```
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.metrics import roc_auc_score
        from sklearn.model_selection import GridSearchCV
        import xgboost
        from sklearn.inspection import permutation_importance

        # 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]

        # Data pre-processing
        X, y = data[data.columns[:-1]].copy(), data[data.columns[-1]].copy()
        X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, rar
        scaler = StandardScaler()
        X_train[num_cols] = scaler.fit_transform(X_train[num_cols])
        X_test[num_cols] = scaler.transform(X_test[num_cols])
```

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

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 [2]:
```
base_est = xgboost.XGBClassifier(tree_method='hist', importance_type='total_
param_grid={'max_depth': [2, 3, 4], 'n_estimators': list(range(20, 41, 5)),
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

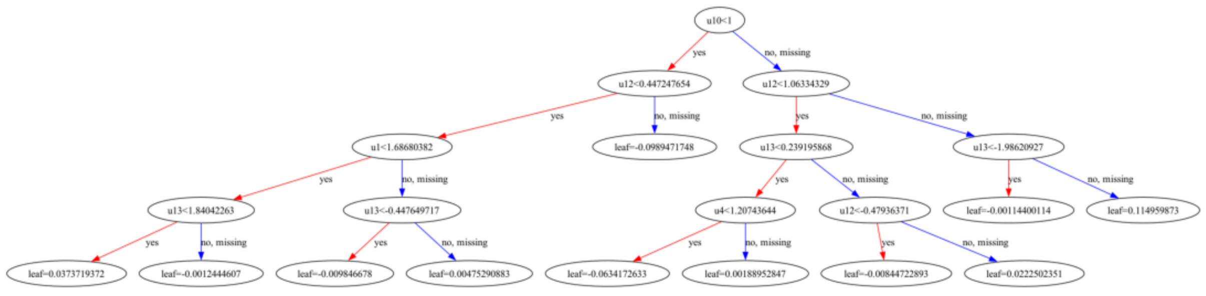
...And for *regularization* (often missing in tree-based models)

- 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 [5]:
```
plt.figure(figsize=figsize)
xgboost.plot_tree(xbm, ax=plt.gca(), tree_idx=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 [6]: xbm_score_cv, xbm_score_test = gscv.best_score_, roc_auc_score(y_test, xbm.p
        print(f'AUC score for {xbm_params}: {xbm_score_cv:.2f} (cross-val.), {xbm_sc
```

```
AUC score for {'max_depth': 4, 'n_estimators': 25, 'reg_lambda': np.float64
(100.0)}: 0.73 (cross-val.), 0.70 (test)
```

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

It seems we finally have a model that we can trust

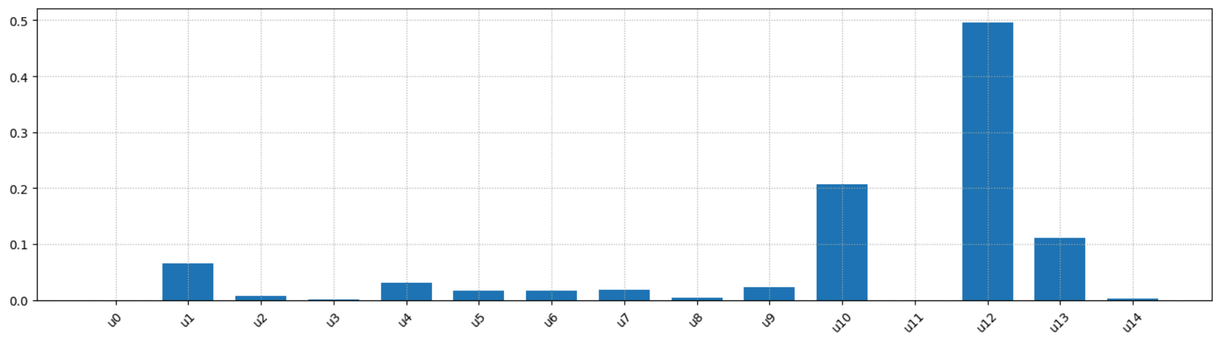
However, we know have an ensemble of many non-linear models

> **How can we make sense of that?**

Feature Importances

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

```
In [7]: 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*

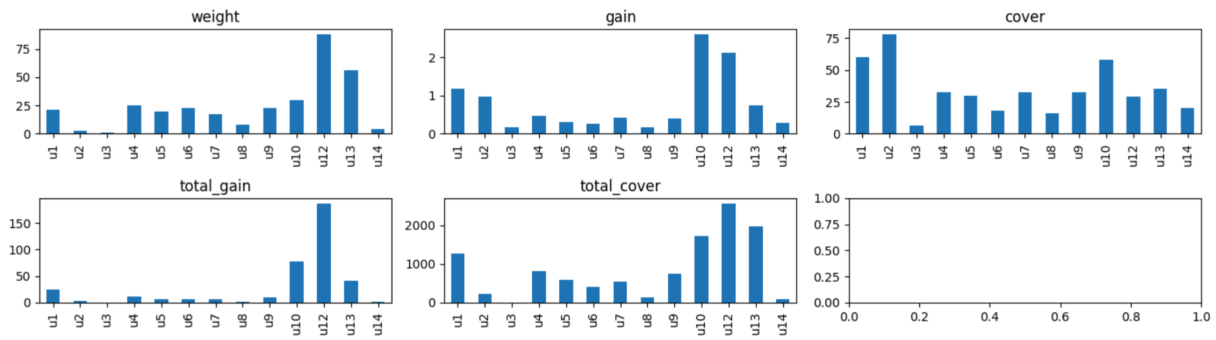
XGBoost supports 5 different approaches:

- "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 [8]:
```
_, axes = plt.subplots(nrows=2, ncols=3, figsize=figsize)
for ax, imp_type in zip(axes.ravel(), ['weight', 'gain', 'cover', 'total_gai
    pd.Series(xbm.get_booster().get_score(importance_type=imp_type)).plot.ba
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

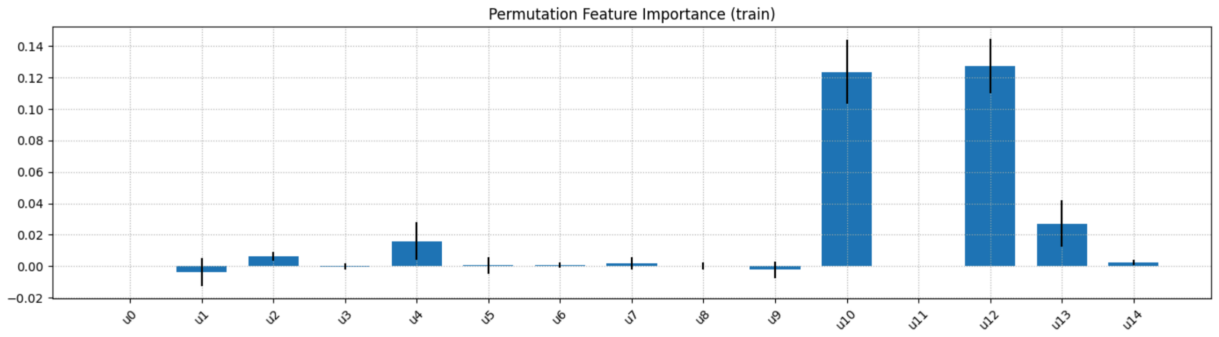
On the *test set*, overfitting will make less of a different

- ...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 [9]: r_train = permutation_importance(xbm, X_train, y_train, n_repeats=30, random
        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, titl
```

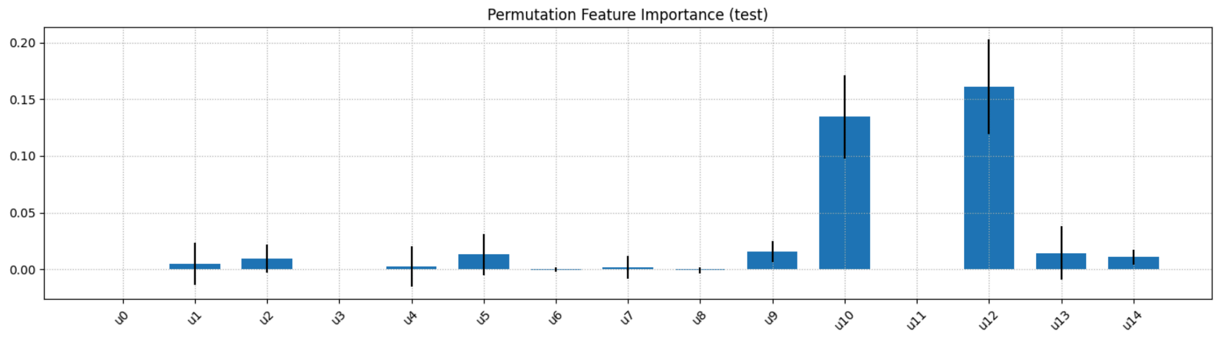


- The closely resemble those XGB "total_gain", but they are more sparse

Permutation Importances, on our Example

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

In [10]:
```
r_test = permutation_importance(xbm, X_test, y_test, n_repeats=30, random_st
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
```



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