Introducing Random Search

HYPERPARAMETER TUNING IN PYTHON

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What you already know

Very similar to grid search:

- Define an estimator, which hyperparameters to tune and the range of values for each hyperparameter.
- We still set a cross-validation scheme and scoring function

BUT we instead *randomly* select grid squares.

Why does this work?

Bengio & Bergstra (2012):

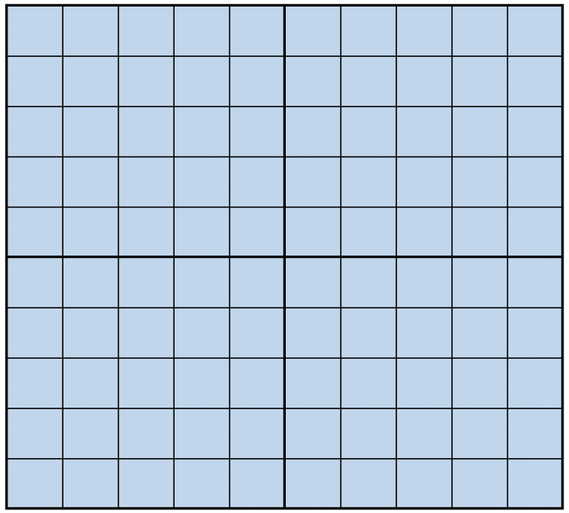
> This paper shows empirically and theoretically that randomly chosen trials are more efficient for hyper-parameter optimization than trials on a grid.

Two main reasons:

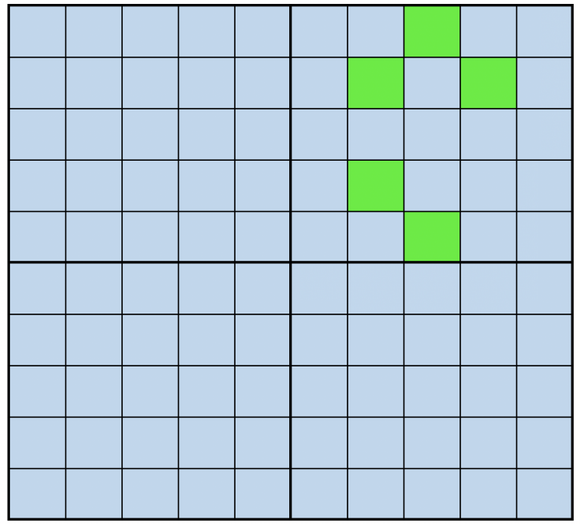
1. Not every hyperparameter is as important
2. A little trick of probability

A probability trick

A grid search:



Our best models:



How many models must we run to have a 95% chance of getting one of the green squares?

A probability Trick

If we randomly select hyperparameter combinations uniformly, let's consider the chance of MISSING every single trial, to show how unlikely that is

- Trial 1 = 0.05 chance of success and (1 - 0.05) of missing
  - Trial 2 = (1-0.05) x (1-0.05) of missing the range
    - Trial 3 = (1-0.05) x (1-0.05) x (1-0.05) of missing again
- In fact, with n trials we have (1-0.05)^n chance that every single trial misses that desired spot.

A probability trick

So how many trials to have a high (95%) chance of getting **in** that region?

- We have (1-0.05)^n chance to miss everything.
- So we must have (1- miss everything) chance to get in there or (1-(1-0.05)^n)
- Solving 1-(1-0.05)^n >= 0.95 gives us **n >= 59**

A probability trick

What does that all mean?

- You are unlikely to keep completely missing the 'good area' for a long time when randomly picking new spots
- A grid search may spend lots of time in a 'bad area' as it covers exhaustively.

Some important notes

Remember:

1. The maximum is still only as good as the grid you set!
2. Remember to fairly compare this to grid search, you need to have the same modeling 'budget'

Creating a random sample of hyperparameters

We can create our own random sample of hyperparameter combinations:

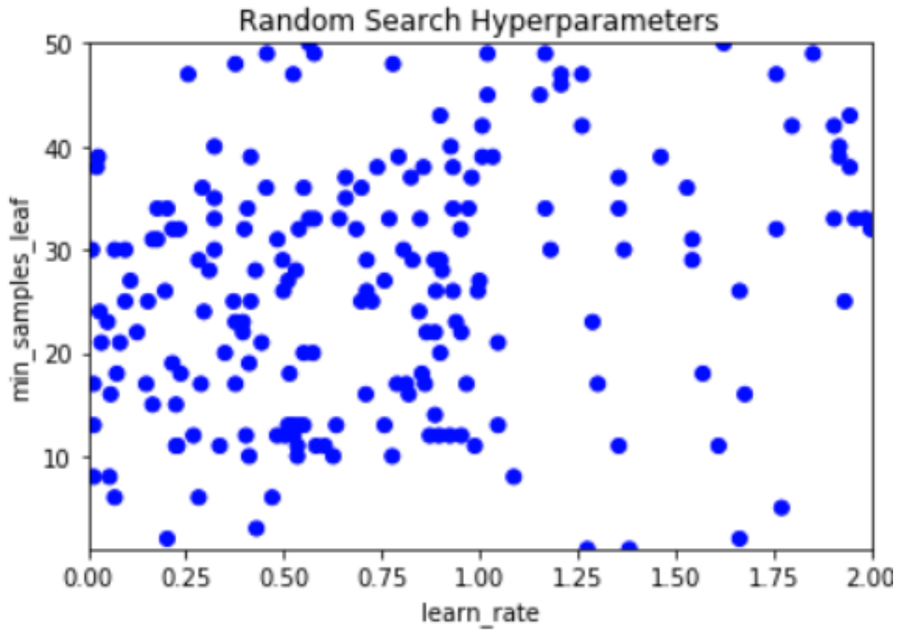
```
# Set some hyperparameter lists
learn_rate_list = np.linspace(0.001,2,150)
min_samples_leaf_list = list(range(1,51))
```

```
# Create list of combinations
from itertools import product
combinations_list = [list(x) for x in product(learn_rate_list, min_samples_leaf_list)]
```

```
# Select 100 models from our larger set
random_combinations_index = np.random.choice(range(0,len(combinations_random)), 100, replace=False)
combinations_random_chosen = [combinations_random[x] for x in random_combinations_index]
```

Visualizing a Random Search

We can also visualize the random search coverage by plotting the hyperparameter choices on an X and Y axis.



Notice how this has a wide range of the scatter but not deep coverage?

Let's practice!

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Random Search in Scikit Learn

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Comparing to GridSearchCV

We don't need to reinvent the wheel. Let's recall the steps for a Grid Search:

1. Decide an algorithm/estimator
2. Defining which hyperparameters we will tune
3. Defining a range of values for each hyperparameter
4. Setting a cross-validation scheme; and
5. Define a score function
6. Include extra useful information or functions

Comparing to Grid Search

There is only one difference:

- Step 7 = Decide how many samples to take (then sample)

That's it! (mostly)

Comparing Scikit Learn Modules

The modules are similar too:

GridSearchCV:

```
sklearn.model_selection.GridSearchCV(estimator, param_grid,
        scoring=None, fit_params=None,
        n_jobs=None,
        iid='warn',
        refit=True, cv='warn', verbose=0,
        pre_dispatch='2*n_jobs',
        error_score='raise-deprecating',
        return_train_score='warn')
```

RandomizedSearchCV:

```
sklearn.model_selection.RandomizedSearchCV(estimator,
        param_distributions, n_iter=10,
        scoring=None, fit_params=None,
        n_jobs=None, iid='warn', refit=True,
        cv='warn', verbose=0,
        pre_dispatch='2*n_jobs',
        random_state=None,
        error_score='raise-deprecating',
        return_train_score='warn')
```

Key differences

Two key differences:

- `n_iter` which is the number of samples for the random search to take from your grid. In the previous example you did 300.
- `param_distributions` is slightly different from `param_grid` , allowing optional ability to set a distribution for sampling.
    - The default is all combinations have equal chance to be chosen.

Build a RandomizedSearchCV Object

Now we can build a random search object just like the grid search, but with our small change:

```
# Set up the sample space
learn_rate_list = np.linspace(0.001,2,150)
min_samples_leaf_list = list(range(1,51))

# Create the grid
parameter_grid = {
    'learning_rate' : learn_rate_list,
    'min_samples_leaf' : min_samples_leaf_list}

# Define how many samples
number_models = 10
```

Build a RandomizedSearchCV Object

Now we can build the object

```
# Create a random search object
random_GBM_class = RandomizedSearchCV(
    estimator = GradientBoostingClassifier(),
    param_distributions = parameter_grid,
    n_iter = number_models,
    scoring='accuracy',
    n_jobs=4,
    cv = 10,
    refit=True,
    return_train_score = True)
# Fit the object to our data
random_GBM_class.fit(X_train, y_train)
```

Analyze the output

The output is exactly the same!

How do we see what hyperparameter values were chosen?

The `cv_results_` dictionary (in the relevant `param_` columns)!

Extract the lists:

```
rand_x = list(random_GBM_class.cv_results_['param_learning_rate'])
rand_y = list(random_GBM_class.cv_results_['param_min_samples_leaf'])
```

Analyze the output

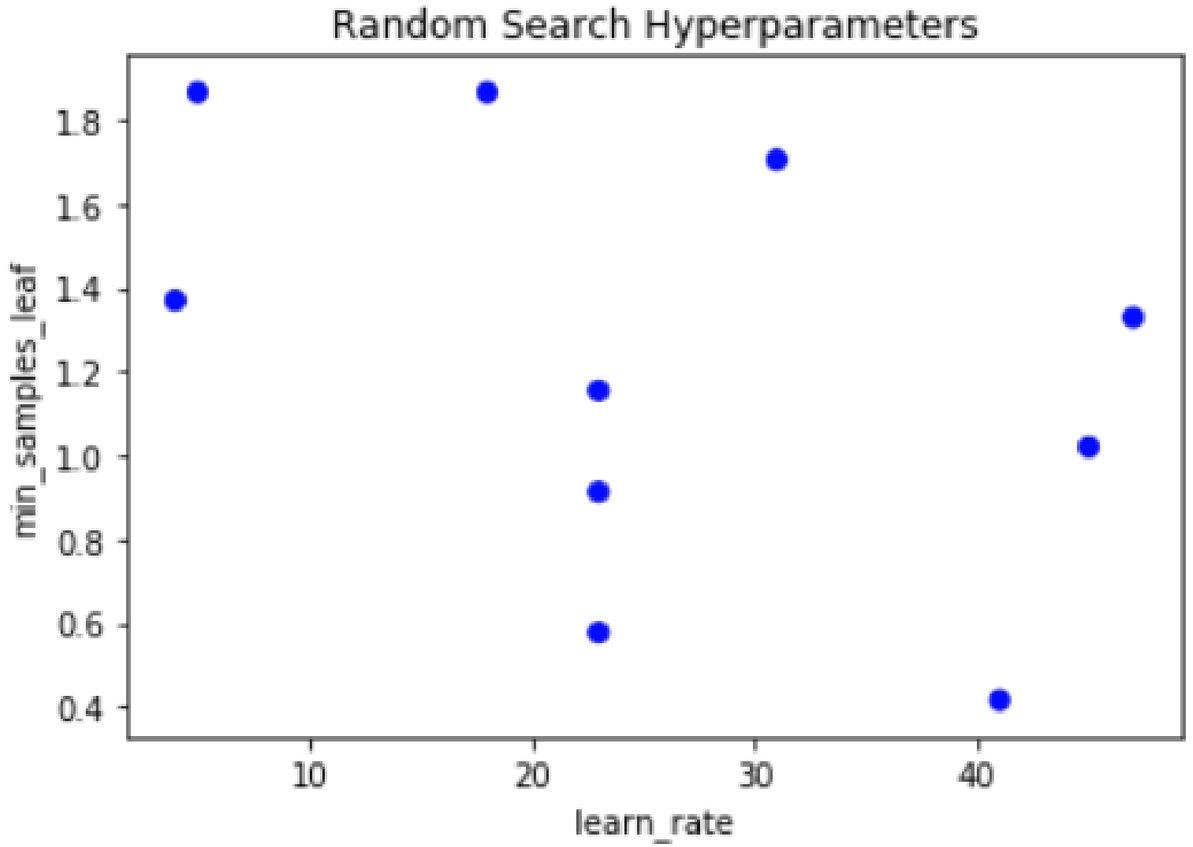
Build our visualization:

```
# Make sure we set the limits of Y and X appriately
x_lims = [np.min(learn_rate_list), np.max(learn_rate_list)]
y_lims = [np.min(min_samples_leaf_list), np.max(min_samples_leaf_list)]

# Plot grid results
plt.scatter(rand_y, rand_x, c=['blue']*10)
plt.gca().set(xlabel='learn_rate', ylabel='min_samples_leaf',
              title='Random Search Hyperparameters')
plt.show()
```

Analyze the output

A similar graph to before:



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Comparing Grid and Random Search

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What's the same?

Similarities between Random and Grid Search?

- Both are automated ways of tuning different hyperparameters
- For both you set the grid to sample from (which hyperparameters and values for each)

Remember to think carefully about your grid!

- For both you set a cross-validation scheme and scoring function

What's different?

Grid Search:

- Exhaustively tries all combinations within the sample space
- No Sampling methodology
- More computationally expensive
- Guaranteed to find the best score in the sample space

Random Search:

- Randomly selects a subset of combinations within the sample space (that you must specify)
- Can select a sampling methodology (other than uniform which is default)
- Less computationally expensive
- Not guaranteed to find the best score in the sample space (but likely to find a *good* one *faster*)

Which should I use?

So which one should I use? What are my considerations?

- How much data do you have?
- How many hyperparameters and values do you want to tune?
- How much resources do you have? (Time, computing power)

- More data means random search may be better option.
- More of these means random search may be a better option.
- Less resources means random search may be a better option.

Let's practice!

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