Biomedical Data Analysis

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Assume we are concated 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 [35]:
```python
data, name_map = util.generate_data(size=500, seed=42)
data
```

Out[35]:

	u0	u1	u2	u3	u4	u5	u6	u7	u8	u9	u10	u11	u12	u13	u1
0	0.0	4.052587	0.0	0.0	1.069842	-0.744702	0.984682	2.069759	-0.859787	1.615419	1.0	0.0	3.905281	1.422892	0.
1	0.0	2.520945	1.0	0.0	-1.924131	-2.340844	4.663292	-1.633941	-0.322910	0.426927	1.0	0.0	1.319270	1.771152	0.
2	0.0	1.061444	0.0	1.0	0.288059	-1.550216	2.641967	0.823806	1.408493	1.498628	1.0	0.0	-1.072016	-0.750879	0.
3	1.0	0.523647	1.0	1.0	1.824137	-3.052719	4.099077	-2.287757	0.293904	1.628930	1.0	1.0	1.299762	2.085999	1.
4	0.0	2.010178	0.0	0.0	-0.050319	-1.734852	3.162254	-0.803245	-1.318084	0.507807	0.0	0.0	0.307414	-0.884796	0.
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	
495	1.0	7.434214	1.0	1.0	-1.948899	-2.436769	2.303599	0.505025	2.199709	1.713777	1.0	0.0	5.451237	0.257810	1.
496	0.0	7.857776	1.0	0.0	0.239719	-0.604961	2.301580	-1.150514	-0.416341	2.100331	0.0	0.0	4.269326	0.760440	0.
497	1.0	3.348010	0.0	0.0	0.147685	-2.913812	2.887376	-0.372831	0.630228	0.967976	0.0	0.0	0.576445	0.450504	0.
498	1.0	2.784484	0.0	0.0	-2.082640	-1.505432	4.271790	-0.269379	0.882540	0.745919	1.0	1.0	0.424243	-1.446797	0.
499	1.0	1.808553	1.0	0.0	-2.458112	-0.539921	3.231171	-2.915948	0.373485	2.988293	1.0	1.0	-0.618186	-0.810217	1.

500 rows × 16 columns

How do we start?

Our Dataset

Let's have a first look at the dataset

In [64]:
```
data.describe()
```

Out[64]:

	u0	u1	u2	u3	u4	u5	u6	u7	u8	
count	500.000000	500.000000	500.000000	500.000000	500.000000	500.000000	500.000000	500.000000	500.000000	500.0000
mean	0.396000	1.828261	0.514000	0.330000	-0.030795	-1.435561	2.995727	-0.361947	0.418395	1.0805
std	0.489554	2.112032	0.500305	0.470684	1.440194	0.964821	1.008219	1.463672	0.977034	1.3008
min	0.000000	0.055230	0.000000	0.000000	-4.699421	-4.185974	0.033381	-5.647642	-2.714647	-2.8838
25%	0.000000	0.547481	0.000000	0.000000	-1.034566	-2.131690	2.289419	-1.295046	-0.244845	0.1887
50%	0.000000	1.127278	1.000000	0.000000	0.023120	-1.446049	3.044132	-0.320448	0.376119	1.0583
75%	1.000000	2.127061	1.000000	1.000000	0.927888	-0.754598	3.714111	0.561467	1.077532	1.9744
max	1.000000	13.486418	1.000000	1.000000	3.747794	1.144399	5.906263	4.334036	3.374752	5.5265

- 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"
- They are called U, which stands for "unknown"

Categorial and Numerical Variables

Some of the potential correlates are numeric, others are categorical

```
In [65]: # Identify numeric and categorical columns
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: {num_cols}')
```

```
Numeric: ['u1', 'u4', 'u5', 'u6', 'u7', 'u8', 'u9', 'u12', 'u13']
Categorical: ['u1', 'u4', 'u5', 'u6', 'u7', 'u8', 'u9', 'u12', 'u13']
```

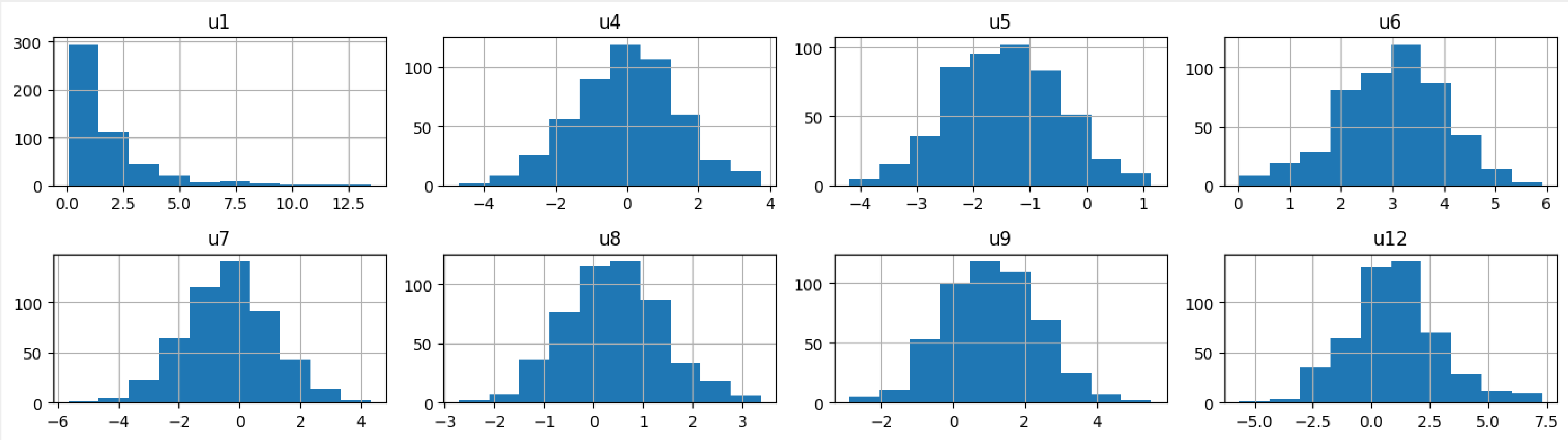
- In this synthetic dataset, all categorical variables are binary
- ...Which explains the simple filter we used to identify them

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 [66]:
```
_, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(num_cols)//2)), figsize=figsize)
for ax, cname in zip(axes.ravel(), num_cols):
    data.hist(cname, ax=ax)
plt.tight_layout()
```



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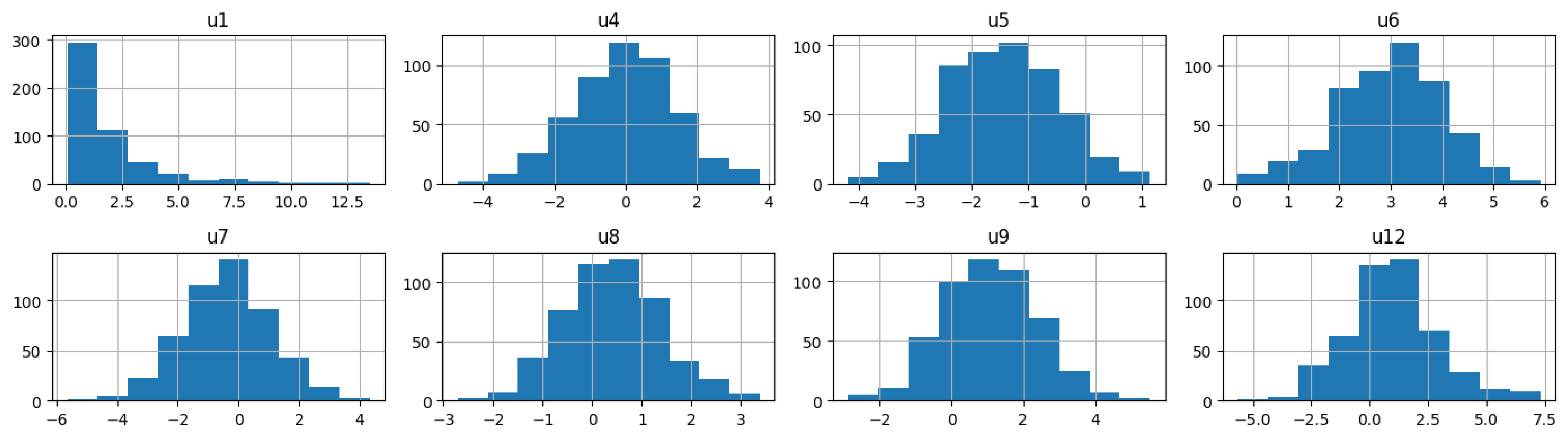

Most of them seem to follow a Normal distribution

Checking the Distributions

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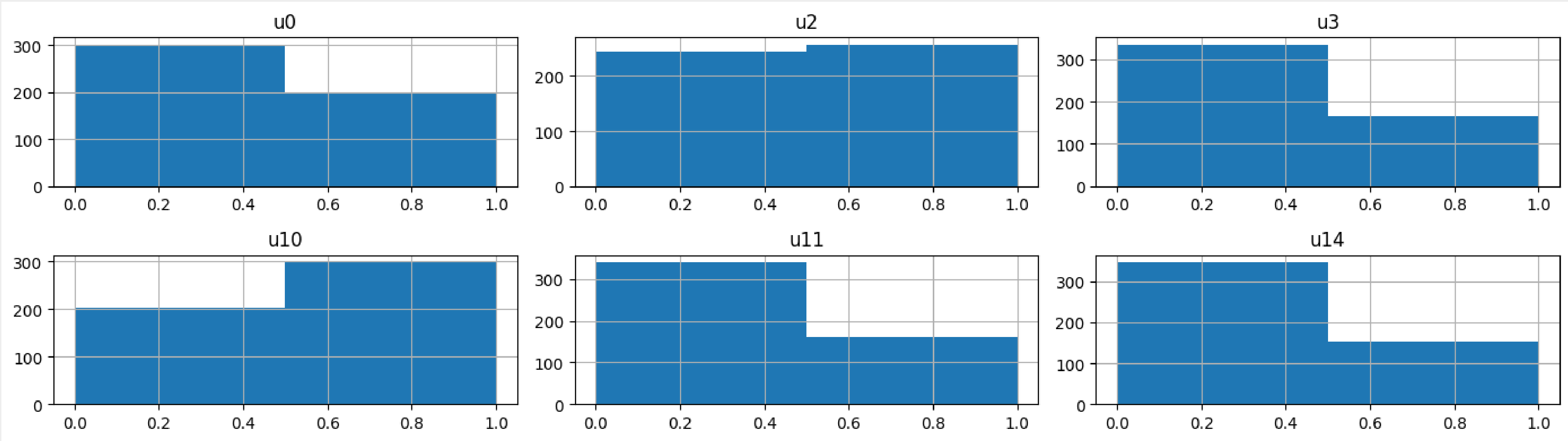
for ax, cname in zip(axes.ravel(), cat_cols):
    data.hist(cname, ax=ax, bins=2)
plt.tight_layout()
```



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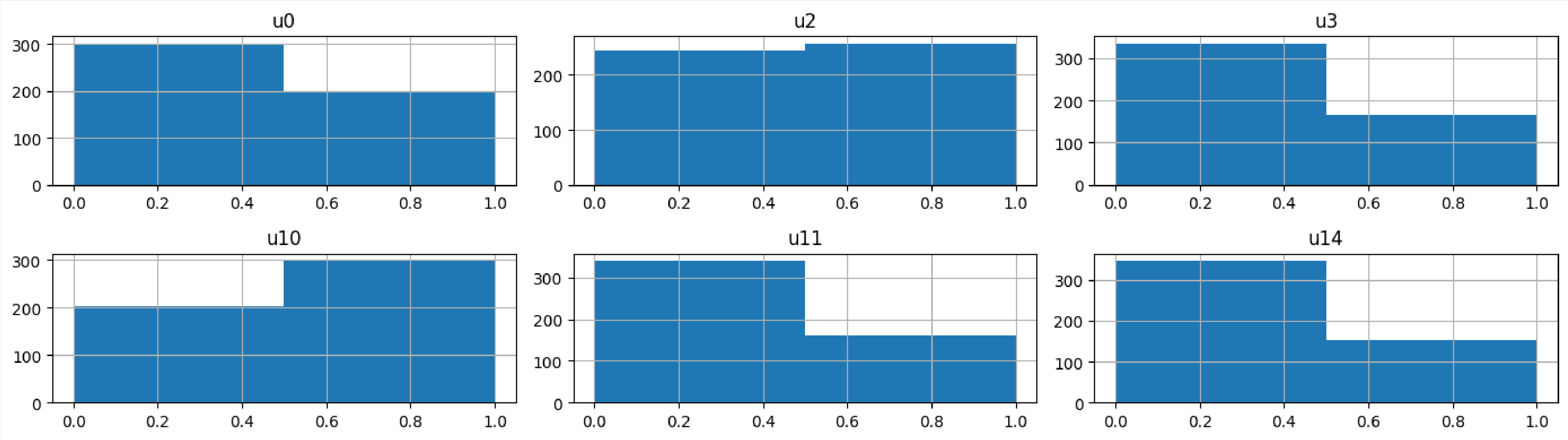
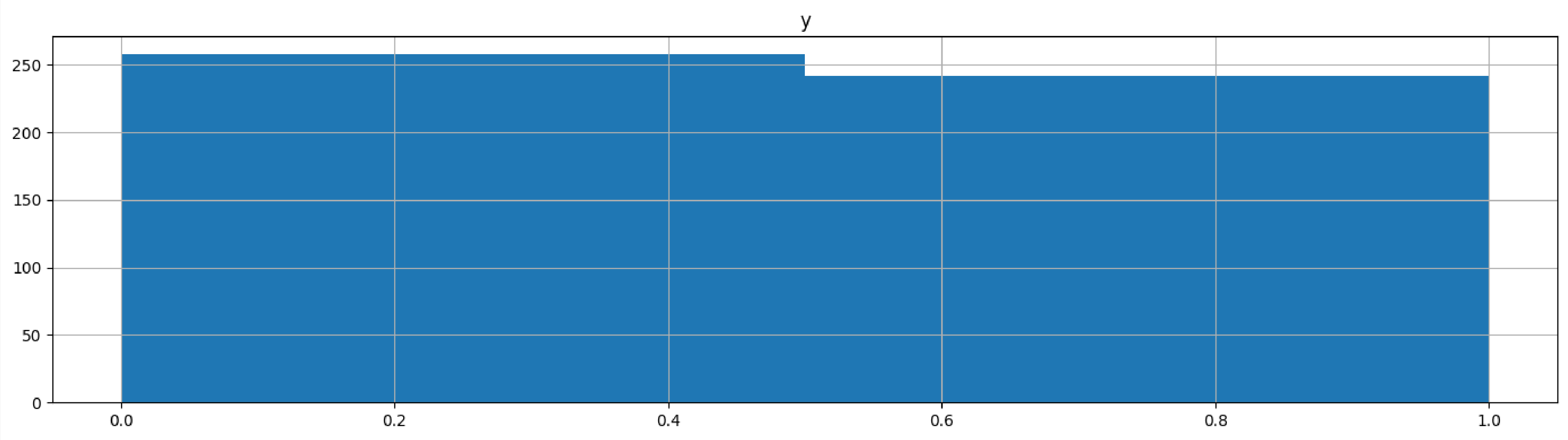


Some are well balanced, othere less so

Checking the Distributions

Let's check the target distribution

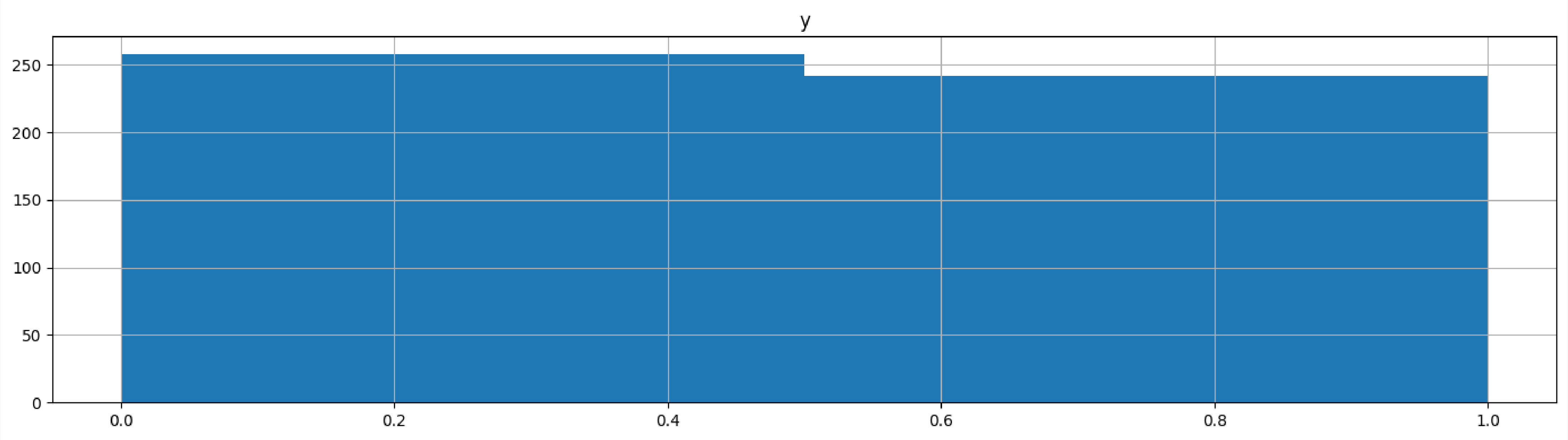
In [53]:
```
data.hist('y', bins=2, figsize=figsize)
plt.tight_layout()
```



Checking the Distributions

Let's check the target distribution

```
In [53]: data.hist('y', bins=2, figsize=figsize)
         plt.tight_layout()
```

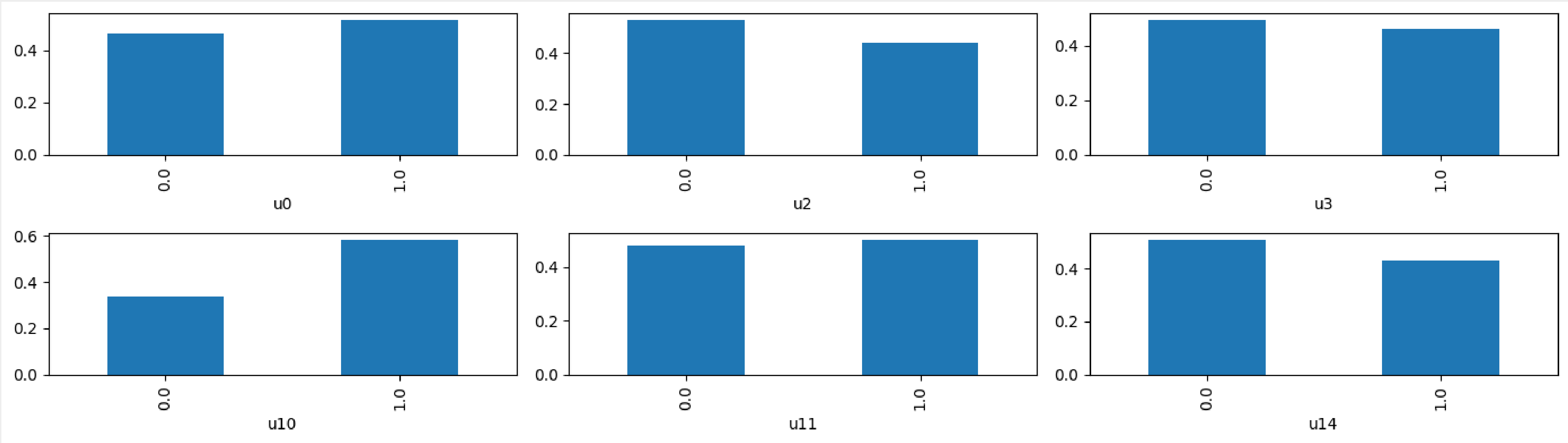


The target distribution quite balanced

Checking Univariate Dependencies

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

In [56]:
```
_, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(cat_cols)//2)), figsize=figsize)
for ax, cname in zip(axes.ravel(), cat_cols):
    data.groupby(cname)['y'].mean().plot.bar(ax=ax)
plt.tight_layout()
```



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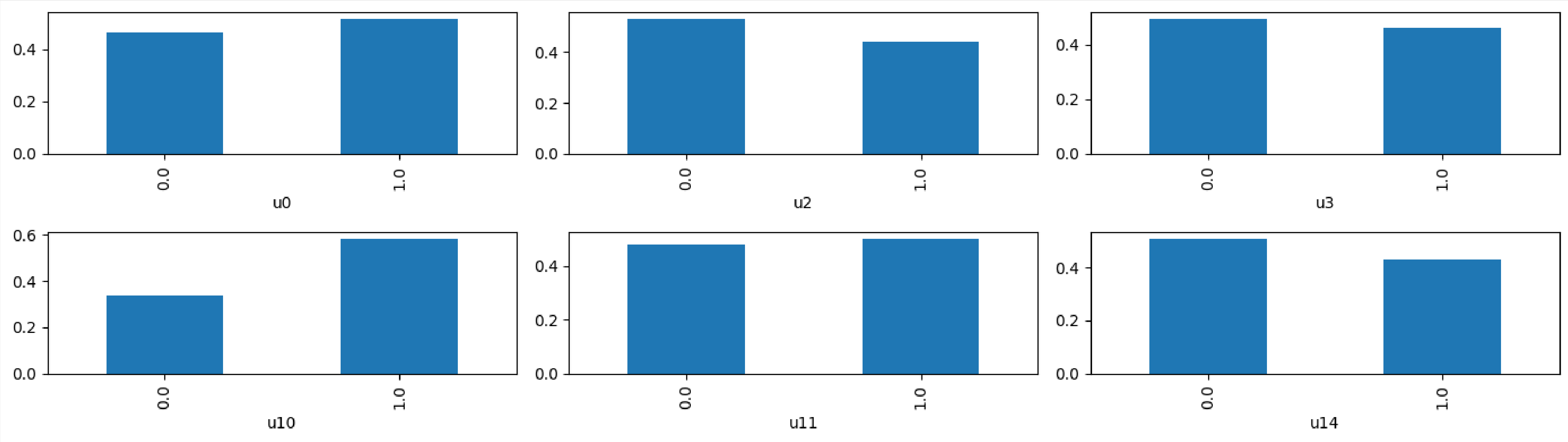
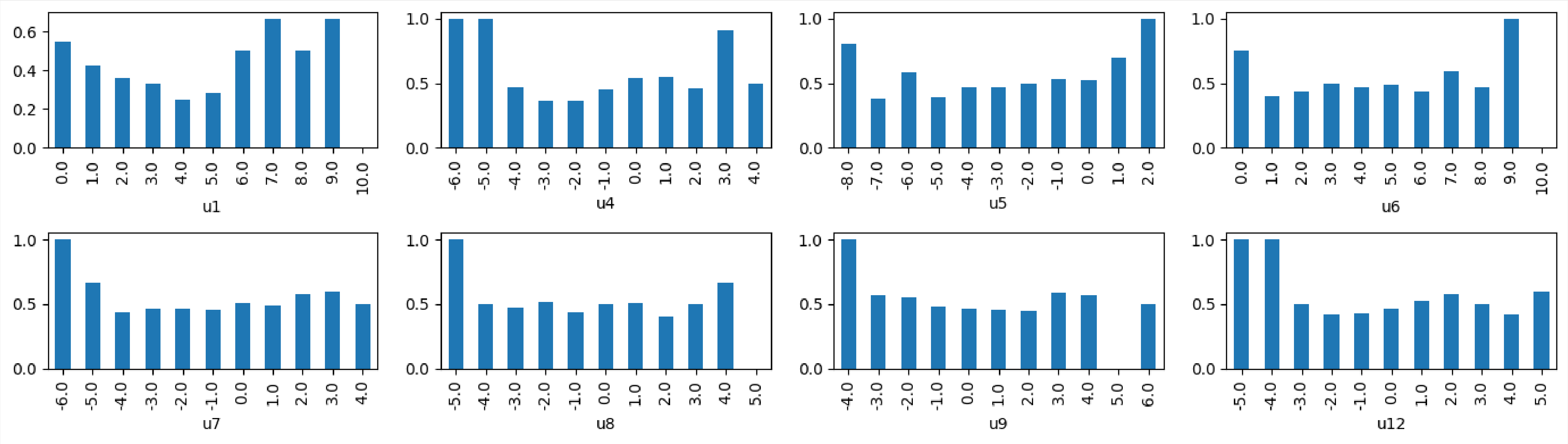


A few of them seems to have a correlation, other cases are less clear

Checking Univariate Dependencies

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

In [57]:
```
_, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(num_cols)//2)), figsize=figsize)
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()
```



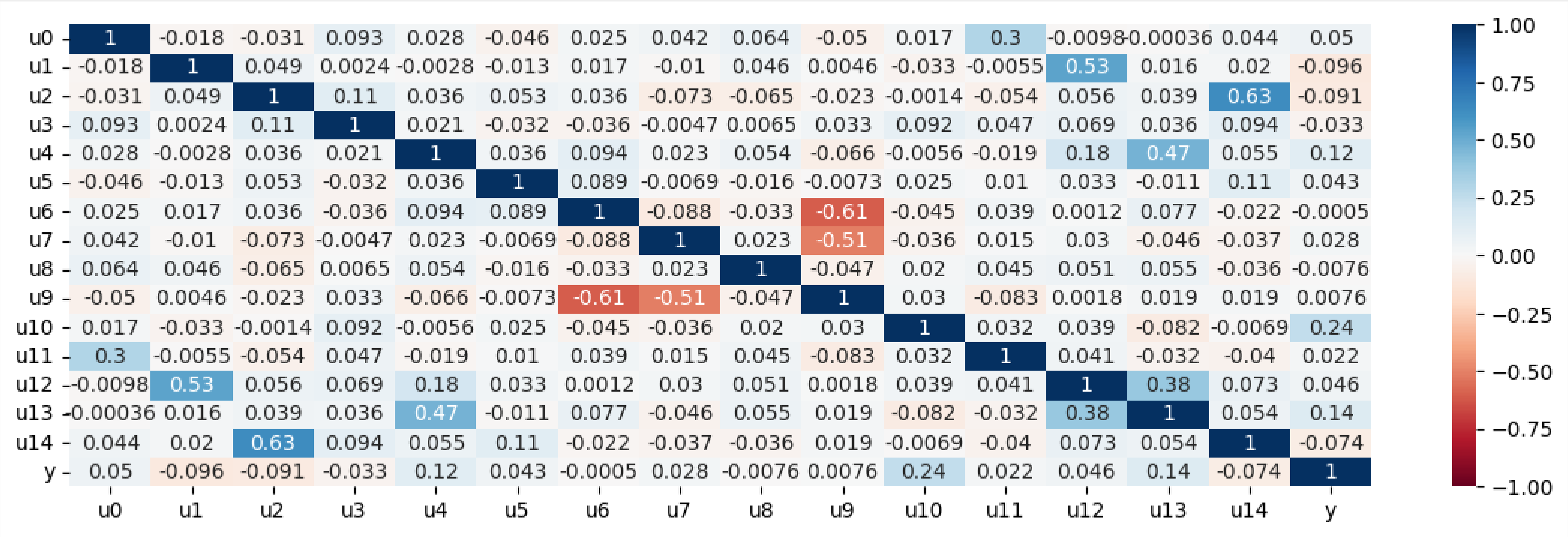
Most of them appear to have some non-linear correlation

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



- 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 a mature tool available

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