Automatic Differentiation as a Tool for Computational Science

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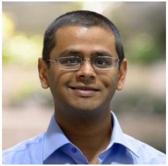
Welcome

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- First time we are giving a virtual tutorial
- Special thanks to those who are up late or early!

What do we have in store

- Session 1:
  - Introduction
  - Seed matrices
  - Demo & Hands on: AD basics
- Session 2:
  - Memory requirements
  - AD for parallel programs
  - Know what you are differentiating
  - Adding AD to existing code
  - Demo & Hands on: Using AD for optimization

Resources: `https://tinyurl.com/siamcse21ad`

Our goals for this tutorial

Participants will ...

- situate AD in contrast to other approaches to derivatives,
- be able to use AD tools effectively,
- imagine what ML frameworks do "behind the scenes",
- understand enough about AD concepts that they can diagnose problems,

... and, why not, at least one participant might be inspired to contribute to AD research?

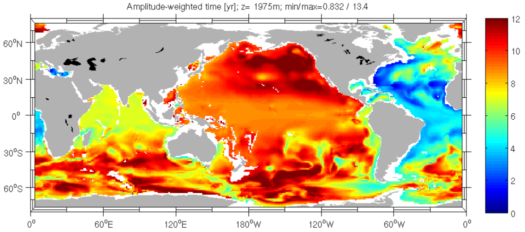
What we assume about you

Computational scientists facing challenging problems, through advanced modeling and simulation, using the most capable computers.

- large complex codes
- continuously developed
- including sophisticated math/physics
- using multiple libraries
- performance is essential
- parallelism involved

Why derivatives?

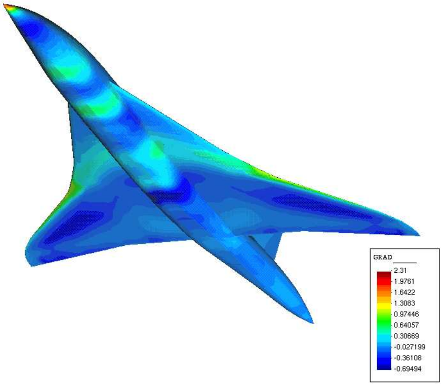
Sensitivity Analysis:



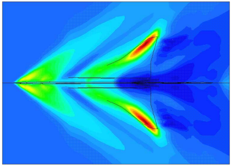
Find sensitivity of the computed field *wrt* one input parameter

Why derivatives?

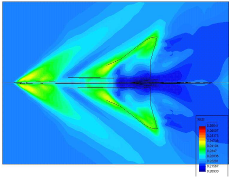
Gradient-driven optimization



before:



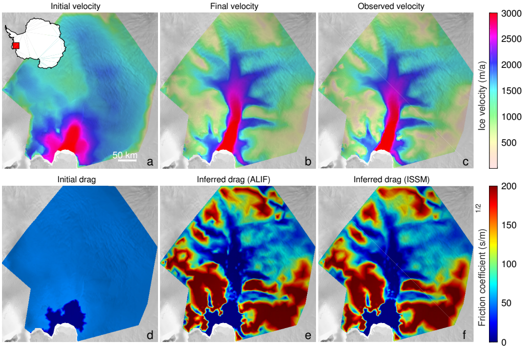
after:



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:

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

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
```

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

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 :

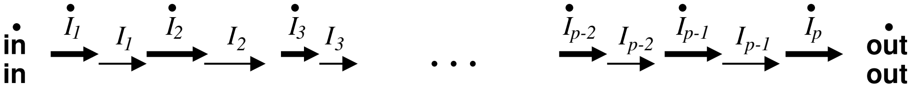
```
xb = 0.0_8
tempb = 2*(x(1:n)-x(0:n-1)**2)*100.d0*yb
xb(0:n-1) = xb(0:n-1) - 2*(1-x(0:n-1))*yb
xb(1:n) = xb(1:n) + tempb
xb(0:n-1) = xb(0:n-1) - 2*x(0:n-1)*tempb
```

```
$ 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!

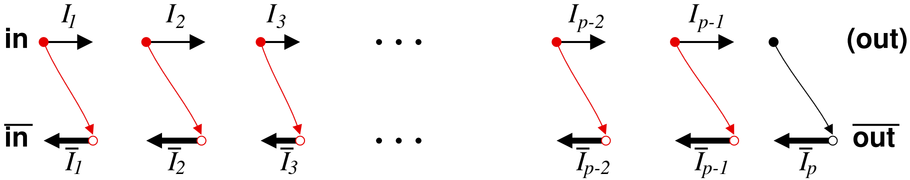


Focus on reverse mode: $\overline{V_p} \times F'$

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

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

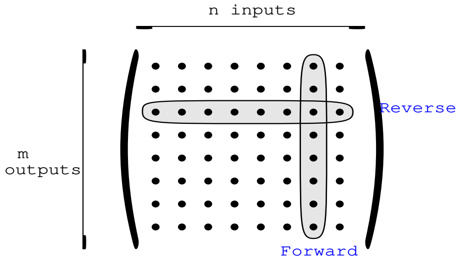
The derivative instructions form the backward sweep

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

Cost model

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

$F' =$



- 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 !