Statistical Machine Learning from Data

Statistical Learning Theory

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The Data

Available training data

- Let $Z_1, Z_2, \cdots, Z_n$ be an n-tuple random sample of an unknown distribution of density $p(z)$.
- All Z_i are independently and identically distributed (iid).
- Let D_n be a particular instance $= \{z_1, z_2, \cdots, z_n\}$.

Various forms of the data

- Classification: $Z = (X, Y) \in \mathbb{R}^d \times \{-1, 1\}$
  objective: given a new x, estimate $P(Y|X = x)$
- Regression: $Z = (X, Y) \in \mathbb{R}^d \times \mathbb{R}$
  objective: given a new x, estimate $E[Y|X = x]$
- Density estimation: $Z \in \mathbb{R}^d$
  objective: given a new z, estimate $p(z)$

The Function Space

Learning: search for a good function in a function space $\mathcal{F}$

Examples of functions $f(\cdot;\theta) \in \mathcal{F}$:

- Regression:

$$\hat{y} = f(x; a, b) = a \cdot x + b$$

- Classification:

$$\hat{y} = f(x; a, b) = \mathrm{sign}(a \cdot x + b)$$

- Density estimation

$$\hat{p}(z) = f(z; \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{|z|}{2}}\sqrt{|\Sigma|}} \exp\left(-\frac{1}{2}(z-\mu)^T\Sigma^{-1}(z-\mu)\right)$$

The Loss Function

Learning: search for a good function in a function space $\mathcal{F}$

Examples of loss functions $L : \mathcal{Z} \times \mathcal{F}$

- Regression:

$$L(z, f) = L((x, y), f) = (f(x) - y)^2$$

- Classification:

$$L(z, f) = L((x, y), f) = \begin{cases} 0 & \text{if } f(x) = y \\ 1 & \text{otherwise} \end{cases}$$

- Density estimation:

$$L(z, f) = -\log p(z)$$

The Risk and the Empirical Risk

Learning: search for a good function in a function space $\mathcal{F}$

- Minimize the Expected Risk on $\mathcal{F}$, defined for a given f as

$$R(f) = E_Z[L(z,f)] = \int_Z L(z,f)p(z)dz$$

- Induction Principle:
  - select $f^\star = \arg\min_{f \in \mathcal{F}} R(f)$
  - problems: $p(z)$ is unknown, and we don't have access to all $L(z,f)$!!!
- Empirical Risk:

$$\hat{R}(f, D_n) = \frac{1}{n}\sum_{i=1}^{n} L(z_i, f)$$

The Empirical Risk

The empirical risk is an unbiased estimate of the risk

$$
\begin{aligned}
E\left[\hat{R}(f,D)\right] &= E\left[\frac{1}{n}\sum_{i=1}^{n} L(f,Z_i)\right] \\
&= \frac{1}{n}\sum_{i=1}^{n} E\left[L(f,Z_i)\right], \quad Z_i s \text{ are independent} \\
&= \frac{1}{n}\sum_{i=1}^{n} E\left[L(f,Z)\right], \quad Z_i s \text{ are identically distributed} \\
&= \frac{1}{n} nE\left[L(f,Z)\right] \\
&= R(f)
\end{aligned}
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Empirical Risk Minimization

The principle of empirical risk minimization (ERM):

$$f^\star(D_n) = \arg\min_{f \in \mathcal{F}} \hat{R}(f, D_n)$$

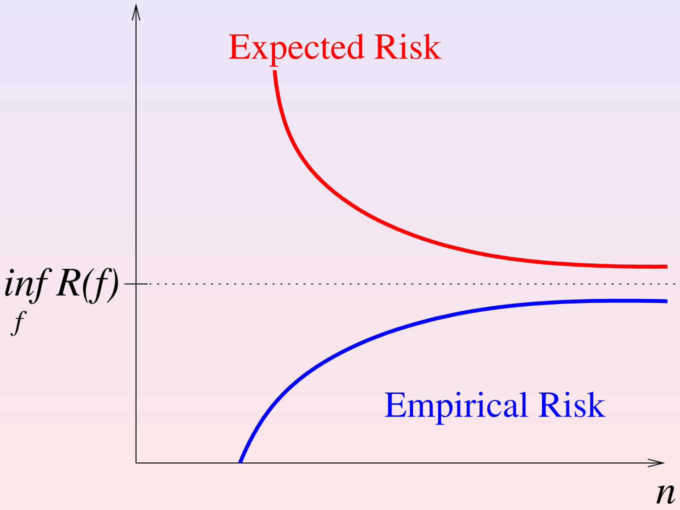
Consistency of the principle of ERM

- Let $f^\star = \arg\min_{f \in \mathcal{F}} R(f)$ and $f^\star(D_n) = \arg\min_{f \in \mathcal{F}} \hat{R}(f, D_n)$
- We say that the principle of ERM is consistent for $\mathcal{F}$ if

$$R(f^\star(D_n)) \quad \xrightarrow[n \to \infty]{P} \quad R(f^\star)$$

$$\text{and} \quad \hat{R}(f^\star(D_n), D_n) \quad \xrightarrow[n \to \infty]{P} \quad R(f^\star)$$

Consistency of the ERM



The Risk and the Training Error

- Training error:

$$\hat{R}(f^\star(D_n), D_n) = \min_{f \in \mathcal{F}} \hat{R}(f, D_n)$$

- Is the training error a biased estimate of the risk? YES.

$$E[R(f^\star(D_n)) - \hat{R}(f^\star(D_n), D_n)] \geq 0$$

- The solution $f^\star(D_n)$ found by minimizing the training error is better on D_n than on any other set $D_n^{'}$ drawn from $p(z)$.

Bounding the Risk

Can we bound the difference between the training error and the generalization error?

$$|R(f^\star(D_n)) - \hat{R}(f^\star(D_n), D_n)| \leq ?$$

- Answer: under certain conditions on $\mathcal{F}$, yes.
- These conditions depend on the notion of capacity h of $\mathcal{F}$.

The Capacity

- The capacity $h(\mathcal{F})$ is a measure of its size, or complexity.
- Classification:

  > *The capacity $h(\mathcal{F})$ is the largest n such that there exist a set of examples D_n such that one can always find an $f \in \mathcal{F}$ which gives the correct answer for all examples in D_n, for any possible labeling.*

- Example: for the set of linear functions ($y = w \cdot x + b$) in d dimensions, the capacity is $d + 1$.
- Regression and density estimation: capacity exists also, but more complex to derive (for instance, we can always reduce a regression problem to a classification problem).

Bounding the Risk

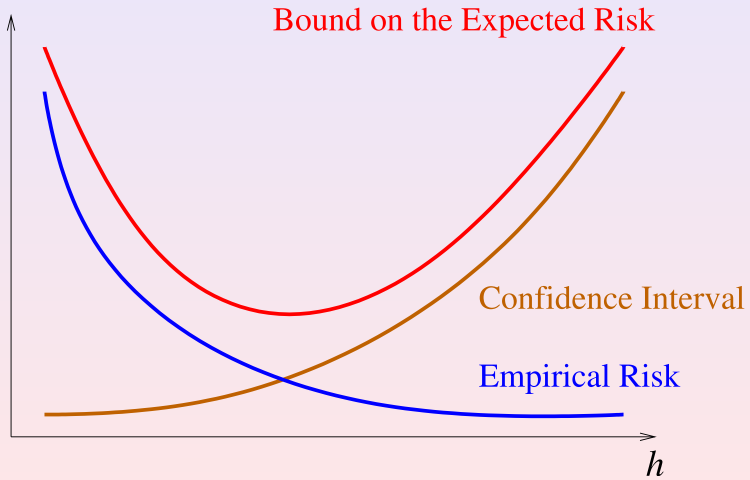
Bound on the expected risk:

- let $\tau = \sup L - \inf L$.
- $\forall \eta$ we have

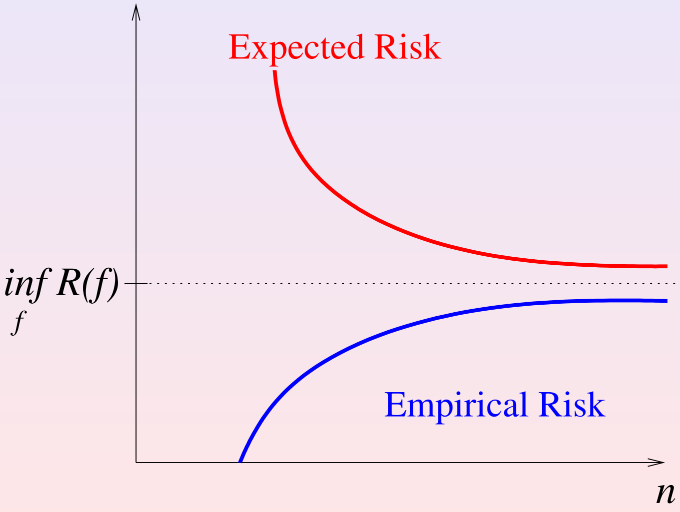
$$P\left(\sup_{f \in \mathcal{F}} |R(f) - \hat{R}(f, D_n)| \leq 2\tau \sqrt{\frac{h\left(\ln \frac{2n}{h} + 1\right) - \ln \frac{\eta}{9}}{n}}\right) \geq 1 - \eta$$

- with h the capacity of $\mathcal{F}$ and n the number of training examples in D_n

Structural Risk Minimization - Fixed n



Consistency - Fixed h

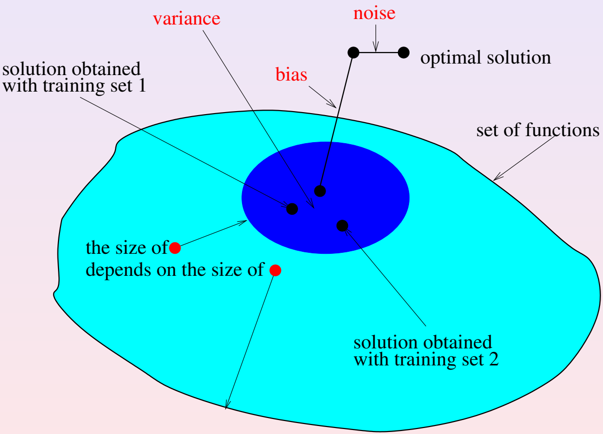


The Bias-Variance Dilemma

The generalization error can be decomposed into 3 parts:

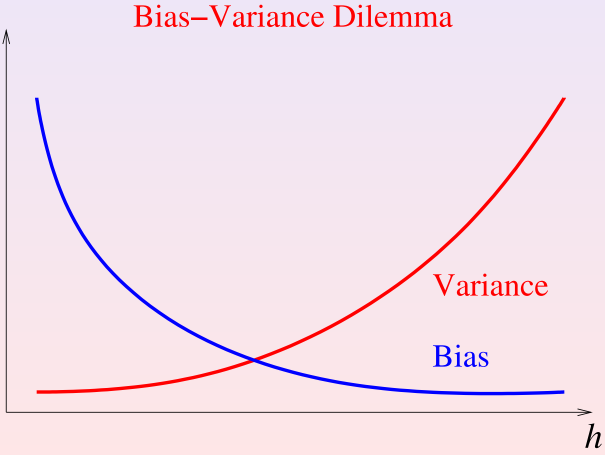
- the bias: due to the fact that the set of functions $\mathcal{F}$ does not contain the optimal solution,
- the variance: due to the fact that if we had been using another set D_n' drawn from the same distribution $p(Z)$, we would have obtained a different solution,
- the noise: even the optimal solution could be wrong! (for instance if for a given x there are more than one possible y)

The Bias-Variance Dilemma (Graphical View)



The Bias-Variance Dilemma (Graphical View)

Intrinsic dilemma: when the capacity $h(\mathcal{F})$ grows, the bias goes down, but the variance goes up!



Regularization

- We have seen that learning = searching in a set of functions
- This set should not be too small (underfitting)
- This set should not be too large (overfitting)
- One solution: regularization
- Penalize functions f according to a prior knowledge
- For instance, penalize functions that have large parameters

$$f^\star(D_n) = \arg\min_{f \in \mathcal{F}} \hat{R}(f, D_n) + H(f)$$

  with $H(f)$ a function that penalizes according to your prior
- For example, in some models:
  small parameters $\longrightarrow$ simpler solutions $\longrightarrow$ less capacity

Early Stopping

- Another method for regularization: early stopping.
- Works when training is an iterative process.
- Instead of selecting the function that minimizes the empirical risk on D_n, we can do:
  - divide your training set D_n into two parts
    - train set $D^{tr} = \{z_1, z_2, \cdots, z_{tr}\}$
    - validation set $D^{va} = \{z_{va+1}, z_{tr+2}, \cdots, z_{tr+va}\}$
    - $tr + va = n$
  - let $f^t(D^{tr})$ be the current function found at iteration t
  - let $\hat{R}(f^t(D^{tr}), D^{va}) = \frac{1}{va} \sum_{z_i \in D^{va}} L(z_i, f^t(D^{tr}))$
  - stop training at iteration $t^\star$ such that

$$t^\star = \arg\min_t \hat{R}(f^t(D^{tr}), D^{va})$$

    and return function $f(D_n) = f^{t^\star}(D^{tr})$

1. Data, Functions, Risk
2. The Capacity
3. **Methodology**

Methodology

- First: identify the goal! It could be
  1. to give the best model you can obtain given a training set?
  2. to give the expected performance of a model obtained by empirical risk minimization given a training set?
  3. to give the best model and its expected performance that you can obtain given a training set?
- If the goal is (1): use need to do model selection
- If the goal is (2), you need to estimate the risk
- If the goal is (3): use need to do both!
- There are various methods that can be used for either risk estimation or model selection:
  - simple validation
  - cross validation (k-fold, leave-one-out)

Model Selection - Validation

- Select a family of functions with hyper-parameter θ
- Divide your training set D_n into two parts
  - $D^{tr} = \{z_1, z_2, \cdots, z_{tr}\}$
  - $D^{va} = \{z_{tr+1}, z_{tr+2}, \cdots, z_{tr+va}\}$
  - $tr + va = n$
- For each value θ_m of the hyper-parameter θ
  - select $f^{\star}_{\theta_m}(D^{tr}) = \arg\min_{f \in \mathcal{F}_{\theta_m}} \hat{R}(f, D^{tr})$
  - estimate $R(f^{\star}_{\theta_m})$ with $\hat{R}(f^{\star}_{\theta_m}, D^{va}) = \frac{1}{va} \sum_{z_i \in D^{va}} L(z_i, f^{\star}_{\theta_m}(D^{tr}))$
- select $\theta^{\star}_m = \arg\min_{\theta_m} R(f^{\star}_{\theta_m})$
- return $f^{\star}(D_n) = \arg\min_{f \in \mathcal{F}_{\theta^{\star}_m}} \hat{R}(f, D_n)$

Model Selection - Cross-validation

- Select a family of functions with hyper-parameter θ
- Divide your training set D_n into K distinct and equal parts $D^1, \cdots, D^k, \cdots, D^K$
- For each value θ_m of the hyper-parameter θ
  - For each part D^k (and its counterpart $\bar{D}^k$)
    - select $f^\star_{\theta_m}(\bar{D}^k) = \arg\min_{f \in \mathcal{F}_{\theta_m}} \hat{R}(f, \bar{D}^k)$
    - estimate $R(f^\star_{\theta_m}(\bar{D}^k))$ with
      $$\hat{R}(f^\star_{\theta_m}(\bar{D}^k), D^k) = \frac{1}{|D^k|} \sum_{z_i \in D^k} L(z_i, f^\star_{\theta_m}(\bar{D}^k))$$
  - estimate $R(f^\star_{\theta_m}(D_n))$ with $\displaystyle\frac{1}{K} \sum_k R(f^\star_{\theta_m}(\bar{D}^k))$
- select $\theta^\star_m = \arg\min_{\theta_m} R(f^\star_{\theta_m}(D))$
- return $f^\star(D_n) = \arg\min_{f \in \mathcal{F}_{\theta^\star_m}} \hat{R}(f, D_n)$

Estimation of the Risk - Validation

- Divide your training set D_n into two parts
  - $D^{tr} = \{z_1, z_2, \cdots, z_{tr}\}$
  - $D^{te} = \{z_{tr+1}, z_{tr+2}, \cdots, z_{tr+te}\}$
  - $tr + te = n$
- select $f^\star(D^{tr}) = \arg\min_{f \in \mathcal{F}} \hat{R}(f, D^{tr})$

  (this optimization process could include model selection)
- estimate $R(f^\star(D^{tr}))$ with

$$\hat{R}(f^\star(D^{tr}), D^{te}) = \frac{1}{te} \sum_{z_i \in D^{te}} L(z_i, f^\star(D^{tr}))$$

Estimation of the Risk - Cross-validation

- Divide your training set D_n into K distinct and equal parts $D^1, \cdots, D^k, \cdots, D^K$
- For each part D^k
  - let $\bar{D}^k$ be the set of examples that are in D_n but not in D^k
  - select $f^\star(\bar{D}^k) = \arg\min_{f \in \mathcal{F}} \hat{R}(f, \bar{D}^k)$

    (this process could include model selection)

  - estimate $R(f^\star(\bar{D}^k))$ with $\hat{R}(f^\star(\bar{D}^k), D^k) = \frac{1}{|D^k|} \sum_{z_i \in D^k} L(z_i, f^\star(\bar{D}^k))$
- estimate $R(f^\star(D_n))$ with $\frac{1}{K} \sum_k R(f^\star(\bar{D}^k))$
- When $k = n$: leave-one-out cross-validation

Estimation of the Risk and Model Selection

- When you want both the best model and its expected risk.
- You then need to merge the methods already presented. For instance:
  - train-validation-test: 3 separate data sets are necessary
  - cross-validation + test: cross-validate on train set, then test on separate set
  - double-cross-validation: for each subset, need to do a second cross-validation with the $K - 1$ other subsets
- Other important methodological aspects:
  - compare your results with other methods!!!!
  - use statistical tests to verify significance
  - verify your model on more than one datasets

Train - Validation - Test

- Select a family of functions with hyper-parameter θ
- Divide your training set D_n into three parts D^{tr}, D^{va}, and D^{te}
- For each value θ_m of the hyper-parameter θ
    - select $f^\star_{\theta_m}(D^{tr}) = \arg\min_{f \in \mathcal{F}_{\theta_m}} \hat{R}(f, D^{tr})$
    - let $\hat{R}(f^\star_{\theta_m}(D^{tr}), D^{va}) = \frac{1}{va} \sum_{z_i \in D^{va}} L(z_i, f^\star_{\theta_m}(D^{tr}))$
- select $\theta^\star_m = \arg\min_{\theta_m} \hat{R}(f^\star_{\theta_m}(D^{tr}), D^{va})$
- select $f^\star(D^{tr} \cup D^{va}) = \arg\min_{f \in \mathcal{F}_{\theta^\star_m}} \hat{R}(f, D^{tr} \cup D^{va})$
- estimate $R(f^\star(D^{tr} \cup D^{va}))$ with $\frac{1}{te} \sum_{z_i \in D^{te}} L(z_i, f^\star(D^{tr} \cup D^{va}))$

Cross-validation + Test

- Select a family of functions with hyper-parameter θ
- Divide you dataset D_n into two parts:

  a training set D^{tr} and a test set D^{te}

- For each value θ_m of the hyper-parameter θ

  estimate $R(f^\star_{\theta_m}(D^{tr}))$ with D^{tr} using cross-validation

- select $\theta^\star_m = \arg\min_{\theta_m} R(f^\star_{\theta_m}(D^{tr}))$
- retrain $f^\star(D^{tr}) = \arg\min_{f \in \mathcal{F}_{\theta^\star_m}} \hat{R}(f, D^{tr})$
- estimate $R(f^\star(D^{tr}))$ with $\displaystyle\frac{1}{te} \sum_{z_i \in D^{te}} L(z_i, f^\star(D^{tr}))$

Double Cross-validation

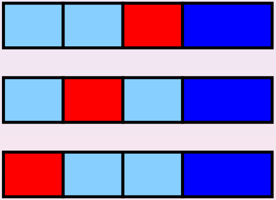
- Select a family of functions with hyper-parameter θ
- Divide your training set D_n into K distinct and equal parts $D^1, \cdots, D^k, \cdots, D^K$
- For each part D^k
  - select the best model $f^\star(\bar{D}^k)$ by cross-validation on $\bar{D}^k$
  - estimate $R(f^\star(\bar{D}^k))$ with

$$\hat{R}(f^\star(\bar{D}^k), D^k) = \frac{1}{|D^k|} \sum_{z_i \in D^k} L(z_i, f^\star(\bar{D}^k))$$

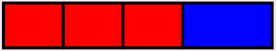
- estimate $R(f^\star(D))$ with $\frac{1}{K} \sum_k R(f^\star(\bar{D}^k))$
- Note: this process only gives you an estimate of the risk, but not a model. If you need the model as well, you have to perform a separate model selection process!

Double Cross-validation

the whole dataset is cut into 3 parts



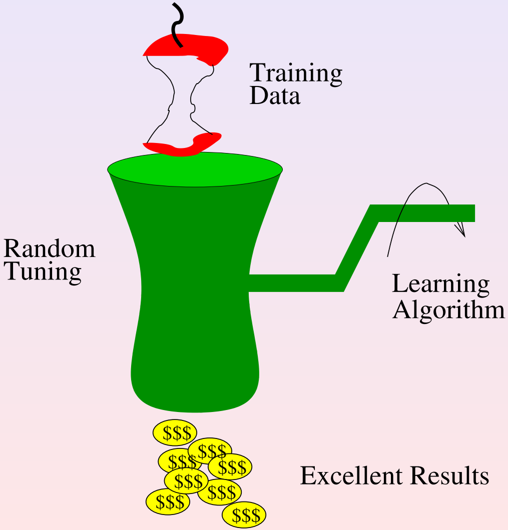
the first 2 parts are cut into 3 parts then perform a 3–fold cross–valid to select the best hyper–parameter



the best hyper–parameter is used to retrain on the 2 original parts and test on the other one

... and do the same for each part to estimate risk

Beware of the Machine Learning Magic



Beware of the Machine Learning Magic (con't)