Lambda School Data Science — Tree Ensembles

## **Random Forests**

#### Pre-read

- Scikit-Learn User Guide, Ensemble Methods (https://scikitlearn.org/stable/modules/ensemble.html)
- <u>Coloring with Random Forests</u>
   (http://structuringtheunstructured.blogspot.com/2017/11/coloring-with-random-forests.html)
- Beware Default Random Forest Importances (https://explained.ai/rf-importance/index.html)

### More

- <u>Machine Learning Explainability: Permutation Importance</u>
   (<a href="https://www.kaggle.com/dansbecker/permutation-importance">https://www.kaggle.com/dansbecker/permutation-importance</a>)
- <u>eli5: Permutation Importance</u>
   (<a href="https://eli5.readthedocs.io/en/latest/blackbox/permutation\_importance.html">https://eli5.readthedocs.io/en/latest/blackbox/permutation\_importance.html</a>)
- <u>eli5: Explaining XGBoost predictions on the Titanic dataset</u> (<a href="https://eli5.readthedocs.io/en/latest/">https://eli5.readthedocs.io/en/latest/</a> notebooks/xgboost-titanic.html)
- The Mechanics of Machine Learning: Categorically Speaking (https://mlbook.explained.ai/catvars.html)

<u>Selecting good features – Part III: random forests (https://blog.datadive.net/selecting-good-features-part-iii-random-forests/)</u>

There are a few things to keep in mind when using the impurity based ranking. Firstly, feature selection based on impurity reduction is biased towards preferring variables with more categories.

Secondly, when the dataset has two (or more) correlated features, then from the point of view of the model, any of these correlated features can be used as the predictor, with no concrete preference of one over the others. But once one of them is used, the importance of others is significantly reduced since effectively the impurity they can remove is already removed by the first feature. As a consequence, they will have a lower reported importance. This is not an issue when we want to use feature selection to reduce overfitting, since it makes sense to remove features that are mostly duplicated by other features. But when interpreting the data, it can lead to the incorrect conclusion that one of the variables is a strong predictor while the others in the same group are unimportant, while actually they are very close in terms of their relationship with the response variable.

An Introduction to Statistical Learning (http://www-bcf.usc.edu/~gareth/ISL/), Chapter 8.2.1, Out-of-Bag Error Estimation

It turns out that there is a very straightforward way to estimate the test error of a bagged model, without the need to perform cross-validation or the validation set approach.

Recall that the key to bagging is that trees are repeatedly fit to bootstrapped subsets of the observations. One can show that on average, each bagged tree makes use of around two-thirds of the observations. The remaining one-third of the observations not used to fit a given bagged tree are referred to as the out-of bag (OOB) observations.

We can predict the response for the ith observation using each of the trees in which that observation was OOB. This will yield around B/3 predictions for the ith observation. In order to obtain a single prediction for the ith observation, we can average these predicted responses (if regression is the goal) or can take a majority vote (if classification is the goal).

This leads to a single OOB prediction for the ith observation. An OOB prediction can be obtained in this way for each of the n observations, from which the overall OOB MSE (for a regression problem) or classification error (for a classification problem) can be computed. The resulting **OOB error is a valid estimate of the test error for the bagged model, since the response for each observation is predicted using only the trees that were not fit using that observation.** ...

It can be shown that with B sufficiently large, OOB error is virtually equivalent to leave-one-out cross-validation error. The OOB approach for estimating the test error is particularly **convenient when performing bagging on large data sets** for which cross-validation would be computationally onerous.

### Libraries

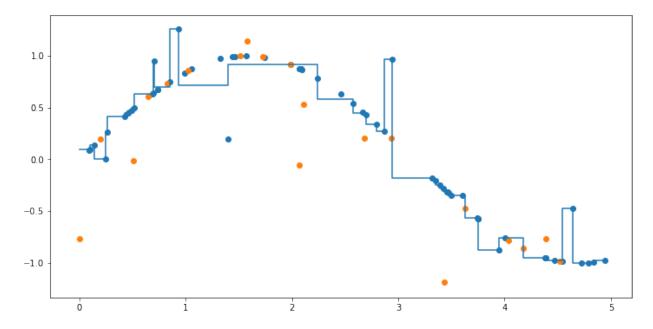
- <u>eli5 (https://github.com/TeamHG-Memex/eli5)</u>: conda install -c conda-forge eli5 / pip install eli5
- category encoders (https://github.com/scikit-learn-contrib/categorical-encoding): conda install -c conda-forge category\_encoders / pip install category encoders
- <u>mlxtend (https://github.com/rasbt/mlxtend)</u>: pip install mlxtend
- <u>ipywidgets (https://ipywidgets.readthedocs.io/en/stable/examples/Using%20Interact.html)</u>: included with Anaconda, doesn't work on Google Colab

# ipywidgets revisited: Decision Tree vs Random Forest

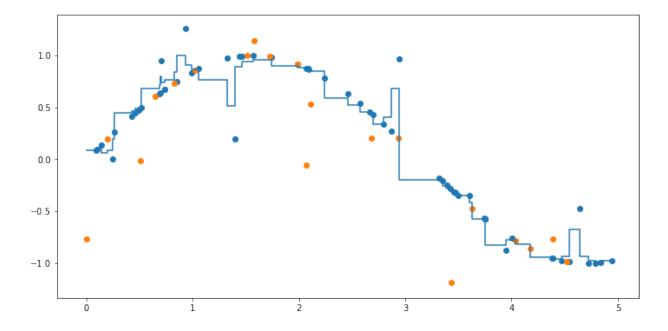
```
In [3]: %matplotlib inline
        from ipywidgets import interact
        import matplotlib.pyplot as plt
        from sklearn.ensemble import RandomForestRegressor
        from sklearn.model selection import train test split
        from sklearn.tree import DecisionTreeRegressor
        # Example from http://scikit-learn.org/stable/auto examples/tree/plot tr
        def make data():
            import numpy as np
            rng = np.random.RandomState(1)
            X = np.sort(5 * rng.rand(80, 1), axis=0)
            y = np.sin(X).ravel()
            y[::5] += 2 * (0.5 - rng.rand(16))
            return X, y
        X, y = make data()
        X_train, X_test, y_train, y_test = train_test_split(
            X, y, test size=0.25, random state=42)
        def regress wave(max depth):
            dt = DecisionTreeRegressor(max depth=max depth)
            dt.fit(X train, y train)
            print('Decision Tree train R^2:', dt.score(X_train, y_train))
            print('Decision Tree test R^2:', dt.score(X test, y test))
            plt.gcf().set size inches(12, 6)
            plt.scatter(X train, y train)
            plt.scatter(X test, y test)
            plt.step(X, dt.predict(X))
            plt.show()
            rf = RandomForestRegressor(max depth=max depth, n estimators=100, n
            rf.fit(X train, y train)
            print('Random Forest train R^2:', rf.score(X train, y train))
            print('Random Forest test R^2:', rf.score(X test, y test))
            plt.gcf().set size inches(12, 6)
            plt.scatter(X train, y train)
            plt.scatter(X test, y test)
            plt.step(X, rf.predict(X))
            plt.show()
        interact(regress wave, max depth=(1,8,1));
```

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Decision Tree train R^2: 0.9846072146401021 Decision Tree test R^2: 0.6675139268793822



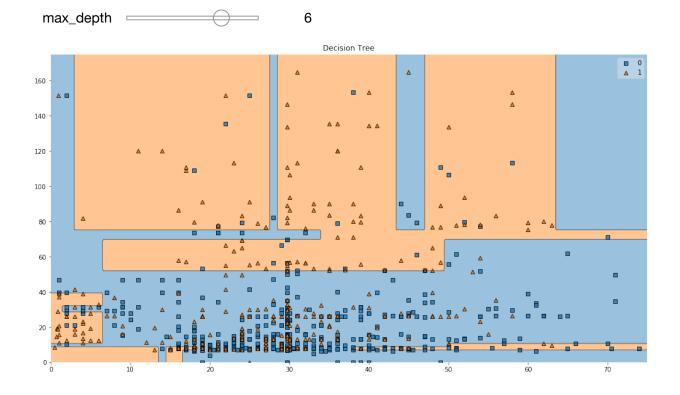
Random Forest train R^2: 0.9833229991881686 Random Forest test R^2: 0.7150540416259283

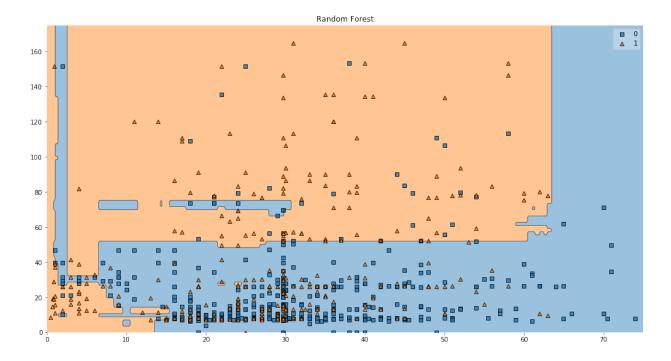


### Regressing a wave

## Titanic survival, by Age & Fare

```
from mlxtend.plotting import plot decision regions
In [2]:
        import seaborn as sns
        from sklearn.ensemble import RandomForestClassifier
        from sklearn.impute import SimpleImputer
        from sklearn.tree import DecisionTreeClassifier
        titanic = sns.load dataset('titanic')
        X = SimpleImputer().fit transform(titanic[['age', 'fare']])
        y = titanic['survived'].values
        def classify titanic(max depth):
            dt = DecisionTreeClassifier(max depth=max depth)
            dt.fit(X, y)
            plot decision regions(X, y, dt)
            plt.gcf().set_size_inches(17, 9)
            plt.title('Decision Tree')
            plt.axis((0,75,0,175))
            plt.show()
            rf = RandomForestClassifier(max depth=max depth, n estimators=100, n
            rf.fit(X, y)
            plot decision regions(X, y, rf)
            plt.gcf().set size inches(17, 9)
            plt.title('Random Forest')
            plt.axis((0,75,0,175))
            plt.show()
        interact(classify titanic, max depth=(1,8,1));
```





## **Lending Club**

Read csv files downloaded from Kaggle (https://www.kaggle.com/c/ds2-tree-ensembles/data)

```
In [34]:
    import pandas as pd
    pd.options.display.max_columns = 200
    pd.options.display.max_rows = 200

X_train = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_
    X_test = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/test_fe
    y_train = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_
    sample_submission = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_
    sample_submission = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_
    Systime
    import pandas as pd
    pd.options.display.max_columns = 200
    pd.options.display.max_rows = 200

    X_train = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_
    sample_submission = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_
    System = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_
    sample_submission = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_
    System = pd.read_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_csv('/Users/wel51x/Downloads/ds2-tree-ensembles/train_csv('/Users/wel51x/Do
```

Wrangle X\_train and X\_test in the same way

```
In [35]: def wrangle(X):
    X = X.copy()

# Drop some columns
    X = X.drop(columns='id') # id is random
    X = X.drop(columns=['member id', 'url', 'desc']) # All null
```

```
X = X.drop(columns='title') # Duplicative of purpose
X = X.drop(columns='grade') # Duplicative of sub grade
# Transform sub grade from "A1" - "G5" to 1.1 - 7.5
def wrangle sub grade(x):
    first digit = ord(x[0]) - 64
    second digit = int(x[1])
    return first digit + second digit/10
X['sub grade'] = X['sub grade'].apply(wrangle sub grade)
# Convert percentages from strings to floats
X['int rate'] = X['int rate'].str.strip('%').astype(float)
X['revol util'] = X['revol util'].str.strip('%').astype(float)
# Transform earliest cr line to an integer: how many days it's been
X['earliest cr line'] = pd.to datetime(X['earliest cr line'], infer
X['earliest cr line'] = pd.Timestamp.today() - X['earliest cr line']
X['earliest cr line'] = X['earliest cr line'].dt.days
# Create features for three employee titles: teacher, manager, owner
X['emp_title'] = X['emp_title'].str.lower()
X['emp title teacher'] = X['emp title'].str.contains('teacher', na=F
X['emp title manager'] = X['emp title'].str.contains('manager', na=F
X['emp title owner'] = X['emp title'].str.contains('owner', na=Fal
# Drop categoricals with high cardinality
X = X.drop(columns=['emp title', 'zip code'])
# Transform features with many nulls to binary flags
many nulls = ['sec app mths since last major derog',
              'sec app revol util',
              'sec app earliest cr line',
              'sec_app mort acc',
              'dti joint',
              'sec app collections 12 mths ex med',
              'sec app chargeoff within 12 mths',
              'sec app num rev accts',
              'sec app open act il',
              'sec app open acc',
              'revol bal joint',
              'annual_inc_joint',
              'sec app ing last 6mths',
              'mths since last record',
              'mths since recent bc dlq',
              'mths since last major derog',
              'mths since recent revol deling',
              'mths since last deling',
              'il util',
              'emp length',
```

```
'mths since recent ing',
                             'mo sin old il acct',
                             'mths since rcnt il',
                             'num tl 120dpd 2m',
                             'bc util',
                             'percent bc gt 75',
                             'bc open to buy',
                             'mths since recent bc']
              for col in many_nulls:
                  X[col] = X[col].isnull()
              # For features with few nulls, do mean imputation
              for col in X:
                  if X[col].isnull().sum() > 0:
                      X[col] = X[col].fillna(X[col].mean())
              # Return the wrangled dataframe
              return X
          X train = wrangle(X train)
          X_test = wrangle(X_test)
          X_train.shape, X_test.shape
Out[35]: ((1309457, 98), (26724, 98))
         Now X train (and X test) have no nulls
In [36]: null_counts = X_train.isnull().sum()
          all(null counts == 0)
Out[36]: True
         And no high cardinality categoricals
In [37]: cardinality = X train.select dtypes(exclude='number').nunique()
          all(cardinality <= 50)</pre>
Out[37]: False
```

In [38]: cardinality 2 Out[38]: term emp length 2 home ownership 6 purpose 14 addr state 51 2 mths since last deling 2 mths since last record initial\_list\_status 2 mths since last major derog 2 2 application type annual inc joint 2 2 dti joint 2 mths since rcnt il 2 il util 2 bc\_open\_to\_buy bc util 2 mo\_sin\_old\_il\_acct 2 2 mths since recent bc 2 mths since recent bc dlq 2 mths since recent inq mths since recent revol deling 2 2 num tl 120dpd 2m 2 percent bc gt 75 2 revol bal joint 2 sec app earliest cr line 2 sec app inq last 6mths 2 sec\_app\_mort\_acc 2 sec app open acc sec\_app\_revol\_util 2 2 sec app open act il 2 sec app num rev accts 2 sec\_app\_chargeoff\_within\_12\_mths 2 sec app collections 12 mths ex med 2 sec app mths since last major derog 2 disbursement method 2 emp title teacher 2 emp title manager emp title owner 2 dtype: int64

### **Decision Tree**

```
In [39]: | %%time
       import category_encoders as ce
        from sklearn.model selection import cross val score
        from sklearn.pipeline import make pipeline
        from sklearn.tree import DecisionTreeClassifier
       pipe = make pipeline(
           ce.OrdinalEncoder(),
           DecisionTreeClassifier(max depth=5, class weight='balanced')
        )
        cross val score(pipe, X train, y train, cv=5, scoring='roc auc')
       CPU times: user 4min 44s, sys: 44.5 s, total: 5min 28s
       Wall time: 5min 58s
In [40]: | %%time
        from sklearn.ensemble import RandomForestClassifier
       pipe = make_pipeline(
           ce.OrdinalEncoder(),
           RandomForestClassifier(
              n estimators=100,
              class weight='balanced',
              min samples leaf=0.005,
              oob score=True,
              n jobs=-1)
       cross val score(pipe, X train, y train, cv=5, scoring='roc auc', verbose
       [Parallel(n jobs=1)]: Using backend SequentialBackend with 1 concurren
       t workers.
       [CV] .....
       [CV] ....., score=0.714071853559479, total= 4.8min
            [Parallel(n jobs=1)]: Done 1 out of 1 | elapsed: 4.8min remaining
         0.0s
        [CV] ....., score=0.712632525364129, total= 4.8min
        [CV] .......
       [Parallel(n jobs=1)]: Done 2 out of 2 | elapsed: 9.6min remaining
           0.0s
        [CV] ....., score=0.7128238788575855, total= 4.4min
```

## **Out-of-Bag estimated score**

Out-of-bag is a faster way to get an estimated score with Random Forest, using the parameter oob score=True

### **Random Forest**

Improves ROC AUC compared to Decision Tree

```
In [41]: from sklearn.metrics import roc_auc_score
In [42]: %%time
    pipe.fit(X_train, y_train)
    y_pred_proba = pipe.named_steps['randomforestclassifier'].oob_decision_f
    print('ROC AUC, Out-of-Bag estimate:', roc_auc_score(y_train, y_pred_pro)

ROC AUC, Out-of-Bag estimate: 0.71302387007396
```

CPU times: user 13min 15s, sys: 22.9 s, total: 13min 38s

Wall time: 4min 31s

```
In [43]: pipe.named steps
Out[43]: {'ordinalencoder': OrdinalEncoder(cols=['term', 'home ownership', 'pur
         pose', 'addr state', 'initial list status', 'application type', 'disbu
         rsement method'],
                  drop invariant=False, handle unknown='impute', impute missing
         =True,
                  mapping=[{'col': 'term', 'mapping': [(' 36 months', 1), (' 60
         months', 2)]}, {'col': 'home ownership', 'mapping': [('MORTGAGE', 1),
         ('RENT', 2), ('OWN', 3), ('ANY', 4), ('OTHER', 5), ('NONE', 6)]}, {'co
         l': 'purpose', 'mapping': [('home improvement', 1), ('debt consolidati
         on', 2), ('major purchase', ... 1), ('Joint App', 2)]}, {'col': 'disbu
         rsement method', 'mapping': [('Cash', 1), ('DirectPay', 2)]}],
                  return df=True, verbose=0),
          'randomforestclassifier': RandomForestClassifier(bootstrap=True, clas
         s weight='balanced',
                      criterion='gini', max depth=None, max features='auto',
                      max leaf nodes=None, min impurity decrease=0.0,
                      min impurity split=None, min samples leaf=0.005,
                      min samples split=2, min weight fraction leaf=0.0,
                      n estimators=100, n jobs=-1, oob_score=True, random_state
         =None,
                      verbose=0, warm start=False)}
```

###You can explore hyperparameter values

```
In [44]:
         %%time
         \max depths = list(range(2, 12, 2)) + [None]
         for max depth in max depths:
             pipe = make pipeline(
                 ce.OrdinalEncoder(),
                 RandomForestClassifier(
                      n estimators=100,
                      class weight='balanced',
                      max depth=max depth,
                      oob score=True,
                      n jobs=-1
                 )
             )
             pipe.fit(X train, y train)
             y pred proba = pipe.named steps['randomforestclassifier'].oob decisi
             print('Max Depth:', max depth)
             print('ROC AUC, OOB:', roc auc score(y train, y pred proba))
```

```
Max Depth: 2
ROC AUC, OOB: 0.6985295117020649
Max Depth: 4
ROC AUC, OOB: 0.7074454057927698
Max Depth: 6
ROC AUC, OOB: 0.712182426840721
Max Depth: 8
ROC AUC, OOB: 0.716150086711317
Max Depth: 10
ROC AUC, OOB: 0.7182985911393234
Max Depth: None
ROC AUC, OOB: 0.6980663211203326
CPU times: user 1h 31min 6s, sys: 2min 56s, total: 1h 34min 3s
Wall time: 35min 43s
```

## **Feature Importances**

We can look at feature importances. <u>But remember: (https://blog.datadive.net/selecting-good-features-part-iii-random-forests/)</u>

Firstly, feature selection based on impurity reduction is biased towards preferring variables with more categories.

Secondly, when the dataset has two (or more) correlated features, then from the point of view of the model, any of these correlated features can be used as the predictor, with no concrete preference of one over the others.

## **Drop Column Importance / "Ablation Study"**

sub\_grade and int\_rate are highly correlated. If we drop one of those features, the model uses the other more, so the score remains similar.

```
In [45]: def show_feature_importances(
    pipe, X, y, estimator_name='randomforestclassifier',
    n=20, figsize=(8, 8), color='blue'):

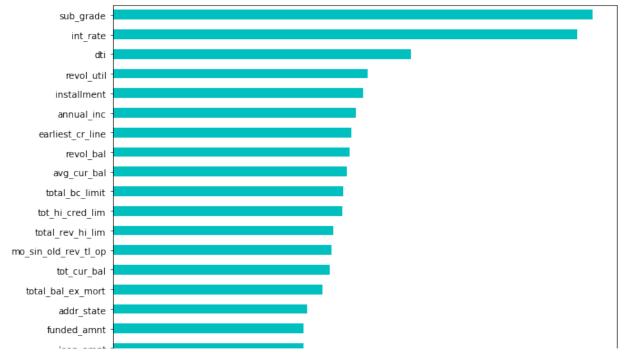
# pipe must not change dimensions of X dataframe
    pipe.fit(X, y)

importances = pd.Series(
        pipe.named_steps[estimator_name].feature_importances_,
        X.columns)

top_n = importances.sort_values(ascending=False)[:n]

plt.figure(figsize=figsize)
    top_n.sort_values().plot.barh(color=color)

show_feature_importances(pipe, X_train, y_train, color='c')
```

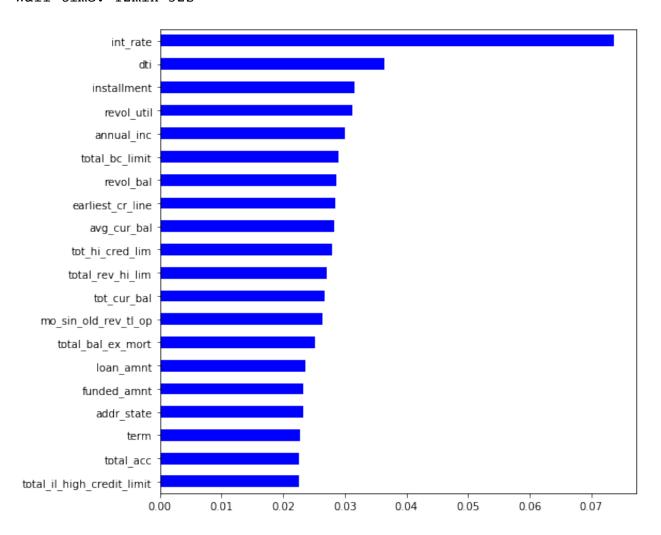


```
In [46]: cross_val_score(pipe, X_train.drop(columns='sub_grade'), y_train, cv=5,
```

Out[46]: array([0.71519181, 0.71073021, 0.71369791, 0.71529829, 0.7136068])

In [47]: %%time
 show\_feature\_importances(pipe, X\_train.drop(columns='sub\_grade'), y\_trai

CPU times: user 31min 16s, sys: 1min 7s, total: 32min 24s Wall time: 12min 52s



But if we drop both features, then the score decreases:

```
In [0]: cross_val_score(pipe, X_train.drop(columns=['sub_grade', 'int_rate']), y
```

Out[16]: array([0.70238724, 0.69620403, 0.69929053, 0.70917935, 0.69917305])

For more information, see <u>Beware Default Random Forest Importances (https://explained.ai/rfimportance/index.html)</u>.

## **Permutation Importance**

Permutation Importance is a compromise between Feature Importance based on impurity reduction (which is the fastest) and Drop Column Importance (which is the "best.")

<u>The ELI5 library documentation explains</u>, (<a href="https://eli5.readthedocs.io/en/latest/blackbox/permutation\_importance.html">https://eli5.readthedocs.io/en/latest/blackbox/permutation\_importance.html</a>)

Importance can be measured by looking at how much the score (accuracy, F1, R^2, etc. - any score we're interested in) decreases when a feature is not available.

To do that one can remove feature from the dataset, re-train the estimator and check the score. But it requires re-training an estimator for each feature, which can be computationally intensive. ...

To avoid re-training the estimator we can remove a feature only from the test part of the dataset, and compute score without using this feature. It doesn't work as-is, because estimators expect feature to be present. So instead of removing a feature we can replace it with random noise - feature column is still there, but it no longer contains useful information. This method works if noise is drawn from the same distribution as original feature values (as otherwise estimator may fail). The simplest way to get such noise is to shuffle values for a feature, i.e. use other examples' feature values - this is how permutation importance is computed.

The method is most suitable for computing feature importances when a number of columns (features) is not huge; it can be resource-intensive otherwise.

For more documentation on using this library, see:

- <u>eli5.sklearn.PermutationImportance</u> (<a href="https://eli5.readthedocs.io/en/latest/autodocs/sklearn.html#eli5.sklearn.permutation\_importance">https://eli5.readthedocs.io/en/latest/autodocs/sklearn.html#eli5.sklearn.permutation\_importance</a>
- <u>eli5.show\_weights</u>
   (https://eli5.readthedocs.io/en/latest/autodocs/eli5.html#eli5.show\_weights)

/Library/anaconda3/lib/python3.7/site-packages/lightgbm/\_\_init\_\_.py:46 : UserWarning: Starting from version 2.2.1, the library file in distribution wheels for macOS is built by the Apple Clang (Xcode\_8.3.1) compiler.

This means that in case of installing LightGBM from PyPI via the ``pip install lightgbm`` command, you don't need to install the gcc compiler anymore.

Instead of that, you need to install the OpenMP library, which is required for running LightGBM on the system with the Apple Clang compiler. You can install the OpenMP library by the following command: ``brew in stall libomp``.

"You can install the OpenMP library by the following command: ``brew install libomp``.", UserWarning)

```
CPU times: user 49min 41s, sys: 2min 14s, total: 51min 56s Wall time: 20min 49s
```

In [49]: eli5.show\_weights(permuter, top=None, feature\_names=X\_train\_transformed.

Out[49]:	Weight	Feature
	0.0325 ± 0.0000	sub_grade
	$0.0128 \pm 0.0000$	int_rate
	$0.0114 \pm 0.0000$	term
	$0.0032 \pm 0.0000$	dti
	$0.0022 \pm 0.0000$	acc_open_past_24mths
	$0.0013 \pm 0.0000$	avg_cur_bal
	$0.0013 \pm 0.0000$	annual_inc
	$0.0011 \pm 0.0000$	loan_amnt
	$0.0010 \pm 0.0000$	tot_hi_cred_lim
	$0.0009 \pm 0.0000$	funded_amnt
	$0.0009 \pm 0.0000$	mort_acc
	$0.0008 \pm 0.0000$	home_ownership
	$0.0008 \pm 0.0000$	total_bc_limit
	$0.0006 \pm 0.0000$	installment
	$0.0006 \pm 0.0000$	num_tl_op_past_12m
	$0.0006 \pm 0.0000$	num_rev_tl_bal_gt_0
	$0.0005 \pm 0.0000$	tot_cur_bal
	$0.0005 \pm 0.0000$	all_util
	$0.0005 \pm 0.0000$	num_actv_rev_tl
	$0.0004 \pm 0.0000$	emp_length
	$0.0004 \pm 0.0000$	total_rev_hi_lim
	$0.0004 \pm 0.0000$	revol_util
	0 0004 + 0 0000	mtha ainea rant il

We can use Permutation Importance weights for feature selection. For example, we can remove features with zero weight. The model trains faster and the score does not decrease.

```
In [51]:
         subset = X train.columns[permuter.feature importances > 0]
         cross_val_score(pipe, X_train[subset], y_train, cv=5, scoring='roc_auc',
         [Parallel(n jobs=1)]: Using backend SequentialBackend with 1 concurren
         t workers.
         [CV]
         /Library/anaconda3/lib/python3.7/site-packages/sklearn/model selection
         / validation.py:542: FutureWarning: From version 0.22, errors during f
         it will result in a cross validation score of NaN by default. Use erro
         r score='raise' if you want an exception raised or error score=np.nan
         to adopt the behavior from version 0.22.
           FutureWarning)
         KeyError
                                                    Traceback (most recent call
         last)
         /Library/anaconda3/lib/python3.7/site-packages/pandas/core/indexes/bas
         e.py in get loc(self, key, method, tolerance)
            3077
                             try:
         -> 3078
                                 return self. engine.get loc(key)
 In [ ]:
```