

# Machine Learning for Predictive Auto-Tuning with Boosted Regression Trees

James Bergstra

Rowland Institute at Harvard  
Harvard University  
Cambridge MA, USA  
bergstra@rowland.harvard.edu

Nicolas Pinto

Rowland Institute at Harvard  
McGovern Institute at MIT  
Cambridge MA, USA  
pinto@rowland.harvard.edu

David Cox

Rowland Institute at Harvard  
Harvard University  
Cambridge MA, USA  
cox@harvard.rowland.edu

## ABSTRACT

The rapidly evolving landscape of multicore architectures makes the construction of efficient libraries a daunting task. A family of methods known collectively as “auto-tuning” has emerged to address this challenge. Two major approaches to auto-tuning are *empirical* and *model-based*: empirical auto-tuning is a generic but slow approach that works by measuring runtimes of candidate implementations, model-based auto-tuning predicts those runtimes using simplified abstractions designed by hand. We show that machine learning methods for non-linear regression can be used to estimate timing models from data, capturing the best of both approaches. A statistically-derived model offers the speed of a model-based approach, with the generality and simplicity of empirical auto-tuning. We validate our approach using the filterbank correlation kernel described in Pinto and Cox [2012], where we find that 0.1 seconds of hill climbing on the regression model (“*predictive* auto-tuning”) can achieve almost the same speed-up as is brought by minutes of empirical auto-tuning. Our approach is not specific to filterbank correlation, nor even to GPU kernel auto-tuning, and can be applied to almost any templated-code optimization problem, spanning a wide variety of problem types, kernel types, and platforms.

## 1. INTRODUCTION

Due to power consumption and heat dissipation concerns, scientific applications have shifted from computing platforms where performance had been primarily driven by rises in the clock frequency of a single “heavy-weight” processor (with complex out-of-order control and cache structures) to a platform with ever increasing numbers of “light-weight” cores. Interestingly, this shift is now not only relevant to computational sciences but to the development of all computer systems: from ubiquitous consumer-facing devices (e.g. phones) to high-end computer farms for web-scale applications (e.g. social networks).

Although the future lies in low-power multi-core hardware designs, the field lacks consensus on exactly how the different subsystems (memory, communication and computation) should be efficiently integrated, modeled and programmed. These systems have exhibited varying degrees of memory hierarchy and multi-threading complexity and, as a consequence, they have been increasingly relying on flexible but low-level software-controlled cache management and parallelism [Asanovic et al., 2006] in order to better control and understand the various trade-offs among performance, reliability, energy efficiency, production costs, etc. This evo-

lution has profoundly altered the landscape of application development: programmers are now facing a wide diversity of low-level architectural issues that must be carefully balanced if they are to write code that is both high-performance and portable.

### 1.1 Motivation

In this rapidly evolving landscape, the construction of general development tools and libraries that fully utilize system resources remains a daunting task. Even within specialized architectures from the *same* vendor, such as NVIDIA’s Graphics Processing Units (GPUs) and the Compute Unified Device Architecture (CUDA) [Nickolls et al., 2008, NVIDIA, 2011], many developers apply massive amounts of manual labor to optimize CUDA code to specific input domains. This hand-tuning rarely generalizes well to new hardware generations or different input domains, is prone to error, results in unmaintainable code, and does not even guarantee optimal performance. One of the reasons is that GPU kernels can yield staggeringly large optimization spaces [Datta et al., 2008]. The problem is further compounded by the fact that these spaces can be highly discontinuous [Ryoo et al., 2008], difficult to explore, and optimal performance is often realized at the edge of “performance cliffs” induced by hard device-specific constraints (e.g. register file size or low-latency cache size).

### 1.2 Auto-Tuning

One strategy for addressing these challenges is to use one of a variety of automatic methods known collectively as “auto-tuning.” Two major auto-tuning approaches have emerged in the extensive literature covering the subject (see surveys in e.g. [Vuduc et al., 2001, Demmel et al., 2005, Vuduc et al., 2005, Williams, 2008, Datta et al., 2008, Cavazos, 2008, Li et al., 2009, Park et al., 2011]): analytical model-driven optimization and empirical optimization [Yotov et al., 2003].

The model-driven optimization approach uses analytical abstractions to model the hardware architectures, in order to identify possible code transformations and their complex interactions. Even though highly-accurate analytical models are generally difficult to build, this approach has been quite successful in the past, especially for accelerating serial code, utilizing simplified but general abstractions. However, large speed-ups for parallel code require more accurate high-dimensional models and since this approach is bound by the quality and scalability of its abstraction, it has been less suited for highly-specialized kernels. This approach has been

well-developed in the compiler community, and as a result, it has most often been applied at compile-time where important run-time characteristics such as input domains may be missing. These limitations render the model-driven optimization approach less attractive in many high-performance library development settings.

The empirical optimization approach, in contrast, seeks to find the best performing code configuration by automatically generating many versions of a parametrized kernel and benchmarking them on the actual hardware (possibly at runtime, when contextual information about the hardware and software stack is the richest). This method directly optimizes the metric(s) of interest (e.g. performance) and does not rely on surrogates. A significant advantage of such approaches is that they allow any metric to be optimized without loss of generality. Indeed, it is possible to formulate a multi-objective optimization that minimize both run time *and* power consumption [Rahman et al., 2011], a feat that would be even more difficult using an analytical model-driven approach. Due to its flexibility, empirical auto-tuning has been successfully applied to build a variety of high-performance domain-specific libraries including dense linear algebra [Clint Whaley et al., 2001, Bilmes et al., 1997], sparse linear algebra [Vuduc et al., 2005], signal processing [Frigo and Johnson, 2005], sorting [Li et al., 2004], general stencil operations [Kamil et al., 2010], etc.

The empirical approach is very sensitive to the choice of instrumented optimizations *and* to the search method. The size of the search space is often so large that the current best empirical auto-tuners typically only consider highly-specialized functions with a limited set of code transformations and compiler options, on a limited set of input domains [Ganapathi et al., 2009]. Although searches for good code configurations in highly-discontinuous spaces can be made “embarrassingly” parallel, and thus benefit from parallel execution across many devices, it remains a prohibitively expensive combinatorial optimization problem, as many variants of the code must be generated, compiled, and benchmarked on specific input domains with meaningful statistics (that may require multiple runs). Consequently, most proposed methods prune the space with hard-coded heuristics that offer little generalization guarantees. This has been a key drawback of the empirical approach as compared to the model-driven approach, where good code configurations can be directly derived from the analytical model.

To address this weakness, it is intuitively appealing to combine the two approaches by first constraining the search space with an analytical model and then exploring the reduced space empirically [Chen et al., 2005, Li et al., 2009]. Unfortunately, such a hybrid approach is still bound by the quality of the analytical model, which remains hard to build by hand.

In this paper, we show that it is possible to *learn the model* using non-linear regression modeling techniques instead of constructing a model manually. By learning the model, one can hope to achieve elements of the best of both approaches: the search speed of model-based auto-tuning with the broad applicability and ease of implementation of empirical auto-tuning.

Various statistical prediction techniques have been applied with success at compile-time for general programs on various CPU architectures [Monsifrot et al., 2002, Stephenson et al., 2003, Yotov et al., 2003, Kulkarni et al., 2004, Cooper et al.,

2005, Franke et al., 2005, Hutter et al., 2006, Cavazos et al., 2007, Cavazos, 2008, Hartono et al., 2009, Park et al., 2011, Fursin et al., 2008]. Relative to this work, our contribution is to show how to do fast predictive auto-tuning that satisfies the requirements to: (a) handle the variety of recent multi-core architectures like GPUs [Schaa and Kaeli, 2009], (b) provide high-performance domain-specific libraries [Nukada and Matsuoka, 2009, Li et al., 2009, Kamil et al., 2010], (c) that select good implementations at run-time [Klöckner et al., 2011, Pinto and Cox, 2012], and (d) for the full input domain of a library routine [Liu et al., 2009, Grauer-Gray and Cavazos, 2011].

The paper is organized as follows: Section 2 describes the boosted regression tree model and the procedure for fitting it to empirical timing data. Section 3 details the data-parallel image processing algorithm we use to illustrate our auto-tuning framework. Section 4 describes the sort of kernel we employ for our benchmarking. Section 5 and 6 present the results of our benchmarking experiments, which compare a reference implementation to a) empirical auto-tuning over a domain-specific grid, b) empirical auto-tuning over a hill-climbing search, and c) predictive auto-tuning. Section 7 provides discussion and concluding remarks, while Section 8 outlines directions for future work.

## 2. PREDICTIVE AUTO-TUNING

<b>AUTOTUNE_EMPIRICAL</b> ( <i>shapes, strides</i> )	
1	$a \leftarrow TaskFeatures(shapes, strides)$
2	$c \leftarrow PlatformFeatures()$
3	$b^* \leftarrow \operatorname{argmin}_{b \in \mathcal{B}} MeasureTime(a, b, c) \triangleright slow$
4	<b>return</b> $b^*$
<b>AUTOTUNE_PREDICTIVE</b> ( <i>shapes, strides</i> )	
1	$a \leftarrow TaskFeatures(shapes, strides)$
2	$c \leftarrow PlatformFeatures()$
3	$f \leftarrow TimingModel()$
4	$b^* \leftarrow \operatorname{argmin}_{b \in \mathcal{B}} f(a, b, c) \triangleright fast$
5	<b>return</b> $b^*$

**Figure 1: Pseudo-code template for empirical and predictive auto-tuning. Empirical auto-tuning (above) is inevitably slow because dynamically-generated code must be compiled and run on a number of actual-size inputs. Predictive auto-tuning (below) can be orders of magnitude faster. We show that it can also be accurate.**

This work shows that auto-tuning can be accelerated by orders of magnitude by using a regression model built offline as a surrogate for actual computations on the real hardware. The general form of an auto-tuning based library routine is illustrated in Figure 1 (top). An auto-tuning based routine must operate on three sets of variables:

- A**: task description (argument shapes, physical layout)
- B**: implementation description (auto-tuning parameters)
- C**: platform description (capabilities, micro-benchmarks)

The hypothetical auto-tuning routine described at the top of Figure 1 might take many minutes or hours to perform the *argmin* at step 3 (during which it computes the desired result many times!) so it would not be suitable for a normal library routine implementation. However, the form of the auto-tuning routine suggests the potential for enormous acceleration: if only there were a fast (even approximate) surrogate for the costly *MeasureTime*( $\cdot$ ) function, then the *argmin* could be done in a fraction of a second and the routine could be used normally (Figure 1, bottom).

## 2.1 Learning a Regression Model

The heart of our predictive auto-tuning is a regression model that acts as surrogate for a hand-crafted hardware model or empirical timing estimates. In our experiments, this regression model fits empirically measured timing information for a *subset* of the configuration space and interpolates / extrapolates that timing across the remainder of the space. To fit this model, we form a training set  $\mathcal{X}, \mathcal{Y}$  where each point  $x^{(i)} \in \mathcal{X}$  is a tuple  $(a^{(i)}, b^{(i)}, c^{(i)})$  and each target  $y^{(i)} \in \mathcal{Y}$  reflects the speed of implementation  $b^{(i)}$  on inputs  $a^{(i)}$  on platform  $c^{(i)}$ .

The effectiveness of predictive auto-tuning depends on the mapping between the raw kernel timings  $t(a, b, c)$  (i.e. in seconds) and the utility  $y$  associated with that timing. Anticipating that regression involves minimizing the squared error of our predictor (see Eq. 1) it is important to choose  $y$  so that differences of a given numerical *magnitude* correspond to *improvements* of a certain utility. In program optimization we are interested in improving the speedup over a reference implementation  $b^{(\text{ref})}$ , so it is natural to choose

$$y^{(i)} = \log \left( \frac{\text{speed}(a, b, c)}{\text{speed}(a, b^{(\text{ref})}, c)} \right) = \log \left( \frac{t(a, b^{(\text{ref})}, c)}{t(a, b, c)} \right) \quad (1)$$

One unique aspect of our setting compared with standard regression is that not all kernel implementations ( $b$ ) are *valid* for all input configurations. One option for dealing with these invalid configurations would be to simply omit them from  $\mathcal{X}$  and  $\mathcal{Y}$ , but that would lead to a regression model that suggests invalid configurations. Instead, we chose to associate invalid  $(a, b, c)$  tuples with a constant  $y = \zeta$ . It makes sense to choose  $\zeta < 0$  so that invalid configurations are treated as being worse than the reference, but the question of how much worse is an empirical one. In our experiments we compare  $\zeta$  in the range  $\log(0.01) \leq \zeta \leq \log(.99)$ .

## 2.2 Regression Trees

A regression tree is a piece-wise constant function from one vector space to another, that works by recursively subdividing the input space into constant regions [Breiman et al., 1984, Hastie et al., 2001]. They are widely used in statistics and data-mining applications because the fitting algorithm is quick and reliable, and the form of the tree can provide insight into the relevant input variables. We use a standard fitting procedure, which takes a set of  $(x, y) \in \mathbb{R}^k \times \mathbb{R}$  pairs and constructs a tree with a low mean squared error. To construct each node of a regression tree, we sort the set  $\mathcal{D}$  of  $(x, y)$  pairs along each of the  $k$  features to find the best partitioning  $f_{i, \gamma}$  of the input space along feature  $i$  at point

$\gamma$  (Eqs. 2, 3).

$$f_{i, \gamma}(x) = \begin{cases} \alpha & \text{if } x_i < \gamma \\ \beta & \text{if } x_i \geq \gamma \end{cases} \quad (2)$$

$$i^*, \gamma^* = \underset{i, \gamma}{\operatorname{argmin}} \hat{\mathbb{E}} [(y - f_{i, \gamma}(x))^2] \quad (3)$$

One disadvantage of the regression tree is that it does not make full use of broad patterns in the data – each partition formed by the fitting procedure is fit independently in the recursive training procedure, so it impossible for the model to extract more than one bit of information from each training partition. This disadvantage is mitigated to a significant extent by the practice of *boosting*.

## 2.3 Boosted Regression Trees

Boosting is an iterative procedure for constructing an *ensemble* of regression trees that is coordinated to fit training examples as accurately as possible. [Schapire, 2001, Friedman, 2002] In a recent empirical study of a range of machine learning regression problems, boosted decision trees were found to be among the best and easiest models to apply [Caruana and Niculescu-Mizil, 2006]. On each boosting iteration, a regression tree is fit to the residual error remaining after all previously-fit models have made their predictions. There are essentially three parameters that control the boosted regression tree training procedure: 1) the depth of tree constructed on each boosting iteration, 2) the minimum number of examples to allow at a regression tree leaf, and 3) the number of trees constructed by boosting. We did not attempt a systematic study of the effect of these variables on performance. We chose a maximum depth of 4, so that each new tree would be a *weak* learner without too much capacity; a minimum number of examples per leaf of 10, so that the ensemble would resist over-fitting; and 100 iterations of boosting, after which the residual error on training data appeared to have reached a minimum. Test examples were not used to choose these values.

## 2.4 Search Algorithms

Once an accurate regression model has been fit to the data, it remains to be optimized for novel arguments (Fig. 1, bottom, step 4). An exhaustive search is the most reliable if it can be afforded, but in our experiments (as in general) an exhaustive search is prohibitively expensive. In our experiments we compare two strategies: (1) a generic stochastic hill-climbing search, and (2) a hand-chosen grid provided by the authors of the kernel used in our experiments [Pinto and Cox, 2012]. The *hill-climbing* (HC) search algorithm starts from the reference implementation and resamples each of the parameters of the current best implementation randomly with probability 0.25 (keeping the current best setting with probability 0.75). On each hill-climbing iteration, if the predicted speed of the newly sampled point is greater than the previous point, then it becomes the current point. We show results for search variants HC25, HC50, and HC75, which correspond do hill-climbing for 25, 50, and 75 iterations respectively. The *grid* algorithm is specific to the kernel used in our case study, the details of the grid are provided with our experimental results in Section 4.1

### 3. FILTERBANK CORRELATION

Filterbank correlation is a simple spatial image filtering operation that is an important subroutine in many image processing applications. It has a relatively high arithmetic intensity which makes it a natural fit for GPU platforms [Pinto and Cox, 2012].

Mathematically, we define filterbank correlation in terms of an image  $x$  and a filterbank  $f$ . The image  $x$  has  $R$  rows,  $C$  columns, and  $D$  channels (e.g. color channels) that we call its *depth*. We index  $x$  like  $\mathbf{x}[i, j, d]$  where  $0 \leq i < R$ ,  $0 \leq j < C$ , and  $0 \leq d < D$ . The filterbank  $f$  has  $F$  filters that are like little images: each has a height  $H$ , a width  $W$ , and  $D$  channels. We will restrict ourselves to what are called *valid* correlations, in which the image is larger in both rows and columns than the filters. The result of filterbank correlation of  $x$  with  $f$  is an image-like array  $z$  with  $R-H+1$  rows,  $C-W+1$  columns, and depth  $F$ , whose elements are defined according to Equation 4:

$$\mathbf{z}[r, c, k] = \sum_{w=0}^{W-1} \sum_{h=0}^{H-1} \sum_{d=0}^{D-1} \mathbf{x}[r+h, c+h, d] \mathbf{f}[k, h, w, d]. \quad (4)$$

In terms of floating point operations (FLOP), a filterbank correlation requires the inner sums to be computed for each output pixel, yielding the quantity in Eq. 5:

$$\text{FLOP} = 2FHWD(R-H+1)(C-W+1) \quad (5)$$

The multiplicative factor of 2 arises because we must first multiply an element of  $x$  with an element of  $f$  and then add the result to an element of  $z$ .

The memory transfer requirements of filterbank correlation are more difficult to quantify. Assuming three kinds of non-register memory – constant, shared, and global – and assuming optimistically that the entire filterbank fits into the GPU’s constant memory, then we can establish a lower bound (Eq. 6) on the amount of memory that must be moved in order to store the computed result to global memory starting from arguments in global memory:

$$\begin{aligned} \text{Bytes} &= 4RCD \\ &+ 4FHWD \\ &+ 4(R-H+1)(C-W+1)F. \end{aligned} \quad (6)$$

In short, we must read the filterbank and image once, and store the result.

The arithmetic intensity of filterbank correlation, assuming our lower bound on memory transfers is therefore approximately

$$\text{intensity} \approx \frac{FDHW}{2(D+F)}, \quad (7)$$

for images that are large relative to filters. Each  $F$  output writes corresponds to approximately  $D$  input reads and  $F$  inner products between  $DHW$  elements.

The high potential for arithmetic intensity makes the GPU an ideal platform for computing filterbank correlations, and filterbank correlation is used extensively in image and video processing, where it is often a computational bottleneck. One might expect then, that it would be easy to implement a library providing this operation as a simple function that takes pointers and strides for  $x$ ,  $f$ , and  $z$  and performs the computation. However, as shown in Pinto and Cox [2012] it is challenging to provide an implementation or even an

implementation strategy that provides satisfactory performance across the range of inputs (shapes, physical layouts) that occur in typical usage. Kamil et al. [2009] summarize a related situation related to general stencil computations in their abstract: “Although the auto-tuning strategy has been successfully applied to libraries, generalized stencil kernels are not amenable to packaging as libraries.”

### 4. GPU IMPLEMENTATION

The strategy we use for computing filterbank correlation on the GPU using CUDA follows Pinto and Cox [2012]. The overall strategy is to load the filterbank into constant memory, which is relatively fast and visible to all threads, and then launch a grid of blocks that tiles the output image. Each thread computes  $4 \times n\_output\_4s$  channels for some column and row of  $z$ . Each block of threads computes  $4 \times n\_output\_4s$  channels for a sub-rectangle of the output image ( $z$ ). When there are more than  $4 \times n\_output\_4s$  channels in  $z$ , or if the filterbank is too large to fit into constant memory, then multiple kernel executions perform the full computation. Our approach permits splitting the filterbank along the number-of-filters dimension ( $F$ ) and the height dimension ( $H$ ). All the filterbanks in our study are small enough that at least one row of a single filter can fit into constant memory. Pseudo-code for the kernel is given in Figure 2.

```

THREAD_FBCORR( $gX, cF, gZ$ )
1   shared  $sX \leftarrow$  all channels of region ( $\beta$ ) of  $gX$ 
2    $x, y \leftarrow$  position of this thread in output image
3   _syncthreads()
4    $v[0 : N] \leftarrow 0$ , for  $N = 4 \times n\_output\_4s$ 
5   for  $d \leftarrow 0$  to  $D$ ,
6     for  $h \leftarrow 0$  to  $H/n\_filter\_r$ ,
7       for  $w \leftarrow 0$  to  $W$ ,
8          $u \leftarrow sX[x+h, y+w, d]$ 
9         for  $n \leftarrow 0$  to  $n\_output\_4s - 1$ ,
10           $v[n] \leftarrow v[n] + cF[n, h, w, d]$ 
11        for  $n \leftarrow 0$  to  $n\_output\_4s - 1$ ,
12           $gZ[x][y][4n:4n+n] += v[4n:4n+n]$ , (float4)

```

**Figure 2: Kernel pseudo-code for filterbank correlation.** Input  $gX$  is a pointer to  $x$  in global memory, input  $cF$  is a pointer to  $f$  in either constant or texture memory, and output  $gZ$  is a pointer to  $z$  in global memory. Each block of threads modifies  $4 \times n\_output\_4s$  channels of a rectangle (called  $\beta$  in code listing) within  $z$ . A grid of blocks covers all rows and columns of  $z$ . Multiple calls can be used to apply all filters of a large filterbank  $f$  to  $x$ .

The kernel is parametrized by 10 parameters:

`block_h`  $\in$  (4, 8, 16, 32, 64, 128)  
`block_w`  $\in$  (4, 8, 16, 32, 64, 128)  
`n_filter_r`  $\in$  (1, 2)  
`n_output_4s`  $\in$  (all, 1, 2)  
`spill`  $\in$  (*False*, *True*)  
`imul_fast`  $\in$  (*False*, *True*)  
`pad_shared`  $\in$  (*False*, *True*)  
`use_tex1d`  $\in$  (*False*, *True*)  
`maxrreg`  $\in$  (8, 16, 20, 24, 28, 32,  $\infty$ )  
`fast_math`  $\in$  (*False*, *True*)

The block height (“`block_h`”) and block width (“`block_w`”) parameters control the number of threads that run within each block. Each kernel call loads some number of filter rows (“`n_filter_r`”) into constant memory and processes the correlation of the image with just those rows, incrementing the output buffer. Each thread can compute several output elements at once, in multiples (“`n_output_4s`”) of 4; this increases the efficiency of each thread, but can lead to lower occupancy. Registers are a precious commodity on the GPU, and this kernel accumulates elements of  $v$  in registers. The “`spill`” parameter controls whether the current thread’s output position in  $gZ$  is stored in a register (faster access) or in shared memory (frees up a register). The “`imul_fast`” parameter controls whether integer multiplication is done in 24-bit (True) or 32-bit (False) precision. The “`pad_shared`” parameter controls whether the  $sX$  shared memory buffer is padded, which wastes space in shared memory but reduces bank conflicts. The “`use_tex1d`” parameter controls whether the image is loaded into shared memory with global pointer dereferences or texture fetches. The “`maxrreg`” and “`fast_math`” parameters are passed to the `nvcc` compiler to limit the number of registers available to each thread, and to enable more aggressive instruction selection, respectively.

When the entire filterbank does not fit into the GPU’s constant memory,  $P$  passes are necessary to compute all of  $z$ , where

$$P = \frac{FH}{4 \cdot n\_output\_4s \cdot n\_filter\_r}.$$

In such cases, the number of bytes moved to and from global memory is much higher than the theoretical lower limit.

$$\begin{aligned} \text{Bytes} = & 4RCDP \\ & + 4FHWD \\ & + 8(R - H + 1)(C - W + 1)FP. \end{aligned}$$

These passes make the I/O requirements increase quadratically in  $F$  and  $H$ . At the same time, the total number of floating-point operations (Eq. 5) is quadratic in  $H$  and  $W$ . In our experiments, we only considered square filters so in our setting the total number of flops is proportional to  $H^4$ .

Critically: what makes this kernel interesting as a case study is that the arithmetic intensity, shared storage, and register requirements of this kernel change significantly and in a complicated platform-dependent way with the argument parameters ( $R, C, D, F, H, W$ ) and with the implementation parameters, especially “`block_w`”, “`block_h`”, “`n_output_4s`” and “`n_filter_rows`.”

## 4.1 Reference and Grid

Pinto and Cox [2012] recommend as a reference implementation: `block_w = 8`, `block_h = 8`, `n_filter_rows = 1`, `n_output_4s = all`, `spill = False`, `imul_fast = True`, `pad_shared = True`, `use_tex1d = True`, `maxrreg =  $\infty$` , and `fast_math = False`. This reference implementation was chosen manually based on good performance across a range of platforms from older-generation cards such as the 8600GT all the way to current-generation flagship cards such as the GTX 580 and C2070. Given that parameters were hand-chosen for the reference kernel, no claims are made as to the optimality nor universality of this reference (indeed, different programmers would undoubtedly arrive at different results). We use this kernel configuration as a reasonable indicator of typical performance made possible by ad hoc experimentation with parameters.

Additionally, Pinto and Cox [2012] advocate a particular grid search over what was estimated to be the most relevant part of the configuration space. This grid iterates over all combinations of `n_filter_rows`, `n_output_4s`, `spill_l`, `pad_shared_l` for three different `block_h`, `block_w` choices: (16, 8), (16, 16), and (32, 8). In our experiments, we call this algorithm the *grid* search procedure. The grid included 72 points in addition to the reference implementation, for a total of 73 points.

## 4.2 Software Stack

This kernel was implemented in the meta-programming style advocated in Pinto and Cox [2012] in Python using Cheetah for string processing and PyCUDA [Klöckner et al., 2011] for dynamic kernel compilation and interfacing with CUDA.

## 5. EXPERIMENTAL SETUP

Recall from the introduction (Eq. 1) that auto-tuning can be seen as a conditional optimization problem in which we seek an implementation ( $b \in \mathcal{B}$ ) that minimizes runtime or some other scalar-valued cost function for given arguments ( $a \in \mathcal{A}$ ) on a particular platform ( $c \in \mathcal{C}$ ). In order to perform predictive auto-tuning with a regression model, it is necessary to characterize these three types of variables with *features*. We describe the arguments to a filterbank correlation with the 6-tuple ( $R, C, D, F, H, W$ ). We randomly sampled arguments (uniformly) from the following product space:

$$\begin{aligned} R = C & \in \{256, 512, 1024, 2048, 4096\} \\ H = W & \in \{3, 5, 7, 9, 11\} \\ D & \in \{1, 4, 8, 16, 32, 64, 128, 256\} \\ F & \in \{1, 4, 8, 16, 32, 64, 128, 256\} \end{aligned}$$

A library implementation of this operation would ideally support all image and filter sizes as well as variations due to strided memory layouts. In such a setting it would be useful to characterize the arguments with features such as whether the inputs are Fortran-style contiguous, C-style contiguous, or row-padded to various byte alignments. These additional options would make our approach of automatic auto-tuning even more important, because there would be a greater variety in the kinds of computations and memory transfers to perform. Our experiments consider a somewhat simplified setting in which the arguments are always stored with depth

channels being contiguous in memory, followed by columns, then rows, and then filters having the largest stride.

The product space in our study includes 1600 argument combinations, but we restricted our experiments to correlations that represented between 1 and 50 gigaflops (GFLOP) of arithmetic. Smaller problems do not fully utilize GPU hardware and are handled equally well by many kernel settings. Larger take so long to evaluate that there is negligible inefficiency in implementing them via multiple calls with smaller images and fewer filters. With the experiments searched an argument space included 602 configurations with between 1 and 50 GFLOP.

For the implementation features  $b$ , we directly used the integer and binary values (block\_w, block\_h, etc.) that paraded the kernels. We did not use platform features ( $c$ ) in our experiments. We leave the investigation of cross-platform predictive auto-tuning for future work.

## 6. RESULTS

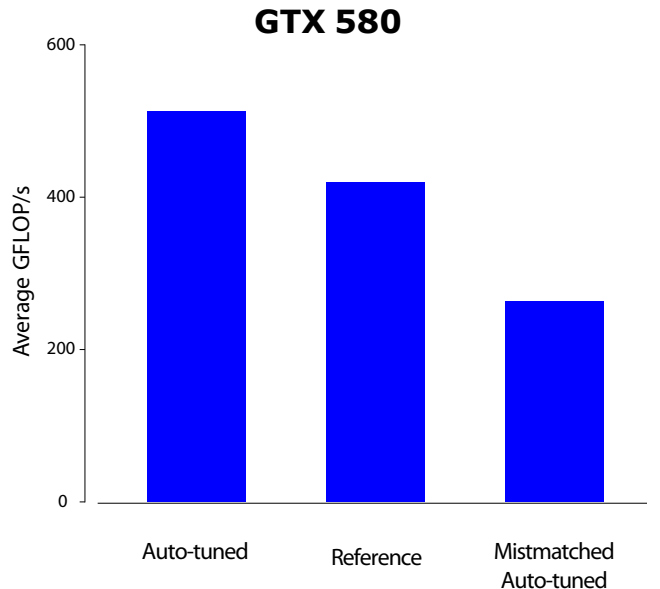
Figure 4 shows the effectiveness of empirical auto-tuning is in this setting. Taking the GTX 580 as an example, and averaging across the range of problem configurations in our study, we find that empirically auto-tuned implementations are on average about 50% faster than the reference implementation. The reference in turn, is about 50% faster than implementations that were empirically auto-tuned for a *randomly chosen* different argument configuration. This shows that it is generally not enough to auto-tune for particular argument configurations; instead it is important to choose the right kernel for the job for each unique argument configuration (input-dependent auto-tuning).

Comparing the *grid* to *HC25*, *HC50* and *HC75* we found very little difference in performance. The HC25 was slightly poorer, but the grid, HC50, and HC75 algorithms delivered similar average results. None of the algorithms was strictly better than the others. In our predictive auto-tuning experiments we used HC75.

Figure 3 shows how accurate predictive auto-tuning is compared with empirical auto-tuning. The training set ( $\mathcal{X}$ ,  $\mathcal{Y}$ ) for the regression model comprised all of the  $((a, b, c), y)$  pairs observed during grid search and hill-climbing search. So for each training argument configuration  $a, c$  there were 148 different values of  $b$  and thus 148 training points. Figure 3 (a) shows that as more argument configurations are used for training, the performance of predictive auto-tuning on test configurations  $(a', c)$  quickly approaches the average performance of empirical auto-tuning. We took care to partition the train and test sets so that there were no overlapping configurations. The key difference between the predictive and empirical auto-tuning, is that predictive auto-tuning typically took about 0.1 seconds per test example, whereas empirical auto-tuning took about 1-3 minutes.

Figure 3 (b) and (c) show that the implementation speeds found by predictive auto-tuning correlates very well with the speed of empirical auto-tuning across all of the devices we tested: GeForce GTX 295, Tesla C1060, GeForce GTX 580, GeForce GTX 480 and Tesla C2070 which span two generations of NVIDIA CUDA platforms.

In some cases, predictive auto-tuning yields an invalid implementation. We dealt with this scenario by backtracking through the various best-estimates found during the hill-climbing search. Some invalid kernels can only be discovered after compiling code and attempting to run the compiled



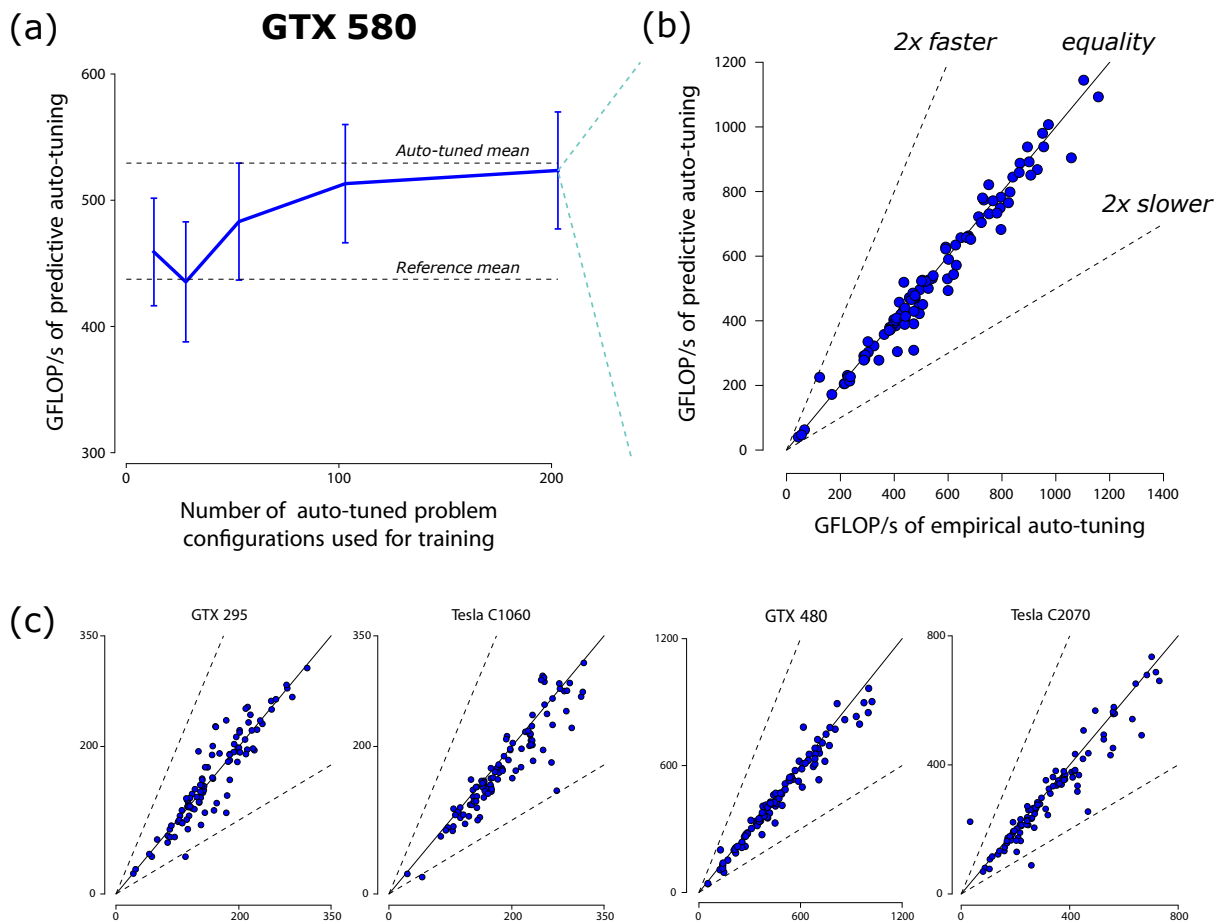
**Figure 4: Different arguments call for different kernels: *left* is the average argument-specific empirical auto-tuned performance across 100 random argument configurations, *middle* is the average speed of our reference implementation, *right* is the average speed of kernels auto-tuned for different argument configurations than the one being tested. For 38 out of 100 random configurations, the kernel auto-tuned for another problem could not even run on the GTX 295 hardware. These points contributed a speed of 0, bringing down the average much lower than the reference. Good performance across a variety of inputs requires *input-dependent auto-tuning*.**

code, so in these cases predictive auto-tuning took up to 3 seconds. Even in these cases the predictive model is much faster than empirical auto-tuning because the first kernel that runs successfully is still typically a fast one.

Figure 5 shows how the training set size and the value of  $\zeta$  affect the accuracy of predictive auto-tuning. All candidates timed during the grid and hill-climbing search procedures were used as training examples, so the training set sizes ranged from an average of 1,480 (10 problem configurations) to 29,600 (200 problem configurations). Training from the largest training sets took approximately 30 seconds. Training 50 or more problem configurations yielded quite accurate predictions with  $\zeta = \log(0.5)$ , which was the best value for  $\zeta$  across the range of devices in our study.

## 7. DISCUSSION

In this paper, we have demonstrated a boosted regression tree-based auto-tuning method, wherein empirical performance data is used to train a machine learning model of performance for an instrumented GPU kernel. In contrast to traditional model-based auto-tuning, where an explicit model of performance is built on the basis of an understanding of hardware inner workings, and empirical auto-tuning, where an exhaustive set of implementation configurations are tried, the present approach generates, from scratch, a model of kernel performance on the basis of timing data



**Figure 3: Computation speed for novel problem configurations using predictive vs. empirical auto-tuning.** (a) As more problem configurations are used to train the regression model, the performance of predictive auto-tuning approaches that of empirical auto-tuning despite taking only 0.1 seconds instead of minutes. (b) and (c) For a wide range of devices, implementation speeds found by predictive auto-tuning correlate tightly with implementation speeds found by empirical auto-tuning.

from a user-definable number of kernel evaluations. This approach allows significant flexibility to navigate trade-offs between offline and run-time costs, and final auto-tuning performance. Importantly, this method treats kernels as black-boxes, allowing the user to auto-tune in the absence of deep knowledge of hardware details (which may even be unknowable, in the case of hardware not available at the time of kernel creation). This approach also frees auto-tuning performance from a strong dependency on the accuracy (or inaccuracy) of a pre-defined analytical model.

An important use case for the tools described here is in the development of user-facing numerical libraries. Such libraries are a critical component of scientific computing infrastructure, since they abstract away implementation details and make algorithms available to a much wider audience. However, the abstraction provided by libraries represents a double-edged sword: one hand, *using* the library is easier, because it presents a unified abstraction of related functionality. However, at the same time, any given library routine might represent a wide range of substantially different problem configurations, each with distinct computational issues and bottlenecks. Auto-tuning has long pro-

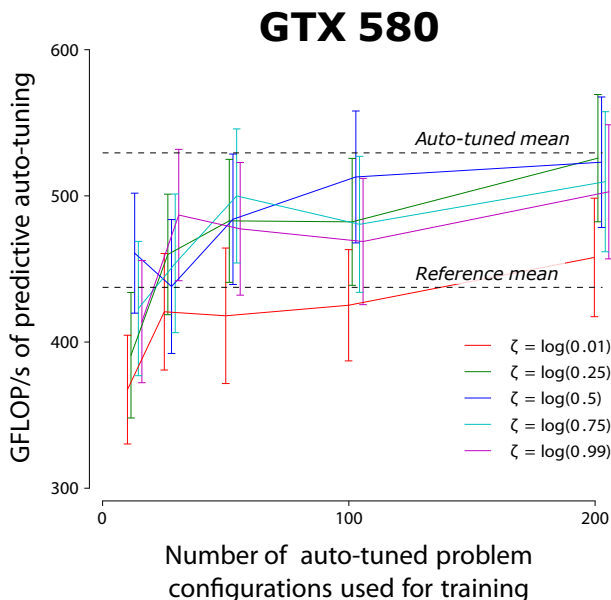
vided a solution that finesses these two issues, providing multiple implementations under the hood, for multiple problem settings, and then using heuristics or explicit, hand-crafted models to select the appropriate implementation for a given set of inputs. The development of such auto-tuned libraries, while extremely successful, is also very difficult. The machine-learning-based techniques described here provide a middle ground, where a library developer can simply create an instrumented kernel, and allow generic tools to automatically generate appropriate auto-tuned implementations, with small (and controllable) run-time costs.

## 8. FUTURE WORK

While the present work serves as a basic demonstration of the value of using machine learning models to predict optimal implementation parameters on a specific application, there are many avenues for taking these ideas further.

A natural route to extend of our current approach is to include more features as inputs to the predictive model. In addition to further instrumentation of the kernel in question, input features could include a much broader range of hardware-related information, from more detailed informa-





**Figure 5: The effect of the invalid configuration score ( $\zeta$ ) and training set size on predictive auto-tuning. Models trained on as few as 25 configurations outperformed the reference. Models trained on 50 or more configurations rivalled empirical auto-tuning. Moderate values of  $\zeta$  between  $\log(0.25)$  and  $\log(0.75)$  are best.**

tion about device capabilities to micro-benchmarks [Wong et al., 2010], and results from performance limiter analyses [Micikevicius, 2010]. Such additional features would increase the predictive model’s ability to adapt to a wide range of different kinds of hardware, including new devices not available at the time of kernel creation.

Another potentially interesting avenue of research is in interpreting the model learned by predictive auto-tuning. While traditional model-based auto-tuning approaches by design assume a given model, and empirical auto-tuning approaches are completely model free, the predictive approach described here *generates* a model from performance data. Because this generated model can be interrogated by a variety of means, a significant opportunity exists to learn about the factors that drive the performance of a given kernel. These insights can be used to further guide the development and instrumentation of the kernel, potentially yielding even greater gains.

Other directions will include the validation of our predictive auto-tuning framework to other domains and environments, in particular general data-parallel primitives and non data-parallel applications, other multi-core architectures, and heterogeneous software platforms such as OpenCL.

## 9. ACKNOWLEDGMENTS

This work was funded by the Rowland Institute of Harvard, the NVIDIA Graduate Fellowship, and the National Science Foundation (IIS 0963668). Hardware support was generously provided by the NVIDIA Corporation.

## References

- K. Asanovic, R. Bodik, B. Catanzaro, J. Gebis, P. Husbands, K. Keutzer, D. Patterson, W. Plishker, J. Shalf, S. Williams, et al. The landscape of parallel computing research: A view from berkeley. *EECS UC Berkeley Tech Rep*, 2006.
- J. Bilmes, K. Asanovic, C. Chin, and J. Demmel. Optimizing matrix multiply using phipac: a portable, high-performance, ansi c coding methodology. In *SC*, 1997.
- L. Breiman, J. H. Friedman, R. A. Olshen, and C. J. Stone. *Classification and Regression Trees*. Wadsworth & Brooks/Cole Advanced Books & Software, 1984.
- R. Caruana and A. Niculescu-Mizil. An empirical comparison of supervised learning algorithms. In *ICML*, 2006.
- J. Cavazos. Intelligent compilers. In *IEEE Cluster Computing*. IEEE, 2008.
- J. Cavazos, G. Fursin, F. Agakov, E. Bonilla, M. O’Boyle, and O. Temam. Rapidly selecting good compiler optimizations using performance counters. In *IEEE CGO*, 2007.
- C. Chen, J. Chame, and M. Hall. Combining models and guided empirical search to optimize for multiple levels of the memory hierarchy. In *IEEE CGO*, 2005.
- R. Clint Whaley, A. Petitet, and J. Dongarra. Automated empirical optimizations of software and the atlas project. *Parallel Computing*, 2001.
- K. Cooper, A. Grosul, T. Harvey, S. Reeves, D. Subramanian, L. Torczon, and T. Waterman. Acme: adaptive compilation made efficient. In *ACM SIGPLAN*, 2005.
- K. Datta, M. Murphy, V. Volkov, S. Williams, J. Carter, L. Oliker, D. Patterson, J. Shalf, and K. Yelick. Stencil computation optimization and auto-tuning on state-of-the-art multi-core architectures. In *SC*, 2008.
- J. Demmel, J. Dongarra, V. Eijkhout, E. Fuentes, A. Petitet, R. Vuduc, R. Whaley, and K. Yelick. Self-adapting linear algebra algorithms and software. *IEEE*, 2005.
- B. Franke, M. O’Boyle, J. Thomson, and G. Fursin. Probabilistic source-level optimisation of embedded programs. In *ACM SIGPLAN*, 2005.
- J. H. Friedman. Stochastic gradient boosting. *Computational Statistics & Data Analysis*, 2002.
- M. Frigo and S. Johnson. The design and implementation of fftw3. *IEEE*, 2005.
- G. Fursin, C. Miranda, O. Temam, M. Namolaru, E. Yom-Tov, A. Zaks, B. Mendelson, E. Bonilla, J. Thomson, H. Leather, et al. Milepost gcc: machine learning based research compiler. 2008.
- A. Ganapathi, K. Datta, A. Fox, and D. Patterson. A case for machine learning to optimize multicore performance. In *HotPar*, 2009.
- S. Grauer-Gray and J. Cavazos. Optimizing and auto-tuning belief propagation on the gpu. *Languages and Compilers for Parallel Computing*, 2011.
- A. Hartono, B. Norris, and P. Sadayappan. Annotation-based empirical performance tuning using orio. In *IEEE IPDPS*, 2009.
- T. Hastie, R. Tibshirani, and J. H. Friedman. *The Elements of Statistical Learning*. Springer Verlag, New York, 2001.
- F. Hutter, Y. Hamadi, H. Hoos, and K. Leyton-Brown. Performance prediction and automated tuning of randomized and parametric algorithms. *Principles and Practice of Constraint Programming-CP 2006*, 2006.



- S. Kamil, C. Chan, S. Williams, L. Oliker, J. Shalf, M. Howison, and P. E. W. Bethel. A generalized framework for auto-tuning stencil computations. In *Cray User Group Conference*, 2009.
- S. Kamil, C. Chan, L. Oliker, J. Shalf, and S. Williams. An auto-tuning framework for parallel multicore stencil computations. In *IEEE IPDPS*, 2010.
- A. Klöckner, N. Pinto, Y. Lee, B. Catanzaro, P. Ivanov, and A. Fasih. Pycuda and pyopencl: A scripting-based approach to gpu run-time code generation. *Parallel Computing*, 2011.
- P. Kulkarni, S. Hines, J. Hiser, D. Whalley, J. Davidson, and D. Jones. Fast searches for effective optimization phase sequences. In *ACM SIGPLAN*, 2004.
- X. Li, M. Garzarán, and D. Padua. A dynamically tuned sorting library. In *IEEE CGO*, 2004.
- Y. Li, J. Dongarra, and S. Tomov. A note on auto-tuning gemm for gpus. *IICS*, 2009.
- Y. Liu, E. Zhang, and X. Shen. A cross-input adaptive framework for gpu program optimizations. In *IEEE IPDPS*, 2009.
- P. Micikevicius. Analysis-driven optimization. In *GPU Technology Conference*. NVIDIA, 2010.
- A. Monsifrot, F. Bodin, and R. Quiniou. A machine learning approach to automatic production of compiler heuristics. *Artificial Intelligence: Methodology, Systems, and Applications*, 2002.
- J. Nickolls, I. Buck, M. Garland, and K. Skadron. Scalable parallel programming with cuda. *ACM Queue*, 2008.
- A. Nukada and S. Matsuoka. Auto-tuning 3-d fft library for cuda gpus. In *Conference on High Performance Computing Networking, Storage and Analysis*. ACM, 2009.
- NVIDIA. Compute unified device architecture (cuda) programming guide. 2011.
- E. Park, S. Kulkarni, and J. Cavazos. An evaluation of different modeling techniques for iterative compilation. In *ACM CASES*, 2011.
- N. Pinto and D. D. Cox. GPU metaprogramming: A case study in biologically inspired machine vision. In *GPU Computing Gems*. Morgan Kaufmann, 2012.
- S. Rahman, J. Guo, and Q. Yi. Automated empirical tuning of scientific codes for performance and power consumption. In *ACM International Conference on High Performance and Embedded Architectures and Compilers*, 2011.
- S. Ryoo, C. Rodrigues, S. Stone, S. Baghsorkhi, S. Ueng, J. Stratton, and W. Hwu. Program optimization space pruning for a multithreaded gpu. In *ACM CGO*, 2008.
- D. Schaa and D. Kaeli. Exploring the multiple-gpu design space. In *IEEE IPDPS*, 2009.
- R. Schapire. The boosting approach to machine learning: An overview. In *MSRI Workshop on Nonlinear Estimation and Classification*. 2001.
- M. Stephenson, S. Amarasinghe, M. Martin, and U. O'Reilly. Meta optimization: Improving compiler heuristics with machine learning. *ACM SIGPLAN*, 2003.
- R. Vuduc, J. Demmel, and J. Bilmes. Statistical models for automatic performance tuning. *ICCS*, 2001.
- R. Vuduc, J. Demmel, and K. Yelick. Oski: A library of automatically tuned sparse matrix kernels. In *Journal of Physics: Conference Series*, 2005.
- S. Williams. *Auto-tuning performance on multicore computers*. ProQuest, 2008.
- H. Wong, M. Papadopoulou, M. Sadooghi-Alvandi, and A. Moshovos. Demystifying gpu microarchitecture through microbenchmarking. In *IEEE ISPASS*, 2010.
- K. Yotov, X. Li, G. Ren, M. Cibulskis, G. DeJong, M. Garzaran, D. Padua, K. Pingali, P. Stodghill, and P. Wu. A comparison of empirical and model-driven optimization. In *ACM SIGPLAN*, 2003.