Transformation pipelines

A transformation pipeline is a a sequence (sometimes called a *pipeline*) of independent transformations $T_1, T_2, \ldots, T_t$

$$
\begin{aligned}
\tilde{\mathbf{x}}_{(1)} &= T_1(\mathbf{x}) \\
\tilde{\mathbf{x}}_{(2)} &= T_2(\tilde{\mathbf{x}}_{(1)}) \\
&\vdots \\
\tilde{\mathbf{x}}_{(l+1)} &= T_{(l+1)}(\tilde{\mathbf{x}}_{(l)})
\end{aligned}
$$

The final transformed $\tilde{\mathbf{x}}$ can be implemented as a function T that is the composition of each transformation function

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

Pipelines in sklearn

`sklearn` has created a generic architecture called `Pipeline` to simplify this for you.

This module is **not meant to be a tutorial**, only to highlight a very convenient tool in `sklearn`.

Here (https://scikit-learn.org/stable/modules/compose.html) is a link to `sklearn`'s manual.

Let's illustrate with a two-step sequence of transformations on numeric features

- Missing data imputation
  - If feature j is missing for example i ($\mathbf{x}_j^{(\mathbf{i})}$ not defined)
  - Replace it with the median (over all m examples) of $\mathbf{x}_j$
- Add a second order polynomial feature to each example

Here is some illustrative code

```
# Illustrative code: this cell is NOT executable from sklearn import pipeline from sklearn.impute import
SimpleImputer from sklearn.preprocessing import PolynomialFeatures # Create transformers
polynomial_features = PolynomialFeatures(2) imputed_features = SimpleImputer(strategy='median') # Put
the transformers into a Pipeline num_pipe = pipeline.Pipeline( [ ("imputer", imputed_features),
("polynomial_features", polynomial_features), ]
```

Each individual transformation has a `fit` and `transform` method, just like a model (e.g., `LinearRegression`)

- `fit` on the transformation `SimpleImputer(strategy='median')` computes the median value of each feature
  - Computes $\Theta_{\text{transform}}$, the parameters of this transformation
- `transform` applies the transformation, after it has been fit
  - creates $\tilde{\mathbf{x}}$ from $\mathbf{x}$

The Pipeline `num_pipe` defines a *sequence* of transformations

- Each element of the Pipeline is a tuple
    - name of the transformation (for your convenience in referencing it)
    - the transformer

The Pipeline *also* has methods `fit` and `transform`

- `fit` on a Pipeline applies `fit` to each component transformation in turn
- `transform` on a Pipeline applies `transform` to each component transformation in turn

The `Pipeline` is thus a composition of the individual transformations

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

Observe that transformers and models both respond to the `fit` and `transform` methods.

This means that you can include a model as the final element of a Pipeline !

```
# Illustrative code: this cell is NOT executable from sklearn import datasets, linear_model linear_regression = linear_model.LinearRegression() full_pipe = pipeline.Pipeline( [ ("imputer", imputed_features), ("polynomial_features", polynomial_features), ("model", linear_regression) ]
```

You can fit the transformations *and* the model in one step

- `full_pipe.fit(X, y)`

In addition to being a concise and convenient notation, pipelines with models as final elements

- Can be used in Cross Validation to avoid "cheating"
- The cross validation code passes in *only* the folds that are the training examples

Example: Pipeline with model as final element

Let's apply a Pipeline to solve an example encountered in a previous module

- Linear Regression model
- With a second order feature added

Let's get the data again:

In [4]:

```
# I will give you the data via a function (so I can easily alter the data in sub
sequent examples)
v1, a1 = 1, .005
lin = recipe_helper.Recipe_Helper(v = v1, a = a1)

X_lin, y_lin = lin.gen_data(num=50)

v2, a2 = v1, a1*2
curv = recipe_helper.Recipe_Helper(v = v2, a = a2)
X_curve, y_curve = curv.gen_data(num=50)

X_train, X_test, y_train, y_test = rh.split(X_curve,y_curve)
```

And here's the model, implemented via a Pipeline in `sklearn`

In [5]:

```python
from sklearn.preprocessing import PolynomialFeatures
import sklearn.preprocessing as pre_proc

# Create the Pipeline
from sklearn.pipeline import make_pipeline
poly_model = make_pipeline(pre_proc.PolynomialFeatures(2),
                           linear_model.LinearRegression())

# Fit the model, running the data transformation first
_= poly_model.fit(X_train.reshape(-1,1), y_train)
```

The `PolynomialFeatures(2)` transformer

- Replace each $\mathbf{x}$
- With 3 features: $\mathbf{x}^0, \mathbf{x}^1, \mathbf{x}^2$

That is: it creates an "intercept" dummy ($\mathbf{x}^0 == 1$) plus first and second order features.

A pipeline successively applies transformations, with the result of transformation $(i-1)$ fed as input to transformation i.

Let's look "inside" the pipeline at the stages, and apply them manually.

In [6]:

```python
# Examine the "stages" of the pipeline
print("Input shape: {shp}".format(shp=X_test.reshape(-1,1).shape)  )

# First stage: Create First and Second Order polynomial features
(label_0, model_0) = poly_model.steps[0]
transf_0 = model_0.transform(X_test.reshape(-1,1))
print("{lab:s} returns shape: {shp}".format(lab=label_0, shp=transf_0.shape) )

# Second stage: Linear Regression
(label_1, model_1) = poly_model.steps[1]
transf_1 = model_1.predict( transf_0 )
print("{lab:s} returns shape: {shp}".format(lab=label_1, shp=transf_1.shape) )
```

```
Input shape: (10, 1)
polynomialfeatures returns shape: (10, 3)
linearregression returns shape: (10, 1)
```

In [7]:

```
# Prediction based on test set
y_pred = poly_model.predict(X_test.reshape(-1,1))

# In and out of sample scores
print("Score (train): ", poly_model.score(X_train.reshape(-1,1), y_train))
print("Score (test): ",  poly_model.score(X_test.reshape(-1,1),  y_test))
```

```
Score (train):  1.0
Score (test):  1.0
```

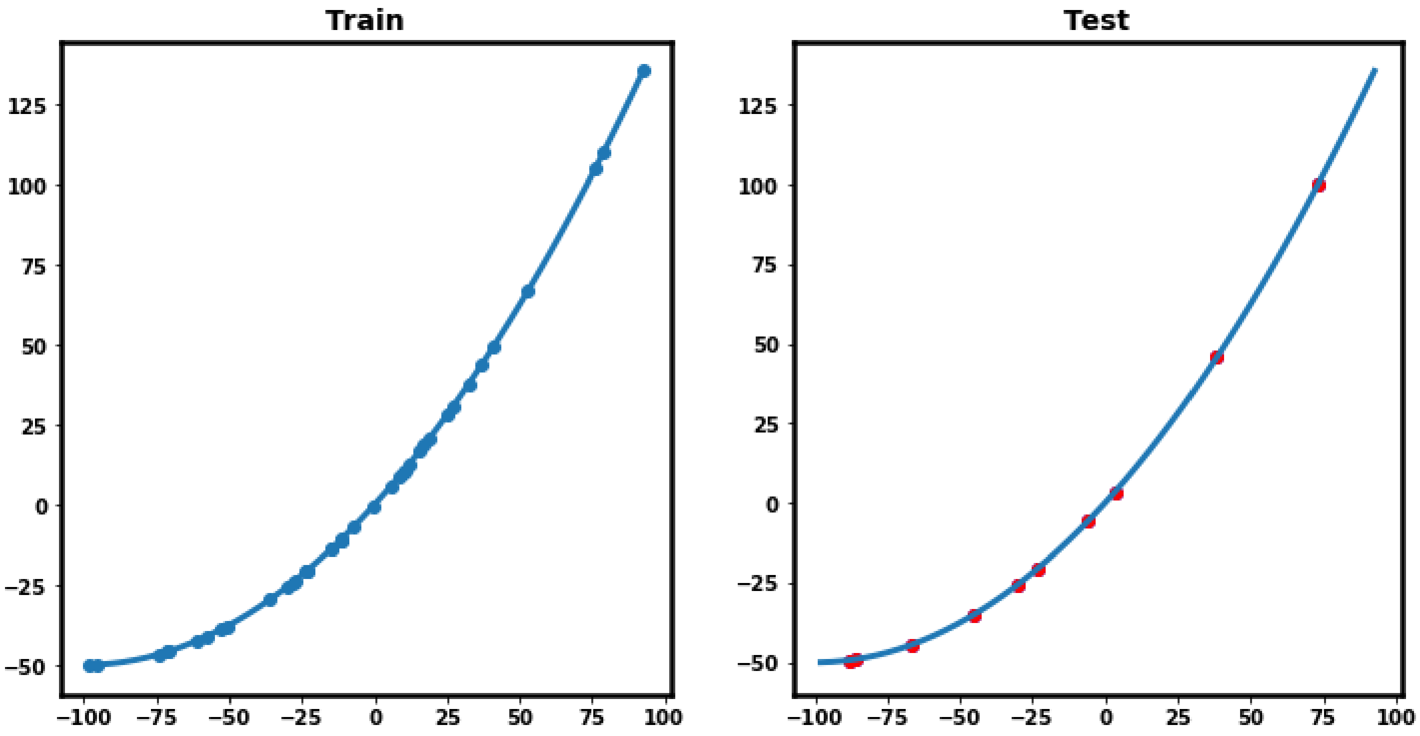
In [8]:

```
# Plot the results
# Create a figure
fig, axs = plt.subplots(1,2, figsize=(12,6))

_= axs[0].scatter(X_train,y_train)

xfit = np.linspace( X_train[:,0].min(), X_train[:,0].max()).reshape(-1,1)
yfit = poly_model.predict(xfit)
_= axs[0].plot(xfit, yfit);
_= axs[0].set_title("Train")

_ = axs[1].scatter(X_test, y_test, color="blue")
_ = axs[1].scatter(X_test, y_pred, color="red")

_= axs[1].plot(xfit, yfit)
_= axs[1].set_title("Test")


print("R-squared score (test): {:.2f}".format(r2_score(y_test, y_pred)) )

# Hide the figure for now, will show it in the next slide
plt.close(fig)
```

```
R-squared score (test): 1.00
```

In [9]:
```
fig
```

Out[9]:



Here's (external/PythonDataScienceHandbook/notebooks/05.04-Feature-Engineering.ipynb#Feature-Pipelines) a slightly longer pipeline from VanderPlas.

- `Imputer` to deal with misssing values
- `PolynomialFeatures(degree=2)`
- `LinearRegression()`

Nested Pipelines

A Pipeline responds to the same methods (`fit`, `transform`) as its elements.

This means that a Pipeline can also be used as a *nested* element of an outer Pipeline.

This is very convenient: we will illustrate this in our detailed example for Classification.

Advanced Pipelines

An issue with Pipelines is that each transformation is applied to *all* the features in an example.

But some transformations need to be applied to *selected* features

- Can't apply numeric transformations to non-numeric data, and vice-versa
- May want to apply a particular transformation to only a subset of features

`sklearn` facilitates this by

- Allowing you to create "filters" that restrict features to a subset
- Applying one pipeline per subset
- Creating a union of transformed features at the end

`FeatureUnion`

`sklearn` allows you to create complex Pipelines with the `FeatureUnion` Pipeline

- "glue together" the features of separate Pipelines. For example
    - Create one pipeline to be applied only to numeric features
    - Create one pipeline to be applied only to non-numeric features

Here is some illustrative code:

num_pipeline = Pipeline([("select_numeric", DataFrameSelector(["Age", "SibSp", "Parch", "Fare"])), ("imputer", SimpleImputer(strategy="median")),]) cat_pipeline = Pipeline([("select_cat", DataFrameSelector(["Pclass", "Sex", "Embarked"])), ("imputer", MostFrequentImputer()), ("cat_encoder", OneHotEncoder(sparse=False)),]) from sklearn.pipeline import FeatureUnion preprocess_pipeline = FeatureUnion(transformer_list=[("num_pipeline", num_pipeline), ("cat_pipeline", cat_pipeline),]) The first element in each pipeline (`DataFrameSelector`)

- restricts each example to a selected subset of features

So the numeric and categorical pipelines above transform disjoint groups of features.

The `FeatureUnion` concatenates (along the horizontal axis) the result of the separate transformations.

`ColumnTransformer`

There is an *experimental* Pipeline object in `sklearn` called Column Transformers, that is a simplification of the `FeatureUnion` paradigm

- No need to filter the features with `DataFrameSelector`
    - just provide a list of feature names
- No need to use `FeatureUnion'

This object *only works* for collections of examples in which we can access features *by name*

- Panda DataFrames !

Here is some illustrative code

cat_features = ["Sex", "Pclass"] cat_transformers= Pipeline(steps=[('imputer', MostFrequentImputer()), ('sex_encoder', SexToInt())]) cat_pipeline = ColumnTransformer(transformers=[("categorical", cat_transformers, cat_features)])

Creating your own transformations

In addition to supplying a number of built-in transformers, `sklearn` let's use build your own.

- Create an object that is subclass of the types used by built-in transformer
- Provide your own implementation of `fit` and `transform`

Here's a transformation for imputation of missing values using the most frequent value as the substitute.

- Similar in function to the built-in `SimpleImputer(strategy="most_frequent")`

In [10]:

```
# Inspired from stackoverflow.com/questions/25239958
from sklearn.base import BaseEstimator, TransformerMixin

class MostFrequentImputer(BaseEstimator, TransformerMixin):
    def fit(self, X, y=None):
        self.most_frequent_ = pd.Series([X[c].value_counts().index[0] for c in
X],
                                        index=X.columns)
        return self

    def transform(self, X, y=None):
        return X.fillna(self.most_frequent_)
```

Example

We will use Pipelines in our Classification task.

In [11]:

```
print("Done")
```

```
Done
```