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 [2]:
```
data, name_map = util.generate_data(size=500, seed=42)
data
```

Out[2]:

	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 [3]: data.describe()
```

Out[3]:

	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	1.08053
std	0.489554	2.112032	0.500305	0.470684	1.440194	0.964821	1.008219	1.463672	0.977034	1.30085
min	0.000000	0.055230	0.000000	0.000000	-4.699421	-4.185974	0.033381	-5.647642	-2.714647	-2.88385
25%	0.000000	0.547481	0.000000	0.000000	-1.034566	-2.131690	2.289419	-1.295046	-0.244845	0.18874
50%	0.000000	1.127278	1.000000	0.000000	0.023120	-1.446049	3.044132	-0.320448	0.376119	1.05831
75%	1.000000	2.127061	1.000000	1.000000	0.927888	-0.754598	3.714111	0.561467	1.077532	1.97444
max	1.000000	13.486418	1.000000	1.000000	3.747794	1.144399	5.906263	4.334036	3.374752	5.52651

- 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 [4]: 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']
```

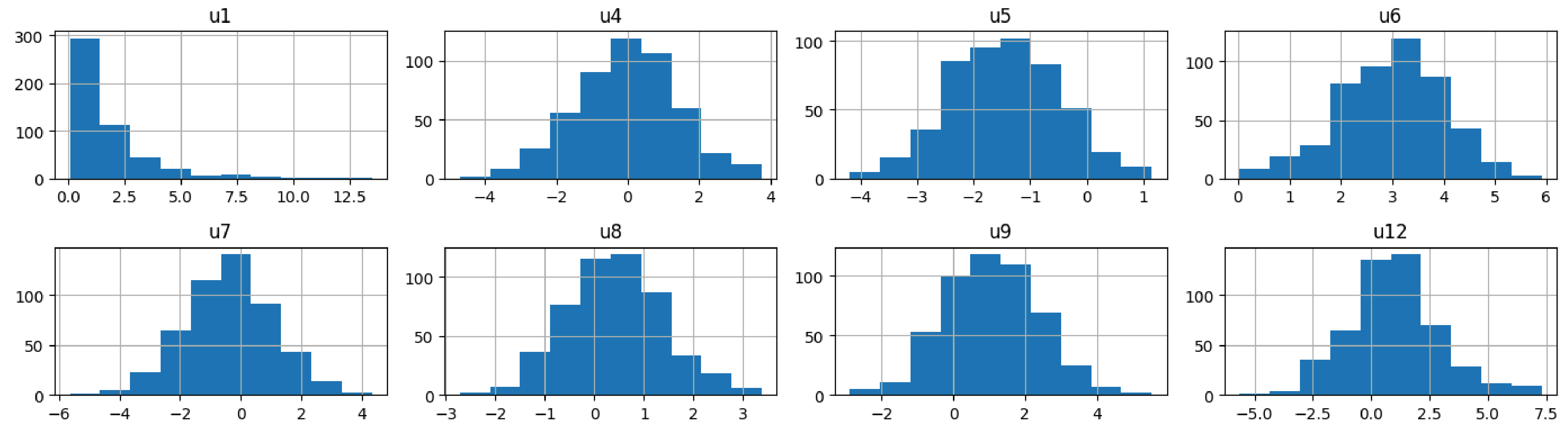
- In this synthetic dataset, all categorical variables are binary
- ...Which explains the simple filter we used to identify them

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 [5]: _, 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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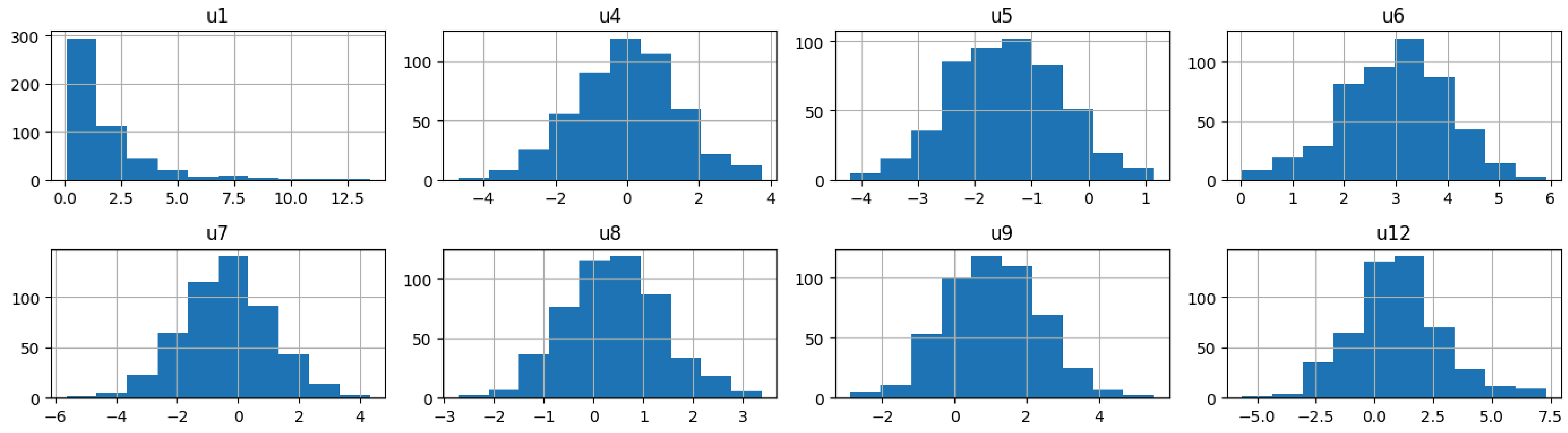
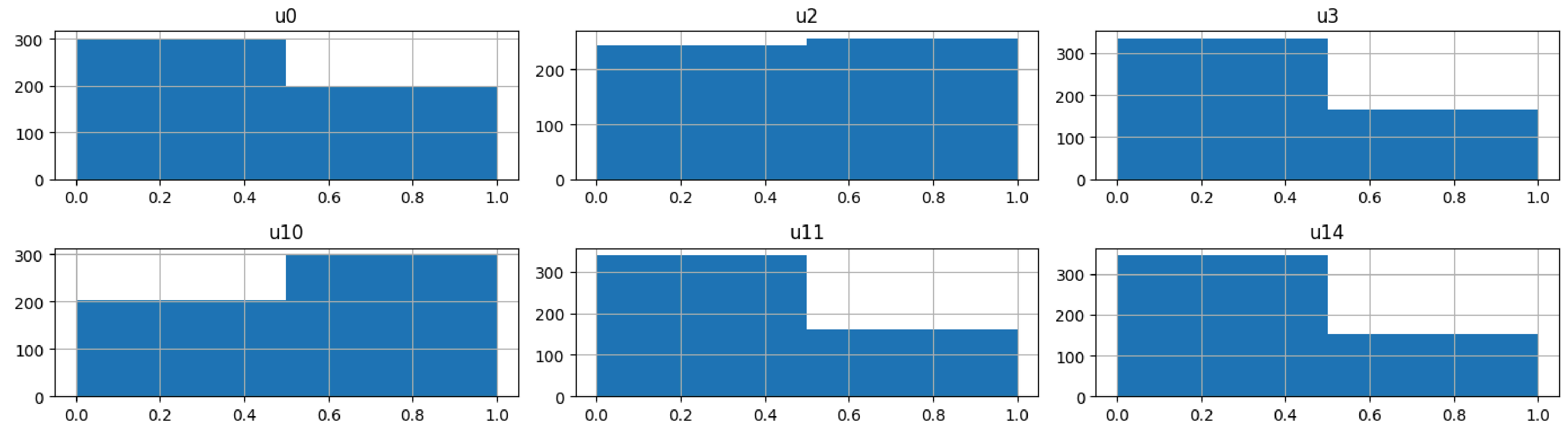


Most of them seem to follow a Normal distribution

Checking the Distributions

Let's check the distribution of the binary candidate correlates

```
In [6]: _, 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.hist(cname, ax=ax, bins=2)
        plt.tight_layout()
```



Checking the Distributions

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In [6]: _, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(cat_cols)//2)), figsize=figsize)
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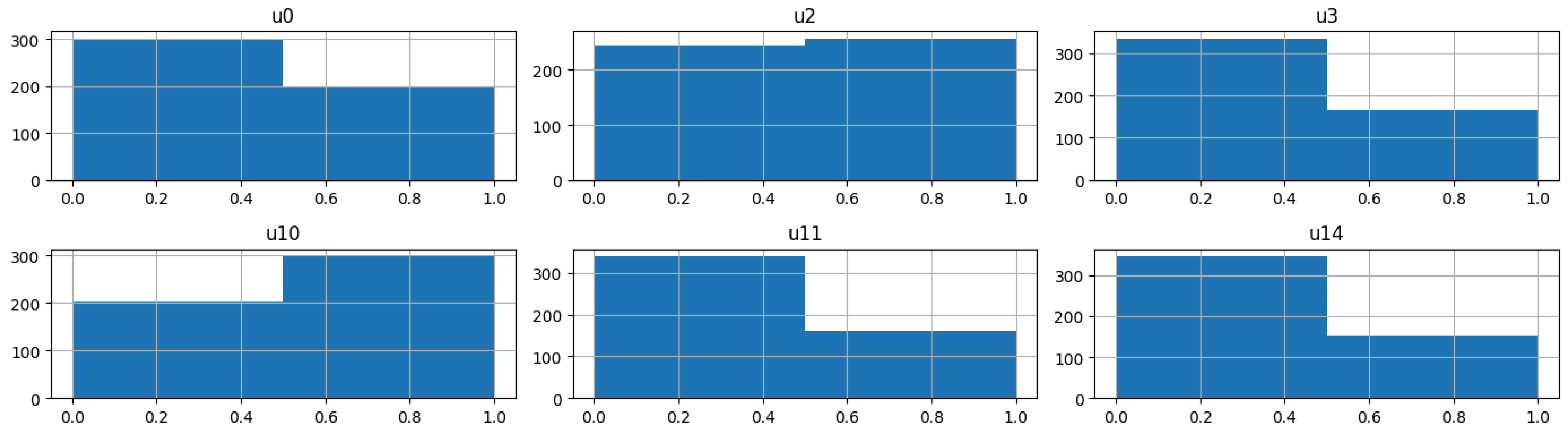
        plt.tight_layout()
```

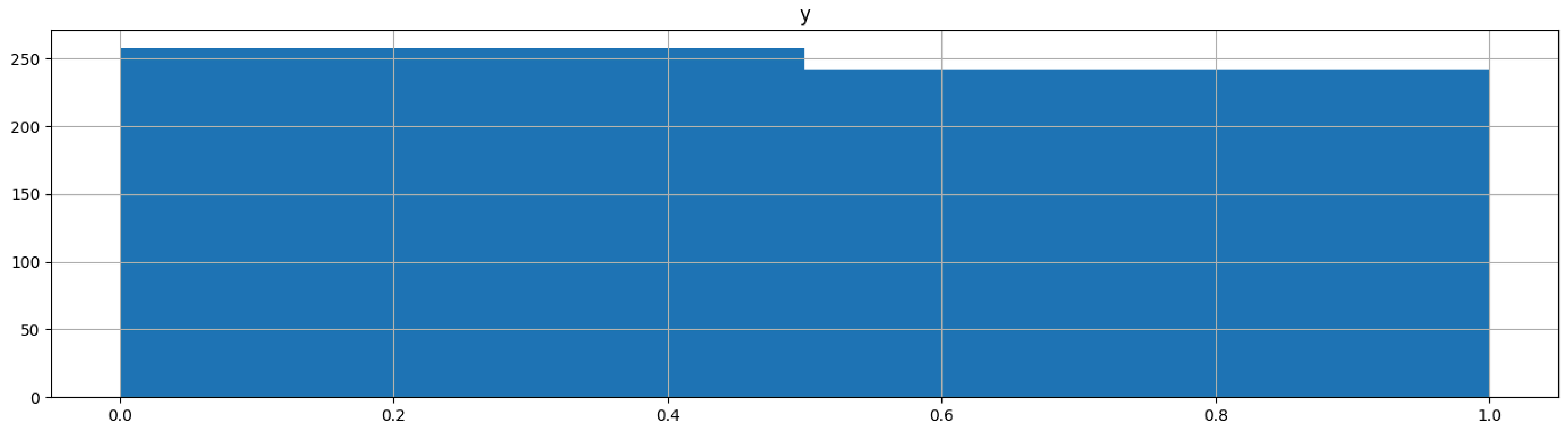


Some are well balanced, othere less so

Checking the Distributions

Let's check the target distribution

```
In [7]: data.hist('y', bins=2, figsize=figsize)
        plt.tight_layout()
```



Checking the Distributions

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In [7]: data.hist('y', bins=2, figsize=figsize)
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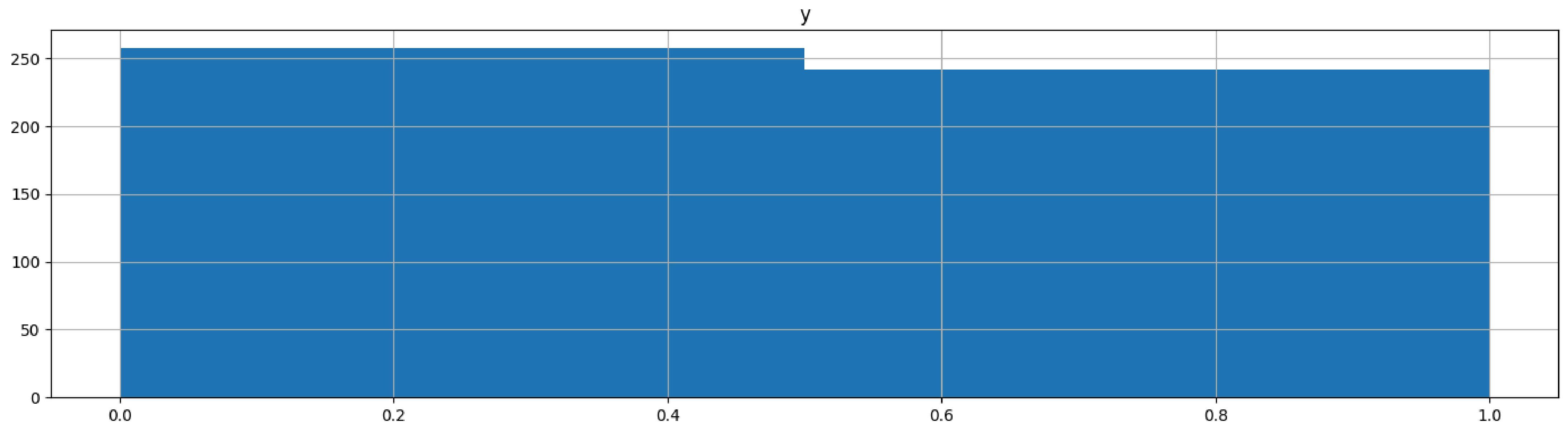
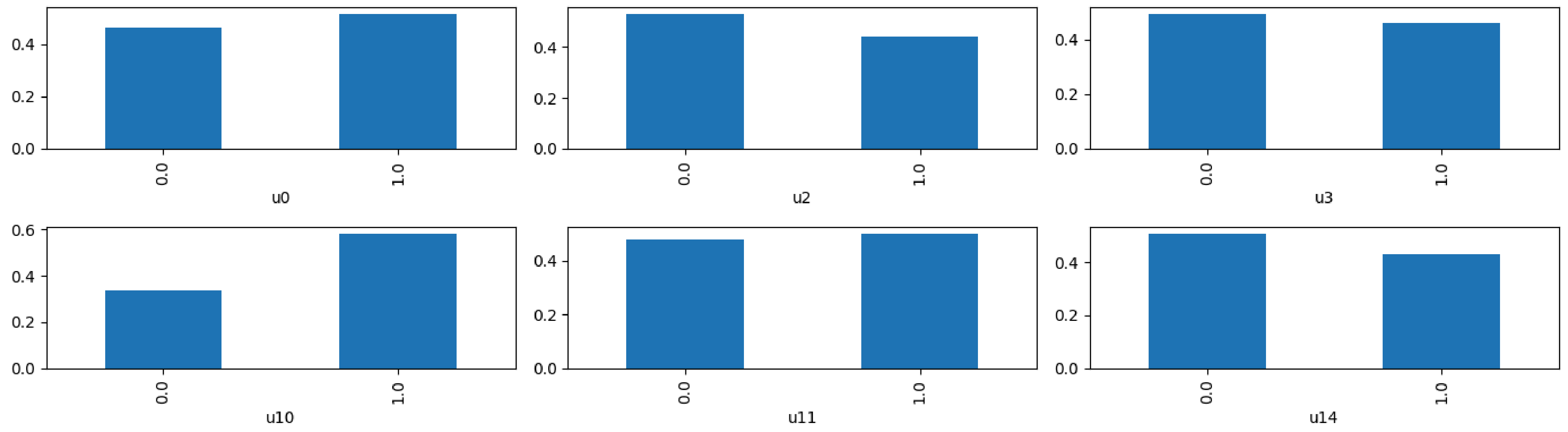


The target distribution is quite balanced

Checking Univariate Dependencies

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

```
In [8]: _, 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()
```



Checking Univariate Dependencies

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In [8]: _, axes = plt.subplots(nrows=2, ncols=int(np.ceil(len(cat_cols)//2)), figsize=figsize)
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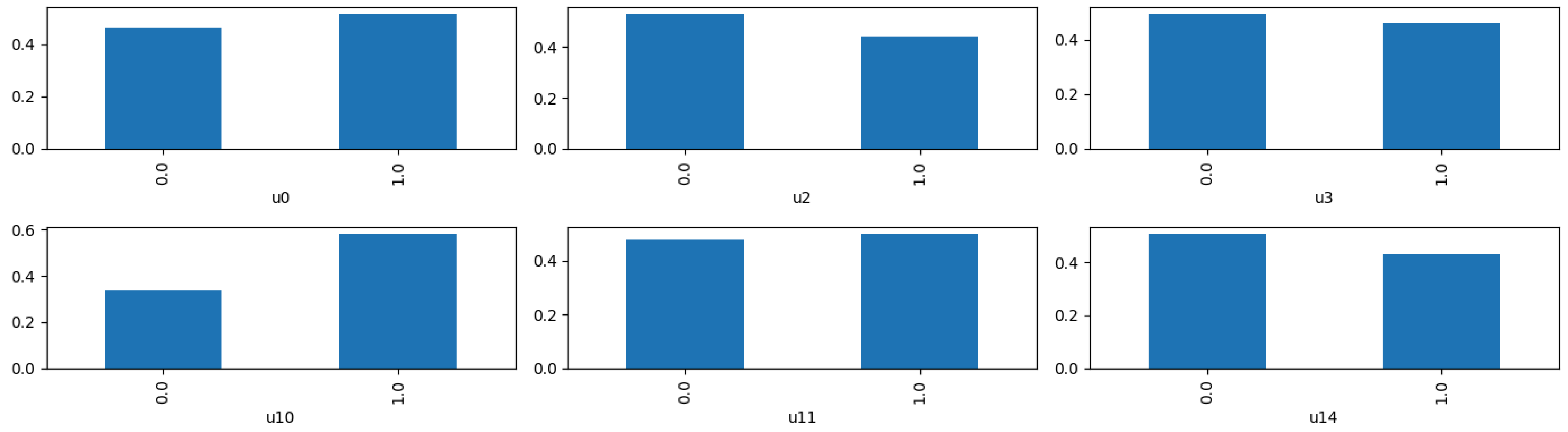
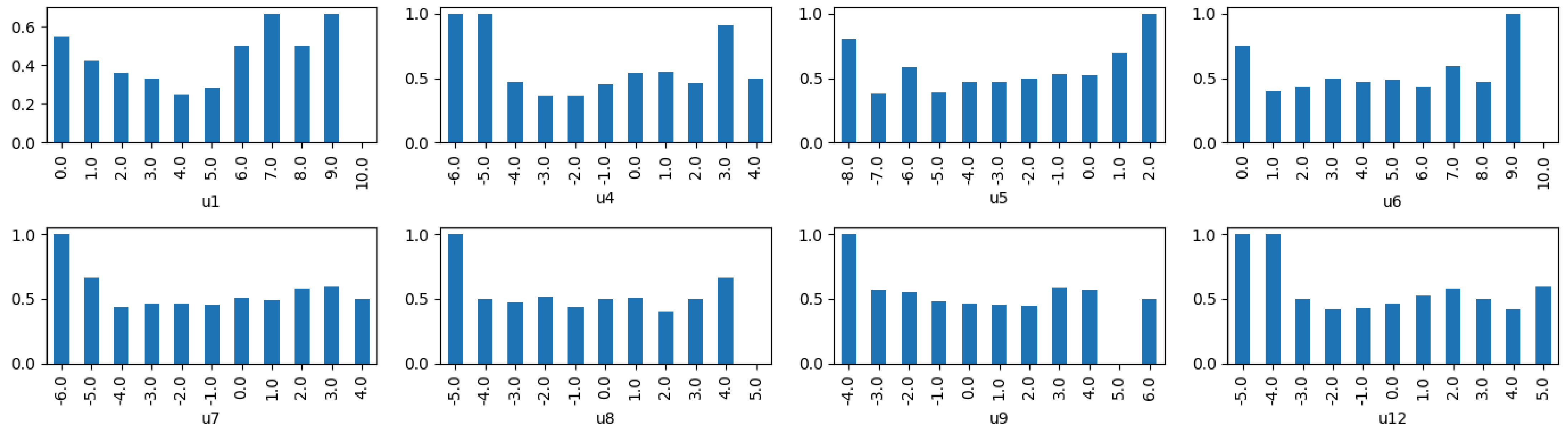


A few of them seems to have a correlation, other cases are less clear

Checking Univariate Dependencies

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

```
In [9]: _, 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()
```



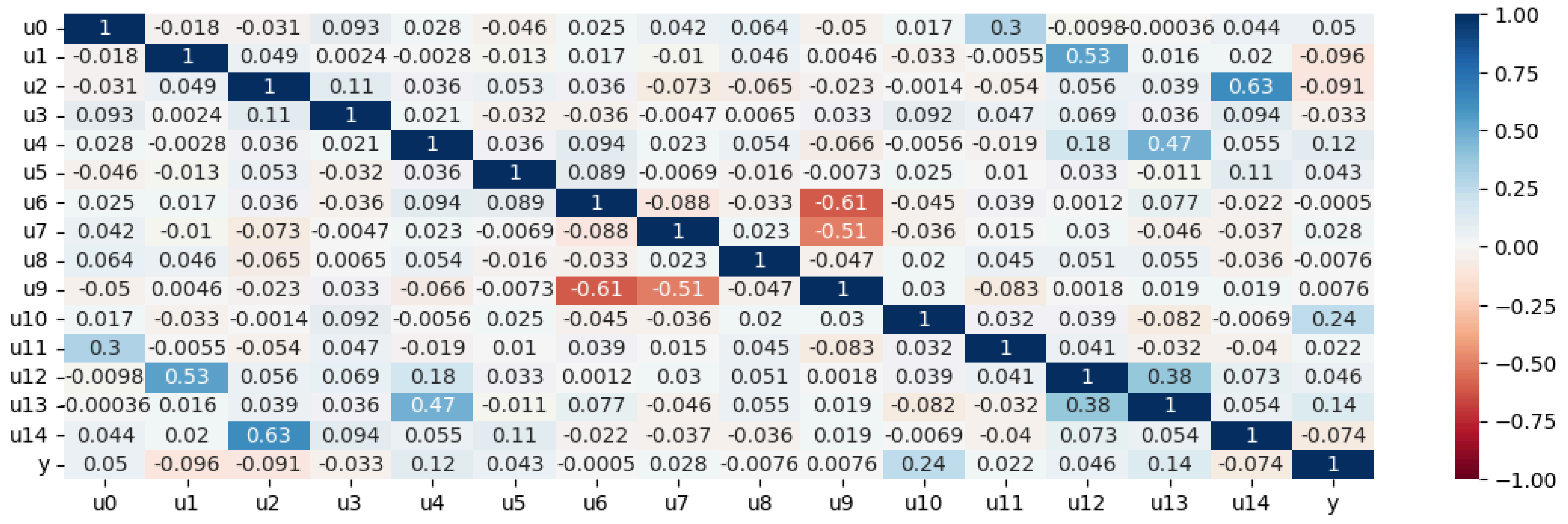
Most of them appear to have some non-linear correlation

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



	u0	u1	u2	u3	u4	u5	u6	u7	u8	u9	u10	u11	u12	u13	u14	y
u0	1	-0.018	-0.031	0.093	0.028	-0.046	0.025	0.042	0.064	-0.05	0.017	0.3	-0.0098	-0.00036	0.044	0.05
u1	-0.018	1	0.049	0.0024	-0.0028	-0.013	0.017	-0.01	0.046	0.0046	-0.033	-0.0055	0.53	0.016	0.02	-0.096
u2	-0.031	0.049	1	0.11	0.036	0.053	0.036	-0.073	-0.065	-0.023	-0.0014	-0.054	0.056	0.039	0.63	-0.091
u3	0.093	0.0024	0.11	1	0.021	-0.032	-0.036	-0.0047	0.0065	0.033	0.092	0.047	0.069	0.036	0.094	-0.033
u4	0.028	-0.0028	0.036	0.021	1	0.036	0.094	0.023	0.054	-0.066	-0.0056	-0.019	0.18	0.47	0.055	0.12
u5	-0.046	-0.013	0.053	-0.032	0.036	1	0.089	-0.0069	-0.016	-0.0073	0.025	0.01	0.033	-0.011	0.11	0.043
u6	0.025	0.017	0.036	-0.036	0.094	0.089	1	-0.088	-0.033	-0.61	-0.045	0.039	0.0012	0.077	-0.022	-0.0005
u7	0.042	-0.01	-0.073	-0.0047	0.023	-0.0069	-0.088	1	0.023	-0.51	-0.036	0.015	0.03	-0.046	-0.037	0.028
u8	0.064	0.046	-0.065	0.0065	0.054	-0.016	-0.033	0.023	1	-0.047	0.02	0.045	0.051	0.055	-0.036	-0.0076
u9	-0.05	0.0046	-0.023	0.033	-0.066	-0.0073	-0.61	-0.51	-0.047	1	0.03	-0.083	0.0018	0.019	0.019	0.0076
u10	0.017	-0.033	-0.0014	0.092	-0.0056	0.025	-0.045	-0.036	0.02	0.03	1	0.032	0.039	-0.082	-0.0069	0.24
u11	0.3	-0.0055	-0.054	0.047	-0.019	0.01	0.039	0.015	0.045	-0.083	0.032	1	0.041	-0.032	-0.04	0.022
u12	-0.0098	0.53	0.056	0.069	0.18	0.033	0.0012	0.03	0.051	0.0018	0.039	0.041	1	0.38	0.073	0.046
u13	-0.00036	0.016	0.039	0.036	0.47	-0.011	0.077	-0.046	0.055	0.019	-0.082	-0.032	0.38	1	0.054	0.14
u14	0.044	0.02	0.63	0.094	0.055	0.11	-0.022	-0.037	-0.036	0.019	-0.0069	-0.04	0.073	0.054	1	-0.074
y	0.05	-0.096	-0.091	-0.033	0.12	0.043	-0.0005	0.028	-0.0076	0.0076	0.24	0.022	0.046	0.14	-0.074	1

- 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!