

(Adjoint) Algorithmic Differentiation [(A)AD]

A Hands-On Introduction

Uwe Naumann

LuFG Informatik 12: Software and Tools for
Computational Engineering, RWTH Aachen University,
Germany

and

The Numerical Algorithms Group Ltd., Oxford, UK

Introduction

First-Order(A)AD

- Prerequisites

- Tangents

- Adjoint

Second-(and Higher-)Order (A)AD

- Tangents of Tangents

- Tangents of Adjoint

“Getting Serious” with AAD

- Implementation by Overloading

- Checkpointing

- Symbolic Adjoint

- Adjoint Code Design Patterns

Progress

Introduction

First-Order(A)AD

- Prerequisites

- Tangents

- Adjoint

Second-(and Higher-)Order (A)AD

- Tangents of Tangents

- Tangents of Adjoint

"Getting Serious" with AAD

- Implementation by Overloading

- Checkpointing

- Symbolic Adjoint

- Adjoint Code Design Patterns

...

For differentiation, is there anything else?

Perturbing the inputs – can't imagine this fails.

I pick a small Epsilon, and I wonder ...

...



from: “Optimality” (Lyrics: Naumann; Music: Think of Fool’s Garden’s “Lemon Tree”) in Naumann: [The Art of Differentiating Computer Programs](#). An Introduction to Algorithmic Differentiation. Number 24 in Software , Environments, and Tools, SIAM, 2012. Page xvii



- ▶ inspired by sensitivity analysis, uncertainty quantification, calibration / optimization
- ▶ finite differences (first- and second-order), symbolic, algorithmic
- ▶ implementation by overloading, source trafo, hand-coding
- ▶ real code
- ▶ sensitivity analysis as modelling and software engineering tool
- ▶ what matters
 - ▶ user expertise
 - ▶ tool quality
 - ▶ tool sustainability and support

Let $y = F(\mathbf{x})$, $F : \mathbb{R}^n \rightarrow \mathbb{R}$:

1. tangent AD: $y^{(1)} = \nabla F \cdot \mathbf{x}^{(1)} \Rightarrow \nabla F$ at $O(n) \cdot \text{Cost}(F)$
2. adjoint AD: $\mathbf{x}_{(1)} = \nabla F^T \cdot y_{(1)} \Rightarrow \nabla F$ at $O(1) \cdot \text{Cost}(F)$
3. 2nd-order tangent AD: $y^{(1,2)} = \mathbf{x}^{(1)T} \cdot \nabla^2 F \cdot \mathbf{x}^{(2)} \Rightarrow \nabla^2 F$ at $O(n^2) \cdot \text{Cost}(F)$
4. 2nd-order adjoint AD: $\mathbf{x}_{(1)}^{(2)} = y_{(1)} \cdot \nabla F^2 \cdot \mathbf{x}^{(2)} \Rightarrow \nabla^2 F$ at $O(n) \cdot \text{Cost}(F)$ and $\nabla^2 F \cdot \mathbf{x}^{(2)}$ at $O(1) \cdot \text{Cost}(F)$

Aims of this Course

You will learn how to

- ▶ implement tangent and adjoint versions of a Monte Carlo / Euler-Maruyama solver for parameterized scalar SDEs
- ▶ ensure feasibility of adjoint Monte Carlo simulation through pathwise adjoints
- ▶ “get serious” with AAD (tools, checkpointing, symbolic adjoints, design patterns, ...)

We are looking for the expected value $\mathbb{E}(x)$ of the solution $x(\mathbf{p}, T), T > 0$ of the scalar stochastic initial value problem

$$dx = f(x(\mathbf{p}, t), \mathbf{p}, t)dt + g(x(\mathbf{p}, t), \mathbf{p}, t)dW$$

with Brownian Motion dW and for $x(\mathbf{p}, 0) = x^0$.

Forward finite differences in time with time step $0 < \delta t \ll 1$ yield the explicit Euler-Maruyama evolution

$$x^{i+1} := x^i + \delta t \cdot f(x^i, \mathbf{p}, i \cdot \delta t) + \sqrt{\delta t} \cdot g(x^i, \mathbf{p}, i \cdot \delta t) \cdot dW^i$$

for $i = 0, \dots, n - 1$, target time $T = n \cdot \delta t$, parameter vector $\mathbf{p} \in \mathbb{R}^l$, and with random numbers dW^i drawn from the standard normal distribution $N(0, 1)$.

The solution $\mathbb{E}(x)$ is approximated using Monte Carlo simulation over (a sufficiently large number of) Euler-Maruyama paths.

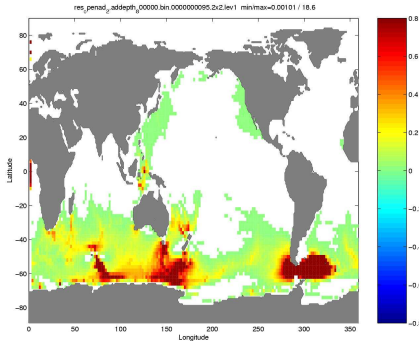
We are interested in sensitivities of the final state $\mathbb{E}(x)$ wrt. \mathbf{p} .

Race (Euler-Maruyama $m = 10^4, n = 10^2, l = 10^2$)

- ▶ **primal**: primal.cpp (inspect)
- ▶ **bumping**: fd.cpp (inspect)
- ▶ **tangent**: tangent.cpp (live)
- ▶ **vector tangent**: tangent_vector.cpp (inspect)
- ▶ **adjoint**: adjoint.cpp (live)
- ▶ **pathwise adjoint**: adjoint_pathwise.cpp (inspect)

mode	run time (s)	memory size (b)	accuracy
bump	$10.9 \sim O(l)$	$\sim P$	-
tangent	$21.5 \sim O(2 \cdot l)$	$\sim 2 \cdot P$	+
vector tangent	$13.6 \sim O(2 \cdot l)$	$\sim P + P \cdot l$	+
adjoint	$0.3 \sim O(1)$	$\sim 2 \cdot P + 2 \cdot m \cdot n \cdot 8$	+
pathwise adjoint	$0.5 \sim O(1)$	$\sim 2 \cdot P + 2 \cdot (m + n) \cdot 8$	+

where P denotes the memory requirement of the primal code.



MITgcm, (EAPS, MIT)

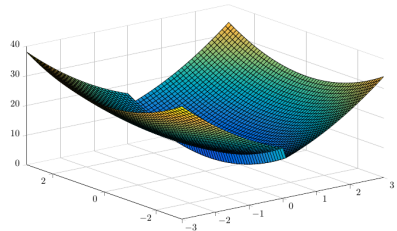
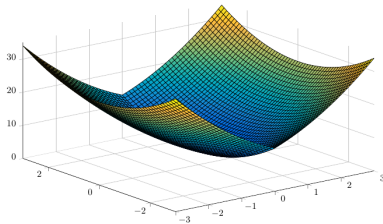
in collaboration with ANL, MIT,
Rice, UColorado

J. Utke, U.N. et al: [OpenAD/F: A modular, open-source tool for automatic differentiation of Fortran codes](#) . ACM TOMS 34(4), 2008.

Plot: A tangent computation / finite difference approximation for 64,800 grid points at 1 min each would keep us waiting for **a month and a half ... :-(((** We can do it in **less than 10 minutes thanks to adjoints computed by a differentiated version of the MITgcm :-)**

Fundamental Mathematics

- ▶ continuity
- ▶ differentiability?



- ▶ gradient, Jacobian, Hessian, higher-order derivative tensors
- ▶ Taylor expansion
- ▶ chain rule

Progress

Introduction

First-Order(A)AD

- Prerequisites

- Tangents

- Adjoint

Second-(and Higher-)Order (A)AD

- Tangents of Tangents

- Tangents of Adjoint

"Getting Serious" with AAD

- Implementation by Overloading

- Checkpointing

- Symbolic Adjoint

- Adjoint Code Design Patterns

1. The given implementation of $F : \mathbb{R}^n \rightarrow \mathbb{R}^m : \mathbf{y} = F(\mathbf{x})$, can be decomposed into a single assignment code (SAC)

$$\begin{aligned}v_i &= \varphi_i(x_i) = x_i & i &= 0, \dots, n-1 \\v_j &= \varphi_j((v_k)_{k \prec j}) & j &= n, \dots, n+q-1 \\y_k &= \varphi_{n+q+k}(v_{n+p+k}) = v_{n+p+k} & k &= 0, \dots, m-1\end{aligned}$$

where $q = p + m$ and $k \prec j$ denotes a direct dependence of v_j on v_k as an argument of φ_j .

2. All elemental functions φ_j possess continuous partial derivatives

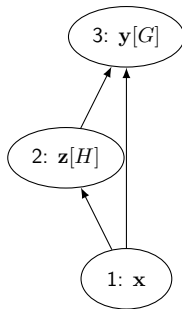
$$d_{j,i} \equiv \frac{d\varphi_j}{dv_i}(v_k)_{k \prec j}$$

with respect to their arguments $(v_k)_{k \prec j}$ at all points of interest.

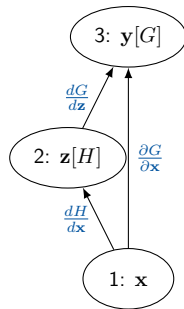
3. A **linearized SAC (ISAC)** is obtained by augmenting the elemental assignments with computations of the local partial derivatives $d_{j,i}$.
4. The SAC induces a directed acyclic graph (DAG) $G = G(F) = (V, E)$ with integer vertices $V = \{0, \dots, n + q\}$ and edges $V \times V \supseteq E = \{(i, j) : i \prec j\}$.
5. The set of vertices representing the n inputs is denoted as $X \subseteq V$. The m outputs are collected in $Y \subseteq V$. All remaining **intermediate vertices** belong to $Z \subsetneq V$.
6. A **linearized DAG (IDAG)** is obtained by attaching the $d_{j,i}$ to the corresponding edges (i, j) in the DAG.

SAC: $\mathbf{z} := H(\mathbf{x})$
 $\mathbf{y} := G(\mathbf{z}, \mathbf{x})$

DAG:



IDAG:



$$\nabla F(\mathbf{x}) \equiv \frac{d\mathbf{y}}{d\mathbf{x}} = \sum_{\text{path} \in \text{IDAG}} \prod_{(i,j) \in \text{path}} d_{j,i}$$

- ▶ U. N.: *Optimal Jacobian accumulation is NP-complete*. Math. Prog. 112(2):427–441, Springer, 2008.

Proof by reduction from ENSEMBLE COMPUTATION

- ▶ U. N.: *Optimal accumulation of Jacobian matrices by elimination methods on the dual computational graph*. Math. Prog. 99(3):399–421, Springer, 2004.

Example: **bat graph** in STCE logo

- ▶ A. Griewank and U. N.: *Accumulating Jacobians as chained sparse matrix products*. Math. Prog. 95(3):555–571, Springer, 2003.

Example: $\mathbb{R}^4 \rightarrow \mathbb{R}^2 \rightarrow \mathbb{R}^2 \rightarrow \mathbb{R}^2 \rightarrow \mathbb{R}^4$

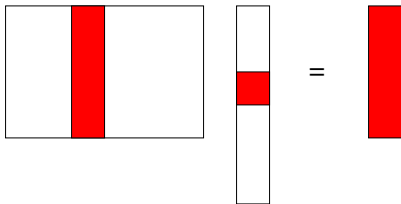
A first-order tangent model $F^{(1)} : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^m \times \mathbb{R}^m$,

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{y}^{(1)} \end{pmatrix} = F^{(1)}(\mathbf{x}, \mathbf{x}^{(1)}),$$

defines a directional derivative alongside with the function value:

$$\mathbf{y} = F(\mathbf{x})$$

$$\mathbf{y}^{(1)} = \nabla F(\mathbf{x}) \cdot \mathbf{x}^{(1)}$$



... definition of the whole Jacobian column-wise by input directions $\mathbf{x}^{(1)} \in \mathbb{R}^n$ equal to the Cartesian basis vectors in \mathbb{R}^n .

A first-order tangent code $F^{(1)} : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^{\tilde{n}} \rightarrow \mathbb{R}^m \times \mathbb{R}^m \times \mathbb{R}^{\tilde{m}}$

$$\begin{pmatrix} \mathbf{z} \\ \mathbf{z}^{(1)} \\ \tilde{\mathbf{z}} \\ \mathbf{y} \\ \mathbf{y}^{(1)} \\ \tilde{\mathbf{y}} \end{pmatrix} := F^{(1)}(\mathbf{x}, \mathbf{x}^{(1)}, \tilde{\mathbf{x}}, \mathbf{z}, \mathbf{z}^{(1)}, \tilde{\mathbf{z}}),$$

computes a Jacobian \times vector product alongside with the function value:

$$\mathbb{R}^m \times \mathbb{R}^{\tilde{m}} \ni \begin{pmatrix} \mathbf{z} \\ \tilde{\mathbf{z}} \\ \mathbf{y} \\ \tilde{\mathbf{y}} \end{pmatrix} := F(\mathbf{x}, \tilde{\mathbf{x}}, \mathbf{z}, \tilde{\mathbf{z}})$$

$$\mathbb{R}^m \ni \begin{pmatrix} \mathbf{z}^{(1)} \\ \mathbf{y}^{(1)} \end{pmatrix} := \nabla F(\mathbf{x}, \tilde{\mathbf{x}}, \mathbf{z}, \tilde{\mathbf{z}}) \cdot \begin{pmatrix} \mathbf{x}^{(1)} \\ \mathbf{z}^{(1)} \end{pmatrix}$$

Variables for which derivatives are computed are referred to as **active**; \mathbf{x} and \mathbf{z} are **active inputs**; \mathbf{z} and \mathbf{y} are **active outputs**.

Variables which depend on active inputs are referred to as **varied**.

Variables for which no derivatives are computed are referred to as **passive**; $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{z}}$ are **passive inputs**; $\tilde{\mathbf{z}}$ and $\tilde{\mathbf{y}}$ are **passive outputs**.

Variables on which active outputs depend are referred to as **useful**.

Active variables are both varied and useful.

The whole (dense) Jacobian can be **harvested** column-wise from the active output directions $(\mathbf{z}^{(1)}, \mathbf{y}^{(1)})^T \in \mathbb{R}^m$ by **seeding** active input directions $(\mathbf{x}^{(1)}, \mathbf{z}^{(1)})^T \in \mathbb{R}^n$ with the Cartesian basis vectors in \mathbb{R}^n .

A first-order tangent code $F^{(1)} : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^m \times \mathbb{R}^m$,

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{y}^{(1)} \end{pmatrix} := F^{(1)}(\mathbf{x}, \mathbf{x}^{(1)}),$$

computes a Jacobian \times vector product alongside with the function value:

$$\begin{aligned} \mathbf{y} &:= F(\mathbf{x}) \\ \mathbf{y}^{(1)} &:= \nabla F(\mathbf{x}) \cdot \mathbf{x}^{(1)} \end{aligned}$$

For $i = 0, \dots, n - 1$

$$\begin{pmatrix} v_i \\ v_i^{(1)} \end{pmatrix} := \begin{pmatrix} x_i \\ x_i^{(1)} \end{pmatrix} \quad (\text{seed})$$

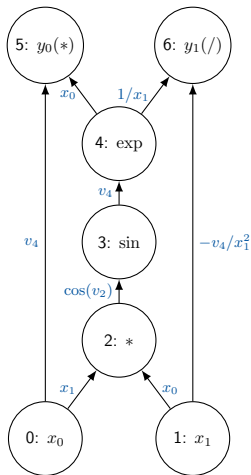
For $i = n, \dots, q - 1$

$$\begin{pmatrix} v_i \\ v_i^{(1)} \end{pmatrix} := \begin{pmatrix} \varphi_i(v_k)_{k \prec i} \\ \sum_{j \prec i} \frac{d\varphi_i(v_k)_{k \prec i}}{dv_j} \cdot v_j^{(1)} \end{pmatrix} \quad (\text{propagate})$$

For $i = 0, \dots, m - 1$

$$\begin{pmatrix} y_i \\ y_i^{(1)} \end{pmatrix} := \begin{pmatrix} v_{n+p+i} \\ v_{n+p+i}^{(1)} \end{pmatrix} \quad (\text{harvest})$$

Tangent assignments augment primal ...



$$\dot{t} = \dot{x}_0 \cdot x_1 + x_0 \cdot \dot{x}_1$$

$$t := x_0 \cdot x_1$$

$$\dot{t} = \cos(t) \cdot \dot{t}$$

$$t := \sin(t)$$

$$t := e^t$$

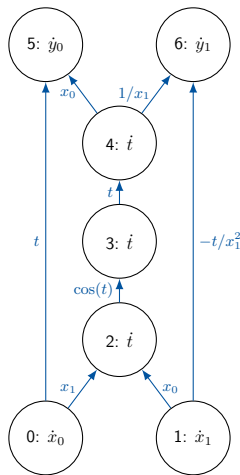
$$\dot{t} = t \cdot \dot{t}$$

$$\dot{y}_0 = \dot{x}_0 \cdot t + x_0 \cdot \dot{t}$$

$$y_0 := x_0 \cdot t$$

$$\dot{y}_1 = \dot{t}/x_1 - t \cdot \dot{x}_1/x_1^2$$

$$y_1 := t/x_1$$



Euler-Maruyama live ...

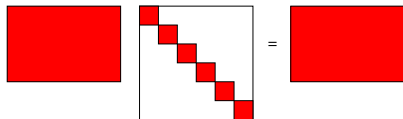
A first-order vector tangent code $F^{(1)} : \mathbb{R}^n \times \mathbb{R}^{n \times l} \rightarrow \mathbb{R}^m \times \mathbb{R}^{m \times l}$,

$$\begin{pmatrix} \mathbf{y} \\ Y^{(1)} \end{pmatrix} := F^{(1)}(\mathbf{x}, X^{(1)}),$$

computes a Jacobian \times matrix product alongside with the function value:

$$\mathbf{y} := F(\mathbf{x})$$

$$Y^{(1)} := \nabla F(\mathbf{x}) \cdot X^{(1)}$$



... harvesting of the whole Jacobian by seeding input directions $X^{(1)}[i] \in \mathbb{R}^n$, $i = 0, \dots, n-1$, with the Cartesian basis vectors in \mathbb{R}^n . Note concurrency!

Euler-Maruyama live ...

Adjoint

The Jacobian is a linear operator $\nabla F : \mathbb{R}^n \rightarrow \mathbb{R}^m$.

Its adjoint is defined as $(\nabla F)^* : \mathbb{R}^m \rightarrow \mathbb{R}^n$ where

$$\langle (\nabla F)^* \cdot \mathbf{y}_{(1)}, \mathbf{x}^{(1)} \rangle_{\mathbb{R}^n} = \langle \mathbf{y}_{(1)}, \nabla F \cdot \mathbf{x}^{(1)} \rangle_{\mathbb{R}^m} ,$$

and where $\langle \cdot, \cdot \rangle_{\mathbb{R}^n}$ and $\langle \cdot, \cdot \rangle_{\mathbb{R}^m}$ denote appropriate scalar products in \mathbb{R}^n and \mathbb{R}^m , respectively.

Theorem

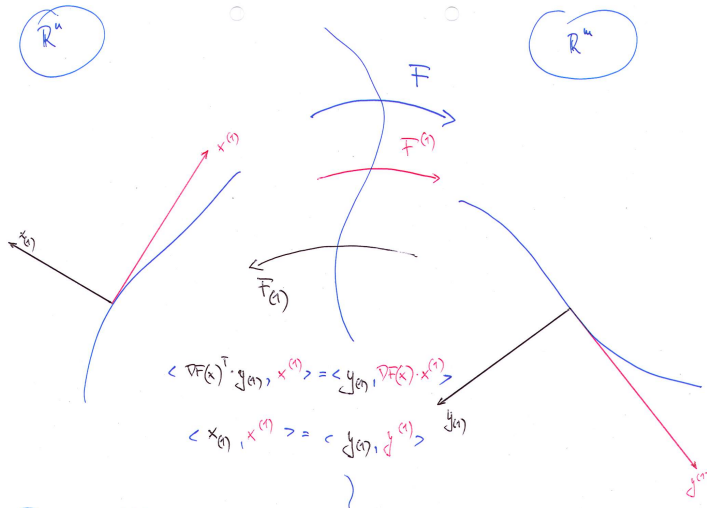
$$(\nabla F)^* = (\nabla F)^T.$$

$$\langle (\nabla F)^T \cdot \mathbf{y}_{(1)}, \mathbf{x}^{(1)} \rangle_{\mathbb{R}^n} = \langle \mathbf{y}_{(1)}, \nabla F \cdot \mathbf{x}^{(1)} \rangle_{\mathbb{R}^m}$$

$\underset{[=: \mathbf{x}_{(1)}]}$
 $\underset{[=: \mathbf{y}^{(1)}]}$

Note invariant at each point in the program execution → [validation](#).

Adjoint



Eq. $y = \sin(x)$; $y = x_0 \cdot x_1$; ...

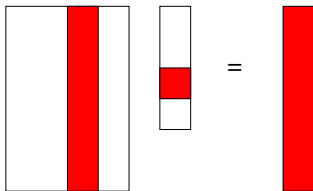
A first-order adjoint model $F_{(1)} : \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^m \times \mathbb{R}^n$,

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{x}_{(1)} \end{pmatrix} = F_{(1)}(\mathbf{x}, \mathbf{y}_{(1)}),$$

defines an adjoint directional derivative alongside with the function value:

$$\mathbf{y} = F(\mathbf{x})$$

$$\mathbf{x}_{(1)} = \nabla F(\mathbf{x})^T \cdot \mathbf{y}_{(1)}$$



... definition of the whole Jacobian row-wise through input directions $\mathbf{y}_{(1)} \in \mathbb{R}^m$ equal to the Cartesian basis vectors in \mathbb{R}^m .

In

$$\left(\frac{dF}{d\mathbf{x}} \right)^T \cdot \mathbf{y}_{(1)}$$

the subscript on \mathbf{y} denotes the first directional differentiation of F performed in adjoint mode in direction $\mathbf{y}_{(1)} \in \mathbb{R}^m$.

Enumeration of derivatives and distinction of super- and subscripts will become relevant in the discussion of higher derivatives computed by combinations of tangent and adjoint modes.

$$F_{(1)} : \mathbb{R}^n \times \mathbb{R}^{n_x} \times \mathbb{R}^m \times \mathbb{R}^{\tilde{n}} \rightarrow \mathbb{R}^m \times \mathbb{R}^n \times \mathbb{R}^{m_y} \times \mathbb{R}^{\tilde{m}},$$

$$\begin{pmatrix} \mathbf{z} & \tilde{\mathbf{z}} & \mathbf{y} & \tilde{\mathbf{y}} & \mathbf{x}_{(1)} & \mathbf{z}_{(1)} & \mathbf{y}_{(1)} \end{pmatrix}^T := F_{(1)}(\mathbf{x}, \mathbf{x}_{(1)}, \tilde{\mathbf{x}}, \mathbf{z}, \mathbf{z}_{(1)}, \tilde{\mathbf{z}}, \mathbf{y}_{(1)}),$$

computes a shifted transposed Jacobian \times vector product alongside with the function value:

$$\begin{aligned} \mathbb{R}^m \times \mathbb{R}^m \ni \begin{pmatrix} \mathbf{z} \\ \tilde{\mathbf{z}} \\ \mathbf{y} \\ \tilde{\mathbf{y}} \end{pmatrix} &:= F(\mathbf{x}, \tilde{\mathbf{x}}, \mathbf{z}, \tilde{\mathbf{z}}) \\ \begin{pmatrix} \mathbf{x}_{(1)} \\ \mathbf{z}_{(1)} \end{pmatrix} &:= \begin{pmatrix} \mathbf{x}_{(1)} \\ 0 \end{pmatrix} + \nabla F(\mathbf{x}, \tilde{\mathbf{x}}, \mathbf{z}, \tilde{\mathbf{z}})^T \cdot \begin{pmatrix} \mathbf{z}_{(1)} \\ \mathbf{y}_{(1)} \end{pmatrix} \\ \mathbf{y}_{(1)} &:= 0 \end{aligned}$$

The whole (dense) Jacobian can be harvested from the active input adjoints

$$\begin{pmatrix} \mathbf{x}_{(1)} \\ \mathbf{z}_{(1)} \end{pmatrix} \in \mathbb{R}^m$$

row-wise by seeding active output adjoints

$$\begin{pmatrix} \mathbf{z}_{(1)} \\ \mathbf{y}_{(1)} \end{pmatrix} \in \mathbb{R}^m$$

with the Cartesian basis vectors in \mathbb{R}^m and for $\mathbf{x}_{(1)} := 0$ on input.

A first-order adjoint code $F_{(1)} : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \rightarrow \mathbb{R}^m \times \mathbb{R}^n$,

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{x}_{(1)} \end{pmatrix} := F_{(1)}(\mathbf{x}, \mathbf{x}_{(1)}, \mathbf{y}_{(1)}),$$

computes a shifted transposed Jacobian \times vector product alongside with the function value:

$$\begin{aligned} \mathbf{y} &:= F(\mathbf{x}) \\ \mathbf{x}_{(1)} &:= \mathbf{x}_{(1)} + \nabla F(\mathbf{x})^T \cdot \mathbf{y}_{(1)} \end{aligned}$$

... harvesting of the whole Jacobian row-wise by seeding input directions $\mathbf{y}_{(1)} \in \mathbb{R}^m$ with the Cartesian basis vectors in \mathbb{R}^m and for $\mathbf{x}_{(1)} = 0$ on input.

1. Augmented Primal (enable data flow reversal)

For $i = 0, \dots, n - 1$

$$v_i := x_i$$

record $i \in V$ ($v_{i_{(1)}} := x_{i_{(1)}}$)

For $i = n, \dots, q - 1$

$$v_i := \varphi_i(v_k)_{k \prec i}$$

record $i \in V$ ($v_{i_{(1)}} := 0$)

For $j \prec i$: record $(i, j) \in E$ ($d_{j,i} := \frac{d\varphi_i(v_k)_{k \prec i}}{dv_j}$)

For $i = 0, \dots, m - 1$

$$y_i := v_{n+p+i}$$

2. Adjoint

For $i = 0, \dots, m-1$

$$v_{n+p+i_{(1)}} := y_{i_{(1)}}$$

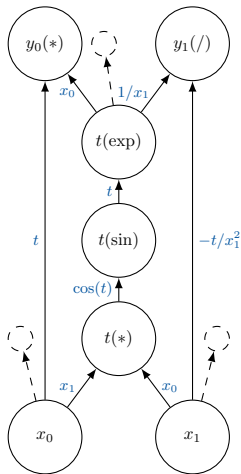
For $i = q-1, \dots, n$

$$\forall (j, i) \in E : v_{j_{(1)}} := v_{j_{(1)}} + v_{i_{(1)}} \cdot d_{i,j}$$

For $i = 0, \dots, n-1$

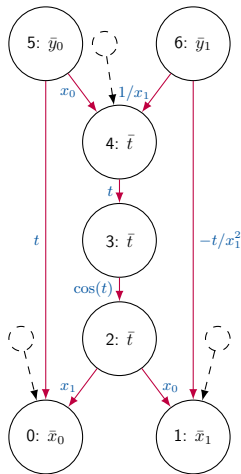
$$x_{i_{(1)}} := v_{i_{(1)}}$$

Mind overwrites and context ...



$t := x_0 \cdot x_1$
 $\text{push}(t); t := \sin(t)$
 $t := e^t$
 $y_0 := x_0 \cdot t$
 $y_1 := t/x_1$

$\bar{x}_1 += -t/x_1^2 \cdot \bar{y}_1$
 $\bar{t} += 1/x_1 \cdot \bar{y}_1$
 $\bar{y}_1 := 0$
 $\bar{t} += x_0 \cdot \bar{y}_0$
 $\bar{x}_0 += t \cdot \bar{y}_0$
 $\bar{y}_0 := 0$
 $\bar{t} := t \cdot \bar{t}$
 $\text{pop}(t); \bar{t} := \cos(v_2) \cdot \bar{t}$
 $\bar{x}_1 += x_0 \cdot \bar{t}$
 $\bar{x}_0 += x_1 \cdot \bar{t}$



Euler-Maruyama live ...

Progress

Introduction

First-Order(A)AD

- Prerequisites

- Tangents

- Adjoint

Second-(and Higher-)Order (A)AD

- Tangents of Tangents

- Tangents of Adjoint

"Getting Serious" with AAD

- Implementation by Overloading

- Checkpointing

- Symbolic Adjoint

- Adjoint Code Design Patterns

Initially we consider multivariate scalar functions

$y = F(\mathbf{x}) : D_F \subseteq \mathbb{R}^n \rightarrow I_F \subseteq \mathbb{R}$ in order to simplify the notation.

We assume F to be twice continuously differentiable over its domain D_F implying the existence of the Hessian

$$\nabla^2 F(\mathbf{x}) \equiv \frac{d^2 F}{d\mathbf{x}^2}(\mathbf{x}).$$

For multivariate vector functions the Hessian is a three-tensor complicating the notation slightly due to the need for tensor arithmetic; see later.

A second-order *central finite difference* quotient

$$\frac{d^2 F}{dx_i dx_j}(\mathbf{x}^0) \approx \left[F(\mathbf{x}^0 + (\mathbf{e}_j + \mathbf{e}_i) \cdot h) - F(\mathbf{x}^0 + (\mathbf{e}_j - \mathbf{e}_i) \cdot h) \right. \\ \left. - F(\mathbf{x}^0 + (\mathbf{e}_i - \mathbf{e}_j) \cdot h) + F(\mathbf{x}^0 - (\mathbf{e}_j + \mathbf{e}_i) \cdot h) \right] / (4 \cdot h^2) \quad (1)$$

yields an approximation of the second directional derivative

$$y^{(1,2)} = \mathbf{x}^{(1)T} \cdot \nabla^2 F(\mathbf{x}) \cdot \mathbf{x}^{(2)} \quad (\text{w.l.o.g. } m = 1)$$

as

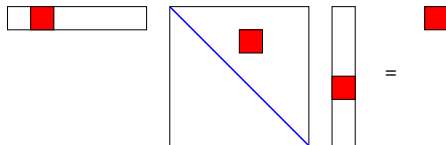
$$\frac{d^2 F}{dx_i dx_j}(\mathbf{x}^0) \approx \frac{\frac{dF}{dx_i}(\mathbf{x}^0 + \mathbf{e}_j \cdot h) - \frac{dF}{dx_i}(\mathbf{x}^0 - \mathbf{e}_j \cdot h)}{2 \cdot h} \\ = \left[\frac{F(\mathbf{x}^0 + \mathbf{e}_j \cdot h + \mathbf{e}_i \cdot h) - F(\mathbf{x}^0 + \mathbf{e}_j \cdot h - \mathbf{e}_i \cdot h)}{2 \cdot h} \right. \\ \left. - \frac{F(\mathbf{x}^0 - \mathbf{e}_j \cdot h + \mathbf{e}_i \cdot h) - F(\mathbf{x}^0 - \mathbf{e}_j \cdot h - \mathbf{e}_i \cdot h)}{2 \cdot h} \right] / (2 \cdot h).$$

A second derivative code $F^{(1,2)} : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R} \times \mathbb{R} \times \mathbb{R} \times \mathbb{R}$, generated in **Tangent-over-Tangent (ToT) mode** computes

$$\begin{pmatrix} y \\ y^{(2)} \\ y^{(1)} \\ y^{(1,2)} \end{pmatrix} = F^{(1,2)}(\mathbf{x}, \mathbf{x}^{(2)}, \mathbf{x}^{(1)}, \mathbf{x}^{(1,2)}),$$

as follows:

$$\begin{pmatrix} y \\ y^{(2)} \\ y^{(1)} \\ y^{(1,2)} \end{pmatrix} := \begin{pmatrix} F(\mathbf{x}) \\ \nabla F(\mathbf{x}) \cdot \mathbf{x}^{(2)} \\ \nabla F(\mathbf{x}) \cdot \mathbf{x}^{(1)} \\ \mathbf{x}^{(1)T} \cdot \nabla^2 F(\mathbf{x}) \cdot \mathbf{x}^{(2)} + \nabla F(\mathbf{x}) \cdot \mathbf{x}^{(1,2)} \end{pmatrix}.$$



$$\mathbf{x}^{(1)T} \cdot \nabla^2 F(\mathbf{x}) \cdot \mathbf{x}^{(2)}$$

... accumulation of the whole Hessian element-wise by *seeding* input directions $\mathbf{x}^{(1)} \in \mathbb{R}^n$ $\mathbf{x}^{(2)} \in \mathbb{R}^n$ independently with the Cartesian basis vectors in \mathbb{R}^n for $\mathbf{x}^{(1,2)} = 0$; harvesting from $y^{(1,2)}$.

Note: [Approximate Tangents of Tangents](#)

A second derivative code

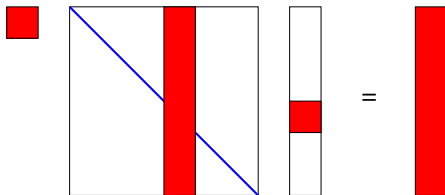
$$F_{(1)}^{(2)} : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R} \times \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n,$$

generated in **Tangent-over-Adjoint (ToA) mode** computes

$$\begin{pmatrix} y \\ y^{(2)} \\ \mathbf{x}_{(1)}^{(2)} \\ \mathbf{x}_{(1)}^{(2)} \end{pmatrix} = F_{(1)}^{(2)}(\mathbf{x}, \mathbf{x}^{(2)}, \mathbf{x}_{(1)}, \mathbf{x}_{(1)}^{(2)}, y_{(1)}, y_{(1)}^{(2)}),$$

as follows:

$$\begin{pmatrix} y \\ y^{(2)} \\ \mathbf{x}_{(1)}^{(2)} \\ \mathbf{x}_{(1)}^{(2)} \end{pmatrix} := \begin{pmatrix} F(\mathbf{x}) \\ \nabla F(\mathbf{x}) \cdot \mathbf{x}^{(2)} \\ \mathbf{x}_{(1)} + \nabla F(\mathbf{x})^T \cdot y_{(1)} \\ \mathbf{x}_{(1)}^{(2)} + y_{(1)} \cdot \nabla^2 F(\mathbf{x}) \cdot \mathbf{x}^{(2)} + \nabla F(\mathbf{x})^T \cdot y_{(1)}^{(2)} \end{pmatrix}$$



$$y_{(1)} \cdot \nabla^2 F(\mathbf{x}) \cdot \mathbf{x}^{(2)}$$

... accumulation of the whole Hessian column-wise by seeding input directions $\mathbf{x}^{(2)} \in \mathbb{R}^n$ with the Cartesian basis vectors in \mathbb{R}^n for $\mathbf{x}_{(1)}^{(2)} = 0$, $y_{(1)} = 1$ and $y_{(1)}^{(2)} = 0$; harvesting from $\mathbf{x}_{(1)}^{(2)}$.

Note: [Approximate Tangents of Adjoint](#)

Progress

Introduction

First-Order(A)AD

- Prerequisites

- Tangents

- Adjoint

Second-(and Higher-)Order (A)AD

- Tangents of Tangents

- Tangents of Adjoint

“Getting Serious” with AAD

- Implementation by Overloading

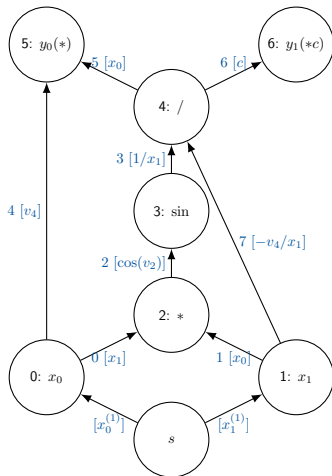
- Checkpointing

- Symbolic Adjoint

- Adjoint Code Design Patterns

dco/c++ features

- ▶ tangents and adjoints of arbitrary order through recursive template instantiation for numerical simulation code implemented in C++
- ▶ front-ends for Fortran, C#, Matlab, Python (3x alpha)
- ▶ optimized assignment-level gradient code through expression templates
- ▶ cache-optimized internal representation in various incarnations
- ▶ vector modes / detection and exploitation of sparsity
- ▶ external adjoint / Jacobian interfaces
- ▶ user-defined intrinsics
- ▶ intrinsic NAG Library functions (e.g. Linear Algebra, Interpolation, Root Finding, Nearest Correlation Matrix)
- ▶ support for parallelism: thread-safe data structures, adjoint MPI library, GPU coupling, meta adjoint programming (map)



Tangent IDAG

We consider

$$\begin{pmatrix} y_0 \\ y_1 \end{pmatrix} = \begin{pmatrix} x_0 * \sin(x_0 * x_1) / x_1 \\ \sin(x_0 * x_1) / x_1 * c \end{pmatrix}$$

implemented as

$$t := \sin(x_0 * x_1) / x_1$$

$$y_0 := x_0 * t; y_1 := t * c$$

yielding SAC

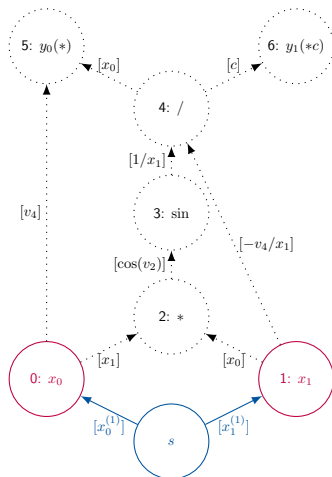
$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4; y_1 := v_4 * c$$

for some *passive* value c , i.e., no derivatives of or with respect to required; x , y , and t are *active*.

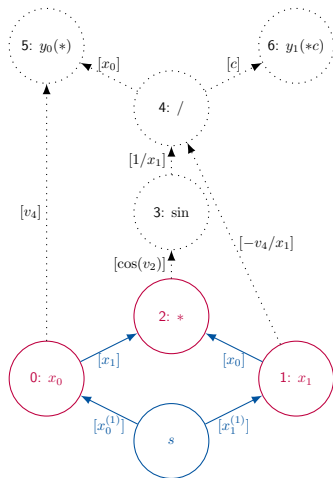


$x_0 := ?$

$x_1 := ?$

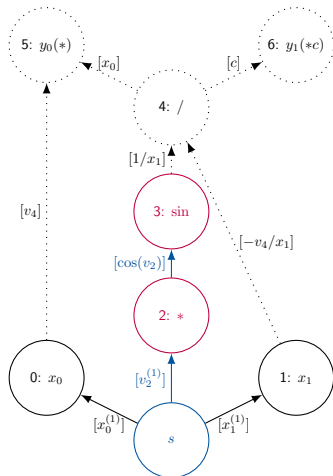
$x_0^{(1)} := ?$

$x_1^{(1)} := ?$

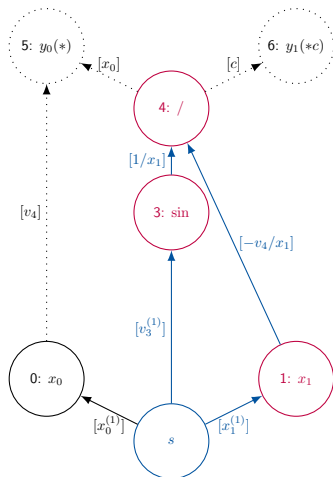


$$v_2 := x_0 * x_1$$

$$v_2^{(1)} := x_1 * x_0^{(1)} + x_0 * x_1^{(1)}$$



$$\begin{aligned}
 v_2 &:= x_0 * x_1 \\
 v_2^{(1)} &:= x_1 * x_0^{(1)} + x_0 * x_1^{(1)} \\
 v_3 &:= \sin(v_2) \\
 v_3^{(1)} &:= \cos(v_2) * v_2^{(1)}
 \end{aligned}$$



$$v_2 := x_0 * x_1$$

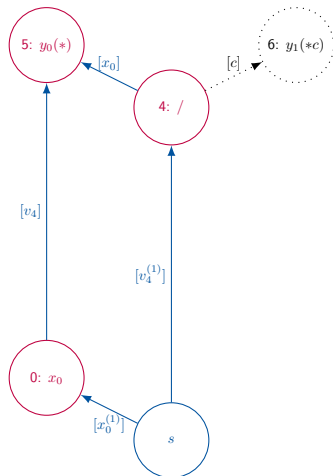
$$v_2^{(1)} := x_1 * x_0^{(1)} + x_0 * x_1^{(1)}$$

$$v_3 := \sin(v_2)$$

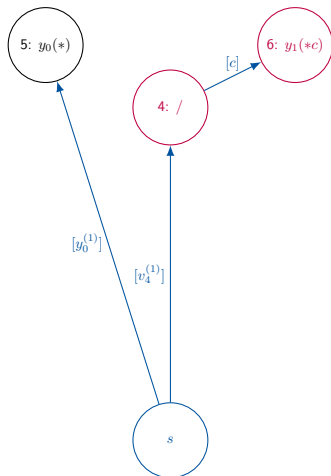
$$v_3^{(1)} := \cos(v_2) * v_2^{(1)}$$

$$v_4 := v_3 / x_1$$

$$v_4^{(1)} := (v_3^{(1)} - v_4 * x_1^{(1)}) / x_1$$



$$\begin{aligned}
 v_2 &:= x_0 * x_1 \\
 v_2^{(1)} &:= x_1 * x_0^{(1)} + x_0 * x_1^{(1)} \\
 v_3 &:= \sin(v_2) \\
 v_3^{(1)} &:= \cos(v_2) * v_2^{(1)} \\
 v_4 &:= v_3 / x_1 \\
 v_4^{(1)} &:= (v_3^{(1)} - v_4 * x_1^{(1)}) / x_1 \\
 y_0 &:= x_0 * v_4 \\
 y_0^{(1)} &:= v_4 * x_0^{(1)} + x_0 * v_4^{(1)}
 \end{aligned}$$



$$v_2 := x_0 * x_1$$

$$v_2^{(1)} := x_1 * x_0^{(1)} + x_0 * x_1^{(1)}$$

$$v_3 := \sin(v_2)$$

$$v_3^{(1)} := \cos(v_2) * v_2^{(1)}$$

$$v_4 := v_3 / x_1$$

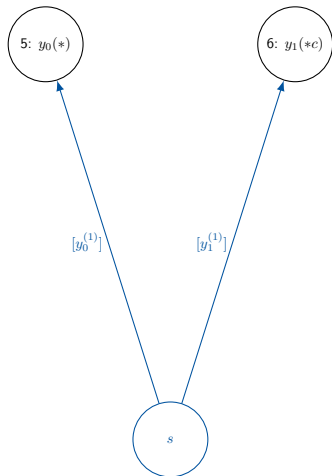
$$v_4^{(1)} := (v_3^{(1)} - v_4 * x_1^{(1)}) / x_1$$

$$y_0 := x_0 * v_4$$

$$y_0^{(1)} := v_4 * x_0^{(1)} + x_0 * v_4^{(1)}$$

$$y_1 := v_4 * c$$

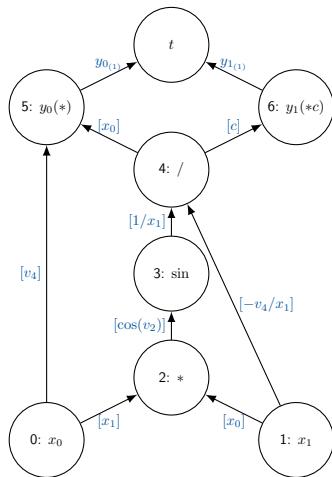
$$y_1^{(1)} := c * v_4^{(1)}$$



$$\begin{aligned}
 v_2 &:= x_0 * x_1 \\
 v_2^{(1)} &:= x_1 * x_0^{(1)} + x_0 * x_1^{(1)} \\
 v_3 &:= \sin(v_2) \\
 v_3^{(1)} &:= \cos(v_2) * v_2^{(1)} \\
 v_4 &:= v_3 / x_1 \\
 v_4^{(1)} &:= (v_3^{(1)} - v_4 * x_1^{(1)}) / x_1 \\
 y_0 &:= x_0 * v_4 \\
 y_0^{(1)} &:= v_4 * x_0^{(1)} + x_0 * v_4^{(1)} \\
 y_1 &:= v_4 * c \\
 y_1^{(1)} &:= c * v_4^{(1)}
 \end{aligned}$$

User Guide: $\mathbf{y}^{(1)} := \nabla F(\mathbf{x}) \cdot \mathbf{x}^{(1)}$

```
1 void driver(const vector<double>& xv, double &yv, vector<double> &g) {
2     typedef dco::gt1s<double>::type DCO_T;
3     size_t n=xv.size();
4     DCO_T y=0;
5     for (size_t i=0;i<n;i++) {
6         vector<DCO_T> x(n,0);
7         for (size_t j=0;j<n;j++) x[j]=xv[j];
8         dco::derivative(x[i])=1; // seed directions
9         f(x,y); // overloaded primal
10        g[i]=dco::derivative(y); // harvest directional derivatives
11    }
12    yv=dco::value(y); // extract function value
13 }
```



Adjoint IDAG

We consider

$$\begin{pmatrix} y_0 \\ y_1 \end{pmatrix} = \begin{pmatrix} x_0 * \sin(x_0 * x_1) / x_1 \\ \sin(x_0 * x_1) / x_1 * c \end{pmatrix}$$

implemented as

$$t := \sin(x_0 * x_1) / x_1$$

$$y_0 := x_0 * t$$

$$y_1 := t * c$$

yielding SAC

$$v_2 := x_0 * x_1$$

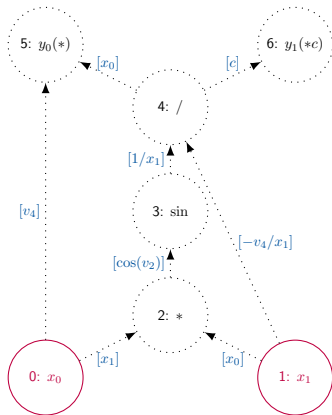
$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$

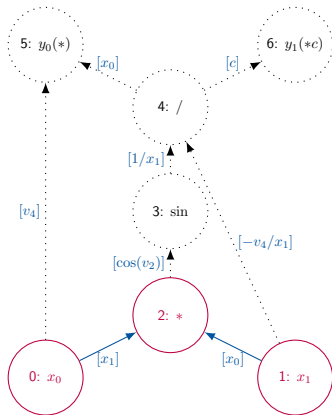
$$y_1 := v_4 * c$$

for some passive value c .

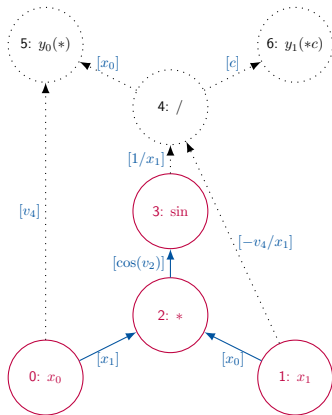


$x_0 := ?$

$x_1 := ?$

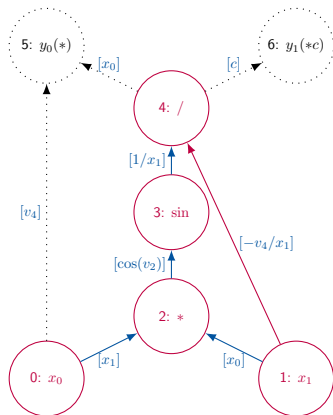


$$v_2 := x_0 * x_1$$



$$v_2 := x_0 * x_1$$

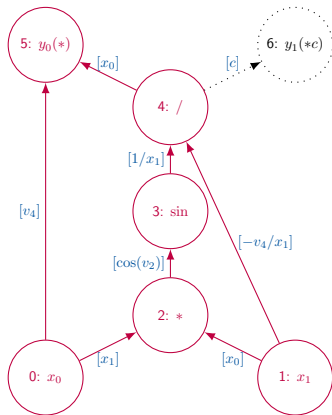
$$v_3 := \sin(v_2)$$



$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

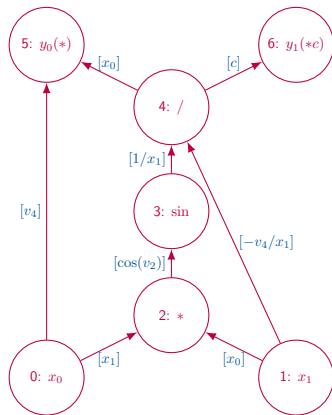


$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$



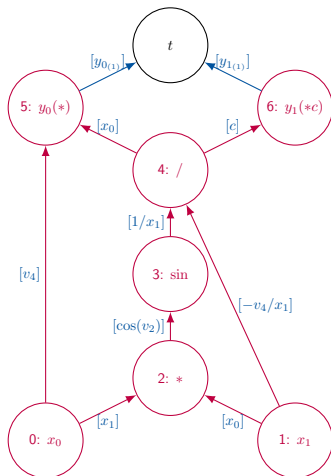
$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$

$$y_1 := v_4 * c$$



$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$

$$y_1 := v_4 * c$$

$$y_{0(1)} := ?$$

$$y_{1(1)} := ?$$

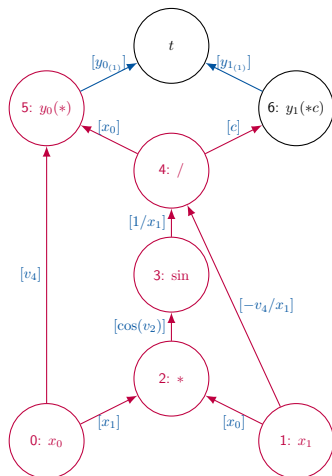
$$x_{0(1)} := ?$$

$$x_{1(1)} := ?$$

$$v_{2(1)} := 0$$

$$v_{3(1)} := 0$$

$$v_{4(1)} := 0$$



$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$

$$y_1 := v_4 * c$$

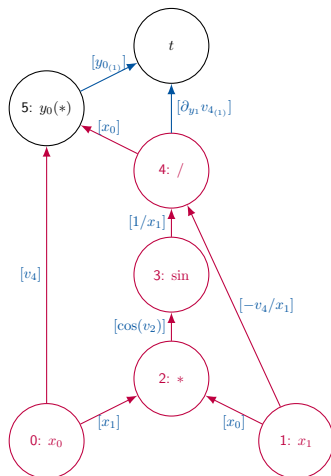
$$v_{4(1)} + = c * y_{1(1)}$$

Note C++ Syntax:

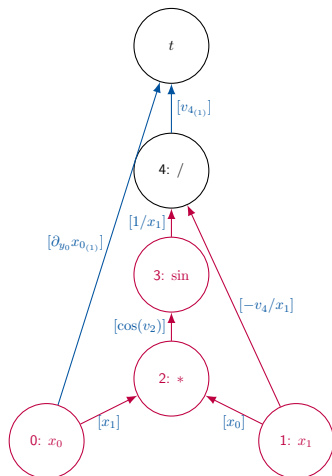
$$v_{4(1)} + = c * y_{1(1)}$$

\Leftrightarrow

$$v_{4(1)} := v_{4(1)} + c * y_{1(1)}.$$



$$\begin{aligned}
 v_2 &:= x_0 * x_1 \\
 v_3 &:= \sin(v_2) \\
 v_4 &:= v_3 / x_1 \\
 y_0 &:= x_0 * v_4 \\
 y_1 &:= v_4 * c \\
 v_{4(1)} + &= c * y_{1(1)} \\
 v_{4(1)} + &= x_0 * y_{0(1)} \\
 x_{0(1)} + &= v_4 * y_{0(1)}
 \end{aligned}$$



$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$

$$y_1 := v_4 * c$$

$$v_{4(1)} + = c * y_{1(1)}$$

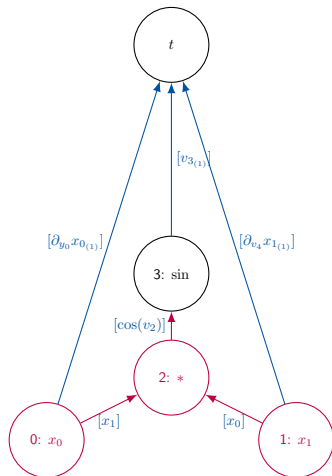
$$v_{4(1)} + = x_0 * y_{0(1)}$$

$$x_{0(1)} + = v_4 * y_{0(1)}$$

$$u := 1/x_1$$

$$v_{3(1)} + = u * v_{4(1)}$$

$$x_{1(1)} - = v_4 * u * v_{4(1)}$$



$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$

$$y_1 := v_4 * c$$

$$v_{4(1)} + = c * y_{1(1)}$$

$$v_{4(1)} + = x_0 * y_{0(1)}$$

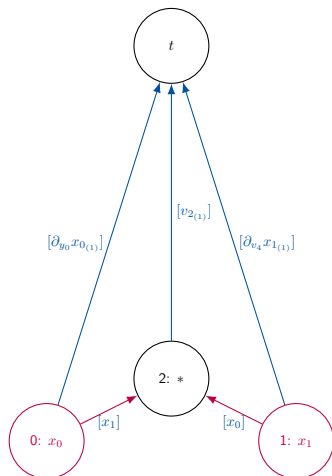
$$x_{0(1)} + = v_4 * y_{0(1)}$$

$$u := 1/x_1$$

$$v_{3(1)} + = u * v_{4(1)}$$

$$x_{1(1)} - = v_4 * u * v_{4(1)}$$

$$v_{2(1)} + = \cos(x_2) * v_{3(1)}$$



$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$

$$y_1 := v_4 * c$$

$$v_{4(1)} + = c * y_{1(1)}$$

$$v_{4(1)} + = x_0 * y_{0(1)}$$

$$x_{0(1)} + = v_4 * y_{0(1)}$$

$$u := 1/x_1$$

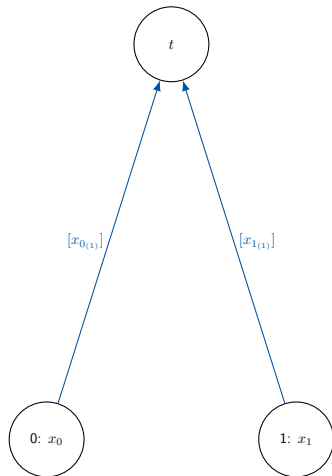
$$v_{3(1)} + = u * v_{4(1)}$$

$$x_{1(1)} - = v_4 * u * v_{4(1)}$$

$$v_{2(1)} + = \cos(x_2) * v_{3(1)}$$

$$x_{0(1)} + = x_1 * v_{2(1)}$$

$$x_{1(1)} + = x_0 * v_{2(1)}$$



$$v_2 := x_0 * x_1$$

$$v_3 := \sin(v_2)$$

$$v_4 := v_3 / x_1$$

$$y_0 := x_0 * v_4$$

$$y_1 := v_4 * c$$

$$v_{4(1)} + = c * y_{1(1)}$$

$$v_{4(1)} + = x_0 * y_{0(1)}$$

$$x_{0(1)} + = v_4 * y_{0(1)}$$

$$u := 1/x_1$$

$$v_{3(1)} + = u * v_{4(1)}$$

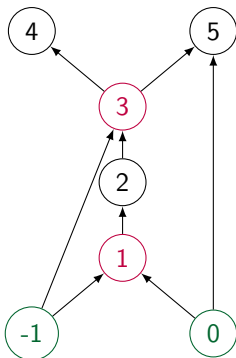
$$x_{1(1)} - = v_4 * u * v_{4(1)}$$

$$v_{2(1)} + = \cos(x_2) * v_{3(1)}$$

$$x_{0(1)} + = x_1 * v_{2(1)}$$

$$x_{1(1)} + = x_0 * v_{2(1)}$$

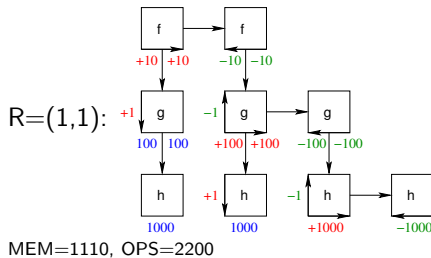
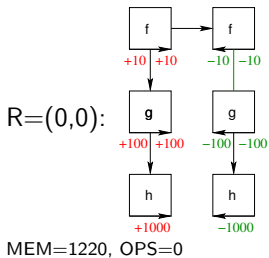
©Uwe Naumann, 2017



v_5, v_4, \dots, v_{-1}

- ▶ U.N.: **DAG REVERSAL** is NP-Complete, J. Disc. Alg. 7(4), 402-410 (2009).
- ▶ U.N.: **CALL TREE REVERSAL** is NP-Complete, LNCSE 64, 13-22 (2008).
- ▶ J. Lotz et al.: **Mixed Integer Programming for Call Tree Reversal**, SIAM CSC (2016).

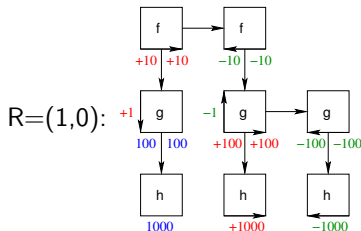
Example: Let $\overline{\text{MEM}} = 1110 \dots$



Example: Let $\overline{\text{MEM}} = 1110 \dots$ Greedy Heuristics

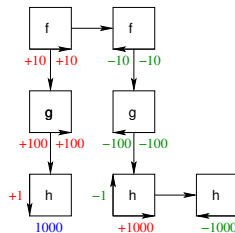
Smallest Memory Increase starts from $R = 1$ and yields \dots

Largest Memory Decrease (LMD) starts from $R = 0$ and yields \dots



MEM=1120, OPS=1200

$R=(0,1):$

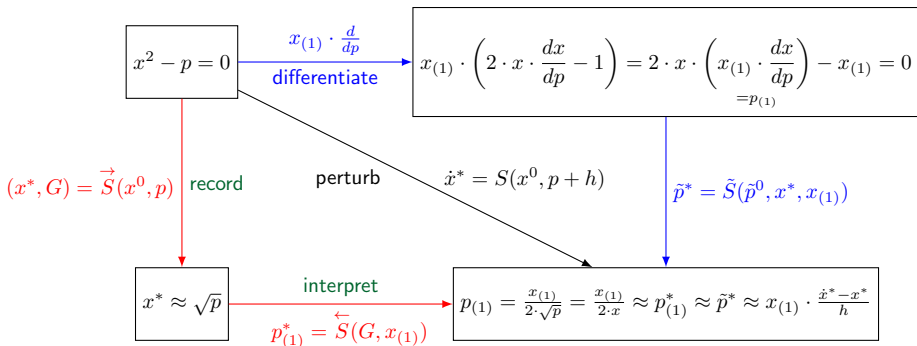


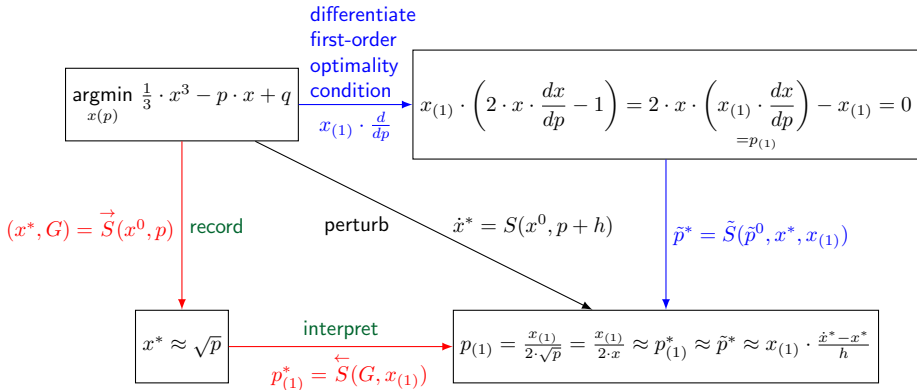
MEM=1110, OPS=1000

Largest Memory Increase (LMI) remains at $R = 1$ as $R = (1, 0)$ infeasible

Algorithmic Differentiation (AD) is based on Symbolic Differentiation (SD).
AD approaches vary in terms of choice of SD level.

- ▶ U.N. et al.: [Algorithmic differentiation of numerical methods: Tangent and adjoint solvers for parameterized systems of linear equations](#), RWTH Technical Report AIB-2012-10 (2012).
- ▶ U.N. et al.: [Algorithmic differentiation of numerical methods: Tangent and adjoint solvers for parameterized systems of nonlinear equations](#), ACM TOMS 41 (4), 26 (2015).
- ▶ N. Safiran et al.: [Algorithmic Differentiation of Numerical Methods: Second-Order Adjoint Solvers for Parameterized Systems of Nonlinear Equations](#), Procedia Computer Science 80, 2231-2235 (2016).
- ▶ J. Lotz et al.: [A Case Study in Adjoint Sensitivity Analysis of Parameter Calibration](#), Procedia Computer Science 80, 201-211 (2016).





Visual Paradigm Standard Edition (RWTH-Aachen University)

