

Machine Learning for Networks: Regression (continued) and Classification

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May 16, 2023



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:

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

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

$$\theta_0$$

- Powers of features

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

- Mixed terms of power 2:

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

- Mixed terms of power 3

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

- ...

- Mixed terms of power p

Hyper-parameter tuning

5 / 42

BufferHealth	BufferProgress	BufferValid	label	label_num
10.241165	0.015357	true	q360p	360
4.446780	0.007103	true	q144p	144
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Hyper-parameter tuning

5 / 42

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{ TRAINING SET }

{ TEST SET }

- Divide training and test sets

Hyper-parameter tuning

5 / 42

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SET

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- Use only training set

Hyper-parameter tuning

5 / 42

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- For all the hyper-parameter values
 - Construct a model with such values
 - Compute cross-validation error

Hyper-parameter tuning

5 / 42

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Hyper-parameter tuning

5 / 42

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

Hyper-parameter tuning

5 / 42

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- Divide training and test sets
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 - Construct a model with such values
 - Compute cross-validation error
- Select the model with the smallest cross-validation error
- Train the selected model on the training set
- Test error on the test set

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

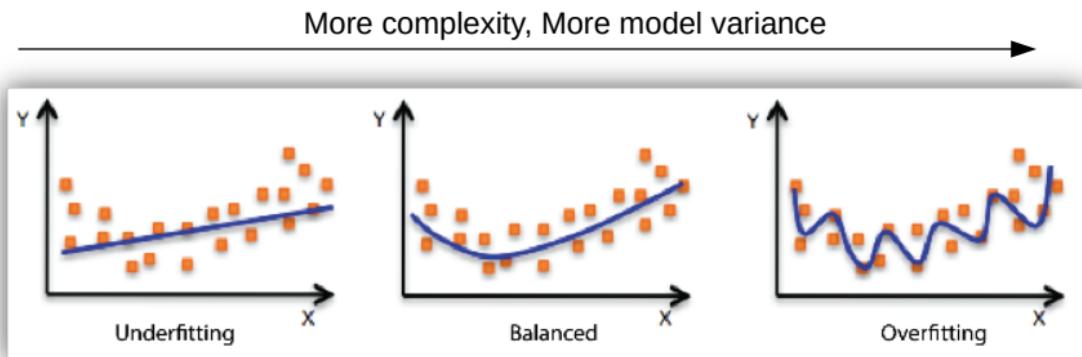


Go to notebook

03.regression_contd-and-classification/a.polynomial-regression.ipynb

Complexity and Variance

7 / 42



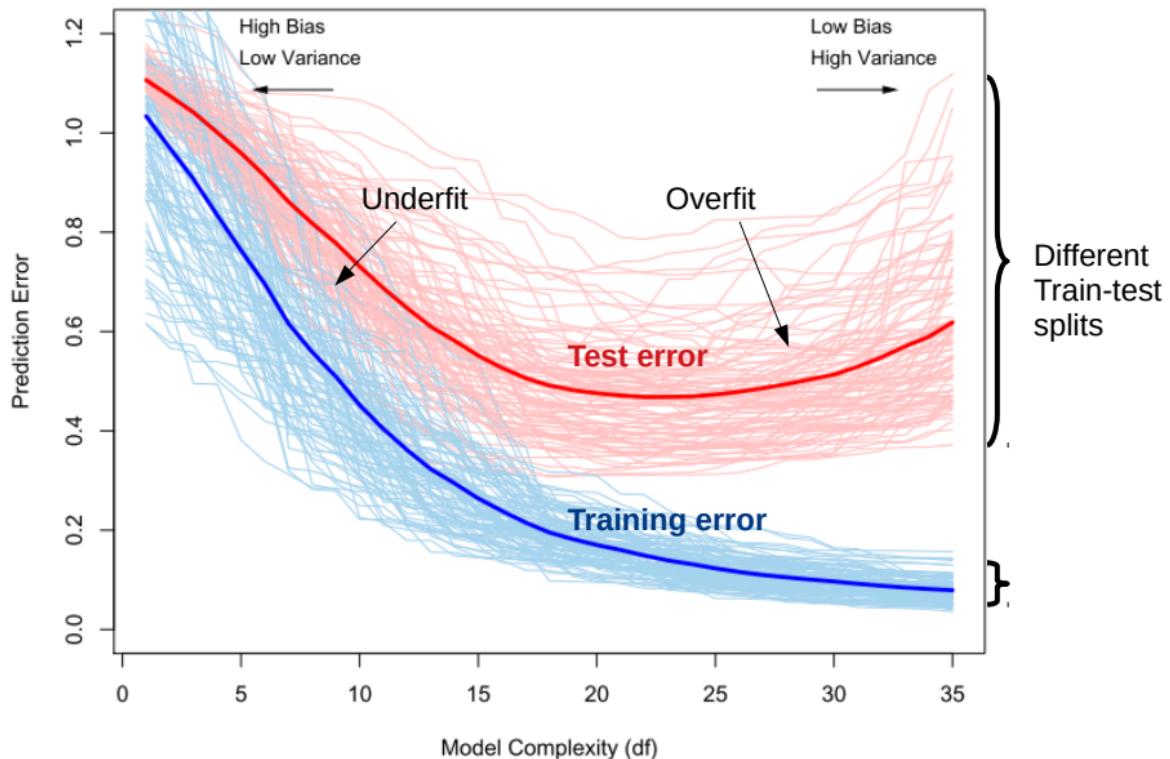
Example of polynomial regression with degree 1 (linear), and then higher degrees

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)

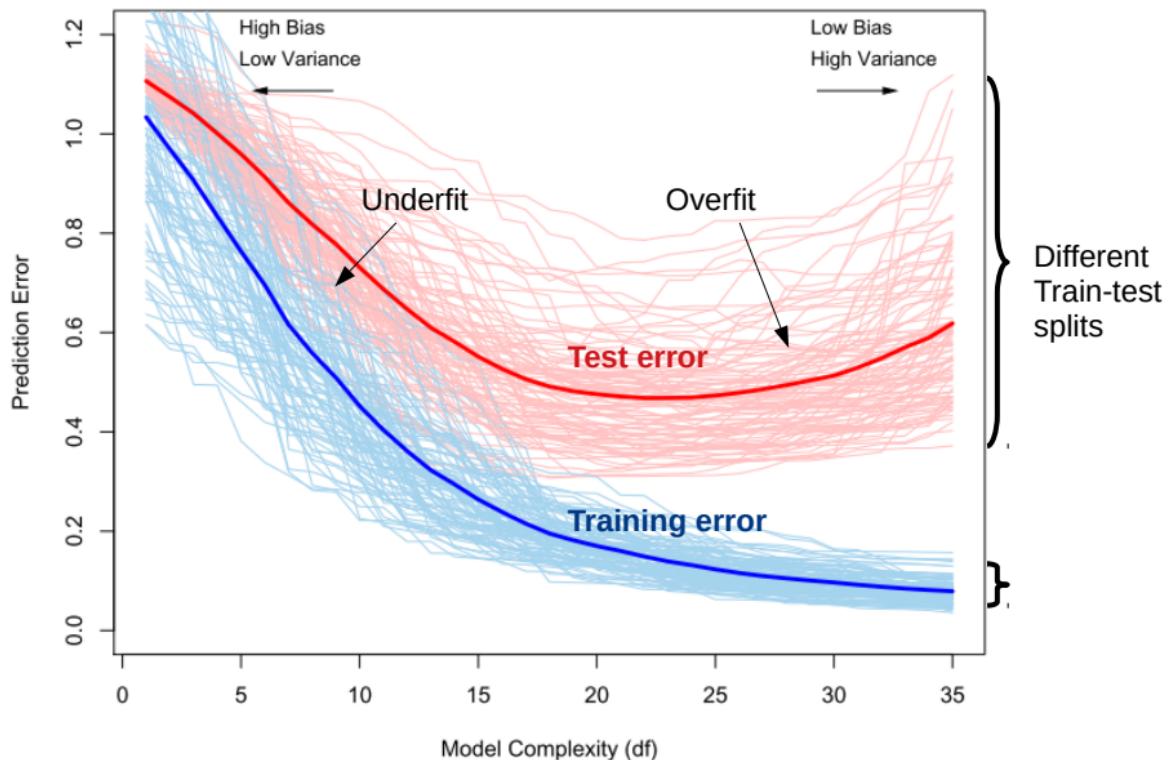


Bias-Variance trade-off

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:

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

- Parameters forced to be small \implies less overfit
- Bias term θ_0 not regularized. Why?

Regularization

10 / 42

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Regularization

10 / 42

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- Parameters forced to be small \implies less overfit
- Bias term θ_0 not regularized. Why?
 - It is just an offset. It does not add complexity.
- Should regularization term considered when evaluating test error?

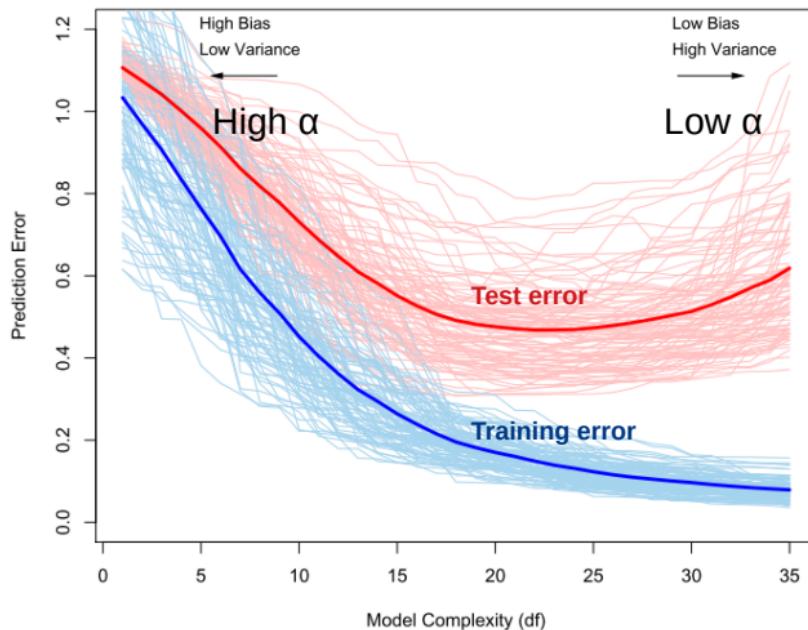
$$J_{\text{train}} = \frac{1}{|\mathcal{D}^{\text{train}}|} \sum_{i \in \mathcal{D}^{\text{train}}} \left(y^{(i)} - h_{\theta}(\mathbf{x}^{(i)}) \right)^2 + \alpha \underbrace{\sum_{j=1}^N \theta_j^2}_{\text{regularization term}}$$

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

Effects of α

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

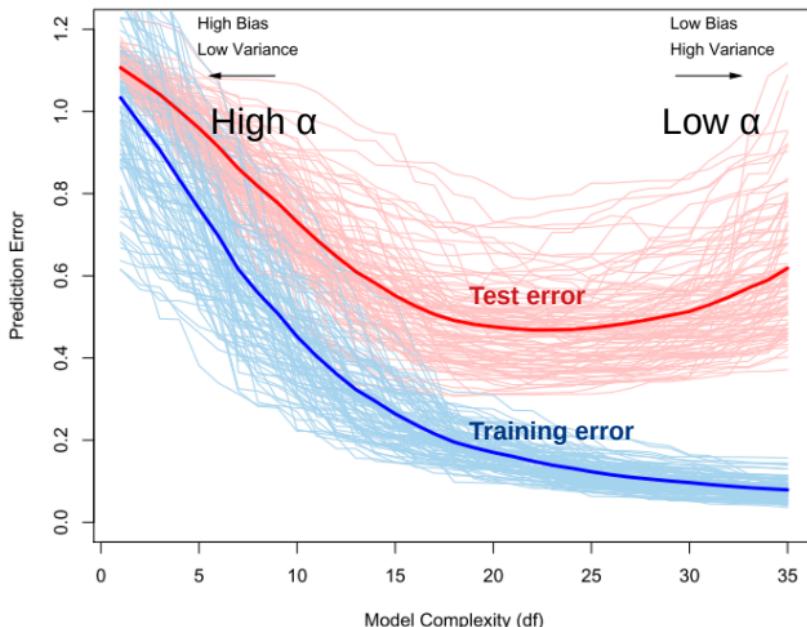
- And if $\alpha \rightarrow +\infty$?

Only θ_0

Effects of α

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 θ_0

- Suppose

- you try different α 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



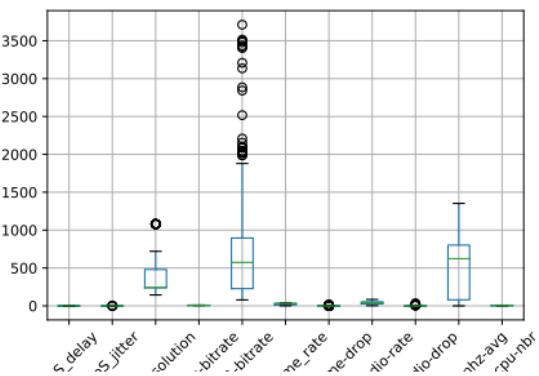
Section 3

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 μ_j is avg of j -feature and σ_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
 $(\mathbf{X}, \mathbf{y}) \rightarrow (\mathbf{X}_{\text{train}}, \mathbf{y}_{\text{train}}), (\mathbf{X}_{\text{test}}, \mathbf{y}_{\text{test}})$
- $\mathbf{X}_{\text{train}'} = \text{scale}(\mathbf{X}_{\text{train}})$
- $\mathbf{X}_{\text{test}'} = \text{scale}(\mathbf{X}_{\text{test}})$
- 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
- $\mathbf{X}' = \text{scale}(\mathbf{X})$
- 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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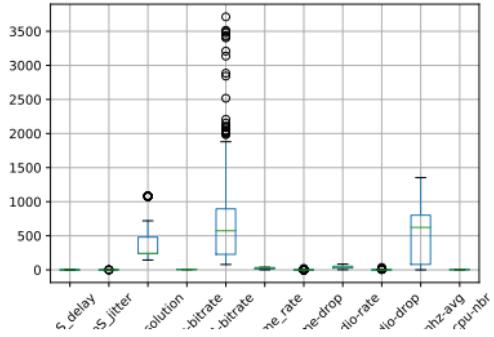
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Data Leakage (Ch.8 of [Teo19])

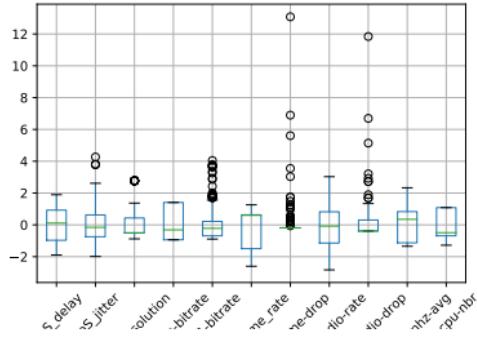
In the 2nd case we would calculate $\mu_j, \sigma_j, \min_j, \max_j$ using data from test set

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

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

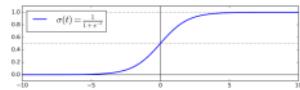
- The predicted probability of being negative is

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

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

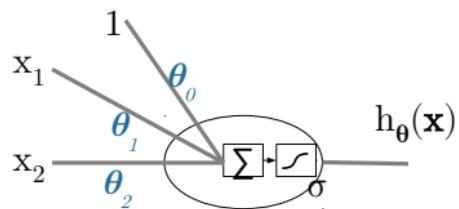


Picture from [Gér17]

- The predicted label is:

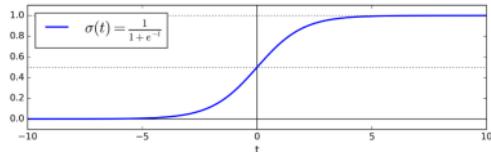
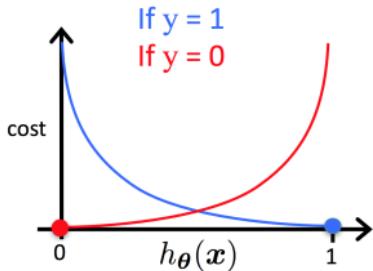
$$\hat{y}^{(i)} = \begin{cases} 1 & \text{if } \hat{p}_1^{(i)} \geq 0.5 \\ 0 & \text{if } \hat{p}_1^{(i)} < 0.5 \end{cases}$$

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 $(\mathbf{x}^{(i)}, y^{(i)})$:

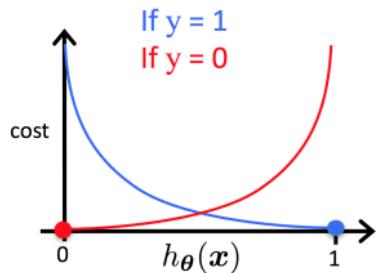
$$\begin{aligned} J(\theta, \mathbf{x}^{(i)}, y^{(i)}) &\triangleq \begin{cases} -\ln(\hat{p}_1^{(i)}) & \text{if } y^{(i)} = 1 \\ -\ln(\hat{p}_0^{(i)}) & \text{if } y^{(i)} = 0 \end{cases} \\ &= \begin{cases} -\ln(\sigma(\theta^T \cdot \mathbf{x}^{(i)})) & \text{if } y^{(i)} = 1 \\ -\ln(1 - \sigma(\theta^T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

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

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

Log-Loss function

25 / 42



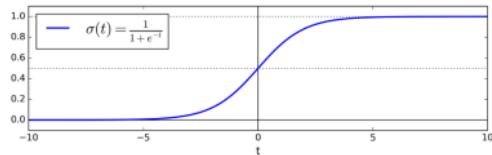
Picture from stackexchange

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

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

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

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- How can we find:

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

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

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

- $\implies J(\boldsymbol{\theta}, \mathbf{X}, \mathbf{y})$ 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 that¹ (No need to learn it by heart):

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

¹Eq. 4.18 of [Gér17]

- At each iteration

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

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- 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 that¹ (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

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

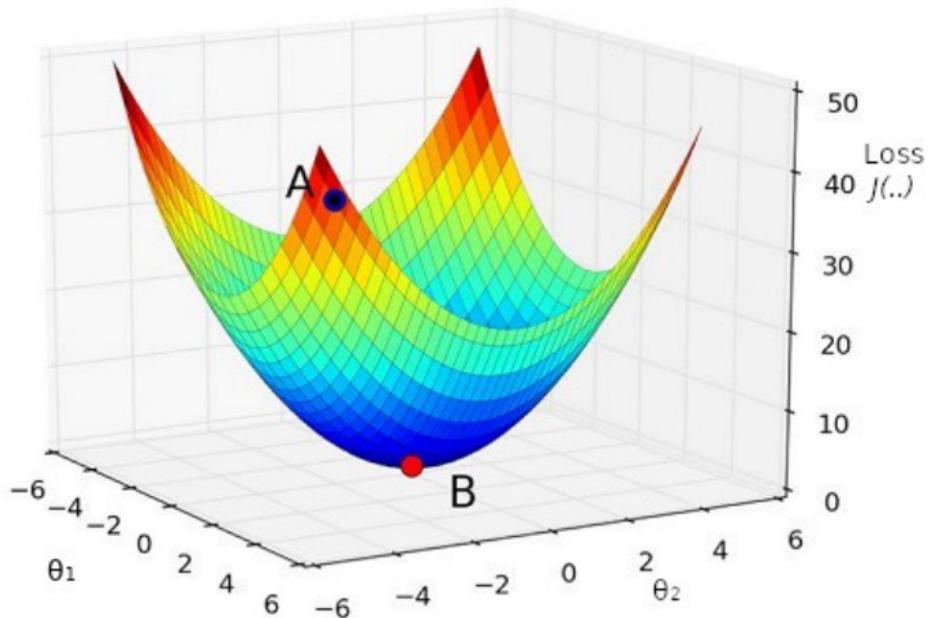
¹Eq. 4.18 of [Gér17]

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 θ
- 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

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

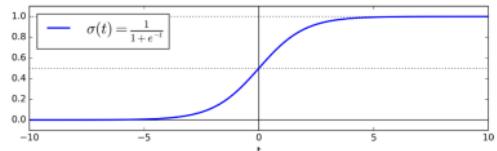
\iff

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

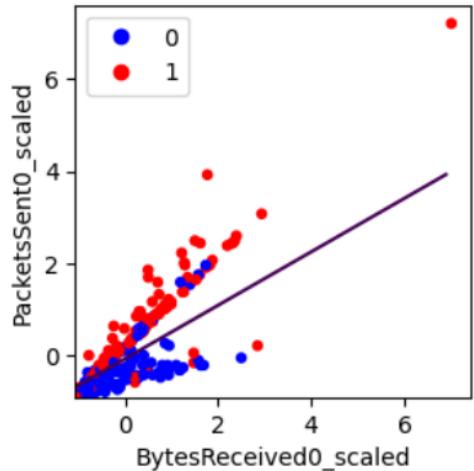
Therefore, the boundary decision is the set of \mathbf{x} such that

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

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

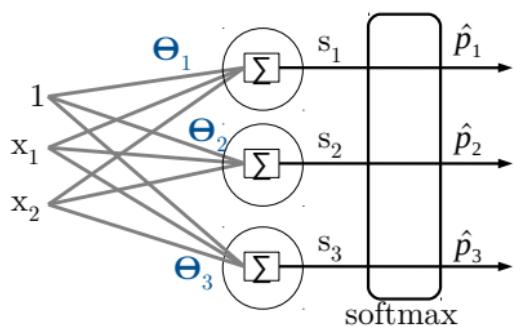
$$s_1(\mathbf{x}), \dots, s_K(\mathbf{x})$$

- 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:

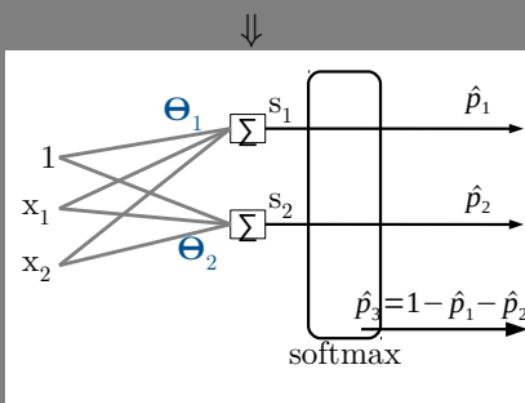
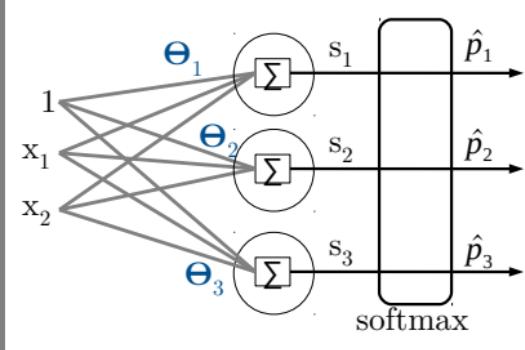
$$k^* = \arg \max_k \text{softmax}(\theta_k^T \cdot \mathbf{x}) = \arg \max_k \theta_k^T \cdot \mathbf{x}$$



Multinomial Logistic Regression (2)

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

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



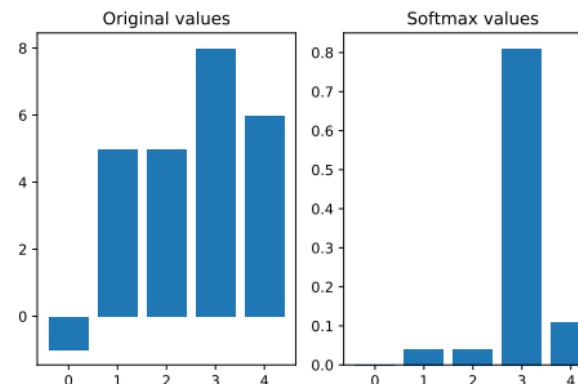
- The loss function for each sample is the cross-entropy

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

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

- We want $\hat{p}_{y^{(i)}}^{(i)}$ 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.



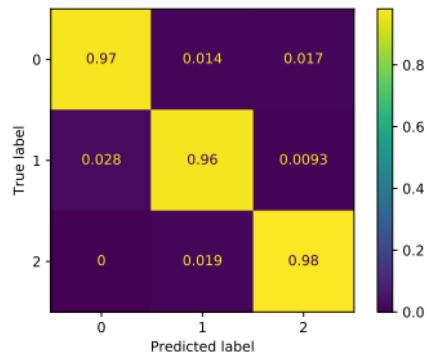
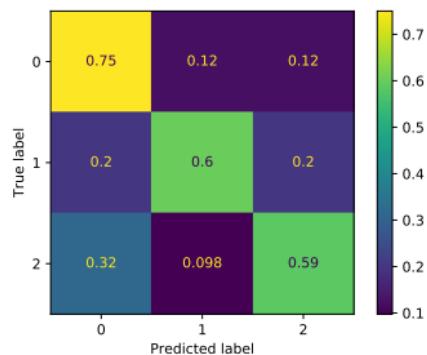
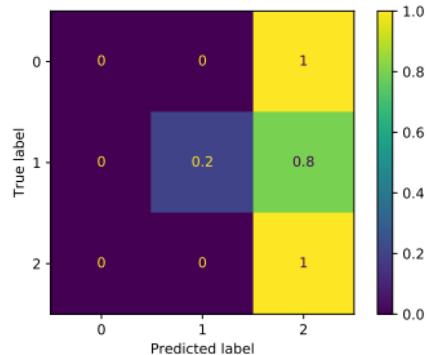
Go to notebook 03.regression_contd-and-classification.ipynb

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](#)].

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<https://docs.aws.amazon.com/machine-learning/>.
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An introduction to Statistical Learning, vol. 7, 2013.
- [KW96] Ron Kohavi and David H. Wolpert, *Bias plus variance decomposition for zero-one loss functions*, International Conference on Machine Learning (ICML96), 1996.

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42 / 42

- [Mic] Microsoft, *Principles of Machine Learning | Loss Function for Classification*, <https://youtu.be/r-vYJqcFxBI>.
- [Teo19] Jake Teo, *Data Science Documentation*, 2019.