

# The Basic Idea

**Vector function** in C/C++:  $F : \mathbb{R}^n \rightarrow \mathbb{R}^m : x \mapsto y = F(x)$

$\Downarrow$  Operator overloading (C++)

**Internal representation** of  $F$  ( $\equiv \text{tape}$ )

$\Downarrow$

Interpretation

$\Downarrow$

## Forward mode

$$x(t) = \sum_{j=0}^d x_j t^j$$

$\Downarrow$

$$y(t) = \sum_{j=0}^d y_j t^j + O(t^{d+1})$$

$\Rightarrow$  **Directional derivatives**

## Reverse mode

$$y_j = y_j(x_0, x_1, \dots, x_j)$$

$\Downarrow$

$$\frac{\partial y_j}{\partial x_i} = \frac{\partial y_{j-i}}{\partial x_0}$$

$$= A_{j-i}(x_0, x_1, \dots, x_{j-i})$$

$\Rightarrow$  **Gradients (adjoints)**

$$y_0 = F(x_0)$$

$$y_1 = F'(x_0) x_1$$

$$y_2 = F'(x_0) x_2 + \frac{1}{2} F''(x_0) x_1 x_1$$

$$y_3 = F'(x_0) x_3 + F''(x_0) x_1 x_2 + \frac{1}{6} F'''(x_0) x_1 x_1 x_1$$

...

$$\frac{\partial y_0}{\partial x_0} = \frac{\partial y_1}{\partial x_1} = \frac{\partial y_2}{\partial x_2} = \frac{\partial y_3}{\partial x_3} = A_0 = F'(x_0)$$

$$\frac{\partial y_1}{\partial x_0} = \frac{\partial y_2}{\partial x_1} = \frac{\partial y_3}{\partial x_2} = A_1 = F''(x_0) x_1$$

$$\frac{\partial y_2}{\partial x_0} = \frac{\partial y_3}{\partial x_1} = A_2 = F''(x_0) x_2 + \frac{1}{2} F'''(x_0) x_1 x_1$$

$$\frac{\partial y_3}{\partial x_0} = A_3 = F''(x_0) x_3 + F'''(x_0) x_1 x_2 + \frac{1}{6} F^{(4)}(x_0) x_1 x_1 x_1$$

...

# Application

## Operator overloading concept $\Rightarrow$ Code modification

- Inclusion of appropriate ADOL-C headers
- Retyping of all involved variables to active data type **adouble**
- Marking active section to be “taped” (**trace\_on/trace\_off**)
- Specification of independent and dependent variables (**<<=**/**>>=**)
- Specification of differentiation task(s)
- Recompile and Linking with ADOL-C library **libad.a**

### Example:

```
#include "adolc.h"                // inclusion of ADOL-C headers
...
adouble foo ( adouble x )         // some activated function
{ adouble tmp;
  tmp = log(x);
  return 3.0*tmp*tmp + 2.0;
}
...
int main (int argc, char* argv[]) // main program or other procedure
{ ...
  double  x[2], y;
  adouble ax[2], ay;              // declaration of active variables
  x[0]=0.3; x[1]=2.3;
  trace_on(1);                    // starting active section
  ax[0]<<=x[0]; ax[1]<<=x[1];      // marking independent variables
  ay=ax[0]*sin(ax[1])+ foo(ax[1]); // function evaluation
  ay>>=y;                         // marking dependend variables
  trace_off();                    // ending active section
  ...
  double g[2];
  gradient(1,2,x,g);              // application of ADOL-C routine
  ...
  x[0]+=0.1; x[1]+=0.3;           // application at different argument
  gradient(1,2,x,g);
  ...
}
```

# Drivers for Optimization and Nonlinear Equations (C/C++)

$$\min_x f(x), \quad f: \mathbb{R}^n \rightarrow \mathbb{R}$$

$$F(x) = 0_m, \quad F: \mathbb{R}^n \rightarrow \mathbb{R}^m$$

<code>function(tag,m,n,x[n],y[m])</code>	$F(x_0)$
<code>gradient(tag,n,x[n],g[n])</code>	$\nabla f(x_0)$
<code>hessian(tag,n,x[n],H[n][n])</code>	$\nabla^2 f(x_0)$
<code>jacobian(tag,m,n,x[n],J[m][n])</code>	$F'(x_0)$
<code>vec_jac(tag,m,n,repeat?,x[n],u[m],z[n])</code>	$u^T F'(x_0)$
<code>jac_vec(tag,m,n,x[n],v[n],z[m])</code>	$F'(x_0) v$
<code>hess_vec(tag,n,x[n],v[n],z[n])</code>	$\nabla^2 f(x_0) v$
<code>lagra_hess_vec(tag,m,n,x[n],v[n],u[m],h[n])</code>	$u^T F''(x_0) v$
<code>jac_solv(tag,n,x[n],b[n],sparse?,mode?)</code>	$F'(x_0) w = b$

Example:     Solution of  $F(x) = 0$  by Newton's method

```

...
double x[n], r[n];
int i;
...
initialize(x);                                // setting up the initial x
...
function(ftag,n,n,x,r);                       // compute residuum r
while (norm(r) > EPSILON)                     // terminate if small residuum
{ jac_solv(ftag,n,x,r,0,2);                   // compute r:=F'(x)^(-1)*r
  for (i=0; i<n; i++)                         // update x
    x[i] -= r[i];
  function(ftag,n,n,x,r);                     // compute residuum r
}
...

```

# Lowest-level Differentiation Routines

$$F : \mathbb{R}^n \rightarrow \mathbb{R}^m$$

## Forward Mode (C/C++)

```
zos_forward(tag,m,n,keep,x[n],y[m])
```

- zero-order scalar forward; computes  $y = F(x)$
- $0 \leq \text{keep} \leq 1$ ;  $\text{keep} = 1$  prepares for `fos_reverse` or `fov_reverse`

```
fos_forward(tag,m,n,keep,x0[n],x1[n],y0[m],y1[m])
```

- first-order scalar forward; computes  $y_0 = F(x_0)$ ,  $y_1 = F'(x_0)x_1$
- $0 \leq \text{keep} \leq 2$ ;  $\text{keep} = \begin{cases} 1 & \text{prepares for fos\_reverse or fov\_reverse} \\ 2 & \text{prepares for hos\_reverse or hov\_reverse} \end{cases}$

```
fov_forward(tag,m,n,p,x[n],X[n][p],y[m],Y[m][p])
```

- first-order vector forward; computes  $y = F(x)$ ,  $Y = F'(x)X$

```
hos_forward(tag,m,n,d,keep,x[n],X[n][d],y[m],Y[m][d])
```

- higher-order scalar forward; computes  $y_0 = F(x_0)$ ,  $y_1 = F'(x_0)x_1, \dots$ , where  $x = x_0$ ,  $X = [x_1, x_2, \dots, x_d]$  and  $y = y_0$ ,  $Y = [y_1, y_2, \dots, y_d]$
- $0 \leq \text{keep} \leq d+1$ ;  $\text{keep} \begin{cases} = 1 & \text{prepares for fos\_reverse or fov\_reverse} \\ > 1 & \text{prepares for hos\_reverse or hov\_reverse} \end{cases}$

```
hov_forward(tag,m,n,d,p,x[n],X[n][p][d],y[m],Y[m][p][d])
```

- higher-order vector forward; computes  $y_0 = F(x_0)$ ,  $Y_1 = F'(x_0)X_1, \dots$ , where  $x = x_0$ ,  $X = [X_1, X_2, \dots, X_d]$  and  $y = y_0$ ,  $Y = [Y_1, Y_2, \dots, Y_d]$

## Reverse Mode (C/C++)

```
fos_reverse(tag,m,n,u[m],z[n])
```

- first-order scalar reverse; computes  $z^T = u^T F'(x)$
- after calling `zos_forward`, `fos_forward`, or `hos_forward` with `keep = 1`

```
fov_reverse(tag,m,n,q,U[q][m],Z[q][n])
```

- first-order vector reverse; computes  $Z = UF'(x)$
- after calling `zos_forward`, `fos_forward`, or `hos_forward` with `keep = 1`

```
hos_reverse(tag,m,n,d,u[m],Z[n][d+1])
```

- higher-order scalar reverse; computes the adjoints  $z_0^T = u^T F'(x_0) = u^T A_0$ ,  $z_1^T = u^T F''(x_0) x_1 = u^T A_1, \dots$ , where  $Z = [z_0, z_1, \dots, z_d]$
- after calling `fos_forward` or `hos_forward` with `keep = d + 1 > 1`

```
hov_reverse(tag,m,n,d,q,U[q][m],Z[q][n][d+1],nz[q][n])
```

- higher-order vector reverse; computes the adjoints  $Z_0 = UF'(x_0) = UA_0$ ,  $Z_1 = UF''(x_0) x_1 = UA_1, \dots$ , where  $Z = [Z_0, Z_1, \dots, Z_d]$
- after calling `fos_forward` or `hos_forward` with `keep = d + 1 > 1`
- optional nonzero pattern `nz` ( $\Rightarrow$  manual)

Example:

```
...
double x[n], y[m], **I, **J;
I=myallocI2(m);           // allocation of identity matrix
J=myalloc2(m,n);          // allocation of Jacobian matrix
...
initialize(x);             // setting up the argument x
...
zos_forward(ftag,m,n,1,x,y); // computing the Jacobian by
fos_reverse(ftag,m,n,m,I,J); // reverse mode of AD
...
```

# Low-level Differentiation Routines

## Forward Mode (C++ interfaces)

<code>forward(tag,m,n,d,keep,X[n][d+1],Y[m][d+1])</code>	hos, fos, zos
<code>forward(tag,m=1,n,d,keep,X[n][d+1],Y[d+1])</code>	hos, fos, zos
<code>forward(tag,m,n,d=0,keep,x[n],y[m])</code>	zos
<code>forward(tag,m,n,keep,x[n],y[m])</code>	zos
<code>forward(tag,m,n,p,x[n],X[n][p],y[m],Y[m][p])</code>	fov
<code>forward(tag,m,n,d,p,x[n],X[n][p][d], y[m],Y[m][p][d])</code>	hov

## Reverse Mode (C++ interfaces)

<code>reverse(tag,m,n,d,u[m],Z[n][d+1])</code>	hos
<code>forward(tag,m=1,n,d,u,Z[n][d+1])</code>	hos
<code>reverse(tag,m,n,d=0,u[m],z[n])</code>	fos
<code>reverse(tag,m=1,n,d=0,u,z[n])</code>	fos
<code>reverse(tag,m,n,d,q,U[q][m],Z[q][n][d+1],nz[q][n])</code>	hov
<code>reverse(tag,m=1,n,d,q,U[q],Z[q][n][d+1],nz[q][n])</code>	hov
<code>reverse(tag,m=1,n,d,Z[m][n][d+1],nz[m][n]) (<math>U = I_m</math>)</code>	hov
<code>reverse(tag,m,n,d=0,q,U[q][m],Z[q][n])</code>	fov
<code>reverse(tag,m,n,q,U[q][m],Z[q][n])</code>	fov
<code>reverse(tag,m=1,n,d=0,q,U[q],Z[q][n])</code>	fov

# Drivers for Ordinary Differential Equations (C/C++)

**ODE:**  $x'(t) = y(t) = F(x(t)), \quad x(0) = x_0$

```
forodec(tag,n,tau,dold,d,X[n][d+1])
```

- recursive forward computation of  $x_{d_{old}+1}, \dots, x_d$  from  $x_0, \dots, x_{d_{old}}$  (by  $x_{i+1} = \frac{1}{1+i}y_i$ )
- application with  $d_{old} = 0$  delivers truncated Taylor series  $\sum_0^d x_j t^j$  at base point  $x_0$

```
hov_reverse(tag,n,n,d-1,n,I[n][n],A[n][n][d],nz[n][n])
```

- reverse computation of  $A_j = \frac{\partial y_j}{\partial x_0}, j = 0, \dots, d$  after calling `forodec` with degree  $d$
- optional nonzero pattern `nz` ( $\Rightarrow$  manual)

```
accodec(n,tau,d-1,A[n][n][d],B[n][n][d],nz[n][n])
```

- accumulation of total derivatives  $B_j = \frac{dx_j}{dx_0}, j = 0, \dots, d$  from the partial derivatives  $A_j = \frac{\partial y_j}{\partial x_0}, j = 0, \dots, d$  after calling `hov_reverse`
- optional nonzero pattern `nz` ( $\Rightarrow$  manual)

C++: Special C++ interfaces can be found in file `SRC/DRIVERS/odedrivers.h!`

Example:

```
...
double x[n], **I, **X, ***A, ***B;
I=myallocI2(n); // allocation of identity matrix
X=myalloc2(n,5); // allocation of matrix X
A=myalloc3(n,n,4); B=myalloc3(n,n,4); // allocation of tensors A and B
...
initialize(X); // setting up the argument x_0
...
forodec(ftag,n,1.0,0,4,X); // compute x_1,...,x_4
hov_reverse(ftag,n,n,3,n,I,A,NULL); // compute A_0,...,A_3
accodec(ftag,n,1.0,3,A,B,NULL); // accumulate B_0,...,B_3
...
```

## ADOL-C provides

- Low-level differentiation routines (**forward/reverse**)
- Easy-to-use driver routines for
  - the solution of optimization problems and nonlinear equations
  - the integration of ordinary differential equations
  - the evaluation of higher derivative tensors ( $\Rightarrow$  manual)
- Derivatives of implicit and inverse functions ( $\Rightarrow$  manual)
- Forward and backward dependence analysis ( $\Rightarrow$  manual)

## Recent developments

- Efficient detection of Jacobian/Hessian sparsity structure
- Exploitation of Jacobian/Hessian sparsity by matrix compression
- Integration of checkpointing routines
- Exploitation of fixpoint iterations
- Differentiation of OpenMP parallel programs

## Future developments

- Internal optimizations to reduce storage needed for reverse mode
- Recovery of structure for internal function representation
- Differentiation of MPI parallel programs

## Contact/Resources

- E-mail: `adol-c@tu-dresden.de`
- WWW: `http://www.math.tu-dresden.de/~adol-c`