5 Basic Practice (part 1 of 3)

Feature Engineering

Feature engineering is the transforming of data into a set of labeled examples of selected features.

One-Hot Encoding

For an algorithm requiring only numerical features,¹ use *one-hot encoding* to transform a categorical feature into several binary features.

e.g. Transform categorical color feature into three binary features; only one is hot at a time:

(input)	(output)		
color	green	red	yellow
green	1	0	0
yellow	0	0	1
red	0	1	0
green	1	0	0

(Encoding color as green=0, yellow=1, red=2 causes trouble because red isn't twice yellow, etc.)

This causes collinearity, in which one feature can be predicted from others, leading to numerically unstable computations. Address this by removing one column from the set of one-hot columns.

Python

import pandas as pd

Make one-hot dummy variables from column(s) in DataFrame (or array) data: pd.get_dummies(data, drop_first=False) # also try drop_first=True

```
# Join columns from other DataFrame:
df.join(other)
```

```
# Do both:
df.join(pd.get_dummies(df['column_to_encode'], drop_first=False))
```

- User guide: https://pandas.pydata.org/docs/user_guide/reshaping.html#reshaping-dummies
- Reference manual:

https://pandas.pydata.org/docs/reference/api/pandas.get_dummies.html

```
https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.join.html
```

¹Scikit-learn requres numerical features, but some of its algorithms convert categorical features automatically. Best practice does not rely on this conversion.

Binning

Binning (or bucketing) converts a numeric feature to categorical.

		[0, 3):	baby
e.g. Map numeric ag	umoria aros.	[3, 18):	child
	umeric ages:	[18, 65):	adult
		$[65,\infty)$:	senior

This can reduce the number of necessary training examples by reducing the complexity of the model and telling it values within a bin should be treated the same.

Python

- import pandas as pd
- pd.cut(x, bins, right=True, labels=None) puts values from x (array-like) into bins bins, if bins is a number, or into bins whose edges are in the sequence bins, that (by default) include the rightmost edge. Use provided labels (if not None).
- User guide: https://pandas.pydata.org/docs/user_guide/reshaping.html#tiling
- Reference manual: https://pandas.pydata.org/docs/reference/api/pandas.cut.html

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Rescaling via Normalization or Standardization

• Normalization converts a numeric range into a standard range.

e.g. Min-max normalization replaces $x^{(j)}$ with $\frac{x^{(j)} - \min^{(j)}}{\max^{(j)} - \min^{(j)}} \in [0, 1].$

This can improve training speed by preventing a large-scale feature from dominating a smallscale one early in a gradient descent search. It can help prevent numeric underflow or overflow. It can improve performance.

• Standardization (or z-score normalization) replaces $x^{(j)}$ with $\frac{x^{(j)} - \mu^{(j)}}{\sigma^{(j)}}$. If $x^{(j)} \sim N(\mu^{(j)}, \sigma^{(j)})$, where $\mu^{(j)}$ and $\sigma^{(j)}$ are the feature mean and standard deviation, then the standardized values follow the standard normal distribution N(0, 1).

Experiment with both, considering:

- standardization often works better for:
 - unsupervised algorithms
 - an \approx normal feature
 - a feature with outliers (as normalization would squeeze values into a small range)
- normalization often works better otherwise
- rescaling often helps

Python

• from sklearn.preprocessing import MinMaxScaler

```
scaler = MinMaxScaler()
scaler.fit_transform(X) # do scaling
scaler.inverse_transform(X) # undo scaling
```

• from sklearn.preprocessing import StandardScaler

```
scaler = StandardScaler()
scaler.fit_transform(X) # do scaling
scaler.inverse_transform(X) # undo scaling
```

- User guide: https://scikit-learn.org/stable/modules/preprocessing.html
- Reference manual:

```
https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.MinMaxScaler.html
https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.StandardScaler.html
```

Missing Features and Data Imputation

Three options for handling missing features:

- Remove examples with missing features.
- Use an algorithm (or implementation) that can handle missing features.
- Use data imputation, which replaces a missing feature value $x_i^{(j)}$ with a computed value:
 - the feature mean, $\frac{1}{M} \sum_{i=1}^{M} x_i^{(j)}$, where M < N is the number of examples with feature j present and the sum is over non-missing values
 - a value outside the feature's normal range; e.g. if the range is [0, 1], use -1 or 2 (then the model can learn how to handle the non-normal value)
 - the midpoint of the feature's normal range; e.g. if the range is [0, 1], use 0.5 (hoping this will not significantly affect the prediction)
 - the predicted value from a regression model for $y = x^{(j)}$ trained from the remaining features over the examples not missing $x^{(j)}$
 - 0 (or some other value) while adding a feature with values in $\{0,1\}$ to say for each example whether $x_i^{(j)}$ is present

When predicting y for a new \mathbf{x} , apply the same imputation method.

Python

- df.dropna() drops rows missing at least one element. For more on what you can drop, see https://pandas.pydata.org/docs/reference/api/pandas.DataFrame.dropna.html.
 Missing data user guide: https://pandas.pydata.org/docs/user_guide/missing_data.html.
- from sklearn.impute import SimpleImputer
- imp = SimpleImputer(missing_values=nan, strategy='mean', fill_value=None) makes an imputer that uses the mean;
 - strategy='median' uses the median
 - strategy='constant' uses fill_value
 - strategy='most_frequent' uses the (smallest) most frequent feature value, which may be useful with strings or numeric data
- imp.fit_transform(X) does the imputation
- User guide: https://scikit-learn.org/stable/modules/impute.html
- Reference manual:

https://scikit-learn.org/stable/modules/generated/sklearn.impute.SimpleImputer.html

Feature Selection

Feature selection is the process of choosing a subset of features for use in a model. It can:

- Improve accuracy by reducing overfitting
- Improve computing performance (time, memory, disk space)
- Make model easier to interpret

Python

For each of the following methods:

- Import METHOD via from sklearn.feature_selection import METHOD
- Set selector = METHOD() (with appropriate parameters)
- Call selector.fit_transform(X) or ...transform(X, y) to get a smaller feature array

Here are some options for METHOD:

- VarianceThreshold(threshold=0.0) removes features with variance less than threshold. The return value includes variances_, an array of variances of the features.
 - e.g. threshold=0.0 removes features that do not vary.

e.g. For $B \sim \text{Bernoulli}(p)$, VAR(B) = p(1-p), so we could remove binary features with $p = P(y = 1) \leq 0.1$ or $p \geq 0.9$ with threshold=0.09.

- Methods based on univariate statistics use a score_func(X, y) which returns an array of scores or a pair of arrays of scores and p-values.
 - SelectKBest(score_func, k=10) retains the k best-scoring features.
 - SelectPercentile(score_func, percentile=10) retains the proportion percentile of features ranked by their scores.

Available score_func include:

- For regression, $r_regression$, whose return value includes correlation_coefficient, an array of correlations between the *j*th feature and *y*. This is problematic because *r* tending toward 1 or -1 indicates predictive power, but "highest score" neglects -1.
- For regression, f_regression, which returns a pair of arrays, f_statistic of scores and p_values of p-values.

Recall: $R^2 = \frac{SSR}{SST}$, $1 - R^2 = \frac{SSE}{SST}$, and $F = \frac{MSR}{MSE} = \frac{SSR/1}{SSE/(n-2)} = \frac{R^2SST}{(1-R^2)SST}(n-2) = \frac{R^2}{1-R^2}(n-2)$ and $R^2 = r^2$. So f_regression is computed from r_regression (if D = 1). Since F > 0, it does not suffer from the r_regression problem.

- For classification, chi2 finds a χ^2 statistic between each non-negative feature and y.

To learn more:

- User guide: https://scikit-learn.org/stable/modules/feature_selection
- API reference: https://scikit-learn.org/stable/modules/classes.html#module-sklearn.feature_selection
- Examples: https://scikit-learn.org/stable/auto_examples/index.html#feature-selection

Feature Importance

The *permutation feature importance* of feature j relative to a model is the decrease in the model score when the feature is randomly shuffled, breaking the relationship between it and \mathbf{y} .

Cautions:

- A feature could be of low importance in one model but high in another.
- Small groups of correlated features may be favored over larger groups.
- None of a set of collinear features may show importance.

Retaining only one of each cluster (§9) of correlated features addresses the last two problems.

Python

- from sklearn.inspection import permutation_importance
- permutation_importance(estimator, X, y, scoring=None, random_state=None)
 - estimator is already fit
 - X, y are the data (training or validation) on which importance is calculated
 - scoring is the scorer to use; if None, the estimator's default
 - The return value contains importances_mean, importances_std, and importances

To learn more:

- User guide: https://scikit-learn.org/stable/modules/permutation_importance.html
- API reference:

https://scikit-learn.org/stable/modules/generated/sklearn.inspection.permutation_importance.html

• Examples:

https://scikit-learn.org/stable/auto_examples/inspection/plot_permutation_importance_multicollinear.html