

# Machine Learning for Networks: Regression (continued) and Classification

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# Regression (continued)

- Polynomial Regression
- Variance vs. Bias Trade-Off
- Regularization
- Scaling
- Feature Selection

# Classification

- Logistic Regression
- Classification Performance
- Class imbalance

## Section 1

# **Polynomial Regression and hyper-parameter tuning**

# Univariate Polynomial Regressions

3 / 42

- A univariate polynomial regression of degree  $p$  is

$$h_{\theta}(x) = \theta_0 + \theta_1 \cdot x + \theta_2 \cdot x^2 + \dots + \theta_p \cdot x^p$$

- $p = 1$ : linear
- $p = 2$ : quadratic
- $p = 3$ : cubic
- $\dots$
- Equivalent to linear regression with features

$$x, x^2, \dots, x^p$$

- $p$  is a *hyper-parameter*: parameter of the learning algorithm.
- How to choose  $p$ ?

# Multi-variate polynomial regression

4 / 42

- With  $j = 1 \dots N$  features, all terms of degree 2 are included:

$$\begin{aligned} h_{\theta}(\mathbf{x}) = & \theta_0 + \theta_1 \cdot x_1 + \cdots + \theta_N \cdot x_N \\ & + \theta_{N+1} \cdot x_1^2 + \cdots + \theta_{N+N} \cdot x_N^2 \\ & + \theta_{1,2} \cdot x_1 x_2 + \theta_{1,3} \cdot x_1 x_3 + \cdots + \theta_{1,N} \cdot x_1 x_N \\ & + \theta_{2,3} \cdot x_2 x_3 + \theta_{2,4} \cdot x_2 x_4 + \dots \end{aligned}$$

- A pol. regression of degree  $p$  includes the following terms:
  - Bias term

$$\theta_0$$

- Powers of features

$$x_j^k \quad k = 1, \dots, p$$

- Mixed terms of power 2:

$$x_j \cdot x_{j'} \quad j' > j$$

- Mixed terms of power 3

$$x_j \cdot x_{j'} \cdot x_{j''} \quad j'' > j' > j$$

- ...

- Mixed terms of power  $p$

# Hyper-parameter tuning

5 / 42

BufferHealth	BufferProgress	BufferValid	label	label_num
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5 / 42

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{ TRAINING SET }

{ TEST SET }

- Divide training and test sets

# Hyper-parameter tuning

5 / 42

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5 / 42

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  - Construct a model with such values
  - Compute cross-validation error

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5 / 42

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5 / 42

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  - Construct a model with such values
  - Compute cross-validation error
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- Train the selected model on the training set
- Test error on the test set

# Hyper-parameter tuning

5 / 42

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We have only used the training set to select the best parameter

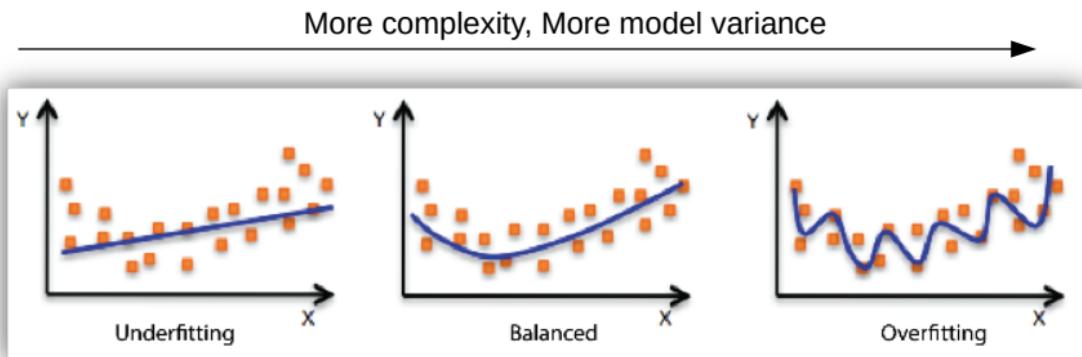


Go to notebook

03.regression\_contd-and-classification/a.polynomial-regression.ipynb

# Complexity and Variance

7 / 42



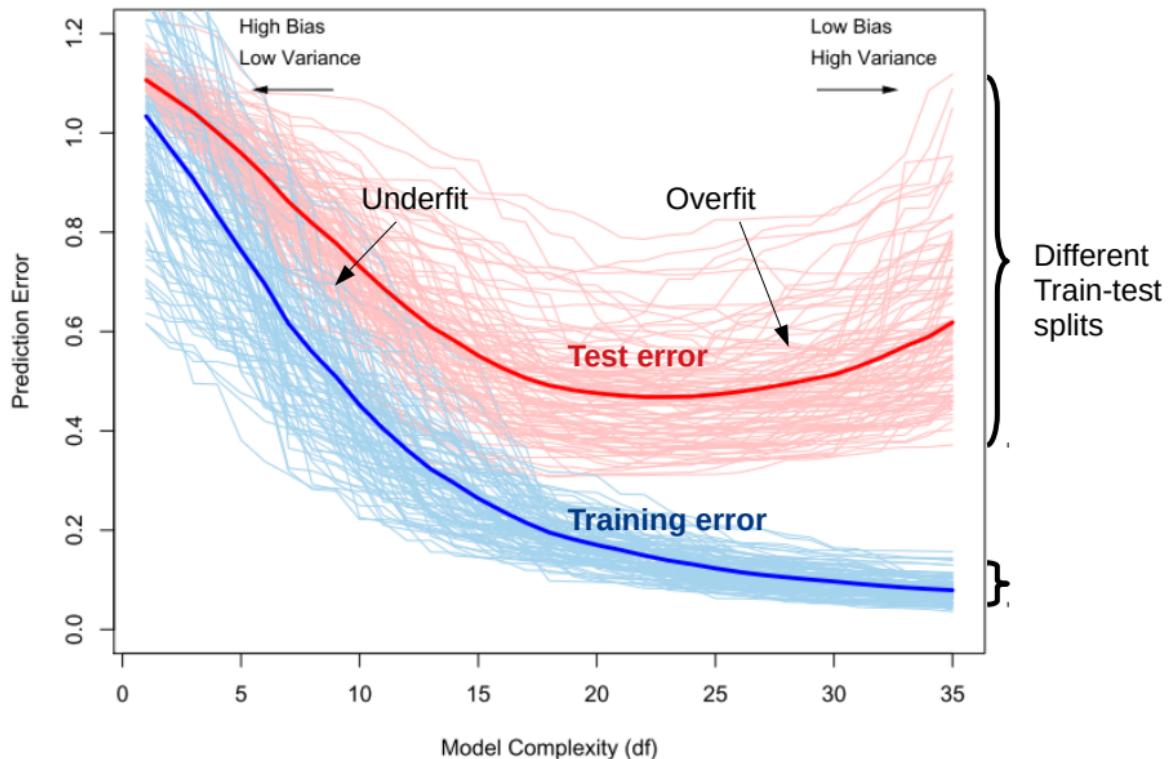
Example of polynomial regression with degree 1 (linear), and then higher degrees

Image from [[AWS](#)].

# Complexity and Variance

7 / 42

Higher  $p \Rightarrow$  higher complexity  $\Rightarrow$  higher variance  
(the model adapts too flexibly to the training data)

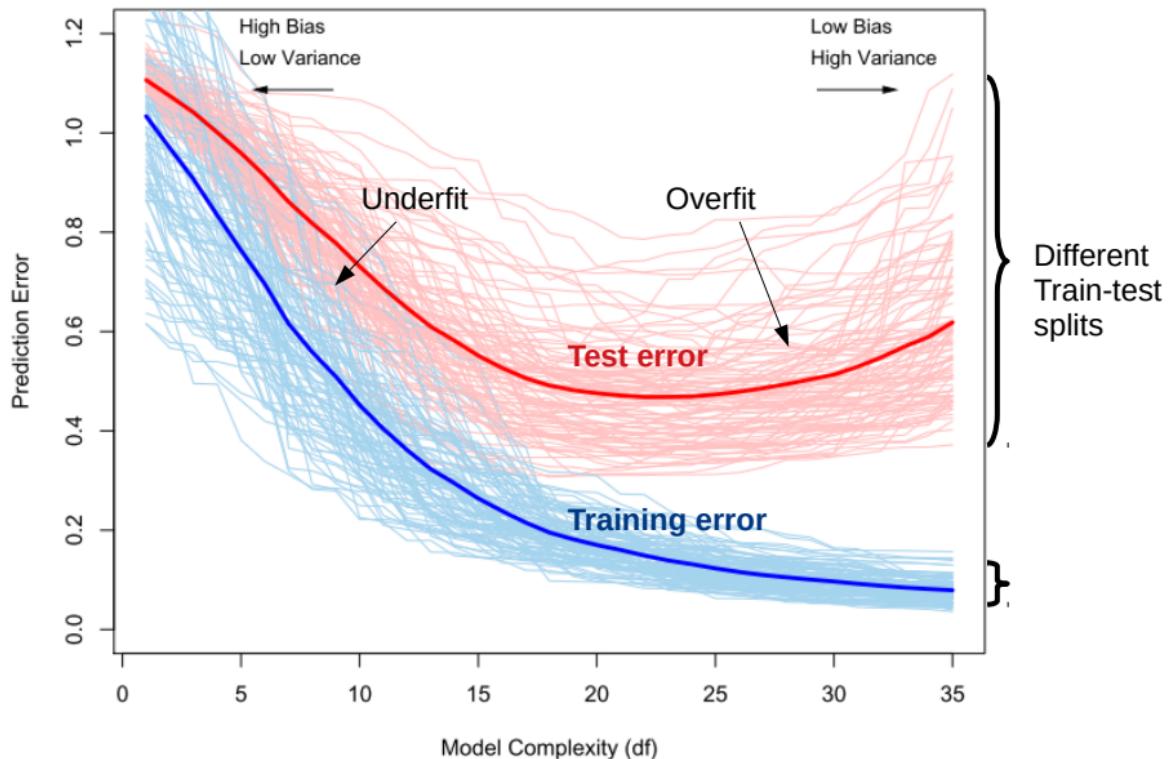


# Bias-Variance trade-off

8 / 42

If you reduce bias (on the training set) you increase the variance. And vice-versa.

This is a fundamental limit of Machine Learning [KW96].



## Section 2

# Regularization

# Regularization

10 / 42

- Force the model to be simple.

Cost function:

$$J(\theta, \mathbf{X}, \hat{\mathbf{y}}) = \frac{1}{M} \sum_{i=1}^M \left( y^{(i)} - h_{\theta}(\mathbf{x}^{(i)}) \right)^2 + \underbrace{\alpha \sum_{j=1}^N \theta_j^2}_{\text{regularization term}}$$

- Parameters forced to be small  $\implies$  less overfit
- Bias term  $\theta_0$  not regularized. Why?

# Regularization

10 / 42

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10 / 42

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- Parameters forced to be small  $\implies$  less overfit
- Bias term  $\theta_0$  not regularized. Why?
  - It is just an offset. It does not add complexity.
- Should regularization term considered when evaluating test error?

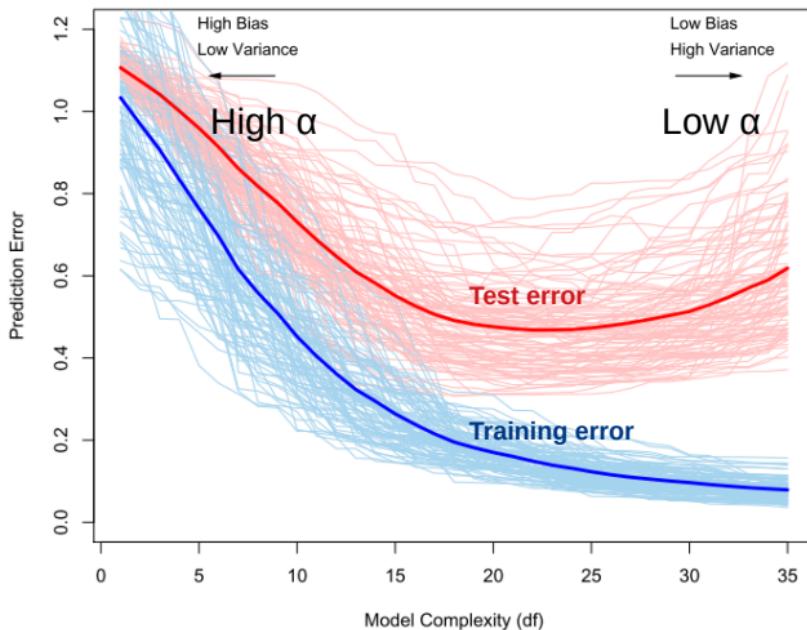
$$J_{\text{train}} = \frac{1}{|\mathcal{D}^{\text{train}}|} \sum_{i \in \mathcal{D}^{\text{train}}} \left( y^{(i)} - h_{\theta}(\mathbf{x}^{(i)}) \right)^2 + \alpha \underbrace{\sum_{j=1}^N \theta_j^2}_{\text{regularization term}}$$

$$J_{\text{test}} = \frac{1}{|\mathcal{D}^{\text{test}}|} \sum_{i \in \mathcal{D}^{\text{test}}} \left( y^{(i)} - h_{\theta}(\mathbf{x}^{(i)}) \right)^2$$

# Effects of $\alpha$

11 / 42

$$J_{\text{train}} = \frac{1}{|\mathcal{D}_{\text{train}}|} \sum_{i \in \mathcal{D}_{\text{train}}} \left( y^{(i)} - h_{\theta}(\mathbf{x}^{(i)}) \right)^2 + \underbrace{\alpha \sum_{j=1}^N \theta_j^2}_{\text{regularization term}}$$



- What if  $\alpha \rightarrow 0$  ?

Linear regression

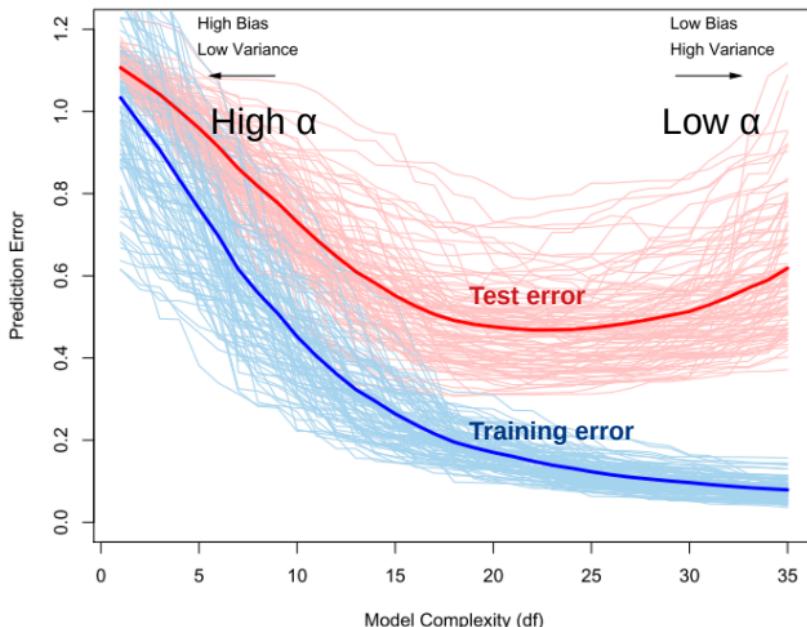
- And if  $\alpha \rightarrow +\infty$  ?

Only  $\theta_0$

# Effects of $\alpha$

11 / 42

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- What if  $\alpha \rightarrow 0$  ?

Linear regression

- And if  $\alpha \rightarrow +\infty$  ?

Only  $\theta_0$

- Suppose

- you try different  $\alpha$  and
  - the best error is with  $\alpha \rightarrow +\infty$ .

What do you conclude?

In this case, the best model is the simple average of  $y$ .

Let's code ...

12 / 42



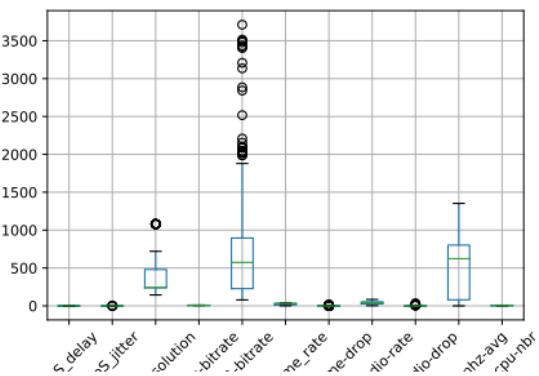
## Section 3

### Scaling

# Regularization and scaling

14 / 42

Features may have different magnitudes



- Regularization squashes blindly all features uniformly.
- “Small” features would need instead larger
- Need to scale features before applying regularization.

$$J(\theta, \mathbf{X}, \mathbf{y}) = \frac{1}{M} \sum_{i=1}^M \left( y^{(i)} - h_{\theta}(\mathbf{x}^{(i)}) \right)^2 + \underbrace{\alpha \sum_{j=1}^N \theta_j^2}_{\text{regularization term}}$$

$$\theta^* = \arg \min_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$

- If  $\mu_j$  is avg of  $j$ -feature and  $\sigma_j$  the stdev:  
Standard Scaler

$$x_j^{(i)'} = \frac{x_j^{(i)} - \mu_j}{\sigma_j}$$

Which is the correct way of applying scaling?

vs.

- Divide  
 $(\mathbf{X}, \mathbf{y}) \rightarrow (\mathbf{X}_{\text{train}}, \mathbf{y}_{\text{train}}), (\mathbf{X}_{\text{test}}, \mathbf{y}_{\text{test}})$
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- Train the model using  
 $(\mathbf{X}_{\text{train}'}, \mathbf{y}_{\text{train}})$
- Test using  $(\mathbf{X}_{\text{test}'}, \mathbf{y}_{\text{test}})$  using  
 $\mu_j, \sigma_j, \min_j, \max_j$  found in training
- $\mathbf{X}' = \text{scale}(\mathbf{X})$
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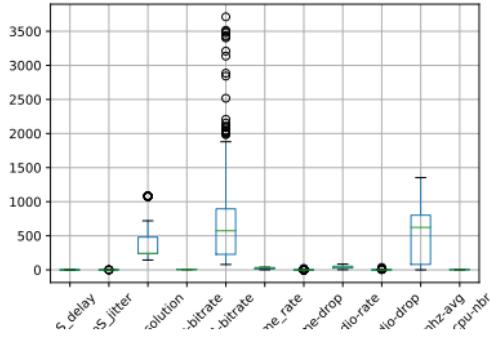
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## Data Leakage (Ch.8 of [Teo19])

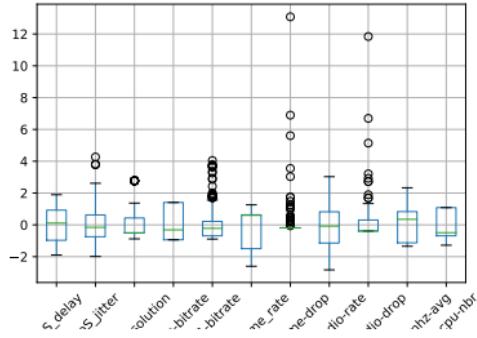
In the 2nd case we would calculate  $\mu_j, \sigma_j, \min_j, \max_j$  using data from test set

# Effect of scaling

16 / 42



⇒



# When is scaling important

17 / 42

Is scaling important in a linear regression?

Is scaling important in a linear regression?

- It does not affect the accuracy of the model
  - Because coefficients can scale based on the feature magnitude.
- But it's good for interpretability, **when features are standardized**
  - Since we impose the stddev of all features to be 1, the value of the coefficient is an indication of **feature importance**
    - (how much a variation of a feature impacts the target)

Is scaling important in a polynomial regression?

## Section 4

### **Feature selection**

- We have already seen some methods:
  - Check the Pearson's correlation
  - Run a lin.regr. on the scaled dataset and check the magnitude of the coefficients.
  - See if a model improves/deteriorates when removing a feature
- Another method: **Recursive Feature Elimination (RFE)**
  - Standardize your features
  - Train your model with all features
  - Remove the feature with the smallest coeff
  - Train the model again
  - Remove the feature with the smallest coeff
  - ...
  - Repeat until you are left with  $N$  features.
- Why do we need to standardize the features?

Otherwise the coefficient weights are not an indication of feature importance.
- RFE + Cross Validation (RFECV)
  - Repeat the process for different  $N$  and select the  $N$  providing the smallest cross-validation error.



Go to notebook 03.regression\_contd-and-classification/b.regularization

## Section 5

# **Classification: Logistic Regression**

Supervised ML task where the labels are in a finite set.

- Ex.: Classify video resolution based on network information  
Labels are 144p, 360p, etc.

# Binomial Logistic Regression

23 / 42

- Classes  $k = 0$  (negative) and  $1$  (positive).
- We do not predict directly the class  $k$  of sample  $\mathbf{x}$
- We instead predict probabilities
  - The predicted probability of being positive is

$$\begin{aligned}\hat{p}_1^{(i)} &= \mathbb{P} \left[ \mathbf{x}^{(i)} \text{ is of class } 1 \right] \\ &= h_{\Theta}(\mathbf{x}^{(i)}) = \sigma(\boldsymbol{\theta}^T \cdot \mathbf{x}^{(i)})\end{aligned}$$

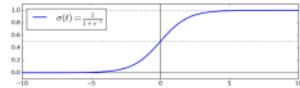
- The predicted probability of being negative is

$$\hat{p}_0^{(i)} = 1 - \hat{p}_1^{(i)}$$

- If  $y^{(i)}$  is the true class of sample  $\mathbf{x}^{(i)}$ , the predicted probability of being of the true class is

$$\hat{p}_{y^{(i)}}^{(i)}$$

- Sigmoid  $\sigma(t) = \frac{1}{1+e^{-t}}$

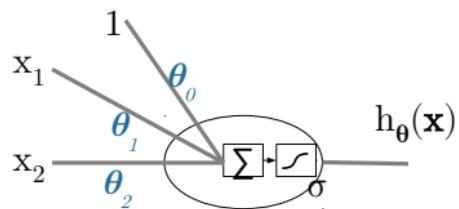


Picture from [Gér17]

- The predicted label is:

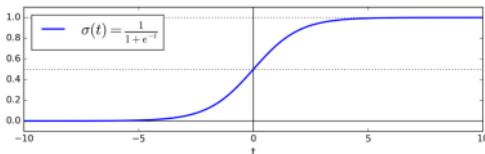
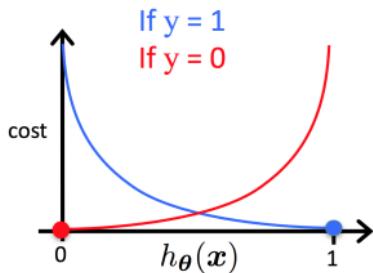
$$\hat{y}^{(i)} = \begin{cases} 1 & \text{if } \hat{p}_1^{(i)} \geq 0.5 \\ 0 & \text{if } \hat{p}_1^{(i)} < 0.5 \end{cases}$$

Logistic regression is a NN with one neuron



# Log-Loss function

25 / 42



- How can we find:

$$\theta^* = \arg \min_{\theta} J(\theta, \mathbf{X}, \mathbf{y})?$$

- For any sample  $(\mathbf{x}^{(i)}, y^{(i)})$ :

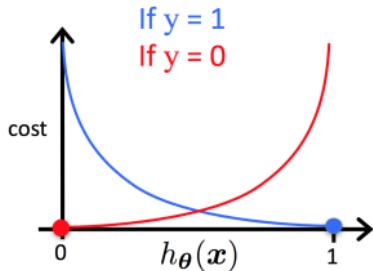
$$\begin{aligned} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) &\triangleq -\ln \left( \hat{p}_{y^{(i)}}^{(i)} \right) = \begin{cases} -\ln \left( \hat{p}_1^{(i)} \right) & \text{if } y^{(i)} = 1 \\ -\ln \left( \hat{p}_0^{(i)} \right) & \text{if } y^{(i)} = 0 \end{cases} \\ &= \begin{cases} -\ln \left( \sigma(\theta^T \cdot \mathbf{x}^{(i)}) \right) & \text{if } y^{(i)} = 1 \\ -\ln \left( 1 - \sigma(\theta^T \cdot \mathbf{x}^{(i)}) \right) & \text{if } y^{(i)} = 0 \end{cases} \end{aligned}$$

- For the entire dataset  $(\mathbf{X}, \mathbf{y})$ :

$$J(\theta, \mathbf{X}, \mathbf{y}) \triangleq \frac{1}{M} \sum_{i=1}^M J(\theta, \mathbf{x}^{(i)}, y^{(i)}) \quad (1)$$

# Log-Loss function

25 / 42

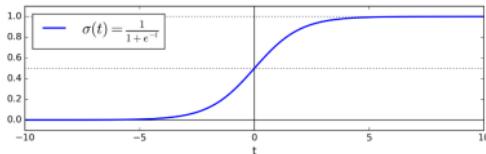
Picture from [stackexchange](#)

- For any sample  $(\mathbf{x}^{(i)}, y^{(i)})$ :

$$\begin{aligned} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) &\triangleq -\ln(\hat{p}_{y^{(i)}}^{(i)}) = \begin{cases} -\ln(\hat{p}_1^{(i)}) & \text{if } y^{(i)} = 1 \\ -\ln(\hat{p}_0^{(i)}) & \text{if } y^{(i)} = 0 \end{cases} \\ &= \begin{cases} -\ln(\sigma(\theta^T \cdot \mathbf{x}^{(i)})) & \text{if } y^{(i)} = 1 \\ -\ln(1 - \sigma(\theta^T \cdot \mathbf{x}^{(i)})) & \text{if } y^{(i)} = 0 \end{cases} \end{aligned}$$

- For the entire dataset  $(\mathbf{X}, \mathbf{y})$ :

$$J(\theta, \mathbf{X}, \mathbf{y}) \triangleq \frac{1}{M} \sum_{i=1}^M J(\theta, \mathbf{x}^{(i)}, y^{(i)}) \quad (1)$$



- How can we find:

$$\theta^* = \arg \min_{\theta} J(\theta, \mathbf{X}, \mathbf{y})?$$

- For any  $(\mathbf{x}^{(i)}, y^{(i)})$ , the loss function is derivable and convex:

$$\begin{aligned} \nabla J(\theta, \mathbf{x}^{(i)}, y^{(i)}) &= \begin{cases} \nabla \left[ -\ln(\sigma(\theta^T \cdot \mathbf{x}^{(i)})) \right] & \text{if } y^{(i)} = 1 \\ \nabla \left[ -\ln(1 - \sigma(\theta^T \cdot \mathbf{x}^{(i)})) \right] & \text{if } y^{(i)} = 0 \end{cases} \end{aligned}$$

- $\implies J(\theta, \mathbf{X}, \mathbf{y})$  is also derivable and convex
- $\implies$  We can use gradient descent.

- At each iteration

$$\theta := \theta - \eta \cdot \nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$

where (see (1))

$$\nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y}) = \frac{1}{M} \sum_{i=1}^M \nabla_{\theta} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = \frac{1}{M} \sum_{i=1}^M \begin{bmatrix} \frac{\partial}{\partial \theta_0} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) \\ \vdots \\ \frac{\partial}{\partial \theta_N} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) \end{bmatrix}$$

- For any sample  $i$  we can compute that<sup>1</sup> (No need to learn it by heart):

$$\frac{\partial}{\partial \theta_j} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = \left( \underbrace{\sigma(\theta^T \cdot \mathbf{x}^{(i)}) - y^{(i)}}_{\text{---}} \right) \cdot x_j^{(i)}$$

---

<sup>1</sup>Eq. 4.18 of [Gér17]

- At each iteration

$$\theta := \theta - \eta \cdot \nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$

where (see (1))

$$\nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y}) = \frac{1}{M} \sum_{i=1}^M \nabla_{\theta} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = \frac{1}{M} \sum_{i=1}^M \begin{bmatrix} \frac{\partial}{\partial \theta_0} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) \\ \vdots \\ \frac{\partial}{\partial \theta_N} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) \end{bmatrix}$$

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- For any sample  $i$  we can compute that<sup>1</sup> (No need to learn it by heart):

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---

<sup>1</sup>Eq. 4.18 of [Gér17]

- At each iteration

$$\theta := \theta - \eta \cdot \nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$

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- For any sample  $i$  we can compute that<sup>1</sup> (No need to learn it by heart):

$$\frac{\partial}{\partial \theta_j} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = \left( \underbrace{\sigma(\theta^T \cdot \mathbf{x}^{(i)}) - y^{(i)}}_{\hat{p}^{(i)}} \underbrace{- \epsilon^{(i)}}_{-\epsilon^{(i)}} \right) \cdot x_j^{(i)}$$

- Therefore

$$\nabla_{\theta} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = -\epsilon^{(i)} \cdot \mathbf{x}^{(i)}$$

---

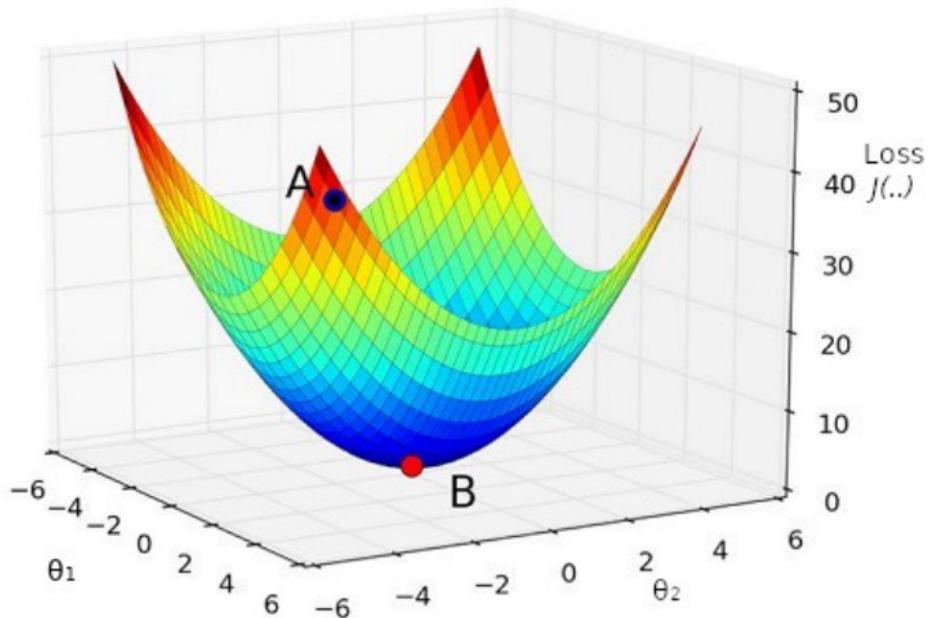
<sup>1</sup>Eq. 4.18 of [Gér17]

# Gradient Descent

27 / 42

At each iteration

$$\theta := \theta - \eta \cdot \nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y})$$



## 1. Full Gradient Descent:

- Initialize a random  $\theta$
- Compute  $h_\theta(\mathbf{x}^{(i)})$  for all  $(\mathbf{x}^{(i)}, y^{(i)}) \in \mathcal{D}^{\text{train}}$
- Compute the residuals

$$\varepsilon^{(i)} = h_\theta(\mathbf{x}) - y^{(i)}$$

- Apply the update:

$$\theta := \theta - \eta \cdot \underbrace{\frac{1}{M} \sum_{i=1}^M \varepsilon^{(i)} \cdot \mathbf{x}^{(i)}}_{\nabla_{\theta} J(\theta, \mathbf{X}, \mathbf{y})}$$

- Repeat several **epochs**.

The more the error on a  $\mathbf{x}^{(i)}$ , the more its contribution to the update.

**Problem:** what happens if  $\mathcal{D}^{\text{train}}$  is huge?

## 2. Stochastic gradient descent

- Randomly select one sample  $(\mathbf{x}^{(i)}, y^{(i)})$
- Directly update

$$\theta := \theta - \eta \cdot \underbrace{\varepsilon^{(i)} \cdot \mathbf{x}^{(i)}}_{\nabla_{\theta} J(\theta, \mathbf{x}^{(i)}, y^{(i)})} \nabla$$

- Why *stochastic*:  
we apply a quantity which on expectation is equal to the actual gradient

## 3. Batch gradient descent

- Partition  $\mathcal{D}^{\text{train}}$  into batches
  - For each batch
  - Predict all the data

# Logistic Regression is a linear classifier

29 / 42

**Decision boundary:** Surface of  $\mathbb{R}^{N+1}$  that divides the region in which the classifier predicts 1 and the region in which it predicts 0.

## Theorem

The decision boundary of Logistic Regression is a hyperplane

Logistic regression predicts 1 if

$$\hat{p}_1^{(i)} = h_{\theta}(\mathbf{x}) = \sigma(\boldsymbol{\theta}^T \cdot \mathbf{x}^{(i)}) \geq 0.5$$

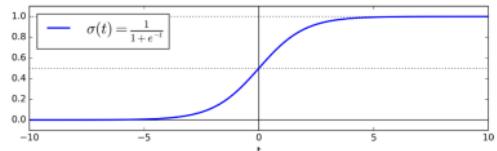
$\iff$

$$\boldsymbol{\theta}^T \cdot \mathbf{x}^{(i)} \geq 0$$

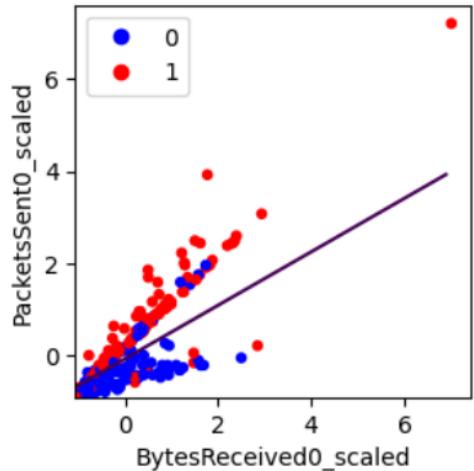
Therefore, the boundary decision is the set of  $\mathbf{x}$  such that

$$\boldsymbol{\theta}^T \cdot \mathbf{x} = 0$$

This surface is described by a linear equation, and thus it is a hyperplane.



Picture above from [Gér17]



# Multinomial Logistic Regression

30 / 42

Extension to multiple classes.

- Each class has its weight parameter  $\theta_k \in \mathbb{R}^{N+1}$ , except the last
- Compute a *score*  $s_k(\mathbf{x}) \triangleq \theta_k^T \cdot \mathbf{x}$
- For any  $\mathbf{x}$ , we have the score of all classes

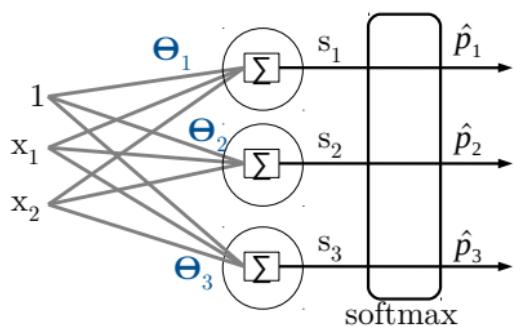
$$s_1(\mathbf{x}), \dots, s_K(\mathbf{x})$$

- We define that:

$$\begin{aligned}\hat{p}_k &= \mathbb{P}[\mathbf{x} \in \text{class } k] = \text{softmax}(s_k(\mathbf{x})) \\ &\triangleq \frac{\exp s_k(\mathbf{x})}{\sum_{z=1}^K \exp s_z(\mathbf{x})} = \frac{\exp (\theta_k^T \cdot \mathbf{x})}{\sum_{z=1}^K \exp (\theta_z^T \cdot \mathbf{x})}\end{aligned}$$

- Predicted Class:

$$k^* = \arg \max_k \text{softmax}(\theta_k^T \cdot \mathbf{x}) = \arg \max_k \theta_k^T \cdot \mathbf{x}$$

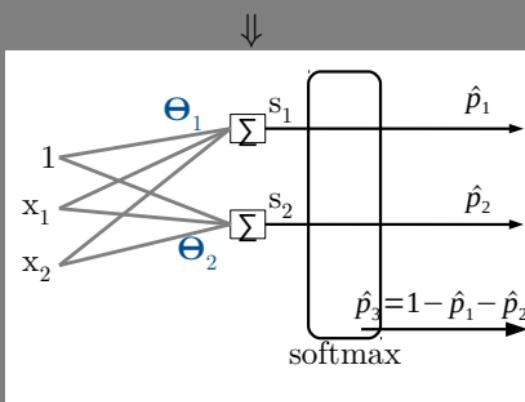
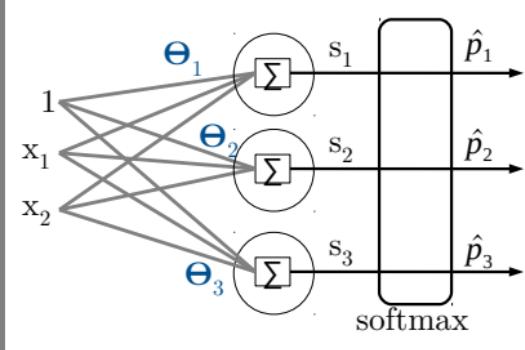


## Multinomial Logistic Regression (2)

31 / 42

We just need to compute  $K - 1$  parameter vectors:

$$\begin{aligned}\hat{p}_k^{(i)} &= \frac{\exp(-\theta_K)}{\exp(-\theta_K)} \cdot \frac{\exp(\theta_k^T \cdot \mathbf{x})}{\sum_{z=1}^K \exp(\theta_z^T \cdot \mathbf{x})} \\ &= \frac{\exp((\theta_k - \theta_K)^T \cdot \mathbf{x})}{\sum_{z=1}^K \exp\left(\underbrace{(\theta_z - \theta_K)^T \cdot \mathbf{x}}_{\theta'_z}\right)} \\ &= \frac{\exp(\theta'^T_k \cdot \mathbf{x})}{1 + \sum_{z=1}^{K-1} \exp(\theta'^T_z \cdot \mathbf{x})}\end{aligned}$$



# Log-loss function (cross-entropy)

32 / 42

- The log-loss function on each sample is

$$J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = -\ln \hat{p}_{y^{(i)}}$$

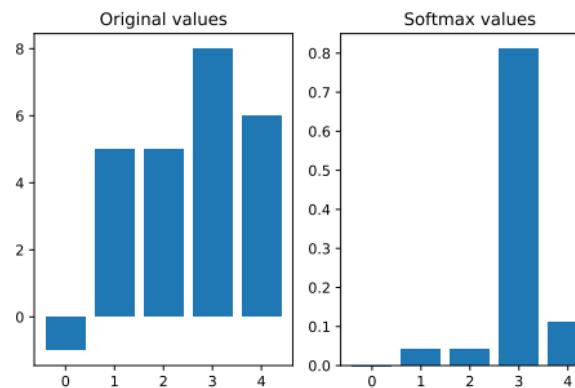
where  $y_k^{(i)} = 1 \iff \mathbf{x}^{(i)} \in \text{class } k$

- The loss function is also called *cross-entropy*

See ([Ger19, Eq. 4-22] and [Wikipedia - section “Estimation”](#))

- We want  $\hat{p}_{y^{(i)}}$  to be as high as possible.

- Softmax “amplifies” the most probable class.



## Assignment

Show that the Multinomial Logistic Regression with  $K = 2$  is equivalent to Binary Logistic Regression.

In other words, show that

$$\mathbb{P}[\mathbf{x} \in \text{class 1}] = \text{softmax}(\boldsymbol{\theta}^T \cdot \mathbf{x})$$

is equivalent to the binomial case

$$\mathbb{P}[\mathbf{x} \in \text{class 1}] = \sigma(\boldsymbol{\theta}^T \cdot \mathbf{x})$$

Then show that the loss function is also equivalent.



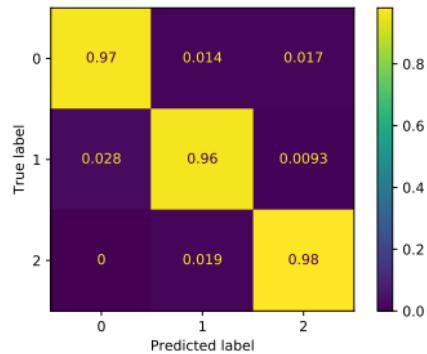
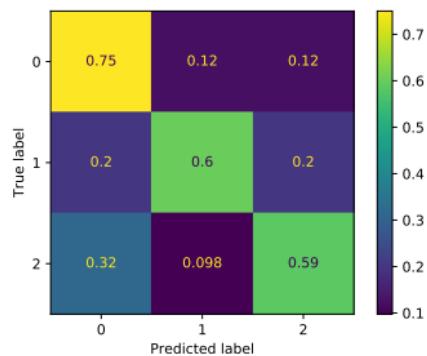
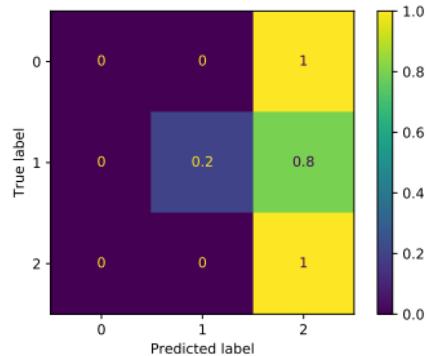
Go to notebook 03.regression\_contd-and-classification.ipynb

## Section 6

### **Class imbalance and performance metrics**

# Confusion Matrix

36 / 42



When there are classes with many samples and other with less samples.

How to cope with it:

- Synthetic Minority Over-Sampling TEchnique (SMOTE) [CBHK02]
  - 10 K citations!
- Others (you can explore yourself, if you want)
  - Under-sampling majority class
  - Use different weights in the loss function
  - Others: see [this blog](#).

# Classification Report

38 / 42

	precision	recall	f1-score	support
0	0.29	0.75	0.41	8
1	0.55	0.60	0.57	10
2	0.89	0.59	0.71	41
accuracy			0.61	59
macro avg	0.57	0.65	0.56	59
weighted avg	0.75	0.61	0.64	59

- **Precision:** 29% of samples classified as 0 are actually 0
- **Recall:** 75% of class 0 samples are correctly classified
- **Accuracy:** 61% of classifications are correct
- **Support:** 8 samples in the test set are of class 0
- **f1-score:** A combination of precision and recall:

$$F_1 = \frac{2}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}}$$

↑ precision, ↑ recall  $\implies$  ↑  $F_1$

## Regression (continued)

- Polynomial Regression
- Variance vs. Bias Trade-Off
- Regularization
- Scaling
- Feature Selection

## Classification

- Logistic Regression
- Classification Performance
- Class imbalance

- Video about [feature scaling](#).
- More on [feature selection](#).
- Several loss functions for classification (Video) [[Mic](#)]
- Another way of looking at Logistic Regression, based on likelihood: Sec. 4.3 of [[JWHT13](#)].

- [AWS] *Amazon Machine Learning Developer Guide*,  
<https://docs.aws.amazon.com/machine-learning/>.
- [CBHK02] N. Chawla, K. W. Bowyer, L. O. Hall, and W. P. Kegelmeyer,  
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