Automatic Differentiation

Jason Boisvert
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Outline

1. Introduction
2. Modes of automatic differentiation
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A numerical algorithm may require

- derivatives
- gradients
- Jacobians
- Hessian matrices
- Taylor polynomials
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Differentiation in numerical software

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Methods to compute derivatives

Functions can be differentiated in several ways
- finite differences
- symbolic differentiation
- automatic differentiation
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- automatic differentiation
What is automatic differentiation?

Automatic differentiation is a set of techniques to numerically differentiate a function through the use of exact formulas and floating-point values. The resulting numerical value involves no approximation error.
Other names for automatic differentiation

- computational differentiation
- algorithmic differentiation
Other names for automatic differentiation

- computational differentiation
- algorithmic differentiation
Several modes of automatic differentiation

- forward automatic differentiation
- reverse automatic differentiation
- a combination of forward and reverse modes of automatic differentiation
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Forward mode

Forward automatic differentiation divides the expression into a sequence of differentiable elementary operations.

The chain rule and well-known differentiation rules are then applied to each elementary operation.
Using forward automatic differentiation on an example

For example, forward automatic differentiation can be used to differentiate the expression

\[ f(x_1, x_2) = \cos(x_1) + x_1 \exp(x_2). \]
Elementary operations

The expression can be divided into the following elementary operations

\[ w_1 = x_1, \]
\[ w_2 = x_2, \]
\[ w_3 = \exp(w_2), \]
\[ w_4 = w_1 w_3, \]
\[ w_5 = \cos(w_1), \]
\[ w_6 = w_4 + w_5, \]
\[ f(x_1, x_2) = w_6. \]
A computational graph
Finding the derivatives of the example

We can find the numerical value of the derivatives to $f(x_1, x_2)$ by using some differentiation rules and applying the chain rule to each of the elementary operations.

\[
\begin{align*}
w'_1 &= \text{seed} \in \{0, 1\} \\
w'_2 &= \text{seed} \in \{0, 1\} \\
w'_3 &= \exp(w_2)w'_2 \\
w'_4 &= w'_1w_3 + w_1w'_3 \\
w'_5 &= -\sin(w_1)w'_1 \\
w'_6 &= w'_4 + w'_5 \\
f'(x_1, x_2) &= w'_6
\end{align*}
\]
In order to find a value for the partial derivative of $f'(x_1, x_2)$ with respect to $x_1$, we set

\[ w'_1 = 1, \]
\[ w'_2 = 0. \]
Introduction

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Implementation of AD
Popular AD packages

Forward automatic differentiation
Reverse automatic differentiation
A combination of forward and reverse modes

A computational graph of the forward mode
- Only one sweep is necessary to compute derivatives for functions $f : \mathbb{R} \rightarrow \mathbb{R}^m$.

Therefore, this mode is efficient for $m \gg 1$.

- It is not necessary to save values for intermediate expressions.

- Implementation is simple due to how expressions are normally evaluated by computers.
Notes on forward automatic differentiation

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The reverse mode computes a series of adjoints

\[ \tilde{w}_i = \sum_{j \in \pi(i)} \tilde{w}_j \frac{\partial w_j}{\partial w_i}, \quad i = N, N - 1, \ldots, 1, \]

where the \( \pi(i) \) are the indices of elementary operations that immediately proceed the elementary operation \( w_i \) in the computational process.

An initial value of

\[ \tilde{w}_N = 1 \]

is used.
Reverse mode

The partial derivatives for a function \( f : \mathbb{R}^n \to \mathbb{R} \) can be obtained from

\[
\frac{\partial f}{\partial x_i} = \bar{w}_i.
\]
Applying reverse mode to example

Recall that \( f(x_1, x_2) = \cos(x_1) + x_1 \exp(x_2) \) can be broken down into the following elementary operations

\[
\begin{align*}
    w_1 &= x_1, \\
    w_2 &= x_2, \\
    w_3 &= \exp(w_2), \\
    w_4 &= w_1 w_3, \\
    w_5 &= \cos(w_1), \\
    w_6 &= w_4 + w_5.
\end{align*}
\]
Computing the adjoints

The adjoints for this example are

\[ \tilde{w}_6 = 1, \]
\[ \tilde{w}_5 = 1, \]
\[ \tilde{w}_4 = 1, \]
\[ \tilde{w}_3 = w_1, \]
\[ \tilde{w}_2 = w_1 \exp(w_2), \]
\[ \tilde{w}_1 = -\sin(w_1) + \exp(w_2). \]
A computational graph of the reverse mode

\( f(x_1, x_2) \)

\( w_1 = w_{1a} + w_1b \)

\( w_2 = \exp(w_2) \)

\( w_3 = w_1 \)

\( \exp \)

\( \cos \)

\( + \)

\( w_4 = 1 \)

\( w_5 = 1 \)

\( \sin \)

\( \times \)

\( x_1 \)

\( x_2 \)
Notes on reverse automatic differentiation

- Only one sweep is required to compute all partial derivatives for \( f : \mathbb{R}^n \to \mathbb{R} \).
  - Therefore, this mode is efficient for \( n \gg 1 \).
- Adjoint must be saved in order to compute partial derivatives.
- A forward sweep through the expression must be performed before a reverse sweep used to compute adjoints is performed.
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A combination of modes

Forward and reverse modes may be combined to more efficiently compute a Jacobian matrix for a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ depending on the sparsity structure of the matrix.

- For example, $n$ sweeps of the forward mode will compute the columns of the Jacobian matrix . . .

- whereas $m$ sweeps of the reverse mode will compute the rows of the Jacobian matrix.

- Depending on the Jacobian matrix, a combination of the forward and reverse modes may require fewer sweeps than either mode alone.
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Methods of implementation

- Source-to-source transformation
- Operator overloading
Methods of implementation

- Source-to-source transformation
- Operator overloading
Uses a compiler to convert source code with mathematical expressions to source code with automatic differentiation expressions.
Notes on source-to-source transformation

- Requires minimal (if any) changes to the original code.
- The resulting automatic differentiation code can be optimized.
- Knowledge of compiler concepts are required, and therefore implementation can be difficult.
- Additional tools must be installed in order for users to apply automatic differentiation to their code.
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User-defined data types and the operator overloading features of a language are used to implement automatic differentiation.
Notes on operator overloading

- Users must modify their code in order to make use of automatic differentiation data types.
- Operator overloading can slow down runtime, and therefore operator overloading automatic differentiation can be slow when compared to source-to-source transformation.
- Implementation of forward mode is much more intuitive than source-to-source transformation. However, implementation of reverse mode can be difficult.
- Other than the language libraries, no additional tools are required for the application of automatic differentiation.
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Some source-to-source AD packages

- openAD
- ADiMat
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openAD

A source-to-source transformation automatic differentiation tool for the Fortran 90 language.
Notes on openAD

- Allows for both forward and reverse automatic differentiation.
- Implemented with an open-source Open64 compiler toolset.
- Used in software that models ocean circulation.
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ADiMat

A source-to-source transformation automatic differentiation tool for Matlab.
Notes on ADiMat

- Supports first- and second-order automatic differentiation with forward mode.
- Supports first-order automatic differentiation with reverse mode.
- Performs code optimization.
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Some operator overloading AD packages

- MAD
- ADOLC
Some operator overloading AD packages

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- ADOLC
An operator-overloading automatic differentiation tool for Matlab.
Notes on ADiMat

- Implements a class called fmad that supports operator overloading.
- Performance has been optimized for Matlab.
- Detects sparsity patterns of matrices for faster derivative calculation at runtime.
- Used along with bvp4c to solve BVODEs.
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ADOLC

An operator-overloading automatic differentiation tool for C++.
Notes on ADOLC

- Supports both forward and reverse automatic differentiation modes.
- Can be used to compute derivatives of any order.
- When evaluating expressions, it records information, e.g., adjoints, on a tape. The tape can later be used for faster automatic differentiation calculations.
- Can be used to calculate sparsity patterns.
- Can be used to solve certain ordinary differentiation equations.
Notes on ADOLC

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