Why do we care?

- Why should cost be symmetric?
- All data is imbalanced
- Detect rare events

Changing Thresholds

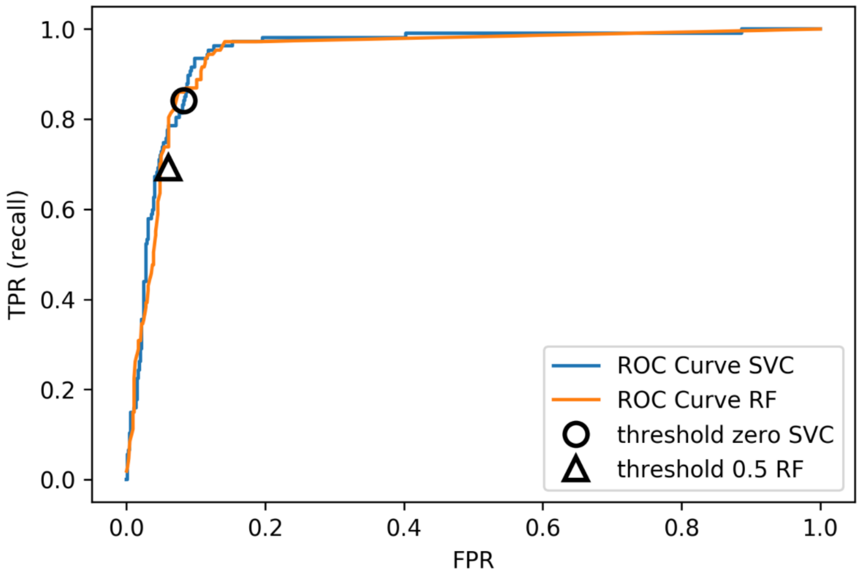
```
data = load_breast_cancer()

X_train, X_test, y_train, y_test = train_test_split(
    data.data, data.target, stratify=data.target, random_state=0)

lr = LogisticRegression().fit(X_train, y_train)
y_pred = lr.predict(X_test)

classification_report(y_test, y_pred)
```

```
          precision   recall  f1-score  support
0              0.91     0.92      0.92       53
1              0.96     0.94      0.95       90
avg/total      0.94     0.94      0.94      143
```

```
y_pred = lr.predict_proba(X_test)[:, 1] > .85

classification_report(y_test, y_pred)
```

```
          precision   recall  f1-score  support
0              0.84     1.00      0.91       53
1              1.00     0.89      0.94       90
avg/total      0.94     0.93      0.93      143
```

Roc Curve


1.0
0.8
0.6
0.4
0.2
0.0
TPR (recall)
0.0
0.2
0.4
0.6
0.8
1.0
FPR
ROC Curve SVC
ROC Curve RF
threshold zero SVC
threshold 0.5 RF

Remedies for the model

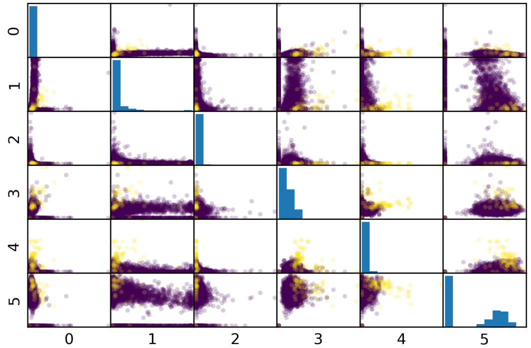
Mammography Data

```
import openml
# mammography dataset
# https://www.openml.org/d/310
data = openml.datasets.get_dataset(310)
X, y = data.get_data(target='class')
X.shape
```

(11183, 6)

```
np.bincount(y)
```

array([10923, 260])



Mammography Data

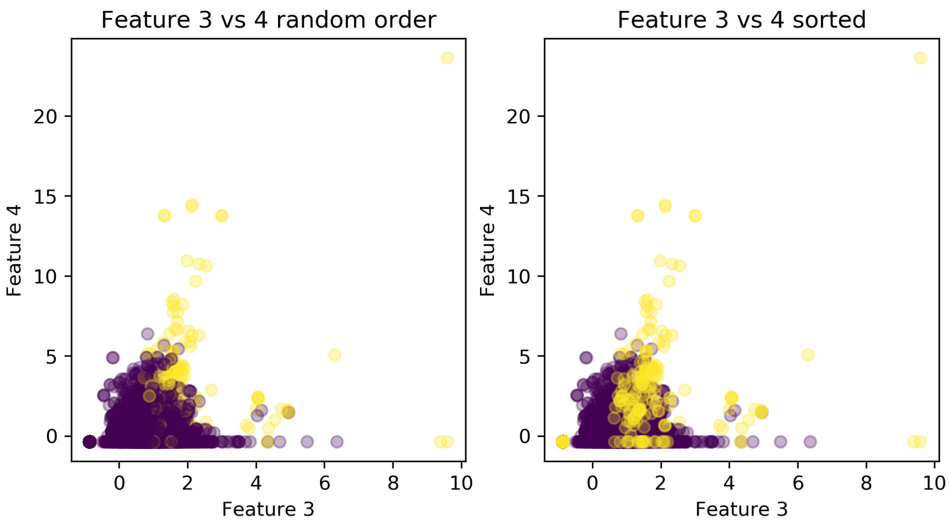
```
from sklearn.model_selection import cross_validate
from sklearn.linear_model import LogisticRegression

scores = cross_validate(LogisticRegression(),
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
```

0.920, 0.630

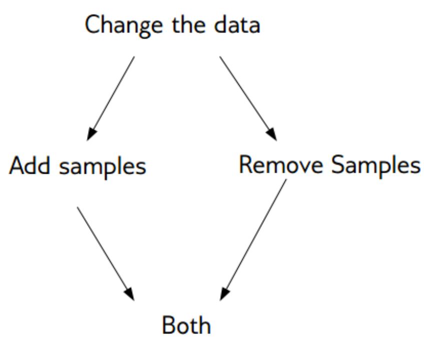
```
from sklearn.ensemble import RandomForestClassifier
scores = cross_validate(RandomForestClassifier(n_estimators=100),
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
```

0.939, 0.722

Mammography Data

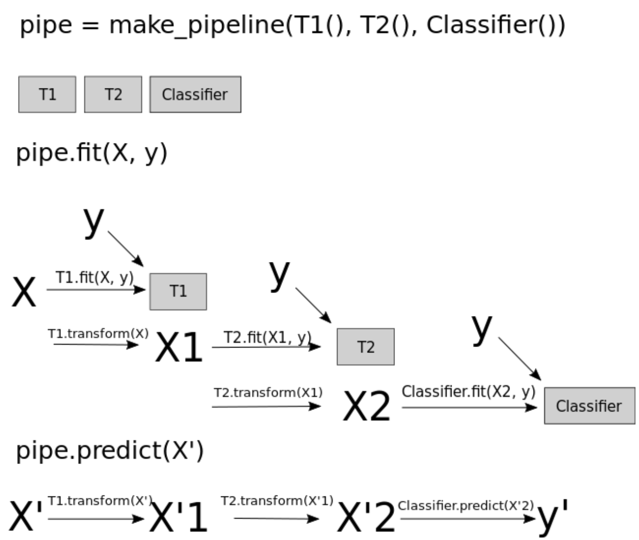


Basic Approaches



Change the training procedure

Sckit-learn vs resampling



Imbalance-Learn

http://imbalanced-learn.org

```
pip install -U imbalanced-learn
```

Extends `sklearn` API

Sampler

To resample a data sets, each sampler implements:

```
data_resampled, targets_resampled = obj.sample(data, targets)
```

Fitting and sampling can also be done in one step:

```
data_resampled, targets_resampled = obj.fit_sample(data, targets)
```

Sampler

To resample a data sets, each sampler implements:

```
data_resampled, targets_resampled = obj.sample(data, targets)
```

Fitting and sampling can also be done in one step:

```
data_resampled, targets_resampled = obj.fit_sample(data, targets)
```

In Pipelines: Sampling only done in `fit`!

Random Undersampling

```
from imblearn.under_sampling import RandomUnderSampler
rus = RandomUnderSampler(replacement=False)
X_train_subsample, y_train_subsample = rus.fit_sample(
    X_train, y_train)
print(X_train.shape)
print(X_train_subsample.shape)
print(np.bincount(y_train_subsample))
```

```
(8387, 6)
(390, 6)
[195 195]
```

Random Undersampling

```
from imblearn.pipeline import make_pipeline as make_imb_pipeline

undersample_pipe = make_imb_pipeline(RandomUnderSampler(), LogisticRegressionCV())
scores = cross_validate(undersample_pipe,
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
# was 0.920, 0.630 without
```

```
0.927, 0.527
```

Random Undersampling

```
from imblearn.pipeline import make_pipeline as make_imb_pipeline

undersample_pipe = make_imb_pipeline(RandomUnderSampler(), LogisticRegressionCV())
scores = cross_validate(undersample_pipe,
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
# was 0.920, 0.630 without
```

```
0.927, 0.527
```

```
undersample_pipe_rf = make_imb_pipeline(RandomUnderSampler(),
                                        RandomForestClassifier())
scores = cross_validate(undersample_pipe_rf,
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
# was 0.939, 0.722 without
```

```
0.951, 0.629
```

Random Oversampling

```python
from imblearn.over_sampling import RandomOverSampler
ros = RandomOverSampler()
X_train_oversample, y_train_oversample = ros.fit_sample(
    X_train, y_train)
print(X_train.shape)
print(X_train_oversample.shape)
print(np.bincount(y_train_oversample))
```

```
(8387, 6)
(16384, 6)
[8192 8192]
```

Random Oversampling

```
oversample_pipe = make_imb_pipeline(RandomOverSampler(), LogisticRegression())
scores = cross_validate(oversample_pipe,
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
```

0.917, 0.585

Random Oversampling

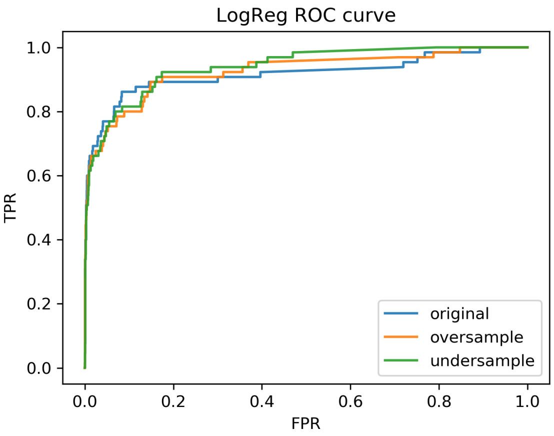
```
oversample_pipe = make_imb_pipeline(RandomOverSampler(), LogisticRegression())
scores = cross_validate(oversample_pipe,
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
```

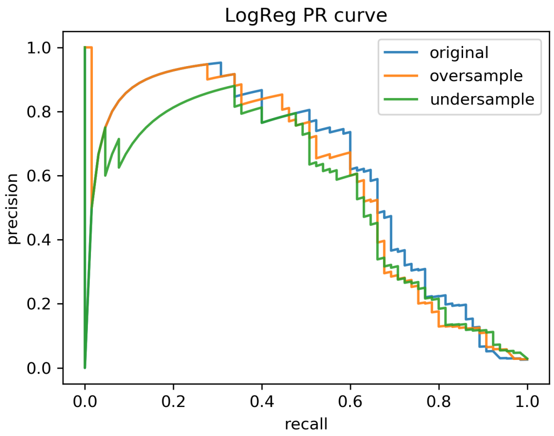
0.917, 0.585

```
oversample_pipe_rf = make_imb_pipeline(RandomOverSampler(),
                                       RandomForestClassifier())
scores = cross_validate(oversample_pipe_rf,
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
```

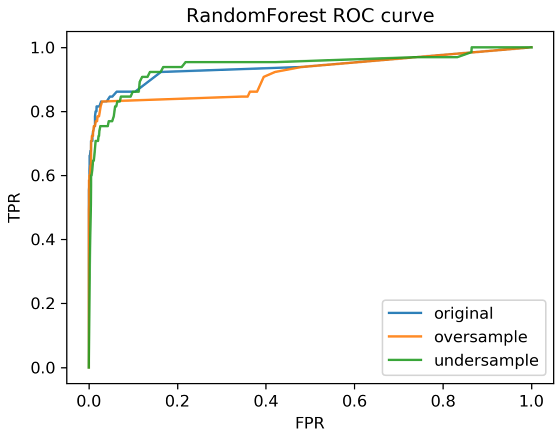
0.926, 0.715

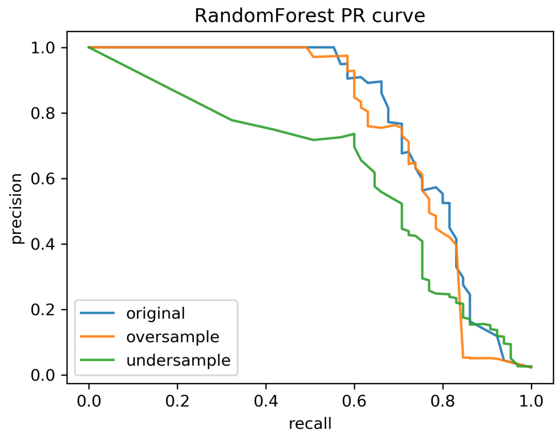
Curves for LogReg





Curves for Random Forest





ROC or PR?

FPR or Precision?

$$\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{FP} + \mathrm{TN}}$$

$$\mathrm{Precision} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

Class-weights

- Instead of repeating samples, re-weight the loss function.
- Works for most models!
- Same effect as over-sampling (though not random), but not as expensive (dataset size the same).

Class-weights in linear models

$$\min_{w \in \mathbb{R}^p} -C \sum_{i=1}^{n} \log(\exp(-y_i w^T \mathbf{x}_i) + 1) + ||w||_2^2$$

$$\min_{w \in \mathbb{R}^p} -C \sum_{i=1}^{n} c_{y_i} \log(\exp(-y_i w^T \mathbf{x}_i) + 1) + ||w||_2^2$$

Similar for linear and non-linear SVM

Class weights in trees

Gini Index:

$$H_{\text{gini}}(X_m) = \sum_{k \in \mathcal{Y}} p_{mk}(1 - p_{mk})$$

$$H_{\text{gini}}(X_m) = \sum_{k \in \mathcal{Y}} c_k p_{mk}(1 - p_{mk})$$

Prediction:

Weighted vote

Using Class-Weights

```
scores = cross_validate(LogisticRegression(class_weight='balanced'),
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
```

0.918, 0.587

```
scores = cross_validate(RandomForestClassifier(n_estimators=100, class_weight='bala
                        X_train, y_train, cv=10, scoring=('roc_auc', 'average_preci
scores['test_roc_auc'].mean(), scores['test_average_precision'].mean()
```

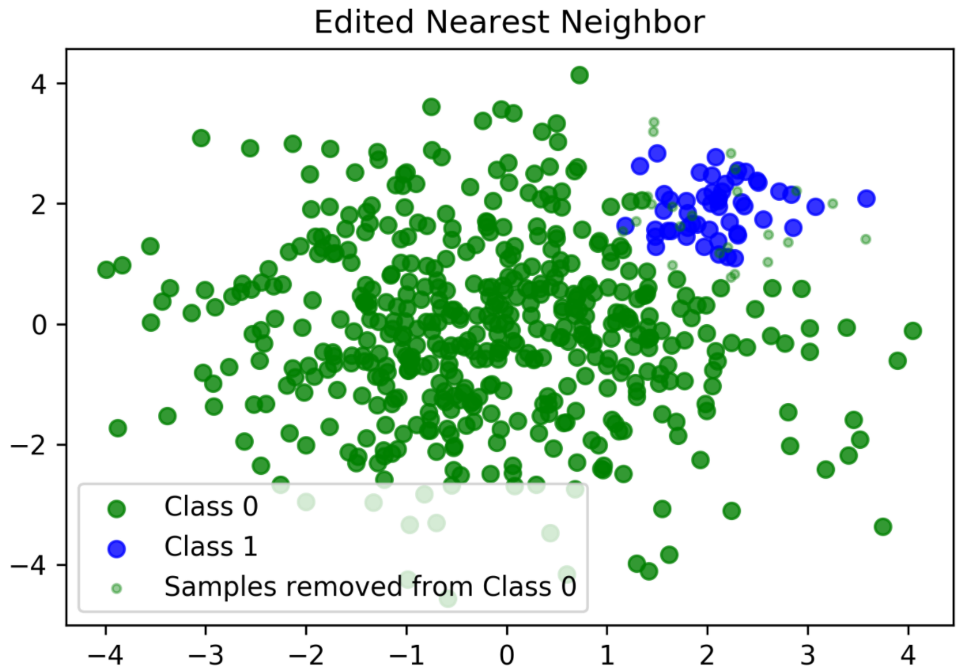
0.917, 0.701

Smart resampling

(based on nearest neighbour heuristics from the 70's)

Edited Nearest Neighbours

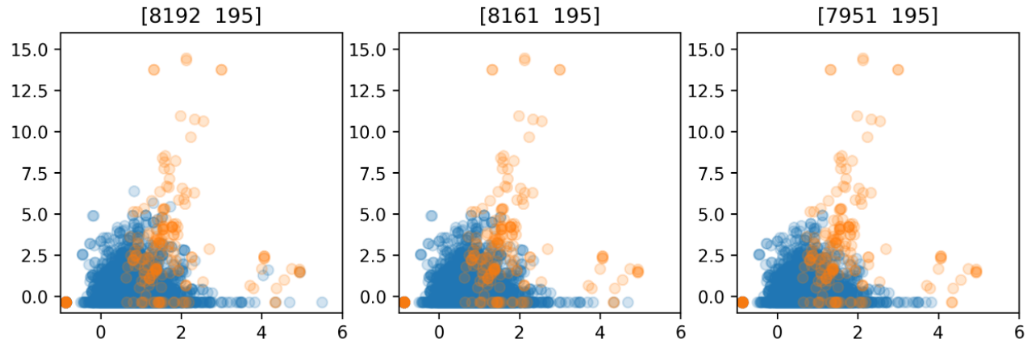
- Originally as heuristic for reducing dataset for KNN
- Remove all samples that are misclassified by KNN from training data (mode) or that have any point from other class as neighbor (all).
- “Cleans up” outliers and boundaries.



Edited Nearest Neighbor
4
2
0
−2
−4
−4
−3
−2
−1
0
1
2
3
4
Class 0
Class 1
Samples removed from Class 0

Edited Nearest Neighbours

```python
from imblearn.under_sampling import EditedNearestNeighbours
enn = EditedNearestNeighbours(n_neighbors=5)
X_train_enn, y_train_enn = enn.fit_sample(X_train, y_train)

enn_mode = EditedNearestNeighbours(kind_sel="mode", n_neighbors=5)
X_train_enn_mode, y_train_enn_mode = enn_mode.fit_sample(X_train, y_train)
```



```python
enn_pipe = make_imb_pipeline(EditedNearestNeighbours(n_neighbors=5),
                             LogisticRegression())
scores = cross_val_score(enn_pipe, X_train, y_train, cv=10, scoring='roc_auc')
np.mean(scores)
```

0.920

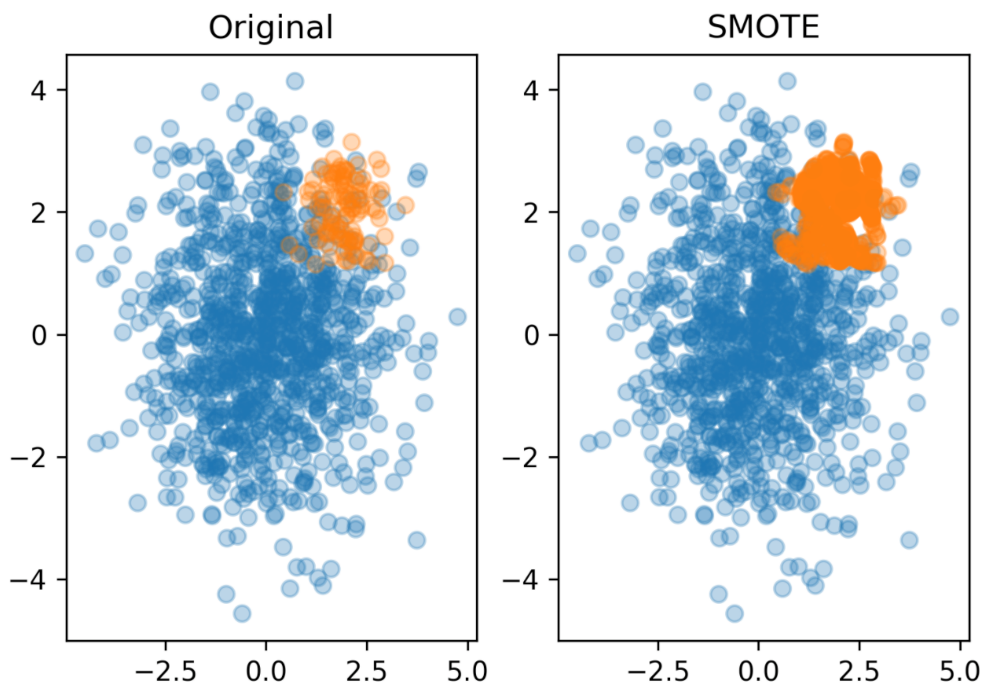
```python
enn_pipe_rf = make_imb_pipeline(EditedNearestNeighbours(n_neighbors= 5),
                                  RandomForestClassifier(n_estimators=100))
scores = cross_val_score(enn_pipe_rf, X_train, y_train, cv=10, scoring='roc_auc')
np.mean(scores)
```

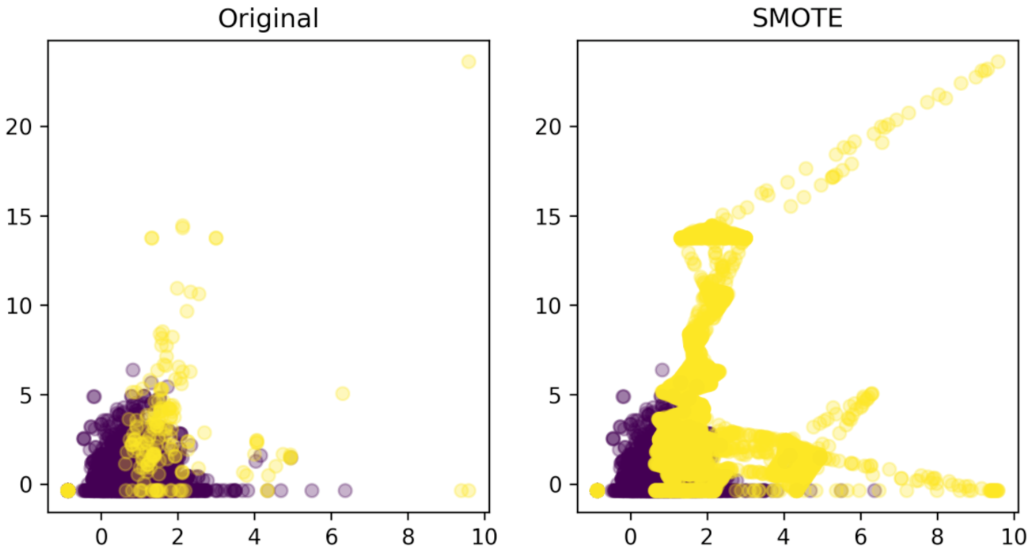
0.944

Synthetic Sample Generation

Synthetic Minority Oversampling Technique (SMOTE)

- Adds synthetic interpolated data to smaller class
- For each sample in minority class:
  - – Pick random neighbor from k neighbors.
  - – Pick point on line connecting the two uniformly
  - – Repeat.


Original
SMOTE
4
2
0
−2
−4
−2.5
0.0
2.5
5.0


Original
SMOTE
20
15
10
5
0
0
2
4
6
8
10

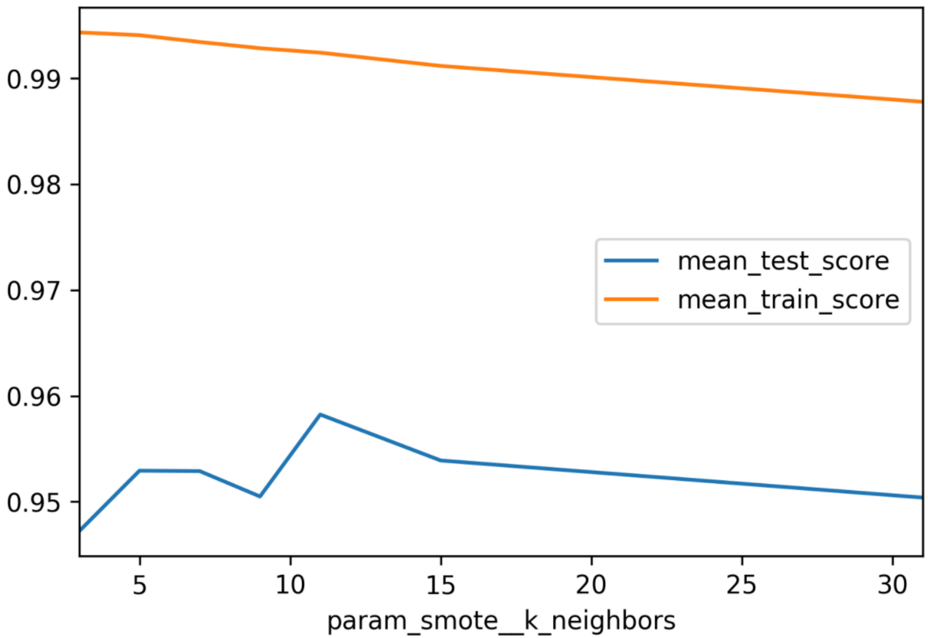
```
smote_pipe = make_imb_pipeline(SMOTE(), LogisticRegression())
scores = cross_val_score(smote_pipe, X_train, y_train, cv=10, scoring='roc_auc')
np.mean(scores)
```

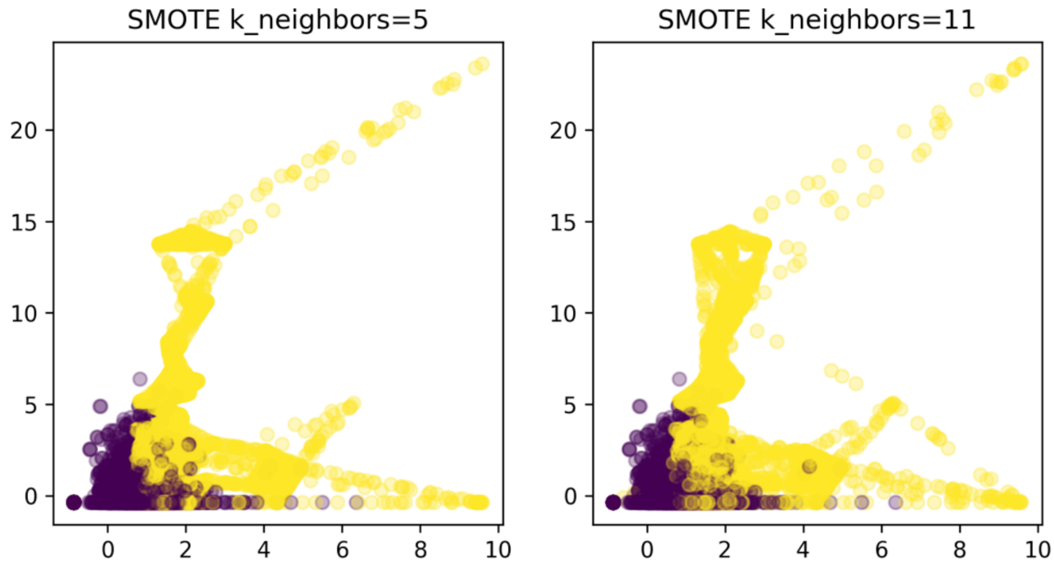
0.919

```
smote_pipe_rf = make_imb_pipeline(SMOTE(),RandomForestClassifier(n_estimators=100))
scores = cross_val_score(smote_pipe_rf,X_train,y_train, cv=10, scoring='roc_auc')
np.mean(scores)
```

0.947

```
param_grid = {'smote__k_neighbors': [3, 5, 7, 9, 11, 15, 31]}
search = GridSearchCV(smote_pipe_rf, param_grid, cv=10, scoring="roc_auc")
search.fit(X_train, y_train)
```


0.99
0.98
0.97
0.96
0.95
5
10
15
20
25
30
param_smote__k_neighbors
mean_test_score
mean_train_score


SMOTE k_neighbors=5
SMOTE k_neighbors=11
0
5
10
15
20
0
2
4
6
8
10

Summary

- Always check roc_auc, look at curve
- Undersampling is very fast and can help!
- Undersampling + Ensembles is very powerful!
- Many smart sampling strategies, mixed outcomes
- SMOTE allows adding new interpolated samples, works well in practice
- More advanced variants of SMOTE available