Mathematical Foundations of ML

Philipp Grohs

universität wien
Faculty of Mathematics

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Short Reading List

1. Felipe Cucker and Ding Yuan Zhou: Learning Theory: An Approximation Theory Viewpoint, 2001
2. Luc Devroye, Laszlo Gyorfi, Gabor Lugosi: A Probabilistic Theory of Pattern Recognition; Springer, 2013.
3. Aurelien Geron: Hands-On Machine Learning with Scikit-Learn and TensorFlow; O'Reilley, 2017
4. Brian Steele and John Chandler and Swarna Reddy: Algorithms for Data Science; Springer, 2017

Syllabus

1. Basic Concepts
2. Mathematical Foundations of General Regression Problems

1. Mathematical Foundations of Machine Learning

1.1 Basic Concepts

Definition of Learning

Definition [Mitchell (1997)]

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E"

The Task T

Classification

Compute $f : \mathbb{R}^n \to \{1, \dots, k\}$ which maps data $x \in \mathbb{R}^n$ to a category in $\{1, \dots, k\}$. Alternative: Compute $f : \mathbb{R}^n \to \mathbb{R}^k$ which maps data $x \in \mathbb{R}^n$ to a histogram with respect to k categories.

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$x =$  $\mapsto f(x) = 5.$

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- Expected claim of insured person
- Algorithmic trading

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- Useful for many tasks in data processing, for example if we observe corrupted data $\tilde{x}$ we may estimate the original x as the argmax of $p(\tilde{x}|x)$.

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- If these data points are not labeled (for example in the classification problem, the algorithm would have to find the clusters itself from the given dataset) we speak of *unsupervised learning*.

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- Often the given dataset is split into a *training set* on which the algorithm operates and a *test set* on which its performance is measured.

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The Performance Measure

Given test data $((x_i^{test}, y_i^{test}))_{i=1}^n$ we evaluate the performance of an estimator $f : \mathbb{R}^d \to \mathbb{R}$ as the *mean squared error*

$$\frac{1}{n}\sum_{i=1}^{n} |f(x_i^{test}) - y_i^{test}|^2.$$

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Define a *Hypothesis Space*

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We let our algorithm find the minimizer (a.k.a. *empirical regression function*)

$$\widehat{f}_{\mathcal{H},\mathbf{z}} := \mathrm{argmin}_{f \in \mathcal{H}} \mathcal{E}_{\mathbf{z}}(f).$$

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- We get that
$$\mathcal{E}_{\mathbf{z}}(f) = \|\mathbf{A}\mathbf{w} - \mathbf{y}\|^2 .$$
- A minimizer is given by $\mathbf{w}_* := \mathbf{A}^\dagger\mathbf{y}$, and we get our estimate
$$f_* := \sum_{i=1}^{l} (\mathbf{w}_*)_i\varphi_i.$$

Proof.

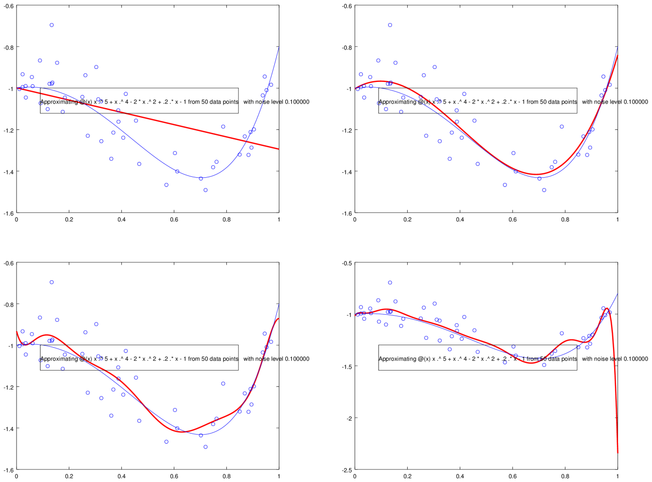
We want to minimize the function

$$\mathcal{X}(\mathbf{w}) := \mathbf{w} \mapsto \|\mathbf{A}\mathbf{w} - \mathbf{y}\|^2,$$

which is (more or less...) equivalent to setting its first derivative to zero. It holds that

$$\frac{d\mathcal{X}(\mathbf{w})}{d\mathbf{w}} = 2\mathbf{A}^\dagger(\mathbf{A}\mathbf{w} - \mathbf{y}),$$

which, if set to zero, are precisely the normal equations. $\square$


Approximating @(x) x .^ 5 + x .^ 4 - 2 * x .^ 2 + .2 .* x - 1 from 50 data points   with noise level 0.100000
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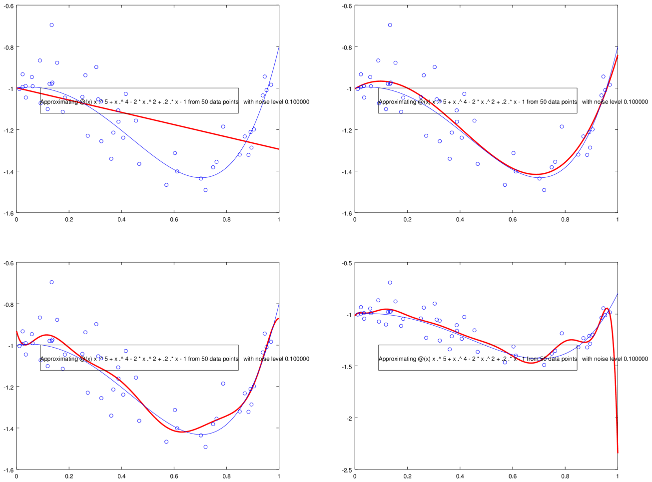

Degree too low: underfitting. Degree to high: overfitting!

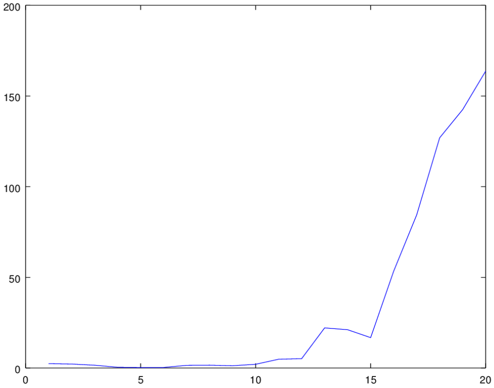

Figure: Error with Polynomial Degree

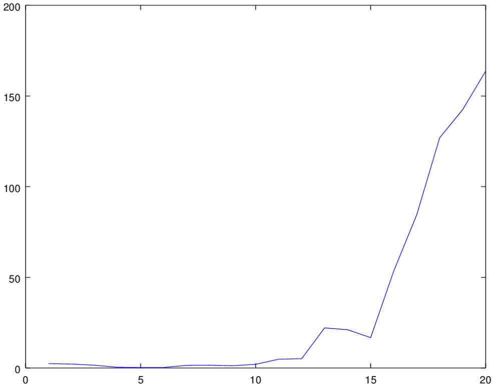

Figure: Error with Polynomial Degree

Bias-Variance Problem

"Capacity" of the hypothesis space has to be adapted to the complexity of the target function and the sample size!

1.2 Mathematical Foundations of General Regression Problems

1.2.1 Basic Definitions

The Mathematical Learning Problem

The Mathematical Learning Problem

Let $(\Sigma, \mathcal{G}, \mathbb{P})$ probability space. Given (Borel measurable) random vectors $X : \Sigma \to \mathbb{R}^d$, $Y : \Sigma \to \mathbb{R}^k$ with $\mathrm{im}(X) \subseteq \Omega$ for $\Omega \subset \mathbb{R}^d$ compact.

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- We have that

$$\begin{aligned}
\mathcal{E}(g) &= \mathbb{E}[(g(X) - Y)^2] = \mathbb{E}[(g(X) - f(X) - \xi)^2] \\
&= \mathbb{E}[(f(X) - g(X))^2] + 2\mathbb{E}[(g(X) - f(X))\xi] + \mathbb{E}\xi^2 \\
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- The learning problem finds f!

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- Now, a function f as above will in general not exist for our problem. But we can look for the function $\widehat{f}$ which minimizes the least squares error $\mathcal{E}$ – this will be the optimal explanation of the measurements in terms of a functional relation between X and Y!

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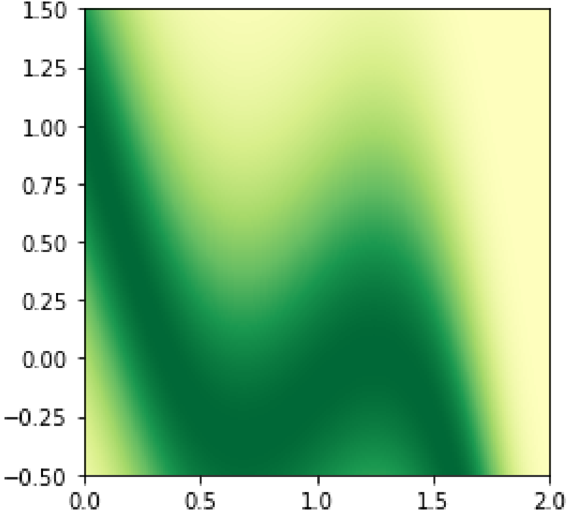

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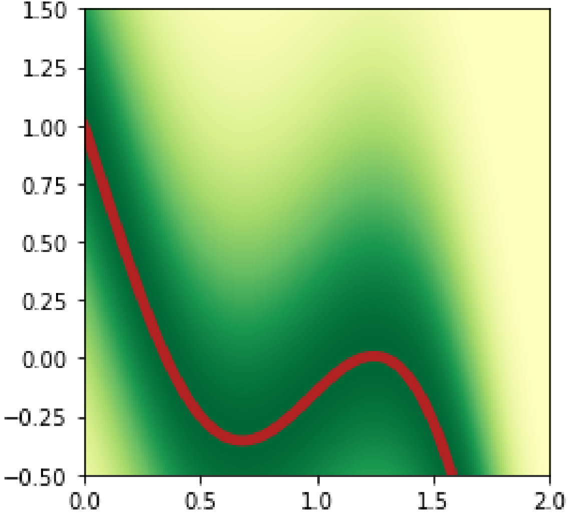
If we knew the data distribution (X, Y), the best functional relation between X and Y would simply be $\mathbb{E}[Y|X = x]$!



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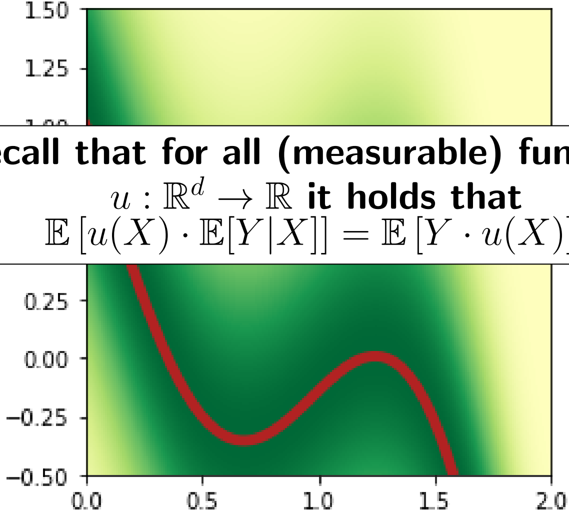

Recall that for all (measurable) functions $u : \mathbb{R}^d \to \mathbb{R}$ it holds that $\mathbb{E}\left[u(X) \cdot \mathbb{E}[Y|X]\right] = \mathbb{E}\left[Y \cdot u(X)\right]$.

Regression Function

Theorem (Main Regression Theorem)

Let $\widehat{f} := \mathbb{E}[Y|X]$ be the regression function and $\sigma^2 := \mathcal{E}(\widehat{f})$. It holds that

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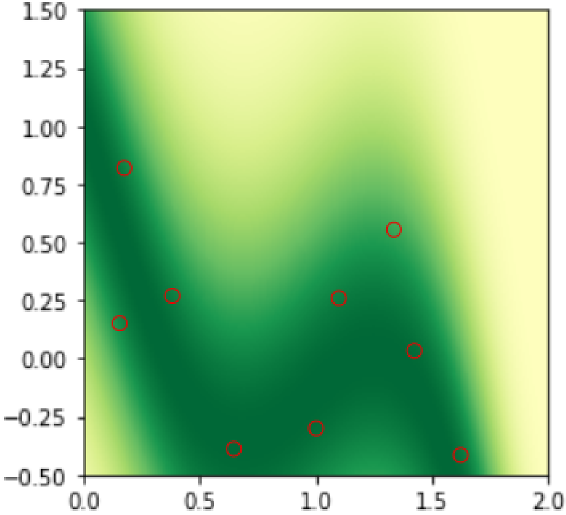

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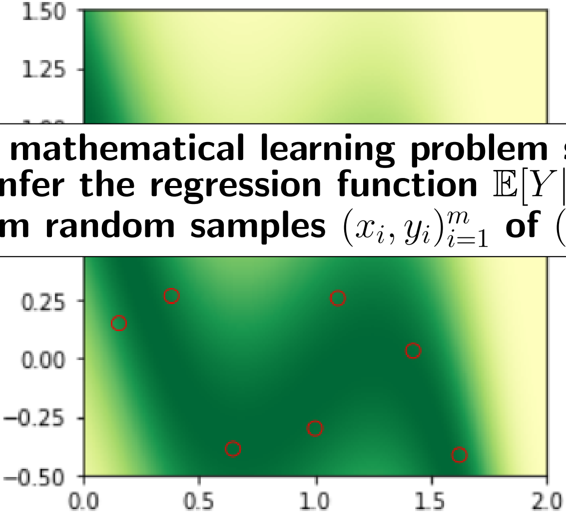

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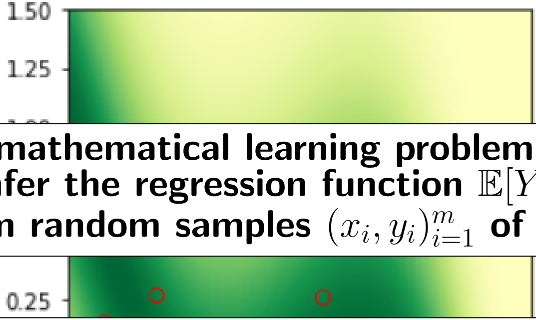

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More generally we would like to minimize

$$\mathbb{E}[\mathcal{L}(f(X), Y)]$$

with general loss function.

$\mathcal{L}(y, y') = (y - y')^2 \rightsquigarrow$ **quadratic loss**

$\mathcal{L}(y, y') = y \log(y') + (1 - y) \log(1 - y') \rightsquigarrow$ **cross-entropy loss.**

1.2.2 Empirical Minimization and Hypothesis Space

Sampling

Empirical Error

Given $\mathbf{z} = ((X^{(1)}, Y^{(1)}), \ldots, (X^{(m)}, Y^{(m)}))$ be i.i.d. with $(X^{(1)}, Y^{(1)}) \sim (X, Y)$. Define the *empirical error*

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Can we control the defect? If yes, we actually have some hope of approximating the regression function.

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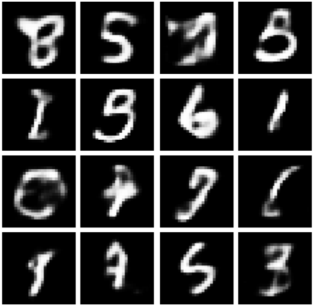
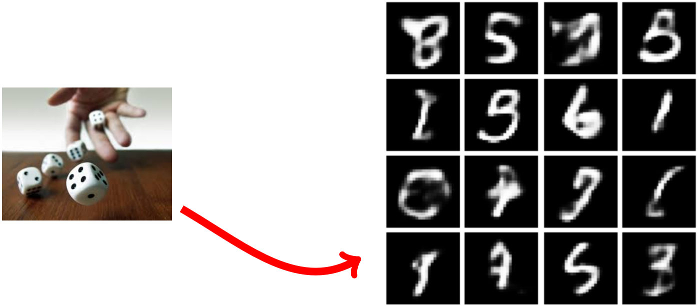


Data Generating Distribution

We suppose that there exists a probability distribution on $\mathbb{R}^{784}$ that randomly generates handwritten digits.



$\rightsquigarrow$ **Variational Autoencoder Demo**

Concentration Inequalities

Bernstein Inequality

Suppose that $(\xi^{(i)})_{i=1}^m$ i.i.d. with $\xi^{(1)} \sim \xi$ with mean $\mathbb{E}(\xi) = \mu$ and $\mathbb{V}(\xi) = \sigma^2$. Suppose that $|\xi - \mu| \leq M$ with probability 1. Then

$$\mathbb{P}\left\{\left|\frac{1}{m}\sum_{i=1}^{m}\xi^{(i)} - \mu\right| \geq \varepsilon\right\} \leq 2e^{-\frac{m\varepsilon^2}{2\left(\sigma^2 + \frac{1}{3}M\varepsilon\right)}}.$$

Bounding the Defect

Theorem A

Let $f : \mathbb{R}^d \to \mathbb{R}^k$ and let $\sigma_f^2 = \mathbb{V}[(f(X) - Y)^2]$. Suppose that $|f(X) - Y| \leq M$ almost everywhere. Then, for all $\varepsilon > 0$,

$$\mathbb{P}\left\{|L_{\mathbf{z}}(f)| \leq \varepsilon\right\} \geq 1 - 2e^{-\frac{m\varepsilon^2}{2\left(\sigma_f^2 + \frac{1}{3}M\varepsilon\right)}}.$$

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Proof.

Apply Bernstein Inequality to $\xi = (f(X) - Y)^2$. $\square$

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Are we done?? We could just minimize the empirical error and bound the defect...

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Proof.

Apply Bernstein Inequality to $\xi = (f(X) - Y)^2$. $\square$

Are we done?? We could just minimize the empirical error and bound the defect...

☹ Any f vanishing on the sample points makes the empirical error vanish!!!

Hypothesis Space

Definition

Let $\mathcal{H}$ be a compact subset of the Banach space $\{f : X \to Y, \text{ continuous}\}$ with norm $\|f\| := \max_{x \in X} |f(x)|$. We call $\mathcal{H}$ *hypothesis space* or *model space*.

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Best Approximation in $\mathcal{H}$

Define the *best approximation in $\mathcal{H}$* via

$$\widehat{f}_{\mathcal{H}} := \operatorname{argmin}_{f \in \mathcal{H}} \mathcal{E}(f) = \operatorname{argmin}_{f \in \mathcal{H}} \|\widehat{f} - f\|_{L^2(\mathbb{R}^d, d\mathbb{P}_X)}.$$

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Empirical Regression Function

Given $\mathbf{z}$ define the *empirical regression function* as

$$\widehat{f}_{\mathcal{H},\mathbf{z}} := \operatorname{argmin}_{f\in\mathcal{H}} \mathcal{E}_{\mathbf{z}}(f).$$

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 The empirical regression function can be computed!

1.2.3. Bias-Variance Decomposition

Generalization- and Approximation Error

Theorem (Bias-Variance Decomposition)

It holds that

$$\|\widehat{f}_{\mathcal{H},\mathbf{z}} - \widehat{f}\|^2_{L^2(\mathbb{R}^d, d\mathbb{P}_X)} = \left(\mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}})\right) + \|\widehat{f}_{\mathcal{H}} - \widehat{f}\|^2_{L^2(\mathbb{R}^d, d\mathbb{P}_X)}.$$

The first term is called *generalization error* and the second term is called *approximation error*.

Generalization- and Approximation Error

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The first term is called *generalization error* and the second term is called *approximation error*.

Proof.

By the Main Regression Theorem

$$\begin{aligned}\|\widehat{f}_{\mathcal{H},\mathbf{z}} - \widehat{f}\|^2_{L^2(\mathbb{R}^d, d\mathbb{P}_X)} &= \mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}) \\ &= \mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}}) + \mathcal{E}(\widehat{f}_{\mathcal{H}}) - \mathcal{E}(\widehat{f}) \\ &= \Big(\mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}})\Big) + \|\widehat{f}_{\mathcal{H}} - \widehat{f}\|^2_{L^2(\mathbb{R}^d, d\mathbb{P}_X)}.\end{aligned}$$

□

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Proof.

By the M

$\|\widehat{f}_{\mathcal{H},}$

Our goal is to make the empirical error

$$\|\widehat{f}_{\mathcal{H},\mathbf{z}} - \widehat{f}\|^2_{L^2(\mathbb{R}^d,d\mathbb{P}_X)}$$

as small as possible.

$$= \left(\mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}})\right) + \|\widehat{f}_{\mathcal{H}} - \widehat{f}\|^2_{L^2(\mathbb{R}^d,d\mathbb{P}_X)}.$$

□

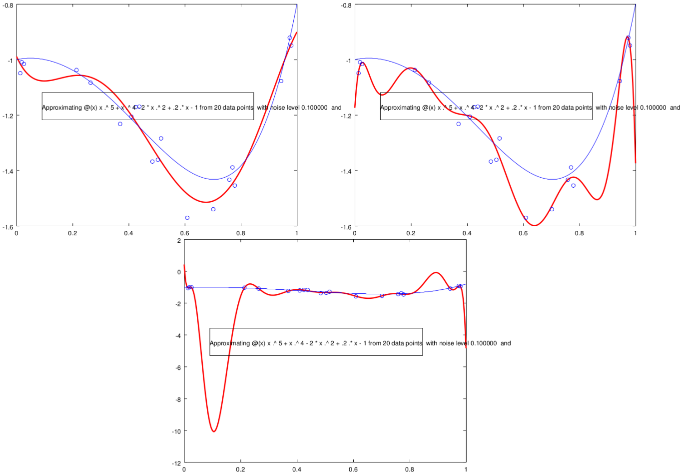

Figure: Blue: $f_{\mathcal{H}}$, Red: $f_{\mathcal{H},\mathbf{z}}$, $m = 10$, $\mathcal{H} =$ polynomials of degree $5, 15, 20$ (from top left to bottom).

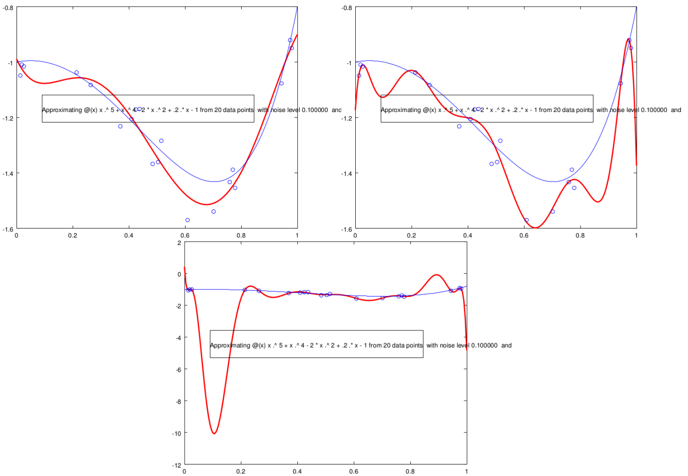

Figure: Blue: $f_{\mathcal{H}}$, Red: $f_{\mathcal{H},\mathbf{z}}$, $m = 10$, $\mathcal{H} =$ polynomials of degree $5, 15, 20$ (from top left to bottom).

If $\mathcal{H}$ is too complex, the sampling error increases.

The Bias-Variance Trade-Off

If we keep the sample size m fixed and enlarge the hypothesis space $\mathcal{H}$, the approximation error will certainly decrease, BUT the sample error will increase – this is exactly what we observed experimentally!

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Bishop [Neural Networks for Pattern Recognition (1995)]

> *"A model which is too simple, or too inflexible, will have a large bias, while one which has too much flexibility in relation to the particular data set will have a large variance. Bias and variance are complementary quantities, and the best generalization is obtained when we have the best compromise between the conflicting requirements of small bias and small variance."*

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Bias-Variance Problem

What are the precise relations between the number of samples m and the "capacity" of our hypothesis space $\mathcal{H}$?

1.2.4 Bounds on the Generalization Error $\mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}})$.

Covering Numbers

Definition

Let S be a metric space and $s > 0$. Define the *covering number* $\mathcal{N}(S, s)$ to be the minimal $l \in \mathcal{N}$ such that there exist l disks in S with radius s covering S.

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Scaling of $\mathcal{N}(S, s)$ with s is a measure of complexity of S termed *metric entropy*.

Abstract Analysis of Generalization Error

Theorem B

Let $\mathcal{H} \subset C(X)$ be a hypothesis class. Assume that for all $f \in \mathcal{H}$ it holds that $|f(X) - Y| < M$ a.e. Then, for all $\varepsilon > 0$,

$$\mathbb{P}\left(\sup_{f\in\mathcal{H}} |L_{\mathbf{z}}(f)| \leq \varepsilon\right) \geq 1 - \mathcal{N}(\mathcal{H}, \frac{\varepsilon}{8M}) 2e^{-\frac{m\varepsilon^2}{4(2\sigma^2 + \frac{1}{3}M^2\varepsilon)}},$$

where $\sigma^2 := \sup_{f\in\mathcal{H}} \sigma_f^2$.

Proof.

First show that for all f, g with $\|f - g\| \leq \tau$ it holds that

$$|\mathcal{E}(f) - \mathcal{E}(g)| \leq 2M\tau \quad \text{and} \quad |\mathcal{E}_{\mathbf{z}}(f) - \mathcal{E}_{\mathbf{z}}(g)| \leq 2M\tau.$$

Cover $\mathcal{H}$ with balls $(U_i)_{i=1}^{\mathcal{N}(\mathcal{H},\epsilon/(8M))}$ with center f_i of radius $\frac{\epsilon}{8M}$. By the estimate above it holds that

$$\left(\sup_{f\in U_i} |\mathcal{E}_{\mathbf{z}}(f) - \mathcal{E}(f)| > \varepsilon\right) \Rightarrow (|\mathcal{E}_{\mathbf{z}}(f_i) - \mathcal{E}(f_i)| > \varepsilon/2)$$

Then by this fact and Theorem A it holds that

$$\begin{aligned}\mathbb{P}\left(\sup_{f\in\mathcal{H}} |L_{\mathbf{z}}(f)| > \varepsilon\right) &\leq \sum_{i=1}^{\mathcal{N}(\mathcal{H},\epsilon/(8M))} \mathbb{P}\left(\sup_{f\in U_i} |\mathcal{E}_{\mathbf{z}}(f) - \mathcal{E}(f)| > \varepsilon\right) \\ &\leq \sum_{i=1}^{\mathcal{N}(\mathcal{H},\epsilon/(8M))} \mathbb{P}\left(|\mathcal{E}_{\mathbf{z}}(f_i) - \mathcal{E}(f_i)| > \varepsilon/2\right) \\ &\leq \mathcal{N}(\mathcal{H}, \epsilon/(8M)) 2e^{-\frac{m\varepsilon^2}{4(2\sigma^2+\frac{1}{3}M^2\varepsilon)}}.\end{aligned}$$

□

Abstract Analysis of Generalization Error

Lemma

Let $\varepsilon > 0$ and $0 < \delta < 1$ such that

$$\mathbb{P}(\sup_{f \in \mathcal{H}} |L_{\mathbf{z}}(f)| \leq \varepsilon) \geq 1 - \delta.$$

Then

$$\mathbb{P}(\mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}}) \leq 2\varepsilon) \geq 1 - \delta.$$

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Proof.

Suppose that $\sup_{f \in \mathcal{H}} |L_{\mathbf{z}}(f)| \leq \varepsilon$. Then $|\mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}})| \leq \varepsilon$, $|\mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}})| \leq \varepsilon$ and $\mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H}}) \leq 0$. It follows that

$$\begin{aligned}
\mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}}) = \mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H},\mathbf{z}}) + \mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H}}) + \\
\mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}}) \\
\leq |\mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}})| + |\mathcal{E}_{\mathbf{z}}(\widehat{f}_{\mathcal{H}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}})| \leq 2\epsilon.
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$\square$

Abstract Analysis of Generalization Error

Theorem C

Let $\mathcal{H}$ be a hypothesis class. Assume that for all $f \in \mathcal{H}$ it holds that $|f(X) - Y| < M$ a.e. Then, for all $\varepsilon > 0$,

$$\mathbb{P}\left(\mathcal{E}(\widehat{f}_{\mathcal{H},\mathbf{z}}) - \mathcal{E}(\widehat{f}_{\mathcal{H}}) \leq \varepsilon\right) \geq 1 - \mathcal{N}(\mathcal{H}, \frac{\varepsilon}{16M})2e^{-\frac{m\varepsilon^2}{8(2\sigma^2 + \frac{1}{3}M^2\varepsilon)}},$$

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where $\sigma^2 := \sup_{f\in\mathcal{H}} \sigma_f^2$.

Proof.

Apply Lemma and Theorem B with $\epsilon \leftrightarrow \epsilon/2$. $\square$

Abstract Analysis of Generalization Error

Question

Given $\varepsilon, \delta > 0$, how many samples m do we need such that the probability that the generalization error is $\leq \varepsilon$ is at least $1 - \delta$?

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Answer

By the previous theorem it suffices to choose

$$m \geq \frac{8(4\sigma^2 + \frac{1}{3}M^2\varepsilon)}{\varepsilon^2} \left(\ln(2\mathcal{N}(\mathcal{H}, \frac{\varepsilon}{16M})) + \ln(\frac{1}{\delta}) \right).$$

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Question

How to bound the covering number?

1.2.5 A Simple Example

Unit Balls

For $R \in (0, \infty)$ and $n \in \mathbb{N}$ let

$$B_{R,n} := \{w \in \mathbb{R}^n : \ \|w\|_\infty \le R\}.$$

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Proof.

Just decompose $B_{R,n}$ into $\left\lceil \frac{R}{\tau} \right\rceil^n$ cubes... $\square$

Parametrized Hypothesis Classes

Let $\mathcal{F} : B_{R,n} \to C(\Omega)$ and $L \in (0, \infty)$ with

$$\|\mathcal{F}(v) - \mathcal{F}(w)\|_{L^\infty(\Omega)} \leq L\|v - w\|_\infty$$

for all $v, w \in B_{R,n}$.

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Lemma

We have

$$\mathcal{N}(\mathcal{F}(B_{R,n}), \tau) \leq \left\lceil \frac{LR}{\tau} \right\rceil^n .$$

Proof.

Use the Lipschitz property to deduce that a τ/L cover of $B_{R,n}$ induced a τ cover of $\mathcal{F}(B_{R,n})$. $\square$

Example: Linear Regression

Let $\mathcal{F}(w) := \sum_{i=1}^{n} w_i \varphi_i$, as in the linear Regression example.

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Corollary

Let $\mathcal{H} = \{\sum_{i=1}^{n} w_i \varphi_i : \ \|w\|_\infty \leq R\}$. Then

$$\mathcal{N}(\mathcal{H}, \tau) \leq \left\lceil \frac{R\| \sum_{i=1}^{n} |\varphi_i|\|_{L^\infty(\Omega)}}{\tau} \right\rceil^n.$$

Analysis of Linear Regression

Theorem

Consider linear regression as above and suppose that we have the approximation error estimate

$$\inf_{f \in \mathcal{H}} \|\widehat{f} - f\|^2_{L^2(\mathbb{R}^d, d\mathbb{P}_X)} \leq \frac{\epsilon}{2}.$$

Then

$$m \gtrsim \frac{\left(n \cdot \mathrm{polylog}(\epsilon) + \ln(\frac{1}{\delta})\right)}{\epsilon^2}$$

independent training samples suffice to get an empirical error ϵ with probability $\geq 1 - \delta$.

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Rule of Thumb to avoid Overfitting

If we double the dimension (for example polynomial degree) we need to double the number of training samples!

More Advanced Topics

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- Better sampling procedures (see for example Cohen, Migliorati: Optimal Weighted Least Squares Methods)