Statistical Natural Language Processing

Machine learning: evaluation

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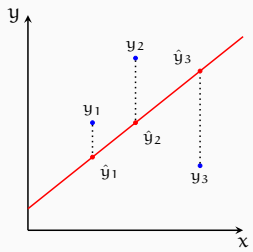
Measuring success/failure in regression

Root mean squared error (RMSE)

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_i^n (y_i - \hat{y}_i)^2}$$

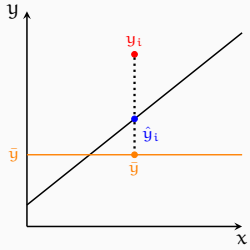


- Measures average error in the units compatible with the outcome variable

Measuring success/failure in regression

Coefficient of determination

$$R^2 = \frac{\sum_i^n (\hat{y}_i - \bar{y})^2}{\sum_i^n (y_i - \bar{y})^2} = 1 - \frac{\text{MSE}}{\sigma_y^2}$$



- r^2 is a standardized measure in range $[0, 1]$
- Indicates the ratio of variance of y explained by x
- For single predictor it is the square of the correlation coefficient r

Measuring success in classification

Accuracy

- In classification, we do not care (much) about the average of the error function
- We are interested in how many of our predictions are correct
- Accuracy measures this directly

$$\text{accuracy} = \frac{\text{number of correct predictions}}{\text{total number of predictions}}$$

Accuracy may go wrong

- Think about a 'dummy' search engine that always returns an empty document set (no results found)
- If we have
  - 1 000 000 documents
  - 1000 relevant documents (including the term in the query)

  the accuracy is:

$$\frac{999\,000}{1\,000\,000} = 99.90\,\%$$

- In general, if our class distribution is *skewed* accuracy will be a bad indicator of success

Measuring success in classification

Precision, recall, F-score

$$\text{precision} = \frac{TP}{TP + FP}$$

$$\text{recall} = \frac{TP}{TP + FN}$$

$$F_1\text{-score} = \frac{2 \times \text{precision} \times \text{recall}}{\text{precision} + \text{recall}}$$

		true value	
		positive	negative
predicted	pos.	TP	FP
	neg.	FN	TN

Example: back to the search engine

- We had a 'dummy' search engine that returned false for all queries
- For a query
  - 1 000 000 documents
  - 1000 relevant documents

$$\text{accuracy} = \frac{999\,000}{1\,000\,000} = 99.90\,\%$$

$$\text{precision} = \frac{0}{1\,000\,000} = 0\,\%$$

$$\text{recall} = \frac{0}{1\,000\,000} = 0\,\%$$

Precision and recall are asymmetric,
the choice of the 'positive' class is important.

Classifier evaluation: another example

Consider the following two classifiers:

		true value		true value	
		positive	negative	positive	negative
predicted	pos.	7	9	1	3
	neg.	3	1	9	7

Accuracy both $8/20 = 0.4$
Precision $7/16 = 0.44$ and $1/4 = 0.25$
Recall $7/10 = 0.7$ and $1/10 = 0.1$
F-score 0.54 and 0.14

Multi-class evaluation

- For multi-class problems, it is common to report average precision/recall/f-score
- For C classes, averaging can be done two ways:

$$\text{precision}_M = \frac{\sum_i^C \frac{TP_i}{TP_i+FP_i}}{C} \qquad \text{recall}_M = \frac{\sum_i^C \frac{TP_i}{TP_i+FN_i}}{C}$$

$$\text{precision}_\mu = \frac{\sum_i^C TP_i}{\sum_i^C TP_i + FP_i} \qquad \text{recall}_\mu = \frac{\sum_i^C TP_i}{\sum_i^C TP_i + FN_i}$$

(M = macro, μ = micro)

- The averaging can also be useful for binary classification, if there is no natural positive class

Confusion matrix

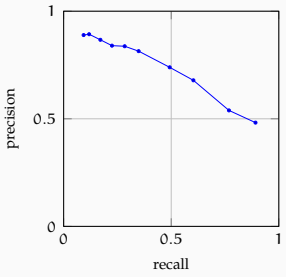
- A confusion matrix is often useful for multi-class classification tasks

		true class		
		a	b	c
predicted	a	10	3	4
	b	2	12	8
	c	0	7	7

- Are the classes balanced?
- What is the accuracy?
- What is per-class, and averaged precision/recall?

Precision–recall trade-off

- Increasing precision (e.g., by changing a hyperparameter) results in decreasing recall
- Precision–recall graphs are useful for picking the correct models
- *Area under the curve* (AUC) is another indication of success of a classifier



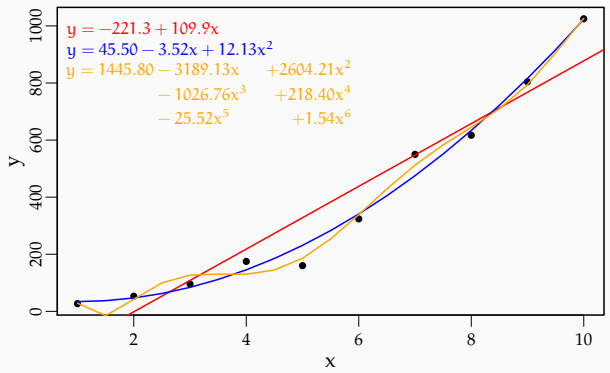
Performance metrics a summary

- Accuracy does not reflect the classifier performance when class distribution is skewed
- Precision and recall are binary and asymmetric
- For multi-class problems, calculating accuracy is straightforward, but others measures need averaging
- These are just the most common measures: there are more
- You should understand what these metrics measure, and use/report the metric that is useful for the purpose

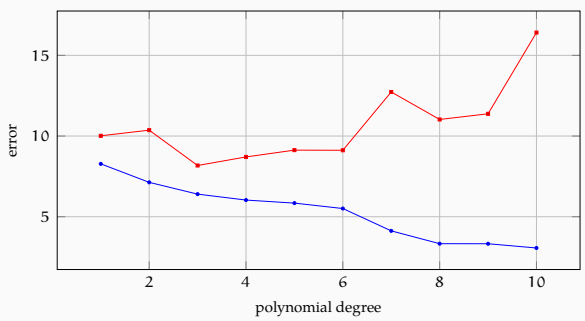
Model selection/evaluation

- Our aim is to fit models that are (also) useful outside the training data
- Evaluating a model on the training data is wrong: complex models tend to fit to the noise in the training data
- The results should always be tested on a test set that does not overlap with the training data
- Test set is ideally used only once - to evaluate the final model
- Often, we also need to tune the model, find best *hyperparameters* (e.g., regularization constant)
- Tuning has to be done on a separate development set

Back to polynomial regression



Training/test error



Bias and variance (revisited)

Bias of an estimate is the difference between the value being estimated, and the expected value of the estimate

$$B(\hat{\boldsymbol{w}}) = E[\hat{\boldsymbol{w}}] - \boldsymbol{w}$$

- An *unbiased* estimator has 0 bias

Variance of an estimate is, simply its variance, the value of the squared deviations from the mean estimate

$$\text{var}(\hat{\boldsymbol{w}}) = E\left[(\hat{\boldsymbol{w}} - E[\hat{\boldsymbol{w}}])^2\right]$$

$\boldsymbol{w}$ is the parameters that define the model

Bias–variance relationship is a trade-off:
models with low bias result in high variance.

Some issues with bias and variance

- *Overfitting* occurs when the model learns the idiosyncrasies of the training data
- *Underfitting* occurs when the model is not flexible enough for the data at hand
- Complex models tend to overfit – and exhibit high variance
- Simple models tend to show low variance, but likely to have (high) bias

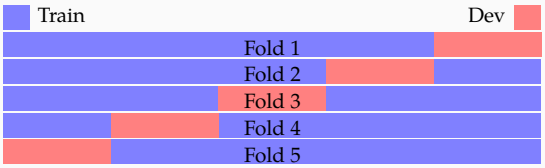
Model selection & hyperparamater tuning

- Our aim is to reduce the test error
- We can estimate the test error on a *development set*, or *held-out* data:
  - Split the data at hand as *training* and *development* set
  - Train alternative models (different hyperparameters) on the training set
  - Choose the model with best development set performance

Cross validation

- To avoid overfitting, we want to tune our models on a *development set*
- But (labeled) data is valuable
- Cross validation is a technique that uses all the data, for both training and tuning with some additional effort
- Besides tuning hyper-parameters, we may also want to get 'average' parameter estimates over multiple folds

K-fold Cross validation



- At each fold, we hold part of the data for testing, train the model with the remaining data
- Typical values for k is 5 and 10
- In *stratified* cross validation each fold contains (approximately) the same proportions of class labels.
- A special case, when k is equal to n (the number of data points is called *leave-one-out cross validation*

The choice of k in k-fold CV

- Increasing k
  - reduces the bias: the estimates converge to true value of the measure (e.g., accuracy) in the limit
  - increases the variance: smaller held-out sets produce more varied parameter estimates
  - is generally computationally expensive
- 5- or 10-fold cross validation is common practice (and found to have a good balance between bias and variance)

Comparing with a basline

- The performance measures are only meaningfull if we have something to compare against

random	does the model do anything useful at all?
majority class	does the classifier better than predicting the majority class all the time?
state-of-the-art	how does your model compare against known (non-trivial) models?

- Diferences between models are reliable only if the same data set is used
- Differences are stable if your test set size is large enough
- Use statistical tests when comparing different models/methods

Summary

The first principle is that you must not fool yourself and you are the easiest person to fool. – Richard P. Feynman

- The measures of success in ML systems include
  - RMSE / r^2
  - Accuracy
  - Precision / recall / F-score
- We want models with low bias and low variance
- Evaluating ML system requires special care:
  - Never use your test set during training / development
  - Tuning your system on a development set
  - Cross-validation allows efficient use of labeled data

Next:

- Have good holiday! We'll start with sequence learning after the break.