# Introduction to Statistical Machine Learning


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# Mathematical Description of Data

Notations

- input - output relation
  - $x$: inputs, feature vectors, predictors, independent variables.
  - $y$: output, response, dependent variable.
- $\mathcal{X}$ and $\mathcal{Y}$ denote the spaces of the generic $x$ and $y$ variables, respectively.
  - Generally $\mathcal{X} = \mathbb{R}^p$; qualitative features are coded using, for example, dummy variables (such as 0,1, -1, etc).
  - Typically $\mathcal{Y} \in \mathbb{R}^1$ is a scalar, or takes a finite number of values as a subset of $\mathbb{N}$ ; it can be a vector in some scenarios.
- The random variable $(X, Y)$ has the joint distribution $p(x, y)$ on the sample space $\mathcal{X} \times \mathcal{Y}$.

# Ground truth

- It is usually assumed that the ground truth for the relation between from input to the output is a deterministic input-output mapping from $x \in \mathcal{X}$ to $y_{\text{true}} \in \mathcal{Y}$:

$$y_{\text{true}} = f^{\star}(x)$$

where the ground truth $f^*$ is an unknown function and has to be approximated by learning from the training dataset.

# Data as iid r.v.

- In **supervised learning**, the data ( observations ) are given as the collection of the pairs [1]

$$\mathtt{D} = \left\{ (x^{(i)}, y^{(i)}) : 1 \leq i \leq N \right\} \subset (\mathcal{X} \times \mathcal{Y})^N$$

  which is assumed iid samples of the r.v. $(X, Y)$ with an unknown joint distribution $p(x, y)$ on the product space $\mathcal{X} \times \mathcal{Y}$.
  - Regression: $\mathcal{Y}$ is continuous/quantitiative, e.g., $\mathbb{R}^d$ or its subset.
  - Classification: $\mathcal{Y}$ is discrete and finite (categorical variable), encoded by a finite number $\{1, \ldots, K\}$. In this case, "$y$" is usually called "label".
- In **unsupervised learning**, the observations only have $\left\{x^{(i)}\right\}$, the information $y^{(i)}$ is zero or there is no definition of $y$ variable. The purpose is to identify the pattern of $\left\{x^{(i)}\right\}$ itself, such as model reduction.

[1] sometimes it is denoted as $\mathtt{D} = \{(x_i, y_i) : 1 \leq i \leq n\}$ if the subindex has no ambiguity.

# Output as perturbed truth

- The observed $x^{(i)} \in \mathcal{X}$ are samples from the marginal distribution $p_X$, i.e., $x^{(i)} \sim X$; in some cases, they are deterministic and assigned by a procedure of experiment design.
- The corresponding observed $y^{(i)}$ are assumed to be the *perturbed* truth $f^\star(x^{(i)})$ with additional measurement error $\varepsilon^{(i)}$ which are assumed to be iid and independent from $X$.

$$y^{(i)} = f^\star(x^{(i)}) + \varepsilon^{(i)}.$$

  $\left\{\varepsilon^{(i)}\right\}$ are assumed iid and distributed as a generic r.v. $\varepsilon$.
- The effect of the noise $\varepsilon$ can never be eliminated by any statistical learning algorithms (irreducible error).

- So, the joint distribution $p(x, y)$ of $(X, Y)$ is completely determined by the triplet:

$$(p_X, f^\star, p_\varepsilon)$$

  - $p_X$: the distribution of the input
  - $f^\star$: the input-output function,
  - $p_\varepsilon$: the distribution of error.

- The joint distribution $p(x, y)$ manifests by the available dataset $\mathtt{D}$. Given $X, Y$ random variables $\sim p$, how to identify $f^\star$?

# Statistics and machine learning

Different views and terminologies:

| **Machine Learning** | **Statistics** |
|---|---|
| Supervised learning | Classification/regression |
| Unsupervised learning | Clustering |
| Semisupervised learning | Classification/regression with missing responses |
| Features/outcomes | Covariates/responses |
| Training set/testing set | Sample/population |
| Learner | Statistical model |
| Generalization error | Misclassification error/prediction error |

# Suggestion

Learn machine learning like a statistician or an applied mathematician, not a software engineer

- Start from stating a problem, not show an algorithm first: Many times, the students think the methods/algorithms/procedures as the problem itself.
- Pay close attentions to the "modelling" process: how to turn the data problem into the statistical model. In particularly the underlying principle which applies very general.
- Try to rigorously ( and in most general context) understand (like a math theorem) the heuristic arguments used in practice, even for some toy examples.
- Draw strict boundaries between general principles and specific methods. In between, computational method survives and thrives.
- Diagnose and rationalize your results of numerical experiments. Test different dataset/parameters/methods.

# Learning Theory: An Approximation Theory Viewpoint

Reference:

Learning Theory: An Approximation Theory Viewpoint; by F. Cucker and D.X. Zhou, Cambridge University Press 2007

Given r.v.s $X$ and $Y$, find a function $f : \mathcal{X} \to \mathcal{Y}$ so that $f(X)$ can explain $Y$ best in certain sense.

# Conditional Expectation as Optimal Prediction

The best $L^2$ approximation of a function $f$ of the r.v. $X$ to a r.v. $Y$ is achieved by the conditional probability. The **(generalized) squared error**[1]

$$\mathcal{E}(f) := \mathbb{E}\,|Y - f(X)|^2 \tag{1}$$

has a minimum at

$$f^*(x) = \mathbb{E}(Y|X = x).$$

i.e.,

$$\mathbb{E}\,|Y - f^*(X)|^2 = \min_{f\text{: a Borel function}} \mathbb{E}(|Y - f(X)|^2)$$

[1] also named as generalization risk, mean square error, $L_2$ error, etc.

## Proof.

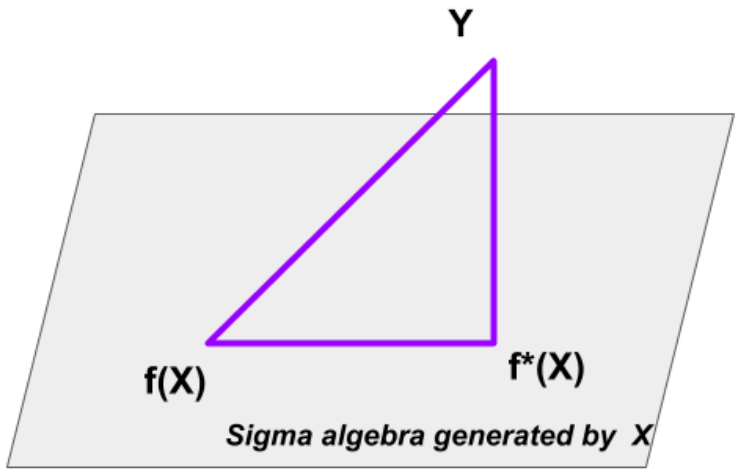
- We show first that $\mathbb{E}[(Y - f^*(X))h(X)] = 0$ is true for any function $h$. Using the double expectation theorem, we have

$$\begin{aligned}\mathbb{E}[(Y - f^*(X))h(X)] &= \mathbb{E}\left[\mathbb{E}[Y - f^*(X))|X]h(X)\right] \\ &= \mathbb{E}\left[\mathbb{E}(Yh(X)|X) - f^*(X)h(X)\right] = 0.\end{aligned}$$

- Note that
  $(y - f(x))^2 = (y - f^*(x))^2 + (f(x) - f^*(x))^2 - 2(y - f^*(x))h(x)$
  where $h(x) = f(x) - f^*(x)$, then for any $f$

$$\boxed{\mathbb{E}(|f(X) - Y|^2) = \mathbb{E}(|f^*(X) - Y|^2) + \mathbb{E}\left[|f(X) - f^*(X)|^2\right]} \quad (2)$$

□




reference for elementary math: Understanding Conditional Expectation via Vector Projection

The following exercise is to use the viewpoint of variational calculus: minimizing in functional space

**Exercise**

*Use the method of Calculus of Variation to solve*

$$\inf_f \iint (f(x)-y)^2 p_{X,Y}(x,y)dxdy$$

*where* $p_{X,Y}$ *is the joint pdf of the r.v.s* $(X,Y)$*. The optimal* $f^*$ *satisfies*

$$\int (f^*(x)-y)p_{X,Y}(x,y)dy = 0, \qquad \forall x$$

*i.e.,* $\mathbb{E}\, Y = \mathbb{E}\, f^*(X)$

What if generalized the $L_2$ norm to $L_p$ norm ?

## Exercise (Conditional distribution of multivariate Gaussian r.v.)

*Suppose that* $X = (X_1, X_2)$ *is a two dimensional Gaussian random variable with mean* $\mu = (\mu_1, \mu_2)$ *and the covariance matrix* $\Sigma = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$. *What is the conditional pdf* $p(x_1|x_2)$ *of* $X_1$ *given* $X_2 = x_2$*? What is the expectation of* $X_1$ *given* $X_2 = x_2$*? What is the general result in* $n$ *dimension ?*

$$X_1|_{X_2=x_2} \sim \mathcal{N}(\mu_1 + \rho\frac{\sigma_1}{\sigma_2}(x_2 - \mu_2), \sigma_1^2(1-\rho^2))$$

- The objective function $\mathcal{E}(f)$ is also called loss function, risk, etc.
- $\mathbb{E}\, f^*(X) = \mathbb{E}\, Y$: $f^*(X)$ is an unbiased estimate of $Y$;
- The variance of the difference between $Y$ and the optimal prediction $f^*(X)$ is

$$\sigma_*^2(x) := \mathbb{E}\left[(Y - f^*(X))^2 | X = x\right]$$

- Take average of $\sigma^2(x)$ over $x$, then the averaged uncertainty is

$$\sigma_*^2 := \mathbb{E}_X\, \sigma^2(X) = \mathbb{E}\left[|Y - f^*(X)|^2\right] = \mathcal{E}(f^*)$$

is the variance of the measurement error $Y - f^*(X)$: irreducible error

# Notations

We have shown that (2)

$$\begin{aligned}\mathbb{E}_{X,Y}(|f(X)-Y|^2) &= \mathbb{E}_{X,Y}(|f^*(X)-Y|^2) + \mathbb{E}_X\left[|f(X)-f^*(X)|^2\right] \\ &= \text{Bayes error} + \text{model error}\end{aligned} \tag{3}$$

where $f^*(x) = \mathbb{E}(Y|X=x)$ is called **Bayes rule**.

# Application to classification with 0-1 loss

- Assume $Y \in \{1, \ldots, K\}$ and $X \in \mathbb{R}^p$.
- $f : \mathcal{X} \to \mathcal{Y}$ is a piece-wise constant function.
- A Loss function $\ell(Y, f(Y))$ for penalizing errors in misclassification.
- Most Common choice is the 0-1 loss

$$\ell(Y, f(X)) = I(Y \neq f(X)).$$

- The expected prediction error, or the generalization error, is

$$\mathcal{E}(f) = \mathbb{E}\, I(Y \neq f(X)) = \mathbb{P}(Y \neq f(X)) = 1 - \mathbb{P}(Y = f(X)).$$

- The Bayes rule minimizing $\mathcal{E}(f)$ is the one maximizing $\mathbb{P}(Y = f(X)) = \int_{\mathcal{X}} \mathbb{P}(Y = f(x)|X = x) p_X(x) dx$, which is

$$f^*(x) = \underset{k}{\operatorname{argmax}}\, \mathbb{P}(Y = k|X = x).$$

since $\mathbb{P}(Y = k|X = x) \leq \mathbb{P}(Y = f^*(x)|X = x), \forall k$

# How do we estimate $f^*$ ?

- direction method by definition of conditional expectation;
- optimization method by minimization of generalization error;

# Nearest neighbors method to approximate condition expectation

A natural way to approximate the function $\mathbb{E}(Y|X=x)$ is to replace the expectation by the average:

$$f^*(x) = \mathbb{E}(Y|X=x) \approx \text{AVE}\{y_i : \text{ where } x_i = x\}, \quad \forall x \in \mathcal{X}$$

Question: Would this work well in practice ? in high dimension ?
(1) this formula is defined point-wisely; (2) one does not have an accurate estimation of the expectation or the joint distribution $p(x,y)$, particularly in high dimension.

- Use windows with size $\Delta$

$$\mathbb{E}(Y|X=x) \approx \text{AVE}\{y_i : \text{ where } |x_i - x| \leq \Delta\}$$

- Use $k$ -nearest neighbors: have a look at its neighbors, and take a vote:

$$\mathbb{E}(Y|X=x) \approx \text{AVE}\{y_i : x_i \in \mathcal{N}_k(x)\}$$

  where $\mathcal{N}_k(x)$ is a neighborhood of $x$ that contains exactly $k$ neighbors (k-nearest neighbors).

# Curse of dimensionality

k-NN can fail in high dimensions, because it becomes difficult to gather $k$ observations close to a target point $x_0$.

- Neighborhoods tend to be spatially large, and estimates are biased.
- Reducing the spatial size of the neighborhood means reducing $k$, and the variance of the estimate increases.

In general (see Figure 2.6),

- Most points are at the boundary, and points tend to be equidistant (Hall et al., JRSS-B, 2005).
- Sampling density is proportional to $n^{1/p}$: the number of sample size increases exponentially in dimension $p$: If 100 points are sufficient to estimate a function in $\mathbb{R}^1$, $100^{10}$ are needed to achieve similar accuracy in $\mathbb{R}^{10}$.

This is similar to the curse of dimensionality in using the mesh grid based method to solve high dimension PDE.

# Minimizing the generalization error: learning as minimization

- Loss function $\ell(y, \hat{y}) : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}^+$
  - $L_2$, $L_1$ norm
  - 0-1 loss: $\ell(y, \hat{y}) = I(y \neq \hat{y})$.
  - ...
- $\mathcal{E}(f) = \mathbb{E}\, \ell(Y, f(X))$

The direct approach of minimizing the risk

$$\min_f \mathcal{E}(f) = \mathbb{E}\, \ell(Y, f(X))$$

where $f$ can be in a very general class of functions, such as continuous function on $\mathcal{X}$, or even piecewise continuous function.

1. the function space of $f$ to search: hypothesis space(model class) $\mathcal{H}$. It is important to specify a hypothesis space $\mathcal{H}$ to restrict the search space.
2. approximate the expectation $\mathbb{E}$ in $\mathcal{E}$ with the use of data $\mathtt{D} = \{x_i, y_i\}$.

# Notations

1. The minimizer of
$$\min_{f\in\mathcal{H}} \mathcal{E}(f)$$
is denoted by $f_{\mathcal{H}}$.

2. $$\mathcal{E}(f) = \mathbb{E}\left[|Y - f(X)|^2\right] \approx \mathcal{E}_N(f) = \frac{1}{N}\sum_i \ell(y_i, f(x_i))$$
The learning algorithm produces the learnt function $\hat{f}_{\mathtt{D}}$ ( regression function) as the solution to
$$\mathcal{E}_N(\hat{f}_{\mathtt{D}}) = \min_{f\in\mathcal{H}} \mathcal{E}_N(f) = \min_{f\in\mathcal{H}} \frac{1}{N} \sum_{(x_i,y_i)\in\mathtt{D}} \ell(y_i, f(x_i))$$
The **training error** (empirical risk) is $\mathcal{E}(\hat{f}_{\mathtt{D}})$ .

- $\hat{f}_{\mathtt{D}}$ depends on *three* elements: the hypothesis space $\mathcal{H}$, the (training) data $\mathtt{D}$ ( random ! ) and the loss function $\ell$. So, $\hat{f}_{\mathtt{D}}$ is a random function to approximate the ground truth $f$.
- For the fixed $\mathcal{H}$ and $\ell$, $\hat{f}_{\mathtt{D}}$ is essentially a mapping from $\mathtt{D}$ to the function space $\mathcal{H}$. As $N \to \infty$, $\hat{f}_{\mathtt{D}} \to f_{\mathcal{H}}$ by the law of large number.

# Hypothesis space: representation of the function $f$

- parametric approach: e.g. $f(x) = \theta \cdot x$ with a set of finite and (usually fixed) number of parameters $\theta$
- non-parametric approach: functional analysis viewpoint, $f$ is only in some function space. (such as in the traditional computational math for representing the solution to some PDE )
- there is no rigorous boundary between parametric/non-parametric: eventually the computer represents a function $f$ only by a finite number of freedoms.
- need to be restricted to certain model class in practice. Examples: linear model, polynomial, spline, kernel machine, neural network, etc.

# some examples of $\mathcal{H}$

- Linear function (chapter 3 , ESL)
- Basis functions and dictionary methods (chapter 5, ESL)

$$f_\theta(x) = \sum_{m=1}^{M} \theta_m h_m(x),$$

where $h_m$'s are pre-specified basis functions.

- Kernel methods and local regression (chapter 6, ESL)

$$RSS(f, x_0) = \sum_{i=1}^{n} K(x_0, x_i)(y_i - f(x_i))^2,$$

where $K$ is a kernel measuring the closeness between points.

- Roughness penalty (chapter 5, ESL)

$$\text{Penalized RSS}(f; \lambda) = \text{RSS}(f) + \lambda J(f),$$

where $J(f)$ is a regularization term on the model complexity.

The generalization error is then decomposed into

$$\mathcal{E}(f^*) = \underbrace{\mathcal{E}(f^*) - \mathcal{E}(f_{\mathcal{H}})}_{\textbf{approximation error}} + \underbrace{\mathcal{E}(f_{\mathcal{H}}) - \mathcal{E}_N(\hat{f}_{\mathtt{D}})}_{\textbf{sampling error}} + \underbrace{\mathcal{E}_N(\hat{f}_{\mathtt{D}})}_{\textbf{training error}}$$

- Approximation error: characterized how large (complex) the hypothesis space $\mathcal{H}$ is. analogy to the interpolation inequality in finite element method. A larger space of $\mathcal{H}$ indicates
  - A larger effective dimension of this space;
  - A smaller approximation error; lower bias
  - More difficult for numerical optimization;
- Sampling error: vanishes if the number of data points is infinity. This error may be analyzed by probability inequality (e.g. Chebychev); analysis method used for Monte Carlo simulation. A larger sample size for training data indicates:
  - Smaller sampling error; lower variance;
  - more challenges for data collection and Big Data techniques;
- Training error: optimization method

These three topics are not completely separate. For example, the necessary number of sample size $N$ may depend on the complexity of hypothesis space, which further depends on the dimension of $\mathcal{X}, \mathcal{Y}$ and the specific representation form of functions in $\mathcal{H}$.

# Generalization Gap

The optimal function in theory is $f^*$; the optimal function in practical computation is $\hat{f}_{\mathtt{D}}$. The difference in risks of these two:

$$\mathcal{E}(\hat{f}_{\mathtt{D}}) - \mathcal{E}(f^*)$$

is called **generalization gap**: it measures to which extent the performance of the algorithm learnt from a given training data set $\mathtt{D}$ is valid for the whole distribution $p(x, y)$.

# First inequality for Generalization Gap

## Exercise

*Prove the upper bound of the generalization gap:*

$$\mathcal{E}(\hat{f}_{\mathtt{D}}) - \mathcal{E}(f^*) \leq 2 \sup_{f \in \mathcal{H}} |\mathcal{E}_N(f) - \mathcal{E}(f)|$$

$$\approx 2 \sup_{f \in \mathcal{H}} \frac{1}{\sqrt{N}} \mathbb{V}(\ell(Y, f(X)))$$

The first RHS depends on the hypothesis space $\mathcal{H}$ and the dataset $\mathtt{D}$ of size $N$ in $\mathcal{E}_N$; and the second depends on $\mathcal{H}$ and the joint distribution $p(x, y)$ of $(X, Y)$.

The supremum in the above inequality can describe the **complexity** of hypothesis space $\mathcal{H}$, which increases when $\mathcal{H}$ is "larger". WARNING: this upper bound is not sharp. A good lower bound is extremely difficult to obtain.

# Statistical Learning: Viewpoint of Bias-Variance Trade-off

# Bias-Variance Decomposition / Trade-off

Let $f$ be a given deterministic function $\mathcal{X} \to \mathcal{Y}$.
Assume that the response r.v. $Y$ is defined by

$$Y = f(X) + \varepsilon$$

where the r.v. $\varepsilon$ is independent of $X$ and has mean $0$ and variance $\sigma_\varepsilon^2$.
Then $f^*(x) = \mathbb{E}[Y|X = x] = f(x)$ is the optimal approximation in the square error sense.

# test error decomposition

Based on a training dataset $\mathtt{D} = \{x_i, y_i\}$ where $y_i = f(x_i) + \varepsilon_i$ and $\varepsilon_i \sim \varepsilon$, one learns a regression function, denoted by $\hat{f}_{\mathtt{D}}(\cdot)$, then the **test error** at a new input $x_0$ (with a new independent measurement error $\varepsilon_0 \sim \varepsilon$) is

$$\mathbb{E}[(Y - \hat{f}_{\mathtt{D}}(X))^2 | X = x_0] = \mathbb{E}_{\varepsilon_0, \mathtt{D}}[(f(x_0) + \varepsilon_0 - \hat{f}_{\mathtt{D}}(x_0))^2]$$

$$= \sigma_\varepsilon^2 + \mathbb{E}_{\mathtt{D}}[\Big(f(x_0) - \hat{f}_{\mathtt{D}}(x_0)\Big)^2] \quad \because \mathbb{E}(\varepsilon_0) = 0, \text{ and } \mathtt{D} \perp \varepsilon_0$$

$$= \sigma_\varepsilon^2 + \mathbb{E}_{\mathtt{D}}[\Big(f(x_0) - \mathbb{E}\,\hat{f}_{\mathtt{D}}(x_0) + \mathbb{E}\,\hat{f}_{\mathtt{D}}(x_0) - \hat{f}_{\mathtt{D}}(x_0)\Big)^2]$$

$$= \sigma_\varepsilon^2 + \underbrace{(f(x_0) - \mathbb{E}\,\hat{f}_{\mathtt{D}}(x_0))^2}_{\text{Bias}^2} + \underbrace{\mathbb{V}(\hat{f}_{\mathtt{D}}(x_0))}_{\text{Variance}}$$

Sometimes, this quantity should be taken expectation w.r.t. $x_0 \sim p_X$.

- low bias: large model space, low training error, overfitting, bad generalization ability (high variance);
- low variance: rigid model space, insensitive to the perturbation of the dataset used in fitting; good generalization for the new data from the same distribution.
- BAD news: it is almost impossible to decrease the bias and variance terms simultaneously!
- Criteria for model assessment or variable selection: **good trade-off between the bias and variance**
  - Analyse the bias or variance or model complexity to have analytical results (very limited cases)
  - A practical method is to estimate $\mathbb{E}[(Y - \hat{f}_{\mathtt{D}}(X))^2] \approx \frac{1}{n}\sum_j (Y'_j - \hat{f}_{\mathtt{D}}(X'_j))$ where $X'_j$ are not from $\mathtt{D}$ but an independent dataset $\mathtt{D}'$.
  - Where is the "new" dataset $\mathtt{D}'$? cross-validation (split 1 cent into 1/2 cents) and bootstrap (1 cent used twice ) .

# Model assessment

Typical objectives:

- Choose a value of a tuning parameter (hyperparameter) used in the model (such as $k$ in k-NN)
- Estimate the prediction performance (test error) of a given model

Remarks:

- For both objectives, the best approach is to run the procedure on an independent test set, if one is available.
- If possible, one should use different test data for (1) and (2) above: a *validation set* for (1) and a *test set* for (2).
- Often there is insufficient data to create a separate validation or test set. In this case, *Cross-Validation* is useful.

# K-fold cross validation

Denote the hyper-parameter by $\lambda$. K-fold cross validation is the most popular method for estimating a tuning parameter $\lambda$.

Divide the dataset (of size $N$) into $K$ subsets: $\mathcal{A}_1, \ldots, \mathcal{A}_K$ ($K = 2, 5, 10$ or $N$)

- For each $k = 1, \ldots, K$, fit the model with parameter $\lambda$ to $\{\mathcal{A}_1, \ldots, \mathcal{A}_{k-1}, \mathcal{A}_{k+1}, \ldots, \mathcal{A}_K\}$ giving $f_\lambda^{-k}(\cdot)$, and compute its prediction error on $\mathcal{A}_k$:

$$E_k(\lambda) = \sum_{x_i \in \mathcal{A}_k} \ell(y_i, f_\lambda^{-k}(x_i)).$$

- The average of these $K$ values $E_k(\lambda)$ give the cross-validation error (per sample)

$$CV(\lambda) := \frac{1}{N} \sum_{k=1}^{K} E_k(\lambda).$$

- Choose the optimal $\lambda^*$ yielding the smallest $CV(\lambda)$.

# K-fold cross validation

- Cross-validation is often abbreviated as CV.
- In the subset selection procedure, $\lambda$ is the subset size
- $f^{-k}(\lambda)$ is the best model of size $\lambda$, found from the training set that leaves out the $k$-th part of the data
- $E_k(\lambda)$ is its estimated test error on the $k$-th part.
- Using $K$-fold CV, the $K$ test error estimates are averaged to give the final CV estimated test error.
- The output is the model associated with $\lambda^*$, typically, computed by using all $N$ data.

# Bootstrap

- Bootstrap works by sampling $N$ times with replacement from the training set to form a “bootstrap" data set. Then model is estimated on the bootstrap data set, and predictions are made on the original training set.
- This process is repeated many times and the results are averaged.
- *Bootstrap is most useful for estimating standard errors of predictions.*
- Can also use modified versions of the bootstrap to estimate prediction error. Sometimes produces better estimates than CV (still an open question!)