Tutorial 2

Decision Tree, Cross-validation, Precision and Recall

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Mar. 2021

Objectives

1. Evaluation Metrics: Accuracy, Precision, Recall and F1 score
2. ROC curve and AUC
3. Should you trust the results?
4. Parametric Tests VS. Non-parametric Tests
5. Regression and Least Square Problem
6. Ensemble Methods

Confusion Matrix

Confusion Matrix can be applied to **binary** classification as well as for **multiclass** classification problems.

		Predicted	
		Positive	**Negative**
Actual	**Positive**	True Positive	False Negative
	Negative	False Positive	True Negative

- True Positive (TP): Correctly classified.
- True Negative (TN): Correctly rejected.
- False Positive (FP): Incorrectly classified. Type I Error.
- False Negative (FN): Incorrectly rejected. Type II Error.

$$\text{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}}$$

Confusion Matrix

How many selected items are relevant? Selected Elements $= \mathrm{TP} + \mathrm{FP}$

$$\text{Precision (P)} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

How many relevant items are selected? Relevant Elements $= \mathrm{TP} + \mathrm{FN}$

$$\text{Recall (R)} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

F_1 score is the **harmonic mean** between Precision and Recall.

$$F_1 = 2 \times \frac{P \times R}{P + R}$$

Example – Weather Prediction

Build a logistic regression model to predict the weather based on the humidity.
Recorded 10 days in total.

Class	Prediction
P	P
N	P
P	N
P	P
N	P
P	P
N	P
N	N
N	N
P	P

Caveat: A model with high Recall may also has high FPR (Type I Error).

		Predicted P	Predicted N	Total
Actual	**P**	4	1	5
	N	3	2	5
	Total	7	3	**10**

$$\text{Acc.} = \frac{6}{10} = 0.6$$

$$\text{Precision (P)} = \frac{\text{TP}}{\text{TP}+\text{FP}} = \frac{4}{4+3} \approx 0.571$$

$$\text{Recall (R)} = \frac{\text{TP}}{\text{TP}+\text{FN}} = \frac{4}{4+1} \approx 0.8$$

$$F_1 = 2\frac{P \times R}{P+R} = 2 \times \frac{0.571 \times 0.8}{0.571+0.8} \approx 0.667$$

Precision-Recall (PR) Curve (Optional)

Average precision (AP) summarizes such a plot as the weighted mean of precisions achieved at each threshold.

$$AP = \sum_n (R_n - R_{n-1}) P_n$$

- Where P_n and R_n are the precision and recall at the n-th threshold.
- A pair (P_n, P_k) is referred to as an *operating point*.

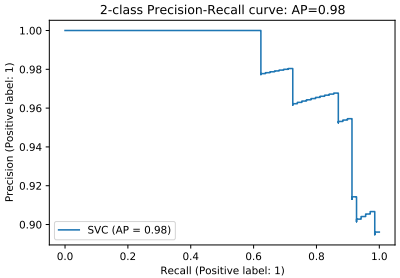


Figure: A SVM classifier trained on the Breast Cancer dataset

Receiver Operating Characteristic (ROC) Curve

- The ROC curve is created by plotting the true positive rate (TPR) against the false positive rate (FPR) at various threshold settings.
- Area Under Curve (AUC): The integration of the ROC function between 0 and 1.

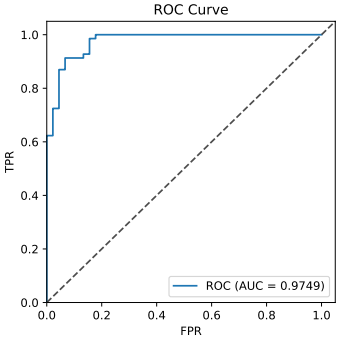


Figure: A SVM classifier trained on the Breast Cancer dataset

Example – Weather Prediction

Build a logistic regression model to predict the weather based on the humidity.
Recorded 10 days in total.

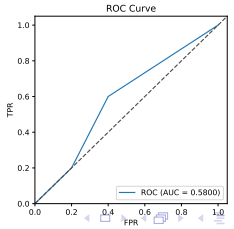
		Thresholds					
Class	**Prediction**	**0**	**0.2**	**0.4**	**0.6**	**0.8**	**1**
P	0.95	1	1	1	1	1	0
N	0.85	1	1	1	1	1	0
P	0.78	1	1	1	1	0	0
P	0.66	1	1	1	1	0	0
N	0.6	1	1	1	1	0	0
P	0.55	1	1	1	0	0	0
N	0.53	1	1	1	0	0	0
N	0.52	1	1	1	0	0	0
N	0.51	1	1	1	0	0	0
P	0.4	1	1	1	0	0	0

Counting TP and FP:

Threshold	**0**	**0.2**	**0.4**	**0.6**	**0.8**	**1**
TPR	1	1	1	0.60	0.2	0
FPR	1	1	1	0.4	0.2	0

Sort the results:

Threshold	**0**	**0.2**	**0.4**	**0.6**	**0.8**	**1**
TPR	0	0.2	0.6	1	1	1
FPR	0	0.2	0.4	1	1	1



Should you trust the results?

Scenario 1 from Page 48 in Week 2 slides

- I built a model based on the data you gave me
- It classified your data with 98% accuracy
- It should get 98% accuracy on the rest of your data

Should you trust them?

- They are reporting training error
- This might have nothing to do with test error
- E.g., They could have
  t a very deep decision tree

Why?

- If they only tried a few very simple models, the 98% might be reliable
- E.g., They only considered decision stumps with simple 1-variable rules

Should you trust the results?

Scenario 2 from Page 49 in Week 2 slides

- I built a model based on half of the data you gave me
- It classified the other half of the data with 98% accuracy
- It should get 98% accuracy on the rest of your data

Probably

- They computed the validation error once
- This is an unbiased approximation of the test error
- Trust them if you believe they did not violate the golden rule

Should you trust the results?

Scenario 4 from Page 51 in Week 2 slides

- I built 1 billion models based on half of the data you gave me
- One of them classified the other half of the data with 98% accuracy
- It should get 98% accuracy on the rest of your data

Probably not

- They computed the validation error a huge number of times
- They tried so many models, one of them is likely to work by chance

Why?

- If the 1 billion models were all extremely-simple, 98% might be reliable.

Regression and Least Square Problem

There are n samples, each sample has d features

$$w = \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix}, y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, x_i = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$$

X is a matrix which represents all samples. Such that:

$$\hat{y} = Xw = \begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix} = \begin{bmatrix} x_{11} & \cdots & x_{1d} \\ \vdots & \ddots & \vdots \\ x_{n1} & \cdots & x_{nd} \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix} = \begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_n \end{bmatrix}$$

Mean Squared Error:

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Cross Validation Questions

Question 1

If you do 2-fold cross validation, 10-fold cross validation or leave-one-out, or use a 70/30 percent train/validation single split. What effect will this have on your results?

- Leave-one-out means that you have a bigger training set and a bigger validation set. Also you have N repetitions where N is the size of your dataset.
- 2-fold gives you a much smaller training set but a bigger validation set. A bigger validation set is good but a smaller training set is not – high bias.
- 10-fold validation gives you a bigger training set but an even smaller validation set than 2-fold – high variance.

Question 2

Which will give you the best representative value to the "unseen test set"?

Probably leave-one-out, with 2-fold the training set might be too small and with 10-fold then validation set might be too small, but tenfold is typically better than 2-fold.

Cross Validation Questions

Question 3

Does it matter how large your original dataset is?
Will you get a different answer for a very big or a very small dataset?

- For a very big dataset – all will probably give you the same answer
- For a very small dataset – you would probably have to do 10-fold or leave-one-out to get good results

Question 4

Which will be the fastest in terms of computation?

- Leave-one-out is the most expensive, you have to learn N models.
- 10-fold CV means you need to learn 10 models and 2-fold means you have to learn 2 models.

Ensemble Questions

Question 1

What are the two key factors an ensemble must have?

- Each tree must perform better than random guess/ average.
- Must be uncorrelated.

Question 2

Which will be the fastest in terms of computation?

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Ensemble Questions

Question 3

Does Error Correcting code work better when there are many classes or when there are few? Why?

It will work better with many classes with 3 classes there are very few codes.

Question 4

4. If you are going to choose with replacement can you then make your training set as big as you want? Will this work?

You cannot make a million instances out of 100, but if you are short on data you can use this to try and bolster your results – especially in ensembles.

Ensemble Questions

Question 5

What is one of the main differences between random forest and bagging?

- What will the effect be of having a dataset with a larger or smaller number of instances?
- What will the effect be of having a dataset with a larger or smaller number of features?

Ensemble Questions

Question 5

What is one of the main differences between random forest and bagging? Random forest samples the features.

- What will the effect be of having a dataset with a larger or smaller number of instances?
  The effect on bagging and random forest will be the same – they both sample the instance space with replacement.
- What will the effect be of having a dataset with a larger or smaller number of features?
  Since random forests sample the features you might get better results when there are a lot of features because you got rid of a lot of noise – but with a data set with only a few features you might do worse because you are not left with enough features to make a good classifier

Ensemble Questions

Question 6

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Which of the "methods for constructing ensembles" does random forest use?

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Question 7

Which of the "methods for constructing ensembles" does random forest use?

Manipulating the training set, Manipulating the input features (columns), Injecting Randomness

Ensemble Questions

Question 8

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Question 9

What is one of the main differences between XG Boost and Random Forests?

Ensemble Questions

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Question 9

What is one of the main differences between XG Boost and Random Forests?

XG Boost chooses without replacement so does not change the distribution of the dataset – also Boosting will have to use a smaller training set by definition; also RF uses democratic voting and XG Boost uses weighted voting

Ensemble Questions

Question 10

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AdaBoost weights the data instances, and XGBoost weights the trees added into the ensemble – non-democratic voting.