Machine Learning
EDS

Approximation-Estimation Error decomposition and first results on generalisation error of a learnt predictor

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So far

- Because ideal predictors rely on the unknown joint distribution of features/outputs, they do not provide a practical way of making predictions
- We have introduced learning rules (e.g. ERM) to select predictors “best fitting” a given observed sample
- Will they provide accurate predictions for new unseen data?
- We need to quantify their generalisation abilities.

1. Approximation and Estimation errors
   - Approximation error
   - Estimation error
   - Decomposition of the excess risk

2. Upper-bounding the estimation error in ERM
   - Zero-error classification with finite models
   - Beyond the zero-error case: global upper-bounds
   - Non-deterministic case with finite models

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Intuition

- When introducing predictors minimising the empirical risk, we straightaway saw that extreme overfitting could occur if no constraints were imposed.

- More generally, when selecting a predictor based on the sample, a structure has to be imposed: we search for predictors within certain families, certain models.

- What if a model that we impose is "far from reality"? Intuitively: even the best predictor within this model will have a poor performance.

The **discrepancy between** 1) the best performance any predictor within a given model can achieve, 2) the perf. of ideal predictors is called the approximation error.

Approximation error

Definition: Approximation error of a model

For a given model $S \subset \mathcal{F}$, the quantity denoted

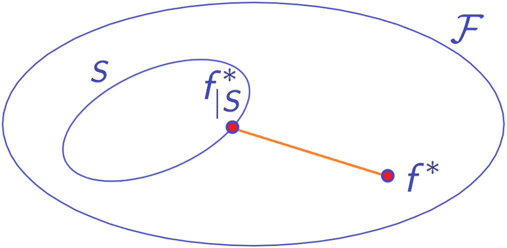
$$\ell(f^*, S) := \inf_{f \in S} \ell(f^*, f) = \inf_{f \in S} \mathcal{R}_P(f) - \mathcal{R}_P^* \geq 0,$$

is called the approximation error of the model S.
Any predictor in S achieving the infimum will be denoted $f^*_{|S}$.
If such a predictor exists, then by definition $\ell(f^*, S) = \ell(f^*, f^*_{|S})$.

Reminder

$\mathcal{R}_P^* := \inf_{f \in \mathcal{F}} \mathcal{R}_P(f)$ is Bayes risk,
i.e. the risk of ideal predictors, i.e. the lowest possible generalisation error achievable by any predictor $f \in \mathcal{F}$.

Approximation error

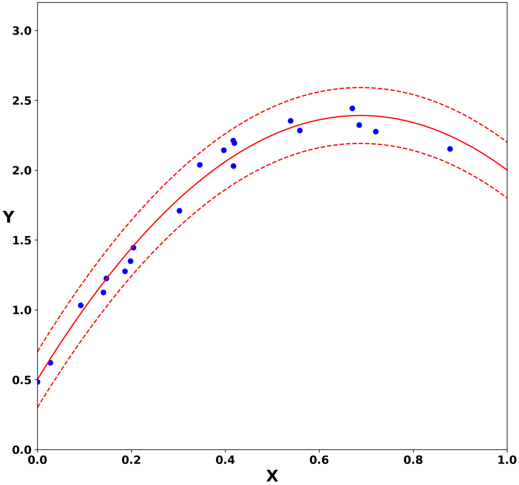


f^*: Bayes predictor $\qquad \mathcal{R}_P(f^*) = \inf_{f \in \mathcal{F}} \mathcal{R}_P(f)$

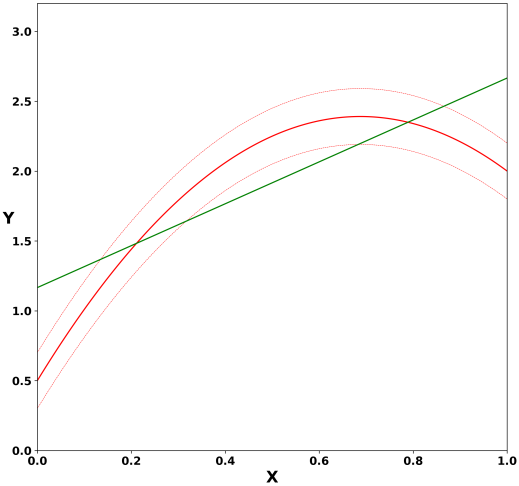
$f^*_{|S}$: theoretical best predictor within model S $\qquad \mathcal{R}_P(f^*_{|S}) = \inf_{f \in S} \mathcal{R}_P(f)$

$$\text{Approximation error} = \inf_{f \in S} \mathcal{R}_P(f) - \inf_{f \in \mathcal{F}} \mathcal{R}_P(f)$$

Illustration



Best linear approximation of a non-linear relationship



Approximation error

- The approximation error measures how accurately a given model is, in theory, able to capture a certain feature/output relationship.
- It is a property of the model and of the prediction problem addressed.
- It depends on the feature/output joint distribution P and on the model S, but not on the sample D_n.

Example: Neural Network as universal approximators

- Artificial neural networks constitute a class of popular models which had recent successes in pattern recognition and NLP
- Recall that neural networks have a long history:
    - 1943: McCulloch and Pitts propose a first formalisation of biology-inspired neural networks
    - 1958: Rosenblatt introduces the Perceptron
    - 1970s and 1980s: Emergence, formalisation and implementation of the back-propagation algorithm
    - Starting 2009-2012: Computational power and larger architectures (known as *deep* networks) enabled to reach human performance in several tasks

Neural networks are a family of nonlinear functions mapping features $x \in \mathcal{X}$ to outputs $y \in \mathcal{Y}$ which are known since 1989 to feature a ***Universal Approximation*** property

Example: Neural Network as universal approximators

Single hidden-layer feedforward neural networks

Consider the regression framework with $\mathcal{X} = \mathbb{R}^p$, $\mathcal{Y} = \mathbb{R}$. Formally, single hidden-layer feedforward NN are functions of the form:

$$NN(x) = \sum_{j=1}^{m} \beta_j \Psi\big(\boldsymbol{w}_j^\top x + b_j\big), \qquad \text{for } x \in \mathbb{R}^p,$$

- $m \geq 1$: number of units in the hidden layer (or *neurons*)
- $\boldsymbol{w}_1, \dots, \boldsymbol{w}_m \in \mathbb{R}^p$ and $b_1, \dots, b_m \in \mathbb{R}$ are weights defining an affine mapping of the inputs to the hidden layer
- $\Psi : \mathbb{R} \to [0, 1]$ is the activation function of the units, assumed here to be non-decreasing with $\Psi(x) \underset{x \to +\infty}{\longrightarrow} 1$, $\Psi(x) \underset{x \to -\infty}{\longrightarrow} 0$
- $\beta_1, \dots, \beta_m$ are weights mapping the hidden layer to the output of the neural network

Example: Neural Network as universal approximators

Proposition: NN are universal approximators
Hornik, Stinchombe and White (1989)

Let $p \geq 1$, Ψ be any activation function, and $f : \mathbb{R}^p \to \mathbb{R}$ be any continuous function.

Then, for any accuracy level $\varepsilon > 0$ and any $[a, b]^p \subset \mathbb{R}^p$, there exists a feedforward neural network NN with single hidden-layer and activation function Ψ such that:

$$\sup_{x \in [a,b]^p} |f(x) - NN(x)| < \varepsilon.$$

Neural networks with as little as one hidden layer are able to approximate any continuous function with arbitrary accuracy.

(See the paper if you are interested in the proof)

Example: Neural Network as universal approximators

Advnaced exercise: Approximation error of neural networks

Consider the regression framework $\mathcal{X} = \mathbb{R}^p$ and $\mathcal{Y} = \mathbb{R}$. Let c be the quadratic cost, let P denote joint distribution of features/outputs and assume the following:

- The features are bounded: there is a bounded set $K \subset \mathbb{R}^d$ such that $\mathbb{P}(X \in K) = 1$.
- There exists a Bayes predictor which is continuous, i.e. there is a continuous predictor f^* such that $\mathcal{R}_P(f^*) = \inf_{f \in \mathcal{F}} \mathcal{R}_P(f)$.

Let S_{NN} be the set of feedforward neural networks with single-hidden layer. Show that in this context, the approximation error is zero:

$$\inf_{g \in S_{\mathrm{NN}}} \ell(f^*, g) = 0.$$

Are Universal Approximators a guarantee of success?

From Hornik, Stinchombe and White's (1989) article:

"*Any lack of success in applications [of neural networks] must arise from inadequate learning, insufficient numbers of hidden units or the lack of a deterministic relationship between input and target.*"

- "*lack of a deterministic relationship between input and target*": Bayes risk is high, i.e. even ideal predictors are not performing well
- "*insufficient numbers of hidden units*": chosen model S is too small
- *"inadequate learning"*: the selected predictor within model S is suboptimal

The last point introduces estimation error.

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Intuition

- When a model has been chosen, we will select a predictor within this model according to some procedure or algorithm.
- There is no reason to believe that we will necessarily select a best performing predictor within this model: we might select a suboptimal one.
- Question: Will the predictor selected be close (in terms of performance) to the best predictor in the chosen model?

The **discrepancy between** 1) the performance of a sample-based predictor over a model, 2) the theoretical best performance of any predictor within this model is called the estimation error.

Estimation error

Definition: Estimation error

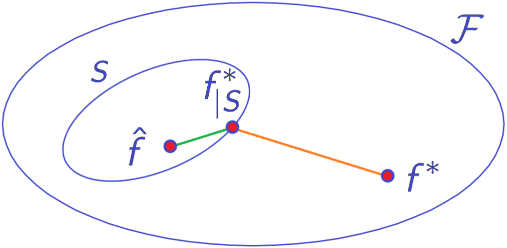
Let $S \subset \mathcal{F}$ be a model and $\hat{f}_S(D_n) \in S$ be a sample-based predictor (e.g. minimising the empirical risk over S). The quantity denoted

$$\mathcal{R}_P(\hat{f}_S(D_n)) - \inf_{f \in S} \mathcal{R}_P(f) = \ell(f^*, \hat{f}_S(D_n)) - \ell(f^*, S) \geq 0,$$

is called the estimation error of $\hat{f}_S(D_n)$. From now on D_n in $\hat{f}_S(D_n)$ is supressed and we write $\hat{f}_S$.

- The estimation error is related to the difficulty of finding/estimating a good predictor in the model S.
- More complex models makes it harder to find a good predictor.
- In regression with quadratic cost, the order of magnitude of the estimation error is typically *the number of parameters*.

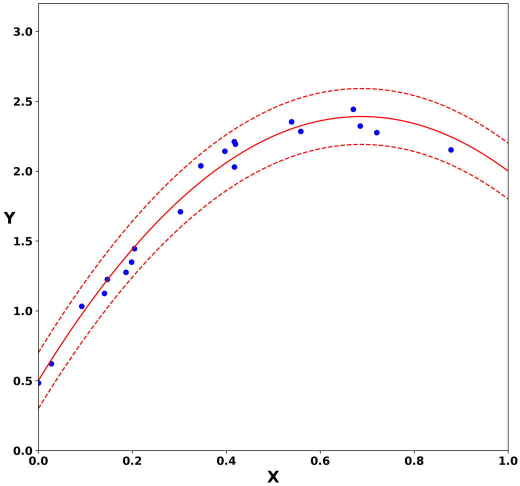
Estimation error



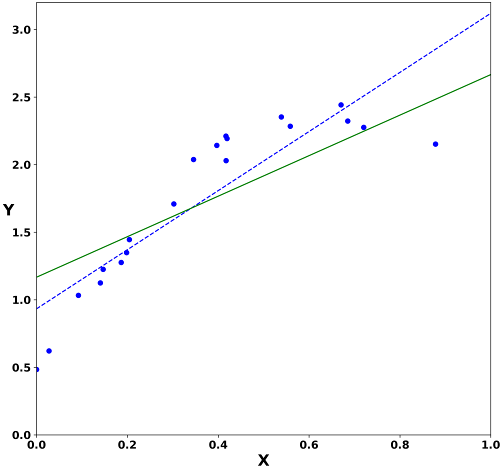
$\hat{f}$: Selected predictor within model S (e.g. by ERM)

$$\text{Estimation error} = \mathcal{R}_P(\hat{f}) - \inf_{f \in S} \mathcal{R}_P(f)$$

Illustration



ERM-selected linear predictor on the sample (dashed blue) vs theoretical best linear predictor (solid green)



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Approximation and Estimation error decomposition

Definition: Approximation and Estimation error decomposition

Let $S \subset \mathcal{F}$ be a model and $\hat{f}_S \in S$ be a sample-based predictor. Then, the excess risk of $\hat{f}_S$ can be written as:

$$\underbrace{\mathcal{R}_P(\hat{f}_S) - \mathcal{R}_P^*}_{\substack{\text{Excess risk of } \hat{f}_S \\ \text{compared to Bayes risk}}} = \underbrace{\mathcal{R}_P(\hat{f}_S) - \inf_{f \in S} \mathcal{R}_P(f)}_{\text{Estimation error}} + \underbrace{\inf_{f \in S} \mathcal{R}_P(f) - \mathcal{R}_P^*}_{\text{Approximation error}}$$

or equivalently

$$\underbrace{\ell(f^*, \hat{f}_S)}_{\substack{\text{Excess risk of } \hat{f}_S \\ \text{compared to Bayes risk}}} = \underbrace{\ell(f^*, \hat{f}_S) - \ell(f^*, S)}_{\text{Estimation error}} + \underbrace{\ell(f^*, S)}_{\text{Approximation error}}$$

Remarks

Remark: non-negativeness of the errors

As mentioned in their definitions, both the approximation and estimation errors are **non-negative**.

Remark: *Bias/Variance* decomposition

The previous decomposition is also sometimes referred to as a *bias/variance* decomposition:

The approximation error is then called *bias (of model S)*, and the estimation error is then called *variance*.

Trade-off between estimation and approximation

- The estimation error measures how far a selected (or *estimated*) predictor is from the best performance possible within the model S.

- When choosing a model S and looking for a sample-based predictor $\hat{f}_S \subset S$, we would like to minimise both errors.

Trade-off between estimation and approximation

- Intuitively: Bigger/more flexible models always allow to reduce approximation error:
  Let $S_1, S_2 \subset \mathcal{F}$ be two nested models such that $S_1 \subset S_2$. Then:
  $$\ell(f^*, S_2) \leq \ell(f^*, S_1).$$

But: Bigger/more flexible models might be complex, depend on many parameters (possibly infinitely many, e.g. non-parametric)

- Practically finding a best predictor within this model can be challenging: estimation error may be very high
- Might be prone to overfitting, mistaking noise in the data for structure

Trade-off between estimation and approximation

Approximation and estimation errors trade-off

Finding a good predictor involves adequatly choosing the model S to find a favorable trade-off between approximation and estimation errors.

- In some cases, it is possible to provide analytical expressions for the approximation error of a model.
- But in general, it is not easily accessible and other methods are used to realise the trade-off (e.g. penalisation of the empirical risk or cross-validation). See Chapter 4 of Mohri et al. (2018) for more details.

Ahead

- We will focus the estimation error in the ERM framework. Essentially, we will try to answer the question:

How close to the best performance possible within a given model can we hope a predictor selected by ERM to be?

- We will introduce several notions of flexibility (the standard term is *complexity*) of a model which will be useful to study the generalisation error of sample-based predictors.

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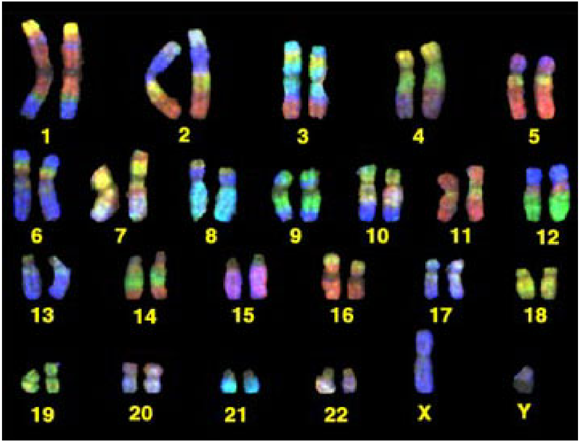
Zero-error classification

- Zero-error classification is one of the simplest frameworks in machine learning.
- Assume the label $Y \in \{0, 1\}$ is a deterministic function of the features $X \in \mathcal{X}$, i.e. there is a function $f^* \in \mathcal{F}$ such that
$$Y = f^*(X) \quad \text{almost surely.}$$
- Its generalisation error is zero and f^* is obviously a target function (an ideal predictor). With c the 0-1 cost:
$$\mathcal{R}_P(f^*) = \mathbb{E}\big[c\big(f^*(X), Y\big)\big] = \mathbb{P}\big(f^*(X) \neq Y\big) = 0.$$
- Although the label is a deterministic function of the features, the relationship may not be obvious neither theoretically, nor based on the data.

Zero-error classification: genetic example

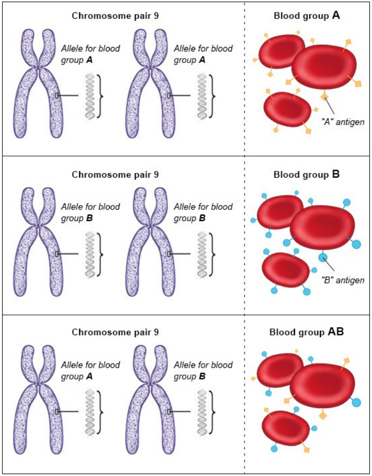
- Example: $X \in \mathcal{X}$ encodes the human genome and $Y \in \{0, 1\}$ encodes whether a person has a particular hereditary disease
- Note that the feature space is large but finite: the human genome is estimated to be composed of 20,000 genes, each having a finite number of distinct versions.
  $\Longrightarrow$ there is a (large but) finite numbers of possible predictors associating X and Y.
- With current genome sequencing techniques, it could be envisionable to gather enough data to study the relationship between X and Y.
- This can be framed as a zero-error classification problem over a finite model, for which we will show that ERM predictors can achieve a good performance.

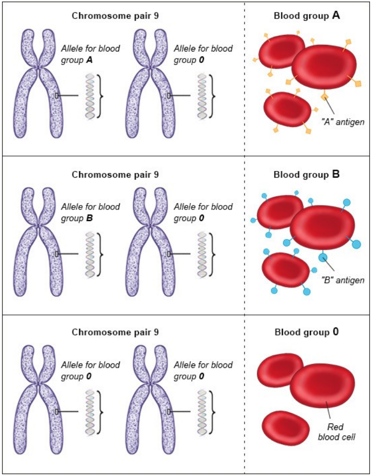
The human genome



Source: http://www.yorku.ca/kdenning/++2140%202006-7/2140-17oct2006.htm

ABO blood types : Alleles on Chromosome Pair 9





https://www.informedhealth.org/how-are-genes-passed-on.html

Finite and Infinite models

Definition: Finite and Infinite models

Let $\mathcal{X}$ be a feature space, $\mathcal{Y}$ be an output space, $\mathcal{F}$ the set of all predictors from $\mathcal{X}$ into $\mathcal{Y}$, and $S \subset \mathcal{F}$ a model.

If S contains a finite number of predictors, i.e. $\text{Card}(S) < +\infty$, then S is said to be a finite model.

If S contains an infinite number of predictors, i.e. $\text{Card}(S) = +\infty$, then S is said to be an infinite model.

Remark: Finite and Infinite models

Remark: Finite and Infinite models

The number of predictors a model contains is different in general from the *number of parameters* of the model.

For instance, the set of linear predictors from $\mathbb{R}^p$ into $\mathbb{R}$:

$$S_{\text{lin}} = \{f_{\boldsymbol{w}} : x \mapsto \boldsymbol{w}^\top x : \quad \boldsymbol{w} \in \mathbb{R}^p\},$$

is defined by p continous *parameters*, but contains an uncountably infinite number of predictors.

Upper-bound for zero-error classification with a finite model

Proposition: Upper-bound for zero-error classification

- Let $\mathcal{Y} = \{0, 1\}$ and P be a zero-error distribution in the sense that $Y = f^*(X)$ a.s. for some $f^* \in \mathcal{F}$.
- Let $D_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ be a sample, c the 0-1 cost.
- Let $S \subset \mathcal{F}$ be a finite model and $\hat{f}_S$ be an ERM learning rule over S.

Then, if $f^* \in S$, we have for any $n \geq 1$ and $\delta > 0$:

$$\mathbb{P}\left(\underbrace{\mathcal{R}_P^c(\hat{f}_S)}_{\substack{\text{Generalisation} \\ \text{error of } \hat{f}_S}} \leq \frac{\ln(\frac{1}{\delta}) + \ln(\operatorname{Card} S)}{n} \right) \geq 1 - \delta.$$

Recall that $\mathcal{R}_P^c(\hat{f}_S)$ is a random variable depending on the sample D_n.

Interpretation

Interpretation

The ERM predictor $\hat{f}_S$ is being computed based on the sample D_n. If we are lucky with the drawn sample, ERM may enable us to pick a good $\hat{f}_S$.

But we may get unlucky and only get observations dramatically oversampled from a certain region of the feature space $\mathcal{X}$. $\hat{f}_S$ will then generalise very poorly for predictions outside this region.

The proposition quantitifies the probability of $\hat{f}_S$ being a "good" predictor for a randomly drawn sample D_n, "good" in the sense that its generalisation error is below some value.

Interpretation: example

If we want $\hat{f}_S$ to have a generalisation error of at most $\varepsilon = 5\%$ in at least 99% of the cases when drawing a sample D_n at random, i.e. with probability $1 - \delta = 99\%$, then we seek

$$\mathbb{P}\Big(\mathcal{R}_P(\hat{f}_S) \leq \varepsilon\Big) \geq 1 - \delta,$$

with $\dfrac{\ln(\frac{1}{\delta}) + \ln(\mathrm{Card} S)}{n} \leq \varepsilon = 5\%$ and $\delta = 1\%$.

To achieve such requirements, the proposition tells us that we would need a sample of size n such that

$$n \geq 20\big(\ln(\mathrm{Card} S) + \ln 100\big).$$

Example: Learning a relation between genes and phenotype

- A person's genetic code can be described as a point $x \in \mathcal{X}$ in the set of all possible genomes.
- The human genome is characterised by $\sim$20,000 genes, each gene coming with a certain number of distinct possible versions called alleles, let's say at most p, for some $p \geq 1$.
- Focusing on persons for whom chromosomes go by pairs, a person's genome is thus characterised by the given of the two (possibly different) alleles of gene 1 it has, the two (possibly different) copies of gene 2 it has, etc.
- A person's genome could thus be encoded as a vector of size $40,000$ (2 alleles of each 20,000 genes), each entry being a number between 1 and p numbering the different alleles of each gene.

Example: Learning a relation between genes and phenotype

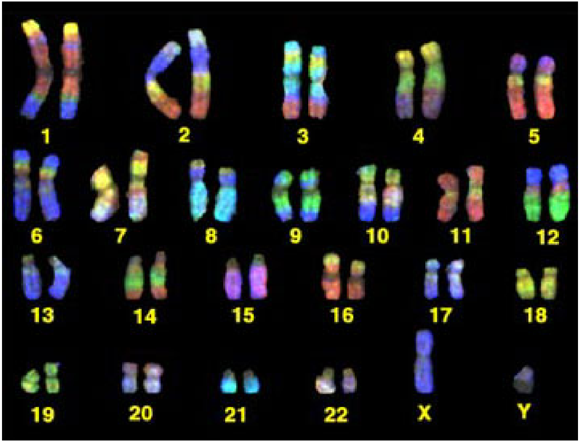
- A person's genome could thus be thought of as a point X in the (large but finite) set $\mathcal{X} = \{1, \ldots, p\}^{40000}$.
- Let's assume that a certain disease is suspected to be triggered ($Y = 1$) deterministically by a certain precise combination of at most 100 genes:

for a certain number q, $1 \leq q \leq 100$, certain distinct gene indexes $1 \leq g_1 < \ldots < g_q \leq 40000$, and certain versions $1 \leq v_1, \ldots, v_q \leq p$

$$Y = f^*(X) := \prod_{j=1}^{q} \mathbb{1}_{X_{g_j} = v_j}, \qquad \text{for } X \in \{1, \ldots, p\}^{40000}$$

The number q, the indexes, g_i's and the versions v_i's are unknown and we would like to find them.

The human genome



Source: http://www.yorku.ca/kdenning/++2140%202006-7/2140-17oct2006.htm

Example: Learning a relation between genes and phenotype

Question

How many genome examples n would we need in order to pin down the relationship between the genome and the disease with 95%-accuracy and 99%-confidence?

Framed as such, we are in a zero-error classification framework with (large but) finite model.

- Let S be the model containing all the functions of the above form.
- What is the cardinal of the set S? With some combinatorics, one can show (check it) that

$$\mathrm{Card} S = \sum_{q=1}^{100} p^q \frac{40000!}{(40000-q)!q!} = \sum_{q=1}^{100} p^q \binom{40000}{q}$$

- We would like $\hat{f}_S$ to have a generalisation error of at most $\varepsilon = 5\%$ with probability at least $1 - \delta = 99\%$ (in 99% of the cases when drawing a sample D_n at random)

- Then, by the proposition, the sample size n should satisfy

$$\frac{\ln \frac{1}{\delta} + \ln(\mathrm{Card}\, S)}{n} \leq \varepsilon,$$

- Assuming each gene has at most $p = 100$ possible versions, then $\mathrm{Card}\, S \approx 1.5 \cdot 10^{502}$, so $\ln(\mathrm{Card}\, S) \approx 1156$ and the sample size should be at least

$$n \geq \frac{1}{\varepsilon}\big[\ln(\mathrm{Card}\, S) - \ln \delta\big] \approx 23000.$$

Not such a big sample size: some companies proposing genome sequencing services had already more than 10 million clients.

Proof of the proposition (1/5).

Strategy of the proof:

1. Notice that f^* is a particular minimiser of the empirical risk, achieving zero empirical risk over the sample.
2. Deduce that any other empirical risk minimiser, in particular $\hat{f}_S$, must also achieve zero empirical risk.
3. Consider the probability $\mathbb{P}\big(\mathcal{R}_P(\hat{f}_S) \geq \varepsilon\big)$, i.e. the probability that the generalisation error of $\hat{f}_S$ is greater than some ε.
4. Bound this quantity by the probability that any other predictor $f \in S$ could have both zero empirical risk over the sample and generalisation risk greater than ε.

Proof (2/5).

Because $f^* \in S$ and we are in the zero-error case:

$$\inf_{f \in S} \mathcal{R}_P(f) = \mathcal{R}_P(f^*) = 0.$$

As $f^*(X) = Y$ a.s., it is immediately clear that $\widehat{\mathcal{R}}_n(f^*) = 0$ a.s. and thus, as risk is non-negative, $f^* \in S$ minimises the empirical risk over S.

Because $\hat{f}_S$ is by definition a minimiser of the empirical risk over S, it necessarily holds as well that

$$\widehat{\mathcal{R}}_n(\hat{f}_S) = 0, \quad a.s.$$

Proof (3/5).

Thus, for any $\varepsilon \geq 0$ we have on the one hand by the union bound:

$$\begin{aligned}
\mathbb{P}\Big(\mathcal{R}_P(\hat{f}_S) \geq \varepsilon\Big) &\leq \mathbb{P}\Big(\{\exists f \in S :\ \widehat{\mathcal{R}}_n(f) = 0 \text{ and } \mathcal{R}_P(f) \geq \varepsilon\}\Big) \\
&= \mathbb{P}\Big(\bigcup_{f \in S} \{\widehat{\mathcal{R}}_n(f) = 0 \text{ and } \mathcal{R}_P(f) \geq \varepsilon\}\Big) \\
&\leq \sum_{f \in S} \mathbb{P}\big(\widehat{\mathcal{R}}_n(f) = 0 \text{ and } \mathcal{R}_P(f) \geq \varepsilon\big) \\
&= \sum_{f \in S} \mathbb{P}\big(\widehat{\mathcal{R}}_n(f) = 0\big) \mathbb{1}_{\mathcal{R}_P(f) \geq \varepsilon}.
\end{aligned}$$

Proof (4/5).

Furthermore:

$$\begin{aligned}\mathbb{P}\big(\widehat{\mathcal{R}}_n(f)=0\big) &= \mathbb{P}\left(\frac{1}{n}\sum_{i=1}^{n}\mathbb{1}_{f(X_i)\neq Y_i}=0\right)\\ &= \mathbb{P}\big(\{\forall i=1,\dots,n:\ f(X_i)=Y_i\}\big)\\ &= \prod_{i=1}^{n}\mathbb{P}\big(f(X_i)=Y_i\big)\\ &= \prod_{i=1}^{n}\big(1-\mathcal{R}_P(f)\big)=\big(1-\mathcal{R}_P(f)\big)^n.\end{aligned}$$

Proof (5/5).

Hence

$$\begin{aligned}\mathbb{P}\Big(\mathcal{R}_P(\hat{f}_S) \geq \varepsilon\Big) &\leq \sum_{f \in S} \mathbb{P}\big(\widehat{\mathcal{R}}_n(f) = 0\big) \mathbb{1}_{\mathcal{R}_P(f) \geq \varepsilon} \\ &= \sum_{f \in S} \underbrace{\big(1 - \mathcal{R}_P(f)\big)^n \mathbb{1}_{\mathcal{R}_P(f) \geq \varepsilon}}_{\leq (1-\varepsilon)^n} \\ &\leq (1-\varepsilon)^n \operatorname{Card} S.\end{aligned}$$

Using the general inequality $1 + u \leq e^u$ for all $u \in \mathbb{R}$, we deduce:

$$\mathbb{P}\Big(\mathcal{R}_P(\hat{f}_S) \geq \varepsilon\Big) \leq e^{-\varepsilon n} \mathrm{Card} S.$$

Thus $\mathbb{P}\Big(\mathcal{R}_P(\hat{f}_S) \leq \varepsilon\Big) \geq 1 - e^{-\varepsilon n}\mathrm{Card} S$. Defining $\delta := e^{-\varepsilon n}\mathrm{Card} S$ and substituting ε in the probability concludes the proof.

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Beyond the zero-error case

- In general, we are not in a zero-error framework
- There is likely some irreducible noise in the data that even ideal predictors cannot predict
- Can we quantify the probability that an ERM predictor will be close, in terms of generalisation error, to the best performance possible within a given model?

A global upper-bound of the estimation error in ERM

Proposition: A global upper-bound of the estimation error

Let $S \subset \mathcal{F}$ be a model (not necessarily finite) and $\hat{f}_S$ be an empirical risk minimiser over the model S. Then:

$$\mathcal{R}_P(\hat{f}_S) - \inf_{f \in S} \mathcal{R}_P(f) \leq 2 \sup_{f \in S} \left| \mathcal{R}_P(f) - \widehat{\mathcal{R}}_n(f) \right|$$

Proof (1/1).

For any predictor $g \in S$, we have

$$\begin{aligned}
&\mathcal{R}_P(\hat{f}_S) - \mathcal{R}_P(g) \\
&\quad = \underbrace{\mathcal{R}_P(\hat{f}_S) - \widehat{\mathcal{R}}_n(\hat{f}_S)}_{\leq \sup_{f \in S} |\mathcal{R}_P(f) - \widehat{\mathcal{R}}_n(f)|} + \underbrace{\widehat{\mathcal{R}}_n(\hat{f}_S) - \widehat{\mathcal{R}}_n(g)}_{\leq 0} + \underbrace{\widehat{\mathcal{R}}_n(g) - \mathcal{R}_P(g)}_{\leq \sup_{f \in S} |\mathcal{R}_P(f) - \widehat{\mathcal{R}}_n(f)|} \\
&\quad \leq 2 \sup_{f \in S} \left| \mathcal{R}_P(f) - \widehat{\mathcal{R}}_n(f) \right|
\end{aligned}$$

By taking the supremum over $g \in S$ on both sides of the inequality, and since only the term $-\mathcal{R}_P(g)$ depends on g:

$$\sup_{g \in S} \left[\mathcal{R}_P(\hat{f}_S) - \mathcal{R}_P(g) \right] = \mathcal{R}_P(\hat{f}_S) - \inf_{g \in S} \mathcal{R}_P(g) \leq 2 \sup_{f \in S} |\mathcal{R}_P(f) - \widehat{\mathcal{R}}_n(f)|.$$

Interpretation

Remark: Interpretation of the previous bound

The term $2\sup_{f\in S}\left|\mathcal{R}_P(f)-\widehat{\mathcal{R}}_n(f)\right|$ is interpreted as a global measure of the complexity of the model S. This comes from the observations that:

- It is an increasing function of the model: for $S_1 \subset S_2$,

$$\sup_{f\in S_1}\left|\mathcal{R}_P(f)-\widehat{\mathcal{R}}_n(f)\right| \leq \sup_{f\in S_2}\left|\mathcal{R}_P(f)-\widehat{\mathcal{R}}_n(f)\right|$$

- It measures the maximum discrepancy possible between generalisation error and empirical error for predictors in S.

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Estimation error upper-bound for ERM with finite models and bounded cost function

Proposition

- Let $D_n = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ be an iid sample
- $S \subset \mathcal{F}$ be a finite model
- c be a bounded cost function $c(y, y') \leq C$ for all $y, y' \in \mathcal{Y}$
- $\hat{f}_S$ be a predictor minimising the empirical risk over S.

Then, for any confidence level $\delta > 0$, and sample size $n \geq 1$

$$\mathbb{P}\left(\mathcal{R}_P(\hat{f}_S) \leq \inf_{f \in S} \mathcal{R}_P(f) + C\sqrt{\frac{2\ln\frac{2}{\delta} + 2\ln\left(\text{Card } S\right)}{n}}\right) \geq 1 - \delta$$

Recall that the generalisation error $\mathcal{R}_P(\hat{f}_S)$ is a random variable because the predictor $\hat{f}_S$ depends on the sample D_n.

Proof (1/6).

Strategy of the proof:

1. Use the global bound from the previous proposition
2. Notice that for any $f \in S$, $\widehat{\mathcal{R}}_n(f) - \mathcal{R}_P(f)$ is a sum of independent, bounded, centered random variables
3. Apply Hoeffding's inequality
4. Rearrange terms

Proof (2/6).

Because $\hat{f}_S$ is an empirical risk minimiser over S, we have the upper-bound:

$$\mathcal{R}_P(\hat{f}_S) - \inf_{f \in S} \mathcal{R}_P(f) \leq 2 \sup_{f \in S} \left| \mathcal{R}_P(f) - \widehat{\mathcal{R}}_n(f) \right|,$$

and it is sufficient to upper-bound the right-hand side.

For any fixed predictor $f \in S$:

$$\begin{aligned} \widehat{\mathcal{R}}_n(f) - \mathcal{R}_P(f) &= \frac{1}{n} \sum_{i=1}^{n} c\big(f(X_i), Y_i\big) - \mathbb{E}\big[c\big(f(X), Y\big)\big] \\ &= \sum_{i=1}^{n} \frac{1}{n} \Big(c\big(f(X_i), Y_i\big) - \mathbb{E}\Big[c\big(f(X_i), Y_i\big)\Big] \Big), \end{aligned}$$

Hence, $\widehat{\mathcal{R}}_n(f) - \mathcal{R}_P(f)$ is the centered sum of n independent random variables, each with values in the interval $[0, C/n]$.

Proof (3/6).

Lemma: Hoeffding's inequality

Let $Z_1, \ldots, Z_n$ be independent bounded random variables such that for all $i = 1, \ldots, n$, $a_i \leq Z_i \leq b_i$ almost surely for some real constants a_i, b_i. Define

$$S_n = \sum_{i=1}^{n} \Big(Z_i - \mathbb{E}[Z_i] \Big).$$

Then for any $\varepsilon > 0$

$$\mathbb{P}\Big(\big| S_n \big| \geq \varepsilon \Big) \leq 2 \exp\left(- \frac{2\varepsilon^2}{\sum_{i=1}^{n} (b_i - a_i)^2} \right).$$

Proof: Omitted (see solutions of problem 3 of problem set 1)

Proof (4/6).

Using Hoeffding's inequality with $Z_i = \frac{c(f(X_i),Y_i)}{n} \in [0, C/n]$, we get for all $z \geq 0$

$$\mathbb{P}\left(\left|\widehat{\mathcal{R}}_n(f) - \mathcal{R}_P(f)\right| \geq z\right) \leq 2\exp\left(\frac{-2z^2}{\sum_{i=1}^n (C/n)^2}\right) = 2\exp\left(\frac{-2z^2 n}{C^2}\right).$$

By the union bound:

$$\begin{aligned}
\mathbb{P}\left(\sup_{f\in S}\left|\widehat{\mathcal{R}}_n(f) - \mathcal{R}_P(f)\right| \geq z\right) &= \mathbb{P}\left(\bigcup_{f\in S}\left\{\left|\widehat{\mathcal{R}}_n(f) - \mathcal{R}_P(f)\right| \geq z\right\}\right)\\
&\leq \sum_{f\in S}\mathbb{P}\left(\left|\widehat{\mathcal{R}}_n(f) - \mathcal{R}_P(f)\right| \geq z\right)\\
&\leq \sum_{f\in S} 2\exp\left(\frac{-2z^2 n}{C^2}\right),
\end{aligned}$$

Proof (5/6).

Thus:

$$\mathbb{P}\left(\sup_{f \in S} \left| \widehat{\mathcal{R}}_n(f) - \mathcal{R}_P(f) \right| \geq z \right) \leq 2 \, \mathrm{Card} S \ \exp\left(\frac{-2z^2 n}{C^2} \right).$$

Because

$$\mathcal{R}_P(\hat{f}_S) - \inf_{f \in S} \mathcal{R}_P(f) \leq 2 \sup_{f \in S} \left| \mathcal{R}_P(f) - \widehat{\mathcal{R}}_n(f) \right|,$$

it holds for all $z \geq 0$ that

$$\begin{aligned} \mathbb{P}\left(\mathcal{R}_P(\hat{f}_S) - \inf_{f \in S} \mathcal{R}_P(f) \geq 2z \right) &\leq \mathbb{P}\left(2 \sup_{f \in S} \left| \mathcal{R}_P(f) - \widehat{\mathcal{R}}_n(f) \right| \geq 2z \right) \\ &\leq 2 \, \mathrm{Card} S \ \exp\left(\frac{-2z^2 n}{C^2} \right) \end{aligned}$$

Proof (6/6).

Therefore:

$$1 - \mathbb{P}\Big(\mathcal{R}_P(\hat{f}_S) - \inf_{f \in S} \mathcal{R}_P(f) \leq 2z\Big) \leq 2 \operatorname{Card} S \ \exp\left(\frac{-2z^2 n}{C^2}\right)$$
$$\iff \mathbb{P}\Big(\mathcal{R}_P(\hat{f}_S) - \inf_{f \in S} \mathcal{R}_P(f) \leq 2z\Big) \geq 1 - 2 \operatorname{Card} S \ \exp\left(\frac{-2z^2 n}{C^2}\right).$$

Finally, defining

$$\delta := 2 \operatorname{Card} S \ \exp\left(\frac{-2z^2 n}{C^2}\right),$$

and substituting for z in the left-hand side yields the conclusion.

Interpretation

Interpretation

In this setting there is no deterministic relationship between features and output.

The proposition quantifies the probability of $\hat{f}_S$ being a "good" predictor for a randomly drawn sample D_n, "good" in the sense that its generalisation error does not exceed the lowest achievable risk over S by more than some specified value.

The interpretation is thus very similar to that for the zero-error case, but the result is less favourable regarding the performance of ERM predictors.

Interpretation: a much weaker guarantee

- In the zero-error case, the requirement to guarantee that $\hat{f}_S$ has a generalisation error of at most $\varepsilon = 5\%$ in at least 99% of the cases when drawing a sample D_n at random ($\delta = 1\%$) was

$$n \geq \frac{1}{\varepsilon}\big(\ln(\mathrm{Card}\, S) + \ln(1/\delta)\big) = 20\big(\ln(\mathrm{Card}\, S) + \ln 100\big)$$

- However, in the setting of the last proposition, asking for similar requirements leads to

$$C\sqrt{\frac{2\ln\frac{1}{\delta} + 2\ln\left(2\mathrm{Card}\, S\right)}{n}} \leq \varepsilon$$

that is (using that $C = 1$ for the 0-1 cost):

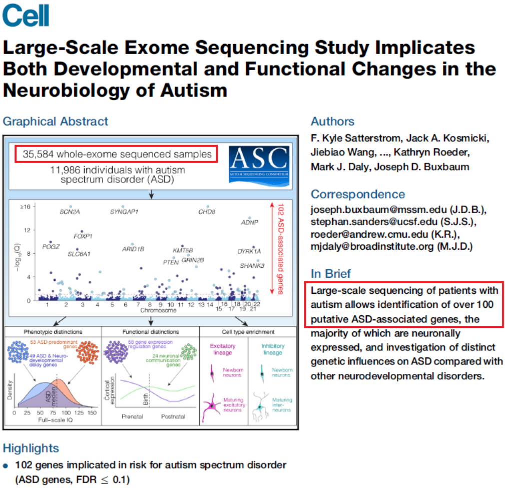
$$n \geq \frac{2}{\varepsilon^2}\big(\ln(2\mathrm{Card}\, S) + \ln(1/\delta)\big) = 800\big(\ln(2\mathrm{Card}\, S) + \ln(100)\big)$$

Interpretation: a less favourable guarantee

A much weaker bound

- To achieve the *same generalisation guarantees*, the sample needs to be more than 40 times larger than in the zero-error case.
- In the genetics example given before, this would mean that to identify a potentially non-deterministic relationship between gene combinations and disease (for instance if non-accounted environmental factor played a role), we would need more than 929 000 examples instead of 23 000.

Published in *Cell* (2020): 102 genes linked to autism identified based on $n \approx 35,000$



Cell

Large-Scale Exome Sequencing Study Implicates Both Developmental and Functional Changes in the Neurobiology of Autism

Graphical Abstract

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In Brief

Large-scale sequencing of patients with autism allows identification of over 100 putative ASD-associated genes, the majority of which are neuronally expressed, and investigation of distinct genetic influences on ASD compared with other neurodevelopmental disorders.

Highlights

- 102 genes implicated in risk for autism spectrum disorder (ASD genes, FDR $\leq$ 0.1)

Wrap-up

We have looked at the decomposition of excess risk into:

- Approximation error, discrepancy performance ideal predictor and theoretically best predictor in model,
- Estimation error, discrepancy between performance of sample-based predictor and theoretically best predictor in model.

We have established learning guarantees for:

- Zero-error classification for finite models,
- Non-deterministic setting with bounded cost and finite models.

Next week:

- We will see how to quantify complexity of infinite models,
- Learning guarantee for infinite models.

Assignment

- You can now make questions 1 and 2 of Assignment Part II
- I encourage you to already start working on it (deadline of Part II is March 18th at 23:59)
- **Important:** recall that the deadline of Assignment Part I is this Thursday (February 29th) at 23:59