Algorithm 984: ADiGator, a Toolbox for the Algorithmic Differentiation of Mathematical Functions in MATLAB Using Source Transformation via Operator Overloading

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A toolbox called ADiGator is described for algorithmically differentiating mathematical functions in MATLAB. ADiGator performs source transformation via operator overloading using forward mode algorithmic differentiation and produces a file that can be evaluated to obtain the derivative of the original function at a numeric value of the input. A convenient by-product of the file generation is the sparsity pattern of the derivative function. Moreover, because both the input and output to the algorithm are source codes, the algorithm may be applied recursively to generate derivatives of any order. A key component of the algorithm is its ability to statically exploit derivative sparsity at the MATLAB operation level to improve runtime performance. The algorithm is applied to four different classes of example problems and is shown to produce runtime efficient derivative code. Due to the static nature of the approach, the algorithm is well suited and intended for use with problems requiring many repeated derivative computations.

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1 INTRODUCTION

Algorithmic differentiation (AD) is the process of determining accurate derivatives of a function defined by computer programs using the rules of differential calculus (Griewank 2008, 2014). AD exploits the fact that a user program may be broken into a sequence of elementary operations, and the derivative of the program is obtained by a systematic application of the calculus chain rule. AD can be performed either using the forward or reverse mode, where the fundamental difference between the two modes is the order in which the chain rule is applied. In the forward mode, the chain rule is applied from the input independent variables of differentiation to the final output dependent variables of the program, while in the reverse mode the chain rule is applied from the final output dependent variables of the program back to the independent variables of differentiation. Forward and reverse mode AD 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 and derivative values 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. In a source transformation approach, typically a compiler-type software is required to transform a user-defined function source code into a derivative source code, where the new program contains derivative statements interleaved with the function statements of the original program. The generated derivative source code may then be evaluated numerically to compute the desired derivatives. Runtime efficiency in computing the AD-generated derivative is gained either by performing optimization at the time of transformation or by exploiting derivative sparsity.

In recent years, MATLAB (Mathworks 2014) has become extremely popular as a platform for numerical computing due largely to its built in high-level matrix operations and user-friendly interface. The interpreted nature of MATLAB and its high-level language make programming intuitive and debugging easy. The qualities that make MATLAB appealing from a programming standpoint, however, tend to pose problems for AD tools. In the MATLAB language, there exist many ambiguous operators (for example, +, *) that perform different mathematical procedures depending on the shapes (for example, scalar, vector, matrix, etc.) of the inputs to the operators. Moreover, user variables are not required to be of any fixed size or shape. Thus, the proper mathematical procedure of each ambiguous operator must be determined at runtime by the MATLAB interpreter. This mechanism poses a major problem for both source transformation and operator overloaded AD tools. Source transformation tools must determine the proper rules of differentiation for all function operations at the time of transformation. Given an ambiguous operation, however, the corresponding differentiation rule is also ambiguous. To cope with this uncertainty, MATLAB source transformation AD tools must either determine fixed shapes for all variables or print derivative procedures that behave differently depending on the meaning of the corresponding ambiguous function operations. As operator overloading is applied at runtime, operator ambiguity is not an issue when employing an operator overloaded AD tool. The mechanism that the MATLAB interpreter uses to determine the meanings of ambiguous operators, however, imposes a great deal of runtime overhead on operator overloaded tools. Several MATLAB AD tools have been developed over the years, including ADMAT (Coleman and Verma 1998a, 1998b), INTLAB (Rump 1999), MAD (Forth 2006), which rely solely on operator overloading; ADiMat (Bischof et al. 2002), which relies on a combination of source transformation and operator overloading; and, most recently, MSAD (Kharche and Forth 2006), which relies solely on source transformation.

In this article, a new open-source MATLAB algorithmic differentiation toolbox called ADiGator (**A**utomatic **Di**fferentiation by **Gator**s) is described. ADiGator performs source transformation

via the non-classical methods of operator overloading and source reading for the forward mode algorithmic differentiation of MATLAB programs. Motivated by the iterative nature of many applications that require numerical derivative computation (for example, nonlinear optimization, ordinary differential equations), a great deal of emphasis is placed on performing an *a priori* analysis of the problem at the time of transformation to minimize derivative computation runtime. Moreover, the algorithm neither relies on sparse data structures at runtime nor relies on matrix compression to exploit derivative sparsity. Instead, an overloaded class is used at transformation time to determine sparse derivative structures for each MATLAB operation. Simultaneously, the sparse derivative structures are exploited to print runtime efficient derivative procedures to an output source code. The printed derivative procedures may then be evaluated numerically to compute the desired derivatives. Finally, it is noted that the previous research given in Patterson et al. (2013) and Weinstein and Rao (2016) focused on the methods on which the ADiGator tool is based, while this article focuses on the software implementation of these previous methods and the utility of the software.

This article is organized as follows. In Section 2, a row/column/value triplet notation used to represent derivative matrices is introduced. In Section 3, an overview of the implementation of the algorithm is given to grant the reader a better understanding of how to efficiently utilize the software as well as to identify various coding restrictions to which the user must adhere. Key topics such as the used overloaded class and the handling of flow control are discussed. In Section 4, a discussion is given on the use of overloaded objects to represent cell and structure arrays. In Section 5, a special class of vectorized functions is considered, where the algorithm may be used to transform vectorized function codes into vectorized derivative codes. In Section 6, the user interface to the ADiGator algorithm is described. In Section 7, the algorithm is tested against other well-known MATLAB AD tools on a variety of examples. In Section 8, a discussion is given on the efficiency of the algorithm and, finally, in Section 9, conclusions are drawn.

2 SPARSE DERIVATIVE NOTATIONS

The algorithm of this article utilizes a row/column/value triplet representation of derivative matrices. In this section, the triplet representation is given for a general matrix function of a vector, $\mathbf{F}(\mathbf{x}) : \mathbb{R}^{n_x} \to \mathbb{R}^{q_f \times r_f}$. The derivative of $\mathbf{F}(\mathbf{x})$ is the three-dimensional (3D) object, $\partial\mathbf{F}/\partial\mathbf{x} \in \mathbb{R}^{q_f \times r_f \times n_x}$. To gain a more tractable two-dimensional derivative representation, we first let $\mathbf{f}(\mathbf{x}) \in \mathbb{R}^{m_f}$ be the one-dimensional transformation of the function $\mathbf{F}(\mathbf{x}) \in \mathbb{R}^{q_f \times r_f}$,

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} \mathbf{F}_1(\mathbf{x}) \\ \vdots \\ \mathbf{F}_{r_f}(\mathbf{x}) \end{bmatrix}, \quad \mathbf{F}_k = \begin{bmatrix} F_{1,k}(\mathbf{x}) \\ \vdots \\ F_{q_f,k}(\mathbf{x}) \end{bmatrix}, \quad (k = 1, \ldots, r_f),$$

where $m_f = q_f r_f$. The *unrolled* representation of the three-dimensional derivative $\partial\mathbf{F}/\partial\mathbf{x}$ is then given by the two-dimensional Jacobian

$$\frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_{n_x}} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_{n_x}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_{m_f}}{\partial x_1} & \frac{\partial f_{m_f}}{\partial x_2} & \cdots & \frac{\partial f_{m_f}}{\partial x_{n_x}} \end{bmatrix} \in \mathbb{R}^{m_f \times n_x}.$$

Assuming the first derivative matrix $\partial\mathbf{f}/\partial\mathbf{x}$ contains $p_x^f \leq m_f n_x$ *possible* non-zero elements (that is, there exist $m_f n_x - p_x^f$ elements of $\partial\mathbf{f}/\partial\mathbf{x}$ that must be zero due to lack of dependence), the row

and column locations of the possible non-zero elements of $\partial \mathbf{f}/\partial \mathbf{x}$ are denoted by the index vector pair $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}}) \in \mathbb{Z}_+^{p^f_x} \times \mathbb{Z}_+^{p^f_x}$, where

$$\mathbf{i}^{\mathbf{f}}_{\mathbf{x}} = \begin{bmatrix} i^{\mathbf{f}}_{\mathbf{x}}(1) \\ \vdots \\ i^{\mathbf{f}}_{\mathbf{x}}(p^f_x) \end{bmatrix}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}} = \begin{bmatrix} j^{\mathbf{f}}_{\mathbf{x}}(1) \\ \vdots \\ j^{\mathbf{f}}_{\mathbf{x}}(p^f_x) \end{bmatrix}$$

correspond to the row and column locations, respectively. To ensure uniqueness of the row/column pairs $(i^{\mathbf{f}}_{\mathbf{x}}(k), j^{\mathbf{f}}_{\mathbf{x}}(k))$ (where $i^{\mathbf{f}}_{\mathbf{x}}(k)$ and $j^{\mathbf{f}}_{\mathbf{x}}(k)$ refer to the kth elements of the vectors $\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}$ and $\mathbf{j}^{\mathbf{f}}_{\mathbf{x}}$, respectively, $k = 1, \ldots, p^f_x$), the following column-major restriction is placed on the order of the index vectors:

$$i^{\mathbf{f}}_{\mathbf{x}}(1) + m_f\left(j^{\mathbf{f}}_{\mathbf{x}}(1) - 1\right) < i^{\mathbf{f}}_{\mathbf{x}}(2) + m_f\left(j^{\mathbf{f}}_{\mathbf{x}}(2) - 1\right) < \ldots < i^{\mathbf{f}}_{\mathbf{x}}\left(p^f_x\right) + m_f\left(j^{\mathbf{f}}_{\mathbf{x}}\left(p^f_x\right) - 1\right).$$

Henceforth, it shall be assumed that this restriction is always satisfied for row/column index vector pairs of the form of $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}})$; however, it may not be explicitly stated. To refer to the possible non-zero *elements* of $\partial \mathbf{f}/\partial \mathbf{x}$, the vector $\mathbf{d}^{\mathbf{f}}_{\mathbf{x}} \in \mathbb{R}^{p^f_x}$ is used such that

$$d^{\mathbf{f}}_{\mathbf{x}}(k) = \frac{\partial f_{[i^{\mathbf{f}}_{\mathbf{x}}(k)]}}{\partial x_{[j^{\mathbf{f}}_{\mathbf{x}}(k)]}}, \quad (k = 1, \ldots, p^f_x),$$

where $d^{\mathbf{f}}_{\mathbf{x}}(k)$ refers to the kth element of the vector $\mathbf{d}^{\mathbf{f}}_{\mathbf{x}}$. Using this sparse notation, the Jacobian $\partial \mathbf{f}/\partial \mathbf{x}$ may be fully defined given the row/column/value triplet $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{d}^{\mathbf{f}}_{\mathbf{x}}) \in \mathbb{Z}_+^{p^f_x} \times \mathbb{Z}_+^{p^f_x} \times \mathbb{R}^{p^f_x}$ together with the dimensions m_f and n_x. Moreover, the three-dimensional derivative matrix $\partial \mathbf{F}(\mathbf{x})/\partial \mathbf{x}$ is uniquely defined given the triplet $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{d}^{\mathbf{f}}_{\mathbf{x}})$ together with the dimensions q_f, r_f, and n_x.

3 OVERVIEW OF THE ADIGATOR ALGORITHM

Without loss of generality, consider a function $\mathbf{f}(\mathbf{v}(\mathbf{x}))$, where $\mathbf{f} : \mathbb{R}^{m_v} \to \mathbb{R}^{m_f}$ and $\partial \mathbf{v}/\partial \mathbf{x}$ is defined by the triplet $(\mathbf{i}^{\mathbf{v}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{v}}_{\mathbf{x}}, \mathbf{d}^{\mathbf{v}}_{\mathbf{x}}) \in \mathbb{Z}_+^{p^v_x} \times \mathbb{Z}_+^{p^v_x} \times \mathbb{R}^{p^v_x}$. Assume now that $\mathbf{f}(\cdot)$ has been coded as a MATLAB function, `F`, where the function `F` takes $\mathbf{v} \in \mathbb{R}^{m_v}$ as its input and returns $\mathbf{f} \in \mathbb{R}^{m_f}$ as its output. Given the MATLAB function `F`, together with the index vector pair $(\mathbf{i}^{\mathbf{v}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{v}}_{\mathbf{x}})$ and the dimensions m_v and n_x, the ADiGator algorithm determines the index vector pair $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}})$ and the dimension m_f. Moreover, a MATLAB derivative function, `DF`, is generated such that `DF` takes $\mathbf{v}$ and $\mathbf{d}^{\mathbf{v}}_{\mathbf{x}}$ as its inputs, and returns $\mathbf{f}$ and $\mathbf{d}^{\mathbf{f}}_{\mathbf{x}}$ as its outputs. To do so, the algorithm uses a process that we have termed source transformation via operator overloading. This process begins by transforming the original user-defined source code into an intermediate source code where the new source code is augmented to contain calls to ADiGator specific transformation routines while preserving the original code's mathematical operations. The forward mode of AD (which is used by ADiGator) is then affected by performing three passes on the intermediate program. On the first pass, a record of all operations, variables, and flow control statements is built. On the second pass, derivative sparsity patterns are propagated, and overloaded unions are performed where code branches join.[1] On the third and final pass, derivative sparsity patterns are again propagated forward, while the procedures required to compute the output non-zero derivatives are printed to the derivative program. For a more detailed description of the method, the reader is referred to Weinstein and Rao (2016) and Patterson et al. (2013).

[1]This second pass is only required if there exists flow control in the user-defined program.

3.1 User Source to Intermediate Source Transformations

The first step in the ADiGator algorithm is to transform the user-defined source code into an intermediate source code. This process is applied to the user provided main function, as well as any user-defined external functions (or sub-functions) that it calls. For each function contained within the user-defined program, a corresponding intermediate function, `adigatortempfunc#`, is created such that # is a unique integer identifying the function. The initial transformation process is carried out by reading the user-defined function, line by line, and searching for keywords. The algorithm looks for the following code behaviors and routines: variable assignments, flow control, external function calls, global variables, code comments, and error statements. If the user-defined source code contains any statements that are not listed above (with the exception of operations defined in the overloaded library), then the transformation will produce an error stating that the algorithm cannot process the statement.

3.2 Overloaded Operations

Once the user-defined program has been transformed to the intermediate program, the forward mode of AD is affected by performing multiple passes on the intermediate program. In the presence of flow control, three passes (parsing, overmapping, and printing) are required, otherwise only two (parsing and printing) are required. In each pass, all overloaded objects are tracked by assigning each object a unique integer `id` value. In the parsing evaluation, information similar to conventional data flow graphs and control flow graphs is obtained by propagating overloaded objects with unique `id` fields. In the overmapping evaluation, forward mode AD is used to propagate derivative sparsity patterns, and overloaded unions are performed in areas where flow control branches join. In the printing evaluation, each basic block of function code is evaluated on its set of overmapped input objects. In this final pass, the overloaded operations perform two tasks: propagating derivative sparsity patterns and printing the procedures required to compute the non-zero derivatives at each link in the forward chain rule. In this section, we briefly introduce the overloaded `cada` class, the manner in which it is used to exploit sparsity at transformation-time, a specific type of known numeric objects, and the manner in which the overloaded class handles logical references/assignments.

3.2.1 The Overloaded `cada` *Class.* The overloaded class is introduced by first considering a variable $\mathbf{Y}(\mathbf{x}) \in \mathbb{R}^{q_y \times r_y}$, where $\mathbf{Y}(\mathbf{x})$ is assigned to the identifier 'Y' in the user's code. It is then assumed that there exist some elements of $\mathbf{Y}(\mathbf{x})$ that are identically zero for any $\mathbf{x} \in \mathbb{R}^{n_x}$. These elements are identified by the strictly increasing index vector $\bar{\mathbf{i}}^{\mathbf{y}} \in \mathbb{Z}_+^{\bar{p}^f}$, $0 \leq \bar{p}^f \leq m_y$, where

$$\mathbf{y}_{[\bar{i}^y(k)]} = 0, \quad \forall \mathbf{x} \in \mathbb{R}^{n_x} \quad (k = 1, \ldots, \bar{p}^f),$$

and $\mathbf{y}(\mathbf{x})$ is the unrolled column-major vector representation of $\mathbf{Y}(\mathbf{x})$. It is then assumed that the possible non-zero elements of the unrolled Jacobian, $\partial \mathbf{y}/\partial \mathbf{x} \in \mathbb{R}^{m_y \times n_x}$ ($m_y = q_y r_y$), are defined by the row/column/value triplet $(\mathbf{i}_{\mathbf{x}}^{\mathbf{y}}, \mathbf{j}_{\mathbf{x}}^{\mathbf{y}}, \mathbf{d}_{\mathbf{x}}^{\mathbf{y}}) \in \mathbb{Z}_+^{p_x^y} \times \mathbb{Z}_+^{p_x^y} \times \mathbb{R}^{p_x^y}$. The corresponding overloaded object, denoted $\mathcal{Y}$, would then have the following function and derivative properties:

Function		Derivative	
name:	'Y.f'	name:	'Y.dx'
size:	(q_y, r_y)	nzlocs:	(i_x^y, j_x^y)
zerolocs:	$\bar{i}^y$		

Assuming that the object $\mathcal{Y}$ is instantiated during the printing pass, the procedures will have been printed to the derivative file such that, on evaluation of the derivative file, `Y.f` and `Y.dx` will

be assigned the values of $\mathbf{Y}$ and $\mathbf{d}_{\mathbf{x}}^{\mathbf{y}}$, respectively. It is important to stress that the values of (q_y, r_y), $\bar{\mathbf{i}}^{\mathbf{y}}$, and $(\mathbf{i}_{\mathbf{x}}^{\mathbf{y}}, \mathbf{j}_{\mathbf{x}}^{\mathbf{y}})$ are all assumed to be fixed at the time of derivative file generation. Moreover, by adhering to the assumption that these values are fixed, it is the case that all overloaded operations must result in objects with fixed sizes and fixed derivative sparsity patterns (with the single exception to this rule given in Section 3.2.4). It is also noted that all user objects are assumed to be scalars, vectors, or matrices. Thus, while MATLAB allows for one to use n-dimensional arrays, the ADiGator algorithm may only be used with two-dimensional arrays.

3.2.2 Exploiting Sparsity at the Operation Level. Holding to the assumption that all input sizes and sparsity patterns are fixed, any files that are generated by the algorithm are only valid for a single input size and derivative sparsity pattern. Fixing this information allows the algorithm to accurately propagate derivative sparsity patterns during the generation of derivative files. Moreover, rather than relying on compression techniques to exploit sparsity of the program as a whole, sparsity is exploited at *every* link in the forward chain rule. Typically, this is achieved by only applying the chain rule to vectors of non-zero derivatives (for example, $\mathbf{d}_{\mathbf{x}}^{\mathbf{y}}$). To illustrate this point, we consider the simple function line:

```
W = sin(Y);.
```

The chain rule for the corresponding operation $\mathbf{W}(\mathbf{x}) = \sin(\mathbf{Y}(\mathbf{x}))$ is then given by

$$\frac{\partial \mathbf{w}}{\partial \mathbf{x}} = \begin{bmatrix} \cos(y_1) & 0 & \cdots & 0 \\ 0 & \cos(y_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \cos(y_{m_y}) \end{bmatrix} \frac{\partial \mathbf{y}}{\partial \mathbf{x}}, \tag{1}$$

where $\mathbf{w} \in \mathbb{R}^{m_y}$ is the unrolled column-major vector representation of $\mathbf{W}$. Given $(\mathbf{i}_{\mathbf{x}}^{\mathbf{y}}, \mathbf{j}_{\mathbf{x}}^{\mathbf{y}}) \in \mathbb{Z}_+^{p_x^y} \times \mathbb{Z}_+^{p_x^y}$, Equation (1) may sparsely be carried out by the procedure

$$d_{\mathbf{x}}^{\mathbf{w}}(k) = \cos(y_{[i_{\mathbf{x}}^{y}(k)]}) d_{\mathbf{x}}^{\mathbf{y}}(k), \quad k = 1, \ldots, p_x^y. \tag{2}$$

Moreover, the index vector pair that identifies the possible non-zero locations of $\partial \mathbf{w}/\partial \mathbf{x}$ is identical to that of $\partial \mathbf{y}/\partial \mathbf{x}$. During the printing evaluation, the overloaded `sin` routine would have access to $(\mathbf{i}_{\mathbf{x}}^{\mathbf{y}}, \mathbf{j}_{\mathbf{x}}^{\mathbf{y}})$ and print the procedures of Equation (2) to the derivative file as the MATLAB procedure

```
W.dx = cos(Y(Index1)).*Y.dx;,
```

where the variable `Index1` would be assigned the value of the index vector $\mathbf{i}_{\mathbf{x}}^{\mathbf{y}}$ and written to memory at the time the derivative procedure is printed. Thus, sparsity is exploited at transformation time, such that the chain rule is carried out at runtime by only operating on vectors of non-zero derivatives. Similar derivative procedures are printed for all array operations (for instance `sqrt`, `log`, `+`, `.*`).

The case where the chain rule is not simply applied to vectors of non-zero derivatives at runtime is that of matrix operations (for example, summation, matrix multiplication, etc.). In general, the inner derivative matrices of such operations contain rows with more than one non-zero value. Thus, the chain rule may not, in general, be carried out by performing element-wise array multiplications on vectors. Derivative sparsity, however, may still be exploited for such operations. For instance, consider the matrix operation $\mathbf{Z}(\mathbf{x}) = \mathbf{A}\mathbf{Y}(\mathbf{x})$, $\mathbf{A} \in \mathbb{R}^{q_z \times q_y}$, where $\mathbf{A}$ is a constant matrix. The chain rule associated with this operation is given as

$$\frac{\partial \mathbf{Z}}{\partial x_k} = \mathbf{A} \frac{\partial \mathbf{Y}}{\partial x_k}, \quad (k = 1, \ldots, n_x).$$

Suppose now that

$$\mathbf{B} \equiv \left[\frac{\partial \mathbf{Y}}{\partial x_1} \cdots \frac{\partial \mathbf{Y}}{\partial x_{n_x}} \right] \in \mathbb{R}^{q_y \times r_y n_x}.$$

Then

$$\mathbf{C} \equiv \mathbf{AB} = \left[\mathbf{A}\frac{\partial \mathbf{Y}}{\partial x_1} \cdots \mathbf{A}\frac{\partial \mathbf{Y}}{\partial x_{n_x}} \right] = \left[\frac{\partial \mathbf{Z}}{\partial x_1} \cdots \frac{\partial \mathbf{Z}}{\partial x_{n_x}} \right] \in \mathbb{R}^{q_z \times r_y n_x}, \tag{3}$$

where the matrices $\mathbf{B}$ and $\mathbf{C}$ have the same column-major linear indices as $\partial \mathbf{y}/\partial \mathbf{x}$ and $\partial \mathbf{z}/\partial \mathbf{x}$, respectively. Now consider that, given the index vector pair $(\mathbf{i}_{\mathbf{x}}^{\mathbf{y}}, \mathbf{j}_{\mathbf{x}}^{\mathbf{y}})$, the sparsity pattern of $\mathbf{B}(\mathbf{x})$ is known. Moreover, if there exist any columns of $\mathbf{B}$ that are known to be zero, then the matrix multiplication of Equation (3) performs redundant computations on columns whose entries are all zero. We now allow the strictly increasing index vector $\mathbf{k}_{\mathbf{x}}^{\mathbf{y}} \in \mathbb{Z}_+^{s_x^y}$, $s_x^y \leq r_y n_x$, to denote the columns of $\mathbf{B}$ that are *not* zero, and let

$$\mathbf{D} \equiv \left[\mathbf{B}_{[k_{\mathbf{x}}^{\mathbf{y}}(1)]} \cdots \mathbf{B}_{[k_{\mathbf{x}}^{\mathbf{y}}(s_x^y)]} \right] \in \mathbb{R}^{q_y \times s_x^y}$$

be the collection of possibly non-zero columns of $\mathbf{B}$. All of the elements of $\mathbf{d}_{\mathbf{x}}^{\mathbf{z}}$ must then be contained within the matrix

$$\mathbf{AD} = \left[\mathbf{C}_{[k_{\mathbf{x}}^{\mathbf{y}}(1)]} \cdots \mathbf{C}_{[k_{\mathbf{x}}^{\mathbf{y}}(s_x^y)]} \right] \in \mathbb{R}^{q_z \times s_x^y}. \tag{4}$$

The ADiGator algorithm takes advantage of this fact and produces derivative procedures corresponding to Equation (4), where the resulting values of $\mathbf{d}_{\mathbf{x}}^{\mathbf{z}}$ may be referenced directly from the result of Equation (4).

3.2.3 Known Numeric Objects. A common error that occurs when using operator overloading in MATLAB is given as

‘`Conversion to double from someclass not possible`.’

This typically occurs when attempting to perform a subscript-index assignment such as `y(i) = x`, where `x` is overloaded and `y` is of the `double` class. To avoid this error and to properly track all variables in the intermediate program, the ADiGator algorithm ensures that *all* active variables in the intermediate program are overloaded. Moreover, immediately after a numeric variable (`double`, `logical` etc.) is created, it is transformed into a “known numeric object,” whose only relevant properties are its stored numeric value, string name and `id`. The numeric value is then assumed to be fixed. As a direct consequence, *all* operations performed in the intermediate program are forced to be overloaded. At times, this consequence may be adverse as redundant auxiliary computations may be printed to the derivative file. Moreover, in the worst case, one of the operations in question may not have an overloaded routine written, and thus produce an error.

3.2.4 Logical References and Assignments. As stated in Section 3.2.1, the algorithm only allows for operations that result in variables of a fixed size (given a fixed dimensional input). It is often the case, however, that one wishes to perform operations on only certain elements of a vector, where the element locations are determined by the values of the entries of the vector. To allow for such instances, the algorithm allows for unknown logical array references under the condition that, if a logical index reference is performed, the result of the logical reference must be assigned to a variable via a logical index assignment. Moreover, the same logical index variable must be used for both the reference and assignment. This method of handling logical array references and assignments allows for all variables of the derivative program to be of a fixed dimension, yet can result in some unnecessary computation.

3.3 Handling of Flow Control

The ADiGator algorithm handles flow control by performing overloaded unions where code fragments join. Namely, the unions are performed on the exit of conditional `if/elseif/else` statements, on the entrance of `for` loop statements, and on both the entrance and exit of user-defined external functions and `while` loops. While this approach allows the software to differentiate routines containing flow control and to transcribe the flow control to the derivative program, it does introduce some limitations and adverse effects. The negative consequences of this approach are summarized as follows. The software is limited in that it cannot differentiate programs that recursively call the same routines, nor is the software entirely robust to different instances of the same variable changing sizes. It is also the case that sparsity cannot always be fully exploited in the presence of flow control. Furthermore, derivative file generation times will be proportional to the number of loop iterations in a program, as loops must be unrolled for purposes of analysis. For a more in-depth analysis of of the methods used to differentiate programs containing flow control, the reader is referred to Weinstein and Rao (2016).

4 OVERLOADED CELL AND STRUCTURE ARRAYS

In Section 3, it was assumed that all user variables in the originating program are of class `double`. In the intermediate program, all such objects are effectively replaced by objects of the `cada` class (Patterson et al. 2013), where each `cada` object is tracked by a unique `id` value. It is sometimes the case, however, that a user code is made to contain cell and/or structure arrays, where the elements of the arrays contain objects of the `double` class. In the intermediate program, it is then desirable to track the outermost cell and/or structure arrays, rather than each of the objects of which the array is composed. To this end, all cell and structure arrays are replaced with objects of the `cadastruct` class during the overloaded analysis. Each `cadastruct` object is then assigned a unique `id` value, assuming it does not correspond to a scalar structure. In the event that a scalar structure is built, then each of the fields of the scalar structure is treated as a unique variable. The `cadastruct` objects are themselves made to contain objects of the `cada` class; however, the embedded `cada` objects are not tracked (assuming the object does not correspond to a scalar structure). The handling of cell and structure arrays in this manner allows the algorithm to perform overloaded unions of cell and structure arrays and to print loop iteration-dependent cell/structure array references and assignments.

5 VECTORIZATION OF THE CADA CLASS

In this section, the differentiation of a special class of vectorized functions is considered, where we define a vectorized function as any function of the form of $\mathbf{F} : \mathbb{R}^{n_x \times N} \to \mathbb{R}^{m_f \times N}$ that performs the vector valued function $\mathbf{f} : \mathbb{R}^{n_x} \to \mathbb{R}^{m_f}$ on each column of its input. That is,

$$\mathbf{F}(\mathbf{X}) = [\,\mathbf{f}(\mathbf{X}_1)\ \mathbf{f}(\mathbf{X}_2)\ \cdots\ \mathbf{f}(\mathbf{X}_N)\,] \in \mathbb{R}^{m_f \times N}, \tag{5}$$

where $\mathbf{X}_k \in \mathbb{R}^{n_x}$, $k = 1, \ldots, N$,

$$\mathbf{X} = [\,\mathbf{X}_1\ \mathbf{X}_2\ \cdots\ \mathbf{X}_N\,] \in \mathbb{R}^{n_x \times N}.$$

It is stressed that the vectorized functions of this section are not limited to a single operation but rather may be coded as a sequence of operations. Similarly to array operations, vectorized functions have a sparse block-diagonal Jacobian structure due to the fact that

$$\frac{\partial F_{l,i}}{\partial X_{j,k}} = 0, \quad \forall i \neq k,\ l = 1, \ldots, m_f,\ j = 1, \ldots, n_x.$$

Allowing

$$\mathbf{X}^{\dagger} = \begin{bmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \\ \vdots \\ \mathbf{X}_N \end{bmatrix} \in \mathbb{R}^{n_x N}, \quad \mathbf{F}_k = \mathbf{f}(\mathbf{X}_k) \in \mathbb{R}^{m_f}$$

and

$$\mathbf{F}^{\dagger}(\mathbf{X}) = \begin{bmatrix} \mathbf{F}_1 \\ \mathbf{F}_2 \\ \vdots \\ \mathbf{F}_N \end{bmatrix} \in \mathbb{R}^{m_f N},$$

the two-dimensional Jacobian $\partial \mathbf{F}^{\dagger}/\partial \mathbf{X}^{\dagger}$ is given by the block-diagonal matrix

$$\frac{\partial \mathbf{F}^{\dagger}}{\partial \mathbf{X}^{\dagger}} = \begin{bmatrix} \frac{\partial \mathbf{F}_1}{\partial \mathbf{X}_1} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \frac{\partial \mathbf{F}_2}{\partial \mathbf{X}_2} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \frac{\partial \mathbf{F}_N}{\partial \mathbf{X}_N} \end{bmatrix} \in \mathbb{R}^{m_f N \times n_x N}, \tag{6}$$

where

$$\frac{\partial \mathbf{F}_i}{\partial \mathbf{X}_i} = \begin{bmatrix} \frac{\partial F_{1,i}}{\partial X_{1,i}} & \frac{\partial F_{1,i}}{\partial X_{2,i}} & \cdots & \frac{\partial F_{1,i}}{\partial X_{n_x,i}} \\ \frac{\partial F_{2,i}}{\partial X_{1,i}} & \frac{\partial F_{2,i}}{\partial X_{2,i}} & \cdots & \frac{\partial F_{2,i}}{\partial X_{n_x,i}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial F_{m_f,i}}{\partial X_{1,i}} & \frac{\partial F_{m_f,i}}{\partial X_{2,i}} & \cdots & \frac{\partial F_{m_f,i}}{\partial X_{n_x,i}} \end{bmatrix} \in \mathbb{R}^{m_f \times n_x}, \quad i = 1, \ldots, N. \tag{7}$$

Such functions commonly occur when utilizing collocation methods (Ascher et al. 1995) to obtain numerical solutions of ordinary differential equations, partial differential equations, or integral equations. In such cases, it is the goal to obtain the values of $\mathbf{X} \in \mathbb{R}^{n_x \times N}$ that solve the equation

$$\mathbf{c}(\mathbf{F}(\mathbf{X}), \mathbf{X}) = \mathbf{0} \in \mathbb{R}^{m_c}, \tag{8}$$

where $\mathbf{F}(\mathbf{X})$ is of the form of Equation (5). Now, one could apply AD directly to Equation (8); however, it is often the case that it is more efficient to instead apply AD separately to the function $\mathbf{F}(\mathbf{X})$, where the specific structure of Equation (6) may be exploited. The results may then be used to compute the derivatives of Equation (8).

Due to the block-diagonal structure of Equation (6), it is the case that the vectorized problem has an inherently compressible Jacobian with a maximum column dimension of n_x. This compression may be performed via the pre-defined Curtis-Powell-Reid seed matrix

$$\mathbf{S} = \begin{bmatrix} \mathbf{I}_{n_x} \\ \mathbf{I}_{n_x} \\ \vdots \\ \mathbf{I}_{n_x} \end{bmatrix} \in \mathbb{R}^{n_x N \times n_x}, \tag{9}$$

where $\mathbf{I}_{n_x}$ is the $n_x \times n_x$ identity matrix. The ADiGator algorithm in the vectorized mode does not, however, rely on matrix compression but rather utilizes the fact that the structure of the Jacobian of Equation (6) is determined by the structure of the Jacobian of Equation (7). To exhibit this point,

the row/column pairs of the derivative of $\mathbf{f}$ with respect to its input are now denoted by $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}}) \in \mathbb{Z}_+^{p^f_x} \times \mathbb{Z}_+^{p^f_x}$. The N derivative matrices, $\partial \mathbf{F}_i / \partial \mathbf{X}_i$, may then be represented by the row/column/value triplets $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{d}^{\mathbf{F}_i}_{\mathbf{X}_i}) \in \mathbb{Z}_+^{p^f_x} \times \mathbb{Z}_+^{p^f_x} \times \mathbb{R}^{p^f_x}$ together with the dimensions m_f and n_x. All possible non-zero derivatives of $\partial \mathbf{F} / \partial \mathbf{X}$ are then given by

$$\mathbf{D}^{\mathbf{F}}_{\mathbf{X}} = \left[\begin{array}{cccc} \mathbf{d}^{\mathbf{F}_1}_{\mathbf{X}_1} & \mathbf{d}^{\mathbf{F}_2}_{\mathbf{X}_2} & \cdots & \mathbf{d}^{\mathbf{F}_N}_{\mathbf{X}_N} \end{array} \right] \in \mathbb{R}^{p^f_x \times N}. \tag{10}$$

Furthermore, $\partial \mathbf{F} / \partial \mathbf{X}$ may be fully defined given the vectorized row/column/value triplets $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{D}^{\mathbf{F}}_{\mathbf{X}}) \in \mathbb{Z}_+^{p^f_x} \times \mathbb{Z}_+^{p^f_x} \times \mathbb{R}^{p^f_x \times N}$, together with the dimensions n_x, m_f, and N. Thus, to print derivative procedures of a vectorized function as defined in Equation (5), it is only required to propagate row/column index vector pairs $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}}) \in \mathbb{Z}_+^{p^f_x} \times \mathbb{Z}_+^{p^f_x}$ corresponding to the non-vectorized problem, and to print procedures that compute vectorized non-zero derivatives, $\mathbf{D}^{\mathbf{F}}_{\mathbf{X}} \in \mathbb{R}^{p^f_x \times N}$.

To identify vectorized `cada` objects, all vectorized `cada` instances are made to have a value of `Inf` located in the size field corresponding to the vectorized dimension. Then, at each vectorized `cada` operation, sparsity patterns of the non-vectorized problem are propagated (that is, $(\mathbf{i}^{\mathbf{f}}_{\mathbf{x}}, \mathbf{j}^{\mathbf{f}}_{\mathbf{x}})$) and procedures are printed to the derivative file to compute the vectorized function and vectorized derivative values (that is, $\mathbf{F}$ and $\mathbf{D}^{\mathbf{F}}_{\mathbf{X}}$). It is then the case that any operations performed on a vectorized `cada` object must be of the form given in Equation (5).

Here is is noted that, given a fixed value of N, the non-vectorized mode may easily be used to print the procedures required to compute the non-zero derivatives of $\mathbf{F}(\mathbf{X})$. Typically the derivative files generated by the vectorized and non-vectorized modes will perform the exact same floating point operations at runtime. One may then question the advantages of utilizing the vectorized mode, particularly when more work is required of the user to separate vectorized functions. The advantages of the vectorized mode are given as follows:

(1) *Derivative files are vectorized.* Typically, functions of the form of Equation (5) are coded such that the value of N may be any positive integer. By utilizing the vectorized mode, it is the case that the derivative files are generated such that N may be any positive integer. In contrast, any files generated using the non-vectorized mode are only valid for fixed input sizes. Allowing the dimension N to change is particularly helpful when using collocation methods together with a process known as mesh refinement (Betts 2009), because in such instances the problem of Equation (8) must often be re-solved for different values of N.

(2) *Transformation time is reduced.* By taking advantage of the fact that the sparsity of the vectorized problem (that is, $\mathbf{F}(\mathbf{X})$) is determined entirely by the sparsity of the non-vectorized problem (that is, $\mathbf{f}(\mathbf{x})$), it is the case that sparsity propagation costs are greatly reduced when using the vectorized mode over the non-vectorized mode.

(3) *Runtime overhead is reduced.* To exploit sparsity, the algorithm prints derivative procedures that perform many subscript index references and assignments at runtime. Unfortunately, these reference and assignment operations incur runtime penalties proportional to the length of the reference/assignment index vectors (Menon and Pingali 1999). Moreover, the lengths of the used reference and assignment indices are proportional to the number of non-zero derivatives at each link in the chain rule. When printing derivative procedures in the vectorized mode, however, the ":" character is used as a reference to *all* elements in the vectorized dimension. Thus, the lengths of the required index vectors are proportional to the number of non-zero derivatives of the non-vectorized problem (that is, $\partial \mathbf{f} / \partial \mathbf{x}$) rather than the vectorized problem (that is, $\partial \mathbf{F} / \partial \mathbf{X}$). Indexing reference/assignment runtime overheads are therefore reduced by an order of N when using the vectorized mode rather than the non-vectorized.

6 USER INTERFACE TO ADIGATOR

The computation of derivatives using the ADiGator package is carried out in a multi-step process. First, the user must code their function as a MATLAB program that conforms to the restrictions discussed in Section 3. The user must then fix information pertaining to the inputs of the program (that is, input variable sizes and derivative sparsity patterns). The ADiGator algorithm is then called to transform the user-defined function program into a derivative program, where the derivative program is only valid for the fixed input information. The ADiGator tool is then no longer used and the generated derivative program may be evaluated on non-overloaded objects to compute the desired derivatives.

To begin the transformation process, the ADiGator algorithm must create overloaded objects of the form discussed in Section 3.2.1. Thus, the user must provide certain information for each input to their program. Assuming temporarily that all user inputs to the original function program are of the `double` class, then all user inputs must fall into one of three categories:

- *Derivative inputs.* Derivative inputs are any inputs that are a function of the variable of differentiation. Derivative inputs must have a fixed size and fixed derivative sparsity pattern.
- *Known numeric inputs.* Known numeric inputs are any inputs whose values are fixed and known. These inputs will be transformed into the known numeric objects discussed in Section 3.2.3.
- *Unknown auxiliary inputs.* Unknown auxiliary inputs are any inputs that are not a function of the variable of differentiation nor are they of a fixed value. It is required, however, that unknown auxiliary inputs have a fixed size.

For each of the user-defined input variables, the user must identify to which category the input belongs and create an ADiGator input variable. Under the condition that a user-defined program takes a structure or cell as an input, the corresponding ADiGator input variable is made to be a structure or cell where each cell/structure element corresponding to an object of the `double` class must be identified as one of the three different input types. The ADiGator input variables are thus made to contain all fixed input information and are passed to the ADiGator transformation algorithm. The ADiGator transformation algorithm is then carried out using the `adigator` command that requires the created ADiGator input variables, the name of the main function file of the user-defined program, and the name of which the generated derivative file is to be titled. The generated derivative program then has the same input structure as the originating program with the exception that derivative inputs must be replaced by structures containing derivative input function values and non-zero derivative values. Moreover, the generated derivative program returns, for each output variable, the function values, possible non-zero derivative values, and locations of the possible non-zero derivatives. The user interface thus allows a great deal of flexibility for the user-defined function program input/output scheme. Moreover, the user is granted the ability to use any desired input seed matrices. For more information on how to use the ADiGator package, the reader is referred to the user's guide and examples that accompany the code.

7 EXAMPLES

In this section, the ADiGator tool is tested by solving four different classes of problems. In Section 7.1, the developed algorithm is used to integrate an ordinary differential equation with a large sparse Jacobian. In Section 7.2, a set of three fixed-dimension non-linear system of equations problems are investigated, and in Section 7.3, a large sparse unconstrained minimization problem is presented. Last, in Section 7.4, the vectorized mode of ADiGator is showcased by solving the large-scale non-linear programming problem that arises from the discretization of an

optimal control problem. For each of the tested problems, comparisons are drawn against methods of finite-differencing, the well-known MATLAB AD tools ADiMat version 0.6.0, INTLAB version 6, and MAD version 1.4, and, when available, hand-coded derivative files. All computations were performed on an Apple Mac Pro with Mac OS-X 10.9.2 (Mavericks) and a 2×2.4GHz Quad-Core Intel Xeon processor with 24GB 1066MHz DDR3 RAM using MATLAB version R2014a. All reported times were computed using MATLAB's tic/toc routines and averaging over 1,000 iterations.

7.1 Stiff Ordinary Differential Equation

In this section, the well-known Burgers' equation is solved using a moving mesh technique as presented in Huang et al. (1994). The form of Burgers' equation used for this example is given by

$$\dot{u} = \alpha \frac{\partial^2 u}{\partial y^2} - \frac{\partial}{\partial y}\left(\frac{u^2}{2}\right), \quad 0 < y < 1, \; t > 0, \; \alpha = 10^{-4} \tag{11}$$

with boundary conditions and initial conditions

$$\begin{aligned} u(0,t) &= u(1,t) = 0, && t > 0, \\ u(y,0) &= \sin(2\pi y) + \tfrac{1}{2}\sin(\pi y), && 0 \le y \le 1. \end{aligned} \tag{12}$$

The partial differential equation (PDE) of Equation (11) is then transformed into an ordinary differential equation (ODE) via a central difference discretization together with the moving mesh PDE, MMPDE6 (with $\tau = 10^{-3}$), and spatial smoothing is performed with parameters $\gamma = 2$ and $p = 2$. The result of the discretization is then a stiff ODE of the form

$$\mathbf{M}(t,x)\dot{\mathbf{x}} = \mathbf{f}(t,\mathbf{x}), \tag{13}$$

where $\mathbf{M} : \mathbb{R} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x \times n_x}$ is a mass-matrix function and $\mathbf{f} : \mathbb{R} \times \mathbb{R}^{n_x} \to \mathbb{R}^{n_x}$ is the ODE function. This problem is given as an example problem for the MATLAB ODE suite and is solved with the stiff ODE solver, `ode15s` (Shampine and Reichelt 1997), which allows the user to supply the Jacobian $\partial\mathbf{f}/\partial\mathbf{x}$.

Prior to actually solving the ODE, a study is performed on the efficiency of differentiation of the function $\mathbf{f}(t,\mathbf{x})$ for varying values of n_x, where the code for the function $\mathbf{f}(t,\mathbf{x})$ has been taken verbatim from the MATLAB example file `burgersode`. The Jacobian $\partial\mathbf{f}/\partial\mathbf{x}$ is inherently sparse and compressible, where a Curtis-Powell-Reid seed matrix $\mathbf{S} \in \mathbb{Z}_+^{n_x \times 18}$ may be found for all $n_x \ge 18$. Thus, the Jacobian $\partial\mathbf{f}/\partial\mathbf{x}$ becomes increasingly more sparse as the dimension of n_x is increased. A test was first performed by applying the AD tools ADiGator, ADiMat, INTLAB, and MAD to the function code for $\mathbf{f}(t,\mathbf{x})$. It was found, however, that all tested AD tools perform quite poorly, particularly when compared to the theoretical efficiency of a sparse finite difference.[2] The reason for the poor performance is due to the fact that the code used to compute $\mathbf{f}$ contains four different explicit loops, each of which runs for $\frac{n_x}{2} - 2$ iterations and performs scalar operations. When dealing with the explicit loops, all tested AD tools incur a great deal of runtime overhead penalties. To quantify these runtime overheads, the function file that computes $\mathbf{f}$ was modified such that all loops (and scalar operations within the loops) were replaced by the proper corresponding array operations and vector reference/assignment index operations.[3] A test was then performed by applying AD to the resulting modified file. The results obtained by applying AD to both the original

[2]Forward difference approximations with respect to n variables may be accomplished by $n + 1$ function evaluations, one for the perturbation of each variable and one for the function at the input value. When utilizing matrix compression, one may replace n with the second dimension of the seed matrix $\mathbf{S}$.

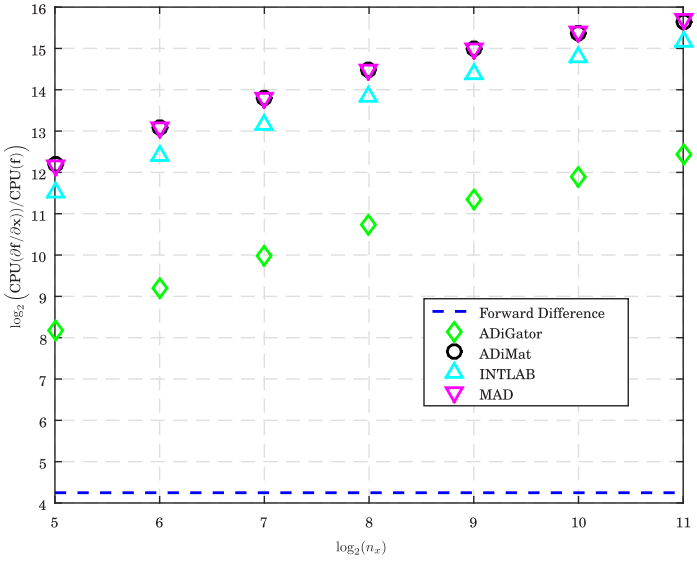
[3]This process of replacing loops with array operations is often referred to as "vectorization." In this article the term "vectorized" has already been used to refer to a specific class of functions in Section 5. Thus, to avoid any confusion, use of the term "vectorization" is avoided when referring to functions whose loops have been replaced.

Table 1. Burgers' ODE Function CPU and ADiGator Generation CPU Times

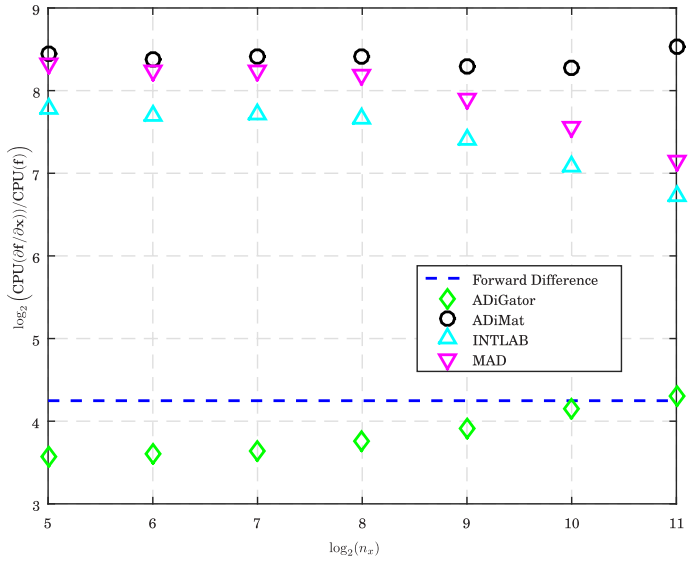
n_x:	32	64	128	256	512	1,024	2,048
Function File Computation Time (ms)							
with loops:	0.2046	0.2120	0.2255	0.2449	0.2895	0.3890	0.5615
without loops:	0.2122	0.2190	0.2337	0.2524	0.2973	0.3967	0.5736
ADiGator Derivative File Generation Time (s)							
with loops:	2.410	4.205	7.846	15.173	30.130	62.754	137.557
without loops:	0.682	0.647	0.658	0.666	0.670	0.724	0.834

and modified files are given in Figure 1. Results were obtained using ADiGator in the default mode, ADiMat in the scalar compressed forward mode, INTLAB's `gradient` class, and MAD in the compressed forward mode. Within this figure it is seen that all tested AD tools greatly benefit from the removal of the loop statements. Moreover, it is seen that the ADiGator tool performs relatively well compared to that of a theoretical finite difference. To further investigate the handling of explicit loops, absolute function CPU times and ADiGator file generation times are given in Table 1. Within this table, it is seen that the reason the original Burgers' ODE function file is written with loops is that it is slightly more efficient than when the loops are removed. It is, however, also seen that when using the ADiGator tool to generate derivative files, the cost of the transformation of the original code containing loops increases immensely as the value of n_x increases. This increase in cost is due to the fact that the ADiGator tool effectively unrolls loops for the purpose of analysis and thus must perform a number of overloaded operations proportional to the value of n_x. When applying the ADiGator tool to the file containing no explicit loops, however, the number of required overloaded operations stays constant for all values of n_x. From this analysis, it is clear that explicit loops should largely be avoided whenever using any of the tested AD tools. Moreover, it is clear that the efficiency of applying AD to a MATLAB function is not necessarily proportional to the efficiency of the original function.

The efficiency of the ADiGator tool is now investigated by solving the ODE and comparing solution times obtained by supplying the Jacobian via the ADiGator tool versus supplying the Jacobian sparsity pattern and allowing `ode15s` to use the `numjac` finite-difference tool to compute the required derivatives. It is important to note that the `numjac` finite-difference tool was specifically designed for use with the MATLAB ODE suite, where a key component of the algorithm is to choose perturbation step-sizes at one point based off of data collected from previous time steps (Shampine and Reichelt 1997). Moreover, it is known that the algorithm of `ode15s` is not extremely reliant on precise Jacobian computations, and thus the `numjac` algorithm is not required to compute extremely accurate Jacobian approximations (Shampine and Reichelt 1997). For these reasons, it is expected that when using `numjac` in conjunction with `ode15s`, Jacobian to function CPU ratios should be near the theoretical values shown in Figure 1. To present the best case scenarios, tests were performed by supplying `ode15s` with the more efficient function file containing loop statements. When the ADiGator tool was used, Jacobians were supplied by the files generated by differentiating the function whose loops had been removed. In both cases, the ODE solver was supplied with the mass matrix, the mass matrix derivative sparsity pattern, and the Jacobian sparsity pattern. Moreover, absolute and relative tolerances were set equal to 10^{-5} and 10^{-4}, respectively, and the ODE was integrated on the interval $t = [0, 2]$. Test results may be seen in Table 2, where it is seen that the ODE may be solved more efficiently when using `numjac` for all test cases except $n_x = 2,048$. It is also seen that the number of Jacobian evaluations required when using either finite differences or AD are roughly equivalent. Thus, the `ode15s` algorithm, in this case, is largely unaffected by supplying a more accurate Jacobian.



(a) With Explicit Loops



(b) Without Explicit Loops

Fig. 1. Burgers' ODE Jacobian to function CPU ratios. All ratios presented in binary logarithm format. (a) Ratios obtained by differentiating the original implementation of $\mathbf{f}$ containing explicit loops. (b) Ratios obtained by differentiating the modified implementation of $\mathbf{f}$ containing no explicit loops. In both cases, the dashed line represents the binary logarithm of the theoretical ratio for a sparse forward difference given by $\log_2\left(\text{CPU}(\partial\mathbf{f}/\partial\mathbf{x})\right)/\text{CPU}(\mathbf{f})\right) = log_2(19) \approx 4.25$.

Table 2. Burgers' ODE Solution Times

n_x:	32	64	128	256	512	1,024	2,048
ODE Solve Time (s)							
ADiGator:	1.471	1.392	2.112	4.061	10.472	36.386	139.813
`numjac`:	1.383	1.284	1.958	3.838	9.705	32.847	140.129
Number of Jacobian Evaluations							
ADiGator:	98	92	126	197	305	495	774
`numjac`:	92	92	128	194	306	497	743

Table 3. Jacobian to Function CPU Ratios for CPF, HHD, and CTS Problems

Problem:	CPF	HHD	CTS
Jacobian to Function CPU Ratios, CPU($\partial f/\partial x$)/CPU(f)			
ADiGator:	8.0	21.3	7.3
ADiMat:	197.0	226.3	56.3
INTLAB:	298.5	436.5	85.9
MAD:	474.8	582.6	189.8
hand:	1.3	1.2	11.3
sfd:	12.0	9.0	7.0

7.2 Fixed-Dimension Nonlinear Systems of Equations

In this section, analysis is performed on a set of fixed-dimension nonlinear system of equations problems taken from the MINPACK-2 problem set (Averick et al. 1992). While originally coded in Fortran, the implementations used for the tests of this section were obtained from Lenton (2005). The specific problems chosen for analysis are those of the "combustion of propane fuel" (CPF), "human heart dipole" (HHD), and "coating thickness standardization" (CTS). The CPF and HDD problems represent systems of nonlinear equations $\mathbf{f}:\mathbb{R}^n \to \mathbb{R}^n$ ($n = 11$ and $n = 8$, respectively), where it is desired to find $\mathbf{x}^*$ such that $\mathbf{f}(\mathbf{x}^*) = \mathbf{0}$. The CTS problem represents a system of nonlinear equations $\mathbf{f}:\mathbb{R}^{134} \to \mathbb{R}^{252}$, where it is desired to find $\mathbf{x}^*$ that minimizes $\mathbf{f}(\mathbf{x})$ in the least-squared sense. The standard methods used to solve such problems are based on Newton iterations and thus require iterative Jacobian computations.

Prior to solving the nonlinear problems, a test is first performed to gauge the efficiency of the Jacobian computation compared to the other well-known MATLAB AD tools. The implementation of Lenton (2005) provides hand-coded Jacobian files that also provide a convenient baseline for computation efficiency. For each of the problems the ADiGator tool was tested against the ADiMat tool in the scalar compressed forward mode, the INTLAB tool's `gradient` class, the MAD tool in the compressed forward mode, and the hand-coded Jacobian as provided by Lenton (2005). Moreover, it is noted that the Jacobians of the CPF and HHD functions are incompressible while the Jacobian of the CTS function is compressible with a column dimension of six. Thus, for the CPF and HHD tests, the ADiMat and MAD tools are essentially used in the full modes. The resulting Jacobian to function CPU ratios are given in Table 3 together with the theoretical ratio for a sparse finite difference (sfd). From Table 3, it is seen that the ADiGator algorithm performs relatively better on the sparser CPF and CTS functions (whose Jacobians contain 43.8% and 2.61% non-zero entries, respectively) than on the denser HHD problem (whose Jacobian contains 81.25% non-zero entries). Moreover, it is seen that, on the incompressible CPF problem, the ADiGator algorithm performs more efficiently than a theoretical sparse finite difference. Furthermore, in the case of

Table 4. Solution Times for Fixed Dimension Nonlinear Systems

Problem:	CPF	HHD	CTS
Solution Time (s)			
ADiGator:	0.192	0.100	0.094
sfd:	0.212	0.111	0.091
Number of Iterations			
ADiGator:	96	38	5
sfd:	91	38	5
ADiGator File Generation Time (s)			
	0.429	0.422	0.291

the compressible CTS problem, the ADiGator tool performs more efficiently than the hand-coded Jacobian file.

Next, the three test problems were solved using the MATLAB optimization toolbox functions `fsolve` (for the CPF and HHD nonlinear root-finding problems) and `lsqnonlin` (for the CTS nonlinear least-squares problem). The problems were tested by supplying the MATLAB solvers with the Jacobian files generated by the ADiGator algorithm and by simply supplying the Jacobian sparsity patterns and allowing the optimization toolbox to perform sparse finite differences. Default tolerances of the optimization toolbox were used. The results of the test are shown in Table 4, which shows the solution times, number of required Jacobian evaluations, and ADiGator file generation times. From this table, it is seen that the CPF, HHD, and CTS problems solve in about the same amount of time whether supplied with the Jacobian via the ADiGator generated files or the MATLAB sparse finite-differencing routine. It is also noted that the time required to generate the ADiGator derivative files is actually greater than the time required to solve the problems. For this class of problems, however, the dimensions of the inputs are fixed, and thus the ADiGator generated derivative files must only be generated a single time.

7.3 Large-Scale Unconstrained Minimization

In this section, the 2D Ginzburg-Landau (GL2) minimization problem is tested from the MINPACK-2 test suite (Averick et al. 1992). The problem is to minimize the Gibbs free energy in the discretized Ginzburg-Landau superconductivity equations. The objective, f, is given by

$$f = \sum_{i=1}^{n_x} \sum_{j=1}^{n_y} -|v_{i,j}|^2 + \frac{1}{2}|v_{i,j}|^4 + \phi_{i,j}(\mathbf{v}, \mathbf{a}^{(1)}, \mathbf{a}^{(2)}), \tag{14}$$

where $\mathbf{v} \in \mathbb{C}^{(n_x+1)\times(n_y+1)}$ and $(\mathbf{a}^{(1)}, \mathbf{a}^{(2)}) \in \mathbb{R}^{(n_x+1)\times(n_y+1)} \times \mathbb{R}^{(n_x+1)\times(n_y+1)}$ are discrete approximations to the order parameter $\mathbf{V} : \mathbb{R}^2 \to \mathbb{C}$ and vector potential $\mathbf{A} : \mathbb{R}^2 \to \mathbb{R}^2$ at the equally spaced grid points $((k-1)h_x, (l-1)h_y), 1 \le k \le n_x + 1, 1 \le l \le n_y + 1$. Periodicity conditions are used to express the problem in terms of the variables $v_{k,l}$, $a^{(1)}_{k,l}$, and $a^{(2)}_{k,l}$ for $1 \le k \le n_x + 1, 1 \le l \le n_y + 1$. Moreover, both the real and imaginary components of $\mathbf{v}$ are treated as variables. Thus, the problem has $4n_xn_y$ variables. For the study conducted in this section, it was allowed that $n = 4n_xn_y$, $n_x = n_y$. Moreover, the Ginzburg-Landau constant, κ, and number of vortices, n_v, were set to $\kappa = 5$ and $n_v = 8$. The code used for the tests of this section was obtained from Lenton (2005), which also contains a hand-coded gradient file.[4] For the remainder of this section, the objective

[4]The files obtained from Lenton (2005) unpacked the decision vector by projecting into a three-dimensional array. The code was slightly modified to project only to a two-dimensional array to allow for use with the ADiGator tool.

Table 5. Different Derivative to Function CPU Ratios for 2D Ginzburg-Landau Problem for Increasing Values of n, where $n = 4n_x n_y$ and $n_x = n_y$

n:	16	64	256	1024	4096	16384
Ratios CPU($\partial f/\partial x$)/CPU(f)						
ADiGator:	6.3	6.3	7.0	9.6	10.9	12.0
ADiMat:	86.9	84.6	80.9	68.7	52.9	21.3
INTLAB:	67.9	67.1	65.4	60.1	57.7	41.0
MAD:	123.6	121.2	118.3	112.9	142.3	240.9
fd:	17.0	65.0	257.0	1025.0	4097.0	16385.0
hand:	3.8	4.2	4.2	3.8	3.8	2.5
Ratios CPU($\partial g/\partial x$)/CPU(f)						
ADiGator:	33.0	38.0	39.1	39.3	49.6	50.4
ADiMat:	632.5	853.1	935.6	902.1	731.4	420.4
INTLAB:	518.7	530.4	514.7	460.0	414.1	249.1
MAD:	896.2	876.9	838.9	724.3	579.8	267.8
sfd:	64.9	87.3	100.5	99.8	95.6	66.2
Ratios CPU($\partial^2 f/\partial x^2$)/CPU($f$)						
ADiGator:	9.7	10.7	13.1	20.5	45.4	62.9
ADiMat:	944.5	926.5	889.2	819.9	727.4	393.0
INTLAB:	102.4	102.3	138.4	2102.4	47260.0	-
MAD:	531.1	527.5	584.3	1947.6	19713.8	-
fd:	289.0	1365.0	6168.0	26650.0	102425.0	426010.0
Hessian Information						
# colors:	16	20	23	25	24	25
% non-zero:	62.50	19.53	4.88	1.22	0.31	0.08

function will be denoted by f, where $f : \mathbb{R}^n \to \mathbb{R}$ and the gradient function will be denoted $\mathbf{g}$, where $\mathbf{g} : \mathbb{R}^n \to \mathbb{R}^n$.

To test the efficiency of the ADiGator tool at both the first and second derivative levels, both the objective and gradient functions, f and $\mathbf{g}$, were differentiated. Thus, three different tests were performed by computing (1) the first derivative of the objective, $\partial f/\partial \mathbf{x}$; (2) the first derivative of the gradient, $\partial \mathbf{g}/\partial \mathbf{x}$; and (3) the second derivative of the objective, $\partial^2 f/\partial \mathbf{x}^2$, where $\partial \mathbf{g}/\partial \mathbf{x} = \partial^2 f/\partial \mathbf{x}^2$. The aforementioned derivatives were computed using the ADiGator, ADiMat, INTLAB, and MAD tools and results are given in Table 5. Additionally, Table 5 provides the theoretical derivative-to-function CPU ratios that would be required if a finite difference was to be used along with the derivative-to-function ratio of the hand-coded gradient file. The results presented in Table 5 were obtained as follows. For the gradient computation, $\partial f/\partial \mathbf{x}$, the tested AD tools were applied to the objective function where ADiMat was used in the reverse scalar mode, and INTLAB and MAD were used in the sparse forward modes. Additionally, the hand-coded gradient $\mathbf{g}$ was evaluated to compute the hand-coded ratios, and the ratio given for a finite difference is equal to $n + 1$. For the Jacobian computation, $\partial \mathbf{g}/\partial \mathbf{x}$, the tested AD tools were applied to the hand-coded gradient function where ADiMat was used in the forward compressed scalar mode, INTLAB was used in the sparse forward mode, and MAD was used in the forward compressed mode. The ratios given for a sparse finite difference are given as $(c + 1)$ times those of the hand-coded gradient ratios, where c is the number of Hessian colors provided in the table. For the Hessian computation, $\partial^2 f/\partial \mathbf{x}^2$, the tested AD tools were applied again to the objective function where ADiMat was used in the

Table 6. Adigator File Generation Times and Objective Function Evaluation Times for 2D Ginzburg-Landau Problem

n:	16	64	256	1,024	4,096	16,384
ADiGator File Generation Time (s)						
$\partial f/\partial x$:	0.51	0.51	0.52	0.53	0.58	0.90
$\partial g/\partial x$:	2.44	2.51	2.51	2.57	2.89	4.33
$\partial^2 f/\partial x^2$:	2.12	2.13	2.23	2.33	4.85	37.75
Objective Function Evaluation Time (ms)						
f:	0.2795	0.2821	0.2968	0.3364	0.4722	1.2611

Shown is the time required for ADiGator to perform the transformations: objective function f to an objective gradient function $\partial f/\partial \mathbf{x}$, gradient function $\mathbf{g}$ to Hessian function $\partial \mathbf{g}/\partial \mathbf{x}$, and gradient function $\partial f/\partial \mathbf{x}$ to Hessian function $\partial^2 f/\partial \mathbf{x}^2$.

compressed forward over scalar reverse mode (with operator overloading for the forward computation, `t1rev` option of `admHessian`), INTLAB was used in the sparse second-order forward mode, and MAD was used in the compressed forward mode over sparse forward mode. The ratios given for a finite-difference are equal to $(n+1)(c+1)$, the number of function evaluations required to approximate the Hessian via a central difference. As witnessed from Table 5, the ADiGator tool performs quite well at runtime compared to the other methods. While the hand-coded gradient may be evaluated faster than the ADiGator generated gradient file, the ADiGator generated file is, at worst, only 5 times slower and is generated automatically.

As seen in Table 5, the files generated by ADiGator are quite efficient at runtime. Moreover, the derivative files generated by ADiGator are only valid for a fixed dimension. Thus, one cannot disregard file generation times. To investigate the efficiency of the ADiGator transformation routine, absolute derivative file generation times together with absolute objective file evaluation times are given in Table 6. This table shows that the cost of generation of the objective gradient file, $\partial f/\partial \mathbf{x}$, and gradient Jacobian file, $\partial \mathbf{g}/\partial \mathbf{x}$, are relatively small, while the cost of generating the objective Hessian file becomes quite expensive at $n = 16384$. Simply revealing the file generation times, however, does not fully put into perspective the tradeoff between file generation time costs and runtime efficiency gains. To do so, a "cost of derivative computation" metric is formed, based off of the number of Hessian evaluations required to solve the GL2 minimization problem. To this end, the GL2 problem was solved using the MATLAB unconstrained minimization solver, `fmincon`, in the full-Newton mode with ADiGator supplied derivatives, and the number of required Hessian computations was recorded. Using the data of Tables 5 and 6, the metric was computed as the total time to perform the k required Hessian computations, using all of the tested AD tools. The results from this computation are given in Table 7, where two costs are given for using the ADiGator tool, one of which takes into account the time required to generate the derivative files. Due to the relatively low number of required Hessian evaluations, it is seen that the ADiGator tool is not always the best option when one factors in the file generation time. That being said, for this test example, files that compute the objective gradient and Hessian sparsity pattern are readily available, and thus the time required to generate them (automatically or otherwise) is not considered. Moreover, when using the ADiGator tool, one obtains the Hessian sparsity pattern and an objective gradient file as a direct result of the Hessian file generation.

7.4 Large Scale Nonlinear Programming

Consider the following nonlinear program (NLP) that arises from the discretization of a scaled version of the minimum time to climb (of a supersonic aircraft) optimal control problem described

Table 7. Cost of Differentiation for 2D Ginzburg-Landau Problem

n:	16	64	256	1,024	4,096	16,384
# Hes Eval:	9	11	26	21	24	26
# colors:	16	20	23	25	24	25
Cost of Differentiation: sfd over AD (s)						
ADiGator:	0.27	0.41	1.29	1.76	3.08	10.23
ADiGator*:	0.78	0.92	1.81	2.29	3.66	11.13
ADiMat:	3.71	5.51	14.99	12.63	15.00	18.19
INTLAB:	2.90	4.37	12.11	11.04	16.36	34.94
MAD:	5.29	7.90	21.90	20.73	40.33	205.34
hand:	0.16	0.27	0.78	0.70	1.08	2.17
Cost of Differentiation: AD over Hand-Coded (s)						
ADiGator:	0.08	0.12	0.30	0.28	0.56	1.65
ADiGator*:	2.52	2.63	2.81	2.85	3.45	5.98
ADiMat:	1.59	2.65	7.22	6.37	8.29	13.79
INTLAB:	1.30	1.65	3.97	3.25	4.69	8.17
MAD:	2.25	2.72	6.47	5.12	6.57	8.78
Cost of Differentiation: AD over AD (s)						
ADiGator:	0.02	0.03	0.10	0.14	0.51	2.06
ADiGator*:	2.65	2.68	2.85	3.01	5.94	40.71
ADiMat:	2.38	2.87	6.86	5.79	8.24	12.88
INTLAB:	0.26	0.32	1.07	14.85	535.61	†
MAD:	1.34	1.64	4.51	13.76	223.42	†

*Includes the cost of ADiGator file generation.
† Could not be computed due to memory overruns.
A "cost of differentiation" metric is given as the time required to perform k Hessian evaluations, where k is the number of Hessian evaluations required to solve the GL2 optimization problem using `fmincon` with a trust-region algorithm and function tolerance of $\sqrt{\epsilon_{machine}}$. Results are presented for three cases of computing the Hessian: sparse-finite differences over AD, AD over the hand-coded gradient, and AD over AD. Times listed for ADiGator* are the times required to compute k Hessians plus the time required to generate the derivative files, as given in Table 6.

in Darby et al. (2011). The problem is discretized using the multiple-interval formulation of the Legendre-Gauss-Radau (LGR) orthogonal collocation method as described in Garg et al. (2010). This problem was studied in Weinstein and Rao (2016) and is revisited in this article as a means of investigating the use of the vectorized mode of the ADiGator algorithm. The problem is to determine the values of the vectorized variable $\mathbf{X} \in \mathbb{R}^{4\times N}$,

$$\mathbf{X} = \begin{bmatrix} \mathbf{Y} \\ \mathbf{U} \end{bmatrix}, \quad \mathbf{Y} \in \mathbb{R}^{3\times N}, \quad \mathbf{U} \in \mathbb{R}^{1\times N}, \tag{15}$$

the support points $\mathbf{s} \in \mathbb{R}^3$, and the parameter β, which minimize the cost function

$$J = \beta \tag{16}$$

subject to the nonlinear algebraic constraints

$$\mathbf{C}(\mathbf{X}, \mathbf{s}, \beta) = [\mathbf{Y}\,\mathbf{s}]\,\mathbf{D}^{\mathsf{T}} - \frac{\beta}{2}\mathbf{F}(\mathbf{X}) = \mathbf{0} \in \mathbb{R}^{3\times N} \tag{17}$$

and simple bounds

$$\mathbf{X}_{\min} \leq \mathbf{X} \leq \mathbf{X}_{\max}, \quad \mathbf{s}_{\min} \leq \mathbf{s} \leq \mathbf{s}_{\max}, \quad \beta_{\min} \leq \beta \leq \beta_{\max}. \tag{18}$$

The matrix $\mathbf{D}^{N\times(N+1)}$ of Equation (17) is the LGR differentiation matrix (Garg et al. 2010), and the function $\mathbf{F}(\mathbf{X}) : \mathbb{R}^{4\times N} \rightarrow \mathbb{R}^{3\times N}$ of Equation (17) is the vectorized function

$$\mathbf{F}(\mathbf{X}) = [\,\mathbf{f}(\mathbf{X}_1)\ \mathbf{f}(\mathbf{X}_2)\ \cdots\ \mathbf{f}(\mathbf{X}_N)\,], \tag{19}$$

where $\mathbf{X}_i \in \mathbb{R}^4$ refers to the ith column of $\mathbf{X}$ and $\mathbf{f} : \mathbb{R}^4 \rightarrow \mathbb{R}^3$ is defined as

$$\begin{aligned} f_1(\mathbf{x}) &= x_2 \sin x_3, \\ f_2(\mathbf{x}) &= \tfrac{1}{c_1}\left(\zeta\left(T(x_1), x_1, x_2\right) - \theta\left(T(x_1), \rho(x_1), x_1, x_2\right)\right) - c_2 \sin x_3, . \\ f_3(\mathbf{x}) &= \tfrac{c_2}{x_2}\,(x_4 - \cos x_3) \end{aligned} \tag{20}$$

The functions $\zeta(T, x_1, x_2)$ and $\theta(T, \rho, x_1, x_2)$, respectively, compute coefficients of thrust and drag, as described in Seywald et al. (1994). Moreover, the functions $T(h)$ and $\rho(h)$ are modified from the smooth functions of Darby et al. (2011) to the following piecewise continuous functions taken from NOAA (1976):

$$\rho(h) = c_3 \frac{p(h)}{T(h)}, \tag{21}$$

where

$$(T(h), p(h)) = \begin{cases} \left(c_4 - c_5 h, c_6 \left[\frac{T(h)}{c_7}\right]^{c_8}\right), & h < 11, \\ \\ \left(c_9, c_{10} e^{c_{11} - c_{12} h}\right), & \text{otherwise.} \end{cases} \tag{22}$$

Unlike the implementation considered in Weinstein and Rao (2016), Equation (22) is implemented as a sequence of logical reference and assignment operations.

In the first portion of the analysis of this problem, the NLP of Equations (16)–(18) is solved for increasing values of N. The number of LGR points in each interval is fixed to four and the number of mesh intervals, K, is varied. The number of LGR points is thus $N = 4K$. The NLP is first solved on an initial mesh with $K = 4$ intervals. The number of mesh intervals is then doubled sequentially, where the result of the solution of the previous NLP is used to generate an initial guess to the next NLP. Mesh intervals are equally spaced for all values of $K = 4, 8, 16, 32, 64, 128, 256, 512, 1024$ and the NLP is solved with the NLP solver IPOPT (Biegler and Zavala 2008; Waechter and Biegler 2006) in both the quasi-Newton (first-derivative) and full-Newton (second-derivative) modes. Moreover, derivatives of the NLP were computed via ADiGator using two different approaches. In the first, non-vectorized, approach, the ADiGator tool is applied directly to the function that computes $\mathbf{C}(\mathbf{X}, \mathbf{s}, \beta)$ of Equation (17) to compute the constraint Jacobian and the Lagrangian Hessian. In the second, vectorized, approach, the ADiGator tool is applied in the vectorized mode to the function that computes $\mathbf{F}(\mathbf{X})$. The ADiGator computed derivatives of $\mathbf{F}(\mathbf{X})$ are then used to construct the NLP constraint Jacobian and Lagrangian Hessian (using discretization separability as described in Betts (2009)). Results of the tests are shown in Table 8. In the presented table, solution times are broken into two different categories, initialization time and NLP solve time. When using the non-vectorized approach, the initialization time is the time required to generate derivative files prior to solving each NLP. When using the vectorized approach, derivative files must only be generated a single time (shown as mesh # 0). The initialization time required of the vectorized approach at each subsequent mesh iteration is the time required to compute the derivative of the linear portion of $\mathbf{C}$ (that is, $[\mathbf{X}\,\mathbf{s}]\,\mathbf{D}^{\mathsf{T}}$) plus the time required to determine sparsity patterns of the constraint Jacobian and Lagrangian Hessian, given sparsity patterns of $\partial\mathbf{f}/\partial\mathbf{x}$ and $\partial^2\mathbf{f}/\partial\mathbf{x}^2$. It is seen in Table 8 for both quasi-Newton and full-Newton solutions that the use of the vectorized mode reduces both

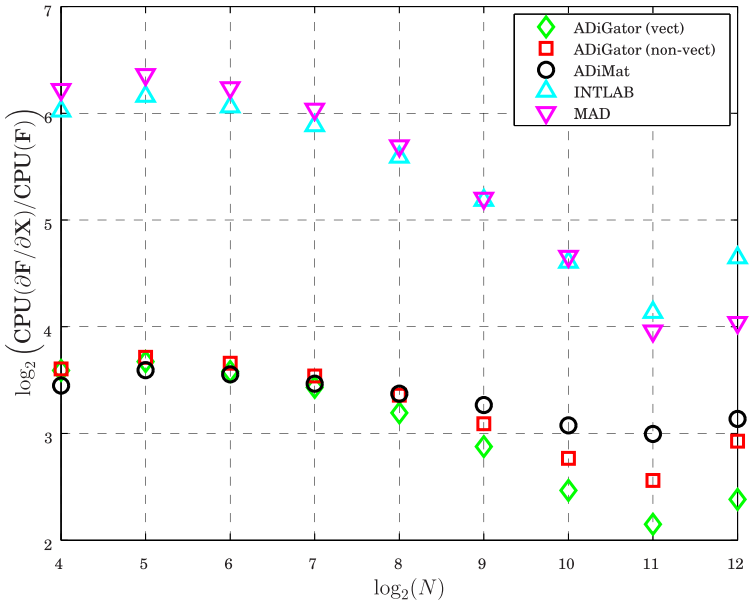
Table 8. NLP Solution Times for Minimum Time to Climb Using IPOPT and ADiGator

	mesh #:	0	1	2	3	4	5	6	7	8	9	**Total**
	K:		4	8	16	32	64	128	256	512	1024	
Quasi-Newton	# jac eval:	-	63	63	93	92	92	71	62	145	52	**733**
	Initialization Time (s)											
	non-vect:	-	1.18	1.17	1.18	1.18	1.19	1.23	1.35	1.62	2.27	**12.4**
	vect:	0.97	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	**1.0**
	NLP Solve Time (s)											
	non-vect:	-	0.59	0.61	0.96	1.12	1.45	1.65	2.37	9.41	7.00	**25.2**
	vect:	-	0.56	0.51	0.82	0.95	1.21	1.35	1.95	7.82	5.80	**21.0**
Full-Newton	# jac eval:	-	41	14	17	17	18	18	20	20	23	**188**
	# hes eval:	-	40	13	16	16	17	17	19	19	22	**179**
	Initialization Time (s)											
	non-vect:	-	5.37	5.38	5.43	5.47	5.64	6.06	7.40	11.09	24.04	**75.9**
	vect:	4.59	0.00	0.00	0.00	0.00	0.01	0.03	0.13	0.46	1.78	**7.0**
	NLP Solve Time (s)											
	non-vect:	-	0.86	0.40	0.48	0.52	0.66	0.89	1.48	2.50	5.73	**13.5**
	vect:	-	0.85	0.23	0.30	0.32	0.41	0.54	0.90	1.51	3.33	**8.4**

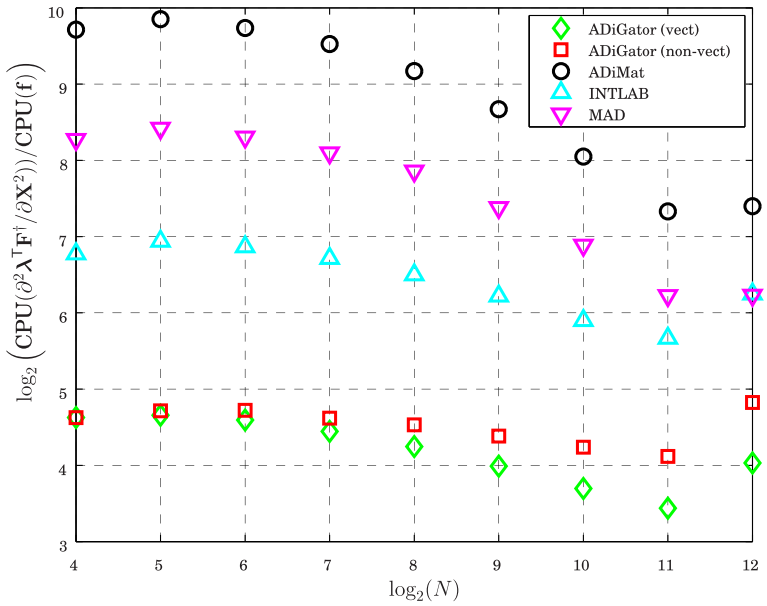
The NLP is solved for increasing values of K using IPOPT in both the quasi-Newton and full-Newton modes. For both modes, the ADiGator tool is used in two different ways. In the non-vectorized case (labeled non-vect), ADiGator is applied directly to the functions of the NLP. In the vectorized case (labeled vect), ADiGator is applied in the vectorized mode to the function $\mathbf{F}(\mathbf{X})$.

initialization times and NLP runtimes. The reason for the reduction in initialization times is fairly straightforward: when using the vectorized mode, derivative files are valid for any value of N and thus must only be generated a single time. The reason for the reduction in runtimes is twofold. First, by separating the nonlinear portion of $\mathbf{C}$ from the linear portion of $\mathbf{C}$, the first derivatives of the linear portion must only be computed a single time for each mesh rather than at runtime. Next, as discussed in Section 5, runtime indexing overheads are effectively reduced by an order of N when using the vectorized mode over the non-vectorized. This reduction of runtime indexing overheads is greatly emphasized in the results from the full-Newton mode, where many more indexing operations are required at the second derivative level than at the first.

In the next part of the analysis of this example the vectorized function $\mathbf{F}(\mathbf{X})$ was differentiated for increasing values of N using a variety of well-known MATLAB AD tools. At the first-derivative level, the ADiGator tool was used in the vectorized and non-vectorized modes, ADiMat was used in the compressed scalar forward mode, INTLAB was used in the sparse forward mode, and MAD was used in the compressed forward mode. At the second-derivative level, the ADiGator tool was again used in the vectorized and non-vectorized modes, ADiMat was used in the compressed forward over scalar reverse mode (with operator overloading for the forward computation), INTLAB was used in the sparse second-order forward mode, and MAD was used in the compressed forward over compressed forward mode. Results are shown in Figure 2. At the second-derivative level, the ADiMat tool was used to compute $\partial^2\lambda^{\mathsf{T}}\mathbf{F}^{\dagger}/\partial\mathbf{X}^2$, where $\lambda \in \mathbb{R}^{3N}$ and $\mathbf{F}^{\dagger} \in \mathbb{R}^{3N}$ is the one-dimensional transformation of $\mathbf{F}$. All other tools were used entirely in the forward mode and thus were simply used to compute $\partial^2\mathbf{F}/\partial\mathbf{X}^2$. The computation time CPU$(\partial^2\lambda^{\mathsf{T}}\mathbf{F}^{\dagger}/\partial\mathbf{X}^2)$ was then computed as the time required to compute $\partial^2\mathbf{F}/\partial\mathbf{X}^2$ plus the time required to pre-multiply $\partial^2\mathbf{F}^{\dagger}/\partial\mathbf{X}^2$ by λ^{T}. It is noted that, where relevant, the number of colors used for both the first and second derivative is always equal to four as the vectorized problem has the convenient pre-defined seed



(a) $\log_2\left(\text{CPU}(\partial\mathbf{F}/\partial\mathbf{X})/\text{CPU}(\mathbf{F})\right)$ vs. $\log_2(N)$



(b) $\log_2\left(\text{CPU}(\partial^2\boldsymbol{\lambda}^\mathsf{T}\mathbf{F}^\dagger/\partial\mathbf{X}^2))/\text{CPU}(\mathbf{f})\right)$ vs. $\log_2(N)$

Fig. 2. Jacobian and Hessian to Function CPU Ratios for Minimum Time to Climb Vectorized Function. All ratios given in binary logarithm format.

matrix given in Equation (9). As seen in Figure 2, the ratios for all tested tools tend to decrease as the value of N is increased. This increase in efficiency is due to a reduction in the relevance of runtime overheads (this is very apparent for the operator overloaded INTLAB and MAD tools at the first derivative) together with the fact that the derivatives become sparser as N is increased (and the number of colors remains constant). When comparing the results obtained from using ADiGator in the vectorized mode versus the non-vectorized mode, it is seen that the ratios diverge as the dimension of the problem is increased. These differences in computation times are due strictly to runtime overheads associated with reference and assignment indexing.

8 DISCUSSION

The presented algorithm has been designed to perform a great deal of analysis at transformation-time to generate the most efficient derivative files possible. The results of Section 7 show these ADiGator generated derivative files to be quite efficient at runtime when compared to other well-known MATLAB AD tools. The presented results also show, however, that transformation times can become quite large as problem dimensions increase. This is particularly the case when dealing with functions containing explicit loops (for example, Burgers' ODE) or those that perform matrix operations (for example, the GL2 minimization problem). Even so, the ADiGator algorithm is well suited for applications requiring many repeated derivative computations, where the cost of file generation becomes less significant as the number of required derivative computations is increased.

The fact that the method has been implemented in the MATLAB language is both an advantage and a hindrance. Due to MATLAB's high level array and matrix operations, the corresponding overloaded operations are granted a great deal of information at transformation time. The overloaded operations can thus print derivative procedures that are optimal for the sequence of elementary operations that the high-level operation performs rather than printing derivative procedures that are optimal for each of the individual elementary operations. To exploit derivative sparsity, however, the overloaded operations print derivative procedures that typically only operate on vectors of non-zero derivatives. Moreover, the derivative procedures rely heavily on index array reference and assignment operations (for example, `a(ind)`, where `ind` is a vector of integers). Due to the interpreted nature of the MATLAB language, such reference and assignment operations are penalized at runtime by MATLAB's array bounds checking mechanism, where the penalty is proportional to the length of the index vector (for example, `ind`) (Menon and Pingali 1999). Moreover, the length of the used index vectors are proportional to the number of non-zero derivatives at each link in the chain rule. Thus, as problem sizes increase, so do the derivative runtime penalties associated with the array bounds checking mechanism. The increase in runtime overheads is manifested in the the results of Figure 1 and Table 5 of Sections 7.1 and 7.3, respectively. For both problems, the Jacobians become relatively more sparse as the problem dimensions are increased. One would thus expect the Jacobian to function CPU ratios to decrease as problem dimensions increase. The witnessed behavior of the ADiGator tool is, however, the opposite and is attributed to the relative increase in runtime overhead due to indexing operations. When studying the vectorized problem of Section 7.4, the indexing runtime overheads may actually be quantified as the difference in runtimes between the vectorized and non-vectorized generated files. From the results of Figure 2, it is seen that, at small values of N, the differences in runtimes are negligible. At $N = 4096$, however, the non-vectorized ADiGator-generated first and second derivative files spent *at least* 32% and 42%, respectively, of the computation time performing array bounds checks from indexing operations.

9 CONCLUSIONS

A toolbox called *ADiGator* has been described for algorithmically differentiating mathematical functions in MATLAB. ADiGator statically exploits sparsity at each link in the chain rule to produce runtime efficient derivative files, and does not require any *a priori* knowledge of derivative sparsity but instead determines derivative sparsity as a direct result of the transformation process. The algorithm is described in detail and is applied to four examples of varying complexity. It is found that the derivative files produced by ADiGator are quite efficient at runtime when compared to other well-known AD tools. The generated derivative files are, however, valid only for fixed dimensional inputs and thus the cost of file generation cannot be overlooked. Finally, it is concluded that the ADiGator tool is well suited for applications requiring many repeated derivative computations.

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