In [1]:
```
# ============================================================
# Notebook setup
# ============================================================

%load_ext autoreload
%autoreload 2

# Control figure size
figsize=(14, 4)

from util import util
from matplotlib import pyplot as plt
import numpy as np
import seaborn as sn
```

Biomedical Data Analysis

Biomedical Data Analysis

Assume we are contacted by a bio-medical lab

- They have collected data about patients with a certain condition
- ...And they want to get a better *understanding* of the involved process

Our Dataset

This use case is based on a real-world example

...But for privacy and simplicity reasons we are going to use synthetic data

In [3]:
```
data, name_map = util.generate_data(size=500, seed=42)
data
```

Out[3]:

	u0	u1	u2	u3	u4	u5	u6	u7	u8
0	0.0	4.052587	0.0	0.0	1.069842	-0.744702	0.984682	2.069759	-0.859787
1	0.0	2.520945	1.0	0.0	-1.924131	-2.340844	4.663292	-1.633941	-0.322910
2	0.0	1.061444	0.0	1.0	0.288059	-1.550216	2.641967	0.823806	1.408493
3	1.0	0.523647	1.0	1.0	1.824137	-3.052719	4.099077	-2.287757	0.293904
4	0.0	2.010178	0.0	0.0	-0.050319	-1.734852	3.162254	-0.803245	-1.318084
...	...	...	...	...	...	...	...	...	...
495	1.0	7.434214	1.0	1.0	-1.948899	-2.436769	2.303599	0.505025	2.199709
496	0.0	7.857776	1.0	0.0	0.239719	-0.604961	2.301580	-1.150514	-0.416341
497	1.0	3.348010	0.0	0.0	0.147685	-2.913812	2.887376	-0.372831	0.630228
498	1.0	2.784484	0.0	0.0	-2.082640	-1.505432	4.271790	-0.269379	0.882540
499	1.0	1.808553	1.0	0.0	-2.458112	-0.539921	3.231171	-2.915948	0.373485

500 rows × 16 columns

How do we start?

Our Dataset

Let's have a first look at the dataset

In [4]:

```
data.describe()
```

Out[4]:

	u0	u1	u2	u3	u4	u5
count	500.000000	500.000000	500.000000	500.000000	500.000000	500.000000
mean	0.396000	1.828261	0.514000	0.330000	-0.030795	-1.435561
std	0.489554	2.112032	0.500305	0.470684	1.440194	0.964821
min	0.000000	0.055230	0.000000	0.000000	-4.699421	-4.185974
25%	0.000000	0.547481	0.000000	0.000000	-1.034566	-2.131690
50%	0.000000	1.127278	1.000000	0.000000	0.023120	-1.446049
75%	1.000000	2.127061	1.000000	1.000000	0.927888	-0.754598
max	1.000000	13.486418	1.000000	1.000000	3.747794	1.144399

- There is one target binary variable Y, representing the condition under study
- All other columns represent potentially correlate variables
- We are going to refer to them as "potential correlates"

Categorial and Numerical Variables

Some of the potential correlates are numeric, others are categorical

In [5]:
```
num_cols = [c for c in data.columns[:-1] if len(data[c].unique()) > 2]
cat_cols = [c for c in data.columns[:-1] if len(data[c].unique()) == 2]
print(f'Numeric: {num_cols}')
print(f'Categorical: {cat_cols}')
```

```
Numeric: ['u1', 'u4', 'u5', 'u6', 'u7', 'u8', 'u9', 'u12', 'u13']
Categorical: ['u0', 'u2', 'u3', 'u10', 'u11', 'u14']
```

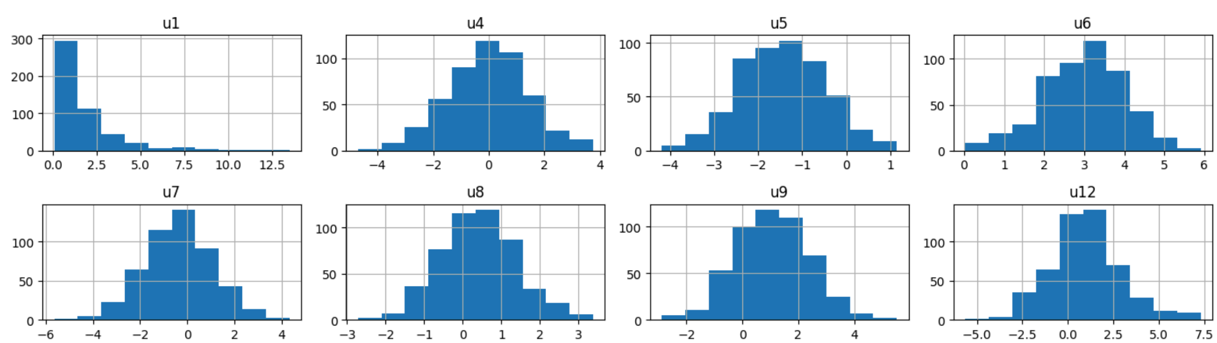
- In this synthetic dataset, all categorical variables are binary
- ...Which explains the simple filter we used to identify them

In a real world setting, you'd need to talk to a domain expert for this

Checking the Distributions

Let's check the distribution of the *numerical* candidate correlates

In [6]:
```
_, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(num_cols)//2)), figsiz
for ax, cname in zip(axes.ravel(), num_cols):
    data.hist(cname, ax=ax)
plt.tight_layout()
```

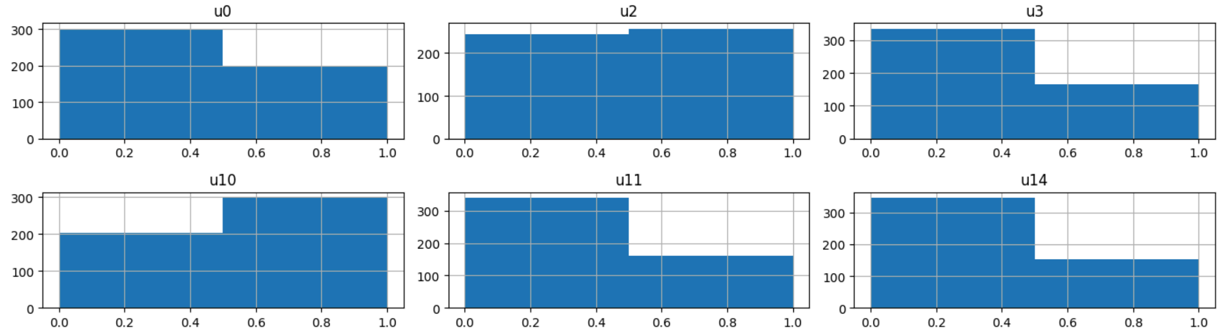


Most of them seem to follow a Normal distribution

Checking the Distributions

Let's check the distribution of the *binary* candidate correlates

In [7]:
```
_, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(cat_cols)//2)), figsiz
for ax, cname in zip(axes.ravel(), cat_cols):
    data.hist(cname, ax=ax, bins=2)
plt.tight_layout()
```

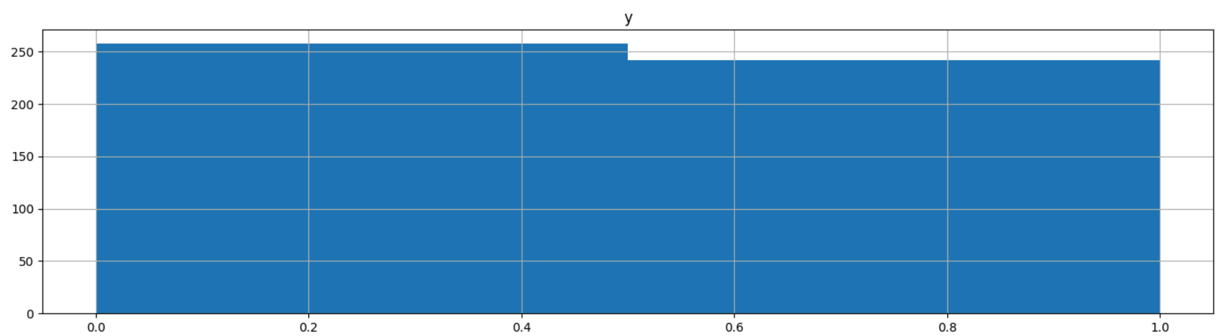


Some are well balanced, othere less so

Checking the Distributions

Let's check the *target* distribution

In [8]:
```
data.hist('y', bins=2, figsize=figsize)
plt.tight_layout()
```

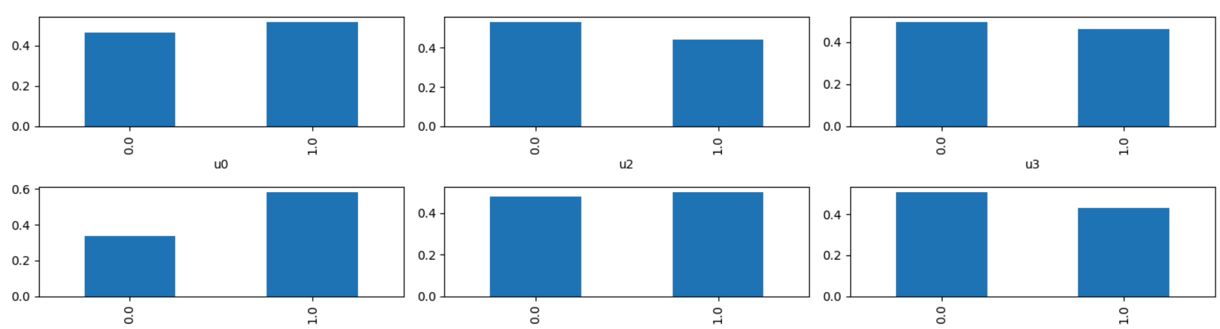


The target distribution is quite balanced

Checking Univariate Dependencies

Let's check the fraction of $Y = 1$ for the *categorical* candidates

In [9]:
```
_, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(cat_cols)//2)), figsiz
for ax, cname in zip(axes.ravel(), cat_cols):
    data.groupby(cname)['y'].mean().plot.bar(ax=ax)
plt.tight_layout()
```

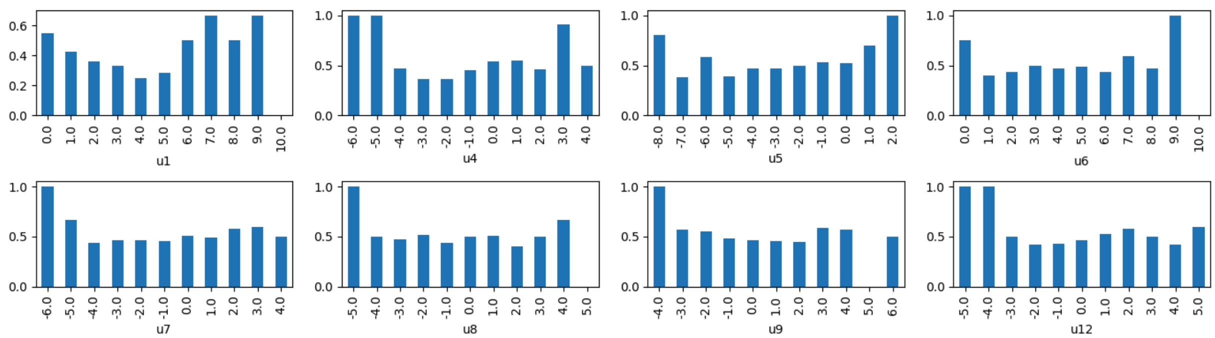


A few of them seems to have a correlation, other cases are less clear

Checking Univariate Dependencies

Let's check the fraction of $y = 1$ for the *numerical* candidates

In [10]:
```
_, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(num_cols)//2)), figsiz
for ax, cname in zip(axes.ravel(), num_cols):
    bin_size = (data[cname].max() - data[cname].min()) / 10
    data['y'].groupby(data[cname] // bin_size).mean().plot.bar(ax=ax)
plt.tight_layout()
```



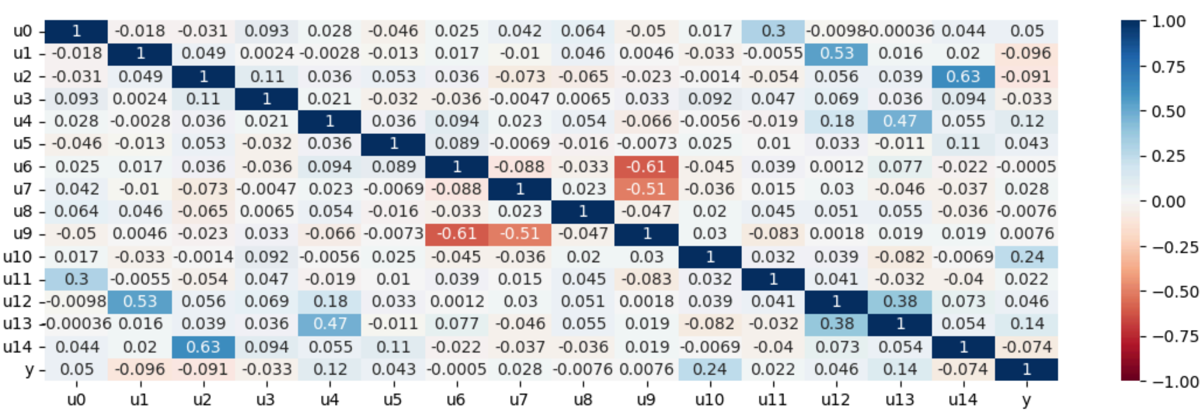
Most of them appear to have some non-linear correlation

Checking Linear Correlations

It's worth checking how all features are correlated

One way to do it is by plotting a correlation matrix (e.g. Pearson)

In [11]:
```
plt.figure(figsize=figsize)
sn.heatmap(data.corr(method='pearson'), annot=True, vmin=-1, vmax=1, cmap='F
```



- Sparse correlations in general, weak (linear) correlations for Y

So far we have just inspected our dataset, but...
what is exactly our goal?

Use Case Objective

Unlike in classical ML tasks, we don't have an *estimation* problem

Rather, our goal is *understanding* the process behind the data

- We want to identify the true *correlates* among our candidates
- We want to see *how* they are linked to the target y

In an ideal world, we'd like to know about *causal* relationships

...But in practice, we'll need to be happy with correlations

- Studying causality is indeed possible (a good start is Judea Pearl's book)
- ...But also very challenging, and there's no general and real-world ready tool available

So, we'll count on the domain expert to check the correlations

Use Case Objective

Our setup also explains a quirk in the dataset

All variables except the target are called U_j, for "unknown"

- This is synthetic data, so nothing is really unknown
- In fact, the ground truth process linking Y to U is avaialable

However, for the sake of the lecture, such process will be hidden

- We will analyze the data pretending we have no such knowledge
- *At the end* of our exercise we'll check the ground truth

...And we'll see how close we got to the truth!