Transform Your Workflow with `scikit-learn`

Sam Ballerini

KPMG D&A Super Day 2018

scikit
learn

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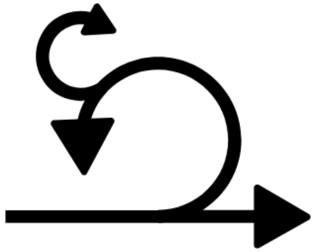
Speed

scikit learn

Speed



Agility

scikit learn

Speed

Agility

Accuracy

Agenda

1. API Overview
2. Pipelines
3. Cross-validation
4. Customization

Why `scikit-learn`?

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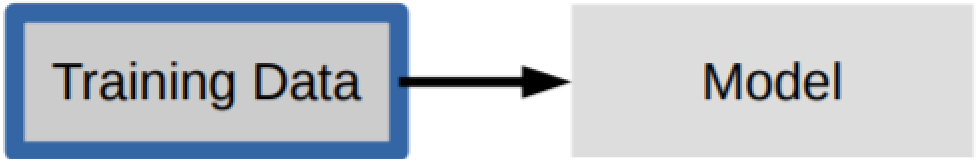
Transformers

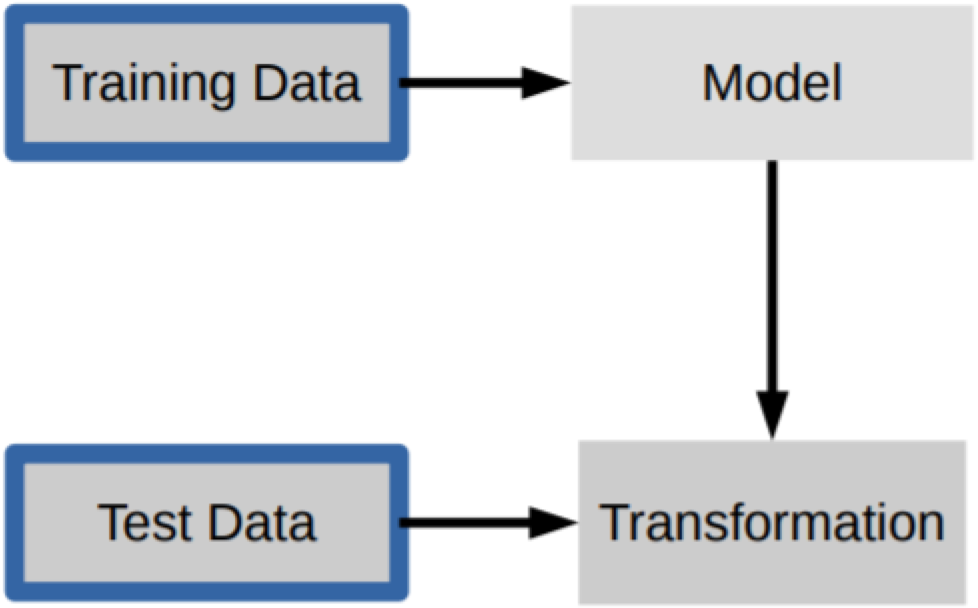
Estimators

`scikit-learn` Transformers



`fit` – find parameters from training data (if needed)

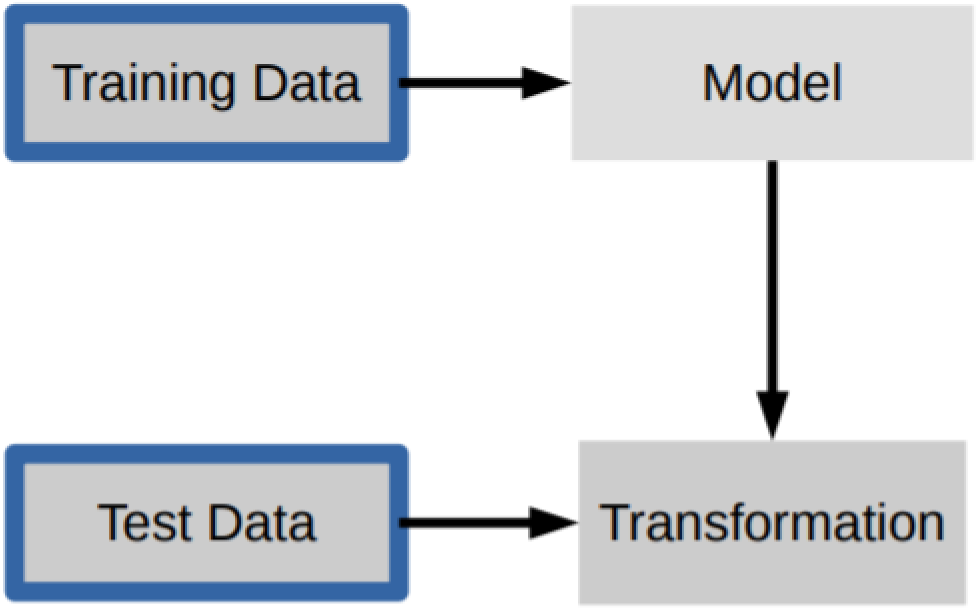
`scikit-learn` Transformers



`fit` – find parameters from training data (if needed)

`transform` – apply to training or test data

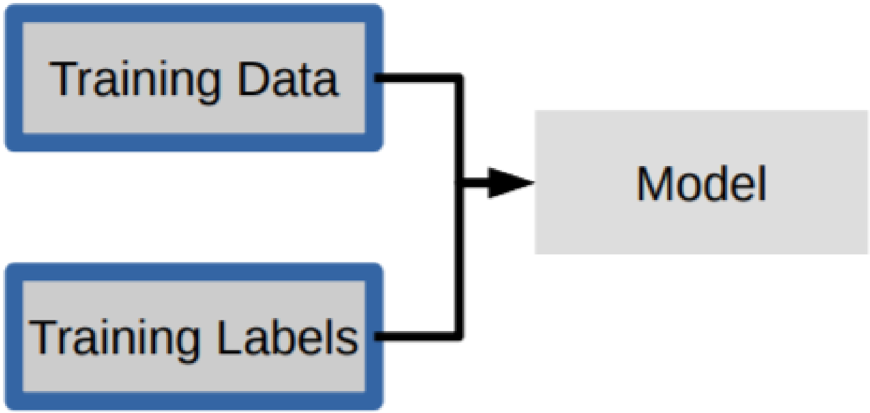
scikit-learn StandardScaler



`fit` – find mean, standard deviation of each feature

`transform` – subtract mean then divide by sd

`scikit-learn` Estimators



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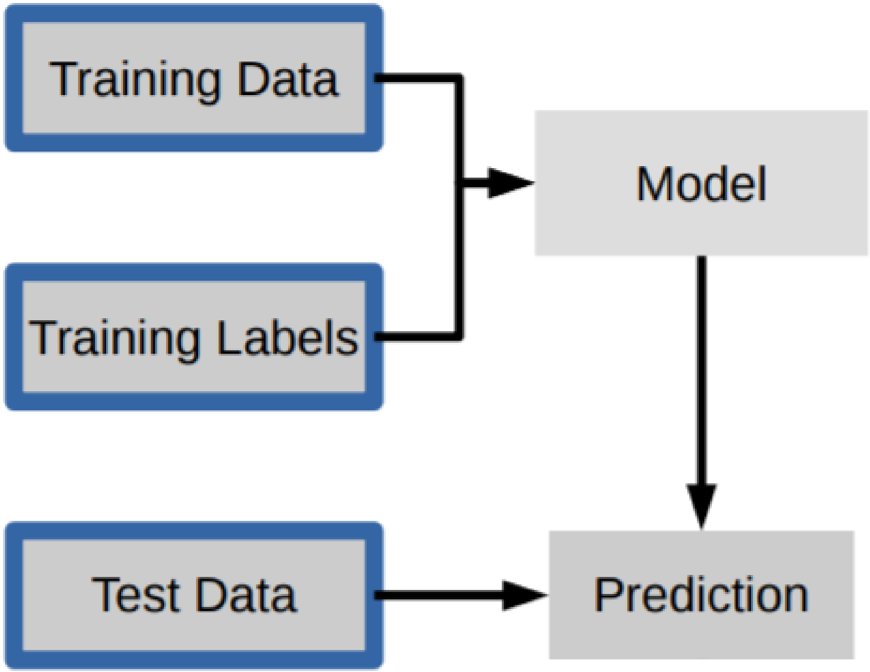
scikit-learn Estimators



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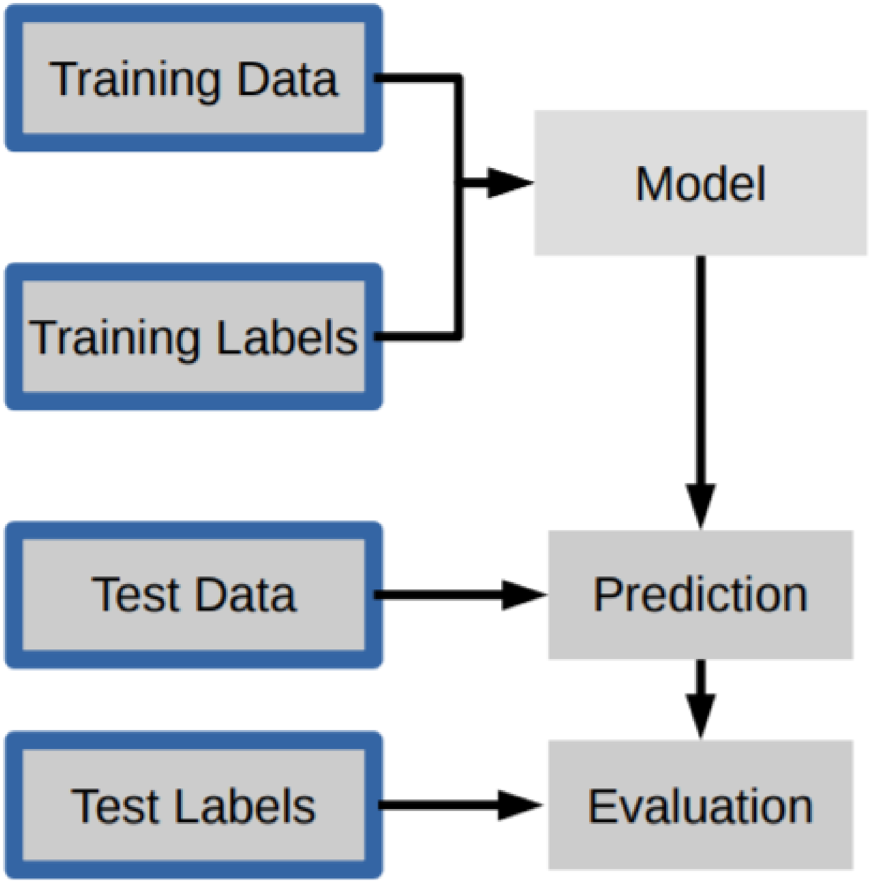
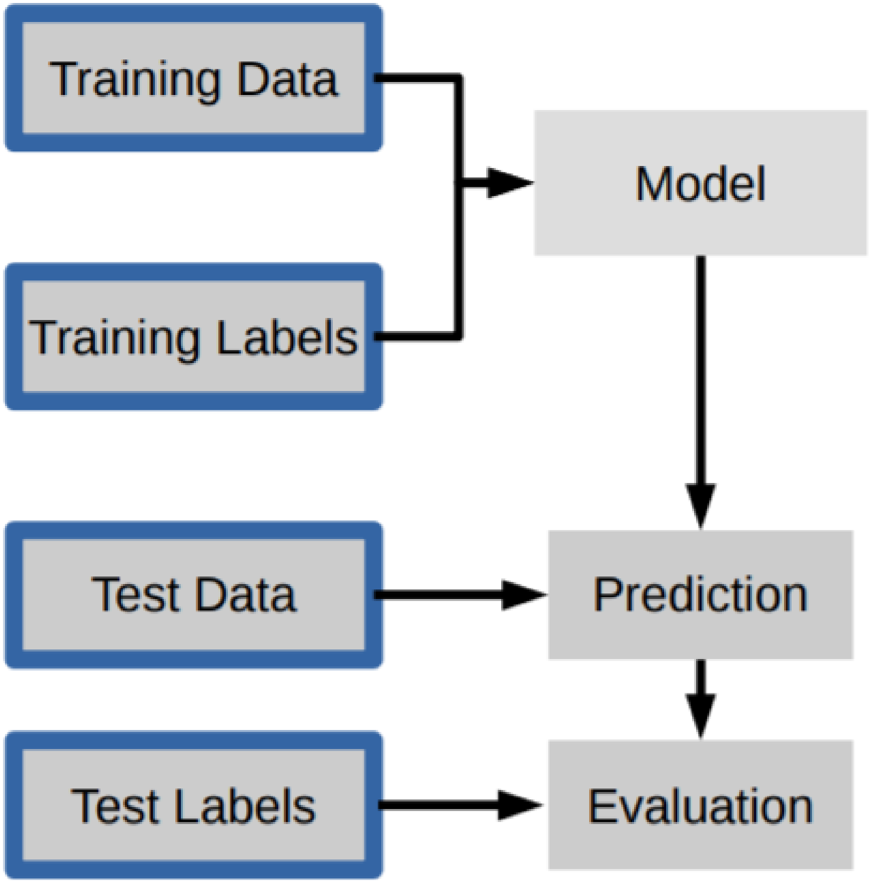


`fit` – find parameters from training data

`predict` – apply to training or test data

`score` – assess model fit

`scikit-learn` `LogisticRegression`



`fit` – find coefficients in logistic regression formula

`predict` – plug into formula, get predicted class

`score` – assess model fit

Alright then…let’s see some code!

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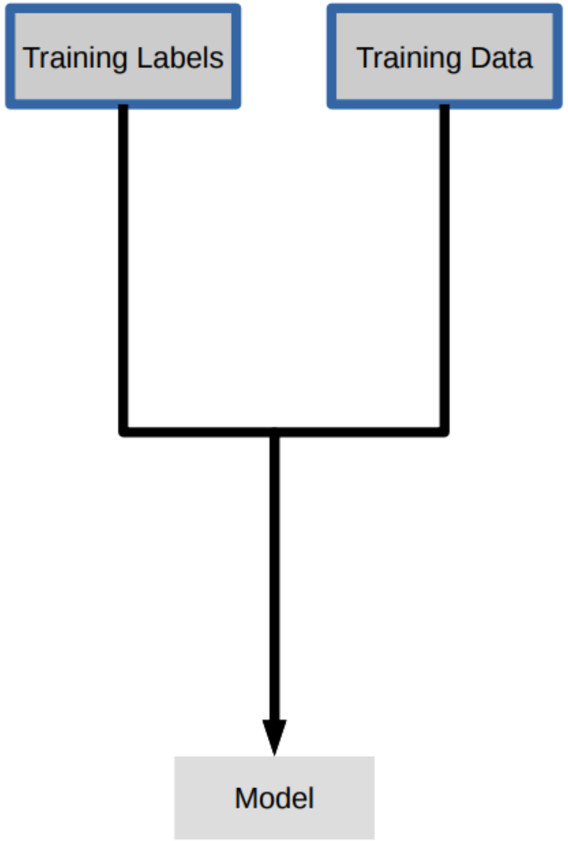
Pipelines to the rescue!

`scikit-learn` Pipelines



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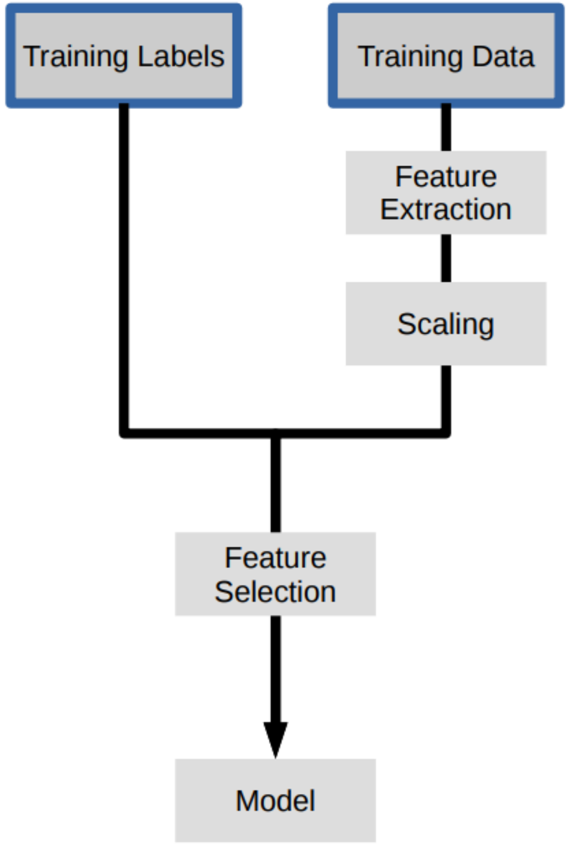

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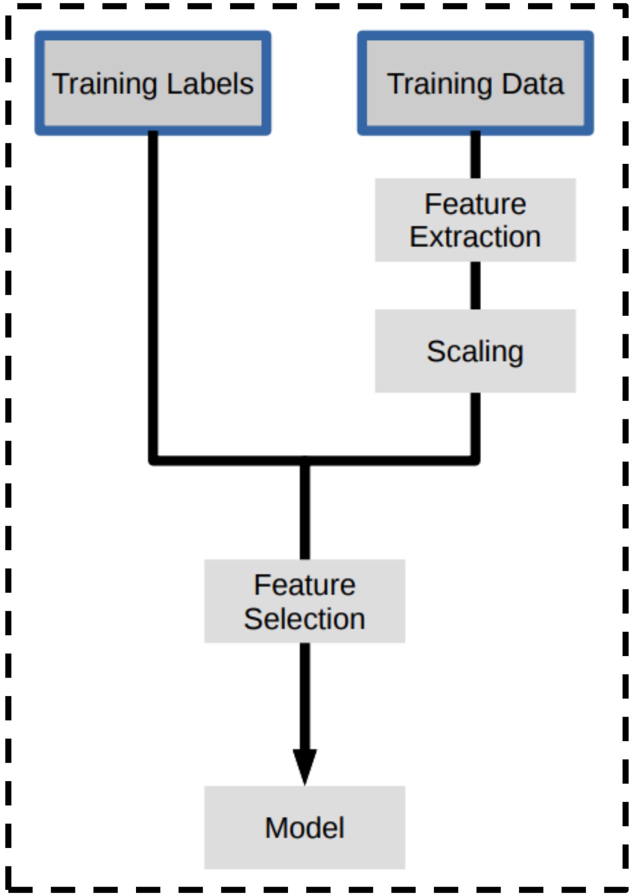
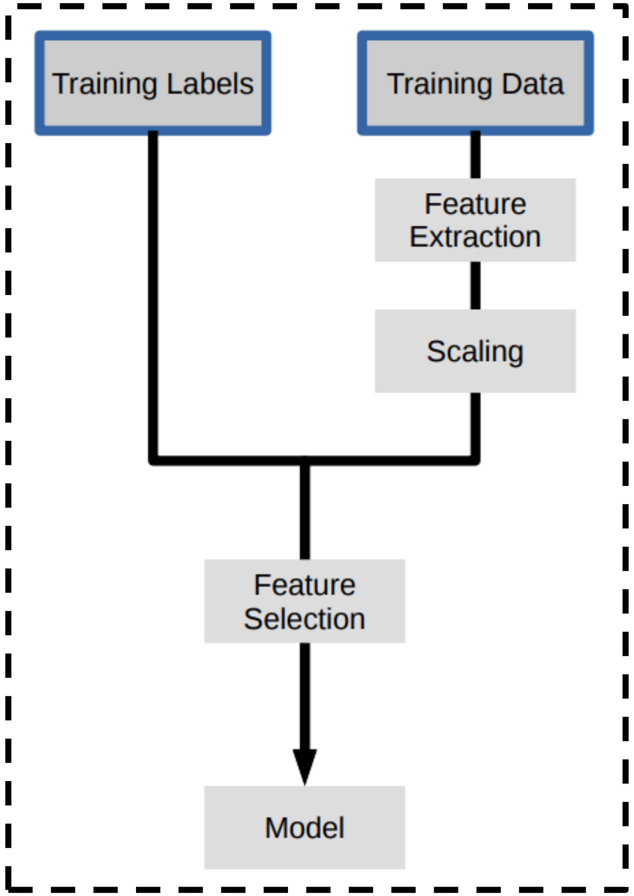


- Encapsulate the modeling process

`scikit-learn` Pipelines



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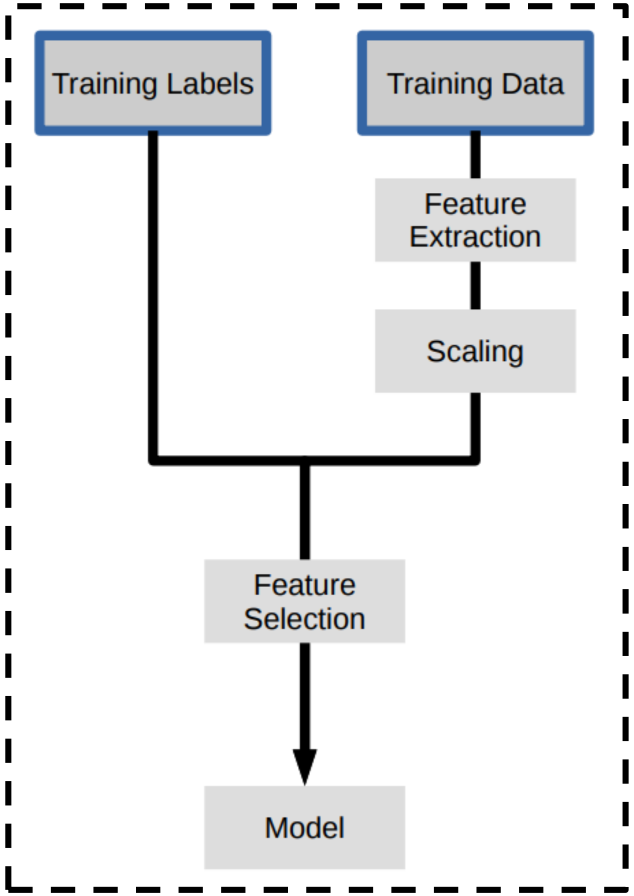

- Encapsulate the modeling process
- Avoid repetitive code
- Hot-swap algorithms

Back to the code

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`scikit-learn` Pipelines

- Instead…use a pipeline!

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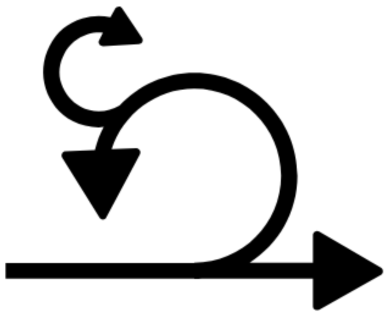
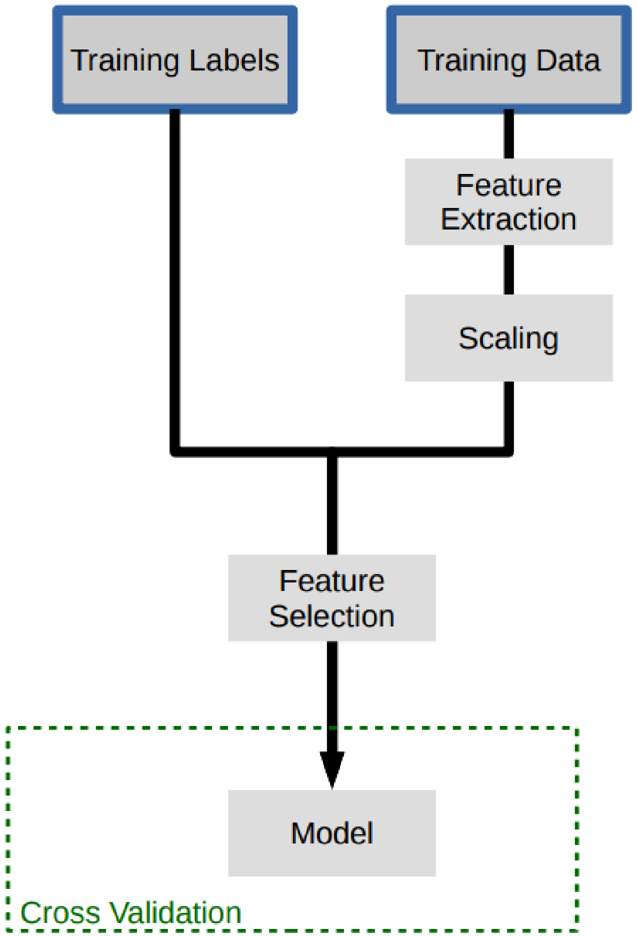
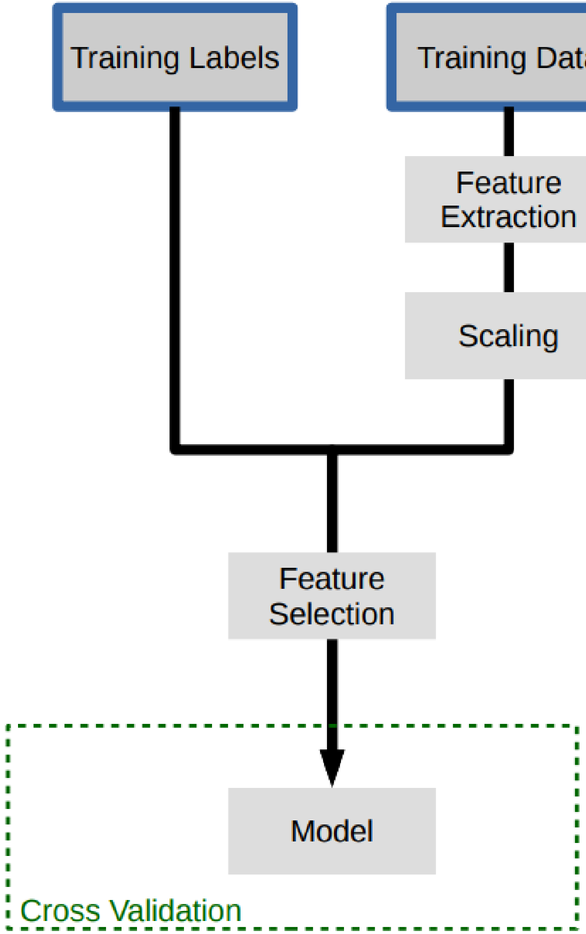
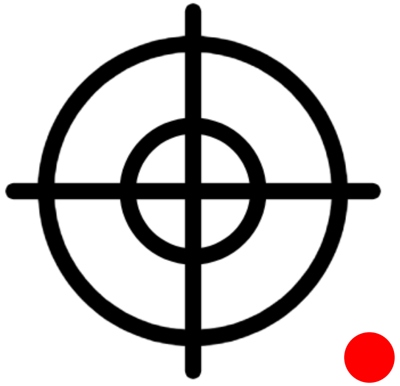


Cross-validation the Wrong Way



Cross-validation the Wrong Way





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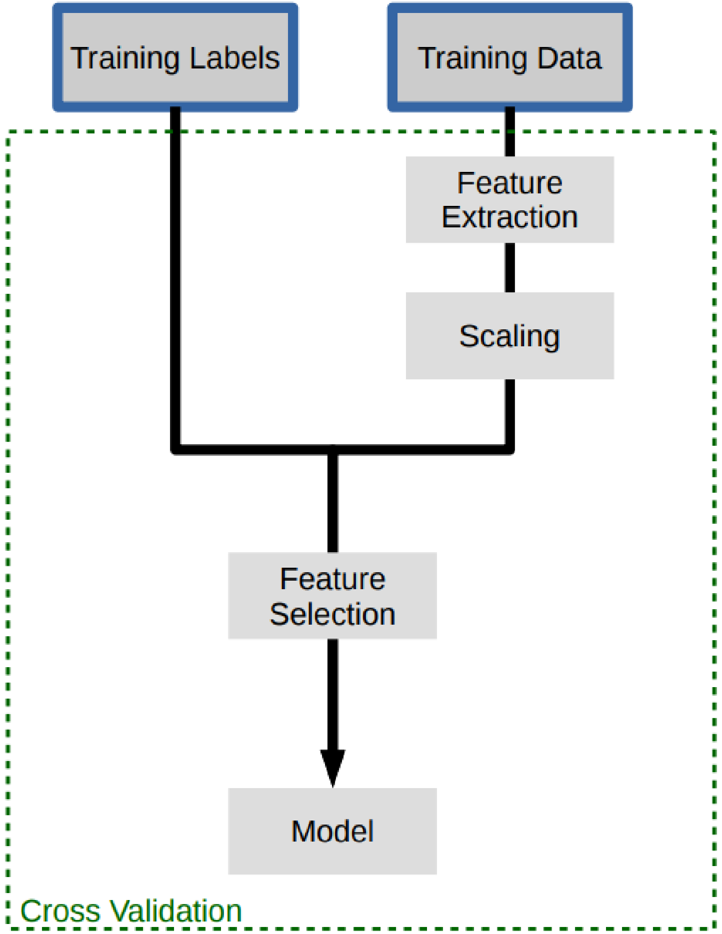

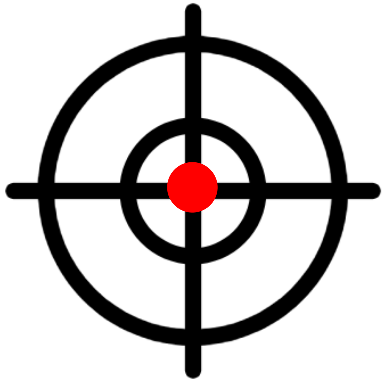

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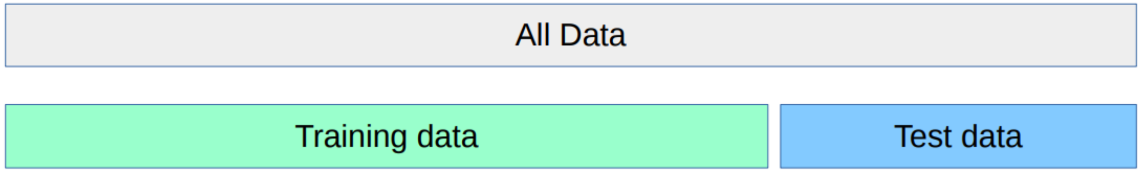

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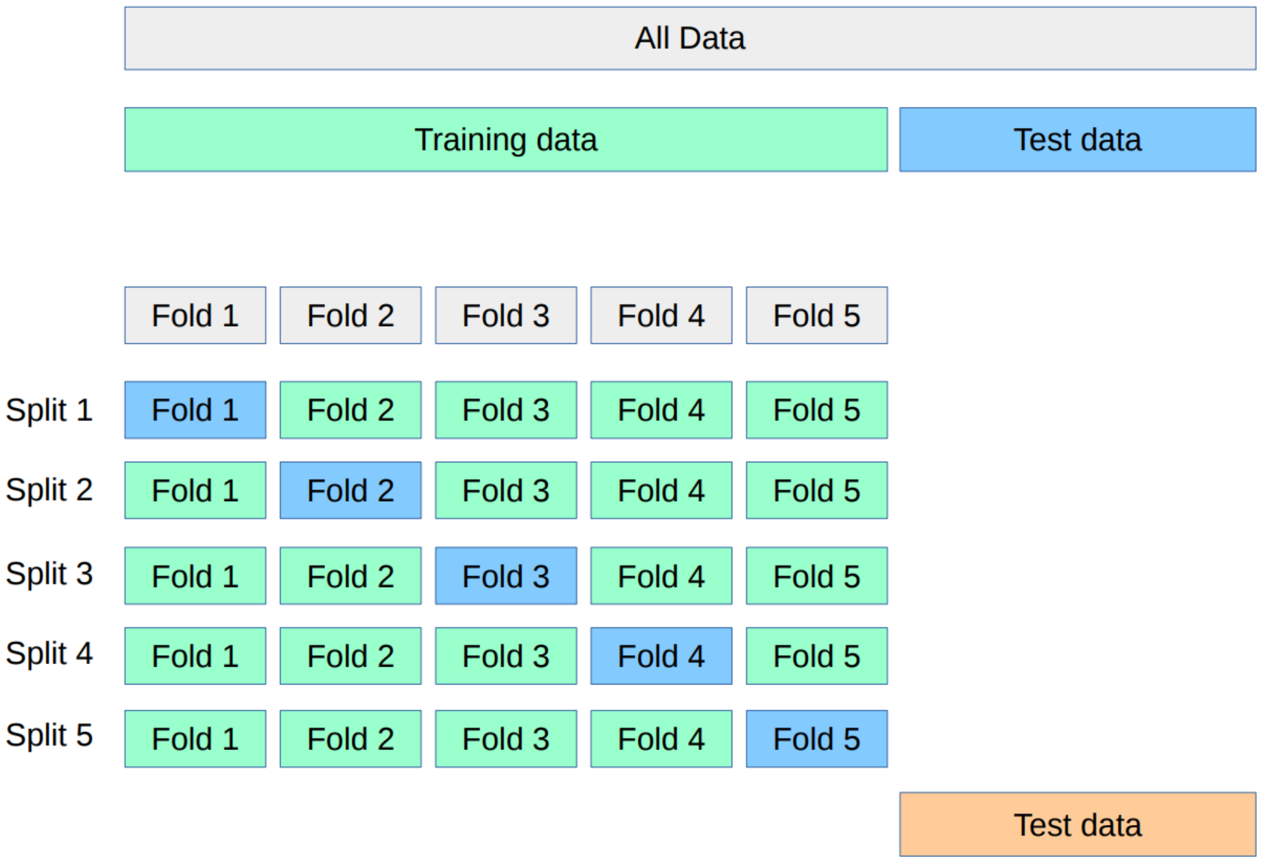

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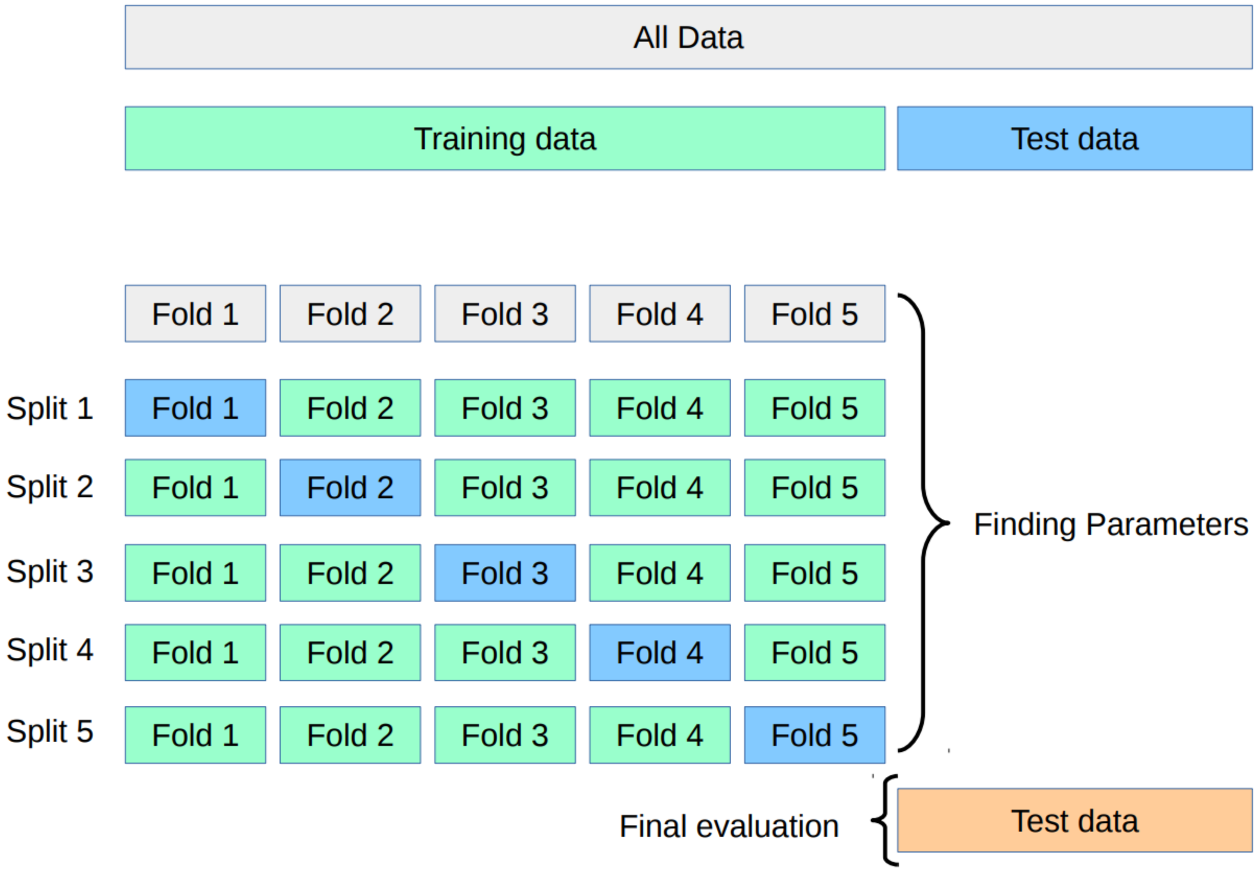
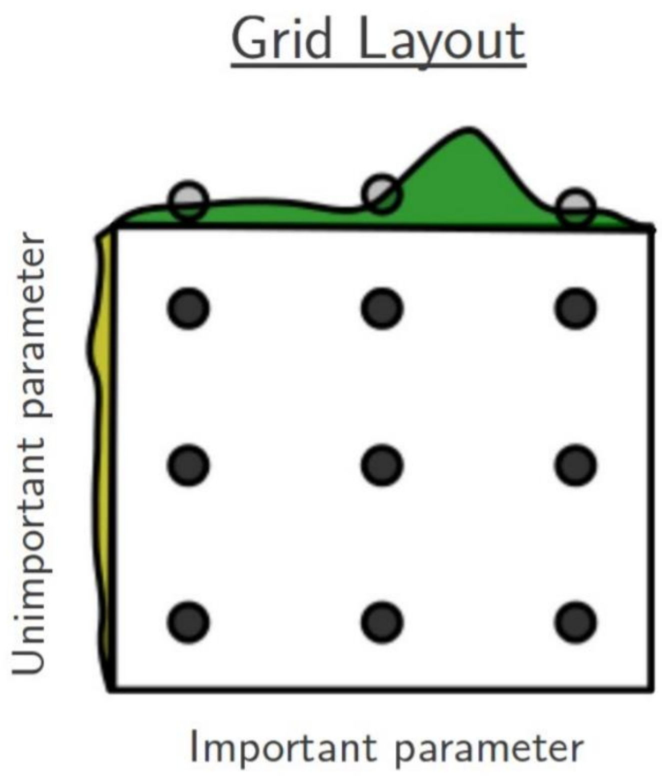


Hyperparameter Tuning



Source: Bergstra and Bengio

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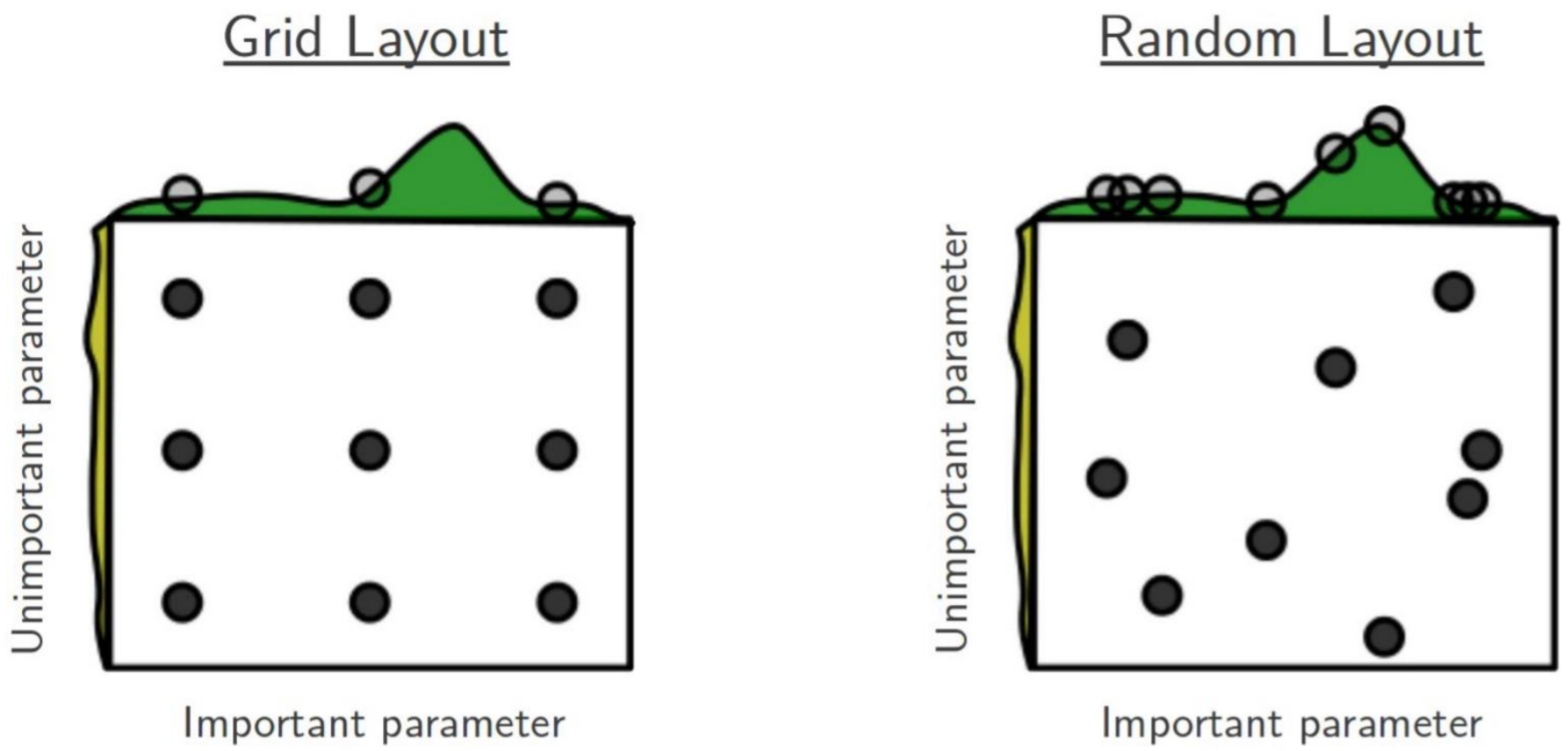

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Extend the API!

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Custom Transformer Use Cases

- Encoding multiple categorical variables
- Extracting columns by type
- Extracting units of time

`DictVectorizer`

- Handles new and unseen levels of categorical variables in test data
- Prevents mismatch of train and test data dimensions

Nested Pipeline with Custom Transformers

```
pipeline = Pipeline([
    ('drop_column', ColumnDropper(col=['service_cd', 'diagnosis_cd', 'county_calc'])),
    ('preproc', FeatureUnion([
        ('continuous', Pipeline([
            ('extract', ColumnExtractor(dtype='number')),
            ('impute', Imputer()),
            ('nearzero', VarianceThreshold())
        ])),
        ('factors', Pipeline([
            ('extract', ColumnExtractor(dtype='object')),
            ('labencode', MultiColumnLabelEncoder()),
            ('impute', Imputer(strategy='most_frequent')),
            ('onehot', OneHotEncoder(handle_unknown='ignore')),
        ])),
    ])),
    ('to_dense', DenseTransformer()),
    ('model', ExtraTreesRegressor(bootstrap=False))
])
```

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More ML Tools

- Yellowbrick – ML visualizations
- Lime – Explain ML predictions
- imbalanced-learn – Over- and under-sampling
- sklearn-pandas – Pandas integration with sklearn

Special Thanks

- Andreas Mueller, Machine Learning Scientist at Columbia University
  - Machine Learning with Scikit-learn, PyData NYC 2015
- Stephen Hoover, Lead Data Scientist at Civis Analytics
  - Scaling Scikit-learn, PyData Seattle 2017
- Julie Michelman, Data Scientist at zulily
  - Pandas, Pipelines, and Custom Transformers, PyData Seattle 2017
- Zac Stewart, Software Developer
  - Using scikit-learn Pipelines and FeatureUnions
- Zen Pursuits
  - Pipelines, FeatureUnions, GridSearchCV, and Custom Transformers