

# Feature Engineering

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# Feature engineering

- In reality, data won't be as nicely represented as we've seen thus far
- Many of the algorithms that we've seen are greatly affected by *how* data is represented
- Examples: Scaling, numeric/categorical values, missing values, feature selection/construction
- We typically need chain together different algorithms
  - Many *preprocessing* steps
  - Possibly many models
- This is called a *pipeline* (or *workflow*)
- The best way to represent data depends not only on the semantics of the data, but also on the kind of model you are using.

# Overview

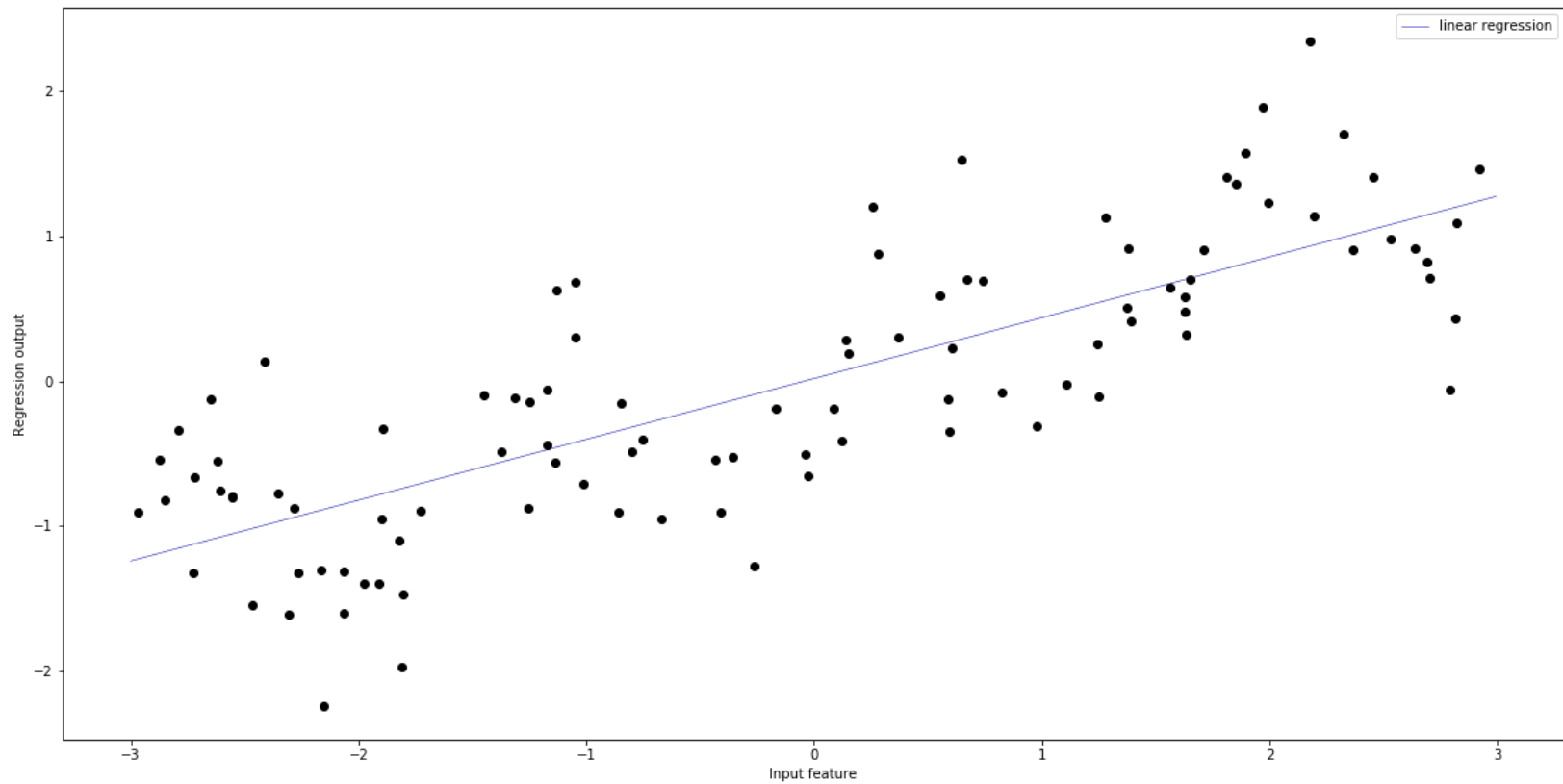
- Feature generation
  - **Polynomial features:** turn linear regression into polynomial regression
  - **Binning:** split a feature into multiple dimensions
  - **Product features:** model interactions between features
  - **Non-linear transformations:** log, sin,...
- Feature selection
  - Univariate techniques (e.g. ANOVA)
  - Model-based feature selection
  - Forward/backward selection
- Scaling
- Missing value imputation
- Pipelines
- Practical advice

# Polynomials

- We can make linear models behave more flexibly by adding polynomials of the original continuous features (also called a *basis expansion*).
- For a given feature  $x$ , we might want to consider  $x^2$ ,  $x^3$ ,  $x^4$ , and so on.
  - This happens implicitly in *kernelization* (SVMs, GLMs, Gaussian Processes,...)
- We can do it explicitly in scikit-learn, through `PolynomialFeatures` in the preprocessing module
  - `degree` is the max. degree of the polynomials, requires some searching
  - `include_bias` adds the 0-th polynomial, i.e.  $x^0$

```
poly = PolynomialFeatures(degree=10, include_bias=False)
X_poly = poly.fit(X).transform(X)
```

Linear regression can't capture the 'wave' in this data



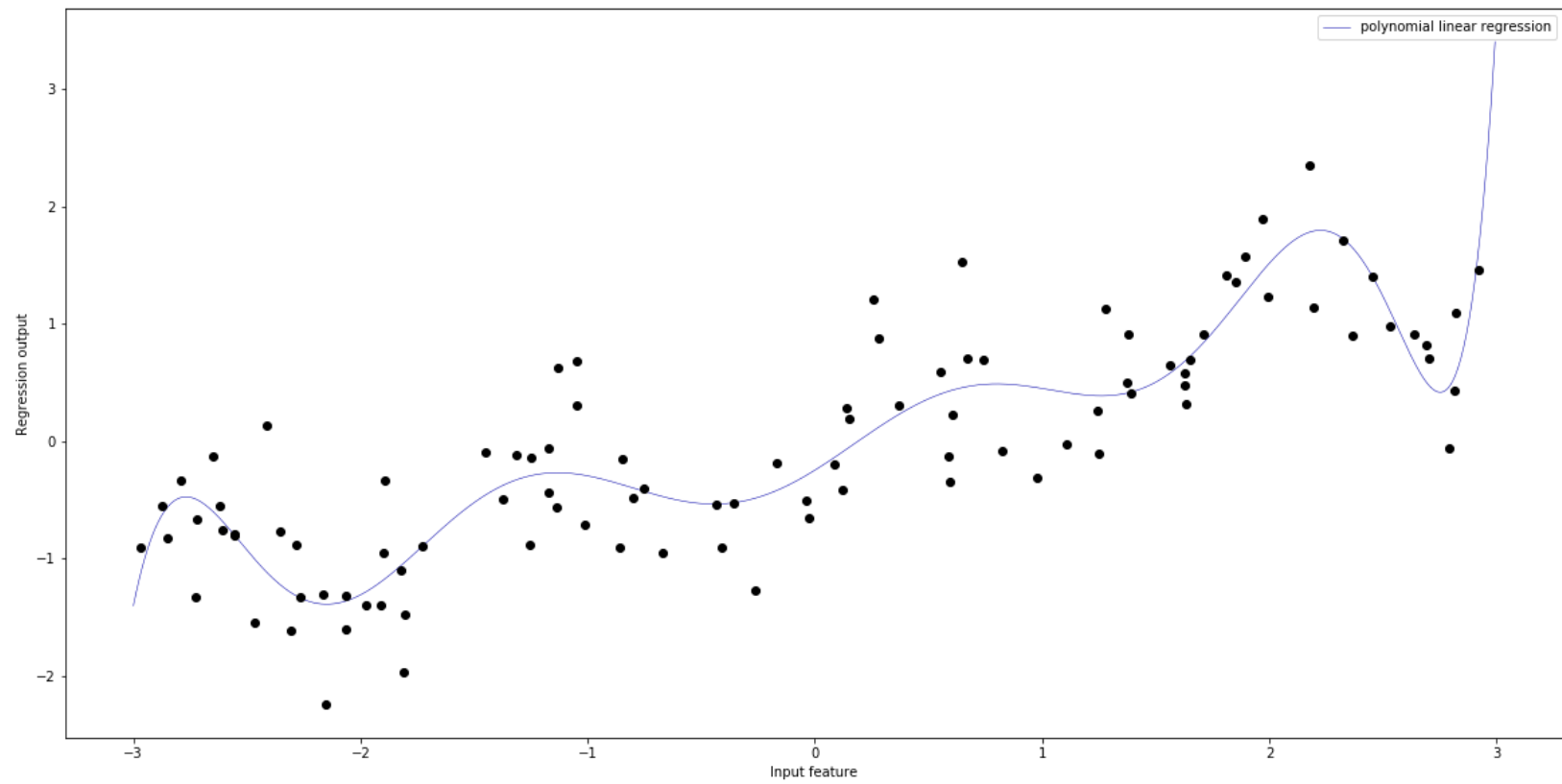
Using a degree of 10 yields 10 features, with the original value raised to the n-th power.

Out[4]:

	x0	x0^2	x0^3	x0^4	x0^5	x0^6	x0^7	x0^8	x0^9	x0^10
0	-0.75	0.57	-0.43	0.32	-0.24	0.18	-0.14	0.1	-0.078	0.058
1	2.7	7.3	20	53	1.4e+02	3.9e+02	1.1e+03	2.9e+03	7.7e+03	2.1e+04
2	1.4	1.9	2.7	3.8	5.2	7.3	10	14	20	27
3	0.59	0.35	0.21	0.12	0.073	0.043	0.025	0.015	0.0089	0.0053
4	-2.1	4.3	-8.8	18	-37	77	-1.6e+02	3.3e+02	-6.8e+02	1.4e+03

Modelling polynomial features with linear regression yields *polynomial regression*.

- The model is still a hyperplane (in a 10-dimensional space)
- The predictions are now a non-linear function of the original variable  $X$
- Fits the wave shape a lot better





## Binning (Discretization)

Sometimes we need a different model for different *ranges* of the input data

- Partition (numeric) feature values into  $n$  intervals (bins)
- Replace each feature with  $n$  features
  - Value is 1 if the original feature value falls in the corresponding bin
  - Value is 0 otherwise
- Train the model on those  $n$  features

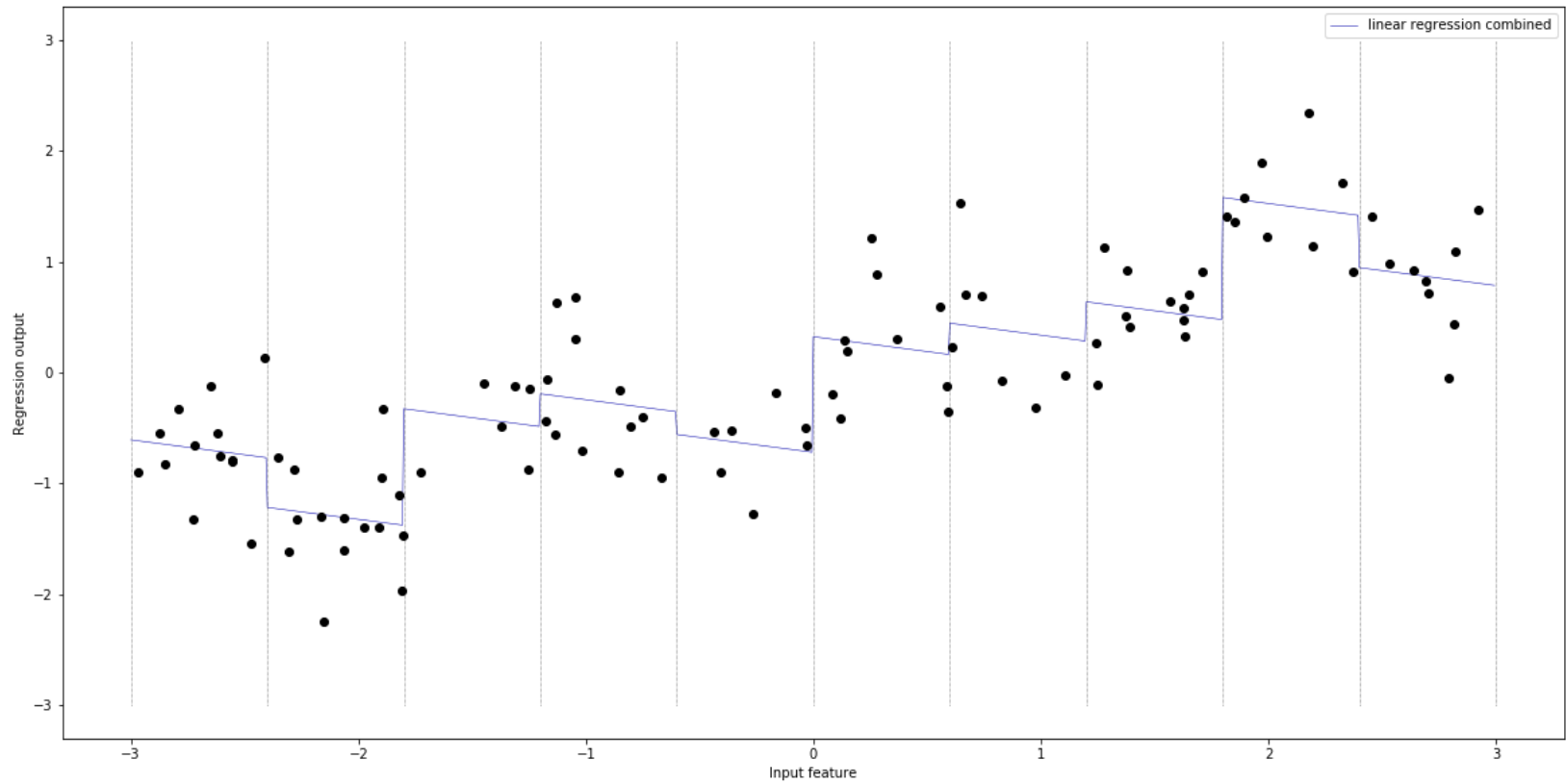
- No handy sklearn function. You need to use:
  - `numpy.digitize` to assign values to bins
  - `OneHotEncoder` to convert a feature of  $n$  numbers to  $n$  binary features
  - `numpy.stack` to add the original feature

```
which_bin = numpy.digitize(X, bins=np.linspace(-3, 3, 11))
X_binned = OneHotEncoder(sparse=False).fit_transform(which_bin)
X_combined = np.hstack([X, X_binned])
```

Out[6]:

	orig	[-3.0,-2.4]	[-2.4,-1.8]	[-1.8,-1.2]	[-1.2,-0.6]	[-0.6,0.0]	[0.0,0.6]	[0.6,1.2]	[1.2,1.8]	[1.8,2.4]
0	-0.75	0	0	0	1	0	0	0	0	0
1	2.7	0	0	0	0	0	0	0	0	0
2	1.4	0	0	0	0	0	0	0	1	0
3	0.59	0	0	0	0	0	1	0	0	0
4	-2.1	0	1	0	0	0	0	0	0	0

- Our linear model learned a fixed slope for each bin in the wave dataset
  - Because we learn a single weight for feature  $x$



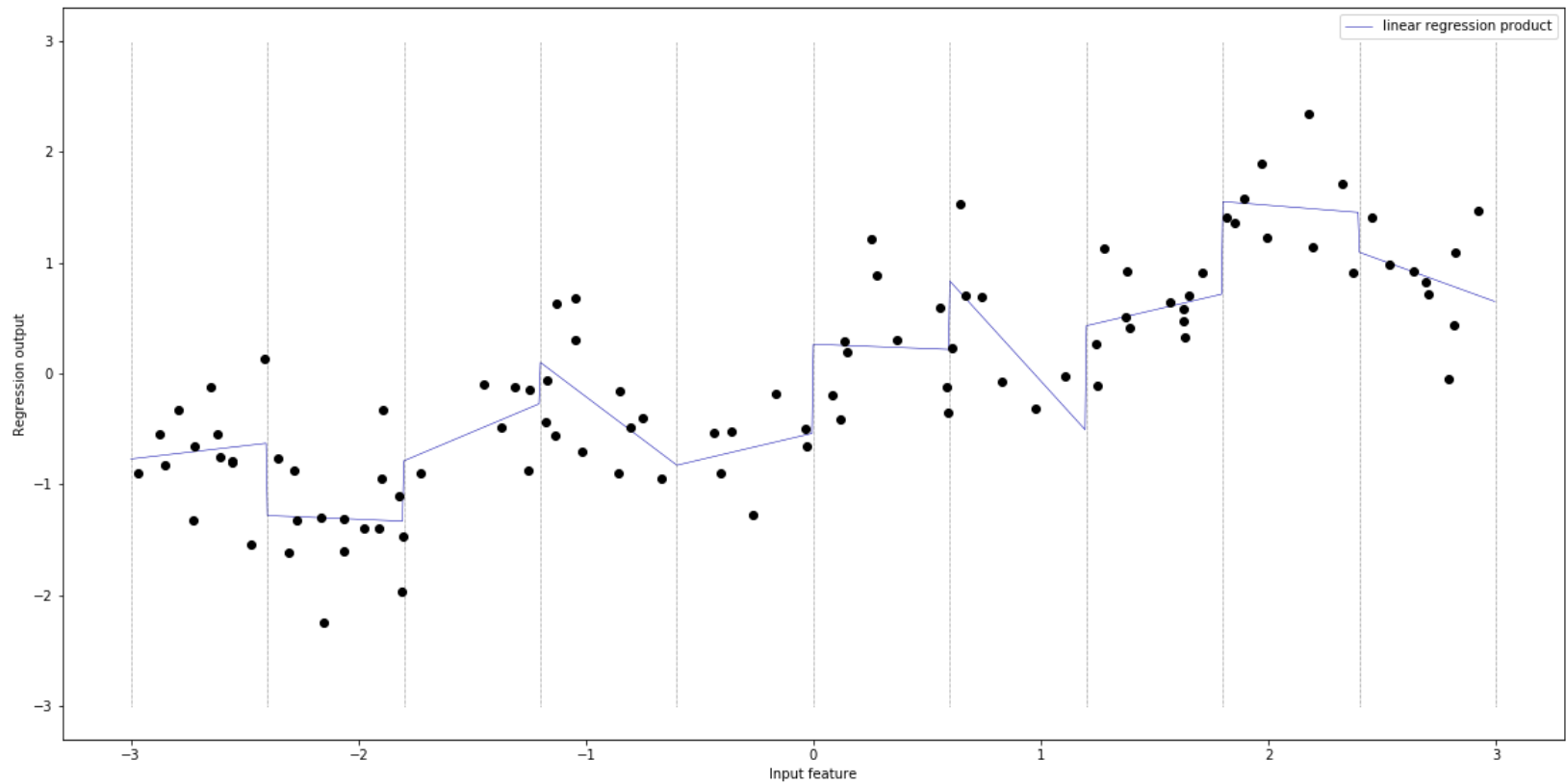
## Interaction features

- If we want a different slope per bin, we need *interaction features* (or *product features*)
- These are the product of the bin encoding and the original feature value

Out[8]:

	b0	b1	b2	b3	b4	b5	b6	b7	b8	b9	X*b0	X*b1	X*b2	X*b3	X*b4	X*b5	X*b6	X*b7
0	0	0	0	1	0	0	0	0	0	0	-0	-0	-0	-0.75	-0	-0	-0	-0
1	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	1.4
3	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0.59	0	0
4	0	1	0	0	0	0	0	0	0	0	-0	-2.1	-0	-0	-0	-0	-0	-0

The interaction features allow the linear model to learn a weight (slope) per bin



## Non-linear transformations

There are other transformations that often prove useful for transforming certain features.

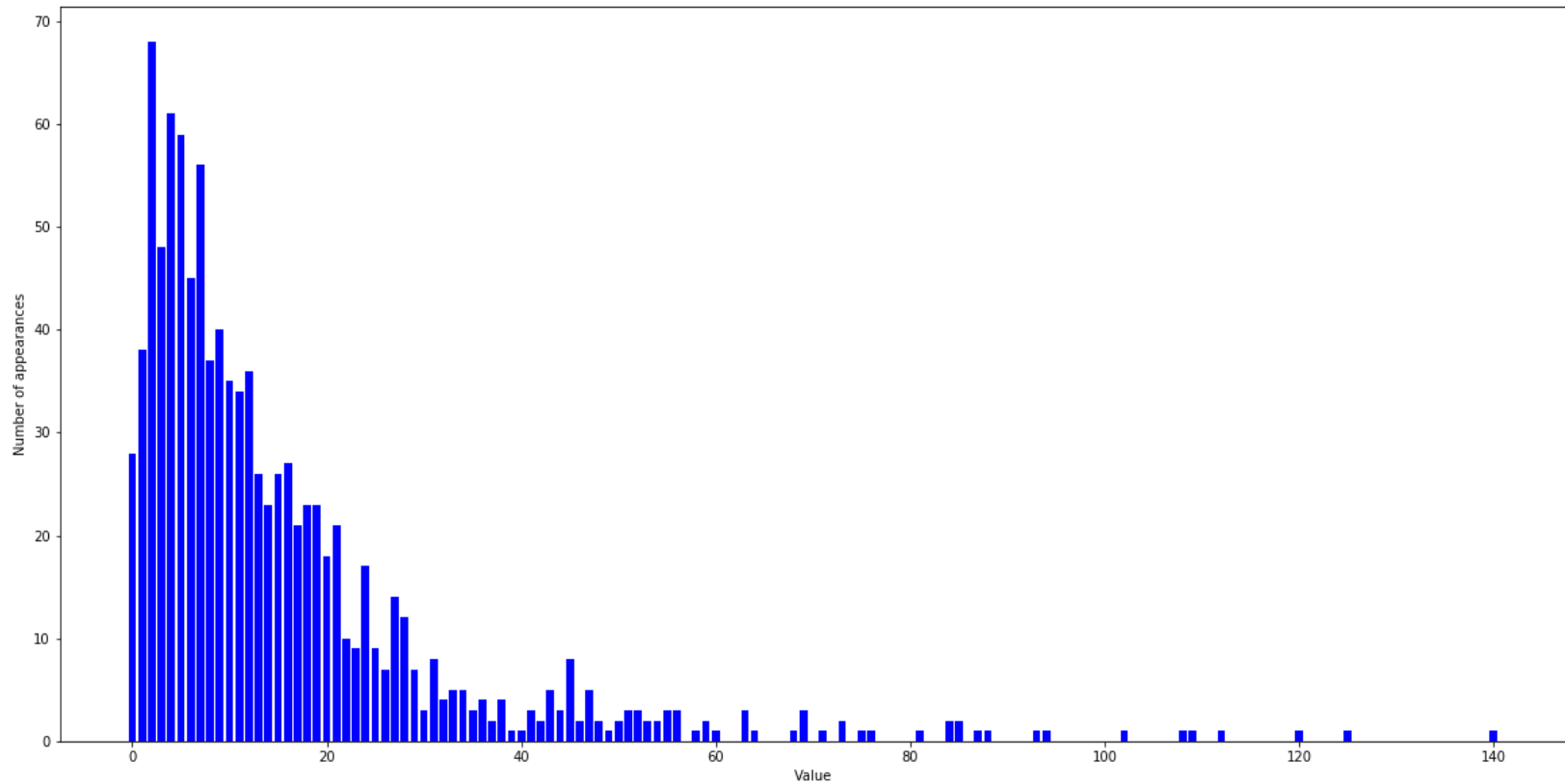
For instance, `log` or `exp` are very useful to better scale your data. This is useful for models that are sensitive to feature scales, such as linear models, SVMs and neural networks.

The functions `log` and `exp` can help by adjusting the relative scales, transforming them to more Gaussian-like value distributions.

Finding the transformation that works best for each combination of dataset and model is somewhat of an art.

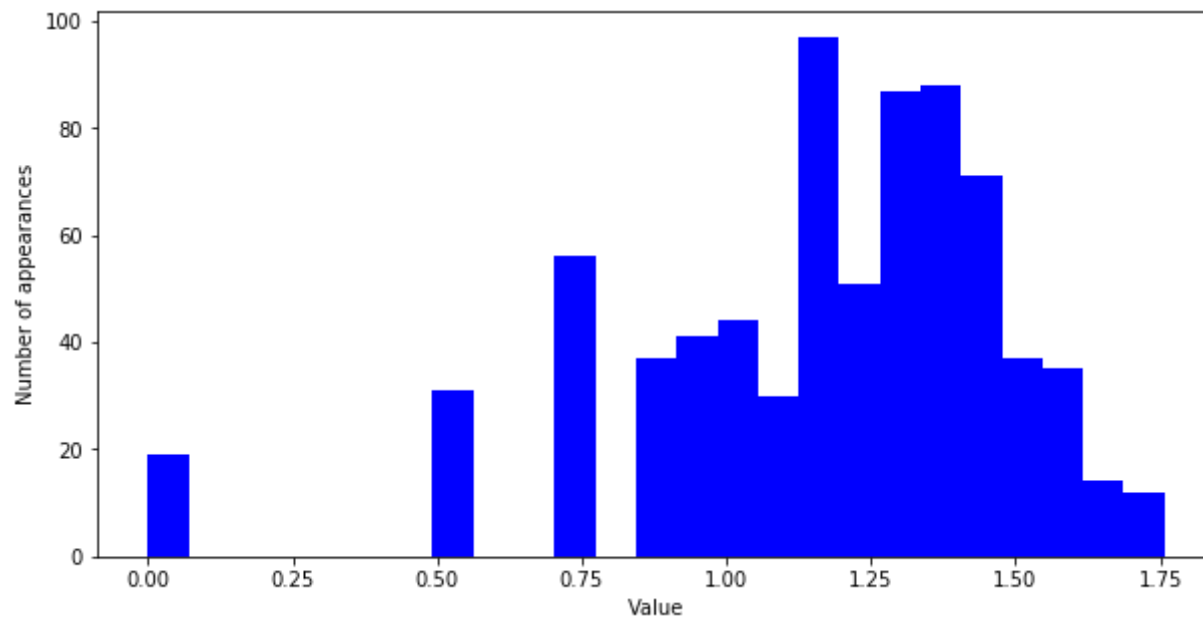
### *Example: Poisson distributions*

Imagine a process where many outcomes are rare (only occur 1 or 2 times) while others occur hundreds of times



Applying a logarithmic transformation can help to create a more normal distribution

```
X_train_log = np.log(X_train + 1)  
X_test_log = np.log(X_test + 1)
```





# Poisson Regression

Most linear models can't handle non-normal distributions well:

```
score = Ridge().fit(X_train, y_train).score(X_test, y_test)
```

Ridge regression (original data) test score (R2): 0.622

But do a lot better if the data is transformed:

```
score = Ridge().fit(X_train_log, y_train).score(X_test_log, y_test)
```

Ridge regression (transformed data) test score (R2): 0.875

# Automatic Feature Selection

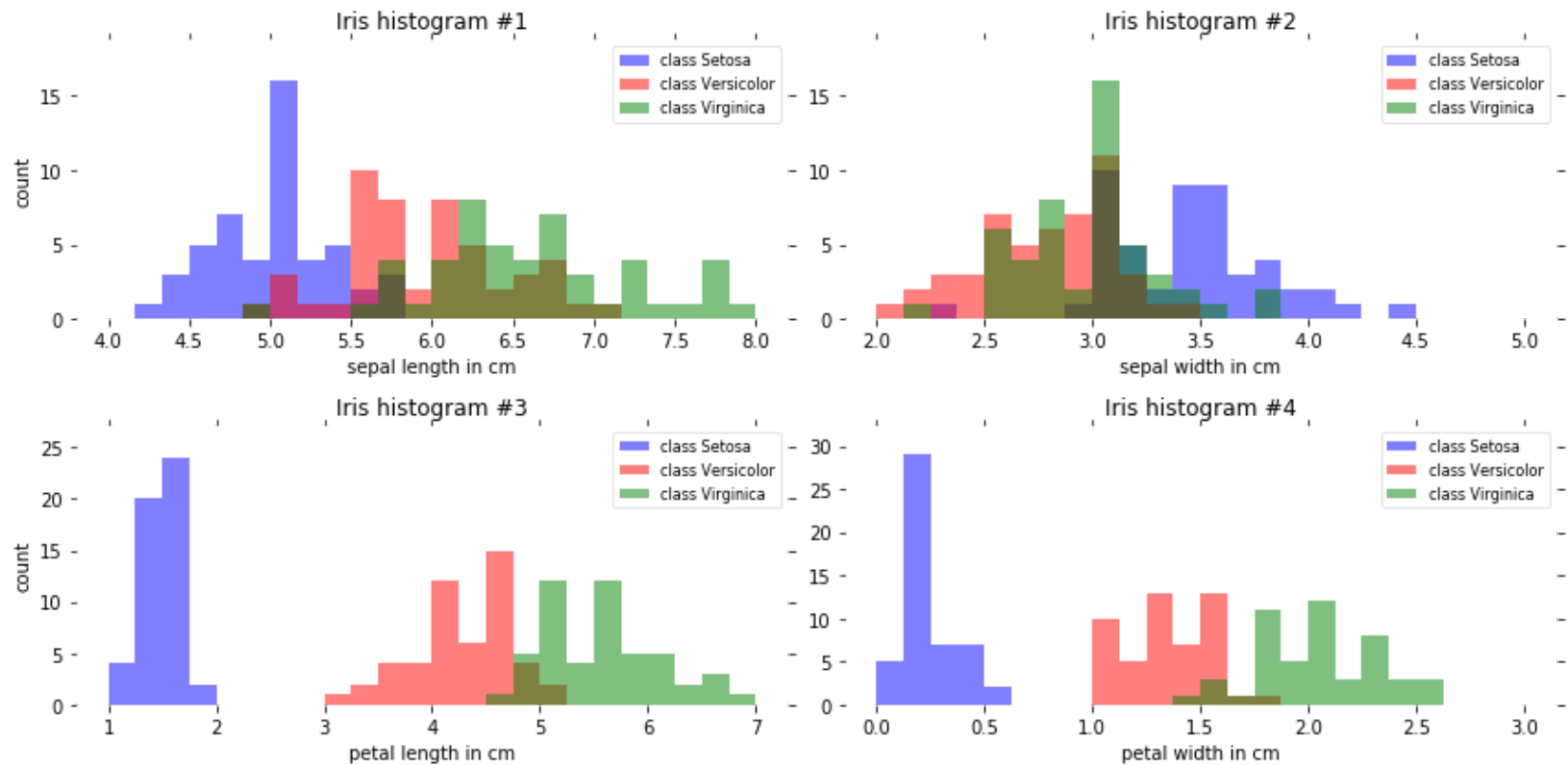
It can be a good idea to reduce the number of features to only the most useful ones

- Simpler models that generalize better (less overfitting)
  - Even models such as RandomForest can benefit from this
- Help algorithms that are sensitive to the curse of dimensionality
  - e.g. kNN and many other distance-based methods
- Sometimes it is one of the main methods to improve models (e.g. gene expression data)

## Example: Iris

Below are the distributions (histograms) of every class according to every feature.

Which of the four features is most informative?



## Univariate statistics

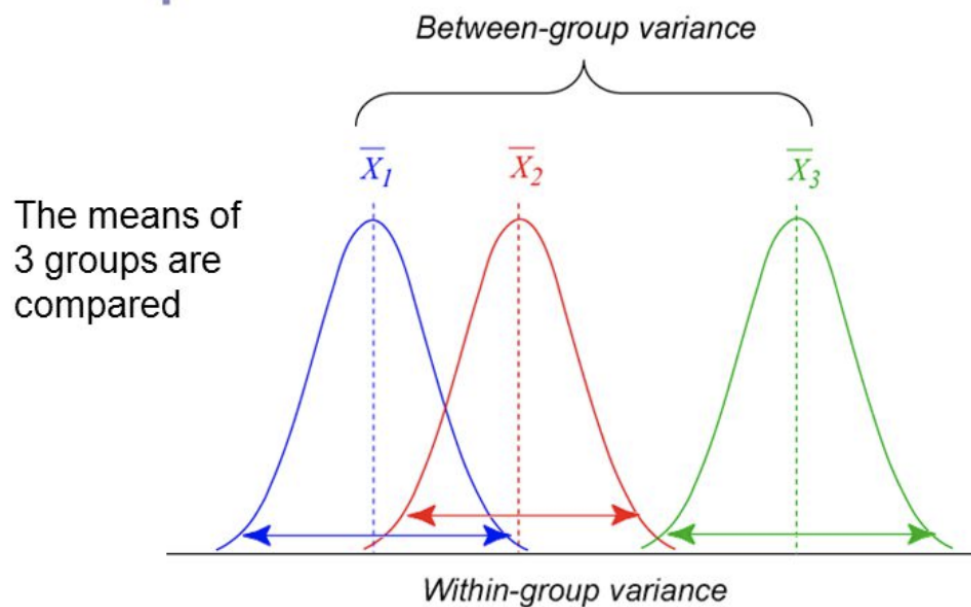
- Keep features for which there is a **statistically significant relationship** between it and the target.
- Consider each feature individually (univariate), independent of the model that you might want to apply afterwards.
- We can use different tests to measure how informative a feature is:

`f_regression` : For numeric targets. Measures the performance of a linear regression model trained on only one feature.

`f_classif` : For categorical targets. Measures the *F-statistic* from one-way Analysis of Variance (ANOVA), or the proportion of total within-class variance explained by one feature.

`chi2` : For categorical features and targets. Performs the chi-square ( $\chi^2$ ) statistic. Similar results as F-statistic, but less sensitive to nonlinear relationships.

- Both the F-statistic and  $\chi^2$  methods use the p-value under the F- and  $\chi^2$  distribution, respectively.
- F-statistic =  $\frac{var(\mu_i)}{var(X_i)}$  (higher is better)
  - $X_i$ : all samples with class i.
  - Better if per-class distributions separate well: means are far apart and variance is small.



Chi-squared for a feature with  $c$  categories and  $k$  classes:

$$\chi^2 = \sum_{i=0}^c \sum_{j=0}^k \frac{(O_{ij} - E_{ij})^2}{E_{ij}}$$

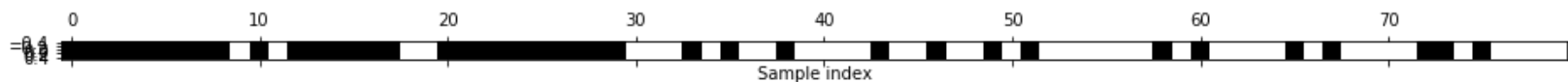
where  $O_{ij}$  is the number of observations of feature category  $i$  and class  $j$ , and  $E_{ij}$  is the expected number of observations of category  $i$  and class  $j$  if there was no relationship between the feature and the target (number of samples of category  $i$  \* ratio of class  $j$ ).

## In practice

- Given a feature ranking, sklearn has two general ways to remove features :
- `SelectKBest` will only keep the  $k$  features with the lowest p values.
- `SelectPercentile` selects a fixed percentage of features.
- Retrieve the selected features with `get_support ( )`

## Visualization:

- Classification dataset with 30 real features, and add 50 random noise features.
  - Ideally, the feature selection removes at least the last 50 noise features.
- Selected features in black, removed features in white
- Results for `SelectPercentile` with `f_classif` (ANOVA):
  - OK, but fails to remove several noise features



Impact on performance: check how the transformation affects the performance of our learning algorithms.

LogisticRegression score with all features: 0.919

LogisticRegression score with only selected features: 0.912



## Model-based Feature Selection

Model-based feature selection uses a supervised machine learning model to judge the importance of each feature, and keeps only the most important ones. They consider all features together, and are thus able to capture interactions: a feature may be more (or less) informative in combination with others.

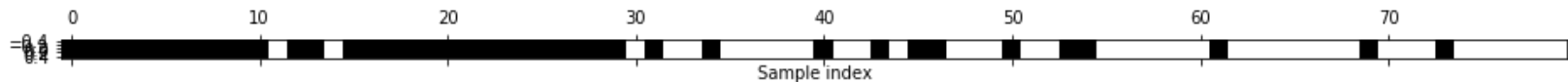
The supervised model that is used for feature selection doesn't need to be the same model that is used for the final supervised modeling, it only needs to be able to measure the (perceived) importance for each feature:

- Decision tree-based models return a `feature_importances_` attribute
- Linear models return coefficients (`coef_`), whose absolute values also reflect feature importance

In scikit-learn, we can do this using `SelectFromModel`. It requires a model and a threshold. `Threshold='median'` means that the median observed feature importance will be the threshold, which will remove 50% of the features.

```
select = SelectFromModel(  
    RandomForestClassifier(n_estimators=100, random_state=42),  
    threshold="median")
```

- Random Forests are known to produce good estimates of feature importance
  - Based on how often a feature is used high up in the trees
  - Based on Information Gain or Mean Decrease in Impurity (MDI)
  - Use with care: Beware Default Random Forest Importances (<https://explained.ai/rf-importance/index.html>)
  - Tune the RandomForest (e.g. `min_samples_leaf`)
  - Use permutation importance (coming up)
- In our example, all but two of the original features were selected, and most of the noise features removed.
- Our logistic regression model improves further



LogisticRegression test score: 0.940

## Iterative feature selection

Instead of building a model to remove many features at once, we can also just ask it to remove the worst feature, then retrain, remove another feature, etc. This is known as *recursive feature elimination* (RFE).

```
select = RFE(RandomForestClassifier(n_estimators=100, random_state=42),  
             n_features_to_select=40)
```

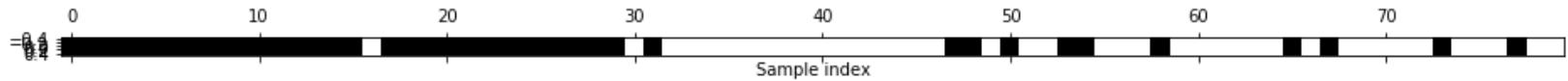
Vice versa, we could also ask it to iteratively add one feature at a time. This is called *forward selection*.

In both cases, we need to define beforehand how many features to select. When this is unknown, one often considers this as an additional hyperparameter of the whole process (pipeline) that needs to be optimized.

Can be rather slow.

RFE result:

- Fewer noise features, only 1 original feature removed
- LogisticRegression performance about the same



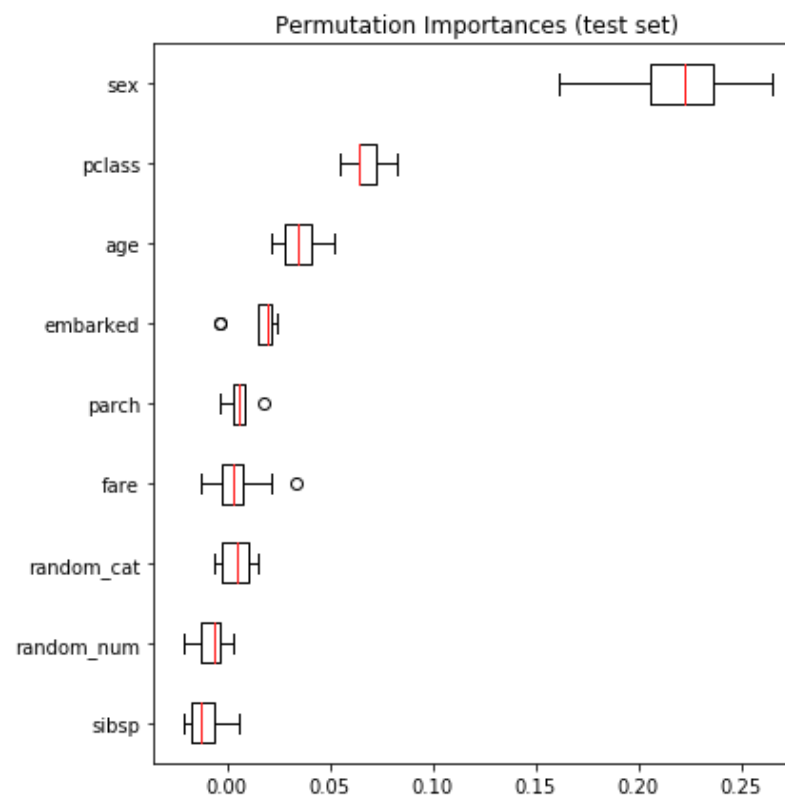
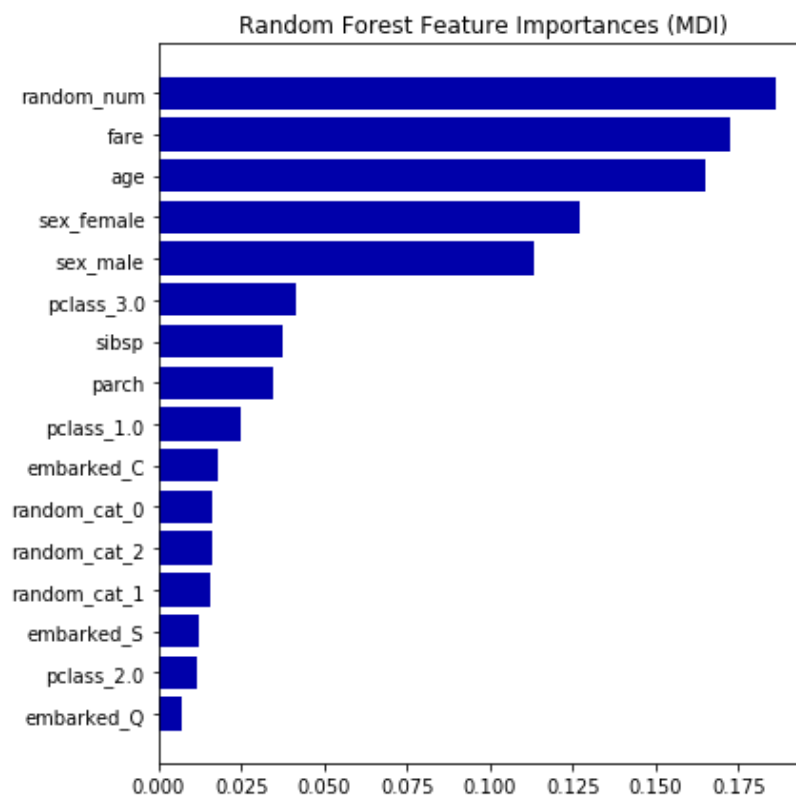
LogisticRegression Test score: 0.930

## Permutation feature importance

- Model inspection technique, especially useful for non-linear or opaque estimators.
- Defined as **the decrease in a model score when a single feature value is randomly shuffled**.
- This breaks the relationship between the feature and the target, thus the drop in the model score is indicative of how much the model depends on the feature.
- Model agnostic, metric agnostic, and can be calculated many times with different permutations.
- The problem with impurity based techniques (e.g. Random Forest)
  - Gives importance to features not predictive on unseen data.
    - Permutation feature importance can be applied to unseen data.
  - Strong bias towards high cardinality features (e.g. numerical features).
    - Permutation feature importances do not exhibit such a bias.

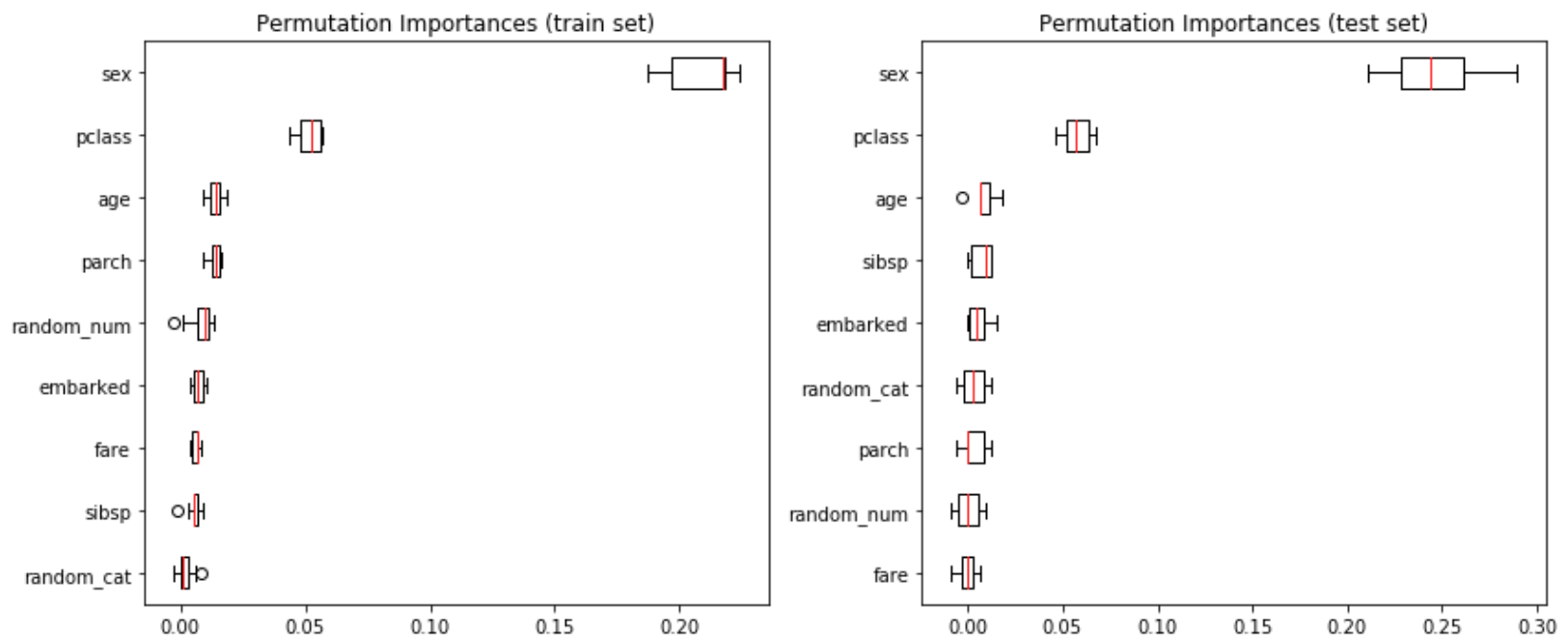
### *Example (Titanic dataset)*

- We add a random feature as well: Random Forest deems it important!
- Low cardinality feature `sex` and `pclass` are actually more important
- Note: this requires the development version of sklearn



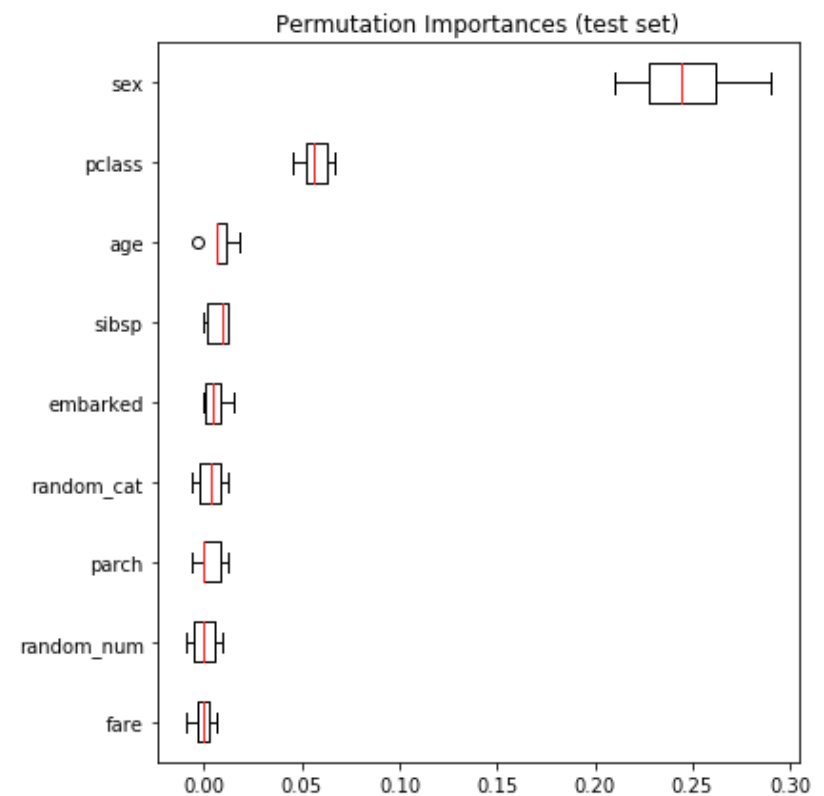
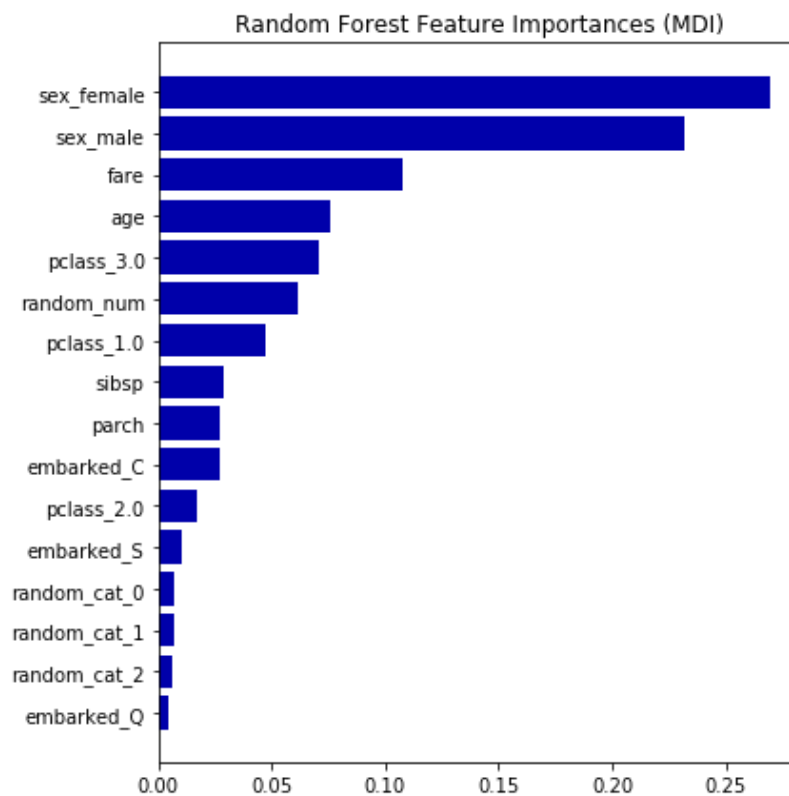
We can also compute the permutation importances on the training set.

- `random_num` gets a significantly higher importance ranking than when computed on the test set.
- This shows that the RF model has enough capacity to use that random numerical feature to overfit.





Let's rerun this with a more regularized Random Forest  
(`min_samples_leaf=10`):



## Feature selection wrap-up

Automatic feature selection can be helpful when:

- You expect some inputs to be uninformative
- Your model does not select features internally (as tree-based models do)
  - Even then it may help
- You need to speed up prediction without losing much accuracy
- You want a more interpretable model (with fewer variables)

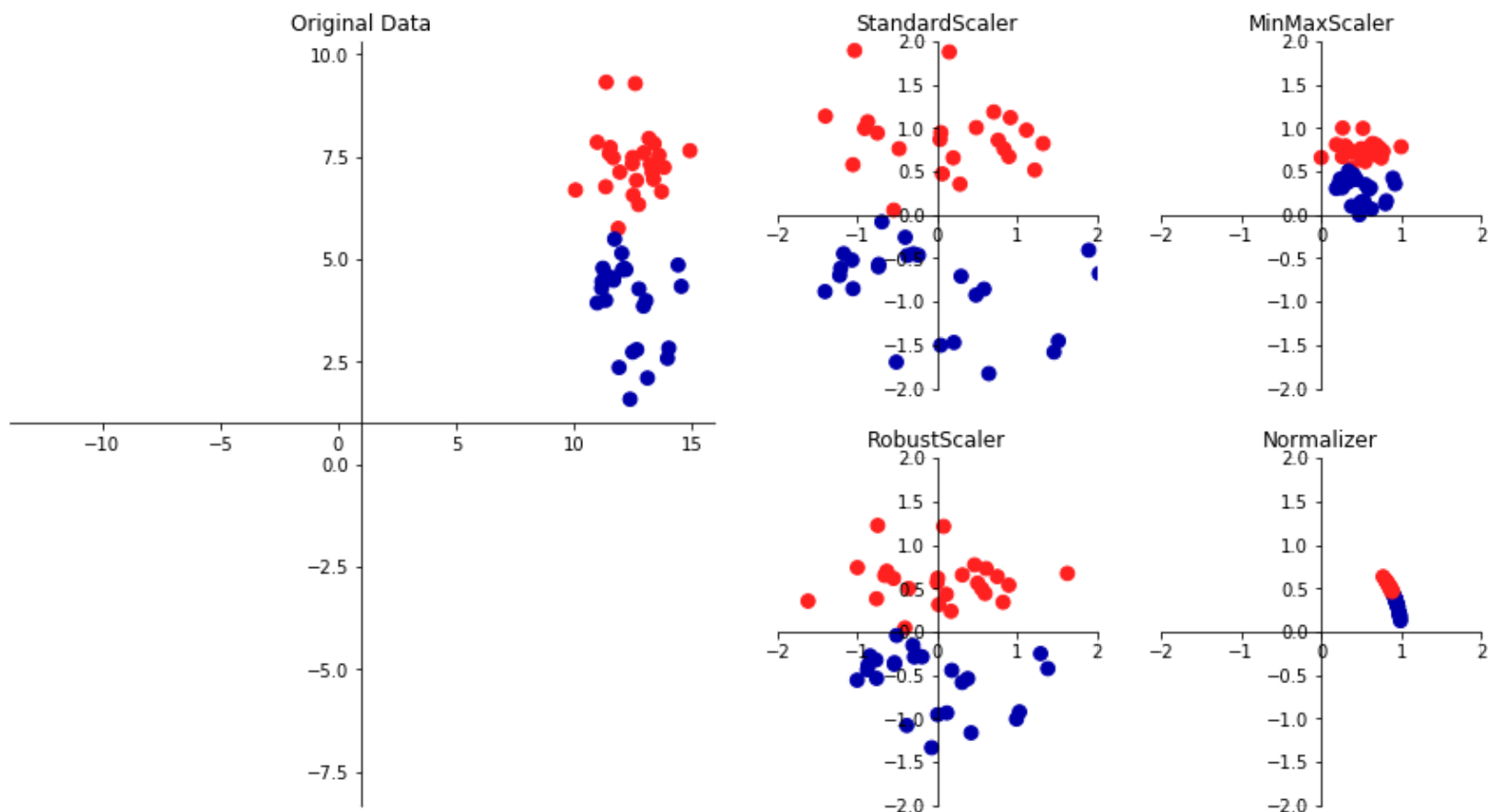
# Scaling

When the features have different scales (their values range between very different minimum and maximum values), it makes sense to scale them to the same range. Otherwise, one feature will overpower the others, especially when raised to the  $n$ th power.

- We can rescale features between 0 and 1 using `MinMaxScaler`.
- Remember to `fit_transform` the training data, then `transform` the test data

Several scaling techniques are available:

- `StandardScaler` rescales all features to mean=0 and variance=1
  - Does not ensure and min/max value
- `RobustScaler` uses the median and quartiles
  - Median  $m$ : half of the values  $< m$ , half  $> m$
  - Lower Quartile  $lq$ : 1/4 of values  $< lq$
  - Upper Quartile  $uq$ : 1/4 of values  $> uq$
  - Ignores *outliers*, brings all features to same scale
- `MinMaxScaler` brings all feature values between 0 and 1
- `Normalizer` scales data such that the feature vector has Euclidean length 1
  - Projects data to the unit circle
  - Used when only the direction/angle of the data matters



## Applying scaling transformations

- Lets apply a scaling transformation *manually*, then use it to train a learning algorithm
- First, split the data in training and test set
- Next, we `fit` the preprocessor on the **training data**
  - This computes the necessary transformation parameters
  - For `MinMaxScaler`, these are the min/max values for every feature
- After fitting, we can `transform` the training and test data

```
scaler = MinMaxScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
```

Training data per-feature minimum after scaling:

[illegible]

Training data per-feature maximum after scaling:

[illegible]

- After scaling the test data, the values are not exactly between 0 and 1
- This is correct: we used the min/max values from the training data only
- We are still interested in how well our preprocessing+learning model generalizes from the training to the test data

```
x_test_scaled = scaler.transform(X_test)
```

Test data per-feature minimum after scaling:

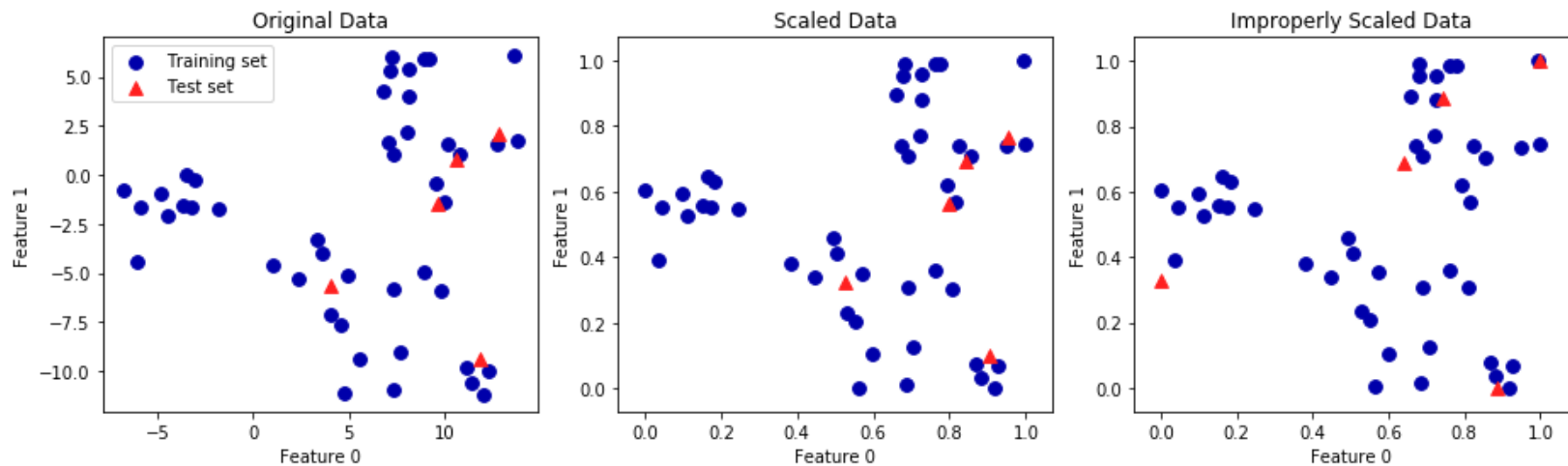
```
[ 0.034  0.023  0.031  0.011  0.141  0.044  0.      0.      0.154 -0.006
 -0.001  0.006  0.004  0.001  0.039  0.011  0.      0.     -0.032  0.007
  0.027  0.058  0.02   0.009  0.109  0.026  0.      0.     -0.     -0.002]
```

Test data per-feature maximum after scaling:

```
[0.958 0.815 0.956 0.894 0.811 1.22  0.88  0.933 0.932 1.037 0.427 0.498
 0.441 0.284 0.487 0.739 0.767 0.629 1.337 0.391 0.896 0.793 0.849 0.745
 0.915 1.132 1.07  0.924 1.205 1.631]
```



- Remember to `fit` and `transform` on the training data, then `transform` the test data
- 2nd figure: `fit` on training set, `transform` on training and test set
- 3rd figure: `fit` and `transform` on the training data
  - Test data points nowhere near same training data points
  - Trained model will have a hard time generalizing correctly



- Note: you can fit and transform the training together with `fit_transform`
- To transform the test data, you always need to `fit` on the training data and transform the test data

```
scaler = StandardScaler()  
# calling fit and transform in sequence (using method chaining)  
X_scaled = scaler.fit(X).transform(X)  
# same result, but more efficient computation  
X_scaled_d = scaler.fit_transform(X)
```

## How great is the effect of scaling?

- First, we train the (linear) SVM without scaling

LinearSVC test set accuracy: 0.93

- With scaling, we get a much better model

LinearSVM (with scaling) test set accuracy: 0.97

# Missing value imputation

- Many sci-kit learn algorithms cannot handle missing value
- `Imputer` replaces specific values
  - `missing_values` (default 'NaN') placeholder for the missing value
  - `strategy`:
    - `mean`, replace using the mean along the axis
    - `median`, replace using the median along the axis
    - `most_frequent`, replace using the most frequent value
- Many more advanced techniques exist, but not yet in scikit-learn
  - e.g. low rank approximations (uses matrix factorization)

```
imp = SimpleImputer(missing_values=np.nan, strategy='mean')  
imp.fit_transform(X1_train)
```

Missing data:

```
[[ 1.  2.]
```

```
[nan  3.]
```

```
[ 7. nan]]
```

Imputed data:

```
[[1.  2. ]
```

```
[4.  3. ]
```

```
[7.  2.5]]
```

# Building Pipelines

- In scikit-learn, a `pipeline` combines multiple processing *steps* in a single estimator
- All but the last step should be transformer (have a `transform` method)
  - The last step can be a transformer too (e.g. `Scaler+PCA`)
- It has a `fit`, `predict`, and `score` method, just like any other learning algorithm
- Pipelines are built as a list of steps, which are (name, algorithm) tuples
  - The name can be anything you want, but can't contain '\_\_\_'
  - We use '\_\_\_' to refer to the hyperparameters, e.g. `svm__C`
- Let's build, train, and score a `MinMaxScaler + LinearSVC` pipeline:

```
pipe = Pipeline([("scaler", MinMaxScaler()), ("svm", LinearSVC())])  
pipe.fit(X_train, y_train).score(X_test, y_test)
```

Test score: 0.97

- Now with cross-validation:

```
scores = cross_val_score(pipe, cancer.data, cancer.target)
```

Cross-validation scores: [0.982 0.974 0.965 0.965 0.991]

Average cross-validation score: 0.98

- We can retrieve the trained SVM by querying the right step indices

```
pipe.steps[1][1]
```

```
SVM component: LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True,  
                           intercept_scaling=1, loss='squared_hinge', max_iter=1000,  
                           multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,  
                           verbose=0)
```

- Or we can use the named\_steps dictionary

```
pipe.named_steps['svm']
```

```
SVM component: LinearSVC(C=1.0, class_weight=None, dual=True, fit_intercept=True,  
                           intercept_scaling=1, loss='squared_hinge', max_iter=1000,  
                           multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,  
                           verbose=0)
```



- When you don't need specific names for specific steps, you can use `make_pipeline`
  - Assigns names to steps automatically

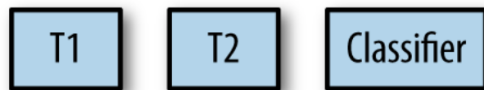
```
pipe_short = make_pipeline(MinMaxScaler(), LinearSVC(C=100))  
print("Pipeline steps:\n{}".format(pipe_short.steps))
```

Pipeline steps:

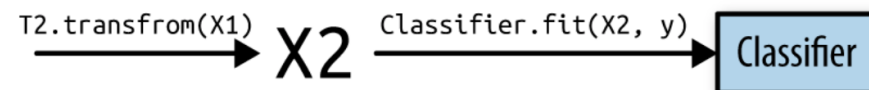
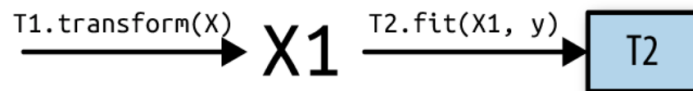
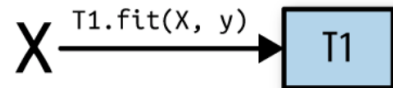
```
[('minmaxscaler', MinMaxScaler(copy=True, feature_range=(0, 1))), ('linear  
svc', LinearSVC(C=100, class_weight=None, dual=True, fit_intercept=True,  
intercept_scaling=1, loss='squared_hinge', max_iter=1000,  
multi_class='ovr', penalty='l2', random_state=None, tol=0.0001,  
verbose=0))]
```

## Visualization of a pipeline fit and predict

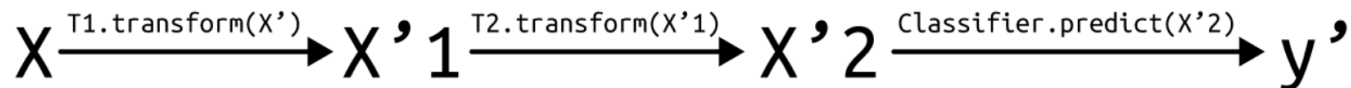
```
pipe = make_pipeline(T1(), T2(), Classifier())
```



```
pipe.fit(X, y)
```



```
pipe.predict(X')
```



# Hyperparameter Selection with Preprocessing

- If we also want to optimize our hyperparameters, things get more complicated
- Indeed, when we `fit` the preprocessor (`MinMaxScaler`), we used *all* the training data.
- The cross-validation splits in `GridSearchCV` will have training sets preprocessed with information from the test sets (data leakage)

Best cross-validation accuracy: 0.98

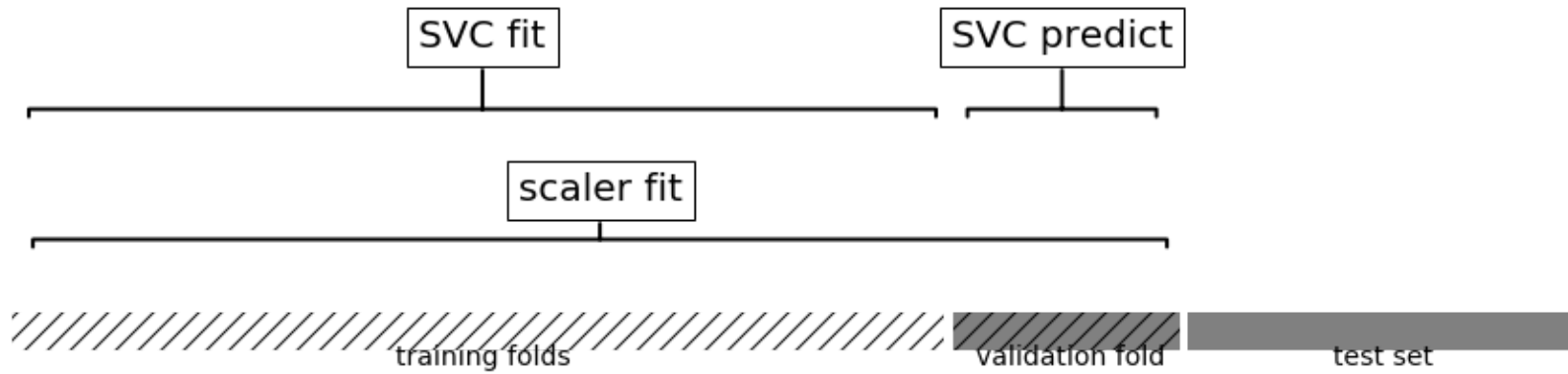
Best set score: 0.97

Best parameters: {'C': 1, 'gamma': 1}

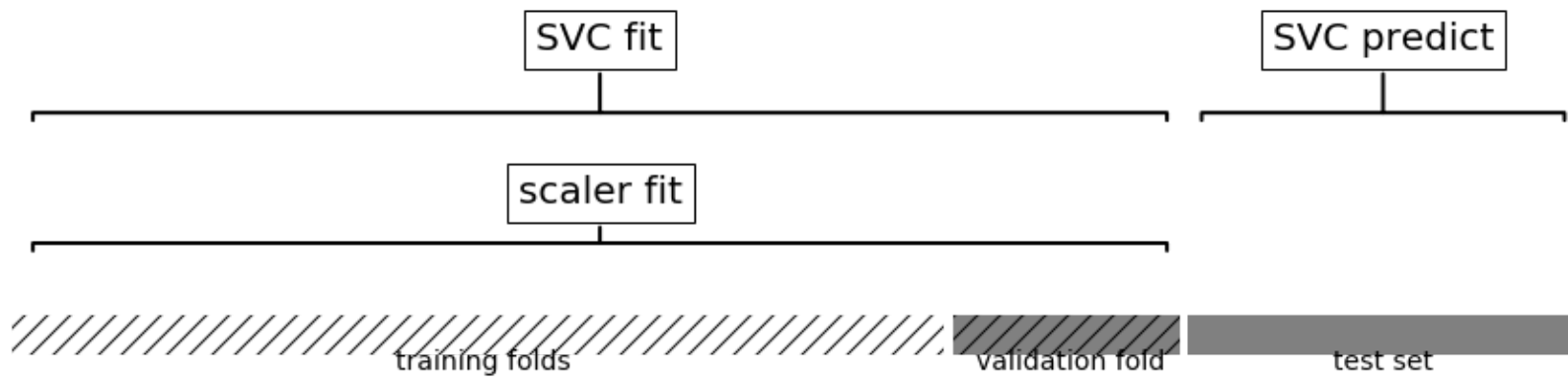
## Visualization of what happens in this code

- During cross-validation (grid search) we evaluate hyperparameter settings on a validation set that was preprocessed with information in that validation set
- This will lead to overly optimistic results during cross-validation
- When we want to use the optimized hyperparameters on the held-out test data, the selected hyperparameters may be suboptimal.
- To solve this, we need to *glue* the preprocessing and learning algorithms together by building a pipeline

Cross validation



Test set prediction



## Using Pipelines in Grid-searches

- We can use the pipeline as a single estimator in `cross_val_score` or `GridSearchCV`
- To define a grid, refer to the hyperparameters of the steps
  - Step `svm`, parameter `C` becomes `svm__C`

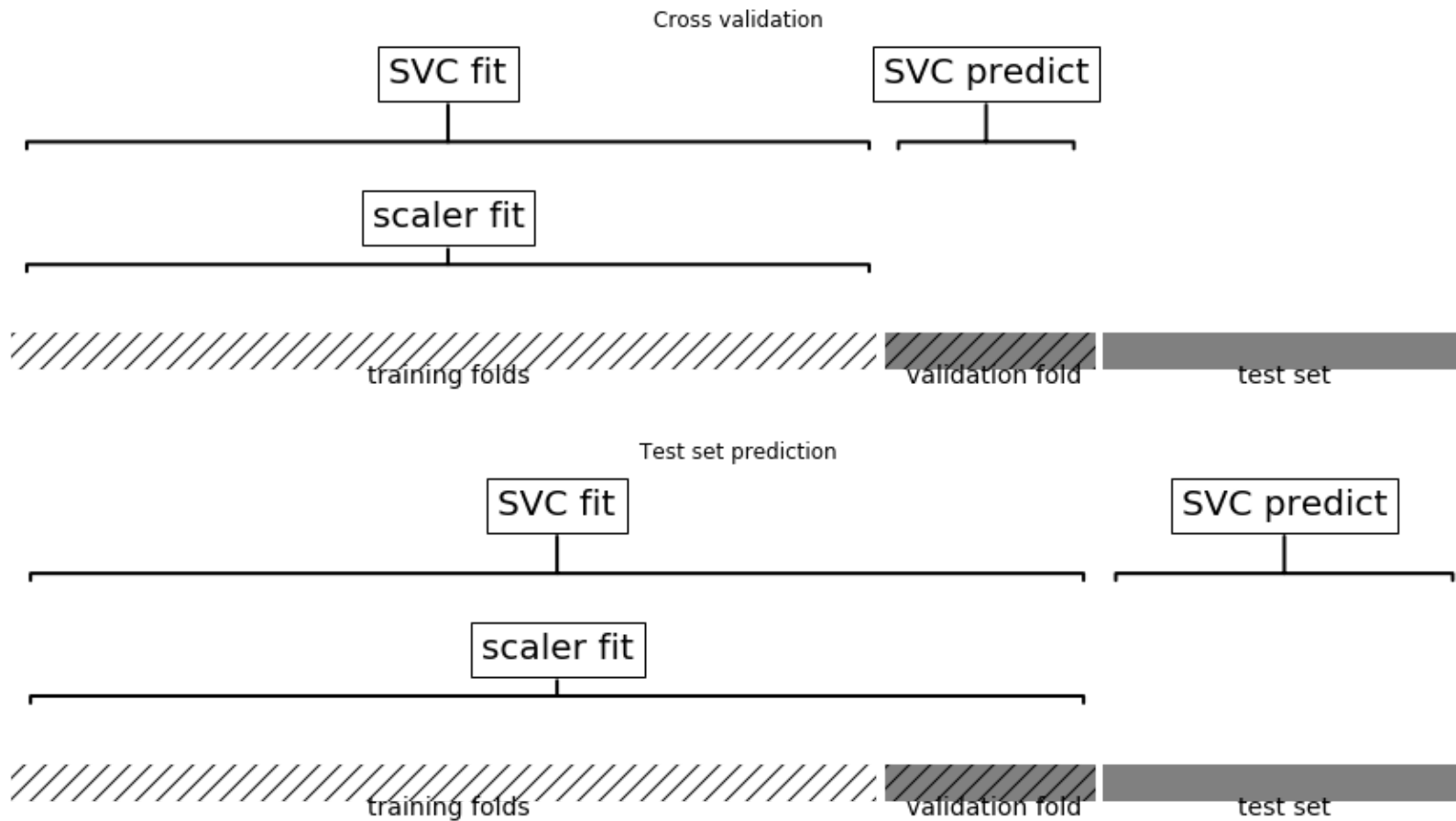
```
param_grid = {'svm__C': [0.001, 0.01, 0.1, 1, 10, 100],  
              'svm__gamma': [0.001, 0.01, 0.1, 1, 10, 100]}  
pipe = pipeline.Pipeline([("scaler", MinMaxScaler()), ("svm", SVC(C=100  
))])  
grid = GridSearchCV(pipe, param_grid=param_grid, cv=5)
```

Best cross-validation accuracy: 0.98

Test set score: 0.97

Best parameters: {'svm\_\_C': 1, 'svm\_\_gamma': 1}

- Now, the preprocessors are refit with only the training data in each cross-validation split.



- When we request the best estimator of the grid search, we'll get the best pipeline

```
grid.best_estimator_
```

Best estimator:

```
Pipeline(memory=None,
          steps=[('scaler', MinMaxScaler(copy=True, feature_range=(0, 1))),
                 ('svm',
                  SVC(C=1, break_ties=False, cache_size=200, class_weight=None,
                      coef0=0.0, decision_function_shape='ovr', degree=3,
                      gamma=1, kernel='rbf', max_iter=-1, probability=False,
                      random_state=None, shrinking=True, tol=0.001,
                      verbose=False))],
          verbose=False)
```

- And we can drill down to individual components and their properties

```
grid.best_estimator_.named_steps["svm"]
```

SVM step:

```
SVC(C=1, break_ties=False, cache_size=200, class_weight=None, coef0=0.0,
    decision_function_shape='ovr', degree=3, gamma=1, kernel='rbf', max_iter=-1,
    probability=False, random_state=None, shrinking=True, tol=0.001,
    verbose=False)
```



## Grid-searching preprocessing steps and model parameters

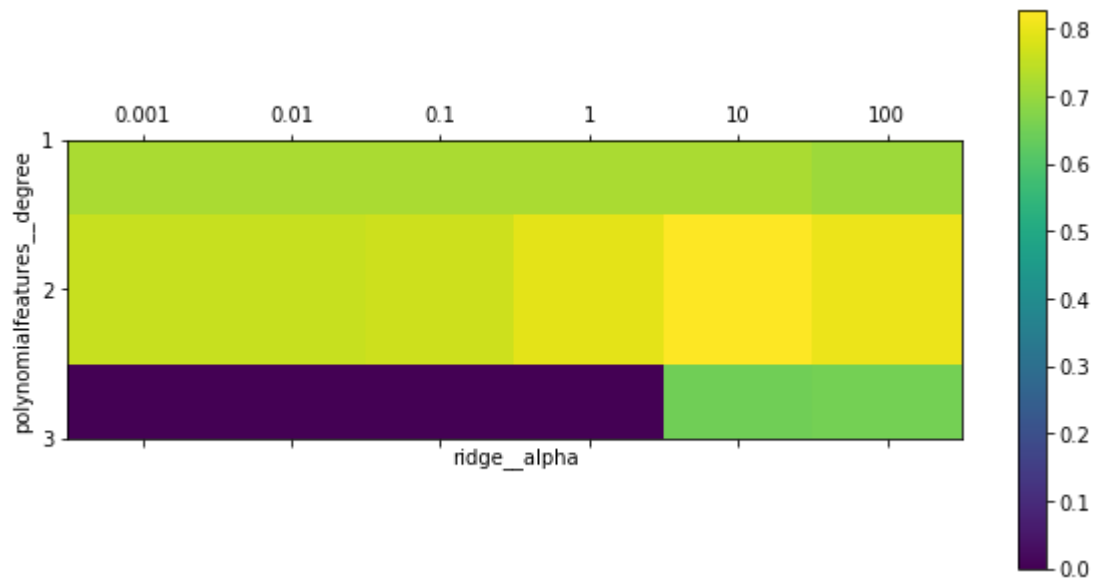
- We can use grid search to optimize the hyperparameters of our preprocessing steps and learning algorithms at the same time
- Consider the following pipeline:
  - `StandardScaler`, without hyperparameters
  - `PolynomialFeatures`, with the max. *degree* of polynomials
  - Ridge regression, with L2 regularization parameter *alpha*

```
pipe = pipeline.make_pipeline(  
    StandardScaler(),  
    PolynomialFeatures(),  
    Ridge())
```

- We don't know the optimal polynomial degree or alpha value, so we use a grid search (or random search) to find the optimal values

```
param_grid = {'polynomialfeatures__degree': [1, 2, 3],  
              'ridge__alpha': [0.001, 0.01, 0.1, 1, 10, 100]}  
grid = GridSearchCV(pipe, param_grid=param_grid, cv=5, n_jobs=1)  
grid.fit(X_train, y_train)
```

- Visualizing the  $R^2$  results as a heatmap:



- Here, degree-2 polynomials help (but degree-3 ones don't), and tuning the alpha parameter helps as well.
- Not using the polynomial features leads to suboptimal results (see the results for degree 1)

Best parameters: {'polynomialfeatures\_\_degree': 2, 'ridge\_\_alpha': 10}  
Test-set score: 0.77

# Approaching machine learning problems

- Running your favourite algorithm on every problem is usually not a great way to start
- Consider the problem at large
  - Do you want exploratory analysis or (black box) modelling?
  - How to define and measure success? Are there costs involved?
  - Do you have the right data? How can you make it better?
- Build prototypes early-on to evaluate the above.
- Analyse your model's mistakes
  - Should you collect more, or additional data?
  - Should the task be reformulated?
  - Often a higher payoff than endless grid searching
- Technical debt
  - Very complex machine learning prototypes are hard/impossible to put into practice
  - There is a creation-maintenance trade-off
  - See 'Machine Learning: The High Interest Credit Card of Technical Debt'

## Real world evaluations

- Accuracy is seldomly the right measure. Usually, costs are involved.
- Don't just evaluate your predictions themselves, also evaluate how the outcome improves *after* you take actions based on them
- Beware of non-representative samples. You often don't have the data you really need.
- Adversarial situations (e.g. spam filtering) can subvert your predictions
- Data leakage: the signal your model found was just an artifact of your data
  - See 'Why Should I Trust You?' by Marco Ribeiro et al.
- A/B testing to evaluate algorithms in the wild
  - More advanced: bandit algorithms

# Summary

- Transforming the features can drastically impact performance
  - Constructing new features makes linear models more powerful
  - Selecting features can reduce overfitting and improve performance
  - Scaling is important for many distance-based methods (e.g. kNN, SVM)
- Pipelines allow us to encapsulate multiple steps into a single estimator
  - Has `fit`, `transform`, and `predict` methods
- Avoids data leakage, hence crucial for proper evaluation
- Choosing the right combination of feature extraction, preprocessing, and models is somewhat of an art.
- Pipelines + Grid/Random Search help, but search space is huge
  - Smarter techniques are being researched (see later)
- Real world applications require careful thought, prototyping, and tireless evaluation.