All Relevant Feature Selection

Racapping Our Path So Far

We started with a somewhat clear goal

- Given data containing candidate correlates and a discrete target
- ...We aimed at identifying the most relevant correlates

We applied a baseline approach (Lasso) to:

- Obtain a surrogate for our data-generation process
- Analyze the impact of each candidate correlate (feature)
- Identify the most relevant correlates

Our baseline turned out to be largely insufficient, so we:

- Trained a non-linear model to obtain a more reliable surrogate
- Learn to assess importance via a permutation-based method
- Learned to explain individual examples via SHAP

We still have a couple of major open problems...

Open Problems

There's a mistmatch between local and global explanations

- We are using SHAP to assess local feature effects
- ...And permutation importance for global feature effects

As a side effect, there may be inconsistences in our analysis

We still don't know how to identify the most relevant features

- Like in the Lasso appproach we could think of using a threshold
- ...But we still don't know how such threshold should be calibrated

It's time that we fix both of them

Global Feature Analysis via SHAP

SHAP explanations can be aggregated to get global importance scores

By default, this is done by averaring absolute SHAP values:

$$\bar{\phi}_j(x) = \frac{1}{n} \sum_{i=1}^{m} |\phi_j(x_i)|$$

- Other aggregation functions can also be used (e.g. max)

By using aggregated SHAP scores

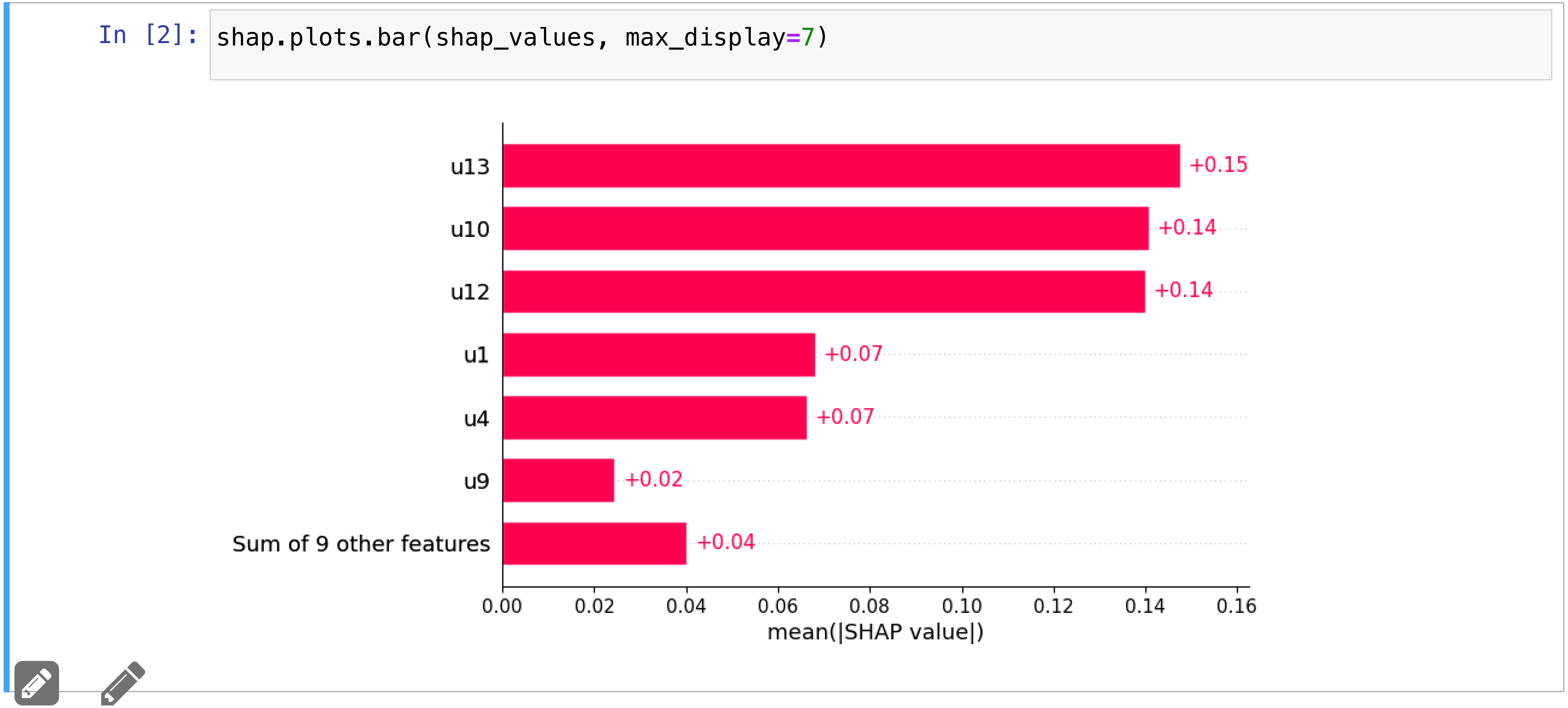
...We can attempt to identify the most important correlates

- I.e. we can used SHAP scores like we were using permutation importances
- In fact, both approaches are sound and well defined

Global Feature Analysis via SHAP

The SHAP library provide convenience functions to plot aggregated values

Here's how to plot mean (absolute) SHAP values:



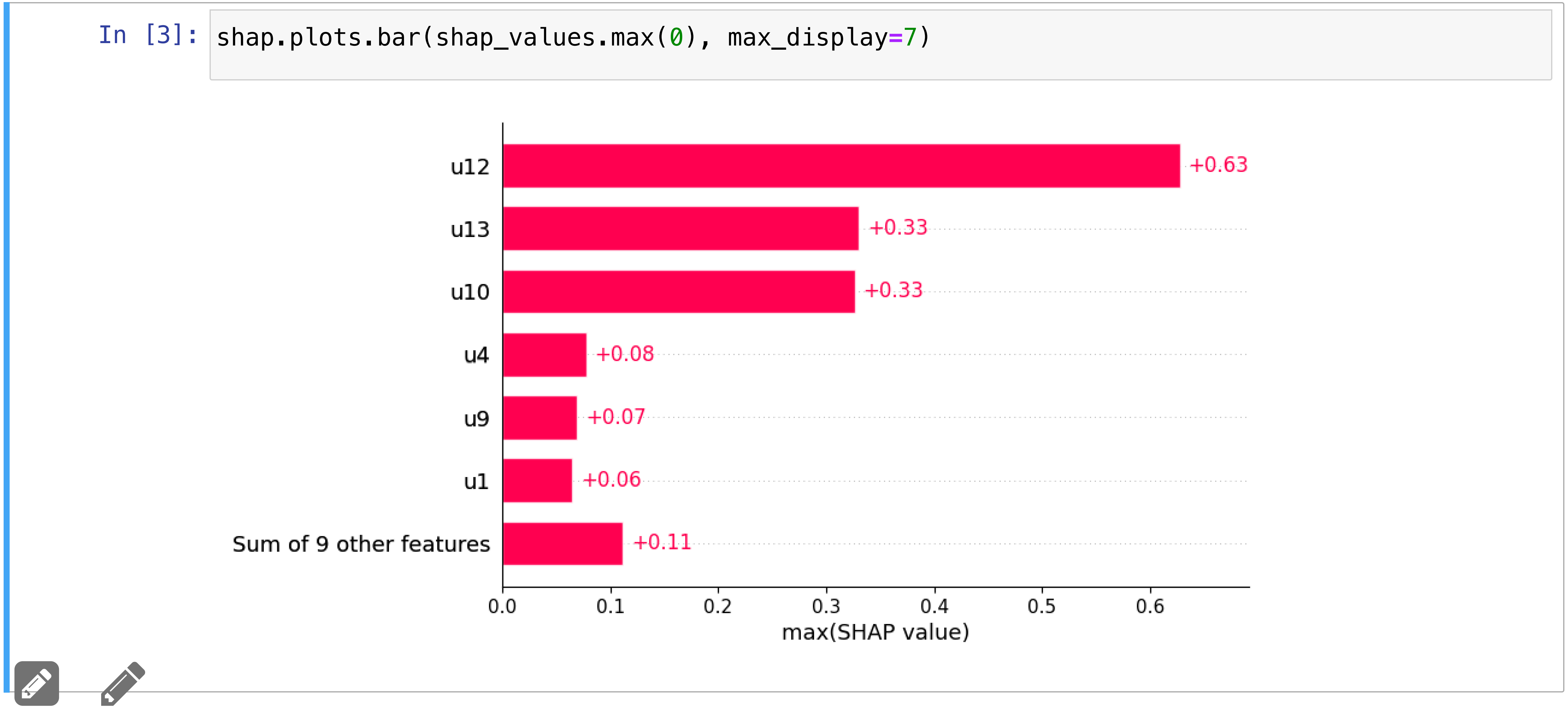
In [2]:

```
shap.plots.bar(shap_values, max_display=7)
```

Global Feature Analysis via SHAP

The SHAP library provide convenience functions to aggregated values

Here's how to display the maximum (absolute) SHAP values:



In [3]:
```
shap.plots.bar(shap_values.max(0), max_display=7)
```

Semantics for Feature Selection

A viable approach for feature selection consists in solving:

$$\mathop{\text{argmin}}_{S \subseteq \mathcal{X}} \left\{ |S| : \hat{y} = \hat{f}_S(x_S), L\left(y, \hat{y}\right) \leq \theta \right\}$$

Where $\boldsymbol{x}, \boldsymbol{y}$ denote all the training data. Intuitively:

- We search for the smallest subset of features $\boldsymbol{S}$
- ...Such that a model $\hat{f}_S$ trained over only over them
- ...Still has an acceptable (cross-validation) accuracy

Heuristics (e.g. greedy search) can be used to improve scalability

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This optimization-driven approach

- ...Can be customized by adjusting the constraint and cost function
- ...Can reduce data storage and location costs on the deployed model

Semantics for Feature Selection

If we care just about cost and accuracy, the optimization approach is perfect

But it is not suitable for our current case study...
Can you tell why?

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Can you tell why?

For a number of reasons:

- We care about finding all the relevant features, not a minimal set
- How should the accuracy threshold be calibrated?
- What about the noise induced by retraining?

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If we wish to use ML for data analysis, we need another approach

...In particular, we will rely on statistical hypothesis testing (HT)

Statistical Hypothesis Testing

HT builds evidence for a hypothesis by refuting a competing one:

We start with:

- a random variable X
- a hypothesis $H(X)$

We define:

- a competing null hypothesis $H_0(X)$
- a experimental statistics $T[X]$, e.g. an expected value, an estimate probability

In most cases:

- H_0 is often the negation of our original hypothesis
- $T[X]$ is a quantity that, if large enough, supports our hypothesis

Statistical Hypothesis Testing

We reject the null hypothesis by checking what happens when H_0 is true

In particular, we need to compute:

- the empirical value t of $T[x \mid H_0]$ on a sample x
- the theoretical probability of the computed value, i.e. $P(T[X \mid H_0] \geq t)$

The former usually requires dedicated experiments (e.g. with a control group)

The probability $P(T[X \mid H_0] = t)$ is called a p-value

- If p is small enough, we can say that H_0 is likely false
- ...Which in turn provides support for our original hypothesis

This is probably very confusing...

Let's make an example for our case

Hypothesis, Data, and Null-Hypothesis

First, we need to define our variable and hypothesis

We care about identifying correlates, so a possible choice might be:

- The variable will be the pair (X, Y), i.e. observable and target
- $H \equiv \text{"}X \text{ is important to predict } Y$, according to some indicator $r[X, Y]$

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Now we need a competing null hypothesis

A good choice might be $H_0 \equiv$ "the importance of X is due to chance

- In this case, refuting H_0 lends directly support for H
- Other situations might be more complicated

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The real difficulty is defining the test statistics

Towards a Test Statistics

Let's consider the desired properties for the test statistics

- It should be related to both H and H_0
- It should be a measurable experimental outcome
- We should be able to run experiments, assuming that H_0 is true
- We shoudd be able to compute probabilities, assuming that H_0 is true

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...And let's consider out situation

- We care about importance, both in H and in H_0
- We can measure importance via the $r[X, Y]$ indicator
- We already have a sample (x, y) where r has a larg-ish value

...But what about the other desired properties?

Towards a Test Statistics

Let's consider this inequality

$$r[\tilde{x}, \tilde{y}] \leq r^* \qquad \text{with: } r^* = r[x, y]$$

- $r[x, y]$ is the correlation value measured on our data
- $(\tilde{x}, \tilde{y})$ is a sample from $(\tilde{X}, \tilde{Y})$
- ...Where $(\tilde{X}, \tilde{Y})$ are similar to (X, Y), but uncorrelated

Later, we will need to find a way to sample from $(\tilde{X}, \tilde{Y})$

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Then:

- If X and Y are correlated, we would expect the inequality to be usually true
- Otherwise, the inequality might be true or false, depending on chance

Towards a Test Statistics

In other words, we use a statistics the expectation

...Which can be estimated via the expectation:

$$T[X, Y \mid H_0] \equiv \sum_{i=1}^{m} P(r[\tilde{X}, \tilde{Y}] \leq r^*)$$

- I.e. the number of times the inequality holds when sampling m times $(\tilde{X}, \tilde{Y})$

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For this statistics, we need do two things

- Computing the theoretical distribution $P(T[X, Y \mid H_0])$
- Computing the empirical value $P(T[x, y \mid H_0])$

Test Statistic and Theoretical Probability

Let's consider again our test $r[\tilde{X}, \tilde{Y}] \leq r^*$

Since it has a binary outcome, it will follow a Bernoulli distribution

- If we assume that the result is due to chance...
- ...Then the associated probability should be ${}^1/_2$

If we make repeated experiments with samples $(\tilde{x}, \tilde{y})$

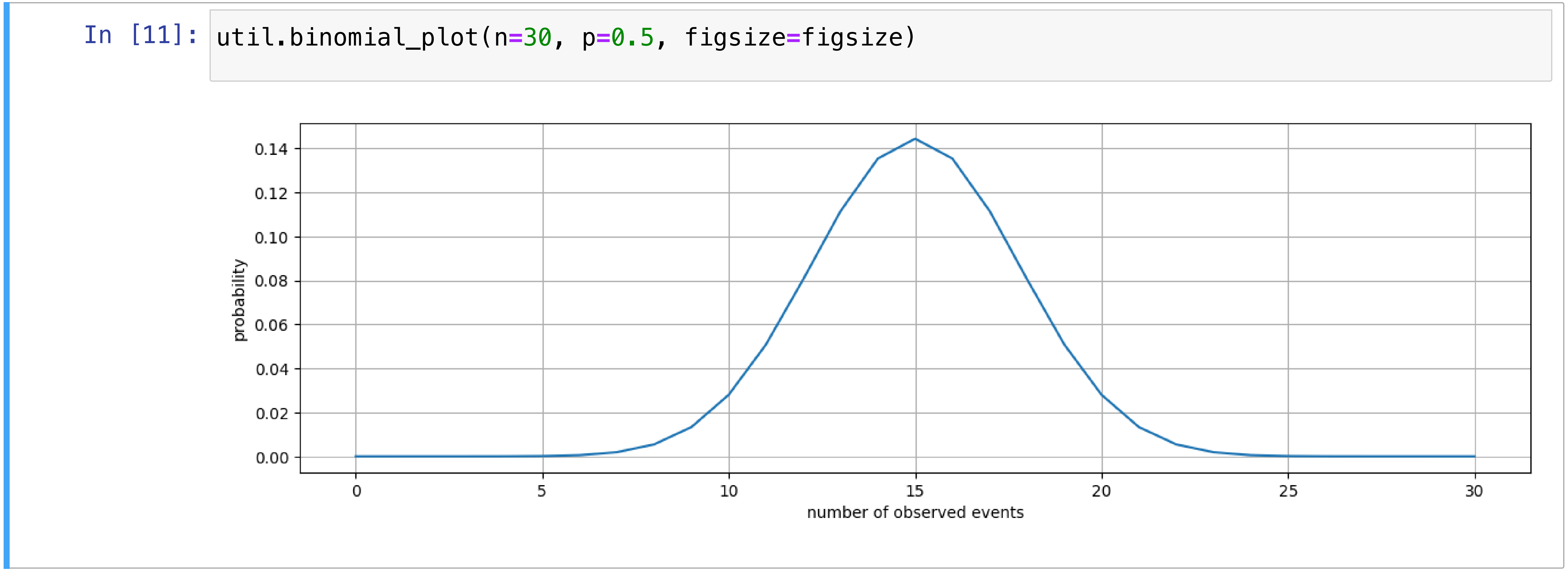
...The number of observed events $\boldsymbol{r[\tilde{x}, \tilde{y}] \leq r^*}$ will follow a binomial distribution

- Given the number of experiments $\boldsymbol{n}$
- ...The probability of $\boldsymbol{T[X, Y \mid H_0]}$ should be $\boldsymbol{B(n, {}^1/_2)}$

Hence, $B(n, {}^1/_2)$ is the theoretical distribution under H_0 for our statistics

Theoretical Probability Computation

We can easily compute and plot the distribution



```
In [11]: util.binomial_plot(n=30, p=0.5, figsize=figsize)
```

- This tells us how likely we are to observe a certain number of events
- ...Assuming that the null hypothesis is true

...But how do we run the experiments?

We need to simulate lack of correlation in (X, Y)

...Without additional assumptions

Empirical Probability Computation

We can use a Monte-Carlo approach

The trick is once again relying on permutations

- If we shuffle the values of one variable (say the values x of X)
- ...We can get a correlation with Y only by chance
- ...But we otherwise preserve the distribution of the sample

Empirical Probability Computation

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- ...But we otherwise preserve the distribution of the sample

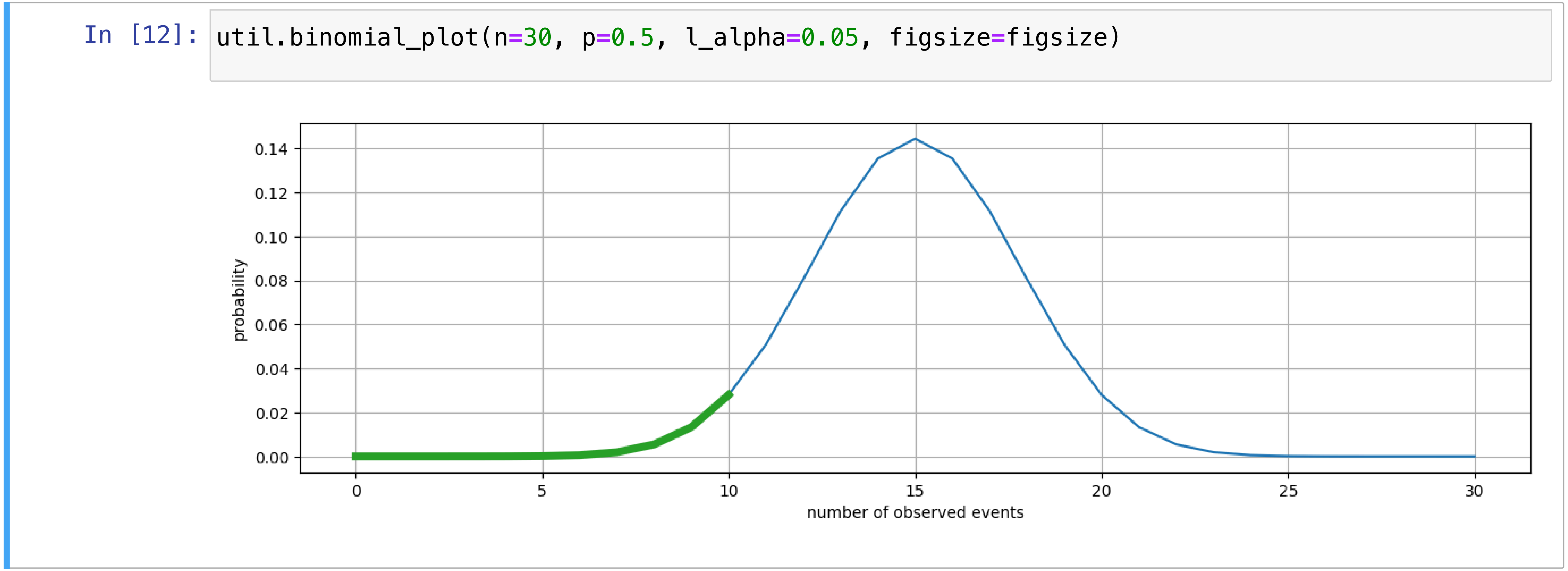
We can mitigate sampling noise via repeated experiments

- Then, we take our empirically observed number $t = T[X, Y \mid H_0]$ of events
- ...And we match it against the theoretical probability

Any sufficiently low probability will allow use to reject H_0

p-Value and the Statistical Test

Basically, there is a "target interval" in the distribution



```
In [12]: util.binomial_plot(n=30, p=0.5, l_alpha=0.05, figsize=figsize)
```

- For any value t in the interval, we have $P(T[X, Y \mid H_0] = t) \leq 1 - \alpha$
- ...Where α is our desired confidence level

p-Value and the Statistical Test

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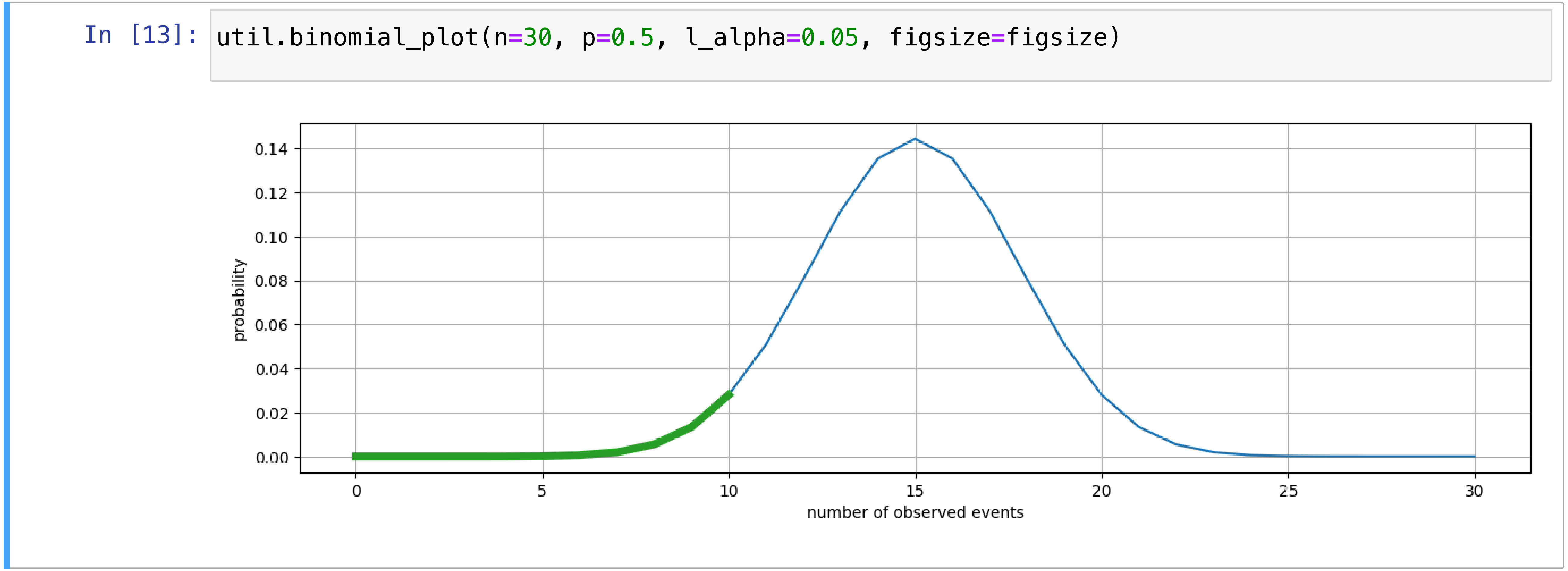

```
In [13]: util.binomial_plot(n=30, p=0.5, l_alpha=0.05, figsize=figsize)
```

- In practice it's more common to compute the p-value $P(T(X,Y) \geq t \mid H_0)$
- ...Which can then be immediately compared with $1 - \alpha$

Back to the Procedure Description

The procedure should be clearer now

Let's recap the steps:

- We define our random variable X the hypothesis H
- We formulate a competing null hypothesis H_0
- We define a test statistics $T[X]$, linked to H and H_0
- Assuming that H_0 holds:
  - We define the theoretical probability $P(T[X, Y \mid H_0])$
  - We compute the empirical value $T[x, y \mid H_0]$
- We compute the p value $P(T[x, y \mid H_0])$
- If $p \leq 1 - \alpha$ for some confidence α, we reject the null hypothesis

Testing a Hypothesis and Its Negation

In our case, the method works also for testing the opposite hypothesis

- Our hypothesis becomes $\neg H* \equiv "X \text{ is not important to predict } Y$
- The null hypothesis is the same as before
- The test statistics is just $n - T[X, Y \mid H_=]$, for the same T as before

Then we can proceed as in the previous case

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Then we can proceed as in the previous case

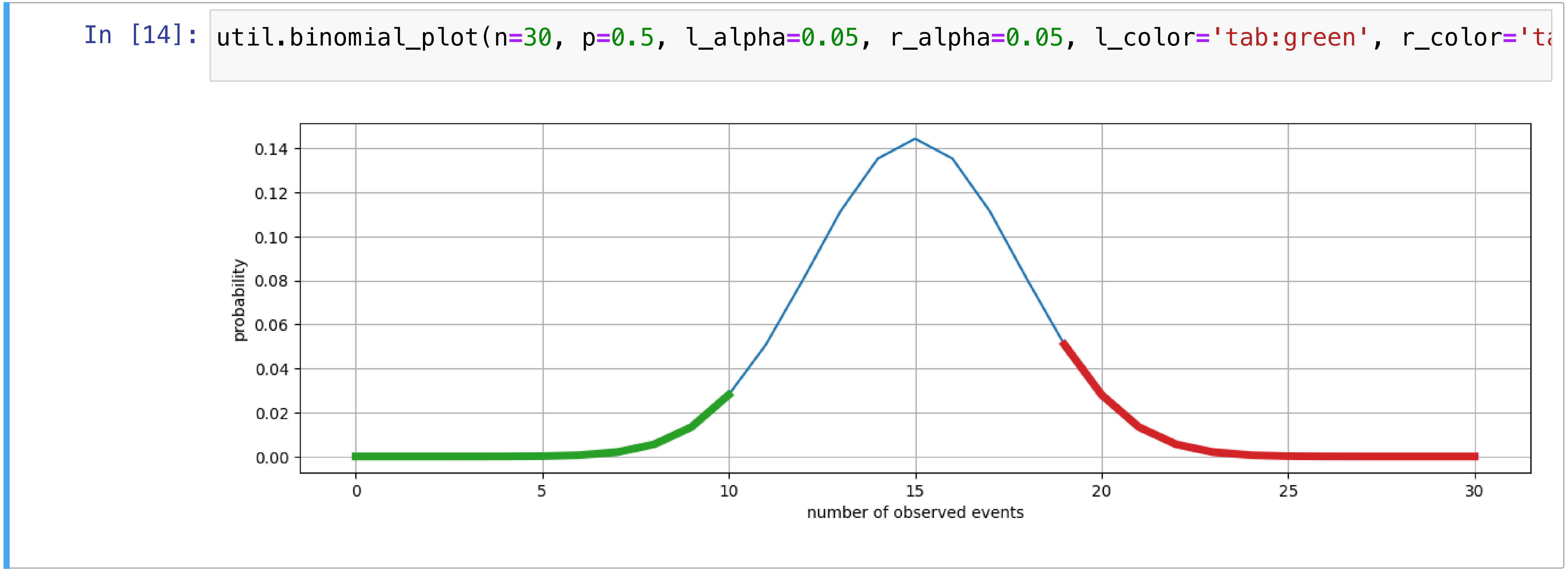
Since we are relying on the same test statistics

...We can use the same set of experiments to test both hypotheses

- Intuitively, in both cases we look at the number of times $r[\tilde{x}, \tilde{y}] \leq r^*$
- If hits is sufficiently high, it's likely that the H holds
- ...If this is sufficiently low, it's likely that $\neg H$ holds

Testing a Hypothesis and Its Negation

In other words, we will end up having two target intervals



```
In [14]: util.binomial_plot(n=30, p=0.5, l_alpha=0.05, r_alpha=0.05, l_color='tab:green', r_color='ta
```

- If T is in the green region, we support H (e.g. confirmed importance)
- If T is in the red region, we support $\neg H$ (e.g. confirmed non-importance)
- If T lands in the center region, we support no claim

Boruta

The approach we have just seen is the backbone of the Boruta algorithm

- The Boruta algorithm is a SotA feature selection method
- ...That relies in statistical HT to determine relevant features

Like in our analysis, the method relies on surrogate models

...And in particular on tree ensembles (the name refers to a Slavic forest spirit)

- As a consequence, the algorithm can deal with non-linear correlations
- ...And accounts for interactions between multiple features

Boruta is an all-relevant feature selector

- This makes it particularly well suited for scientific analyses
- ...But it can be used to reduce data collection costs or improve generalization

Tested Hypothesis in Boruta

Boruta relies on a measure of feature importance

- The original algorithm and the BorutaPy package use permutation importance
- An unmaintained version based on SHAP is also available

In both cases, importance is computed w.r.t. a reference dataset

The hypothesis H being tested is more general than ours and consists in:

> *"Feature j is important among those in the dataset,*
> *according to the chosen metric"*

- This is bit more general than the one we considered
- ...And it require as slighly more sophisticated test statistics

Test Statistics in Boruta

The main idea is stil to rely on permuted features

Let (x, y) be our original dataset

- First, we augmented it by introducing permuted versions $\tilde{X}$ of all features
- These are called shadow features by the algorithm. Let their values be $\tilde{x}$

Then, we train a predictive model on $(x, \tilde{x}, y)$

Let $\phi_j((x, \tilde{x}), y)$ be the importance of feature j, on the augmented dataset

- If the feature is important, its ϕ_j should beat the shadow features
- Therefore, we can consider the event

$$\phi_j((x, \tilde{x}), y) > \max_{j \in \tilde{X}} \phi_j((x, \tilde{x}), y)$$

Test Statistics in Boruta

Then the testing statistics T is similar to the one we used:

- The algorithms performs multiple experiments (retraining the model)
- ...And counts the number of times the event is satisfied ("hits")

The thereotical distribution for T under H_0 is mostly a binomial

- The algorithm needs to apply some statistical corrections
- ...Since we are testing multiple features together (we have a $\max$)

Boruta tests both the positive and negative hypothesis

Therefore, at the end of the process:

- Some features will be confirmed important
- Some features will be confirmed unimportant
- Some features will be remain tentative

Using Boruta in Practice

We'll use Boruta through the BorutaPy package

```
In [20]: bfs = BorutaPy(xbm, n_estimators='auto', max_iter=100, verbose=0, random_state=42)
         bfs.fit(X=X, y=y);
```

- We can choose how many samples to use
- The algorithm also determines the best number of estimators

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Let's see which features have been selected

```
In [35]: print('Confirmed important:', X.columns[bfs.ranking_ == 1].values)
         print('Uncomfirmed:', X.columns[bfs.ranking_ == 2].values)
         print('Confirmed unimportant:', X.columns[bfs.ranking_ > 2].values)
```

```
Confirmed important: ['u1' 'u10' 'u12' 'u13']
Uncomfirmed: ['u4']
Confirmed unimportant: ['u0' 'u2' 'u3' 'u5' 'u6' 'u7' 'u8' 'u9' 'u11' 'u14']
```

Ok, but... Did it work?

What we Have Discovered

So far, by using Boruta we found that:

- There seem to be 4 relevant features, i.e. $U_1, U_{10}, U_{12}, U_{13}$

By inspecting the data we found that:

- U_{12} and U_{13} are roughly Normally distributed
- U_1 is not Normally distributed
- U_{10} is binary

By using SHAP we found that:

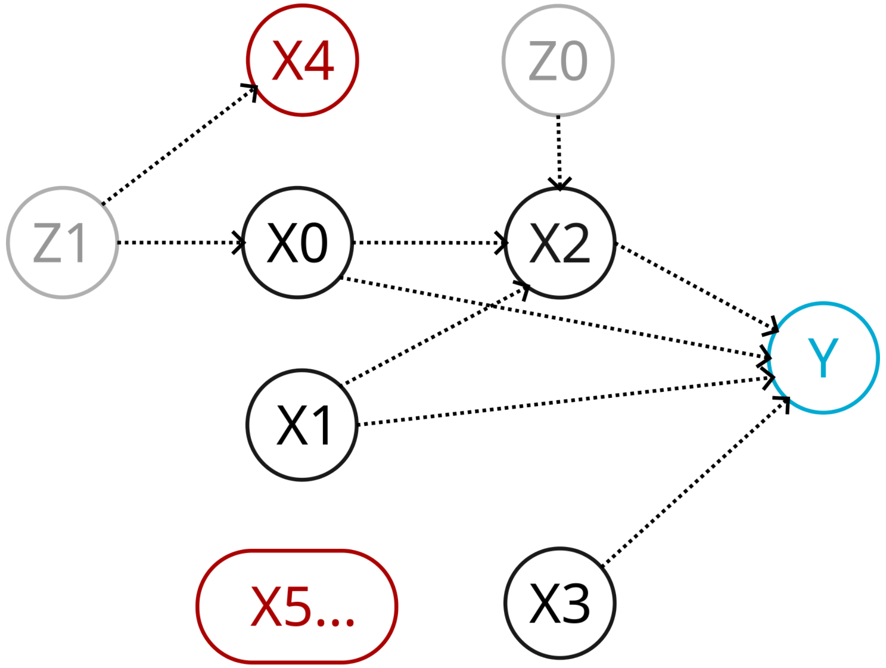
- U_{13} has a mostly monotonic effect
- U_{12} has a complex effect, which seems to be modulated by U_{10}
- U_1 seems to have mostly an anti-monotonic effect

We can now inspect the ground truth process

So we can check whether our results actually hold

Checking the Ground Truth

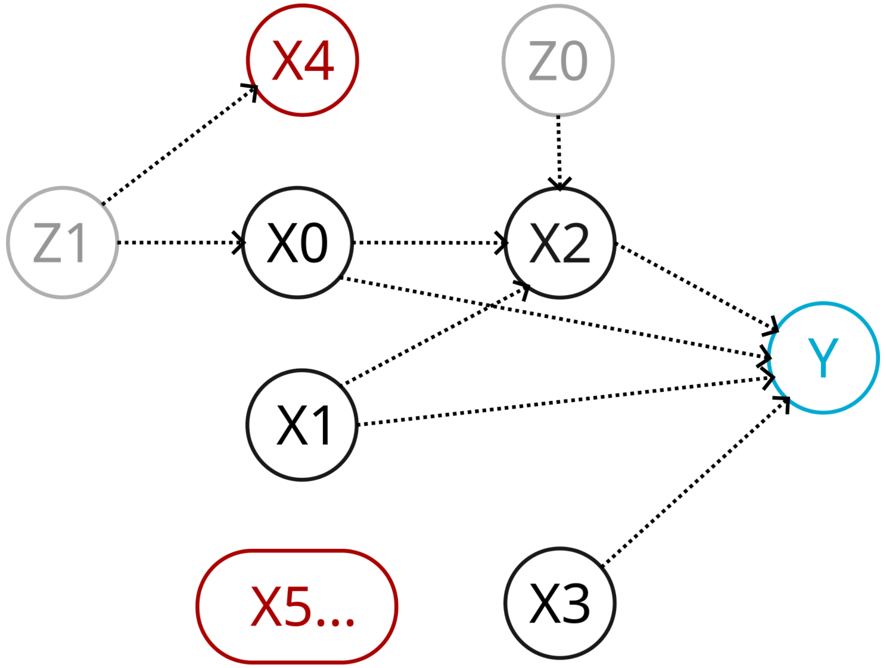
The ground-truth process is described by this causal graph:



- The Y variable (in **blue**) is the target
- The variables in **black** are those that are relevant
- The variables in **gray** are not observable, i.e. latent
- The variables in **red** are irrelevant

Checking the Ground Truth

The process was engineered to contain several classical cases



X_2 is a mediator beween X_0, X_1 and Y

- The variable partially hides the effect of X_0 and X_1
- If it does that completely, even Boruta cannot mark X_0 and X_1 as important
- Depending on the use case, this might be an issue

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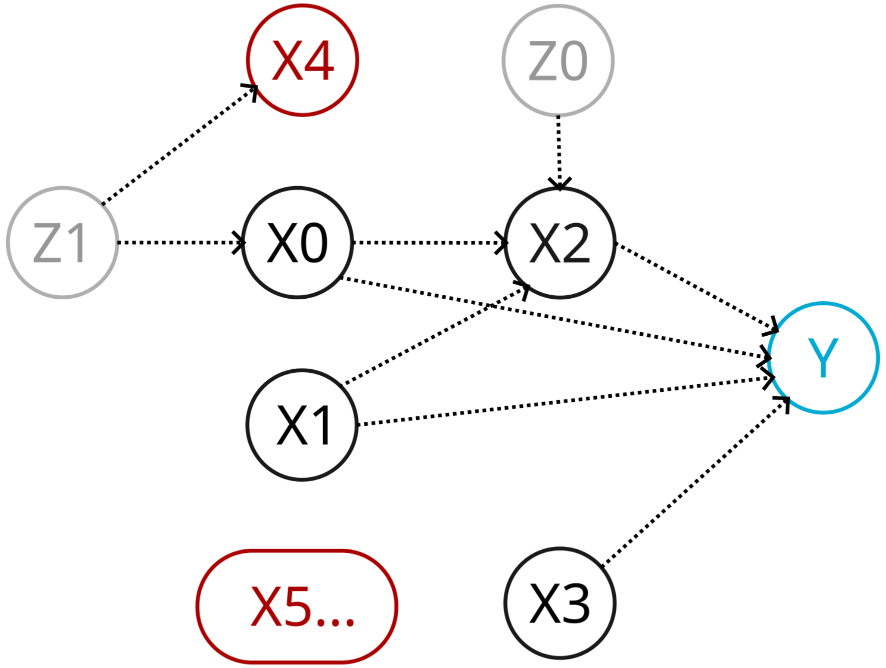
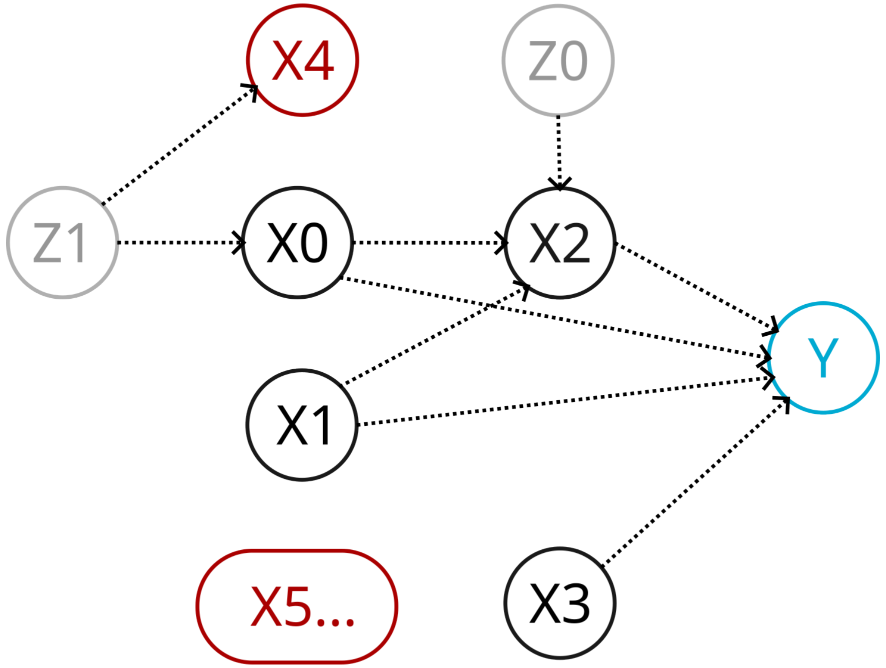


X_2 is also a complete mediator for Z_0

- ...But in this case it is a good thing!
- Z_0 is not observed, but we can account for that at least indirectly

Checking the Ground Truth

The process was engineered to contain several classical cases



Z_1 is a confounder and causes a correlation between X_1 and X_0

- It is totally mediated by X_1, which is a good thing
- ...But it also causes a correlation between X_0 and X_4
- This might trick a model into considering X_4 as important

Checking the Ground Truth

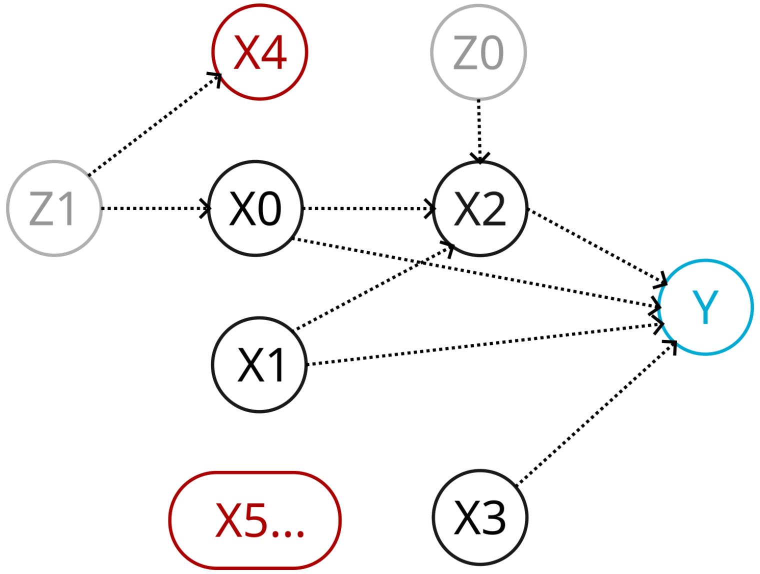
In detail, the data is generated as follows:

$$\begin{aligned}
Z_0 &\sim \mathcal{N}(\mu = 0, \sigma = 1.5) \\
Z_1 &\sim \mathcal{N}(\mu = 0, \sigma = 1) \\
X_0 &\sim \mathcal{N}(\mu = 0, \sigma = 1) + Z_1 \\
\log X_1 &\sim \mathcal{N}(\mu = 0, \sigma = 1) \\
X_2 &= {}^1/_2(X_0 + X_1) + Z_0 \\
X_3 &\sim B(p = 0.6) \\
\operatorname{logit}(Y) &\sim (-1 + 2X_3)X_2 + 0.4X_0 - 0.4X_1
\end{aligned}$$

- All other variables are follow either a Normal or Bernoulli distribution
- ...And they have sparse correlations among themselves

Checking the Ground Truth

Now let's check how accurate our importance estimate is:



In [37]:

```
print(f'The accepted feature are {X.columns[bfs.ranking_ == 1].values}')
print(f'...Which correspond to {[name_map[f] for f in X.columns[bfs.ranking_ == 1].values]}
```

```
The accepted feature are ['u1' 'u10' 'u12' 'u13']
...Which correspond to ['X1', 'X3', 'X2', 'X0']
```

What we Have Discovered

Now, let's check our findings, with the due substitutions:

- The relevant features are X_0, X_1, X_2, X_3 → **correct!**
- All claims on distributions → **mostly correct!**
  - X_2 is a sum of 3 variables, two of which are Normal
- X_0 has a mostly monotonic effect → **correct!**
  - Direct monotonic effect on Y + a complex one mediated by X_2
- X_1 has a mostly anti-monotonic effect → **correct!**
  - Direct anti-monotonic effect on Y + a complex one mediated by X_2
- X_2 has complex effect modulated by X_3 → **correct!**
  - X_3 decides the sign of the X_2 contribution

A Few Final Remarks

ML models are not just for prediction!

- They can be used for generation, anomaly detection, decision support
- ...And also as tools for a scientific analysis!

Explainability is an important topic in AI

- It is one of the main approaches to make an AI model transparent
- This critical when AI systems need to interact with human users
- ...And for some domains it is also required by existing regulations

Beware of correlated features

- Strongly correlated features (e.g mediated-mediator) may mislead algorithms
- Dealing with those is still a partially open problem!