Automatic Differentiation as a Tool for Computational Science

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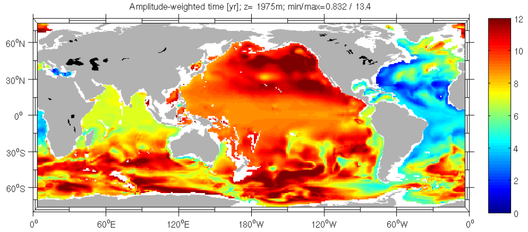
What do we have in store

- Presented Today:
  - Introduction
  - Demo & Hands on: AD basics
  - Demo & Hands on: Using AD for optimization
- Further Material:
  - Seed matrices
  - Memory requirements
  - AD for parallel programs
  - Know what you are differentiating
  - Adding AD to existing code

Resources: `https://tinyurl.com/siaman24ad`

Why derivatives?

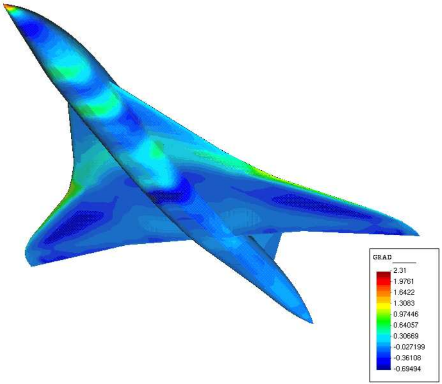
Sensitivity Analysis:



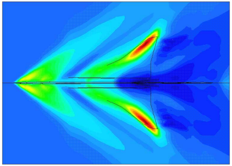
Find sensitivity of the computed field *wrt* one input parameter

Why derivatives?

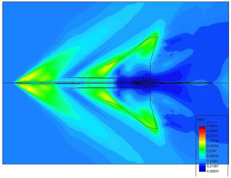
Gradient-driven optimization



before:



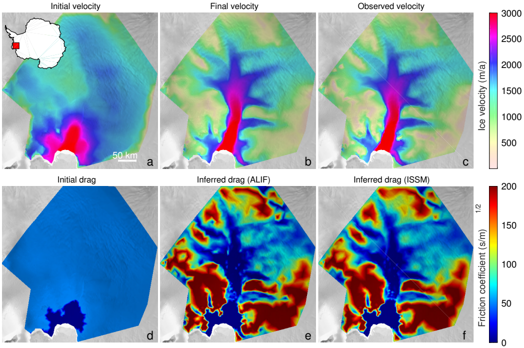
after:



Why derivatives?

Inverse problems:

from measurements and model, estimate hidden parameters



Other uses: Reduced models, Error estimation, Mesh adaption, Uncertainty Quantification, Backpropagation for ML training. . .

What is AD?

The chain rule applied to algorithms

See any algorithm/program $\mathtt{P}:\{I_1; I_2; \ldots I_p;\}$ as:

$$F : \mathbb{R}^n \rightarrow \mathbb{R}^m \qquad F = f_p \circ f_{p-1} \circ \cdots \circ f_1$$

Define for short:

$$V_0 = \textbf{input} \quad \text{and} \quad V_k = f_k(V_{k-1})$$

Apply the chain rule:

$$F'(V_0) = f'_p(V_{p-1}) \times f'_{p-1}(V_{p-2}) \times \cdots \times f'_1(V_0)$$

...and transform P to make it compute that.

Cost considerations

$$F'(V_0) = f'_p(V_{p-1}) \times f'_{p-1}(V_{p-2}) \times \cdots \times f'_1(V_0)$$

is often expensive:

- in computation time
- in storage space

What can save us:

- The shapes of the f'_k matter
- The final usage may not require the full F' but only a projection

Classical projections of F'

- $F' \times \dot{V}_0$, “forward” or “tangent” mode
- $\overline{V_p} \times F'$ “reverse” or “adjoint” mode

When full F' needed, use multi-directional AD
$\rightarrow F' \times Id$ (or $Id \times F'$),
$\rightarrow$ possibly compressed as $F' \times S$ (or $S \times F'$)

For higher-order derivatives, differentiate F'
If directional, differentiate $F' \times \dot{V}_0$

Demo (with Tapenade)

rosenbrock.f90 :

```
REAL*8 FUNCTION ROSENBROCK(x,n) RESULT(y)
  INTEGER ::  n
  REAL*8 ::  x(0:n)
  y = SUM(100.d0*(x(1:n) - x(0:n-1)**2)**2
            + (1-x(0:n-1))**2)
END FUNCTION ROSENBROCK
```

- $n + 1$ inputs x, scalar output y
- Looking for $\frac{dy}{dx}$

Demo with Tapenade: tangent

```
$ tapenade rosenbrock.f90
$>   -head "rosenbrock(y)/(x)" -d
```

rosenbrock_d.f90 :

```
arg1d(:)  = 100.d0*2*(x(1:n)-x(0:n-1)**2)
               *(xd(1:n)-2*x(0:n-1)*xd(0:n-1))
          - 2*(1-x(0:n-1))*xd(0:n-1)
arg1 = 100.d0*(x(1:n) - x(0:n-1)**2)**2
          + (1-x(0:n-1))**2
yd = SUM(arg1d(:))
y = SUM(arg1(:))
```

`driverTgt.f90` initializes `xd` to 0,0,0,0,1,0,0,0,0,0 (`n`=9)

```
$ gfortran rosenbrock_d.f90 driverTgt.f90 -o tangent.exe
$ ./tangent.exe
Rosenbrock tangent:  -260.4622
```

Demo with Tapenade: gradient

```
$ tapenade rosenbrock.f90
$>   -head "rosenbrock(y)/(x)" -b
```

rosenbrock_b.f90 :

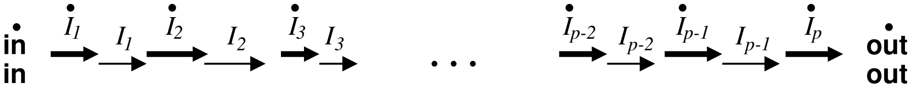
```
xb = 0.0_8
tempb = 2*(x(1:n)-x(0:n-1)**2)*100.d0*yb
xb(0:n-1) = xb(0:n-1) - 2*(1-x(0:n-1))*yb
xb(1:n) = xb(1:n) + tempb
xb(0:n-1) = xb(0:n-1) - 2*x(0:n-1)*tempb
```

```
$ gfortran rosenbrock_b.f90 driverGrad.f90 -o gradient.exe
$ ./gradient.exe
Rosenbrock gradient:  15.9751 50.3524
-109.0627 -447.2795 -260.4622 -113.7724
-421.9504 -121.0793 66.6307 6.3868
```

Focus on forward mode: $F' \times \dot{V}_0$

$$F' \times \dot{V}_0 = f'_p(V_{p-1}) \times f'_{p-1}(V_{p-2}) \times \cdots \times f'_1(V_0) \times \dot{V}_0$$

$\dot{V}_0$ is a vector $\Rightarrow$ compute from right to left!
This corresponds to `P`'s original order
$\Rightarrow$ interleave derivative and primal computation.
Easy!

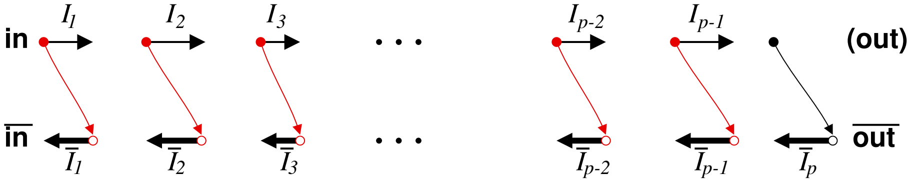


Focus on reverse mode: $\overline{V_p} \times F'$

$$\overline{V_p} \times F' = \overline{V_p} \times f'_p(V_{p-1}) \times f'_{p-1}(V_{p-2}) \times \cdots \times f'_1(V_0)$$

Vector now on the left $\Rightarrow$ compute from left to right

Not so easy, but worth the effort!



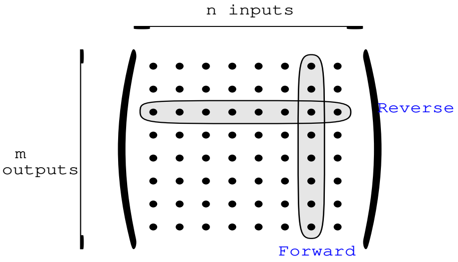
A forward sweep, and then a backward sweep

The derivative instructions form the backward sweep

"Data-flow reversal" to get V_k's in reverse order

Cost model

$$F \;:\; \textbf{in} \in \mathbb{R}^{n} \;\rightarrow\; \textbf{out} \in \mathbb{R}^{m}$$

$F' =$ 

- full F' cost grows like n using the forward mode
  Good if $n <= m$
- full F' cost grows like m using the reverse mode
  Good if $n >> m$ (e.g. $m = 1$ for a gradient)

Alternatives to AD

- Symbolic differentiation, Continuous adjoint...
  Uses equations, not code ;
  Duplicates discretization & coding work
- Finite Differences
  Robust wrt coding style & non-differentiable code ;
  inaccurate (2nd order contributions) ; only forward mode
- Complex-step
  Astute use of Complex arithmetics ;
  similar to AD ; only forward mode

Tool landscape

- Various AD models $\Rightarrow$ various AD tools:
  Store derivatives stuck to primals or in separate variables ;
  Tape all forward computation or only chosen values ;

  Preaccumulate partials ; Prefer recomputation to storage
- Various languages $\Rightarrow$ Various tool interfaces:
  AD by separate tool or embedded in application language ;
  AD in the compiler ; Differentiated code visible or not ;

  AD on restricted language or DSL

End of basics

Let's look in detail !