

Robust Evaluation of Machine Learned Models

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Goals for Building Reliable Models

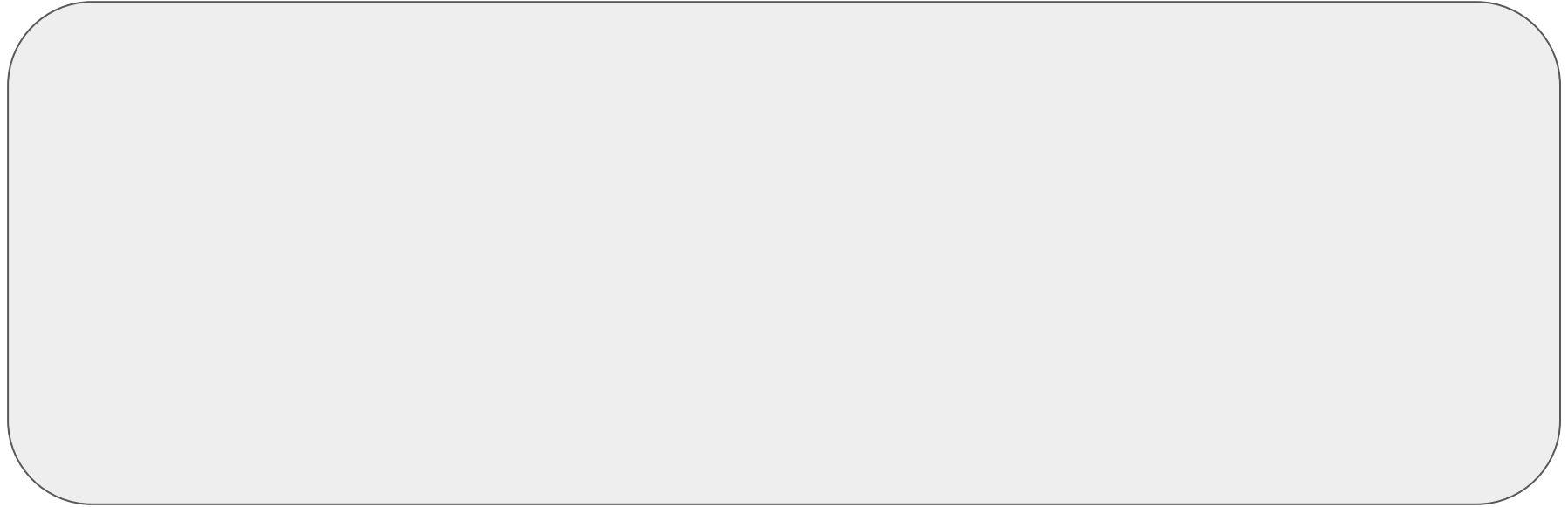
We want:

- Models that will work well with future data
- A sense of how sensitive our model performance is to:
 - The specific training data that we are using
 - The amount of training data that we have
- Formal ways of selecting model hyper-parameters
- Formal ways of comparing two (or more) different model types (the bake off!)

Definitions

- **Parameters:** parameters that are selected by a learning algorithms
- **Hyper-parameters:** parameters that are selected outside the learning algorithm, but affect how it behaves
 - Regularization
 - Structure: number of layers, number of computing elements within a layer, ...
- **Model type:** broad category of models (e.g., deep network vs a support vector machine)

Data Universe



Contains all possible data samples, including all time

A First Approach

Ideal process:

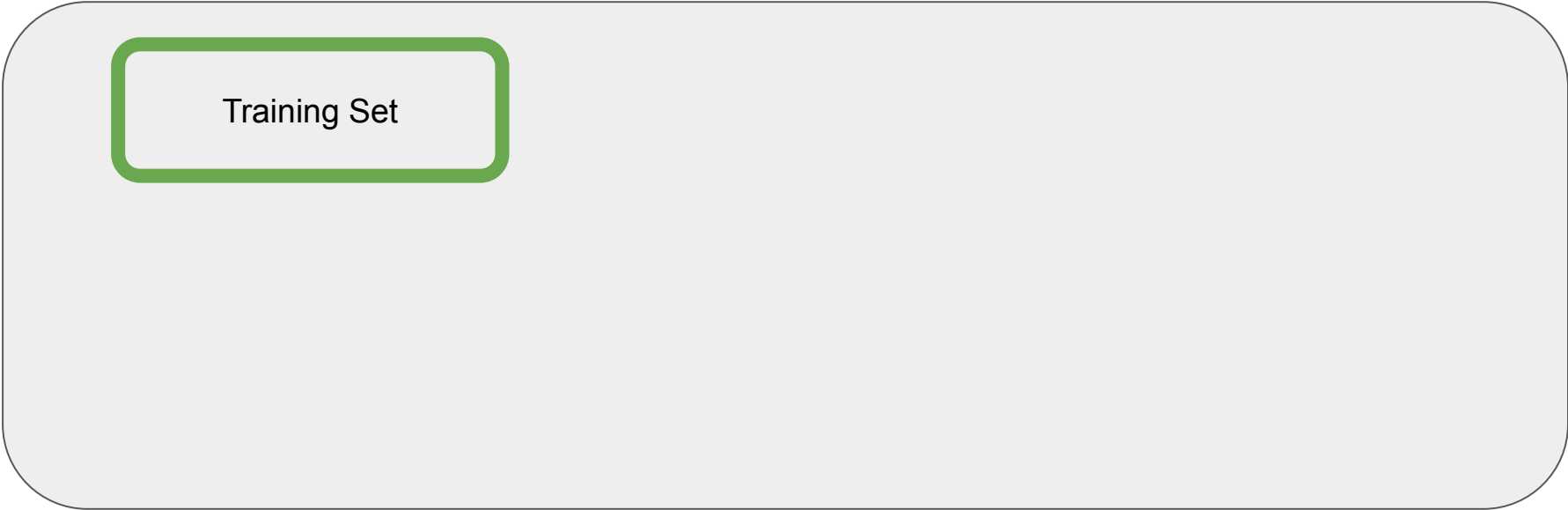
- We can observe the entire data universe
- Construct a model that explains all of these samples
- Done

A First Approach

Challenges:

- Sampling the universe is typically not feasible
- Even when we can sample the universe, it may not be feasible to use with our learning algorithm

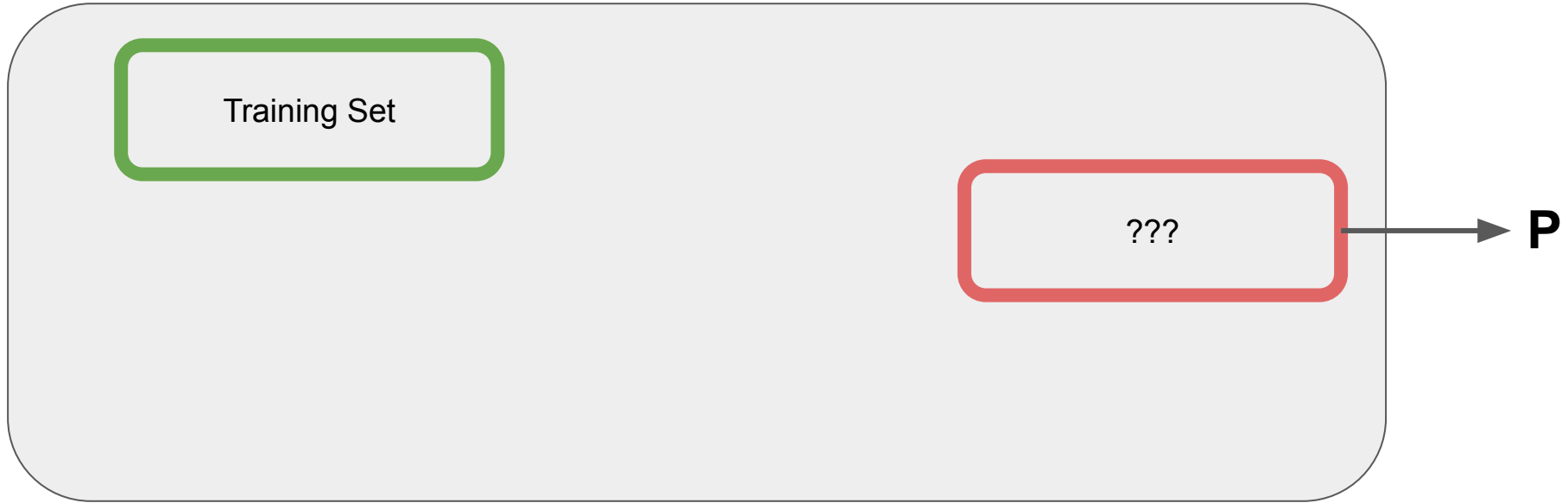
A Second Approach

A diagram consisting of a large, light gray rounded rectangle. Inside the top-left corner of this rectangle is a smaller, white rounded rectangle with a thick green border. The text 'Training Set' is centered within the white rectangle.

Training Set

Take a sample from the universe for the purpose of training the model

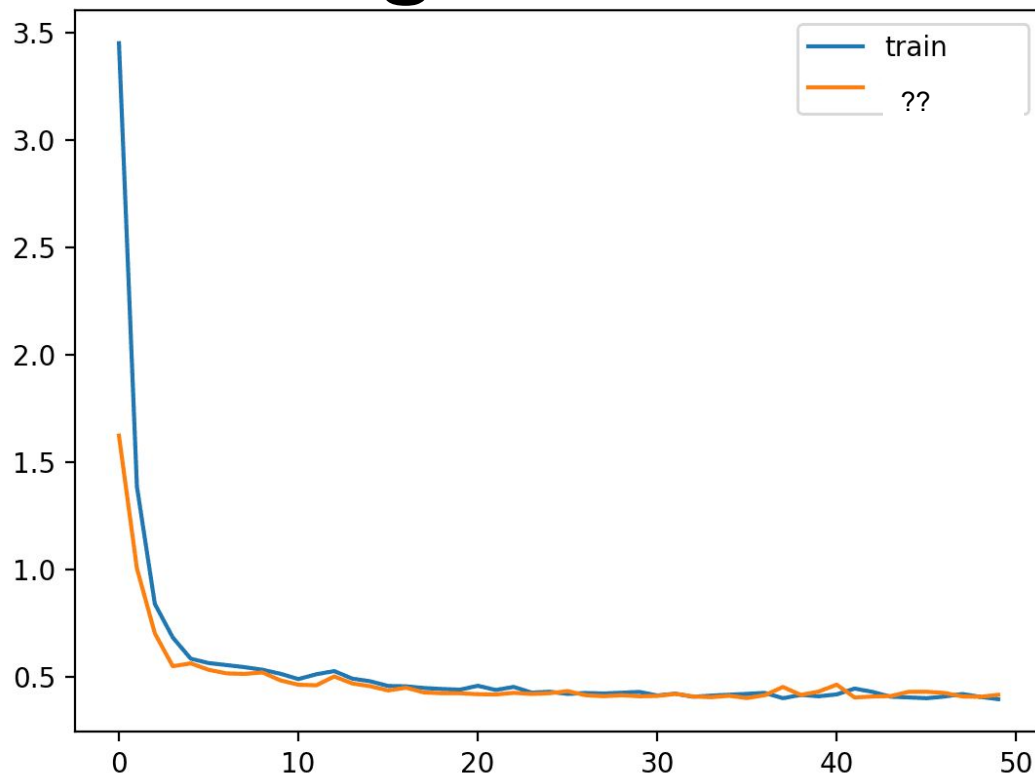
A Second Approach



P is the performance of the learned model on independent data set

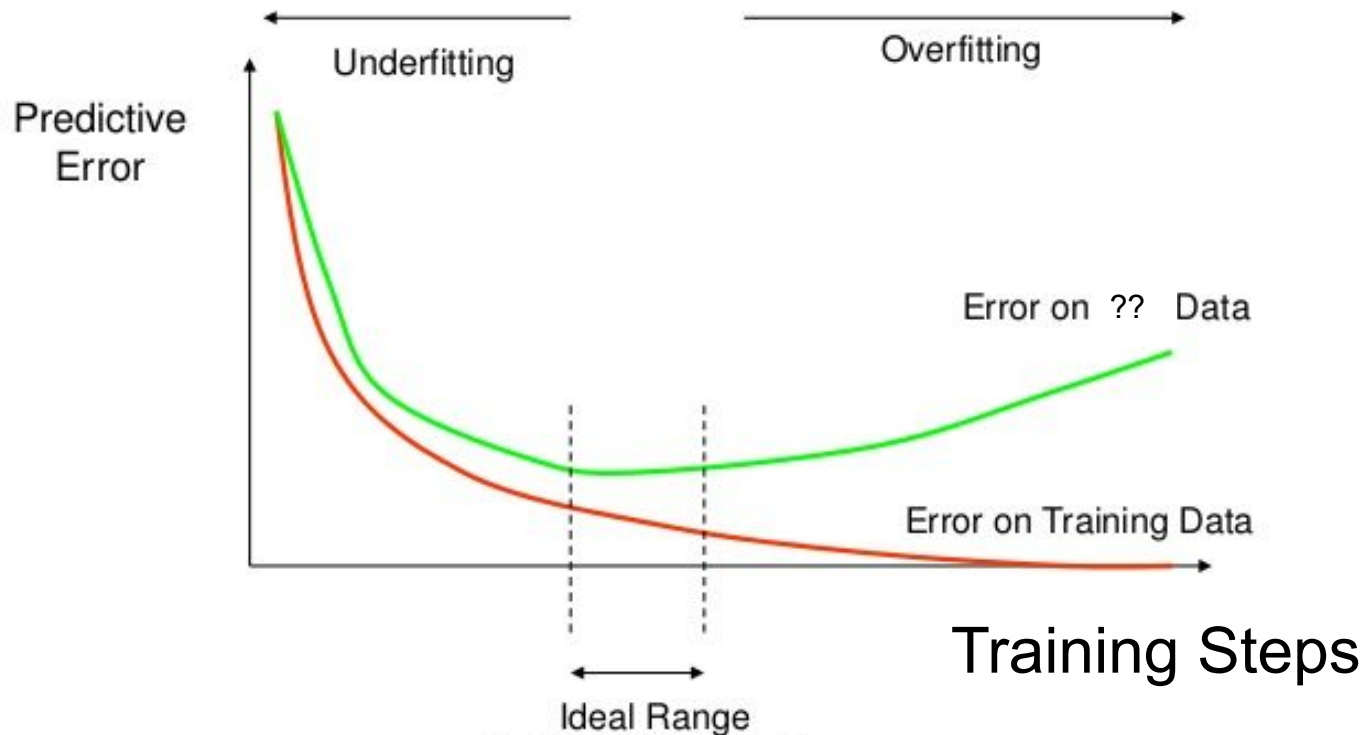
Learning Curves: Ideal

Prediction
Error



Training Steps

Learning Curves: Overfitting



Combating Overfitting

- Increase training set size
- Reduce number of parameters
- Regularization techniques: force simpler models
 - Explicit: add model complexity to cost function
 - Implicit: random reduction in model complexity (e.g., dropout)
- Early stopping: use independent data set performance to halt the gradient descent process

Building a Model is a Stochastic Process

- Sampling a data set from the universe
- Learning algorithms often have stochastic elements
 - Initial parameter choices are often selected from a distribution
 - Approximate gradient descent using a subset of training set examples (batches)
 - Sampling question types in a decision tree

Building a Model is a Stochastic Process

- We need to treat all performance measures as random variables
- So, a single observation is not sufficient to conclude anything, especially if we want to formally compare model types
- And - we need a sufficient number of observations to apply our hypothesis testing tools

A Third Approach



Statistically independent training and evaluation data sets

A Third Approach

- N performance measures are also statistically independent
- Can treat as a set of IID samples from a distribution. Can then answer:
 - Did we learn anything?
 - How does this model type compare with another model type?
 - If we use the same training / evaluation data set pairs for the different model types, then can use a paired statistical test

Challenges of the Third Approach

- Each model type has many possible hyper-parameters
- Before we compare model types, we need to choose the appropriate hyper-parameter set for each
- But, how to make this choice?
 - Hyper-parameters often affect the degree of overfitting, so training set data cannot be used to make this choice
 - But, using the same Test Data Set, we run the risk of overfitting the hyper-parameters to this data set

Three Different Data Set Types

Data sets that are IID:

- **Training set:** used by the learning algorithm to select parameters
- **Validation set:**
 - Select an early stopping point for training
 - Make hyper-parameter choices
- **Test set:**
 - Reporting results
 - Formal comparison between model types

A Fourth Approach

M 0

Training Set

Validation Set

Test Set

V0, Te0

M 1

Training Set

Validation Set

Test Set

**V1,
Te1**

⋮

⋮

⋮

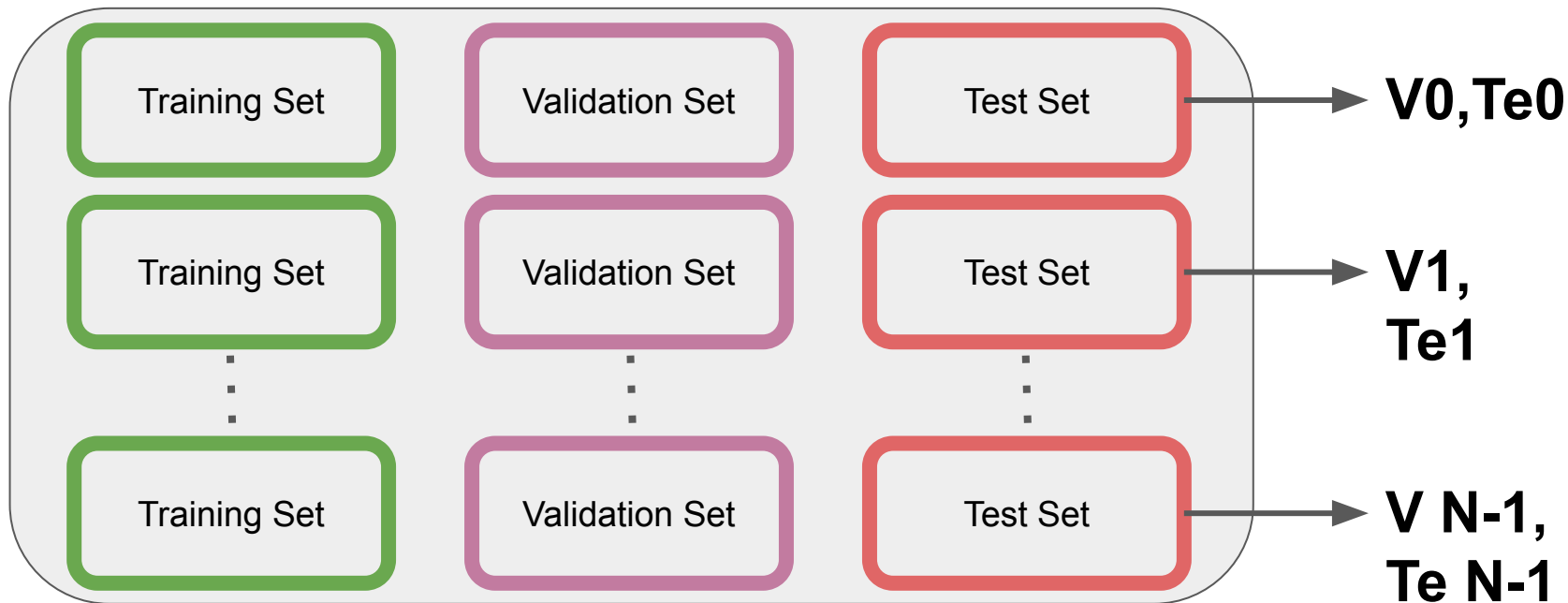
M N-1

Training Set

Validation Set

Test Set

**V N-1,
Te N-1**



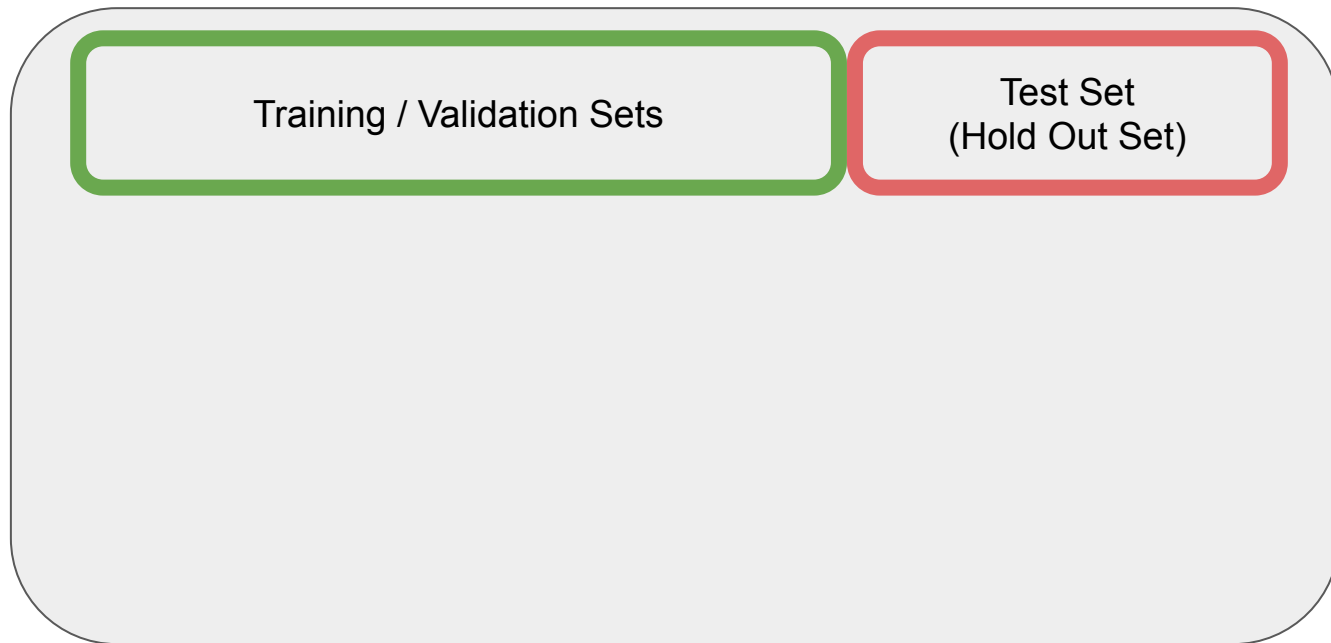
Specifics

- For each model i : use V_i to determine the end of the training process
- Use $\bar{V}$ to compare different hyper-parameter choices
 - Pick the one best performing set of hyper-parameters
- For the selected hyper-parameters: use Te_i 's for:
 - Final evaluation
 - Comparison with other models using hypothesis testing

Challenges

- So far, we have assumed that sampling from the universe is easy / inexpensive
- In practice, this is not the case:
 - Real limitations in our ability to collect / label data
- But still want sound approaches to:
 - Selecting hyper-parameters
 - Comparing model types
- And: want some way to understand sensitivity of model performance with respect to training set size

A Fifth Approach: N-Fold Cross-Validation



Sample what we can from the universe & split into two pieces

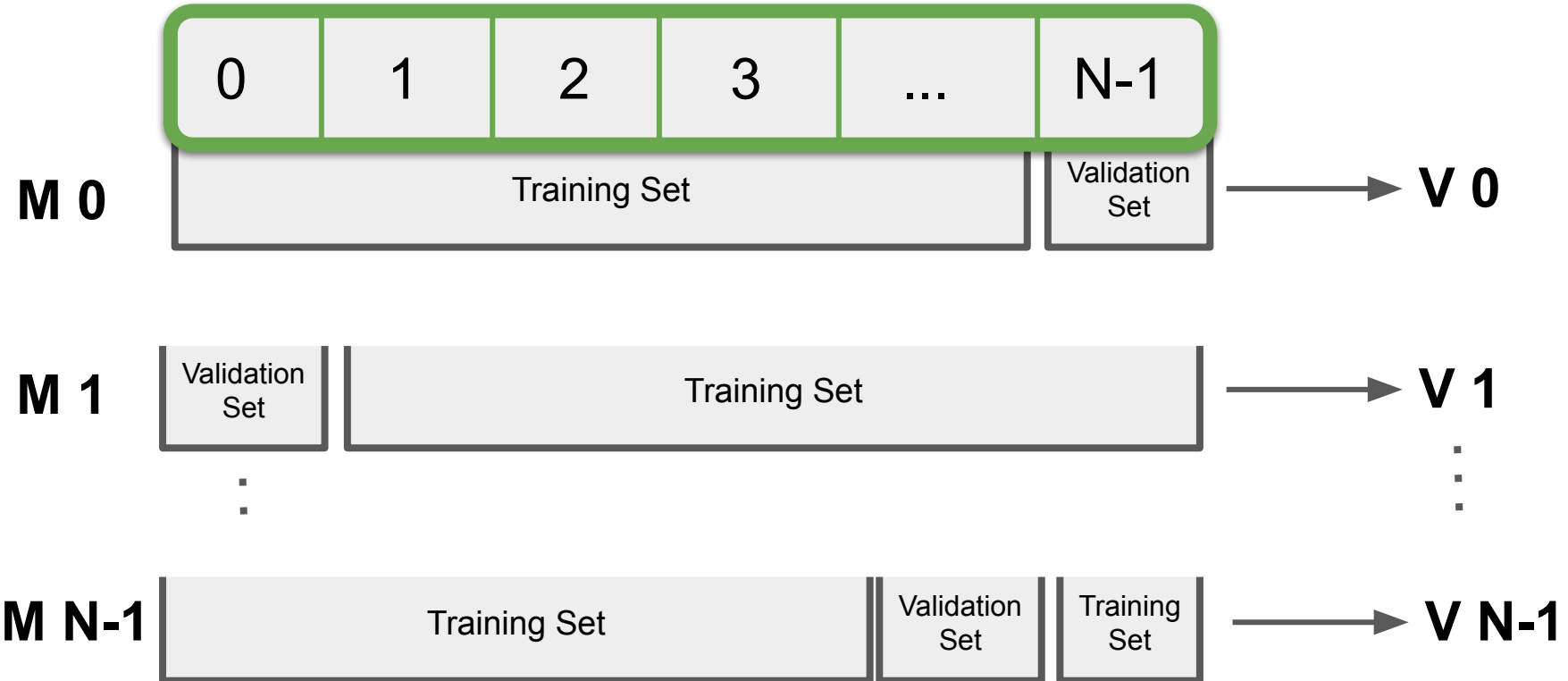
N-Fold Cross-Validation

Cut training/validation set into N independent folds



Construct N different models with different subsets of the folds

N-Fold Cross-Validation



Specifics

- A single sample occurs in exactly one fold
- For model i : use V_i for early stopping
- Use $\bar{V}$ to compare different hyper-parameter choices
 - Pick the one best performing set of hyper-parameters
 - Call this H^*

Evaluating

Comparing model types:

- Evaluate each of the N models with the same Test Data Set.
 - This gives us N metrics: Te_i
- Use this set of N measures for:
 - Final evaluation
 - Comparison with other models using hypothesis testing

Reporting Performance / Future Use

A common final step for production situations:

- Use all N folds to train a new model using hyper-parameters H^*
- Evaluate this new model using the Test Data Set. Report this performance
- Use this model with future data

N-Fold Cross-Validation

Dominant approach

- Many papers, blog posts, books
- Built into standard toolkits, including SciKit Learn (e.g., `cross_val_predict()`)

But there is a problem...

N-Fold Cross-Validation

But there is a problem...

- Because the same Test Data Set is used to compute all N performance measures (the Te_i 's), they are not independent from one-another
- This precludes our use of many standard hypothesis testing tools

N-Fold Cross-Validation

How do we repair this?

- Could cut the Test Data Set into N independent folds and use a different one to evaluate each of the N models
 - Potentially increase the variance of the performance metrics (especially a problem if the Test Data are already small or sparse)
- Draw the Test Data Set from the original set of folds

“Holistic” N-Fold Cross-Validation

- Cut available data into N independent folds
- For each model, use
 - $N-2$ folds for training
 - 1 fold for validation
 - 1 fold for testing

Holistic N-Fold Cross-Validation



Specifics

- A single sample occurs in exactly one fold
 - So it occurs in exactly one validation and one test set
- For model i : use V_i for early stopping
- Use $\bar{V}$ to compare different hyper-parameter choices
 - Pick the one best performing set of hyper-parameters
 - Call this H^*

Evaluating

Comparing model types:

- Evaluate each of the N models **with its Test Data Set**.
 - This gives us N metrics: Te_i
- Use this set of N measures for:
 - Final evaluation
 - Comparison with other models using hypothesis testing

Notes

- A single data set example is used exactly once for validation and once for testing
- If the samples are independent, this means that our test folds are independent from one-another
- This means that the Te_i 's are independent (maybe)
- So, can use our standard hypothesis testing tools (maybe)

Caveats

- Holistic cross-validation uses one less fold for training than the previous approach
 - But does not require a hold-out set
- In either case, the training sets are **NOT** independent
 - Means that the models themselves are not independent
 - So... the Te_i 's may not be truly independent
 - In practice, if the folds individually reflect the distribution of the universe, then this is probably not a problem (will return to this)

Sensitivity to Training Set Size

- Want to understand how sensitive a model type is to training size
- We might choose different hyper-parameters for different sizes

Implementation with Holistic N-Fold Cross-Validation

- Use only k of the available $N-2$ training folds
- These k rotate with the validation and test data sets

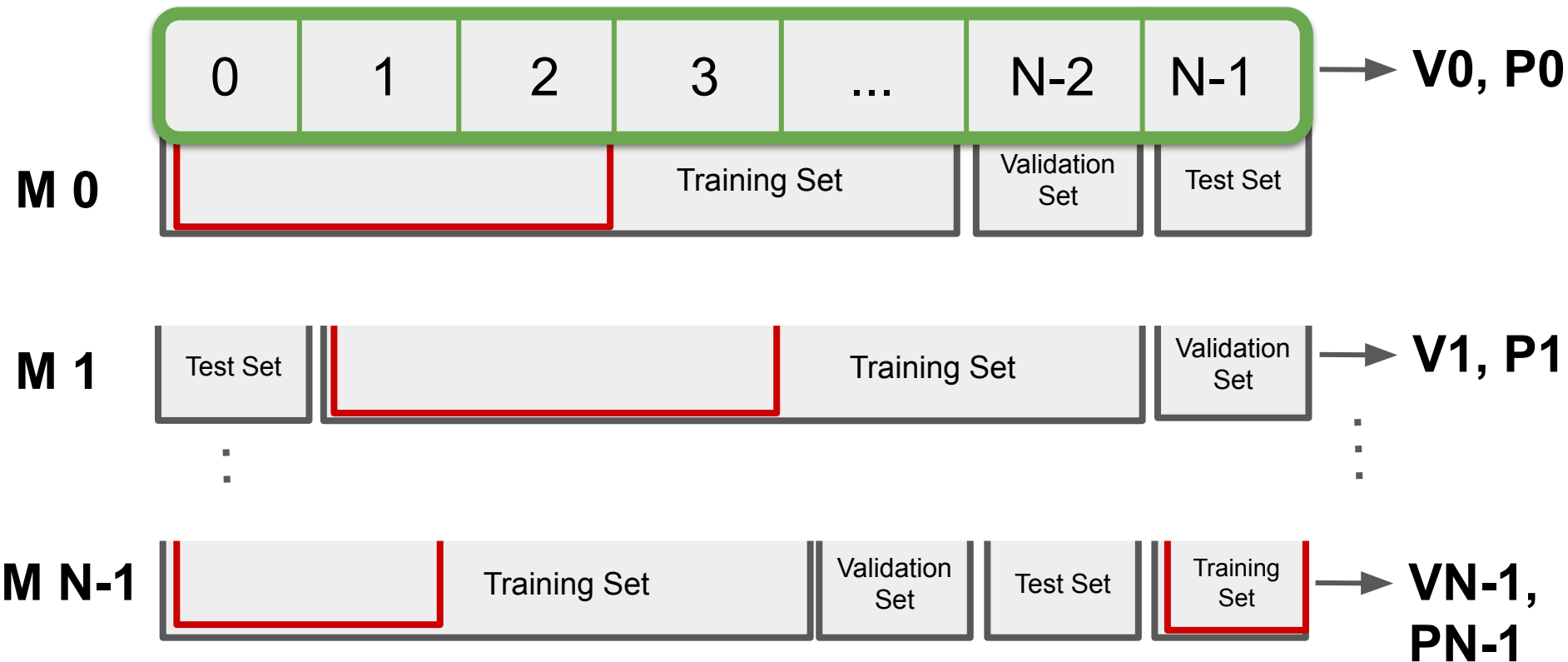
Training Size: 1 Fold



Training Size: 2 Folds



Training Size: 3 Folds



A Little Code ...

- `nfolds` = Total number of folds
- `trainsize` = Number of folds used for the training set:
1, 2, ... `nfolds`-2
- `rotation` = one of: 0, 1, ... `nfolds`-1

```
trainfolds = (range(trainsize) + rotation) % nfolds
valfold = (nfolds - 2 + rotation) % nfolds
testfold = (nfolds - 1 + rotation) % nfolds
```

Details

- For a single model type, a total of $N \times M \times L$ models are learned & evaluated
 - N folds (so, N rotations) **20**
 - M hyper-parameter sets **???**
 - L choices for training set size **factors of 2 or 10?**
- We typically reserve this process for formal evaluation
- And: do a lot of informal work ahead of time to explore hyper-parameter possibilities and training set sizes

Practicalities

- How small can we make N ?
 - 20-30 is nice; 10 is not uncommon; 5?
- Training data set size sensitivity analysis is often done informally
 - Interacts with hyper-parameter selection

Challenges with Holistic Cross-Validation

- For a given rotation, the testing fold is independent of the training and validation folds
- However, to make decisions about hyperparameters, we don't look at validation performance for a single rotation, but the mean across all validation folds
- One can argue that because validation fold for rotation $k+1 \pmod N$ is the same as test fold for rotation k , that the performance measures are not truly independent

Orthogonalized Cross-Validation

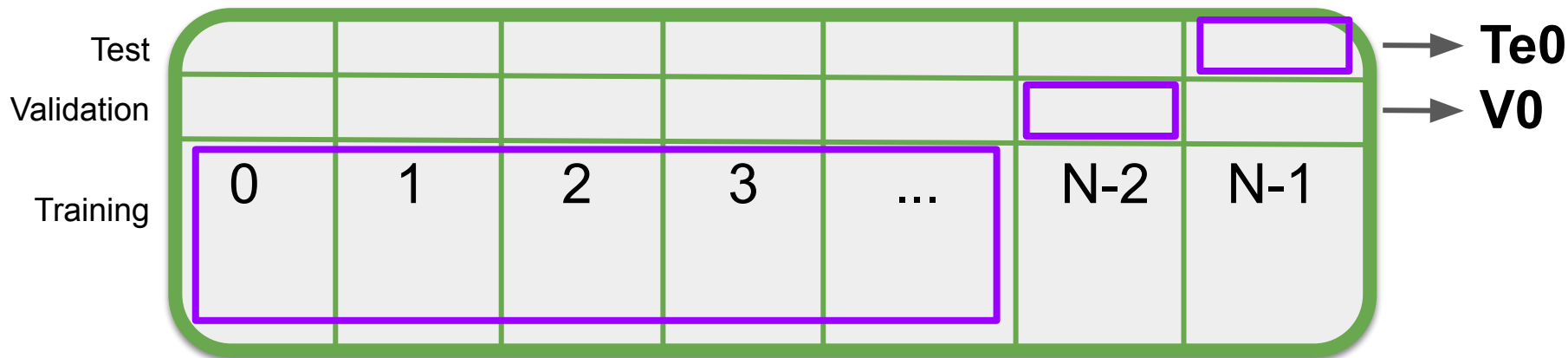
- Goal: fully independent validation and testing measures while using as much of the data for any rotation as possible
- Variety of solutions
- One approach:
 - Hold-out sets for both validation and testing
 - Cut each hold-out set into N folds

Orthogonal N-Fold Cross-Validation

Test							
Validation							
Training	0	1	2	3	...	N-2	N-1

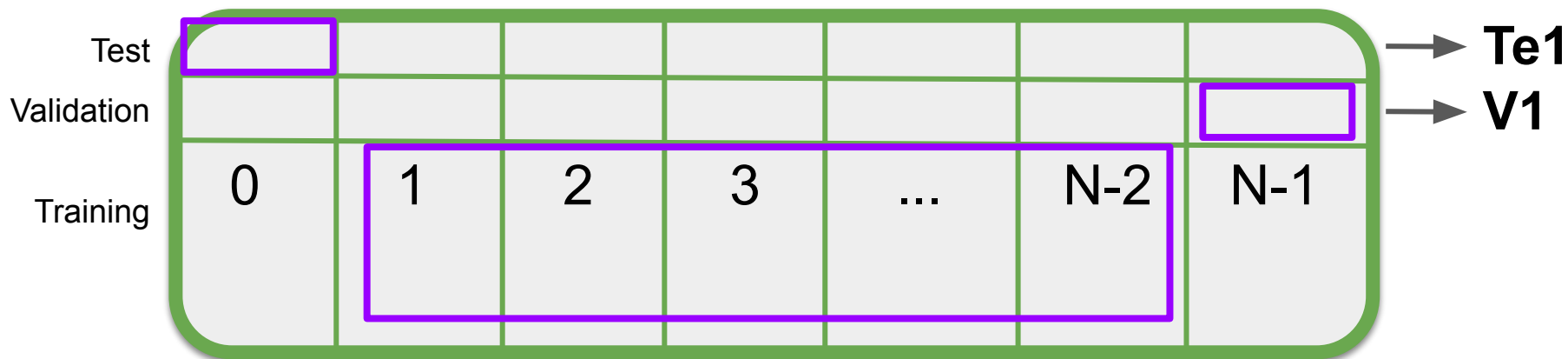
Orthogonal N-Fold Cross-Validation

Rotation 0

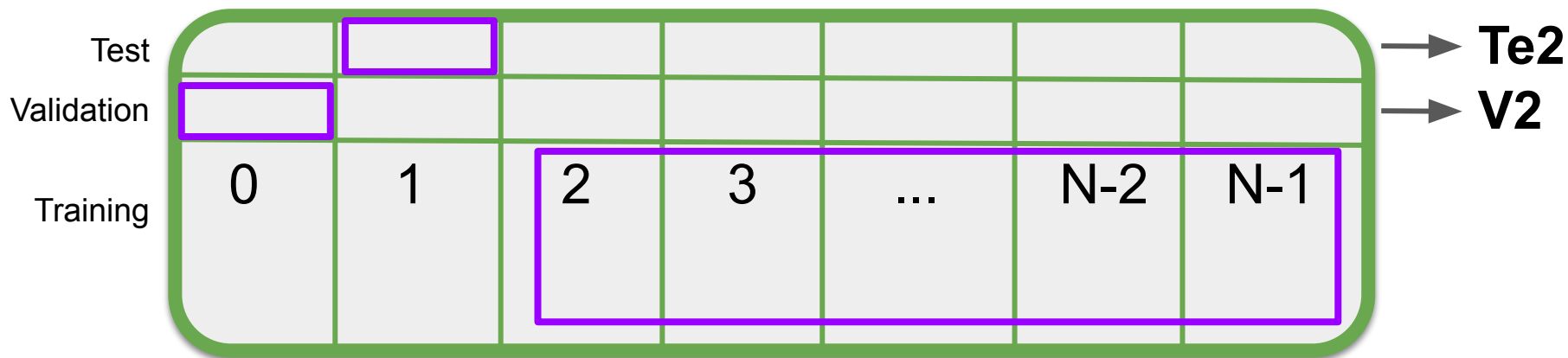


Orthogonal N-Fold Cross-Validation

Rotation 1



Orthogonal N-Fold Cross-Validation Rotation 2



Orthogonal N-Fold Cross-Validation

- For each rotation
 - Leaving some of the available data untouched
 - Using less data for training, validation and/or testing
- But, we feel more confident in the independence of the testing measures

Take-Aways

- Statistical evaluation matters
- There isn't one solution to this
- Don't confuse validation and test data sets
 - Can't look at test data performance until the very end (though it is often convenient to compute on the fly for all and save the results for future use)
- Work to ensure independence of the individual folds (not always easy)

Creating Folds

- Folds should be independent of one another
- But, may have to take steps to make sure that the distribution of samples within each fold reflects the distribution of the universe
- For classification tasks, we often use ***stratification***:
 - Ensure that the samples for a given class are evenly distributed across the folds

Creating Folds with Time-series Data

- Samples that are near in time to one-another are often not statistically independent
- Can't randomly assign samples from the time-series to folds
- Instead, we typically cut the time-series into folds
 - Must be careful: take steps to make sure that the samples on either side of the cut are independent
 - A common approach: cut out some samples between the end of one fold and the start of the next