A Source Transformation via Operator Overloading Method for the Automatic Differentiation of Mathematical Functions in MATLAB

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A source transformation via operator overloading method is presented for computing derivatives of mathematical functions defined by MATLAB computer programs. The transformed derivative code that results from the method of this article computes a sparse representation of the derivative of the function defined in the original code. As in all source transformation automatic differentiation techniques, an important feature of the method is that any flow control in the original function code is preserved in the derivative code. Furthermore, the resulting derivative code relies solely upon the native MATLAB library. The method is useful in applications where it is required to repeatedly evaluate the derivative of the original function. The approach is demonstrated on several examples and is found to be highly efficient when compared to well-known MATLAB automatic differentiation programs.

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1. INTRODUCTION

Automatic differentiation, or as it has more recently been termed, *algorithmic differentiation* (AD), is the process of determining accurate derivatives of a function defined by computer programs [Griewank 2008] using the rules of differential calculus. The objective of AD is to employ the rules of differential calculus in an algorithmic manner to efficiently obtain a derivative that is accurate to machine precision. AD exploits the fact that a computer program containing an implementation of a mathematical function $\mathbf{y} = \mathbf{f}(\mathbf{x})$ can be decomposed into a sequence of elementary function operations. The derivative is then obtained by applying the standard differentiation rules (e.g., product, quotient, and chain rules).

The most well known methods for automatic differentiation are *forward* and *reverse modes*. In either forward or reverse mode, each link in the calculus chain

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rule is implemented until the derivative of the dependent output(s) with respect to the independent input(s) is encountered. The fundamental difference between forward and reverse modes is the direction in which the derivative calculations are performed. In the forward mode, the derivative calculations are performed from the dependent input variables of differentiation to the output independent variables of the program, whereas in reverse mode, the derivative calculations are performed from the independent output variables of the program back to the dependent input variables.

Forward and reverse mode automatic differentiation methods are classically implemented using either operator overloading or source transformation. In an operator-overloaded approach, a custom class is constructed and all standard arithmetic operations and mathematical functions are defined to operate on objects of the class. Any object of the custom class typically contains properties that include the function value and derivatives of the object at a particular numerical value of the input. Furthermore, when any operation is performed on an object of the class, both function and derivative calculations are executed from within the overloaded operation. Well-known implementations of forward and reverse mode AD that utilize operator overloading include MXYZPTLK [Michelotti 1991], ADOL-C [Griewank et al. 1996], COSY INFINITY [Berz et al. 1996], ADOL-F [Shiriaev and Griewank 1996], FADBAD [Bendtsen and Stauning 1996], IMAS [Rhodin 1997], AD01 [Pryce and Reid 1998], ADMIT-1 [Coleman and Verma 1998b], ADMAT [Coleman and Verma 1998a], INTLAB [Rump 1999], FAD [Aubert et al. 2001], MAD [Forth 2006], and CADA [Patterson et al. 2013].

In a source transformation approach, a function source code is transformed into a derivative source code, where, when evaluated, the derivative source code computes a desired derivative. An AD tool based on source transformation may be thought of as an AD preprocessor, consisting of both a compiler and a library of differentiation rules. As with any preprocessor, source transformation is achieved via four fundamental steps: parsing of the original source code, transformation of the program, optimization of the new program, and the printing of the optimized program. In the parsing phase, the original source code is read and transformed into a set of data structures that define the procedures and variable dependencies of the code. This information may then be used to determine which operations require a derivative computation, and the specific derivative computation may be found by means of the mentioned library. In doing so, the data representing the original program is augmented to include information on new derivative variables and the procedures required to compute them. This transformed information then represents a new derivative program, which after an optimization phase may be printed to a new derivative source code. Although the implementation of a source transformation AD tool is much more complex than that of an operator overloaded tool, it usually leads to faster runtime speeds. Moreover, considering that a source transformation tool produces source code, it may, in theory, be applied recursively to produce n^{th}-order derivative files, although Hessian symmetry may not be exploited. Well-known implementations of forward and reverse mode AD that utilize source transformation include DAFOR [Berz 1987], GRESS [Horwedel 1991], PADRE2 [Kubota 1991], Odysée [Rostaing-Schmidt 1993], TAF [Giering and Kaminski 1996], ADIFOR [Bischof et al. 1992, 1996], PCOMP [Dobmann et al. 1995], ADiMat [Bischof et al. 2002], TAPENADE [Hascoët and Pascual 2004], ELIAD [Tadjouddine et al. 2003], and MSAD [Kharche and Forth 2006].

In recent years, MATLAB [Mathworks 2010] has become extremely popular as a platform for developing automatic differentiation tools. ADMAT/ADMIT [Coleman and Verma 1998a, 1998b] was the first automatic differentiation program written in MATLAB. The ADMAT/ADMIT package utilizes operator overloading to implement both the forward and reverse modes to compute either sparse or dense Jacobians and Hessians. The next operator overloading approach was developed as a part of the INTLAB toolbox

[Rump 1999], which implements the sparse forward mode to compute first and second derivatives. The MAD package [Forth 2006] was developed a few years later. Although MAD also employs operator overloading, unlike previously developed MATLAB AD tools, MAD utilizes the *derivvec* class to store directional derivatives within instances of the *fmad* class. In addition to operator overloaded methods that evaluate derivatives at a numeric value of the input argument, the hybrid source transformation and operator overloaded ADiMat package [Bischof et al. 2003] was developed. ADiMat employs source transformation to create a derivative source code. The derivative code may then be evaluated in a few different ways. If only a single directional derivative is desired, then the generated derivative code may be evaluated independently on numeric inputs to compute the derivative; this is referred to as the scalar mode. Thus, a Jacobian may be computed by a process known as strip mining, where each column of the Jacobian matrix is computed separately. To compute the entire Jacobian in a single evaluation of the derivative file, it is required to use either an overloaded derivative class or a collection of ADiMat-specific runtime functions. Here it is noted that the derivative code used for both the scalar and overloaded modes is the same, but the generated code required to evaluate the entire Jacobian *without* overloading is slightly different, as it requires that different ADiMat function calls be printed. The most recent MATLAB source transformation AD tool to be developed is MSAD, which was designed to test the benefits of using source transformation together with MAD's efficient data structures. The first implementation of MSAD [Kharche and Forth 2006] was similar to the overloaded mode of ADiMat in that it utilized source transformation to generate derivative source code that could then be evaluated using the *derivvec* class developed for MAD. The current version of MSAD [Kharche 2011], however, does not depend upon operator overloading but still maintains the efficiencies of the *derivvec* class.

The interpreted nature of MATLAB makes programming intuitive and easy; however, it also makes source transformation AD quite difficult. For example, the operation `c = a*b` takes on different meanings depending upon whether `a` or `b` is a scalar, vector, or matrix, and the differentiation rule is different in each case. ADiMat deals with such ambiguities differently depending upon which ADiMat-specific runtime environment is being used. In both the scalar and overloaded modes, a derivative rule along the lines of `dc = da*b + a*db` is produced. Then, if evaluating in the scalar mode, `da` and `db` are numeric arrays of the same dimensions as `a` and `b`, respectively, and the expression `dc = da*b + a*db` may be evaluated verbatim. In the overloaded vector mode, `da` and `db` are overloaded objects, thus allowing the overloaded version of `mtimes` to determine the meaning of the `*` operator. In its nonoverloaded vector mode, ADiMat instead produces a derivative rule along the lines of `dc = adimat_mtimes(da,a,db,b)`, where `adimat_mtimes` is a runtime function that distinguishes the proper derivative rule. Different from the vector modes of ADiMat, the most recent implementation of MSAD does not rely on an overloaded class or a separate runtime function to determine the meaning of the `*` operator. Instead, MSAD utilizes shape and size propagation rules to attempt to determine the dimensions of `a` and `b`. In the event that the dimensions cannot be determined, MSAD places conditional statements on the dimensions of `a` and `b` directly within the derivative code, where each branch of the conditional statement contains the proper differentiation rule given the dimension information.

In this research, a new method is described for automatic differentiation in MATLAB. The method performs source transformation via operator overloading and source reading techniques such that the resulting derivative source code can be evaluated using commands from only the native MATLAB library. The approach developed in this article utilizes the recently developed operator overloaded method described in Patterson et al. [2013]. Different from traditional operator overloading in MATLAB where the derivative is obtained at a particular numeric value of the input, the method

of Patterson et al. [2013] uses the forward mode of automatic differentiation to print to a file a derivative function, which when evaluated computes a sparse representation of the derivative of the original function. Thus, by evaluating a function program on the overloaded class, a reusable derivative program that depends solely upon the native MATLAB library is created. Different from a traditional source transformation tool, the method of Patterson et al. [2013] requires that all object sizes be known, and thus ambiguities such as the meaning of the $*$ operator are eliminated, as the sizes of all variables are known at the time of code generation. This approach was shown to be particularly appealing for problems where the same user program is to be differentiated at a set of different numeric inputs, where the overhead associated with the initial overloaded evaluation becomes less significant with each required numerical evaluation of the derivative program.

The method of Patterson et al. [2013] is limited in that it cannot transform MATLAB function programs that contain flow control (i.e., conditional or iterative statements) into derivative programs containing the same flow control statements. Indeed, a key issue that arises in any source code generation technique is the ability to handle flow control statements that may be present in the originating program. In a typical operator overloaded approach, flow is dealt with during execution of the program on the particular instance of the class. In other words, because any typical overloaded objects contain numeric function information, any flow control statements are evaluated in the same manner as if the input argument had been numeric. In a typical forward mode source transformation approach, flow control statements are simply copied over from the original program to the derivative program. In the method of Patterson et al. [2013], however, the differentiation routine has no knowledge of flow control nor is any numeric function information known at the time the overloaded operations are performed. Thus, a function code that contains conditional statements that depend upon the numeric values of the input cannot be evaluated on instances of the class. Furthermore, if an iterative statement exists in the original program, all iterations will be evaluated on overloaded objects and separate calculations corresponding to each iteration will be printed to the derivative file.

In this article, a new approach for generating derivative source code in MATLAB is described. The approach of this work combines the previously developed overloaded *cada* class of Patterson et al. [2013] with source-to-source transformation in such a manner that any flow control in the original MATLAB source code is preserved in the derivative code. Two key aspects of the method are developed to allow for differentiation of programs that contain flow control. First, because the method of Patterson et al. [2013] is not cognizant of any flow control statements that may exist in a function program, it is neither possible to evaluate conditional statements nor is it possible to differentiate the iterations of a loop without unrolling the loop and printing each iteration of the loop to the resulting derivative file. In this work, however, an intermediate source program is created where flow control statements are replaced by transformation routines. These transformation routines act as a pseudo-overloading of the flow control statements that they replace, thus enabling evaluation of the intermediate source program on instances of the *cada* class, where the control of the flow of the program is given to the transformation routines. Second, due to the sparse nature of the *cada* class, the result of any overloaded operation is limited to a single derivative sparsity pattern, where different sparsity patterns may arise depending upon conditional branches or loop iterations. This second issue is similar to the issues experienced when applying the vertex elimination tool ELIAD to Fortran programs containing conditional branches. The solution using ELIAD was to determine the union of derivative sparsity patterns across each conditional branch [Tadjouddine et al. 2003]. Similarly, in this article, an overloaded union operator is developed that is used to determine the union of

the derivative sparsity patterns generated by all possible conditional branches and/or loop iterations in the original source code, thus making it possible to print derivative calculations that are valid for all possible branches/loop iterations.

This article is organized as follows. In Section 2, the notation and conventions used throughout the work are described. In Section 3, brief reviews are provided of the previously developed CADA differentiation method and *cada* class. In Section 4, the concepts of overloaded unions and overmapped objects are described. In Section 5, a detailed explanation is provided of the method used to perform user source to derivative source transformation of user functions via the *cada* class. In Section 6, four examples are given to demonstrate the capabilities of the proposed method and to compare the method against other well-known MATLAB AD tools. In Section 7, a discussion is given of the results obtained in Section 6. Finally, in Section 8, conclusions on our work are given.

2. NOTATION AND CONVENTIONS

In this article, we employ the following notation. First, without loss of generality, consider a vector function of a vector $\mathbf{f}(\mathbf{x})$, where $\mathbf{f} : \mathbb{R}^n \longrightarrow \mathbb{R}^m$, and where a vector is denoted by a lowercase bold letter. Thus, if $\mathbf{x} \in \mathbb{R}^n$, then $\mathbf{x}$ and $\mathbf{f}(\mathbf{x})$ are column vectors with the following forms, respectively:

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{R}^n. \tag{1}$$

Consequently, $\mathbf{f}(\mathbf{x})$ has the form

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \\ \vdots \\ f_m(\mathbf{x}) \end{bmatrix} \in \mathbb{R}^m, \tag{2}$$

where $x_i,\ (i = 1, \ldots, n)$ and $f_j(\mathbf{x}),\ (j = 1, \ldots, m)$ are the elements of $\mathbf{x}$ and $\mathbf{f}(\mathbf{x})$, respectively. The *Jacobian* of the vector function $\mathbf{f}(\mathbf{x})$, denoted $\mathbf{Jf}(\mathbf{x})$, is then an $m \times n$ matrix

$$\mathbf{Jf}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_1}{\partial x_m} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{m \times n}. \tag{3}$$

Assuming that the Jacobian $\mathbf{Jf}(\mathbf{x})$ contains N_{nz} nonzero elements, we denote $\mathbf{i}_{\mathbf{x}}^{\mathbf{f}} \in \mathbb{Z}_+^{N_{nz}}$, $\mathbf{j}_{\mathbf{x}}^{\mathbf{f}} \in \mathbb{Z}_+^{N_{nz}}$, to be the row and column locations of the nonzero elements of $\mathbf{Jf}(\mathbf{x})$. Furthermore, we denote $\mathbf{d}_{\mathbf{x}}^{\mathbf{f}} \in \mathbb{R}^{N_{nz}}$ to be the nonzero elements of $\mathbf{Jf}(\mathbf{x})$ such that

$$d_{\mathbf{x}}^{\mathbf{f}}(k) = \frac{\partial f_{[i_{\mathbf{x}}^{\mathbf{f}}(k)]}}{\partial x_{[j_{\mathbf{x}}^{\mathbf{f}}(k)]}}, \quad (k = 1 \ldots N_{nz}), \tag{4}$$

where $d_{\mathbf{x}}^{\mathbf{f}}(k)$, $i_{\mathbf{x}}^{\mathbf{f}}(k)$, and $j_{\mathbf{x}}^{\mathbf{f}}(k)$ refer to the k^{th} elements of the vectors $\mathbf{d}_{\mathbf{x}}^{\mathbf{f}}$, $\mathbf{i}_{\mathbf{x}}^{\mathbf{f}}$, and $\mathbf{j}_{\mathbf{x}}^{\mathbf{f}}$, respectively.

Because the method described in this article performs both the analysis and overloaded evaluation of source code, it is necessary to develop conventions and notation for these processes. First, MATLAB variables will be denoted using typewriter text (e.g., `y`). Next, when referring to a MATLAB source code fragment, uppercase nonbold text will be used (e.g., A), where a subscript may be added to distinguish between multiple similar code fragments (e.g., A_i, $A_{i,j}$). Then, given a MATLAB source code fragment A of a program P, the fragments of code that are evaluated before and after the evaluation of A are denoted $Pred(A)$ and $Succ(A)$, respectively, where $Pred(A)$, A, and $Succ(A)$ are mutually disjoint sets such that $Pred(A) \cap A = A \cap Succ(A) = Pred(A) \cap Succ(A) = \emptyset$ and $Pred(A) \cup A \cup Succ(A) = P$. Next, any overloaded object will be denoted using a calligraphic character (e.g., $\mathcal{Y}$). Furthermore, an overloaded object that is assigned to a variable is referred to as an *assignment object*, whereas an overloaded object that results from an overloaded operation but is not assigned to a variable is referred to as an *intermediate object*. It is noted that an intermediate object is not necessarily the same as an *intermediate variable* as defined in Griewank [2008]. Instead, intermediate objects as defined in this article are the equivalent of statement-level intermediate variables. To clarify, consider the evaluation of the line of MATLAB code `y = sin(x) + x` evaluated on the overloaded object $\mathcal{X}$. This evaluation will first result in the creation of the intermediate object $\mathcal{V} = \sin(\mathcal{X})$ followed by the assignment object $\mathcal{Y} = \mathcal{V} + \mathcal{X}$, where $\mathcal{Y}$ is then assigned to the variable `y`.

3. REVIEW OF THE CADA DIFFERENTIATION METHOD

Patterson et al. [2013] describes a forward mode operator overloading method for transforming a mathematical MATLAB program into a new MATLAB program, which when evaluated computes the nonzero derivatives of the original program. The method of Patterson et al. [2013] relies upon a MATLAB class called *cada*. Unlike conventional operator overloading methods that operate on numerical values of the input argument, the CADA differentiation method does not store numeric function and derivative values. Instead, instances of the *cada* class store only the size of the function, nonzero derivative locations, and symbolic identifiers. When an overloaded operation is called on an instance of the *cada* class, the proper function and nonzero derivative calculations are printed to a file. It is noted that the method of Patterson et al. [2013] was developed for MATLAB functions that contain no flow control statements and whose derivative sparsity pattern is fixed (i.e., the nonzero elements of the Jacobian of the function are the same on each call to the function). In other words, given a MATLAB program containing only a single basic block and with fixed input sizes and derivative sparsity patterns, the method of Patterson et al. [2013] can generate a MATLAB code that contains the statements that compute the nonzero derivative of the original function. In this section, we provide a brief description of a slightly modified version of the *cada* class and the method used by overloaded operations to print derivative calculations to a file.

3.1. The *cada* Class

During the evaluation of a user program on *cada* objects, a derivative file is simultaneously being generated by storing only sizes, symbolic identifiers, and sparsity patterns within the objects themselves and writing the computational steps required to compute derivatives to a file. Without loss of generality, we consider an overloaded object $\mathcal{Y}$, where it is assumed that there is a single independent variable of differentiation, $\mathbf{x}$. The properties of such an object are given in Table I. Assuming that the overloaded object $\mathcal{Y}$ has been created, then the proper calculations will have been printed to a file to compute both the value of $\mathbf{y}$ and the nonzero derivatives $\mathbf{d}_{\mathbf{x}}^{\mathbf{y}}$ (if any) of the Jacobian $\mathbf{Jy}(\mathbf{x})$. In this article, we refer to the printed variable assigned the value of $\mathbf{y}$ as a

Table I. Properties of an Overloaded Object $\mathcal{Y}$

`id`	Unique integer value that identifies the object	
`func`	Structure containing the following information on the function variable associated with this object:	
	`name`	String representation of function variable.
	`size`	1×2 array containing the dimensions of $\mathbf{y}$.
	`zerolocs`	$N_z \times 1$ array containing the linear index of any known zero locations of $\mathbf{y}$, where N_z is the number of known zero elements (this field is only used if the function variable is strictly symbolic).
	`value`	If the function variable is *not* strictly symbolic, then this field contains the values of each element of $\mathbf{y}$.
`deriv`	Structure array containing the following information on the derivative variable associated with this object:	
	`name`	String representation of what the derivative variable is called.
	`nzlocs`	$N_{nz} \times 2$ array containing the row and column indices, $\mathbf{i}_{\mathbf{x}}^{\mathbf{y}} \in \mathbb{Z}_+^{N_{nz}}$ and $\mathbf{j}_{\mathbf{x}}^{\mathbf{y}} \in \mathbb{Z}_+^{N_{nz}}$, of any possible nonzero entries of the Jacobian $\mathbf{J}\mathbf{y}(\mathbf{x})$.

Note: Each overloaded object has the fields `id`, `func`, and `deriv`. The `func` field contains information of the function variable that is assigned the value of $\mathbf{y}$ in the generated program, and the `deriv` field contains information on the derivative variable that is assigned the value of $\mathbf{d}_{\mathbf{x}}^{\mathbf{y}}$ in the generated program (where $\mathbf{x}$ is the independent variable of differentiation).

function variable and the printed variable assigned the value of $\mathbf{d}_{\mathbf{x}}^{\mathbf{y}}$ as a *derivative variable*. We also make the distinction between strictly symbolic and not strictly symbolic function variables, where if a function variable is *strictly symbolic*, at least one element of the function variable is unknown at the time of code generation. Thus, a function variable that is *not strictly symbolic* is considered to be a constant with no associated derivative (where constants are propagated within overloaded operations and calculations are still printed to file). Furthermore, it is noted that the value assigned to any derivative variable may be mapped into a two-dimensional Jacobian using the row and column indices stored in the `deriv.nzlocs` field of the corresponding overloaded object.

3.2. Example of the CADA Differentiation Method

The *cada* class utilizes forward-mode AD to propagate derivative sparsity patterns while performing overloaded evaluations on a section of user written code. All standard unary mathematical functions (e.g., polynomial, trigonometric, exponential), binary mathematical functions (e.g., plus, minus, times), and organizational functions (e.g., reference, assignment, concatenation, transpose) are overloaded. These overloaded functions result in the appropriate function and nonzero derivative calculations being printed to a file while simultaneously determining the associated sparsity pattern of the derivative function. In this section, the CADA differentiation method is explained by considering a MATLAB function such that $\mathbf{x} \in \mathbb{R}^n$ is the input and is the variable of differentiation. Let $\mathbf{v}(\mathbf{x}) \in \mathbb{R}^m$ contain $N_{nz} \leq m \times n$ nonzero elements in the Jacobian, $\mathbf{J}\mathbf{v}(\mathbf{x})$, and let $\mathbf{i}_{\mathbf{x}}^{\mathbf{v}} \in \mathbb{R}^{N_{nz}}$ and $\mathbf{j}_{\mathbf{x}}^{\mathbf{v}} \in \mathbb{R}^{N_{nz}}$ be the row and column indices corresponding to the nonzero elements of $\mathbf{J}\mathbf{v}(\mathbf{x})$, respectively. Furthermore, let $\mathbf{d}_{\mathbf{x}}^{\mathbf{v}} \in \mathbb{R}^{N_{nz}}$ be a vector of the nonzero elements of $\mathbf{J}\mathbf{v}(\mathbf{x})$. Assuming that no zero function locations are known in $\mathbf{v}$, the *cada* instance, $\mathcal{V}$, would posses the following relevant properties: (1) `func.name='v.f'`; (2) `func.size=`$[m \;\; 1]$; (3) `deriv.name='v.dx'`; and (4) `deriv.nzlocs=`$[\mathbf{i}_{\mathbf{x}}^{\mathbf{v}} \; \mathbf{j}_{\mathbf{x}}^{\mathbf{v}}]$. It is assumed that since the object $\mathcal{V}$ has been created, the function variable, `v.f`, and the derivative variable, `v.dx`, have been printed to a file in such a manner that upon evaluation, `v.f` and `v.dx` will be assigned the numeric values of $\mathbf{v}$ and $\mathbf{d}_{\mathbf{x}}^{\mathbf{v}}$, respectively. Suppose now that the unary array operation $g : \mathbb{R}^m \to \mathbb{R}^m$ (e.g., `sin`, `sqrt`, etc.) is encountered during the evaluation of the MATLAB function code. If we consider the function $\mathbf{w} = g(\mathbf{v}(\mathbf{x}))$, it can easily be seen that $\mathbf{J}\mathbf{w}(\mathbf{x})$ and

$\mathbf{Jv}(\mathbf{x})$ will contain possible nonzero elements in the same locations. Additionally, the nonzero derivative values $\mathbf{d}_{\mathbf{x}}^{\mathbf{w}}$ may be calculated as

$$d_{\mathbf{x}}^{\mathbf{w}}(k) = g'(v_{[i_{\mathbf{x}}^{\mathbf{v}}(k)]})d_{\mathbf{x}}^{\mathbf{v}}(k), \quad (k = 1 \ldots N_{nz}), \tag{5}$$

where $g'(\cdot)$ is the derivative of $g(\cdot)$ with respect to the argument of the function g. In the file that is being created, the derivative variable, `w.dx`, would be written as follows. Assume that the index $\mathbf{i}_{\mathbf{x}}^{\mathbf{v}}$ is printed to a file such that it will be assigned to the variable `findex` within the derivative program. Then the derivative computation would be written as `w.dx = dg(v.f(findex)).*v.dx;`, and the function computation would simply be written as `w.f = g(v.f);`, where `dg(·)` and `g(·)` represent the MATLAB operations corresponding to $g'(\cdot)$ and $g(\cdot)$, respectively. The resulting overloaded object, $\mathcal{W}$, would then have the same properties as $\mathcal{V}$ with the exception of `id`, `func.name`, and `deriv.name`. Here we emphasize that, in the preceding example, the derivative calculation is only valid for a vector, $\mathbf{v}$, whose nonzero elements of $\mathbf{Jv}(\mathbf{x})$ lie in the row locations defined by $\mathbf{i}_{\mathbf{x}}^{\mathbf{v}}$, and that the values of $\mathbf{i}_{\mathbf{x}}^{\mathbf{v}}$ and m are known at the time of the overloaded operation.

3.3. Motivation for a New Method to Generate Derivative Source Code

The aforementioned discussion identifies the fact that the CADA method as developed in Patterson et al. [2013] may be used to transform a mathematical program containing a simple basic block into a derivative program, which when executed in MATLAB will compute the nonzero derivatives of a fixed input size version of the original program. The method may also be applied to programs containing unrollable loops, where if evaluated on *cada* objects, the resulting derivative code would contain an unrolled representation of the loop. Function programs containing indeterminable conditional statements (i.e., conditional statements that are dependent upon strictly symbolic objects), however, cannot be evaluated on instances of the *cada* class, as multiple branches may be possible. The remainder of this article focuses on developing the methods to allow for the application of the *cada* class to differentiate function programs containing indeterminable conditional statements and loops, where the flow control of the originating program is preserved in the derivative program.

4. OVERMAPS AND UNIONS

Before proceeding to the description of the method, it is important to describe an overmap and a union, both which are integral parts of the method itself. Specifically, due to the nature of conditional blocks and loop statements, it is often the case that different assignment objects may be written to the same variable, where the determination of which object is assigned depends upon which conditional branch is taken or which iteration of the loop is being evaluated. The issue is that any overloaded operation performed on such a variable may print different derivative calculations depending upon which object is assigned to the variable. To print calculations that are valid for all objects that may be assigned to the variable (i.e., all of the variable's immediate predecessors), a *cada overmap* is assigned to the variable, where an overmap has the following properties:

- *Function size*: The function row/column size is the maximum row/column size of all possible row/column sizes.
- *Function sparsity*: The function is only considered to have a known zero element if every possible function is known to have same known zero element.
- *Derivative sparsity*: The Jacobian is only considered to have a known zero element if every possible Jacobian has the same known zero element.

Table II. Overloaded Variable Properties for Overloaded Union Example

Object Property	$\mathcal{U}$	$\mathcal{V}$	$\mathcal{W} = \mathcal{U} \cup \mathcal{V}$
Function size	m_u	m_v	m_w
Possible function nonzero locations	$\mathbf{i}^{\mathbf{u}}$	$\mathbf{i}^{\mathbf{v}}$	$\mathbf{i}^{\mathbf{w}}$
Possible derivative nonzero locations	$[\mathbf{i}^{\mathbf{u}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{u}}_{\mathbf{x}}]$	$[\mathbf{i}^{\mathbf{v}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{v}}_{\mathbf{x}}]$	$[\mathbf{i}^{\mathbf{w}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{w}}_{\mathbf{x}}]$

Furthermore, the overmap is defined as the union of all possible objects that may be assigned to the variable.

Example of an Overloaded Union. To illustrate the concept of the union of two overloaded objects, consider two configurations of the same variable, $\mathbf{y} = \mathbf{u}(\mathbf{x}) \in \mathbb{R}^{m_u}$ or $\mathbf{y} = \mathbf{v}(\mathbf{x}) \in \mathbb{R}^{m_v}$, where $\mathbf{x} \in \mathbb{R}^n$. Suppose further that $\mathcal{U}$ and $\mathcal{V}$ are *cada* instances that possess the properties shown in Table II, and that $\mathcal{W} = \mathcal{U} \cup \mathcal{V}$ is the union of $\mathcal{U}$ and $\mathcal{V}$. Then the size property of $\mathcal{W}$ will be $m_w = \max(m_u, m_v)$. The nonzero function locations of $\mathcal{W}$ are then determined as follows. Let $\bar{\mathbf{u}}$ and $\bar{\mathbf{v}}$ be vectors of length m_w, where

$$\begin{aligned} \bar{\mathbf{u}}_i &= \begin{cases} 1, & i \in \mathbf{i}^{\mathbf{u}}, \\ 0, & \text{otherwise}, \end{cases} \\ \bar{\mathbf{v}}_i &= \begin{cases} 1, & i \in \mathbf{i}^{\mathbf{v}}, \\ 0, & \text{otherwise}, \end{cases} \end{aligned} \qquad i = 1, \ldots, m_w. \tag{6}$$

The possible nonzero function locations of $\mathcal{W}$, $\mathbf{i}^{\mathbf{w}}$, are then defined by the nonzero locations of $\bar{\mathbf{w}} = \bar{\mathbf{u}} + \bar{\mathbf{v}}$.

Next, the locations of all possible nonzero *derivatives* of $\mathcal{W}$ can be determined in a manner similar to the approach used to determine the nonzero function locations of $\mathcal{W}$. Specifically, let $\bar{\mathbf{U}}^{\mathbf{x}}$, $\bar{\mathbf{V}}^{\mathbf{x}}$ be $m_w \times m_x$ matrices whose elements are given as

$$\begin{aligned} \bar{U}^{\mathbf{x}}_{i,j} &= \begin{cases} 1, & (i,j) \in [\mathbf{i}^{\mathbf{u}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{u}}_{\mathbf{x}}], \\ 0, & \text{otherwise}, \end{cases} \\ \bar{V}^{\mathbf{x}}_{i,j} &= \begin{cases} 1, & (i,j) \in [\mathbf{i}^{\mathbf{v}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{v}}_{\mathbf{x}}], \\ 0, & \text{otherwise}, \end{cases} \end{aligned} \qquad \begin{aligned} i &= 1, \ldots, m_w, \\ j &= 1, \ldots, m_x. \end{aligned} \tag{7}$$

Finally, suppose that we let $\bar{\mathbf{W}}^{\mathbf{x}} = \bar{\mathbf{U}}^{\mathbf{x}} + \bar{\mathbf{V}}^{\mathbf{x}}$. Then the possible nonzero derivative locations of $\mathcal{W}$, $[\mathbf{i}^{\mathbf{x}}_{\mathbf{w}}, \mathbf{j}^{\mathbf{x}}_{\mathbf{w}}]$, are defined to be the row and column indices corresponding to the nonzero locations of the matrix $\bar{\mathbf{W}}^{\mathbf{x}}$.

5. SOURCE TRANSFORMATION VIA THE OVERLOADED *CADA* CLASS

A new method is now described for generating derivative files of mathematical functions implemented in MATLAB, where the function source code may contain flow control statements. Source transformation on such function programs is performed using the overloaded *cada* class together with unions and overmaps as described in Section 4. In other words, all function/derivative computations are printed to the derivative file as described in Section 3 while flow control is preserved by performing overloaded unions where code fragments join, for example, on the output of conditional fragments, on the input of loops, and so forth. The method thus has the feature that the resulting derivative code depends solely on the functions from the native MATLAB library (i.e., derivative source code generated by the method does *not* depend upon overloaded statements or separate runtime functions). Furthermore, the structure of the flow control statements is transcribed to the derivative source code. In this section, we describe in detail the various processes that are used to carry out the source transformation. An outline of the source transformation method is shown in Figure 1.

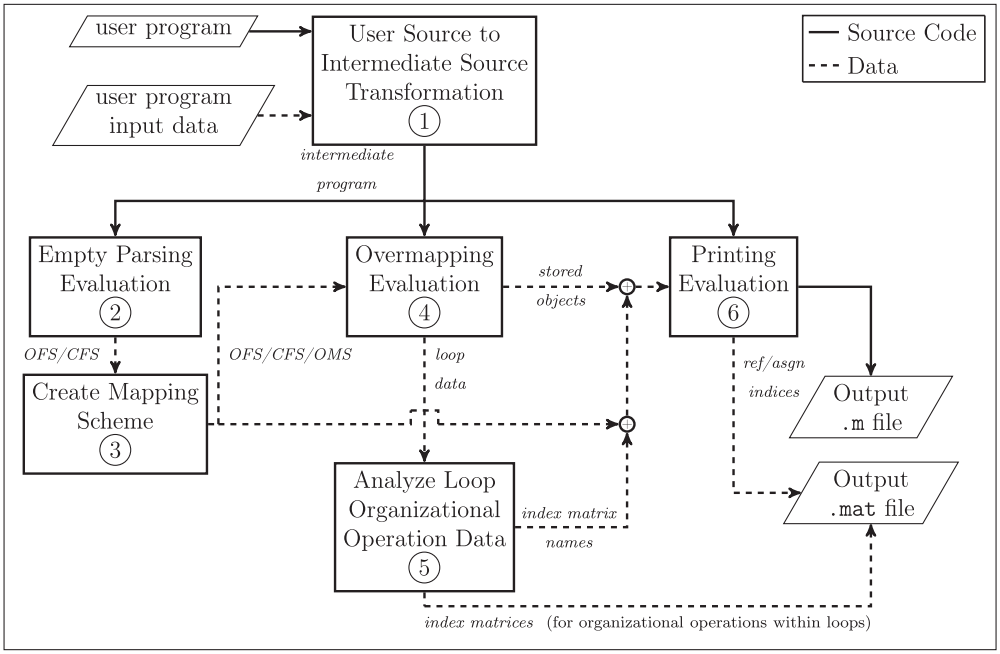
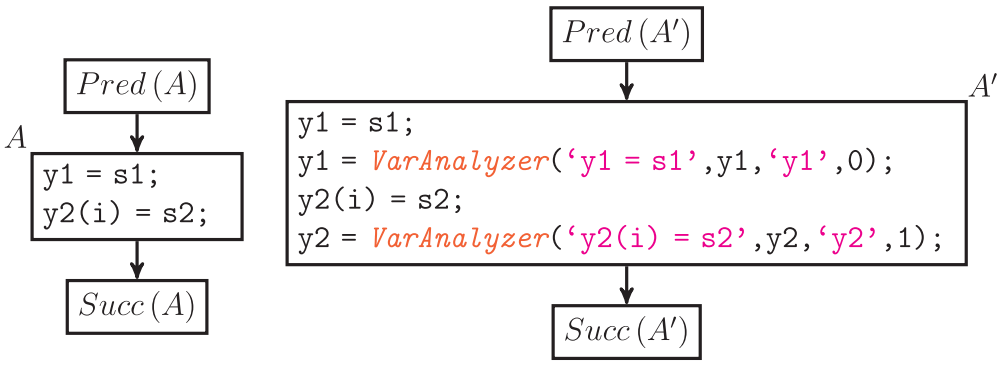


Fig. 1. Source transformation via operator overloading process.

From Figure 1, it is seen that the inputs to the transformation process are the user program to be differentiated together with the information required to create *cada* instances of the inputs to the user program. Using Figure 1 as a guide, the source transformation process starts by performing a transformation of the original source code to an intermediate source code (process ①). This initial transformation then results in a source code on which an overloaded analysis may be performed. Automatic differentiation is then effected by performing *three* overloaded evaluations of the intermediate source code. During the first evaluation (process ②), a record of all objects and locations relative to flow control statements is built to form an object flow structure (OFS) and a control flow structure (CFS), but no derivative calculations are performed. Next, an object mapping scheme (OMS) is created (process ③) using the DFS and CFS obtained from the first evaluation, where the OMS defines where overloaded unions must be performed and where overloaded objects must be saved. During the second evaluation (process ④), the intermediate source code is evaluated on *cada* instances, where each overloaded *cada* operation does not print any calculations to a file. During this second evaluation, overmaps are built and stored in global memory (shown as *stored objects* output of process ④) while data is collected regarding any organizational operations contained within loops (shown as *loop data* output of process ④). The organizational operation data is then analyzed to produce special derivative mapping rules for each operation (process ⑤). During the third evaluation of the intermediate source program (process ⑥), all of the data produced from processes ② through ⑤ is used to print the final derivative program to a file. In addition, a MATLAB binary file is written that contains the reference and assignment indices required for use in the derivative source code. The details of the steps required to transform a function program containing no function/subfunction calls into a derivative program are given in Sections 5.1 through 5.6 and correspond to processes ① through ⑥,



(a) Original basic block (b) Transformed basic block

Fig. 2. Transformation of user source basic block A to intermediate source basic block A'. The quantities `s1` and `s2` represent generic MATLAB expressions.

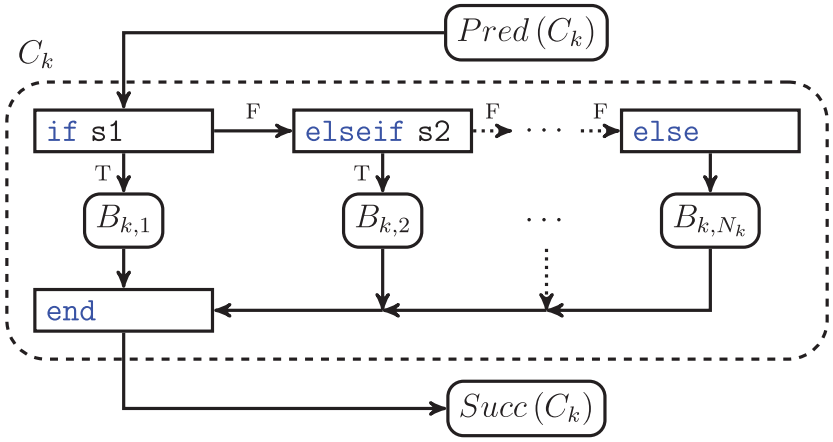
respectively, shown in Figure 1. Section 5.7 then shows how the methods developed in Sections 5.1 through 5.6 are applied to programs containing multiple function calls.

5.1. User Source to Intermediate Source Transformation

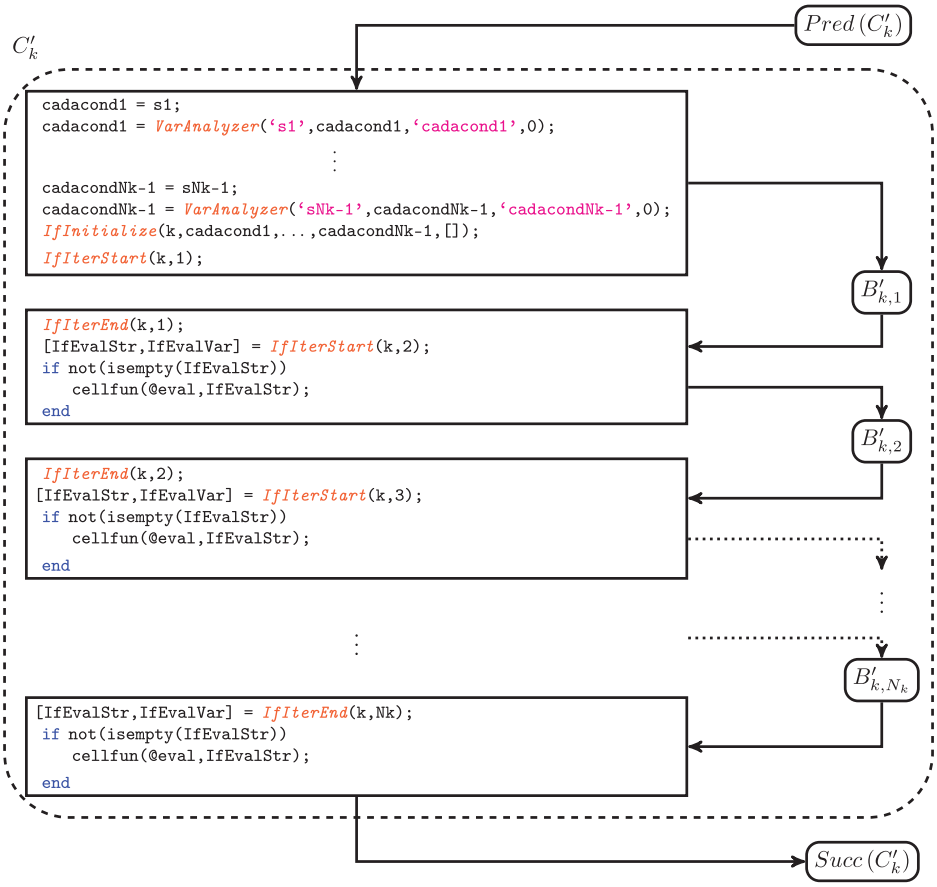
The first step in generating derivative source code is to perform source-to-source transformation on the original program to create an intermediate source code, where the intermediate source code is an augmented version of the original source code that contains calls to transformation routines. The resulting intermediate source code may then be evaluated on overloaded objects to effectively analyze and apply AD to the program defined by the original user code. This initial transformation is performed via a purely lexical analysis within MATLAB, where first the user code is parsed line by line to determine the location of any flow control keywords (i.e., `if`, `elseif`, `else`, `for`, `end`). The code is then read again, line by line, and the intermediate program is printed by copying sections of the user code and applying different augmentations at the statement and flow control levels.

Figure 2 shows the transformation of a basic block in the original program, A, into the basic block of the intermediate program, A'. At the basic block level, it is seen that each user assignment is copied exactly from the user program to the intermediate program, but it is followed by a call to the transformation routine `VarAnalyzer`. It is also seen that after any object is written to a variable, the variable analyzer is provided the assignment object, the string of code whose evaluation resulted in the assignment object, the name of the variable to which the object was written, and a flag stating whether or not the assignment was an array subscript assignment. After each assignment object is sent to the `VarAnalyzer`, the corresponding variable is immediately rewritten on the output of the `VarAnalyzer` routine. By sending all assigned variables to the variable analyzer, it is possible to distinguish between assignment objects and intermediate objects and determine the names of the variables to which each assignment object is written. Additionally, by rewriting the variables on the output of the variable analyzer, full control over the overloaded workspace (i.e., the collection of all variables active in the intermediate program) is given to the source transformation algorithm. Consequently, all variables (and any operations performed on them) are forced to be overloaded.

Figure 3 shows the transformation of the k^{th} conditional fragment encountered in the original program to a transformed conditional fragment in the intermediate program. In the original conditional fragment, C_k, each branch contains the code fragment



(a) Original conditional fragment



(b) Transformed conditional fragment

Fig. 3. Transformation of user source conditional fragment C_k to intermediate source conditional fragment C'_k. Here, C_k is the k^{th} conditional fragment encountered in the user program; $B_{k,i}$ $(i = 1, \ldots, N_k)$ are the fragments of code contained within each branch of the conditional fragment C_k; and the quantities `s1`, `s2`, and `sNk-1` represent MATLAB logical expressions.

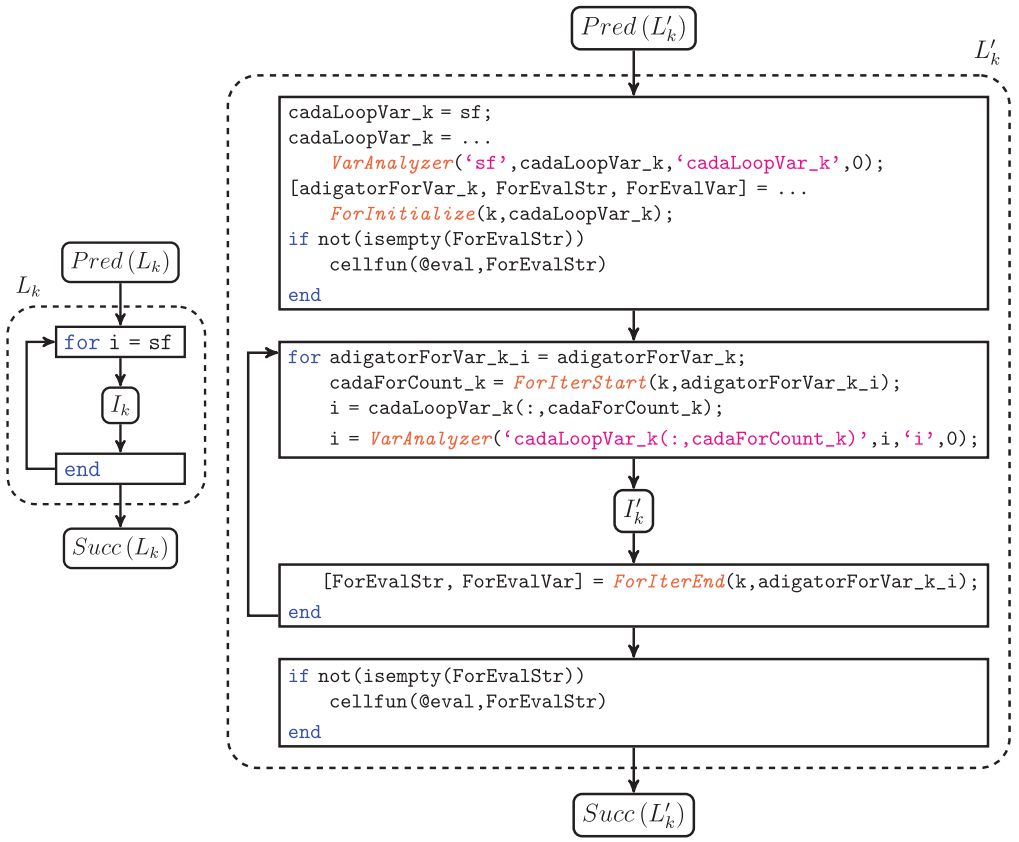
$B_{k,i}$ $(i = 1, \ldots, N_k)$, where the determination of which branch is evaluated depends upon the logical values of the statements `s1,s2,...,sNk-1`. In the transformed conditional fragment, it is seen that no flow control surrounds any of the branches. Instead, all conditional variables are evaluated and sent to the *IfInitialize* transformation routine. The transformed branch fragments $B'_{k,1}, \ldots, B'_{k,N_k}$ are then evaluated in a linear manner, with a call to the transformation routines *IfIterStart* and *IfIterEnd* before and after the evaluation of each branch fragment. By replacing all conditional statements with transformation routines, the control of the flow is given to the transformation routines. When the intermediate program is evaluated, the *IfInitialize* routine can determine whether each conditional variable returns true, false, or indeterminate, and then the *IfIterStart* routine can set different global flags prior to the evaluation of each branch to emulate the conditional statements. As the overloaded analysis of each branch $B'_{k,i}$ is performed in a linear manner, it is important to ensure that each branch is analyzed independent of the others. Thus, prior to any `elseif/else` branch, the overloaded workspace may be modified using the outputs, `IfEvalStr` and `IfEvalVar`, of the *IfIterStart* transformation routine. Furthermore, following the overloaded evaluation and analysis of the conditional fragment C'_k, it is often the case that overmapped outputs must be brought into the overloaded workspace. Thus, the final *IfIterEnd* routine has the ability to modify the workspace via its outputs, `IfEvalStr` and `IfEvalVar`.

Figure 4 shows an original loop fragment, L_k, and the corresponding transformed loop fragment L'_k, where k is the k^{th} loop encountered in the original program. Similar to the approach used for conditional statements, Figure 4 shows that control over the flow of the loop is given to the transformation routines. Transferring control to the transformation routines is achieved by first evaluating the loop index expression and feeding the result to the *ForInitialize* routine. The loop is then run on the output, `adigatorForVar_k`, of the *ForInitialize* routine, with the loop variable being calculated as a reference on each iteration. Thus, the *ForInitialize* routine has the ability to unroll the loop for the purposes of analysis, or to evaluate the loop for only a single iteration. Furthermore, the source transformation algorithm is given the ability to modify the inputs and outputs of the loop. This modification is achieved via the outputs, `ForEvalStr` and `ForEvalVar`, of the transformation routines *ForInitialize* and *ForIterEnd*.

It is important to note that the code fragments $B_{k,i}$ of Figure 3 and I_k of Figure 4 do not necessarily represent basic blocks but may themselves contain conditional fragments and/or loop fragments. To account for nested flow control, the user source to intermediate source transformation is performed in a recursive process. Consequently, if the fragments $B_{k,i}$ and/or I_k contain loop/conditional fragments, then the transformed fragments $B'_{k,i}$ and/or I'_k are made to contain transformed loop/conditional fragments.

5.2. Parsing of the Intermediate Program

After generating the intermediate program, the next step is to build a record of all objects encountered in the intermediate program and locations of any flow control statements. Building this record results in an OFS and a CFS. In this article, the OFS and CFS are analogous to the data flow graphs and control flow graphs of conventional compilers. Unlike conventional data flow graphs and control flow graphs, however, the OFS and the CFS are based on the locations and dependencies of all overloaded objects encountered in the intermediate program, where each overloaded object is assigned a unique integer value. The labeling of overloaded objects is achieved by using the global integer variable `OBJECTCOUNT`, where `OBJECTCOUNT` is set to unity prior to the evaluation of the intermediate program. Then, as the intermediate program is evaluated on overloaded objects, each time an object is created the `id` field of the



(a) Original loop fragment (b) Transformed loop fragment

Fig. 4. Transformation of user source loop fragment L_k to intermediate source loop fragment L'_k. The quantity L_k refers to the k^{th} loop fragment encountered in the user program, I_k is the fragment of code contained within the loop, and the quantity `sf` denotes an arbitrary loop index expression.

created object is assigned the value of `OBJECTCOUNT`, and `OBJECTCOUNT` is incremented. As control flow has been removed from the intermediate program, there exists only a single path that it may take, and thus if an object takes on the `id` field equal to i on one evaluation of the intermediate program, then that object will take on the `id` field equal to i on *any* evaluation of the intermediate program. Furthermore, if a loop is to be evaluated for multiple iterations, then the value of `OBJECTCOUNT` prior to the first iteration is saved, and `OBJECTCOUNT` is set to the saved value prior to the evaluation of *any* iteration of the loop. By resetting `OBJECTCOUNT` at the start of each loop iteration, we ensure that the `id` assigned to all objects within a loop are iteration independent.

Because it is required to know the OFS and CFS *prior* to performing any derivative operations, the OFS and CFS are built by evaluating the intermediate program on a set of empty overloaded objects. During this evaluation, no function or derivative properties are built. Instead, only the `id` field of each object is assigned, and the OFS and CFS are built. Using the unique `id` assigned to each object, the OFS is built as follows:

- Whenever an operation is performed on an object $\mathcal{O}$ to create a new object, $\mathcal{P}$, we record that the $\mathcal{O}.\texttt{id}^{th}$ object was last used to create the $\mathcal{P}.\texttt{id}^{th}$ object. Thus, after the

entire program has been evaluated, the location (relative to all other created objects) of the last operation performed on $\mathcal{O}$ is known.
- If an object $\mathcal{O}$ is written to a variable, `v`, it is recorded that the $\mathcal{O}$.`id`th object was written to a variable with the name '`v.`' Furthermore, it is noted if the object $\mathcal{O}$ was the result of an array subscript assignment or not.

Similarly, the CFS is built based on the `OBJECTCOUNT` in the following manner:

- Before and immediately after the evaluation of each branch of each conditional fragment, the value of `OBJECTCOUNT` is recorded. Using these two values, it can be determined which objects are created within each branch (and subsequently which variables are written, given the OFS).
- Before and immediately after the evaluation of a single iteration of each `for` loop, the value of `OBJECTCOUNT` is recorded. Using the two recorded values, it can then be determined which objects are created within the loop.

The OFS and CFS then contain *most* of the information contained in conventional data flow graphs and control flow graphs but are more suitable to the recursive manner in which flow control is handled in this work.

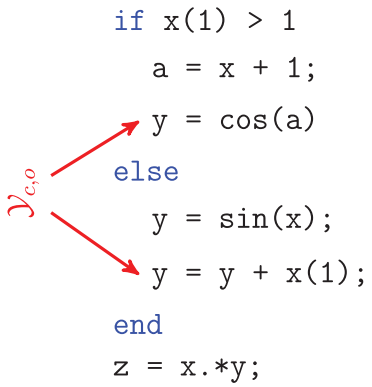
5.3. Creating an Object Overmapping Scheme

Using the OFS and CFS obtained from the empty evaluation, it is then required that an OMS be built, where the OMS will be used in both the overmapping and printing evaluations. The OMS is used to tell the various transformation routines when an overloaded union must be performed to build an overmap, where the overmapped object is being stored, and when the overmapped object must be written to a variable in the overloaded workspace. The determination of where unions must be performed is based on where in the original user code the program joins. In other words, unions must be performed at the exit of conditional fragments and at the entrance of loops. Similarly, the OMS must also tell the transformation routines when an object must be saved, to where it will be saved, and when the saved object must be written to a variable in the overloaded workspace. We now look at how the OMS must be built to deal with both conditional branches and loop statements.

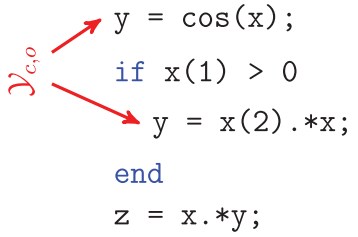
5.3.1. Conditional Statement Mapping Scheme. It is required to print conditional fragments to the derivative program such that different branches may be taken depending upon numerical input values. The difficulty that arises using the *cada* class is that given a conditional fragment, different branches can write different assignment objects to the same output variable, and each of these assignment objects can contain differing function and/or derivative properties. To ensure that any operations performed on these variables *after* the conditional block are valid for any of the conditional branches, a conditional overmap must be assigned to all variables defined within a conditional fragment and used later in the program (i.e., the outputs of the conditional fragment). Given a conditional fragment C'_k containing N_k branches, where each branch contains the fragment $B'_{k,i}$ (as shown in Figure 3), the following rules are defined:

Mapping Rule 1. If a variable `y` is written within C'_k and read within $Succ(C'_k)$, then a single conditional overmap, $\mathcal{Y}_{c,o}$, must be created and assigned to the variable `y` prior to the execution of $Succ(C'_k)$.

Mapping Rule 1.1. For each branch fragment $B'_{k,i}$ $(i = 1, \ldots, N_k)$ within which `y` is written, the last object assigned to `y` within $B'_{k,i}$ must belong to $\mathcal{Y}_{c,o}$. Figure 5(a) provides an illustrative example.



(a) Example of Mapping Rule 1.1



(b) Example of Mapping Rule 1.2

Fig. 5. Illustrative examples of Mapping Rule 1. (a) The marked variables belong to the conditional overmap $\mathcal{Y}_{c,o}$ as a result of Mapping Rule 1.1. Since the unmarked variables are not outputs of the conditional fragment, they do not belong to a conditional overmap. (b) The marked variables belong to the conditional overmap $\mathcal{Y}_{c,o}$ as a result of Mapping Rule 1.2.

Mapping Rule 1.2. If there exists a branch fragment $B'_{k,i}$ within which y is *not* written, *or* there exists no `else` branch, then the last object that is written to y within $Pred(C'_k)$ must belong to $\mathcal{Y}_{c,o}$. Figure 5(b) provides an illustrative example.

Using Mapping Rule 1, for each conditional fragment, it is determined which variables require a conditional overmap and which assignment objects belong to which conditional overmaps. By adhering to Mapping Rule 1, it is the case that each conditional fragment is analyzed independently of the others. For instance, if a program contains two successive conditional fragments C_1 and C_2, $C_2 \not\subset C_1$, containing N_1 and N_2 branches, respectively, then the program contains N_1N_2 possible branches (assuming both C_1 and C_2 contain `else` branches). Rather than analyzing all N_1N_2 possible branches, the proposed mapping rule states to first analyze the N_1 branches of C_1 and to then use the overmapped outputs to analyze the N_2 branches of C_2. Similarly, if a program contains a nested conditional fragment $C_2 \subset C_1$, then the inner fragment C_2 is first analyzed and the overmapped outputs are used for the analysis of the outer fragment C_1.

The second issue with evaluating transformed conditional fragments of the form shown in Figure 3(b) stems from the fact that flow control is removed in the intermediate program. Thus, each branch is analyzed via overloaded evaluation in a successive order. To properly emulate the flow control and force each transformed conditional branch to be analyzed independently, the following mapping rule is defined for each transformed conditional fragment C'_k:

Mapping Rule 2. If a variable y is written within $Pred(C'_k)$, rewritten within a branch fragment $B'_{k,i}$ and read within a branch fragment $B'_{k,j}$ $(i < j)$, then the last object written to y within $Pred(C'_k)$ must be saved. Furthermore, the saved object must be assigned to the variable y prior to the evaluation of the fragment $B'_{k,j}$. Figure 6 provides an illustrative example.

To adhere to Mapping Rule 2, we use the OFS and CFS to determine the `id` of all objects that must be saved, to where they will be saved, and the `id` of the assignment objects that must be replaced with the saved objects.

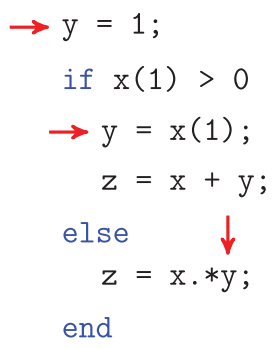


Fig. 6. Illustrative example of Mapping Rule 2. The variable y is an input to the else branch but is rewritten in the if branch. Since both branches are analyzed successively, the input version of y (y = 1) must be saved prior to the overloaded evaluation of the if branch and brought back into the overloaded workspace prior to the overloaded evaluation of the else branch.

5.3.2. Loop Mapping Scheme. To print derivative calculations within loops in the derivative program, a single loop iteration must be evaluated on a set of overloaded inputs to the loop, where the input function sizes and/or derivative sparsity patterns may change with each loop iteration. To print calculations that are valid for all possible loop inputs, a set of loop overmapped inputs are found by analyzing all possible loop iterations (i.e., unrolling for the purpose of analysis) in the overmapping evaluation phase. The loop may then be printed as a rolled loop to the derivative program by evaluating on the set of overmapped loop inputs. The first mapping rule is now given for a transformed loop L'_k of the form shown in Figure 4:

Mapping Rule 3. If a variable is written within I'_k, then it must belong to a *loop overmap*. Moreover, during the printing evaluation of I'_k, the overloaded workspace must only contain loop overmaps.

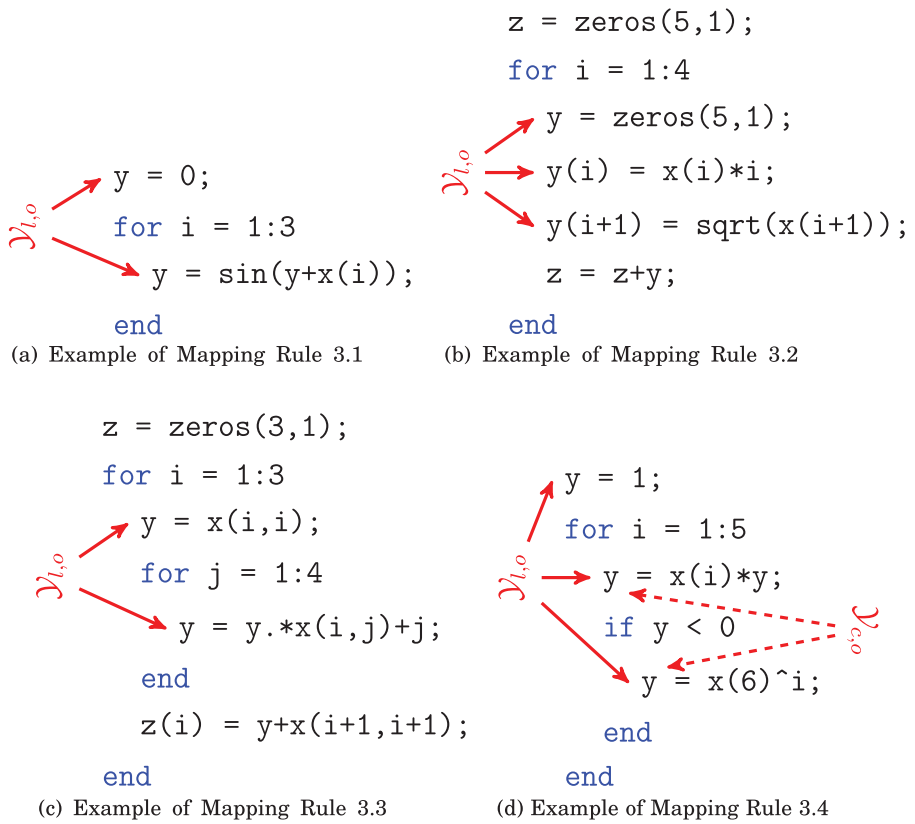
Mapping Rule 3.1. If a variable y is written within $Pred(L'_k)$, read within I'_k, and then rewritten within I'_k (i.e., y is an iteration-dependent input to I'_k), then the last objects written to y within $Pred(L'_k)$ and I'_k must share the same loop overmap. Furthermore, during the printing evaluation, the loop overmap must be written to the variable y prior to the evaluation of I'_k. Figure 7(a) provides an illustrative example.

Mapping Rule 3.2. Any assignment object that results from an array subscript assignment belongs to the same loop overmap as the last object that was written to the same variable. Figure 7(b) provides an illustrative example.

Mapping Rule 3.3. If an assignment object is created within multiple nested loops, then it still only belongs to one loop overmap. Figure 7(c) provides an illustrative example.

Mapping Rule 3.4. Any object belonging to a conditional overmap within a loop must share the same loop overmap as all objects that belong to the conditional overmap. Figure 7(d) provides an illustrative example.

Using this set of rules together with the developed OFS and CFS, it is determined, for each loop L'_k, which assignment objects belong to which loop overmaps. Unlike the handling of conditional fragments, outer loops are made to dominate the overloaded analysis as a result of Mapping Rule 3. Although this rule may result in the collection of unnecessary data, it simplifies the analysis of any flow control nested within the loop. For instance, in the case of a conditional fragment nested within a loop (such as that shown in Figure 7(d)), the loop overmap is always made to contain the



(a) Example of Mapping Rule 3.1 (b) Example of Mapping Rule 3.2

(c) Example of Mapping Rule 3.3 (d) Example of Mapping Rule 3.4

Fig. 7. Illustrative examples of Mapping Rule 3. (a) The variable `y` is an iteration-dependent input to the loop, and thus the objects assigned to the marked variables must be joined to create the corresponding overmapped input. During the overmapping evaluation phase, this is achieved by joining the four different objects assigned to `y`: the original input together with the result of `sin(y + x(i))` for the three values of `i`. (b) Since the variable `y` is initialized to zero and then assigned to via subscript index assignment twice, the objects that result from all three assignments are made to belong to the loop overmap $\mathcal{Y}_{l,o}$. Thus, the loop overmap $\mathcal{Y}_{l,o}$ is built by joining 12 overloaded objects, 3 for each loop iteration. (c) In this example, the variable `y` is written within a nested loop and is also an iteration-dependent input to the nested loop. As a result of Mapping Rules 3.1 and 3.3, the corresponding loop overmap is made to contain the 15 different objects written to `y`: 3 from the outer loop assignment and 12 from the nested loop assignment. (d) As a result of Mapping Rule 1.2, the conditional overmap $\mathcal{Y}_{c,o}$ is made to contain the objects assigned to `y` at both places within the loop, where a new conditional overmap is built on each iteration of the loop in the overmapping evaluation. As a result of Mapping Rule 3.4, the loop overmap $\mathcal{Y}_{l,o}$ is made to contain the object assigned to `y` prior to the loop, as well as the objects assigned to `y` across all overloaded evaluations of the loop.

iteration-dependent conditional overmap. In the overmapping evaluation of such a code fragment, the iteration-dependent conditional overmaps would be built on each iteration to properly propagate sparsity patterns. In the printing evaluation, however, conditional overmaps are unnecessary, as it is ensured that all possible conditional overmaps belong to the loop overmap. Additionally, this provides a measure of safety for the printing evaluation by ensuring that all assignment objects created within loops are in the overmapped form.

The second mapping rule associated with loops results from the fact that the overmapped outputs of a loop are not necessarily the same as the *true* outputs of a loop. Loop overmaps are eliminated from the overloaded workspace by replacing them

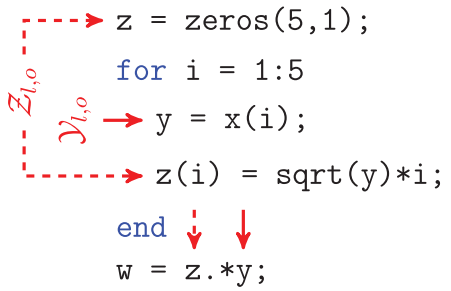


Fig. 8. Illustrative example of Mapping Rule 4. In this example, both variables y and z are outputs of the loop. Thus, the objects assigned to the variables y and z on the fifth and final iteration of the loop must be stored in the overmapping evaluation phase and returned as outputs in both the overmapping evaluation and printing evaluation of the loop. Here it can be seen that the derivative sparsity pattern of the *true* overloaded output corresponding to y will contain fewer nonzeros than the loop overmap $\mathcal{Y}_{l,o}$, whereas the true overloaded output corresponding to z is equal to the loop overmap $\mathcal{Z}_{l,o}$.

with assignment objects that result from the overloaded evaluation of all iterations of the loop. This final mapping rule is stated as follows:

Mapping Rule 4. For any outer loop L'_k (i.e., there does not exist L'_j such that $L'_k \subset L'_j$), if a variable y is written within I'_k, and read within $Succ(L'_k)$, then the last object written to y within the loop during the overmapping evaluation must be saved. Furthermore, the saved object must be written to y prior to the evaluation of $Succ(L'_k)$ in both the overmapping and printing evaluations. Figure 8 provides an illustrative example.

The `id` field of any assignment objects subject to Mapping Rule 4 are marked so that the assignment objects may be saved at the time of their creation and accessed at a later time.

It is noted that the presented mapping rules do not address cases of loops containing `break` or `continue` statements. We now briefly introduce how the proposed method handles such cases. For the sake of conciseness, however, they will neither be discussed in detail nor addressed in the remaining sections. In the presence of `break`/`continue` statements, the *true* outputs of the loop (as addressed in Mapping Rule 4) are considered to be the union between all possible outputs of the loop (i.e., the outputs that result from any `break` statement firing across all iterations, the outputs that result from any `continue` statement firing on the final iteration, and the outputs that result from no `break` statements firing on any iteration and no `continue` statements firing on the final iteration). In the presence of `continue` statements, the overmapped loop inputs (as addressed in Mapping Rule 3.1) must be made to contain all possible inputs to the loop (i.e., any initial inputs together with any iteration-dependent inputs that result from a `continue` statement firing, or no `continue` statements firing).

5.4. Overmapping Evaluation

The purpose of the overmapping evaluation is to build the aforementioned conditional overmaps and loop overmaps, as well as to collect data regarding organizational operations within loop statements. This overmapping evaluation is performed by evaluating the intermediate program on overloaded *cada* objects, where no calculations are printed to file but rather only data is collected. Recall now from Mapping Rules 1 and 3 that any object belonging to a conditional and/or loop overmap must be an assignment object. Additionally, all assignment objects are sent to the `VarAnalyzer` routine immediately after they are created. Thus, building the conditional and loop overmaps may be achieved by

performing overloaded unions within the variable analyzer routine immediately after the assignment objects are created. The remaining transformation routines must then control the flow of the program and manipulate the overloaded workspace such that the proper overmaps are built. We now describe the tasks performed by the transformation routines during the overmapping evaluation of conditional and loop fragments.

5.4.1. Overmapping Evaluation of Conditional Fragments. During the overmapping evaluation of a conditional fragment, it is required to emulate the corresponding conditional statements of the original program. First, those branches on which overmapping evaluations are performed must be determined. This determination is made by analyzing the conditional variables given to the `IfInitialize` routine (`cadacond1,...,cadacondn-1` of Figure 3), where each of these variables may take on a value of true, false, or indeterminate. Any value of *indeterminate* implies that the variable may take on the value of either *true* or *false* within the derivative program. Using this information, it can be determined if overmapping evaluations are *not* to be performed within any of the branches. For any such branches within which overmapping evaluations are not to be performed, empty evaluations are performed in a manner similar to those performed in the parsing evaluation. Next, it is required that all branches of the conditional fragment be evaluated independently (i.e., we must adhere to Mapping Rule 2). Thus, for a conditional fragment C'_k, if a variable is written within $Pred(C'_k)$, rewritten within $B'_{k,i}$, and then read within $B'_{k,j}$ $(i < j)$, then the variable analyzer will use the developed OMS to save the last assignment object written to the variable within $Pred(C'_k)$. The saved object may then be written to the overloaded workspace prior to the evaluation of any dependent branches using the outputs of the `IfIterStart` routines corresponding to the dependent branches. Finally, to ensure that any overmaps built after the conditional fragment are valid for all branches of the conditional fragment, all conditional overmaps associated with the conditional fragment must be assigned to the overloaded workspace. For some conditional overmap, these assignments are achieved ideally within the `VarAnalyzer` at the time the last assignment object belonging to the conditional overmap is assigned. If, however, such assignments are not possible (due to the variable being read prior to the end of the conditional fragment), then the conditional overmap may be assigned to the overloaded workspace via the outputs of the last `IfIterEnd` routine.

5.4.2. Overmapping Evaluation of Loops. As seen from Figure 4, all loops in the intermediate program are preceded by a call to the `ForInitialize` routine. In the overmapping evaluation, this routine determines the size of the second dimension of the object to be looped upon and returns `adigatorForVar_k` such that all loop iterations will be analyzed successively. During these loop iterations, the loop overmaps are built and organizational operation data is collected. Here we stress that at no time during the overmapping evaluation are any loop overmaps active in the overloaded workspace. Thus, after the loop has been evaluated for all iterations, the objects resulting from the evaluation of the last iteration of the loop will be active in the overloaded workspace. Furthermore, on this last iteration, the `VarAnalyzer` routine saves any objects subject to Mapping Rule 4 for use in the printing evaluation.

5.5. Organizational Operations within `For` Loops

Consider that all organizational operations may be written as one or more references or assignments: horizontal or vertical concatenation can be written as multiple subscript index assignments, reshapes can be written as either a reference or a subscript index assignment, and so forth. Consider now that the derivative operation corresponding to a function reference/assignment is given by performing the same reference/assignment

on the first dimension of the Jacobian. In the method of this article, however, derivative variables are written as vectors of nonzeros rather than full Jacobians. Thus, the derivative procedures corresponding to function references/assignments cannot be written in terms of *function* reference/assignment indices. Instead, separate *derivative* reference/assignment indices are determined to write the derivative procedure. Moreover, when dealing with loops, it is often the case that function reference/assignment indices change on loop iterations, and thus the corresponding derivative reference/assignment indices must be made to be iteration dependent. In this section, we describe how organizational operations are handled within loops.

Example of an Organizational Operation within a Loop. Consider the following example that illustrates the method used to deal with organizational operations within loops. Suppose that within a loop there exists an organizational operation

$$\mathbf{w}_i = \mathbf{f}\big(\mathbf{v}_i, \mathbf{j}_i^{\mathbf{v}}, \mathbf{j}_i^{\mathbf{w}}\big), \tag{8}$$

where on iteration $i \in [1, \ldots, N]$, the elements $\mathbf{j}_i^{\mathbf{v}}$ of $\mathbf{v}_i$ are assigned to the elements $\mathbf{j}_i^{\mathbf{w}}$ of $\mathbf{w}_i$. Let the overmapped versions of $\mathcal{V}_i$ and $\mathcal{W}_i$, across all calls to the overloaded organizational operation, $\mathcal{F}$, be denoted by $\bar{\mathcal{V}}$ and $\bar{\mathcal{W}}$ with associated overmapped Jacobians, $\mathbf{J}\bar{\mathbf{v}}(\mathbf{x})$ and $\mathbf{J}\bar{\mathbf{w}}(\mathbf{x})$, respectively. Further, let the nonzeros of the overmapped Jacobians be defined by the vectors $\mathbf{d}_{\mathbf{x}}^{\bar{\mathbf{v}}} \in \mathbb{R}^{nz_{\bar{\mathbf{v}}}}$ and $\mathbf{d}_{\mathbf{x}}^{\bar{\mathbf{w}}} \in \mathbb{R}^{nz_{\bar{\mathbf{w}}}}$.

Now, given the overmapped sparsity patterns of $\bar{\mathcal{V}}$ and $\bar{\mathcal{W}}$, together with the reference and assignment indices, $\mathbf{j}_i^{\mathbf{v}}$ and $\mathbf{j}_i^{\mathbf{w}}$, the derivative reference and assignment indices $\mathbf{k}_i^{\bar{\mathbf{v}}}$, $\mathbf{k}_i^{\bar{\mathbf{w}}} \in \mathbb{Z}^{m_i}$ are found such that on iteration i, the elements $\mathbf{k}_i^{\bar{\mathbf{v}}}$ of $\mathbf{d}_{\mathbf{x}}^{\bar{\mathbf{v}}}$ are assigned to the elements $\mathbf{k}_i^{\bar{\mathbf{w}}}$ of $\mathbf{d}_{\mathbf{x}}^{\bar{\mathbf{w}}}$. In other words, on iteration i, the valid derivative rule for the operation $\mathcal{F}$ is given as

$$d^{\bar{\mathbf{w}}}_{\mathbf{x}[k_i^{\bar{\mathbf{w}}}(l)]} = d^{\bar{\mathbf{v}}}_{\mathbf{x}[k_i^{\bar{\mathbf{v}}}(l)]} \quad l = 1, \ldots, m_i. \tag{9}$$

To write these calculations to file as concisely and efficiently as possible, a sparse *index matrix* $\mathbf{K} \in \mathbb{Z}^{nz_{\bar{\mathbf{w}}} \times N}$ is defined such that in the i^{th} column of $\mathbf{K}$, the elements of $\mathbf{k}_i^{\bar{\mathbf{v}}}$ lie in the row locations defined by the elements of $\mathbf{k}_i^{\bar{\mathbf{w}}}$. The following derivative rule may then be written to a file:

```
w.dx(logical(K(:,i))) = v.dx(nonzeros(K(:,i)));,
```
(10)

where `K` corresponds to the *index matrix* $\mathbf{K}$, `i` is the loop iteration, and `w.dx` and `v.dx` are the derivative variables associated with $\bar{\mathcal{W}}$ and $\bar{\mathcal{V}}$, respectively.

5.5.1. Collecting and Analyzing Organizational Operation Data. As seen in the preceding example, derivative rules for organizational operations within loops rely on index matrices to print valid derivative variable references and assignments. Here it is emphasized that given the proper index matrix, valid derivative calculations are printed to file in the manner shown in Equation (10) for *any* organizational operation contained within a loop. The aforementioned example also demonstrates that the index matrices may be built given the overmapped inputs and outputs (e.g., $\bar{\mathcal{W}}$ and $\bar{\mathcal{V}}$), together with the iteration-dependent function reference and assignment indices (e.g., $\mathbf{j}_i^{\mathbf{v}}$ and $\mathbf{j}_i^{\mathbf{w}}$). Although there exists no single operation in MATLAB that is of the form of Equation (8), it is noted that the function reference and assignment indices may be easily determined for *any* organizational operation by collecting certain data at each call to the operation within a loop. For instance, for any single call to an organizational operation, any input reference/assignment indices and function sizes of all inputs and outputs are collected for each iteration of a loop within which the operation is contained. Given this information, the function reference and assignment indices are then determined for each

iteration to rewrite the operation to one of the form presented in Equation (8). To collect this data, each overloaded organizational operation must have a special routine written to store the required data when it is called from within a loop during the overmapping evaluations. Additionally, in the case of multiple nested loops, the data from each child loop must be neatly collected on each iteration of the parent loop's `ForIterEnd` routine. Furthermore, because it is required to obtain the overmapped versions of all inputs and outputs and it is sometimes the case that an input and/or output does not belong to a loop overmap, it is also sometimes the case that unions must be performed within the organizational operations themselves to build the required overmaps.

After having collected all of this information in the overmapping evaluation, it is then required that it be analyzed and derivative references and/or assignments be created prior to the printing of the derivative file. This analysis is done by first eliminating any redundant indices/sizes by determining upon which loops the indices/sizes are dependent. Index matrices are then built according to the rules of differentiation of the particular operation. These index matrices are then stored to memory, and the proper string references/assignments are stored to be accessed by the overloaded operations. Additionally, for operations embedded within multiple loops, it is often the case that the index matrix is built to span multiple loops, and additionally that prior to an inner loop, a reference and/or reshape must be printed for the inner loop to have an index matrix of the form given in the presented example. For example, consider an object $\mathcal{W}$ that results from an organizational operation embedded within two loops, where the overmapped object $\bar{\mathcal{W}}$ contains n possible nonzero derivatives. If the outer loop runs for $i_1 = 1, \ldots, m_1$ iterations, the inner loop runs for $i_2 = 1, \ldots, m_2$ iterations, and the function reference/assignment indices are dependent upon both loops, then an index matrix $\mathbf{K}_1 \in \mathbb{Z}^{nm_2 \times m_1}$ will be built. Then, prior to the printing of the inner loop, a statement such as

```
K2 = reshape(K1(:,i1),n,m2);                    (11)
```

must be printed, where `K1` is the outer index matrix, `i1` is the outer loop iteration, and `n` and `m2` are the dimensions of the inner index matrix `K2`. The strings that must be printed to allow for such references/reshapes are then also stored into memory to be accessed prior to the printing of the nested `for` loop statements.

5.6. Printing Evaluation

During the printing evaluation, we finally print the derivative code to a file by evaluating the intermediate program on instances of the *cada* class, where each overloaded operation prints calculations to the file in the manner presented in Section 3. To print `if` statements and `for` loops to the file that contains the derivative program, the transformation routines must both print flow control statements and ensure that the proper overloaded objects exist in the overloaded workspace. Manipulating the overloaded workspace in this manner enables all overloaded operations to print calculations that are valid for the given flow control statements. Unlike in the overmapping evaluations, if the overloaded workspace is changed, then the proper remapping calculations must be printed to the derivative file such that all function variables and derivative variables within the printed file reflect the properties of the objects within the active overloaded workspace. We now introduce the concept of an overloaded remap and explore the various tasks performed by the transformation routines to print derivative programs containing both conditional and loop fragments.

5.6.1. Remapping of Overloaded Objects. During the printing of the derivative program, it is often the case that an overloaded object must be written to a variable in the intermediate program by means of the transformation routines, where the variable

was previously written by the overloaded evaluation of a statement copied from the user program. Because the derivative program is simultaneously being printed as the intermediate program is being evaluated, any time a variable is rewritten by means of a transformation routine, the printed function and derivative variable must be made to reflect the properties of the new object being written to the overloaded workspace. If an object $\mathcal{O}$ is currently assigned to a variable in the intermediate program, and a transformation routine is to assign a different object, $\mathcal{P}$, to the same variable, then the overloaded operation that prints calculations to transform the function variable and derivative variable(s) that reflect the properties of $\mathcal{O}$ to those that reflect the properties of $\mathcal{P}$ is referred to as the remap of $\mathcal{O}$ to $\mathcal{P}$. To describe this process, consider the case where both $\mathcal{O}$ and $\mathcal{P}$ contain derivative information with respect to an input object $\mathcal{X}$. Furthermore, let `o.f` and `o.dx` be the function variable and derivative variable that reflect the properties of $\mathcal{O}$. Here it can be assumed that because $\mathcal{O}$ is active in the overloaded workspace, the proper calculations have been printed to the derivative file to compute `o.f` and `o.dx`. If it is desired to *remap* $\mathcal{O}$ to $\mathcal{P}$ such that the variables `o.f` and `o.dx` are used to create the function variable, `p.f`, and derivative variable, `p.dx`, which reflect the properties of $\mathcal{P}$, the following steps are executed:

- Build the function variable, `p.f`:
  Remapping Case 1.A. If `p.f` is to have a *greater* row and/or column dimension than those of `o.f`, then `p.f` is created by appending zeros to the rows and/or columns of `o.f`.
  Remapping Case 1.B. If `p.f` is to have a *lesser* row and/or column dimension than those of `o.f`, then `p.f` is created by removing rows and/or columns from `o.f`.
  Remapping Case 1.C. If `p.f` is to have the same dimensions as those of `o.f`, then `p.f` is set equal to `o.f`.
- Build the derivative variable, `p.dx`:
  Remapping Case 2.A. If $\mathcal{P}$ has more possible nonzero derivatives than $\mathcal{O}$, then `p.dx` is first set equal to a zero vector and then `o.dx` is assigned to elements of `p.dx`, where the assignment index is determined by the mapping of the derivative locations defined by $\mathcal{O}$`.deriv.nzlocs` into those defined by $\mathcal{P}$`.deriv.nzlocs`.
  Remapping Case 2.B. If $\mathcal{P}$ has fewer possible nonzero derivatives than $\mathcal{O}$, then `p.dx` is created by referencing off elements of `o.dx`, where the reference index is determined by the mapping of the derivative locations defined by $\mathcal{P}$`.deriv.nzlocs` into those defined by $\mathcal{O}$`.deriv.nzlocs`.
  Remapping Case 2.C. If $\mathcal{P}$ has the same number of possible nonzero derivatives as $\mathcal{O}$, then `p.dx` is set equal to `o.dx`.

It is noted that in the 1.A and 2.A cases, the object $\mathcal{O}$ is being remapped to the overmapped object $\mathcal{P}$, where $\mathcal{O}$ belongs to $\mathcal{P}$. In the 1.B and 2.B cases, the overmapped object, $\mathcal{O}$, is being remapped to an object $\mathcal{P}$, where $\mathcal{P}$ belongs to $\mathcal{O}$. Furthermore, the remapping operation is only used to either map an object to an overmapped object to which it belongs, or to map an overmapped object to an object that belongs to the overmap.

5.6.2. Printing Evaluation of Conditional Fragments. Printing a valid conditional fragment to the derivative program requires that the following tasks must be performed. First, it is necessary to print the conditional statements—that is, print the statements `if`, `elseif`, `else`, and `end`. Second, it is required that each conditional branch is evaluated independently (as was the case with the overmapping evaluation). Third, after the conditional fragment has been evaluated in the intermediate program (and printed to the derivative file), all associated conditional overmaps must be assigned to the proper variables in the intermediate program. In addition, all of the proper remapping

calculations must be printed to the derivative file such that when each branch of the derivative conditional fragment is evaluated, it will calculate derivative variables and function variables that reflect the properties of the active conditional overmaps in the intermediate program. These three aforementioned tasks are now explained in further detail.

The printing of the conditional branch headings is fairly straightforward due to the manner in which all expressions following the `if`/`elseif` statements in the user program are written to a conditional variable in the intermediate program (as seen in Figure 3). Thus, each *`IfIterStart`* routine may simply print the branch heading as such: `if cadacond1, elseif cadacond2, else,` and so on. As each branch of the conditional fragment is then evaluated, the overloaded *cada* operations will print derivative and function calculations to the derivative file in the manner described in Section 3. As was the case with the overmapping evaluations, each of the branch fragments must be evaluated independently, where this evaluation is performed in the same manner as described in Section 5.4.1. Likewise, it is ensured that the overloaded workspace will contain all associated conditional overmaps in the same manner as in the overmapping evaluation. Unlike the overmapping evaluation, however, conditional overmaps are not built during the printing evaluations. Instead, the conditional overmaps are stored within memory and may be accessed by the transformation routines to print the proper remapping calculations to the derivative file. For some conditional fragment C'_k within which the variable `y` has been written, the following calculations are required to print the function variable and derivative variable that reflect the properties of the conditional overmap $\mathcal{Y}_{c,o}$:[1]

- If an object $\mathcal{Y}$ belongs to $\mathcal{Y}_{c,o}$ as a result of Mapping Rule 1.1 and *is not* to be operated on from within the branch it is created, then $\mathcal{Y}$ is remapped to $\mathcal{Y}_{c,o}$ from within the *`VarAnalyzer`* routine at the time that $\mathcal{Y}$ is assigned to `y`.
- If an object $\mathcal{Y}$ belongs to $\mathcal{Y}_{c,o}$ as a result of Mapping Rule 1.1 and *is* to be operated on from within the branch it is created, then $\mathcal{Y}$ is stored from within the *`VarAnalyzer`* and the *`IfIterEnd`* routine corresponding to the branch performs the remap of $\mathcal{Y}$ to $\mathcal{Y}_{c,o}$.
- For each branch within which `y` is not written, the *`IfIterEnd`* routine accesses both $\mathcal{Y}_{c,o}$ and the last object written to `y` within $Pred(C'_k)$ (where this will have been saved previously by the *`VarAnalyzer`* routine). The *`IfIterEnd`* routine then remaps the previously saved object to the overmap.
- If the fragment C'_k contains no `else` branch, an `else` branch is imposed and the *last* *`IfIterEnd`* routine again accesses both $\mathcal{Y}_{c,o}$ and the last object written to `y` within $Pred(C'_k)$. This routine then remaps the previously saved object to the overmap within the imposed `else` branch.

Finally, the last *`IfIterEnd`* routine prints the `end` statement.

5.6.3. Printing Evaluation of Loops. To print a valid loop fragment to the derivative program, an overloaded evaluation of a single iteration of the transformed loop is performed in the intermediate program. To ensure that all printed calculations are valid for each iteration of the loop in the derivative program, these overloaded evaluations are performed only on loop overmaps. The printing evaluation of loops is then completed as follows. When an *outermost* loop is encountered in the printing evaluation of the intermediate program, the *`ForInitialize`* routine must first use the OMS

[1]This is assuming that the conditional fragment is not nested within a loop. In the case of a conditional fragment nested within a loop, Mapping Rule 3 takes precedence over Mapping Rule 1 in the printing evaluation.

to determine which, if any, objects belong to loop overmaps but are created prior to the loop (i.e., loop inputs that are loop iteration dependent). Any of these previously created objects will have been saved within the *VarAnalyzer* routine, and the *ForInitialize* routine may then access both the previously saved objects and the loop overmaps to which they belong and then remap the saved objects to their overmapped form. As it is required that the overmapped inputs to the loop be active in the overloaded workspace, the *ForInitialize* then uses its outputs, `ForEvalStr` and `ForEvalVar`, to assign the overmapped objects to the proper variables in the overloaded workspace. Next, the *ForIterStart* routine must print out the outermost `for` statement. Here we note that all outer loops must evaluate for a fixed number of iterations, so if the loop is to be run for 10 iterations, then the `for` statement would be printed as `for cadaforcount = 1:10`. The `cadaforcount` variable will then be used in the derivative program to reference columns off of the index matrices presented in Section 5.5 and to reference the user-defined loop variable. As the loop is then evaluated on loop overmaps, all overloaded operations will print function and derivative calculations to file in the manner presented in Section 3, with the exception being the organizational operations. The organizational operations will instead use stored global data to print derivative references and assignments using the *index matrices* as described in Section 5.5. Moreover, during the evaluation of the loop, only organizational operations are cognizant of the fact that the evaluations are being performed within the loop. Thus, when operations are performed on loop overmaps, the resulting assignment objects can sometimes be computed to be different from their overmapped form. To adhere to Mapping Rule 3, after each variable assignment within the loop, the assignment object is sent to the *VarAnalyzer* routine, which then remaps the assigned object to the stored loop overmap to which it belongs.

Nested loops are handled different from nonnested loops. When a nested loop is reached during the printing evaluation, the active overloaded workspace will only contain loop overmaps, and thus it is not required to remap any nested loop inputs to their overmapped form. What is required, however, is that the *ForInitialize* routine checks to see if any index matrix references and/or reshapes must be printed, where if this is the case, the proper references and/or reshapes are stored during the organizational operation data analysis. These references/reshapes are then accessed and printed to file. The printing of the actual nested loop statements is then handled by the *ForIterStart* routine, where, unlike outer loops, nested loops may run for a number of iterations, which is dependent upon a parent loop. If it is the case that a nested loop changes size depending upon a parent loop's iteration, then the loop statement is printed as such: `for cadaforcount2 = 1:K(cadaforcount1)`, where `cadaforcount2` takes on the nested loop iteration, `cadaforcount1` is the parent loop iteration, and `K` is a vector containing the sizes of the nested loop. Any evaluations performed within the nested loop are then handled exactly as if they were within an outer loop, and when the *ForIterEnd* routine of the nested loop is encountered, it prints the `end` statement.

After the outer loop has been evaluated, the outermost *ForIterEnd* routine then prints the `end` statement and must check to see if it needs to perform any remaps as a result of Mapping Rule 4. In other words, the OMS is used to determine which variables defined within the loop will be read after the loop (i.e., which variables are outputs of the loop). The objects that were written to these variables as a result of the last iteration of the loop in the overmapping evaluation are saved and are now accessible by the *ForIterEnd* routine. The loop overmaps are then remapped to the saved objects, and the outputs of *ForIterEnd*, `ForEvalStr` and `ForEvalVar`, are used to assign the saved objects to the overloaded workspace. Printing loops in this manner ensures that all calculations printed within the loop are valid for all iterations of the

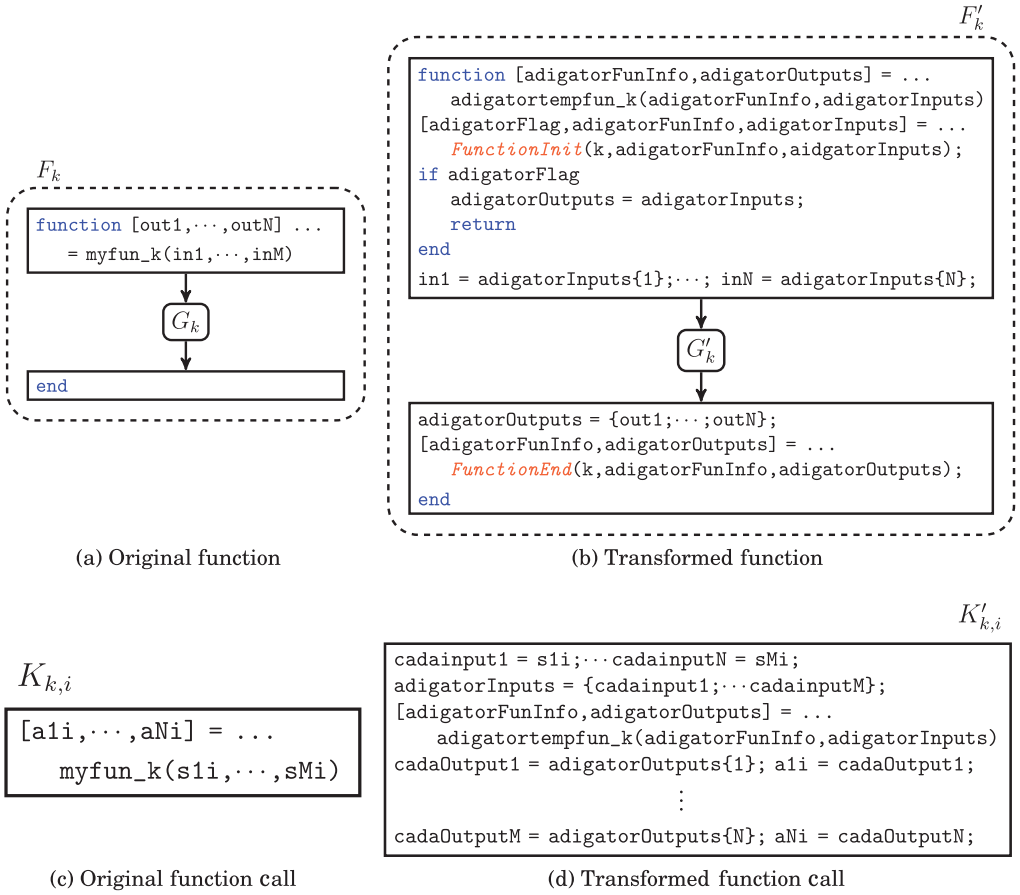
loop. Furthermore, this printing process ensures that any calculations printed after the loop are valid only for the result of the evaluation of all iterations of the loops (thus maintaining sparsity).

5.6.4. Storage of Global Data Required to Evaluate the Derivative File. Because the method presented in this article is geared toward applications in which the derivative is required at a number of different values, it is most efficient to determine all references and assignment indices required to evaluate the derivative file only once prior to all evaluations of the derivative file for a particular application. Thus, unlike the method of Patterson et al. [2013], where all reference and assignment indices are embedded within the derivative program itself, in the method of this article these reference and assignment indices are written as variable names to a MATLAB binary file (which is an output of the process shown in Figure 1). These variable names are then used within the derivative program itself and are recalled from global MATLAB memory. Furthermore, in the case where the associated global structure is cleared, it is restored on an ensuing call to the derivative program by loading the aforementioned MATLAB binary file associated with the derivative program. Using this aforementioned approach to keeping track of reference and assignment indices, the overhead associated with reading the indices is incurred only once. Furthermore, the derivative program is printed much more concisely than it would have been had the indices themselves been printed to the derivative file.

5.7. Multiple User Functions

At this point, the methods have been described that transform a program containing only a single function into a derivative program containing only a single function. It is often the case, however, that a user program consists of multiple functions and/or subfunctions. The method of this article handles both the cases of called functions and subfunctions in the same manner. To deal with programs containing multiple function calls, the transformations of Figure 9 are applied during the user source to intermediate source transformation phase. In the parsing phase, it is then determined which functions F'_k are called more than a single time. If a function is called only once, then the input and output objects are saved during the overmapping evaluation phase. Then, in the printing evaluation phase, when the function F'_k is called, the `FunctionInit` routine returns the saved outputs and sets the `adigatorFlag` true, returning the outputs to the calling function. After the calling function has been printed, the function F'_k is then evaluated in the manner discussed in Section 5.6.

In the case that a function F'_k is called multiple times, it is required to build a set of overmapped inputs and overmapped outputs of the function. The building of overmapped inputs and outputs is performed during the overmapping evaluation phase by joining the inputs across each function call, evaluating the called function on each unique set of inputs, and joining all possible outputs. Moreover, the outputs of *each* call are stored in memory for use in the printing evaluation phase. To allow for function call–dependent organizational operations, each call is assigned an iteration count and organizational operations are then handled in the manner presented in Section 5.5. During the printing phase, when the function F'_k is called, the `FunctionInit` routine remaps the given inputs for the particular call to the overmapped inputs, prints the function call, remaps the overmapped outputs to the stored outputs, and then returns the stored outputs. The function is then *not* evaluated by setting the `adigatorFlag` to true. After the calling function has finished printing, the function F'_k is then evaluated on the set of stored overmapped inputs and all organizational operations are treated as if they were being called from within a loop.



(a) Original function (b) Transformed function

(c) Original function call (d) Transformed function call

Fig. 9. Transformation of original function F_k to transformed function F'_k and transformation of the i^{th} call to function F_k, $K_{k,i}$, to the i^{th} call to function F'_k, $K'_{k,i}$.

6. EXAMPLES

The method described in Section 5 (which is implemented in the ADiGator software) is now applied to four examples. The first example provides a detailed examination of the process that ADiGator uses to handle conditional statements. The second example is the well-known Speelpenning problem of Speelpenning [1980] and demonstrates the ability of ADiGator to handle a `for` loop while simultaneously providing a comparison between a rolled loop and an unrolled loop. The third example is a polynomial data fitting example that contains a `for` loop and provides a comparison between the efficiency of ADiGator with the previously developed operator overloaded tool MAD [Forth 2006] and the combination source transformation and operator overloading tool ADiMat [Bischof et al. 2003]. The fourth example is a large-scale nonlinear programming problem (NLP) whose constraint function contains multiple levels of flow control. This fourth example is used to compare the efficiency of the first- and second-order derivative code generated by ADiGator against the previously developed software tools INTLAB [Rump 1999], MAD [Forth 2006], and ADiMat [Bischof et al. 2003]. Comparisons were performed against INTLAB version 6, MAD version 1.4, and ADiMat version 0.5.9. All computations were performed on an Apple Mac Pro with Mac OS-X 10.9.2 (Mavericks)

User Program

```
function z = myfun(x)

N  = 5;
x1 = x(1);
xN = x(N);

if x1 > xN
  y = x*x1;
else
  y = x*xN;
end

z = sin(y);
```

Intermediate Program

```
function [adigatorFunInfo, adigatorOutputs] = ...
    adigatortempfunc1(adigatorFunInfo,adigatorInputs)
[adigatorFlag, adigatorFunInfo, adigatorInputs] = ...
   FunctionInit(1,adigatorFunInfo,adigatorInputs);
if adigatorFlag; adigatorOutputs = adigatorInputs; return; end;
x = adigatorInputs{1};

N  = 5;
N  = VarAnalyzer('N  = 5;',N,'N',0);
x1 = x(1);
x1 = VarAnalyzer('x1 = x(1);',x1,'x1',0);
xN = x(N);
xN = VarAnalyzer('xN = x(N);',xN,'xN',0);

% ADiGator IF Statement #1: START
cadacond1 = x1 > xN;
cadacond1 = VarAnalyzer('cadacond1 = x1 > xN',cadacond1,'cadacond1',0);
IfInitialize(1,cadacond1,[]);
IfIterStart(1,1);
    y = x*x1;
    y = VarAnalyzer('y = x*x1;',y,'y',0);
IfIterEnd(1,1);
[IfEvalStr, IfEvalVar] = IfIterStart(1,2);
if not(isempty(IfEvalStr)); cellfun(@eval,IfEvalStr); end
    y = x*xN;
    y = VarAnalyzer('y = x*xN;',y,'y',0);
[IfEvalStr, IfEvalVar] = IfIterEnd(1,2);
if not(isempty(IfEvalStr)); cellfun(@eval,IfEvalStr); end
% ADiGator IF Statement #1: END

z = sin(y);
z = VarAnalyzer('z = sin(y);',z,'z',0);

adigatorOutputs = {z};
[adigatorFunInfo, adigatorOutputs] = ...
    FunctionEnd(1,adigatorFunInfo,adigatorOutputs);
```

Fig. 10. User source to intermediate source transformation for Example 1.

and a 2 × 2.4 GHz quad-core Intel Xeon processor with 24GB 1,066MHz DDR3 RAM using MATLAB version R2014a.

Example 1: Conditional Statement

In this example, we investigate the transformation of a user program containing a conditional statement into a derivative program containing the same conditional statement. The original user program and the transformed intermediate program is shown in Figure 10, where it is seen that the variable `y` is written within both the `if` branch and the `else` branch. Furthermore, because the variable `y` is read after the conditional fragment, a conditional overmap, $\mathcal{Y}_{c,o}$, is required to print derivative calculations that are valid for both the `if` and `else` branches.

Now let $\mathcal{Y}_{\texttt{if}}$ and $\mathcal{Y}_{\texttt{else}}$ be the overloaded objects written to `y` as a result of the overloaded evaluation of the `if` and `else` branches, respectively, in the intermediate program. Using this notation, the required conditional overmap is $\mathcal{Y}_{c,o} = \mathcal{Y}_{\texttt{if}} \cup \mathcal{Y}_{\texttt{else}}$, where this conditional overmap is built during the overmapping evaluation of the intermediate program shown in Figure 10. Fixing the input to be a vector of length five, the sparsity patterns of the Jacobians defined by $\mathcal{Y}_{\texttt{if}}$, $\mathcal{Y}_{\texttt{else}}$, and $\mathcal{Y}_{c,o}$ are shown

$$\begin{bmatrix} d_1 & 0 & 0 & 0 & 0 \\ d_2 & d_6 & 0 & 0 & 0 \\ d_3 & 0 & d_7 & 0 & 0 \\ d_4 & 0 & 0 & d_8 & 0 \\ d_5 & 0 & 0 & 0 & d_9 \end{bmatrix} \quad \begin{bmatrix} d_1 & 0 & 0 & 0 & d_5 \\ 0 & d_2 & 0 & 0 & d_6 \\ 0 & 0 & d_3 & 0 & d_7 \\ 0 & 0 & 0 & d_4 & d_8 \\ 0 & 0 & 0 & 0 & d_9 \end{bmatrix} \quad \begin{bmatrix} d_1 & 0 & 0 & 0 & d_9 \\ d_2 & d_6 & 0 & 0 & d_{10} \\ d_3 & 0 & d_7 & 0 & d_{11} \\ d_4 & 0 & 0 & d_8 & d_{12} \\ d_5 & 0 & 0 & 0 & d_{13} \end{bmatrix}$$

(a) $\mathbf{struct}(\mathcal{Y}_{\texttt{if}}.\texttt{deriv})$ (b) $\mathbf{struct}(\mathcal{Y}_{\texttt{else}}.\texttt{deriv})$ (c) $\mathbf{struct}(\mathcal{Y}_{c,o}.\texttt{deriv})$

Fig. 11. Derivative sparsity patterns of $\mathcal{Y}_{\texttt{if}}$, $\mathcal{Y}_{\texttt{else}}$, and $\mathcal{Y}_{c,o} = \mathcal{Y}_{\texttt{if}} \cup \mathcal{Y}_{\texttt{else}}$.

in Figure 11, and the final transformed derivative program is seen in Figure 12. From Figure 12, it is seen that remapping calculations are required from within both the `if` and `else` branches, where these remapping calculations represent the mapping of the nonzero elements of the Jacobians shown in Figure 11(a) and (b) into those shown in Figure 11(c). More precisely, in the `if` branch of the derivative program, the assignment indices `Gator1Indices.Index4` maps the derivative variable of $\mathcal{Y}_{\texttt{if}}$ into elements [1, 2, 3, 4, 5, 6, 7, 8, 13] of the derivative variable of $\mathcal{Y}_{c,o}$. Similarly, in the `else` branch of the derivative program, the assignment index `Gator1Indices.Index8` maps the derivative variable of $\mathcal{Y}_{\texttt{else}}$ into the [1, 6, 7, 8, 9, 10, 11, 12, 13] elements of the derivative variable of $\mathcal{Y}_{c,o}$. Thus, the evaluation of the derivative program shown in Figure 12 always produces a 13-element derivative variable, `z.dx`, which is mapped into a Jacobian of the form shown in Figure 11(c) using the mapping index written to `z.dx_location`. Due to the nature of the `if` and `else` branches of the derivative program, at least 4 elements of the derivative variable `z.dx` will always be identically zero, where the locations of the zero elements will depend upon which branch of the conditional block is taken.

Example 2: Speelpenning Problem

This example demonstrates the transformation of a function program containing a `for` loop into a derivative program containing the same `for` loop. The function program to be transformed computes the Speelpenning function [Speelpenning 1980] given as

$$y = \prod_{i=1}^{N} x_i, \tag{12}$$

where Equation (12) is implemented using a `for` loop as shown in Figure 13. From Figure 13, two major challenges of transforming the loop are identified. First, it is seen that the variable `y` is an input to the loop, rewritten within the loop, and read after the loop (as the output of the function), and thus a loop overmap, $\mathcal{Y}_{c,o}$ must be built to print valid derivative calculations within the loop. Second, it is seen that the reference `x(I)` depends upon the loop iteration, where the object assigned to `x` has possible nonzero derivatives. Thus, an index matrix, $\mathbf{K}$, and an overmapped `subsref` output, $\mathcal{R}_o$, must be built to allow for the iteration-dependent derivative reference corresponding to the function reference `x(I)`. To further investigate, let $\mathcal{Y}_i$ be the object written to `y` after the evaluation of the i^{th} iteration of the loop from within the intermediate program. Furthermore, we allow R_i to be the intermediate object created as a result of the overloaded evaluation of `x(I)` within the intermediate program. The overmapped objects $\mathcal{Y}_{l,o}$ and $\mathcal{R}_o$ are now defined as

$$\mathcal{Y}_{l,o} = \bigcup_{i=0}^{N} \mathcal{Y}_i \tag{13}$$

FunctionInit

```
function z = myderiv(x)
global ADiGator_myderiv
if isempty(ADiGator_myderiv); ADiGator_LoadData(); end
Gator1Indices = ADiGator_myderiv.myderiv.Gator1Indices;
Gator1Data = ADiGator_myderiv.myderiv.Gator1Data;
% ADiGator Start Derivative Computations
```

Overloaded Operations

```
N.f =  5;                          %User Line: N  = 5;
x1.dx = x.dx(1); x1.f = x.f(1);    %User Line: x1 = x(1);
xN.dx = x.dx(5); xN.f = x.f(N.f); %User Line: xN = x(N);
cadacond1 = gt(x1.f,xN.f);         %User Line: cadacond1 = x1 > xN
```

IfIterStart

```
if cadacond1
```

Overloaded Operation

```
    cada1tempdx = x1.dx(Gator1Indices.Index1);
    cada1td1 = zeros(9,1);
    cada1td1(Gator1Indices.Index2) = x1.f.*x.dx;
    cada1td1(Gator1Indices.Index3) = ...
        cada1td1(Gator1Indices.Index3) + x.f(:).*cada1tempdx;
    y.dx = cada1td1;
    y.f = x.f.*x1.f;               %User Line: y = x*x1;
```

Remapping Operation

```
    cada1tempdx = y.dx;
    y.dx = zeros(13,1);
    y.dx(Gator1Indices.Index4,1) = cada1tempdx;
```

IfIterStart

```
else
```

Overloaded Operations

```
    cada1tempdx = xN.dx(Gator1Indices.Index5);
    cada1td1 = zeros(9,1);
    cada1td1(Gator1Indices.Index6) = xN.f.*x.dx;
    cada1td1(Gator1Indices.Index7) = ...
        cada1td1(Gator1Indices.Index7) + x.f(:).*cada1tempdx;
    y.dx = cada1td1;
    y.f = x.f.*xN.f;               %User Line: y = x*xN;
```

Remapping Operation

```
    cada1tempdx = y.dx;
    y.dx = zeros(13,1);
    y.dx(Gator1Indices.Index8,1) = cada1tempdx;
```

IfIterEnd

```
end
```

Overloaded Operations

```
cada1tf1 = y.f(Gator1Indices.Index9);
z.dx = cos(cada1tf1(:)).*y.dx;
z.f = sin(y.f);                    %User Line: z = sin(y);
```

FunctionEnd

```
z.dx_size = [5,5];
z.dx_location = Gator1Indices.Index10;
end

function ADiGator_LoadData()
global ADiGator_myderiv
ADiGator_myderiv = load('myderiv.mat');
return
end
```

Fig. 12. Transformed derivative program for Example 1 showing from where each line is printed.

User Program

```
function y = SpeelFun(x)

y = 1;

for I = 1:length(x)

  y = y*x(I);

end
```

Intermediate Program

```
function [adigatorFunInfo, adigatorOutputs] = ...
    adigatortempfun_1(adigatorFunInfo,adigatorInputs)
[flag, adigatorFunInfo, adigatorInputs] = ...
    FunctionInit(1,adigatorFunInfo,adigatorInputs);
if flag; adigatorOutputs = adigatorInputs; return; end;
x = adigatorInputs{1};

y = 1;
y = VarAnalyzer('y = 1;',y,'y',0);

% ADiGator FOR Statement #1: START
cadaLoopVar_1 = 1:length(x);
cadaLoopVar_1 = ...
    VarAnalyzer('cadaLoopVar_k = 1:length(x);',cadaLoopVar_k,'cadaLoopVar_k',0);
[adigatorForVar_1, ForEvalStr, ForEvalVar] = ForInitialize(1,cadaLoopVar_1);
if not(isempty(ForEvalStr)); cellfun(@eval,ForEvalStr); end
for adigatorForVar_1_i = adigatorForVar_1
    cadaForCount_1 = ForIterStart(1,adigatorForVar_1_i);
    I = cadaLoopVar_1(:,cadaForCount_1);
    I = VarAnalyzer('I = cadaLoopVar_1(:,cadaForCount_1);',I,'I',0);
    y = y*x(I);
    y = VarAnalyzer('y = y*x(I);',y,'y',0);
    [ForEvalStr, ForEvalVar]= ForIterEnd(1,adigatorForVar_1_i);
end
if not(isempty(ForEvalStr)); cellfun(@eval,ForEvalStr); end
% ADiGator FOR Statement #1: END

adigatorOutputs = {y};
[adigatorFunInfo, adigatorOutputs] = ...
    FunctionEnd(1,adigatorFunInfo,adigatorOutputs);
```

Fig. 13. User source to intermediate source transformation for the Speelpenning problem.

and

$$\mathcal{R}_o = \bigcup_{i=1}^{N} \mathcal{R}_i, \tag{14}$$

where $\mathcal{Y}_0$ represents the object written to y prior to the evaluation of the loop in the intermediate program. Now, as the input object, $\mathcal{X}$, has a Jacobian with a diagonal sparsity pattern (which does not change), then each object $\mathcal{R}_i$ will have a $1 \times N$ gradient where the i^{th} element is a possible nonzero. Thus, the union of all such gradients over i results in all N elements being possibly nonzero—that is, a full gradient. Within the derivative program, the reference operation must then result in a derivative variable of length N, where on iteration i, the i^{th} element of the derivative variable corresponding to $\mathcal{X}$ must be assigned to the i^{th} element of the derivative variable corresponding to $\mathcal{R}_o$. This reference and assignment is done as described in Section 5.5 using the index matrix $\mathbf{K} \in \mathbb{Z}^{N \times N}$, where

$$K_{i,j} = \begin{cases} i, & i = j \\ 0, & i \neq j \end{cases} \quad \begin{matrix} i = 1, \ldots, N \\ j = 1, \ldots, N \end{matrix}. \tag{15}$$

Now, because $\mathcal{R}_i$ contains a possible nonzero derivative in the i^{th} location of the gradient and $\mathcal{Y}_i = \mathcal{Y}_{i-1} * \mathcal{R}_i$, $\mathcal{Y}_i$ will contain i possible nonzero derivatives in the first i locations. Furthermore, the union of $\mathcal{Y}_i$ over $i = 0, \ldots, N$ results in an object $\mathcal{Y}_{l,o}$ containing N possible nonzero derivatives (i.e., a full gradient). Thus, in the derivative program, the object $\mathcal{Y}_0$ must be remapped to the object $\mathcal{Y}_{l,o}$ prior to the printing evaluation of the loop in the intermediate program. The result of the printing evaluation of the intermediate program for $N = 10$ is seen in Figure 14. In particular, Figure 14 shows the remapping of the object $\mathcal{Y}_0$ to $\mathcal{Y}_{l,o}$ immediately prior to the loop. Additionally, it is seen that the derivative variable `cada1f1dx` (which results from the aforementioned reference

```
FunctionInit
                function y = SpeelDer(x)
                global ADiGator_SpeelDer
                if isempty(ADiGator_SpeelDer); ADiGator_LoadData(); end
                Gator1Indices = ADiGator_SpeelDer.SpeelDer.Gator1Indices;
                Gator1Data = ADiGator_SpeelDer.SpeelDer.Gator1Data;
                % ADiGator Start Derivative Computations

Overloaded
Operations
Remapping
Operation       y.f =  1;                   %User Line: y = 1;
                cada1f1 = length(x.f);
                cadaforvar1.f = 1:cada1f1;  %User Line: cadaforvar1 = 1:length(x);

                y.dx = zeros(10,1);

ForInitialize   for cadaforcount1 = 1:10

Overloaded
Operation           I.f = cadaforvar1.f(:,cadaforcount1);
                    %User Line: I = cadaforvar1(:,cadaforcount1);

Organizational
Overloaded
Operation           cada1td1 = zeros(10,1);
                    cada1td1(logical(Gator1Indices.Index1(:,cadaforcount1))) =...
                      x.dx(nonzeros(Gator1Indices.Index1(:,cadaforcount1)));
                    cada1f1dx = cada1td1;
                    cada1f1 = x.f(I.f);

Overloaded
Operation           cada1td1 = cada1f1*y.dx;
                    cada1td1 = cada1td1 + y.f*cada1f1dx;
                    y.dx = cada1td1;
                    y.f = y.f*cada1f1;
                    %User Line: y = y*x(I);

ForIterEnd      end

                y.dx_sizy.dx_size = 10;
                y.dx_location = Gator1Indices.Index2;
                end

FunctionEnd     function GatorAD_LoadData()
                global GatorAD_mymax2D_deriv
                GatorAD_mymax2D_deriv = load('GatorAD_mymax2D_deriv.mat');
                return
                end
```

Fig. 14. Derivative program for the Speelpenning problem for $N = 10$ showing the origin of each printed line of code.

within the loop) is of length 10, where the reference and assignment of `cada1f1dx` depends upon the loop iteration. This reference and assignment is made possible by the index matrix $\mathbf{K}$ assigned to the variable `Gator1Indices.Index1` within the derivative program.

Rolled Versus Unrolled Loops for the Speelpenning Problem. The following important issue arises in this example because the loop remains rolled in the derivative code. Specifically, by imposing the overmapping scheme and maintaining a rolled loop in the derivative code, all derivative computations are forced to be dense on vectors of length N. If, on the other hand, the loop had been unrolled, all derivative computations on iteration i would have been performed sparsely on vectors of length i. Unrolling the loop, however, increases the size of the derivative program. To investigate the trade-off between between a rolled and an unrolled loop, consider for this example the Jacobian-to-function evaluation ratio, CPU($\mathbf{Jf}$)/CPU($\mathbf{f}$), for different values of N using a derivative code generated with a function code that contains a rolled version of the loop and a second derivative code generated using a function code that contains an unrolled

Table III. Sizes of GatorAD-Generated Derivative Programs and Ratios of Jacobian-to-Function Computation Time, CPU(**Jf**)/CPU(**f**), for the Rolled and Unrolled Speelpenning Function

N	CPU(**Jf**)/CPU(**f**) Ratio with Rolled Loop	CPU(**Jf**)/CPU(**f**) Ratio with Unrolled Loop	Program Sizes (kB) with Rolled Loop	Program Sizes (kB) with Unrolled Loop
10	223	65	1.5	2.9
100	1,255	297	1.9	23.3
1,000	2,522	780	6.3	370.8
10,000	5,960	3,831	60.4	82,170.3

Note: File sizes were computed as the sum of the sizes of the produced `.m` and `.mat` files, and CPU(**Jf**)/CPU(**f**) were obtained by averaging the values obtained over 1,000 Jacobian and function evaluations.

version of the loop. The values of CPU(**Jf**)/CPU(**f**) for both the rolled and unrolled cases are shown in Table III for $N = (10{,}100, 1{,}000, 10{,}000)$. It is seen that unrolling the loops results in a more efficient derivative code, but this increase in computational efficiency comes at the expense of generating a significantly larger derivative file. However, it is seen that in the worst case ($N = 100$), the evaluation of the rolled loop is only about four times slower than that of the unrolled loop.

Example 3: Polynomial Data Fitting

Consider the problem of determining the coefficients of the m-degree polynomial $p(x) = p_1 + p_2x + p_3x^2 + \cdots + p_mx^{m-1}$ that best fits the points $(x_i, d_i),\ (i = 1, \ldots, n),\ (n > m)$, in the least squares sense. This polynomial data fitting problem leads to an overdetermined linear system $\mathbf{Vp} = \mathbf{d}$, where $\mathbf{V}$ is the Vandermonde matrix,

$$\mathbf{V} = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{m-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{m-1} \\ \vdots & \vdots & & \vdots & \\ 1 & x_n & x_n^2 & \cdots & x_n^{m-1} \end{bmatrix}. \tag{16}$$

The problem of computing the Jacobian $\mathbf{Jp}(\mathbf{x})$ was presented by Bischof et al. [2002] as a way of demonstrating both the AD tool ADiMat and powerful MATLAB operators (particularly, `mldivide`). This same example was considered by Forth [2006] to demonstrate the effectiveness of the MAD sparse forward mode AD class `fmad`. In this example, ADiGator is compared to the forward sparse mode of MAD and the overloaded vector forward mode of ADiMat. The code that computes $\mathbf{p}$ and the ADiGator-transformed derivative code for this problem may be seen in Figure 15.

Table IV shows the Jacobian-to-function evaluation times for the ADiGator, MAD, and ADiMat methods. Because the Jacobian $\mathbf{Jp}(\mathbf{x})$ is full, MAD was found to be most efficient in the sparse forward mode, and ADiMat was found to be most efficient when evaluating the forward mode generated code on derivative objects of the `opt_derivclass`. Furthermore, it is seen that for all chosen values of n, the derivative program generated by ADiGator is evaluated in less time than the time required to evaluate the original function file on sparse `fmad` objects or the time required to evaluate the derivative file generated by ADiMat on `opt_derivclass` objects. It is noted, however, that all three AD tools compute the derivative of the backslash operator in a different manner. As seen in Figure 15, the method employed by the ADiGator tool involves squaring the Vandermonde matrix. This approach produces efficient derivative files; however, the accuracy of the computed derivatives deteriorates as the condition number of the Vandermonde matrix increases. To analyze the efficiency of the source

Function Program

```
function p= fit(x, d, m)
% FIT -- Given x and d, fit() returns p
% such that norm(V*p-d) = min, where
% V = [1, x, x.^2, ... x.^(m-1)].

dim_x = size(x, 1);
if dim_x < m
  error('x must have at least m entries');
end

V = zeros(dim_x,m);
for i = 1:m
  V(:,i) = x.^(i-1);
end

p = V \ d;
```

ADiGator-Generated Program

```
function p = fit_x(x,d,m)
global ADiGator_fit_x
if isempty(ADiGator_fit_x); ADiGator_LoadData(); end
Gator1Indices = ADiGator_fit_x.fit_x.Gator1Indices;
Gator1Data = ADiGator_fit_x.fit_x.Gator1Data;
% ADiGator Start Derivative Computations
%User Line: % FIT -- Given x and d, fit() returns p
%User Line: % such that norm(V*p-d) = min, where
%User Line: % V = [1, x, x.^2, ... x.^(m-1)].
dim_x.f = size(x.f,1);
%User Line: dim_x = size(x, 1);
cadaconditional1 = lt(dim_x.f,m);
%User Line: cadaconditional1 = dim_x < m
V.f = zeros(dim_x.f,m);
%User Line: V = zeros(dim_x,m);
cadaforvar1.f = 1:m;
%User Line: cadaforvar1 = 1:m;
V.dx = zeros(30,1);
for cadaforcount1 = 1:4
    i.f = cadaforvar1.f(:,cadaforcount1);
    %User Line: i = cadaforvar1(:,cadaforcount1);
    cada1f1 = i.f - 1;
    cadaconditional1 = cada1f1;
    if cadaconditional1
        cada1f2dx = cada1f1.*x.f(:).^(cada1f1-1).*x.dx;
    else
        cada1f2dx = zeros(10,1);
    end
    cada1f2 = x.f.^cada1f1;
    V.dx(logical(Gator1Indices.Index1(:,cadaforcount1))) = ...
        cada1f2dx(nonzeros(Gator1Indices.Index1(:,cadaforcount1)));
    V.f(:,i.f) = cada1f2;
    %User Line: V(:,i) = x.^(i-1);
end
cada1tf3 = V.f\ d;
cada1td1 = sparse(Gator1Indices.Index2,Gator1Indices.Index3,V.dx,4,100);
cada1td1 = cada1tf3.'*cada1td1;
cada1td1 = cada1td1(:);
cada1td3 = full(cada1td1(Gator1Indices.Index4));
cada1tf4 = V.f.';
cada1td1 = zeros(10,10);
cada1td1(Gator1Indices.Index5) = cada1td3;
cada1td1 = cada1tf4*cada1td1;
cada1td1 = cada1td1(:);
cada1td4 = cada1td1(Gator1Indices.Index6);
cada1tf4 = (V.f*cada1tf3 - d).';
cada1td1 = sparse(Gator1Indices.Index7,Gator1Indices.Index8,V.dx,10,40);
cada1td1 = cada1tf4*cada1td1;
cada1td1 = cada1td1(:);
cada1td5 = full(cada1td1(Gator1Indices.Index9));
cada1td3 = cada1td4;
cada1td3(Gator1Indices.Index10) = cada1td3(Gator1Indices.Index10) + cada1td5;
cada1tf4 = -(V.f.'*V.f);
cada1td1 = zeros(4,10);
cada1td1(Gator1Indices.Index11) = cada1td3;
cada1td1 = cada1tf4\ cada1td1;
cada1td1 = cada1td1(:);
p.dx = cada1td1(Gator1Indices.Index12);
p.f = cada1tf3;
%User Line: p = V \ d
p.dx_size = [4,10];
p.dx_location = Gator1Indices.Index13;
end

function ADiGator_LoadData()
global ADiGator_fit_x
ADiGator_fit_x = load('fit_x.mat');
return
end
```

Fig. 15. Function program and GatorAD-generated derivative program ($m = 4, n = 10$, fixed) for the polynomial data fitting example.

Table IV. Ratio of Jacobian-to-Function Computation Time, CPU($\mathbf{Jp}(\mathbf{x})$)/CPU($\mathbf{p}(\mathbf{x})$), for Example 4 ($m = 4$) Using ADiGator, MAD, and ADiMat Together with ADiGator Code Generation Times and Function Evaluation Times

Problem Size	CPU($\mathbf{Jp}(\mathbf{x})$)/CPU($\mathbf{p}(\mathbf{x})$)			ADiGator File	CPU($\mathbf{p}(\mathbf{x})$)
n	*ADiGator*	*MAD*	*ADiMat*	Gen. Time (s)	(ms)
10	5	49	849	0.114	0.102
20	7	50	1,031	0.116	0.110
40	7	48	1,887	0.120	0.117
80	7	44	4,115	0.118	0.131
160	9	48	23,231	0.120	0.130
320	11	46	103,882	0.124	0.162
640	17	52	604,633	0.140	0.241
1,280	53	139	—	0.227	0.398
2,560	109	300	—	0.474	0.675

Note: MAD was used in the sparse forward mode and ADiMat was used in the vector forward mode with the derivative class `opt_derivclass`. All times CPU($\mathbf{Jp}(\mathbf{x})$) and CPU($\mathbf{p}(\mathbf{x})$) were obtained by averaging over 100 trials, and ADiGator file generation times were obtained by averaging over 10 trials. It is noted that the entries for ADiMat are omitted at $n = 1{,}280$ and $n = 2{,}560$ due to large Jacobian CPU times.

transformation for this problem, the average function evaluation time and the average ADiGator source transformation times are also given in Table IV. It is then seen that as the problem increases in size, the ADiGator source transformation times do not increase significantly, where the increase in times is only due to the increase in nonzero derivative locations that must be propagated via the *cada* class. Although perhaps not the ideal comparison,[2] it is noted that the average time required to perform the source transformation using ADiMat was 0.936s, whereas the source transformation time using AdiGator took a maximum of 0.474s (at $n = 2{,}560$).

An alternative approach for evaluating the efficiency of the ADiGator transformation process is to determine the number of Jacobian evaluations required to overcome the overhead associated with the source transformation. Specifically, Table IV shows that for $n = 10$ and $n = 2{,}560$, the Jacobian would need to be evaluated at least 26 and 4 times, respectively, before ADiGator consumes less time when compared to MAD.

Example 4: Sparse Nonlinear Programming

Consider the following NLP that arises from the discretization of a scaled version of the optimal control problem described in Darby et al. [2011] using a multiple-interval formulation of the Legendre-Gauss-Radau (LGR) orthogonal collocation method as described in Patterson et al. [2013]. The NLP decision vector $\mathbf{z} \in \mathbb{R}^{4N+4}$ is given as

$$\mathbf{z} = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{u}, \beta] \,, \tag{17}$$

where N is a parameter that defines the number of collocation points [Garg et al. 2010, 2011a, 2011b; Patterson and Rao 2012], $\mathbf{x}_1 \in \mathbb{R}^{N+1}$, $\mathbf{x}_2 \in \mathbb{R}^{N+1}$, $\mathbf{x}_3 \in \mathbb{R}^{N+1}$, $\mathbf{u} \in \mathbb{R}^N$, and

[2]To perform source transformation using ADiMat, the original source code must be sent to a transformation server that performs the transformation and then sends back the derivative code. Thus, there are a few unknown factors that may not be accounted for in the direct comparison of ADiMat code generation times to ADiGator code generation times.

$\beta \in \mathbb{R}$. Furthermore, let $\mathbf{f} : \mathbb{R}^{4N+4} \to \mathbb{R}^{3N}$ be defined as

$$\begin{aligned} f_i(\mathbf{z}) &= \left[\sum_{k=1}^{N+1} D_{i,k}x_{1k} - \frac{\beta}{2}x_{2i}\sin x_{3i}\right], \quad (i = 1, \ldots, N), \\ f_{N+i}(\mathbf{z}) &= \left[\sum_{k=1}^{N+1} D_{i,k}x_{2k} - \frac{\beta}{2}\left(\frac{\zeta-\theta}{c_1} - c_2\sin x_{3i}\right)\right], \quad (i = 1, \ldots, N), \\ f_{2N+i}(\mathbf{z}) &= \left[\sum_{k=1}^{N+1} D_{i,k}x_{3k} - \frac{\beta}{2}\frac{c_2}{x_{2i}}(u_i - \cos x_{3i})\right], \quad (i = 1, \ldots, N), \end{aligned} \tag{18}$$

where

$$\begin{aligned} \zeta &= \zeta(T(h), h, v), \\ \theta &= \theta(T(h), \rho(h), h, v), \end{aligned} \tag{19}$$

and the functions ζ, θ, T, and ρ are evaluated at values $h = x_{1i}$ and $v = x_{2i}$, where x_{1i} and x_{2i} are the i^{th} elements of the vectors $\mathbf{x}_1$ and $\mathbf{x}_2$, respectively. Furthermore, the quantity $[D_{ik}] \in \mathbb{R}^{N\times(N+1)}$ in Equation (18) is the LGR differentiation matrix [Garg et al. 2010, 2011a, 2011b; Patterson and Rao 2012]. It is noted that $N = N_k K$, where K is the number of mesh intervals that the problem is divided via using the multiple-interval LGR collocation method. The objective of the NLP that arises from the discretization is to minimize the cost function

$$J = \beta \tag{20}$$

subject to the nonlinear algebraic constraints

$$\mathbf{f}(\mathbf{x}) = \mathbf{0} \tag{21}$$

and the simple bounds on the decision variables

$$\mathbf{z}_{\min} \le \mathbf{z} \le \mathbf{z}_{\max}, \tag{22}$$

where

$$\begin{aligned} x_1 &= b_1, \; x_{N+1} = b_2, \\ x_{N+2} &= b_3, \; x_{2N+2} = b_4 \\ x_{2N+3} &= b_5, \; x_{3N+3} = b_6. \end{aligned} \tag{23}$$

A key aspect of this example is the modification of the functions $T(h)$ and $\rho(h)$ from smooth functions (as used in Darby et al. [2011]) to the following piecewise continuous functions taken from NOAA [1976]:

$$\rho(h) = c_3\frac{p(h)}{T(h)}, \tag{24}$$

where

$$(T(h), p(h)) = \begin{cases} \left(c_4 - c_5 h, c_6\left[\frac{T(h)}{c_7}\right]^{c_8}\right), & h < 11, \\ (c_9, c_{10}e^{c_{11}-c_{12}h}), & \text{otherwise.} \end{cases} \tag{25}$$

In the implementation considered in this example, Equation (25) is represented by a conditional statement nested within a `for` loop. Figure 16 shows the MATLAB code that computes the function $\mathbf{f}(\mathbf{z})$, where it is seen that the source code contains multiple loops, an indeterminate conditional statement (nested within a loop), and a loop iteration–dependent conditional statement. Table V shows the constants and parameters used in this example.

Constraint Function f(z)

```
function C = Constraints(z)
global probinfo

nLGR = probinfo.LGR.nLGR;
D    = probinfo.LGR.Dmatrix;

X  = z(probinfo.map.state);
U  = z(probinfo.map.control);
tf = z(probinfo.map.tf);

F       = Dynamics(X(1:nLGR,:),U);
Defects = D*X - tf/2*F;

C = Defects(:);
```

Lagrangian Function $L(z)$

```
function L = Lagrangian(lambda,z)
global probinfo
tf = z(probinfo.map.tf);
C  = Constraints(z);

L  = tf + lambda.'*C;
```

Dynamics Function

```
function daeout = Dynamics(x,u)
global probinfo

CONSTANTS = probinfo.CONSTANTS;
CoF       = CONSTANTS.CoF;

h = x(:,1); v = x(:,2); fpa = x(:,3);

c1  = 392.4;    c2  = 16818;      c3  = 86.138;
c4  = 288.14;   c5  = 6.49;       c6  = 4.0519e9;
c7  = 288.08;   c8  = 5.256;      c9  = 216.64;
c10 = 9.06e8;   c11 = 1.73;       c12 = 0.157;
c13 = 6e-5;     c14 = 4.00936;    c15 = 2.2;

zeros4over = h*0;
rho  = zeros4over; T    = zeros4over;
for i = 1:length(h)
  hi = h(i);
  if hi < 11
    Ti = c4 - c5*hi;
    p     = c6*(Ti./c7).^c8;
  else
    Ti = c9;
    p     = c10* exp(c11 - c12*hi);
  end
  rho(i)  = c3*p./Ti;
  T(i) = Ti;
end
q = 0.5.*rho.*v.*v.*c13;

a = c14*sqrt(T);       M = v./a;
Mp = cell(1,6);
for i = 1:6
  Mp{i} = M.^(i-1);
end

numeratorCD0 = zeros4over; denominatorCD0 = zeros4over;
numeratorK   = zeros4over; denominatorK   = zeros4over;
for i = 1:6
  Mpi = Mp{i};
  if i < 6
    numeratorCD0   = numeratorCD0   + CoF(1,i).*Mpi;
    denominatorCD0 = denominatorCD0 + CoF(2,i).*Mpi;
    numeratorK     = numeratorK     + CoF(3,i).*Mpi;
  end
  denominatorK = denominatorK  + CoF(4,i).*Mpi;
end
Cd0 = numeratorCD0./denominatorCD0;
K   = numeratorK./denominatorK;
FD  = q.*(Cd0+K.*((c2^2).*(c1^2)./(q.^2)).*(u.^2));

FT = zeros4over;
for i = 1:6
  ei = zeros4over;
  for j = 1:6
    ei = ei + CoF(4+j,i).*Mpj;
  end
  FT = FT + ei.*h.^(i-1);
end
FT = FT.*c1/c15;

hdot   = v.*sin(fpa);
vdot   = (FT-FD)/c2 - c1*sin(fpa);
fpadot = c1*(u-cos(fpa))./v;

daeout = [hdot vdot fpadot];
end
```

Fig. 16. Function program for the NLP in Example 4.

Table V. Constants and Parameters for Example 4

c_1	3.9240×10^2	c_2	1.6818×10^4	c_3	8.6138×10^1
c_4	2.8814×10^2	c_5	6.4900×10^0	c_6	4.0519×10^9
c_7	2.8808×10^2	c_8	5.2560×10^0	c_9	2.1664×10^2
c_{10}	9.0600×10^8	c_{11}	1.7300×10^0	c_{12}	1.5700×10^{-1}
c_{13}	6.0000×10^{-5}	c_{14}	4.00936×10^0	c_{15}	2.2000×10^0
b_1	0	b_2	2.0000×10	b_3	2.6000×10
b_4	5.9000×10^0	b_5	0	b_6	0

Table VI. Ratio of Jacobian-to-Function Computation Time, CPU(**Jf**)/CPU(**f**), for Example 4 Using ADiGator, ADiMat, INTLAB, and MAD

NLP Size		CPU(**Jf**(**z**))/CPU(**f**(**z**))					
K	$N = 4K$	*ADiGator*	*ADiMat* (scalar)	*ADiMat* (vector)	*INTLAB*	*MAD* (comp)	*MAD* (sparse)
4	16	17	79	142	149	188	186
8	32	21	93	210	220	275	276
16	64	29	116	322	332	417	421
32	128	41	151	502	511	636	650

Note: ADiMat was supplied the compressed seed matrix in both the scalar forward and nonoverloaded vector forward modes, and MAD was used in the compressed forward mode and the sparse forward mode. All times CPU(**Jf**) and CPU(**f**) were obtained by taking the average over 100 Jacobian and function evaluations.

To solve the NLP of Equations (20) through (22), typically either a first-derivative (quasi-Newton) or a second-derivative (Newton) NLP solver is used. In a first-derivative solver, the objective gradient and constraint Jacobian, $\mathbf{Jf}(\mathbf{z})$, are used together with a dense quasi-Newton approximation of the Lagrangian Hessian. In a second-derivative solver, the objective gradient and constraint Jacobian are used together with the Hessian of the NLP Lagrangian, where in this case the Lagrangian is given by

$$L = \beta + \boldsymbol{\lambda}^T \mathbf{f}(\mathbf{z}). \tag{26}$$

In this example, we now concern ourselves with the computation of both the constraint Jacobian, $\mathbf{Jf}(\mathbf{z})$, and the Lagrangian Hessian, $\mathbf{H}L(\mathbf{z})$. Moreover, the efficiencies with which the method of this article generates the constraint Jacobian and Lagrangian Hessian source code is presented along with the computational efficiency of the resulting derivative code. To analyze the performance of the method as the aforementioned NLP increases in size, the number of LGR points in each mesh interval is set to four (i.e., $N_k = 4$) and the number of mesh intervals, K, is varied. Thus, in this example, the total number of LGR points is always $N = 4K$. Finally, the comparative performance of the method developed in this work against the well-known MATLAB automatic differentiation tools INTLAB, MAD, and ADiMat is provided.

Table VI shows the ratio of the constraint Jacobian evaluation time to constraint function evaluation time, CPU(**Jf**)/CPU(**f**), using the derivative code generated by ADiGator alongside the values of CPU(**Jf**)/CPU(**f**) using ADiMat, INTLAB, and MAD, where ADiMat is used in both of its nonoverloaded (scalar and vector) modes while being supplied the compressed seed matrix $\mathbf{S} \in \mathbb{R}^{(4N+4)\times 5}$, whereas MAD was used in the compressed mode with the same seed matrix. In addition, it is noted that the compressed seed matrix, $\mathbf{S}$, has a column dimension $1 + \max(N_k) = 5$ for any K used in this example. From Table VI, it is seen that the Jacobian is computed in a smaller amount of time using the ADiGator-generated code than any of the other methods. Moreover, it is seen that for all values of K used, the time required to evaluate the derivative code generated by ADiGator (and produce the entire Jacobian) is slightly greater than the time required

Table VII. Ratio of Hessian-to-Function Computation Time, CPU($\mathbf{H}L(\mathbf{z})$)/CPU($\mathbf{f}(\mathbf{z})$), for Example 4 Using ADiGator, ADiMat, INTLAB, and MAD

NLP Size		CPU($\mathbf{H}L(\mathbf{z})$)/CPU($L(\mathbf{z})$)			
K	$N = 4K$	*ADiGator*	*INTLAB*	*MAD*	*ADiMat*
4	16	32	198	708	5,202
8	32	48	270	1,132	9,590
16	64	93	382	2,287	21,206
32	128	330	573	6,879	55,697

Note: MAD was used in the sparse forward over forward mode, and ADiMat was used in the forward operator overloading over reverse source transformation mode. All times CPU($\mathbf{H}L(\mathbf{z})$) and CPU($L(\mathbf{z})$) were obtained by taking the average over 100 Jacobian and function evaluations.

to evaluate the derivative code generated by ADiMat in the scalar mode (and produce a single column of the compressed Jacobian).

Table VII now shows the ratio of Lagrangian Hessian evaluation time to Lagrangian function evaluation, CPU($\mathbf{H}L$)/CPU(L), using the derivative code generated by ADiGator alongside the values of CPU($\mathbf{H}L$)/CPU(L) using ADiMat, INTLAB, and MAD. Unlike the constraint Jacobian, the Lagrangian Hessian is incompressible, and as such, MAD is only used in the sparse forward over forward mode. The nonoverloaded modes of ADiMat may not be used to compute the Lagrangian Hessian, as only the diagonal elements of Hessians may be computed via strip mining, and currently, source transformation may not be recursively called on ADiMat-generated code produced for the nonoverloaded vector mode (as it is written in terms of ADiMat specific runtime functions). The computation of the Lagrangian Hessian using ADiMat was thus found to be most efficient when evaluating a Lagrangian gradient code generated in the reverse mode on a set of overloaded objects (the default mode of the ADiMat function `admHessian`). From Table VII, it is again seen that the ADiGator-generated code is more efficient than the other methods. It is also seen, however, that this efficiency appears to dissipate (when compared to INTLAB) as the NLP grows in size.

Up to this point in the example, it has been shown that the Jacobian and Hessian programs generated by the method of this article are efficient when compared to other MATLAB AD tools. The expense of the code generation then comes into question. The time required to generate the constraint Jacobian and Lagrangian Hessian derivative files using ADiGator are now given in Table VIII, as well as the constraint and Lagrangian function evaluation times. Unlike the previous example, there are two reasons for the increase in derivative file generation times seen in Table VIII. For instance, the increase in time is both due to an increase in the number of propagated nonzero derivative locations together with an increase in the number of required overloaded operations. In other words, since the dimension N is looped upon in the dynamics function of Figure 16, as N increases the number of required overloaded operations also increases. In an attempt to quantify the efficiency of the transformation process, we first compare the generation times of Table VIII to similar ADiMat source transformations. To do so, we computed the average time to generate constraint Jacobian and Lagrangian Hessian derivative files using the forward mode of ADiMat. These times are now given as 1.40 and 3.42 s, respectively, and are thus less than those required by ADiGator.

To further quantify the efficiency of the method of this article applied to this example, we solved the NLP of Equations (20) through (22) using the NLP solver IPOPT [Biegler and Zavala 2008; Waechter and Biegler 2006]. IPOPT was used in both the

Table VIII. ADiGator Constraint Jacobian and Lagrangian Hessian Code Generation Times with Constraint and Lagrangian Function Evaluation Times

NLP Size		ADiGator Code Generation Times (s)		Function Evaluation Times (ms)	
K	$N = 4K$	$\mathbf{Jf}$	$\mathbf{H}L$	$\mathbf{f}$	L
4	16	1.70	6.87	0.381	0.418
8	32	2.02	8.44	0.400	0.435
16	64	2.72	11.54	0.480	0.482
32	128	4.17	17.90	0.537	0.571

Note: The times taken to generate the constraint Jacobian and Lagrangian Hessian files were averaged over 10 trials, where the Lagrangian Hessian generation time is the time taken to perform two successive source transformations: once on the Lagrangian file and once on the resulting derivative file. The constraint and Lagrangian function evaluation times were averaged over 100 trials.

Table IX. Total Derivative Computation Time to Solve NLP of Example 4 Using IPOPT in First-Derivative Mode

NLP Size		Jacobian	Derivative Computation Time (s)			
K	$N = 4K$	Evaluations	*ADiGator*	*ADiMat*	*INTLAB*	*MAD*
4	16	62	2.1	3.3	3.5	4.4
8	32	98	2.8	5.1	8.6	10.8
16	64	132	4.4	8.2	19.6	24.6
32	128	170	7.9	15.1	46.7	58.1

Note: Derivative computation times were computed as the estimated total time to perform the number of required Jacobian evaluations plus any source transformation overhead. The transformation overhead of ADiGator is the Jacobian code generation time shown in Table VIII, and the transformation overhead of ADiMat is the time required to generate the forward mode Jacobian code (1.40s). Estimated Jacobian evaluation times of ADiMat and MAD were computed by using the average times of the scalar compressed and compressed modes, respectively, from Table VI.

quasi-Newton and Newton modes with the following initial guess of the NLP decision vector:

$$\begin{aligned} \mathbf{x}_1 &= \texttt{linspace}(b_1, b_2, N+1) \\ \mathbf{x}_2 &= \texttt{linspace}(b_3, b_4, N+1) \\ \mathbf{x}_3 &= \texttt{linspace}(b_5, b_6, N+1) \\ \mathbf{u} &= \texttt{linspace}(0, 0, N) \\ \beta &= 175, \end{aligned} \tag{27}$$

where the function $\texttt{linspace}(a, b, M)$ provides a set of M linearly equally spaced points between a and b. The number of constraint Jacobian evaluations required to solve the problem in the quasi-Newton mode and the number of constraint Jacobian and Lagrangian Hessian evaluations required to solve the problem in the Newton mode were then recorded. The recorded values were then used to predict the amount of derivative computation time that would be required when supplying IPOPT with derivatives using the ADiGator, ADiMat, INTLAB, and MAD tools. The results are now given in Tables IX and X, respectively, where the total derivative computation time was computed as the time to evaluate the Jacobian/Hessian the required amount of times (using the average evaluation times of Tables VI and VII) plus any required source transformation overhead. Moreover, it is also noted that the total ADiGator time of Table X does not reflect the time required to generate the constraint Jacobian file, as the constraint

Table X. Total Derivative Computation Time to Solve NLP of Example 4 Using IPOPT in Second-Derivative Mode

NLP Size		Jacobian	Hessian	Derivative Computation Time (s)			
K	$N = 4K$	Evaluations	Evaluations	*ADiGator*	*ADiMat*	*INTLAB*	*MAD*
4	16	31	30	7.5	73.3	4.2	11.1
8	32	39	38	9.6	167.3	7.9	23.0
16	64	53	52	14.5	541.6	17.5	67.2
32	128	152	150	49.5	4790.8	90.8	641.2

Note: Derivative computation times were computed as the total time to perform the number of required Jacobian and Hessian evaluations plus any source transformation overhead. The transformation overhead of ADiGator is the average Hessian code generation time shown in Table VIII, and the transformation overhead of ADiMat is the average time required to generate the forward mode constraint Jacobian code (1.40s) together with the average time required to generate the reverse mode Lagrangian gradient code (5.75s). Estimated Jacobian evaluation times of ADiMat and MAD were computed by using the average times of the scalar compressed and compressed modes, respectively, from Table VI.

Jacobian file is produced in the process of generating the Lagrangian Hessian file. From Table IX, it may be seen that even though the majority of the computation time required by ADiGator is spent in the file generation, the expense of the file generation is worth the time saved in the solving of the NLP. From Table X, it may be seen that for the values of $K = 4$ and $K = 8$, the overhead required to generate the Lagrangian Hessian file using ADiGator outweighs the time savings at NLP solve time, and thus INTLAB is the most efficient. At the values of $K = 16$ and $K = 32$, however, due to a larger number of required Jacobian and Hessian evaluations, ADiGator becomes the more efficient tool.

7. DISCUSSION

The four examples given in Section 6 demonstrate both the utility and the efficiency of the method presented in this article. The first example showed the ability of the method to perform source transformation on a user program containing a conditional statement and gave an in-depth look at the processes that must take place to do so. The second example demonstrated the manner in which a user program that contains a loop can be transformed into a derivative program that contains the same loop. The second example also provided a discussion of the trade-offs between using a rolled and an unrolled loop. In particular, it was seen in the second example that using an unrolled loop led to a more efficient derivative code at the expense of generating a much larger size derivative file, whereas using a rolled loop led to slightly less efficient but much more aesthetically pleasing derivative code and a significantly smaller derivative file. The third example showed the efficiency of the method when applied to a large dense problem and compared to the tools of MAD and ADiMat. It is also seen that the method of this article is not the most preferred choice if it is required to compute the derivative only a smaller number of times. On the other hand, in applications where a large number of function evaluations is required, the method of this article is more efficient than other well-known automatic differentiation tools. The fourth example shows the performance of the method on a large, sparse NLP where the constraint function contains multiple levels of flow control. From this fourth example, it is seen that the method can be used to generate efficient first- and second-order derivative code of programs containing loops and conditional statements. Furthermore, it is shown that the presented method is particularly appealing for problems requiring a large number of derivative evaluations.

One aspect of the CADA method emphasized in Patterson et al. [2013] was its ability to be applied repeatedly to a program, thus creating second- and higher-order derivative files. It is noted that similar to CADA, the method of this article generates

stand-alone derivative code and is thus repeatable if higher-order derivatives are desired. Unlike the method of Patterson et al. [2013], however, ADiGator has the ability to recognize when it is performing source transformation on a file that was created by ADiGator and also has the ability to recognize the naming scheme used in the previously generated file. This awareness enables the method to eliminate any redundant 1^{st} through $(n-1)^{th}$ derivative calculations in the n^{th} derivative file. For example, if source transformation were performed twice on a function `y = sin(x)` such that the second transformation is done *without* knowledge of the first derivative transformation, the source transformation would be performed as follows:

$$\texttt{y = sin(x)} \begin{cases} \texttt{dy = cos(x)} \\ \\ \texttt{y = sin(x)} \end{cases} \begin{cases} \texttt{ddy = -sin(x)} \\ \texttt{dy = cos(x)} \\ \texttt{dy = cos(x)} \\ \texttt{y = sin(x).} \end{cases} \tag{28}$$

It is seen that in the second derivative file, the first derivative would be printed twice: once as a function variable and once as a derivative variable. On the other hand, the method of this article would have knowledge of the naming scheme used in the first derivative file and would thus eliminate this redundant line of code in the file that contains the second derivative.

7.1. Limitations of the Approach

The method of this article utilizes fixed input sizes and sparsity patterns to exploit sparsity at each required derivative computation and to reduce the required computations at runtime. The exact reasons that allow for the proposed method to generate efficient stand-alone derivative code also add limitations to the approach. The primary limitation is that derivative files may only be created for a fixed input size and sparsity pattern. Thus, if one wishes to change the input size, a new derivative file must be created. Moreover, the times required to generate derivative files are largely based upon the number of required overloaded evaluations in the intermediate program. Thus, if a loop is to run for many iterations (as was the case in the fourth example), the time required to generate the derivative files can become quite large. Requiring that all *cada* objects have a fixed size also limits the functions used in the user program to those that result in objects of a fixed size, and thus, in general, logical referencing cannot be used. Another limitation comes from the fact that all objects in the intermediate program are forced to be overloaded, even if they are simply numeric values. Therefore, any operation upon which the intermediate program is dependent must be overloaded, even if it is never used to operate on objects that contain derivative information.

8. CONCLUSIONS

A method has been described for generating derivatives of mathematical functions in MATLAB. Given a user program to be differentiated together with the information required to create *cada* instances of the inputs, the developed method may be used to generate derivative source code. The method employs a source transformation via operator overloading approach such that the resulting derivative code computes a sparse representation of the derivative of the user function whose input is a fixed size. A key aspect of the method is that it allows for the differentiation of MATLAB code where the function contains flow control statements. Moreover, the generated derivative code relies solely on the native MATLAB library, and thus the process may be repeated to obtain n^{th}-order derivative files. The approach has been demonstrated on four examples and is found to be highly efficient at runtime when compared

to well-known MATLAB AD programs. Furthermore, although there does exist an inherent overhead associated with generating the derivative files, the overhead becomes less of a factor as the number of required derivative evaluations is increased.

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