Lecture 6. Data preprocessing

Real-world machine learning pipelines

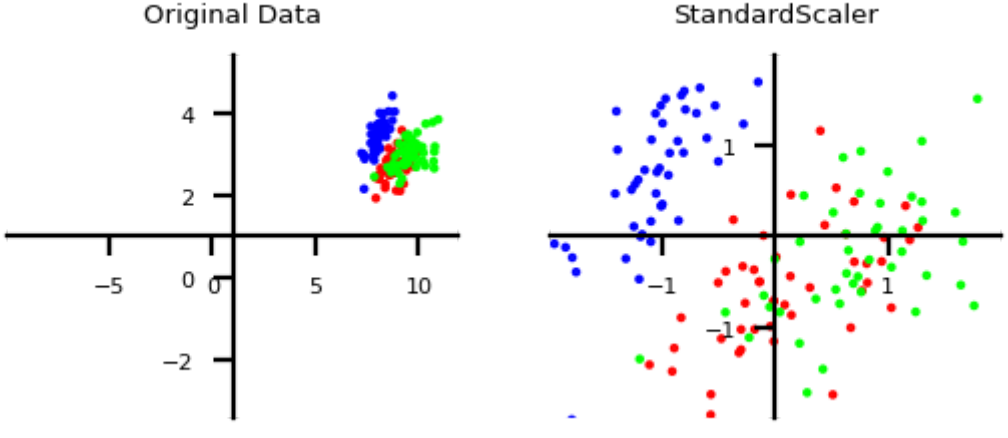
Joaquin Vanschoren

Data transformations

- Machine learning models make a lot of assumptions about the data
- In reality, these assumptions are often violated
- We build *pipelines* that *transform* the data before feeding it to the learners
    - Scaling (or other numeric transformations)
    - Encoding (convert categorical features into numerical ones)
    - Automatic feature selection
    - Feature engineering (e.g. binning, polynomial features,...)
    - Handling missing data
    - Handling imbalanced data
    - Dimensionality reduction (e.g. PCA)
    - Learned embeddings (e.g. for text)
- Seek the best combinations of transformations and learning methods
    - Often done empirically, using cross-validation
    - Make sure that there is no data leakage during this process!

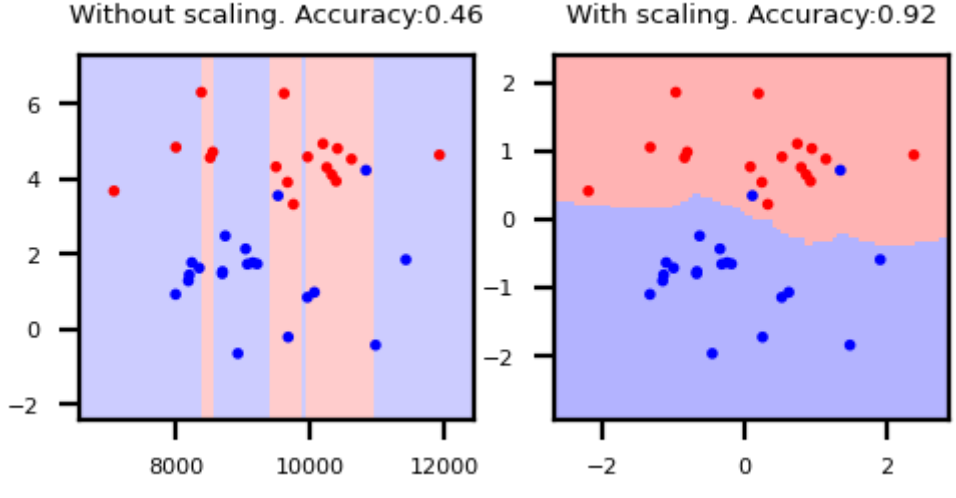
Scaling

- Use when different numeric features have different scales (different range of values)
    - Features with much higher values may overpower the others
- Goal: bring them all within the same range
- Different methods exist



Why do we need scaling?

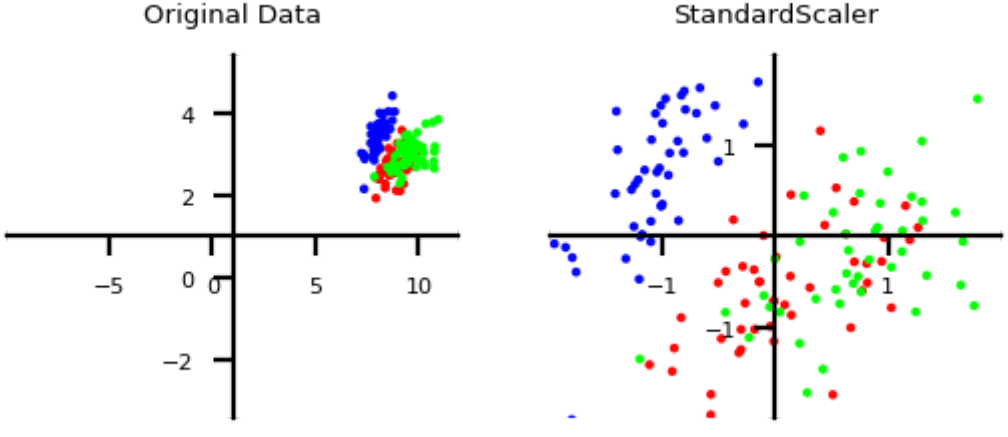
- KNN: Distances depend mainly on feature with larger values
- SVMs: (kernelized) dot products are also based on distances
- Linear model: Feature scale affects regularization
    - Weights have similar scales, more interpretable



Standard scaling (standardization)

- Generally most useful, assumes data is more or less normally distributed
- Per feature, subtract the mean value μ, scale by standard deviation σ
- New feature has $\mu = 0$ and $\sigma = 1$, values can still be arbitrarily large

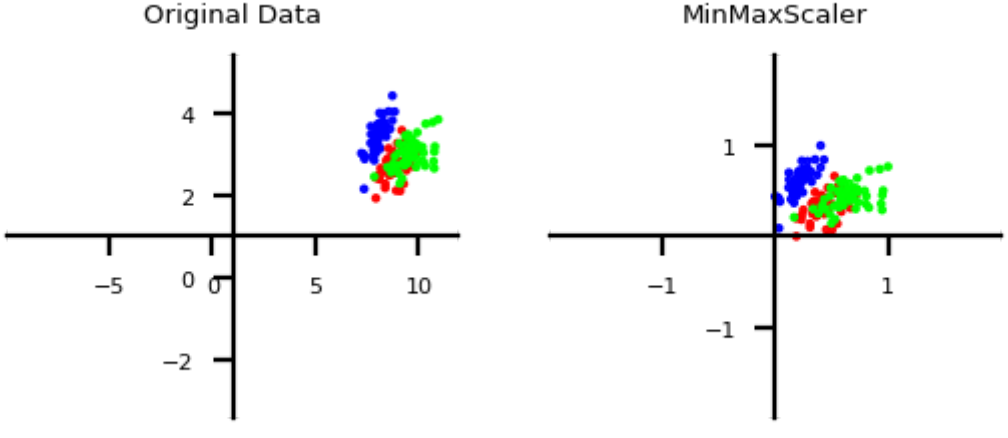
$$\mathbf{x}_{new} = \frac{\mathbf{x} - \mu}{\sigma}$$



Min-max scaling

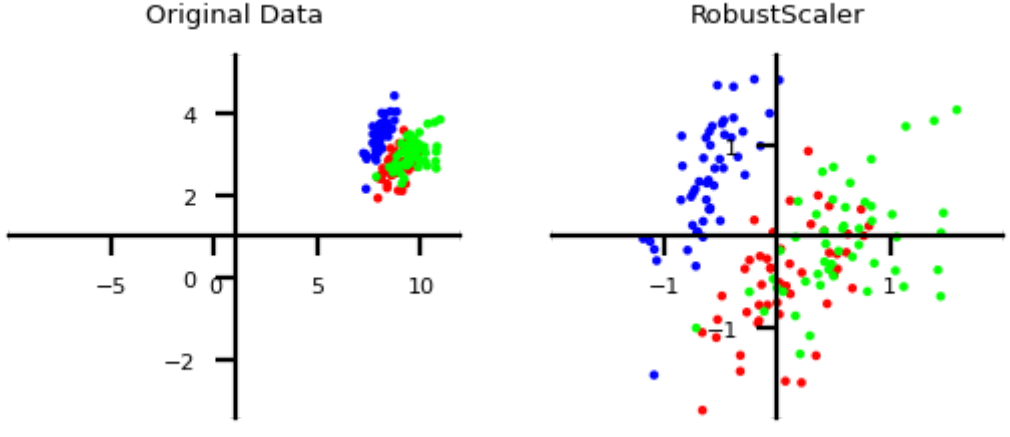
- Scales all features between a given min and max value (e.g. 0 and 1)
- Makes sense if min/max values have meaning in your data
- Sensitive to outliers

$$\mathbf{x}_{new} = \frac{\mathbf{x} - x_{min}}{x_{max} - x_{min}} \cdot (max - min) + min$$



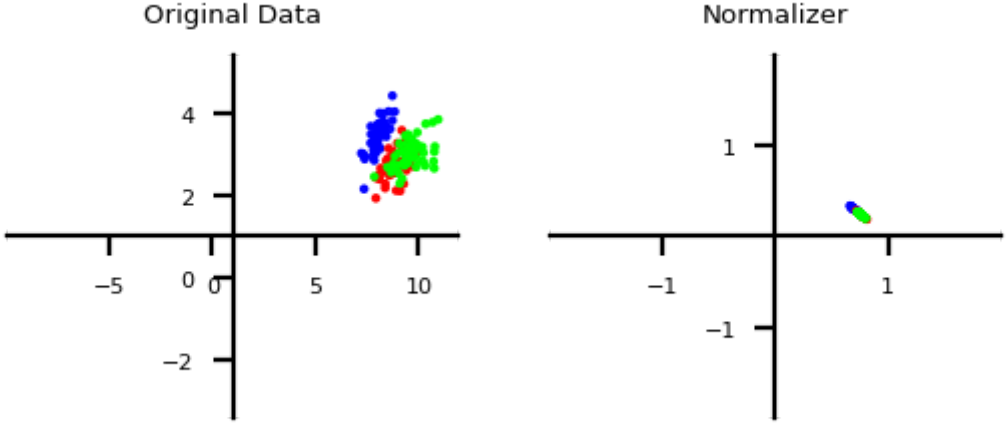
Robust scaling

- Subtracts the median, scales between quantiles q_{25} and q_{75}
- New feature has median 0, $q_{25} = -1$ and $q_{75} = 1$
- Similar to standard scaler, but ignores outliers



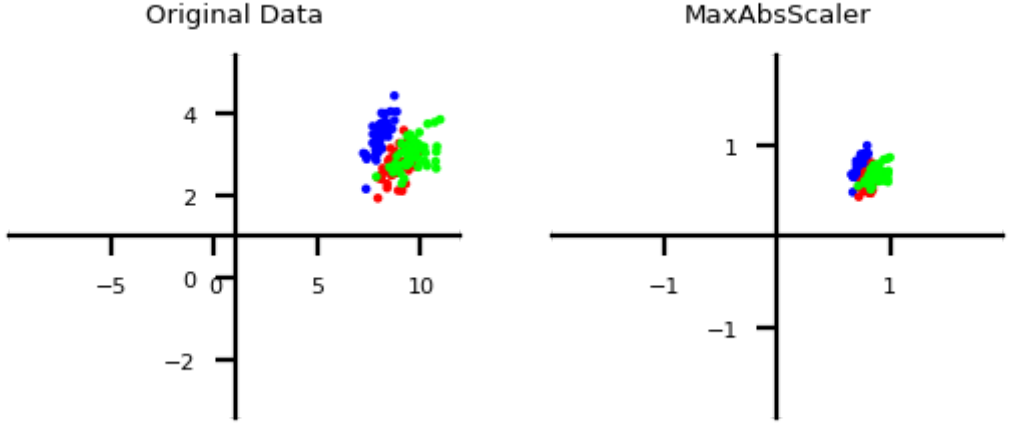
Normalization

- Makes sure that feature values of each point (each row) sum up to 1 (L1 norm)
    - Useful for count data (e.g. word counts in documents)
- Can also be used with L2 norm (sum of squares is 1)
    - Useful when computing distances in high dimensions
    - Normalized Euclidean distance is equivalent to cosine similarity



Maximum Absolute scaler

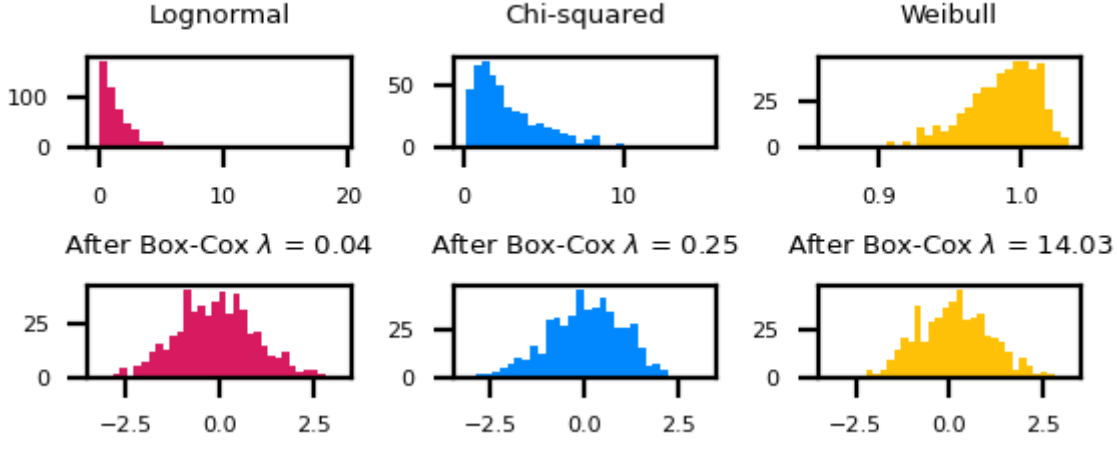
- For sparse data (many features, but few are non-zero)
    - Maintain sparseness (efficient storage)
- Scales all values so that maximum absolute value is 1
- Similar to Min-Max scaling without changing 0 values



Power transformations

- Some features follow certain distributions
    - E.g. number of twitter followers is log-normal distributed
- Box-Cox transformations transform these to normal distributions (λ is fitted)
    - Only works for positive values, use Yeo-Johnson otherwise

$$bc_\lambda(x) = \begin{cases} log(x) & \lambda = 0 \\ \frac{x^\lambda - 1}{\lambda} & \lambda \neq 0 \end{cases}$$



Categorical feature encoding

- Many algorithms can only handle numeric features, so we need to encode the categorical ones

	boro	salary	vegan
0	Manhattan	103	0
1	Queens	89	0
2	Manhattan	142	0
3	Brooklyn	54	1
4	Brooklyn	63	1
5	Bronx	219	0

Ordinal encoding

- Simply assigns an integer value to each category in the order they are encountered
- Only really useful if there exist a natural order in categories
    - Model will consider one category to be 'higher' or 'closer' to another

	boro	boro_ordinal	salary
0	Manhattan	2	103
1	Queens	3	89
2	Manhattan	2	142
3	Brooklyn	1	54
4	Brooklyn	1	63
5	Bronx	0	219

One-hot encoding (dummy encoding)

- Simply adds a new 0/1 feature for every category, having 1 (hot) if the sample has that category
- Can explode if a feature has lots of values, causing issues with high dimensionality
- What if test set contains a new category not seen in training data?
    - Either ignore it (just use all 0's in row), or handle manually (e.g. resample)

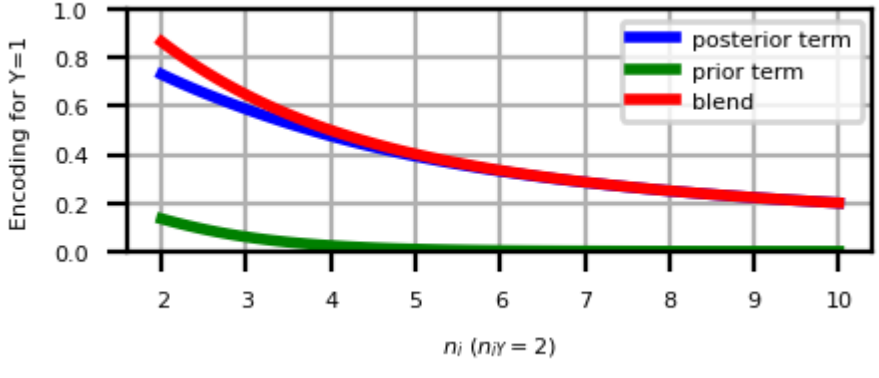
	boro	boro_Bronx	boro_Brooklyn	boro_Manhattan	boro_Queens	salary
0	Manhattan	0	0	1	0	103
1	Queens	0	0	0	1	89
2	Manhattan	0	0	1	0	142
3	Brooklyn	0	1	0	0	54
4	Brooklyn	0	1	0	0	63
5	Bronx	1	0	0	0	219

Target encoding

- Value close to 1 if category correlates with class 1, close to 0 if correlates with class 0
- Preferred when you have lots of category values. It only creates one new feature per class
- Blends posterior probability of the target $\frac{n_{iY}}{n_i}$ and prior probability $\frac{n_Y}{n}$.
  - n_{iY}: nr of samples with category i and class Y=1, n_i: nr of samples with category i
  - Blending: gradually decrease as you get more examples of category i and class Y=0

$$Enc(i) = \frac{1}{1+e^{-(n_i-1)}}\frac{n_{iY}}{n_i} + (1 - \frac{1}{1+e^{-(n_i-1)}})\frac{n_Y}{n}$$

  - Same for regression, using $\frac{n_{iY}}{n_i}$: average target value with category i, $\frac{n_Y}{n}$: overall mean



Example

- For Brooklyn, $n_{iY} = 2, n_i = 2, n_Y = 2, n = 6$
- Would be closer to 1 if there were more examples, all with label 1

$$Enc(Brooklyn) = \frac{1}{1 + e^{-1}} \frac{2}{2} + (1 - \frac{1}{1 + e^{-1}}) \frac{2}{6} = 0,82$$

- Note: the implementation used here sets $Enc(i) = \frac{n_Y}{n}$ when $n_{iY} = 1$

	boro	boro_encoded	salary	vegan
0	Manhattan	0.089647	103	0
1	Queens	0.333333	89	0
2	Manhattan	0.089647	142	0
3	Brooklyn	0.820706	54	1
4	Brooklyn	0.820706	63	1
5	Bronx	0.333333	219	0

In practice (scikit-learn)

- Ordinal encoding and one-hot encoding are implemented in scikit-learn
    - dtype defines that the output should be an integer

```
ordinal_encoder = OrdinalEncoder(dtype=int)
one_hot_encoder = OneHotEncoder(dtype=int)
```

- Target encoding is available in `category_encoders`
    - scikit-learn compatible
    - Also includes other, very specific encoders

```
target_encoder = TargetEncoder(return_df=True)
```

- All encoders (and scalers) follow the `fit-transform` paradigm
    - `fit` prepares the encoder, `transform` actually encodes the features
    - We'll discuss this next

```
encoder.fit(X, y)
X_encoded = encoder.transform(X,y)
```

Applying data transformations

- Data transformations should always follow a fit-predict paradigm
    - Fit the transformer on the training data only
        - E.g. for a standard scaler: record the mean and standard deviation
    - Transform (e.g. scale) the training data, then train the learning model
    - Transform (e.g. scale) the test data, then evaluate the model
- Only scale the input features (X), not the targets (y)
- If you fit and transform the whole dataset before splitting, you get data leakage
    - You have looked at the test data before training the model
    - Model evaluations will be misleading
- If you fit and transform the training and test data separately, you distort the data
    - E.g. training and test points are scaled differently

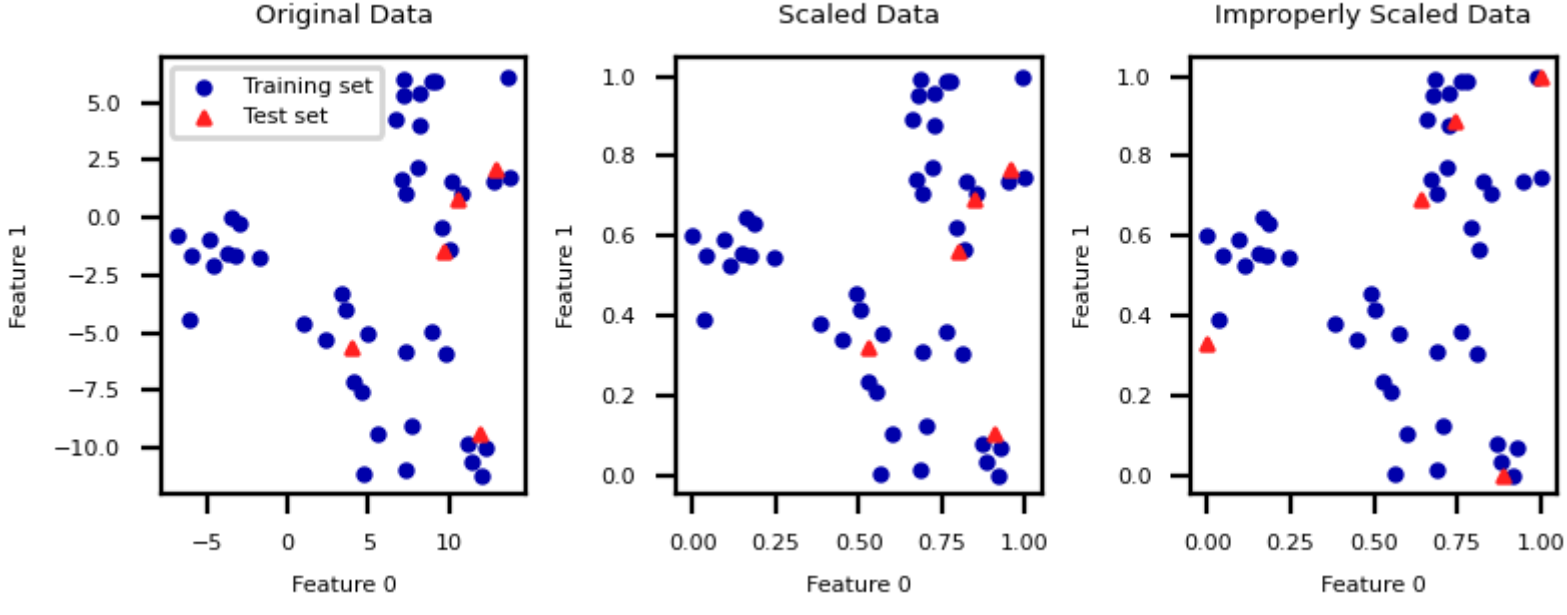
In practice (scikit-learn)

```
# choose scaling method and fit on training data
scaler = StandardScaler()
scaler.fit(X_train)

# transform training and test data
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
```

```
# calling fit and transform in sequence
X_train_scaled = scaler.fit(X_train).transform(X_train)
# same result, but more efficient computation
X_train_scaled = scaler.fit_transform(X_train)
```

Test set distortion

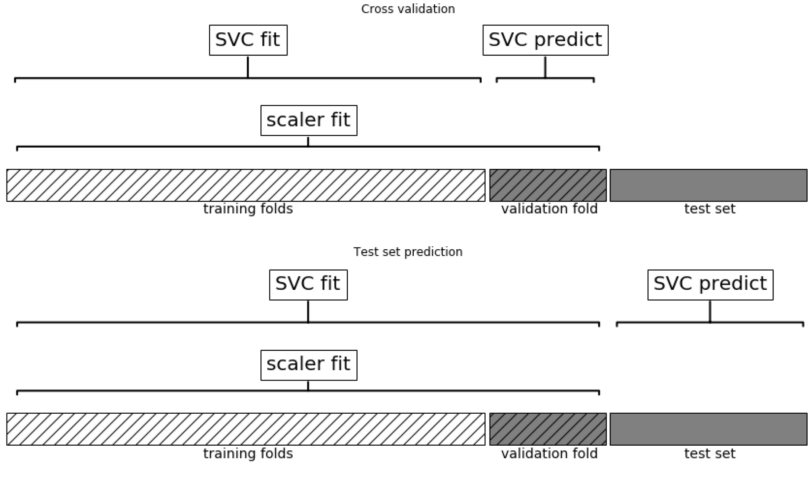
- Properly scaled: `fit` on training set, `transform` on training and test set
- Improperly scaled: `fit` and `transform` on the training and test data separately
    - Test data points nowhere near same training data points



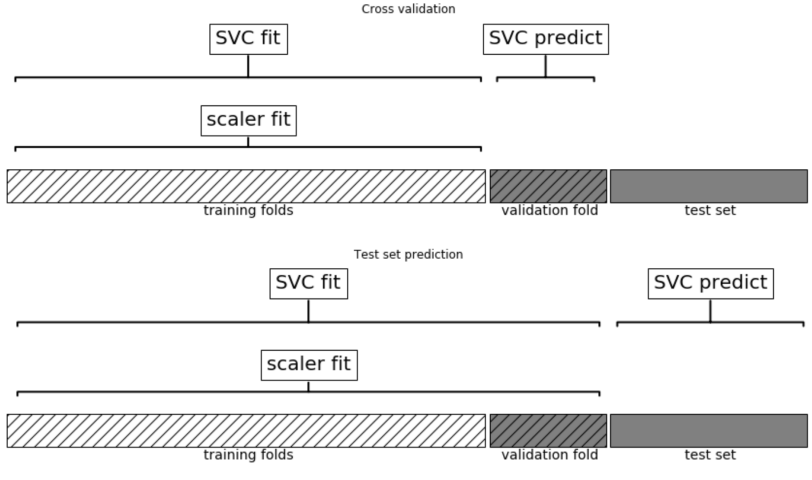
Data leakage

- Cross-validation: training set is split into training and validation sets for model selection
- Incorrect: Scaler is fit on whole training set before doing cross-validation
    - Data leaks from validation folds into training folds, selected model may be optimistic
- Right: Scaler is fit on training folds only

Information Leak



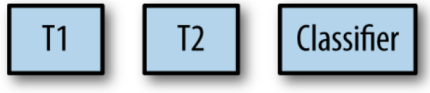
No Information leakage



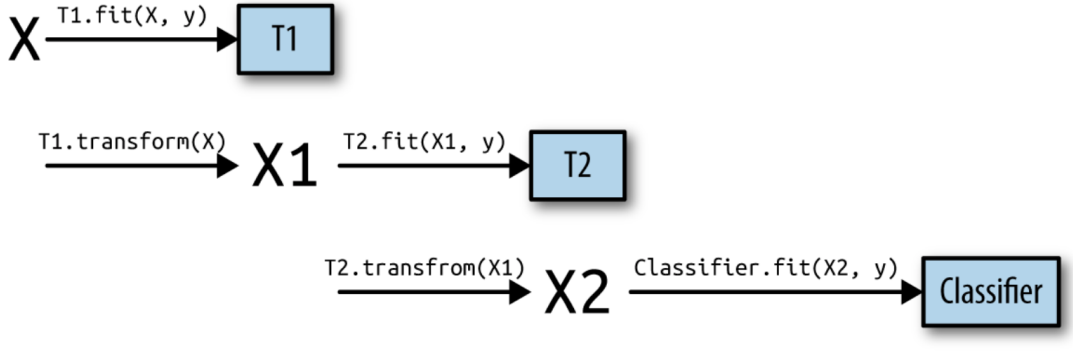
Pipelines

- A pipeline is a combination of data transformation and learning algorithms
- It has a `fit`, `predict`, and `score` method, just like any other learning algorithm
    - Ensures that data transformations are applied correctly

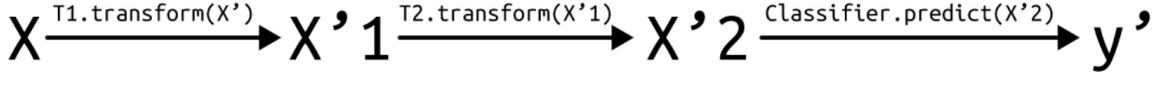
```
pipe = make_pipeline(T1(), T2(), Classifier())
```




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




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



In practice (scikit-learn)

- A `pipeline` combines multiple processing *steps* in a single estimator
- All but the last step should be data transformer (have a `transform` method)

```
# Make pipeline, step names will be 'minmaxscaler' and 'linearsvc'
pipe = make_pipeline(MinMaxScaler(), LinearSVC())
# Build pipeline with named steps
pipe = Pipeline([("scaler", MinMaxScaler()), ("svm", LinearSVC())])

# Correct fit and score
score = pipe.fit(X_train, y_train).score(X_test, y_test)
# Retrieve trained model by name
svm = pipe.named_steps["svm"]
```

```
# Correct cross-validation
scores = cross_val_score(pipe, X, y)
```

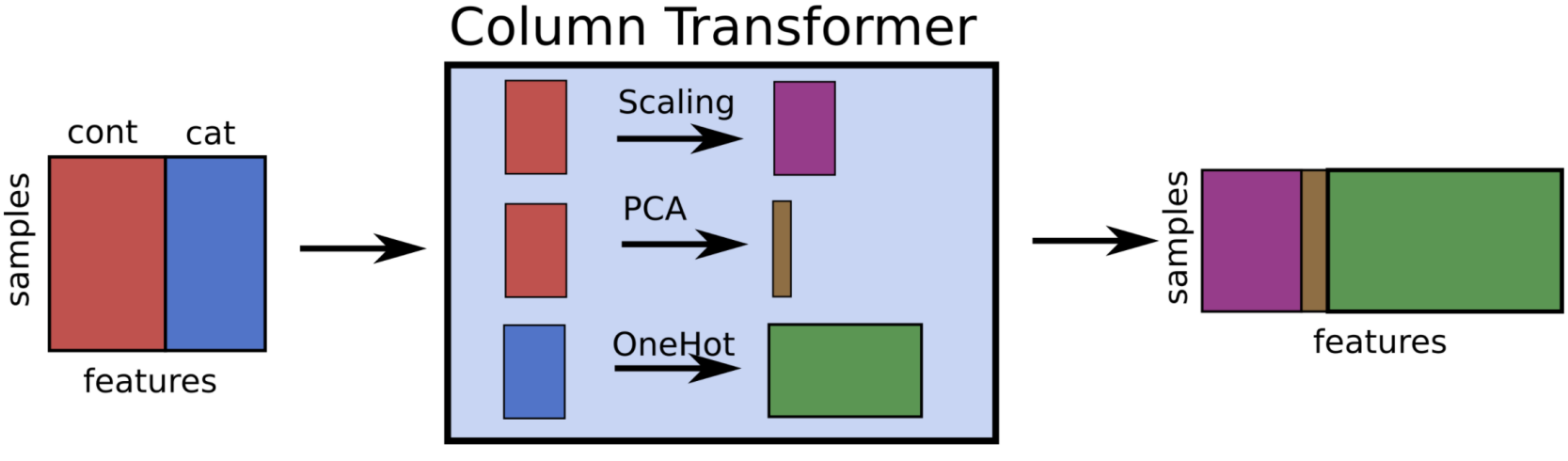
- If you want to apply different preprocessors to different columns, use `ColumnTransformer`
- If you want to merge pipelines, you can use `FeatureUnion` to concatenate columns

```
# 2 sub-pipelines, one for numeric features, other for categorical
ones
numeric_pipe = make_pipeline(SimpleImputer(),StandardScaler())
categorical_pipe = make_pipeline(SimpleImputer(),OneHotEncoder())

# Using categorical pipe for features A,B,C, numeric pipe otherwise
preprocessor = make_column_transformer((categorical_pipe,
                                        ["A","B","C"]),
                                        remainder=numeric_pipe)

# Combine with learning algorithm in another pipeline
pipe = make_pipeline(preprocess, LinearSVC())
```

```
# Feature union of PCA features and selected features
union = FeatureUnion([("pca", PCA()), ("selected", SelectKBest())])
pipe = make_pipeline(union, LinearSVC())
```

- `ColumnTransformer` concatenates features in order

```
pipe = make_column_transformer((StandardScaler(),numeric_features),
                               (PCA(),numeric_features),

(OneHotEncoder(),categorical_features))
```



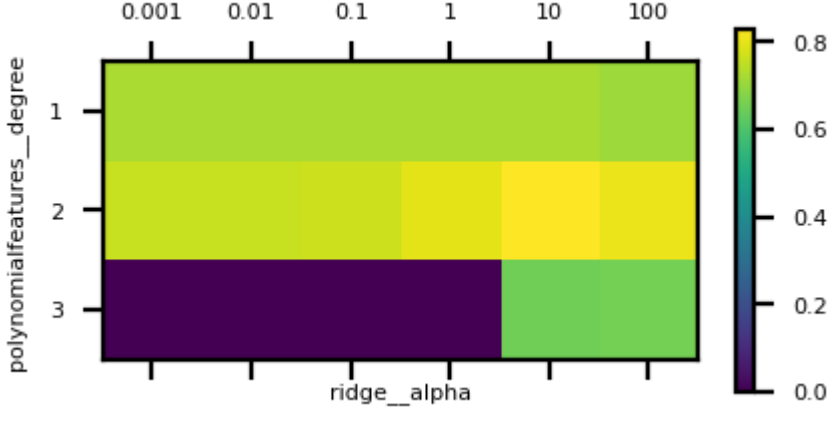
Pipeline selection

- We can safely use pipelines in model selection (e.g. grid search)
- Use `'__'` to refer to the hyperparameters of a step, e.g. `svm__C`

```
# Correct grid search (can have hyperparameters of any step)
param_grid = {'svm__C': [0.001, 0.01],
              'svm__gamma': [0.001, 0.01, 0.1, 1, 10, 100]}
grid = GridSearchCV(pipe, param_grid=param_grid).fit(X,y)
# Best estimator is now the best pipeline
best_pipe = grid.best_estimator_

# Tune pipeline and evaluate on held-out test set
grid = GridSearchCV(pipe,
param_grid=param_grid).fit(X_train,y_train)
grid.score(X_test,y_test)
```

Example: Tune multiple steps at once

```
pipe = make_pipeline(StandardScaler(),PolynomialFeatures(), Ridge())
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).fit(X_train,
y_train)
```



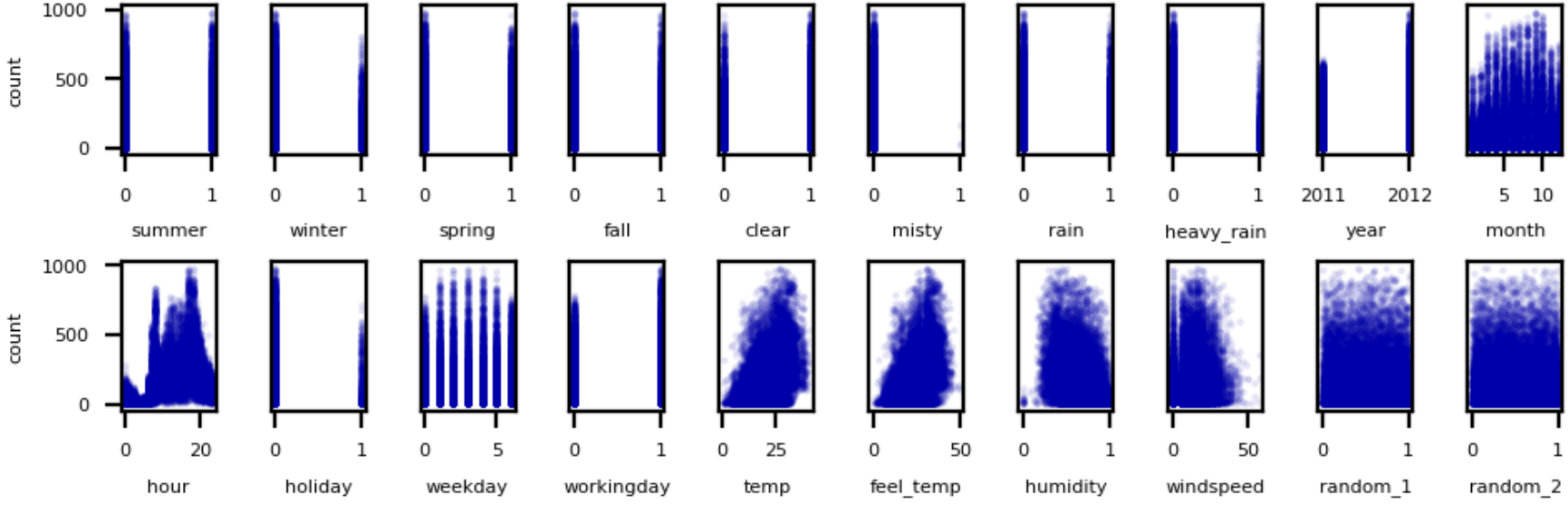
Automatic Feature Selection

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)
    - Curse of dimensionality (e.g. kNN)
    - Even models such as RandomForest can benefit from this
    - Sometimes it is one of the main methods to improve models (e.g. gene expression data)
- Faster prediction and training
    - Training time can be quadratic (or cubic) in number of features
- Easier data collection, smaller models (less storage)
- More interpretable models: fewer features to look at

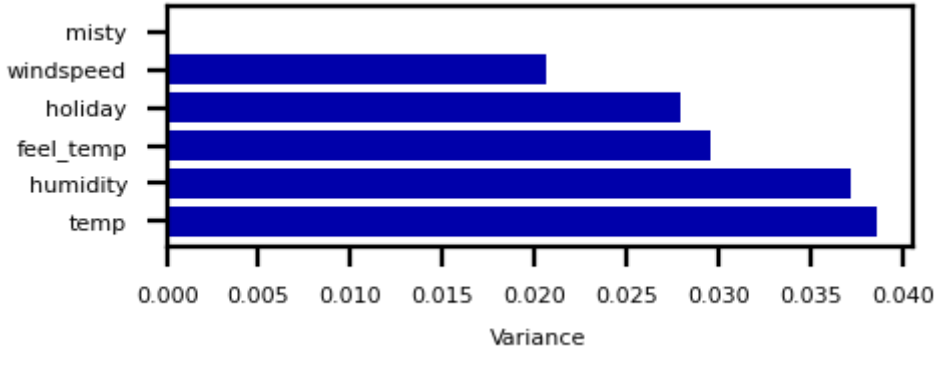
Example: bike sharing

- The Bike Sharing Demand dataset shows the amount of bikes rented in Washington DC
- Some features are clearly more informative than others (e.g. temp, hour)
- Some are correlated (e.g. temp and feel_temp)
- We add two random features at the end



Unsupervised feature selection

- Variance-based
    - Remove (near) constant features
        - Choose a small variance threshold
    - Scale features before computing variance!
    - Infrequent values may still be important
- Covariance-based
    - Remove correlated features
    - The small differences may actually be important
        - You don't know because you don't consider the target

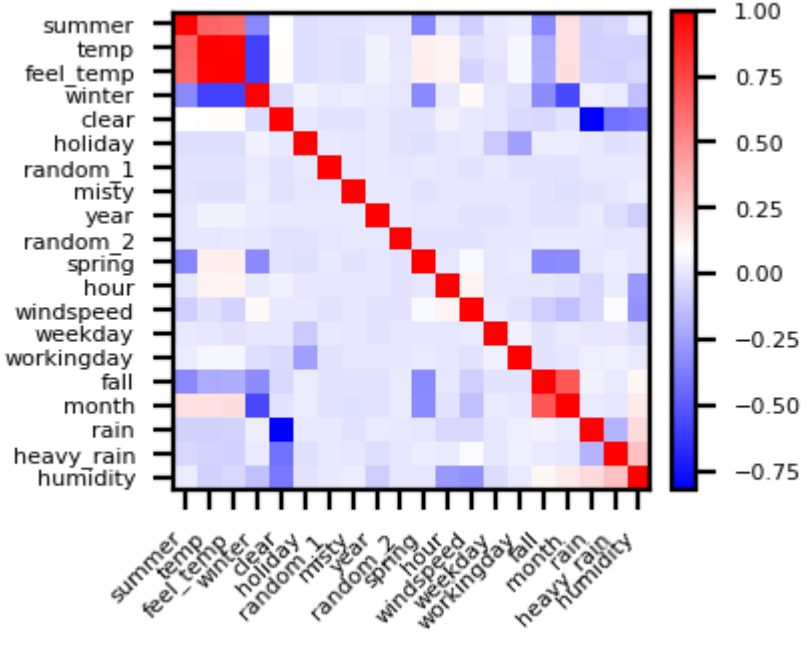


Covariance based feature selection

- Remove features X_i (= $\mathbf{X_{:,i}}$) that are highly correlated (have high correlation coefficient ρ)

$$\rho(X_1, X_2) = \frac{\text{cov}(X_1, X_2)}{\sigma(X_1)\sigma(X_2)} = \frac{\frac{1}{N-1}\sum_i (X_{i,1} - \overline{X_1})(X_{i,2} - \overline{X_2})}{\sigma(X_1)\sigma(X_2)}$$

- Should we remove `feel_temp`? Or `temp`? Maybe one correlates more with the target?

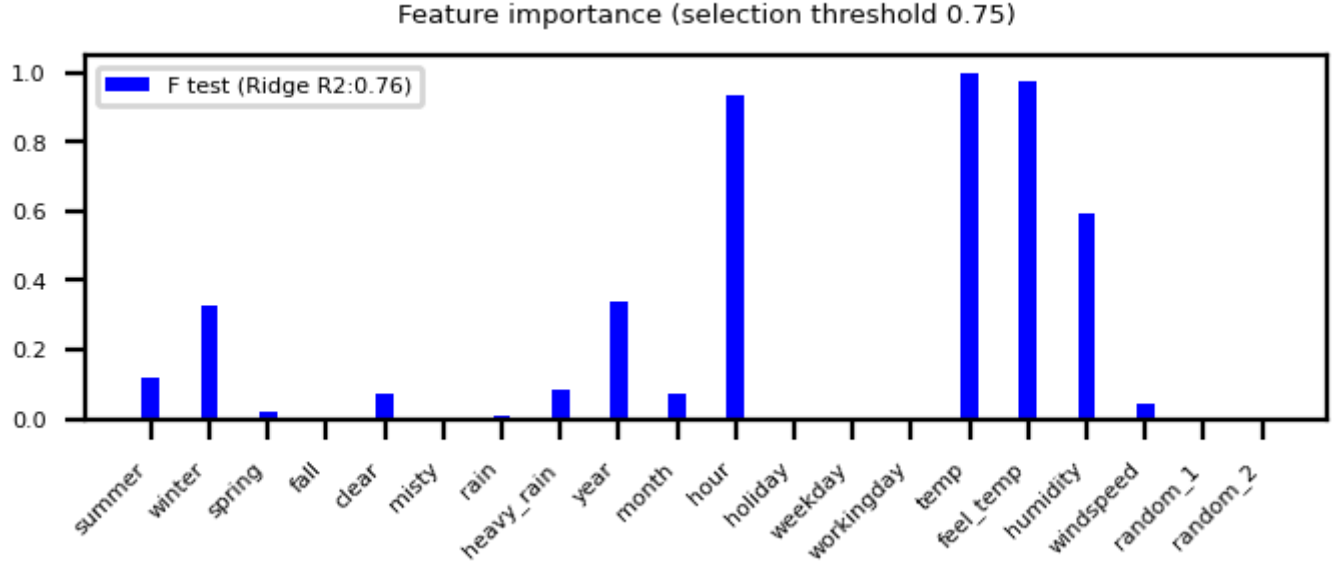


Supervised feature selection: overview

- Univariate: F-test and Mutual Information
- Model-based: Random Forests, Linear models, kNN
- Wrapping techniques (black-box search)
- Permutation importance

Univariate statistics (F-test)

- Consider each feature individually (univariate), independent of the model that you aim to apply
- Use a statistical test: is there a *linear* **statistically significant relationship** with the target?
- Use F-statistic (or corresponding p value) to rank all features, then select features using a threshold
    - Best k, best k %, probability of removing useful features (FPR),...
- Cannot detect correlations (e.g. temp and feel_temp) or interactions (e.g. binary features)



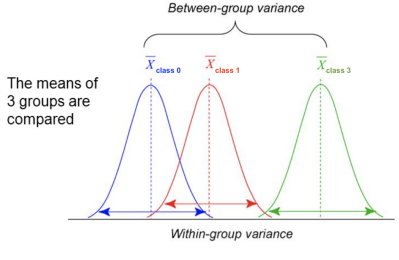
F-statistic

- For regression: does feature X_i correlate (positively or negatively) with the target y?

$$\text{F-statistic} = \frac{\rho(X_i, y)^2}{1 - \rho(X_i, y)^2} \cdot (N - 1)$$

- For classification: uses ANOVA: does X_i explain the between-class variance?
    - Alternatively, use the χ^2 test (only for categorical features)

$$\text{F-statistic} = \frac{\text{within-class variance}}{\text{between-class variance}} = \frac{\overline{var(X_i)}}{\overline{var(X_i)}}$$

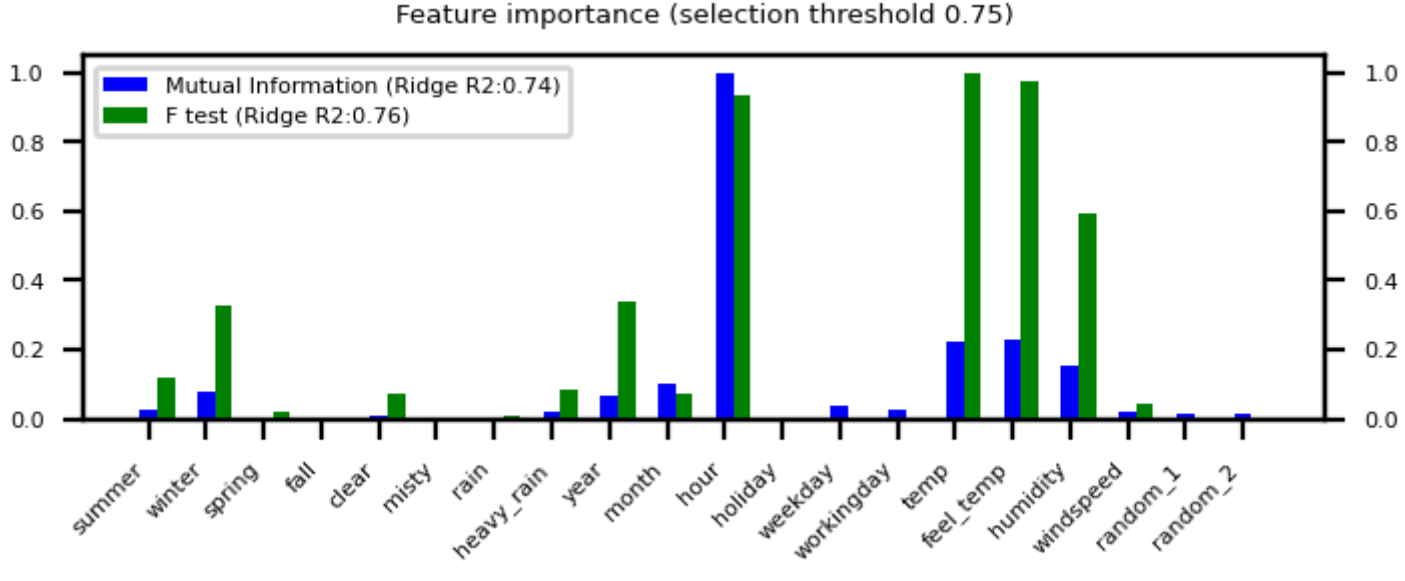


Mutual information

- Measures how much information X_i gives about the target Y. In terms of entropy H:

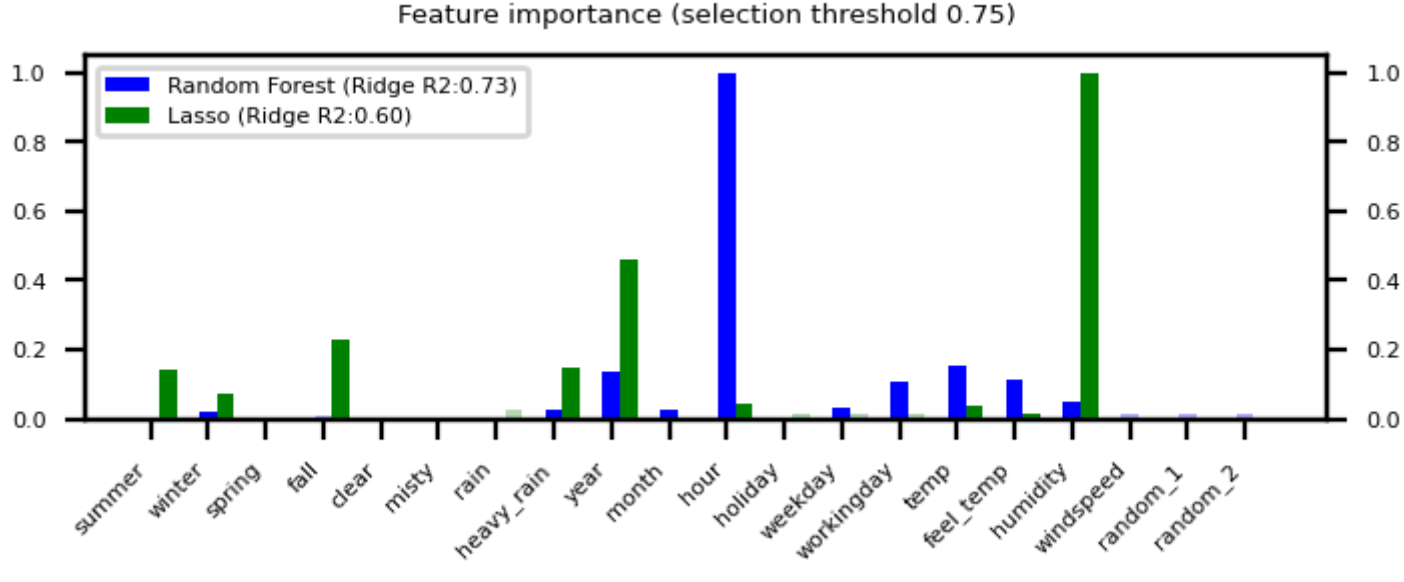
$$MI(X, Y) = H(X) + H(Y) - H(X, Y)$$

- Idea: estimate H(X) as the average distance between a data point and its k Nearest Neighbors
    - You need to choose k and say which features are categorical
- Captures complex dependencies (e.g. hour, month), but requires more samples to be accurate



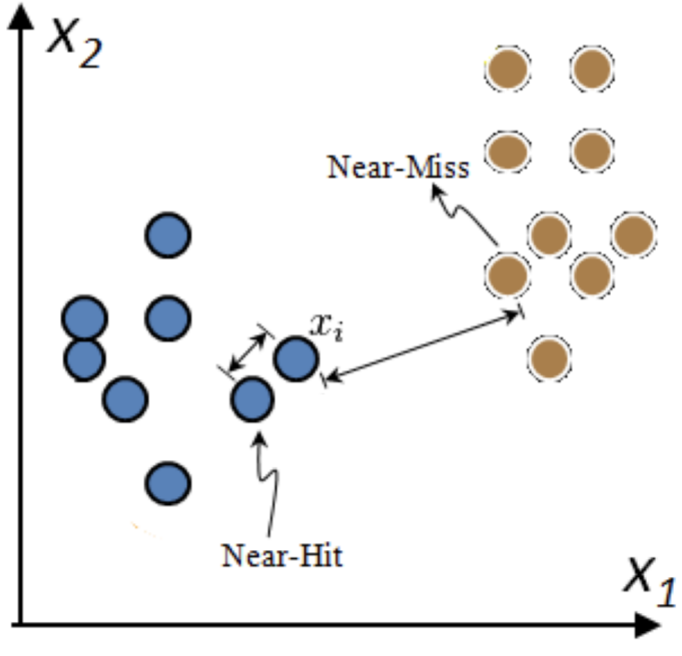
Model-based Feature Selection

- Use a tuned(!) supervised model to judge the importance of each feature
    - Linear models (Ridge, Lasso, LinearSVM,...): features with highest weights (coefficients)
    - Tree–based models: features used in first nodes (high information gain)
- Selection model can be different from the one you use for final modelling
- Captures interactions: features are more/less informative in combination (e.g. winter, temp)
- RandomForests: learns complex interactions (e.g. hour), but biased to high cardinality features



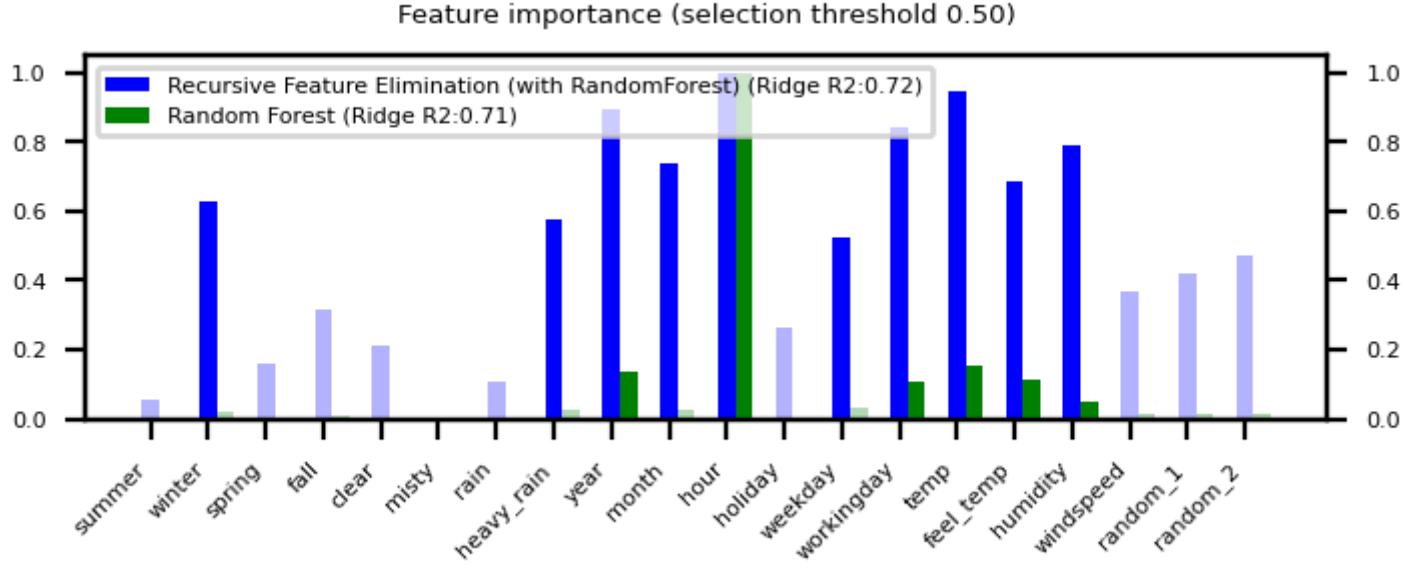
Relief: Model-based selection with kNN

- For I iterations, choose a random point $\mathbf{x_i}$ and find k nearest neighbors $\mathbf{x_k}$
- Increase feature weights if $\mathbf{x_i}$ and $\mathbf{x_k}$ have different class (near miss), else decrease
    - $\mathbf{w_i} = \mathbf{w_{i-1}} + (\mathbf{x_i} - \text{nearMiss}_i)^2 - (\mathbf{x_i} - \text{nearHit}_i)^2$
- Many variants: ReliefF (uses L1 norm, faster), RReliefF (for regression), ...



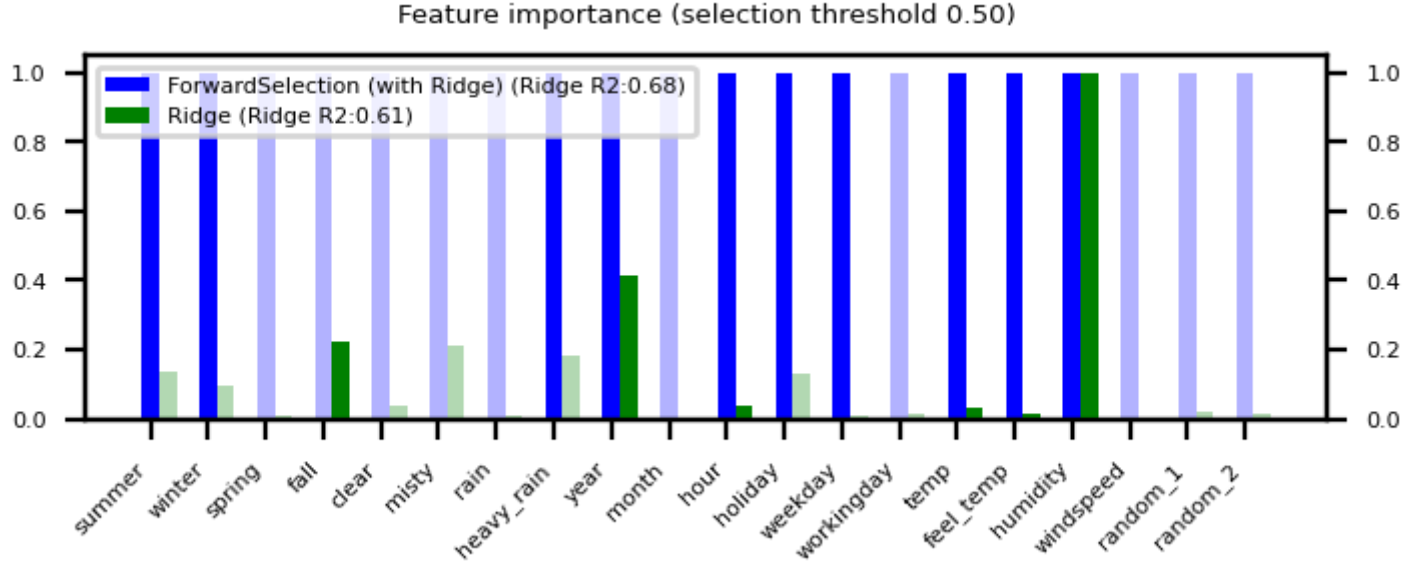
Iterative Model-based Feature Selection

- Dropping many features at once is not ideal: feature importance may change in subset
- Recursive Feature Elimination (RFE)
    - Remove s least important feature(s), recompute remaining importances, repeat
- Can be rather slow



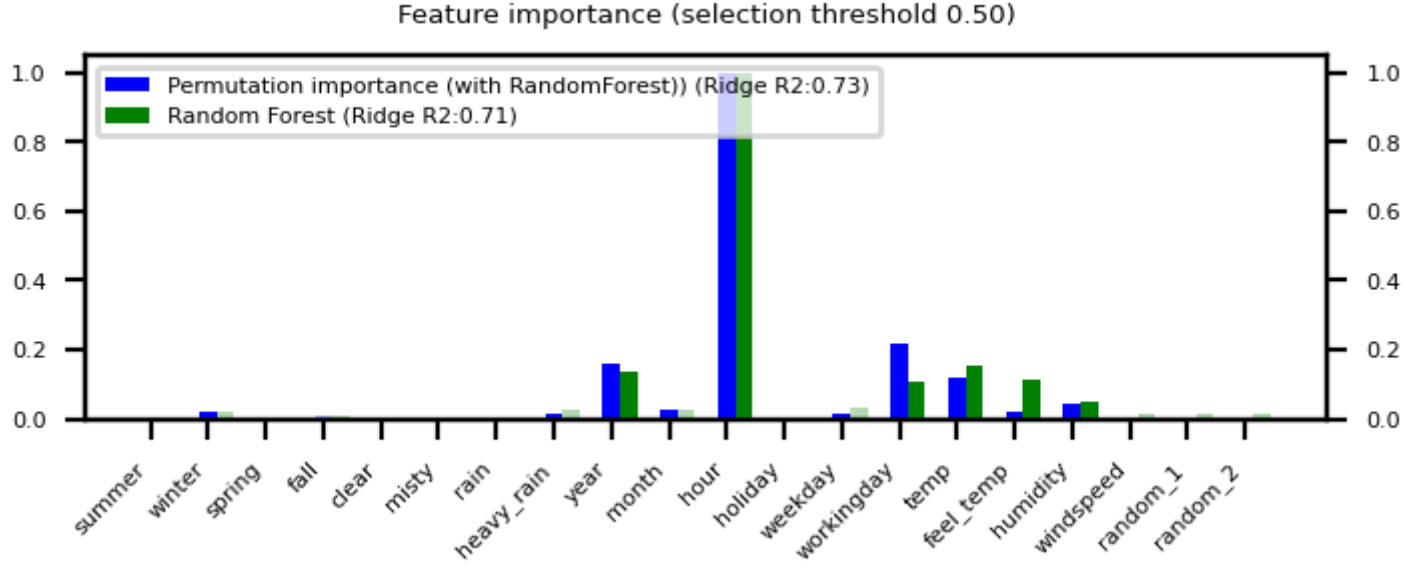
Sequential feature selection (Wrapping)

- Evaluate your model with different sets of features, find best subset based on performance
- Greedy black-box search (can end up in local minima)
    - Backward selection: remove least important feature, recompute importances, repeat
    - Forward selection: set aside most important feature, recompute importances, repeat
    - Floating: add best new feature, remove worst one, repeat (forward or backward)
- Stochastic search: use random mutations in candidate subset (e.g. simulated annealing)



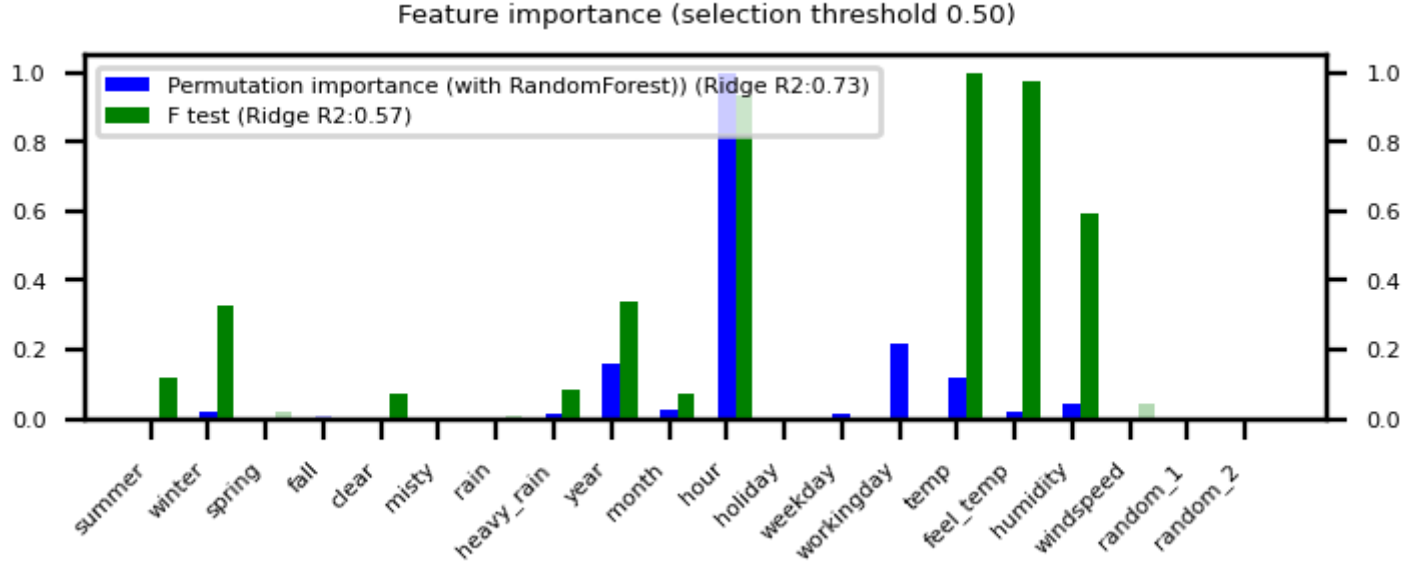
Permutation feature importance

- Defined as the decrease in model performance when a single feature value is randomly shuffled
    - This breaks the relationship between the feature and the target
- Model agnostic, metric agnostic, and can be calculated many times with different permutations
- Can be applied to unseen data (not possible with model-based techniques)
- Less biased towards high-cardinality features (compared with RandomForests)



Comparison

- Feature importances (scaled) and cross-validated R^2 score of pipeline
    - Pipeline contains features selection + Ridge
- Selection threshold value ranges from 25% to 100% of all features
- Best method ultimately depends on the problem and dataset at hand



In practice (scikit-learn)

- Unsupervised: `VarianceTreshold`

```
selector = VarianceThreshold(threshold=0.01)
X_selected = selector.fit_transform(X)
variances = selector.variances_
```

- Univariate:
    - For regression: `f_regression`, `mutual_info_regression`
    - For classification: `f_classification`, `chi2`, `mutual_info_classication`
    - Selecting: `SelectKBest`, `SelectPercentile`, `SelectFpr`,...

```
selector = SelectPercentile(score_func=f_regression, percentile=50)
X_selected = selector.fit_transform(X,y)
selected_features = selector.get_support()
f_values, p_values = f_regression(X,y)
mi_values = mutual_info_regression(X,y,discrete_features=[])
```

- Model-based:
  - `SelectFromModel`: requires a model and a selection threshold
  - `RFE`, `RFECV` (recursive feature elimination): requires model and final nr features

```
selector = SelectFromModel(RandomForestRegressor(),
threshold='mean')
rfe_selector = RFE(RidgeCV(), n_features_to_select=20)
X_selected = selector.fit_transform(X)
rf_importances = Randomforest().fit(X, y).feature_importances_
```

- Sequential feature selection (from `mlxtend`, sklearn-compatible)

```
selector = SequentialFeatureSelector(RidgeCV(), k_features=20,
forward=True,
                                     floating=True)
X_selected = selector.fit_transform(X)
```

- Permutation Importance (in `sklearn.inspection`), no fit-transform interface

```
importances =
permutation_importance(RandomForestRegressor().fit(X,y),
                                     X, y,
n_repeats=10).importances_mean
feature_ids = (-importances).argsort()[:n]
```

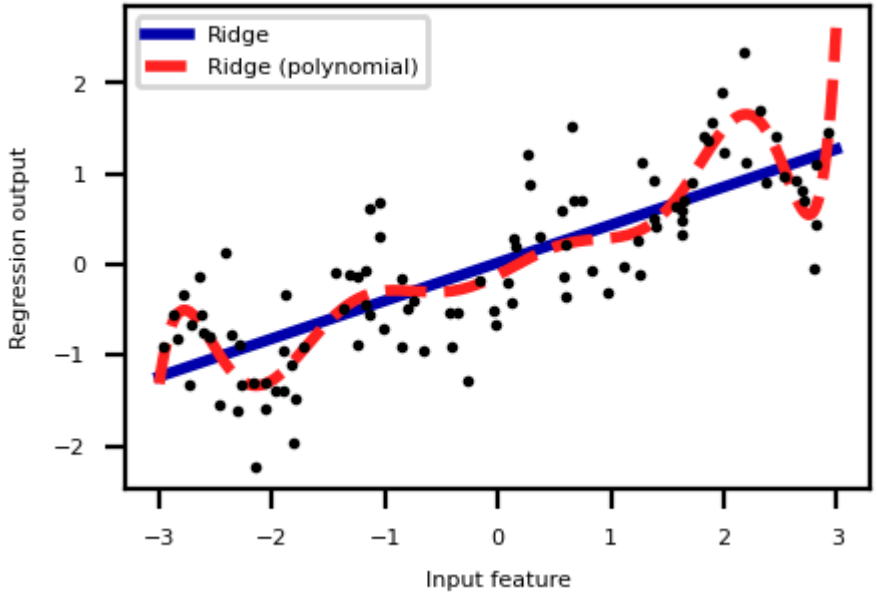
Feature Engineering

- Create new features based on existing ones
    - Polynomial features
    - Interaction features
    - Binning
- Mainly useful for simple models (e.g. linear models)
    - Other models can learn interations themselves
    - But may be slower, less robust than linear models

Polynomials

- Add all polynomials up to degree d and all products
    - Equivalent to polynomial basis expansions

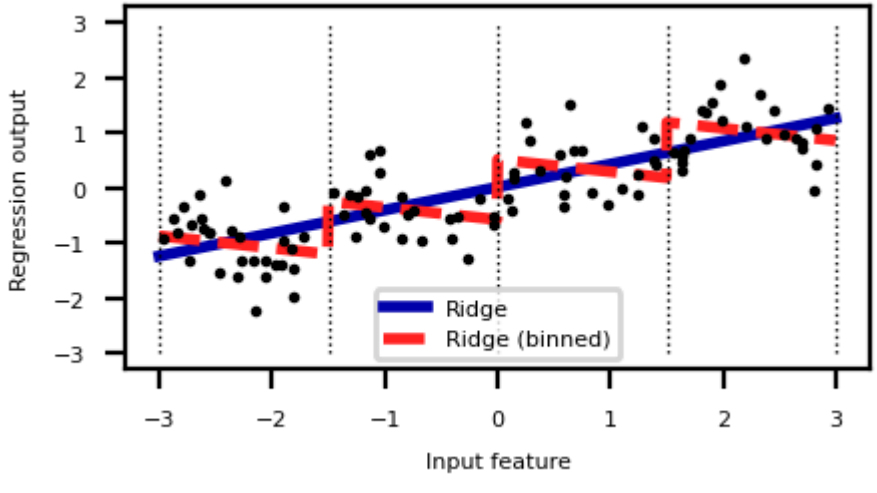
$$[1, x_1, \ldots, x_p] \rightarrow [1, x_1, \ldots, x_p, x_1^2, \ldots, x_p^2, \ldots, x_p^d, x_1 x_2, \ldots, x_{p-1} x_p]$$



Binning

- Partition numeric feature values into n intervals (bins)
- Create n new one-hot features, 1 if original value falls in corresponding bin
- Models different intervals differently (e.g. different age groups)

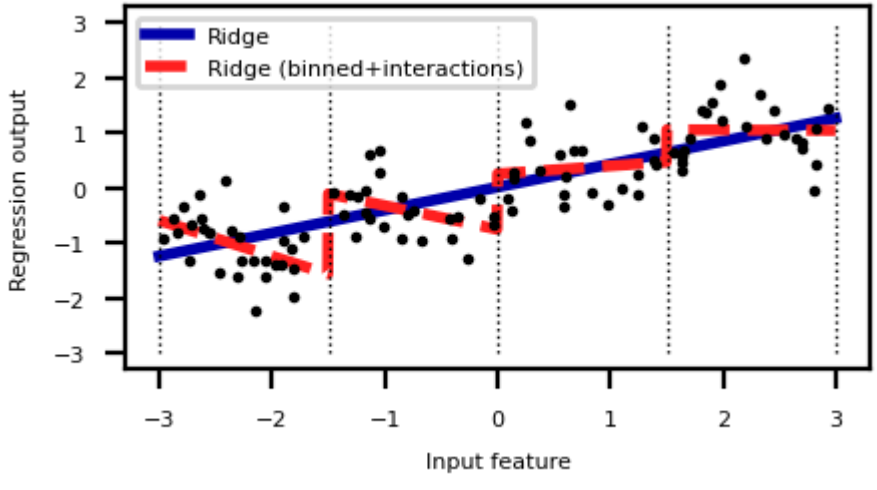
	orig	[-3.0,-1.5]	[-1.5,0.0]	[0.0,1.5]	[1.5,3.0]
0	-0.752759	0.000000	1.000000	0.000000	0.000000
1	2.704286	0.000000	0.000000	0.000000	1.000000
2	1.391964	0.000000	0.000000	1.000000	0.000000



Binning + interaction features

- Add *interaction features* (or *product features*)
  - Product of the bin encoding and the original feature value
  - Learn different weights per bin

	orig	b0	b1	b2	b3	X*b0	X*b1	X*b2	X*b3
0	-0.752759	0.000000	1.000000	0.000000	0.000000	-0.000000	-0.752759	-0.000000	-0.000000
1	2.704286	0.000000	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000	2.704286
2	1.391964	0.000000	0.000000	1.000000	0.000000	0.000000	0.000000	1.391964	0.000000



Categorical feature interactions

- One-hot-encode categorical feature
- Multiply every one-hot-encoded column with every numeric feature
- Allows to built different submodels for different categories

	gender	age	pageviews	time
0	M	14	70	269
1	F	16	12	1522
2	M	12	42	235
3	F	25	64	63
4	F	22	93	21

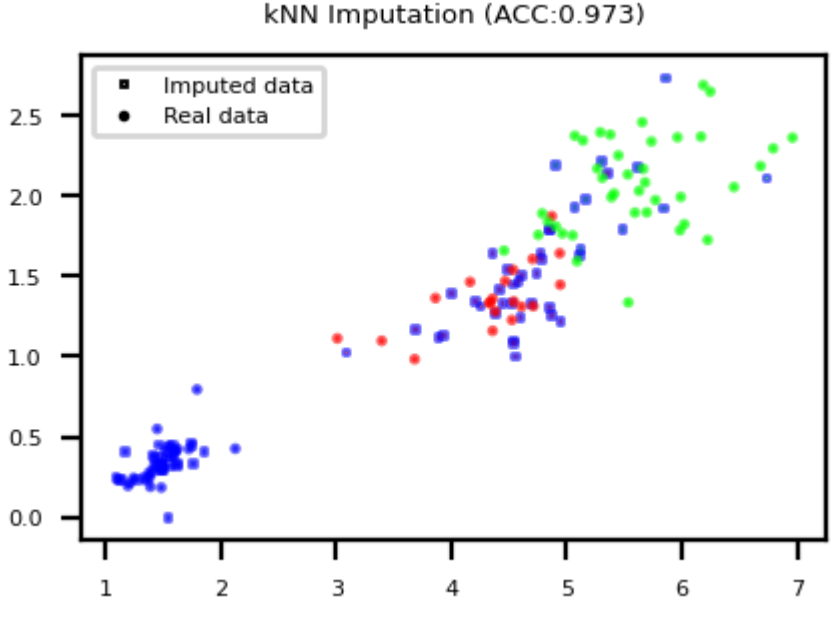
	age_M	pageviews_M	time_M	gender_M_M	age_F	pageviews_F	time_F	gender_F_F
0	14	70	269	1	0	0	0	0
1	0	0	0	0	16	12	1522	1
2	12	42	235	1	0	0	0	0
3	0	0	0	0	25	64	63	1
4	0	0	0	0	22	93	21	1

Missing value imputation

- Data can be missing in different ways:
    - Missing Completely at Random (MCAR): purely random points are missing
    - Missing at Random (MAR): something affects missingness, but no relation with the value
        - E.g. faulty sensors, some people don't fill out forms correctly
    - Missing Not At Random (MNAR): systematic missingness linked to the value
        - Has to be modelled or resolved (e.g. sensor decay, sick people leaving study)
- Missingness can be encoded in different ways:'?', '-1', 'unknown', 'NA',...
- Also labels can be missing (remove example or use semi-supervised learning)

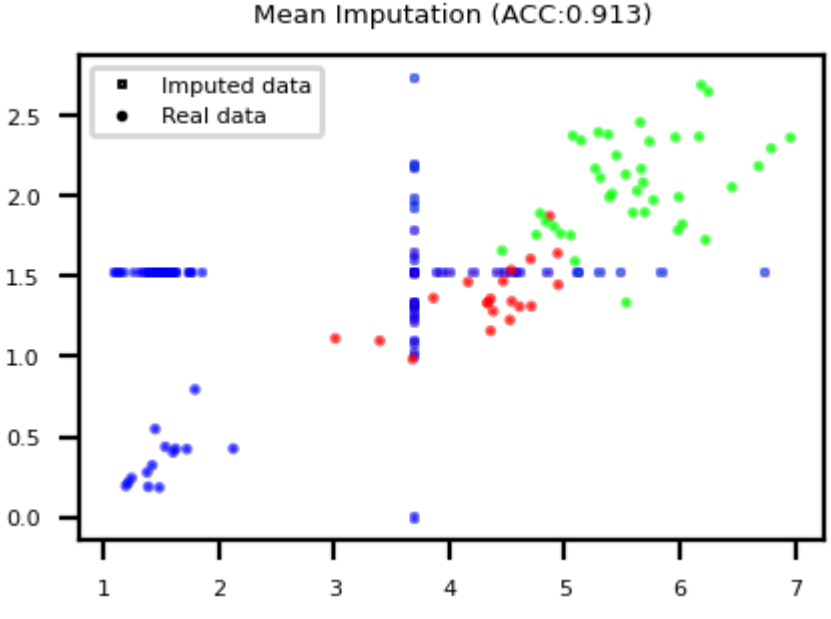
Overview

- Mean/constant imputation
- kNN-based imputation
- Iterative (model-based) imputation
- Matrix Factorization techniques



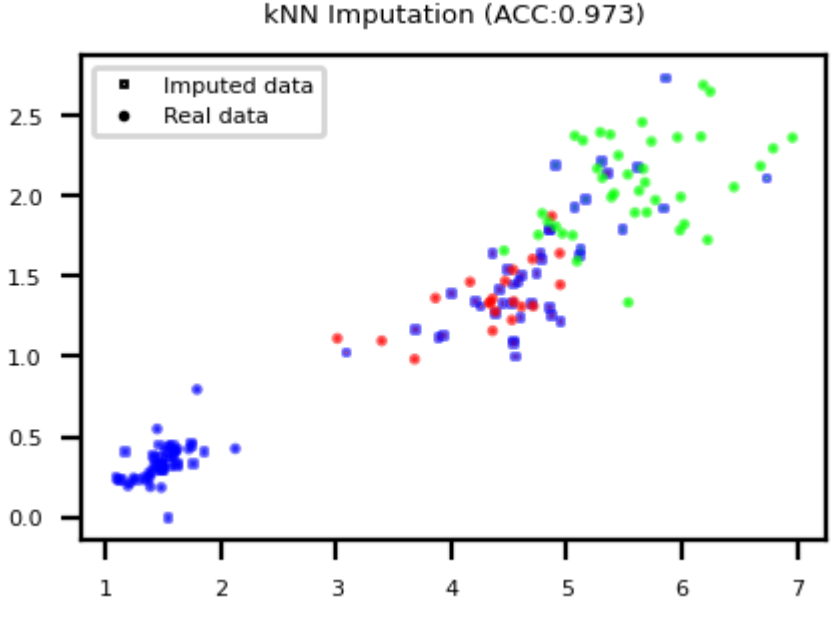
Mean imputation

- Replace all missing values of a feature by the same value
    - Numerical features: mean or median
    - Categorical features: most frequent category
    - Constant value, e.g. 0 or 'missing' for text features
- Optional: add an indicator column for missingness
- Example: Iris dataset (randomly removed values in 3rd and 4th column)



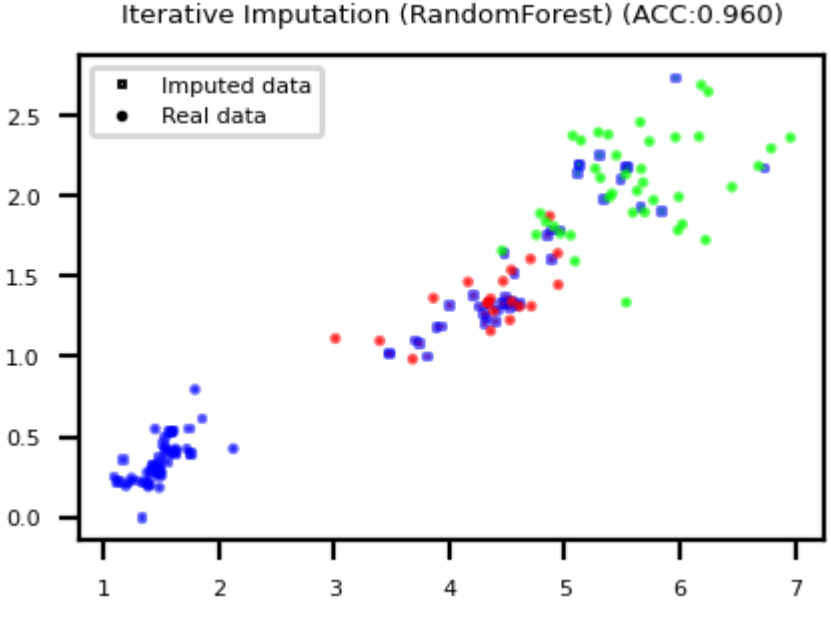
kNN imputation

- Use special version of kNN to predict value of missing points
- Uses only non-missing data when computing distances



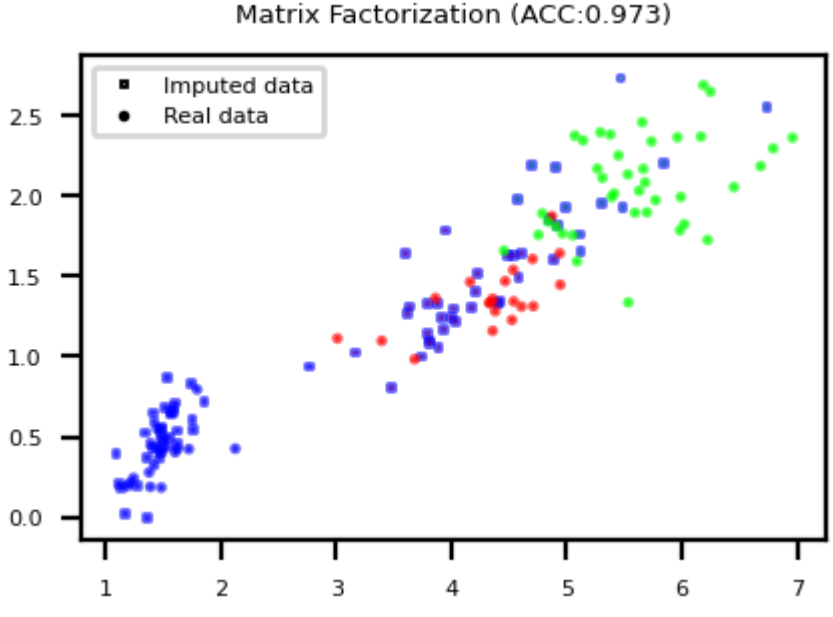
Iterative (model-based) Imputation

- Better known as Multiple Imputation by Chained Equations (MICE)
- Iterative approach
    - Do first imputation (e.g. mean imputation)
    - Train model (e.g. RandomForest) to predict missing values of a given feature
    - Train new model on imputed data to predict missing values of the next feature
        - Repeat m times in round-robin fashion, leave one feature out at a time



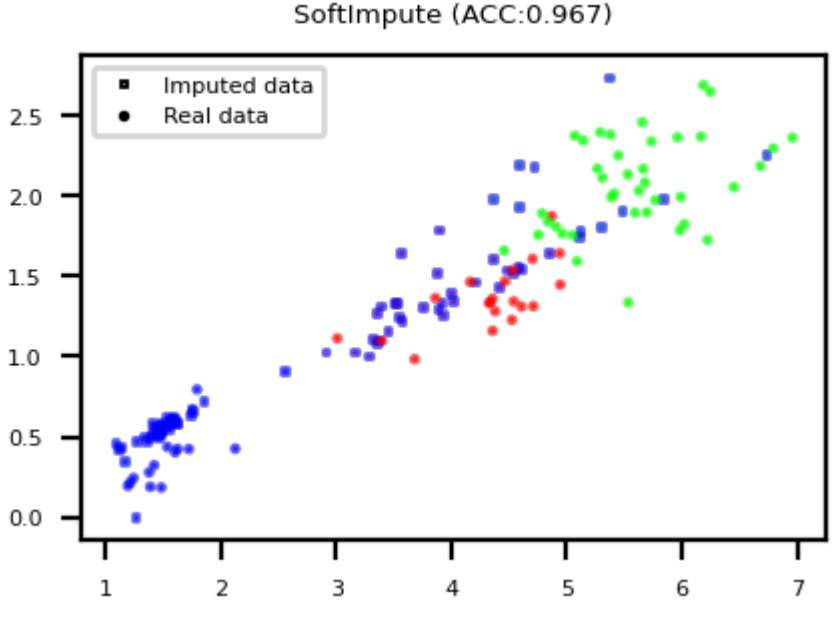
Matrix Factorization

- Basic idea: low-rank approximation
    - Replace missing values by 0
    - Factorize $\mathbf{X}$ with rank r: $\mathbf{X}^{n \times p} = \mathbf{U}^{n \times r}\mathbf{V}^{r \times p}$
        - With n data points and p features
        - Solved using gradient descent
    - Recompute $\mathbf{X}$: now complete



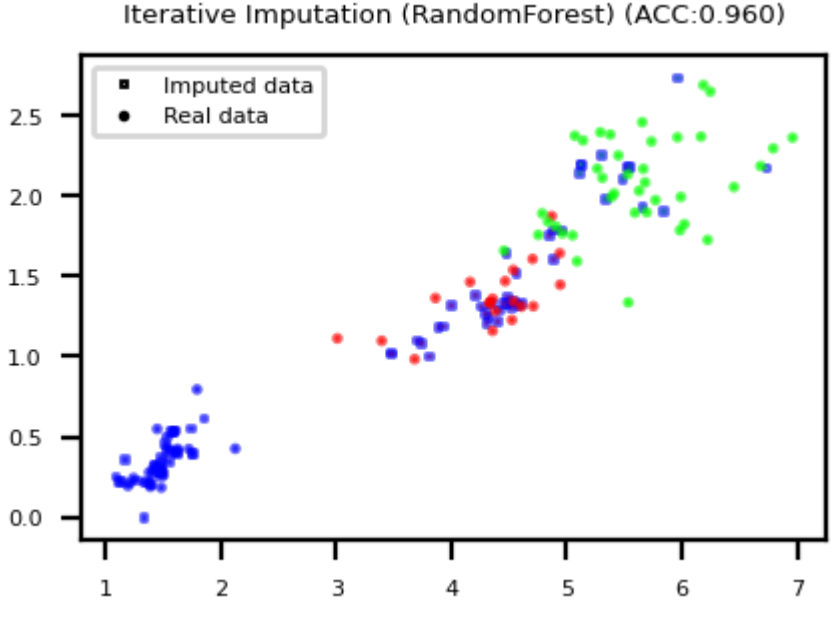
Soft-thresholded Singular Value Decomposition (SVD)

- Same basic idea, but smoother
    - Replace missing values by 0, compute SVD: $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\mathbf{T}}$
        - Solved with gradient descent
    - Reduce eigenvalues by shrinkage factor: $\lambda_i = s \cdot \lambda_i$
    - Recompute $\mathbf{X}$: now complete
    - Repeat for m iterations



Comparison

- Best method depends on the problem and dataset at hand. Use cross-validation.
- Iterative Imputation (MICE) generally works well for missing (completely) at random data
    - Can be slow if the prediction model is slow
- Low-rank approximation techniques scale well to large datasets



In practice (scikit-learn)

- Simple replacement: `SimpleImputer`
  - Strategies: `mean` (numeric), `median`, `most_frequent` (categorical)
  - Choose whether to add indicator columns, and how missing values are encoded

```
imp = SimpleImputer(strategy='mean', missing_values=np.nan,
add_indicator=False)
X_complete = imp.fit_transform(X_train)
```

- kNN Imputation: `KNNImputer`

```
imp = KNNImputer(n_neighbors=5)
X_complete = imp.fit_transform(X_train)
```

- Multiple Imputation (MICE): `IterativeImputer`
  - Choose estimator (default: `BayesianRidge`) and number of iterations (default 10)

```
imp = IterativeImputer(estimator=RandomForestClassifier(),
max_iter=10)
X_complete = imp.fit_transform(X_train)
```

In practice (fancyimpute)

- Cannot be used in CV pipelines (has `fit_transform` but no `transform`)
- Soft-Thresholded SVD: `SoftImpute`
    - Choose max number of gradient descent iterations
    - Choose shrinkage value for eigenvectors (default: $\frac{1}{N}$)

```
imp = SoftImpute(max_iter=10, shrinkage_value=None)
X_complete = imp.fit_transform(X)
```

- Low-rank imputation: `MatrixFactorization`
    - Choose rank of the low-rank approximation
    - Gradient descent hyperparameters: learning rate, epochs,...
    - Several variants exist

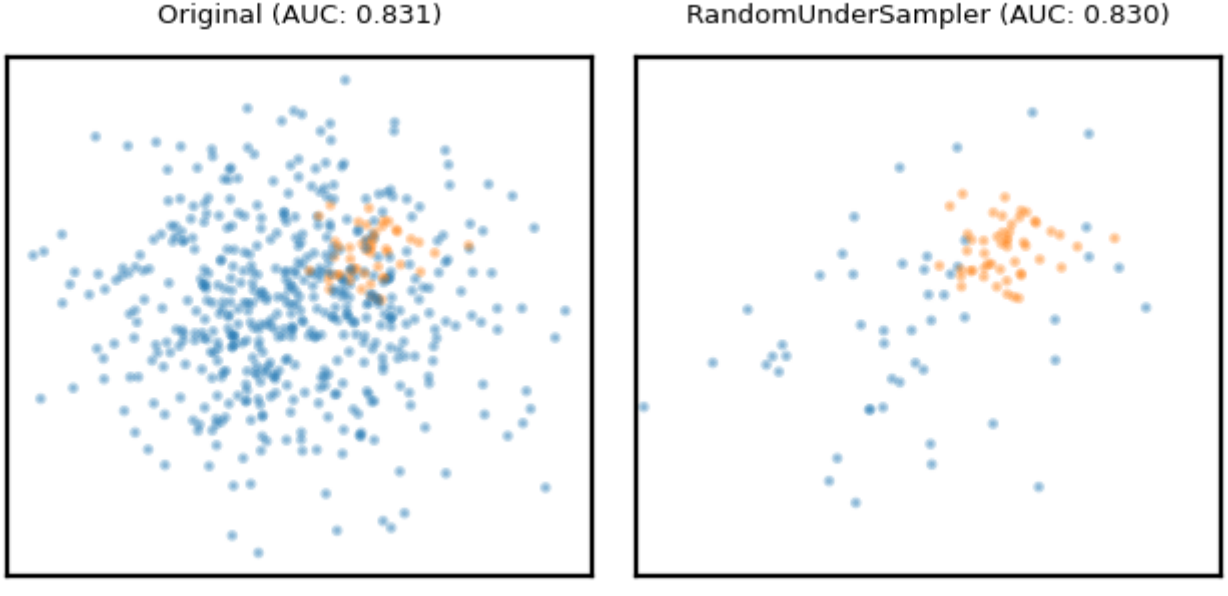
```
imp = MatrixFactorization(rank=10, learning_rate=0.001,
epochs=10000)
X_complete = imp.fit_transform(X)
```

Handling imbalanced data

- Problem:
    - You have a majority class with many times the number of examples as the minority class
    - Or: classes are balanced, but associated costs are not (e.g. FN are worse than FP)
- We already covered some ways to resolve this:
    - Add class weights to the loss function: give the minority class more weight
        - In practice: set `class_weight='balanced'`
    - Change the prediction threshold to minimize false negatives or false positives
- There are also things we can do by preprocessing the data
    - Resample the data to correct the imbalance
        - Random or model-based
    - Generate synthetic samples for the minority class
    - Build ensembles over different resampled datasets
    - Combinations of these

Random Undersampling

- Copy the points from the minority class
- Randomly sample from the majority class (with or without replacement) until balanced
    - Optionally, sample until a certain imbalance ratio (e.g. 1/5) is reached
    - Multi-class: repeat with every other class
- Preferred for large datasets, often yields smaller/faster models with similar performance

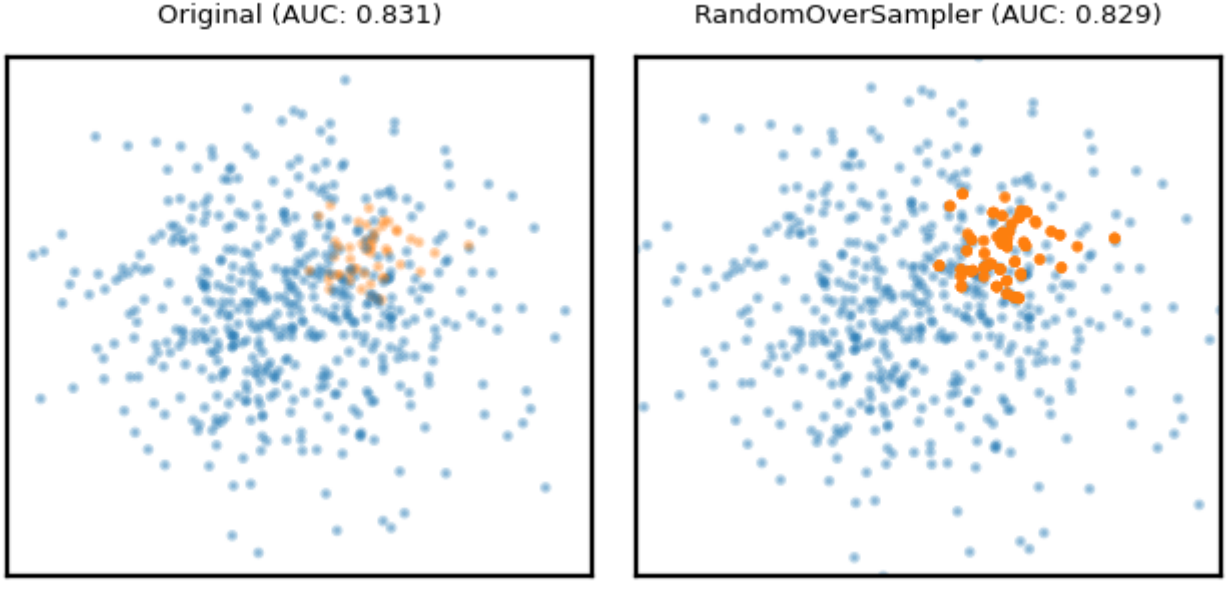


Model-based Undersampling

- Edited Nearest Neighbors
    - Remove all majority samples that are misclassified by kNN (mode) or that have a neighbor from the other class (all).
    - Remove their influence on the minority samples
- Condensed Nearest Neighbors
    - Remove all majority samples that are *not* misclassified by kNN
    - Focus on only the hard samples

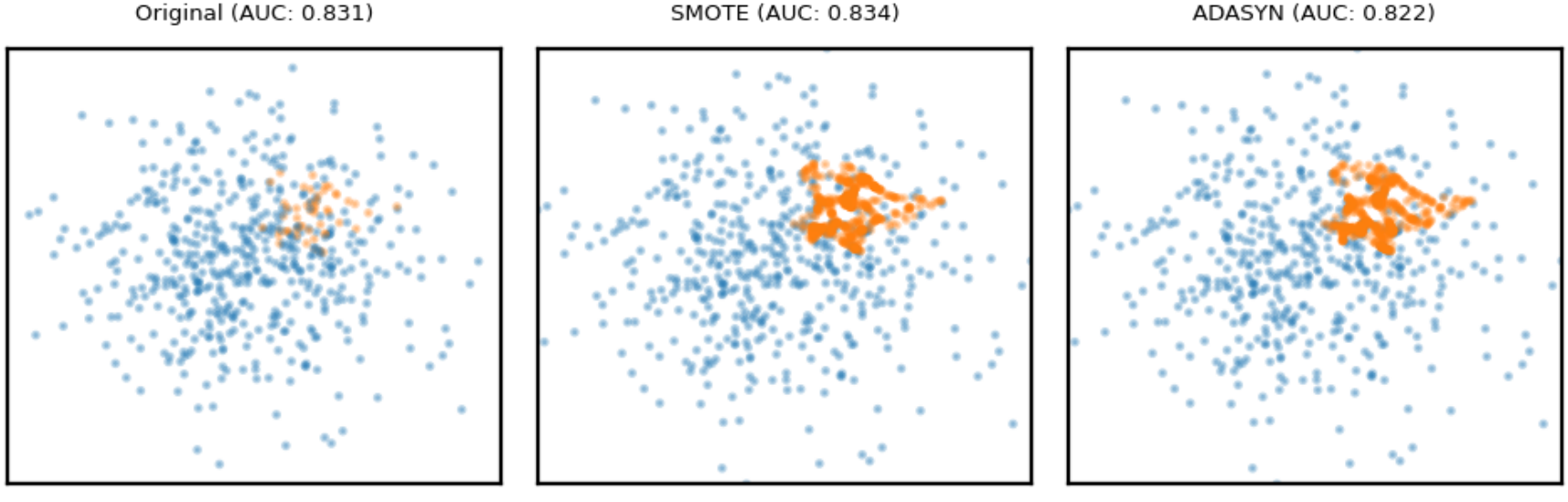
Random Oversampling

- Copy the points from the majority class
- Randomly sample from the minority class, with replacement, until balanced
    - Optionally, sample until a certain imbalance ratio (e.g. 1/5) is reached
- Makes models more expensive to train, doens't always improve performance
- Similar to giving minority class(es) a higher weight (and more expensive)



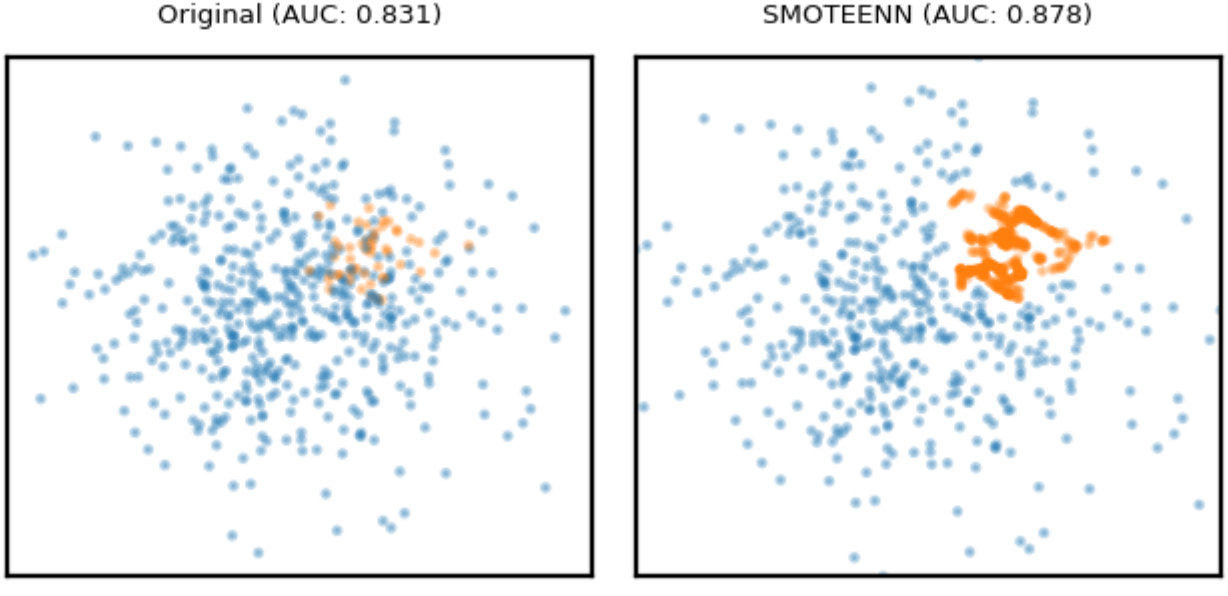
Synthetic Minority Oversampling Technique (SMOTE)

- Repeatedly choose a random minority point and a neighboring minority point
    - Pick a new, artificial point on the line between them (uniformly)
- May bias the data. Be careful never to create artificial points in the test set.
- ADASYN (Adaptive Synthetic)
    - Similar, but starts from 'hard' minority points (misclassified by kNN)



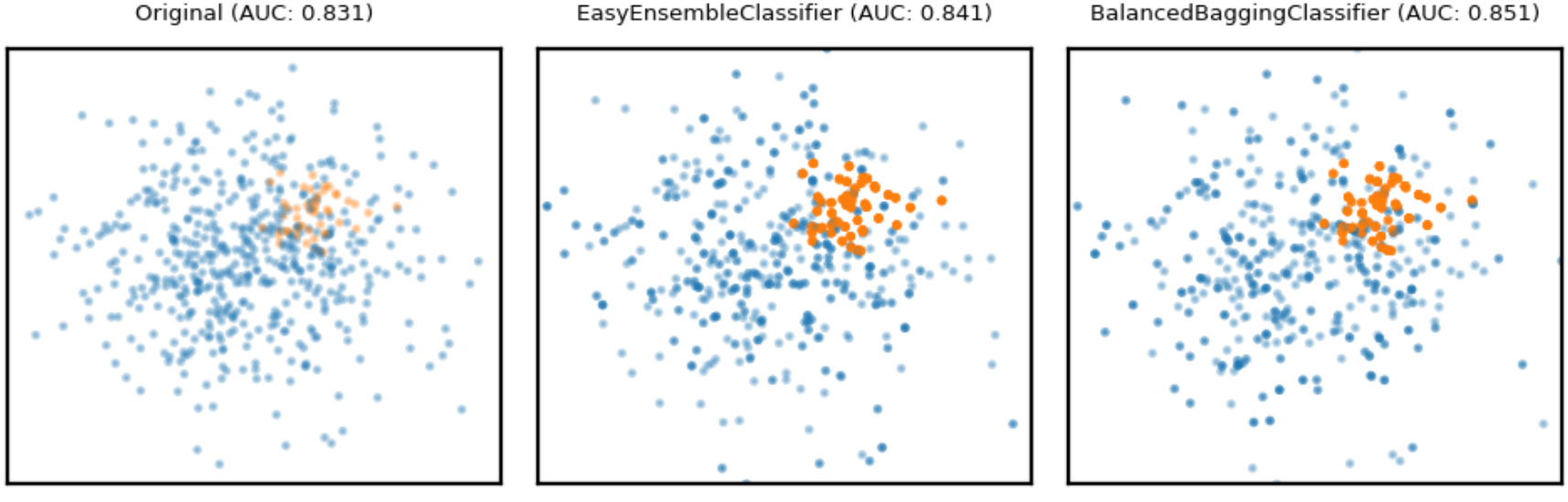
Combined techniques

- Combines over- and under-sampling
- E.g. oversampling with SMOTE, undersampling with Edited Nearest Neighbors (ENN)
    - SMOTE can generate 'noisy' point, close to majority class points
    - ENN will remove up these majority points to 'clean up' the space



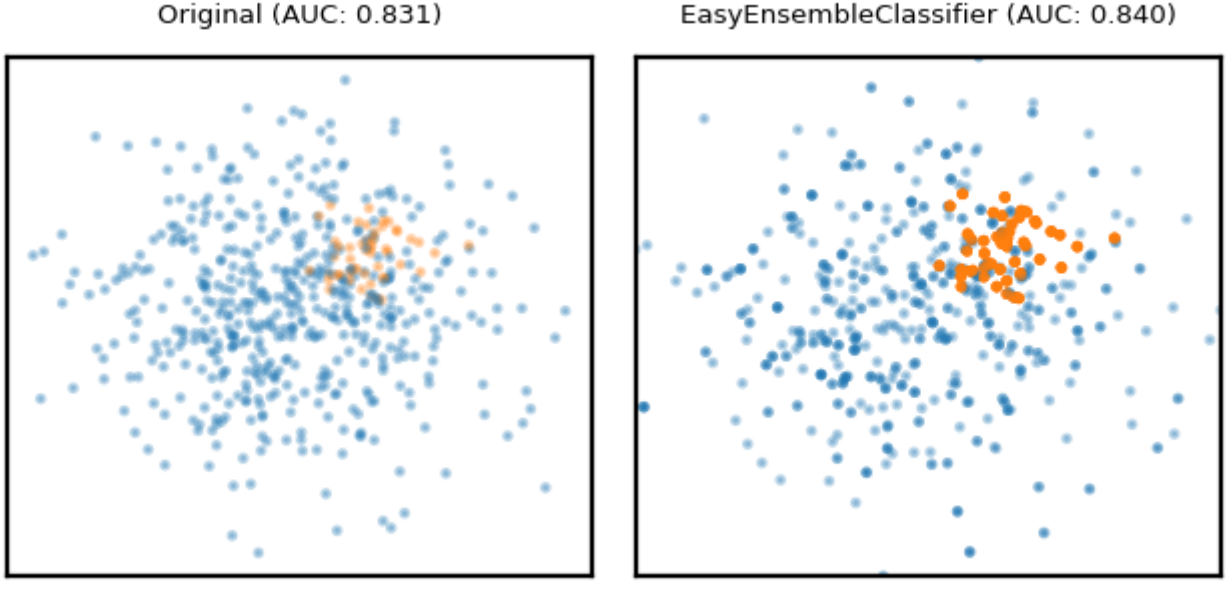
Ensemble Resampling

- Bagged ensemble of balanced base learners. Acts as a learner, not a preprocessor
- BalancedBagging: take bootstraps, randomly undersample each, train models (e.g. trees)
    - Benefits of random undersampling without throwing out so much data
- Easy Ensemble: take multiple random undersamplings directly, train models
    - Traditionally uses AdaBoost as base learner, but can be replaced



Comparison

- The best method depends on the data (amount of data, imbalance,...)
    - For a very large dataset, random undersampling may be fine
- You still need to choose the appropriate learning algorithms
- Don't forget about class weighting and prediction thresholding
    - Some combinations are useful, e.g. SMOTE + class weighting + thresholding



In practice (imblearn)

- Follows fit-sample paradigm (equivalent of fit-transform, but also affects y)
- Undersampling: RandomUnderSampler, EditedNearestNeighbours,...
- (Synthetic) Oversampling: RandomOverSampler, SMOTE, ADASYN,...
- Combinations: SMOTEENN,...

```
X_resampled, y_resampled = SMOTE(k_neighbors=5).fit_sample(X, y)
```

- Can be used in imblearn pipelines (not sklearn pipelines)
    - imblearn pipelines are compatible with GridSearchCV,...
    - Sampling is only done in `fit` (not in `predict`)

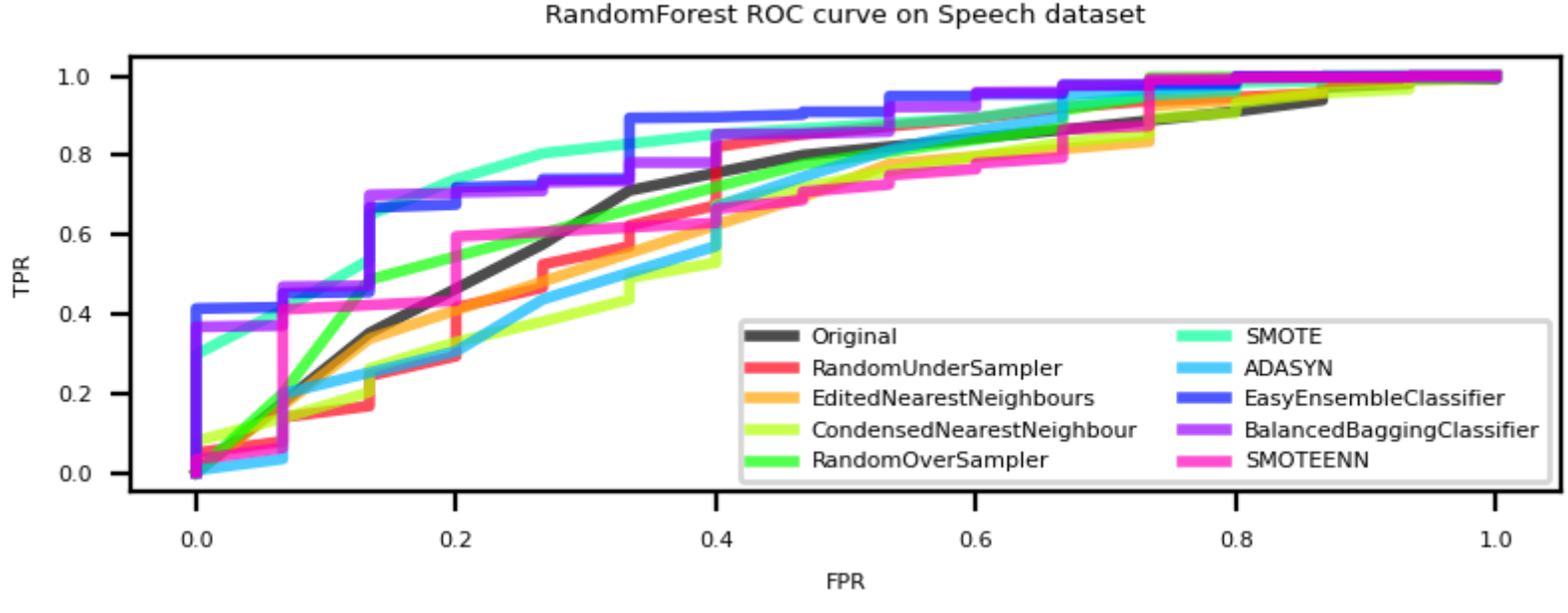
```
smote_pipe = make_pipeline(SMOTE(), LogisticRegression())
scores = cross_validate(smote_pipe, X_train, y_train)
param_grid = {"k_neighbors": [3,5,7]}
grid = GridSearchCV(smote_pipe, param_grid=param_grid, X, y)
```

- The ensembling techniques should be used as wrappers

```
clf = EasyEnsembleClassifier(base_estimator=SVC()).fit(X_train,
y_train)
```

Real-world data

- The effect of sampling procedures can be unpredictable
- Best method can depend on the data and FP/FN trade-offs
- SMOTE and ensembling techniques often work well



Summary

- Data preprocessing is a crucial part of machine learning
    - Scaling is important for many distance-based methods (e.g. kNN, SVM, Neural Nets)
    - Categorical encoding is necessary for numeric methods (or implementations)
    - Selecting features can speed up models and reduce overfitting
    - Feature engineering is often useful for linear models
    - It is often better to impute missing data than to remove data
    - Imbalanced datasets require extra care to build useful models
- Pipelines allow us to encapsulate multiple steps in a convenient way
    - Avoids data leakage, crucial for proper evaluation
- Choose the right preprocessing steps and models in your pipeline
    - Cross-validation helps, but the search space is huge
    - Smarter techniques exist to automate this process (AutoML)