Automatic Differentiation

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Outline

1. Introduction
2. Modes of automatic differentiation
3. Implementation of AD
4. Popular AD packages

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Differentiation in numerical software

A numerical algorithm may require

- derivatives
- gradients
- Jacobians
- Hessian matrices
- Taylor polynomials

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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

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- 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 differentiate the expression

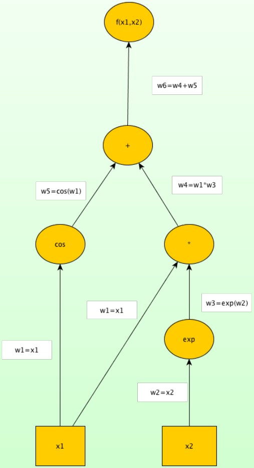
$$f(x_1, x_2) = \cos(x_1) + x_1 \exp(x_2).$$

Elementary operations

The expression can be divided into the following elementary operations

$$
\begin{aligned}
w_1 &= x_1, \\
w_2 &= x_2, \\
w_3 &= \exp(w_2), \\
w_4 &= w_1 w_3, \\
w_5 &= \cos(w_1), \\
w_6 &= w_4 + w_5, \\
f(x_1, x_2) &= w_6.
\end{aligned}
$$

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.

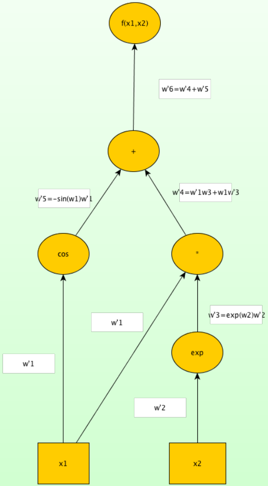
$$
\begin{aligned}
w_1' &= \texttt{seed} \in \{0, 1\} \\
w_2' &= \texttt{seed} \in \{0, 1\} \\
w_3' &= \exp(w_2) w_2' \\
w_4' &= w_1' w_3 + w_1 w_3' \\
w_5' &= -\sin(w_1) w_1' \\
w_6' &= w_4' + w_5' \\
f'(x_1, x_2) &= w_6'
\end{aligned}
$$

Seed values

In order to find a value for the partial derivative of $f'(x_1, x_2)$ with respect to x_1, we set

$$w_1' = 1,$$
$$w_2' = 0.$$

A computational graph of the forward mode



Notes on forward automatic differentiation

- Only one sweep is necessary to compute derivatives for functions $\mathbf{f} : \mathbb{R} \to \mathbb{R}^m$.
  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.

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Reverse mode

The reverse mode computes a series of adjoints

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

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

$$\bar{w}_N = 1$$

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

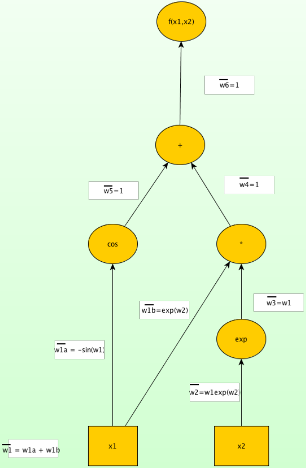
$$
\begin{aligned}
w_1 &= x_1, \\
w_2 &= x_2, \\
w_3 &= \exp(w_2), \\
w_4 &= w_1 w_3, \\
w_5 &= \cos(w_1), \\
w_6 &= w_4 + w_5.
\end{aligned}
$$

Computing the adjoints

The adjoints for this example are

$$\begin{aligned}
\bar{w}_6 &= 1, \\
\bar{w}_5 &= 1, \\
\bar{w}_4 &= 1, \\
\bar{w}_3 &= w_1, \\
\bar{w}_2 &= w_1 \exp(w_2), \\
\bar{w}_1 &= -sin(w_1) + \exp(w_2).
\end{aligned}$$

A computational graph of the reverse mode



Notes on reverse automatic differentiation

- Only one sweep is required to compute all partial derivatives for $f : \mathbb{R}^n \to \mathbb{R}$.
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- Adjoints 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 $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^m$ 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

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Introduction to source-to-source transformation

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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Introduction to operator overloading

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

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- `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.
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- `ADOLC`

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MAD

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.

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