Introduction to Backpropagation aka Reverse Mode of Algorithmic Differentiation

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Artificial Intelligence in Natural Sciences

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Outline

Where are Derivatives Needed?

- Optimization:

unbounded:	$\min f(x)$,	$f : \mathbb{R}^n \to \mathbb{R}$
bounded:	$\min f(x)$,	$f : \mathbb{R}^n \to \mathbb{R}$, $c(x) = 0$, $h(x) \leq 0$

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- Solution of nonlinear equation systems

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

  Newton method requires $F'(x) \in \mathbb{R}^{n \times n}$

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- Sensitivity analysis
- Real-time control
- machine learning (ML), e.g., Stochastic Gradient Descent, Adam, ...
  target functions quite often nonsmooth!

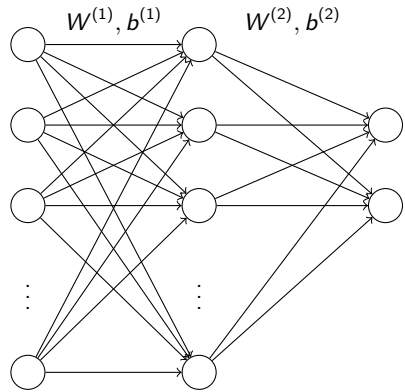
Training of a Deep Neural Network

Goal: Learn weights $W^{(i)}$ and biases $b^{(i)}$ such that the network approximates the true mapping.

Empirical Risk Minimization:

$$\min_{\{W^{(i)},b^{(i)}\}} \frac{1}{M} \sum_{i=1}^{M} l\left(y(x_i),\, y_{\theta,i}^{NN}\right)$$

- Parameters: $\theta = (W^{(i)}, b^{(i)})_{1 \le i \le k}$
- $y(x_i)$: value of true mapping for input x_i
- $y_{\theta,i}^{NN}$: output of the network for input x_i
- l: loss function (e.g. MSE, cross-entropy)



Stochastic Gradient Descent (SGD)

SGD Algorithm

for $t = 0, 1, \ldots$

$$\theta_{t+1} = \theta_t - \eta \nabla_\theta l_{\mathcal{I}}(y(x_{\mathcal{I}}),\, y^{NN}_{\theta_t, \mathcal{I}})$$

where:

- θ_t: parameter vector at step t
- η: learning rate = fixed (!) step size
- $l_{\mathcal{I}}$: part of the loss function for stochastic index/set $\mathcal{I}$ of samples

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Gradients essential!

My Point of View

Munich, March 2018

A (Quite Long) History of Differentiation

- Nasir ad-Din at-Tusi (1201-1274 Iran and Irak) examined positive solvability of
$$c = f(x) = x^2(a - x)$$
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- Hence: Definitely not just the Newton versus Leibniz controversy in 1666-1717

Computing Derivatives

Given:

Description of functional relation as

- formula $y = F(x)$ $\Rightarrow$ explicit expression $y' = F'(x)$
- computer program $\Rightarrow$?

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Task:

Computation of derivatives taking

- requirements on exactness
- computational effort

into account

Finite Differences

Idea: Taylor expansion, $f : \mathbb{R} \to \mathbb{R}$ smooth then

$$
\begin{aligned}
& f(x+h) &&= f(x) + hf'(x) + h^2 f''(x)/2 + h^3 f'''(x)/6 + \dots \\
\Rightarrow \quad & f(x+h) &&\approx f(x) + hf'(x) \\
\Rightarrow \quad & Df(x) &&= \frac{f(x+h) - f(x)}{h}
\end{aligned}
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- simple derivative calculation (only function evaluations!)
- inexact derivatives
- computation cost often too high

  $F : \mathbb{R}^n \to \mathbb{R} \quad \Rightarrow \quad \mathrm{OPS}(\nabla F(x)) \sim (n+1)\mathrm{OPS}(F(x))$

Analytic Differentiation

- symbolic derivatives, e.g.,

$$f(x) = \exp(\sin(x^2)) \Rightarrow$$
$$f'(x) = \exp(\sin(x^2)) * \cos(x^2) * 2x$$

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derivative computation based on

  - sensitivity equation
  - adjoint equation $\qquad \lambda' = -f_x(x,u)^\top \lambda \ + \ \text{TC}$

$\Rightarrow J'(y(u),u)$ based on continuous adjoint

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    consistent derivative information?!

Algorithmic Differentiation (AD)

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Main Products:

- Quantitative dependence information (local):
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  - Error and condition number estimates ...
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Assumption: F differentiable at least in a neighbourhood of current argument x

Historical Development of AD

J. Nolan 1953 →
L. M. Beda et al. 1959 →
A. Gibbons 1960 →
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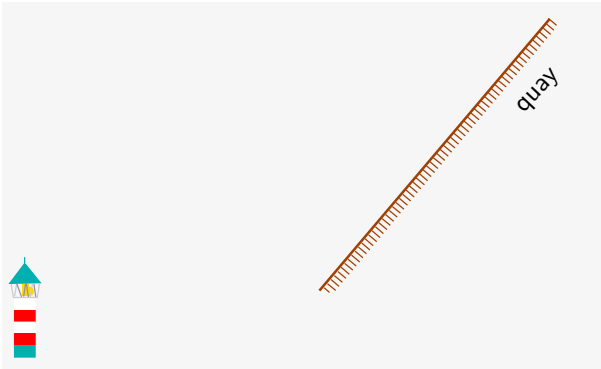
Rumelhart at al. (1986) made backpropagation famous for neural nets

The “Hello-World”-Example of AD



Lighthouse

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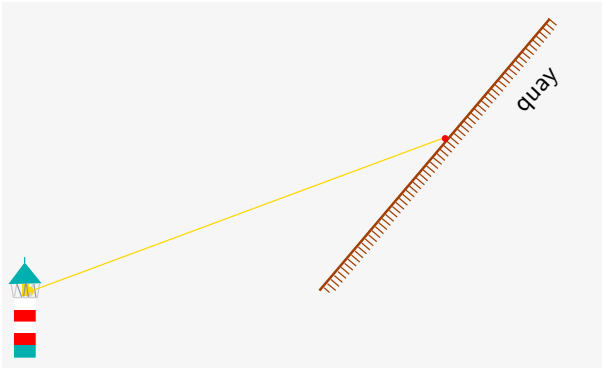

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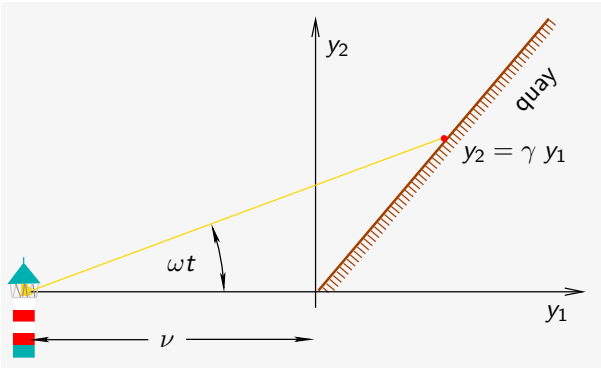

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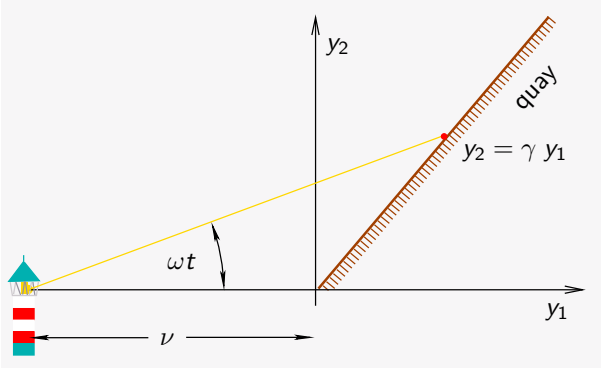

Lighthouse

$$y_1 = \frac{\nu\ \tan(\omega\, t)}{\gamma - \tan(\omega\, t)}$$

and

$$y_2 = \frac{\gamma\,\nu\ \tan(\omega\, t)}{\gamma - \tan(\omega\, t)}$$

Evaluation Procedure (Lighthouse)

$$y_1 = \frac{\nu \tan(\omega\, t)}{\gamma - \tan(\omega\, t)}$$

$$y_2 = \frac{\gamma\, \nu \tan(\omega\, t)}{\gamma - \tan(\omega\, t)}$$

$\Longrightarrow$

v_{-3}	$= x_1 = \nu$	
v_{-2}	$= x_2 = \gamma$	
v_{-1}	$= x_3 = \omega$	
v_0	$= x_4 = t$	
v_1	$= v_{-1} * v_0$	$\equiv \varphi_1(v_{-1}, v_0)$
v_2	$= \tan(v_1)$	$\equiv \varphi_2(v_1)$
v_3	$= v_{-2} - v_2$	$\equiv \varphi_3(v_{-2}, v_2)$
v_4	$= v_{-3} * v_2$	$\equiv \varphi_4(v_{-3}, v_2)$
v_5	$= v_4 / v_3$	$\equiv \varphi_5(v_4, v_3)$
v_6	$= v_5 * v_{-2}$	$\equiv \varphi_6(v_5, v_{-2})$
y_1	$= v_5$	
y_2	$= v_6$	

Function Evaluation in ML

Typical function evaluation (deep neural net):

Propagation of one data point:

$$
\begin{aligned}
x = x^{(1)} \to \tilde{x}^{(1)} = W^{(1)}x^{(1)} + b^{(1)} \quad &\to x^{(2)} = \rho(\tilde{x}^{(1)}) \\
\to \tilde{x}^{(2)} = W^{(2)}x^{(2)} + b^{(2)} \quad &\to x^{(3)} = \rho(\tilde{x}^{(2)}) \to \quad \cdots \\
\to y = W^{(k)}x^{(k)} + b^{(k)}
\end{aligned}
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Empirical risk, loss function, ...

$$f(x_{1\le i\le M}) = \tfrac{1}{M}\sum_{i=1}^{M} l(y_i(x_i), y_{\theta,i}^{NN})$$

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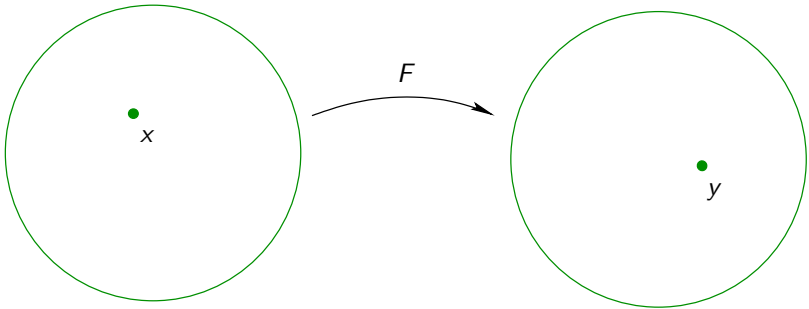
Stochastic gradient descent requires

$$\nabla_{W^1,b^1,\ldots,W^k,b^k} l(y_i(x_i), y_{\theta,i}^{NN})$$

for $i \in \{1,\ldots,M\}$

Forward mode AD = Tangents/Sensitivities



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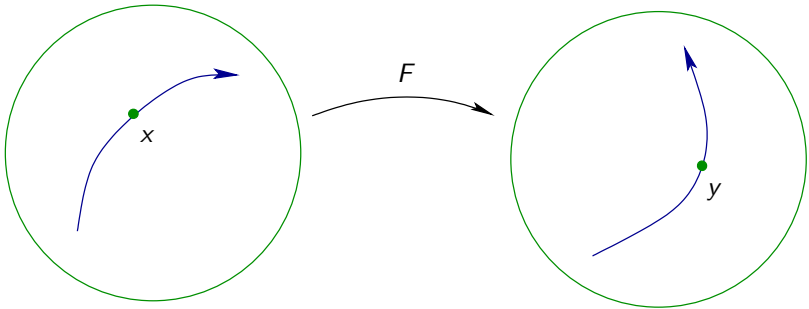

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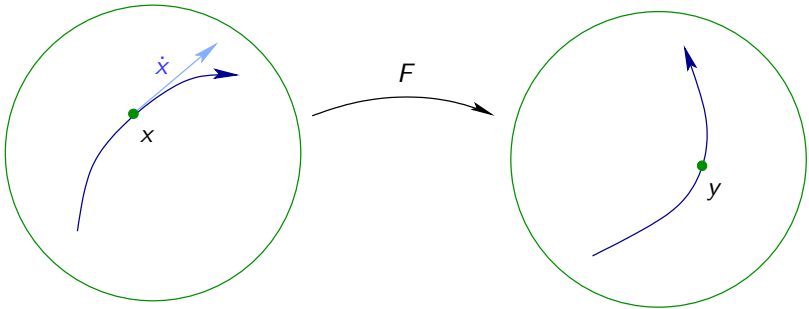

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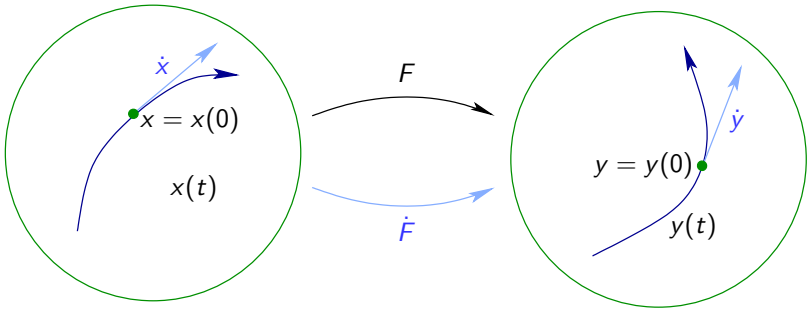

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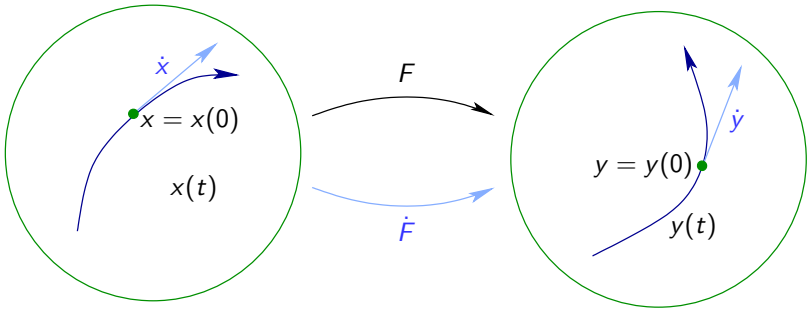

$$\dot{y}(t) \;=\; \frac{\partial}{\partial t} F(x(t)) \;=\; F'(x(t))\,\dot{x}(t) \equiv \;\dot{F}(x, \dot{x})$$

Forward Mode (Lighthouse)

$$
\begin{array}{lcl}
v_{-3} & = & x_1 = \nu \\
v_{-2} & = & x_2 = \gamma \\
v_{-1} & = & x_3 = \omega \\
v_0 & = & x_4 = t \\
\hline
v_1 & = & v_{-1} * v_0 \\
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y_1 & = & v_5 \\
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v_0	$=$	$x_4 = t$	$\dot{v}_0$	$=$	$\dot{x}_4$
v_1	$=$	$v_{-1} * v_0$			
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v_{-1}	$=$	$x_3 = \omega$	$\dot{v}_{-1}$	$=$	$\dot{x}_3$
v_0	$=$	$x_4 = t$	$\dot{v}_0$	$=$	$\dot{x}_4$
v_1	$=$	$v_{-1} * v_0$	$\dot{v}_1$	$=$	$\dot{v}_{-1} * v_0 + v_{-1} * \dot{v}_0$
v_2	$=$	$\tan(v_1)$			
v_3	$=$	$v_{-2} - v_2$			
v_4	$=$	$v_{-3} * v_2$			
v_5	$=$	v_4 / v_3			
v_6	$=$	$v_5 * v_{-2}$			
y_1	$=$	v_5			
y_2	$=$	v_6			

Forward Mode (Lighthouse)

v_{-3}	$=$	$x_1 = \nu$	$\dot{v}_{-3}$	$=$	$\dot{x}_1$
v_{-2}	$=$	$x_2 = \gamma$	$\dot{v}_{-2}$	$=$	$\dot{x}_2$
v_{-1}	$=$	$x_3 = \omega$	$\dot{v}_{-1}$	$=$	$\dot{x}_3$
v_0	$=$	$x_4 = t$	$\dot{v}_0$	$=$	$\dot{x}_4$
v_1	$=$	$v_{-1} * v_0$	$\dot{v}_1$	$=$	$\dot{v}_{-1} * v_0 + v_{-1} * \dot{v}_0$
v_2	$=$	$\tan(v_1)$	$\dot{v}_2$	$=$	$\dot{v}_1 / \cos(v_1)^2$
v_3	$=$	$v_{-2} - v_2$			
v_4	$=$	$v_{-3} * v_2$			
v_5	$=$	v_4 / v_3			
v_6	$=$	$v_5 * v_{-2}$			
y_1	$=$	v_5			
y_2	$=$	v_6			

Forward Mode (Lighthouse)

v_{-3}	$=$	$x_1 = \nu$	$\dot{v}_{-3}$	$=$	$\dot{x}_1$
v_{-2}	$=$	$x_2 = \gamma$	$\dot{v}_{-2}$	$=$	$\dot{x}_2$
v_{-1}	$=$	$x_3 = \omega$	$\dot{v}_{-1}$	$=$	$\dot{x}_3$
v_0	$=$	$x_4 = t$	$\dot{v}_0$	$=$	$\dot{x}_4$
v_1	$=$	$v_{-1} * v_0$	$\dot{v}_1$	$=$	$\dot{v}_{-1} * v_0 + v_{-1} * \dot{v}_0$
v_2	$=$	$\tan(v_1)$	$\dot{v}_2$	$=$	$\dot{v}_1 / \cos(v_1)^2$
v_3	$=$	$v_{-2} - v_2$	$\dot{v}_3$	$=$	$\dot{v}_{-2} - \dot{v}_2$
v_4	$=$	$v_{-3} * v_2$			
v_5	$=$	v_4 / v_3			
v_6	$=$	$v_5 * v_{-2}$			
y_1	$=$	v_5			
y_2	$=$	v_6			

Forward Mode (Lighthouse)

v_{-3}	$=$	$x_1 = \nu$	$\dot{v}_{-3}$	$=$	$\dot{x}_1$
v_{-2}	$=$	$x_2 = \gamma$	$\dot{v}_{-2}$	$=$	$\dot{x}_2$
v_{-1}	$=$	$x_3 = \omega$	$\dot{v}_{-1}$	$=$	$\dot{x}_3$
v_0	$=$	$x_4 = t$	$\dot{v}_0$	$=$	$\dot{x}_4$
v_1	$=$	$v_{-1} * v_0$	$\dot{v}_1$	$=$	$\dot{v}_{-1} * v_0 + v_{-1} * \dot{v}_0$
v_2	$=$	$\tan(v_1)$	$\dot{v}_2$	$=$	$\dot{v}_1 / \cos(v_1)^2$
v_3	$=$	$v_{-2} - v_2$	$\dot{v}_3$	$=$	$\dot{v}_{-2} - \dot{v}_2$
v_4	$=$	$v_{-3} * v_2$	$\dot{v}_4$	$=$	$\dot{v}_{-3} * v_2 + v_{-3} * \dot{v}_2$
v_5	$=$	v_4 / v_3			
v_6	$=$	$v_5 * v_{-2}$			
y_1	$=$	v_5			
y_2	$=$	v_6			

Forward Mode (Lighthouse)

v_{-3}	$=$	$x_1 = \nu$	$\dot{v}_{-3}$	$=$	$\dot{x}_1$
v_{-2}	$=$	$x_2 = \gamma$	$\dot{v}_{-2}$	$=$	$\dot{x}_2$
v_{-1}	$=$	$x_3 = \omega$	$\dot{v}_{-1}$	$=$	$\dot{x}_3$
v_0	$=$	$x_4 = t$	$\dot{v}_0$	$=$	$\dot{x}_4$
v_1	$=$	$v_{-1} * v_0$	$\dot{v}_1$	$=$	$\dot{v}_{-1} * v_0 + v_{-1} * \dot{v}_0$
v_2	$=$	$\tan(v_1)$	$\dot{v}_2$	$=$	$\dot{v}_1 / \cos(v_1)^2$
v_3	$=$	$v_{-2} - v_2$	$\dot{v}_3$	$=$	$\dot{v}_{-2} - \dot{v}_2$
v_4	$=$	$v_{-3} * v_2$	$\dot{v}_4$	$=$	$\dot{v}_{-3} * v_2 + v_{-3} * \dot{v}_2$
v_5	$=$	v_4 / v_3	$\dot{v}_5$	$=$	$(\dot{v}_4 - \dot{v}_3 * v_5) * (1/v_3)$
v_6	$=$	$v_5 * v_{-2}$			
y_1	$=$	v_5			
y_2	$=$	v_6			

Forward Mode (Lighthouse)

v_{-3}	$=$	$x_1 = \nu$	$\dot{v}_{-3}$	$=$	$\dot{x}_1$
v_{-2}	$=$	$x_2 = \gamma$	$\dot{v}_{-2}$	$=$	$\dot{x}_2$
v_{-1}	$=$	$x_3 = \omega$	$\dot{v}_{-1}$	$=$	$\dot{x}_3$
v_0	$=$	$x_4 = t$	$\dot{v}_0$	$=$	$\dot{x}_4$
v_1	$=$	$v_{-1} * v_0$	$\dot{v}_1$	$=$	$\dot{v}_{-1} * v_0 + v_{-1} * \dot{v}_0$
v_2	$=$	$\tan(v_1)$	$\dot{v}_2$	$=$	$\dot{v}_1 / \cos(v_1)^2$
v_3	$=$	$v_{-2} - v_2$	$\dot{v}_3$	$=$	$\dot{v}_{-2} - \dot{v}_2$
v_4	$=$	$v_{-3} * v_2$	$\dot{v}_4$	$=$	$\dot{v}_{-3} * v_2 + v_{-3} * \dot{v}_2$
v_5	$=$	v_4 / v_3	$\dot{v}_5$	$=$	$(\dot{v}_4 - \dot{v}_3 * v_5) * (1/v_3)$
v_6	$=$	$v_5 * v_{-2}$	$\dot{v}_6$	$=$	$\dot{v}_5 * v_{-2} + v_5 * \dot{v}_{-2}$
y_1	$=$	v_5			
y_2	$=$	v_6			

Forward Mode (Lighthouse)

v_{-3}	$=$	$x_1 = \nu$	$\dot{v}_{-3}$	$=$	$\dot{x}_1$
v_{-2}	$=$	$x_2 = \gamma$	$\dot{v}_{-2}$	$=$	$\dot{x}_2$
v_{-1}	$=$	$x_3 = \omega$	$\dot{v}_{-1}$	$=$	$\dot{x}_3$
v_0	$=$	$x_4 = t$	$\dot{v}_0$	$=$	$\dot{x}_4$
v_1	$=$	$v_{-1} * v_0$	$\dot{v}_1$	$=$	$\dot{v}_{-1} * v_0 + v_{-1} * \dot{v}_0$
v_2	$=$	$\tan(v_1)$	$\dot{v}_2$	$=$	$\dot{v}_1 / \cos(v_1)^2$
v_3	$=$	$v_{-2} - v_2$	$\dot{v}_3$	$=$	$\dot{v}_{-2} - \dot{v}_2$
v_4	$=$	$v_{-3} * v_2$	$\dot{v}_4$	$=$	$\dot{v}_{-3} * v_2 + v_{-3} * \dot{v}_2$
v_5	$=$	v_4 / v_3	$\dot{v}_5$	$=$	$(\dot{v}_4 - \dot{v}_3 * v_5) * (1/v_3)$
v_6	$=$	$v_5 * v_{-2}$	$\dot{v}_6$	$=$	$\dot{v}_5 * v_{-2} + v_5 * \dot{v}_{-2}$
y_1	$=$	v_5	$\dot{y}_1$	$=$	$\dot{v}_5$
y_2	$=$	v_6	$\dot{y}_2$	$=$	$\dot{v}_6$

Complexity (Forward Mode)

tang	c	$\pm$	$*$	ψ
MOVES	$1+1$	$3+3$	$3+3$	$2+2$
ADDS	0	$1+1$	$0+1$	$0+0$
MULTS	0	0	$1+2$	$0+1$
NLOPS	0	0	0	$1+1$

Complexity (Forward Mode)

tang	c	$\pm$	$*$	ψ
MOVES	$1+1$	$3+3$	$3+3$	$2+2$
ADDS	0	$1+1$	$0+1$	$0+0$
MULTS	0	0	$1+2$	$0+1$
NLOPS	0	0	0	$1+1$

$$\text{OPS}(F'(x)\dot{x}) \quad \leq \quad c\ \text{OPS}(F(x))$$

with $c \in [2, 5/2]$ platform dependent

Forward Mode AD for ML

Typical function evaluation (deep neural net):

$$x = x^{(1)} \to \tilde{x}^{(1)} = W^{(1)}x^{(1)} + b^{(1)} \quad \to x^{(2)} = \rho(\tilde{x}^{(1)})$$

Attention: Optimization variables W and $b \Rightarrow \dot{W}$ and $\dot{b}$!

Forward Mode AD for ML

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$$x = x^{(1)} \to \tilde{x}^{(1)} = W^{(1)}x^{(1)} + b^{(1)} \quad \to x^{(2)} = \rho(\tilde{x}^{(1)})$$

Attention: Optimization variables W and $b \Rightarrow \dot{W}$ and $\dot{b}$!

$$\begin{aligned} x = x^{(1)} \to \tilde{x}^{(1)} &= W^{(1)}x^{(1)} + b^{(1)} && \to x^{(2)} = \rho(\tilde{x}^{(1)}) \\ \dot{\tilde{x}}^{(1)} &= \dot{W}^{(1)}x^{(1)} + \dot{b}^{(1)} && \to \dot{x}^{(2)} = \rho'(\tilde{x}^{(1)})\dot{\tilde{x}}^{(1)} \end{aligned}$$

Forward Mode AD for ML

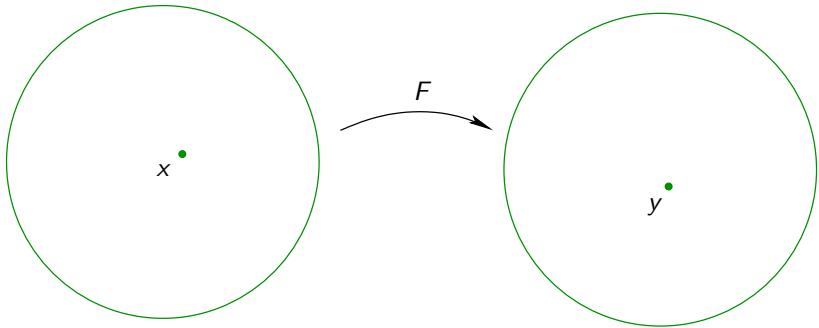
Typical function evaluation (deep neural net):

$$x = x^{(1)} \to \tilde{x}^{(1)} = W^{(1)}x^{(1)} + b^{(1)} \quad \to x^{(2)} = \rho(\tilde{x}^{(1)})$$

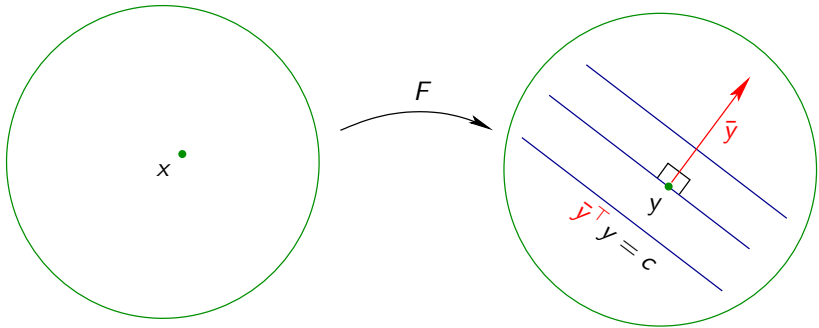
Attention: Optimization variables W and $b \Rightarrow \dot{W}$ and $\dot{b}$!

$$\begin{aligned}
x = x^{(1)} \to \tilde{x}^{(1)} &= W^{(1)}x^{(1)} + b^{(1)} && \to x^{(2)} = \rho(\tilde{x}^{(1)}) \\
\dot{\tilde{x}}^{(1)} &= \dot{W}^{(1)}x^{(1)} + \dot{b}^{(1)} && \to \dot{x}^{(2)} = \rho'(\tilde{x}^{(1)})\dot{\tilde{x}}^{(1)} \\
\to \tilde{x}^{(2)} &= W^{(2)}x^{(2)} + b^{(2)} && \to\ x^{(3)} = \rho(\tilde{x}^{(2)}) \\
\dot{\tilde{x}}^{(2)} &= \dot{W}^{(2)}x^{(2)} + W^{(2)}\dot{x}^{(2)} + \dot{b}^{(2)} && \to\ \dot{x}^{(3)} = \rho'(\tilde{x}^{(3)})\dot{\tilde{x}}^{(3)} \\
\to \cdots & \\
\to y &= W^{(k)}x^{(k)} + b^{(k)} \\
\to \dot{y} &= \dot{W}^{(k)}x^{(k)} + W^{(k)}\dot{x}^{(k)} + \dot{b}^{(k)}
\end{aligned}$$

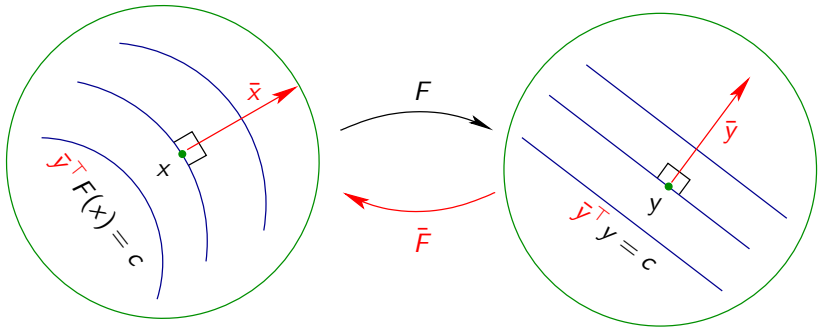
Reverse Mode AD = Discrete Adjoints



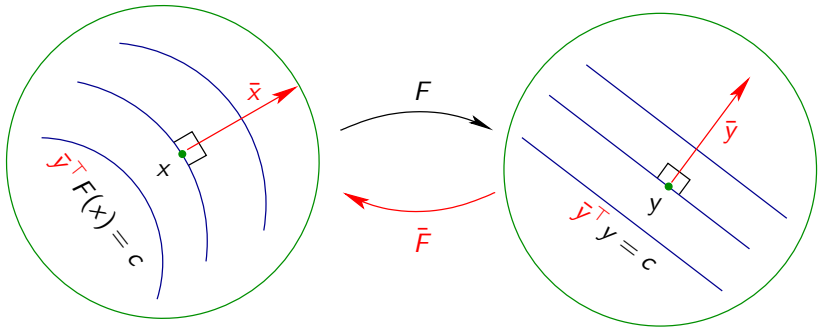
Reverse Mode AD = Discrete Adjoints



Reverse Mode AD = Discrete Adjoints



Reverse Mode AD = Discrete Adjoints



$$\bar{x} \equiv \bar{y}^\top F'(x) = \nabla_x \langle \bar{y}^\top F(x) \rangle \equiv \bar{F}(x, \bar{y})$$

Reverse Mode (Lighthouse)

$$
\begin{aligned}
&v_{-3} = x_1; \quad v_{-2} = x_2; \quad v_{-1} = x_3; \quad v_0 = x_4;\\
&\qquad v_1 = v_{-1} * v_0;\\
&\qquad\qquad v_2 = \tan(v_1);\\
&\qquad\qquad\qquad v_3 = v_{-2} - v_2;\\
&\qquad\qquad\qquad\qquad v_4 = v_{-3} * v_2;\\
&\qquad\qquad\qquad\qquad\qquad v_5 = v_4 / v_3;\\
&\qquad\qquad\qquad\qquad\qquad\qquad v_6 = v_5 * v_{-2};\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad y_1 = v_5; \quad y_2 = v_6;\\
\hline
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad \bar{v}_5 = \bar{y}_1; \quad \bar{v}_6 = \bar{y}_2;\\
&\qquad\qquad\qquad\qquad\qquad\qquad \bar{v}_5 \mathrel{+}= \bar{v}_6 * v_{-2}; \quad \bar{v}_{-2} \mathrel{+}= \bar{v}_6 * v_5;\\
&\qquad\qquad\qquad\qquad\qquad \bar{v}_4 \mathrel{+}= \bar{v}_5 / v_3; \quad \bar{v}_3 \mathrel{-}= \bar{v}_5 * v_5 / v_3;\\
&\qquad\qquad\qquad\qquad \bar{v}_{-3} \mathrel{+}= \bar{v}_4 * v_2; \quad \bar{v}_2 \mathrel{+}= \bar{v}_4 * v_{-3};\\
&\qquad\qquad\qquad \bar{v}_{-2} \mathrel{+}= \bar{v}_3; \; \bar{v}_2 \mathrel{-}= \bar{v}_3;\\
&\qquad\qquad \bar{v}_1 \mathrel{+}= \bar{v}_2 / \cos^2(v_1);\\
&\qquad\quad \bar{v}_{-1} \mathrel{+}= \bar{v}_1 * v_0; \; \bar{v}_0 \mathrel{+}= \bar{v}_1 * v_{-1};\\
&\bar{x}_4 = \bar{v}_0; \quad \bar{x}_3 = \bar{v}_{-1}; \quad \bar{x}_2 = \bar{v}_{-2}; \quad \bar{x}_1 = \bar{v}_{-3};
\end{aligned}
$$

Complexity (Reverse Mode)

grad	c	$\pm$	$*$	ψ
MOVES	$1+1$	$3+6$	$3+8$	$2+5$
ADDS	0	$1+2$	$0+2$	$0+1$
MULTS	0	0	$1+2$	$0+1$
NLOPS	0	0	0	$1+1$

$$\text{OPS}(\bar{y}^\top F'(x)) \leq c\ \text{OPS}(F(x)),\ \text{MEM}(\bar{y}^\top F'(x)) \sim \text{OPS}(F(x))$$

with $c \in [3, 4]$ platform dependent

Complexity (Reverse Mode)

grad	c	$\pm$	$*$	ψ
MOVES	$1+1$	$3+6$	$3+8$	$2+5$
ADDS	0	$1+2$	$0+2$	$0+1$
MULTS	0	0	$1+2$	$0+1$
NLOPS	0	0	0	$1+1$

$$\text{OPS}(\bar{y}^\top F'(x)) \leq c\ \text{OPS}(F(x)),\ \text{MEM}(\bar{y}^\top F'(x)) \sim \text{OPS}(F(x))$$

with $c \in [3, 4]$ platform dependent

Remarks:

- Cost for gradient calculation independent of n
- Memory requirement may cause problem! $\Rightarrow$ Checkpointing

Reverse Mode AD for ML

= a.k.a. backpropagation

Typical function evaluation (deep neural net):

$$
\begin{aligned}
x = x^{(1)} \to \tilde{x}^{(1)} &= W^{(1)}x^{(1)} + b^{(1)} \quad \to x^{(2)} = \rho(\tilde{x}^{(1)}) \\
\to \tilde{x}^{(2)} &= W^{(2)}x^{(2)} + b^{(2)} \quad \to x^{(3)} = \rho(\tilde{x}^{(2)}) \\
&\to \cdots \\
&\to y = W^{(k)}x^{(k)} + b^{(k)}
\end{aligned}
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&\to \cdots \\
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\end{aligned}
$$

With $\bar{y} = 1$ one obtains

$$\bar{W}^{(k)} = [x^{(k)}], \quad \bar{x}^{(k)} = W^{(k)}, \quad \bar{b}^{(k)} = \mathbb{1}$$

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= a.k.a. backpropagation

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\begin{aligned}
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\to \tilde{x}^{(2)} &= W^{(2)}x^{(2)} + b^{(2)} \quad \to x^{(3)} = \rho(\tilde{x}^{(2)}) \\
&\to \cdots \\
&\to y = W^{(k)}x^{(k)} + b^{(k)}
\end{aligned}
$$

With $\bar{y} = 1$ one obtains

$$
\begin{aligned}
&\bar{W}^{(k)} = [x^{(k)}], \quad \bar{x}^{(k)} = W^{(k)}, \quad \bar{b}^{(k)} = \mathbb{1} \\
&\quad \cdots \\
&\bar{\tilde{x}}^{(2)} = \rho'(x^{(2)}) * \bar{x}^{(3)}, \quad \bar{W}^{(2)} = x^{(2)} * \bar{\tilde{x}}^{(2)}, \bar{x}^{(2)} = W^{(2)} * \bar{\tilde{x}}^{(2)}, \quad \bar{b}^{(2)} = \bar{\tilde{x}}^{(2)} \\
&\bar{\tilde{x}}^{(1)} = \rho'(x^{(1)}) * \bar{x}^{(2)}, \quad \bar{W}^{(1)} = x^{(1)} * \bar{\tilde{x}}^{(1)}, \bar{x}^{(1)} = W^{(1)} * \bar{\tilde{x}}^{(1)}, \quad \bar{b}^{(1)} = \bar{\tilde{x}}^{(1)}
\end{aligned}
$$

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&\to \cdots \\
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&\bar{\tilde{x}}^{(2)} = \rho'(x^{(2)}) * \bar{x}^{(3)}, \quad \bar{W}^{(2)} = x^{(2)} * \bar{\tilde{x}}^{(2)}, \bar{x}^{(2)} = W^{(2)} * \bar{\tilde{x}}^{(2)}, \quad \bar{b}^{(2)} = \bar{\tilde{x}}^{(2)} \\
&\bar{\tilde{x}}^{(1)} = \rho'(x^{(1)}) * \bar{x}^{(2)}, \quad \bar{W}^{(1)} = x^{(1)} * \bar{\tilde{x}}^{(1)}, \bar{x}^{(1)} = W^{(1)} * \bar{\tilde{x}}^{(1)}, \quad \bar{b}^{(1)} = \bar{\tilde{x}}^{(1)}
\end{aligned}
$$

very simple to implement!

Numerical Stability

Usually:
No problems with accuracy of computed derivatives

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No problems with accuracy of computed derivatives but:

Example by John Reid shows:
Blow up of derivatives for cross-country mode of AD possible!

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No problems with accuracy of computed derivatives but:

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Blow up of derivatives for cross-country mode of AD possible!

Therefore:
Formal error analysis for forward and reverse mode of AD yielding:
Condition of derivative calculation = condition of function evaluation

(A. Griewank, K. Kulshreshtha, A. Walther, Computing, 2012)

Automatic Differentiation by OverLoading in C++

- ADOL-C version 2.7, available at COIN-OR since 2009
  open source (GPL or ECL)
- based on operator overloading, trace as internal representation
- general-purpose AD tool with focus on functionalities
- interfaces to ColPack (Purdue University) and Ipopt (COIN-OR)
- current developments
  - exploitation of fixed-point structure for second-order derivatives
  - generalized derivatives for nonsmooth functions

Model Generation with ADOL-C

```
double x1, x2, x3, x4;
double v1, v2, v3, v4, v5, v6;
double y1, y2;

x1 = 3.7; x2 = 0.7;
x3 = 0.5; x4 = 0.5;

v1 = x3*x4;
v2 = tan(v1);
v3 = x2-v2;
v4 = x1*v2;
v5 = v4/v3;
v6 = v5*x2

y1 = v5; y2 = v6;
```

Model Generation with ADOL-C

```
double x1, x2, x3, x4;
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v4 = x1*v2;
v5 = v4/v3;
v6 = v5*x2

y1 = v5; y2 = v6;
```
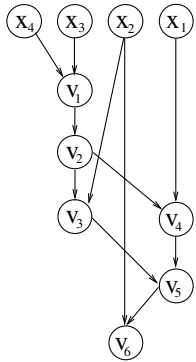
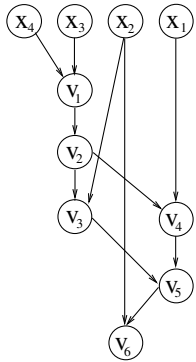



Model Generation with ADOL-C

```
adouble x1, x2, x3, x4;
adouble v1, v2, v3, v4, v5, v6;
double y1, y2;

trace_on(tag);
x1 <<= 3.7; x2 <<= 0.7;
x3 <<= 0.5; x4 <<= 0.5;

v1 = x3*x4;
v2 = tan(v1);
v3 = x2-v2;
v4 = x1*v2;
v5 = v4/v3;
v6 = v5*x2

v5 >>= y1; v6 >>= y2;
trace_off();
```



Model Generation with ADOL-C

```
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v3 = x2-v2;
v4 = x1*v2;
v5 = v4/v3;
v6 = v5*x2

v5 >>= y1; v6 >>= y2;
trace_off();
```

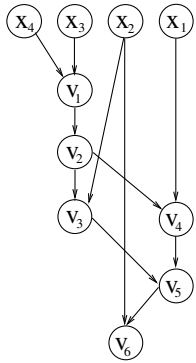

ADOL–C trace

trace_on, tag
<<=, x1, 3.7
<<=, x2, 0.7
<<=, x3, 0.5
<<=, x4, 0.5
*, x3, x4, v1
tan, v1, v2
–, x2, v2, v3
*, x1, v2, v4
/, v4, v3, v5
*, v5, x2, v6
>>=, v5, y1
>>=, v6, y2
trace_off

Easy-to-use Routines

int gradient(tag,n,x[n],g[n]):

tag	= tape number
n	= # indeps
x[n]	= values of indeps
g[n]	= $\nabla f(x)$

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int jacobian(tag,m,n,x[n],J[m][n]):

tag	= tape number
m	= # deps
n	= # indeps
x[n]	= values of indeps
J[m][n]	= $F'(x)$

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- n = # indeps
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- J[m][n] = $F'(x)$

int hessian(tag,n,x[n],H[n][n])

- tag = tape number
- n = # indeps
- x[n] = values of indeps
- H[n][n] = $\nabla^2 f(x)$

Lighthouse Example: Real Code

```
void f(double *x, double*y)
 {

  // intermediates
  double v[2];
  v[0] = tan(x[2]*x[3]);
  v[1] = x[0]*v[0];
  y[0] = v[1]/(x[1]-v[0]);
  y[1] = x[1]*y[0];
  }
```

Lighthouse Example: Real Code for Forward Mode

```
void d1_f(double* x, double* d1_x, double* y, double* d1_y)
//$ad indep x d1_x
//$ad dep y d1_y
 {
  double v[2];                 double d1_v[2];
  double w1_0 = 0;             double d1_w1_0 = 0;
  ...
  double w1_5 = 0;             double d1_w1_5 = 0;

  d1_w1_0 = d1_x[2];           w1_0 = x[2];
  d1_w1_1 = d1_x[3];           w1_1 = x[3];
  d1_w1_2 = w1_1*d1_w1_0 + w1_0*d1_w1_1;
  w1_2 = w1_0*w1_1;
  d1_w1_3 = 1/(cos(w1_2)*cos(w1_2)) * d1_w1_2;
  w1_3 = tan(w1_2);
  ...                          using dcc (U. Naumann, RWTH Aachen)
```

Lighthouse Example: Real Code for Forward Mode

```
void d1_f(double* x, double* d1_x, double* y, double* d1_y)
//$ad indep x d1_x
//$ad dep y d1_y
 {
   double v[2];                 double d1_v[2];
   double w1_0 = 0;             double d1_w1_0 = 0;
   ...
   double w1_5 = 0;             double d1_w1_5 = 0;

   d1_w1_0 = d1_x[2];           w1_0 = x[2];
   d1_w1_1 = d1_x[3];           w1_1 = x[3];
   d1_w1_2 = w1_1*d1_w1_0 + w1_0*d1_w1_1;
   w1_2 = w1_0*w1_1;
   d1_w1_3 = 1/(cos(w1_2)*cos(w1_2)) * d1_w1_2;
   w1_3 = tan(w1_2);
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```

Lighthouse Example: Real Code for Forward Mode

```
void d1_f(double* x, double* d1_x, double* y, double* d1_y)
//$ad indep x d1_x
//$ad dep y d1_y
 {
   double v[2];                 double d1_v[2];
   double w1_0 = 0;             double d1_w1_0 = 0;
   ...
   double w1_5 = 0;             double d1_w1_5 = 0;

   d1_w1_0 = d1_x[2];           w1_0 = x[2];
   d1_w1_1 = d1_x[3];           w1_1 = x[3];
   d1_w1_2 = w1_1*d1_w1_0 + w1_0*d1_w1_1;
   w1_2 = w1_0*w1_1;
   d1_w1_3 = 1/(cos(w1_2)*cos(w1_2)) * d1_w1_2;
   w1_3 = tan(w1_2);
   ...                          using dcc (U. Naumann, RWTH Aachen)
```

Lighthouse Example: Real Code for Reverse Mode

```
void b1_f(int& bmode_1, double* x, double* b1_x, double* y, double* b1_y)
//$ad indep x b1_x b1_y
//$ad dep y b1_x
  { double v[2];            double b1_v[2];
    double w1_0 = 0;        double b1_w1_0 = 0;        ...
    double w1_5 = 0;        double b1_w1_5 = 0;
    int save_cs_c = 0;      save_cs_c = cs_c;
    if (bmode_1==1) { // augmented forward section
     cs[cs_c] = 0;          cs_c = cs_c+1;
     fds[fds_c] = v[0];     fds_c = fds_c+1;    v[0] = tan(x[2]*x[3]);
     ...
     fds[fds_c] = y[1];     fds_c = fds_c+1;    y[1] = x[1]*y[0];
     while (cs_c>save_cs_c) {    // reverse section
        cs_c = cs_c-1;
        if (cs[cs_c]==0) {
           fds_c = fds_c-1;         y[1] = fds[fds_c];
           w1_0 = x[1];             w1_1 = y[0];      w1_2 = w1_0*w1_1;
           b1_w1_2 = b1_y[1];   b1_y[1] = 0; // adjoint assignment
           b1_w1_0 = w1_1*b1_w1_2;    b1_w1_1 = w1_0*b1_w1_2;        ...
```

Lighthouse Example: Real Code for Reverse Mode

```
void b1_f(int& bmode_1, double* x, double* b1_x, double* y, double* b1_y)
//$ad indep x b1_x b1_y
//$ad dep y b1_x
  { double v[2];            double b1_v[2];
    double w1_0 = 0;        double b1_w1_0 = 0;        ...
    double w1_5 = 0;        double b1_w1_5 = 0;
    int save_cs_c = 0;      save_cs_c = cs_c;
    if (bmode_1==1) { // augmented forward section
     cs[cs_c] = 0;          cs_c = cs_c+1;
     fds[fds_c] = v[0];     fds_c = fds_c+1;    v[0] = tan(x[2]*x[3]);
     ...
     fds[fds_c] = y[1];     fds_c = fds_c+1;    y[1] = x[1]*y[0];
     while (cs_c>save_cs_c) {    // reverse section
        cs_c = cs_c-1;
        if (cs[cs_c]==0) {
           fds_c = fds_c-1;         y[1] = fds[fds_c];
           w1_0 = x[1];             w1_1 = y[0];      w1_2 = w1_0*w1_1;
           b1_w1_2 = b1_y[1];   b1_y[1] = 0; // adjoint assignment
           b1_w1_0 = w1_1*b1_w1_2;    b1_w1_1 = w1_0*b1_w1_2;        ...
```

Lighthouse Example: Real Code for Reverse Mode

```
void b1_f(int& bmode_1, double* x, double* b1_x, double* y, double* b1_y)
//$ad indep x b1_x b1_y
//$ad dep y b1_x
 { double v[2];          double b1_v[2];
   double w1_0 = 0;      double b1_w1_0 = 0;      ...
   double w1_5 = 0;      double b1_w1_5 = 0;
   int save_cs_c = 0;    save_cs_c = cs_c;
   if (bmode_1==1) { // augmented forward section
    cs[cs_c] = 0;        cs_c = cs_c+1;
    fds[fds_c] = v[0];   fds_c = fds_c+1;   v[0] = tan(x[2]*x[3]);
    ...
    fds[fds_c] = y[1];   fds_c = fds_c+1;   y[1] = x[1]*y[0];
    while (cs_c>save_cs_c) {    // reverse section
       cs_c = cs_c-1;
       if (cs[cs_c]==0) {
          fds_c = fds_c-1;       y[1] = fds[fds_c];
          w1_0 = x[1];           w1_1 = y[0];     w1_2 = w1_0*w1_1;
          b1_w1_2 = b1_y[1];   b1_y[1] = 0; // adjoint assignment
          b1_w1_0 = w1_1*b1_w1_2;   b1_w1_1 = w1_0*b1_w1_2;      ...
```

Lighthouse Example: Real Code for Reverse Mode

```
void b1_f(int& bmode_1, double* x, double* b1_x, double* y, double* b1_y)
//$ad indep x b1_x b1_y
//$ad dep y b1_x
 { double v[2];          double b1_v[2];
   double w1_0 = 0;      double b1_w1_0 = 0;      ...
   double w1_5 = 0;      double b1_w1_5 = 0;
   int save_cs_c = 0;    save_cs_c = cs_c;
   if (bmode_1==1) { // augmented forward section
    cs[cs_c] = 0;        cs_c = cs_c+1;
    fds[fds_c] = v[0];   fds_c = fds_c+1;   v[0] = tan(x[2]*x[3]);
    ...
    fds[fds_c] = y[1];   fds_c = fds_c+1;   y[1] = x[1]*y[0];
    while (cs_c>save_cs_c) {    // reverse section
       cs_c = cs_c-1;
       if (cs[cs_c]==0) {
          fds_c = fds_c-1;       y[1] = fds[fds_c];
          w1_0 = x[1];           w1_1 = y[0];     w1_2 = w1_0*w1_1;
          b1_w1_2 = b1_y[1];     b1_y[1] = 0; // adjoint assignment
          b1_w1_0 = w1_1*b1_w1_2;    b1_w1_1 = w1_0*b1_w1_2;      ... using again dcc
```

Conclusions Part I

- Differentiation of computer programmes with working accuracy (Griewank, Kulshreshtha, Walther 2012)

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Conclusions Part I

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$$
\begin{array}{lllll}
\text{Forward mode:} & \mathrm{OPS}(F'(x)\dot{x}) & \leq & c\,\mathrm{OPS}(F), & c \in [2, 5/2] \\
\text{Reverse mode:} & \mathrm{OPS}(\bar{y}^\top F'(x)) & \leq & c\,\mathrm{OPS}(F), & c \in [3, 4] \\
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$\Longrightarrow$ Gradients are cheap $\sim$ Function costs!!

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  $\Longrightarrow$ Gradients are cheap $\sim$ Function costs!!
- Consistent derivative information!
- AD-tools: ADOL-C, CoDiPack, Tapenade, INTLAB, ...
- General purpose tools: FEniCS, SU2, JAX, PyTorch, TensorFlow, ...

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(Griewank, Walther 2008), (Naumann 2012), www.autodiff.org