Classification with a control channel

Don't cheat yourself!

Gilles Louppe (@glouppe)
Tim Head (@betatim)

Disclaimer

The following applies only for the learning protocol of the *Flavours of Physics* Kaggle challenge.

See notebook for further details.

Flavours of Physics: Finding $\tau \mapsto \mu\mu\mu$ challenge

Given a learning set $\mathcal{L}$ of

- simulated signal events $(\mathbf{x}, s)$
- real data background events $(\mathbf{x}, b)$,

build a classifier $\varphi : \mathcal{X} \mapsto \{s, b\}$ for distinguishing $\tau \mapsto \mu\mu\mu$ signal events from background events.

Control channel test

The simulation is not perfect: discriminative patterns exist between simulated and real data events.

To avoid exploiting simulation versus real data artefacts to classify signal from background events, we evaluate whether φ behaves differently on simulated signal and real data signal from a control channel $\mathcal{C}$.

Here, the control channel test consists in requiring the Kolmogorov-Smirnov test statistic between $\{\varphi(\mathbf{x})|\mathbf{x} \in \mathcal{C}^{\text{sim}}\}$ and $\{\varphi(\mathbf{x})|\mathbf{x} \in \mathcal{C}^{\text{data}}\}$ to be strictly smaller than some pre-defined threshold t.

Proposition

Assuming that

- control data can be distinguished from training data with high confidence,
- simulated features are more discriminative than they are in real data,

Then, even by chance, φ might exploit simulation versus real data artefacts to classify signal from background events, while still passing the control channel test.

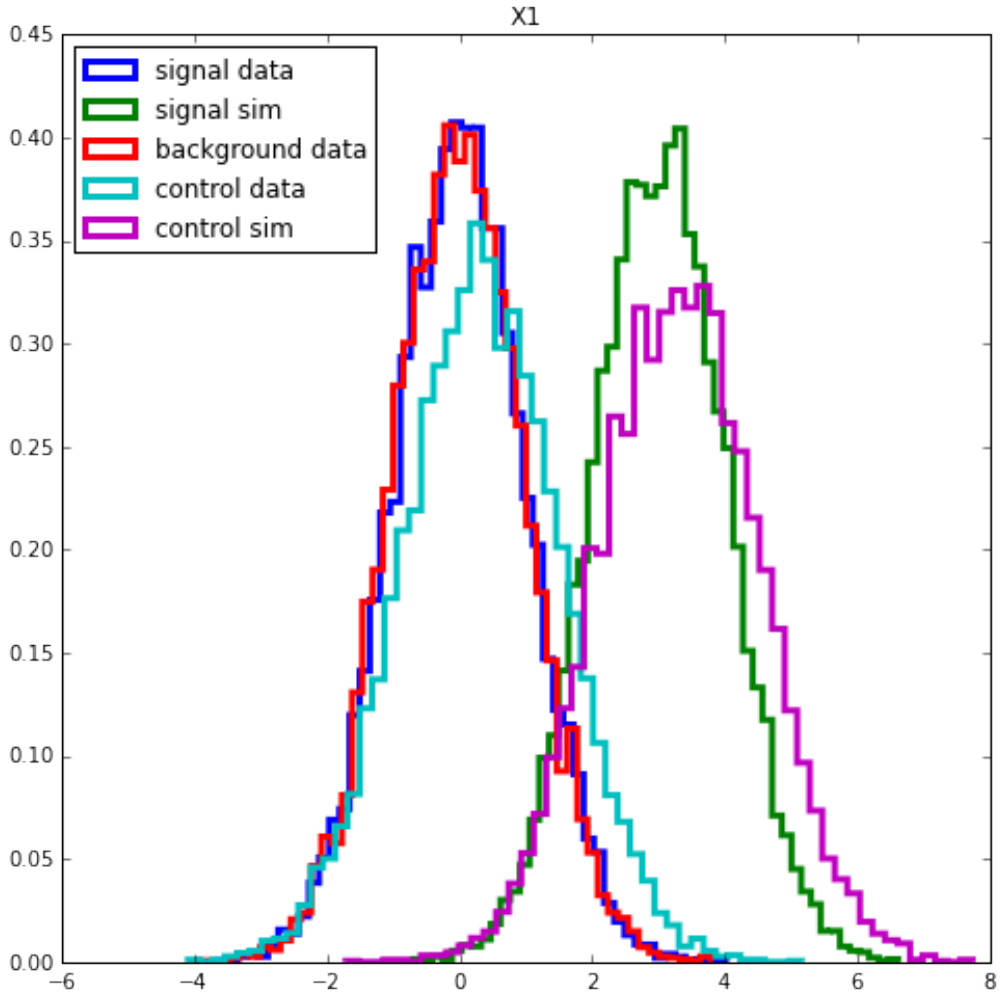
Therefore,

- The true performance of φ on real data may be significantly different (typically lower) than estimated on simulated signal events versus real data background events.
- Passing the KS test does not tell you anything about φ.

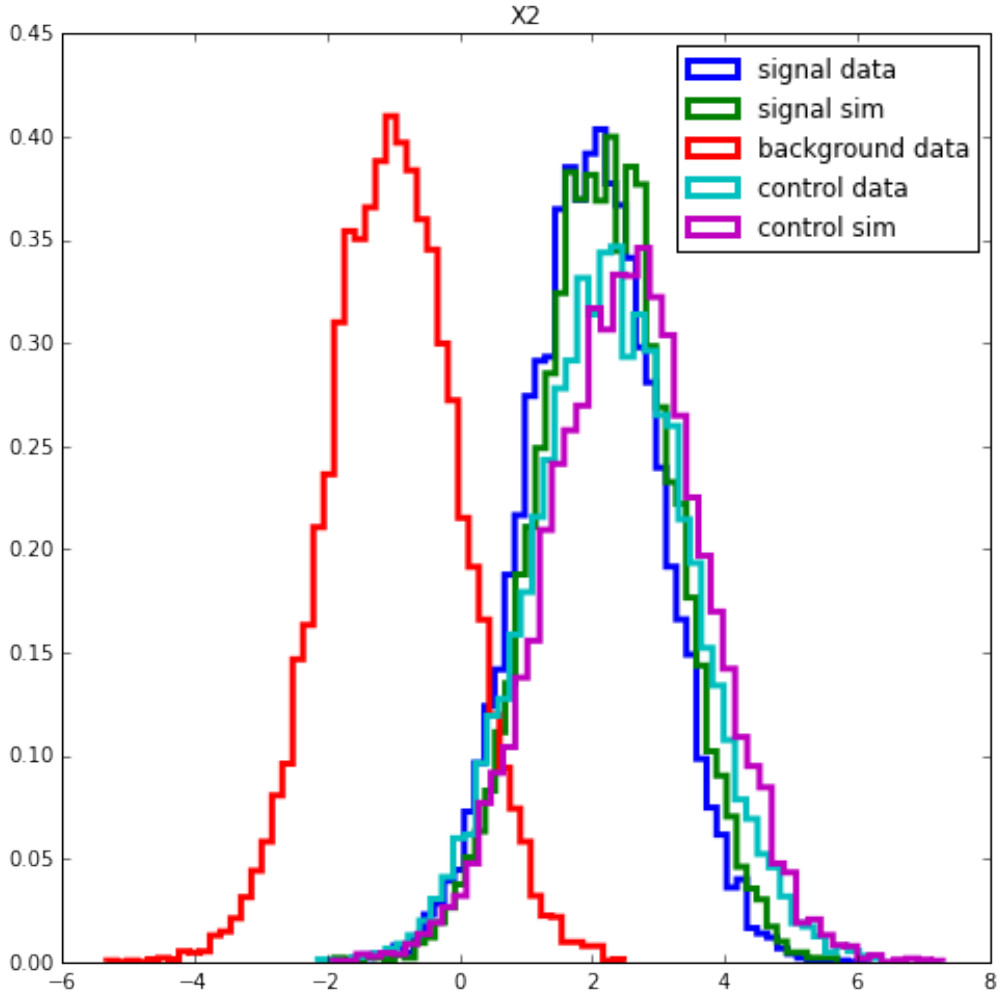
Toy example

Let us consider an artificial classification problem between signal and background events, along with some close control channel data $\mathcal{C}^{\text{sim}}$ and $\mathcal{C}^{\text{data}}$.

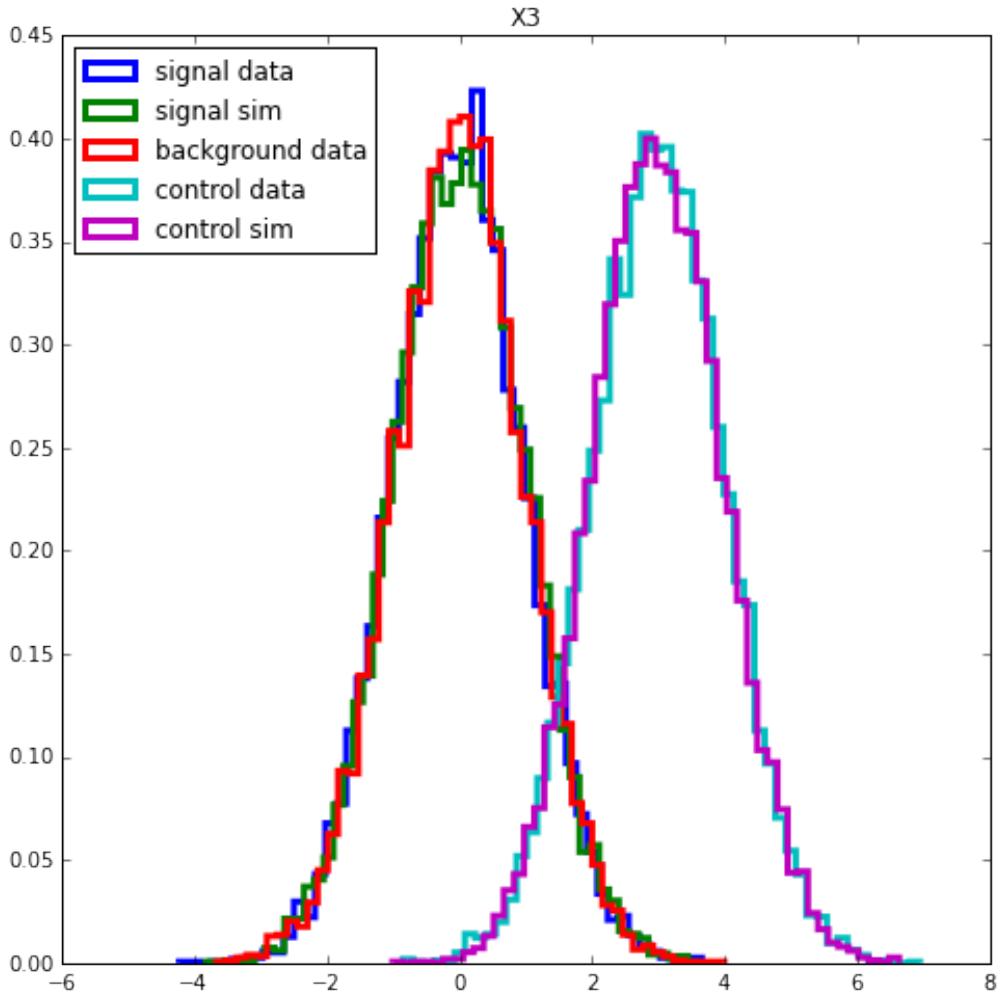
Let us assume an input space defined on three input variables X_1, X_2, X_3 as follows.



X_1 is irrelevant for distinguishing real data signal from real data background but, because of simulation imperfections, has discriminative power between simulated events and real data events.



X_2 is discriminative between signal and background events.



X_3 is discriminative between events from the original problem and the control channel, but has otherwise no discriminative power between signal and background events.

Random exploration

```
from sklearn.ensemble import ExtraTreesClassifier

def find_best_tree(X_train, y_train, X_test, y_test,
                   X_data, y_data, X_control_sim, X_control_data):
    best_auc_test, best_auc_data = 0, 0
    best_ks = 0
    best_tree = None

    for seed in range(2000):
        clf = ExtraTreesClassifier(n_estimators=1, max_features=1,
                                   max_leaf_nodes=5, random_state=seed)
        clf.fit(X_train, y_train)
        auc_test = roc_auc_score(y_test, clf.predict_proba(X_test)[:, 1])
        auc_data = roc_auc_score(y_data, clf.predict_proba(X_data)[:, 1])
        ks = ks_statistic(clf.predict_proba(X_control_sim)[:, 1],
                          clf.predict_proba(X_control_data)[:, 1])

        if auc_test > best_auc_test and ks < 0.09:
            best_auc_test = auc_test
            best_auc_data = auc_data
            best_ks = ks
            best_tree = clf

    return best_auc_test, best_auc_data, best_ks, best_tree
```

Random exploration

```
auc_test, auc_data, ks, tree = find_best_tree(X_train, y_train,
                                              X_test, y_test,
                                              X_data, y_data,
                                              X_control_sim, X_control_data)

print "ROC AUC (simulated signal vs. data background) =", auc_test
print "ROC AUC (data signal vs. data background) =", auc_data
print "KS statistic =", ks
```

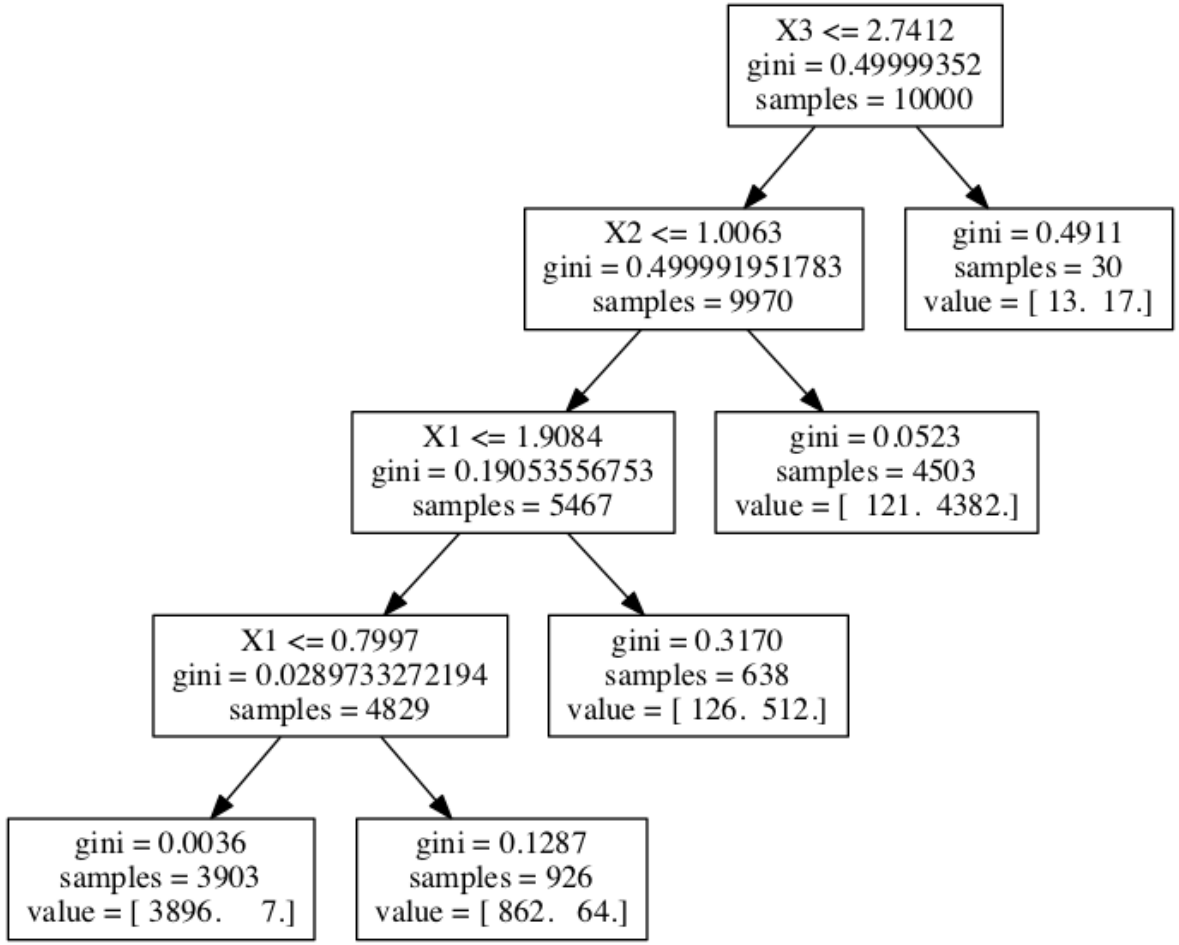
```
>>> ROC AUC (simulated signal vs. data background) = 0.986357983199
>>> ROC AUC (data signal vs. data background) = 0.90973817
>>> KS statistic = 0.0578
```

What just happened? By chance, we have found a classifier that

- has seemingly good test performance (AUC=0.986 on simulated signal versus real data background); and
- passes the control channel test that we have defined.

This classifier appears to be exactly the one we were seeking.

Wrong. The expected ROC AUC of 0.91 on real data signal and real data background is significantly lower than our first estimate, suggesting that there is still something wrong.



φ exploits X_1, i.e. simulation versus real data artefacts to indirectly classify signal from background events, while still passing the control channel test because of its use of X_3!

Winning the challenge

As in the challege, simulation versus real data patterns may be hidden into several variables, making it not possible to detect the problem by eye by looking at variables individually. However, a learning algorithm might still be able to exploit them, either by chance or on purpose.

Recipe for winning the challenge:

1. learn to distinguish between training and control data,
2. build a classifier on training data, with all the freedom to exploit simulation artefacts,
3. assign random predictions to samples predicted as control data, otherwise predict using the classifier found in the previous step.

A better protocol

If differences between simulated and real data events are fixed, then the problem goes away.

One way to do it is to learn a transformation (e.g., a reweighting) from simulation onto real data from the control channel, and then learn on transformed simulated signal events versus real data background events.