Cross-validation

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Review of *k*-Nearest Neighbors

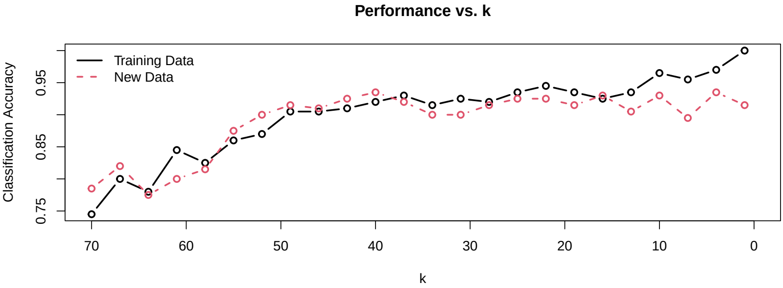
The *k-nearest neighbors* algorithm makes predictions by aggregating the *k* observed samples closest to a new data-point. In order to use the algorithm, we must provide the following:

1. A way of measuring distance
2. A value for *k*
3. If neighbors should contribute uniformly or be weighted by distance

A **parameter** is an unknown value that an algorithm needs to make predictions. A **tuning parameter** (or **hyperparameter**) must be specified before an algorithm is used.

Tuning Parameters

Below is the classification accuracy of various KNN models for our toy data (healthy vs. unhealthy classification):



Small values of *k* will *overfit the training data*, while for large values *k* introduce too much bias.

Tuning Parameters

- We'd like to avoid using the the test data to choose our tuning parameters
  - This would introduce the very same problems we were trying to avoid by using independent training and testing sets
- So, how might we determine good values for tuning parameters using *only the training data*?

Cross-validation

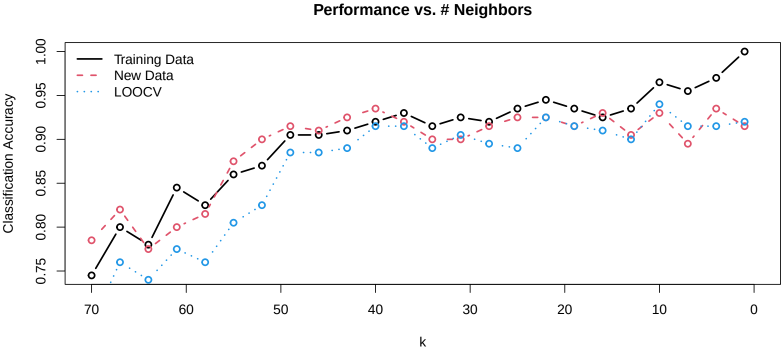
Cross-validation (CV) is a general term describing methods of repeated data-splitting used to evaluate the performance of a model on data that was not used in the training process:

1. Non-exhaustive cross-validation, notably k-fold cross-validation
2. Exhaustive cross-validation, notably leave-one-out cross-validation (LOOCV)

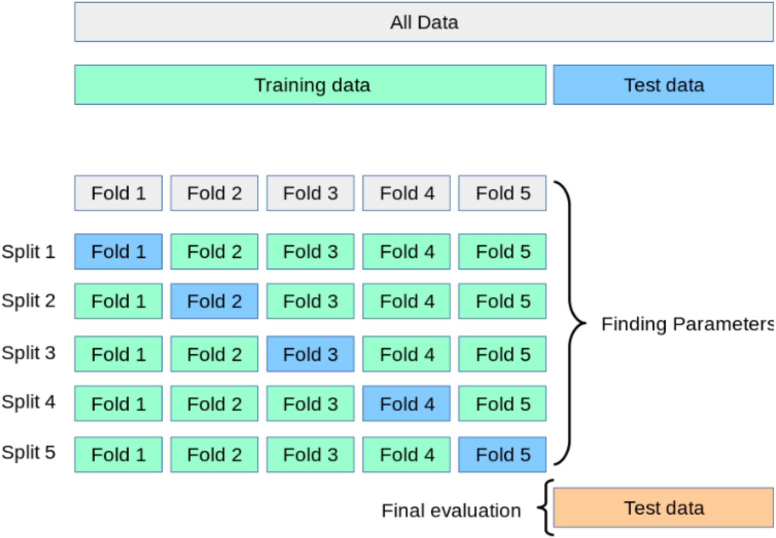
Non-exhaustive CV approaches involve randomness, so they are sometimes applied repeated (we'll generally focus on a single use).

Example - LOOCV

Cross-validation helps us *avoid over-fitting* by producing reasonable estimates of performance without using the test set:



5-fold Cross-validation



All Data

Training data

Test data

	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 1	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 2	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 3	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 4	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5
Split 5	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

Finding Parameters

Final evaluation

Test data

k-fold Cross-validation

Pseudocode of 5-fold cross-validation:

```
## Assign n obs into k folds
fold_id = sample(1:k, size = n)

## Loop through each fold:
for i in 1:k
   train_X = samples[fold_id != i]
   train_y = labels[fold_id != i]
   eval_X = samples[fold_id == i]
   eval_y = labels[fold_id == i]

   model.fit(train_X, train_y)
   pred[fold_id == k] = model.predict(eval_X, eval_y)

## Calculate performance
score(pred)
```

k-fold or LOOCV?

- LOOCV is a special case of k-fold CV using $k = n$ (ie: each fold contains just a single observation)
- Compared to k-fold CV, LOOCV is a *higher variance procedure*
    - Repeating LOOCV on different samples from the same underlying data source will show a greater range of performance estimates
    - Errors are highly correlated in LOOCV due to the high degree of overlap in each training segment

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    - Repeating LOOCV on different samples from the same underlying data source will show a greater range of performance estimates
    - Errors are highly correlated in LOOCV due to the high degree of overlap in each training segment
- k-fold cross-validation offers *better generalization*, but can be unfeasible for small samples
    - Smaller values of k are also more computationally efficient (especially if parallelization can be used)

How many folds?

The bias-variance trade-off governs how the number of folds impacts the reliability of performance estimates:

- More folds allows larger amounts of data to be used during model training, which should reduce bias
  - However, too many folds will lead to highly correlated training errors, which will increase variance
- Conversely, too few folds can also lead to high variance estimates if model training is to the fold assignments and repeated CV is not used

Most practitioners favor 10-fold or 5-fold CV, with deep learning applications sometimes using smaller numbers of folds, such as $k = 3$ or even a single validation set for computational reasons.

Grid Search

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- Cross-validation provides a framework for unbiased performance evaluation *using only the training data*
  - However, it must be combined with other methods in order to determine the best values for a method's tuning parameters (ie: finding the best number of neighbors)
- **Grid search** is a simple (and widely used) approach for finding optimal combinations of tuning parameters using via cross-validation
  - The idea is to systematically and exhaustively search a grid spanning the parameter space

Grid Search (example)

Here's an example parameter grid for KNN that considers $k \in \{3, 4, 5\}$, euclidean or Manhattan distance, and uniform or distance weighting:

k	Distance	Weight
3	euclidean	uniform
4	euclidean	uniform
5	euclidean	uniform
3	manhattan	uniform
4	manhattan	uniform
5	manhattan	uniform
3	euclidean	distance
4	euclidean	distance
5	euclidean	distance
3	manhattan	distance
4	manhattan	distance
5	manhattan	distance

We'd ask Python to train and evaluate each row of this grid using cross-validation to reliably assess performance.

Randomized Search

- Grid search can be computationally expensive, especially when you'd like to tune over a broad range of values for several different tuning parameters
- **Randomized search** is an alternative method that allows you specify distributions to be randomly sampled from for each tuning parameter
  - For kNN, you might specify k as being sampled from a Poisson distribution with $\mu = \sqrt{n}$

Other Approaches

- Randomized search and grid search approaches can be combined to explore large parameter spaces with greater efficiency
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- **Successive halving searches** are also supported in Python's `sklearn` library
  - The main idea is to only allow top scoring parameter values to "survive" into later rounds of the search
  - We will not cover this method, but you may consider using it on your final project