Big Data and Machine Learning with Python

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Feature Engineering, Model Selection and Pipelining

Feature Engineering

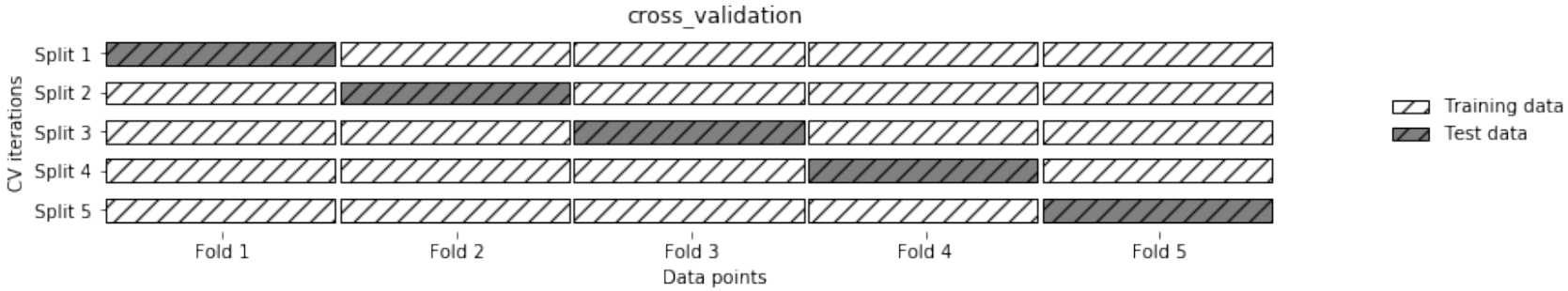
1. Categories into dummies (One-Hot-Encoding)
2. Continuous variables into dummies representing groups (Binning and Discretization)
3. Polynomials
4. Combinations

Cross-Validation

- Learned weights likely specific to training set
- Estimates of generalization affected by random split into training and test
- Solution: Repeat learning on different splits

! ***!! ALWAYS !!*** use this

Cross-Validation, cont.



from: Andreas Müller and Sarah Guido (2016): Introduction to Machine Learning with Python, O'Reilly

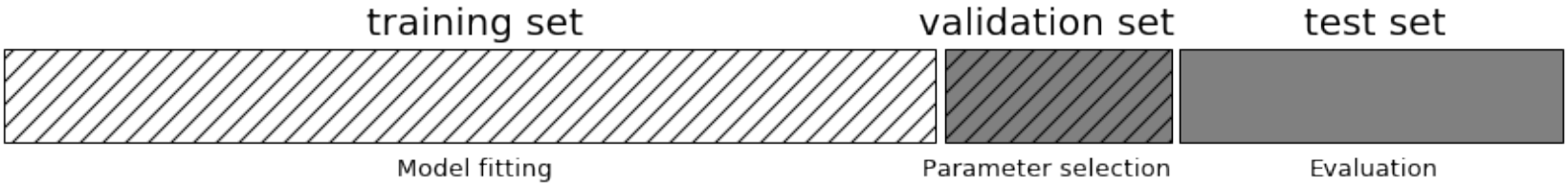
Cross-Validation strategies

- k-Fold CV: Split evenly into k data points, pick one as test set and the rest as training set, repeat k times (data can be shuffled first)
- Stratified k-Fold: Split data k times such that proportions between classes are similar across folds
- Leave-one-out CV: Set K equal to the number of observations
- Shuffle-split CV: In each fold, split data into fixed shares for training and test set (which do not need add up to 1)

Grid Search

- Loop over different combinations of parameters
- Keep the best performing parameter combinations returning
- IMPORTANT: Don't evaluate parameters on training set, but on distinct *validation set*

Validation set



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- Necessary to evaluate parameter combinations on unseen data
- ... for the same reason you do generalize on unseen data, too
- Simply split training set again

Grid Search with Cross Validation

- `GridSearchCV(estimator, param_grid)` (→ Documentation)
  - `estimator` is model class (i.e. `MLPerceptron()`)
  - `param_grid` is dict or list of dict
  - Optionally specify desired evaluation score and CV strategy

Grid Search with Cross Validation

- `GridSearchCV(estimator, param_grid)` (→ Documentation)
  - `estimator` is model class (i.e. `MLPerceptron()`)
  - `param_grid` is dict or list of dict
  - Optionally specify desired evaluation score and CV strategy
- How many computations do you have for a 5-fold Cross-Validation, 2 possibilities for one parameter and 3 for another parameters?

Model Pipelines

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What's wrong about scaling, then folding and then selecting parameters?

- The information used for scaling partly comes from the verification fold
- This is not how new data looks to the model
- $\rightarrow$ Information leakage Right approach: Splitting/Folding before any preprocessing, i.e. in the cross-validation loop
- `Pipeline()` to the rescue ($\rightarrow$ Documentation)

Checklist

- Learn any model *only* using `GridSearchCV`
- Put parameters into dictionary
- If you scale data, you *must* use `Pipeline`