

Cognitive Algorithms

Lecture 3

Linear Regression

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Technische Universität Berlin
Machine Learning Group

Organizational

Tutorials **next week** (changes due to holiday)

Hannah	H2053	Tue 21.05.	12.00
Augustin	FH 314	Tue 21.05.	14.00
Joanina	Zoom	Wed 22.05.	10.00
Jonas	MAR 4.033	Thu 23.05.	10.00

Bi-weekly tutorials **from June onwards**

Joanina	Zoom	Mondays	10.00
Hannah	H2053	Tuesdays	12.00
Augustin		no more tutorials	
Jonas	FH 303	Mondays	14.00

Please remember the Q&A session via Zoom by Ken, each Wednesday at 12.00.

Summary of last lecture

- Correlations between features can affect classification accuracy

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Summary of last lecture

- Correlations between features can affect classification accuracy
- Linear Discriminant Analysis (LDA) maximizes *between class variance* while minimizing *within class variance*
- If data has multivariate normal distribution with equal class covariances, then LDA is the optimal classifier
- We want our model to **generalize** well. We need to test this on data that was not used during training.

Estimating covariance matrices

Given n data points $\mathbf{x}_i \in \mathbb{R}^d$ in a data matrix $X \in \mathbb{R}^{d \times n}$ the empirical estimate of the **covariance matrix** is defined as

$$\hat{\Sigma} = \frac{1}{n} (X - \bar{X})(X - \bar{X})^\top,$$

where the estimate of the expected value is given by the mean

$$\bar{\mathbf{x}} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i, \quad \bar{X} = (\bar{\mathbf{x}}, \bar{\mathbf{x}}, \dots, \bar{\mathbf{x}}) \in \mathbb{R}^{d \times n}$$

The diagonal entries of $\hat{\Sigma}$ are estimates of the variance.

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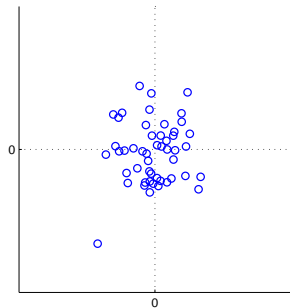
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$$\begin{matrix} D \rightarrow \\ D \downarrow \end{matrix} \begin{matrix} D \rightarrow \\ (X - \bar{X}) \\ \cdot (X - \bar{X})^\top \end{matrix} = \begin{matrix} D \rightarrow \\ D \downarrow \end{matrix} \begin{matrix} N \rightarrow \\ X - \bar{X} \end{matrix} \quad \begin{matrix} D \rightarrow \\ (X - \bar{X})^\top \\ N \downarrow \end{matrix}$$

We call $(X - \bar{X})(X - \bar{X})^\top$ the *empirical scatter matrix*

Correlated data and linear mappings

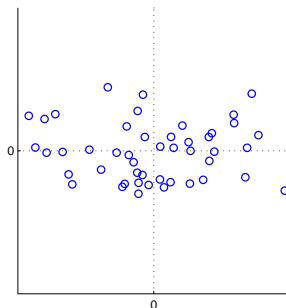
Uncorrelated



$$x \sim \mathcal{N}(0, 1)$$

$$XX^T = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

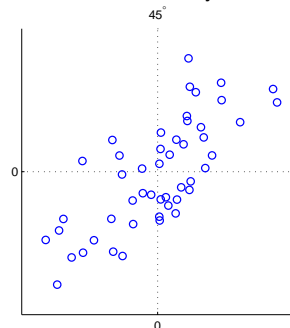
Uncorrelated, scaled



$$\begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} x$$

$$XX^T = \begin{bmatrix} 9 & 0 \\ 0 & 1 \end{bmatrix}$$

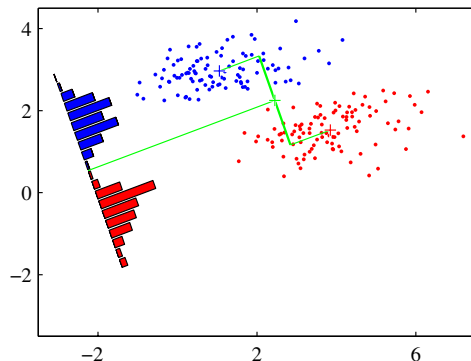
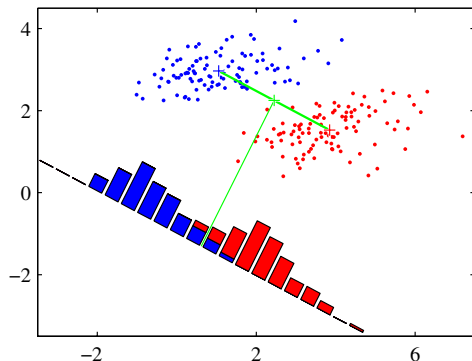
Scaled, rotated by 45°



$$\begin{bmatrix} \cos(\phi) & -\sin(\phi) \\ \sin(\phi) & \cos(\phi) \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} x$$

$$XX^T = \begin{bmatrix} 5 & 4 \\ 4 & 5 \end{bmatrix}$$

Linear Discriminant Analysis (LDA)



Goal: Find a (normal vector of a linear decision boundary) \mathbf{w} that

- Maximizes mean class difference, and
- Minimizes variance in each class

Linear Discriminant Analysis (LDA)

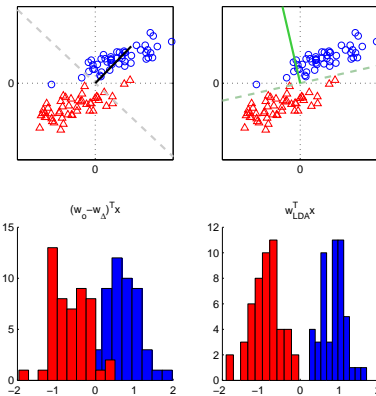
Optimization problem:

$$\operatorname{argmax}_{\mathbf{w}} \frac{\mathbf{w}^{\top} S_B \mathbf{w}}{\mathbf{w}^{\top} S_W \mathbf{w}}$$

Setting the gradient to zero we obtained:

$$\mathbf{w} \propto S_W^{-1}(\mathbf{w}_o - \mathbf{w}_{\Delta})$$

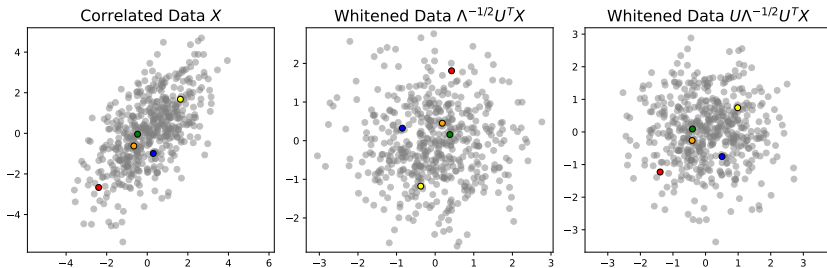
NCC vs. LDA



Whitening

Transforms data to data with covariance matrix that is the identity.

→ Data are decorrelated after whitening



Generalization and model evaluation

The goal of classification is **generalization**: Correct categorization/prediction of new data

How can we estimate generalization performance?

→ **Test set**

- Train model on part of data (training set)
- Test model on other part of data (test set)

From classification to regression

What if our labels are not in $\{-1, +1\}$ but in \mathbb{R} ?

$y \in \{-1, +1\}$ |
Classification

From classification to regression

What if our labels are not in $\{-1, +1\}$ but in \mathbb{R} ?

$y \in \{-1, +1\}$	$y \in \mathbb{R}$
Classification	Regression

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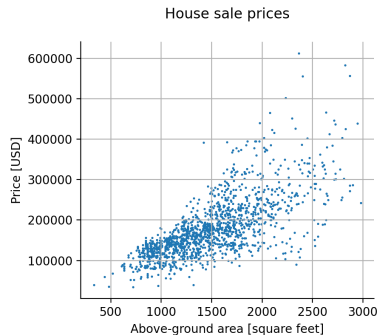
$y \in \{-1, +1\}$	$y \in \mathbb{R}$
Classification	Regression

The most basic and best understood type of regression is **linear regression** (or ordinary least squares (OLS)) using a *least-squares cost function*.

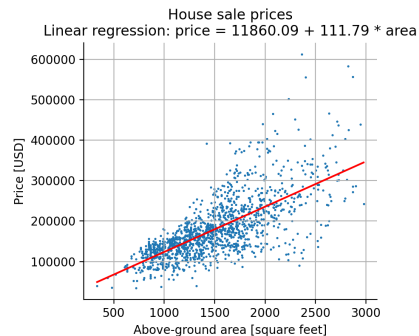
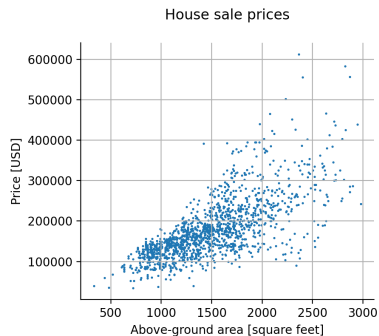
Linear regression - application examples

- Estimate price of a house
- Describe processes in physics/engineering
- Control a hand prosthesis based on electric activity measured on the arm
- Predict sales as a function of advertisement budgets for TV, radio and newspaper.
- Predict stock prices
- ... many, many more...

Simple linear regression



Simple linear regression



How to find the regression line?

(data from kaggle, a great data science platform

<https://www.kaggle.com/competitions/house-prices-advanced-regression-techniques/>)

Simple linear regression (one-dimensional data)

Given data $x_1, \dots, x_n \in \mathbb{R}$ and labels $y_1, \dots, y_n \in \mathbb{R}$, the goal is to predict new y using an (affine) linear function

$$f(x) = w \cdot x + b$$

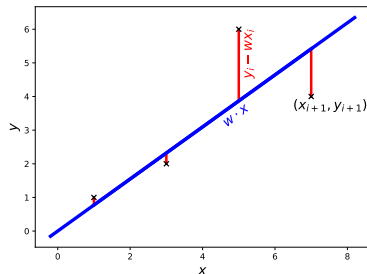
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We will first focus on a simpler version without intercept $f(x) = w \cdot x$.

Approach: Minimize the **squared error** to find the w



$$\mathcal{E}(w) = \sum_{i=1}^n (y_i - w \cdot x_i)^2$$

- differentiable
- analytically solvable
- (optimal under normality assumptions)

Least-squares error: general case

Given data $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$ with $\mathbf{x}_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$ the goal is to find a weight vector $\mathbf{w} \in \mathbb{R}^d$ to predict y for a new \mathbf{x} via

$$y = \mathbf{w}^\top \mathbf{x}.$$

Approach: find \mathbf{w} by minimizing the **least-squares error** [Gauß, 1809; Legendre, 1805], defined as

$$\mathcal{E}_{LSQ}(\mathbf{w}) = \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i)^2 \quad (1)$$



C.F. Gauß (1777–1855)



A.M. Legendre (1752–1833)

Supplementary: optimality of LSE when assuming Gaussian noise

$$\begin{aligned}y &= w \cdot x + \epsilon & \epsilon &\sim \mathcal{N}(0, \sigma_\epsilon^2) \\p(y|w) &= \mathcal{N}(y|w \cdot x, \sigma_\epsilon^2) \\&= \frac{1}{\sqrt{2\pi}\sigma_\epsilon} \exp \left\{ -\frac{1}{2} \left(\frac{y - w \cdot x}{\sigma_\epsilon} \right)^2 \right\}\end{aligned}$$

Maximizing $p(y|w)$ as a function of w is equivalent to maximizing the logarithm of $p(y|w)$ (because it is monotonically increasing).

For more details, see Chapter 1.2.5 in Bishop [2007].

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Simple linear regression: analytical solution

$$\mathcal{E}(w) = \sum_{i=1}^n (y_i - w \cdot x_i)^2$$

Compute the derivative w.r.t. w

$$\frac{\partial \mathcal{E}(w)}{\partial w} = \sum_{i=1}^n 2(y_i - w \cdot x_i) \cdot (-x_i).$$

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Set to zero and solve for w :

$$\sum_{i=1}^n 2(y_i - w \cdot x_i) \cdot (-x_i) = 0 \implies -\sum_{i=1}^n y_i x_i + w \sum_{i=1}^n x_i^2 = 0$$

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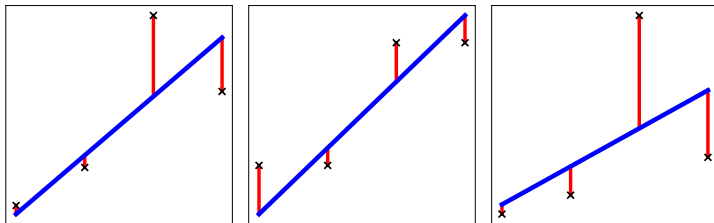
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How does OLS behave?

How does the **predicted label** behave for different samples (marked as \times)?



OLS is sensitive to outliers,
because we minimize the **squared distance** between y and $w \cdot x$.
Therefore, large deviations have a large effect.

Linear regression

Let's look at samples with more than one feature and write everything in matrix notation:

Let n be the number of samples, so $\mathbf{y} \in \mathbb{R}^{1 \times n}$ and $\mathbf{X} \in \mathbb{R}^{d \times n}$.

The prediction $\hat{\mathbf{y}}$ of our Linear Regression model then becomes

$$\mathbf{y} \approx \hat{\mathbf{y}} = \mathbf{w}^T \mathbf{X}.$$

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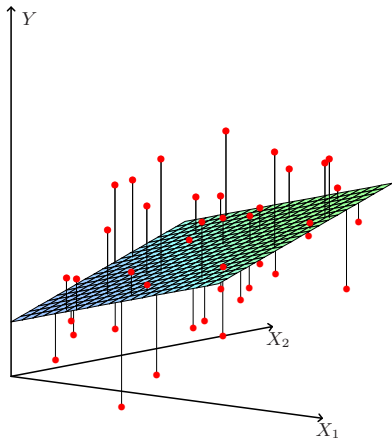
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$$\overset{n \rightarrow}{\text{red box } \hat{\mathbf{y}}} = \overset{d \rightarrow}{\text{gray box } \mathbf{w}^T} \cdot \overset{n \rightarrow}{\underset{d \downarrow}{\text{blue box } \mathbf{X}}}$$

The goal is still to find \mathbf{w} that minimizes the least-squares error.

Linear regression



$$\hat{y} = w_1 \cdot x_1 + w_2 \cdot x_2$$

The target variable $\hat{y} \in \mathbb{R}$ is modeled as a **linear combination** $\mathbf{w} \in \mathbb{R}^d$ of d features $\mathbf{x} \in \mathbb{R}^d$

$$\hat{y} = \mathbf{w}^\top \mathbf{x}$$

Linear regression with basis functions

The target variable $\hat{y} \in \mathbb{R}$ can be modeled as a **linear combination** $\mathbf{w} \in \mathbb{R}^{\tilde{d}}$ of \tilde{d} features $\phi(\mathbf{x}) \in \mathbb{R}^{\tilde{d}}$

$$\hat{y} = \mathbf{w}^\top \phi(\mathbf{x})$$

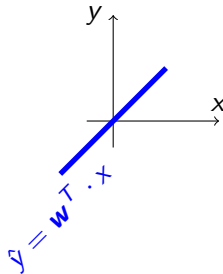
where $\phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \dots, \phi_{\tilde{d}}(\mathbf{x}))$ denotes a vector of (possibly non-linear) *basis functions*.

The basis function can also be $\phi(\mathbf{x}) = \mathbf{x}$.
Generally $\phi(\mathbf{x})$ allows us to model more complex functions.

Intercept term

For non-centered data:
use an *intercept* (often called *bias*) term

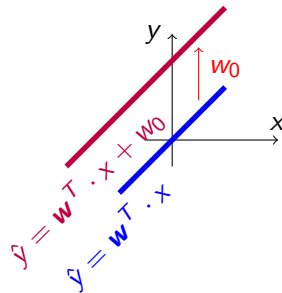
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Intercept term

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$$\hat{y} = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix}^T \cdot \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} + w_0$$

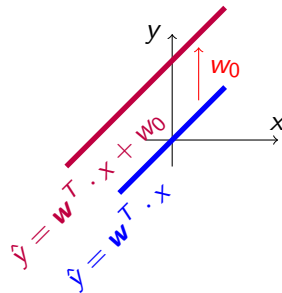


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$$= \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}^T \cdot \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}$$

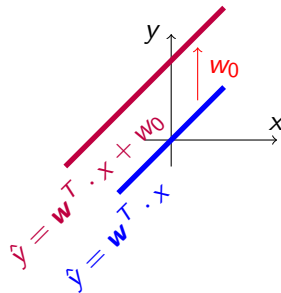


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$$= \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}^T \cdot \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}$$



This unifies the notation. Basis function: $\phi([x_1, x_2, \dots, x_d]^T) = [1, x_1, x_2, \dots, x_d]^T$

Linear Regression: non-linear $\phi(\mathbf{x})$

The general model is $\hat{y} = \mathbf{w}^\top \phi(\mathbf{x})$ with $\hat{y} \in \mathbb{R}$, $\mathbf{w} \in \mathbb{R}^{\tilde{d}}$, $\mathbf{x} \in \mathbb{R}^d$, $\phi : \mathbb{R}^d \rightarrow \mathbb{R}^{\tilde{d}}$.

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Consider the following example:

$$\hat{y} = 0.5x^3 - 3x.$$

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Here $d = 1$, $\tilde{d} = 2$, $\phi(x) = \begin{bmatrix} x^3 \\ x \end{bmatrix}$ and $\mathbf{w} = \begin{bmatrix} 0.5 \\ -3 \end{bmatrix}$.

The feature map ϕ is a fixed part of the model. The vector \mathbf{w} is found via linear regression (it depends on the data!).

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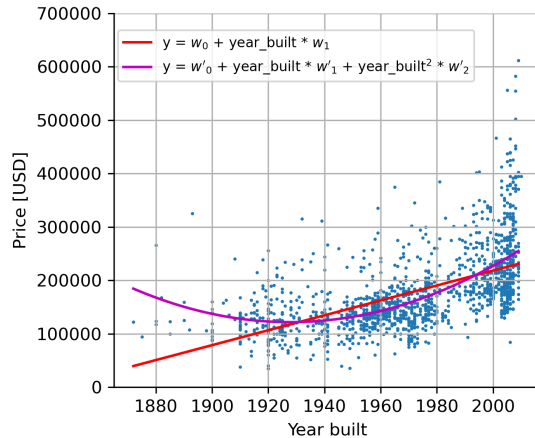
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We can use non-linear basis functions to apply linear regression in higher-dimensional space and predict a non-linear function!

Example with non-linear basis functions

House sale prices



Linear regression: minimizing LSE

To minimize the least-squares loss function in eq. 1

$$\begin{aligned}\mathcal{E}_{LSQ}(\mathbf{w}) &= \sum_{i=1}^n (y_i - \mathbf{w}^\top \mathbf{x}_i)^2 \\ &= \|\mathbf{y} - \mathbf{w}^\top X\|^2 \\ &= \mathbf{y}\mathbf{y}^\top - 2\mathbf{w}^\top X\mathbf{y}^\top + \mathbf{w}^\top XX^\top \mathbf{w}\end{aligned}$$

Linear regression: minimizing LSE

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We compute the derivative with respect to \mathbf{w}

Linear regression: minimizing LSE

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$$\frac{\partial \mathcal{E}_{LSQ}(\mathbf{w})}{\partial \mathbf{w}} = -2X\mathbf{y}^\top + 2XX^\top \mathbf{w}$$

set it to zero and solve for \mathbf{w}

Linear regression: minimizing LSE

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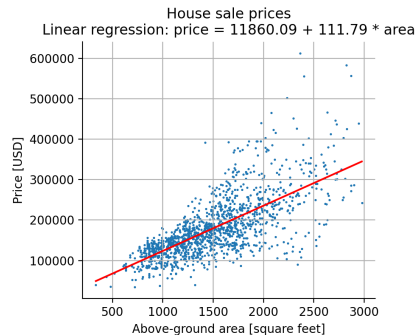
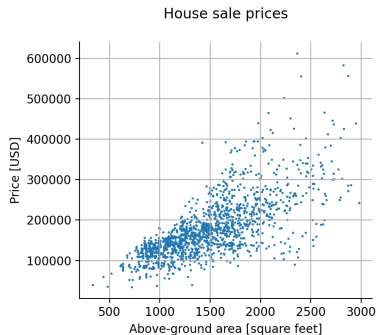
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$$-2X\mathbf{y}^\top + 2XX^\top \mathbf{w} = 0$$

$$XX^\top \mathbf{w} = X\mathbf{y}^\top$$

$$\mathbf{w} = (XX^\top)^{-1} X\mathbf{y}^\top \quad (2)$$

Back to initial example



Now you know how to calculate the regression line.

Data from kaggle, a great data science platform

<https://www.kaggle.com/competitions/house-prices-advanced-regression-techniques/>

Does correlation influence the performance of linear regression?

For a new data point $\mathbf{z} \in \mathbb{R}^d$ and centered data, we have

$$\begin{aligned}\mathbf{z} &\mapsto \mathbf{w}^\top \mathbf{z} \\ \mathbf{w} &= (X X^\top)^{-1} X y^\top\end{aligned}$$

Does correlation influence the performance of linear regression?

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$$\begin{aligned}\mathbf{z} &\mapsto \mathbf{w}^\top \mathbf{z} \\ \mathbf{w} &= (XX^\top)^{-1} X y^\top\end{aligned}$$

We can decompose:

$$\mathbf{w}^\top \mathbf{z} = y X^\top (XX^\top)^{-1} \mathbf{z} = y \underbrace{X^\top U \Lambda^{-1/2}}_{\text{whitened } X^\top} \cdot \underbrace{\Lambda^{-1/2} U^\top \mathbf{z}}_{\text{whitened } \mathbf{z}}$$

where $XX^\top = U \Lambda U^\top$ is the eigenvalue decomposition of XX^\top

Does correlation influence the performance of linear regression?

For a new data point $\mathbf{z} \in \mathbb{R}^d$ and centered data, we have

$$\begin{aligned}\mathbf{z} &\mapsto \mathbf{w}^\top \mathbf{z} \\ \mathbf{w} &= (XX^\top)^{-1} X y^\top\end{aligned}$$

We can decompose:

$$\mathbf{w}^\top \mathbf{z} = y X^\top (XX^\top)^{-1} \mathbf{z} = y \underbrace{X^\top U \Lambda^{-1/2}}_{\text{whitened } X^\top} \cdot \underbrace{\Lambda^{-1/2} U^\top \mathbf{z}}_{\text{whitened } \mathbf{z}}$$

where $XX^\top = U \Lambda U^\top$ is the eigenvalue decomposition of XX^\top

\Rightarrow LR is not susceptible to correlation in the features (different from NCC)
(But note: numerical problems can occur, e.g. if X has near-collinear features)

Linear Regression for vector labels

We now want to predict vector-valued labels $y \in \mathbb{R}^m$

For a measurement $X \in \mathbb{R}^{d \times n}$, $Y \in \mathbb{R}^{m \times n}$ the model is

$$Y = W^T X$$

where $W^T \in \mathbb{R}^{m \times d}$ is a **linear mapping** from data to labels.

Linear Regression for Vector Labels

Given Data $X \in \mathbb{R}^{d \times n}$ and labels $Y \in \mathbb{R}^{m \times n}$, the error function for multiple linear regression is

$$\mathcal{E}_{MLR}(W) = \|Y - W^T X\|_F^2 \quad (3)$$

where $\|A\|_F = \sqrt{\sum_i^n \sum_j^d A_{ij}^2}$ denotes the Frobenius norm and $W^T \in \mathbb{R}^{m \times d}$

Eq. 3 is minimized by (see also eq. 2)

$$W = (XX^T)^{-1}XY^T$$

Linear Regression for Vector Labels

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$$\begin{matrix} m \downarrow & n \rightarrow \\ \text{red box } Y \end{matrix} = \begin{matrix} d \rightarrow & m \downarrow \\ \text{gray box } W^T \end{matrix} \cdot \begin{matrix} d \downarrow & n \rightarrow \\ \text{blue box } X \end{matrix}$$

Application example: myoelectric control of prostheses

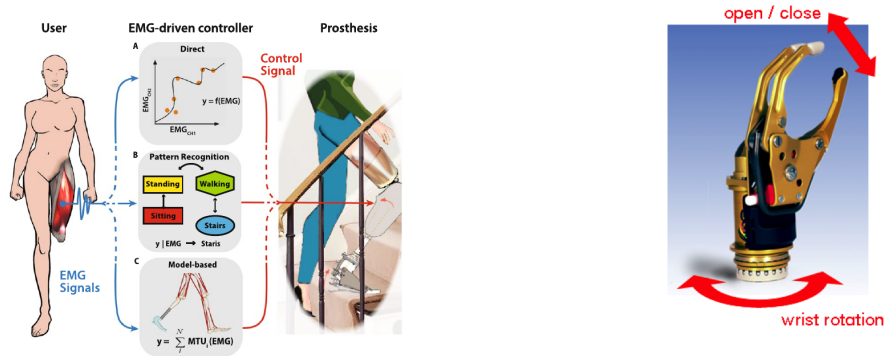


hand prosthesis

Only 2 degrees of freedom are controlled
(open/close, rotate)

Controlled by muscle activity

Application example: myoelectric control of prostheses

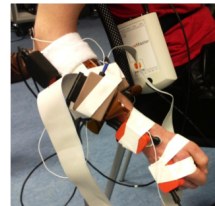
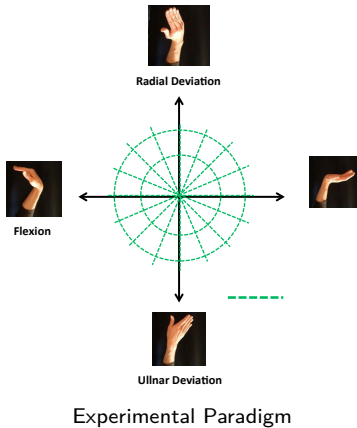


Cimolatto et al. [2022]

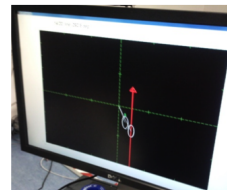
Neurons activate muscles via electric discharges
Electric activity can be measured non-invasively

hand prosthesis
Only 2 degrees of freedom are controlled
(open/close, rotate)
Controlled by muscle activity

Acquisition of training data

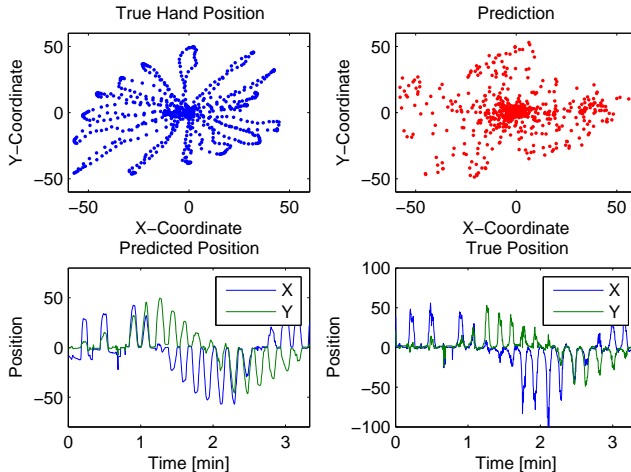


Motion Capture System

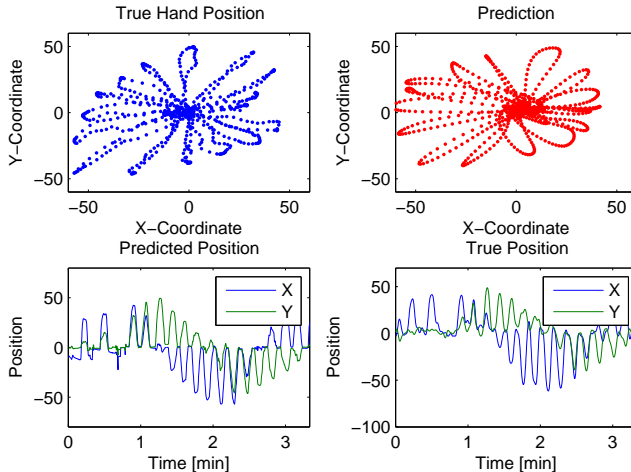


Visual Feedback

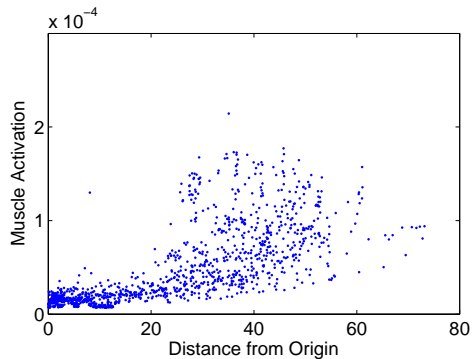
Results from linear regression



Results linear regression - smoothed

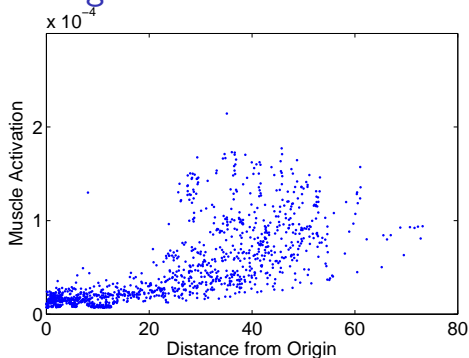


Linear regression

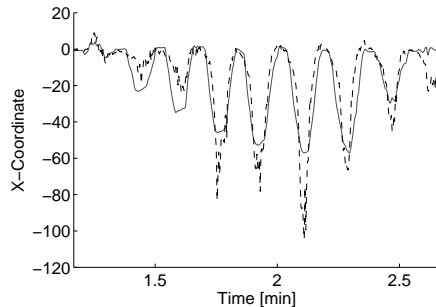


Hand position is a *non-linear* function of muscle activation

Linear regression



Hand position is a *non-linear* function of muscle activation



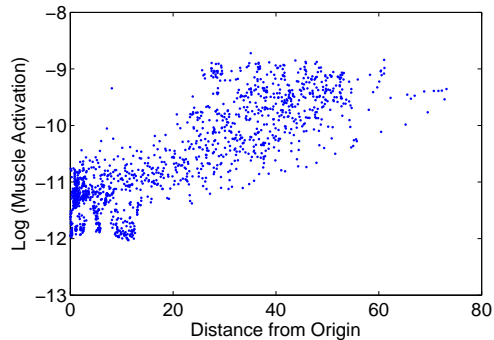
Weak muscle activation

→ True hand position (gray) **underestimated** (dashed)

Strong muscle activation

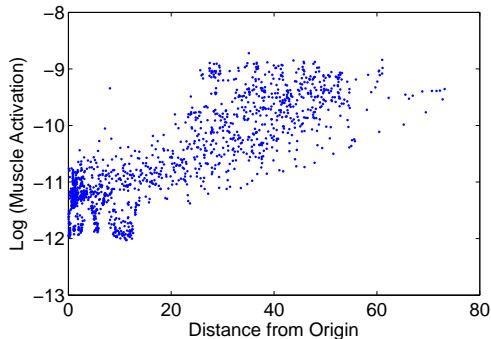
→ True hand position **overestimated**

Linear(ized) Regression

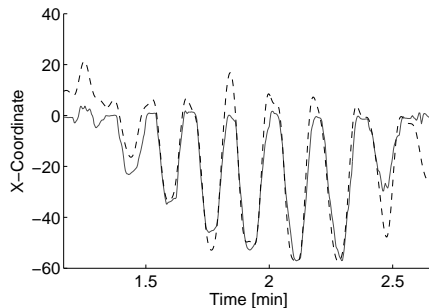


Hand position is *almost linearly*
related to log of muscle activation

Linear(ized) Regression

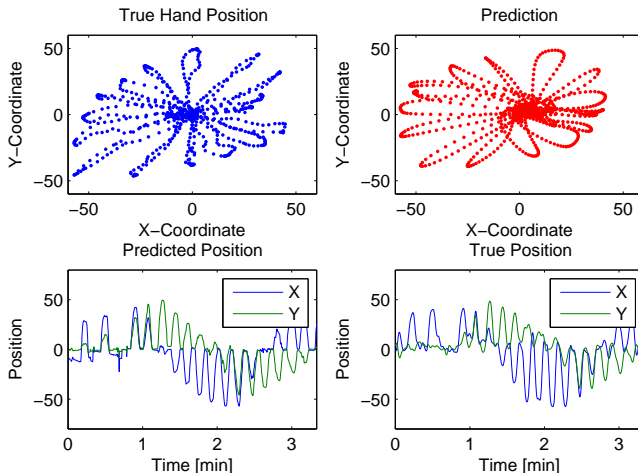


Hand position is *almost linearly* related to log of muscle activation



Strong muscle activation
→ hand position *less overestimated*

Results linear regression - smoothed and log features



The statistical model of linear regression

Linear Model:

$$y = \mathbf{w}^\top \cdot \mathbf{x} + \epsilon$$

Linear Regression: estimates

$$\hat{\mathbf{w}} = (X X^\top)^{-1} X y$$

from given data X, y .

Random variable (recap)

A mapping $X : \Omega \rightarrow \mathbb{R}$ which assigns a real value to every elementary event, is called a real-valued random variable.

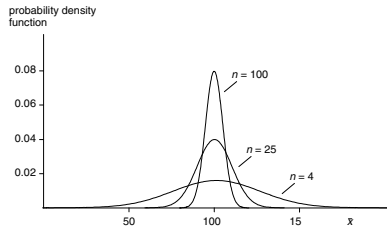
Ω is the sample space, the set of all possible outcomes.

Example: tossing a coin

$$X(\omega) = \begin{cases} 0, & \text{if } \omega = \text{tail} \\ 1, & \text{if } \omega = \text{head} \end{cases} \quad \text{for } \omega \in \Omega$$

The sampling distribution of an estimator

Example: Mean of a random variable



The sampling distribution of an estimator

Example: Mean of a random variable

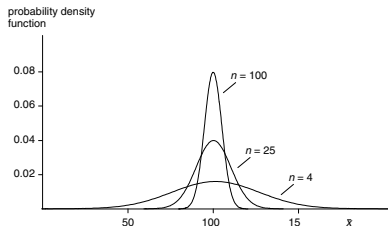
Consider random variables $x_i \sim \mathcal{N}(\mu, \sigma^2)$ independent, identically distributed (i.i.d.).

Draw n data points and *estimate* mean on n data points:

$$\hat{\mu} = \frac{1}{n} \sum_{i=1}^n x_i$$

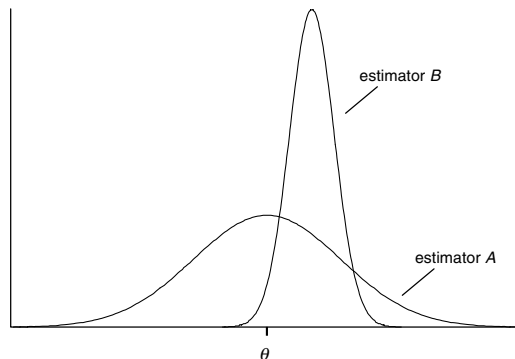
$\hat{\mu}$ is a function of the data and thus itself a random variable.

The sampling distribution is the distribution of values that $\hat{\mu}$ takes.



Desirable properties of estimators

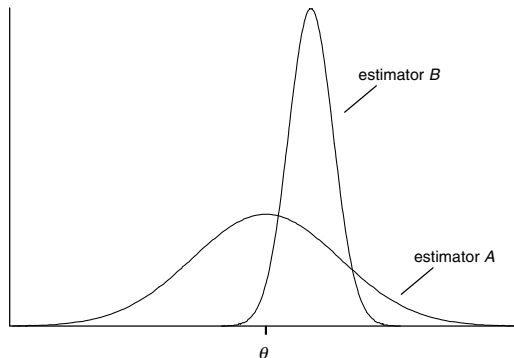
probability density
function



Unbiased The estimator's expected value is the true value of the parameter being estimated (A in the Fig.)

Desirable properties of estimators

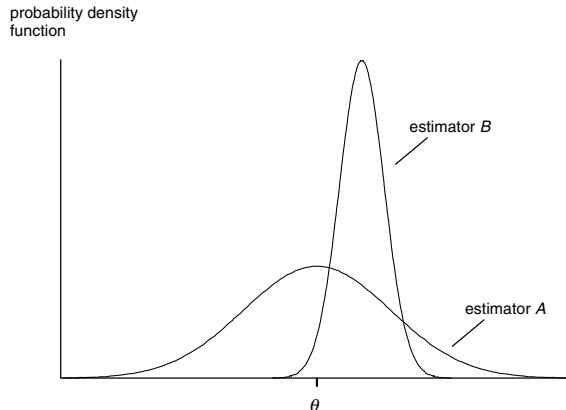
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Small estimator variance
(B has a smaller variance than A)

Desirable properties of estimators

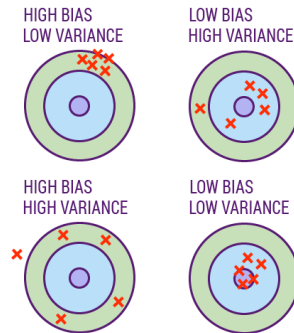


Unbiased The estimator's expected value is the true value of the parameter being estimated (*A* in the Fig.)

Small estimator variance (*B* has a smaller variance than *A*)

Robust not unduly affected by outliers or other small deviations from the model assumptions

Bias and variance



Source: Ikompass [2019]

Gauss-Markov Theorem

Under the model assumption $y = \mathbf{w}^\top \cdot \mathbf{x} + \epsilon$ with uncorrelated noise ϵ , our ordinary least squares estimator $\hat{\mathbf{w}} = (X X^\top)^{-1} X y$ is the Best Linear Unbiased Estimator (BLUE), i.e. the minimum variance unbiased estimator that is linear in y .

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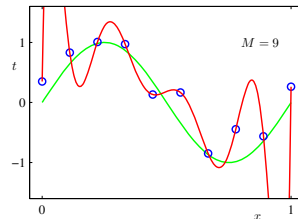
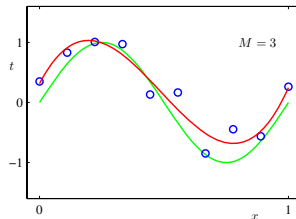
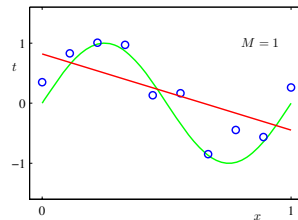
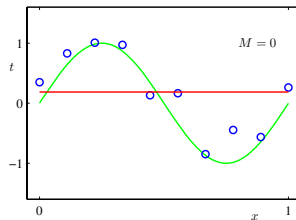
But: in some cases biased estimators with lower variance might be more suitable.

Example: polynomial regression

Higher degrees of polynomials are not necessarily better.

$$\phi_M(x) = [x^0, x^1, \dots, x^M]^T$$

$$\hat{y} = \mathbf{w}^T \phi_M(x)$$



Example: polynomial regression

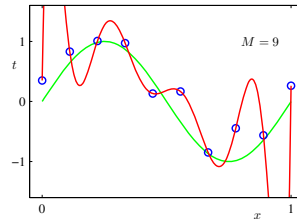
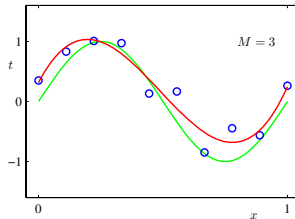
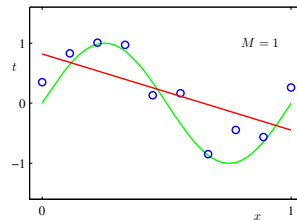
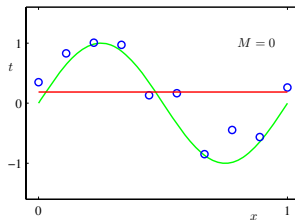
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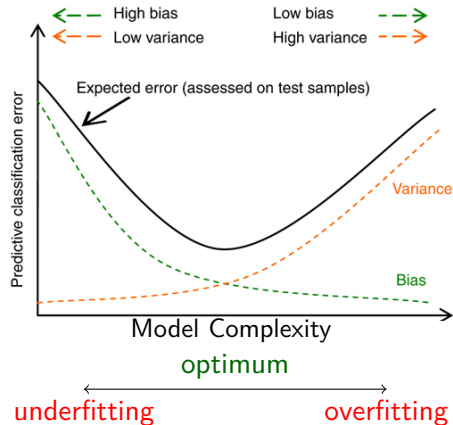
$$\hat{y} = \mathbf{w}^T \phi_M(x)$$

Weights:

	$M = 0$	$M = 1$	$M = 6$	$M = 9$
w_0^*	0.19	0.82	0.31	0.35
w_1^*		-1.27	7.99	232.37
w_2^*			-25.43	-5321.83
w_3^*			17.37	48568.31
w_4^*				-231639.30
w_5^*				640042.26
w_6^*				-1061800.52
w_7^*				1042400.18
w_8^*				-557682.99
w_9^*				125201.43



The bias-variance trade-off



Careful...

Bias and *variance* are terms with multiple (related) usages

- $\mathbf{w}^\top \mathbf{x} + b$, $w \cdot x + b$
- Bias/variance of an estimator
- Bias/variance of a general ML model

Ridge regression

Often it is important to **control the complexity** of the solution \mathbf{w} .

This is done by constraining the norm of \mathbf{w} (regularization)

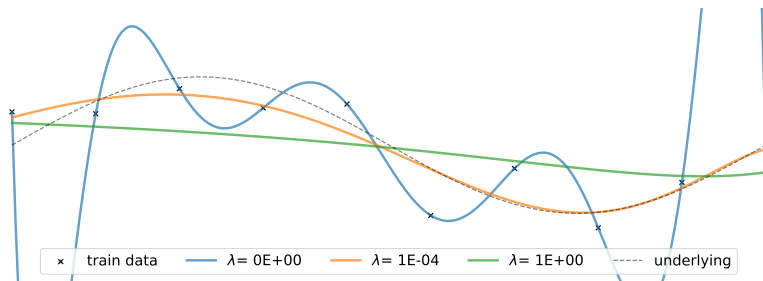
$$\mathcal{E}_{RR}(\mathbf{w}) = \|\mathbf{y} - \mathbf{w}^\top \mathbf{X}\|^2 + \lambda \|\mathbf{w}\|^2$$

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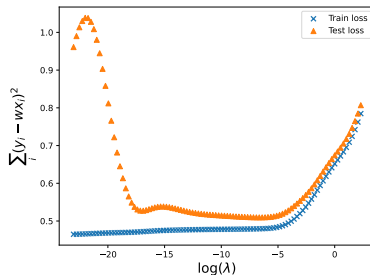


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Ridge regression

Computing the derivative with respect to \mathbf{w} yields

$$\frac{\partial \mathcal{E}_{RR}(\mathbf{w})}{\partial \mathbf{w}} = -2X\mathbf{y}^\top + 2XX^\top \mathbf{w} + 2\lambda \mathbf{w}.$$

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Setting the gradient to zero and rearranging terms, the optimal \mathbf{w} is

$$2XX^\top \mathbf{w} + 2\lambda \mathbf{w} = 2X\mathbf{y}^\top$$

$$(XX^\top + \lambda I)\mathbf{w} = X\mathbf{y}^\top$$

$$\mathbf{w} = (XX^\top + \lambda I)^{-1}X\mathbf{y}^\top$$

Ridge regression

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Setting the gradient to zero and rearranging terms, the optimal \mathbf{w} is

$$\begin{aligned} 2XX^\top \mathbf{w} + 2\lambda \mathbf{w} &= 2X\mathbf{y}^\top \\ (XX^\top + \lambda I)\mathbf{w} &= X\mathbf{y}^\top \\ \mathbf{w} &= (XX^\top + \lambda I)^{-1}X\mathbf{y}^\top \end{aligned}$$

One can show (calculate) that for $\lambda \neq 0$, this estimator is biased and has a smaller variance than the OLS estimator

[Hoerl and Kennar, 1970; Tychonoff, 1943]

(Multi-)linear (ridge) regression algorithm

Computes: Weight matrix W for linear mapping of $\mathbb{R}^{d+1} \rightarrow \mathbb{R}^m$

Input: Data $\{(x_1, y_1), \dots, (x_n, y_n)\}$, $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}^m$, ridge λ
 Include offset parameters (row vector of n ones)

$$X = \begin{bmatrix} \mathbf{1} \\ X \end{bmatrix}$$

$$W = (XX^\top + \lambda I)^{-1}XY^\top$$

Output: W

Bias and variance of y_{test}

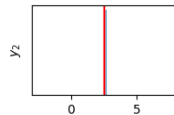
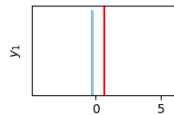
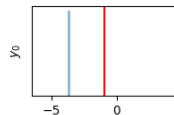
How do bias and variance of
predicted labels behave

→ Let's simulate

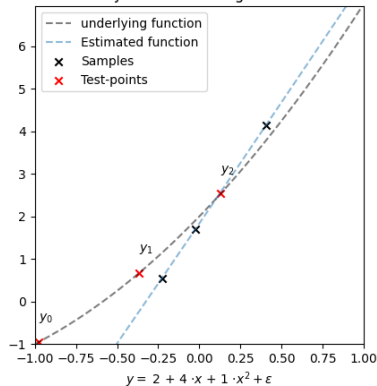
Bias and variance of y_{test}

How do bias and variance of predicted labels behave
→ Let's simulate

Estimates for test labels



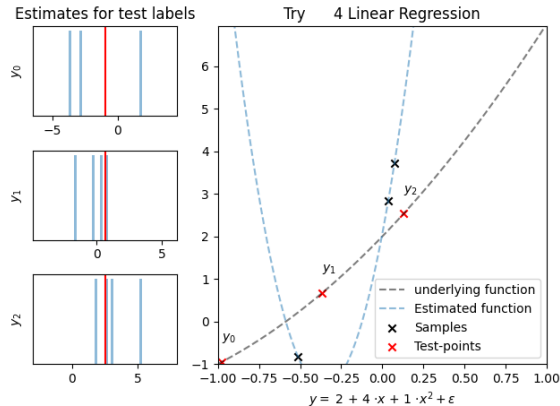
Try 1 Linear Regression



Bias and variance of y_{test}

How do bias and variance of predicted labels behave

→ Let's simulate

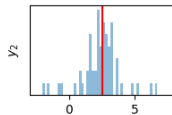
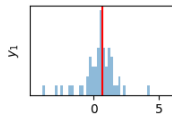
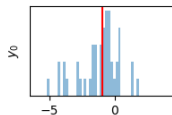


Bias and variance of y_{test}

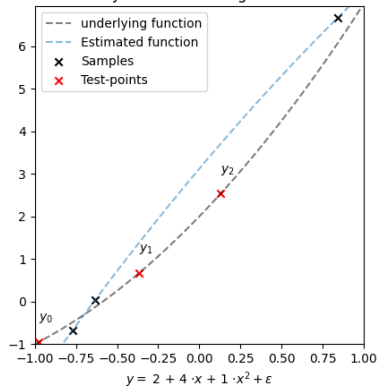
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Estimates for test labels



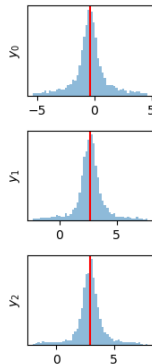
Try 64 Linear Regression



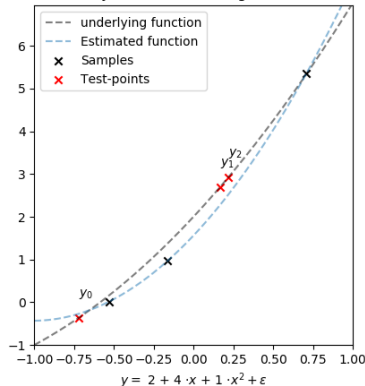
Bias and variance of y_{test}

How do bias and variance of predicted labels behave
→ Let's simulate

Estimates for test labels



Try 4096 Linear Regression



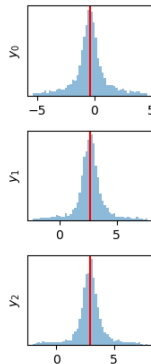
Bias and variance of y_{test}

How do bias and variance of predicted labels behave

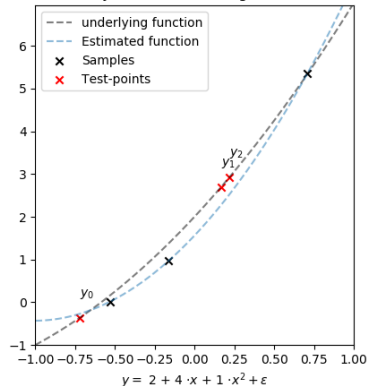
→ Let's simulate

For LR it looks unbiased (on average correct), but high variance

Estimates for test labels



Try 4096 Linear Regression



Bias and variance of y_{test}

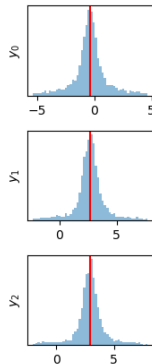
How do bias and variance of predicted labels behave

→ Let's simulate

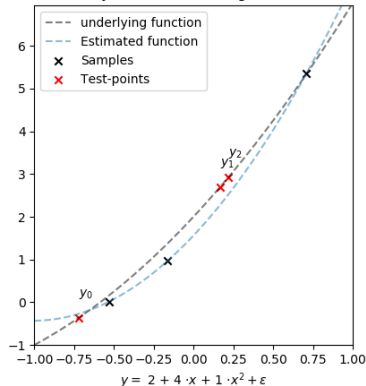
For LR it looks unbiased (on average correct), but high variance

Let's look at the effect of regularization

Estimates for test labels



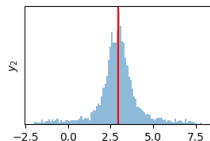
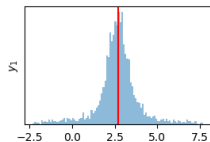
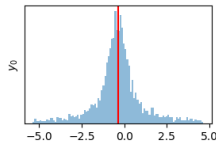
Try 4096 Linear Regression



Effect of λ on bias and variance

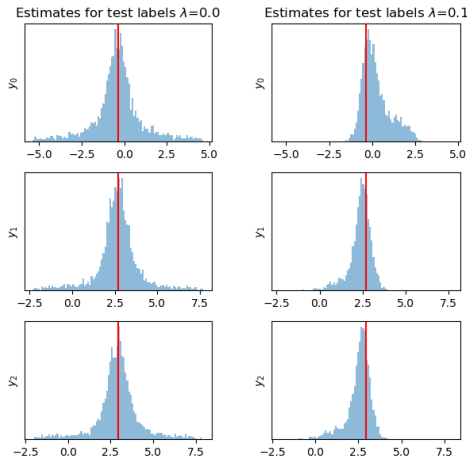
- For RR we see that estimates are biased, but less variance
- How can we choose optimal λ ?

Estimates for test labels $\lambda=0.0$



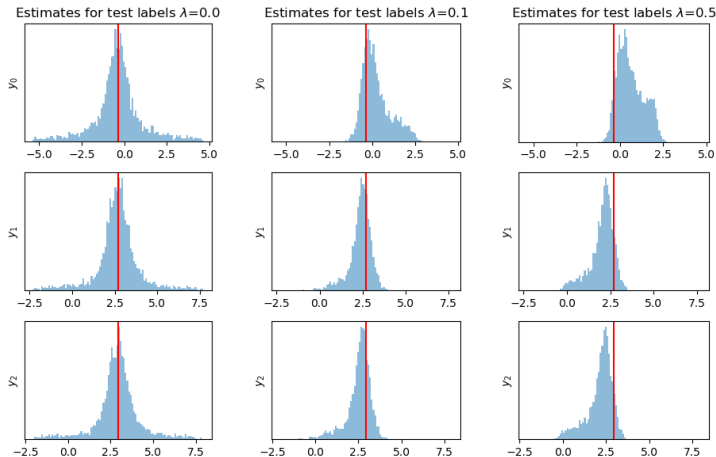
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Effect of λ on bias and variance

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Model selection

How can we find the best λ ?

Model selection

How can we find the best λ ?

One option: grid search

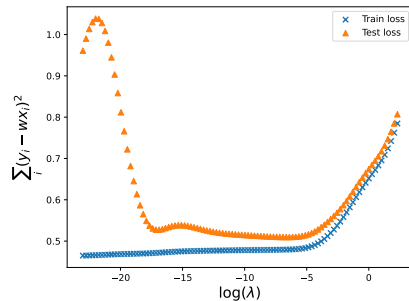
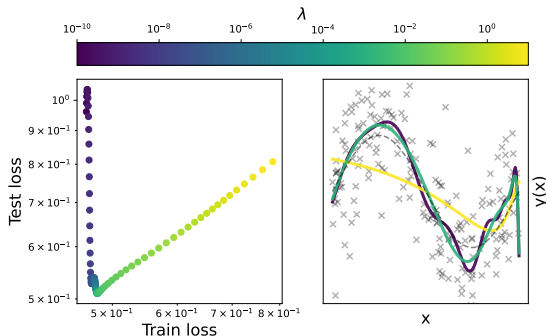
→ try out e.g. $\lambda \in \{0, 0.1, \dots, 0.9, 1.0\}$ and choose the one with the lowest error on test set

Model selection

How can we find the best λ ?

One option: grid search

→ try out e.g. $\lambda \in \{0, 0.1, \dots, 0.9, 1.0\}$ and choose the one with the lowest error on test set



What if we have a small data-set?

Standard approach

Split the data into train and test

$$\underbrace{[X_{i_1}, X_{i_2}, X_{i_3}, X_{i_4}]}_{\text{train}}, \underbrace{[X_{i_5}, X_{i_6}]}_{\text{test}}$$

Then

Train your model on the training data

Test your model on the test data

We are not using the full data-set

Test set could be sampled badly

What if we have a small data-set?

Standard approach

Split the data into train and test

$$\underbrace{[x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}]}_{\text{train}}, \underbrace{[x_{i_5}, x_{i_6}]}_{\text{test}}$$

Then

Train your model on the training data

Test your model on the test data

We are not using the full data-set

Test set could be sampled badly

Solution

k-fold Cross-Validation:

$$\text{fold 1 } \underbrace{[x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}]}_{\mathcal{F}_1^{\text{train}}}, \underbrace{[x_{i_5}, x_{i_6}]}_{\mathcal{F}_1^{\text{test}}}$$

$$\text{fold 2 } \underbrace{[x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}]}_{\mathcal{F}_2^{\text{test}}}, \underbrace{[x_{i_5}, x_{i_6}]}_{\mathcal{F}_2^{\text{train}}}$$

fold 3 ...

For each fold:

Train your model on the training data

Test your model on the test data

Cross-validation

Split data set in k different random **training** and **test** data

$$\text{fold 1 } [x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}, x_{i_5}, x_{i_6}]$$

$$\underbrace{\hspace{10em}}_{\mathcal{F}_1^{\text{train}}} \quad \underbrace{\hspace{10em}}_{\mathcal{F}_1^{\text{test}}}$$

$$\text{fold 2 } [x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}, x_{i_5}, x_{i_6}]$$

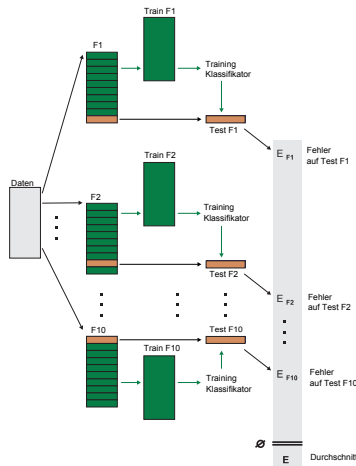
$$\underbrace{\hspace{10em}}_{\mathcal{F}_2^{\text{test}}} \quad \underbrace{\hspace{10em}}_{\mathcal{F}_2^{\text{train}}}$$

fold 3 ...

For each fold:

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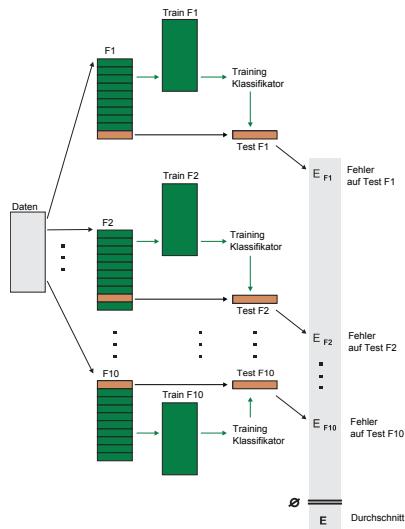


Cross-validation

Algorithm 1: Cross-Validation

Require: Data $(x_1, y_1) \dots, (x_N, y_N)$, Number of CV folds F

- 1: # Split data in F **disjunct** folds
- 2: **for** folds $f = 1, \dots, F$ **do**
- 3: # Train model on folds $\{1, \dots, F\} \setminus f$
- 4: # Compute prediction error on fold f
- 5: **end for**
- 6: # Average prediction error



Cross-validation: Can be used differently

Model Evaluation

"How well does my model perform?"

Report **mean evaluation score**

– e.g. accuracy – across folds

Model Selection

"What hyperparameter should I use?"

Do grid search on every fold.

Take parameter with the highest mean test score across folds

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After CV you still need to train your model on the whole data-set

Comparison of Supervised Algorithms

Algorithm	Solution	Assumption
NCC LDA	$w = Xy^T$ $w = S^{-1}Xy^T$	$y_t \in \left\{ \frac{1}{n_{+1}}, -\frac{1}{n_{-1}} \right\}$ NCC: Isotropic Normal distribution LDA: Equal within-class covariances, Multivariate Normal distribution
Linear Regression	$w = (XX^T)^{-1}Xy^T$	$y_i \in \mathbb{R}$ Gaussian Noise

Summary

Linear Regression

- is a generic framework for prediction
- straightforwardly extends to vector labels
- can model nonlinear dependencies between data and labels
- can be made more robust (Ridge Regression)

Cross-Validation

- Data-efficient method for model selection & model evaluation
- Only use if your bottleneck is data

References

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