Intro to Automatic Differentiation

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Recap

- Derivative information useful for solving inverse problems
  - 1st derivative of cost function for minimisation with gradient algorithm (mean value of posterior PDF)
  - 2nd derivative of cost function for approximation of uncertainties (covariance of posterior PDF)
- This lecture: Construction of efficient derivative code

Outline

- Chain Rule
- Basic Concepts: Active and Required Variables
- Tangent linear and adjoint code
- Verification of derivative code

Intro AD

Example:

$$F \quad : \mathbf{R}^5 \rightarrow \mathbf{R}^1$$

$$\quad : x \rightarrow y$$

$F(x) = f_4 \circ f_3 \circ f_2 \circ f_1(x)$, let each f_i be differentiable

Apply the chain rule for Differentiation!

$$DF = Df_4 \cdot Df_3 \cdot Df_2 \cdot Df_1$$

AD: Forward vs. Reverse

Example function:
N=5 inputs and M=1 output

Forward mode

$$\begin{pmatrix} x & x & x \end{pmatrix}\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}\begin{pmatrix} x & x \\ x & x \\ x & x \end{pmatrix}\begin{pmatrix} x & x & x & x & x \\ x & x & x & x & x \end{pmatrix}$$

$$= \begin{pmatrix} x & x & x \end{pmatrix}\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}\begin{pmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{pmatrix}$$

$$= \begin{pmatrix} x & x & x \end{pmatrix}\begin{pmatrix} x & x & x & x & x \\ x & x & x & x & x \\ x & x & x & x & x \end{pmatrix}$$

$$= \begin{pmatrix} x & x & x & x & x \end{pmatrix}$$

Reverse mode

$$\begin{pmatrix} x & x & x \end{pmatrix}\begin{pmatrix} x & x & x \\ x & x & x \\ x & x & x \end{pmatrix}\begin{pmatrix} x & x \\ x & x \\ x & x \end{pmatrix}\begin{pmatrix} x & x & x & x & x \\ x & x & x & x & x \end{pmatrix}$$

$$= \begin{pmatrix} x & x & x \end{pmatrix}\begin{pmatrix} x & x \\ x & x \\ x & x \end{pmatrix}\begin{pmatrix} x & x & x & x & x \\ x & x & x & x & x \end{pmatrix}$$

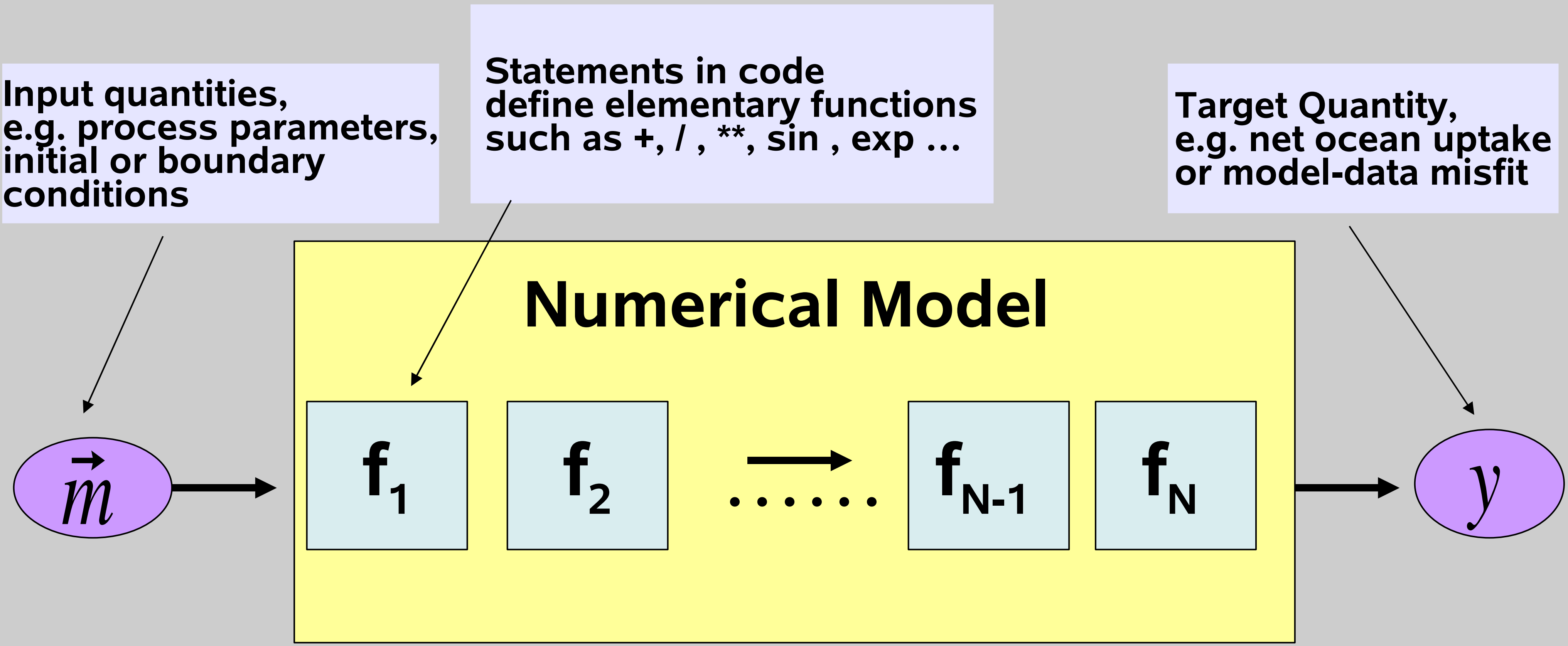
$$= \begin{pmatrix} x & x \end{pmatrix}\begin{pmatrix} x & x & x & x & x \\ x & x & x & x & x \end{pmatrix}$$

$$= \begin{pmatrix} x & x & x & x & x \end{pmatrix}$$

Intermediate Results

- **Forward and reverse mode yield the same result.**
- **Reverse mode: fewer operations (time) and less space for intermediates (memory)**
- **Cost for forward mode grows with N**
- **Cost for reverse mode grows with M**

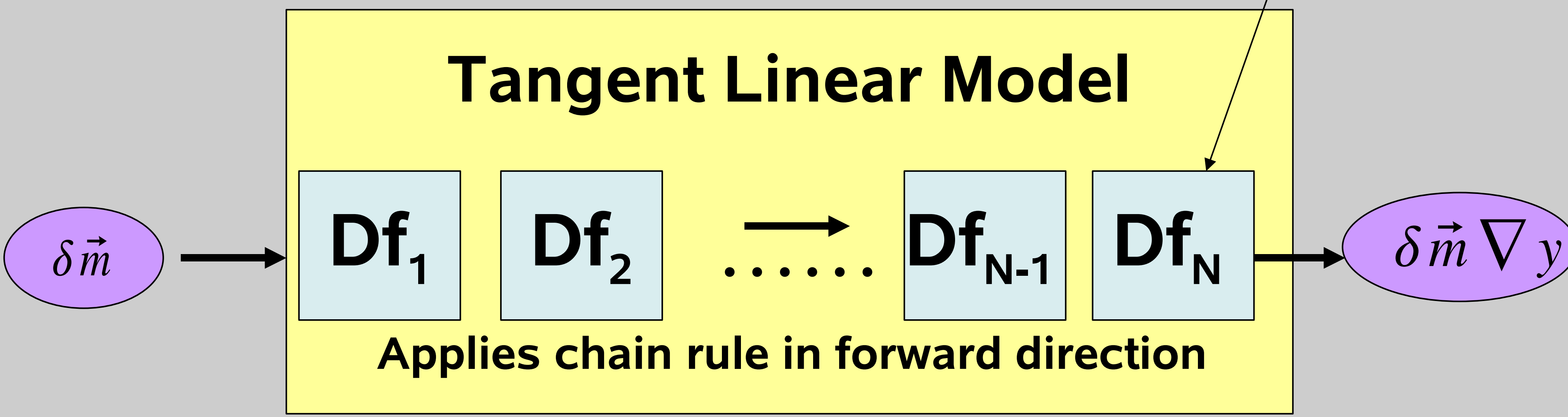
Sensitivities via AD



Sensitivities via AD

Cost of gradient evaluation proportional to # of parameters

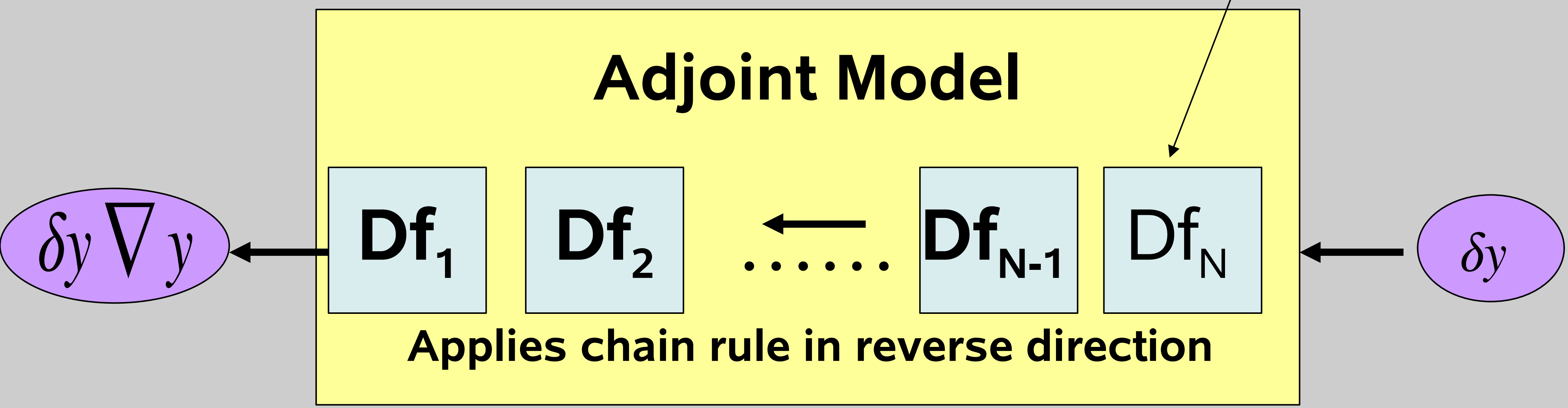
Derivatives of elementary functions are simple, they define local Jacobians



Sensitivities via AD

Cost of gradient evaluation independent of # of inputs

Derivatives of elementary functions are simple, they define local Jacobians



Reverse and Adjoint

$$DF = Df_4 \cdot Df_3 \cdot Df_2 \cdot Df_1 \qquad DF^T = Df_1^T \cdot Df_2^T \cdot Df_3^T \cdot Df_4^T$$

Propagation of Derivatives

Function:

$$x = z_0 \xrightarrow{f_1} z_1 \xrightarrow{f_2} z_2 \xrightarrow{f_3} z_3 \xrightarrow{f_4} z_4 = y$$

Forward:

$$x' = z'_0 \xrightarrow{Df_1} z'_1 \xrightarrow{Df_2} z'_2 \xrightarrow{Df_3} z'_3 \xrightarrow{Df_4} z'_4 = y'$$

$z'_0 \ldots z'_4$ are called tangent linear variables

Reverse:

$$\bar{x} = \bar{z}_0 \xleftarrow{Df_1^T} \bar{z}_1 \xleftarrow{Df_2^T} \bar{z}_2 \xleftarrow{Df_3^T} \bar{z}_3 \xleftarrow{Df_4^T} \bar{z}_4 = \bar{y}$$

$\bar{z}_0 \ldots \bar{z}_4$ are called adjoint variables

Forward Mode
Interpretation of tangent linear variables

Function:

$$x = z_0 \xrightarrow{f_1} z_1 \xrightarrow{f_2} z_2 \xrightarrow{f_3} z_3 \xrightarrow{f_4} z_4 = y$$

Forward:

$$x' = z'_0 \xrightarrow{Df_1} z'_1 \xrightarrow{Df_2} z'_2 \xrightarrow{Df_3} z'_3 \xrightarrow{Df_4} z'_4 = y'$$

x'=Id: $z'_2 = Df_2 \cdot Df_1 \cdot x' = Df_2 \cdot Df_1$

tangent linear variable z'_2 holds derivative of z_2 w.r.t. x: dz_2/dx

x'=v: $z'_2 = Df_2 \cdot Df_1 \cdot v$

tangent linear variable z'_2 holds directional derivative of z_2 w.r.t. x in direction of v

Function y=F(x) defined by Fortran code:

```
u = 3*x(1)+2*x(2)+x(3)
v = cos(u)
w = sin(u)
y = v * w
```

Task: Evaluate **DF** = **dy/dx** in forward mode!

Problem: Identify $\mathbf{f_1}$ $\mathbf{f_2}$ $\mathbf{f_3}$ $\mathbf{f_4}$ $\mathbf{z_1}$ $\mathbf{z_2}$ $\mathbf{z_3}$

Observation: f_3: `w = sin(u)` can't work, dimensions don't match!

Instead:
Just take all variables

$$f_3 : z_2 = \begin{pmatrix} x(1) \\ x(2) \\ x(3) \\ u \\ v \\ w \\ y \end{pmatrix} \longrightarrow z_3 = \begin{pmatrix} x(1) \\ x(2) \\ x(3) \\ u \\ v \\ \sin(u) \\ y \end{pmatrix}$$

A step in forward mode

$$f_3 \quad : \quad z_2 = \begin{pmatrix} x(1) \\ x(2) \\ x(3) \\ u \\ v \\ w \\ y \end{pmatrix} \rightarrow z_3 = \begin{pmatrix} x(1) \\ x(2) \\ x(3) \\ u \\ v \\ \sin(u) \\ y \end{pmatrix}$$

```
w        = sin(u)
```

$$z'_3 = Df_3 \; z'_2$$

$$\begin{pmatrix} x'(1) \\ x'(2) \\ x'(3) \\ u' \\ v' \\ w' \\ y' \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \cos(u) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x'(1) \\ x'(2) \\ x'(3) \\ u' \\ v' \\ w' \\ y' \end{pmatrix}$$

```
gx(1) = gx(1)
gx(2) = gx(2)
gx(3) = gx(3)
gu    = gu
gv    = gv
gw    = gu*cos(u)
gy    = gy
```

Entire Function + required variables

Function code

```
u = 3*x(1)+2*x(2)+x(3)

v = cos(u)

w = sin(u)

y = v * w
```

Forward mode/ tangent linear code

```
  gu = 3*gx(1)+2*gx(2)+gx(3)
u = 3* x(1)+2* x(2)+ x(3)
  gv = -gu*sin(u)
v = cos(u)
  gw = gu*cos(u)
w = sin(u)
  gy = gv*w + v*gw
y = v * w
```

u v w are *required* variables, their values need to be provided to the derivative statements

Active and passive variables

Consider slight modification of code for y = F(x):

```
u   = 3*x(1)+2*x(2)+x(3)
pi  = 3.14
v   = pi*cos(u)
w   = pi*sin(u)
sum = v + u
y   = v * w
```

Observation: Variable **sum** (diagnostic) does not influce the function value y
Variable **pi** (constant) does not depend on the independent variables x

Variables that do influence y and are influenced by x are called *active variables*.
The remaining variables are called *passive variables*

Active and passive variables

Function code

```
u   = 3*x(1)+2*x(2)+x(3)

pi  = 3.14

v   = pi*cos(u)

w   = pi*sin(u)

sum = v + u

y   = v * w
```

Forward mode/ tangent linear code

```
gu = 3*gx(1)+2*gx(2)+gx(3)
u  = 3* x(1)+2* x(2)+ x(3)

pi = 3.14
gv = -gu*pi*sin(u)
v  = pi*cos(u)
gw = gu*pi*cos(u)
w  = pi*sin(u)



gy = gv*w + v*gw
```

For passive variables
- no tangent linear variables needed
- no tangent linear statements for their assignments needed

Reverse Mode

Function:

$$x = z_0 \xrightarrow{f_1} z_1 \xrightarrow{f_2} z_2 \xrightarrow{f_3} z_3 \xrightarrow{f_4} z_4 = y$$

Reverse:

$$\bar{x} = \bar{z}_0 \xleftarrow{Df_1^T} \bar{z}_1 \xleftarrow{Df_2^T} \bar{z}_2 \xleftarrow{Df_3^T} \bar{z}_3 \xleftarrow{Df_4^T} \bar{z}_4 = \bar{y}$$

$\bar{y}$=Id: $\bar{z}_2 = Df_3^T \cdot Df_4^T \cdot \bar{y} = (Df_4 \cdot Df_3)^T$

Adjoint variable $\bar{z}_2$ holds (transposed) derivative of **y** w.r.t. z_2: dy/dz_2

For example: y scalar, i.e. $\bar{y}=1$

A step in reverse mode

$$f_3 \quad : \quad z_2 = \begin{pmatrix} x(1) \\ x(\text{٢}) \\ x(3) \\ u \\ v \\ w \\ y \end{pmatrix} \rightarrow \quad z_3 = \begin{pmatrix} x(\text{١}) \\ x(2) \\ x(3) \\ u \\ v \\ \sin(u) \\ y \end{pmatrix}$$

```
w = sin(u)
```

$$Df_3 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & \cos(u) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

$$\overline{z_2} = Df_3^T \, \overline{z_{\text{٣}}}$$

$$\begin{pmatrix} \bar{x}(1) \\ \bar{x}(2) \\ \bar{x}(3) \\ \bar{u} \\ \bar{v} \\ \bar{w} \\ \bar{y} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & \cos(u) & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \bar{x}(1) \\ \bar{x}(2) \\ \bar{x}(3) \\ \bar{u} \\ \bar{v} \\ \bar{w} \\ \bar{y} \end{pmatrix}$$

```
adx(1) = adx(1)
adx(2) = adx(2)
adx(3) = adx(3)
adu = adu+adw*cos(u)
adv = adv
adw = 0.
ady = ady
```

Function code

```
u = 3*x(1)+2*x(2)+x(3)
v = cos(u)
w = sin(u)
y = v * w
```

Adjoint code

```
   u = 3*x(1)+2*x(2)+x(3)
   v = cos(u)
   w = sin(u)

adv = adv+ady*w
adw = adw+ady*v
ady = 0.

adu = adu+adw*cos(u)
adw = 0.

adu = adu-adv*sin(u)
adv = 0.

adx(3) = adx(3)+3*adu
adx(2) = adx(2)+2*adu
adx(1) = adx(1)+adu
adu    = 0.
```

Function F defined by Fortran code:

```
u = 3*x(1)+2*x(2)+x(3)
v = cos(u)
w = sin(u)
y = v * w
```

Typically, to save memory, variables are used more than once!

```
u = 3*x(1)+2*x(2)+x(3)
v = cos(u)
u = sin(u)
y = v * u
```

Function code

```
u = 3*x(1)+2*x(2)+x(3)
v = cos(u)
u = sin(u)
y = v * u
```

Adjoint code

```
  u = 3*x(1)+2*x(2)+x(3)
  v = cos(u)
  u = sin(u)
adv = adv+ady*u
adu = adu+ady*v
ady = 0.
  u = 3*x(1)+2*x(2)+x(3)
adu = adu*cos(u)
adu = adu-adv*sin(u)
adv = 0.
adx(3) = adx(3)+3*adu
adx(2) = adx(2)+2*adu
adx(1) = adx(1)+adu
adu    = 0.
```

Store and retrieve values

Function code

```
u = 3*x(1)+2*x(2)+x(3)
v = cos(u)
u = sin(u)
y = v * u
```

Adjoint code

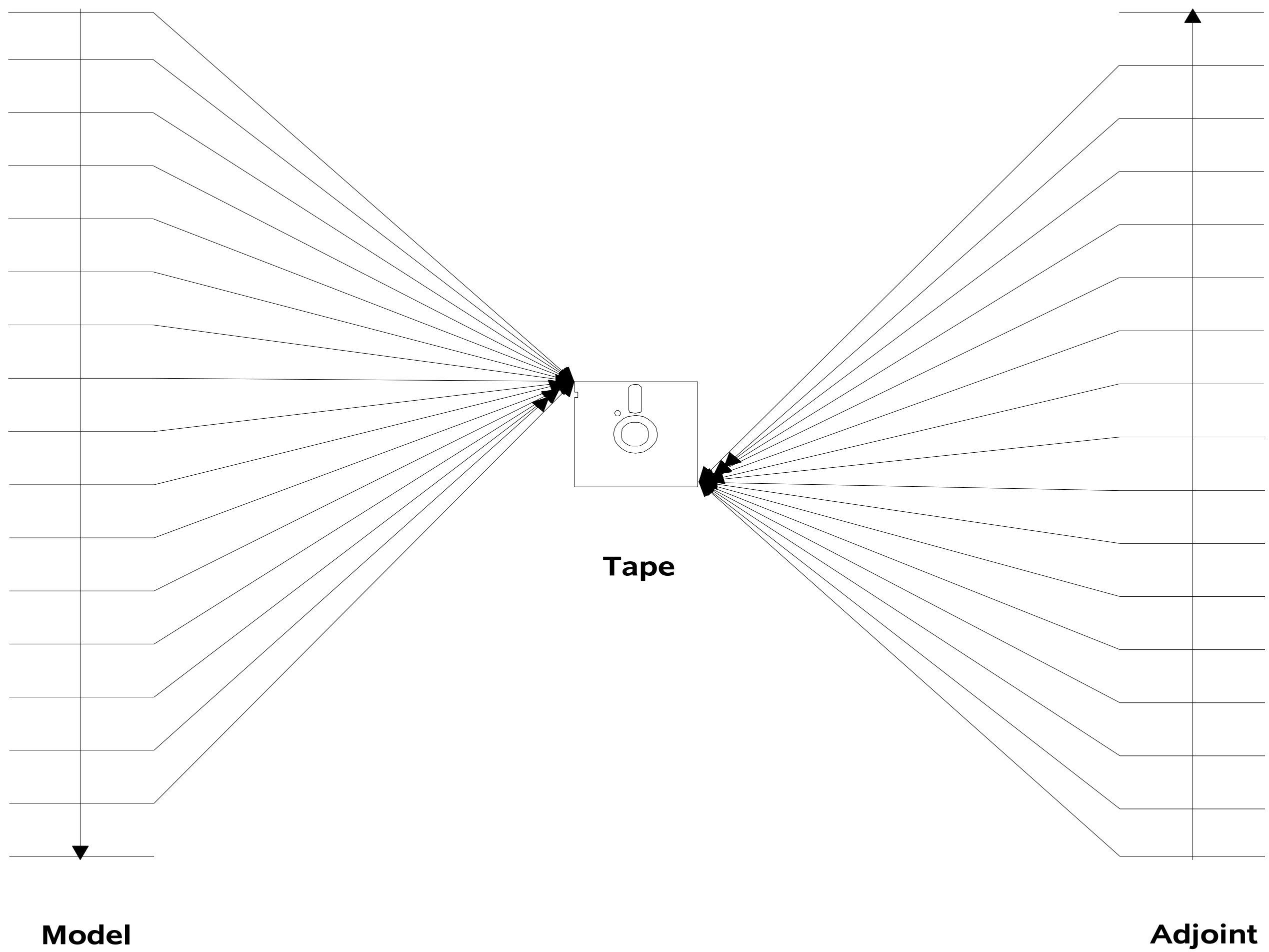
```
u = 3*x(1)+2*x(2)+x(3)
   store (u)
v = cos(u)
u = sin(u)

adv = adv+ady*u
adu = adu+ady*v
ady = 0.

   retrieve (u)
adu = adu*cos(u)

adu = adu-adv*sin(u)
adv = 0.

adx(3) = adx(3)+3*adu
adx(2) = adx(2)+2*adu
adx(1) = adx(1)+adu
adu    = 0.
```

Bookkeeping must be arranged (store / retrieve)

Values can be saved

- **on disc or**
- **in memory**

Storing of required variables



AD Summary

- **AD exploits chain rule**
- **Forward and reverse modes**
- **Active/Passive variables**
- **Required variables: Recomputation vs. Store/Reading**

Further Reading

- AD Book of **Andreas Griewank**: *Evaluating Derivatives: Principles of Algorithmic Differentiation, SIAM, 2000*
- Books on **AD Workshops:**
  Chicago 2004: *Buecker et al. (Eds.), Springer*
  Nice 2000: *Corliss et al. (Eds.), Springer*
  Santa Fe 1996: *Berz et al. (Eds.), SIAM*
  Beckenridge 1991: *Griewank and Corliss (Eds.), SIAM*
- **Olivier Talagrand's** overview article in Santa Fe Book
- **RG/TK** article: *Recipes of Adjoint Code Construction, TOMS, 1998*

AD Tools

- Specific to programming language
- Source-to-source / Operator overloading
- For details check http://www.autodiff.org !

Selected Fortran tools (source to source):

- ADIFOR (M. Fagan, Rice, Houston)
- Odyssee (C. Faure) -> TAPENADE (L. Hascoet, INRIA, Sophia- Antipolis, France)
- TAMC (R. Giering) -> TAF (FastOpt)

Selected C/C++ tools:

- ADOLC (A. Walther, TU-Dresden, Operator Overloading)
- ADIC (P. Hovland, Argonne, Chicago)
- TAC++ (FastOpt)

very simple example

ex1.f90

```
subroutine ex1( x, u, y )
  implicit none
  real x, u, y

  y = 4*x + sin(u)
end
```

drv1tlm.f90

```
program driver
  implicit none
  real x, u, y

  x = 1.2
  u = 0.5
  call ex1( x, u, y )
  print *,' y = ',y
end
```

command line:

taf -f90 -v2 **-forward** -toplevel ex1 -input x,u -ouput y ex1.f90

generated tangent linear code (ex1_tl.f90)

```
subroutine ex1_tl( x, x_tl, u, u_tl, y, y_tl )

implicit none

!===============================================
! declare arguments
!===============================================
real u
real u_tl
real x
real x_tl
real y
real y_tl

!-----------------------------------------------
! TANGENT LINEAR AND FUNCTION STATEMENTS
!-----------------------------------------------
y_tl = u_tl*cos(u)+4*x_tl
y = 4*x+sin(u)

end subroutine ex1_tl
```

driver of tangent linear code

```
program drivertlm
  implicit none
  real x_tl, u_tl, y_tl
  real x, u, y

  x = 1.2     ! initial x
  u = 0.5     ! initial u
  x_tl = 0.0 ! define direction in input space
  u_tl = 1.0 !

  call ex1_tl( x, x_tl, u, u_tl, y, y_tl )

  print *,' y = ',y
  print *,' y_tl = ',y_tl
end
```

```
subroutine ex1_tl( x, x_tl, u, u_tl, y, y_tl )
...
end
```

very simple example

ex1.f90

```
subroutine ex1( x, u, y )
  implicit none
  real x, u, y
  y = 4*x + sin(u)
end
```

command line:

taf -f90 -v2 **-reverse** -toplevel ex1 -input x,u -ouput y ex1.f90

generated adjoint code (ex1_ad.f90)

```
subroutine ex1_ad( x, x_ad, u, u_ad, y, y_ad )

implicit none

!==============================================
! declare arguments
!==============================================
real u
real u_ad
real x
real x_ad
real y
real y_ad

!----------------------------------------------
! FUNCTION AND TAPE COMPUTATIONS
!----------------------------------------------
y = 4*x+sin(u)

!----------------------------------------------
! ADJOINT COMPUTATIONS
!----------------------------------------------
u_ad = u_ad+y_ad*cos(u)
x_ad = x_ad+4*y_ad
y_ad = 0.

end subroutine ex1_ad
```

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driver of adjoint code

```
program driveradm
  implicit none
  real x_ad, u_ad, y_ad
  real x, u, y

  x = 1.2     ! initial x
  u = 0.5     ! initial u
  x_ad = 0.   ! no other influence
  u_ad = 0.   ! no other influence
  y_ad = 1.   ! just some sensitivity

  call ex1_ad( x, x_ad, u, u_ad, y, y_ad )

  print *,' x_ad = ', x_ad
  print *,' u_ad = ', u_ad

end
```

```
subroutine ex1_ad( x, x_ad, u, u_ad, y, y_ad )
...
end
```

Verification of Derivative code

Compare to finite difference approximation:

FD = (f(x+eps)-f(x))/eps

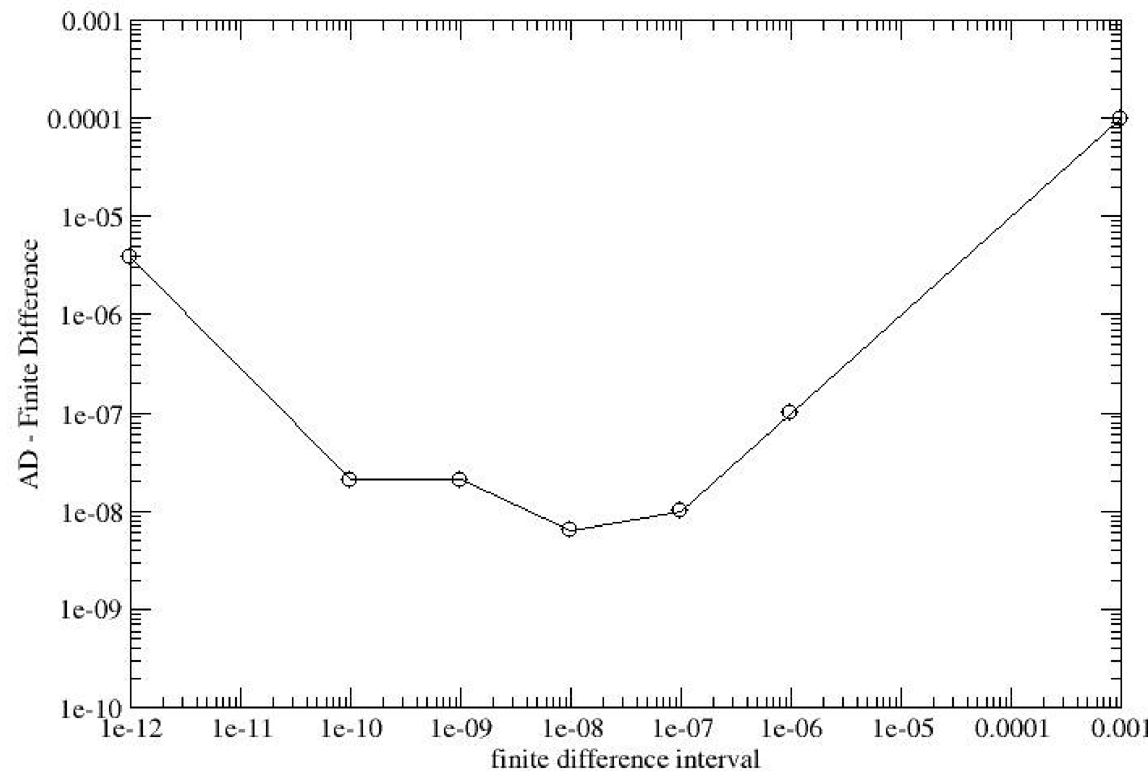
Result depends on eps:

•Too large eps: Non linear terms spoil result

•Too small eps: Rounding error problems:

f(x+eps) = f(x) -> FD = 0.

Example --------------------------->



Exercise

Hand code tangents and adjoints and the respective drivers for:

```
subroutine func( n, x, m, y )
  implicit none
  integer :: n, m
  real    :: x(n), y(m), u, v
  u = cos(x(1))
  v = sqrt(x(2)) + x(1)
  y(1) =  u + v
end subroutine func

program main
  implicit none
  ! dimensions
  integer, parameter :: n = 3
  integer, parameter :: m = 1
  real    :: x(n), y(m)
  ! initialisation
  x(1) = 0.
  x(2) = 1.
  x(3) = 2.
  ! function evaluation
  call func( n, x, m, y )
  ! postprocessing
  print '(a2,3(x,f6.2),a4,f6.2)', 'y(',x,') = ',y
end program main
```