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
import pandas as pd
from sklearn.model_selection import train_test_split
from sklearn.preprocessing import StandardScaler
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import roc_auc_score
from sklearn.model_selection import GridSearchCV

# Generate synthetic data
data, name_map = util.generate_data(size=500, seed=42)
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]
```

A Baseline Approach

A Baseline Approach

Our goal is *understading* the process behind the data

Of of many possible ways to do it consist in:

- Training an approximate model via Machine Learning
- Studying the model as a proxy for the real process

> **Basically, we use a ML model as an *analysis tool***

For this approach to work, we need the ML model to be *explainable*

- A few model naturally enjoy this property (e.g. linear models, simple DTs)
- Explaining other models is not obvious (e.g. Neural Networks, large ensembles)

We will start with the simplest option: Logistic Regression

Data Preprocessing

We start with the usual data preprocessing

We will treat all candidate correlates as inputs

In [2]:
```
# Input-output separation
X, y = data[data.columns[:-1]].copy(), data[data.columns[-1]].copy()
# Train-test split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, rar
# Input standardization
scaler = StandardScaler()
X_train[num_cols] = scaler.fit_transform(X_train[num_cols])
X_test[num_cols] = scaler.transform(X_test[num_cols])
```

Even if we don't care about estimates, we need a *test/validation set*

- This will allow us to check the model for overfitting

We also need to standardize all numeric features

- This will make the model coefficients more easily interpretable

On the Danger of Overfitting

We plan to use our model as proxy for the true process

...Which makes *overfitting is especially bad*

- Our results will stricly apply only to the model
- ...And they will be as general as the model

We will use *L1 regularization* on this purpose

Scikit learn support L1 regularizers for Logistic Regression in the form:

$$\mathrm{argmin}_\theta\, H(y, f(x, \theta)) + \frac{1}{C}\|\theta\|_1$$

- We encourage the weights to be close to 0
- ...And we attempt to sparsify the weights

Training our "Proxy" Model

We can calibrate the C parameter via cross-validation

We'll need the SAGA solver to train our model with L1 regularization

In [3]:
```
base_est = LogisticRegression(penalty='l1', solver='saga')
param_grid={'C': 1. / np.linspace(1e-1, 1e4, 100)}
gscv = GridSearchCV(base_est, param_grid=param_grid, scoring='roc_auc')
```

```
gscv.fit(X_train, y_train)
lr, lr_params = gscv.best_estimator_, gscv.best_params_
```

Then we can check the performance of the refitted estimator

In [4]:
```
lr_score_cv, lr_score_test = gscv.best_score_, roc_auc_score(y_test, lr.prec
print(f'AUC score for C={lr_params["C"]:.2f}: {lr_score_cv:.2f} (cross-valic
```

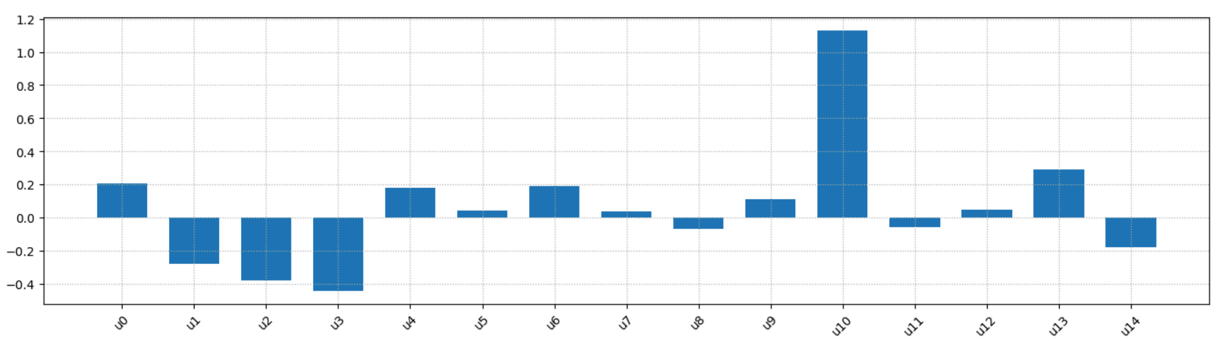
```
AUC score for C=10.00: 0.64 (cross-validation), 0.60 (test)
```

- We use the AUC score, since this is not a deterministic classification problem
- There's no significant overfitting

Coefficient Analysis

Finally, we can analyze the model coefficients

In [5]:
```
lr_coefs = pd.Series(index=X.columns, data=lr.coef_[0])
util.plot_bars(lr_coefs, figsize=figsize)
```



- Some variables seem to be more important than others
- The sign tells us how they are linked to the target

This baseline approach has *many* issues

Can you spot a few ones?

Three Key Issues with our Baseline

Issue 1: our model has *poor accuracy*

- An AUC score of 0.6 is not much above random
- ...Hence, studying our model will say little about the data

Issue 2: our model can only capture *linear correlations*

- We can capture neither non-linear effects
- ...Nor interactions among the variables

Issue 3: the coefficients are not sparse

- The L1 terms needs both to sparsify and to prevent overfitting
- ...And it cannot do both things effectively
- Additionally: it's unclear what a good level of sparsification might be

We'll now get to work to fix them