An Introduction to Statistical Machine Learning - Theoretical Aspects -

Samy Bengio
bengio@idiap.ch

Dalle Molle Institute for Perceptual Artificial Intelligence (IDIAP)
CP 592, rue du Simplon 4
1920 Martigny, Switzerland
http://www.idiap.ch/~bengio

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Statistical Learning Theory

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The Data

- Available training data:
  - $D_n = \{z_1, z_2, \ldots, z_n\} \in \mathcal{Z}$,
  - independently and identically distributed (iid),
  - drawn from unknown distribution $p(Z)$

- 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 $E[Y|X = x]$
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:
    \[
    \hat{y} = f(x; a, b, c) = a \cdot x^2 + b \cdot x + c
    \]
  - Classification:
    \[
    \hat{y} = f(x; a, b, c) = \text{sign}(a \cdot x^2 + b \cdot x + c)
    \]
  - Density estimation
    \[
    \hat{p}(z) = f(z; \mu, \Sigma) = \frac{1}{(2\pi)^{|\Sigma|/2} \sqrt{|\Sigma|}} \exp \left( -\frac{1}{2} (z - \mu)^T \Sigma^{-1} (z - \mu) \right)
    \]
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:
    \[
    L(z, f) = -\log f(z)
    \]
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 $f^* = \arg\min_{f \in \mathcal{F}} R(f)$
  - problem: $p(Z)$ is unknown!!!
- Empirical Risk:
  \[
  \hat{R}(f, D_n) = \frac{1}{n} \sum_{i=1}^{n} L(z_i, f)
  \]
The Risk and the Empirical Risk

- The empirical risk is an unbiased estimate of the risk:
  \[ E_D[\hat{R}(f, D)] = R(f) \]

- The principle of empirical risk minimization:
  \[ f^*(D_n) = \arg \min_{f \in \mathcal{F}} \hat{R}(f, D_n) \]

- Training error:
  \[ \hat{R}(f^*(D_n), D_n) = \min_{f \in \mathcal{F}} \hat{R}(f, D_n) \]

- Is the training error a biased estimate of the risk?
The Training Error

- Is the training error biased? yes.

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

- The solution \( f^*(D_n) \) found by minimizing the training error is better on \( D_n \) than on any other set \( D'_n \) drawn from \( p(Z) \).

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

\[ |R(f^*(D_n)) - \hat{R}(f^*(D_n), D_n)| \leq ? \]

- 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.

- **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).

- **Bound on the expected risk:** let $\tau = \sup L - \inf L$

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

Bound on the Expected Risk

Confidence Interval

Empirical Risk

$h$
Theoretical Curves

Bound on the Expected Risk

\[ \inf R(f) \]

Empirical Risk

\( n \)
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 $y$)
- **Intrinsic dilemma**: when the capacity $h(\mathcal{F})$ grows, the bias goes down, but the variance goes up!
The Bias-Variance Dilemma (Graphical View)

- **Bias**
- **Variance**
- **Noise**
- **Optimal Solution**

- Solution obtained with training set 1
- Solution obtained with training set 2

The size of the set of functions depends on the size of the training set.
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 very large parameters

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

with $H(f)$ a function that penalizes according to your prior
- For example, in some models:
  - small parameters $\rightarrow$ simpler solutions $\rightarrow$ 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 $t^*$ such that
    $$t^* = \arg \min_t \hat{R}(f^t(D^{tr}), D^{va})$$
    and return function $f(D_n) = f^{t^*}(D^{tr})$
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)
  ○ sequential validation (for time series)
Model Selection - Validation

- Select a family of functions with hyper-parameter $\theta$
- Divide your training set $D_n$ into two parts
  - $D^{tr} = \{z_1, z_2, \ldots, z_{tr}\}$
  - $D^{te} = \{z_{tr+1}, z_{tr+2}, \ldots, z_{tr+te}\}$
  - $tr + te = n$
- For each value $\theta_m$ of the hyper-parameter $\theta$
  - select $f^{\ast}_{\theta_m}(D^{tr}) = \arg\min_{f \in F_{\theta_m}} \hat{R}(f, D^{tr})$
  - let $\hat{R}(f^{\ast}_{\theta_m}, D^{te}) = \frac{1}{te} \sum_{z_i \in D^{te}} L(z_i, f^{\ast}_{\theta_m}(D^{tr}))$
- select $\theta^{\ast}_m = \arg\min_{\theta_m} \hat{R}(f^{\ast}_{\theta_m}, D^{te})$
- return $f^{\ast}(D_n) = \arg\min_{f \in F_{\theta^{\ast}_m}} \hat{R}(f, D_n)$
Model Selection - Cross-validation

- Select a family of functions with hyper-parameter $\theta$
- Divide your training set $D_n$ into $k$ distinct and equal parts $D^1, \ldots, D^k$
- For each value $\theta_m$ of the hyper-parameter $\theta$
  - For each part $D^j$ (and its counterpart $\tilde{D}^j$)
    - select $f^{*}_{\theta_m}(\tilde{D}^j) = \arg \min_{f \in \mathcal{F}_{\theta_m}} \hat{R}(f, \tilde{D}^j)$
    - let $\hat{R}(f^{*}_{\theta_m}(\tilde{D}^j), D^j) = \frac{1}{|D^j|} \sum_{z_i \in D^j} L(z_i, f^{*}_{\theta_m}(\tilde{D}^j))$
  - estimate $\hat{R}_{\theta_m}(f) = \frac{1}{k} \sum_{j} \hat{R}(f^{*}_{\theta_m}(\tilde{D}^j), D^j)$
  - select $\theta^{*}_m = \arg \min_{\theta_m} \hat{R}_{\theta_m}(f)$
  - return $f^{*}(D_n) = \arg \min_{f \in \mathcal{F}_{\theta^{*}_m}} \hat{R}(f, D_n)$
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 $f^*(D^{tr}) = \arg\min_{f \in \mathcal{F}} \hat{R}(f, D^{tr})$
  (this optimization process could include model selection)
- estimate $R(f) = \hat{R}(f^*(D^{tr}), D^{te}) = \frac{1}{te} \sum_{z_i \in D^{te}} L(z_i, f^*(D^{tr}))$
Estimation of the Risk - Cross-validation

- Divide your training set $D_n$ into $k$ distinct and equal parts $D^1, \ldots, D^k$
- For each part $D^j$
  - let $\tilde{D}^j$ be the set of examples that are in $D_n$ but not in $D^j$
  - select $f^*(\tilde{D}^j) = \arg\min_{f \in \mathcal{F}} \hat{R}(f, \tilde{D}^j)$
    (this process could include model selection)
  - let $\hat{R}(f^*(\tilde{D}^j), D^j) = \frac{1}{|D^j|} \sum_{z_i \in D^j} L(z_i, f^*(\tilde{D}^j))$
- estimate $R(f) = \frac{1}{k} \sum_j \hat{R}(f^*(\tilde{D}^j), D^j)$
- When $k = n$: leave-one-out cross-validation
Estimation of the Risk - Sequential Validation

- When data is sequential in nature (time series)
- Divide your training set $D_n$ into $k$ distinct and equal sequential blocks $D^1, \ldots, D^k$
- For $j = 1 \rightarrow k - 1$
  - select $f^*(D^1 \rightarrow j) = \arg\min_{f \in \mathcal{F}} \hat{R}(f, \bigcup_{i=1}^{j} D^i)$
    (this process could include model selection)
  - let $\hat{R}(f^*(D^1 \rightarrow j), D^{j+1}) = \frac{1}{|D^{j+1}|} \sum_{z_i \in D^{j+1}} L(z_i, f^*(D^1 \rightarrow j))$
- estimate $R(f) = \frac{1}{k-1} \sum_{j=1}^{k-1} \hat{R}(f^*(D^1 \rightarrow j), D^{j+1})$
Estimation of the Risk - Bootstrap

- Is our estimate of the risk really accurate?
- Let us use Bootstrap to estimate the accuracy of a given statistics:
  - Let us create $N$ bootstraps of $D_n$
  - For each bootstrap $B_i$, get an estimate of the risk $R_i$ (using cross-validation for instance)
  - You can now compute estimates of the mean and the standard deviation of your estimates of the risk:

\[
\bar{R} = \frac{1}{N} \sum_{j=1}^{N} R_j
\]

\[
\sigma = \sqrt{\frac{1}{N-1} \sum_{i=1}^{N} (R_i - \bar{R})^2}
\]
Given a data set $D_n$ with $n$ examples drawn from $p(Z)$

A bootstrap $B_i$ of $D_n$ also contains $n$ examples:

For $j = 1 \rightarrow n$, the $j^{th}$ example of $B_i$ is drawn independently with replacement from $D_n$

Hence,

- some examples from $D_n$ are in multiple copies in $B_i$
- and some examples from $D_n$ are not in $B_i$

Hypothesis: the examples were iid drawn from $p(Z)$

Hence, the datasets $B_i$ are as plausible as $D_n$, but drawn from $D_n$ instead of $p(Z)$.
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 other datasets
Train - Validation - Test

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

Statistical Learning Theory
Cross-validation + Test

- Select a family of functions with hyper-parameter $\theta$

- Divide your dataset $D_n$ into two parts:
  - a training set $D^{tr}$ and a test set $D^{te}$

- For each value $\theta_m$ of the hyper-parameter $\theta$
  - estimate $\hat{R}_{\theta_m}(D^{tr})$ using cross-validation

- select $\theta^*_m = \arg\min_{\theta_m} \hat{R}_{\theta_m}(D^{tr})$

- retrain $f^*(D^{tr}) = \arg\min_{f \in \mathcal{F}_{\theta^*_m}} \hat{R}(f, D^{tr})$

- estimate $R(f) = \frac{1}{te} \sum_{z_i \in D^{te}} L(z_i, f^*(D^{tr}))$
Double Cross-validation

- Select a family of functions with hyper-parameter $\theta$
- Divide your training set $D_n$ into $k$ distinct and equal parts $D^1, \ldots, D^k$
- For each part $D^j$
  - select the best model $f^*(\bar{D}^j)$ by cross-validation on $\bar{D}^j$
  - let $\hat{R}(f^*(\bar{D}^j), D^j) = \frac{1}{|D^j|} \sum_{z_i \in D^j} L(z_i, f^*(\bar{D}^j))$
- estimate $R(f) = \frac{1}{k} \sum_j \hat{R}(f^*(\bar{D}^j), D^j)$
- 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

<table>
<thead>
<tr>
<th>Step</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>the whole dataset is cut into 3 parts</td>
</tr>
<tr>
<td>2</td>
<td>the first 2 parts are cut into 3 parts then perform a 3–fold cross–valid to select the best hyper–parameter</td>
</tr>
<tr>
<td>3</td>
<td>the best hyper–parameter is used to retrain on the 2 original parts and test on the other one</td>
</tr>
<tr>
<td>4</td>
<td>... and do the same for each part to estimate risk</td>
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