Parallel High Performance Bootstrapping in Python

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We use a combination of code-generation, code lowering, and just-in-time compilation techniques called SEJITS (Selective Embedded JIT Specialization) to generate highly performant parallel code for Bag of Little Bootstraps (BLB), a statistical sampling algorithm that solves the same class of problems as general bootstrapping, but which parallelizes better. We do this by embedding a very small domain-specific language into Python for describing instances of the problem and using expert-created code generation strategies to generate code at runtime for a parallel multicore platform. The resulting code can sample gigabyte datasets with performance comparable to hand-tuned parallel code, achieving near-linear strong scaling on a 32-core CPU, yet the Python expression of a BLB problem instance remains source- and performance-portable across platforms. This work represents another case study in a growing list of algorithms we have "packaged" using SEJITS in order to make high-performance implementations of the algorithms available to Python programmers across diverse platforms.

Introduction

A common task domain experts are faced with is performing statistical analysis on data. The most prevalent methods for doing this task (e.g. coding in Python) often fail to take advantage of the power of parallelism, which restricts domain experts from performing analysis on much larger data sets, and doing it much faster than they would be able to with pure Python.

The rate of growth of scientific data is rapidly outstripping the rate of single-core processor speedup, which means that scientific productivity is now dependent upon the ability of domain expert, non-specialist programmers (productivity programmers) to harness both hardware and software parallelism. However, parallel programming has historically been difficult for productivity programmers, whose primary concern is not mastering platform specific programming frameworks. At the same time, the methods available to harness parallel hardware platforms become increasingly arcane and specialized in order to expose maximum performance potential to efficiency programming experts. Several methods have been proposed to bridge this disparity, with varying degrees of success.

High performance natively-compiled scientific libraries (such as SciPy) seek to provide a portable, high-performance interface for common tasks, but the usability and efficiency of an interface often varies inversely to its generality. In addition, SciPy's implementations are sequential, due to both the wide variety of parallel programming models and the difficulty of selecting parameters such as degree of concurrency, thread fan-out, etc.

SEJITS [SEJITS] provides the best of both worlds by allowing very compact Domain-Specific Embedded Languages (DSELs) to be embedded in Python. Specializers are mini-compilers for these DSELs, themselves implemented in Python, which perform code generation and compilation at runtime; the specializers only intervene during those parts of the Python program that use Python classes belonging to the DSEL. BLB is the latest such specializer in a growing collection.

ASP ("ASP is SEJITS for Python") is a powerful framework for bringing parallel performance to Python using targeted just-in-time code transformation. The ASP framework provides a skinny waist interface which allows multiple applications to be built and run upon multiple parallel frameworks by using a single run-time compiler, or specializer. Each specializer is a Python class which contains the tools to translate a function/functions written in Python into an equivalent function/functions written in one or more low-level efficiency languages. In addition to providing support for interfacing productivity code to multiple efficiency code back-ends, ASP includes several tools which help the efficiency programmer lower and optimize input code, as well as define the front-end DSL. Several specializers already use these tools to solve an array of problems relevant to scientific programmers [SEJITS].

Though creating a compiler for a DSL is not a new problem, it is one with which efficiency experts may not be familiar. ASP eases this task by providing accessible interfaces for AST transformation. The `NodeTransformer` interface in the ASP toolkit includes and expands upon CodePy's [CodePy] C++ AST structure, as well as providing automatic translation from Python to C++ constructs. By extending this interface, efficiency programmers can define their DSEL by modifying only those constructs which differ from standard python, or intercepting specialized constructs such as special function names. This frees the specializer writer from re-writing boilerplate for common constructs such as branches or arithmetic operations.

ASP also provides interfaces for managing source variants and platforms, to complete the task of code lowering. The ASP framework allows the specializer writer to specify Backends, which represent distinct parallel frameworks or platforms. Each backend may store multiple specialized source variants, and includes simple interfaces for selecting new or best-choice variants, as well as compiling and running the underlying efficiency source codes. Couple with the Mako templating language and ASP's

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AST transformation tools, efficiency programmers are relieved of writing and maintaining platform-specific boilerplate and tools, and can focus on providing the best possible performance for their specializer.

Related Work

Prior work on BLB includes a serial implementation of the algorithm, as described in "The Big Data Bootstrap" and a Scala implementation that runs on the Spark cluster computing framework, as described in "A Scalable Bootstrap for Massive Data". The first paper shows that the BLB algorithm produces statistically robust results on a small data set with a linear estimator function. The second paper describes how BLB scales with large data sets in distributed environments.

BLB

BLB ("Bag of Little Bootstraps") is a method to assess the quality of a statistical estimator, $\theta(X)$, based upon subsets of a sample distribution X. θ might represent such quantities as the parameters of a regressor, or the test accuracy of a machine learning classifier. In order to calculate θ, subsamples of size K^{γ}, where $K = |X|$ and γ is a real number between 0 and 1, are drawn n times without replacement from X, creating the independent subsets $X_1, X_2, ..., X_n$. Next, K elements are resampled with replacement from each subset X_i, m times. This procedure of resampling with replacement is referred to as bootstrapping. The estimator θ is applied to each bootstrap. These results are reduced using a statistical aggregator (e.g. mean, variance, margin of error, etc.) to form an intermediate estimate $\theta'(X_i)$.Finally, the mean of θ' for each subset is taken as the estimate for $\theta(X)$. This method is statistically rigorous, and in fact reduces bias in the estimate compared to other bootstrap methods [BLB]. In addition, its structural properties lend themselves to efficient parallelization.

DSEL for BLB

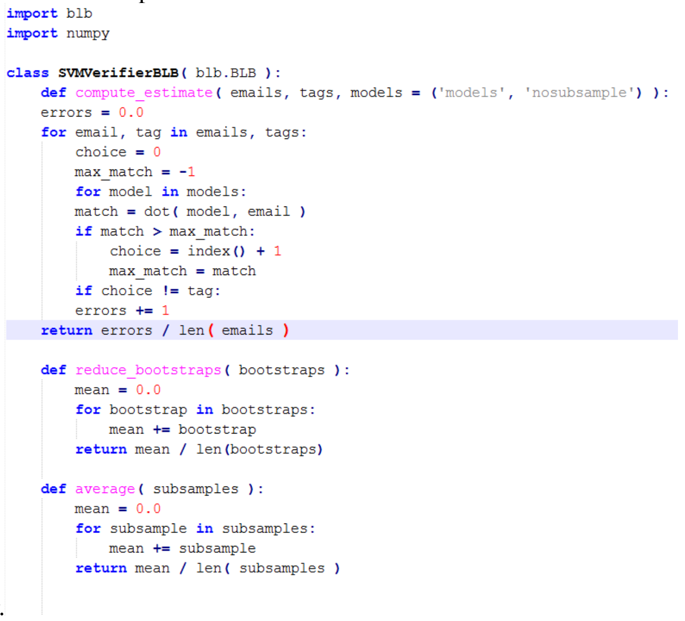
A BLB problem instance is defined by the estimators and reducers it uses, its sampling parameters, and its input data. Our BLB specializer exposes a simple but expressive interface which allows the user to communicate all of these elements using either pure Python or a simple DSEL.

The DSEL, which is formally specified in Appendix A, is designed to concisely express the most common features of BLB estimator computations: position-independent iteration over large data sets, and dense linear algebra. The BLB algorithm was designed for statistical and loss-minimization tasks. These tasks share the characteristic of position-independant computation; they depend only on the number and value of the unique elements of the argument data sets, and not upon the position of these data points within the set. For this reason, the DSEL provides a pythonic interface for iteration, instead of a position-oriented style (i.e., subscripts and incrementing index variables) which is common in lower-level languages. Because most data sets which BLB operates on will have high-dimensional data, the ability to efficiently express vector operations is an important feature of the DSEL. All arithmetic operations and function calls which operate on data are replaced in the final code with optimized, inlined functions which automatically handle data of any size without changes to the source code. In addition to these facilities, common dense linear algebra operations may also be accessed via special function calls in the DSEL.

The next set of problem parameters, the sampling parameters, are not represented directly in the DSEL; In fact, they are not referenced anywhere therein. This is because the sampling parameters, which comprise n, m, and γ, have pattern-level consequences, and have no direct bearing on the executrion of users' computations. These values can be passed as keyword arguments to the specializer object when it is created, or the specializer may be left to choose reasonable defaults.

The final components of a problem instance are the input data. Much of the necessary information about the input data is gleaned by the specializer without referring to the DSEL. However, a major component of what to do with the input data is expressed using the DSEL's annotation capability. Argument annotations, as seen in figure 1 below, are used to determine whether or not a given input should be subsampled as part of the BLB pattern. This is essential for many tasks, because it allows the user to pass in non-data information (e.g. a machine learning model vector) into the computation. Though the annotations are ultimately removed, the information they provide propagates as changes to the pattern within the execution template.

An example application of BLB is to do model verification. Suppose we have trained a classifier $\pi : \mathbb{R}^d \rightarrow C$ where d is the dimension of our feature vectors and C is the set of classes. We can define $\theta[Y]$ to be `error[Y]/|Y|`, where the error function is 1 if $\pi(y)$ is not the true class of y, and 0 elsewhere. If we then choose arithmetic mean as a statistical aggregator, the BLB method using the γ we defined will provide an estimate of the test error of our



```
import blb
import numpy

class SVMVerifierBLB( blb.BLB ):
    def compute_estimate( emails, tags, models = ('models', 'nosubsample') ):
    errors = 0.0
    for email, tag in emails, tags:
        choice = 0
        max_match = -1
        for model in models:
        match = dot( model, email )
        if match > max_match:
            choice = index() + 1
            max_match = match
        if choice != tag:
        errors += 1
    return errors / len( emails )

    def reduce_bootstraps( bootstraps ):
        mean = 0.0
        for bootstrap in bootstraps:
            mean += bootstrap
        return mean / len(bootstraps)

    def average( subsamples ):
        mean = 0.0
        for subsample in subsamples:
            mean += subsample
        return mean / len( subsamples )
```

classifier.

Figure 1. User-supplied code for model verification application using BLB specializer.

The Specializer: A Compiler for the BLB DSEL

The BLB specializer combines various tools, as well as components of the ASP framework and a few thousand lines of custom code, to inspect and lower productivity code at run time.

The BLB DSEL is accessed by creating a new Python class which uses the base specializer class, `blb.BLB`, as a parent. Specific methods corresponding to the estimator and reducer functions are written with the DSEL, allowing the productivity programmer to easily express aspects of a BLB computation which can be difficult to write efficiently. Though much of this code is converted faithfully from Python to C++ by the specializer, two important sets of constructs are intercepted and rewritten in an optimized way when they are lowered to efficiency code. The first such construct is the for loop. In the case of the estimator *theta*, these loops must be re-written to co-iterate over a weight set. As mentioned above, the bootstrap step of the algorithm samples with replacement a number of data points exponentially larger than the size of the set. A major optimization of this operation is to re-write the estimator to work with a weight set the same size as the subsample, who's weights sum to the size of the original data set. This is accomplished within the DSEL by automatically converting for loops over subsampled data sets into weighted loops, with weight sets drawn from an appropriate multinomial distribusion for each bootstrap. When this is done, the specializer converts all the operations in the interior of the loop to weighted operations, which is why only augmented assignments are permitted in the interior of loops Appendix A. The other set of constructs handled specially by the specializer are operators and function calls. These constructs are specialized as described in the previous section.

Introspection begins when a specializer object is instantiated. When this occurs, the specializer uses Python's inspect module to extract the source code from the specializer object's methods named `compute_estimate`, `reduce_bootstraps`, and `average`. The specializer then uses Python's ast module to generate a Python abstract syntax tree for each method.

The next stage of specialization occurs when the specialized function is invoked. When this occurs, the specializer extracts salient information about the problem, such as the size and data type of the inputs, and combines it with information about the platform gleaned using ASP's platform detector. Along with this information, each of the three estimator ASTs is passed to a converter object, which transforms the Python ASTs to C++ equivalents, as well as performing optimizations. The converter objects referred to above perform the most radical code transformations, and more so than any other part of the specializer might be called a run-time compiler (with the possible exception of the C++ compiler invoked later on). Once each C++ AST is produced, it is converted into a python string whose contents are a valid C++ function of the appropriate name. These functions-strings, along with platform and problem-specific data, are used as inputs to Mako templates to generate a C++ source file tailored for the platform and problem instance. Finally, CodePy is used to compile the generate source file and return a reference to the compiled function to Python, which can then be invoked.

In addition to code lowering and parallelization, the specializer is equipped to make pattern-level optimization decisions. These optimizations change the steps of the execution pattern, but do not affect the user's code. The best example of this in the BLB specializer is the decision of whether or not to load in subsamples. Subsamples of the full data set can be accessed by indirection to individual elements (a subsample is an array of pointers) or by loading the subsampled elements into a new buffer (loading in). Loading in subsamples encourages caching, and our experiments showed performance gains of up to 3x for some problem/platform combinations using this technique. However, as data sizes grow, the time spent moving data or contending for shared resources outweighs the caching benefit. Because the specializer has some knowledge of the platform and of the input data sizes, it is able to make predictions about how beneficial loading in will be, and can modify the efficiency level code to decide which inputs should be loaded in and which should not. The specializer determines this by comparing the size of a subsample to the size of the shared L2 cache; if the memory needed for a single thread would consume more than 40% of the resources, then subsamples will not be loaded in. The value of 40% is empirical, and determined for the particular experiments herein. In the future, this and other architecture-level optimizations will be made automatically by specializers by comparing the performance effects of such decisions on past problem instances.

The other major pattern-level decision for a BLB computation is choice of sampling parameters. These constitute the major efficiency/accuracy trade-off of the BLB approach. By default, the specializer sets these parameters conservatively, favoring accuracy heavily over efficiency; The default sampling parameters are n = 25 subsamples, m = 100 bootstraps per subsample, and γ = 0.7. Though each of these values has clear performance implications, the specializer does not adjust them based on platform parameters because it does not include a mechanism to evaluate acceptable losses in accuracy.

Empirical evidence shows that accuracy declines sharply using γ less than 0.5 [BLB], though does not increase much more using a higher value than 0.7. A change of .1 in this value leads to an order-of-magnitude change in subsample size for data sets in the 10-100 GB range, so the smallest value which will attain the desired accuracy should be chosen. The number of subsamples taken also has a major impact on performance. The run time of a specialized computation in these experiments could be approximated to within 5% error using the formula $t = \lceil \frac{n}{c} \rceil s$, where t is the total running time, c is the number of cores in use, and s is the time to compute the bootstraps of a single subsample in serial. Though the result from bootstraps of a given subsample will likely be close to the true estimate, at least 20 subsamples were needed in the experiments detailed here to reduce variance in the estimate to an acceptable level. Finally, the number of bootstraps per subsample determines how accurate an estimate is produced for each subsample. In the experiments described below, 40 bootstraps were used. In experiments not susceptible to noise, as few as 25 were used with acceptable results. Because the primary effect of additional bootstraps is to reduce the effect of noise and improve accuracy, care should be taken not to use too few.

Evaluation

We evaluated the performance gains from using our SEJITS specializer by performing model verification of a SVM classifier on a subset of the Enron email corpus [ENRON]. We randomly selected 10% (Approximately 120,000 emails) from the corpus to serve as our data set. From each email, we extracted the counts of all words in the email, as well as the user-defined directory the email was filed under. We then aggregated the word counts of all the emails to construct a Bag-of-Words model of our data set, and assigned classes based upon directory. In the interest of classification efficiency, we filtered the emails to use only those from the 20 most common classes, which preserved approximately 98% of our original data set. In the final count, our test data consisted of approximately 126,000 feature vectors and tags, with each feature vector composed of approximately 96,000 8-bit features. Using the SVM-Multiclass [SVM] library, we trained a SVM classifier to decide the likeliest storage directory for an email based upon its bag of words representation. We trained the classifier on 10% of our data set, reserving the other 90% as a test set. We then applied the specialized code shown in figure 1 to estimate the accuracy of the classifier. We benchmarked the performance and accuracy of the specializer on a system using 4 Intel X7560 processors.

Our experiments indicate that our specialized algorithm was able to achieve performance gains of up to 31.6x with regards to the serial version of the same algorithm, and up to 22.1x with respect to other verification techniques. These gains did not come at the cost of greatly reduced accuracy; the results from repeated runs of the specialized code were both consistent and very close to the true population statistic.

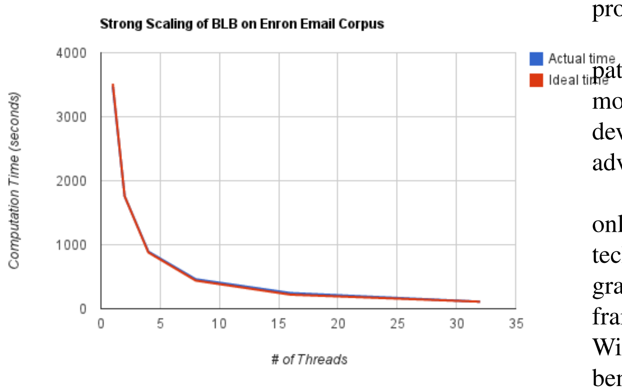


Figure 2. Efficiency gains from specialized code.

As is visible from figure 2 above, our specialized code achieved near-perfect strong scaling. In the serial case, the computation took approximately 3478 seconds. By comparison, when utilizing all 32 available hardware contexts, the exact same productivity level code returned in just under 110 seconds.

We also used SVM Multiclass' native verification utility to investigate the relative performance and accuracy of the specializer. SVM Multiclass' utility differs critically from our own in several ways: The former uses an optimized sparse linear algebra system, whereas the latter uses a general dense system; the former provides only a serial implementation; and the algorithm (traditional cross-validation) is different from ours. All of these factors should be kept in mind as results are compared. Nevertheless, the specializer garnered order-of-magnitude performance improvements once enough cores were in use. SVM Multiclass' utility determined the true population statistic in approximately 2200 seconds, making it faster than the serial incarnation of our specializer, but less efficient than even the dual-threaded version.

The native verification utility determined that the true error rate of the classifier on the test data was 67.86%. Our specializers estimates yielded a mean error rate of 67.24%, with a standard deviation of 0.36 percentage points. Though the true statistic was outside one standard deviation from our estimate's mean, the specializer was still capable of delivering a reasonably accurate estimate very quickly.

Limitations and Future Work

Some of the limitations of our current specializer are that the targets are limited to OpenMP and Cilk. We would like to implement a GPU and a cloud version of the BLB algorithm as additional targets for our specializer. We'd like to explore the performance of a GPU version implemented in CUDA. A cloud version will allow us to apply the BLB sepcializer to problems involving much larger data sets than are currently supported. Another feature we'd like to add is the ability for our specializer to automatically determine targets and parameters based on the input data size and platform specifications.

Conclusion

Using the SEJITS framework, productivity programmers are able to easily express high level computations while simultaneously gaining order-of-magnitude performance benefits. Because the parallelization strategy for a particular pattern of computation and hardware platform is often similar, efficiency expert programmers can make use of DSLs embedded in higher level languages, such as Python, to provide parallel solutions to large families of similar problems.

We were able to apply the ASP framework and the BLB pattern of computation to efficiently perform the high level task of model verification on a large data set. This solution was simple to develop with the help of the BLB specializer, and efficiently took advantage of all available parallel resources.

The BLB specializer provides the productivity programmer not only with performance, but with performance portability. Many techniques for bringing performance benefits to scientific programming, such as pre-compiled libraries, autotuning, or parallel framework languages, tie the user to a limited set of platforms. With SEJITS, productivity programmers gain the performance benefits of a wide variety of platforms without changes to source code.

This specializer is just one of a growing catalogue of such tools, which will bring to bear expert parallelization techniques to a variety of the most common computational patterns. With portable, efficient, high-level interfaces, domain expert programmers will be able to easily create and maintain code bases in the face of evolving parallel hardware and networking trends.

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Appendix A: Formal Specification of DSEL

```
## NAME indicates a valid python name, with the added
## stipulation it not start with '_blb_'
## INT and FLOAT indicate decimal representations of
## 64 bit integers and IEEE floating point numbers,
## respectively
## NEWLINE, INDENT, and DEDENT stand for the respective
## whitespace elements

P ::= OUTER_STMT* RETURN_STMT
AUG ::= '+=' \ '-=' | '*=' | '/='
NUM ::= INT | FLOAT
OP ::= '+' | '-' | '*' | '/' | '**'
COMP ::= '>' | '<' | '==' | '!=' | '<=' | '>='
BRANCH ::= 'if' NAME COMP NAME':'

RETURN_STMT ::= 'return' NAME | 'return' CALL
```

```
CALL ::= 'sqrt(' NAME ')'
      | 'len(' NAME ')'
      | 'mean(' NAME ')'
      | 'pow(' NAME',' INT ')'
      | 'dim(' NAME [',' INT ] ')'
      | 'dtype(' NAME ')'
      | 'MV_solve(' NAME',' NAME',' NAME ')'
      | NAME OP CALL | CALL OP NAME
      | CALL OP CALL | NAME OP NAME
      | NAME '*' NUM | CALL '*' NUM
      | NAME '/' NUM | CALL '/' NUM
      | NAME '**' NUM | CALL '**' NUM

INNER_STMT ::= NAME '=' NUM |
      | NAME = 'vector(' INT [',' INT]*', type='NAME ')'
      | NAME AUG CALL
      | NAME '=' 'index('[INT]')' OP NUM
      | NAME = NUM OP 'index('[INT]')'
      | BRANCH NEWLINE INDENT INNER_STMT* DEDENT
      | 'for' NAME[',' NAME]* 'in' NAME[',' NAME]*':' NEWLINE INDENT INNER_STMT* DEDENT

OUTER_STMT ::= NAME '=' NUM
      | NAME '=' 'vector(' INT [',' INT]*', type='NAME ')'
      | NAME '=' CALL | NAME AUG CALL
      | 'for' NAME[',' NAME]* 'in' NAME[',' NAME]*':' NEWLINE INDENT INNER_STMT* DEDENT
      | BRANCH NEWLINE INDENT OUTER_STMT* DEDENT
```

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