Non-Linear Models and Importances

Dealing with Non-Linearities

We'll start by switching to a non-linear model

By doing so:

- We can still account for non-linear correlations
- We can account for interactions among variables
- We might reach a much better accuracy
- ...And hence have a more representative proxy model

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Of course there is a price to pay

- Non-linear models are less easy to interpret
- ...And they are at a much higher risk of overfitting

Gradient Boosted Trees Model

We'll train a Gradient Bossted Trees model

We'll rely on the Extreme Gradient Boosting package (XGBoost) for this

```
In [73]: base_est = xgboost.XGBClassifier(tree_method='hist', importance_type='total_gain')
         param_grid={'max_depth': [2, 3, 4], 'n_estimators': list(range(20, 41, 5)), 'reg_lambda': n
         gscv = GridSearchCV(base_est, param_grid=param_grid)
         gscv.fit(X, y)
         xbm, xbm_params = gscv.best_estimator_, gscv.best_params_
```

XGBoost is a library for fast, distributed, training of GBT models

It has support for multiple loss functions

- For classification, the default is "reg:logistic", i.e. binary cross-entropy

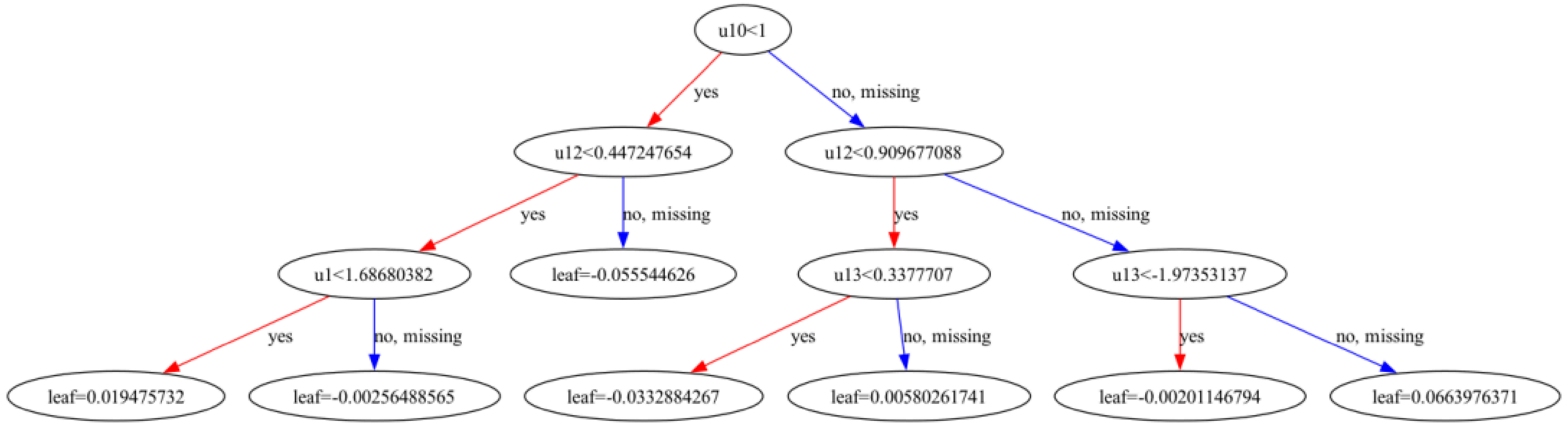
...And for regularization (often missing in tree-based models)

- The "reg_lambda" parameter refers to the weight of an L2 regularization term
- ...Which in GBT is applied to the leaf labels

Gradient Boosted Trees Model

It's easier to see how regularization work by checking a tree in the ensemble

```
In [74]: plt.figure(figsize=figsize)
         xgboost.plot_tree(xbm, ax=plt.gca(), num_trees=0);
```



- Assuming T is the number of leaves and w_j is the label assigned to each leaf
- ...Then the regularization term is in the form $\sum_{k=1}^{T} w_j^2$

Gradient Boosted Trees Model

On our dataset, a GBT model has substantially better performance

```
In [75]: xbm_score_cv, xbm_score_test = gscv.best_score_, roc_auc_score(y_test, xbm.predict(X_test))
         print(f'AUC score for {xbm_params}: {xbm_score_cv:.2f} (cross-val.), {xbm_score_test:.2f} (
```

```
AUC score for {'max_depth': 3, 'n_estimators': 35, 'reg_lambda': np.float64(200.0)}: 0.73
(cross-val.), 0.71 (test)
```

- The AUC score is much higher now
- There is no significant overfitting

It seems we finally have a model that we can trust

Gradient Boosted Trees Model

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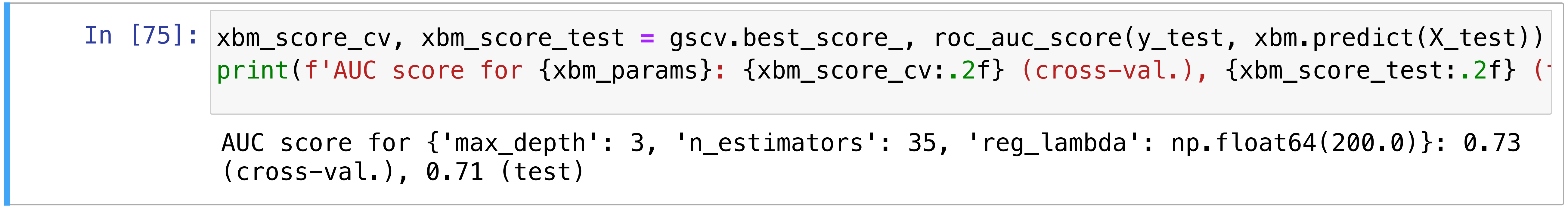

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It seems we finally have a model that we can trust

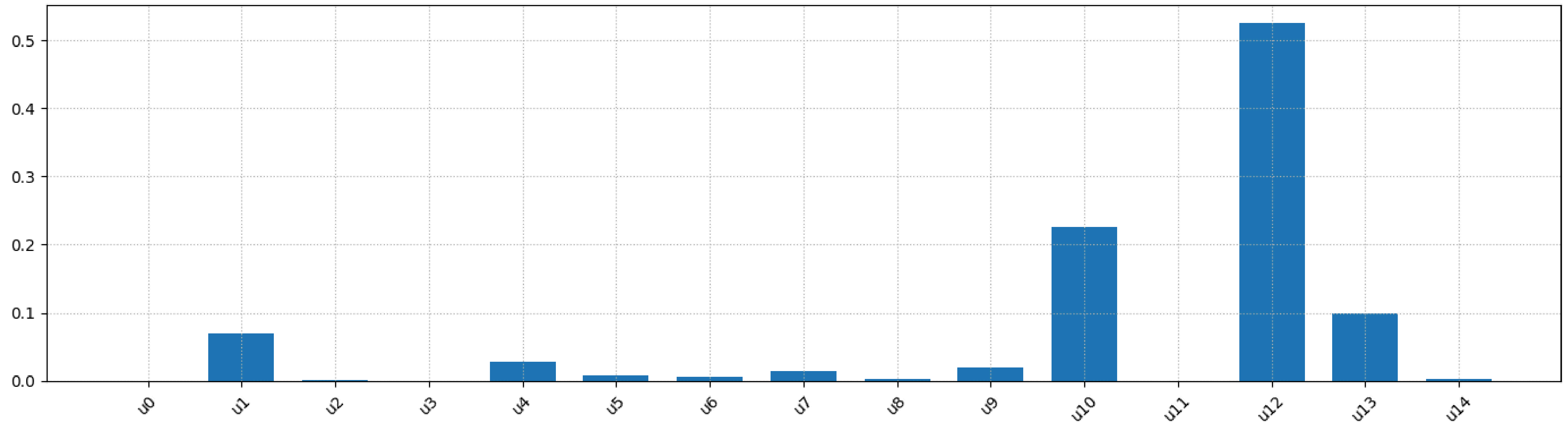
However, we know have an ensemble of many non-linear models

How can we make sense of that?

Feature Importances

The first option one can probably think of is using feature importances

```
In [76]: xbm_imp = pd.Series(index=X.columns, data=xbm.feature_importances_)
         util.plot_bars(xbm_imp, figsize=figsize)
```



- The scores differ significanly from those obtained for linear regression (as expected)
- ...But what do they represent?

Which Feature Importances?

Feature importance is typicaly presented as this:

- For each input x_j, we sum the associated gain at training time
- Once training is over, we normalize the scores so that they sum up to 1

Howver, there are other ways to define importance

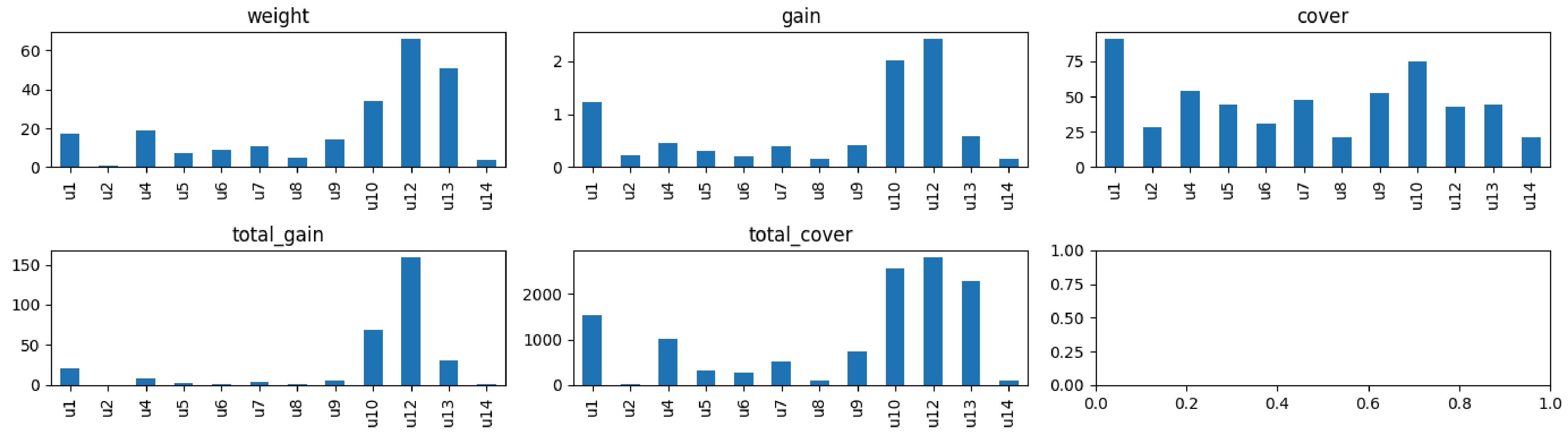
XGBoost supports 5 different approaches:

- "weight": number of times an attribute is used to split
- "gain": average gain associated to splits over an attribute
- "cover": average number of examples for which an attribute is used to decide
- "total_gain": as above, but replacing the average with a sum
- "total_cover": as above, but replacing the average with a sum

Which Feature Importances?

The values of the multiple feature importances can be quite different:

In [77]:
```
_, axes = plt.subplots(nrows=2, ncols=3, figsize=figsize)
for ax, imp_type in zip(axes.ravel(), ['weight', 'gain', 'cover', 'total_gain', 'total_cove
    pd.Series(xbm.get_booster().get_score(importance_type=imp_type)).plot.bar(ax=ax, title=
plt.tight_layout()
```



Importance and Data

Moreover, most importance scores are computed w.r.t. a dataset:

E.g. in XGBoost "gain", "cover", "total_gain", and "total_cover"

- For this reason, they are not really properties of the model
- ...But rather of the model and a reference sample

This means that the score semantic depends on the reference sample

By default, importances are computed on the training set

...Which means they are susceptible to overfitting

- The model might split on an attribute because it really is importance
- ...But also due to a spurious correlation

Permutation Importance

We can improve things by changing the way we compute importance

Given a reference sample $\{x_i, y_i\}_{i=1}^m$

- We can evaluate the performance of our model on the sample
- ...With that of a modified sample where the j-th input is made unimportant

For example, we can achieve that by permuting the values of the input

- This will preserve the distribution of the input
- ...But it will break all its correlations

Then, we look at the change in the model performance

- If it is small, the attribute is really unimportant
- Otherwise, the attribute is important

These scores are known as permutation importances

Permutation Importance

Permutation importances are robust w.r.t. spurious correlations

- We just need to repeat the process multiple times
- ...And record means and standard deviations

It's unlikely that we often get a high score by accident

They allow us to choose our reference sample:

On the training set, the model might have overfit over the data

- The performance gap will be wider
- ...And the score will reflect how the model is using the data

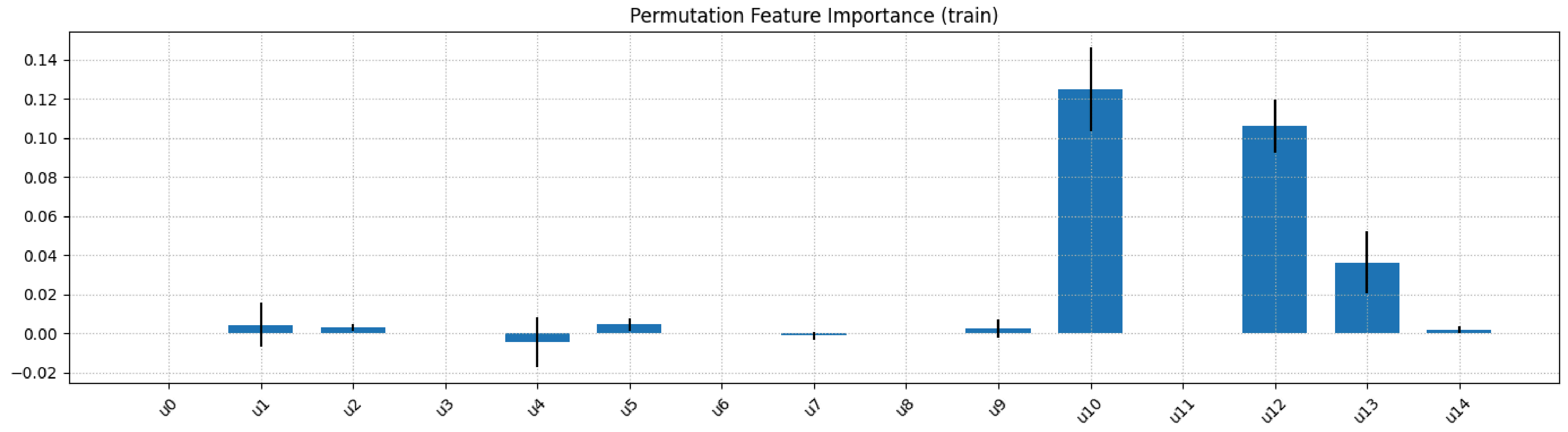
On the test set, overfitting will make less of a different

- ...And the score will reflect how correlated the attribute is with the target

Permutation Importances, on our Example

Let's check the training permutation importances in our case study

```
In [78]: r_train = permutation_importance(xbm, X_train, y_train, n_repeats=30, random_state=42)
         xbm_p_imp = pd.Series(index=X.columns, data=r_train.importances_mean)
         util.plot_bars(xbm_p_imp, figsize=figsize, std=r_train.importances_std, title='Permutation I
```

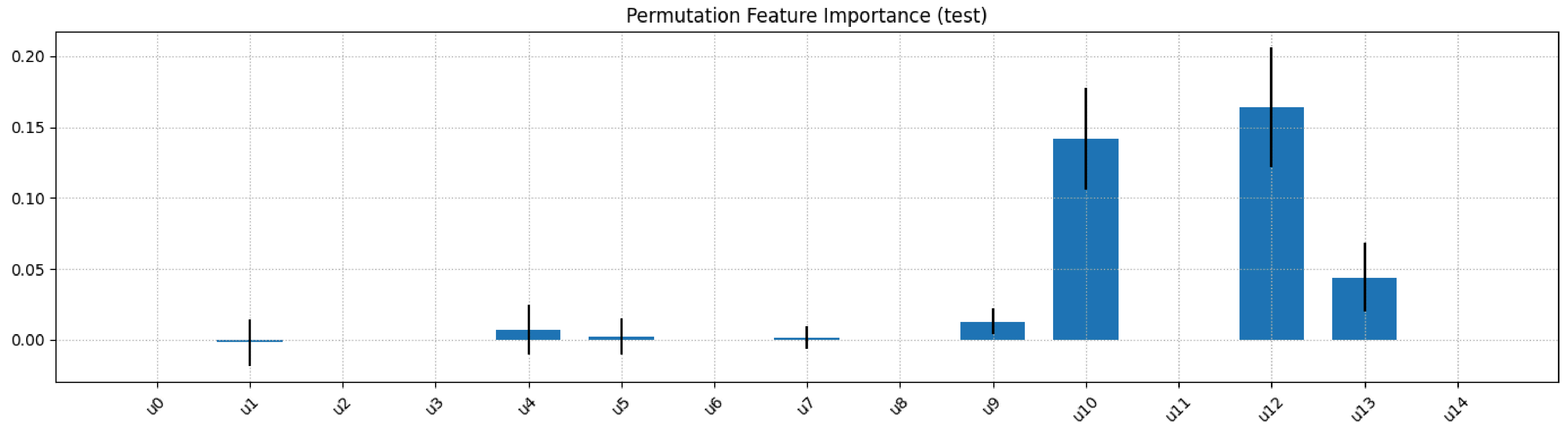


- The closely resemble those XGB "total_gain", but they are more sparse

Permutation Importances, on our Example

Let's check the test permutation importances in our case study

```
In [79]: r_test = permutation_importance(xbm, X_test, y_test, n_repeats=30, random_state=42)
         xbm_p_imp = pd.Series(index=X.columns, data=r_test.importances_mean)
         util.plot_bars(xbm_p_imp, figsize=figsize, std=r_test.importances_std, title='Permutation Fe
```



- A few low-importance features become even less relevant on the test data