Abstract

We propose the use of \( k \)-determinantal point processes in hyperparameter optimization via random search. Compared to conventional approaches where hyperparameter settings are sampled independently, a \( k \)-DPP promotes diversity. We describe an approach that transforms hyperparameter search spaces for efficient use with a \( k \)-DPP. Our experiments show significant benefits over uniform random search in realistic scenarios with a limited budget for training supervised learners, whether in serial or parallel.

1 Introduction

Hyperparameter values—regularization strength, model family choices like depth of a neural network or which nonlinear functions to use, procedural elements like dropout rates, stochastic gradient descent step sizes, and data preprocessing choices—can make the difference between a successful application of machine learning and a wasted effort. To search among many hyperparameter values requires repeated execution of often-expensive learning algorithms, creating a major obstacle for practitioners and researchers alike. Ad hoc methods and inheritance of hyperparameter values from earlier projects have been giving way to specialized techniques for optimizing hyperparameters [Brochu et al., 2010, Li et al., 2017].

Recently, random search has been shown competitive for hyperparameter optimization [Li et al., 2017]. It is especially appealing due to its simplicity: define the domain of hyperparameter values \( \mathcal{Y} \) to be searched, draw a value uniformly from \( \mathcal{Y} \), evaluate it (i.e., train a model with that hyperparameter value and measure its error on development data), and repeat until satisfied. Further, it is straightforward to parallelize evaluations of multiple hyperparameter values.

Here, we are concerned with scenarios where multiple interacting hyperparameters’ values affect an algorithm’s performance, and where we have a fixed budget of \( k \) applications of the learning algorithm. The central idea is that the random draws should not be independent, but rather should seek diversity. This is one of the attractions of earlier approaches based on Bayesian optimization [Snoek et al., 2012], which encouraged exploration of hyperparameter value regions.

The core idea is to replace \( k \) uniform, independent draws with one draw of size \( k \) from a \( k \)-determinantal point process \([k\text{-DPP}; Kulesza et al., 2012]\). We transform a hyperparameter domain
\(\mathcal{Y}\)—which may include real, integer, and categorical dimensions and which may have a tree structure—into the sample space for a \(k\)-DPP that allows efficient sampling. Importantly, we avoid explicit calculation of all of the pairwise similarities between values in \(\mathcal{Y}\) using a computationally efficient and intuitive decomposition. As presented in Kulesza et al. [2012], sampling from a ( discrete ) \(k\)-DPP is as fast as sampling from a DPP, which is \(O(N^3)\), where \(N = |\mathcal{Y}|\) (this computation is dominated by the cost to invert a matrix). On a modern 36 core machine, constructing the DPP using our methods takes less than 30 seconds for \(N\) up to 100,000, and samples can be drawn (with \(k\) up to 200) from DPPs with \(N\) as large as 2,000 in less than a second, and with \(N\) as large as 20,000 in less than ten minutes.

Experimentally, we explore the use of our \(k\)-DPP random search method and find that it significantly outperforms uniform random search in cases where the hyperparameter values have a large effect on performance. Unsurprisingly, when hyperparameter values matter less, it has no effect. Additionally, our experiments demonstrate that the amount by which our method outperforms sampling uniformly increases as the difficulty of the search increases (i.e. as a smaller fraction of the space leads to good results).

An open-source implementation of our methods, as an extension to the hyperopt package [Bergstra et al., 2013] can be found online[1].

2 Method

We begin by reviewing determinantal point processes (DPPs) and \(k\)-DPPs.

Let \(\mathcal{Y}\) be a domain of values from which we would like to sample a finite subset. (In our use of DPPs, this is the set of hyperparameter settings.) In general, \(\mathcal{Y}\) could be discrete or continuous, but here we assume it is discrete with \(N\) values. A DPP defines a probability distribution over \(2^\mathcal{Y}\) (all subsets of \(\mathcal{Y}\)) with the property that two elements of \(\mathcal{Y}\) are more (less) likely to both be chosen the more dissimilar (similar) they are. Let random variable \(Y\) range over finite subsets of \(\mathcal{Y}\).

There are several ways to define the parameters of a DPP. The first, and perhaps most intuitive, uses a symmetric matrix \(K \in \mathbb{R}^{N \times N}\) to represent the DPP. \(K\)'s rows and columns are indexed by elements of \(\mathcal{Y}\). Consider a subset \(A \subseteq \mathcal{Y}\). Under the DPP, the marginal probability that all elements of \(A\) are drawn is:

\[
P(A \subseteq Y) = \det(K_A),
\]

(1)

where \(K_A\) is the submatrix of \(K\) including rows and columns corresponding to elements of \(A\).

The second formulation allows us to define the probability that a specific subset is drawn (i.e., \(P(Y = A)\) for some \(A \subset \mathcal{Y}\)). Let:

\[
L = K(I - K)^{-1}.
\]

(2)

Then it is straightforward to show that

\[
P(Y = A) = \frac{\det(L_A)}{\det(L + I)}.
\]

(3)

As shown in Kulesza et al. [2012], this definition of \(L\) admits a decomposition to terms representing the quality and diversity of the elements of \(\mathcal{Y}\). For any \(y_i, y_j \in \mathcal{Y}\), let:

\[
L[i, j] = q_i \phi_i^\top \phi_j q_j,
\]

(4)

where \(q_i > 0\) is the quality of \(y_i\) and \(\phi_i \in \mathbb{R}^D\) is a featurized representation of \(y_i\), constrained so that \(||\phi_i|| = 1\). (We will discuss how to featurize hyperparameter settings in Section 2.2.) Hence the inner product \(\phi_i^\top \phi_j\) captures (cosine) similarity between the feature vectors (and therefore between \(y_i\) and \(y_j\)). If we stack all \(q_i \phi_i\) as columns of matrix \(B \in \mathbb{R}^{D \times N}\), then \(B^\top B = L\).

Here, we fix all \(q_i = 1\); in future work, iterative variants of our method might make use of \(q_i\) to encode evidence about the quality of particular hyperparameter settings to adapt the DPP’s distribution over time.

[1] https://github.com/dodgejesse/random_search_using_discrete_dpp
2.1 Sampling from a \(k\)-DPP

DPPs have support over all subsets of \(\mathcal{Y}\), including \(\emptyset\) and \(\mathcal{Y}\) itself. In many practical settings, one may have a fixed budget that allows running the training algorithm \(k\) times, so we require precisely \(k\) elements of \(\mathcal{Y}\) for evaluation. \(k\)-DPPs are distributions over subsets of \(\mathcal{Y}\) of size \(k\). Thus,

\[
P(Y = A | |Y| = k) = \frac{\det(L_A)}{\sum \det(L_{A'})}
\]

(Kulesza et al. [2012]) gives an \(O(N^3)\) algorithm for sampling exactly from \(k\)-DPPs. We use an open-source implementation of this method.[3]

In this work, we use discretized values for continuous hyperparameters, to allow a single treatment of all dimensions of our hyperparameter search space using a discrete \(k\)-DPP.

2.2 Constructing \(B\) for hyperparameter optimization

The vector \(\phi_i\) will encode \(y_i\) (an element of \(\mathcal{Y}\)), which in its most general form is an attribute-value mapping assigning values to different hyperparameters.

Let \(\phi_i = \frac{r_i}{\|r_i\|}\) for each \(y_i \in \mathcal{Y}\), and define the unnormalized vector \(r_i\) as a modular encoding of the attribute-value mapping, in which fixed segments of the vector are assigned to each hyperparameter attribute (e.g., the dropout rate, the choice of nonlinearity, etc.). We present two methods for constructing a \(k\)-DPP over hyperparameter values. The first, "\(k\)-DPP-Cos," is based on cosine distance between \(\phi_i\) and \(\phi_j\). The second, "\(k\)-DPP-Hamm," is built from a transformation of the Hamming distance between \(r_i\) and \(r_j\).

2.3 \(k\)-DPP-Cos

For a hyperparameter that takes a numerical value in range \([h_{\text{min}}, h_{\text{max}}]\), we encode value \(h\) using one dimension \((j)\) of \(r\) and project into the range \([0, 1]\):

\[
r[j] = \frac{h - h_{\text{min}}}{h_{\text{max}} - h_{\text{min}}}
\]

This rescaling prevents hyperparameters with greater dynamic range from dominating the similarity calculations for \(B\).

A categorical-valued hyperparameter attribute that takes \(m\) values is given \(m\) elements of \(r\) and a one-hot encoding.

To avoid the trivial value \(r_i = 0\), which would lead to degenerate similarity values, we append a 1 to every \(r_i\).

2.4 \(k\)-DPP-Hamm

The preference for diversity in DPPs tends to encourage a points to be sampled which are far apart, leading to higher density of samples near the extreme regions of the space (i.e., near \(h_{\text{min}}\) or \(h_{\text{max}}\)). Intuitively, if the best value found for some hyperparameter takes an extreme value, then the search should perhaps be widened to trap values that are even better. For this reason, in practice, wide ranges \([h_{\text{min}}, h_{\text{max}}]\) are often constructed deliberately. If this has been done, then the DPP’s preference for extreme values may be a liability.

Using the same unnormalized vector \(r\) as above, we replace the inner product \(\phi_i^T \phi_j\) in the construction of \(L\) with the following:

\[
\frac{2(D - \text{Hamming}(r_i, r_j))}{D} - 1
\]

where Hamming(a, b) is the Hamming distance between two vectors.\(^3\) The expression in Eq. 7 has the range \([-1, 1]\), so will define a valid \(k\)-DPP, but since it has no sense of how far apart \(r_i[k]\) and \(r_j[k]\) are.

\(^3\)Hamming distance is traditionally defined for strings and binary vectors; it applies an elementwise inequality test (for each dimension \(k\), return 1 if \(r_i[k] \neq r_j[k]\), 0 otherwise), then sums the results. We extend the definition to include real vectors.

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[3]: http://www.alexkulesza.com/code/dpp.tgz
\( r_j[k] \) are—it knows only whether they are different—extreme regions won’t be oversampled. In Figure 4 we see empirical evidence of this difference.

### 2.5 Tree-structured hyperparameters

Many real-world hyperparameter search spaces are tree-structured. For example, the number of layers in a neural network is a hyperparameter, and each additional layer adds at least one new hyperparameter which ought to be tuned (the number of nodes in that layer).

For a binary hyperparameter like whether or not to use regularization, we use a one-hot encoding. When this hyperparameter is “on,” we set the associated regularization strength in \( r \) as above, and when it is “off” we set it to zero. Intuitively, with all other hyperparameter settings equal, this causes the "off" setting to be closest (in both cosine distance and Hamming distance) to the least strong regularization.

One can also treat higher-level design decisions as hyperparameters [Komer et al., 2014], such as whether to train a logistic regression classifier, a convolutional neural network, or a recurrent neural network. In this construction, the type of model would be a categorical variable (and thus get a one-hot encoding), and all child hyperparameters for an "off" model setting (such as the convergence tolerance for logistic regression, when training a recurrent neural network) would be set to zero.

### 3 Experiments

In this section we present our experiments. We compare samples drawn using \( k \)-DPP-Hamm and \( k \)-DPP-Cos against samples drawn uniformly at random. In all three cases, we use the same discretization for continuous hyperparameter values. It is worth noting that as \( k \) increases, all sampling methods approach the true optimum in our search space. In our experiments we will use \( k = 20 \) and \( k = 50 \), with \( N \) greater than 4,000.

#### 3.1 Convolutional neural networks for text classification

Our experiments consider a setting where hyperparameters have a large effect on performance: a convolutional neural network for text classification [Kim, 2014]. The task is binary sentiment analysis on the Stanford sentiment treebank [Socher et al., 2013]. On this balanced dataset, random guessing leads to 50% accuracy. We use the CNN-non-static model from Kim [2014], with Word2Vec [Mikolov et al., 2013] vectors. The model architecture consists of a convolutional layer, a max-over-time pooling layer, then a fully connected layer leading to a softmax.

We begin with a search over three hyperparameters, assuming a budget of \( k = 20 \) repetitions of training the convolutional neural net. \( L_2 \) regularization strengths in the range \([e^{-5}, e^{-1}]\) (or no regularization) and dropout rates in \([0, 0.7]\) are considered. We consider three increasingly “easy” ranges for the learning rate:

- **Hard:** 16 values discretizing \([e^{-5}, e^{5}]\). 13 of the values lead to accuracy no better than chance.
- **Medium:** 16 values discretizing \([e^{-5}, e^{-1}]\). Half of the values lead to accuracy no better than chance.
- **Easy:** 16 values discretizing \([e^{-10}, e^{-3}]\). All 16 values lead to models that beat chance.

In each case, discretized points are evenly spaced in the given range (in log space).

We ran 100 trials of hyperparameter optimization for each of the three methods. Table 1 shows means and confidence intervals of the best of the 20 random models considered in each hyperparameter optimization trial. Unsurprisingly, starting with a narrow, good range (“Easy”) allows more effort for searching the other hyperparameter values and leads to better overall accuracies. The \( k \)-DPP-based methods outperform uniform sampling in all cases except \( k \)-DPP-Cos on the easiest setting (where it lags by less than 0.002% average accuracy).

Figure 1 shows the mean accuracy of the best model found after exploring 1, 2, …, \( k \) hyperparameter settings. It compares the sampling methods against a Bayesian optimization technique using a tree-structured Parzen estimator [BO-TPE; Bergstra et al., 2011]. This technique evaluates points


|       | Uniform          | k-DPP-Hamm       | k-DPP-Cos       |
|-------|------------------|------------------|------------------|
| Hard  | 75.911           | (75.897, 75.925) | **77.727**      |
|       | (75.950, 76.971) |                  | (77.117, 77.737)|
| Medium| 78.070           | (78.065, 78.075) | **78.586**      |
|       | (78.295, 78.303) |                  | (78.583, 78.590)|
| Easy  | **82.107**       | (82.106, 82.108) | **82.113**      |
|       | (82.112, 82.114) |                  | (82.104, 82.105)|
| Stable| 82.360           | (82.359, 82.360) | **82.397**      |
|       | (82.397, 82.398) |                  | (82.347, 82.348)|

Table 1: Best-found model accuracy means and 99% confidence intervals averaged across 100 trials of hyperparameter search, on four spaces as defined in Section 3.1 and Section 3.2, with \(k = 20\). All results for \(k\)-DPP-Hamm and \(k\)-DPP-Cos are statistically significantly better than random except \(k\)-DPP-Cos on the easiest two search spaces.

![Figure 1: Average best-found model accuracy by iteration (the rightmost values correspond to Table 1) when training a convolutional neural network on three hyperparameter search spaces (defined in Section 3.1), averaged across 100 trials of hyperparameter optimization, with \(k = 20\).](image)

Note that when sampling uniformly, from \(k\)-DPP-Cos, or from \(k\)-DPP-Hamm, the order of the \(k\) hyperparameter settings in one trial is arbitrary (though this is not the case with BO-TPE as it is an iterative algorithm). The variance of the \(k\)-DPP methods (not shown for clarity) tends to be high in early iterations, simply because the \(k\) samples from a \(k\)-DPP are likely to be more diverse than those sampled uniformly, but in all cases the variance of the best of the \(k\) points when sampled uniformly is as high or higher than those sampled from the \(k\)-DPP-based methods. In all cases, the first half of the \(k\) samples in Figure 1 are not statistically significantly different.

### 3.2 Optimizing within ranges known to be good

Zhang and Wallace [2015] analyzed the stability of convolutional neural networks for sentence classification with respect to a large set of hyperparameters, and found a set of six which they claimed had the largest impact: the number of kernels, the difference in size between the kernels, the size of each kernel, dropout, regularization strength, and the number of filters. After their extensive experiments, they proposed a space over these hyperparameters which should be searched to ensure good results.
Figure 2: Best-found model accuracy by iteration (the rightmost values correspond to Table 1) when training a convolutional neural network on the “Stable” search space (defined in Section 3.2), averaged across 100 trials of hyperparameter optimization, with $k = 20$. Though the range in accuracies is small, $k$-DPP-Hamm still finds better solutions than uniform.

We optimized over their prescribed “Stable” ranges after discretizing continuous variables to five discrete values; average accuracies across 100 trials of hyperparameter optimization, across $k = 20$ iterations, are shown in Figure 2. We find that even in this case where every value gives reasonable performance, $k$-DPP-Hamm outperforms uniform sampling. $k$-DPP-Cos performs similarly to uniform sampling.

Our experiments revealed that while the hyperparameters proposed by Zhang and Wallace [2015] can have an effect, the learning rate, which they don’t analyze, is at least as impactful.

3.3 Logistic regression for text classification

In addition to tuning hyperparameters for a convolutional neural network, we tuned the following hyperparameters to a logistic regression classifier: the type of regularization ($L_1$ vs. $L_2$), convergence tolerance in $[e^{-10}, e^{-1}]$, $n$-grams used as features $\{(1), (1, 2), (1, 3), (2, 2), (2, 3)\}$, whether to use count features or binary features for those $n$-grams, whether or not to apply a tf-idf transform to the counts, and whether or not to remove stop words. In these experiments, we average over 50 trials, with $k = 50$, and we discretized the continuous variables to seven discrete values. Using this different model, on a very different hyperparameter search space, we again see in Figure 3 that $k$-DPP-Cos outperforms sampling uniformly at random. The average best-found model accuracy for $k$-DPP-Cos was 79.15%, and 79.04% for sampling uniformly.

3.4 Further analysis of $k$-DPPs distributions

When tuning hyperparameters for our “Hard” search space in Section 3.1, we note that $k$-DPP-Cos outperforms $k$-DPP-Hamm and uniform sampling, but for less extreme settings, like the “Easy” case in Section 3.1 or the search space with known-to-be-good values in Section 3.2, $k$-DPP-Hamm outperforms the others. To see how these approaches differ in which values they sample, we can examine the proportion of times the two techniques sample a given (discretized) hyperparameter value across 100 trials. Figure 4 shows histograms of hyperparameter values sampled (alongside sensitivity analysis), for the “Hard” convolutional neural net hyperparameter search problem from Section 3.1.

We see that $k$-DPP-Cos samples the points on the edge of the search space more frequently than $k$-DPP-Hamm, while $k$-DPP-Hamm samples more evenly. Since the models are agnostic to the actual values taken on by these hyperparameters (by construction), we expect to see the same distribution when sampling any 16-point space.
(As it happens, the smallest learning rates in this space led to the best values, and \( k \)-DPP-Cos samples those with higher probability, giving it an advantage.)

We also examined the coverage within a single sample of size \( k \) (i.e. how many unique discretized values for a given hyperparameter were evaluated). We set \( k = 20 \), searched over regularization strength, dropout, and learning rate, with 16 discrete values, and averaged over 100 trials. We found that the mean, median, and max coverage did not differ between sampling uniformly and sampling from \( k \)-DPP-Cos, but \( k \)-DPP-Hamm had better coverage. For example, we found sampling uniformly and from \( k \)-DPP-Cos contained an average of 11.55 and 11.6 unique learning rate values, respectively, while sampling from \( k \)-DPP-Hamm had an average of 12.3. The maximum coverage observed in one sample for each hyperparameter was 15 for \( k \)-DPP-Hamm, and 14 for \( k \)-DPP-Cos and sampling uniformly.

4 Related Work

Hyperparameter optimization algorithms abound, as selecting hyperparameters is necessary for any machine learning practitioner. Grid search is the most commonly used hyperparameter optimization algorithm, as it is simple to understand and implement. Performing a grid search quickly becomes intractable as the dimension of the search space increases, however, and coverage of each dimension necessarily decreases; evaluating \( m \) points for each of \( D \) hyperparameters using grid search leads to evaluating \( m^D \) points. With a restricted budget of \( k \) evaluations, this can lead to trying only a small number of points in each dimension. For example, our “Stable” search space described in Section 3.2 covers six dimensions. To evaluate only two points for each hyperparameter using grid search (which would obviously lead to very poor coverage) requires \( 2^6 = 64 \) evaluations, much greater than our budget of \( k = 20 \), while our sampling approach covered a much larger amount of the space with each sample.

Sampling \( k \) points uniformly at random can potentially lead to evaluating \( k \) unique values for each hyperparameter (assuming the hyperparameters can take on at least \( k \) values), irrespective of \( D \), and this increased coverage can lead to better performance. In addition, if some hyperparameters don’t impact the evaluation of the model, then any experiments varying only in those dimensions (as would be commonly seen when performing grid search) would be wasted. Bergstra and Bengio [2012] found that the Sobol sequence has better coverage over continuous spaces (and therefore can lead to better hyperparameters) than sampling uniformly at random. The Sobol sequence is only defined for continuous spaces, so for hyperparameter search which involves discrete dimensions it is not appropriate, and DPPs model global repulsion between all points in a sample, which is not true of the Sobol sequence.
Figure 4: Each plot focuses on one hyperparameter, showing (i) in red, the average accuracy obtained across samples where the hyperparameter took each value—essentially, a sensitivity analysis; (ii) in dark blue, the fraction of samples under $k$-DPP-Cos where the hyperparameter took that value; and (iii) in cyan, the fraction of samples under $k$-DPP-Hamm where the hyperparameter took each value. Note that $k$-DPP-Cos has a tendency to over-sample extreme values for learning rate, regularization strength, and dropout. (Not shown: uniform would have flat distributions across values, by design.)

Both sampling uniformly at random and grid search are trivial to parallelize, which has contributed to their widespread adoption.

Much attention has been paid to sequential model-based optimization techniques such as Bayesian optimization [Snoek et al., 2012, Bergstra et al., 2011], which sample hyperparameter spaces adaptively. These techniques first choose a point in the space of hyperparameters, then train and evaluate a model with the hyperparameter values represented by that point, then sample another point based on how well previous point(s) performed. These methods can become complicated, and while they can lead to improved performance, the differences are frequently small. In addition, it has recently been observed that many Bayesian optimization methods, when run for $k$ iterations, are outperformed by sampling $2k$ points uniformly at random [Li et al., 2017]. Parallelizing Bayesian optimization methods has proven to be nontrivial, and while a number of algorithms exist which sample more than one point at each iteration [Contal et al., 2013, Desautels et al., 2014, González et al., 2016], none can achieve the parallelization that grid search, sampling uniformly, or sampling according to a DPP allow.

So-called configuration evaluation methods have been shown to perform well by adaptively allocating resources to different hyperparameter settings [Swersky et al., 2014, Li et al., 2017]. They initially choose a set of hyperparameters to evaluate (often uniformly), then partially train a set of models for these hyperparameters. After some fixed training budget (e.g. time, or number of training examples observed), they compare the partially trained models against one another and allocate more resources to those which perform best. Eventually, these algorithms produce one (or a small number) of fully trained, high-quality models.
One recent line of research has examined the use of DPPs for optimizing hyperparameters, in the context of parallelizing Bayesian optimization [Kathuria et al., 2016, Wang et al., 2017]. At each iteration within one trial of Bayesian optimization, instead of drawing a single new point to evaluate from the posterior, they use the posterior to define a DPP and sample a set of diverse points. While this can lead to easy parallelization within one iteration of Bayesian optimization, the overall algorithms are still sequential.

5 Conclusions

We have explored two novel approaches to hyperparameter optimization, built on sampling from $k$-DPPs. We described how to construct $k$-DPPs over hyperparameter search spaces, and showed that sampling from these retains the attractive parallelization capabilities of random search. Our experiments demonstrate that, under a limited computation budget, on a number of realistic hyperparameter optimization problems, these approaches perform better than sampling uniformly at random. As we increase the difficulty of our hyperparameter optimization problem (i.e., as values which lead to good model evaluations become more scarce) the improvement over sampling uniformly at random increases. An open-source implementation of our method is available.

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