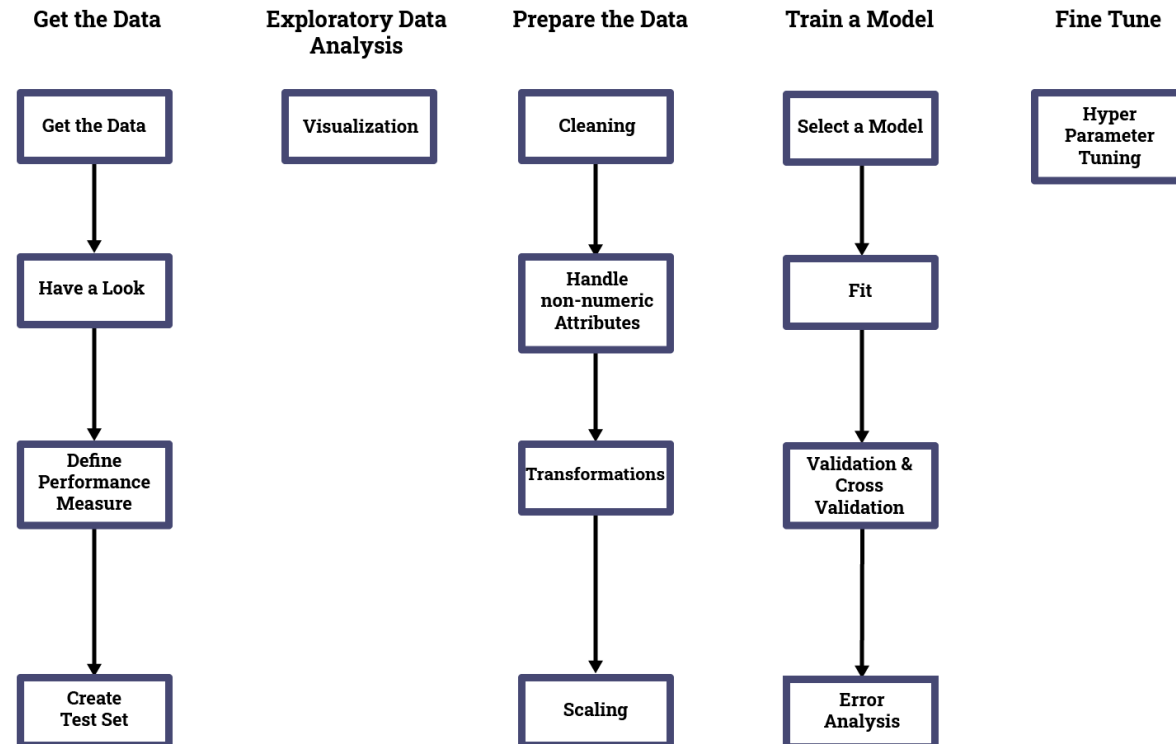


Prepare data: transformations

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

Recipe for Machine Learning

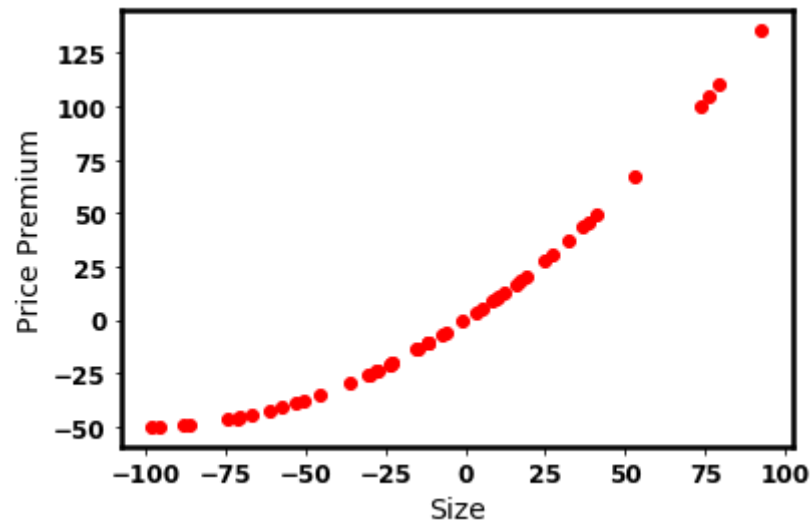


It is often the case that the "raw" features given to us don't suffice

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

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

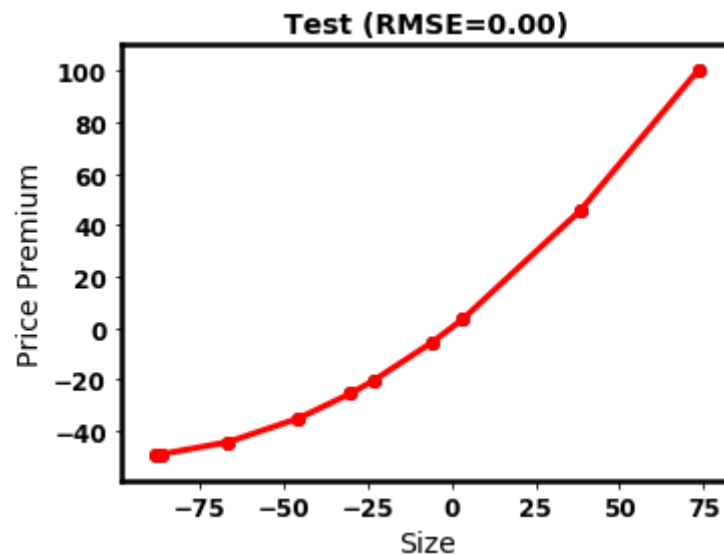
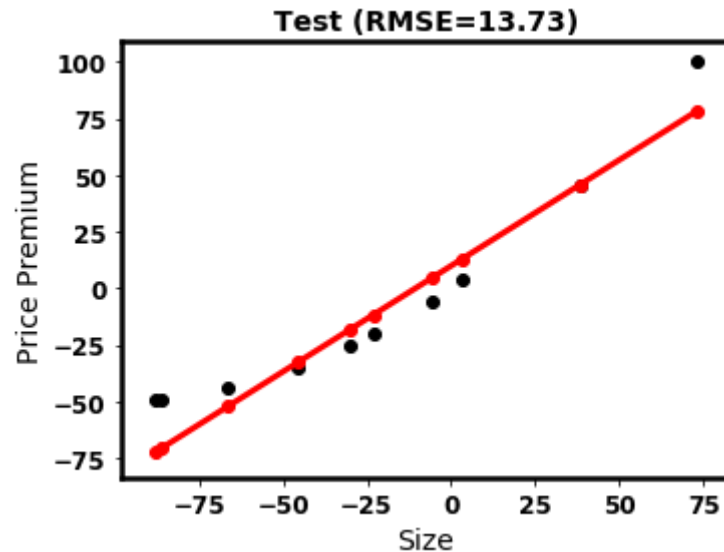
```
In [45]: (xlabel, ylabel) = ("Size", "Price Premium")
v1, a1 = 1, .005
v2, a2 = v1, a1*2
curv = recipe_helper.Recipe_Helper(v = v2, a = a2)
X_curve, y_curve = curv.gen_data(num=50)
_ = curv.gen_plot(X_curve, y_curve, xlabel, ylabel)
```



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=ylabel, visible=True, plot_train=False)
```



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

Feature engineering, or transformations

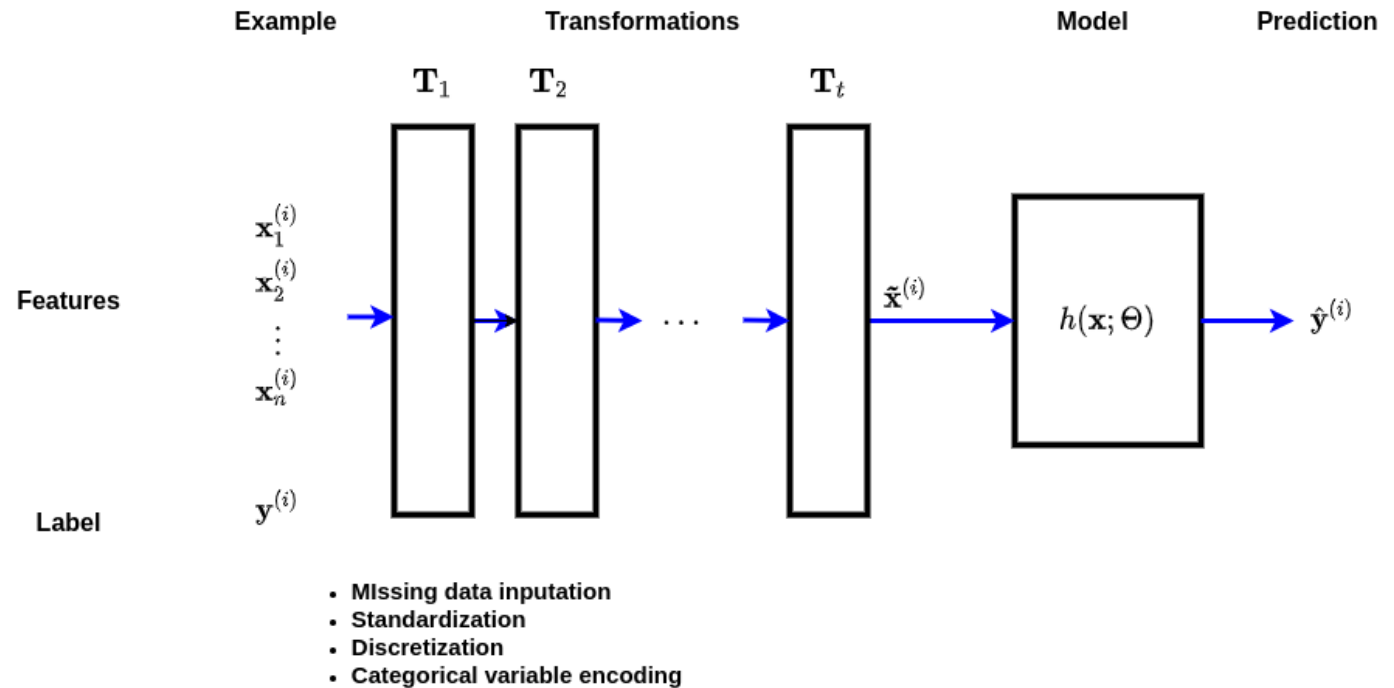
- takes an example: vector $\mathbf{x}^{(i)}$ with n features
- produces a new vector $\tilde{\mathbf{x}}^{(i)}$, with n' features

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

We can apply multiple transformations, each

- Adding new synthetic features
- Further transforming synthetic features

Feature Engineering



The above diagram shows multiple transformations

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

$$\tilde{\mathbf{x}}_{(1)} = T_1(\mathbf{x})$$

$$\tilde{\mathbf{x}}_{(2)} = T_1(\tilde{\mathbf{x}}_{(1)})$$

$$\vdots$$

$$\tilde{\mathbf{x}}_{(l+1)} = T_1(\tilde{\mathbf{x}}_{(l)})$$

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

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

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}

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

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.

#	x_1	x_2
1	1.0	10
2	2.0	20
\vdots	\vdots	\vdots
i	2.0	NaN
\vdots	\vdots	\vdots
m	...	

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

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:

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

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 Θ .

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 Θ , 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

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

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

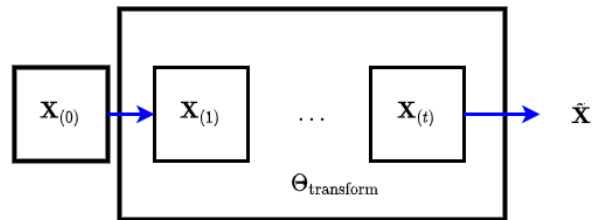
- We would violate the Fundamental Assumption of Machine Learning

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: $\text{min}(\mathbf{X}), \text{max}(\mathbf{X})$
- 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

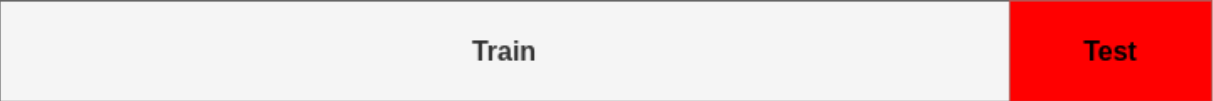
Using pipelines to avoid cheating in cross validation

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/Validation/Test



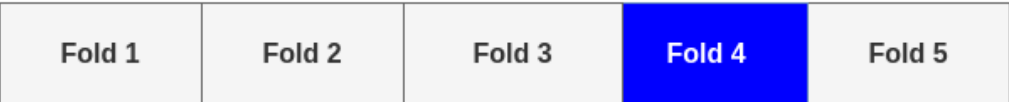
Cross Validation
Split 1



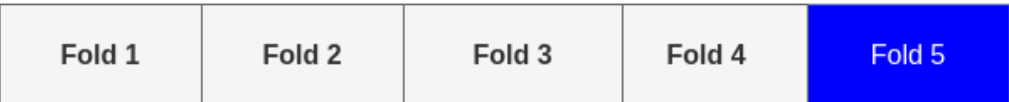
Split 2



Split 3



Split 4



Split 5



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 for training in this fit

For example, when Fold₁ is out of sample

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

versus

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

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