

A Baseline Approach



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Our goal is **understanding** the process behind the data

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, random_state=42)
# 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:

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

- 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.predict_proba(X_test))
        print(f'AUC score for C={lr_params["C"]:.2f}: {lr_score_cv:.2f} (cross-validation), {lr_score_test:.2f} (test)')
```

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

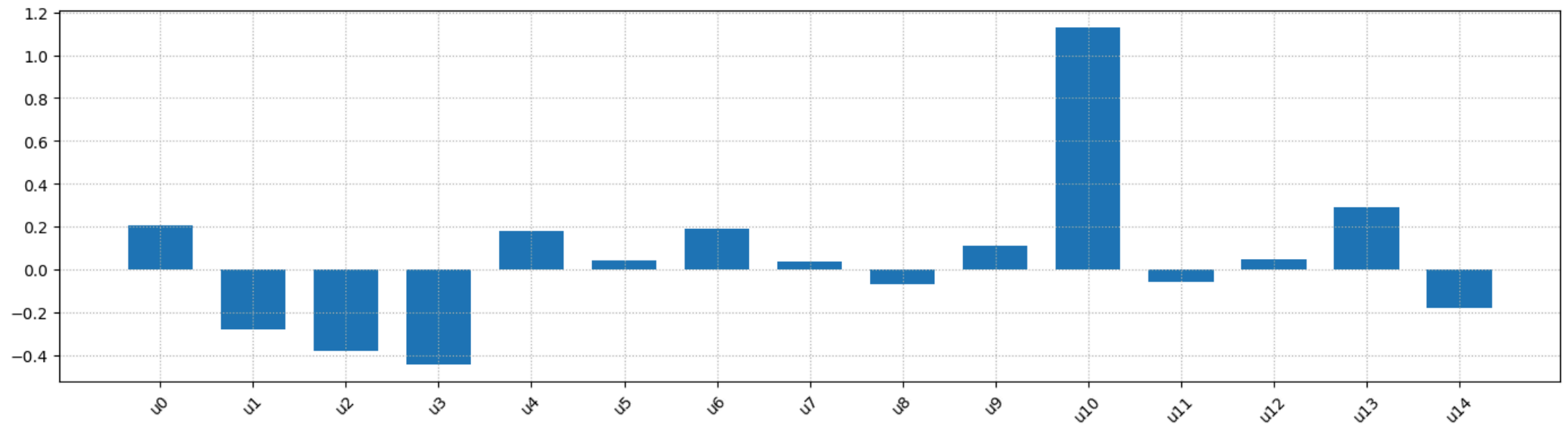
- We use the AUC score, since this is not a deterministic classification problem
- There's no significant overfitting



Coefficient Analysis

Finally, we can analyze the model coefficients

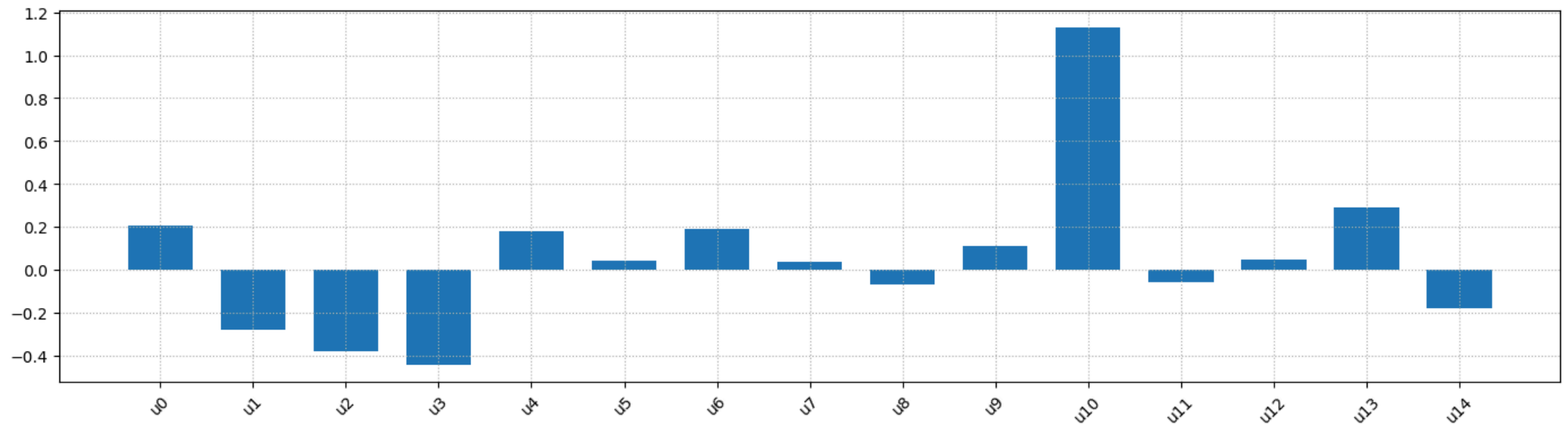
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In [6]: lr_coefs = pd.Series(index=X.columns, data=lr.coef_[0])  
util.plot_bars(lr_coefs, figsize=figsize)
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```



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



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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

