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

- A univariate polynomial regression of degree p is

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

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

$$x, x^2, \ldots, x^p$$

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

Multi-variate polynomial regression

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

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

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

$$\theta_0$$

  - Powers of features

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

  - Mixed terms of power 2:

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

  - Mixed terms of power 3

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

  - ...
  - Mixed terms of power p

Hyper-parameter tuning

BufferHealth	BufferProgress	BufferValid	label	label_num
10.241165	0.015357	true	q360p	360
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5.314732	0.009400	true	q240p	240
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3.633641	0.005897	true	q480p	480
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TRAINING SET

TEST SET

- Divide training and test sets

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- Use only training set

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

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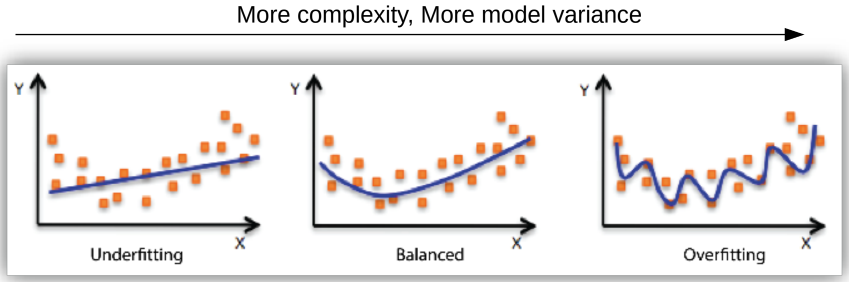
We have only used the training set to select the best parameter

Let's code ...

Go to notebook
03.regression_contd-and-classification/a.polynomial-regression.ipynb

Complexity and Variance

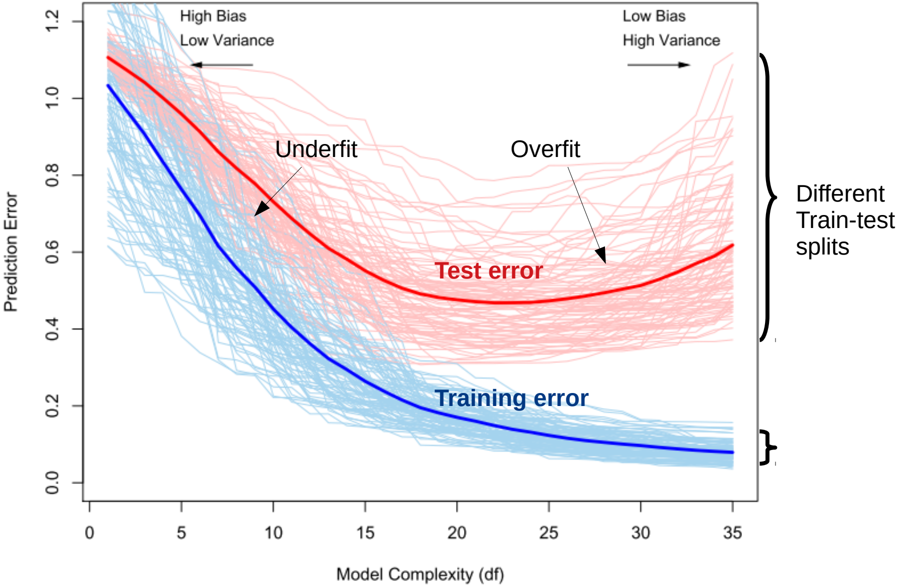


Example of polynomial regression with degree 1 (linear), and then higher degrees

Image from [AWS].

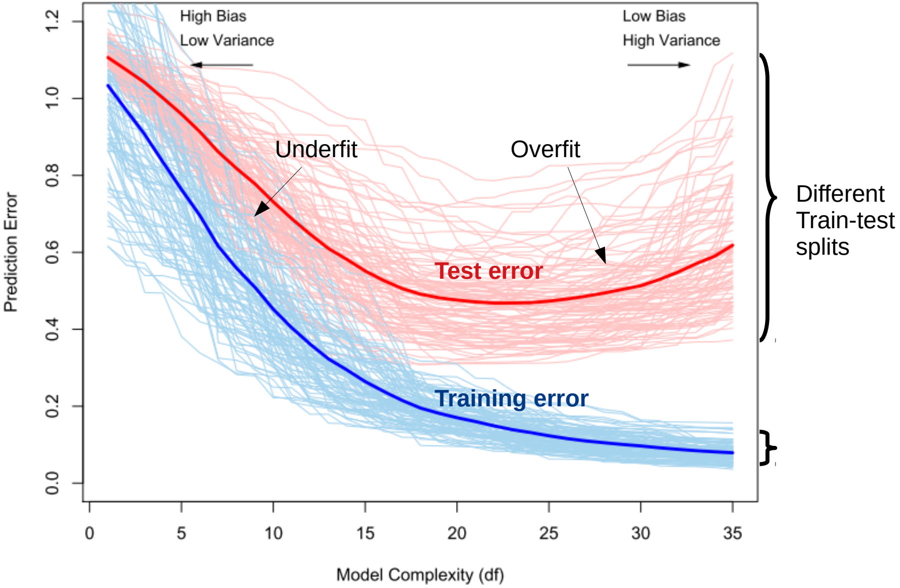
Complexity and Variance

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



Bias-Variance trade-off

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

- 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 $\Longrightarrow$ less overfit
- Bias term θ_0 not regularized. Why?

Regularization

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  Cost function:

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  - It is just an offset. It does not add complexity.

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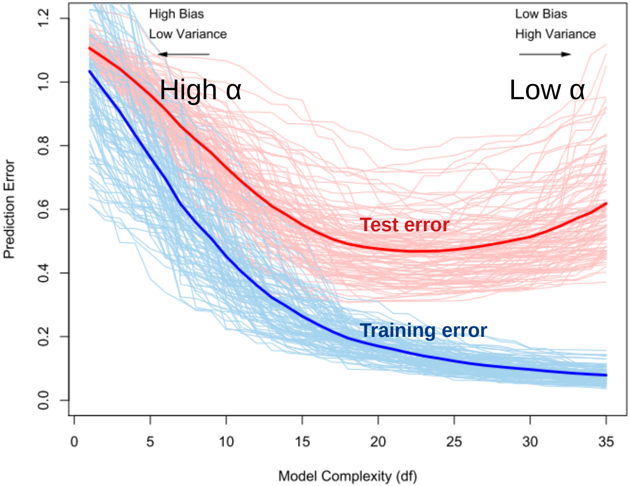
- Parameters forced to be small $\Longrightarrow$ less overfit
- Bias term θ_0 not regularized. Why?
  - It is just an offset. It does not add complexity.
- Should regularization term considered when evaluating test error?

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

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

Effects of α

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



- What if $\alpha \to 0$?

  Linear regression

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

  Only θ_0

Effects of α

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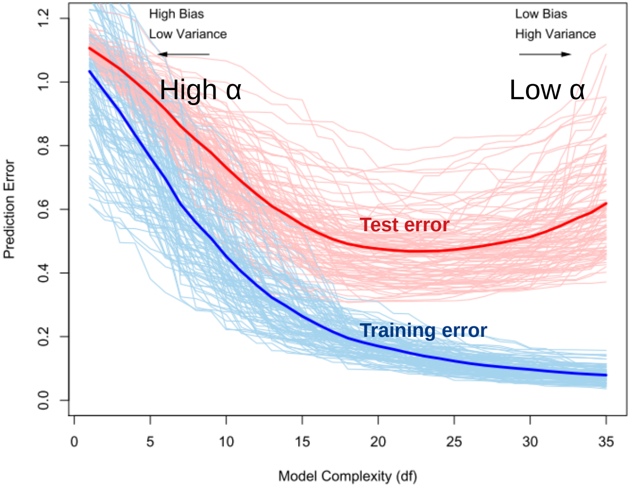

- What if $\alpha \to 0$?

  Linear regression

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

  What do you conclude?

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

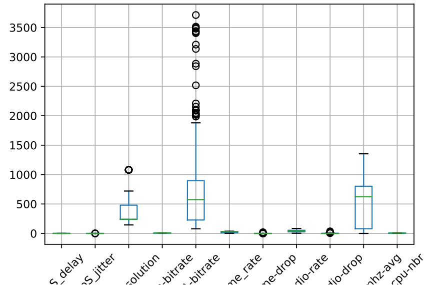
Let’s code ...

Section 3

Scaling

Regularization and scaling

Features may have different magnitudes



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

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

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

Standard scaler

- If μ_j is avg of j-feature and σ_j the stdev:
  Standard Scaler

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

Which is the correct way of applying scaling?

- Divide $(\mathbf{X}, \mathbf{y}) \to (\mathbf{X}_{\text{train}}, \mathbf{y}_{\text{train}}), (\mathbf{X}_{\text{test}}, \mathbf{y}_{\text{test}})$
- $\mathbf{X}_{\text{train}}{}' = \text{scale}(\mathbf{X}_{\text{train}})$
- $\mathbf{X}_{\text{test}}{}' = \text{scale}(\mathbf{X}_{\text{test}})$
- 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

vs.

- $\mathbf{X}' = \text{scale}(\mathbf{X})$
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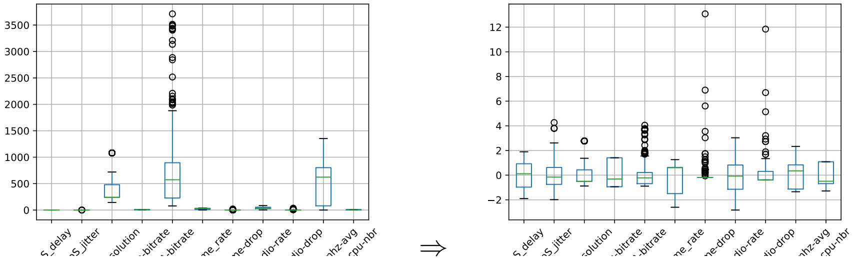
Data Leakage (Ch.8 of [Teo19])

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

Effect of scaling



When is scaling important

Is scaling important in a linear regression?

When is scaling important

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

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.

Let's code ...

Go to notebook 03.regression_contd-and-classification/b.regularization

Section 5

Classification: Logistic Regression

Classification

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

- 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

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

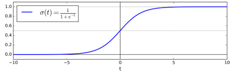
  - The predicted probability of being negative is

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

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



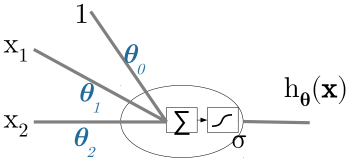
Picture from [Gér17]

- The predicted label is:

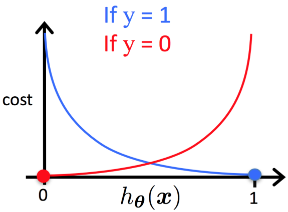
$$\hat{y}^{(i)} = \begin{cases} 1 & \text{if } \hat{p}_1^{(i)} \geq 0.5 \\ 0 & \text{if } \hat{p}_1^{(i)} < 0.5 \end{cases}$$

Neural Network

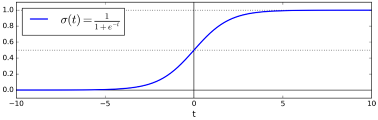
Logistic regression is a NN with one neuron



Log-Loss function



Picture from stackexchange



- How can we find:

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

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

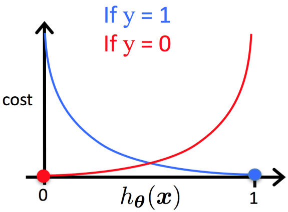
$$J(\theta, \mathbf{x}^{(i)}, y^{(i)}) \triangleq -\ln\left(\hat{p}^{(i)}_{y^{(i)}}\right) = \begin{cases} -\ln\left(\hat{p}^{(i)}_1\right) & \text{if } y^{(i)} = 1 \\ -\ln\left(\hat{p}^{(i)}_0\right) & \text{if } y^{(i)} = 0 \end{cases}$$

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

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

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

Log-Loss function



Picture from stackexchange

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

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

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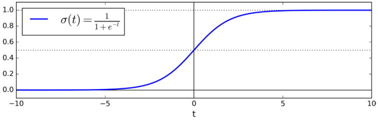

- How can we find:

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

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

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

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

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[1] (No need to learn it by heart):

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

[1] Eq. 4.18 of [Gér17]

- At each iteration

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

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[1] Eq. 4.18 of [Gér17]

Gradient Descent

- 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[1] (No need to learn it by heart):

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

- Therefore

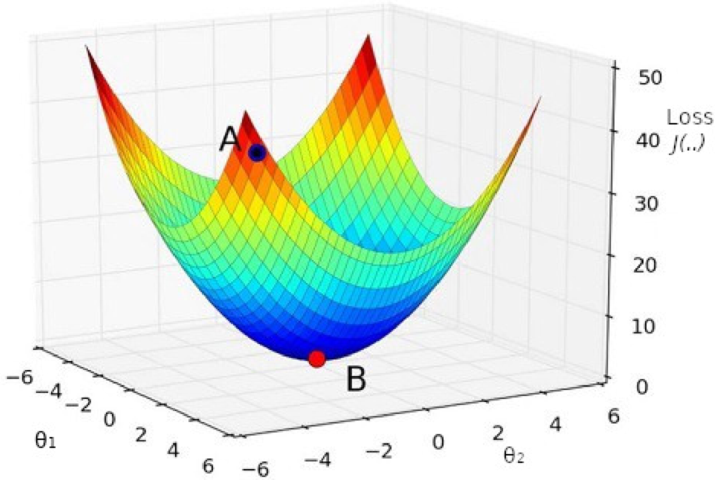
$$\nabla_\theta J(\theta, \mathbf{x}^{(i)}, y^{(i)}) = -\varepsilon^{(i)} \cdot \mathbf{x}^{(i)}$$

[1] Eq. 4.18 of [Gér17]

Gradient Descent

At each iteration

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



Training with Gradient Descent

1. **Full** Gradient Descent:
   - Initialize a random θ
   - Compute $h_\theta(\mathbf{x}^{(i)})$ for all $(\mathbf{x}^{(i)}, y^{(i)}) \in \mathscr{D}^{\text{train}}$
   - 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 $\mathscr{D}^{\text{train}}$ is huge?

2. **Stochastic** gradient descent
   - Randomly select one sample $(\mathbf{x}^{(i)}, y^{(i)})$
   - Directly update

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

   - Why *stochastic*:
     we apply a quantity which on expectation is equal to the actual gradient
3. **Batch** gradient descent
   - Partition $\mathscr{D}^{\text{train}}$ into batches
   - For each batch
     – Predict all the data

Logistic Regression is a linear classifier

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

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

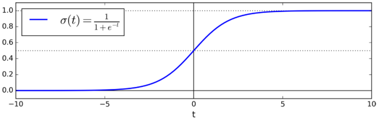
$$\iff$$

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

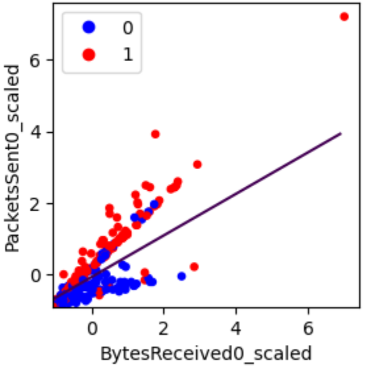
Therefore, the boundary decision is the set of $\mathbf{x}$ such that

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

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



Picture above from [Gér17]



Multinomial Logistic Regression

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

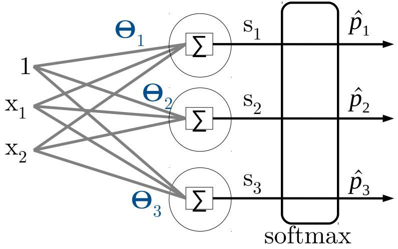
$$s_1(\mathbf{x}), \ldots, s_K(\mathbf{x})$$

- We define that:

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

- Predicted Class:

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



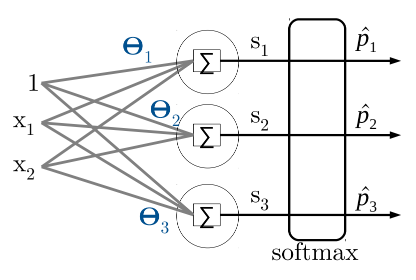
Multinomial Logistic Regression (2)

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

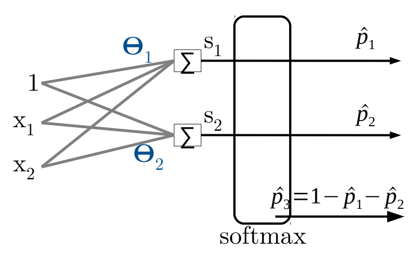
$$\hat{p}_k^{(i)} = \frac{\exp(-\theta_K)}{\exp(-\theta_K)} \cdot \frac{\exp\left(\theta_k{}^T \cdot \mathbf{x}\right)}{\sum_{z=1}^{K} \exp\left(\theta_z{}^T \cdot \mathbf{x}\right)}$$

$$= \frac{\exp\left(\left(\theta_k - \theta_K\right)^T \cdot \mathbf{x}\right)}{\sum_{z=1}^{K} \exp\left(\underbrace{\left(\theta_z - \theta_K\right)^T \cdot \mathbf{x}}_{\theta'_z}\right)}$$

$$= \frac{\exp\left(\theta_k'^{T} \cdot \mathbf{x}\right)}{1 + \sum_{z=1}^{K-1} \exp\left(\theta_z'^{T} \cdot \mathbf{x}\right)}$$



$\Downarrow$



Cross-entropy

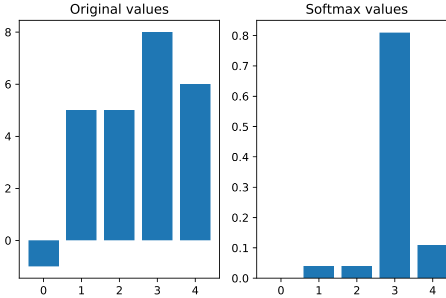
- The loss function for each sample is the cross-entropy

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

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

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

- Softmax "amplifies" the most probable class.



Assignement

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

In other words, show that

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

is equivalent to the binomial case

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

Then show that the loss function is also equivalent.

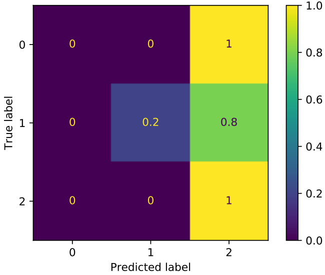
Let's code ...

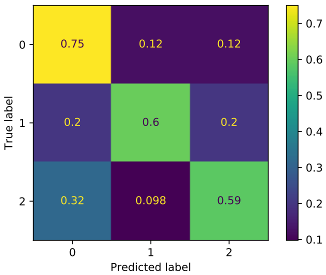
Go to notebook 03.regression_contd-and-classification.ipynb

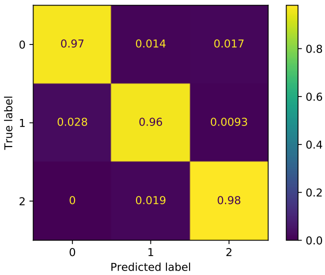
Section 6

Class imbalance and performance metrics

Confusion Matrix







Class imbalance

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

	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:

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

$$\uparrow \text{precision}, \uparrow \text{recall} \Longrightarrow \uparrow F_1$$

Regression (continued)

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

Classification

- Logistic Regression
- Classification Performance
- Class imbalance

To know more

- 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].

References I

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[CBHK02] N. Chawla, K. W. Bowyer, L. O. Hall, and W. P. Kegelmeyer, *SMOTE: Synthetic Minority Over-sampling Technique*, Journal of Artificial Intelligence Research **16** (2002), 321–357.

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[JWHT13] Gareth James, Daniela Witten, Trevor Hastie, and Robert Tibshirani, *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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[Mic] Microsoft, *Principles of Machine Learning | Loss Function for Classification*, https://youtu.be/r-vYJqcFxBI.

[Teo19] Jake Teo, *Data Science Documentation*, 2019.