# Derivative-based Optimization for Applications in Physics

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Keynote Lecture
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MATH+

# Outline

# Where are Derivatives Needed?

- Optimization:

unbounded: $\min f(x), \quad f: \mathbb{R}^n \to \mathbb{R}$

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

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

# Frequent Situation

# 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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Description of functional relation as

- formula $y = F(x)$ $\Rightarrow$ explicit expression $y' = F'(x)$
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**Task:**

Computation of derivatives taking

- requirements on exactness
- computational effort

into account



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# Algorithmic Differentiation (AD)

aka Automatic Differentiation

= Differentiation of computer programs implementing $F : \mathbb{R}^n \mapsto \mathbb{R}^m$

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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 in a neighbourhood of current argument $x$



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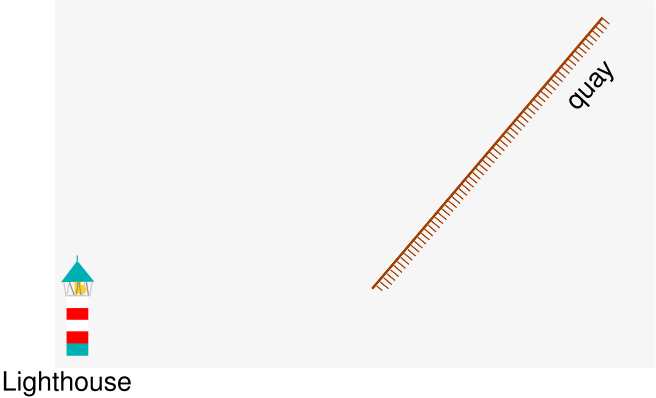
# The “Hello-World”-Example of AD



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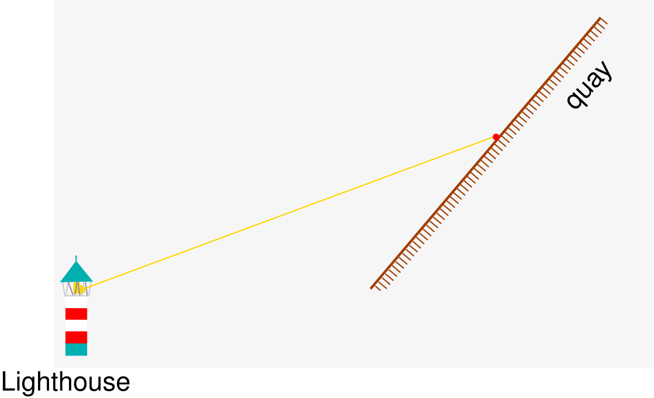

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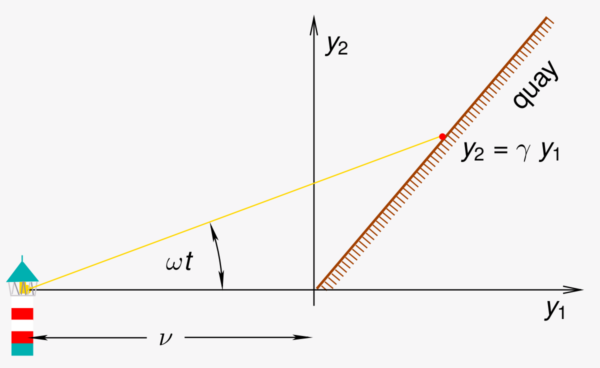


Lighthouse

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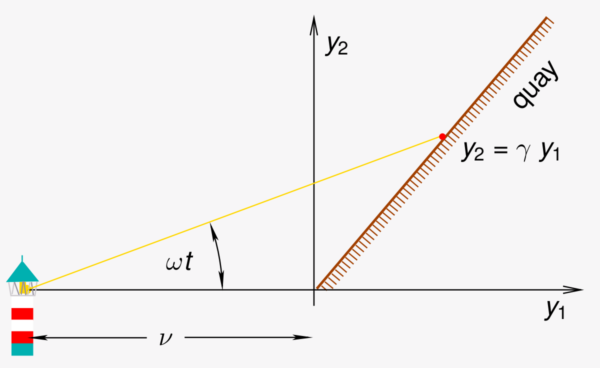


Lighthouse

$$y_1 = \frac{\nu \tan(\omega\, t)}{\gamma - \tan(\omega\, t)} \quad \text{and} \quad y_2 = \frac{\gamma\, \nu \tan(\omega\, t)}{\gamma - \tan(\omega\, t)}$$

# Evaluation Procedure (Lighthouse)

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

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

$$\Longrightarrow$$

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

# Function Evaluation in ML

Typical function evaluation (deep neural net):

Propagation of one data point:

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

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

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Empirical risk, loss function, ...

$$f(x_{1\leq i\leq M}) = \frac{1}{M}\sum_{i=1}^{M} l(y_i(x_i), y_i^{NN})$$

Stochastic gradient descent requires

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



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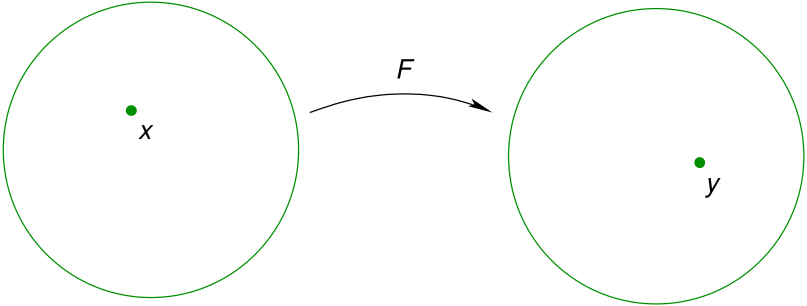
# Forward mode AD = Tangents/Sensitivities



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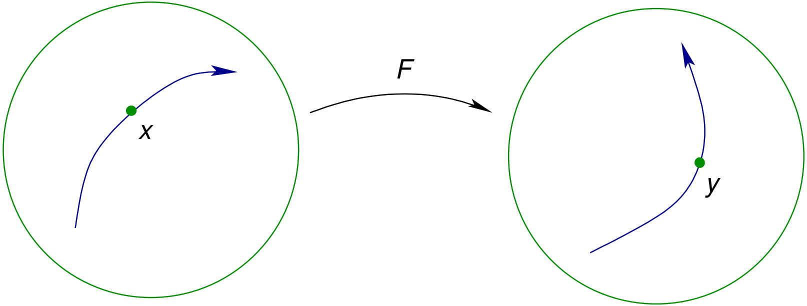

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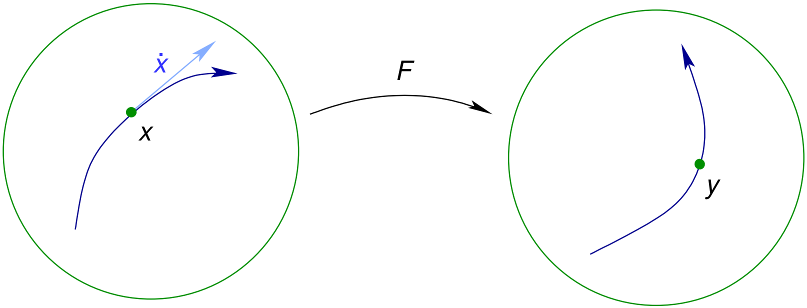

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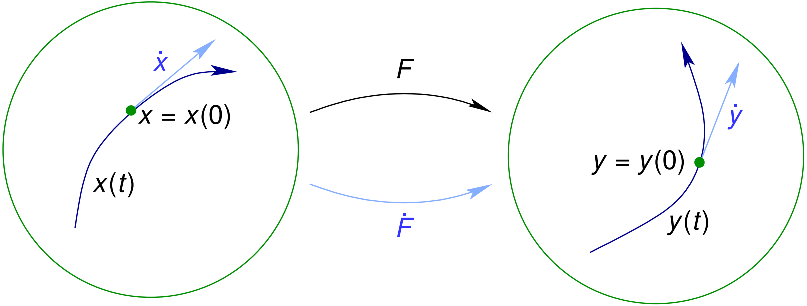

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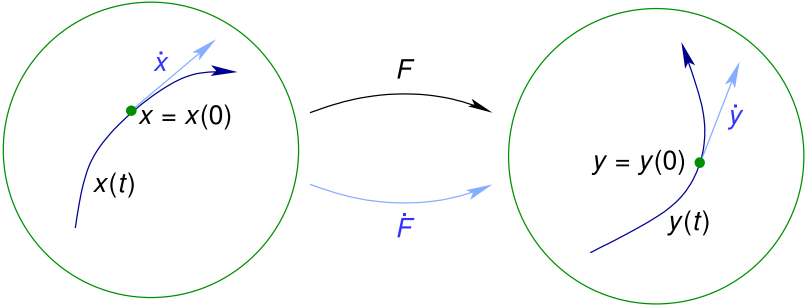


$$\dot{y}(t) \;=\; \frac{\partial}{\partial t} F(x(t)) \;=\; F'(x(t))\,\dot{x}(t) \equiv \dot{F}(x, \dot{x})$$

# Forward Mode (Lighthouse)

$$
\begin{array}{lcl}
v_{-3} & = & x_1 = \nu \\
v_{-2} & = & x_2 = \gamma \\
v_{-1} & = & x_3 = \omega \\
v_0 & = & x_4 = t \\
\hline
v_1 & = & v_{-1} * v_0 \\
v_2 & = & \tan(v_1) \\
v_3 & = & v_{-2} - v_2 \\
v_4 & = & v_{-3} * v_2 \\
v_5 & = & v_4 / v_3 \\
v_6 & = & v_5 * v_{-2} \\
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y_1 & = & v_5 \\
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$$

# Complexity (Forward Mode)

| tang | $c$ | $\pm$ | $*$ | $\psi$ |
|---|---|---|---|---|
| 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 |

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| MULTS | 0 | 0 | $1+2$ | $0+1$ |
| NLOPS | 0 | 0 | 0 | $1+1$ |

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

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

# Forward Mode AD for ML

Typical function evaluation (deep neural net):

$$x = x^{(1)} \rightarrow \tilde{x}^{(1)} = W^{(1)}x^{(1)} + b^{(1)} \quad \rightarrow x^{(2)} = \rho(\tilde{x}^{(1)}) \quad \ldots \quad \rightarrow y = W^{(k)}x^{(k)} + b^{(k)}$$

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

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

# Forward Mode AD for ML

Typical function evaluation (deep neural net):

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\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 & \dots \\
\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}$$



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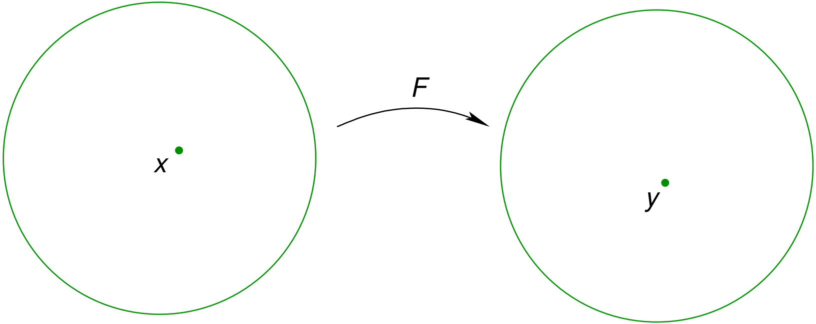
# Reverse Mode AD = Discrete Adjoints



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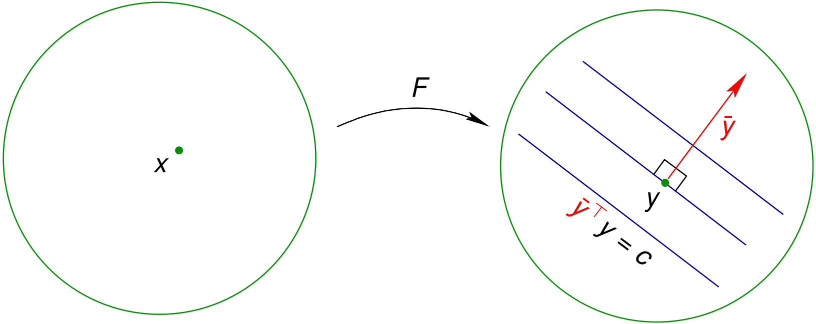

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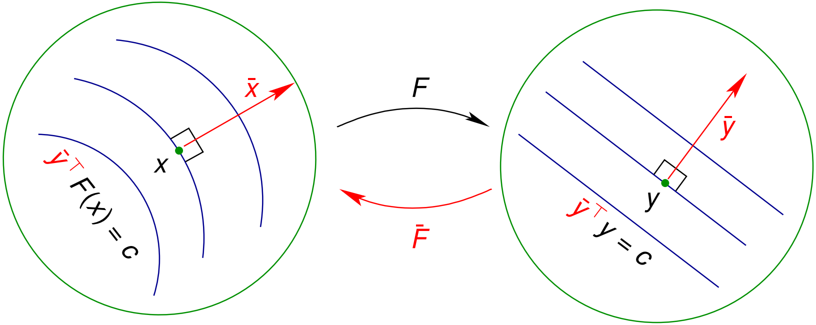

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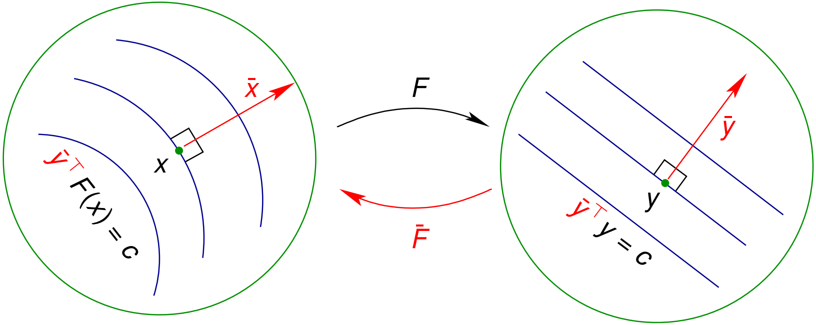


$$\bar{x} \equiv \bar{y}^\top F'(x) = \nabla_x \langle \bar{y}^\top F(x) \rangle \equiv \bar{F}(x, \bar{y})$$

# Reverse Mode (Lighthouse)

$$v_{-3} = x_1; \quad v_{-2} = x_2; \quad v_{-1} = x_3; \quad v_0 = x_4;$$
$$v_1 = v_{-1} * v_0;$$
$$v_2 = \tan(v_1);$$
$$v_3 = v_{-2} - v_2;$$
$$v_4 = v_{-3} * v_2;$$
$$v_5 = v_4 / v_3;$$
$$v_6 = v_5 * v_{-2};$$
$$y_1 = v_5; \quad y_2 = v_6;$$

---

$$\bar{v}_5 = \bar{y}_1; \quad \bar{v}_6 = \bar{y}_2;$$
$$\bar{v}_5 \mathrel{+}= \bar{v}_6 * v_{-2}; \quad \bar{v}_{-2} \mathrel{+}= \bar{v}_6 * v_5;$$
$$\bar{v}_4 \mathrel{+}= \bar{v}_5 / v_3; \quad \bar{v}_3 \mathrel{-}= \bar{v}_5 * v_5 / v_3;$$
$$\bar{v}_{-3} \mathrel{+}= \bar{v}_4 * v_2; \quad \bar{v}_2 \mathrel{+}= \bar{v}_4 * v_{-3};$$
$$\bar{v}_{-2} \mathrel{+}= \bar{v}_3; \; \bar{v}_2 \mathrel{-}= \bar{v}_3;$$
$$\bar{v}_1 \mathrel{+}= \bar{v}_2 / \cos^2(v_1);$$
$$\bar{v}_{-1} \mathrel{+}= \bar{v}_1 * v_0; \; \bar{v}_0 \mathrel{+}= \bar{v}_1 * v_{-1};$$
$$\bar{x}_4 = \bar{v}_0; \quad \bar{x}_3 = \bar{v}_{-1}; \quad \bar{x}_2 = \bar{v}_{-2}; \quad \bar{x}_1 = \bar{v}_{-3};$$

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# Complexity (Reverse Mode)

| grad | $c$ | $\pm$ | $*$ | $\psi$ |
|---|---|---|---|---|
| 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 |



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

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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

Typical function evaluation (deep neural net):

$$
\begin{aligned}
x = x^{(1)} &\rightarrow \tilde{x}^{(1)} = W^{(1)}x^{(1)} + b^{(1)} &&\rightarrow x^{(2)} = \rho(\tilde{x}^{(1)})\\
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With $\bar{y} = 1$ one obtains

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very simple to implement!

# Historical Development of AD

| | | | | | |
|---|---|---|---|---|---|
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Rumelhart at al. (1986) made backpropagation famous for neural nets



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# Overview AD Theory and Tools

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

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  = discrete analogon to sensitivity equation



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



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- current developments
  - Julia interface ADOLC.jl
  - exploitation of fixed-point structure for second-order derivatives
  - generalized derivatives for nonsmooth functions

# Piezoelectricity

Fundamental properties:

- Transformation of **mechanical energy** into **electrical energy**
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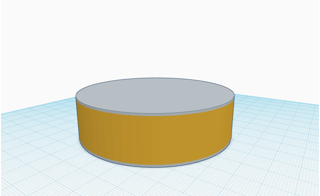
Used in wide range of applications:
Pressure Sensors, Ultrasonic Cleaning, Ultrasound Imaging, Piezoelectric Speakers, Electronic Toothbrushes, Instrument Pickups, Microphones, Piezoelectric Igniters, Electricity Generation, Tennis Racquets, . . .

# The Considered Setting



https://www.piceramic.de/de/produkte/piezokeramische-bauelemente/scheiben-staebe-und-zylinder/piezoelektrische-scheiben-1206710/

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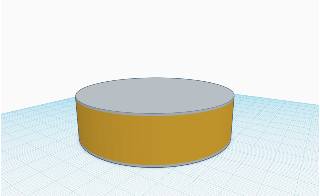

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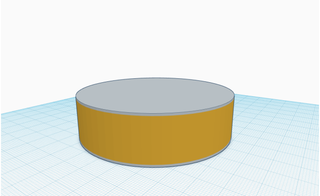

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- Here: Consider only small loads $\Rightarrow$ Disregard thermal effects
  Nonlinear effects $\Rightarrow$ DFG research group NEPTUN

# Inverse Problem - State of the Art

- Sensitivity too small for some parameter
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  Up to 20% error not uncommon

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- Alternative approaches:
  - Use multiple differently shaped piezoceramics
    $\Rightarrow$ Leads to inconsistent datasets
  - Use additional measuremens of surface displacement
    $\Rightarrow$ Very expensive and still low sensitivity
  - Low sensitivity parameters are excluded from parameter identification

# Inverse Problem - State of the Art

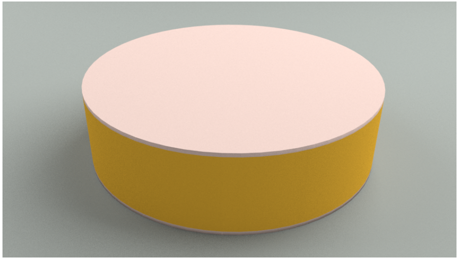
- Sensitivity too small for some parameter
  (using conventional methods or data provided by manufacturer)
  Up to 20% error not uncommon

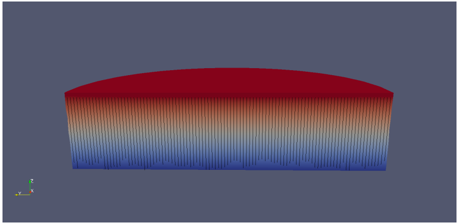
- Alternative approaches:
  - Use multiple differently shaped piezoceramics
    $\Rightarrow$ Leads to inconsistent datasets
  - Use additional measuremens of surface displacement
    $\Rightarrow$ Very expensive and still low sensitivity
  - Low sensitivity parameters are excluded from parameter identification

**Goal:** Identify all parameters using a single piezoceramic and impedance measurements

# AD-enabled Optimization of the Electrodes

Fully covering electrodes

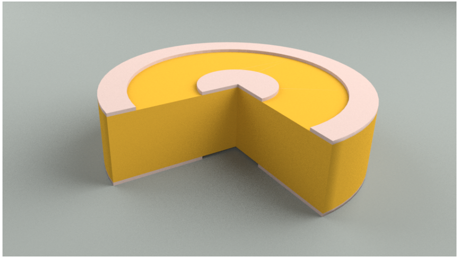


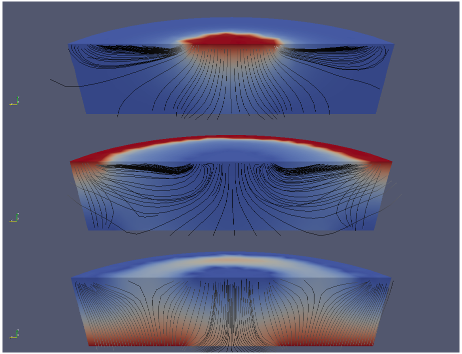


Thanks to B. Jurgelucks

# AD-enabled Optimization of the Electrodes

Triple-ring electrodes





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# Real Measurements

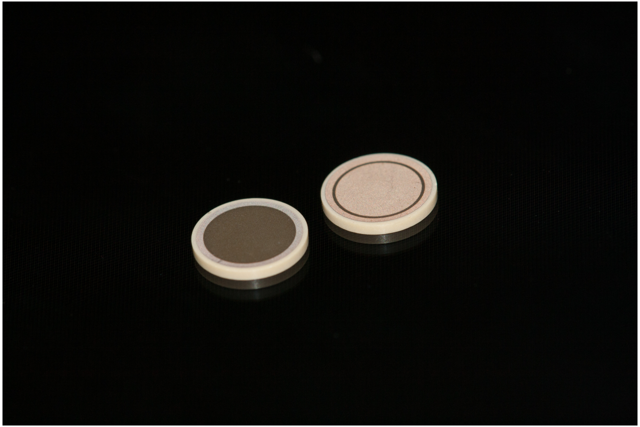
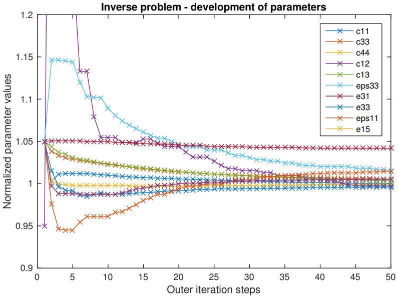
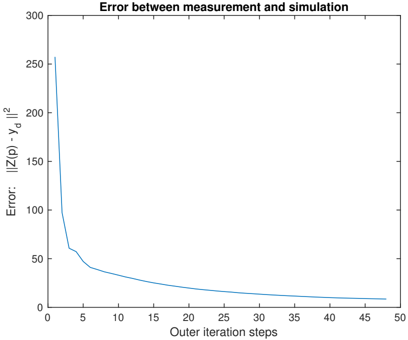


Photo by S. Olfert

# Appropriate Version of AD-enabled Gauss-Newton Method



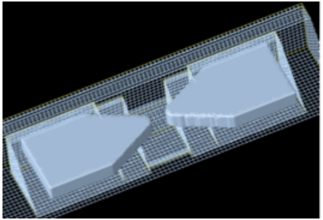

- None of the 10 (!) parameters diverges
- To the best of our knowledge this has not been possible with only one piezoceramic

# Optical Nano-Structures

**State of the art:** Nano-structures are used to confine light

Simple example: Bow-tie antenna

- metallic nano structure
- two triangles and gap
- Size: 100 nm ($< \lambda_{\text{light}}$!)
- intensity enhancement in gap

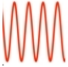


# Possible Configurations

Simple setting:

- different structure

- “simple” excitation



- pure metal
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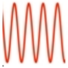

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Advanced setting:

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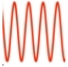

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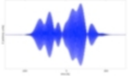

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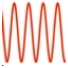

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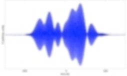

- add resonances in semiconductors

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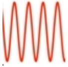

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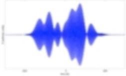
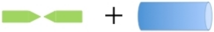


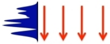
- add resonances in semiconductors
- longer dephasing



# Test Case: Quantum Wire

Cooperation with T. Meier, M. Reichelt, Dep. Physik, Uni Paderborn

Generic configuration:

 $\longleftarrow$ adaptable light puls $E(t)$



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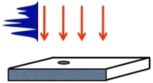

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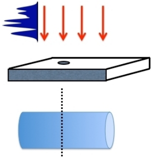

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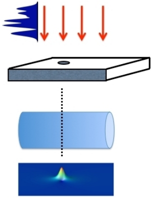

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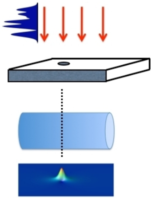

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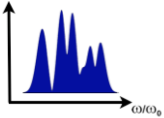
Light puls:




$$\text{with } E(t) = \sum A_i \exp\left(-\left(\frac{t-t_i}{\delta t_i}\right)^2\right)\cos(\omega_i t + \phi_i)$$

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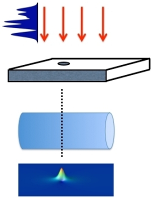

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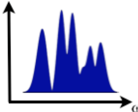


with $E(t) = \sum A_i \exp\left(-\left(\frac{t-t_i}{\delta t_i}\right)^2\right) \cos(\omega_i t + \phi_i)$

Parameter: $A_i, \phi_i, \omega_i, t_i$ $\Rightarrow$ up to 120!

# Mathematical Formulation

**State equation:**

$$
\begin{aligned}
\frac{\partial}{\partial t} p &= \frac{i}{\hbar}(\epsilon_0 - \epsilon_1)p + \frac{i}{\hbar}\mathbf{E}(t)\cdot\mathbf{d}\,(n_0 - n_1) \\
\frac{\partial}{\partial t} n_0 &= \frac{2}{\hbar}\mathrm{Im}\,[\mathbf{E}(t)\cdot\mathbf{d}\,p^*] \\
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1 &= n_1 + n_0
\end{aligned}
$$

$\Rightarrow$ Three complex-valued coupled differential equations $p$, $n_0$ and $n_1$ distributed in space.

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Target:
Maximize energy at given time and given place with constant energy

= Maximize emitted radiation

$$I_{rad} = \left|\omega^2 P(\omega)\right|^2 = \left|\omega^2\, 2\,\mathrm{Re}(d\,p)\right|^2$$

# Function Evaluation of $I_{rad}(f(g(x)))$

```
x[] ← (phase[], amplitude[], width[], point[])

for time=0 to Tfinal do
    if (time >= Tobs && time < Tobs+dt)
        eval_time_step1(x,int_tar)
    else
        eval_time_step2(x,int_tar)
    end if
end for

eval_target(int_tar,fitness)
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scenarios:

# independents $\in \{20, 60, 120\}$ $\Rightarrow$ Reverse mode!

# time steps $\in \{16000, 32000, 160000\}$ $\Rightarrow$ Checkpointing!

# Quantum Wire: Optimization

**So far:** Genetic algorithms

**Now:** L-BFGS and efficient gradient computation

- ADOL-C coupled with hand-coded adjoints
- Checkpointing (160 000 time steps!!)

$\Rightarrow$ TIME(gradient)/TIME(target function) $<$ 7 despite of checkpointing!

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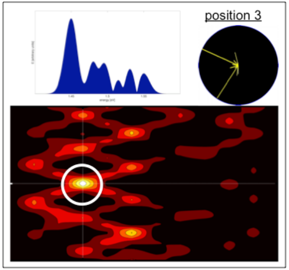
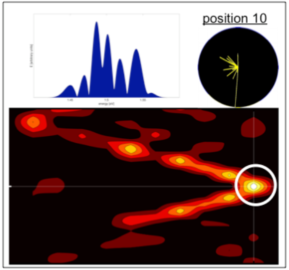



excite
- at **same** position
- at **same** time
- with **same** energy

optimize
- for **same** $t_{opt}$
- **different** positions



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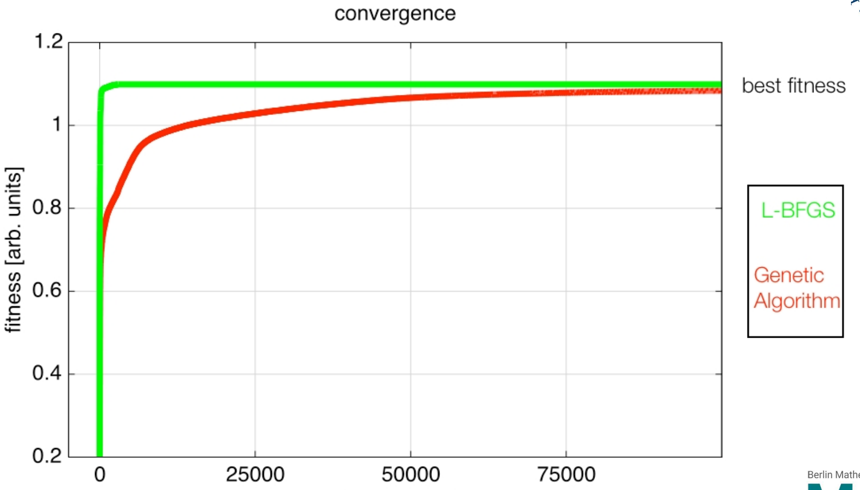
# Quantum Wire: Comparison



# Photonic Nano-Resonators

Joint work with F. Binkowski, J. Kullig, F. Betz, L. Zschiedrich, J. Wiersig, S. Burger

Applications:

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Furter aspects:

- computed by solving the source-free Maxwell's equations
- sensitivities of resonances are of interest for
  - better understanding of the underlying physical effects
  - an efficient optimization of corresponding photonic devices

# Behaviour of Sensitivities at EPs

Exceptional points: spectral degeneracies
(eigenfrequencies and eigenmodes coalesce)

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Exceptional points: spectral degeneracies
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- parametric fine-tuning is needed to achieve such non-Hermitian degeneracies
  $\Rightarrow$ exceptional points (EPs)
- EPs have been connected to many interesting effects including
  - ultra-sensitive sensors
  - control of light transport
  - electromagnetically induced transparency
  - optical amplifiers,...

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Exceptional points: spectral degeneracies
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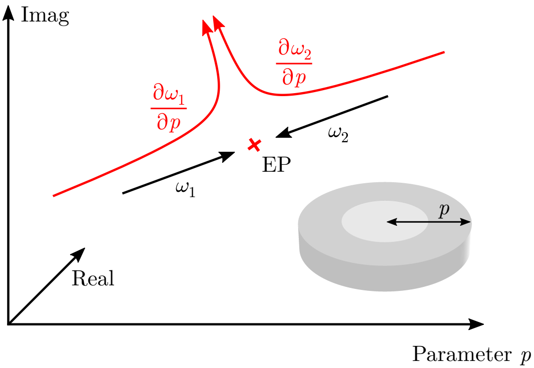
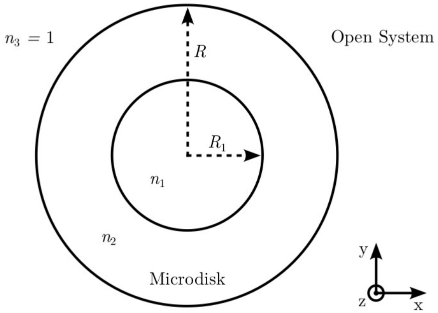
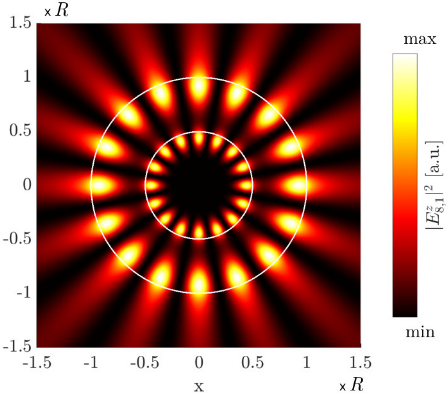


# Calculation of EPs and Their Sensitivities

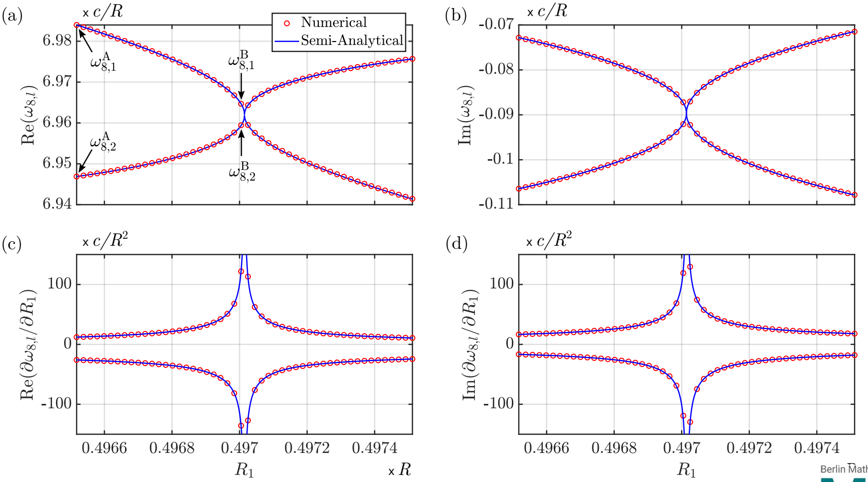
- RPExpand
  Software for Riesz projection expansion of resonance phenomena
  by F. Betz, F. Binkowski, S. Burger
- JCMSuite
  part of JCMWave (commercial software)
  based on FEM combined with efficient contour-integral method
  implements own AD approach

# The Considered Setting



# Eigenfrequencies and Their Sensitivities



# Conclusions

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  - Various tools/implementations available
- Structure exploitation indispensable
- AD for applications in physics:
  - parameter identification for piezoceramics[1]
  - optimized excitation of nano antenna[2]
  - sensitivities of exceptional points of nano-resonators[3]

[1] e.g., L. Claes et al.: Inverse procedure for measuring piezoelectric material parameters using a single multi-electrode sample. J. Sensors and Sensor Systems 12 (1) (2023)

[2] e.g., M. Reichelt, A. Walther, T. Meier: Tailoring the high-harmonic emission in two-level systems and semiconductors by pulse shaping. JOSA B 29 (2) (2012)

[3] F. Binkowski, J. Kullig, F. Betz, L. Zschiedrich, A. Walther, J. Wiersig, S. Burger: Computing eigenfrequency sensitivities near exceptional points,Phys. Rev. Research 6 (2) (2024)