ML Part 2 tutorial

Dimensionality reduction & cross-validation

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Problem setting

$$Y = f(X) + E \quad (1)$$

- $Y \in \mathbb{R}$: output (a.k.a. target, dependent variable) to predict
- $X \in \mathbb{R}^p$: features (a.k.a. inputs, regressors, descriptors, independent variables)
- $E \in \mathbb{R}$: unmodelled noise
- f: the function we try to approximate

Parameter estimation a.k.a. model fitting

Minimize a sum of:

- the empirical risk: error on training data
- a regularization term

Example: logistic regression

$$\underset{\boldsymbol{\beta}, \beta_0}{\operatorname{argmin}} \frac{1}{2} \|\boldsymbol{\beta}\|_2^2 + C \sum_{i=1}^{n} \log(\exp(-y_i \, (\mathbf{X}_i^T \, \boldsymbol{\beta} + \beta_0)) + 1) \tag{2}$$

- $\boldsymbol{\beta}, \beta_0$: parameters to be *estimated*
- C: hyperparameter, *chosen* prior to learning (controls amount of regularization)

`sklearn.linear_model.LogisticRegression`

scikit-learn "estimator API": `fit; predict`

```
estimator = LogisticRegression(C=1)
estimator.fit(X_train, y_train)
predictions = estimator.predict(X_test)
```

https://scikit-learn.org/stable/getting_started.html
sklearn.linear_model.LogisticRegression

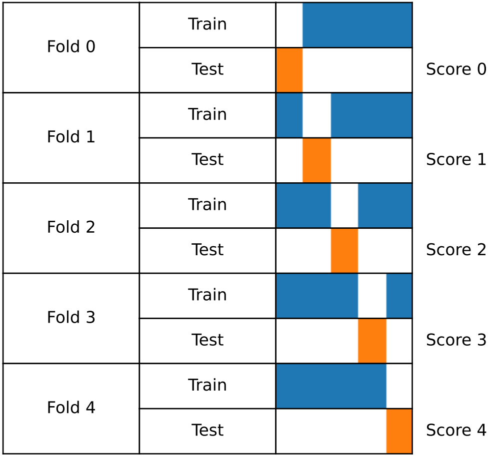
Evaluating performance with `sklearn.metrics`

```
estimator = LogisticRegression(C=1)
estimator.fit(X_train, y_train)
predictions = estimator.predict(X_test)

accuracy = metrics.accuracy_score(y_test, predictions)
```

https://scikit-learn.org/stable/getting_started.html
`sklearn.linear_model.LogisticRegression`
`sklearn.metrics` more info on model evaluation

Cross-validation



scikit-learn.org/stable/modules/cross_validation.html
sklearn.model_selection.cross_validate

Dataset transformations

Typical pipeline

Feature extraction → Standardization → Dim reduction → Estimator

Example: for autism prediction with fMRI from ML part 1

`ConnectivityMeasure` → `StandardScaler` → `PCA` → `LogisticRegression`

scikit-learn "transformer API": `fit; transform`

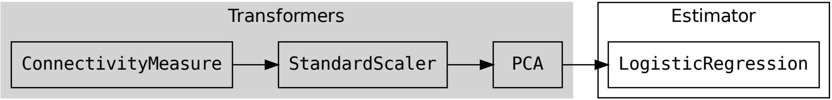
```
transformer = StandardScaler()
transformer.fit(X_train)
transformed_X = transformer.transform(X_train)
```

`sklearn.preprocessing.StandardScaler`
scikit-learn "getting started"
scikit-learn "user guide"

scikit-learn "transformer API": `fit; transform`

```
transformer = StandardScaler()
transformed_X = transformer.fit_transform(X_train)

transformed_X_test = transformer.transform(X_test)
```



`sklearn.preprocessing.StandardScaler`
scikit-learn "getting started"
scikit-learn "user guide"

Example: `preprocessing.StandardScaler`

`fit`:
Compute mean and standard deviation of each column

`transform`:
Subtract mean and divide by standard deviation

`sklearn.preprocessing.StandardScaler`

Example: `feature_selection.SelectKBest`

`fit:`

- Perform ANOVA for each column of X
- Remember the indices of the k columns with highest scores

`transform:`

- Index input to keep only the k selected columns

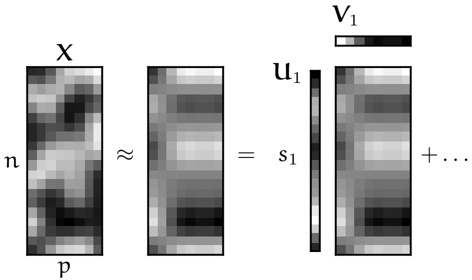
`sklearn.feature_selection.SelectKBest`

Example: `decomposition.PCA`

`fit:`

- Compute Singular Value Decomposition of X

$$X = U\,S\,V^{\top} \tag{3}$$



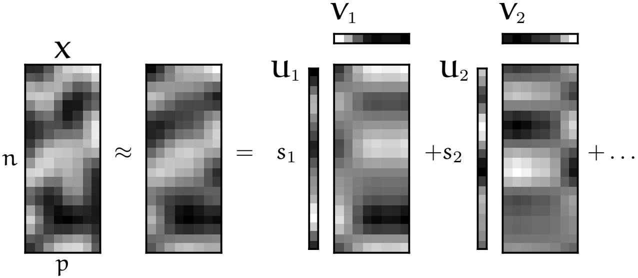
Explained variance: 0.53

Example: `decomposition.PCA`

`fit:`

- Compute Singular Value Decomposition of X

$$\mathsf{X} = \mathsf{U}\, S\, \mathsf{V}^{\intercal} \tag{4}$$



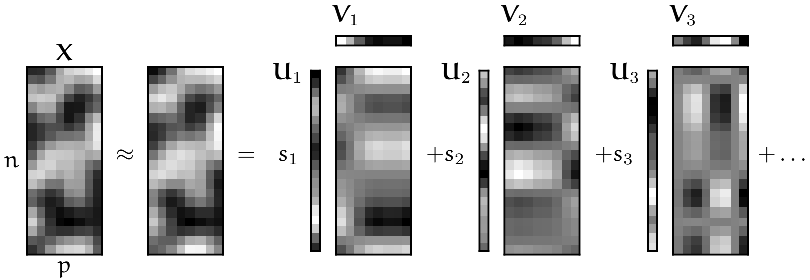
Explained variance: 0.84

Example: `decomposition.PCA`

`fit:`

- Compute Singular Value Decomposition of X

$$X = U S V^{\top} \tag{5}$$



Explained variance: 0.97

Example: `decomposition.PCA`

`fit:`

- Compute Singular Value Decomposition of $\mathbf{X}$
$$\mathbf{X} = \mathbf{U}\,\mathbf{S}\,\mathbf{V}^{\mathsf{T}}$$
- store $\mathbf{V}$

`transform:`
Compute projection on column space of $\mathbf{V}$: simply multiply by $\mathbf{V}^{\mathsf{T}}$

Notes

- `fit_transform`: simply return $\mathbf{U}\,\mathbf{S}$
- $\mathbf{V}^{\mathsf{T}}$ is the ‘components_‘ attribute of a fitted ‘PCA‘ instance

`sklearn.decomposition.PCA`

Chaining transformations

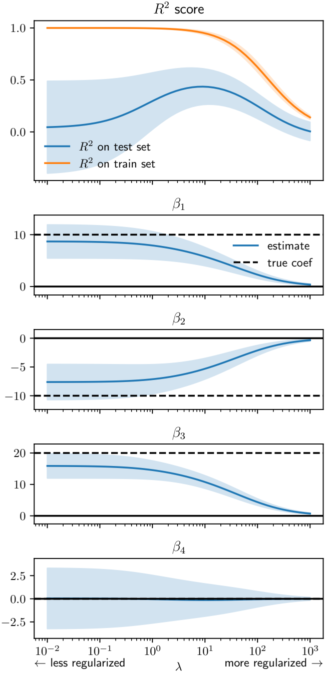
Use `sklearn.pipeline.Pipeline` or `sklearn.pipeline.make_pipeline`:

```
pipe = make_pipeline(
    standardizer, dim_reductor, estimator
)
pipe.fit(X, y)
```

Example:

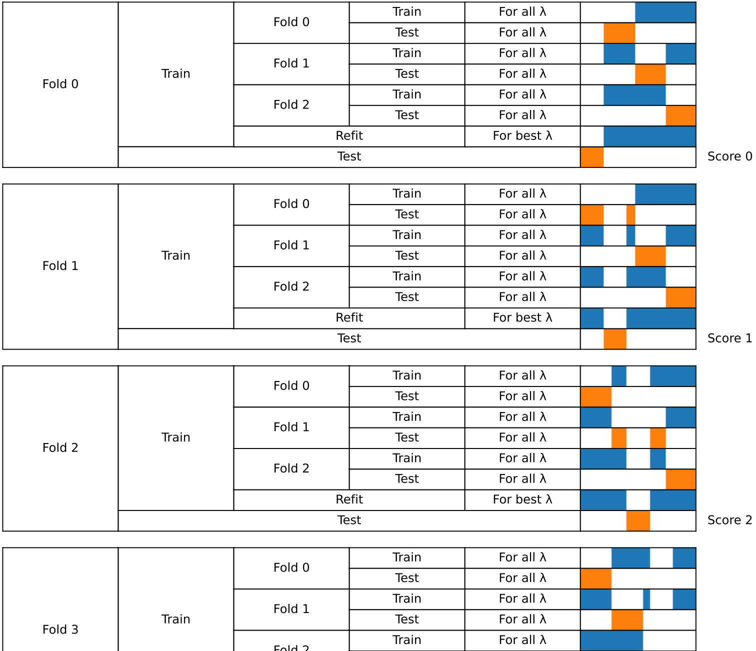
```
make_pipeline(
    StandardScaling(), PCA(), LogisticRegression()
)
```

$$\mathrm{Var}(\hat{\beta}_i) = \mathbb{E}(\hat{\beta}_i - \mathbb{E}(\hat{\beta}_i))^2$$



$$\mathrm{Bias}(\hat{\beta}_i) = \mathbb{E}(\hat{\beta}_i) - \beta_i$$

Nested cross-validation

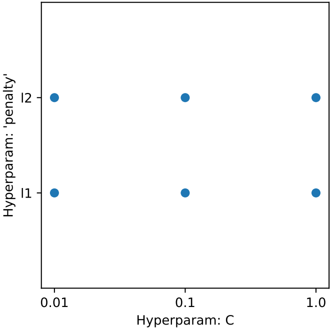


Implementing nested CV

See `nested_cross_validation.py`

Cross-validation and hyperparameter selection in scikit-learn

- `sklearn.pipeline.Pipeline` or `sklearn.pipeline.make_pipeline`
- `sklearn.model_selection.GridSearchCV`
- `sklearn.model_selection.cross_validate`
- use `*CV` estimators! `RidgeCV`, `LogisticRegressionCV`, ...



Cross-validation pitfalls

- fitting part of the pipeline on the whole data: use `Pipeline`
- ignoring some dependencies in the data: use the appropriate cv iterator: https://scikit-learn.org/stable/modules/cross_validation.html#cross-validation-iterators
- good cv scores on one dataset do not guarantee generalization to new data