From workflows to pipelines

DESIGNING MACHINE LEARNING WORKFLOWS IN PYTHON

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Revisiting our workflow

```
from sklearn.ensemble import RandomForestClassifier as rf
X_train, X_test, y_train, y_test = train_test_split(X, y)
```

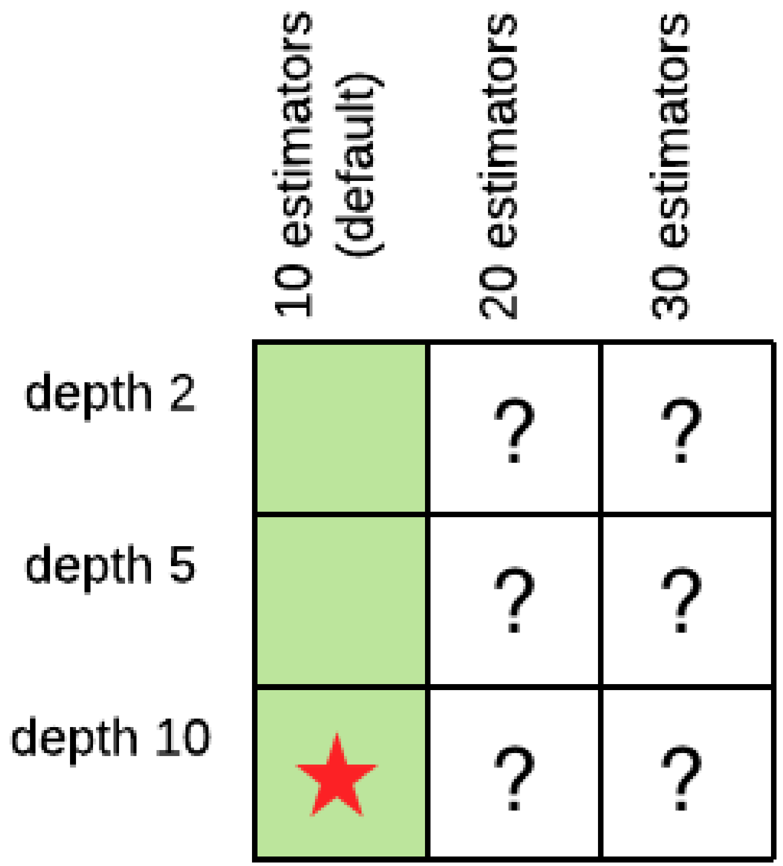
```
grid_search = GridSearchCV(rf(), param_grid={'max_depth': [2, 5, 10]})
grid_search.fit(X_train, y_train)
depth = grid_search.best_params_['max_depth']
```

```
vt = SelectKBest(f_classif, k=3).fit(X_train, y_train)
clf = rf(max_depth=best_value).fit(vt.transform(X_train), y_train)
accuracy_score(clf.predict(vt.transform(X_test), y_test))
```

The power of grid search

Optimize `max_depth` :

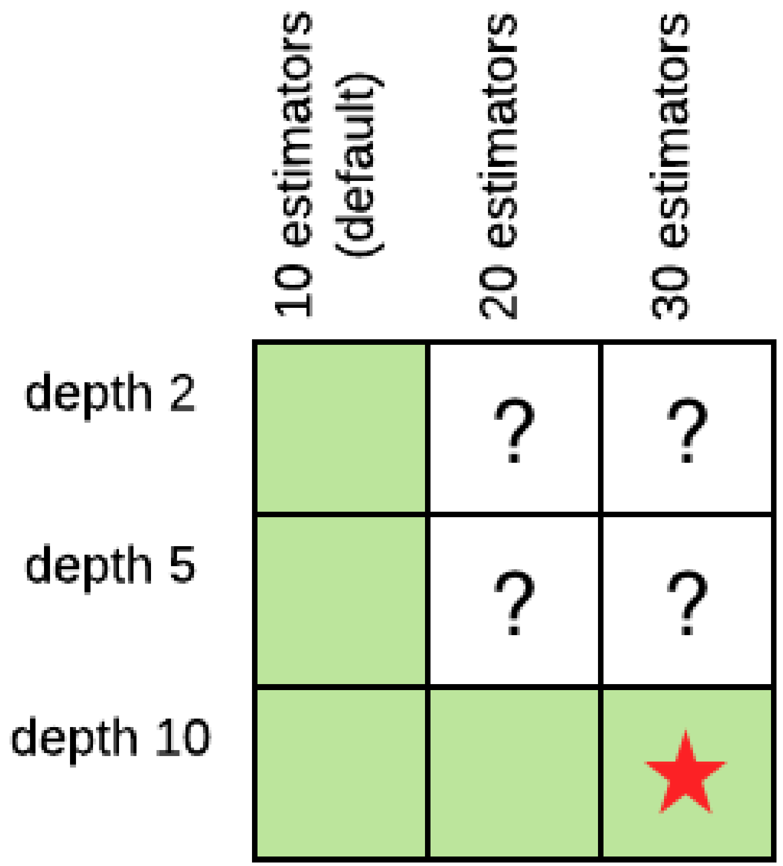
```
pg = {'max_depth': [2,5,10]}
gs = GridSearchCV(rf(),
   param_grid=pg)
gs.fit(X_train, y_train)
depth = gs.best_params_['max_depth']
```



The power of grid search

Then optimize `n_estimators` :

```
pg = {'n_estimators': [10,20,30]}
gs = GridSearchCV(
   rf(max_depth=depth),
   param_grid=pg)
gs.fit(X_train, y_train)
n_est = gs.best_params_[
    'n_estimators']
```

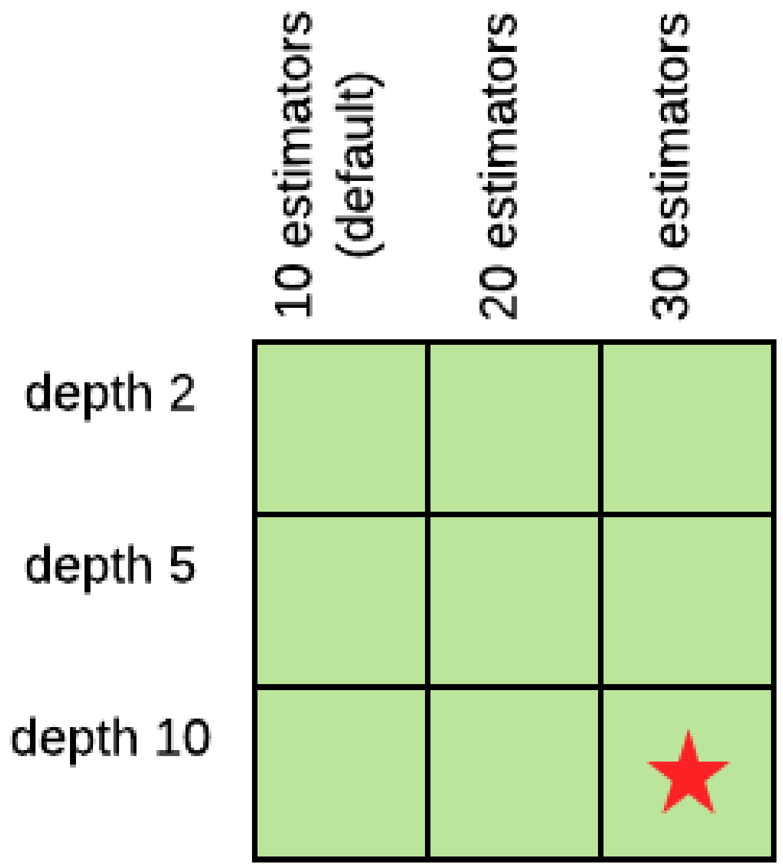


The power of grid search

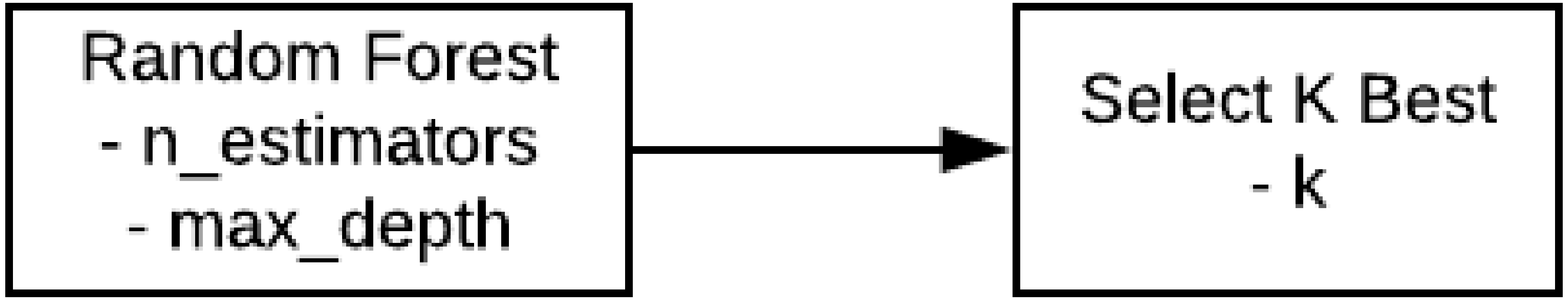
Jointly `max_depth` and `n_estimators` :

```
pg = {
    'max_depth': [2,5,10],
    'n_estimators': [10,20,30]
}
gs = GridSearchCV(rf(),
    param_grid=pg)
gs.fit(X_train, y_train)
print(gs.best_params_)
```

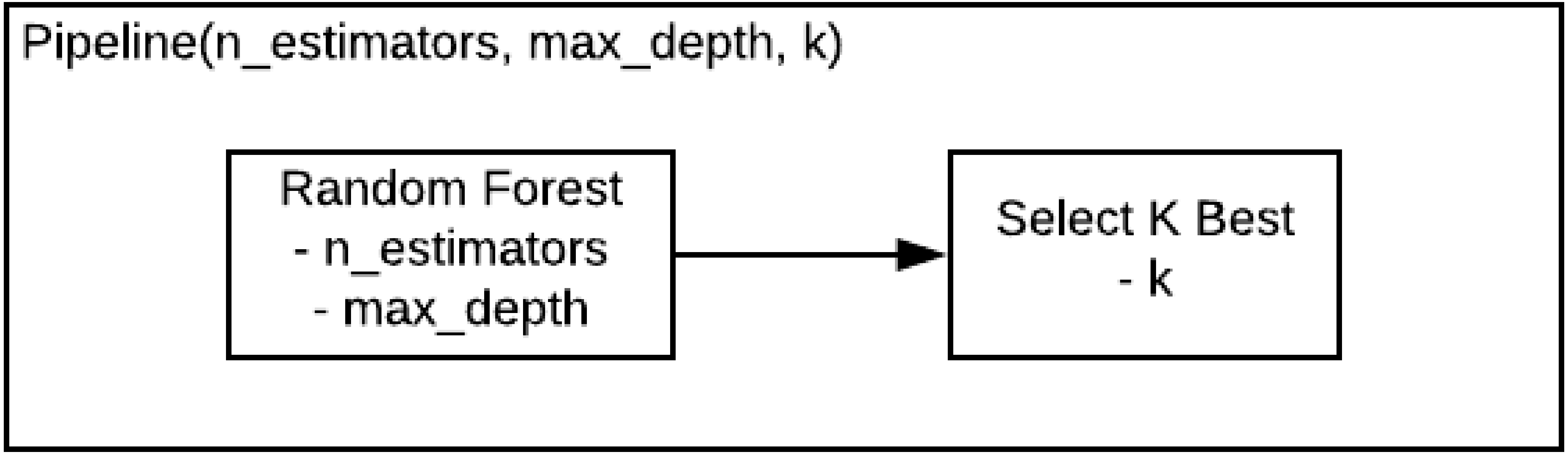
```
{'max_depth': 10, 'n_estimators': 20}
```



Pipelines



Pipelines



Pipeline(n_estimators, max_depth, k)
Random Forest
- n_estimators
- max_depth
Select K Best
- k

Pipelines

```
from sklearn.pipeline import Pipeline
pipe = Pipeline([
    ('feature_selection', SelectKBest(f_classif)),
    ('classifier', RandomForestClassifier())
])
params = dict(
    feature_selection__k=[2, 3, 4],
    classifier__max_depth=[5, 10, 20]
)
grid_search = GridSearchCV(pipe, param_grid=params)
gs = grid_search.fit(X_train, y_train).best_params_
```

```
{'classifier__max_depth': 20, 'feature_selection__k': 4}
```

Customizing your pipeline

```
from sklearn.metrics import roc_auc_score, make_scorer
auc_scorer = make_scorer(roc_auc_score)

grid_search = GridSearchCV(pipe, param_grid=params, scoring=auc_scorer)
```

Don't overdo it

```
params = dict(
    feature_selection__k=[2, 3, 4],
    clf__max_depth=[5, 10, 20],
    clf__n_estimators=[10, 20, 30]
)
grid_search = GridSearchCV(pipe, params, cv=10)
```

3 x 3 x 3 x 10 = 270 classifier fits!

Supercharged workflows

DESIGNING MACHINE LEARNING WORKFLOWS IN PYTHON

Model deployment

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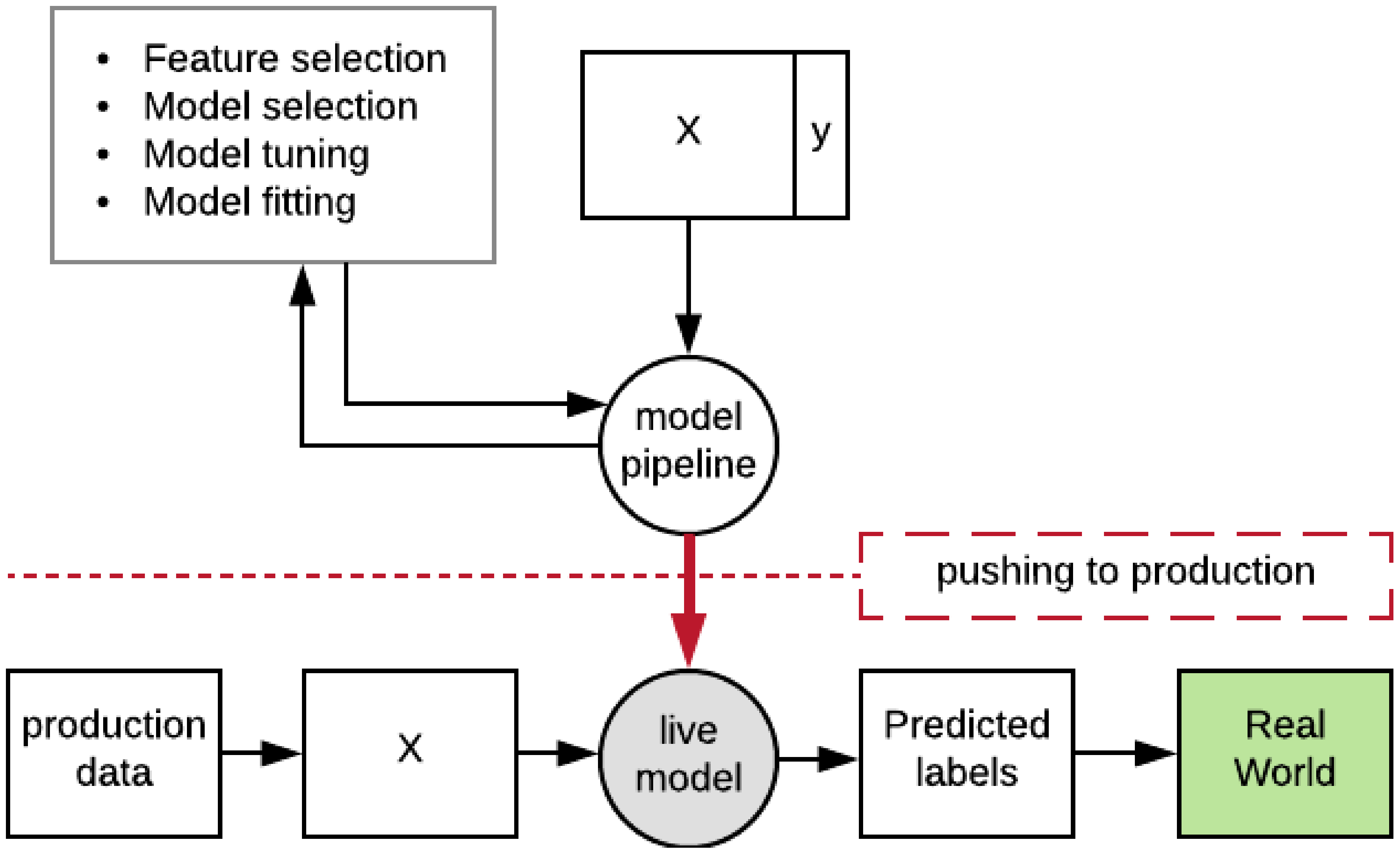

• Feature selection
• Model selection
• Model tuning
• Model fitting
X
y
model pipeline
pushing to production
production data
X
live model
Predicted labels
Real World

Serializing your model

Store a classifier to file:

```
import pickle
clf = RandomForestClassifier().fit(X_train, y_train)
with open('model.pkl', 'wb') as file:
    pickle.dump(clf, file=file)
```

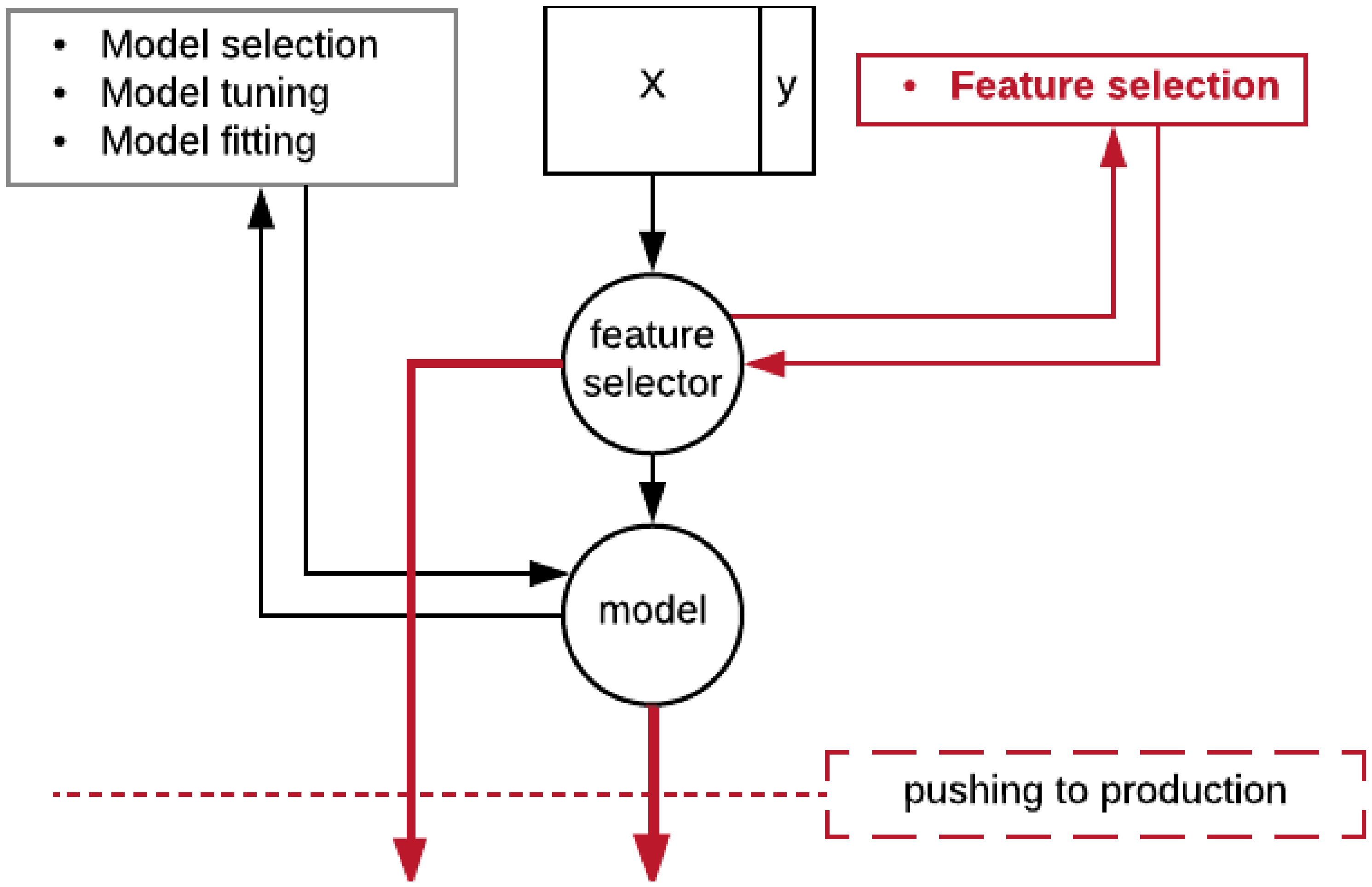
Load it again from file:

```
with open('model.pkl', 'rb') as file:
    clf2 = pickle.load(file)
```

Serializing your pipeline

Development environment:

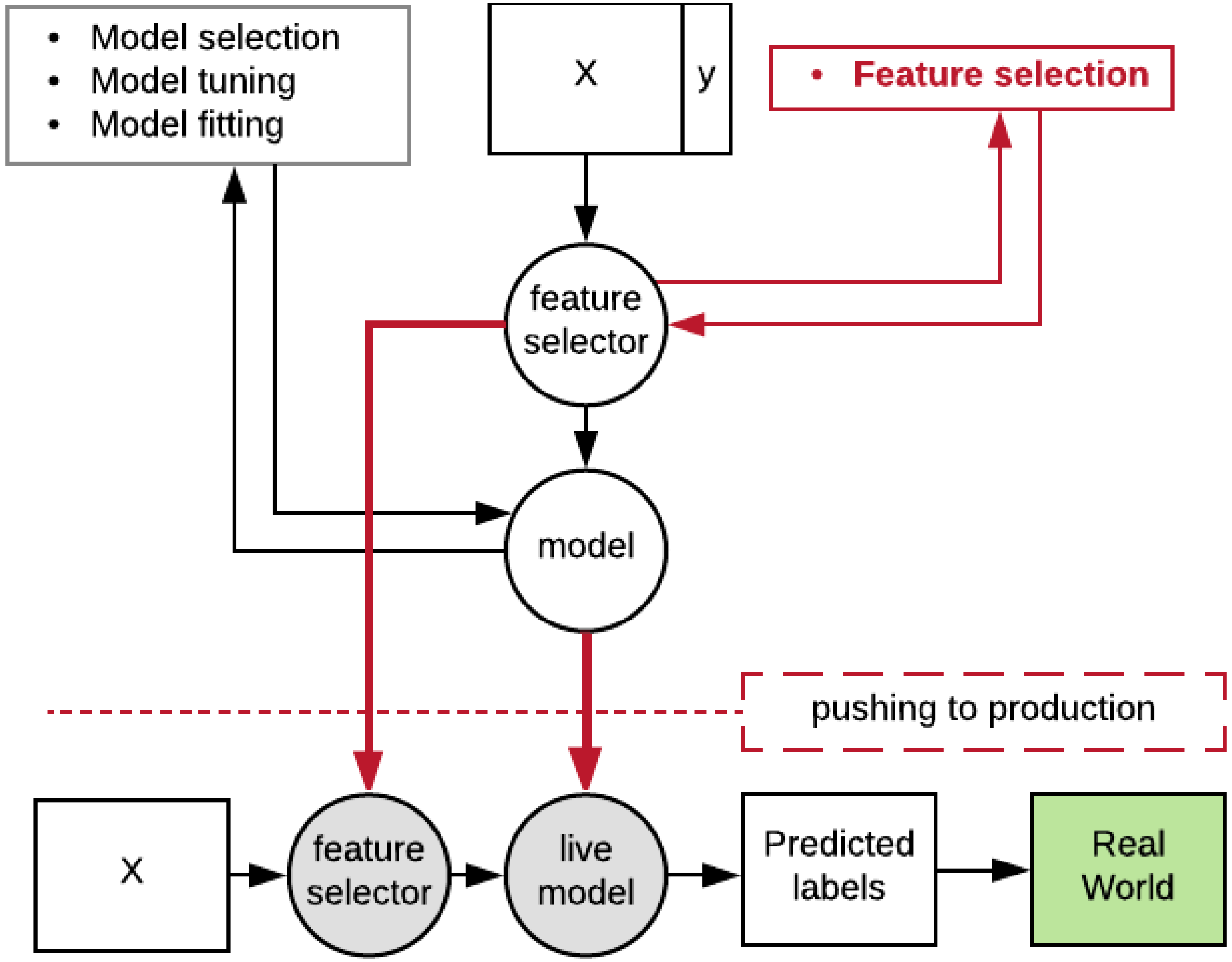
```
vt = SelectKBest(f_classif).fit(
    X_train, y_train)
clf = RandomForestClassifier().fit(
    vt.transform(X_train), y_train)
with open('vt.pkl', 'wb') as file:
     pickle.dump(vt)
with open('clf.pkl', 'wb') as file:
     pickle.dump(clf)
```



Serializing your pipeline

Production environment:

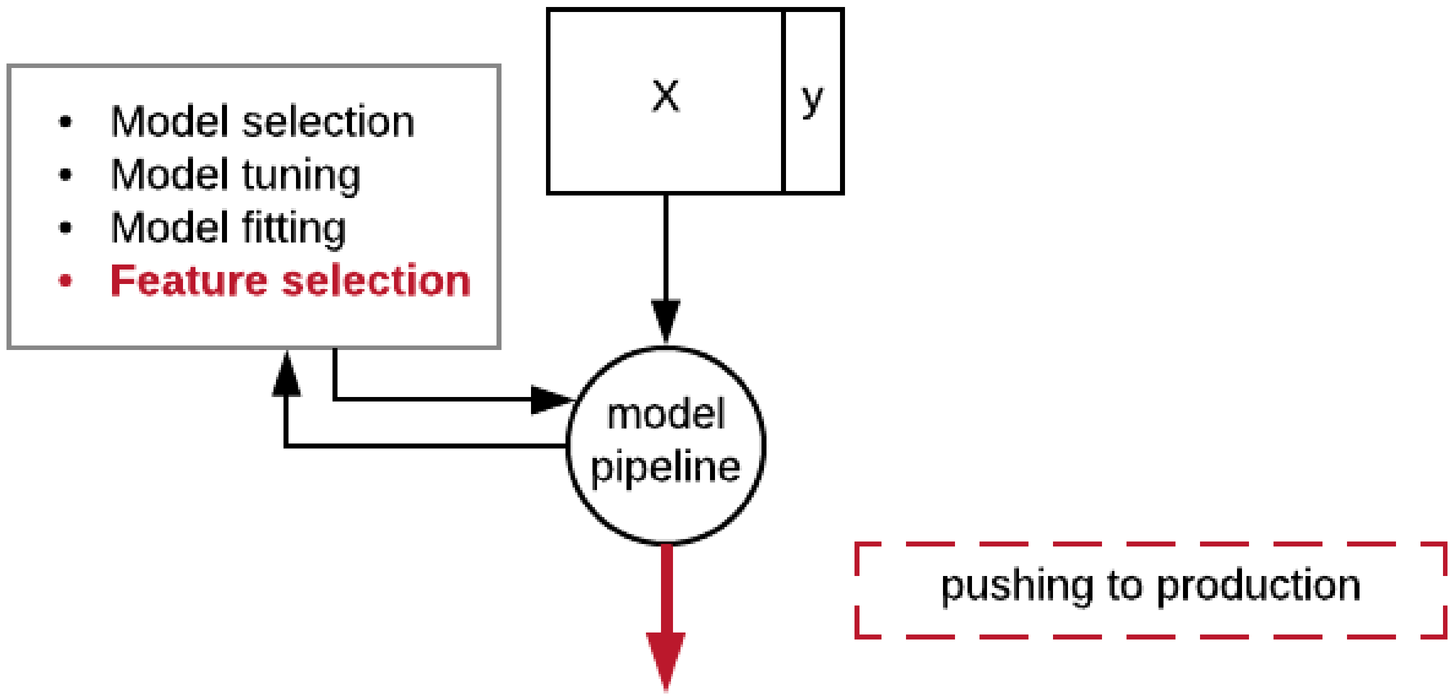
```
with open('vt.pkl', 'rb') as file:
    vt = pickle.load(vt)
with open('clf.pkl', 'rb') as file:
    clf = pickle.load(clf)
clf.predict(vt.transform(X_new))
```



Serializing your pipeline

Development environment:

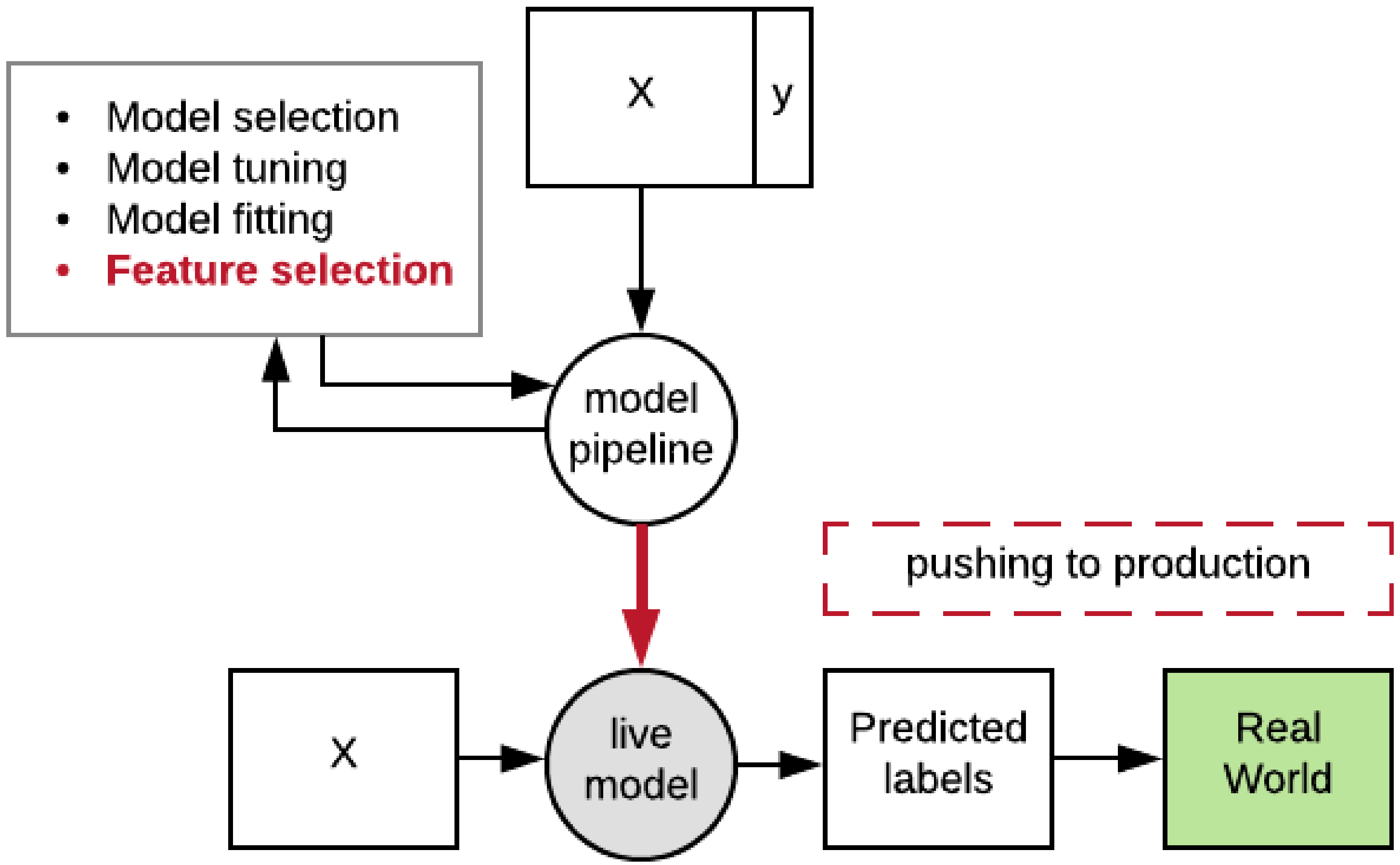
```
pipe = Pipeline([
    ('fs', SelectKBest(f_classif)),
    ('clf', RandomForestClassifier())
])
params = dict(fs__k=[2, 3, 4],
    clf__max_depth=[5, 10, 20])
gs = GridSearchCV(pipe, params)
gs = gs.fit(X_train, y_train)

with open('pipe.pkl', 'wb') as file:
    pickle.dump(gs, file)
```



Serializing your pipeline

Production environment:

```
with open('pipe.pkl', 'rb') as file:
    gs = pickle.dump(gs, file)
gs.predict(X_test)
```



Custom feature transformations

```
   checking_status  duration       ...       own_telephone  foreign_worker
0                1         6       ...                   1               1
1                0        48       ...                   0               1
```

```python
def negate_second_column(X):
    Z = X.copy()
    Z[:,1] = -Z[:,1]
    return Z
```

```python
pipe = Pipeline([('ft', FunctionTransformer(negate_second_column)),
    ('clf', RandomForestClassifier())])
```

Production ready!

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Iterating without overfitting

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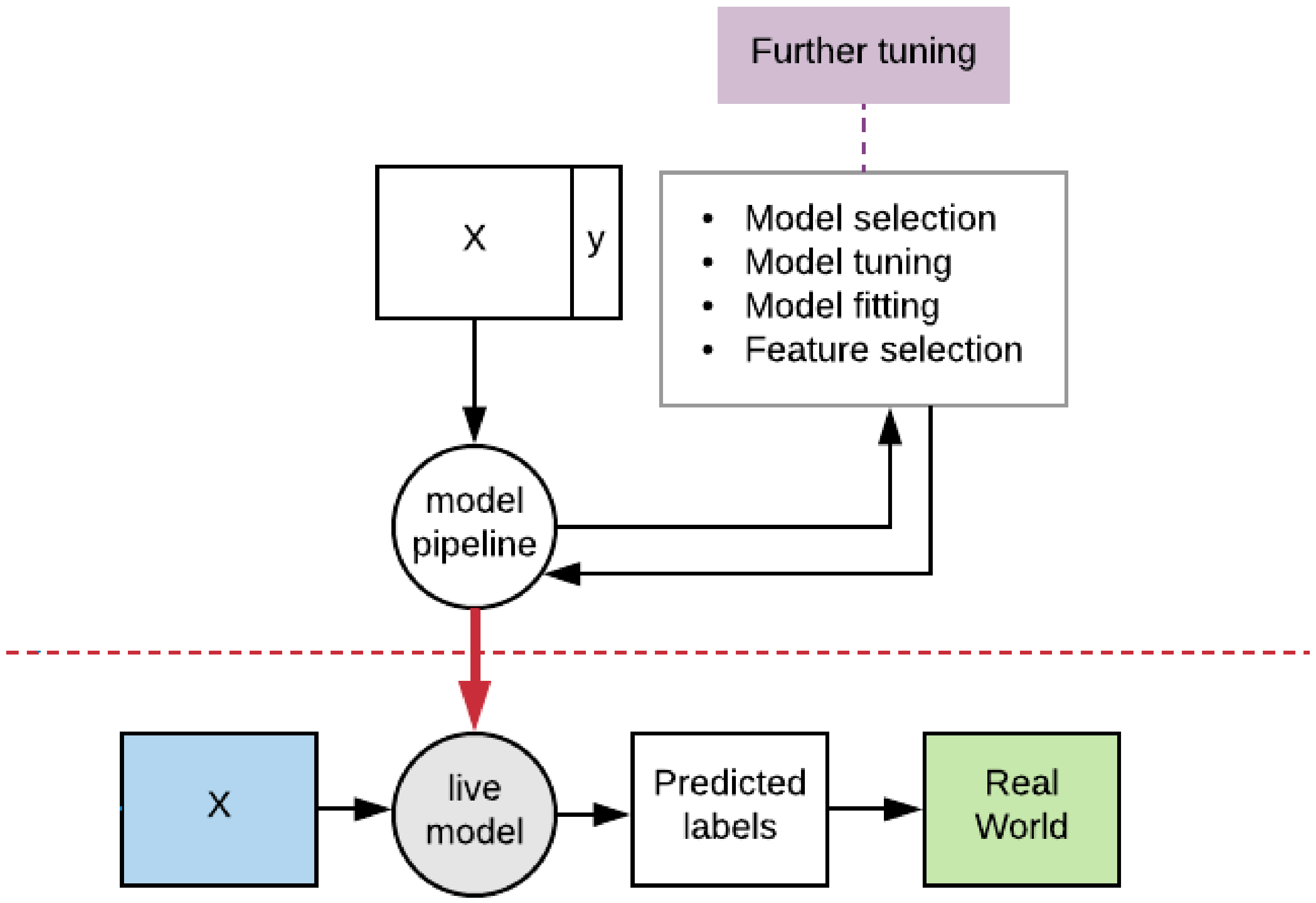
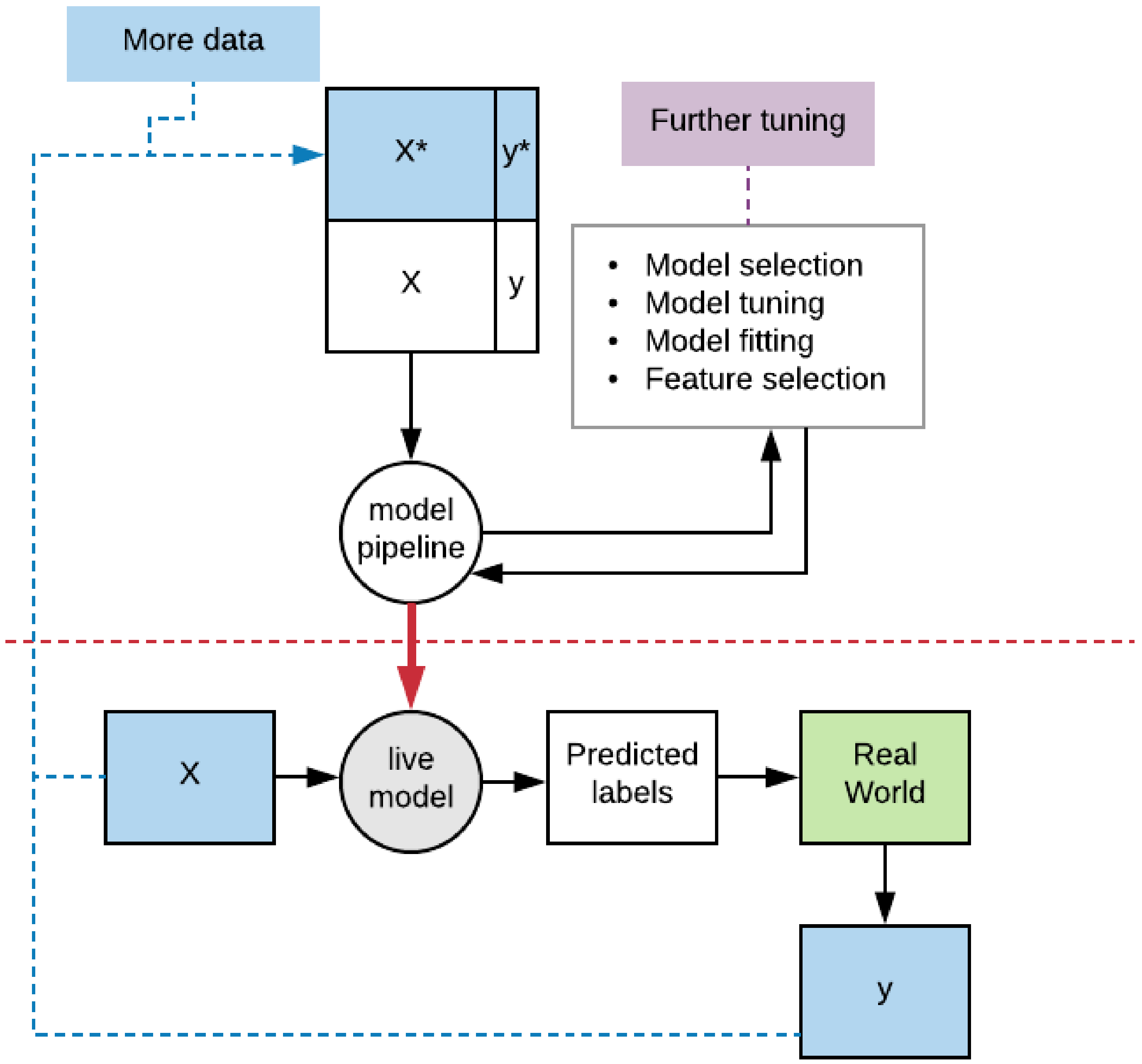
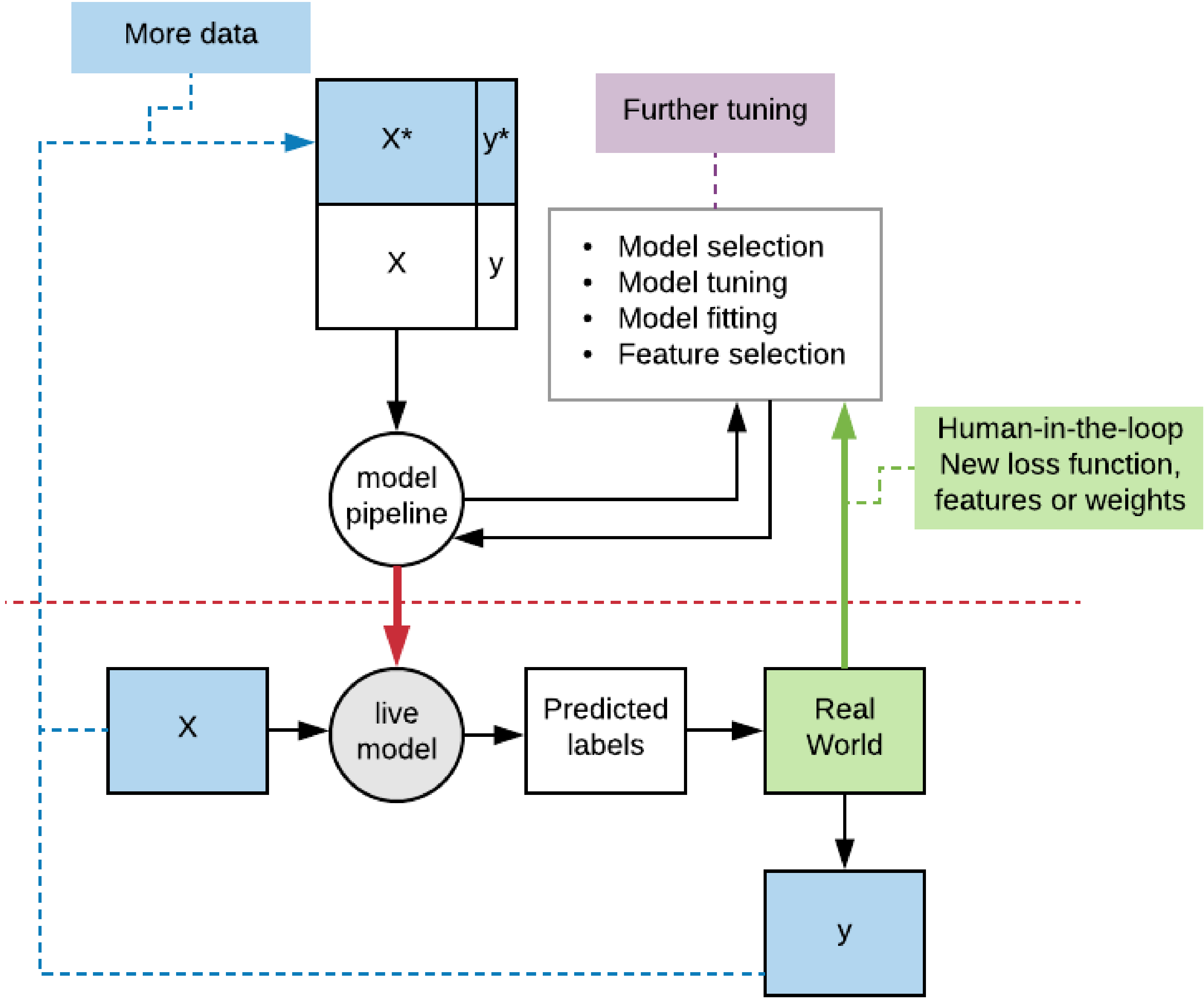
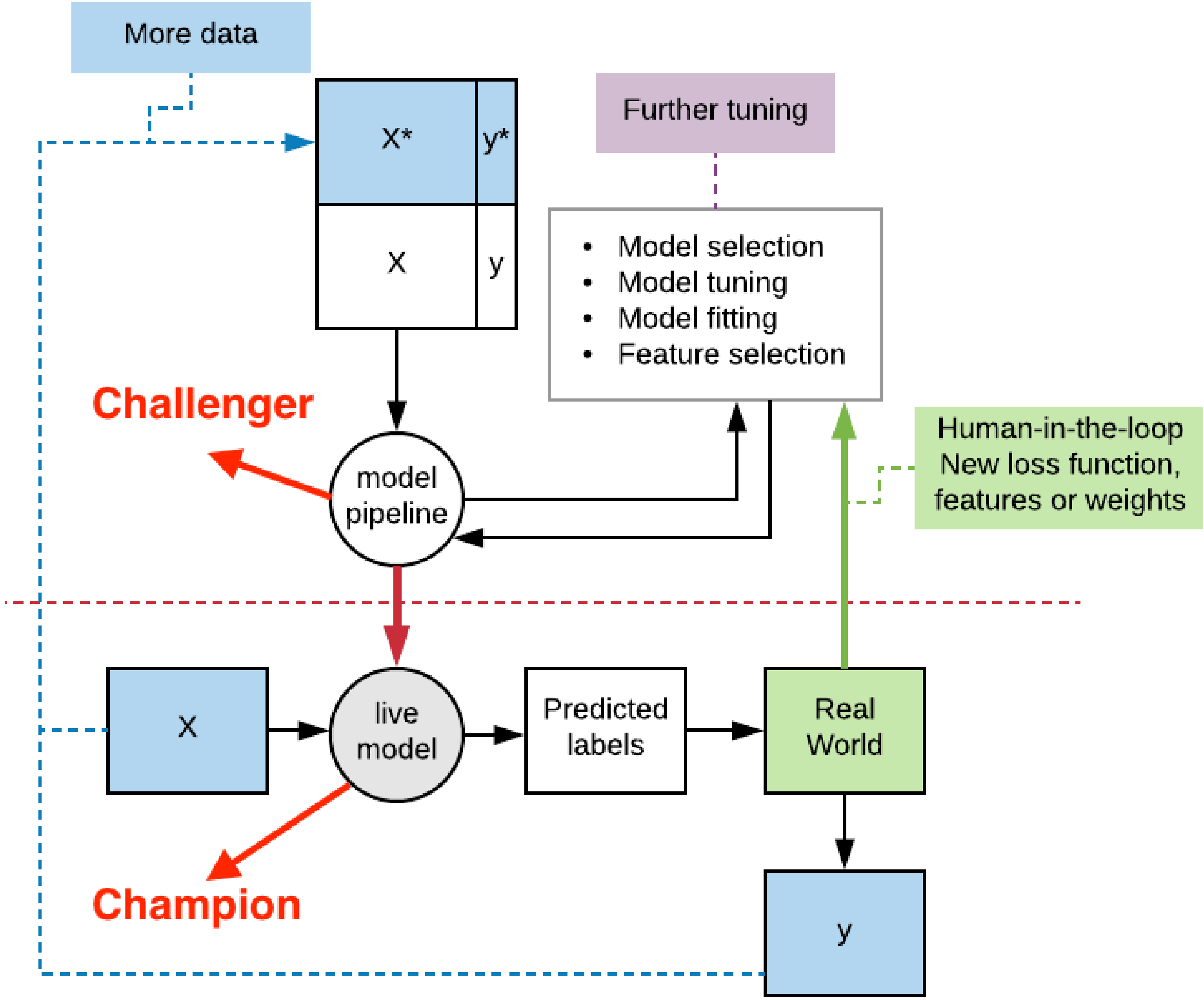

Further tuning
X
y
• Model selection
• Model tuning
• Model fitting
• Feature selection
model pipeline
X
live model
Predicted labels
Real World


More data
X*
y*
X
y
Further tuning
Model selection
Model tuning
Model fitting
Feature selection
model pipeline
X
live model
Predicted labels
Real World
y


More data
X*
y*
X
y
Further tuning
• Model selection
• Model tuning
• Model fitting
• Feature selection
Human-in-the-loop
New loss function,
features or weights
model
pipeline
X
live
model
Predicted
labels
Real
World
y


More data
X*
y*
X
y
Further tuning
Model selection
Model tuning
Model fitting
Feature selection
Challenger
model pipeline
Human-in-the-loop
New loss function,
features or weights
X
live model
Predicted labels
Real World
Champion
y

Cross-validation results

```
grid_search = GridSearchCV(pipe, params, cv=3, return_train_score=True)
gs = grid_search.fit(X_train, y_train)
results = pd.DataFrame(gs.cv_results_)
```

```
results[['mean_train_score', 'std_train_score',
   'mean_test_score', 'std_test_score']]
```

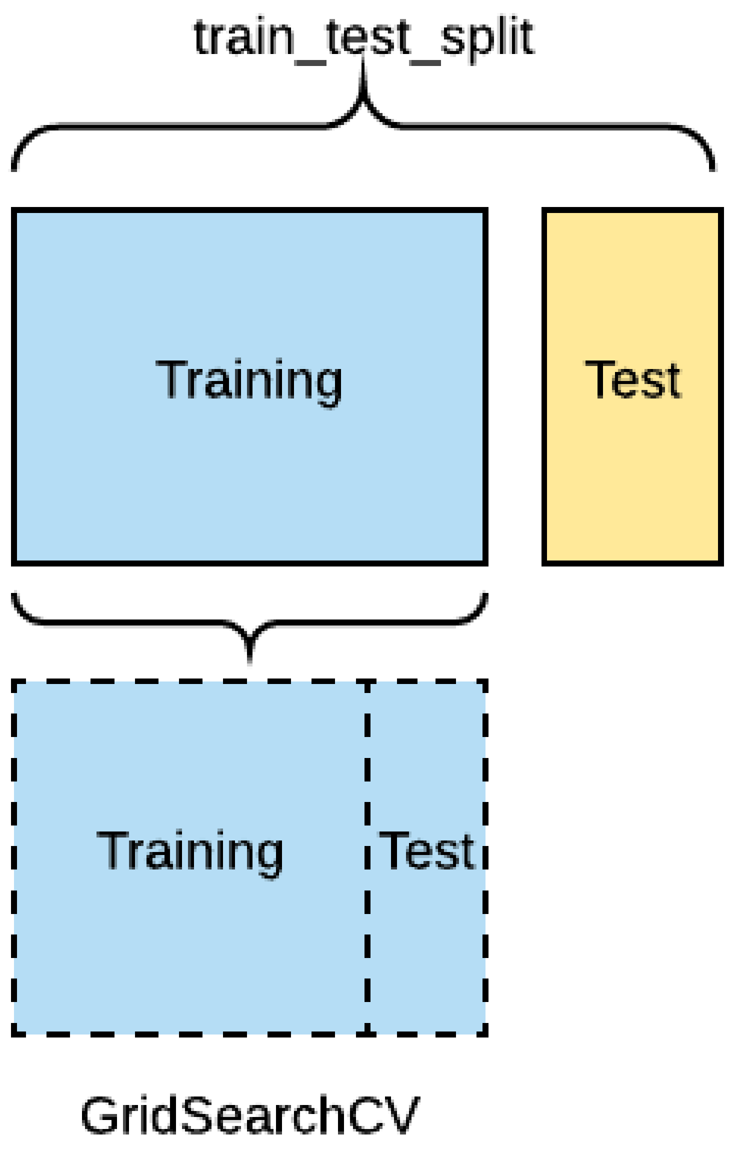
```
   mean_train_score  std_train_score  mean_test_score  std_test_score
0             0.829            0.006            0.735           0.009
1             0.829            0.006            0.725           0.009
2             0.961            0.008            0.716           0.019
3             0.981            0.005            0.749           0.024
...
```

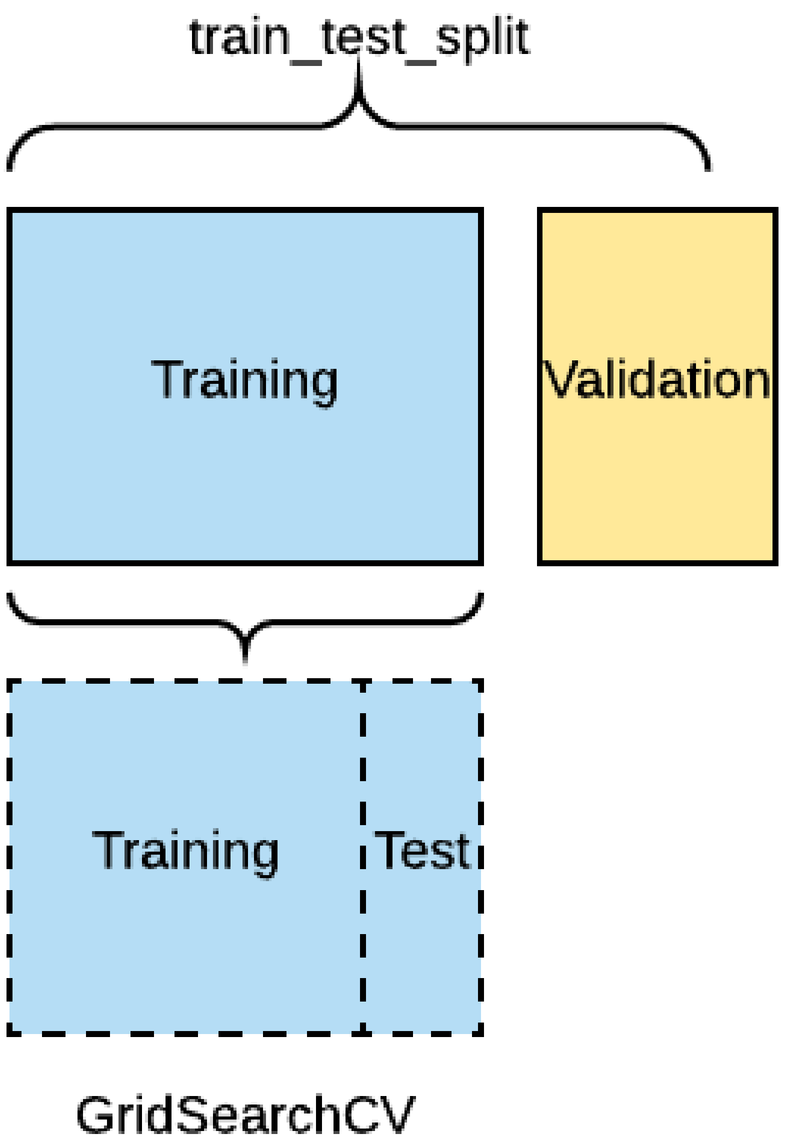
Cross-validation results

	mean_train_score	std_train_score	mean_test_score	std_test_score
0	0.829	0.006	0.735	0.009
1	0.829	0.006	0.725	0.009
2	0.961	0.008	0.716	0.019
3	0.981	0.005	0.749	0.024
4	0.986	0.003	0.728	0.009
5	0.995	0.002	0.751	0.008

Observations:

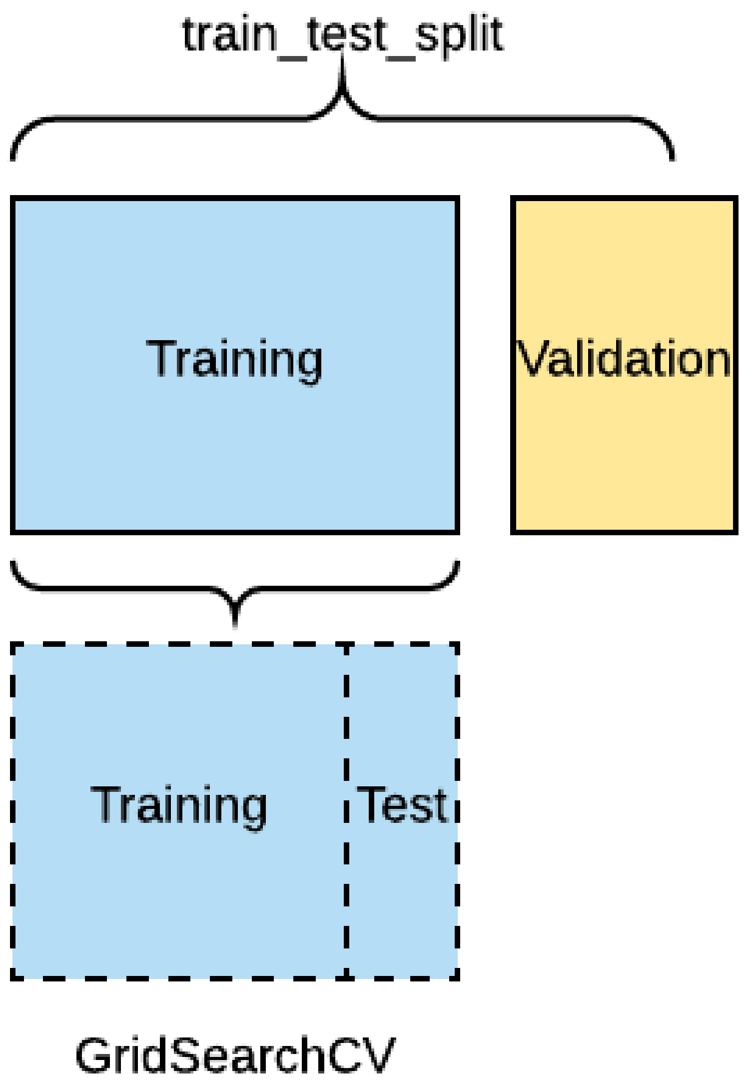
- Training score much higher than test score.
- The standard deviation of the test score is large.

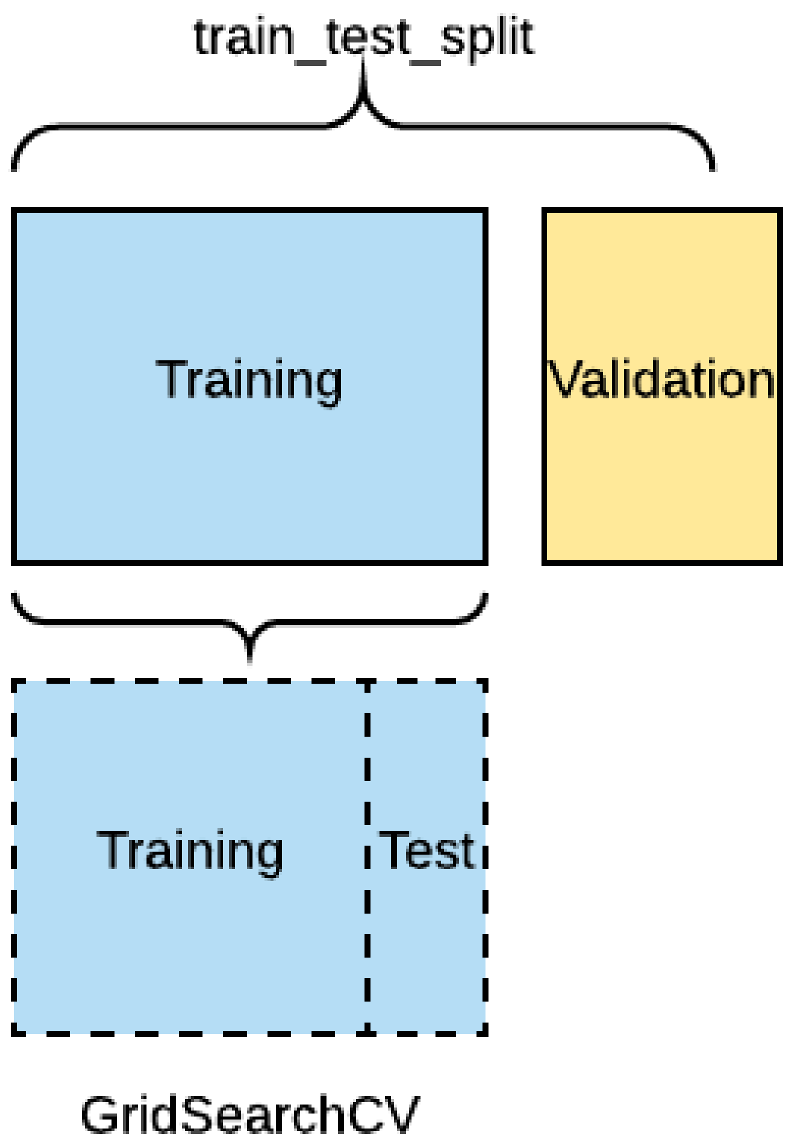

train_test_split
Training
Test
Training
Test
GridSearchCV

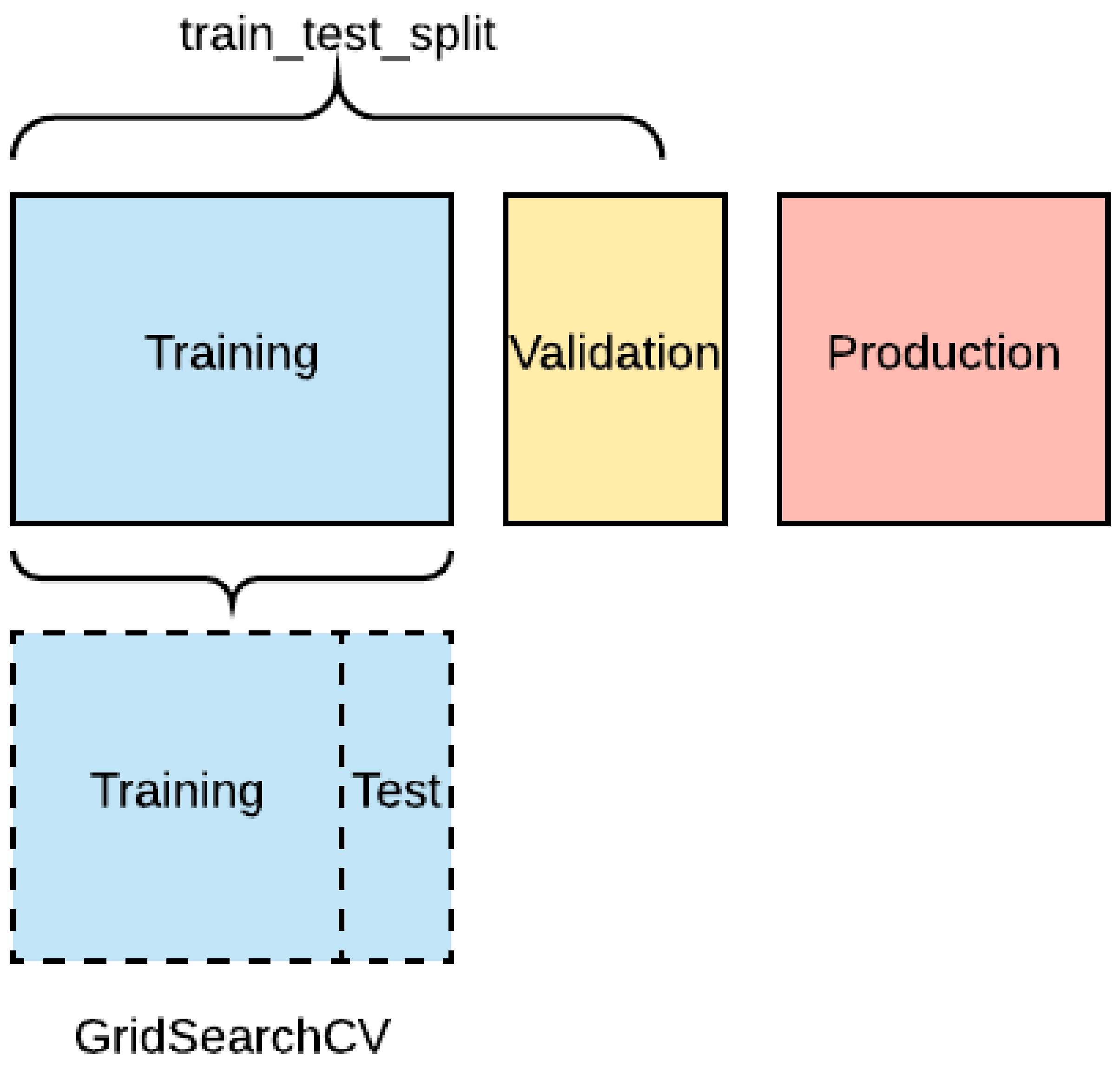

train_test_split
Training
Validation
Training
Test
GridSearchCV

Detecting overfitting

- CV Training Score >> CV Test Score
  - *overfitting in model fitting stage*
  - reduce complexity of classifier
  - get more training data
  - increase cv number
- CV Test Score >> Validation Score
  - *overfitting in model tuning stage*
  - decrease cv number
  - decrease size of parameter grid




train_test_split
Training
Validation
Training
Test
GridSearchCV


train_test_split
Training
Validation
Production
Training
Test
GridSearchCV

"Expert in CV" in your CV!

DESIGNING MACHINE LEARNING WORKFLOWS IN PYTHON

Dataset shift

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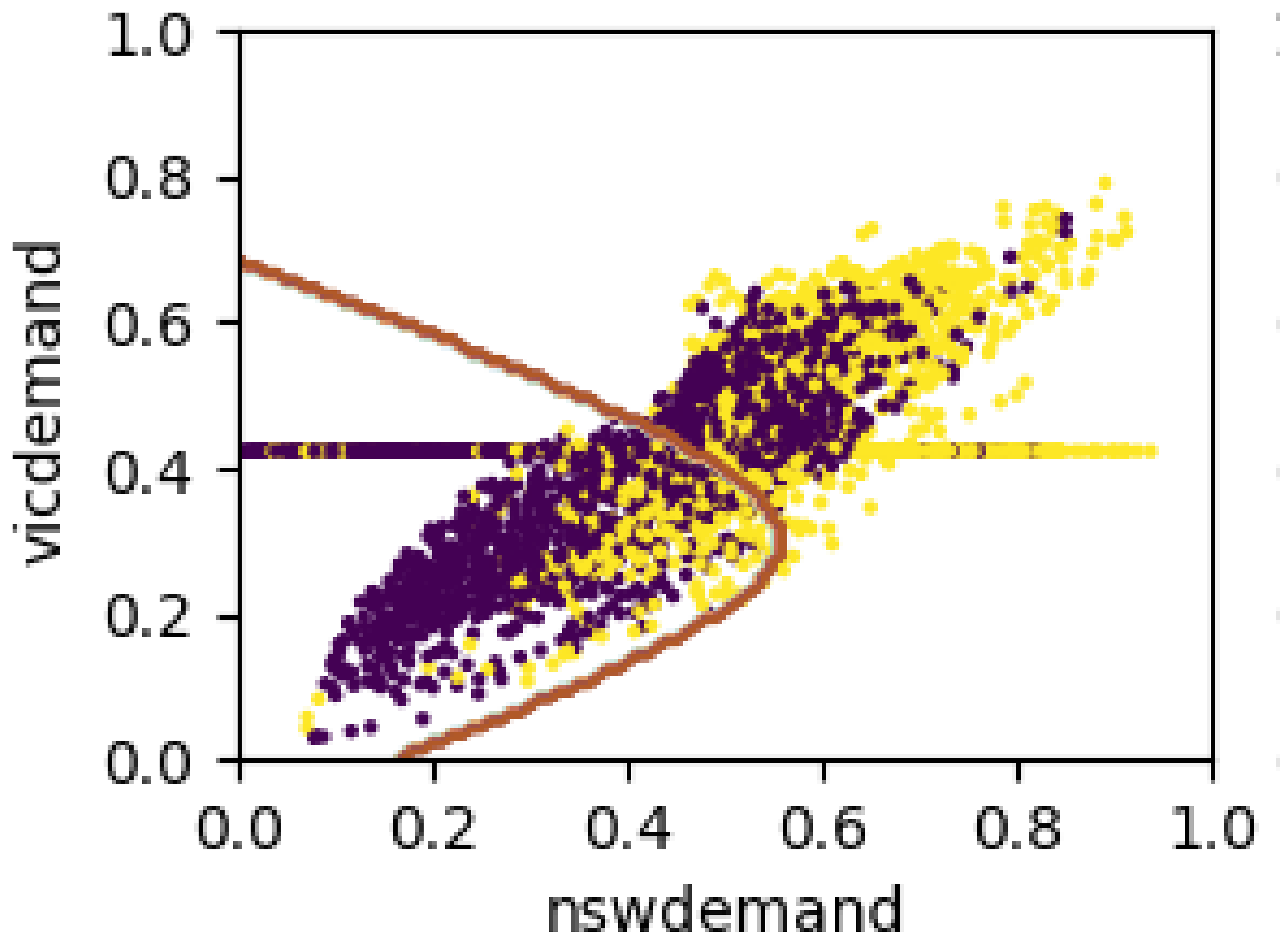
What is dataset shift?

`elec` dataset:

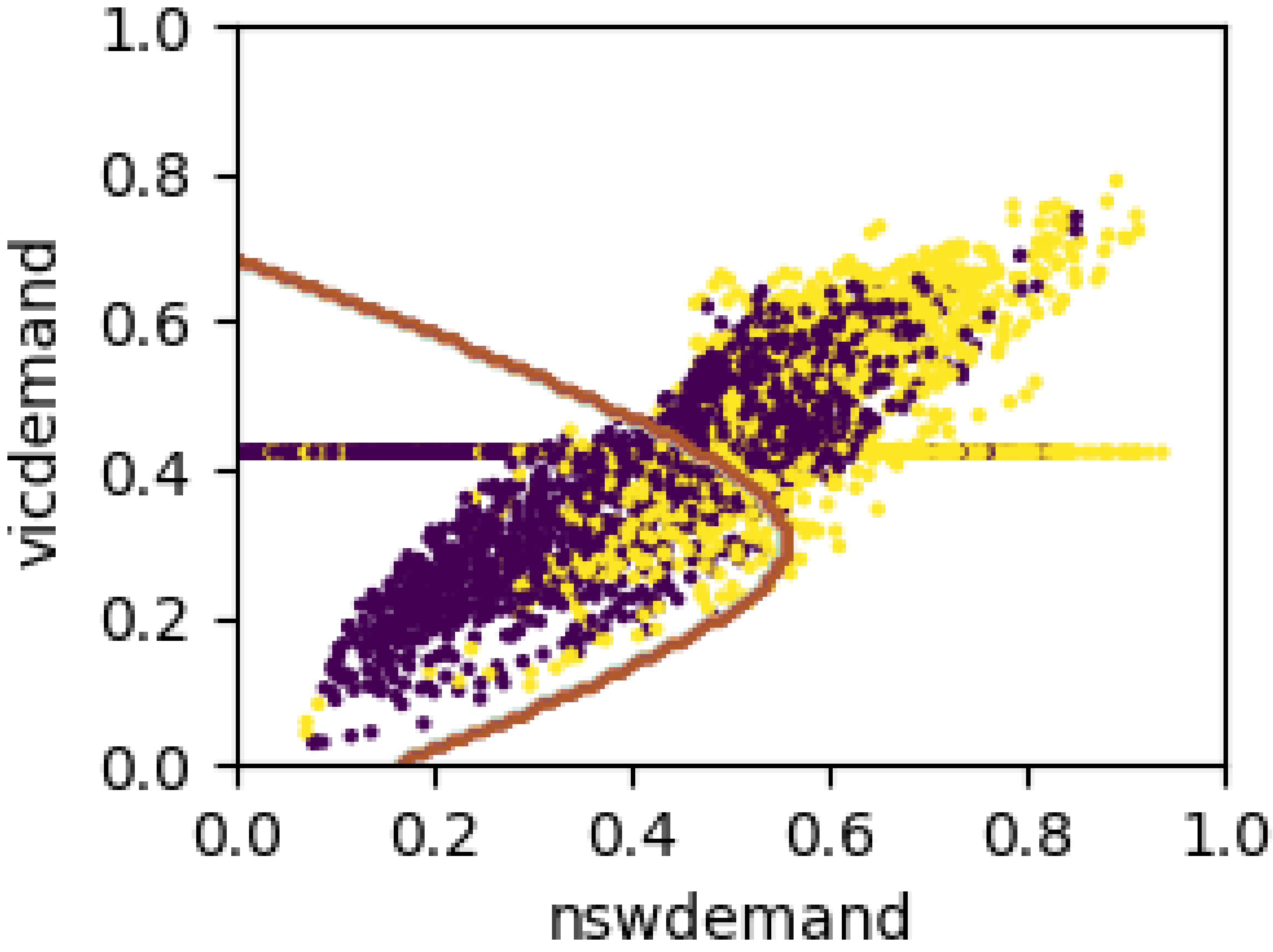
- 2 years worth of data.
- `class=1` represents price went *up* relative to last 24 hours, and `0` means *down*.

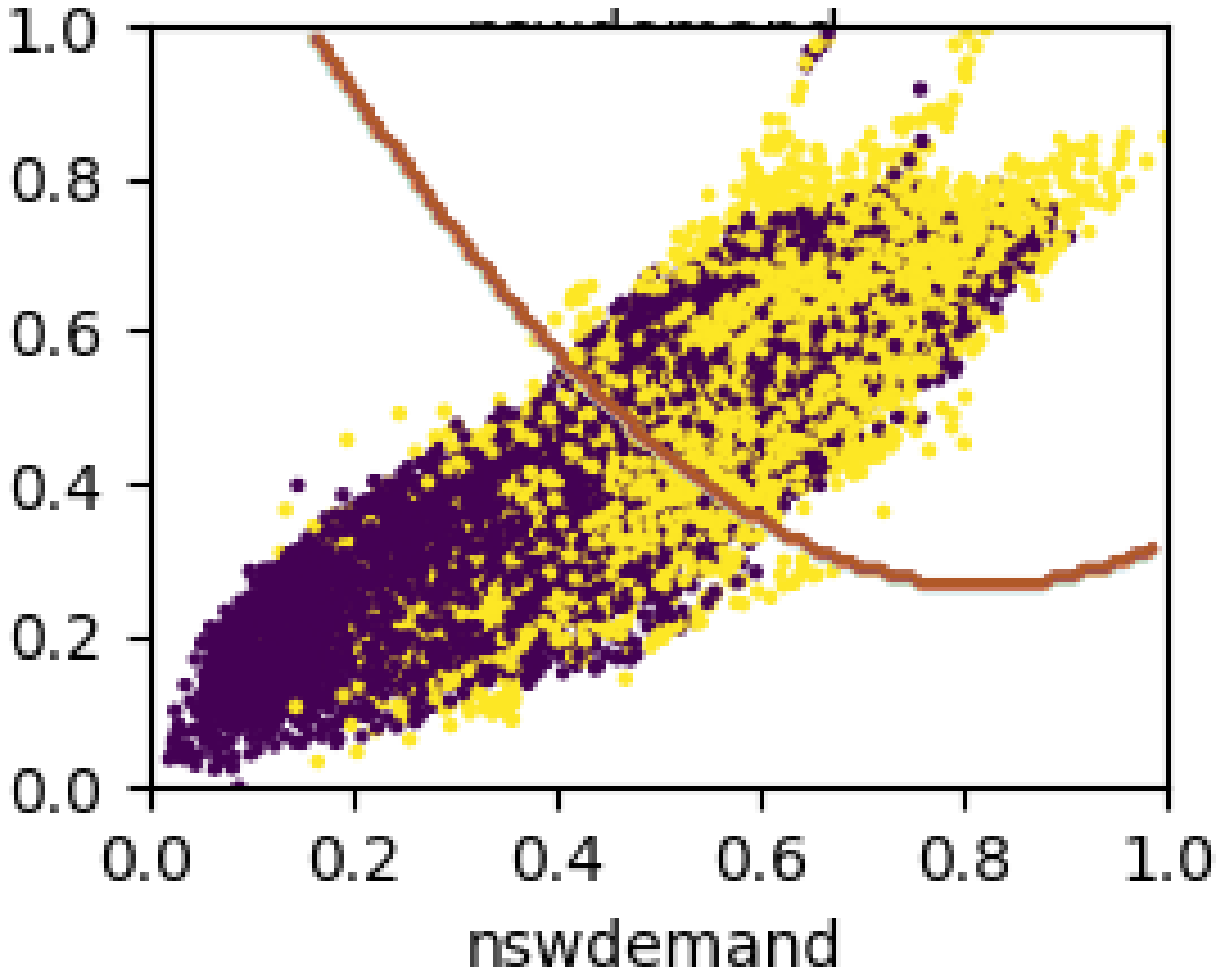
```
   day    period  nswprice  ...    vicdemand  transfer  class
0    2  0.000000  0.056443  ...     0.422915  0.414912      1
1    2  0.553191  0.042482  ...     0.422915  0.414912      0
2    2  0.574468  0.044374  ...     0.422915  0.414912      1

[3 rows x 8 columns]
```

What is shifting exactly?



What is shifting exactly?





Windows

Sliding window

```
window = (t_now-window_size+1):t_now
sliding_window = elec.loc[window]
```

	day	period	nswprice	...	vicdemand	transfer	class
0	2	0.000000	0.056443	...	0.422915	0.414912	1
1	2	0.553191	0.042482	...	0.422915	0.414912	0
2	2	0.574468	0.044374	...	0.422915	0.414912	1
3	2	0.595745	0.044374	...	0.422915	0.414912	1
4	2	0.617021	0.042482	...	0.422915	0.414912	0
5	2	0.638298	0.040861	...	0.422915	0.414912	0
6	2	0.659574	0.041161	...	0.422915	0.414912	0
7	2	0.680851	0.041161	...	0.422915	0.414912	0
8	2	0.702128	0.041161	...	0.422915	0.414912	0
9	2	0.723404	0.042482	...	0.422915	0.414912	0
10	2	0.765957	0.041041	...	0.422915	0.414912	0
11	2	0.787234	0.040711	...	0.422915	0.414912	0
12	2	0.808511	0.040711	...	0.422915	0.414912	0
13	2	0.829787	0.040861	...	0.422915	0.414912	0
14	2	0.851064	0.041041	...	0.422915	0.414912	0
15	2	0.872340	0.042482	...	0.422915	0.414912	0
16	2	0.893617	0.041161	...	0.422915	0.414912	0
17	2	0.914894	0.051489	...	0.422915	0.414912	1
18	2	0.936170	0.056443	...	0.422915	0.414912	1
19	2	0.957447	0.054642	...	0.422915	0.414912	1

Expanding window

```
window = 0:t_now
expanding_window = elec.loc[window]
```

	day	period	nswprice	...	vicdemand	transfer	class
0	2	0.000000	0.056443	...	0.422915	0.414912	1
1	2	0.553191	0.042482	...	0.422915	0.414912	0
2	2	0.574468	0.044374	...	0.422915	0.414912	1
3	2	0.595745	0.044374	...	0.422915	0.414912	1
4	2	0.617021	0.042482	...	0.422915	0.414912	0
5	2	0.638298	0.040861	...	0.422915	0.414912	0
6	2	0.659574	0.041161	...	0.422915	0.414912	0
7	2	0.680851	0.041161	...	0.422915	0.414912	0
8	2	0.702128	0.041161	...	0.422915	0.414912	0
9	2	0.723404	0.042482	...	0.422915	0.414912	0
10	2	0.765957	0.041041	...	0.422915	0.414912	0
11	2	0.787234	0.040711	...	0.422915	0.414912	0
12	2	0.808511	0.040711	...	0.422915	0.414912	0
13	2	0.829787	0.040861	...	0.422915	0.414912	0
14	2	0.851064	0.041041	...	0.422915	0.414912	0
15	2	0.872340	0.042482	...	0.422915	0.414912	0
16	2	0.893617	0.041161	...	0.422915	0.414912	0
17	2	0.914894	0.051489	...	0.422915	0.414912	1
18	2	0.936170	0.056443	...	0.422915	0.414912	1
19	2	0.957447	0.054642	...	0.422915	0.414912	1

Dataset shift detection

```
# t_now = 40000, window_size = 20000
clf_full = RandomForestClassifier().fit(X, y)
clf_sliding = RandomForestClassifier().fit(sliding_X, sliding_y)
```

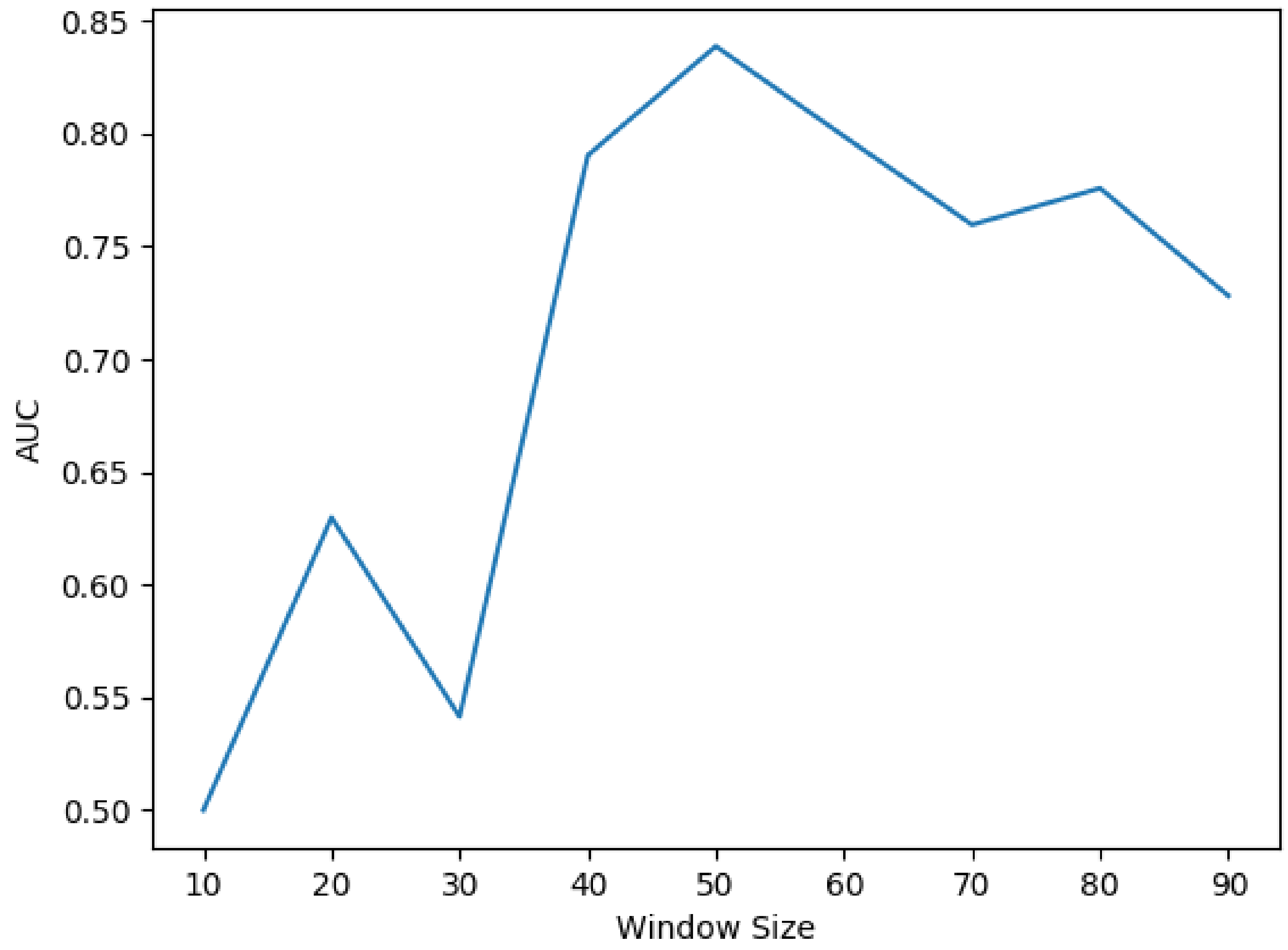
```
# Use future data as test
test = elec.loc[t_now:elec.shape[0]]
test_X = test.drop('class', 1); test_y = test['class']
```

```
roc_auc_score(test_y, clf_full.predict(test_X))
roc_auc_score(test_y, clf_sliding.predict(test_X))
```

```
0.775
0.780
```

Window size

```python
for w_size in range(10, 100, 10):
    sliding = arrh.loc[
      (t_now - w_size + 1):t_now
    ]
    X = sliding.drop('class', 1)
    y = sliding['class']
    clf = GaussianNB()
    clf.fit(X, y)
    preds = clf.predict(test_X)
    roc_auc_score(test_y, preds)
```



Domain shift

`arrhythmia` dataset:

```
   age  sex  height  ...    chV6_TwaveAmp  chV6_QRSA  chV6_QRSTA  class
0   75    0     190  ...              2.9       23.3        49.4      0
1   56    1     165  ...              2.1       20.4        38.8      0
2   54    0     172  ...              3.4       12.3        49.0      0
3   55    0     175  ...              2.6       34.6        61.6      1
4   75    0     190  ...              3.9       25.4        62.8      0

[5 rows x 280 columns]
```

More data is not always better!

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