Mathematical Foundations of ML

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OWA Seminar, Oct. 2018

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
3. Reproducing Kernel Hilbert Spaces
4. Classification
5. Dimensionality Reduction
6. (Kernel) Support Vector Machine

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 $f : \mathbb{R}^n \to \{1, \ldots, k\}$ which maps data $x \in \mathbb{R}^n$ to a category in $\{1, \ldots, k\}$. 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
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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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$$\mathcal{H} = \mathsf{span}\{\varphi_1, \ldots, \varphi_l\} \subset C(\mathbb{R}^d)$$

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

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

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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.

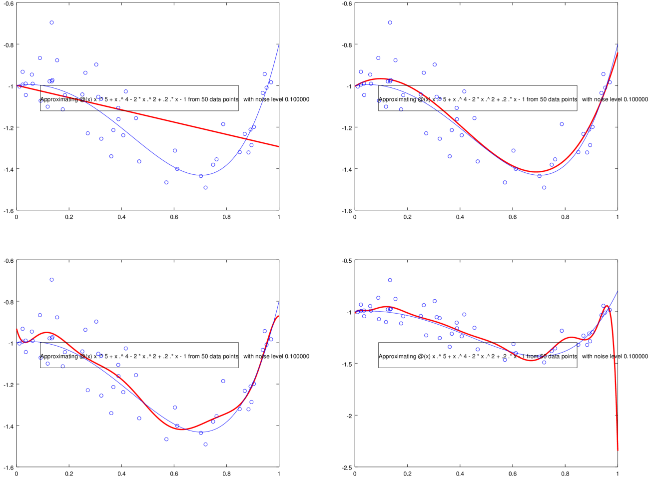
We want to minimize the function

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

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
-0.6
-0.8
-1
-1.2
-1.4
-1.6
-0.5
-1.5
-2
-2.5
0
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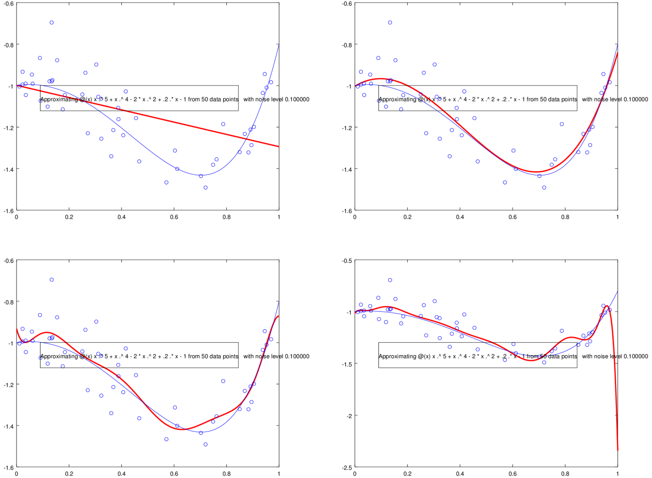
1



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

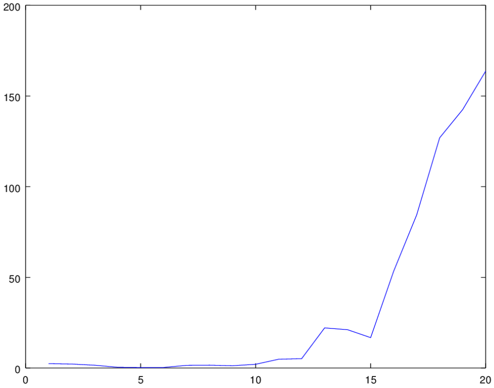


Figure: Error with Polynomial Degree

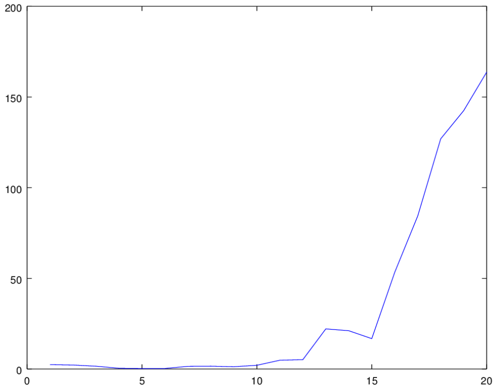


Figure: Error with Polynomial Degree

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

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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

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\mathcal{E}(g) &= \mathbb{E}[(g(X) - Y)^2] = \mathbb{E}[(g(X) - f(X) - \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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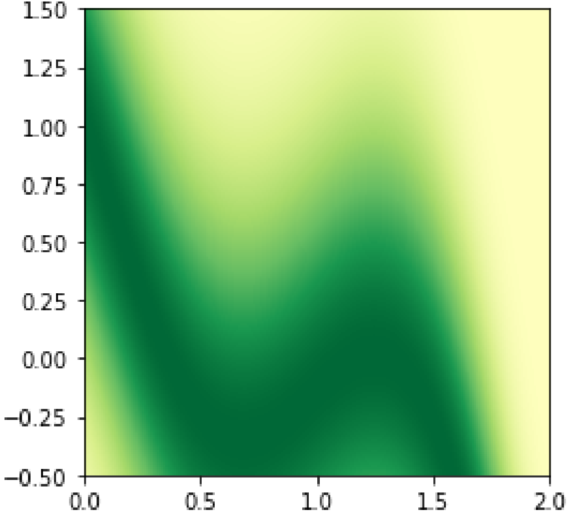

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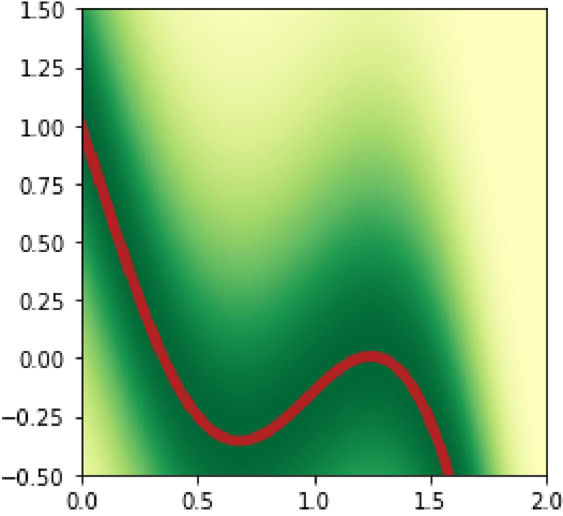

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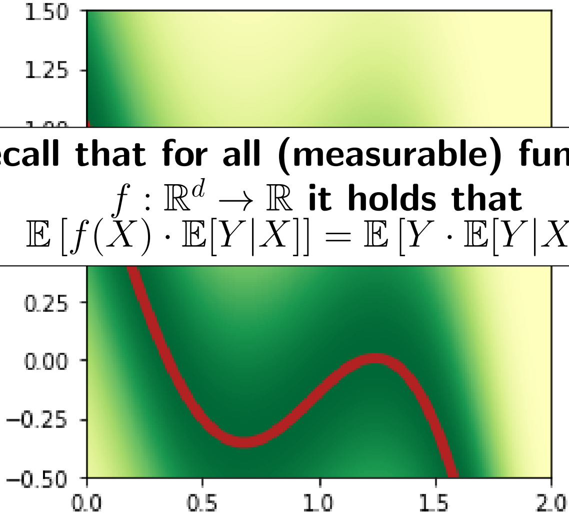

Recall that for all (measurable) functions $f : \mathbb{R}^d \to \mathbb{R}$ it holds that $\mathbb{E}\left[f(X) \cdot \mathbb{E}[Y|X]\right] = \mathbb{E}\left[Y \cdot \mathbb{E}[Y|X]\right]$.

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

$$\mathcal{E}(f) = \|f - \widehat{f}\|^2_{L^2(\mathbb{R}^d, d\mathbb{P}_X)} + \sigma^2$$

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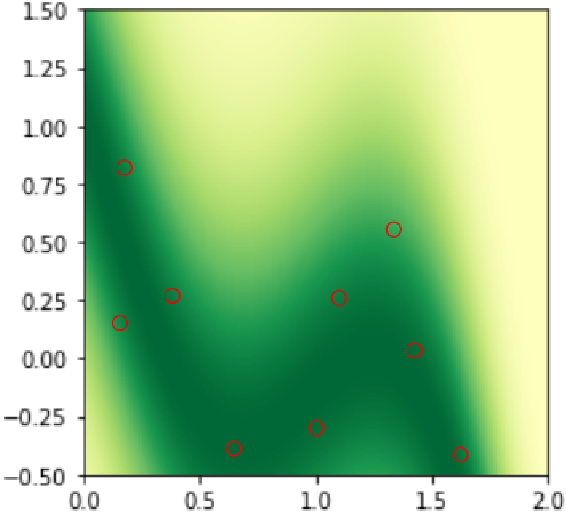

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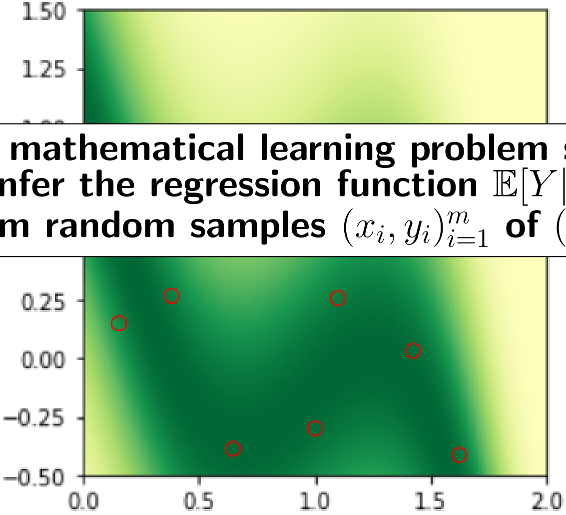

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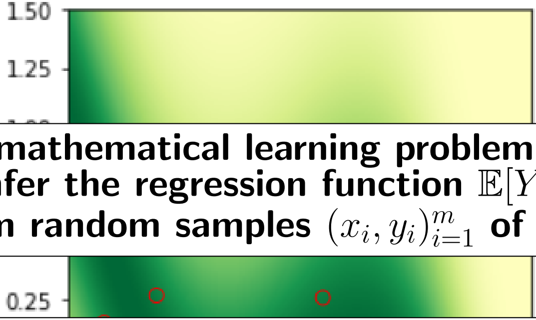

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More generally we would like to minimize

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

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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The defect of f is defined as

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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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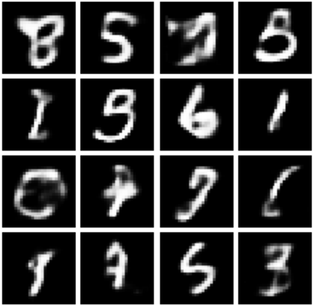

Data Generating Distribution

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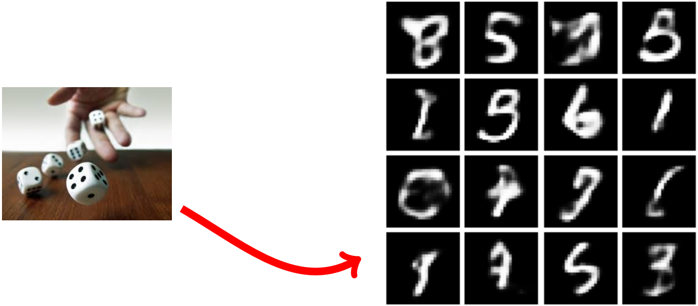

$\rightsquigarrow$ **Variational Autoencoder Demo**

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 $\xi = (f(X) - Y)^2$. □

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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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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

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

$\square$

Generalization- and Approximation Error

Theorem (Bias-Variance Decomposition)

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

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.

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

□

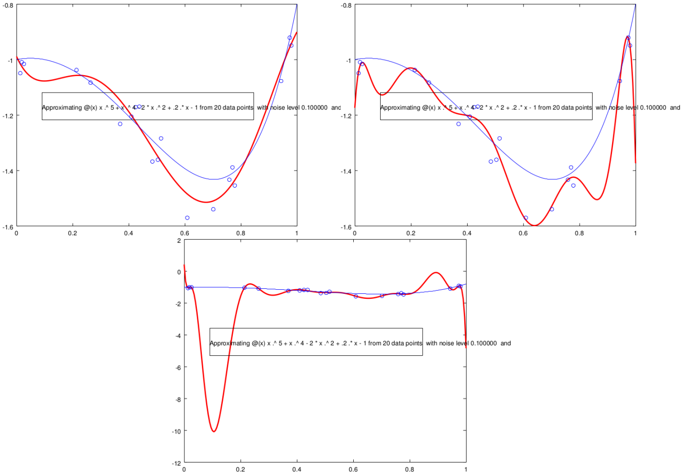

Figure: Blue: $f_{\mathcal{H}}$, Red: $f_{\mathcal{H},\mathbf{z}}$, $m = 10$, $\mathcal{H} =$ polynomials of degree $5, 15, 20$ (from top left to bottom).

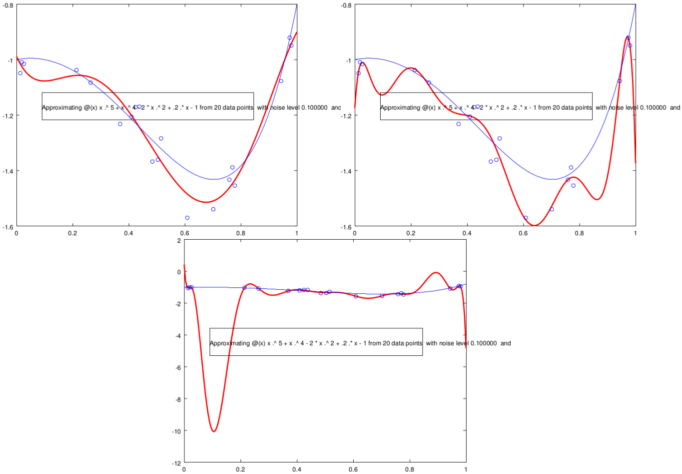

Figure: Blue: $f_{\mathcal{H}}$, Red: $f_{\mathcal{H},\mathbf{z}}$, $m = 10$, $\mathcal{H} =$ polynomials of degree $5, 15, 20$ (from top left to bottom).

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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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.

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 $\varepsilon > 0$,

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

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

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

Then by this fact and Theorem A it holds that

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

$\square$

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

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

$\square$

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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Abstract Analysis of Generalization Error

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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

Linear Regression

Recall

$$\mathcal{H}_{l,R} = \mathsf{span}\,\{\varphi_1, \ldots, \varphi_l\} \cap \{f \in C(\Omega) : \|f\| \leq R\} \subset C(\Omega).$$

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Theorem

Let $T := \| \sum_{j=1}^{l} |\varphi_j| \|$. Then

$$\ln(\mathcal{N}(\mathcal{H}_R, \eta)) \leq l \cdot \ln\left(\frac{4RT}{\eta}\right).$$

Linear Regression

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Let $T := \|\sum_{j=1}^{l} |\varphi_j|\|$. Then

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In the motivational section on linear regression we have seen that $f_{\mathcal{H},\mathbf{z}}$ can be found by solving an l-dimensional linear system.

Analysis of Linear Regression

Theorem

Suppose that we have the approximation error estimate

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

Then

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

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

More Advanced Topics

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- General Loss function (see for example Devroye, Gyorfi, Lugosi: A Probabilistic Theory of Pattern Recognition)

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

1.3 Reproducing Kernel Hilbert Spaces (RKHS)

1.3.1 Definition

Reproducing Kernel Hilbert Spaces (RKHS)

Motivation

Suppose we have a 'similarity measure' $K : \Omega \times \Omega \to \mathbb{R}$ on Ω and we would like to do things like nearest neighbour search, PCA etc. with respect to this measure of similarity. One idea is to associate each $x \in \Omega$ with a *feature map* Φ_x which is an element of a high-dimensional inner-product-space, but which 'linearizes' the similarity measure in the sense that

$$K(x, x') = \langle \Phi_x, \Phi_{x'} \rangle.$$

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Question

Which conditions on K guarantee the existence of a feature map?

Mercer Theorem

Definition

$K : \Omega \times \Omega \to \mathbb{R}$ is symmetric if $K(x, x') = K(x', x)$ for all $x, x' \in \Omega$. Let $\mathbf{x} = \{x_1, \ldots, x_k\} \subset \Omega$ and $K[\mathbf{x}] \in \mathbb{R}^{k \times k}$ with entries $K(x_i, x_j)$ the *Gramian* of K at $\mathbf{x}$. K is called *positive semidefinite* if its Gramian is always positive semidefinite. K is called a *Mercer kernel* if it is symmetric, positive semidefinite and continuous.

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Theorem

There exists a unique Hilbert space $\mathcal{H}_K$ of functions on Ω satisfying

1. The functions $K_x : x' \mapsto K(x, x')$ are in $\mathcal{H}_K$,
2. the span of the K_x's is dense, and
3. for all $f \in \mathcal{H}_K$ we have $f(x) = \langle f, K_k \rangle$.

Mercer Theorem

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3. for all $f \in \mathcal{H}_K$ we have $f(x) = \langle f, K_k \rangle$.

In particular, $K(x, x') = \langle K_x, K_{x'} \rangle$ and in this sense, the RKHS $\mathcal{H}_K$ can be regarded as a feature space.

Proof.

Consider finite sums

$$f(x) = \sum_{i=1}^{m} w_i K(x_i, x), \quad g(x) = \sum_{i=1}^{m} v_i K(x_i, x)$$

with inner product $\langle f, g \rangle = \mathbf{w}^T K[\mathbf{x}]\mathbf{v}$ and complete. $\square$

Examples I

Dot-Product Kernels

Let Ω be the ball of radius T in $\mathbb{R}^d$ and $K(x, x') = \sum_{d=1}^{\infty} a_d(x \cdot x')$, where $a_d \geq 0$ for all d and $\sum_d a_d T^{2d} < \infty$. Then K is a mercer kernel on Ω called a *dot product kernel*.

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Let Ω be the ball of radius T in $\mathbb{R}^d$ and $K(x, x') = \sum_{d=1}^{\infty} a_d(x \cdot x')$, where $a_d \geq 0$ for all d and $\sum_d a_d T^{2d} < \infty$. Then K is a mercer kernel on Ω called a *dot product kernel*.

Example

Suppose that Ω is as above and $K(x, x') = 1 + x \cdot x'$. Then $\{1, x_1, \ldots, x_n\}$ constitutes on ONB of $\mathcal{H}_K$.

Examples II

Translation-Invariant Kernels

Suppose that $k : \mathbb{R}^d \to \mathbb{R}$ is such that its Fourier transform is real-valued and non-negative. Then $K(x, x') := k(x - x')$ is a mercer kernel, called a *translation-invariant kernel*.

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Example

Let $k = \chi_{[-1,1]} * \chi_{[-1,1]}$ the cardinal B-spline of degree one. Then

$$K(x, x') = \begin{cases} 1 - \frac{|x-x'|}{2} & |x - x'| \leq 2 \\ 0 & \text{else} \end{cases} .$$

Examples III

Radial Basis Functions (RBF)

Suppose that $f : \mathbb{R}_+ \to \mathbb{R}$ is completely monotonic (i.e. $(-1)^k f^{(k)} \geq 0$). Then $K(x, x') := f(|x - x'|^2)$ is a mercer kernel, called a *RBF kernel*.

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Example

A Gaussian $f(t) := e^{-t/c^2}$ and an inverse multiquadric $(c^2 + |t|)^{-\alpha}, \alpha > 0$ are completely monotonic and define corresponding RBF kernels.

Covering Numbers

Theorem

For $R > 0$ denote B_R the ball of radius R in a RKHS $\mathcal{H}_K$. Then B_R is a compact subset of $C(\Omega)$ and thus a valid hypothesis space.

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If $K \in C^s$ then

$$\ln(\mathcal{N}(B_R, \eta)) \leq C \cdot \mathsf{diam}(X)^n \|K\|_{C^s}^{n/s} \left(\frac{R}{\eta}\right)^{2n/s}.$$

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For specific kernels (such as Gaussian RBF kernels), much better results exist.

1.3.2 Computation of the Empirical Regression Function

Computational Issues

Question

How can we determine $f_{\mathcal{H},\mathbf{z}}$?

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Let $\mathcal{H}_{K,\mathbf{z}} := \text{span}\{K_{x_1}, \ldots, K_{x_m}\}$ and $P : \mathcal{H}_K \to \mathcal{H}_{K,\mathbf{z}}$ the orthogonal projection. Then, since $f(x_i) = \langle f, K_{x_i} \rangle$ $= \langle P(f), K_{x_i} \rangle = P(f)(x_i)$ we have $\mathcal{E}_{\mathbf{z}}(f) = \mathcal{E}_{\mathbf{z}}(P(f))$!!!

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Theorem

We have $f_{\mathcal{H},\mathbf{z}} = \sum_{i=1}^m c_i^* K_{x_i}$, where (c_i^*) is a minimizer of

$$\frac{1}{m} \sum_{j=1}^m \left(\sum_{i=1}^m c_i K(x_i, x_j) - y_j \right)^2 \quad \text{s.t.} \quad c^T K[\mathbf{x}] c \leq R^2.$$

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This is a convex quadratic program that can be efficiently solved by interior point methods! Check out `http://cvxr.com/cvx/`!

1.3.3 A Bayesian Interpretation

Bayes' Theorem

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$$\mathbb{P}(f|\mathbf{z}) = \frac{\mathbb{P}(\mathbf{z}|f) \cdot \mathbb{P}(f)}{\mathbb{P}(\mathbf{z})}$$

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$$\mathbb{P}(f|\mathbf{z}) = \frac{\mathbb{P}(\mathbf{z}|f) \cdot \mathbb{P}(f)}{\mathbb{P}(\mathbf{z})} \sim \exp(-\frac{1}{2\sigma^2}\sum_{i=1}^{m}(f(x_i) - y_i)^2 - \|f\|^2_{\mathcal{H}_K}).$$

Maximum A Posteriori (MAP) Estimate

MAP Estimate

The MAP Estimate maximizes the a posteriori probability $\mathbb{P}(f|\mathbf{z})$, given an a priori distribution on f and on the noise.

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For the a priori distribution $\mathbb{P}(f) = c \cdot \exp(-\|f\|^2_{\mathcal{H}_K})$ and Gaussian noise, the solution of the regularized least squares problem is also the MAP estimate!

1.4 Classification

The Classification Problem

The Classification Problem

We now aim at classifying data into two classes and thus look for $f : \Omega \to \{-1, 1\}$. Therefore, let's put $Y = \{-1, 1\}$ and $Z := \Omega \times Y$.

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Misclassification Error

Given a distribution (X, Y) and $f : X \to Y$, define the *misclassification error* as

$$\mathcal{R}(f) := \mathbb{P}_{(X,Y)}(f(X) \neq Y).$$

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The classification problem asks to minimize the misclassification error.

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Define the *Bayes rule* as

$$\widehat{f_c} := \mathrm{sgn}(\widehat{f}).$$

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Theorem

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We can re–use everything!

Bayes Rule

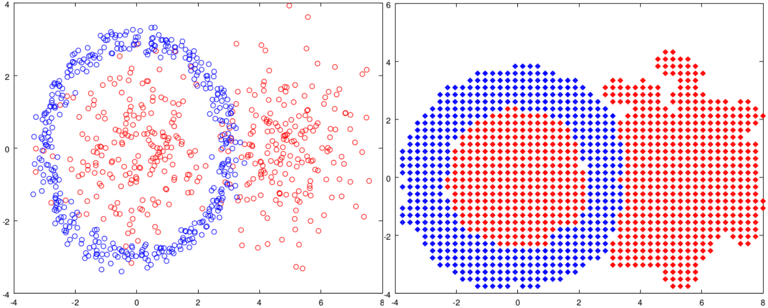

Figure: Bayes Rule for Gaussian Kernel regression. Left: sample data. Right: Estimate using Bayes Rule.

Case Study: Breast Cancer Detection

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Classification Results based on Kernel Regression

Size of dataset $m = 683$ and dimensionality of feature space $d = 10$.

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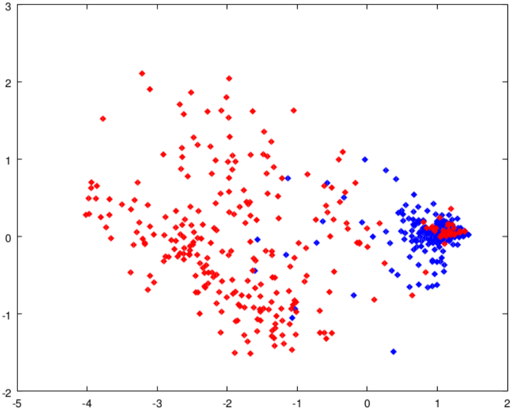
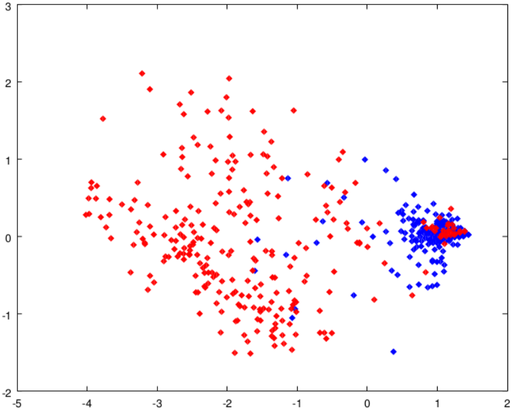
We obtain 95 percent classification accuracy from only 68 training samples and linear kernel!

Visualizing Data



Visualizing Data



Data is very well-clustered...

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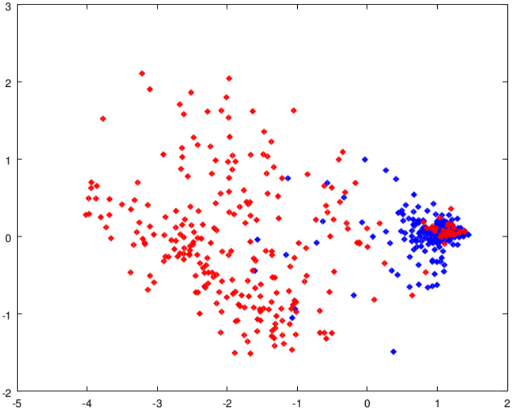

Data is very well-clustered...

But how did we obtain this visualization of our 10-dimensional dataset?

1.5 Dimensionality Reduction

Dimensionality Reduction

Dimensionality Reduction Problem

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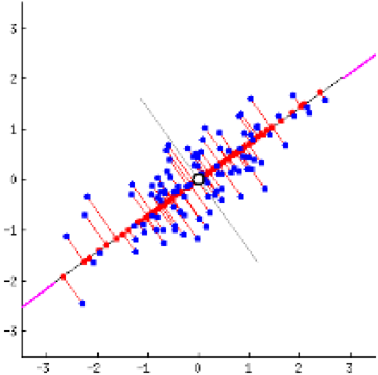
Simplest case: Φ is orthogonal projection onto affine subspace $\rightsquigarrow$ PCA.

What is a good projection?



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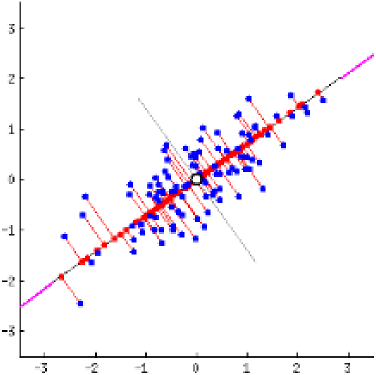

Pick subspace which maximizes variance of the projected dataset.

PCA

PCA Problem

Look for s-dimensional affine subspace with associated orthogonal projection Φ such that the variance $\sum_{i=1}^{m} |\Phi(x_i - \frac{1}{m}\sum_{j=1}^{m} x_j)|^2$ is maximized.

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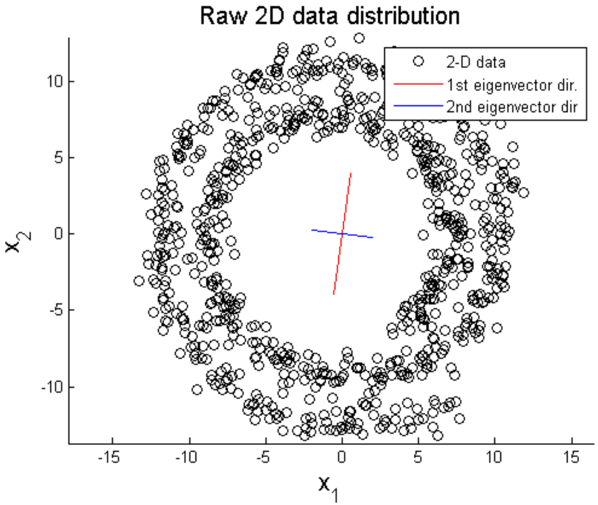
- Define the empirical covariance matrix $G = \frac{1}{m}\sum_{i=1}^{m} x_i x_i^T \in \mathbb{R}^{d\times d}$.
- Then the solution is given by the subspace spanned by the first s normalized Eigenvectors $u_1, \ldots, u_s$ of G and $\Phi(x) = \sum_{l=1}^{s}(x \cdot u_l)u_l$.

It's really simple

```
function z=pca(X)
%project data X on its
%principal components.
C=cov(X);
[U,D,pc] = svd(C);
z = center(X)*pc;
scatter(z(:,1),z(:,2));%plot 2d projection
```

When PCA fails...



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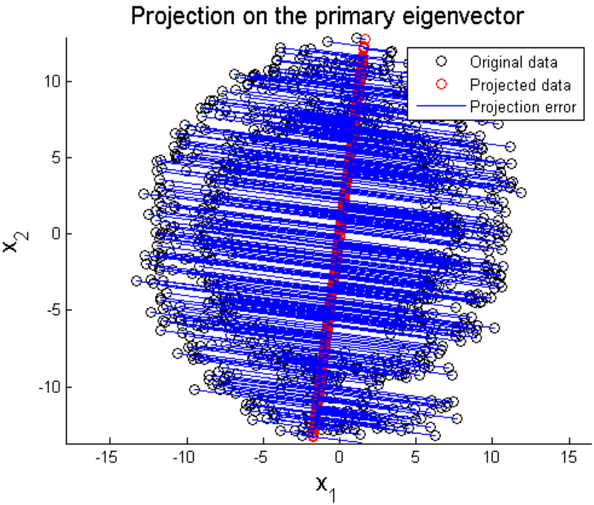

Kernel PCA

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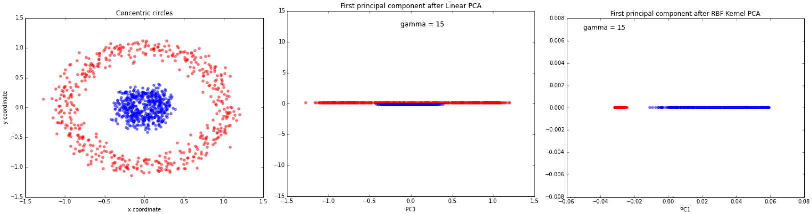
Kernel PCA

Define the matrix
$G = K[\mathbf{x}] - \mathbf{1}_m K[\mathbf{x}] - K[\mathbf{x}]\mathbf{1}_m + \mathbf{1}_m K[\mathbf{x}]\mathbf{1}_m \in \mathbb{R}^{m \times m}$ and $(\mathbf{1}_m)_{i,j} = \frac{1}{m}$ for $i, j \in \{1, \ldots, m\}$ and denote $u_1, \ldots, u_s$ the first s normalized (w.r.t. the inner product $u^T K[\mathbf{x}]u$) Eigenvectors of G. Then the projection Φ is defined as

$$\Phi(x) = \left(\sum_{i=1}^{m} (u_1)_i K(x_i, x), \ldots, \sum_{i=1}^{m} (u_s)_i K(x_i, x) \right)^T .$$

Example



Concentric circles
y coordinate
x coordinate
First principal component after Linear PCA
gamma = 15
PC1
First principal component after RBF Kernel PCA
gamma = 15
PC1

Kernel PCA Denoising

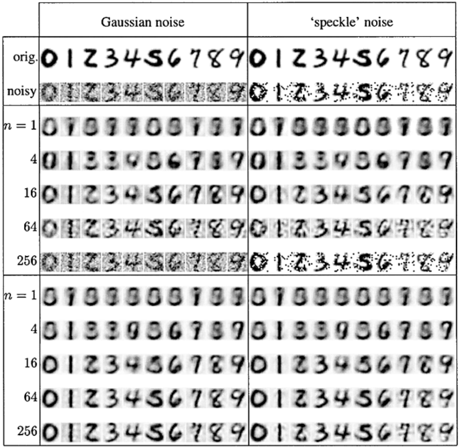


Figure: Top: Linear PCA reconstruction from n principal components. Bottom: Gaussian Kernel Reconstruction from n principal components (find z with $\|K_z - \Phi(x)\|_{\mathcal{H}_K}$ minimal).

- Literature: Sebastian Mika, Bernhard Schölkopf, Alex Smola, Klaus-Robert Müller, Matthias Scholz, Gunnar Rätsch. *Kernel PCA and De-Noising in Feature Space*. NIPS (1999).

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- Other methods: Multidimensional Scaling, Isomap, Diffusion Maps, ...
- Try to appreciate the power of kernelization!
- Go to `https://archive.ics.uci.edu/ml/datasets.html` for further datasets and play around with them!

1.6 (Kernel) Support Vector Machine (SVM)

Basic Idea

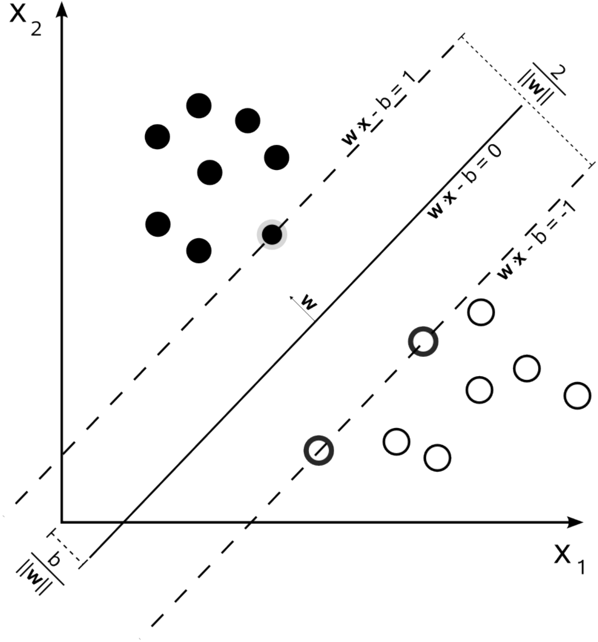
- Suppose that data points $(x_i)_{i=1}^m \subset \mathbb{R}^n$ to be classified are *linearly separable*, i.e. there exists a separating hyperplane defined by $w \in \mathbb{R}^n$, $|w| = 1$ and $b \in \mathbb{R}$ such that

$$y_i = 1 \Leftrightarrow w \cdot x_i > b.$$

- Define the *margin* of a separating hyperplane defined by w, b as above by

$$\Delta(w, b) := \min_{i=1}^{m} |w \cdot x_i - b|.$$

Try to find separating hyperplane with maximal margin!



X 2
X 1
w·x - b = 1
w·x - b = 0
w·x - b = -1
w
2/||w||
b/||w||

The SVM

The SVM problem can be formalized by the following minimization problem

$$\operatorname{argmin}_{w,b} |w| \quad \text{s.t.} \quad y_i(w \cdot x_i - b) \geq 1 \quad \text{for all} \quad i \in \{1, \ldots, m\}.$$

The SVM

The SVM problem can be formalized by the following minimization problem

$$\operatorname{argmin}_{w,b} |w| \quad \text{s.t.} \quad y_i(w \cdot x_i - b) \geq 1 \quad \text{for all} \quad i \in \{1, \ldots, m\}.$$

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Soft Margin SVM

Relax to

$$\operatorname{argmin}_{w,b} \frac{1}{m} \sum_{i=1}^{m} \Phi_{hl}(y_i(w \cdot x_i - b)) + \lambda |w|^2,$$

where $\Phi_{hl}(t) := \max(0, 1-t)$, the *hinge loss*.

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 This is a convex quadratic program that can be efficiently solved!

K-SVM

K-SVM

Kernelization yields the problem

$$\operatorname{argmin}_{f\in\mathcal{H}_K,b}\frac{1}{m}\sum_{i=1}^{m}\Phi_{hl}(y_i(f(x_i)-b))+\lambda\|f\|_{\mathcal{H}_K}^2$$

K-SVM

K-SVM

Kernelization yields the problem

$$\mathrm{argmin}_{f\in\mathcal{H}_K,b}\,\frac{1}{m}\sum_{i=1}^{m}\Phi_{hl}(y_i(f(x_i)-b))+\lambda\|f\|^2_{\mathcal{H}_K}$$

Separable Measures

This provably works for separable measures ρ in the sense that there is $f_s\in\mathcal{H}_K$ with $yf(x)>0$ almost surely. It means that data is separated by the zero level set of f_s. Clearly, the Bayes classifier is that equal to $\mathrm{sgn}(f_s)$.

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 For most data points the hinge loss will be zero which implies that f will be sparse in $\{K_{x_i}: i=1,\ldots,m\}$, resulting in potentially big computational savings!

- Literature: Felipe Cucker and Ding Xuan Zhou. *Learning Theory: An Approximation Theory Viewpoint*. Chapter 9.

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- Main advantage as compared to classification method in Section 1.4 is that solution will be sparse.
- Experiment and Compare!

Further Userful Methods

- Gradient Boosted Trees
- Independent Component Analysis