

Hyperparameter Optimization: A Spectral Approach

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Abstract

We give a simple, fast algorithm for hyperparameter optimization inspired by techniques from the analysis of Boolean functions. We focus on the high-dimensional regime where the canonical example is training a neural network with a large number of hyperparameters. The algorithm— an iterative application of compressed sensing techniques for orthogonal polynomials— requires only uniform sampling of the hyperparameters and is thus easily parallelizable.

Experiments for training deep nets on Cifar-10 show that compared to state-of-the-art tools (e.g., Hyperband and Spearmint), our algorithm finds significantly improved solutions, in some cases matching what is attainable by hand-tuning. In terms of overall running time (i.e., time required to sample various settings of hyperparameters plus additional computation time), we are at least an order of magnitude faster than Hyperband and even more so compared to Bayesian Optimization. We also outperform Random Search $5\times$.

Additionally, our method comes with provable guarantees and yields the first quasi-polynomial time algorithm for learning decision trees under the uniform distribution with *polynomial* sample complexity, the first improvement in over two decades.

1 Introduction

Large scale machine learning and optimization systems usually involve a large number of free parameters for the user to fix according to their application. A timely example is the training of deep neural networks for a signal processing application: the ML specialist needs to decide on an architecture, depth of the network, choice of connectivity per layer (convolutional, fully-connected, etc.), choice of optimization algorithm and recursively choice of parameters inside the optimization library itself (learning rate, momentum, etc.).

Automatically finding a good setting of these parameters— now referred to as hyperparameter optimization— has become an important problem in machine learning and has received significant attention in recent years. For continuous hyperparameters, gradient descent is usually sufficient [MDA15]. Discrete parameters, however, such as choice of architecture, number of layers, connectivity and so forth are significantly more challenging. Existing approaches include Bayesian optimization [SLA12], Multi-armed bandit algorithms [LJD⁺16], and Random search [BB12].

In this paper we introduce a new *spectral* approach to hyperparameter optimization based on harmonic analysis of Boolean functions. At a high level, the idea is to fit a sparse polynomial function to the discrete, high-dimensional function mapping hyperparameters to loss, and then optimize the resulting sparse polynomial.

Using ideas from discrete Fourier analysis and compressed sensing, we can give provable guarantees for a sparse-recovery algorithm that admits an efficient, parallelizable implementation. Here we are concerned with the *tradeoff* between running time and sample complexity for learning Boolean functions f where sampling uniformly from f is very expensive. This approach appears to be new and allows us to give uniform-distribution learning algorithms for Boolean concept classes such as decision trees that match the state-of-the-art in running time and save dramatically in sample complexity.

Our contributions:

- An new spectral method called *Harmonica* that has provable guarantees: sample-efficient recovery if the underlying hyperparameter objective is a sparse (noisy) polynomial and easy to implement on parallel architectures.
- A sample-efficient learning procedure for learning size s decision trees over n variables under the uniform distribution. We improve the two-decades old sample complexity bound of $n^{O(\log(s/\varepsilon))}$, to quadratic in the size of the tree $\tilde{O}(s^2 \log n/\varepsilon)$, while matching the best known quasipolynomial bound in running time.
- We demonstrate significant improvements in accuracy, sample complexity, and running time for deep neural net training experiments. We compare ourselves to state-of-the-art solvers from Bayesian optimization, Multi-armed bandit techniques, and random search. Projecting to even higher numbers of hyperparameters, we perform simulations that show several orders-of-magnitude of speedup versus Bayesian optimization techniques.

2 Setup and definitions

The problem of hyperparameter optimization is that of minimizing a discrete, real-valued function, which we denote by $f : \{-1, 1\}^n \mapsto [-1, 1]$ (we can handle arbitrary inputs, binary is chosen for simplicity of presentation).

In the context of hyperparameter optimization, function evaluation is very expensive, although parallelizable, as it corresponds to training a deep neural net. In contrast, any computation that does not involve function evaluation is considered less expensive, such as computations that require time $\Omega(n^d)$ for “somewhat large” d or are subexponential (we still consider runtimes that are exponential in n to be costly).

2.1 Basics of Fourier analysis

Let $f : \mathcal{X} \mapsto [-1, 1]$ be a function over domain $\mathcal{X} \subseteq \mathbb{R}^n$. Let \mathcal{D} a probability distribution on \mathcal{X} . We write $g \equiv_\varepsilon f$ and say that f, g are ε -close if

$$\mathbb{E}_{x \sim \mathcal{D}}[f(x) - g(x)]^2 \leq \varepsilon.$$

Definition 1. [Rau10] We say a family of functions ψ_1, \dots, ψ_N (ψ_i maps \mathcal{X} to \mathbb{R}) is a *Random Orthonormal Family* with respect to \mathcal{D} if

$$\mathbb{E}_{\mathcal{D}}[\psi_i(X) \cdot \psi_j(X)] = \delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}.$$

The expectation is taken with respect to probability distribution \mathcal{D} . We say that the family is K -bounded if $\sup_{x \in \mathcal{X}} |\psi_i(x)| \leq K$ for every i . Henceforth we assume $K = 1$.

An important example of a random orthonormal family is the class of parity functions with respect to the uniform distribution on $\{-1, 1\}^n$, i.e., functions of the form $\chi_S : \{-1, 1\}^n \mapsto \{-1, 1\}$ where $\chi_S(x) = \prod_{i \in S} x_i$ for any $S \subseteq [n]$. The set of all parities is oftentimes referred to as the Fourier basis, as it is a complete orthonormal basis for the class of Boolean functions. Concretely, for any $f : \{-1, 1\}^n \mapsto \mathbb{R}$, f can be uniquely represented in this basis as

$$f(x) = \sum_{S \subseteq [n]} \hat{f}_S \chi_S(x)$$

where

$$\hat{f}_S = \langle f, \chi_S \rangle = \mathbb{E}_{x \in \{-1, 1\}^n}[f(x) \chi_S(x)]$$

is the Fourier coefficient corresponding to S where x is drawn uniformly from $\{-1, 1\}^n$. Parseval’s identity says that $\mathbb{E}[f^2] = \sum_S \hat{f}_S^2$.

More generally, we have the following definitions for classes of orthogonal polynomials with respect to product spaces:

Definition 2 (Orthonormal Bases of Polynomials). Fix a product distribution \mathcal{D} on $\mathbb{R}^n = \mu_1 \times \dots \times \mu_n$. Let $\{p_{ij}(x)\}_{j=1}^\infty$ be a complete family of orthonormal polynomials with respect to μ_i (depending on μ_i the family may be finite). That is, $\mathbb{E}_{x \sim \mu_i}[p_{ij}(x)p_{ik}(x)] = \delta_{jk}$ and for every function $g : \mathbb{R} \mapsto \mathbb{R}$ with $\mathbb{E}[g^2] \leq \infty$ we have that g can be written uniquely as $\sum_{j=1}^\infty \hat{g}(j)p_{ij}(x)$ and $\lim_{d \rightarrow \infty} \mathbb{E}[(g(x) - \sum_{j=1}^d \hat{g}(j)p_{ij}(x))^2] = 0$. Now we can define n -variate families of orthonormal polynomials as follows: for $S \in \mathbb{N}^n$ let $H_S = \prod_{i=1}^n p_{iS_i}(x)$. Then $\{H_S\}_{S \in \mathbb{N}^n}$ (note that H_S has total degree $|S| = \sum_i S_i$) is a random orthonormal family and a complete orthonormal basis for all $f : \mathbb{R}^n \mapsto \mathbb{R}$ with $E_{\mathcal{D}}[f^2] \leq \infty$. That is, $\lim_{d \rightarrow \infty} \mathbb{E}_{\mathcal{D}}[(f - \sum_{S, |S| \leq d} \hat{f}(S)H_S)^2] = 0$. We call $\{H_S\}$ an *orthonormal polynomial basis* for \mathcal{D} .

We conclude with a definition of low-degree, approximately sparse (bounded L_1 norm) functions:

Definition 3 (Approximately sparse function). Let $\{H_S\}$ be an orthonormal polynomial basis with respect to \mathcal{D} and let \mathcal{C} be a class of functions such that $E[f^2] \leq \infty$ for every $f \in \mathcal{C}$. Thus $f = \sum_S \hat{f}(S)H_S$. We say that a function $f \in \mathcal{C}$ is s -**sparse** if $L_0(f) \leq s$, ie., has at most s nonzero entries in its polynomial expansion. We say f is (ε, d) -**concentrated** if $\mathbb{E}[(f - \sum_{S, |S| \leq d} \hat{f}(S)H_S)^2] \geq 1 - \varepsilon$. We say \mathcal{C} is (ε, d, s) -**bounded** if for every $f \in \mathcal{C}$, f is (ε, d) -concentrated and in addition \mathcal{C} has L_1 norm bounded by s , that is, for every $f \in \mathcal{C}$ we have $\sum_S |\hat{f}(S)| \leq s$.

It is easy to see that the class of functions with bounded L_1 norm is more general than sparse functions. For example, the Boolean AND function has L_1 norm bounded by 1 but is not sparse.

We also have the following simple fact:

Fact 4. [Man94] Let f be such that $L_1(f) \leq s$. Then there exists g such that g is s^2/ε sparse and $E[(f - g)^2] \leq \varepsilon$. The function g is constructed by taking all coefficients of magnitude ε/s or larger in f 's expansion as a polynomial.

2.2 Compressed sensing and sparse recovery

In the problem of *sparse recovery*, a learner attempts to recover a sparse vector $x \in \mathbb{R}^n$ which is s sparse, i.e. $\|x\|_0 \leq s$, from an observation vector $y \in \mathbb{R}^m$ that is assumed to equal

$$y = Ax + e,$$

where e is assumed to be zero-mean, usually Gaussian, noise. The seminal work of [CRT06, Don06] shows how x can be recovered exactly under various conditions on the observation matrix $A \in \mathbb{R}^{m \times n}$ and the noise. The usual method for recovering the signal proceeds by solving a convex optimization problem consisting of ℓ_1 minimization as follows (for some parameter $\lambda > 0$):

$$\min_{x \in \mathbb{R}^n} \{ \|x\|_1 + \lambda \|Ax - y\|_2^2 \}. \quad (1)$$

The above formulation comes in many equivalent forms (e.g., Lasso), where one of the objective parts may appear as a hard constraint.

For our work, the most relevant extension of traditional sparse recovery is due to Rauhut [Rau10], who considers the problem of sparse recovery when the measurements are evaluated according to a *random orthonormal family*. More concretely, fix $x \in \mathbb{R}^n$ with s non-zero entries. For K -bounded random orthonormal family $\mathcal{F} = \{\psi_1, \dots, \psi_N\}$, and m independent draws z^1, \dots, z^m from corresponding distribution \mathcal{D} define the $m \times N$ matrix A such that $A_{ij} = \psi_j(z^i)$. Rauhut gives the following result for recovering sparse vectors x :

Theorem 5 (Sparse Recovery for Random Orthonormal Families). [Rau10] Given as input matrix A and vector y with $y_i = Ax + e_i$ for some vector e with $\|e\|_2 \leq \eta\sqrt{m}$, mathematical program (1) finds a vector x^* such that (for constants c and d)

$$\|x - x^*\|_2 \leq c \frac{\sigma_s(x)_1}{\sqrt{s}} + d\eta$$

with probability $1 - \delta$ as long as, for sufficiently large constant C ,

$$m \geq CK^2 \log K \cdot s \log^3 s \cdot \log^2 N \cdot \log(1/\delta).$$

The term $\sigma_s(x)_1$ is equal to $\min\{\|x - z\|_1, z \text{ is } s \text{ sparse}\}$. Recent [Bou14, HR16] has improved the dependence on the polylog factors in the lower bound for m .

3 Polynomial Recovery Algorithm and Main Theorem

The main component of our spectral algorithm for hyperparameter optimization is given in Algorithm (1). It is essentially an extension of sparse recovery (basis pursuit or Lasso) to the orthogonal basis of polynomials. In the next subsection, we describe how it is called from our main algorithm Harmonica.

Algorithm 1 Polynomial Sparse Recovery (PSR)

- 1: Input: oracle for f , number of samples T , sparsity s , degree d , regularization parameter λ
- 2: Query T random samples: $\{f(x_1), \dots, f(x_T)\}$.
- 3: Solve sparse d -polynomial regression over all polynomials up to degree d

$$\arg \min_{\alpha \in \mathbb{R}^{\binom{n}{d}}} \left\{ \sum_{i=1}^T \left(\sum_{|S| \leq d} \alpha_S \psi_S(x_i) - f(x_i) \right)^2 + \lambda \|\alpha\|_1 \right\} \quad (2)$$

- 4: Let S_1, \dots, S_s be the largest coefficients of $\vec{\alpha}$. Let g be the polynomial

$$g(x) = \sum_{i \in [s]} \alpha_{S_i} \psi_{S_i}(x)$$

- 5: **return** g and $J = \cup_{i=1}^s S_i$
-

The main theorem we prove regarding this subprocedure performance is given as follows.

Theorem 6 (Main). *Fix \mathcal{D} and associated K -bounded orthonormal polynomial family $\{H_S\}$. Assume $f : \mathbb{R}^n \mapsto \mathbb{R}$ is (ε, d, s) -bounded as per definition 3. Then algorithm 1 finds a function $g \equiv_\varepsilon f$ in time $O(n^d)$ and sample complexity $T = \tilde{O}(K^2 s^2 \log N / \varepsilon)$.*

Remark: In this paper we focus on distributions \mathcal{D} that are products of *discrete* univariate distributions. In this case the basis of orthonormal polynomials is the set of all parity functions, see Section 2.1. However, our method encompasses scenarios where μ_i can be continuous (e.g., Gaussian).

In the rest of this section we proceed to prove the main theorem. As a first step, for functions that are computed exactly by a sparse, low-degree polynomial. This is immediately obtainable as a corollary of Theorem 5:

Corollary 7. *Let $\{H_S\}$ be a K -bounded orthonormal polynomial basis for \mathcal{D} . Let f be a $(0, d, s)$ -sparse function with respect to the basis H_S . Then f is recoverable by Algorithm 1 with samples from \mathcal{D} in time $n^{O(d)}$ and sample complexity $m = \tilde{O}(K^2 s d \log n)$.*

Note that in the above corollary the *degree* of f dictates the running time and the sparsity of f controls the sample complexity.

Proof. There are at most $N = n^d$ polynomials H_S with $|S| \leq d$. Let the enumeration of these polynomials be ψ_1, \dots, ψ_N . Draw m labeled examples $\{(z^1, y^1), \dots, (z^m, y^m)\}$ independently from \mathcal{D} and construct an $m \times N$ matrix A with $A_{ij} = \psi_j(z^i)$. Since c can be written as an s sparse linear combination of ψ_1, \dots, ψ_N , there exists an s -sparse vector x such that $Ax = y$

where the i th entry of y is y^i . Hence we can apply Theorem 5 to recover x exactly. These are the s non-zero coefficients of f 's expansion in terms of $\{H_S\}$. \square

We proceed to the more general statement and proof of the main theorem. Recall the Chebyshev inequality:

Fact 8 (Multidimensional Chebyshev inequality). *Let X be an m dimensional random vector, with expected value $\mu = \mathbb{E}[X]$, and covariance matrix $V = \mathbb{E}[(X - \mu)(X - \mu)^T]$.*

If V is a positive definite matrix, for any real number $\delta > 0$:

$$\mathbb{P}(\sqrt{(X - \mu)^T V^{-1} (X - \mu)} > \delta) \leq \frac{m}{\delta^2}$$

Proof of Theorem 6. For ease of notation we assume $K = 1$. Let f be an (ε, s, d) -bounded function written in the orthonormal basis as $\sum_S \hat{f}(S) H_S$. We can equivalently write f as $f = h + g$, where h is a degree d polynomial that only includes coefficients of magnitude at least ε/t and the constant term of the polynomial expansion of f .

Since $L_1(f) = \sum_S |\hat{f}(S)| \leq s$, by Fact 4 we have that h is $1 + s^2/\varepsilon$ sparse. The function g is thus the sum of the remaining $\hat{f}(S) H_S$ terms not included in h .

Draw m (to be chosen later) random labeled examples $\{(z^1, y^1), \dots, (z^m, y^m)\}$ and enumerate all $N = n^d$ basis functions H_S for $|S| \leq d$ as $\{\psi_1, \dots, \psi_N\}$. Form matrix A such that $A_{ij} = \psi_j(z^i)$ and consider the problem of recovering $1 + s^2/\varepsilon$ sparse x given $Ax + e = y$ where x is the vector of coefficients of h , the i th entry of y equals y^i , and $e_i = g(z^i)$.

We will prove that with constant probability over the choice m random examples, $\|e\|_2 \leq O(\sqrt{\varepsilon})$. Applying Theorem 5 and observing that $\sigma_{t^2/\varepsilon}(x)_1 = 0$, we will recover x' such that $\|x - x'\|_2^2 \leq O(\varepsilon)$. As such, for the function $\tilde{f} = \sum_{i=1}^N x'_i \psi_i$ we will have $\mathbb{E}[\|f - \tilde{f}\|^2] \leq O(\varepsilon)$.

It remains to bound $\|e\|_2$. Note that since the examples are chosen independently, the entries $e_i = g(z^i)$ are independent random variables. Since g is a linear combination of orthonormal monomials (not including the constant term), we have $\mathbb{E}_{z \sim D}[g(z)] = 0$. Here we can apply linearity of variance (the covariance of ψ_i and ψ_j is zero for all $i \neq j$) and calculate the variance

$$\mathbf{Var}(g(z^i)) = \left(\sum_{S, |S| > d} \hat{f}(S)^2 + \sum_T \hat{f}(T)^2 \right)$$

where each $\hat{f}(T)$ is of magnitude at most ε/T . By Fact 4 and Parseval's identity we have $\sum_T \hat{f}(T)^2 \leq \varepsilon$. Since f is (ε, d) -concentrated we have $\sum_{S, |S| > d} \hat{f}(S)^2 \leq \varepsilon$. Thus, $\mathbf{Var}(g(z^i))$ is at most 2ε .

Now consider the covariance matrix V of the vector e which equals $\mathbb{E}[ee^T]$ (recall every entry of e has mean 0). Then V is a diagonal matrix (covariance between two independent samples is zero), and every diagonal entry is at most 2ε . Applying Fact 8 we have

$$\mathbb{P}(\|e\|_2 > \sqrt{2\varepsilon}\delta) \leq \frac{m}{\delta^2}.$$

Now let $\nu = \sqrt{2\varepsilon}\delta$ and $\eta = \sqrt{2D\varepsilon}$, we conclude that $\mathbb{P}(\|e\|_2 > \eta\sqrt{m}) \leq \frac{2\varepsilon m}{\eta^2 m} = \frac{1}{2}$. Hence with probability at least $1/2$, we have that $\|e\|_2 \leq O(\sqrt{\varepsilon})$. From Theorem 5, we may choose $m = \tilde{O}(s^2 \log N/\varepsilon)$. This completes the proof. Note that the probability $1/2$ above can be boosted to any constant probability with a constant loss in sample complexity. \square

Prior to this work, the best known algorithm for learning functions as described in Theorem 6 with both non-trivial running time *and* sample complexity was the classic “low-degree algorithm” of Linial, Mansour, and Nisan [LMN93], which requires time $\Omega(N)$ and sample complexity $\Omega(NL_\infty(f)^2/\varepsilon)$ where $L_\infty(f) = \sup_{x \in \mathcal{X}} |f(x)|$. Notice that we have matched their running time but have dramatically reduced the sample complexity.

For the related problem of learning *exactly* k -sparse Boolean functions, Haviv and Regev [H15] have recently shown that $O(nk \log n)$ uniformly random samples suffice. Their result is not algorithmic but does provide an upper bound on the information-theoretic problem of how many samples are required to learn. The best algorithm in terms of running time for learning k -sparse Boolean functions is due to [FGKP09], and requires time $2^{\Omega(n/\log n)}$. It is based on the Blum, Kalai, and Wasserman algorithm for learning parities with noise [BKW03].

3.1 Application: Learning Decision Trees in Quasi-polynomial Time and Polynomial Sample Complexity

Theorem 6 has important applications for learning (in the PAC model [Val84]) well-studied function classes with respect to the uniform distribution on $\{0, 1\}^n$. For example, we obtain the first quasi-polynomial time algorithm for learning decision trees with respect to the uniform distribution on $\{0, 1\}^n$ with *polynomial* sample complexity:

Corollary 9. *Let $\mathcal{X} = \{0, 1\}^n$ and let \mathcal{C} be the class of all decision trees of size s on n variables. Then \mathcal{C} is learnable with respect to the uniform distribution in time $n^{O(\log(s/\varepsilon))}$ and sample complexity $\tilde{O}(s^2 \log n/\varepsilon)$.*

Previous results for learning decision trees required quasi-polynomial running time *and* sample complexity [LMN93]. We remark that our result also holds for decision trees with real values at the leaves. A tree f with s leaves and real valued labels r_1, \dots, r_s will have $L_1(f) \leq \sum_i |r_i|$ and still be $(\varepsilon, \log(Rs/\varepsilon))$ -concentrated where $R = \max_i r_i$.

Proof. It is well known that the orthonormal polynomial basis for the class of Boolean functions with respect to the uniform distribution on $\{0, 1\}^n$ is the class of parity functions $\{\chi_S\}$ for $S \subseteq \{0, 1\}^n$. Further, it is easy to show that for Boolean function f , if $\mathbb{E}[(h - f)^2] \leq \varepsilon$ then $\mathbb{P}[\text{sign}(h(x)) \neq f(x)] \leq \varepsilon$. The corollary now follows by applying Theorem 6 and known structural facts about decision trees: namely that a tree of size s is $(\varepsilon, \log(s/\varepsilon))$ -concentrated and has L_1 norm bounded by s (see e.g., Mansour [Man94]). \square

We also obtain improved sample complexity bounds for learning DNF formulas, a central problem in computational learning theory:

Corollary 10. *Let $\mathcal{X} = \{0, 1\}^n$ and let \mathcal{C} be the class of all DNF formulas of size s on n variables. Then \mathcal{C} is learnable with respect to the uniform distribution in time $n^{O(\log(s/\varepsilon))}$ and sample complexity $\tilde{O}(s^{\log \log s \log(1/\varepsilon)} \log n)$.*

The proof follows by applying Theorem 6 and known structural results due to Mansour [Man95]. Further, assuming Mansour’s conjecture is true [KLW10], we obtain a quasi-polynomial time algorithm for learning DNF formulas with sample complexity $\tilde{O}(s^{\log(1/\varepsilon)} \log n)$.

4 Harmonica: The Full Algorithm

The full algorithm continues to invoke the PSR subroutine until the search space has become sufficiently small, at which point we use a “base” hyperparameter optimizer (in our case either Hyperband or Random Search).

The space of minimizing assignments to a multivariate polynomial is a highly non-convex set that may contain many distinct points. As such, we take an average of several of the best minimizers, and iteratively apply PSR on this average.

In order to describe this formally we need the following definition for restrictions of functions:

Definition 11 (restriction [O’D14]). Let $f \in \{-1, 1\}^n \mapsto \mathbb{R}$, $J \subseteq [n]$, and $z \in \{-1, 1\}^J$ be given. We call (J, z) a restriction pair of function f . We denote $f_{J,z}$ the function over $n - |J|$ variables given by setting the variables of J to z .

We can now describe our main algorithm as follows:

Algorithm 2 Harmonica

- 1: Input: oracle for f , number of samples T , sparsity s , degree d , regularization parameter λ , number of stages q , restriction size t , base hyperparameter optimizer ALG.
 - 2: **for** stage $i = 1$ to q **do**
 - 3: Invoke PSR(f, T, s, d, λ) (Algorithm 1) to obtain (g_i, J_i) , where g_i is a function defined on variables specified by index set $J_i \subseteq [n]$.
 - 4: Let $M_i = \{x_1^*, \dots, x_t^*\} = \arg \min g_i(x)$ be the best t minimizers of g_i .
 - 5: Let $f_i = \mathbb{E}_{k \in [t]} [f_{J_i, x_k^*}]$ be the expected restriction of f according to minimizers M_i .¹
 - 6: Set $f = f_i$.
 - 7: **end for**
 - 8: **return** Search for the global minimizer of f_q using base optimizer ALG
-

5 Algorithm Comparison and Experiments

We compare Harmonica with Spearmint [SLA12], Hyperband [LJD⁺16] and random search, see Table 1. Both Spearmint and Hyperband are state-of-the-art algorithms, and it is observed that random search 2x (random search with doubled time resource) is a very competitive benchmark that beats many algorithms². We defer the detailed explanation of these algorithms and comparisons to Section 6.

5.1 Resnet hyperparameter tuning

Our first experiment runs Harmonica for residual network on Cifar-10 dataset, using degree 3 features. We included 39 binary hyperparameters, including initialization, optimization method, learning rate schedule, momentum rate, etc. Please refer to Table 3 (Section 7.1) for the detailed explanation of those hyperparameters. To make the task more challenging,

¹In order to evaluate f_i , we first sample $k \in [t]$ to obtain f_{J_i, x_k^*} , and then evaluate f_{J_i, x_k^*} .

²E.g., see [Rec16a, Rec16b].

Table 1: Comparison. n : #hyperparameters. m : #samples. d : degree of features

| Properties | Harmonica | Bayesian opt | Hyperband | random search |
|---------------------|---|--------------|---------------|---------------|
| Scalability in n | Best | Fair | Better | Better |
| Optimization time | $O\left(\frac{n^d m}{\varepsilon}\right)$ | Very slow | $O(m \log m)$ | $O(1)$ |
| Parallelizable? | Yes | Difficult | Yes | Yes |
| Feature extraction? | Yes | No | No | No |

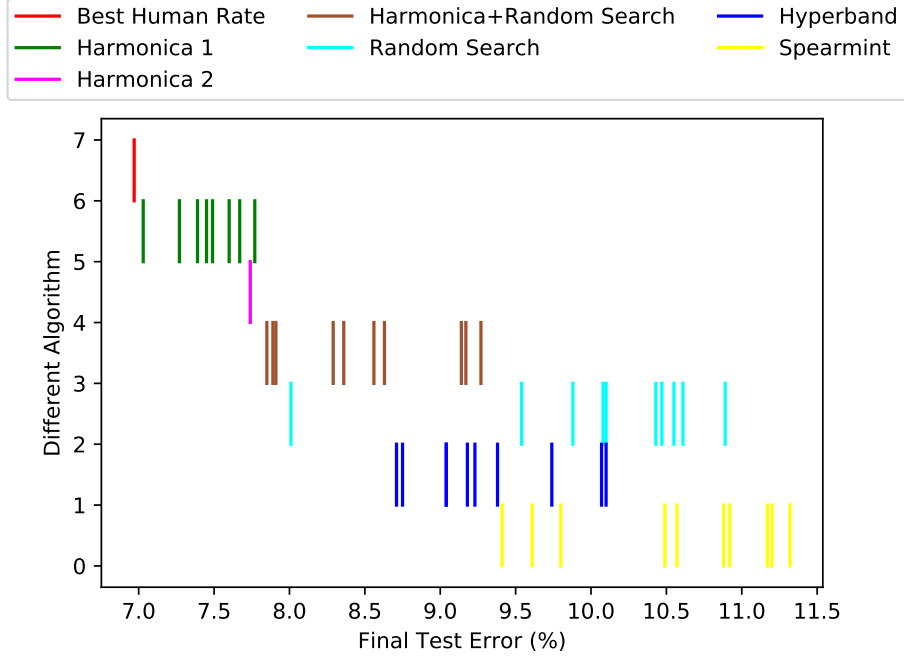


Figure 1: Distribution of the best results.

we also include 21 dummy variables. We run this experiment on 10 NC6 machines on Azure cloud, each has one GPU of Tesla K80.

As most hyperparameters have a consistent effect as the network becomes deeper, a common hand-tuning strategy is “tune on small network, then apply the knowledge to big network”. Harmonica can also exploit this strategy as it selects important features stage-by-stage. More specifically, during its first 2 stages of feature selection, we run Harmonica on an 8 layer neural network for training 30 epochs, with 300 samples, 5 features selected per stage, restriction size $t = 4$ (see Algorithm 1). After that, we fix all the important features, and run the SH algorithm (subroutine of Hyperband [LJD⁺16], 4 stage version) as our base algorithm on the big 56 layer neural network for training the whole 160 epochs³. To clarify, “stage” means the stages of the hyperparameter algorithms, while “epoch” means the epochs for training the neural network.

Top Test Error Distributions See the top 10 test error results of the different algorithms in Figure 1, and running time in Figure 2. We run Harmonica twice, with different total running times: Harmonica 1 uses 10.1 days, while Harmonica 2 uses 3.6 days. They have the

³Other algorithms like random search, hyperband, etc. can be used as base algorithm as well.

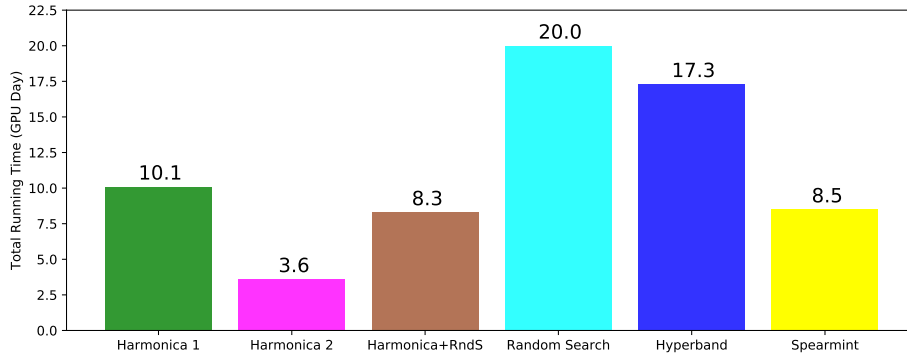


Figure 2: Running time of different algorithms

Table 2: Stable ranges for parameters in Lasso

| Parameter | Stage 1 | Stage 2 | Stage 3 |
|-----------|-------------|------------|------------|
| λ | [0.01, 4.5] | [0.1, 2.5] | [0.5, 1.1] |
| #Samples | ≥ 250 | ≥ 180 | ≥ 150 |

same feature extraction process, while the difference is the time for running the SH algorithm. We show less than 10 test errors for both Harmonica 1 and Harmonica 2 because those are the only final results returned after running the SH algorithm.

Better test error, and faster. Harmonica 2 uses only 1/4 time of Hyperband and 1/5 time compared with random search, but get results better than all the results obtained by these algorithms. In other words, it beats random search 5x benchmark (stronger than random search 2x benchmark of [LJD⁺16]).

Close to human rate. The best one from Harmonica 1 (7.03%) is only 0.06% away from the hand-tuning rate 6.97% reported in [HZRS16], using 10 GPU days, which is 1 day with 10 GPU.

We also tried random search as the base algorithm for Harmonica, which gives slightly worse performance compared with the SH version. However, it is still much better than Hyperband, Random Search and Spearmint. It finds three sets of hyperparameters with less than 8% test error. This indicates that different base algorithms can be used with Harmonica.

Since Spearmint does not have multiple-machine support, we had to run it on a single machine. Due to time constraints, we chose to stop it after running for 8.5 days. The results of Spearmint were not competitive. It seems that for the high dimensional regime, Spearmint is similar to Random Search⁴.

Average Test Error For Each Stage We compute the average test error among 300 random samples for 8 layer network with 30 epochs after each stage. See Figure 3. After selecting 5 features in stage 1, the average test error drops from 60.16 to 33.3, which indicates the top 5 features are very helpful. As we proceed to stage 3, the improvement on test error becomes less significant as the selected features at stage 3 have mild contributions.

⁴We also tried Spearmint on a training a small 8 layer network and observed similar behavior.

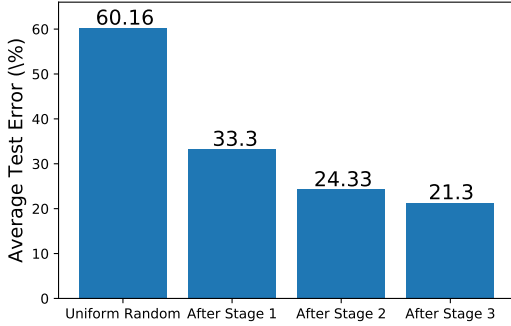


Figure 3: Average test error drops.

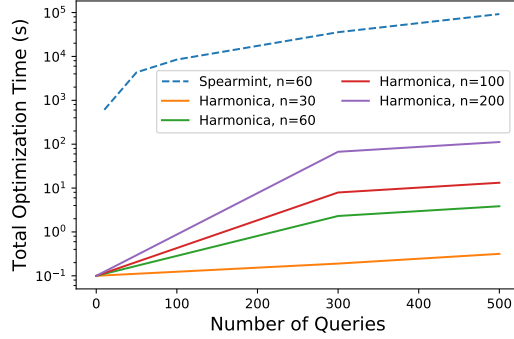


Figure 4: Optimization time comparison

Sensitivities to hyperparameters As a hyperparameter tuning algorithm, Harmonica itself has a few hyperparameters that one needs to set. Fortunately, its performance is not sensitive to those parameters. For example, Table 2 shows the stable ranges for the regularization term λ and the number of samples in Harmonica. Here stable range means as long as the parameters are set in this range, the top 5 features and the signs of their weights do not change. In other words, the feature selection outcome is not affected. See Section 7.3 for discussions on other parameters.

5.2 Synthetic function

Our second experiment considers a synthetic hierarchically bounded function $h(x)$ (see Appendix 7.4 for detailed definition of $h(x)$). We run Harmonica with 100 samples, 5 features selected per stage, for 3 stages, using degree 3 features. See Figure 4 for optimization time comparison. We only plot the running time for Spearmint when $n = 60$, which takes more than one day for 500 samples. Harmonica is several magnitudes faster than Spearmint. In Figure 5 (Section 7.4), we show that Harmonica is able to estimate the hidden function with error proportional to the noise level. For synthetic experiment, Spearmint is able to find equally good results compared with Harmonica⁵.

6 Algorithm Comparisons

6.1 Bayesian optimization: Spearmint

Bayesian optimization (BO) algorithms tune hyperparameters by assuming a prior distribution of the loss function, and then keep updating this prior distribution based on the new observations. Each new observation is selected according to an acquisition function, which balances exploration and exploitation such that either the new observation gives us a better result, or helps us gain more information about the loss function. See e.g., [SLA12, SSA13, SSZA14, GKK⁺14, WZH⁺13]. In this paper, we use one of the most popular Bayesian optimization packages called Spearmint⁶, which combines the results of multiple recent papers [SLA12, SSA13, SSZA14].

⁵We only evaluated a few trials for Spearmint due to time constraint.

⁶<https://github.com/HIPS/Spearmint.git>

6.2 Hyperband algorithm

Hyperband [LJD⁺16] is a general version of the SuccessiveHalving (SH) algorithm [JT16], which is a multi-armed bandit algorithm on randomly selected configurations. The SH algorithm runs in multiple stages, and maintains a hyperparameter configuration set T . Initially T has m random configurations. At each stage, SH runs each configuration from T for r iterations (assuming we are training some machine learning tasks iteratively, and intermediate results are visible). Then based on the intermediate result, only the top 1/3 configurations in T are kept for the next stage. Hyperband algorithm is based on SH algorithm, but automatically tunes m , as well as the number of stages. We implemented a parallel version of Hyperband in Lua.

6.3 Comparing Harmonica with other algorithms

Scalability If the hidden function is s -sparse, Harmonica could find such sparse function using $\tilde{O}(s \log s)$ samples. If at every stage of Harmonica, the target function can be approximated by a s sparse function, we only need $\tilde{O}(ks \log s)$ samples where k is the number of stages. For real world applications like neural network hyperparameter tuning, it seems that the hidden function is indeed sparse at every stage and Harmonica performs well. See Section 5.1.

For Hyperband or random search, even if the function is s -sparse, in order to cover the optimal configuration by random sampling, we need $\Omega(2^s)$ samples. For Bayesian optimization it might be even worse.

Optimization time Harmonica runs Lasso [Tib96] algorithm after each stage to solve (2), which is a well studied convex optimization problem and has very fast implementations. Hyperband is also scalable in n , because it simply runs a quick sort algorithm on m samples after every stage, which is negligible. The running time of Bayesian optimization is cubic in number of evaluations, and is very slow for large n . See Section 5.2.

Parallelizability Harmonica, Hyperband and random search are naturally suitable for parallelization, and have straightforward implementations. In every stage of those algorithms, we could simply run m random samples in parallel. In our experiment $m = 300$, which is enough to gain full speed ups with 10+ machines.

By contrast, it's hard to run Bayesian optimization algorithm in parallel, due to its inherent serial nature. While it is possible to pick multiple points at the same time and evaluate them as a batch in parallel [WF16], the speed ups do not grow linearly in the number of machines, and the batch size is usually limited up to 30. Spearmint does not have multiple machine implementations, therefore in this paper we always run it on a single machine.

Feature Extraction Harmonica is able to extract important features with weights in each stages, which automatically sorts all the features according to their importance. See Section 7.2.1.

7 Experimental details

7.1 Options

Table 3: 60 options used in Section 5.1

| Option Name | Description |
|---------------------------------------|--|
| 01. Weight initialization | Use standard initializations or other initializations? |
| 02. Weight initialization (Detail 1) | Xavier Glorot [GB10], Kaiming [HZRS15], $1/n$, or $1/n^2$? |
| 03. Optimization method | SGD or ADAM? [KB14] |
| 04. Initial learning rate | ≥ 0.01 or < 0.01 ? |
| 05. Initial learning rate (Detail 1) | ≥ 0.1 , < 0.1 , ≥ 0.001 , or < 0.001 ? |
| 06. Initial learning rate (Detail 2) | 0.3, 0.1, 0.03, 0.01, 0.003, 0.001, 0.0003, or 0.0001? |
| 07. Learning rate drop | Do we need to decrease learning rate as we train? Yes or No? |
| 08. Learning rate first drop time | If drop learning rate, when is the first time to drop by $1/10$? Epoch 40 or Epoch 60? |
| 09. Learning rate second drop time | If drop learning rate, when is the second time to drop by $1/100$? Epoch 80 or Epoch 100? |
| 10. Use momentum [SMDH13] | Yes or No? |
| 11. Momentum rate | If use momentum, rate is 0.9 or 0.99? |
| 12. Initial residual link weight | What is the initial residual link weight? All constant 1 or a random number in $[0, 1]$? |
| 13. Tune residual link weight | Do we want to use back propagation to tune the weight of residual links? Yes or No? |
| 14. Tune time of residual link weight | When do we start to tune residual link weight? At the first epoch or epoch 10? |
| 15. Resblock first activation | Do we want to add activation layer after the first convolution? Yes or No? |
| 16. Resblock second activation | Do we want to add activation layer after the second convolution? Yes or No? |
| 17. Resblock third activation | Do we want to add activation layer after adding the residual link? Yes or No? |
| 18. Convolution bias | Do we want to have bias term in convolutional layers? Yes or No? |
| 19. Activation | What kind of activations do we use? ReLU or others? |
| 20. Activation (Detail 1) | ReLU, ReLU, Sigmoid, or Tanh? |
| 21. Use dropout [SHK ⁺ 14] | Yes or No? |
| 22. Dropout rate | If use dropout, rate is high or low? |
| 23. Dropout rate (Detail 1) | If use dropout, the rate is 0.3, 0.2, 0.1, or 0.05? |
| 24. Batch norm [IS15] | Do we use batch norm? Yes or No? |
| 25. Batch norm tuning | If we use batch norm, do we tune the parameters in the batch norm layers? Yes or No? |
| 26. Resnet shortcut type | What kind of resnet shortcut type do we use? Identity or others? |
| 27. Resnet shortcut type (Detail 1) | Identity, Identity, Type B or Type C? |
| 28. Weight decay | Do we use weight decay during the training? Yes or No? |
| 29. Weight decay parameter | If use weight decay, what is the parameter? $1e-3$ or $1e-4$? |
| 30. Batch Size | What is the batch size we should use? Big or Small? |
| 31. Batch Size (Detail 1) | 256, 128, 64, or 32? |

| | |
|------------------------------------|--|
| 32. Optnet | An option specific to the code ⁷ . Yes or No? |
| 33. Share gradInput | An option specific to the code. Yes or No? |
| 34. Backend | What kind of backend shall we use? cudnn or cunn? |
| 35. cudnn running state | If use cudnn, shall we use fastest of other states? |
| 36. cudnn running state (Detail 1) | Fastest, Fastest, default, deterministic |
| 37. nthreads | How many threads shall we use? Many or few? |
| 38. nthreads (Detail 1) | 8, 4, 2, or 1? |
| 39-60. Dummy variables | Just dummy variables, no effect at all. |

See Table 3 for the specific hyperparameter options that we use in Section 5.1. For those variables with k options ($k > 2$), we use $\log k$ binary variables under the same name to represent them. For example, we have two variables (01, 02) and their binary representation to denote four kinds of possible initializations: Xavier Glorot [GB10], Kaiming [HZRS15], $1/n$, or $1/n^2$.

7.2 Importance features

7.2.1 Important features that Harmonica selected

We show the selected important features and their weights during the first 3 stages in Table 4 (Section 7.2), where each feature is a monomial of variables with degree at most 3. We do not include the 4th stage because in that stage there are no features with nonzero weights.

Smart choices on important options. Based on Table 4, Harmonica will fix the following variables (sorted according to their importance): Batch Norm (Yes), Activation (ReLU), Initial learning rate ($[0.001, 0.1]$), Optimization method (Adam), Use momentum (Yes), Resblock first activation (Yes), Resblock third activation (No), Weight decay (No if initial learning rate is comparatively small and Yes otherwise), Batch norm tuning (Yes). Most of these choices match what people are doing in practice.

A metric for the importance of variables. The features that Harmonica finds can serve as a metric for measuring the importance of different variables. For example, Batch Norm turns out to be the most significant variable, more important than any other variables, and ReLU is second important. By contrast, Dropout, when Batch Norm is presented, does not have significant contributions. This actually matches with the observations in [IS15].

No dummy/irrelevant variables selected. Although there are 21/60 dummy variables, we never select any of them. Moreover, the irrelevant variables like cudnn, backend, nthreads, which do not affect the test error, were not selected.

7.3 Sensitivities to hyperparameters

#Stages. We observe that having 2, 3 or 4 stages have similar results for this experiment. If the degree of the features is 1 (no correlations between features), or every stage only 3 or fewer features are selected, then 3 or 4 stages will be better.

⁷<https://github.com/facebook/fb.resnet.torch>

⁸This is an interesting feature. In the code repository that we use, optnet, shared gradInput are two special options of the code and cannot be set true at the same time, otherwise the training becomes unpredictable.

Table 4: Important features

| Stage | Feature Name | Weights |
|-------|--|---------|
| 1-1 | 24. Batch norm | 8.05 |
| 1-2 | 19. Activation | 3.47 |
| 1-3 | 04. Initial learning rate * 05. Initial learning rate (Detail 1) | 3.12 |
| 1-4 | 19. Activation * 24. Batch norm | -2.55 |
| 1-5 | 04. Initial learning rate | -2.34 |
| 1-6 | 28. Weight decay | -1.90 |
| 1-7 | 24. Batch norm * 28. Weight decay | 1.79 |
| 1-8 | 34. Optnet * 35. Share gradInput * 52. Dummy ⁸ | 1.54 |
| 2-1 | 03. Optimization method | -4.22 |
| 2-2 | 03. Optimization method * 10. Use momentum | -3.02 |
| 2-3 | 15. Resblock first activation | 2.80 |
| 2-4 | 10. Use momentum | 2.19 |
| 2-5 | 15. Resblock first activation * 17. Resblock third activation | 1.68 |
| 2-6 | 01. Good initialization | -1.26 |
| 2-7 | 01. Good initialization * 10. Use momentum | -1.12 |
| 2-8 | 01. Good initialization * 03. Optimization method | 0.67 |
| 3-1 | 29. Weight decay parameter | -0.49 |
| 3-2 | 28. Weight decay | -0.26 |
| 3-3 | 06. Initial learning rate (Detail 3) * 28. Weight decay | 0.23 |
| 3-4 | 25. Batch norm tuning | 0.21 |
| 3-5 | 28. Weight decay * 29. Weight decay parameter | 0.20 |

#Features per stage. We observe that selecting 3-5 features per stage works well, and produces similar results. More features per stage brings more noise, and fewer features incurs more stages.

Lasso parameters. For Lasso regression, we need to decide the regularization term λ and the number of samples. See Table 2 for stable range for λ and #samples. Here stable range means as long as the parameters are set in this range, the top 5 features and the signs of their weights (which are what we need for computing $g(x)$ in Algorithm 1) do not change. In other words, the feature selection outcome is not affected. When parameters are outside the stable ranges, usually the top features are still unchanged, and we miss only one or two out of the five features.

Degree of features. As we can see in Table 4, although we set the degree to be 3, almost all the important features Harmonica selected have degree at most 2. The same observation holds for degree 4. We also tried to use degree 1 features, which is significantly faster to optimize in Lasso, but will give slightly worse results ($\approx 7.5\%$ best test error with 3 stages and 12 days total running time), because it does not consider the correlations between features. Therefore, we recommend using degree 2 or degree 3 in practice.

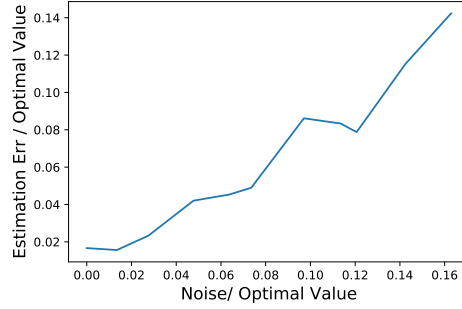


Figure 5: The estimation error of Harmonica is linear in noise level.

7.4 Synthetic function

We define $h(x) \in \{-1, +1\}^n \rightarrow \mathbb{R}$ as follows. $h(x)$ has three stages, and in i -th stage ($i = 0, 1, 2$), it has 32^i sparse vectors $s_{i,j}$ for $j = 0, \dots, 32^i - 1$. Each $s_{i,j}$ contains 5 pairs of weight $w_{i,j}^k$ and feature $f_{i,j}^k$ for $k = 1, \dots, 5$, where $w_{i,j}^k \in [10 + 10^{-i}, 10 + 10^{2-i}]$. and $f_{i,j}^k$ is a monomial on x with degree at most 3. Therefore, for input $x \in \mathbb{R}^n$, the sparse vector $s_{i,j}(x) = \sum_{k=1}^5 w_{i,j}^k f_{i,j}^k(x)$. Since $x \in \{-1, +1\}^n$, $f_{i,j}^k(x)$ is binary. Therefore, $\{f_{i,j}^k(x)\}_{k=1}^5$ contains 5 binaries and represents a integer in $[0, 31]$, denoted as $c_{i,j}(x)$. Let $h(x) = s_{1,1}(x) + s_{2,c_{1,1}(x)}(x) + s_{3,c_{1,1}(x)*32+c_{2,c_{1,1}(x)}}(x) + \xi$, where ξ is the noise uniformly sampled from $[-A, A]$ (A is the noise level). In other words, in every stage i we will get a sparse vector $s_{i,j}$. Based on $s_{i,j}(x)$, we pick a the next sparse function and proceed to the next stage.

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