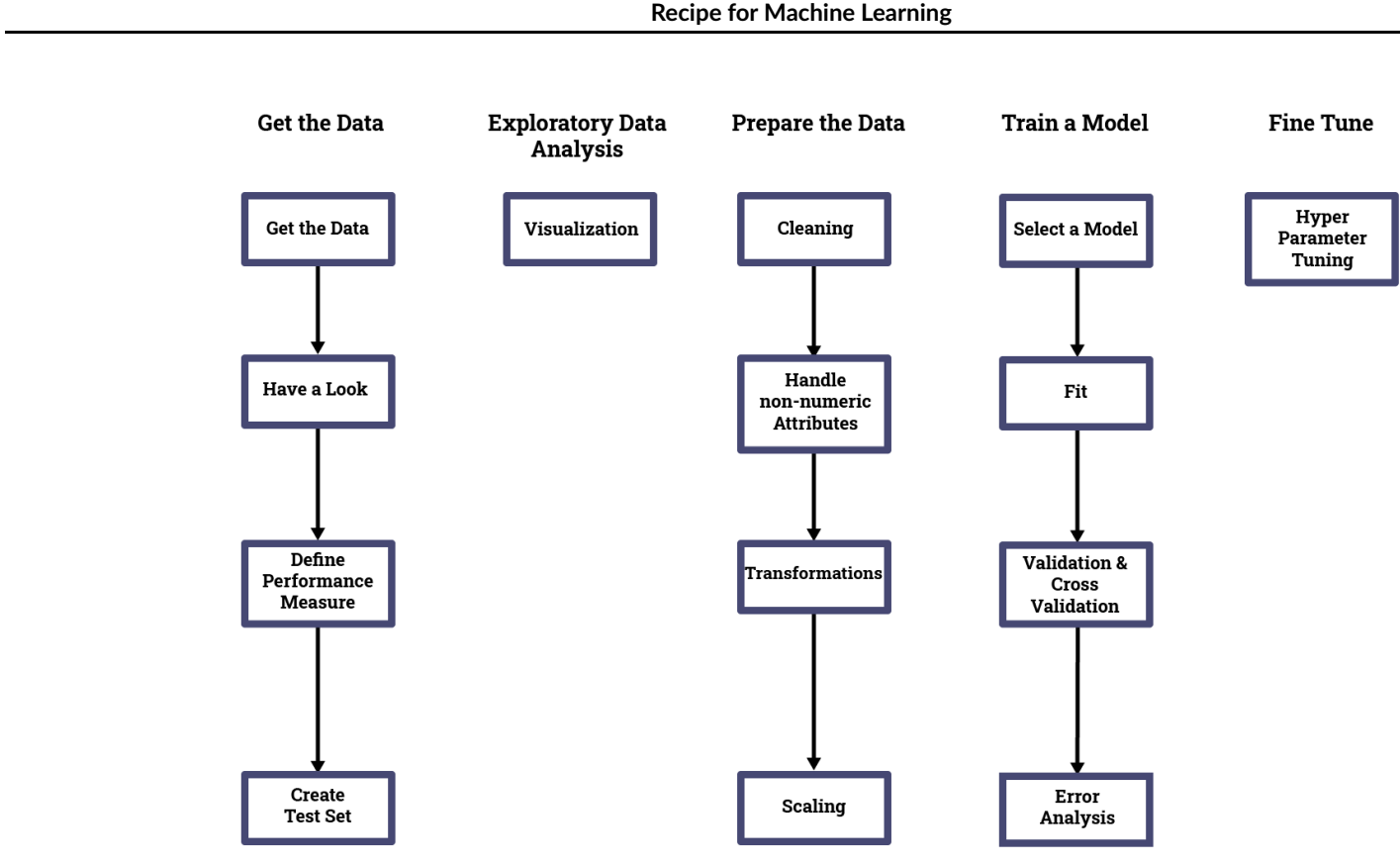
# Prepare data: transformations

Transforming data (Recipe C.3) may be **the most important** step of the multi-step Recipe !



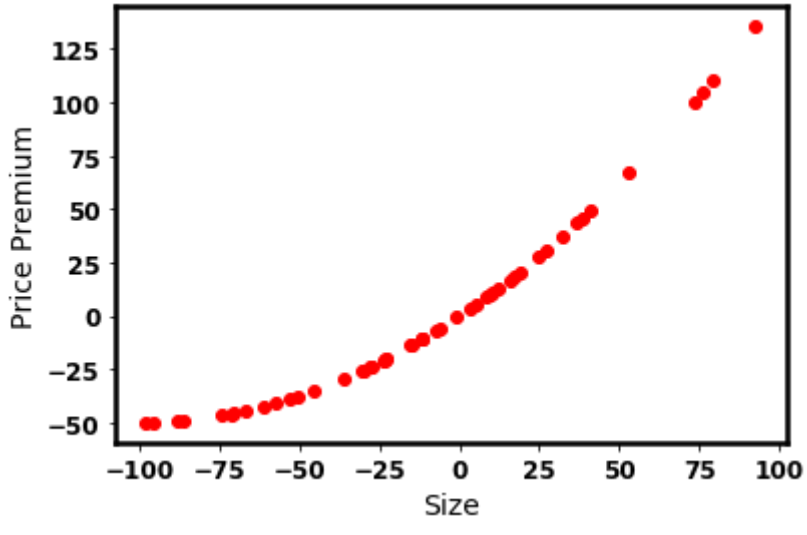
It is often the case that the "raw" features given to us don't suffice

- we may need to create "synthetic" features.
- This is called **feature engineering**.

Recall: our "curvy" data set from the previous lecture:

In [45]:

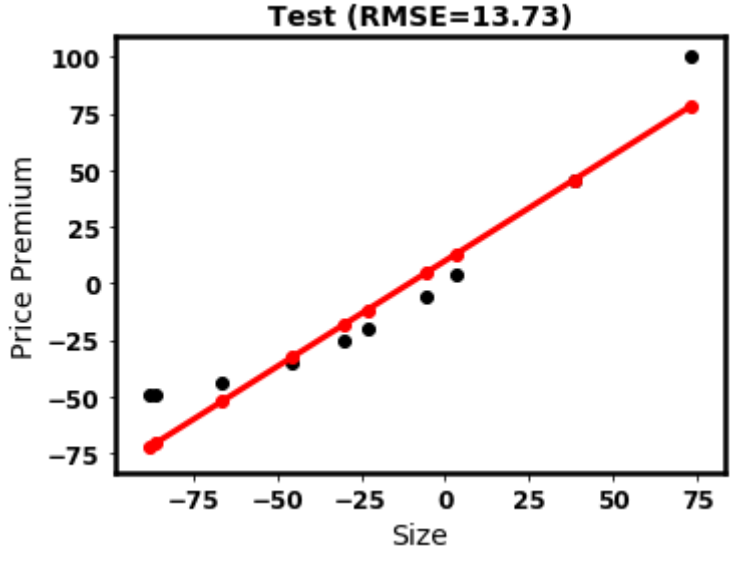
```
(xlabel, ylabel) = ("Size", "Price Premium")
v1, a1 = 1, .005
v2, a2 = v1, a1*2
curv = recipe_helper.Recipe_Helper(v = v2, a = a2)
X_curve, y_curve = curv.gen_data(num=50)
_= curv.gen_plot(X_curve,y_curve, xlabel, ylabel)
```

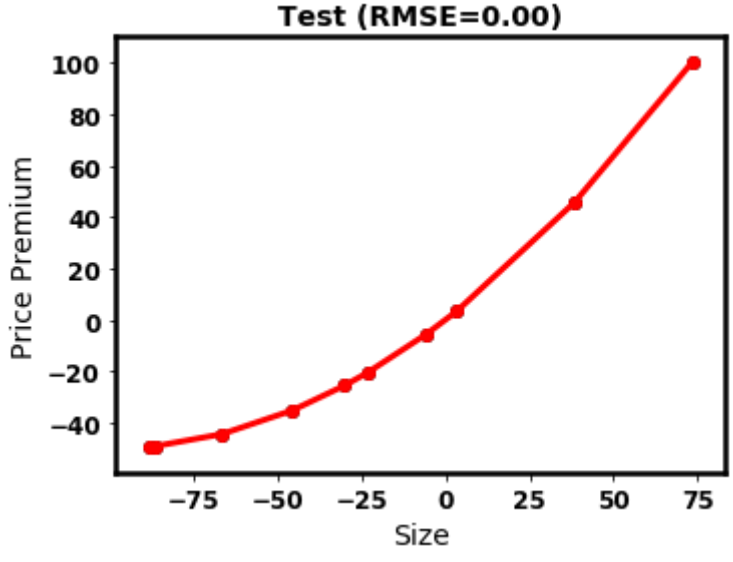


And compare the out of sample performance on this data set

- On a linear model (single, raw feature)
- On a model with a second feature (squared version of raw feature)

In [46]:
```
model_results = curv.compare_regress(X_curve, y_curve, xlabel=xlabel, ylabel=yla
bel, visible=True, plot_train=False)
```



Adding the synthetic feature was key to better performance (lower RMSE).

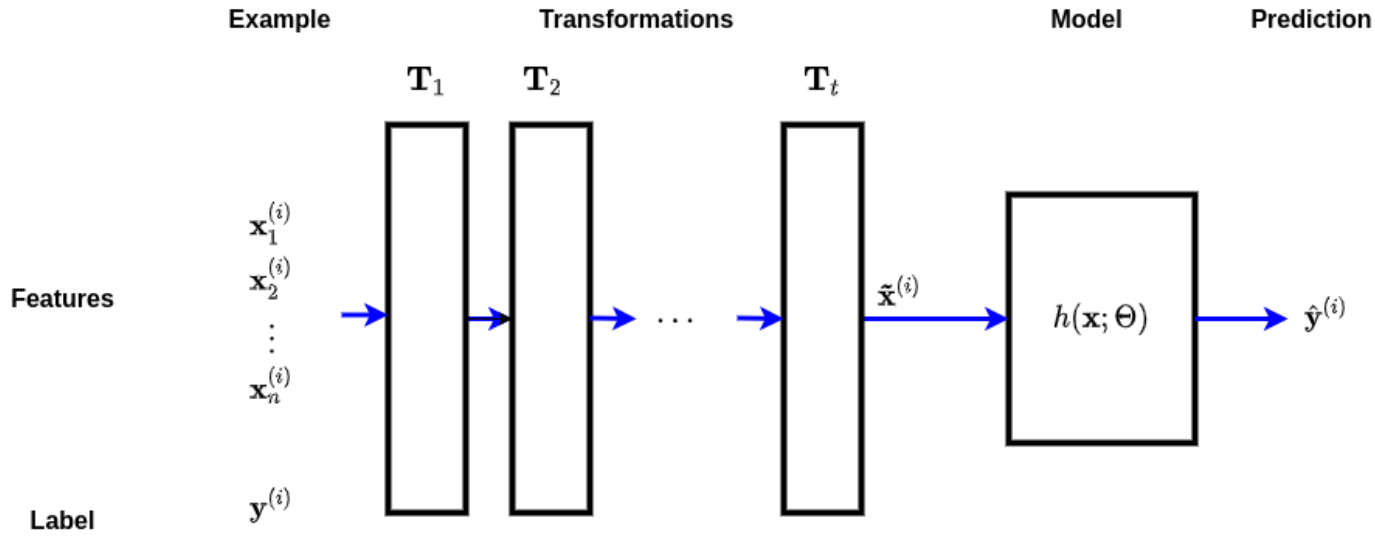
Feature engineering, or transformations

- takes an example: vector $\mathbf{x}^{(\mathbf{i})}$ with $n$ features
- produces a new vector $\tilde{\mathbf{x}}^{(\mathbf{i})}$, with $n'$ features

We ultimately fit the model with the transformed *training* examples.

We can apply multiple transformations, each

- Adding new synthetic features
- Further transforming synthetic features




- MIssing data inputation
- Standardization
- Discretization
- Categorical variable encoding

The above diagram shows multiple tranformations

- organized as a sequence (sometimes called a *pipeline*) of independent transformations $T_1, T_2, \ldots, T_t$

$$\begin{aligned}
\tilde{\mathbf{x}}_{(1)} &= T_1(\mathbf{x}) \\
\tilde{\mathbf{x}}_{(2)} &= T_1(\tilde{\mathbf{x}}_{(1)}) \\
&\vdots \\
\tilde{\mathbf{x}}_{(l+1)} &= T_1(\tilde{\mathbf{x}}_{(l)})
\end{aligned}$$

We write the final transformed $\tilde{\mathbf{x}}$ as a function $T$ that is the composition of each transformation function

$$\tilde{\mathbf{x}} = T(\mathbf{x}) = T_t(\ T_{t-1}(\ldots T_1(\mathbf{x})\ldots)\ )$$

The length of the final transformed vector $\tilde{\mathbf{x}}$ may differ from the $n$, the length of the input $\mathbf{x}$

- may add features
- may drop features

The predictions are now a function of $\tilde{\mathbf{x}}$ rather than $\mathbf{x}$

$$\hat{\mathbf{y}} \quad = \quad h_{\Theta}(\tilde{\mathbf{x}})$$

# Example transformation: Missing data imputation

The first transformation we encountered added a feature ($\mathbf{x}^2$ term) that improved prediction.

Some transformations alter existing features rather than adding new ones.

Transformations in detail will be the subject of a separate lecture but let's cover the basics.

Let's consider a second reason for transformation: filling in (imputing) missing data for a feature.

| # | $\mathbf{x}_1$ | $\mathbf{x}_2$ |
|---|---|---|
| 1 | 1.0 | 10 |
| 2 | 2.0 | 20 |
| ⋮ | ⋮ | ⋮ |
| i | 2.0 | NaN |
| ⋮ | ⋮ | ⋮ |
| m | . . . | |

In the above: feature $\mathbf{x}_2$ is missing a value in example $i$: $\mathbf{x}_2^{(\mathbf{i})} = \mathrm{NaN}$

We will spend more time later discussing the various ways to deal with missing data imputation.

For now: let's adopt the common strategy of replacing it with the median of the defined values:

$$\mathrm{median}(\mathbf{x}_2) = \mathrm{median}(\{\mathbf{x}_2^{(\mathbf{i})} | 1 \leq i \leq m, \mathbf{x}_2^{(\mathbf{i})} \neq \mathrm{NaN}\})$$

This imputation is a kind of data transformation: replacing an undefined value.

Without this transformation: the algorithm that implements our model

- May fail
- May impute a less desirable value, since it lacks specific knowledge of our problem

# "Fitting" transformations

The behavior of our models for prediction have parameters $\Theta$.

It might not be obvious that transformations have parameters $\Theta_{\text{transform}}$ as well

$$\tilde{\mathbf{x}} = T_{\Theta_{\text{transform}}}(\mathbf{x})$$

For example: when missing data imputation for a feature substitutes the mean/median feature value

- $\Theta_{\text{transform}}$ stores this value

We use the term "fitting" to describe the process of solving for $\Theta_{\text{transform}}$

- Unlike $\Theta$, one doesn't usually find a "optimal" value for $\Theta_{\text{transform}}$

Our prediction is thus

$$\begin{aligned} \hat{\mathbf{y}} &= h_{\Theta}(\tilde{\mathbf{x}}) \\ &= h_{\Theta}( T_{\Theta_{\text{transform}}}(\mathbf{x}) ) \end{aligned}$$

The process of Transformations is similar to fitting a model and predicting.

The parameters in $\Theta_{\text{transform}}$

- are "fit" by examining all training data $\mathbf{X}$
- once fit, we can transform ("predict") *any* example (whether it be training/validation or test)

# Applying transformations consistently

Since the prediction is now

$$\hat{\mathbf{y}} \quad = \quad h_\Theta(\,\tilde{\mathbf{x}}\,) \qquad \text{where } \tilde{\mathbf{x}} = T_{\text{transform}}(\mathbf{x})$$

**each and every** input $\mathbf{x}$ must be transformed

- Training examples
- Test examples

That is: the transformation is applied consistently across all examples, regardless of their source

If we didn't apply the same transformation to both training and test examples

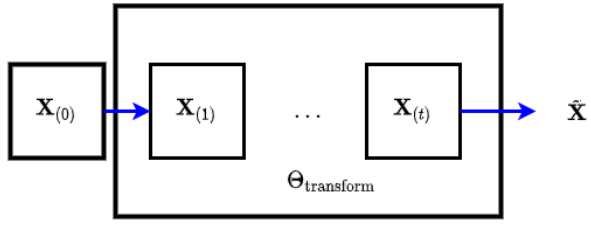
- We would violate the Fundamental Assumption of Machine Learning

However

- $\Theta_{\text{transform}}$ is fit **only** to training examples
- It is **not** recalculated on a set of test examples

Here's the picture

## Feature engineering: fit, then transform




**Train**

$$\text{fit} : \mathbf{X}_{(0)} \mapsto \Theta_{\text{transform}}$$

$$\text{transform}(\mathbf{x}^{(i)}; \Theta_{\text{transform}}) \mapsto \tilde{\mathbf{x}}^{(i)}$$

**Test**

$$\text{transform}(\underline{\mathbf{x}}; \Theta_{\text{transform}}) \mapsto \underline{\mathbf{x}}'$$

**NO fitting at test time, re-use**

$\Theta_{\text{transform}}$

- standardization: $\text{mean}(\mathbf{X}), \text{std-dev}(\mathbf{X})$
- scaling: $\min(\mathbf{X}), \max(\mathbf{X})$
- imputation: $\text{median}(\mathbf{X})$

There are several reasons not to re-fit on test examples

- It would be a kind of "cheating" to see all test examples (required to fit)
- You should assume that you only encounter one test example at a time, not as a group

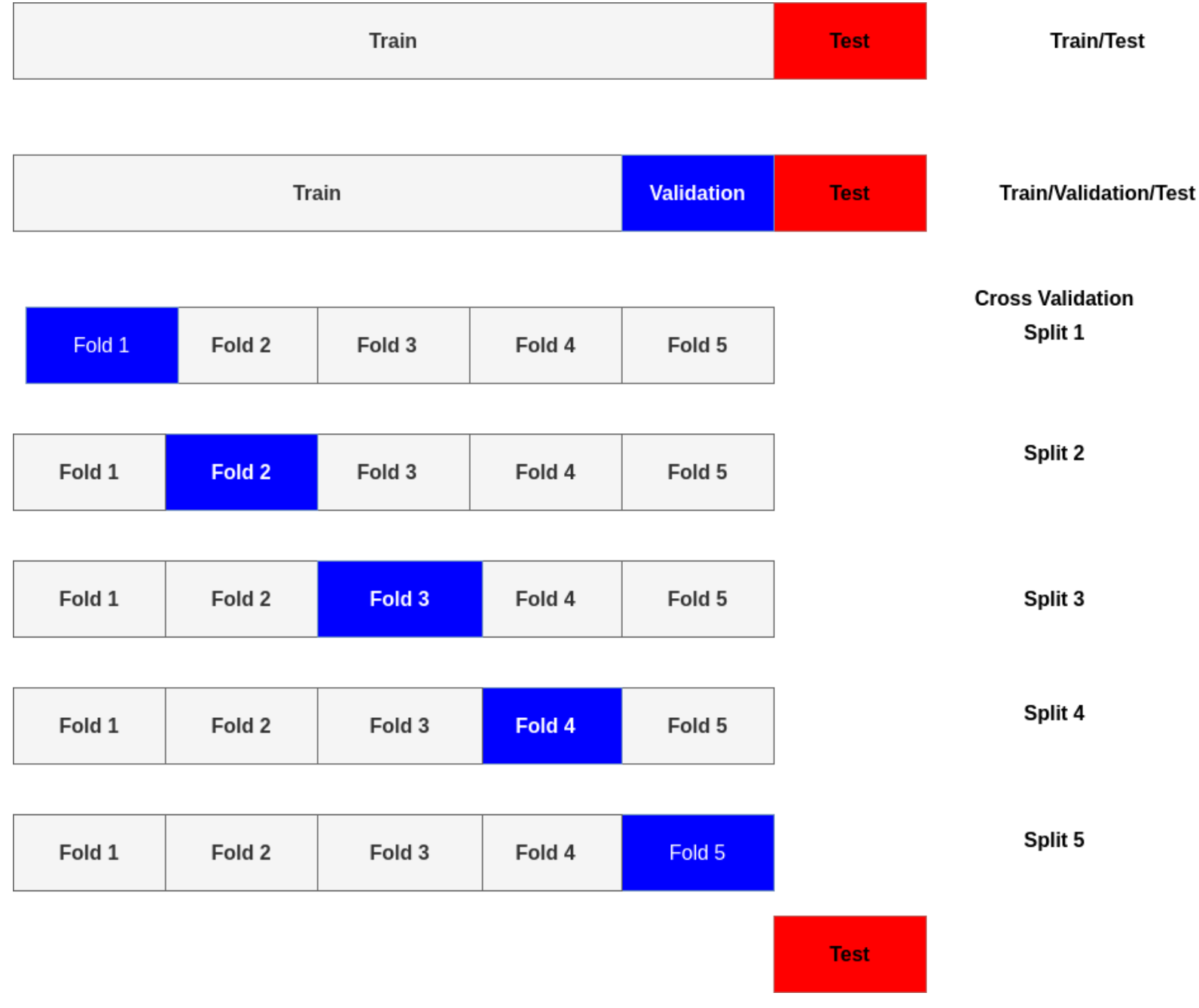
# Using pipelines to avoid cheating in cross validation

Although we start off with the best intentions, it is easy to accidentally "cheat"

- When we combine transformations and cross-validation (to measure out of sample performance)
- Is surprisingly common !

$k$-fold cross-validation:

- Divides the training examples into $k$ "folds"
- A model is fit $k$ times
- Each fit
    - Uses $(k-1)$ folds for training
    - The remaining fold is considered "out of sample" for that fit
- This gives us $k$ Performance Metrics: a distribution of out of sample performance


Train
Test
Train/Test
Train
Validation
Test
Train/Validation/Test
Cross Validation
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
Test

Consider the difference between fitting $\Theta_{\text{transform}}$

- Once, on *all* the training examples, *before* applying cross-validation
- Separately for each of the $k$ fits of Cross-Validation
    - Using the $(k-1)$ folds used fro training in this fit

For example, when $\mathrm{Fold}_1$ is out of sample

$$\tilde{\mathbf{X}} = T_{\Theta_{\text{transform}}}\left(\left[\mathrm{Fold}_1, \mathrm{Fold}_2, \ldots \mathrm{Fold}_{k-1}, \mathrm{Fold}_k\right]\right)$$

$$\text{versus}$$

$$\tilde{\mathbf{X}} = T_{\Theta_{\text{transform}}}\left(\left[\mathrm{Fold}_1, \mathrm{Fold}_2, \ldots \mathrm{Fold}_{k-1}\right]\right)$$

In the first case, we are cheating !

- Fold $k$ is out of sample for this fit
- And should **not** influence $\Theta_{\text{transform}}$

The second case avoids this problem

- With seemingly a lot more work
- Fitting $\Theta_{\text{transform}}$ multiple times

Perhaps the increase in effort is one reason this subtle cheating is overlooked.

Fortunately, a good toolkit for ML (e.g., `sklearn` ) can facilitate proper transformation fitting without extra effort.

Let's explore Transformation pipelines in `sklearn` (Transformations_Pipelines.ipynb)

We will see this in action within the notebook for Classification.

In [2]:
```
print("Done")
```

```
Done
```