Hyperopt-Sklearn: Really Simple Hyperparameter Optimization

by Matthew Emery @lstmemery (https://github.com/lstmemery/hyperopt-sklearn/tree/master/hpsklearn)

About Me

- Master's degree from UBC in Data Science
- Data scientist at Imbellus Inc.
- We build simulations to predict the problem-solving abilities of job applicants
- We are hiring! We pay American!

Table of Questions

1. What are hyperparameters?
2. Why should I care about this talk?
3. How does the Tree Parzen Estimator algorithm work?
4. What does Hyperopt do?
5. Why should I use Hyperopt-Sklearn?
6. What are my other options?

What Are Those Machines Learning?

- Machine learning algorithms find the **parameters** of a model that minimize some **loss function**
- Every algorithm comes with a different set of assumptions about your data
- You can modify the algorithm's assumptions before you minimize by setting **hyperparameters**

In [43]:
```
ols = Lasso(alpha = 0.0001) # Alpha is a hyperparameter
ols.fit(X1_train, y1_train)
print(ols.coef_) # Regression coefficients are parameters
print(f"Score: {mean_absolute_error(y1_test, ols.predict(X1_test)):.2f}")

lasso = Lasso(alpha = 1)
lasso.fit(X1_train, y1_train)
print(lasso.coef_)
print(f"Score: {mean_absolute_error(y1_test, lasso.predict(X1_test)):.2f}")
```

```
[52.44  0.06 73.27 -0.06  9.66 13.49 -0.03 -0.05  0.16 40.06]
Score: 1.70
[51.41  0.   72.26 -0.    8.76 12.45 -0.   -0.    0.   38.98]
Score: 2.35
```

Speaker notes

- I generated two synthetic datasets for regression
- First has 10 features, 5 are informative
- Second has 1000 features, with 5 informative
- Lasso with weak regression does better here

In [57]:
```
# Same generating process, but more uninformative features
ols = Lasso(alpha = 0.0001)
ols.fit(X2_train, y2_train)
print(f"Score: {mean_absolute_error(y2_test, ols.predict(X2_test)):.2f}")

lasso = Lasso(alpha = 1)
lasso.fit(X2_train, y2_train)
print(f"Score: {mean_absolute_error(y2_test, lasso.predict(X2_test)):.2f}")
```

```
Score: 41.83
Score: 2.51
```

Speaker notes

- Even though the processes that made these data sets are similar, the results are radically similar
- Talk about No Free Lunch here

- Imagine that you've been instructed to recreate a 5-minute song on this synth
- Some of the knobs and switches affect others. Some don't do anything at all
- You don't know what you're doing, but a blind DJ tells you how close you are

Speaker notes

what hyperparameter tuning is like
long time

- It's frustrating to do by hand
- You don't get much feedback

- The combination of all hyperparameters is called **Hyperparameter Space**

What do we know about Hyperparameter Space?

1. It's huge. You can expect to be exploring in dozens of dimensions
2. It's costly to explore. Each point in hyperparameter space has to be evaluated by training a model
3. It's not smooth. You can't expect to take the gradient of hyperparameter space
4. Not all dimensions are equal. There are often hyperparameters whose optimal values don't contribute very much minimizing the loss function.
5. (Because of the first 4): Humans are bad at exploring it. Randomized search often outperforms humans. [1]

Speaker notes

- Taking gradient is nice because it gives you a sense of direction
- Very recent work has found some clever ways for you to take the derivative of something like hyperparameter space

Optimization Bias and Getting Rich Quick[5]

- Every weekday for two weeks (10 days) I send you an email predicting whether the Dow Jones will rise or fall
- I'm always right
- Assuming the Dow Jones Index is independent of the past and equally likely to rise or fall:

$$\left(\frac{1}{2}\right)^{10} = \frac{1}{1024}$$

- Is there anything you should know before you give me all your money?

What if I sent out random emails to 10000 different people?

In [8]:
```
emails = binomial(n=10, p=0.5, size=10000)
len(emails[emails == 10]) # Nine lucky recipients!
```

Out[8]: 9

Speaker notes

Make sure to mention How Not to Be Wrong by Jordan Ellenberg.

What does this have to do with hyperparameter optimization?

- Each email is a model that gives a prediction
- The emailer is your hyperparameter optimization algorithm
- The first 10 days if your validation set
- You lose all your money by putting a crappy model in production

How do we defeat optimization bias?

1. **Get more data:** This is almost always the right call.
2. **Cross-validation:** This is like asking the stock picker to predict the direction of multiple indices. Optimization bias is always possible, but it will occur more slowly. Repeat cross-validation with different seeds if you can afford to.
3. **Build fewer models:** This is why the efficiency of the hyperparameter optimization algorithm matters

- Hyperparameter optimization is computationally costly
- Your ideal hyperparameters will shift depending on feature engineering
- Create a few basic models first and see if validation accuracy improves
- **Don't do hyperparameter tuning until you are reasonably sure you won't be making significant changes**

Speaker notes

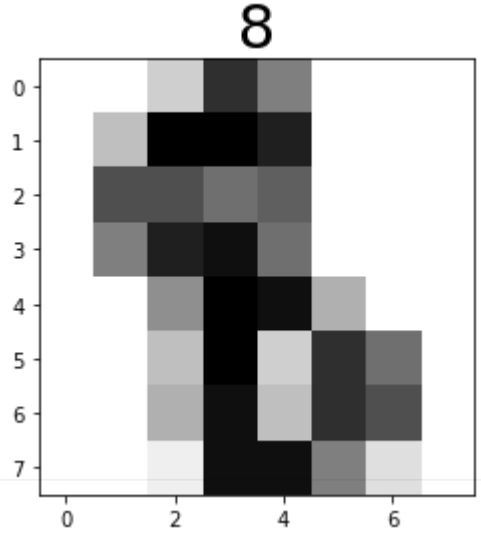
- It's tempting to run this all the time. You shouldn't
- I think of hyperparameter tuning as sending your model off to get laminated

Dessert First: Let's Peek at Hyperopt-Sklearn

In [13]:
```
X, y = load_digits(return_X_y = True) # MNIST Dataset

(train_X, test_X, train_y, test_y) = train_test_split(X, y,
                                     test_size = 0.2,
                                     random_state = 0) # Split the Data
random_image = randint(0, len(train_X))
plt.title(train_y[random_image], fontsize=30)
plt.imshow(train_X[random_image].reshape(8, 8), cmap=plt.cm.gray_r)
```

Out[13]:
```
<matplotlib.image.AxesImage at 0x7f4f56844cf8>
```



Speaker notes

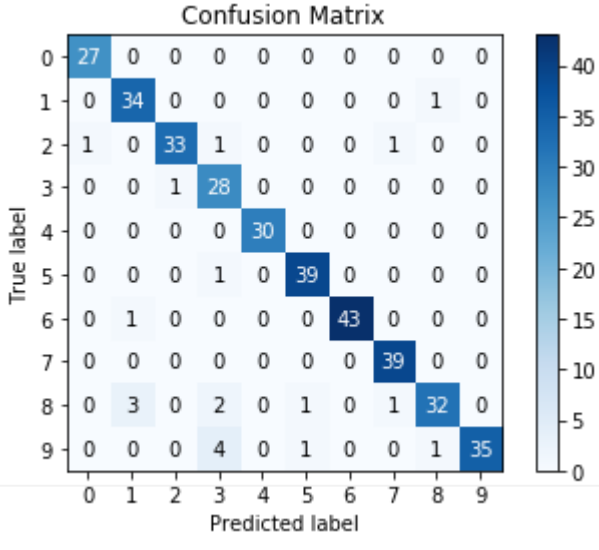
- This is interactive in the notebook version
- I've loaded all the all the libraries ahead of time

In [11]:
```
model = RandomForestClassifier(random_state = 0) # Basic Random Forest
model.fit(train_X, train_y)
print(accuracy_score(test_y, model.predict(test_X)).round(3))

skplt.metrics.plot_confusion_matrix(test_y, model.predict(test_X)) # Lookup Scik
it-plot!
```

```
0.944
```

Out[11]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7efe55a9bdd8>
```



Speaker notes

- This is already really good. (About 1 in 20 wrong)
- I love scikit-plot

In [37]:
```
from hpsklearn import HyperoptEstimator, any_classifier

hyperopt_model = HyperoptEstimator(classifier=any_classifier("mnist"),
                                   max_evals=100,
                                   seed=0)
hyperopt_model.fit(train_X,
                   train_y,
                   n_folds=5,
                   cv_shuffle=True,
                   random_state=0)

from sklearn.externals import joblib

joblib.dump(hyperopt_model, "hyperopt_model.pkl")
```

Out[37]:
```
['hyperopt_model.pkl']
```

Speaker notes

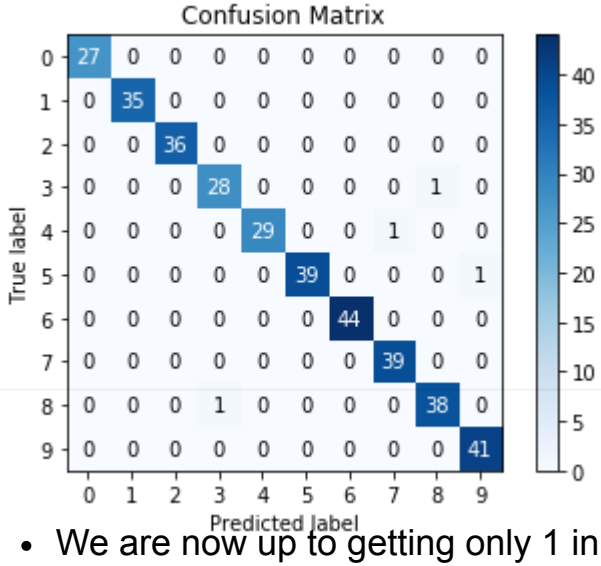
- This took about 30 minutes to run
- I usually run stuff like this overnight or in the cloud
- ALWAYS SAVE YOUR WORK
- You can also specify specific classifiers you want

In [14]:
```
hyperopt_model = joblib.load("hyperopt_model.pkl")
hyperopt_predictions = hyperopt_model.predict(test_X)

print(accuracy_score(test_y, hyperopt_predictions).round(3))
print(hyperopt_model.best_model())
skplt.metrics.plot_confusion_matrix(test_y, hyperopt_predictions)
```

```
0.989
{'learner': KNeighborsClassifier(algorithm='auto', leaf_size=30, metric='eucli
dean',
           metric_params=None, n_jobs=1, n_neighbors=3, p=2,
           weights='distance'), 'preprocs': (Normalizer(copy=True, norm='l
2'),), 'ex_preprocs': ()}
```

Out[14]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7efe505dfcf8>
```

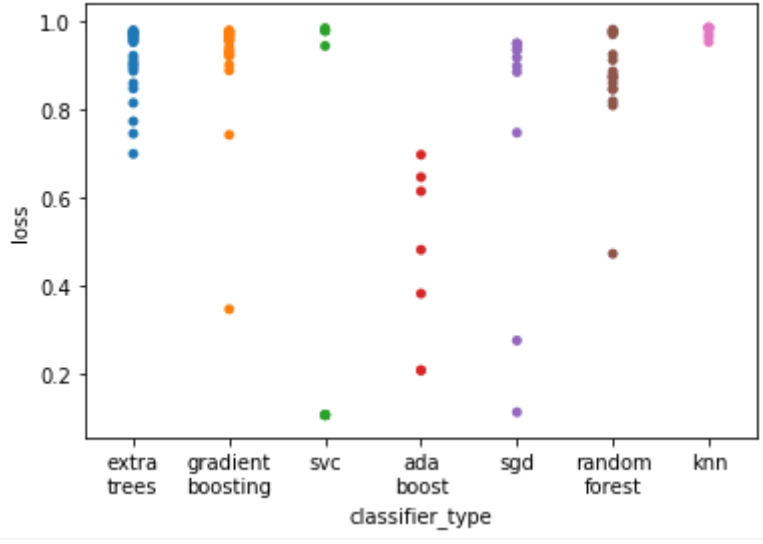


Speaker notes

- We are now up to getting only 1 in 100 wrong
- This model happens to be an excellent solution

In [19]:
```
sns.stripplot(x="classifier_type", y="loss", data= pd.DataFrame(classifier_performance))
```

Out[19]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7efe5038eeb8>
```

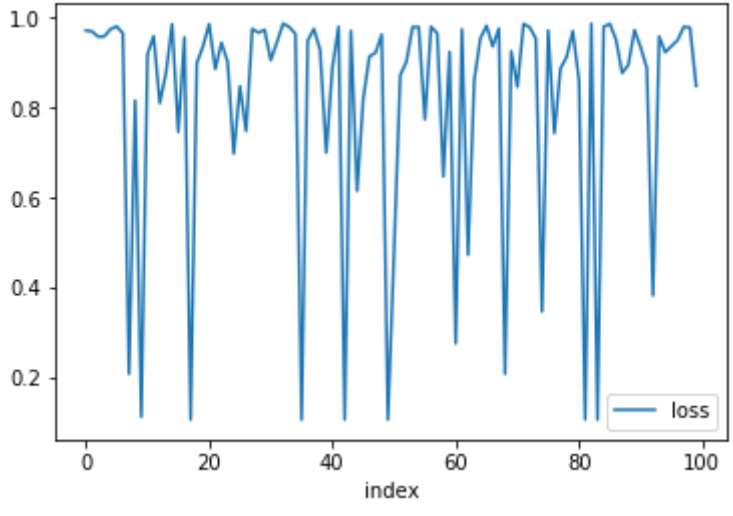


Speaker notes

- This is a plot of performance for the different algorithms tried
- What you can see is some models outperform others
- Why is gradient boosting fine but adaptive not? Who knows

In [20]:
```
pd.DataFrame(classifier_performance).plot.line(x="index", y="loss")
```

Out[20]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7efe5033dcf8>
```



Speaker notes

- In this case, the problem was rather easy, so you don't notice a huge trend
- Over time those deep dips will start to disappear
- That wouldn't happen in random search

Sequential Model-Based Optimization (SMBO)

```
Make a container for your history
For each time step in the total number of time steps
    Find the most promising set of hyperparameters based on a
        *surrogate function* and your *model of the data*
    Evaluate your most promising set with your real, expensive function
    Update your history
    Update your model of the data, given the new history
```

Speaker notes

- Here comes the math
- Begestra did a tremendous amount of work here
- SMBO is a general framework. We have to make up the surrogate function and model.

How should we model the data?

The original paper suggests two options:

1. Gaussian Processes (Maybe next talk?)
2. **Tree-based Parzen Windows (TPE)**

Speaker notes

- Gaussian processes tend to work well with continuous variables
- GPs tend to fail when you have many features that don't matter
- Hyperparameter optimization is still a very open field

What Is a Surrogate Function?

- A surrogate function attempts to put forward the best proposal for the actual function
- The one chosen in the original paper is called expected improvement, but there are other proposals

$$EI_{y^*}(x) = \int_{-\infty}^{\infty} \max(y^* - y, 0) p(y|x) dy$$

- y^* is some threshold value. $p(y|x)$ is the probability of achieving the loss y given the hyperparameters x
- In TPE y^* is a quantile cutoff point of previous values

How do Tree-Based Parzen Estimators Work?

- Imagine you have two distributions
- One distribution contains all of the sets of hyperparameters that give good results
- The other contains all the sets of hyperparameters that are not good

$$p(x|y) = \begin{cases} l(x) \ if \ y<y^* \\ g(x) \ if \ y \geq y^* \end{cases}$$

- Notice that we are modeling $p(x|y)$, not $p(y|x)$, but we have Bayes' thereom

What decides y^*?

- You do! It's a hyper-hyperparameter
- The TPE algorithm contains a parameter γ.
- $\gamma = p(y < y^*)$
- This represents the proportion of "good" ys
- By default, it's 15%

What are $l(x)$ and $g(x)$?

- They start as some prior distribution (uniform, log-uniform, normal, log-normal or discrete)
- If the prior is continuous, then the prior distribution is replaced by a truncated 1D Gaussian mixture
- If the prior is discrete, then add some weight to the value selected
- As far as I can tell, l is for lesser, and g is for greater

What is the TPE algorithm optimizing?

- Begestra[1] shows that

$$EI_y^*(x) \propto \left(\gamma + \frac{g(x)}{l(x)}(1-\gamma)\right)^{-1}$$

- The best point x^* will appear be highly probable in $l(x)$ and highly improbable in $g(x)$
- To find the optimal point x^* we sample x in both mixtures and report the the value that minimizes $\frac{g(x)}{l(x)}$
- Gaussian mixtures are easy to calculate, so this sampling operation is fast

What is a Gaussian Mixture?

- Imagine adding two Gaussian curves together and normalizing

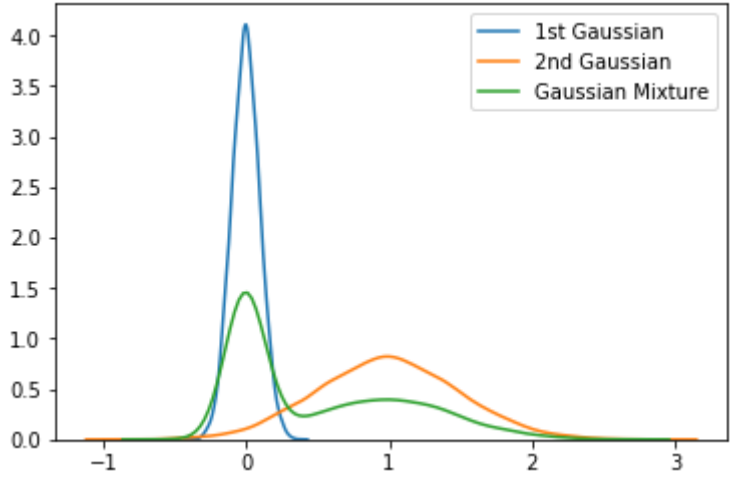
In TPE:

- The mean of each Gaussian is defined as the point sampled from the previous distribution
- The standard deviation is the difference between the new sampled point, and its immediate neighbors. Pick the greater of the two distances.

In [112]:
```
gaussian_example_1 = normal(loc=0, scale=0.1, size=10000)
gaussian_example_2 = normal(loc=1, scale=0.5, size=10000)
mixture_example = choice(np.concatenate([gaussian_example_1, gaussian_example_2
]), size = len(gaussian_example_1))

sns.distplot(gaussian_example_1, kde=True, hist=False, label="1st Gaussian")
sns.distplot(gaussian_example_2, kde=True, hist=False, label="2nd Gaussian")
sns.distplot(mixture_example, kde=True, hist=False, label="Gaussian Mixture")
```

Out[112]:
```
<matplotlib.axes._subplots.AxesSubplot at 0x7f420637f320>
```



Speaker notes

- TPE constructs these mixtures iteratively

What is Hyperopt?

- People assume that hyperopt is the reference implementation of TPE in Python[4]
- That's true, but it's also a general purpose optimization framework

We need:

- A function to minimize
- A defined hyperparameter space
- An object to store our experiments in
- A search algorithm (TPE)

In [10]:

```
def example_experiment(space_arguments):
    # Recall MNIST from near the start of the talk?
    accuracy_results = cross_val_score(space_arguments,
                                       train_X, train_y, scoring=make_scorer(acc
uracy_score))

    try:
        return {"loss": -accuracy_results.mean(), # Negative because hyperopt al
ways minimizes
         "status": hp.STATUS_OK}
    except Exception as e:
        return {"status": hp.STATUS_FAIL,
                "exception": str(e)}
```

In [11]:

```
hp.pyll.scope.define(RandomForestClassifier)
hp.pyll.scope.define(KNeighborsClassifier)


space = hp.hp.pchoice("model", [
    (0.4, hp.pyll.scope.RandomForestClassifier( # Weighted discrete
        criterion=hp.hp.choice(
            "random_forest.criterion", ["gini", "entropy"]),
        n_estimators=hp.pyll.scope.int(
            hp.hp.qloguniform(
                "random_forest.n_estimators", np.log(9.5), np.log(3000.5), 1
))))),
    (0.6, hp.pyll.scope.KNeighborsClassifier(
        n_neighbors=hp.pyll.scope.int(
            hp.hp.qloguniform("knn.n_neighbors", np.log(0.5), np.log(50.5), 1
))))
])
```

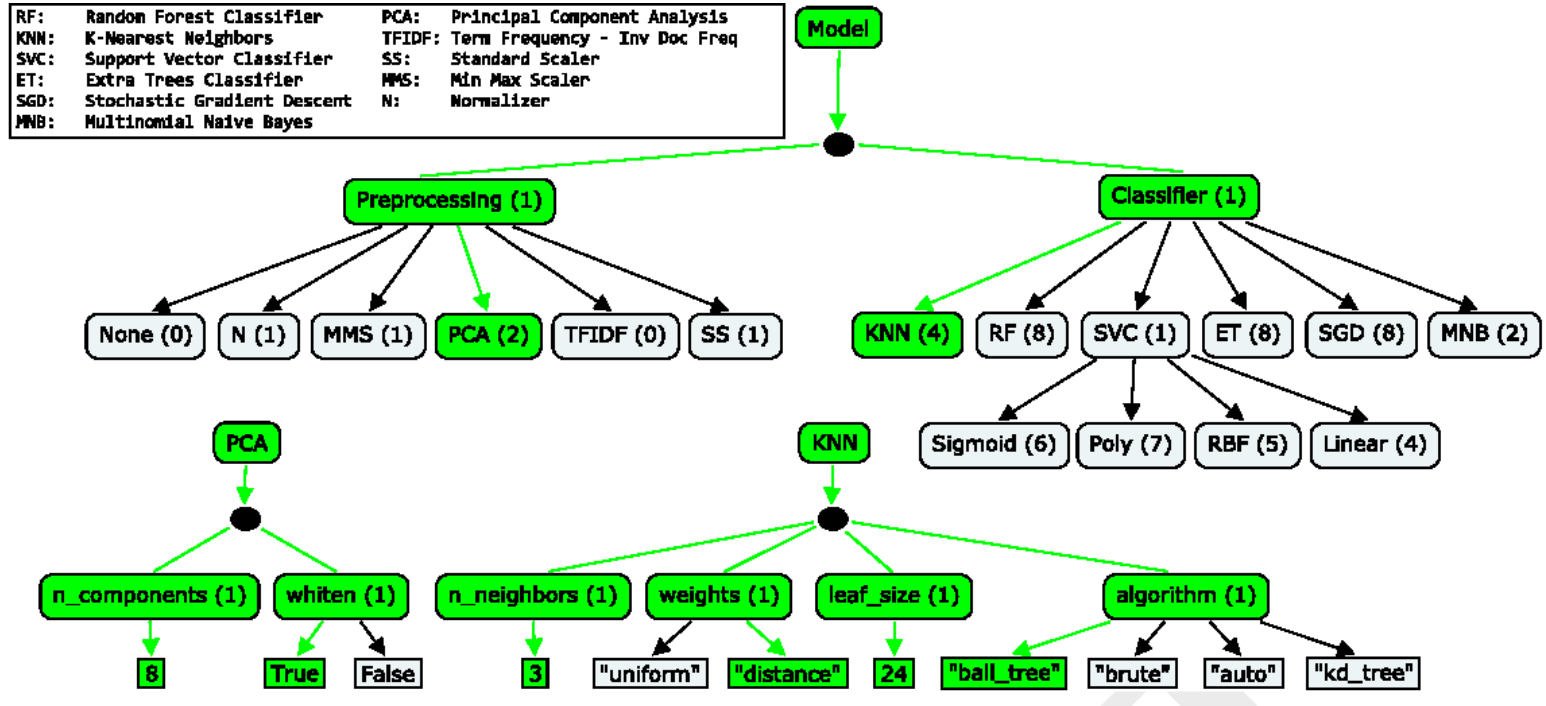
Speaker notes

- scope.define makes a function accessible to space
- pchoice is weighted discrete
- qloguniform just rounds a log-uniform (can't be negative)

In [14]:
```
trials = hp.Trials() # Basicially, a dictionary
best = hp.fmin(example_experiment,
               space,
               algo=hp.tpe.suggest, max_evals=10, trials=trials)
best
trials.trials[0]
```

Out[14]:
```
{'knn.n_neighbors': 3.0, 'model': 1}
```

What is Hyperopt-Sklearn? [3]



eprot-sklearn's full search space ("Any Classifier") consists of a (preprocessing, classsifier) pair. There are 6 possible pr

- A wrapper for Hyperopt compatible with the scikit-learn API
- Also includes reasonable prior distributions for many scikit-learn models (plug and play)
- Supports XGBoost
- Check out my fork of it is here: https://github.com/lstmemery/hyperopt-sklearn (https://github.com/lstmemery/hyperopt-sklearn)
- My main contribution: Fixing cross-validation, adding repeated cross-validation

Speaker notes

This is a way of visualizing hyperopt-sklearn. It selects a preprocessor randomly, then selects the hyperparameters for the preprocessor. This comes image comes from hyperopt-sklearn paper

Other Features

- Parallel Optimization through MongoDB
- Warm Starting (don't start from square one every time)

Speaker notes

- These are both ways of dealing with a more massive datasets
- When in doubt, buy a bigger instance

What about Neural Networks?

- Some kind soul built a keras-compatibility layer called Hyperas (https://github.com/maxpumperla/hyperas)
- Hyperas has a similar syntax to Jinja or any other HTML templating library
- I haven't found anything for PyTorch

Other Hyperparameter Libraries

- Hyperband (subsampling, bandit algorithm random search)
- TPOT (Evolutionary pipeline building)
- Auto-sklearn (Ensemble building and meta-learning)

Speaker notes

- There's a new paper suggesting that you combine Hyperband and Hyperopt

Bibliography

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[2]D. D. Labs, “District Data Labs - Parameter Tuning with Hyperopt.” [Online]. Available: https://districtdatalabs.silvrback.com/parameter-tuning-with-hyperopt (https://districtdatalabs.silvrback.com/parameter-tuning-with-hyperopt). [Accessed: 15-Jul-2018].

[3]B. Komer, J. Bergstra, and C. Eliasmith, “Hyperopt-Sklearn: Automatic Hyperparameter Configuration for Scikit-Learn,” p. 7, 2014.

[4]J. Bergstra, B. Komer, C. Eliasmith, D. Yamins, and D. D. Cox, “Hyperopt: a Python library for model selection and hyperparameter optimization,” Comput. Sci. Disc., vol. 8, no. 1, p. 014008, 2015.

[5]J. Ellenberg, How Not to Be Wrong: The Power of Mathematical Thinking. Penguin Books, 2014.