Cognitive Algorithms
Lecture 3

Linear Regression

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Summary of last lecture

- Correlations between features can affect classification accuracy

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- 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 classifer
- 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 $\boldsymbol{x}_i \in \mathbb{R}^d$ 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

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

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

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

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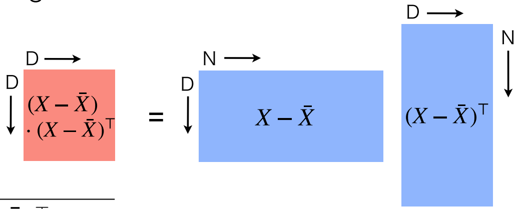

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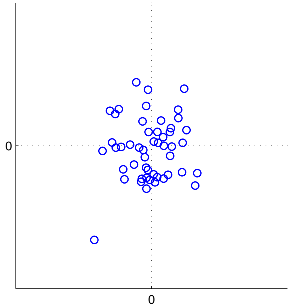
Correlated data and linear mappings

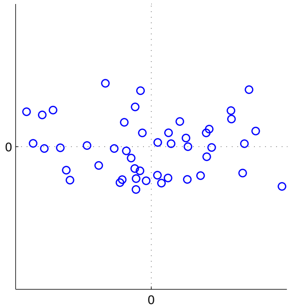
Uncorrelated



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

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

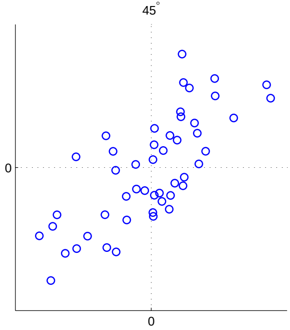
Uncorrelated, scaled



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

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

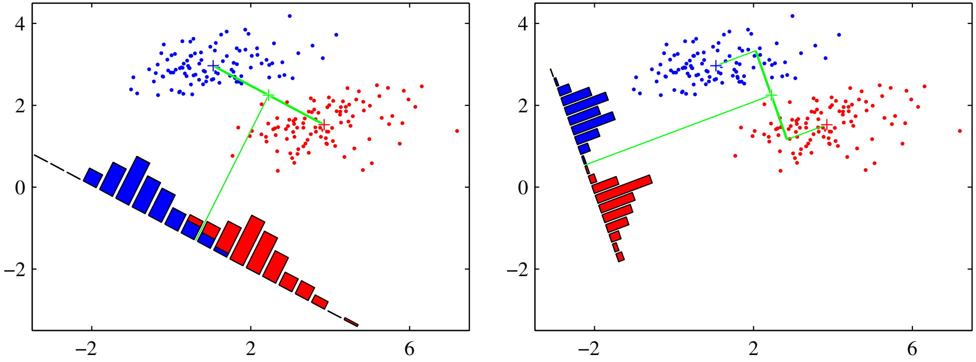
Scaled, rotated by 45°



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

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

Linear Discriminant Analysis (LDA)



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

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

Linear Discriminant Analysis (LDA)

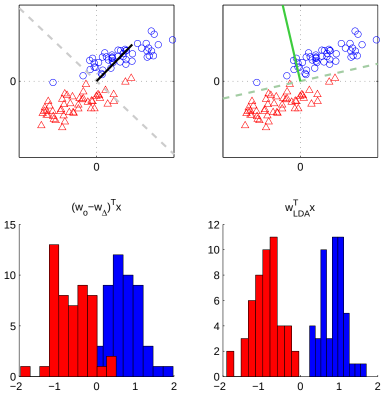
Optimization problem:

$$\underset{\boldsymbol{w}}{\operatorname{argmax}} \frac{\boldsymbol{w}^\top S_B \boldsymbol{w}}{\boldsymbol{w}^\top S_W \boldsymbol{w}}$$

Setting the gradient to zero we obtained:

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

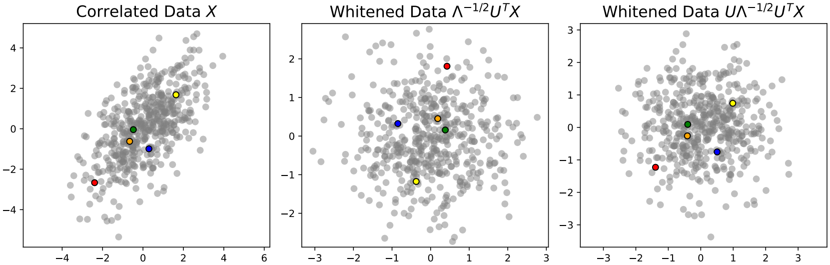
NCC vs. LDA



Whitening

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

$\rightarrow$ 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?

$\rightarrow$ **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

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

From classification to regression

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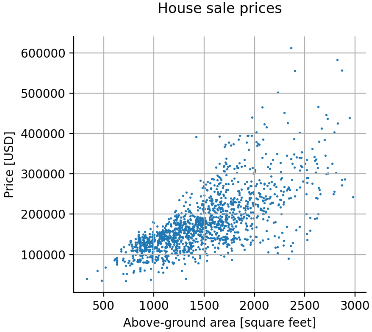
$y \in \{-1, +1\}$	$y \in \mathbb{R}$
Classification	**Regression**

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



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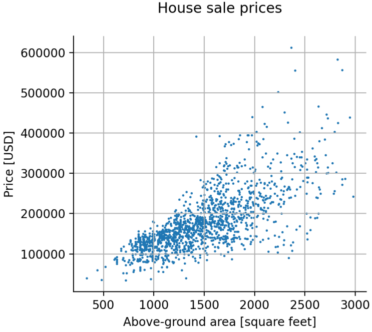

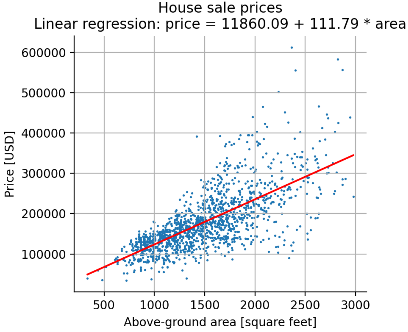

How to find the regression line?

(data from kaggle, a great data science platform
`https://www.kaggle.com/competitions/house-prices-advanced-regression-techniques/`)

Simple linear regression

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

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

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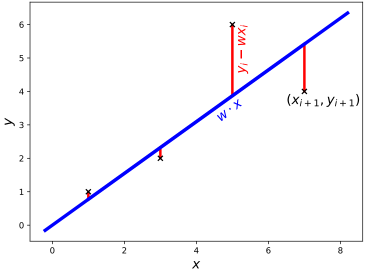
We will first focus on a simpler version without intercept $f(x) = w \cdot x$.
Approach: Minimize the **squared error** to find the w



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

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

Least-squares error: general case

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

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

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

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

C.F. Gauß (1777–1855)

A.M. Legendre (1752–1833)

Supplementary: optimality of LSE when assuming Gaussian noise

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

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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$$\begin{aligned} \underset{w}{\operatorname{argmax}}\, p(y|w) &= \underset{w}{\operatorname{argmax}} \log p(y|w) \\ &= \underset{w}{\operatorname{argmax}} \left(- \underbrace{(y - w \cdot x)^2}_{\text{Least-squares error}} \right) \end{aligned}$$

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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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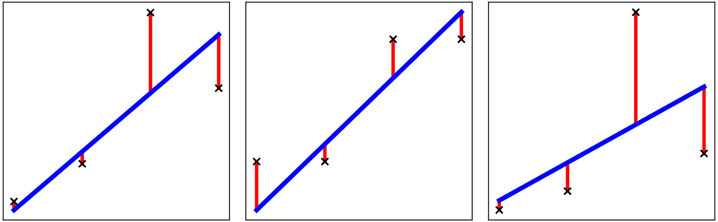
$$\implies w = \frac{\sum_{i=1}^{n} x_i y_i}{\sum_{i=1}^{n} x_i x_i}$$

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 $\boldsymbol{y} \in \mathbb{R}^{1\times n}$ and $X \in \mathbb{R}^{d\times n}$.
The prediction $\hat{y}$ of our Linear Regression model then becomes

$$\boldsymbol{y} \approx \hat{\boldsymbol{y}} = \boldsymbol{w}^\top X.$$

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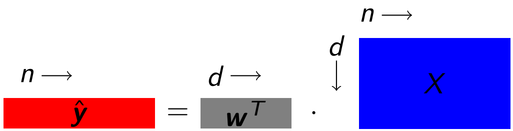
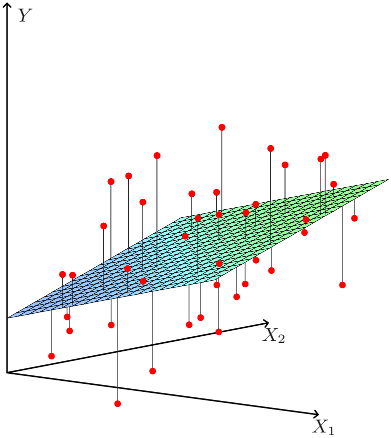


The goal is still to find $\boldsymbol{w}$ that minimizes the least-squares error.

Linear regression

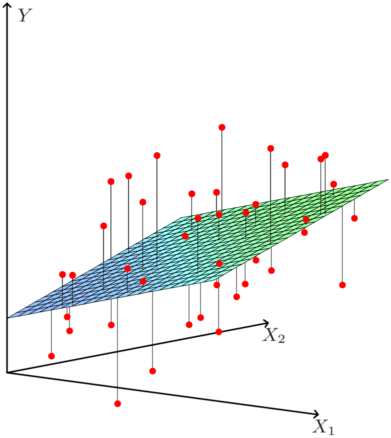


$$\hat{y} = w_1 \cdot x_1 + w_2 \cdot x_2$$

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

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

Linear regression with basis functions



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

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

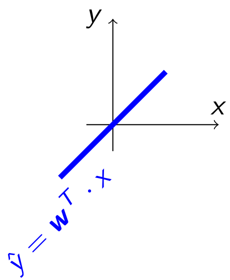
where $\phi(\boldsymbol{x}) = (\phi_1(\boldsymbol{x}), \ldots \phi_{\tilde{d}}(\boldsymbol{x}))$ denotes a vector of (possibly non-linear) *basis functions*.

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

Intercept term

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

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



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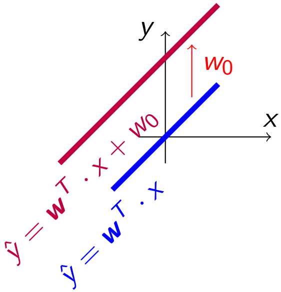

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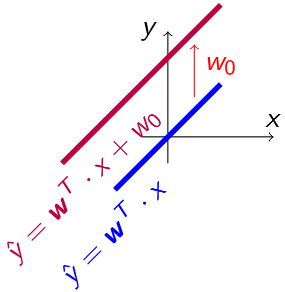
$$= \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_d \end{bmatrix}^T \cdot \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_d \end{bmatrix}$$



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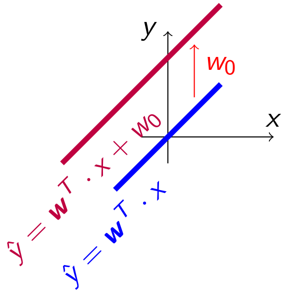
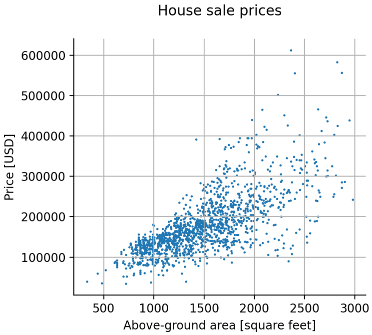
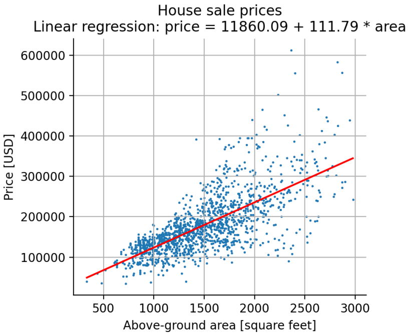


This unifies the notation. Basis function: $\phi([x_1, x_2, \ldots, x_d]^T) = [1, x_1, x_2, \ldots, x_d]^T$

Back to initial example





Now you know how to calculate the regression line.

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

Polynomials as an example for $\phi(\boldsymbol{x})$:

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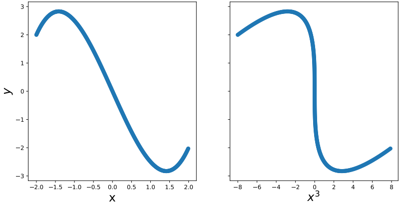

$\hat{y}$ as a function of x and x^3

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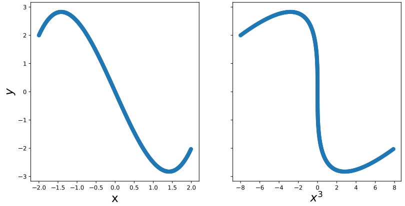

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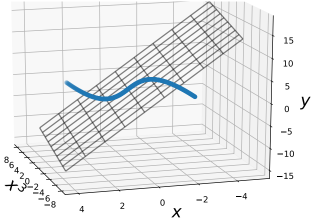

$\hat{y}$ lies on a plane in x, x^3 space

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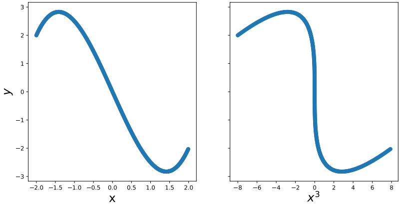
We can use non-linear basis functions to apply linear regression in higher-dimensional space and predict a non-linear function!



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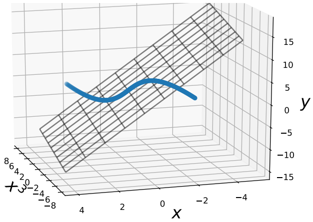

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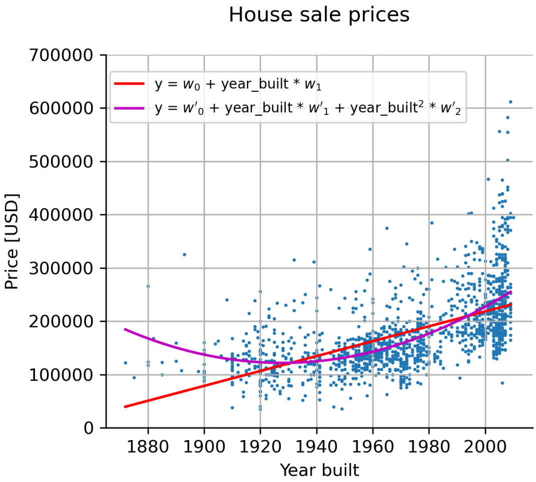
Example with non-linear basis functions



Linear regression: minimizing LSE

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

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

We compute derivative w.r.t. $\boldsymbol{w}$

Linear regression: minimizing LSE

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

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

We compute derivative w.r.t. $\boldsymbol{w}$

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

set it to zero and solve for $\boldsymbol{w}$

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set it to zero and solve for $\boldsymbol{w}$

$$
\begin{aligned}
-2X\boldsymbol{y}^\top + 2XX^\top \boldsymbol{w} &= 0 \\
XX^\top \boldsymbol{w} &= X\boldsymbol{y}^\top \\
\boldsymbol{w} &= (XX^\top)^{-1} X y^\top \qquad (2)
\end{aligned}
$$

Does correlation influence the performance of linear regression?

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

$$\begin{aligned} \mathbf{z} &\mapsto \mathbf{w}^T \cdot \mathbf{z} \\ \boldsymbol{w} &= (XX^\top)^{-1} Xy^\top \end{aligned}$$

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

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

$\Rightarrow$ LR is not susceptible to correlation in the features (different from NCC!)

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

$$Y = W^\top X$$

where $W^\top \in \mathbb{R}^{m \times d}$ 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

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

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

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

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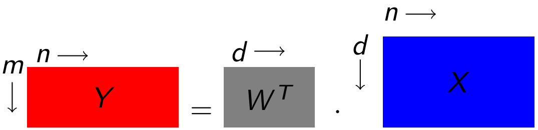

Application example: myoelectric control of prostheses

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

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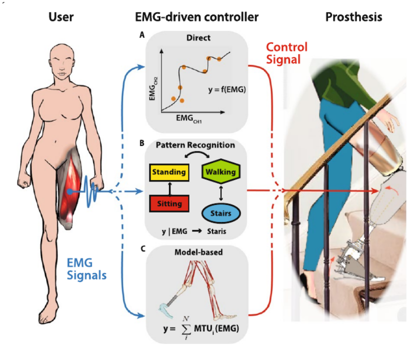

Cimolato et al. [2022]

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

hand prosthesis
Only 2 degrees of freedom are controlled
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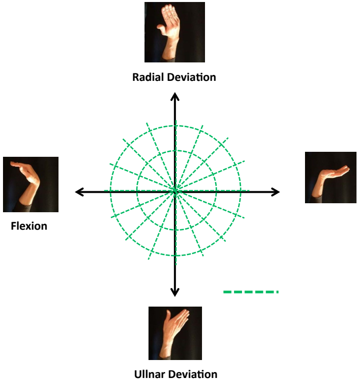
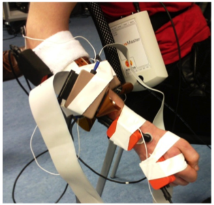
Controlled by muscle activity

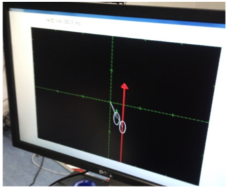
Acquisition of training data



Experimental Paradigm

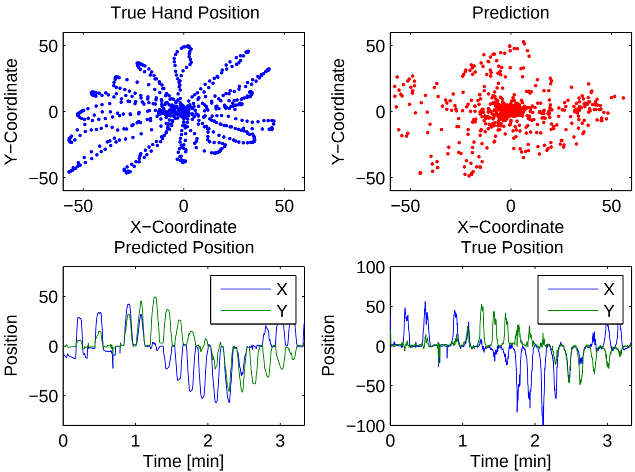


Motion Capture System

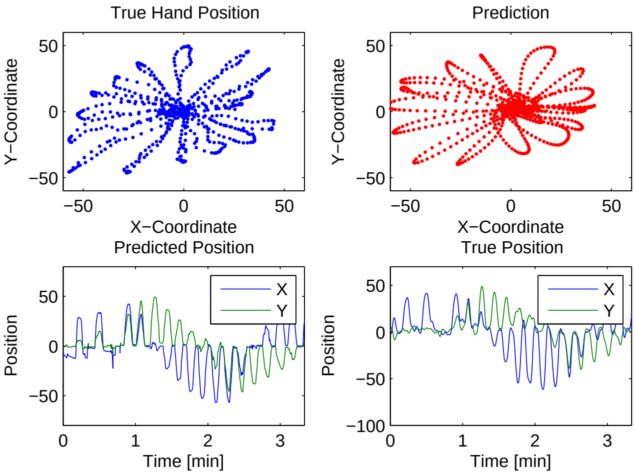


Visual Feedback

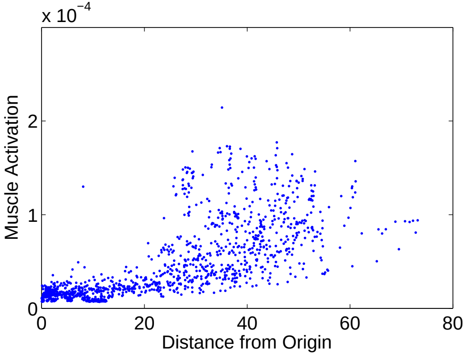
Results from linear regression



Results linear regression - smoothed



Linear regression



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

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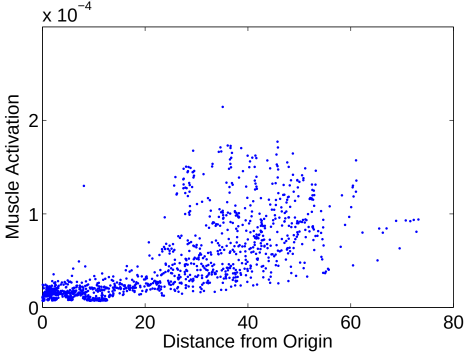

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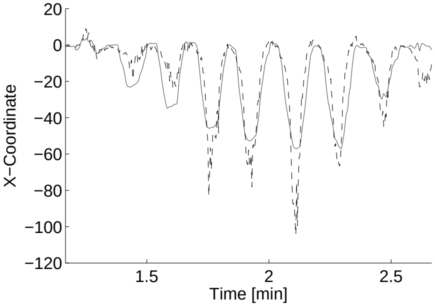
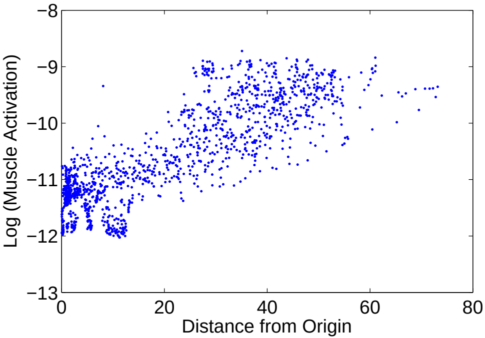


Weak muscle activation
→ True hand position (gray) **under**estimated (dashed)

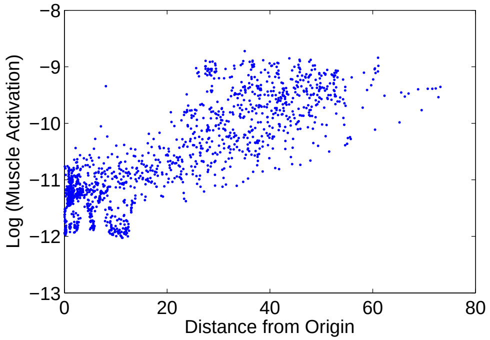
Strong muscle activation
→ True hand position **over**estimated

Linear(ized) Regression



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

Linear(ized) Regression



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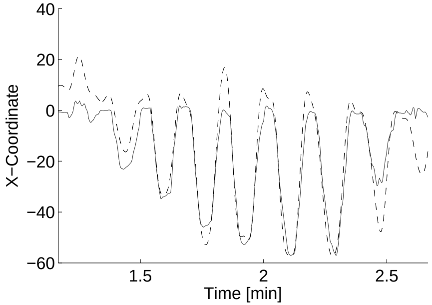
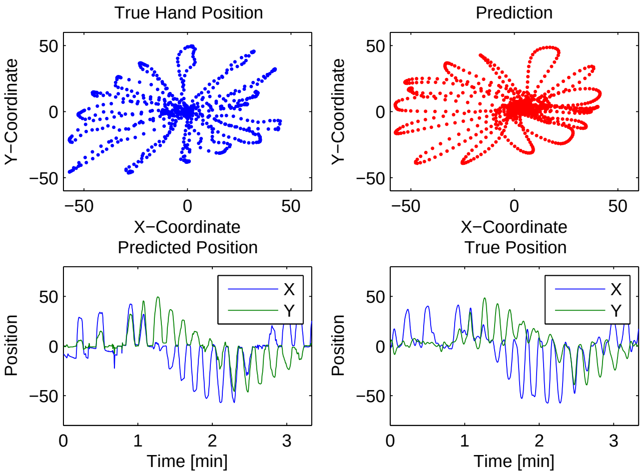


Strong muscle activation
→ hand position *less* **over**estimated

Results linear regression - smoothed and log features



The statistical model of linear regression

Linear Model:

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

Linear Regression: estimates

$$\hat{\boldsymbol{w}} = (XX^\top)^{-1}Xy$$

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.

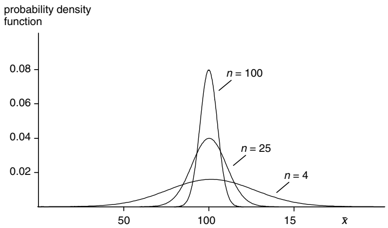
Ω is the sample space, the set of all possible outcomes.

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



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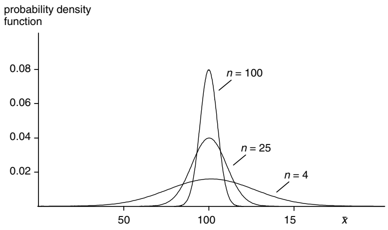


Consider random variables $x_i \sim \mathcal{N}(\mu, \sigma^2)$ independent, identically distributed (i.i.d.).

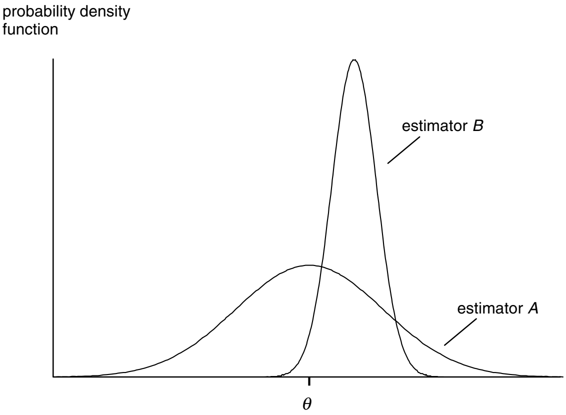
Draw n data points and *estimate* mean on n data points:

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

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

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

Desirable properties of estimators



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

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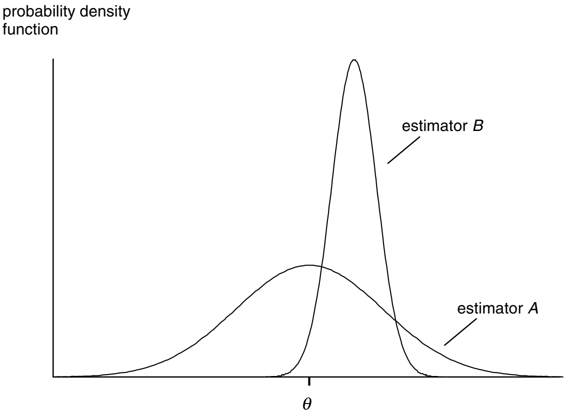

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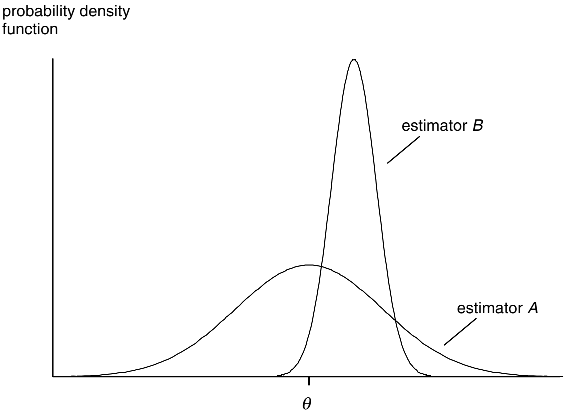

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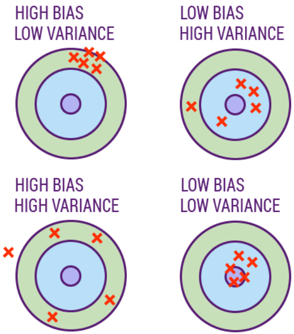
Small estimator variance (B has a smaller variance than A)

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

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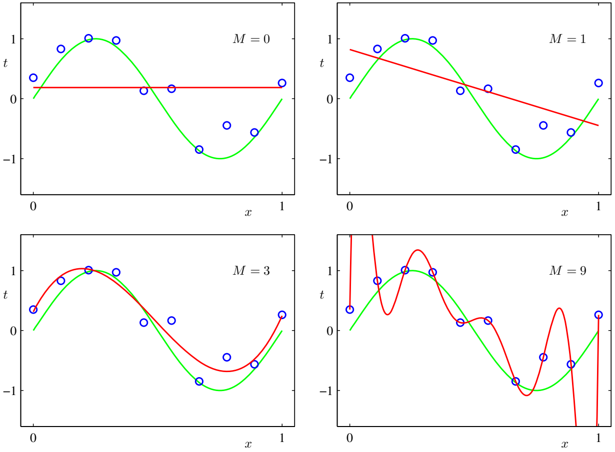
But: in some cases biased estimators with lower variance might be more suitable.

Example: polynomial regression

$$\phi_M(x) = [x^0, x^1, ..., x^M]^T$$
$$\hat{y} = \boldsymbol{w}^T \phi_M(x)$$



Example: polynomial regression

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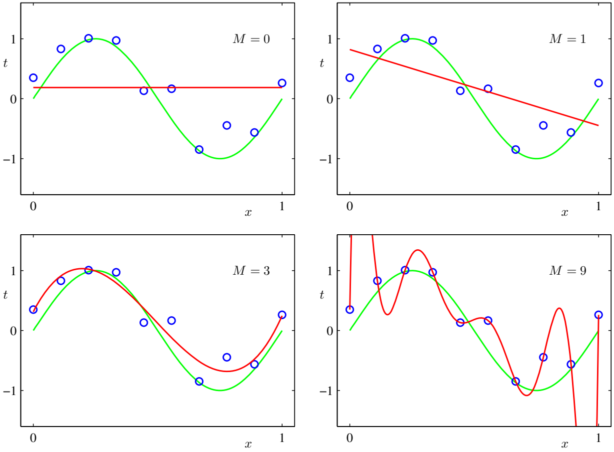
$$\hat{y} = \boldsymbol{w}^T \phi_M(x)$$

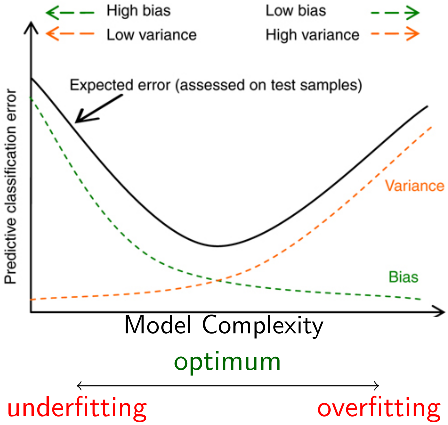
Weights:

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



[Bishop, 2007]

The bias-variance trade-off



Careful. . .

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

- $\boldsymbol{w}^\top \boldsymbol{x} + b$, $w \cdot x + b$
- 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 $\boldsymbol{w}$.

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

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

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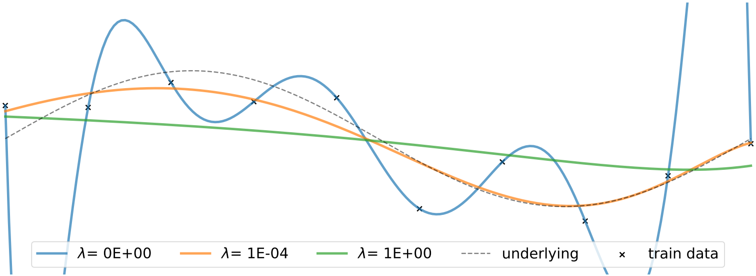

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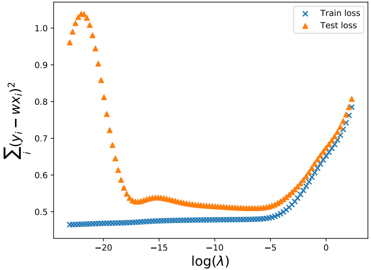

Ridge regression

Computing the derivative with respect to $\boldsymbol{w}$ yields

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

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

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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 $\mathbb{R}^{d+1} \to \mathbb{R}^m$

Input: Data $\{(x_1, y_1), \ldots, (x_n, y_n)\}, x_i \in \mathbb{R}^d,\ y_i \in \mathbb{R}^m$, ridge λ

Include offset parameters (row vector of n ones)

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

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

Output: W

Bias and variance of y_{test}

How do bias and variance of predicted labels behave
$\rightarrow$ Let's simulate

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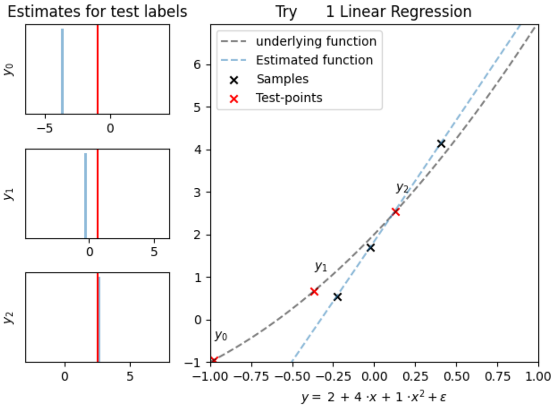

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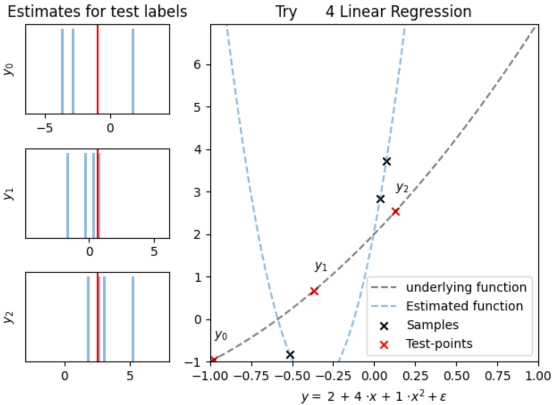

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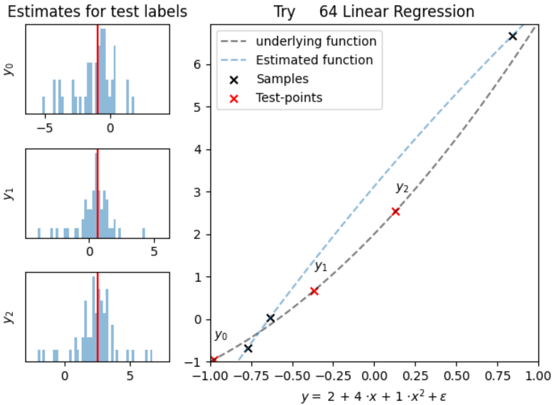

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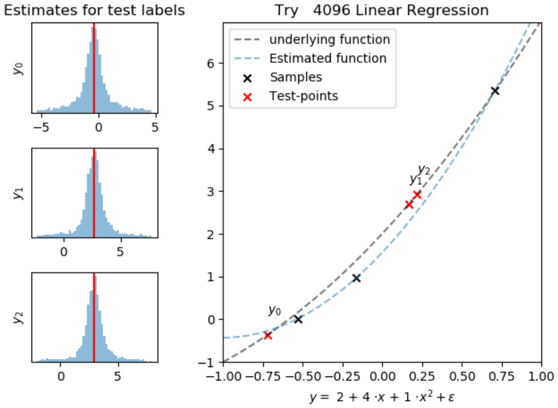

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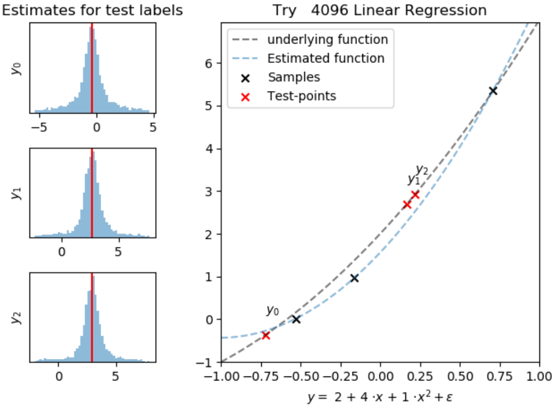
For LR it looks unbiased (on average correct), but high variance



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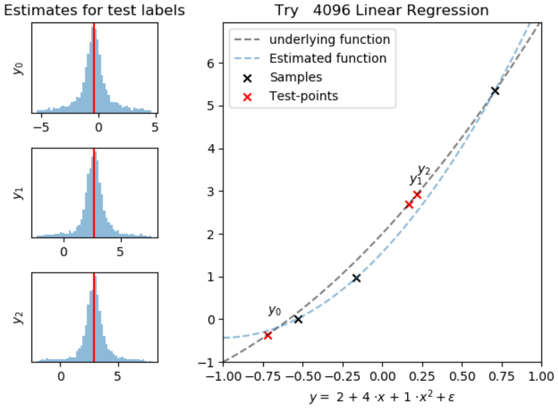
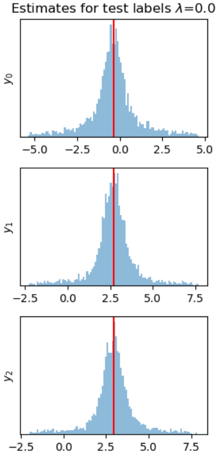
For LR it looks unbiased (on average correct), but high variance
Let's look at the effect of regularization



Effect of λ on bias and variance

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



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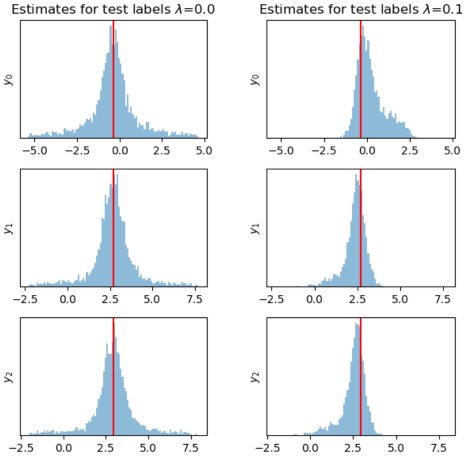

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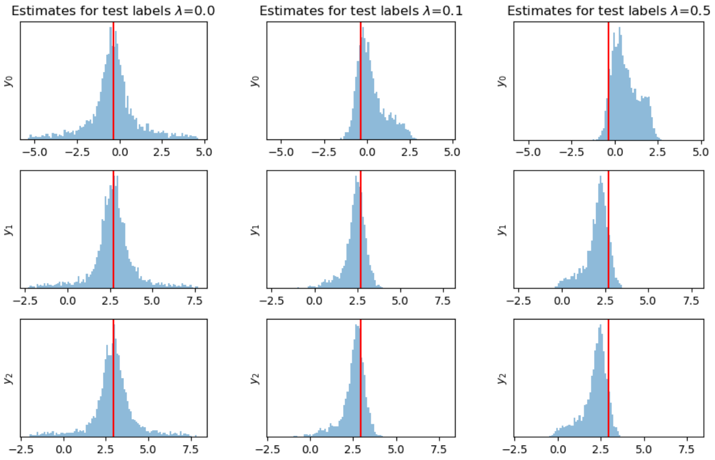

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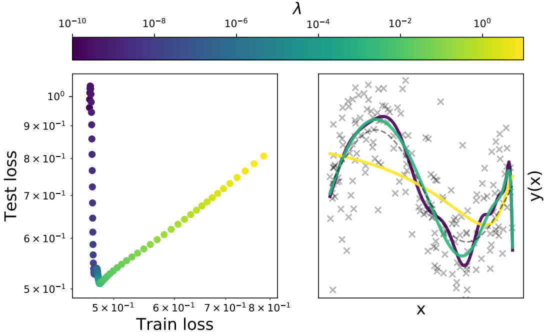
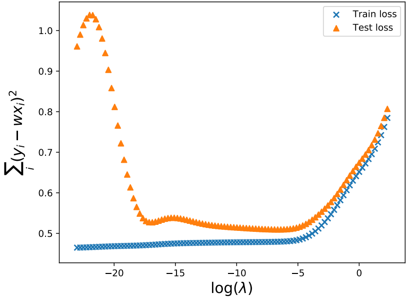




What if we have a small data-set?

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:

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

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

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

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

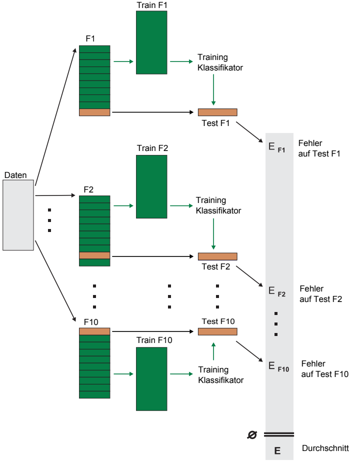
$$\text{fold 2 } [\underbrace{x_{i_1}, x_{i_2}}_{\mathcal{F}_2^{\text{test}}}, \underbrace{x_{i_3}, x_{i_4}, x_{i_5}, x_{i_6}}_{\mathcal{F}_2^{\text{train}}}]$$

fold 3 ...

For each fold:

Train your model on the training data

Test your model on the test data

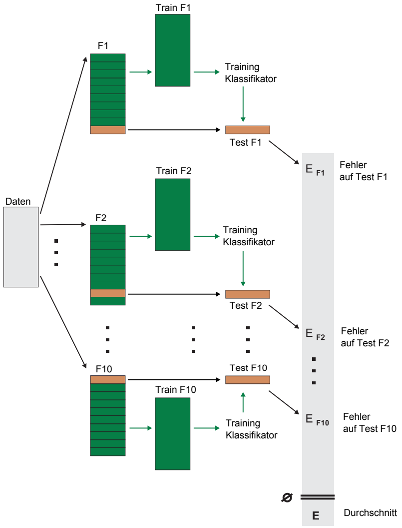


Cross-validation

Algorithm 1: Cross-Validation

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

# Split data in F **disjunct** folds
for folds $f = 1,\ldots,F$ **do**
    # Train model on folds $\{1,\ldots,F\} \setminus f$
    # Compute prediction error on fold f
end for
# 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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If we did both on the same test fold:

We would be too optimistic because we use same test set for optimizing and evaluating

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- If we did both on the same test fold:
  - We would be too optimistic because we use same test set for optimizing and evaluating

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	$w = (XX^\top)^{-1}Xy^\top$	$y_i \in \mathbb{R}$ 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

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