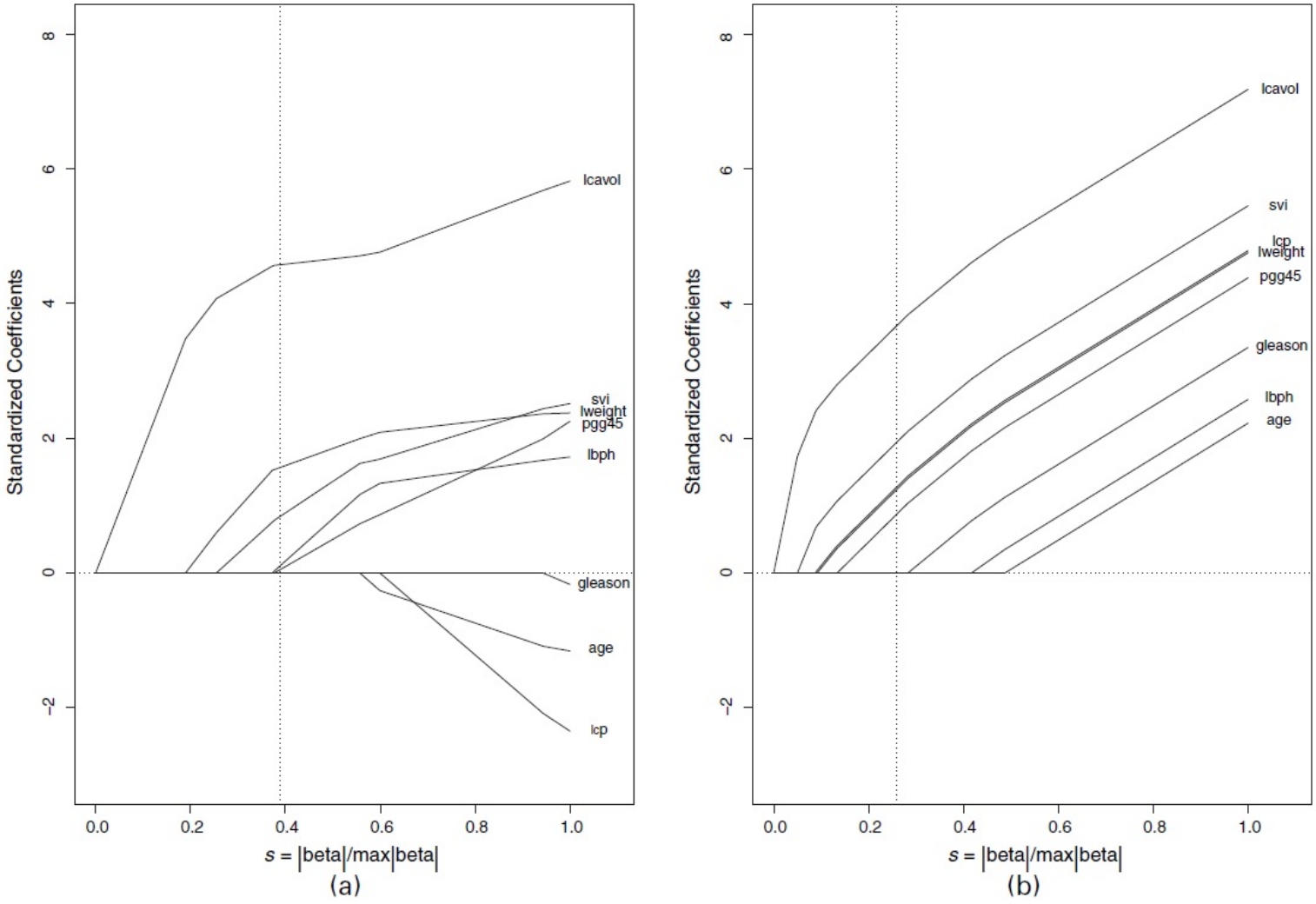
- Rationale (from [Zou and Hastie, 2005])

(a) In the $p > n$ case, the lasso selects at most n variables before it saturates, because of the nature of the convex optimization problem. This seems to be a limiting feature for a variable selection method. Moreover, the lasso is not well defined unless the bound on the L_1-norm of the coefficients is smaller than a certain value.
(b) If there is a group of variables among which the pairwise correlations are very high, then the lasso tends to select only one variable from the group and does not care which one is selected. See Section 2.3.
(c) For usual $n > p$ situations, if there are high correlations between predictors, it has been empirically observed that the prediction performance of the lasso is dominated by ridge regression (Tibshirani, 1996).

- Combination of ℓ_1 and ℓ_2 penalties

$$\widehat{\beta}_\lambda \in \arg\min_{\beta \in \mathbb{R}^d} \left\{ \|\mathbf{Y} - \mathbf{X}\beta\|^2 + \lambda \|\beta\|_1 + \mu \|\beta\|_2^2 \right\}$$

LASSO vs. Elastic Net
Comparison of regularization paths



Tuning the hyperparameters
Cross-validation

- How do we select the parameters λ and μ? These are called hyperparameters or smoothing parameters or regularization parameters.
- This is a universal problem in monitoring the overfitting effect of Machine Learning methods.
- The procedure of cross-validation will be developed later in the course.

Exercise
Comparison of the three penalties

- Consider the following toy problem: $Y \sim \mathcal{N}_1(\beta^*, 1)$ where β is a real-valued parameter ($d = 1$).
- Find the three estimators when minimizing the following three functions:

$$\text{(i)}\frac{1}{2}(Y-\beta)^2+\lambda,\ \text{(ii)}\frac{1}{2}(Y-\beta)^2+\lambda|\beta|,\ \text{(iii)}\frac{1}{2}(Y-\beta)^2+\lambda\beta^2$$

- Show a plot of the estimators as functions of the unconstrained LSE and explain the use of the following terminology for the penalized procedures: hard thresholding, soft thresholding, shrinkage.

B. Examples of generalizations

2. Playing with cost functions: from regression to classification and scoring

Penalized optimization
What about other variations?

- Until now: hypothesis class with linear functions $h \in \mathcal{H}$ and variations on the penalties

$$\text{Criterion}(h) = \text{Training error}(h) + \lambda \, \text{Penalty}(h)$$

- From now on: play with other losses affects the Training error

$$\text{Criterion}(h) = \text{Training error}(h) + \lambda \, \text{Penalty}(h)$$

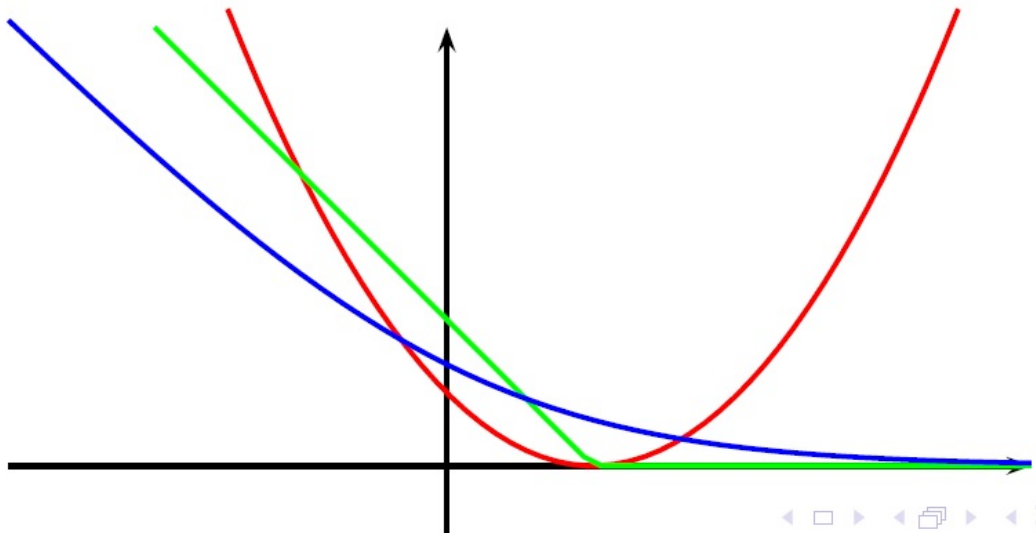
Using other loss functions

A few examples:

Ridge regression:
$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \frac{1}{2}(y_i - \beta^\top \mathbf{x}_i)^2 + \lambda \|\beta\|_2^2.$$

Linear SVM:
$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \max(0, 1 - y_i \beta^\top \mathbf{x}_i) + \lambda \|\beta\|_2^2.$$

Logistic regression:
$$\min_{\beta \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} \log\left(1 + e^{-y_i \beta^\top \mathbf{x}_i}\right) + \lambda \|\beta\|_2^2.$$



B. Examples of generalizations

3. Playing with the hypothesis space: nonlinear dependencies

From nonlinear to linear
Polynomial regression example

- Consider a polynomial regression in dimension $d = 2$: this corresponds to a linear model of dimension $d' = 7$ with feature vector:

$$\Phi(x_1, x_2) = (1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2)^T$$

- Note that:

$$\Phi(x)^T\Phi(x') = (x^Tx' + 1)^2$$

- We call $K(x, x') = (x^Tx' + 1)^2$ a polynomial kernel. A kernel has the property to be represented as a scalar product in a high dimensional feature space. The feature space is the image of the original input space of dimension d through Φ. The feature space can be of huge dimension.

The magic of kernels
Kernel ridge regression

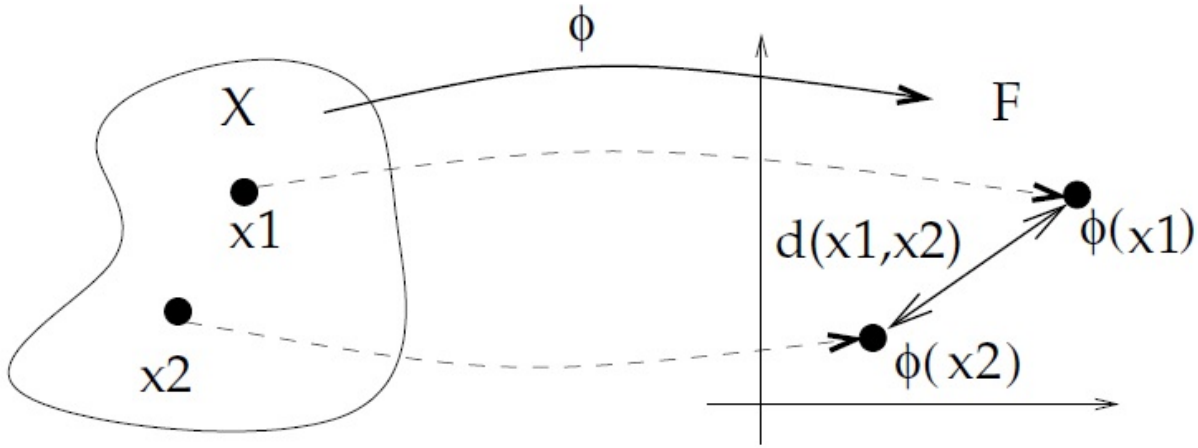
- In the linear case of ridge regression, we have seen that the only data-dependent quantities that matter in both problem formulation and evaluation of predictions are the pairwise scalar products of $X_i^T X_j$ and $x^T X_i$.
- We can basically replace any scalar product by the kernel evaluation of the considered pair without changing at all the algorithmic complexity of resolution. We are then able to estimate the parameters α_i of nonlinear functions of the form:

$$f(x) = \sum_{i=1}^{n} \alpha_i K(x, X_i)$$

Examples of basic kernels

- Linear: $\mathrm{K}(\mathrm{x}, \mathrm{z}) = \mathrm{x} \cdot z$
- Polynomial: $\mathrm{K}(\mathrm{x}, z) = (\mathrm{x} \cdot z)^{\mathrm{d}}$ or $\mathrm{K}(\mathrm{x}, z) = (1 + \mathrm{x} \cdot z)^{\mathrm{d}}$
- Gaussian: $\mathrm{K}(\mathrm{x}, z) = \exp\left[-\frac{\|x-z\|^2}{2\,\sigma^2}\right]$
- Laplace Kernel: $\mathrm{K}(\mathrm{x}, z) = \exp\left[-\frac{\|x-z\|}{2\,\sigma^2}\right]$

How a kernel defines a metric
Definition



$$
\begin{aligned}
d_K(\mathbf{x}_1, \mathbf{x}_2)^2 &= \| \Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2) \|_{\mathcal{H}}^2 \\
&= \langle \Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2), \Phi(\mathbf{x}_1) - \Phi(\mathbf{x}_2) \rangle_{\mathcal{H}} \\
&= \langle \Phi(\mathbf{x}_1), \Phi(\mathbf{x}_1) \rangle_{\mathcal{H}} + \langle \Phi(\mathbf{x}_2), \Phi(\mathbf{x}_2) \rangle_{\mathcal{H}} - 2 \langle \Phi(\mathbf{x}_1), \Phi(\mathbf{x}_2) \rangle_{\mathcal{H}} \\
d_K(\mathbf{x}_1, \mathbf{x}_2)^2 &= K(\mathbf{x}_1, \mathbf{x}_1) + K(\mathbf{x}_2, \mathbf{x}_2) - 2K(\mathbf{x}_1, \mathbf{x}_2)
\end{aligned}
$$

Kernel engineering

- Specific kernels have been design to process structured data such as strings (text, DNA sequence...)
- Example of spectrum kernel used for DNA sequences:

Kernel definition

- The 3-spectrum of

$$\mathbf{x} = \texttt{CGGSLIAMMWFGV}$$

is:

$$(\texttt{CGG},\texttt{GGS},\texttt{GSL},\texttt{SLI},\texttt{LIA},\texttt{IAM},\texttt{AMM},\texttt{MMW},\texttt{MWF},\texttt{WFG},\texttt{FGV}) \ .$$

- Let $\Phi_u(\mathbf{x})$ denote the number of occurrences of u in $\mathbf{x}$. The k-spectrum kernel is:

$$K(\mathbf{x},\mathbf{x}') := \sum_{u \in \mathcal{A}^k} \Phi_u(\mathbf{x}) \Phi_u(\mathbf{x}') \ .$$

Kernel machine learning estimation
Is it doable?

- Nice modeling properties of kernel functions
- The question is whether the penalized optimization in the sense of least squares is feasible?

B. Examples of generalizations

4. Playing with the input space: from vectors to matrices

Motivation
Recommender systems

- One million big ones!

- Given 100 million ratings on a scale of 1 to 5, predict 3 million ratings to highest accuracy

- 17770 total movies
- 480189 total users
- Over 8 billion total ratings

Matrix completion
Problem formulation

	Item 1	Item 2	...	Item 99	Item 100
Customer 1	5	NA	...	NA	3
Customer 2	NA	2	...	3	NA
...	...	...	...	...	...
Customer 49	2	3	...	NA	4
Customer 50	1	NA	...	NA	NA

- **PROBLEM:** Find the matrix of lowest rank has the specified entries

$$\begin{array}{ll} \text{minimize} & \text{rank}(\mathbf{X}) \\ \text{subject to} & X_{ij} = M_{ij} \quad \forall\ (i,j) \in \Omega \end{array}$$

- **When is this problem easy?**
  - Which algorithms?
  - Which sampling sets?
  - Which low-rank matrices?

Matrix completion
Discussion

- Can be used for other matrix estimation problems such as: community detection on social networks, covariance matrix estimation in portfolio management, ...
- Efficient solutions have been developed through relaxation of the initial problem
- Relies on linear algebra techniques (matrix norms, SVD...)
- Interesting to consider structural assumptions on matrices, tensors, depending on the physics of the problem

Next sessions

- From data to information: on the importance of data representation...
- ... and back to sparsity as a means for variable selection
- Insights on optimization problems raised in machine learning
- Main algorithmic principles: kernel machines, ensemble methods, deep learning