A Practical Introduction to Machine Learning in Python Day 4 – Thursday »Supervised Machine Learning«

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Today

The problem of overfitting

Train/validation/test split

Cross-validation

Finding the optimal (hyper-)parameters

Grid search

A typical case for gridsearch: The regularization parameter C

More suggestions for improving your models

Tuning decision thresholds with ROC curves

Exercise

Also re-read chapter 8.5!



Everything clear from this morning?

The problem of overfitting



Isn't training multiple models and then selecting the best one a bit like p-hacking?

Yes. We call this problem "overfitting".

The problem of overfitting

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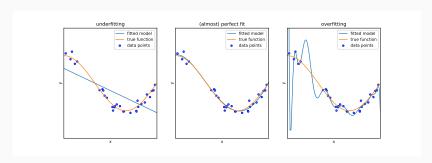


Figure 1: Underfitting and overfitting. Example adapted from https://scikit-

learn.org/stable/auto examples/model selection/plot underfitting overfitting

How to avoid overfitting

- 1. Train/test split. We already do this. It avoids overfitting on the training data.1

¹In classical statistics, the R^2 of an OLS regression is prone to that. Calculating R^2 on a separate test set would be much more conservative.

How to avoid overfitting

The problem of overfitting

- 1. Train/test split. We already do this. It avoids overfitting on the training data.1
- 2. Train/validation/test split. But maybe we overfit on the test data now? We could set aside third dataset.

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How to avoid overfitting

- 1. Train/test split. We already do this. It avoids overfitting on the training data.1
- 2. Train/validation/test split. But maybe we overfit on the test data now? We could set aside third dataset.
- 3. k-fold crossvalidation. Extending the above such that every case is sometimes k-1 times part of the training data and 1 time part of the validation data.

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- 3. k-fold crossvalidation. Extending the above such that every case is sometimes k-1 times part of the training data and 1 time part of the validation data.
- 4. Regularization. (in combination with the above) We "penalize" models for being too complex.

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The problem of overfitting

Train/validation/test split

Train/validation/test split

- When you compare a lot of different models (or (hyper-)parameters), you might want to evaluate (compare) them using a third dataset
- e.g., make 80/20 split (train/test); then split first part again 80/20 (train/validation)
- only use the test data at the very end to get a final estimate of how good your model is.

<u>Train/</u>validation/test split

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In short: Validation data to *select* the best approach; test data to get the accuracy of the approach you chose.

The problem of overfitting

Cross-validation

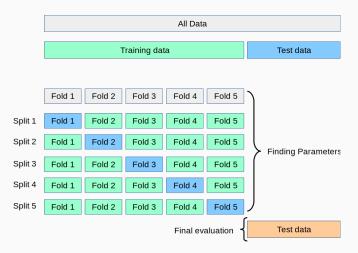


Figure 2: First, we set aside a test dataset for the final evaluation. Then, we split our data into k=5 folds, where each fold is used for validation once (blue) and k-1=4 times for training. $s_{ource:}$ https://scikit-learn.org/stable/_images/grid_search_cross_validation.png

Cross-validation

The problem of overfitting

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```
from sklearn.model_selection import cross_val_score
from sklearn.naive_bayes import MultinomialNB
nb = MultinomialNB() # the classifier we trained last week
scores = cross_val_score(nb, train_features, [r[1] for r in reviews], cv =10)
print(scores)
```

results in:

```
1 [0.858 0.8612 0.8516 0.8528 0.8672 0.8664 0.8576 0.8652 0.8436 0.852 ]
```

We estimate the model 10 times on different trainig/validation data splits and get 10 different evaluation scores (here: accuracy, but we can use precision, recall, F1, etc. – see examples in the book).

Note that a simple 50:50 train/validation split is identical to setting k = 2

Reasons to do Cross-validation

We can get confidence intervals around the scores

- If we have 10 scores instead of one, we can not only get the mean, but also a standarddeviation
- If you have two models, both with a mean accuracy (or F1, or whatever) of .85 but one with a large and one with a low standard deviation, you probably prefer the latter — it generalizes better, less likely to suffer from overfitting

Reasons to do Cross-validation

We do not "waste" too much validation data

- If k = 10 (the most typical value), in each iteration, we use 90% of the data for training.
- We even use all data (except test set, of course) for training at least once.
- With train/validation split, we probably need a larger validation set to be sure (e.g., 80/30)
- Especially relevant when annotation is expensive.

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The problem of overfitting

Simple train/test split

- introductory examples/pedagical reasons
- really small dataset where you cannot afford to set aside validation data
- if for whatever reason you do not compare different models and settings.

Takeaway ii

Train/validation/test split

- To compare different model configurations without overfitting on the test data
- Pedacogical reasons, simple start
- Very large datasets or very complex models where setting k > 2 would lead to prohibitively expensive computations

Takeaway m

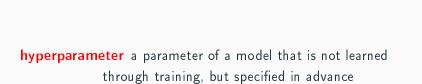
k-fold crossvalidation

 Best option for comparing multiple models, especially when engaging in hyperaparameter tuning (next section)

In other words: whether you have or create a train/validation/test or use cross-validation — just make sure you always set aside one test set for final evaluation that you have never used before.

Finding the optimal

(hyper-)parameters



Finding the optimal

(hyper-)parameters

Grid search

Hyperparameter optimization with grid search

General idea

Rather than arbitrary trying some configurations, let's systematically test and compare.

First idea: Use a for-loop! (Example 11.4 in the book)

```
configurations =
   [('NB with Count', CountVectorizer(min_df=5, max_df=.5), MultinomialNB()
         ),
   ('NB with TfIdf', TfidfVectorizer(min_df=5, max_df=.5), MultinomialNB())
    ('LogReg with Count', CountVectorizer(min_df=5, max_df=.5),
         LogisticRegression(solver='liblinear')),
    ('LogReg with TfIdf', TfidfVectorizer(min_df=5, max_df=.5),
5
         LogisticRegression(solver='liblinear'))]
6
    for description, vectorizer, classifier in configurations:
7
       print(description)
8
9
       X_train = vectorizer.fit_transform(reviews_train)
       X_test = vectorizer.transform(reviews_test)
10
       classifier.fit(X_train, y_train)
11
       y_pred = classifier.predict(X_test)
12
13
       short_classification_report(y_test, y_pred)
14
       print('\n')
```

(where (X_test, y_test) hopefully refers to a validation dataset with another test dataset set aside)

- could simply state this instead of manually creating the list?

A wishlist

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- (especially if we had (NB|LogReg) \times (count|tf· idf) \times (min df=5|min df=1) × (max df=.5|max df=.8 $[\max df=.9) = 2 \times 2 \times 2 \times 3 = 24 \text{ options}]$

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A wishlist

We now tested 2×2 combinations: (NB|LogReg) \times (count|tf· idf).

Wouldn't it be nice if we...

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That's what scikit-learn's gridsearch functionality does! (and the second bullet point is called the grid)

Gridsearch is especially useful for hyperparameter optimization, such as trying out different values for min_df and max_df on the previous slide.

You could also use a combined approach where you first use a handwritten loop to narrow down the number of candidate models and then tune the model(s) you settled on with a grid search.

Finding the optimal (hyper-)parameters

(nyper-)parameters

regularization parameter C

A typical case for gridsearch: The

The regularization parameter λ (or $C = .5n\lambda$)

$$\underset{\beta}{\operatorname{arg\,min}} \left[\sum_{i=1}^{n} \left(Y_i - \beta_0 - \sum_{j=1}^{p} \beta_j X_{ji} \right)^2 + \lambda \sum_{j=1}^{p} \left| \beta_j \right|^q \right]$$

We estimate the β -coefficients of a model by optimizing a so-called loss function, i.e minimizing the "cost" that occurs when the prediction is wrong.

If we simply add the sum of the β coefficients to the model, we "punish" large coefficients.

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If λ is larger, we punish more.

If q=1, we call it L1 regularization. If we add the squared coefficients (q=2), we call it L2 regularization.

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- As always, there is a lot of extra info on the scikit-learn website



How harsh should the penalty be?

Hyperparameter optimization with grid search

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- Think of this term as a penalty for overfitting
- How much weight should our penalty carry? That's determined by a constant, C.

• How to determine the best $C? \Rightarrow \text{grid search}$

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Hyperparameter optimization with grid search

Finding C in a logistic regression using 5-fold cross-validation

- from sklearn.linear_model import LogisticRegressionCV
- logregCV = LogisticRegressionCV(cv=5).fit(train_features, [r[1] for r in reviews])

Finding C in a logistic regression using 5-fold cross-validation

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 - Here, we just need to use LogisticRegressionCV instead of LogisticRegression.
 - But we can use it to test any combination of choices

reviews])

Hyperparameter optimization with grid search

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- Here, we just need to use LogisticRegressionCV instead of LogisticRegression.
- But we can use it to test any combination of choices

```
pipeline = Pipeline(steps = [('vectorizer', TfidfVectorizer()), (')
         classifier', LogisticRegression(solver='liblinear'))])
   grid = {
        'vectorizer__ngram_range' : [(1,1), (1,2)],
3
       'vectorizer__max_df': [0.5, 1.0],
4
       'vectorizer__min_df': [0, 5],
5
       'classifier__C': [0.01, 1, 100]
6
7
8
9
    search = GridSearchCV(estimator=pipeline,
10
                        param_grid=grid,
                        scoring='accuracy',
11
12
                       cv=5.
13
                        n_jobs=-1, # use all cpus
                        verbose=10)
14
    search.fit(reviews_train, y_train)
15
    print(f'Using these hyperparameters {search.best_params_}, we get the
16
         best performance: ')
    print(short_classification_report(y_test, search.predict(reviews_test)))
17
```

Example 11.6 (book)

Note that the grid is specified as a dictionary where the keys are strings with the name of the step in the pipeline followed by two underscores followed by the parameter to tune, and the values are lists of values.

This means that any parameter that the classifier or vectorizer takes can be tuned!

The pipeline notation in scikit learn

You might have notived the Pipeline construct in the last example.

- Machine learning involves multiple steps (e.g., preprocessing \rightarrow vectorizer \rightarrow classification)
- We did all of them seperately before
- Nothing wrong with that, but to ease use and evaluation of the whole process (as needed for the gridsearch), we can define a pipeline.

Example with a pipeline (and add cross-validation)

```
1
    from sklearn.feature_extraction.text import TfidfVectorizer
    from sklearn.linear_model import LogisticRegressionCV
3
    from sklearn.pipeline import make_pipeline
4
    vec = TfidfVectorizer()
    clf = LogisticRegressionCV()
    pipe = make_pipeline(vec, clf)
7
8
    pipe.fit([r[0] for r in reviews], [r[1] for r in reviews])
    predictions = pipe.predict([r[0] for r in test])
10
```

- In principle, just a different way to write what we already did
- ullet The more steps, the more relevant (e.g., preprocessing ovectorizer \rightarrow dimensionality-reduction \rightarrow classification)
- The more you rely on automated evaluation (e.g., grid search) of *multiple* steps in the pipeline, the more useful it is

Grid-search takeaway

- When you want to systematically test what happens when you vary a hyperparameter, use grid-search to automatically do so and select the best value

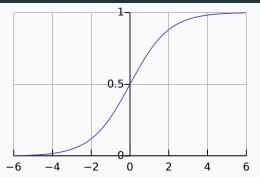
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Grid-search takeaway

- When you want to systematically test what happens when you vary a hyperparameter, use grid-search to automatically do so and select the best value
- sometimes already implemented (e.g., LogisticRegressionCV as direct replacement for LogisticRegression)
- But GridSearchCV is very flexible: can be used in combination with pipeline (wait a minute...) for very different purposes

curves

Tuning decision thresholds with ROC



In logistic regression, we use the sigmoid function to transform the estimates into probabilities.

To transform the probabilities into binary labels, we use a cutoff (default: 0.5).

- It makes most sense (intuitively, mathematically)

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- Maybe it is importance to us that our classifier is balanced and equally good in predicting both classes, even if overall accuracy suffers (slightly)

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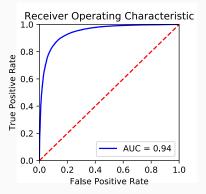
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Why use 0.5 as cutoff?

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Let's see what happens if we plot False Positives against True Positives (ROC-curve)

ROC Curve



- If we choose a threshold such that we get very little false positives, we also get too little true positives.
- Optimum in the upper left corner

So, how to we determine the exact value?

See notebook

https://github.com/damian0604/bdaca/blob/master/12ec/ week 10/Determining %20the %20cutoff-point %20in %20logistic % 20 regression.ipynb

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Some further ideas to look into

Balancing classes

Your classifier probably works better if you have approximately the same amount of annotated training data for both classes (e.g., pos/neg). If getting such data is not an option, you may consider weighing accordingly, e.g. using

LogisticRegression(class_weight='balanced')

More advanced pipelines

Consider constructing advanced pipelines, including a dimension reduction step:

https://scikit-learn.org/stable/tutorial/statistical_inference/ putting together.html

Some further ideas to look into

Combine different feature sets

E.g., use BOW-features as well as features such as sentence length, number of sentences (or whatever)

https://scikit-learn.org/stable/auto examples/hetero feature union.html

Exercise



Any questions?

- Try it yourself! Ideally, on own data! (can also be via Google Dataset Search, Kaggle, ...)
- But you are also free to use datasets from this morning.

Learning goals:

- Apply techniques to new datasets.
- Be able to construct the whole pipeline from ingesting via preprocessing to final prediction

Exercise 0000

Let's exercise!