# Improving model performance:
# Model Selection, Parameter Tuning and Feature Engineering

B. Michel

Ecole Centrale de Nantes

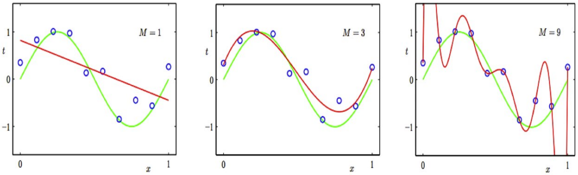
Statistical Learning

# Outline

# Overfitting

- Statistics is not just interpolating between observation points !
- Overfitting occurs when the learning rule too closely corresponds to a particular set of data, and may therefore fail to generalize on future observations.

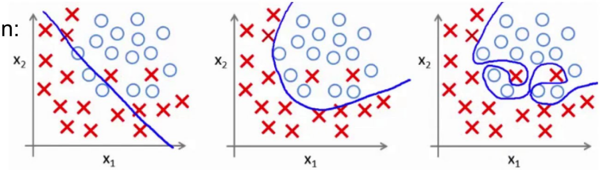
Regression:




predictor too inflexible: cannot capture pattern

predictor too flexible: fits noise in the data

Classification:



# Overfitting

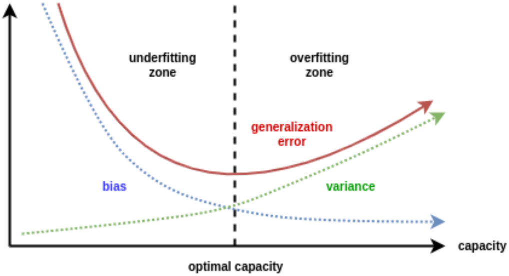
- Statistics is not just interpolating between observation points !
- Overfitting occurs when the learning rule too closely corresponds to a particular set of data, and may therefore fail to generalize on future observations.
- An overfitted model is a statistical model that contains more parameters than can be learned (estimated) by the data.
- Examples :
  - In regression : e.g. a linear model with too many variables (features).
  - In classification : e.g. a k-NN with k too small.
  - In density estimation : an histogram with too many bins.
  - Kernel methods : bandwidth too small
  - ...
- High dimensional statistics : $n$ is of the order (or smaller than) the number of features $p$.

# Bias Variance Tradeoff

- loss $\ell$ : quadratic, logistic, hinge loss ....
- Risk or Generalization error of a learning rule $\hat{f}$ : $\mathbb{E}\ell(Y, \hat{f}(X))$
- Typical decomposition of the generalization error :

Generalization error = (or $\leq$) Approximation error + Estimation error

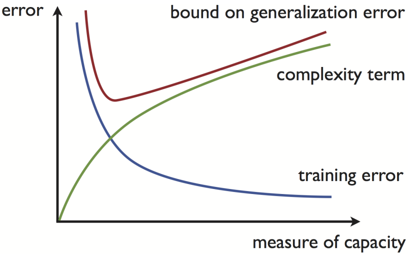
- Estimation error : random term $\approx$ variance term in statistics.
- Approximation error : deterministic term $\approx$ bias term in statistics.




[ Daniel Saunders]

# Training error versus test error

- How can we **estimate** the generalization error from the data ?
- The **learning error** is the average error that results from estimating the performance of a learning rule using the sample **already used** to fit the learning rule.
- The **test error** is the average error that results from estimating the performance of a learning rule using a **different** sample.
- The **learning error** can dramatically **underestimate** the generalization error :




**Question:** Why does the learning error may fail to estimate the generalization error ?

# Outline

# Splitting

- Sample $(X_i, Y_i)_{i=\dots n}$, loss function $\ell$.
- Split the data at random :
  - $I_{\text{train}}$ : observations in the train set ;
  - $I_{\text{test}}$ : observations in the test set.
- Learn a learning rule $\hat{f}$ on $I_{\text{train}}$.
  E.g Empirical Risk Minimization (ERM) on $S$ with loss $\ell$:

$$\hat{f} = \operatorname*{argmin}_{f \in S} \frac{1}{|I_{\text{train}}|} \sum_{i \in I_{\text{train}}} \ell(Y_i, f(X_i))$$

- Compute the test error on $I_{\text{test}}$:

$$\text{Err}_{\text{test}} = \frac{1}{|I_{\text{test}}|} \sum_{i \in I_{\text{test}}} \ell(Y_i, \hat{f}(X_i))$$

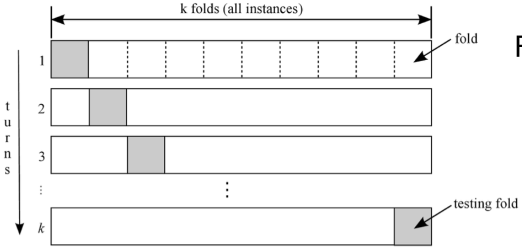
- Split at random $N$ times and average the $N$ test errors.

# Splitting

- For each splitting we compute a learning rule : high computational cost.
- The train sample is smaller than the complete sample : it overestimates the generalization error.
- Alternative : Cross validation methods.

# Cross validation : k-fold cross validation

- k-fold validation: pick a random partition $I_1, \ldots, I_v, \ldots I_k$ of $\{1, \ldots, n\}$ where $|I_v| \sim n/k$.




[Gaiffas]

For each fold $v$ :

- $I_{\text{test},v} = I_v$,
- $I_{\text{train},v} = \{1, \ldots, n\} \setminus I_v$,
- $\hat{f}_v$ : learning rule fitted (trained) on $I_{\text{train},v}$.

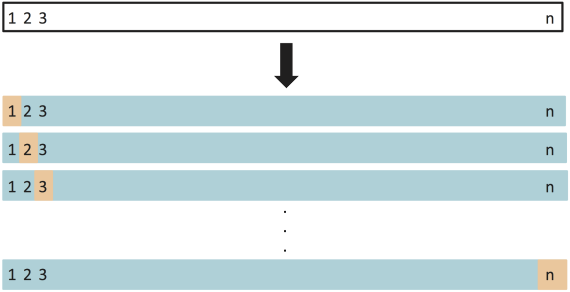
- Compute

$$\text{Err} = \frac{1}{k} \sum_{v=1\ldots k} \frac{1}{|I_v|} \sum_{i \in I_v} \ell(Y_i, \hat{f}_v(X_i)).$$

- Only $k$ learning rules are fitted with this approach.

# Cross validation : Leave one out

- Leave one out (Loo) : $k = n$




[From : The Elements of Stat Learning]

- $I_{\text{test},v} = \{v\}$,
- $I_{\text{train},v} = \{1, \ldots, n\} \setminus \{v\}$,

# Cross validation

- Cross validation aims at estimating the generalization error :
  - Cross validation methods are estimation procedures, they have a bias and a variance.
  - In practice : take $k \approx 5 - 10$.
  - Cross validation with sklearn :
- Cross validation can be used for
  - tuning a parameter, e.g. for regularization.
  - for selecting models in a given collection.

  In both cases: **after tuning the parameters and selecting a model, you should fit the chosen model on the complete dataset (not only on the train dataset).**

# Outline

# Linear regression in high dimension

- Regression, design matrix $X$ of size $n \times p$, target $Y$.
- Linear predictors of $Y$ : $f_\beta(x) = x'\beta$.
- Quadratic loss : $\hat{\beta} = (X'X)^{-1}X'Y$.
- High dim: $n \sim p$ or $n \lesssim p$ : $X'X$ is not inversible.
- Ridge regularization :

$$\hat{\beta}_\lambda^{\text{ridge}} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \|Y - X\beta\|^2 + \lambda \sum_{j=1}^{p} \beta_j^2.$$

  and the solution is

$$\hat{\beta}_\lambda^{\text{ridge}} = (X'X + \lambda \mathrm{Id}_p)^{-1} X'Y.$$

- It can be proved that ridge penalization leads to a better generalization error.

# Penalized Empirical Risk Minimization

- Penalized Empirical Risk Minimization is not restricted to linear models, it consists in finding a solution to

$$\hat{f}_{S,\lambda} := \operatorname*{argmin}_{f \in S} \sum_{i=1\dots n} \ell(Y, f(X_i)) + \lambda \,\mathrm{pen}(f)$$

  where :
  - $S$ is a class of predictors
  - $\mathrm{pen}$ is a (positive) penalization function, which keeps the (statistical) complexity of $f$ under control,
  - $\lambda$ is a tuning or smoothing parameter, that balances goodness-of-fit and penalization.

- $\lambda$ can be chosen by cross validation.

- When $f = f_\beta$ with $\beta \in \mathbb{R}^p$, $\mathrm{pen}(f_\beta) = \mathrm{pen}(\beta)$:
  - the $\ell_0$ penalty $\mathrm{pen}(\beta) = \|\beta\|_0$,
  - the ridge penalty $\mathrm{pen}(\beta) = \|\beta\|_2$,
  - the lasso penalty $\mathrm{pen}(\beta) = \|\beta\|_1$.

- (Data driven penalty, Radamacher, boostrap ...)

# Penalized linear predictors

$$\underset{f \in S}{\operatorname{argmin}} \sum_{i=1 \ldots n} \ell(Y, f(X_i)) + \lambda \operatorname{pen}(f_\beta) \tag{1}$$

with

$$S: \quad f_\beta^{reg}(x) = \langle x, \beta \rangle \quad \text{or} \quad f_\beta^{cla}(x) = \operatorname{sign}(\langle x, \beta \rangle)$$

- When $\beta_j = 0$, then feature $j$ has no impact on the prediction.
- To control overfitting but also to improve interpretation we would like $\beta$ to be sparse : many 0's in $\beta$.

# Penalized linear predictors

$$\underset{f \in S}{\operatorname{argmin}} \sum_{i=1...n} \ell(Y, f(X_i)) + \lambda \operatorname{pen}(f_\beta) \tag{1}$$

with

$$S: \quad f_\beta^{reg}(x) = \langle x, \beta \rangle \quad \text{or} \quad f_\beta^{cla}(x) = \operatorname{sign}(\langle x, \beta \rangle)$$

- First option: the $\ell_0$ penalty $\|\beta\|_0 = \left|\{j \in \{1, \ldots, p\} \ \beta_j \neq 0\}\right|$
  - corresponds to AIC, BIC and Mallows $C_p$ and more recent $\ell_0$ strategies.
  - strong mathematical guarantees.
  - ... but NP hard problem because we have to consider and find the solution for all the possible supports for $\beta$.

# Penalized linear predictors

$$\underset{f \in S}{\operatorname{argmin}} \sum_{i=1 \ldots n} \ell(Y, f(X_i)) + \lambda \operatorname{pen}(f_\beta) \tag{1}$$

with

$$S : \quad f_\beta^{reg}(x) = \langle x, \beta \rangle \quad \text{or} \quad f_\beta^{cla}(x) = \operatorname{sign}(\langle x, \beta \rangle)$$

- The ridge ($\ell_2$) penalty $\|\beta\|_2 = \sqrt{\sum_{j=1}^{p} \beta_j^2}$
  - Lagrange duality:

    (1) $\Leftrightarrow$ minimize $\sum_{i=1 \ldots n} \ell(Y, f(X_i))$ under $\|\beta\|_2 \leq C_\lambda$.

**Question:** Draw the $\ell_2$ unit ball in $\mathbb{R}^2$. How does it intersect with the level sets of the empirical risk ?

  - No strong sparsity induced !

# Penalized linear predictors

$$\operatorname*{argmin}_{f \in S} \sum_{i=1 \ldots n} \ell(Y, f(X_i)) + \lambda \, \mathrm{pen}(f_\beta) \tag{1}$$

with

$$S : \quad f_\beta^{reg}(x) = \langle x, \beta \rangle \quad \text{or} \quad f_\beta^{cla}(x) = \mathrm{sign}(\langle x, \beta \rangle)$$

- The Lasso ($\ell_1$) penalty $\|\beta\|_1 = \sum_{j=1}^{p} |\beta_j|$
  - $\ell_1$ appears as a convex proxy of the $\ell_0$.
  - Lagrange duality :

    (1) $\Leftrightarrow$ minimize $\sum_{i=1 \ldots n} \ell(Y, f(X_i))$ under $\|\beta\|_1 \leq C_\lambda$.

**Question:** Draw the $\ell_1$ unit ball in $\mathbb{R}^2$. How does it intersect with the level sets of the empirical risk ?

  - Sparsity induced. Strong mathematical guarantees.
  - E.g standard Lasso (regression with quadratic loss), logistic Lasso (classification with logistic loss), SVM lasso (hinge loss) ...

# Penalized linear predictors

$$\underset{f \in S}{\text{argmin}} \sum_{i=1 \dots n} \ell(Y, f(X_i)) + \lambda \, \text{pen}(f_\beta) \tag{1}$$

with

$$S : \quad f_\beta^{reg}(x) = \langle x, \beta \rangle \quad \text{or} \quad f_\beta^{cla}(x) = \text{sign}(\langle x, \beta \rangle)$$

- Other options:
  - elastic-net : sum of lasso and ridge,
  - group lasso : select variables by blocks,
  - Fused lasso : penalizes the $\ell_1$ norm of both the coefficients and their successive differences,
  - mixed strategies.

# Penalty shapes

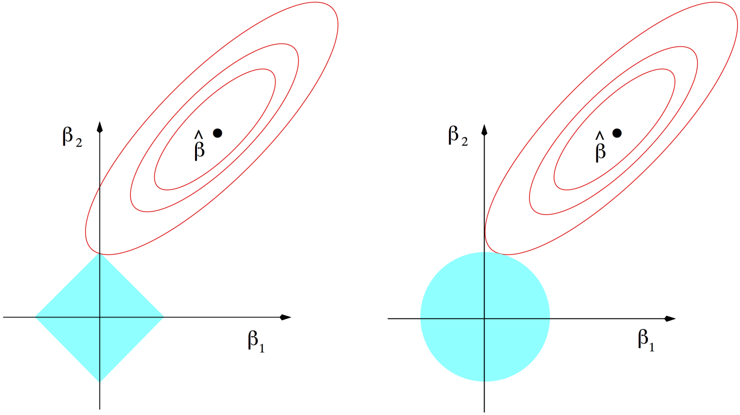
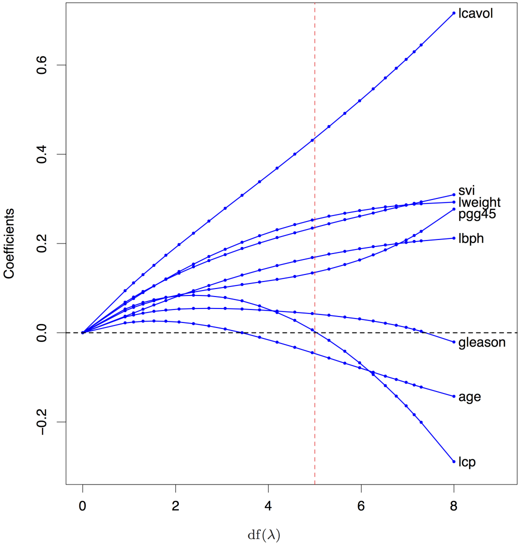



**FIGURE 3.11.** *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses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

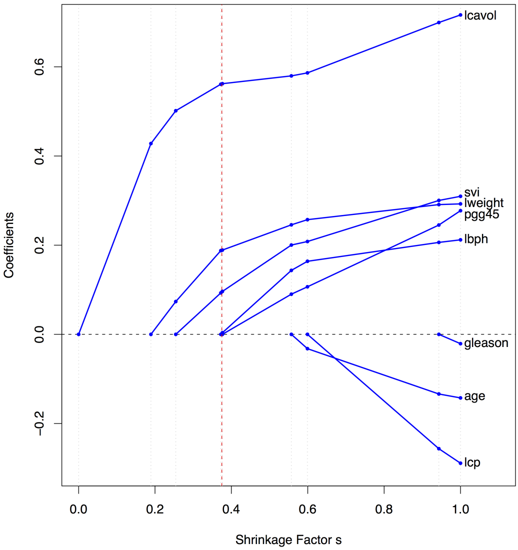
[From The Elements of Stat Learning]

# Regularization path: Ridge




[From The Elements of Stat Learning]

# Regularization path: Lasso




[From The Elements of Stat Learning]

# Outline

# Normalization

- Contrary to the standard least square estimator, ridge and lasso estimators are not scale invariant, even for the quadratic loss.
- We need to normalize the variables :
  - center, include an intercept, standardize
  - min-max scaling
  - binarize the variables
- More generally, these preliminary steps are recommended for most machine learning procedures.

# Feature extraction and feature generation

- Create new variables to improve the prediction performances and use model selection / regularization methods to control the statistical complexity.
- Recipe / list of basic ideas :
  - Transform variables to obtain a better (simpler) relationship with the output : log, exponential, quadratic, sin, cos ..transformations
  - Introduce interaction variables
  - If there exists a model for $Y$ (e.g. physical or biological model), including the corresponding variables will help the machine learning approach.
  - Times series : min / max / min-max / derivatives / spectral pattern
  - Decomposition and projection : PCA, splines, Fourrier, wavelets ...
  - Images : specific pattern
- The python library featuretools generates many classical features, see for instance this blog.
- Take home message: Feature engineering is generally a critical step for machine learning !