# Cognitive Algorithms Lecture 3

#### Linear Regression

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### Summary of last lecture

Recap

- 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

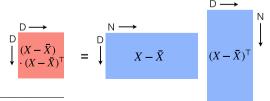
Given n data points  $\mathbf{x}_i \in \mathbb{R}^d$  in a data matrix  $X \in \mathbb{R}^{d \times n}$ the empirical estimate of the covariance matrix is defined as

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

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

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

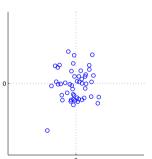
The diagonal entries of  $\hat{\Sigma}$  are estimates of the variance.



### Correlated data and linear mappings

#### Uncorrelated

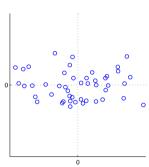
Recap



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

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

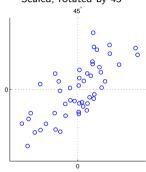
#### Uncorrelated, scaled



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

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

#### Scaled, rotated by $45^{\circ}$

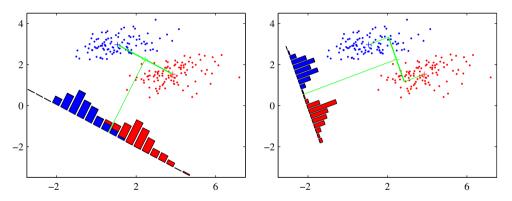


$$\begin{bmatrix} \cos(\phi) & -\sin(\phi) \\ \sin(\phi) & \cos(\phi) \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} X$$

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

# Linear Discriminant Analysis (LDA)

Recap



**Goal:** Find a (normal vector of a linear decision boundary) **w** that

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

Recap 00000000

## Linear Discriminant Analysis (LDA)

Optimization problem:

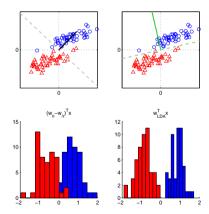
$$\underset{\boldsymbol{w}}{\operatorname{argmax}} \frac{\boldsymbol{w}^{\top} S_{B} \boldsymbol{w}}{\boldsymbol{w}^{\top} S_{W} \boldsymbol{w}}$$

Setting the gradient to zero we obtained:

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

### NCC vs. LDA

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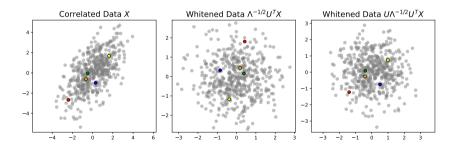


#### Whitening

Recap

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

→ Data are decorrelated after whitening



Recap

#### 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  $\mathbb{R}$ ?

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





#### How to find the regression line?

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

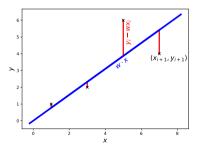
### Simple linear regression

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

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

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

Linear Regression

Given data  $(x_1, y_1), ..., (x_n, y_n)$  with  $x_i \in \mathbb{R}^d$ ,  $y_i \in \mathbb{R}$  the goal is to find a weight vector  $\mathbf{w} \in \mathbb{R}^d$  to predict y for a new x via

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

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

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







A.M. Legendre (1752–1833)

#### Supplementary: optimality of LSE when assuming Gaussian noise

Linear Regression 

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

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

$$\underset{w}{\operatorname{argmax}} p(y|w) = \underset{w}{\operatorname{argmax}} \log p(y|w)$$

$$= \underset{w}{\operatorname{argmax}} \left( -\underbrace{(y - w \cdot x)^2}_{\text{least source error}} \right)$$

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

Linear Regression

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

Compute the derivative w.r.t. w

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

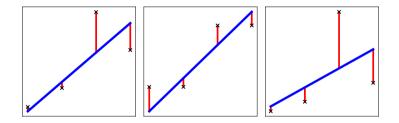
Set to zero and solve for w:

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

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

#### 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

Linear Regression 000000000000000000

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

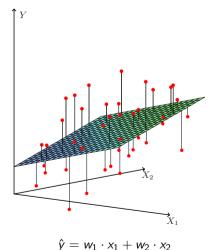
> Let *n* be the number of samples, so  $\mathbf{y} \in \mathbb{R}^{1 \times n}$  and  $X \in \mathbb{R}^{d \times n}$ . The prediction  $\hat{y}$  of our Linear Regression model then becomes

> > $\mathbf{v} \approx \hat{\mathbf{v}} = \mathbf{w}^{\top} X$ .

The goal is still to find **w** that minimizes the least-squares error.

### Linear regression

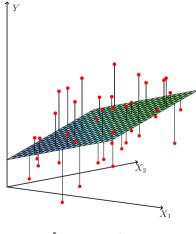
Linear Regression



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

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

### Linear regression with basis functions



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

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

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

where  $\phi(\mathbf{x}) = (\phi_1(\mathbf{x}), ... \phi_{\tilde{d}}(\mathbf{x}))$  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.

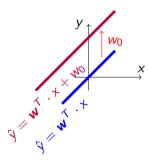
#### Intercept term

Linear Regression 000000000000000000

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

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

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



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

### Back to initial example

Linear Regression





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/

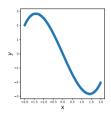
# Linear Regression: non-linear $\phi(\mathbf{x})$

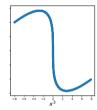
Polynomials as an example for  $\phi(\mathbf{x})$ :

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

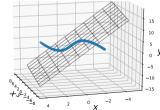
Here 
$$\phi(x) = \begin{bmatrix} x^3 \\ x \end{bmatrix}$$
 and  $\mathbf{w} = \begin{bmatrix} 0.5 \\ -3 \end{bmatrix}$ 

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





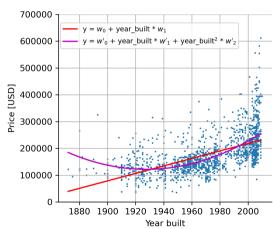
 $\hat{y}$  as a function of x and  $x^3$ 



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

#### Example with non-linear basis functions

#### House sale prices



### Linear regression: minimizing LSE

Linear Regression

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

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

$$= \|\mathbf{y} - \mathbf{w}^{\top} X\|^2$$

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

We compute derivative w.r.t. 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 w

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

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

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

Linear Regression

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

$$\mathbf{z} \mapsto \mathbf{w}^T \cdot \mathbf{z}$$
 $\mathbf{w} = (XX^T)^{-1}Xy^T$ 

We can decompose:

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

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

Linear Regression

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

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

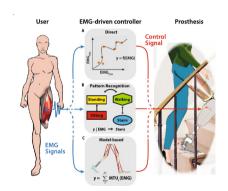
where  $||A||_F = \sqrt{\sum_i^n \sum_j^d A_{ij}^2}$  denotes the Frobenius norm and  $W^{ op} \in \mathbb{R}^{m imes d}$ 

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

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



#### Application example: myoelectric control of prostheses

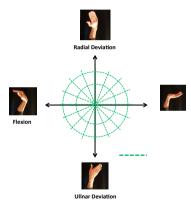


Cimolato et al. [2022] Neurons activate muscles via electric discharges Electric activity can be measured non-invasively

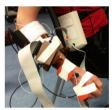


hand prosthesis Only 2 degrees of freedom are controlled (open/close, rotate) Controlled by muscle activity

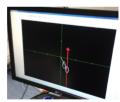
### Acquisition of training data



Experimental Paradigm

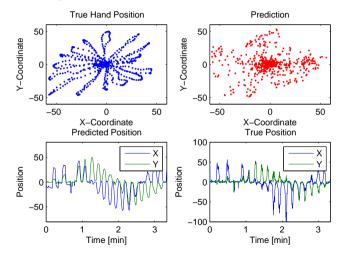


Motion Capture System

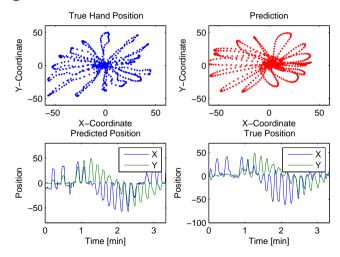


Visual Feedback

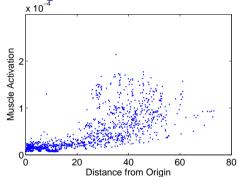
#### Results from linear regression



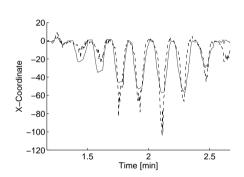
#### Results linear regression - smoothed



# Linear regression



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



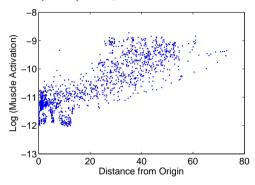
Weak muscle activation

→ True hand position (gray) underestimated (dashed)

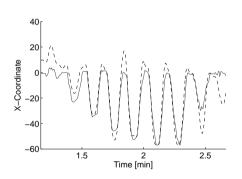
Strong muscle activation

→ True hand position overestimated

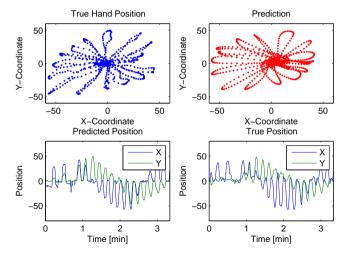
# Linear(ized) Regression



Hand position is almost linearly related to log of muscle activation



Strong muscle activation  $\rightarrow$  hand position *less* **over**estimated



#### The statistical model of linear regression

Linear Model:

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

Linear Regression: estimates

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

from given data X, y.

# Random variable (recap)

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

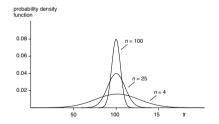
 $\Omega$  is the sample space, the set of all possible outcomes.

Example: tossing a coin

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

## 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.).

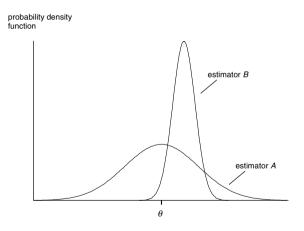
Draw n data points and estimate mean on n data points:

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

 $\hat{\mu}$  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

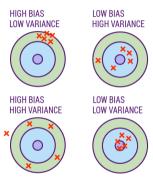


**Unbiased** The estimator's expected value is the true value of the parameter being estimated (*A* in the Fig.)

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

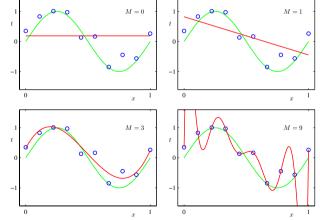
But: in some cases biased estimators with lower variance might be more suitable.

## Example: polynomial regression

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

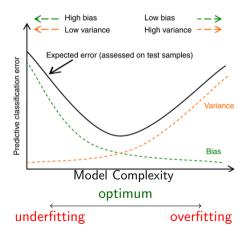
## Weights:

	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

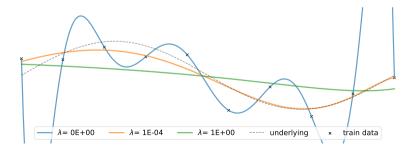
- $\mathbf{w}^{\top}\mathbf{x} + b$ .  $\mathbf{w} \cdot \mathbf{x} + \mathbf{b}$
- Bias/variance of an estimator
- Bias/variance of a general ML model

## Ridge regression

Often it is important to **control the complexity** of the solution w.

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

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



Ridge regression 00000000000000

## Ridge regression

Computing the derivative with respect to **w** yields

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

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

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

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

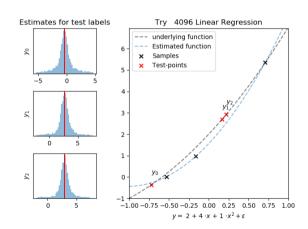
[Hoerl and Kennar, 1970; Tychonoff, 1943]

# (Multi-)linear (ridge) regression algorithm

Computes: Weight matrix W for linear mapping of  $\mathbb{R}^{d+1} \to \mathbb{R}^m$  Input: Data  $\{(x_1,y_1),\dots,(x_n,y_n)\}, x_i \in \mathbb{R}^d, \ y_i \in \mathbb{R}^m, \ \text{ridge } \lambda$  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

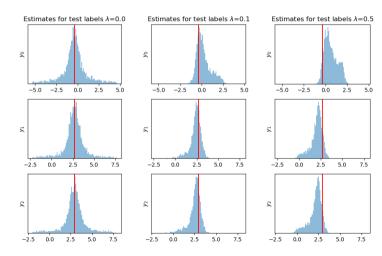
## Bias and variance of $y_{test}$

How do bias and variance of predicted labels behave → Let's simulate
For LR it looks unbiased (on average correct), but high variance Let's look at the effect of regularization



#### Effect of $\lambda$ on bias and variance

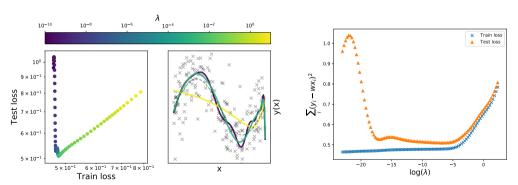
- For RR we see that estimates are biased, but less variance
- How can we choose optimal λ?



#### Model selection

# How can we find the best $\lambda$ ? One option: grid search

ightarrow try out e.g.  $\lambda \in \{0,0.1,...,0.9,1.0\}$  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

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

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:

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

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

fold 3 . . .

For each fold:

**Train** your model on the training data **Test** your model on the test data

#### Cross-validation

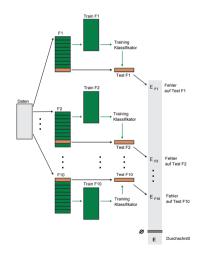
Split data set in k different random training and test data

$$\begin{array}{c} \text{fold 1} \ \underbrace{\left[\underbrace{x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}}_{\mathcal{F}_1^{\text{train}}}, \underbrace{x_{i_5}, x_{i_6}}_{\mathcal{F}_1^{\text{test}}}\right]}_{\mathcal{F}_2^{\text{test}}} \\ \text{fold 2} \ \underbrace{\left[\underbrace{x_{i_1}, x_{i_2}, x_{i_3}, x_{i_4}, x_{i_5}, x_{i_6}}_{\mathcal{F}_2^{\text{train}}}\right]}_{\mathcal{F}_2^{\text{train}}} \end{array}$$

fold 3 ...

For each fold:

**Train** your model on the training data **Test** your model on the test data

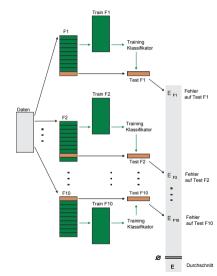


## Cross-validation

#### **Algorithm 1:** Cross-Validation

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

- 1: # Split data in F disjunct folds
- 2: for folds  $f = 1, \ldots, F$  do
- 3: # Train model on folds  $\{1, \ldots, F\} \setminus f$
- 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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You can't do both at the same time with simple cross-validation! 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	$w = Xy^T$ $w = S^{-1}Xy^T$	$y_t \in \left\{ rac{1}{n_{+1}}, -rac{1}{n_{-1}}  ight\}$ 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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