Machine Learning

Lecture 6
Cross Validation and Feature Encoding

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2024

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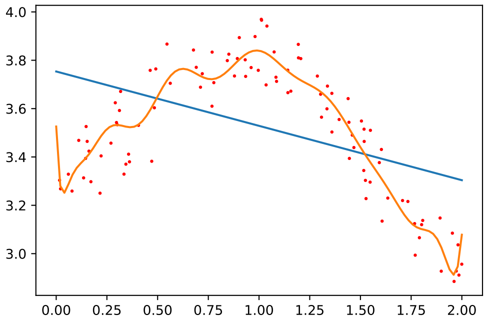
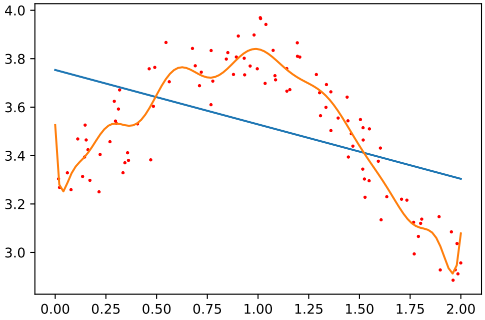
Over Fitting vs Under Fitting



Blue line is under fitting the data, or the model is biased towards solutions that will not explain the data.
Orange line is over-fitting the data, or the model has a high variance. It is trying to model the irregularities in the data.

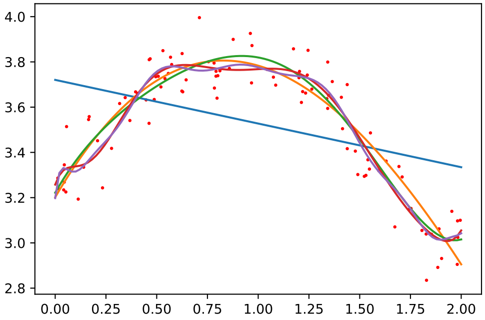
Intution behind high bias



- The basic intuition behind high bias is that the model is not sensitive enough to the training data set in use.
- If there's a slight change in the training data, the model will not change significantly.

Hence high bias . . .

Intution behind high variance



- The basic intuition behind high variance is that the predicted model is too sensitive to the training data set in use.
- If there's a slight change in the training data, the model will change significantly.

Hence high variance . . .

Case with Classification Models

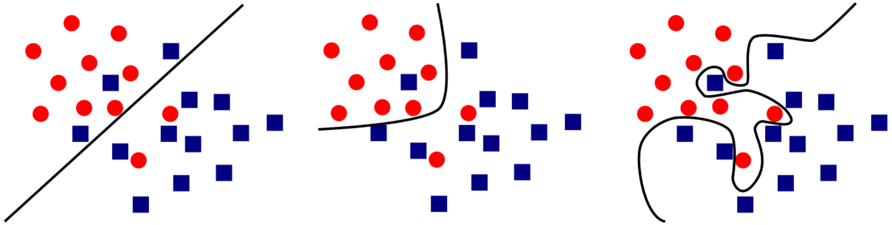


Figure: Under fitting, Just right and Over fitting in classification models

Training and Validation Data

What is the goal of machine learning?

- To predict future values of unknown data.

If you are doing statistics, then you could start making assumptions about your data and start proving theorems.
Machine learning is a often a bit different, you cannot always make sensible assumptions about the distribution of your data.

Training and Validation Data

- Ideally we would like to train our algorithm on all the available data and then evaluate the performance of the model on the future unknown data.
- Since we cannot really do this we have to fake it, by splitting our data into two parts: training and test data.

The function

```
sklearn.model_selection.train_test_split
```

is maybe one most important functions that you will use.

Training and Validation Data

- There are lots of reasons to split, but it avoids over-fitting. It avoids learning how to exactly predict how well you learned your training set.
- When you report how well your learning algorithm does, you should report the score on validation set and not the training set.
- You can compare several learning algorithms and compare their validation errors.
- Statistically it is all about reducing variance.

Training and Validation

- You might use different error metrics for the training and validation set. With logistic regression you would train the model by minimising

$$J(\theta) = \frac{1}{m} \sum_{i=1}^{m} -y \log(\sigma(h_\theta(x))) - (1-y) \log(1 - \sigma(h_\theta(x)))$$

  But you might evaluate the model using accuracy, precision, recall or the F-score from the confusion matrix.

Bias vs Variance

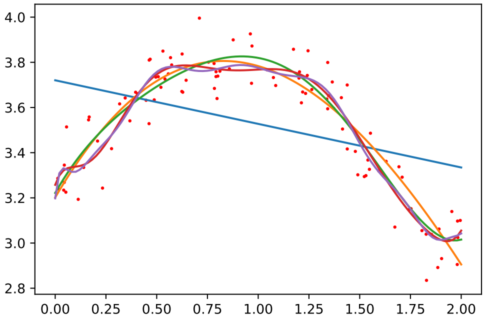
To do this properly you have to do statistics. The following definitions are not really water tight and are intended to give you some intuition.

Model Bias
: A model has high bias if the error/loss/cost function is high on the training data. It makes bad prediction on the training data.

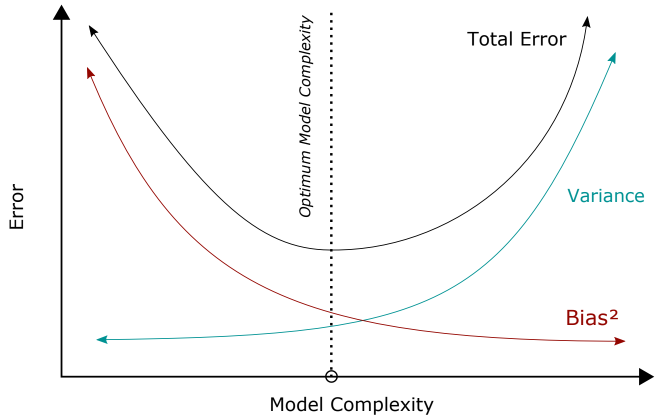
Model Variance
: A model has high variance if the error/loss/cost function is high on the test data compared with the training data.

Overfitting vs Bias again

If you have a series of models that get more and more complex, then how do you know when you are over fitting?



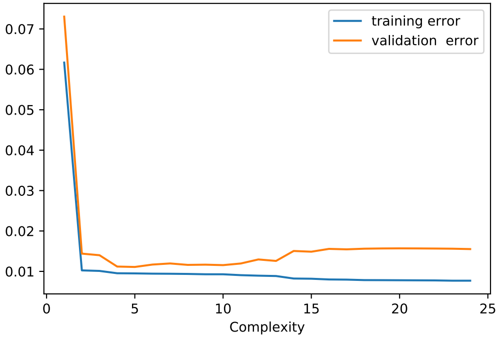
Bias variance trade off



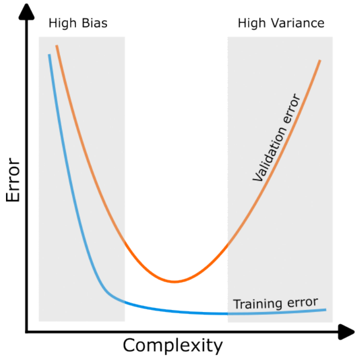
You want to find the sweet spot. Without advanced statistics or something like Bayesian based approaches it can be quite hard.

Overfitting vs Bias

Assuming that you have split the model into training and validation sets then you can look at training and validations errors as your models get more complicated. Andrew Ng calls this the elbow method.



Overfitting vs Bias



- If the test set error and the training set error is very high then you are probably under-fitting.
- When the training error gets smaller and smaller, but your test set error starts increasing you are probably over-fitting.

Overfitting vs Bias

There are lots of problems with this approach including:

- It is not always easy to judge the complexity of your model on a neat straight line.
- What if you picked the wrong division of your data into training and test sets?

Two Goals

Model Selection: estimating the performance of different models in order to chose the best one.

Model assessment: Having chosen a final model, estimate its prediction error on new data.

If we are doing model selection then there is a problem that we might overfit on the validation set.

Hyper parameters and Models

The terminology is a bit unclear but

Hyper-parameters These are parameters to the learning algorithm that do not depend on the data. They are often continuous values such as the regularisation parameter, but not always. Sometimes people refer to the choice of kernel as a hyper parameter.

- In a Bayesian framework it is possible to reason about the value of hyper parameters, but it can get quite complicated.
- The main problem with hyper parameters is that it is hard to use the data to optimise the values of the hyper-parameters.

Non-linear search spaces and other learning parameters

- With for example k-means clustering (see the next lecture), the final result you get also depends on the random initial starting points that you pick.
- There might be other learning parameters that affect how well you converge on a solution.
- The architecture of your neural network is very important.

Regularisation – Again

Regularisation is an attempt to stop learning too complex hypotheses. With linear regression and non-logistic regression we modified the cost function J

$$J(\theta) = \frac{1}{2m}\sum_{i=1}^{m}(h_\theta(x^{(i)}) - y^{(i)})^2 + \lambda\sum_{i=1}^{n}\theta_i^2$$

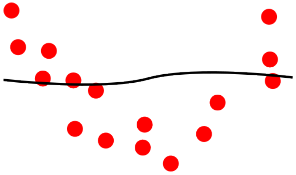
or

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m} -y\log(\sigma(h_\theta(x))) - (1-y)\log(1-\sigma(h_\theta(x))) + \lambda\sum_{i=1}^{n}\theta_i^2$$

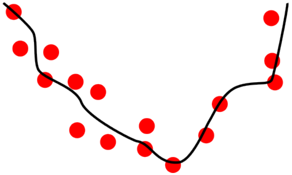
Increasing λ forces the optimisation to consider models with small weights. The λ term is something that you do not learn from the data.

Impact of λ on the model

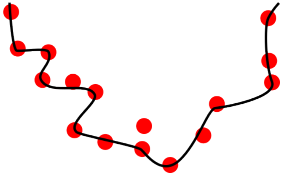
When minimizing the cost function, $\lambda > 0$ and it will penalize every feature weight in the model.



$\lambda = \sim 1000$



$\lambda = \mathit{optimal}$



$\lambda = \sim 0$

More features and Kernels

Yet more hyper parameters.

- Support Vector machines without kernels, linear regression and logistic regression can only learn linear hypotheses.
- Embedding your problem via a kernel function into a higher dimensional space to make the problem more linear is one way of making something learnable. For SVMs you have a lot of choice of different kernels and parameters.
- For linear and logistic regression you can try to invent non-linear features.

Hyper-parameters - Train — Validation — Test

If we have enough data then we can split out data into three parts:

Training	This is what we use to train our different algorithms. Typical split 50%.
Validation	This is what we use to choose our model and hyper-parameters. We pick the model with the best validation score. Typical split 25%.
Test	This is the data that you keep back until you have picked a model. You use this to predict how well you model will do on real data. Typical split 25%.

This avoids overfitting in the model selection. If you are comparing models then you use the validation set to pick the best model, but report the error score on the test set to give an indication on how well the model will generalise.

k-fold cross validation

What if we don't have enough data to split into three parts. Then we can use k-fold validation.

- Split your data randomly into k equal size parts.
- For each part, hold one back as a test set and train on the $k-1$ remaining parts, evaluate on the part you held back.
- Report the average evaluation and use this to set your hyper-parameters or to select the best model.

This effectively generates more training test splits out of your data. The random selection gives you statistically similar splits.

k-fold cross validation

If $k = 5$, then you have 5 parts $T_1, \ldots, T_5$ you would run 5 training runs

- Train on T_1, T_2, T_3, T_4 evaluate on T_5.
- Train on T_1, T_2, T_3, T_5 evaluate on T_4.
- Train on T_1, T_2, T_4, T_5 evaluate on T_3.
- Train on T_1, T_3, T_4, T_5 evaluate on T_2.
- Train on T_2, T_3, T_4, T_5 evaluate on T_1.

Good values of k are 5 or 10. Obviously the larger k is the more time it takes to run the experiments.

A Fold[3]

Sheep near a dry stone sheepfold, one of the oldest types of livestock enclosure.

[3] https://commons.wikimedia.org/wiki/File:Sheep_Fold.jpg

k-fold cross validation

What do you do after *k*-fold cross validation.

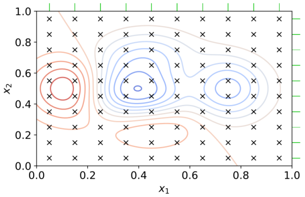
- Cross validation only returns a value that is a prediction of how well the model will do on more data.
- Assuming that you sample of the data is randomly drawn (not biased) then there are good statistical reasons why the *k*-fold valuation is a good idea.

k-fold cross validation

- Once you have decided which model or set of parameters to use, you then train a new model over the whole data set and use that for prediction.
- For example you could test if SVMs and Logistic regression on the same data-set and use *k*-fold cross validation to decide which model would perform best. Once you know this, you can then retrain on the whole data-set and use this model in production.

Estimating Hyper parameters — Grid Search[4]

Very simple idea choose some step size and divide you continuous parameters into a grid. Go through all the combinations and return the parameters that minimise the training error.



With a split into training and validation sets you can find close to optimal values for your hyper-parameters. Of course you will need to combine this with cross-validation to get something meaningful if you are comparing different models.

[4] https://de.wikipedia.org/wiki/Datei:Hyperparameter_Optimization_using_Grid_Search.svg

Summary of methods to avoid overfitting

- Add more training data.
- Regularisation.
- Feature selection. — regularisation will penalize features that are not useful
- Picking hyper-parameters via cross validation or training/validation/test split.

With some learning methods, stopping the training early is often a good way of avoiding over fitting.

Often, just thinking about what your model is doing is a good way.

Some feature engineering — One-Hot Encoding

Remember Categorical data is data that can take on a number of discrete values. For example if your data contains the type of car somebody drives:

- Audi
- Volvo
- Saab

You could pick some coding where you just assign a natural number to the each type of car

- Audi $= 0$
- Volvo $= 1$
- Saab $= 2$

Categorical Data

Car	Year	Sale
Audi	2000	No
Volvo	2001	Yes
Saab	2002	Yes
Saab	2003	Yes
Volvo	2000	No
Saab	2001	Yes
Audi	2002	No
Volvo	2003	Yes

One-Hot Encoding

- But what is special about the values 0,1 and 2? If you where trying to do some sort of regression then learning a weight that made sense.
- If x_c is your variable for your car type, then what sense does

$$h_\theta(x_c, \ldots) = \theta_c x_c + \ldots$$

even make?

One-Hot Encoding

Instead we use binary 0/1 variables to represent the categorical variables.
In our example we would have three variables

- x_a equals 1 if the car is an Audi and 0 otherwise
- x_v equals 1 if the car is an Volvo and 0 otherwise
- x_s equals 1 if the car is an Saab and 0 otherwise

Note that Scikit Learn has functions to do this automatically for you.

One-Hot Encoding

With our binary variables our models are easier to learn

$$h_\theta(x_a, x_v, x_s, \ldots) = \theta_a x_a + \theta_v x_v + \theta x_s$$

One-Hot Encoding

Car	Year	Sale
Audi	2000	No
Volvo	2001	Yes
Saab	2002	Yes
Saab	2003	Yes
Volvo	2000	No
Saab	2001	Yes
Audi	2002	No
Volvo	2003	Yes

$\Rightarrow$

Audi	Volvo	Saab	Year	Sale
1	0	0	2000	0
0	1	0	2001	1
0	0	1	2002	0
0	0	1	2003	1
0	1	0	2000	0
0	0	1	2001	1
1	0	0	2002	0
0	1	0	2003	1

Label Encoding

Car	Year	Sale
Audi	2000	No
Volvo	2001	Yes
Saab	2002	Yes
Saab	2003	Yes
Volvo	2000	No
Saab	2001	Yes
Audi	2002	No
Volvo	2003	Yes

$\Rightarrow$

Car	Year	Sale
0	2000	0
1	2001	1
2	2002	1
2	2003	1
1	2000	0
2	2001	1
0	2002	0
1	2003	1

where 0 = Audi, 1 = Volvo, 2 = Saab and 0 = No, 1 = Yes

Target Encoding

Car	Year	Sale
Audi	2000	No
Volvo	2001	Yes
Saab	2002	Yes
Saab	2003	Yes
Volvo	2000	No
Saab	2001	Yes
Audi	2002	No
Volvo	2003	Yes

$\Rightarrow$

Car	Year	Sale
0	2000	0
0.67	2001	1
1	2002	1
1	2003	1
0.67	2000	0
1	2001	1
0	2002	0
0.67	2003	1

- Bayesian target Encoding *(Overfitting . . .)*
- K-Fold target Encoding