

A New Architecture for Optimization Modeling Frameworks

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Abstract—We propose a new architecture for optimization modeling frameworks in which solvers are expressed as computation graphs in a framework like TensorFlow rather than as standalone programs built on a low-level linear algebra interface. Our new architecture makes it easy for modeling frameworks to support high performance computational platforms like GPUs and distributed clusters, as well as to generate solvers specialized to individual problems. Our approach is particularly well adapted to first-order and indirect optimization algorithms. We introduce `cvxflow`, an open-source convex optimization modeling framework in Python based on the ideas in this paper, and show that it outperforms the state of the art.

I. INTRODUCTION

Optimization offers a principled approach to solving problems in a wide variety of application domains, such as machine learning, statistics, control, signal and image processing, networking, engineering design, finance, and many others [1]. Instead of designing specialized algorithms for each individual problem, the user describes the problem as the minimization of a cost function and the optimal solution with minimal cost is found by the optimization method.

The wealth of applications for this methodology has driven the development of several high-level modeling languages. These languages provide a separation of concerns between the development of mathematical models and the implementation of numerical routines to optimize these models. This is especially useful for rapidly prototyping new applications, allowing practitioners to easily experiment with different cost functions and constraints by writing expressions that closely mimic the mathematical optimization problem. Prominent examples of modeling languages and frameworks include AMPL [2], YALMIP [3], and CVX [4], as well as several tied closely to particular solvers, such as CPLEX’s ILOG [5] and MathProg from GLPK [6].

Despite the popularity of these modeling frameworks, support for modern large-scale computational environ-

ments such as GPUs and distributed clusters is virtually nonexistent. In part, this is due to fundamental challenges in scaling interior point methods, which have historically been the basis for solvers of most modeling frameworks, as these methods require solving sparse linear systems to high accuracy and as such do not benefit greatly from GPU implementation. In addition, distributing such methods beyond a single machine typically requires high bandwidth interconnects such as those available exclusively in HPC environments.

However, there are also highly practical reasons for the lack of support for new environments: mature solvers often require several years to develop and writing entirely new implementations of low-level numerical routines specialized to each environment is unappealing. Traditionally, a degree of platform independence has been provided by implementing on top of low-level linear algebra libraries (*e.g.*, BLAS, LAPACK, and SuiteSparse), but as we discuss in this paper, this architecture is often insufficient, especially for large problems. In addition, such libraries do not handle memory management and data transfer between GPU and CPU or between multiple machines.

The solution that we explore is a new architecture for optimization modeling frameworks based on solvers represented as computation graphs. This architecture is well-suited for solving large optimization problems by taking advantage of problem-specific structure. In particular, the computation graph abstraction naturally represents the composition of structured linear operators which can be significantly more efficient than the standard sparse or dense matrix representation. We develop such a method in this paper and demonstrate that it outperforms the existing state of the art for solving large convex optimization problems, a GPU-enabled version of SCS [7], which itself is one of the few GPU-optimized solvers available, POGS [8] being another example.

A secondary, but not insignificant, benefit of this ap-

proach is automatic support for a wide variety of computational environments (CPU, GPU, distributed clusters, *etc.*), leveraging the considerable momentum and engineering effort of existing computation graph frameworks from the deep learning community. A potential drawback of our approach is that the runtime system must support the necessary mathematical operations to implement numerical optimization algorithms. For first-order and indirect solvers, the many frameworks developed for deep learning, such as TensorFlow [9], Theano [10], [11], Caffe [12], and Torch [13], provide all the necessary functionality. The frameworks have only limited support, however, for the sparse matrix factorization routines used by direct solvers. Thus, given the computation graph implementations available at this time, our architecture tends to favor first-order and indirect methods as opposed to interior point methods.

The outline of the paper is as follows. In §II, we review the traditional architecture for optimization modeling frameworks and discuss its shortcomings. In §III, we explore prior work that addressed the shortcomings of the traditional architecture. In §IV, we describe the new architecture we propose and the computation graph abstraction the architecture is based on. In §V, we present `cvxflow`, an open-source implementation of the ideas in this paper, and numerical results comparing `cvxflow` with the state of the art.

II. TRADITIONAL ARCHITECTURE

The traditional architecture for optimization modeling frameworks dates back to AMPL [2] and GAMS [14] in the 1980s. In this architecture, solving an optimization problem is divided into a three step process, shown in Fig. 1. The process begins with a high-level description of the optimization problem expressed in a modeling language. The first step is canonicalization, in which the problem is transformed through symbolic manipulation into an equivalent problem in a standard form. The second step is matrix stuffing, in which the symbolic representation of the standard form is instantiated so that linear operators are represented by sparse matrices. Often canonicalization and matrix stuffing are combined into a single step. The final step is to call a solver with the sparse matrix representation of the standard form as input and return the solver output as the solution.

The ecosystem of modeling frameworks for convex optimization is an illustrative example of the traditional architecture. Convex optimization modeling languages are built around the principles of disciplined convex programming, a set of rules for constructing optimization problems that make it easy to verify problem convexity.

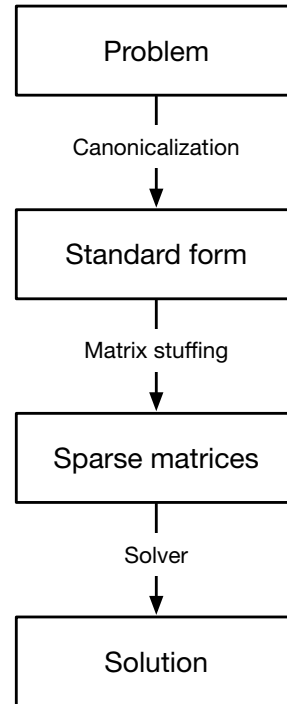


Fig. 1: The traditional architecture for optimization modeling frameworks.

Implementations include CVX [4] and YALMIP [3] in MATLAB, CVXPY [15] in Python, Convex.jl [16] in Julia, and the standalone compilers CVXGEN [17] and QCML [18]. We discuss each component of the traditional architecture in the concrete case of convex modeling frameworks.

A. Canonicalization

The standard form for convex optimization problems is a cone program, an optimization problem of the form

$$\begin{aligned} & \text{minimize} && c^T x \\ & \text{subject to} && Ax + b \in \mathcal{K}, \end{aligned} \quad (1)$$

where $x \in \mathbf{R}^n$ is the optimization variable; $A \in \mathbf{R}^{m \times n}$, $b \in \mathbf{R}^m$, and $c \in \mathbf{R}^n$ are constants; and \mathcal{K} is a nonempty closed convex cone [19]. Convex optimization modeling frameworks symbolically convert problems into cone programs via epigraph transformations [20].

B. Matrix stuffing

In solvers and other software that use the cone program standard form as an input format for problems, c and b are represented by arrays and A is represented by a standard sparse matrix format, such as column compressed storage. Matrix stuffing generates a sparse matrix

representation of A from the symbolic representation generated through canonicalization [21]. Solvers use a sparse matrix representation of A because they generally use algorithms and libraries that exploit sparsity.

C. Solver

A wide variety of solver implementations have been developed for problems in the cone program standard form. Many solvers are written in pure C, including MOSEK [22], SDPA [23], ECOS [24], and SCS [7]. Other solvers are written in higher level languages, such as SeDuMi [25] and SDPT3 [26] in MATLAB and CVXOPT [27] in Python. The solvers rely heavily on low-level linear algebra interfaces like BLAS and LAPACK [28] for basic operations and libraries like SuiteSparse [29] for sparse matrix factorization. Existing cone solvers are almost exclusively restricted to CPU implementations; an exception is SCS which provides GPU support using the cuBLAS library [30].

D. Drawbacks

The traditional approach to optimization modeling frameworks has been enormously successful, allowing modeling languages and solver implementations to be developed independently in the programming languages best suited to their function. The conventional solver implementation is based on interior point methods, for which the dominant computational effort is solving a sparse linear system. Such a solver can be ported relatively easily to new platforms provided the necessary linear algebra libraries (BLAS, LAPACK, SuiteSparse, *etc.*) are available.

However, many optimization problems of interest are too large to be solved with interior point methods and, more generally, any method that requires a direct solution to a linear system involving the A matrix of the cone program standard form (1). In some problem domains the memory requirements even for sparse A matrices can be prohibitive (*e.g.*, 2D convolution in large-scale image reconstruction), while at the same time efficient procedural evaluations of the matrix-vector computations with A and A^T exist (*e.g.*, FFT-based convolution).

A possible solution is a first-order method, such as SCS [7], which only requires solving linear systems to moderate accuracy. This approach can be implemented with either a direct or indirect method for the linear solver subroutine. In the case of a direct solver, the computational cost can be amortized by caching the factorization of the A matrix leading to iterations that are significantly faster than interior point methods. In the indirect case, a matrix-free method such as conjugate

gradient is used, requiring only matrix-vector computations with A and A^T . In the traditional architecture, these computations are simply implemented with sparse matrix multiplies, but the proposed graph-based approach enables taking advantage of specialized linear operator implementations, as we will discuss in detail in the next section.

III. ALTERNATIVE APPROACHES

Prior work has explored alternative approaches to bypassing the limitations of the traditional architecture for optimization modeling frameworks, with a focus on scaling to larger problem sizes. There are two main lines of work that are precursors to the graph-based architecture proposed in this paper: the first replaces the sparse matrix representation of the standard form generated by matrix stuffing with a more general representation, and the second explores new standard forms based on functions with efficient proximal operators. In this section, we review these approaches, providing motivation for our general graph-based framework.

A. Abstract linear operators

In solving many convex optimization problems, the majority of computational time is spent in evaluating linear operators. While the sparse matrix representation of cone programs is fully general, it does not provide the most efficient implementation for many types of linear functions. Matrix-free CVXPY replaces traditional sparse matrix representation of the cone program standard form (1) with a computation graph based representation. The computation graph representation allows the modeling layer to encode information about structured linear operators in the optimization problem that solvers can exploit [21]. The matrix-free CVXPY implementation includes a custom runtime system for computation graphs, as opposed to the `cvxflow` implementation presented in this paper, which is built on TensorFlow.

B. Proximal standard forms

Another line of work explores solvers based on functions with efficient proximal operators. Epsilon [31] introduces the standard form

$$\text{minimize } \sum_{i=1}^N f_i(A_i x), \quad (2)$$

where $x \in \mathbf{R}^n$ is the optimization variable, $A_i \in \mathbf{R}^{m_i \times n}$ are linear operators, and f_i are functions with efficient proximal operators [32]. Epsilon exploits the flexibility of the standard form (2) to rewrite the problem so it can be solved efficiently by a variant of the alternating direction method of multipliers (ADMM) [33]. Along

similar lines, POGS [8] introduces a slightly different standard form, again based on functions with efficient proximal operators, and includes a highly efficient GPU implementation of an ADMM-based algorithm.

The ProxImaL modeling framework also targets the standard form (2), but supports a variety of solver algorithms and applies problem rewritings specialized to optimization problems in imaging [34]. ProxImaL moves towards platform independence by generating solver implementations using Halide [35]. Halide is a language and compiler that allows for platform independent abstraction of individual mathematical operations, but not of full algorithms composed of many operations inside control logic.

These new proximal standard forms are not necessarily incompatible with the traditional architecture based on sparse matrices. However, as opposed to cone solvers and in particular interior point methods, the implementation of algorithms operating on the proximal standard forms is less reliant on sparse linear algebra and thus there is less benefit from building on existing sparse linear algebra libraries. These approaches instead require a library of proximal operator implementations which can benefit greatly from being built on a high-level framework such as Halide or TensorFlow, providing platform independence and a highly optimized runtime system.

IV. GRAPH-BASED ARCHITECTURE

In this section, we propose a new graph-based architecture for optimization modeling frameworks. Our architecture divides the process of solving an optimization problem into three steps, shown in Fig. 2. As with the traditional architecture we begin with a high-level problem description which is canonicalized to a standard form. The solver generation step produces a computation graph representing the solver algorithm, which is executed by the runtime system to produce a solution.

The key difference from the traditional architecture is that the graph-based approach directly generates computation graphs representing the numerical algorithms for solving problems rather than representing all problems with sparse matrices. The first benefit of this approach is support for abstract linear operators with highly efficient implementations, such as convolution, Kronecker products, and others. The second benefit is a closer connection between canonicalization and solver generation, which can now both be implemented in the same high-level language and even in a single library.

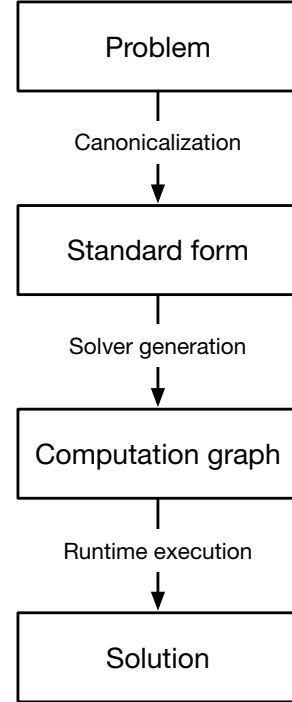


Fig. 2: The proposed graph-based architecture for optimization modeling frameworks.

This more easily allows for supporting different standard forms that incorporate problem-specific structure. Finally, the new architecture severs the link between the solver implementation and computing platform, allowing solvers to take advantage of new computing platforms simply by changing the target of the computation graph runtime system.

We next explain the central abstraction, computation graphs, and describe how such graphs representing solvers are generated.

A. Computation graphs

A computation graph is a directed acyclic graph (DAG) where each vertex represents a mathematical operation and each edge represents data transfer. Input vertices have no incoming edges, while output vertices have no outgoing edges. A vertex is evaluated by applying its operation to the data on the vertex and broadcasting the result on its outgoing edges. The overall graph is evaluated by loading data onto the input vertices, evaluating the vertices in topological order, and reading the results off the output vertices.

For example, Fig. 3 shows a computation graph for the function $f(x, y) = x^2 + 2x + y$. The input vertices represent the variables x and y . The output vertex rep-

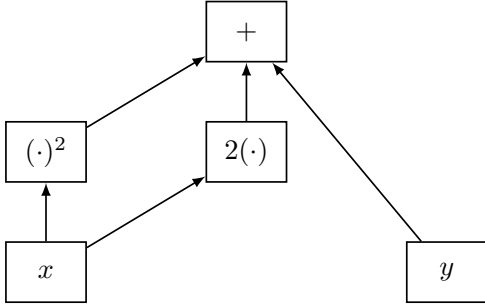


Fig. 3: A computation graph for $f(x, y) = x^2 + 2x + y$.

represent the top level sum. The internal vertices represent the operations $z \rightarrow z^2$ and $z \rightarrow 2z$.

Given a computation graph to evaluate a function, computation graphs for evaluating the function’s gradient or adjoint (for linear functions) can be obtained through simple graph transformations [36], [21]. Function, gradient, and adjoint evaluations are the key operations in first-order and indirect solvers and are even sufficient to precondition a problem [37].

Computation graphs are a useful intermediate representation for solvers because they abstract away the platform-specific details of both computation and memory management. These details are handled by a computation graph runtime system, which has platform-specific code to execute each mathematical operation and to pass data from one operation to the next. By contrast, a solver built on the traditional abstraction of a low-level linear algebra interface must implement its own platform-specific logic for mathematical operations not expressible as linear functions and for memory management.

B. Solver generation

The solver generation step produces a computation graph representing a numerical algorithm for solving an optimization problem. Graph generation is naturally implemented in a high-level functional programming style with modular functions that produce computation graphs implementing numerical algorithms or subroutines. Typically, these functions take as inputs individual nodes or in some cases are naturally parameterized by graph generator functions.

As a concrete example, the Python code snippet for generating a TensorFlow graph representing the conjugate gradient method for the linear system $Ax = b$ is shown below.

```
def cg_solve(A, b, x_init, tol=1e-8):
    delta = tol*norm(b)
```

```
def body(x, k, r_norm_sq, r, p):
    Ap = A(p)
    alpha = r_norm_sq / dot(p, Ap)
    x = x + alpha*p
    r = r - alpha*Ap
    r_norm_sq_prev = r_norm_sq
    r_norm_sq = dot(r, r)
    beta = r_norm_sq / r_norm_sq_prev
    p = r + beta*p
    return (x, k+1, r_norm_sq, r, p)
```

```
def cond(x, k, r_norm_sq, r, p):
    return tf.sqrt(r_norm_sq) > delta
```

```
r = b - A(x_init)
loop_vars = (
    x_init, tf.constant(0),
    dot(r, r), r, r)
return tf.while_loop(
    cond, body, loop_vars)[:3]
```

In this example, the function `cg_solve` is parameterized by the the linear operator A , and vector b with initial starting point, vector x_init . The inputs b and x_init are computation graph nodes and A is a single-argument function such that $A(x)$ produces the computation graph representing the linear operator applied to an arbitrary vector x . Implemented in this fashion, the conjugate gradient method can be applied to any linear operator expressed as a computation graph.

V. NUMERICAL EXAMPLES

In this section, we present numerical examples of solving convex optimization problems in our proposed architecture. As solving linear systems forms the basis for convex methods, we first present results for an indirect linear solver with various linear operators. Using this indirect linear solver as a subroutine, we then implement a version of SCS [7] in the computation graph framework and compare with the native version of SCS implemented in C. We present results for both CPU and GPU environments; all experiments are run on a 32-core Intel Xeon 2.2GHz processor and an nVidia Titan X GPU with 12GB of RAM.

Our implementation builds on CVXPY [15], a convex optimization modeling framework in Python. Using this framework, convex optimization problems can be expressed with minimal code and are automatically converted into the standard conic form (1). As an example,

the nonnegative deconvolution problem we consider in Section V-C is written as the following Python code.

```
from cvxpy import *
x = Variable(n)
f = norm(conv(c, x) - b, 2)
prob = Problem(Minimize(f), [x >= 0])
```

Here c and b are previously-defined problem inputs and n is the size of the optimization variable. Our implementation differs from the existing CVXPY functionality in that instead of solving problems by constructing sparse matrices and calling numerical routines written in C, we build a computation graph, as described in Section IV, and evaluate with TensorFlow. Ultimately, this implementation achieves faster running times than existing methods—for example, on the large nonnegative deconvolution example, our implementation takes roughly 1/10th the time of SCS running on GPU, the existing state-of-the-art method for solving large convex problems to moderate accuracy.

Concurrent with the publication of this paper, we are releasing the `cvxflow` Python library; it is available at

<http://github.com/cvxgrp/cvxflow>

and includes the code for all of the examples in this section. The implementation is general and solves any problem modeled with CVXPY using TensorFlow.

A. Regularized least squares

We begin with solving linear systems using the conjugate gradient method (CG) [38]. CG is matrix-free which makes it a natural fit for linear systems represented as a graph, allowing for specialized implementations of each linear operator including those that are inefficient to represent as sparse matrices such as convolution, Kronecker products, and others. In terms of the graph-based architecture shown in Fig. 2, the standard form in this example is a linear system and the solver generation step generates a graph representing the conjugate gradient method.

In particular, we consider the regularized least squares problem

$$\text{minimize} \quad (1/2)\|Ax - b\|_2^2 + \lambda\|x\|_2^2 \quad (3)$$

where $x \in \mathbf{R}^n$ is the optimization variable, the linear map $A : \mathbf{R}^n \rightarrow \mathbf{R}^m$ and vector $b \in \mathbf{R}^m$ are problem data, and $\lambda > 0$ is the regularization parameter. This problem has the solution

$$x^* = (\lambda I + A^T A)^{-1} A^T b, \quad (4)$$

which can be computed by solving a linear system.

	dense matrix	sparse matrix	convolution
variables n	3000	3000	3000
nonzeros in A	18000000	180000	4095000
spsolve			
solve time	255 secs	28 secs	41 secs
memory usage	2.2 GB	1.06 GB	1.5 GB
objective	5.97×10^{-1}	5.97×10^{-1}	7.68×10^{-1}
CG TensorFlow			
solve time, CPU	3.0 secs	0.9 secs	2.9 secs
solve time, GPU	2.0 secs	0.7 secs	1.0 secs
graph build time	0.4 secs	0.1 secs	0.1 secs
memory usage	1.8 GB	755 MB	946 MB
objective	5.97×10^{-1}	5.97×10^{-1}	7.68×10^{-1}
CG iterations	49	49	71

TABLE I: Results for regularized least squares.

It is often the case that A takes the form of a sparse or dense matrix; for example, in a statistical problem each row of A may represent an observation of multiple variables weighted by x in order to predict the response variable. However, A can also be an abstract linear operator; for example, a convolution with a vector c , written as $Ax = c * x$. We present results for each of these examples: a sparse matrix, a dense matrix, and convolution.

In the matrix examples, entries are sampled from $\mathcal{N}(0, 1)$ with 1% nonzero in the sparse case. For convolution, we apply the Gaussian kernel with standard deviation $n/10$. In all cases, the response variable is formed by $b = A\hat{x} + v$ where v has entries sampled from $\mathcal{N}(0, 0.01^2)$ and \hat{x} from $\mathcal{N}(0, 1)$. The conjugate gradient method is run until the residual satisfies $\|(\lambda I + A^T A)x^k - A^T b\|_2 \leq 10^{-8} \|A^T b\|_2$.

Table I shows the results for these experiments, demonstrating that conjugate gradient on TensorFlow is significantly faster than the baseline method, `scipy.sparse.spsolve`. This is a somewhat weak baseline as `spsolve` does not run on GPU and is not well-suited for dense matrices. Nonetheless, this comparison highlights the difference in architecture exploited by TensorFlow which can take advantage of dedicated implementations for the linear operators leading to significantly faster solve times.

B. Lasso

Next we solve a convex problem with SCS [7]. In this case, the canonicalization step produces a problem in the standard cone form (1) and solver generation produces a graph implementing the SCS iterations. In essence, the algorithm iterates between projections onto a linear subspace and a convex cone; the former is done through solving a linear system with a computation

	dense matrix	sparse matrix	convolution
variables n	6001	6001	6001
constraints m	12002	12002	12001
nonzeros in A	18012002	1812002	4107002
SCS native			
solve time, CPU	29 secs	3.4 secs	6.4 secs
solve time, GPU	27 secs	3.8 secs	7.6 secs
matrix build time	13 secs	1.4 secs	2.8 secs
memory usage	3.1 GB	663 MB	927 MB
objective	3.36×10^1	3.19×10^1	2.02×10^0
SCS iterations	40	40	60
avg. CG iterations	2.66	2.71	2.72
SCS TensorFlow			
solve time, CPU	23 secs	25 secs	24 secs
solve time, GPU	9.9 secs	7.1 secs	5.3 secs
graph build time	1.8 secs	2.0 secs	0.8 secs
memory usage	8.7 GB	4.6 GB	1.2 GB
objective	3.36×10^1	3.19×10^1	2.02×10^0
SCS iterations	60	40	180
avg. CG iterations	3.35	3.55	1.93

TABLE II: Results for lasso.

	small	medium	large
variables n	101	1001	10001
constraints m	300	3000	30000
nonzeros in A	9401	816001	69220001
SCS native			
solve time, CPU	0.1 secs	2.2 secs	260 secs
solve time, GPU	2.0 secs	2.0 secs	105 secs
matrix build time	0.01 secs	0.6 secs	52 secs
memory usage	360 MB	470 MB	10.4 GB
objective	1.38×10^0	4.57×10^0	1.41×10^1
SCS iterations	380	100	160
avg. CG iterations	8.44	2.95	3.01
SCS TensorFlow			
solve time, CPU	3.4 secs	5.7 secs	88 secs
solve time, GPU	5.7 secs	3.2 secs	13 secs
graph build time	0.8 secs	0.8 secs	0.9 secs
memory usage	895 MB	984 MB	1.3 GB
objective	1.38×10^0	4.57×10^0	1.41×10^1
SCS iterations	480	100	160
avg. CG iterations	2.75	2.00	2.00

TABLE III: Results for nonnegative deconvolution.

graph representing the CG method as in the previous section. The SCS method is appealing in this context as it works well with approximate solutions to linear systems, such as those produced by CG.

We consider the lasso problem

$$\text{minimize } (1/2)\|Ax - b\|_2^2 + \lambda\|x\|_1, \quad (5)$$

where the regularization term $\|x\|_1$ replaces the $\|x\|_2^2$ in the regularized least squares problem from the previous section. This problem is convex but no longer has a closed-form solution.

To generate problem instances, we construct example linear operators A as in the previous section. We set the regularization parameter to $\lambda = 0.1\|A^T b\|_\infty$ where $\|A^T b\|_\infty$ is the smallest value of λ such that the solution is zero.

Table II compares the TensorFlow version of SCS to the native implementation and demonstrates that in the dense matrix and convolution cases, the solve time on GPU is faster with TensorFlow. This highlights the benefit of the computation graph, taking advantage of specialized implementations for dense matrix multiplication and convolution. In contrast, when the input linear operator A is a sparse matrix, native SCS is faster.

C. Nonnegative deconvolution

As a final example further illustrating the benefit of abstract linear operators, we consider the nonnegative deconvolution problem

$$\begin{aligned} &\text{minimize } \|c * x - b\|_2 \\ &\text{subject to } x \geq 0 \end{aligned} \quad (6)$$

where $x \in \mathbf{R}^n$ is the optimization variable, and $c \in \mathbf{R}^n$, $b \in \mathbf{R}^{2n-1}$ are problem data. As in the previous example, the canonicalization step transforms the problem to the standard form (1) and solver generation produces a computation graph for the SCS algorithm.

We generate problem instances by taking c to be the Gaussian kernel with standard deviation $n/10$ and convolving it with a sparse signal \hat{x} with 5 nonzero entries sampled uniformly from $[0, n/10]$. We set the response $b = c * \hat{x} + v$ with $v \sim \mathcal{N}(0, 0.01^2)$.

Table III shows that on large problem sizes, the SCS TensorFlow implementation performs significantly better than the native implementation, requiring 13 seconds as compared to 105 seconds. This difference is largely due to differences in architecture, as the matrix-based SCS requires a considerable amount of time (52 seconds) to simply construct the sparse matrix representing the convolution operator. As many linear operators benefit from from specialized implementations (see *e.g.*, [39], [40], [41], [42]), one could easily demonstrate an even more significant gap between the proposed architecture and existing methods simply by choosing more egregious examples that highlight this difference.

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