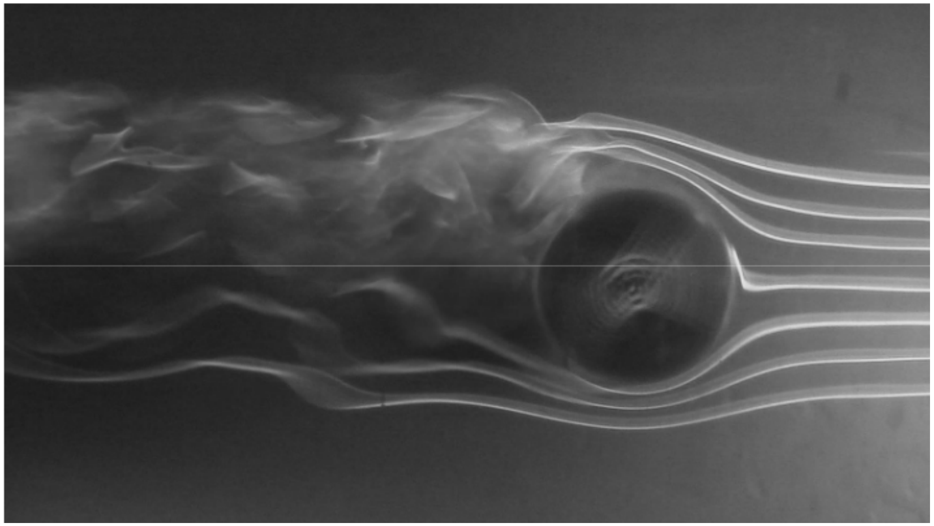


Physics based learning for forward and inverse problems

Amuthan Ramabathiran
Dept. of Aerospace Engineering, IIT Bombay.
E-mail: amuthan@aero.iitb.ac.in

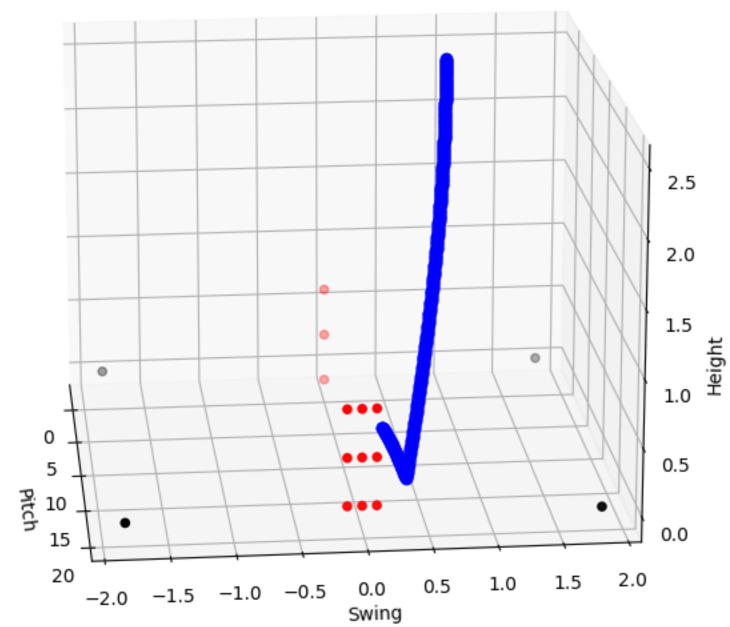
Code: https://github.com/Amuthan/AICTEworkshop2021

ATAL-AICTE Online Workshop (Dec 6-10, 2021)
Multi-Disciplinary Design Optimization in Engineering: Basics

Outline

- Differentiable physics
- Review of Optimization
- Automatic Differentiation
- Deep Neural Networks
- Application: ODEs

- **Hands-on session:**
    - Simple examples with PyTorch
    - *Competition:* Who is the best bowler?



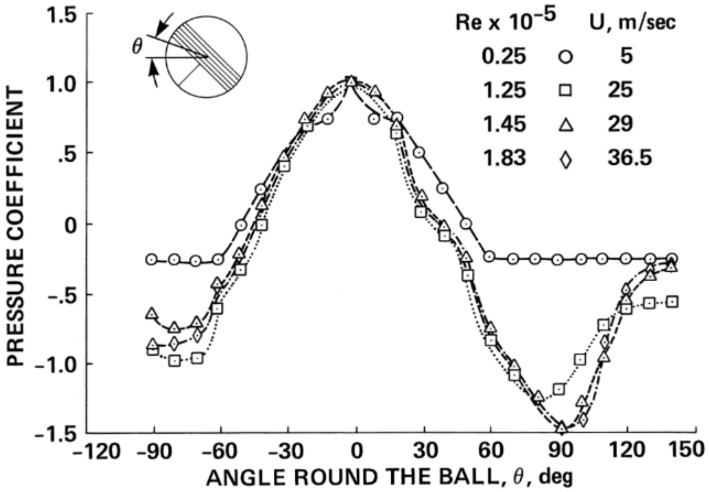
Working knowledge of Python required!

Data based vs physics based modeling

How do we predict the swing of a cricket ball?

Data based approach:
Use data from experiments or numerical simulations directly

Physics based approach:
Use known physics about fluid flow around ball



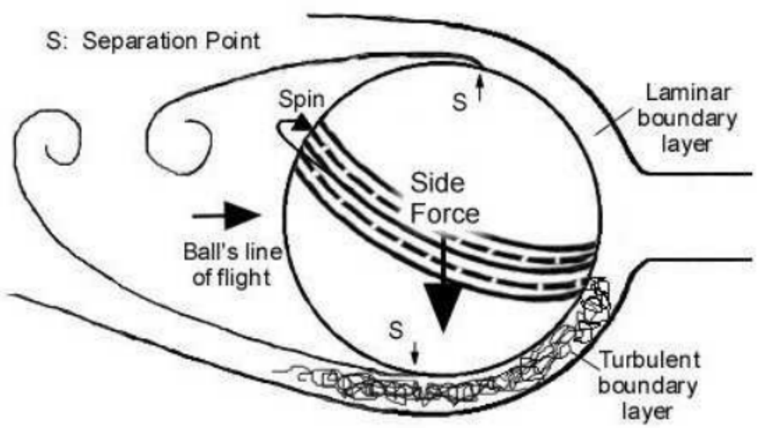
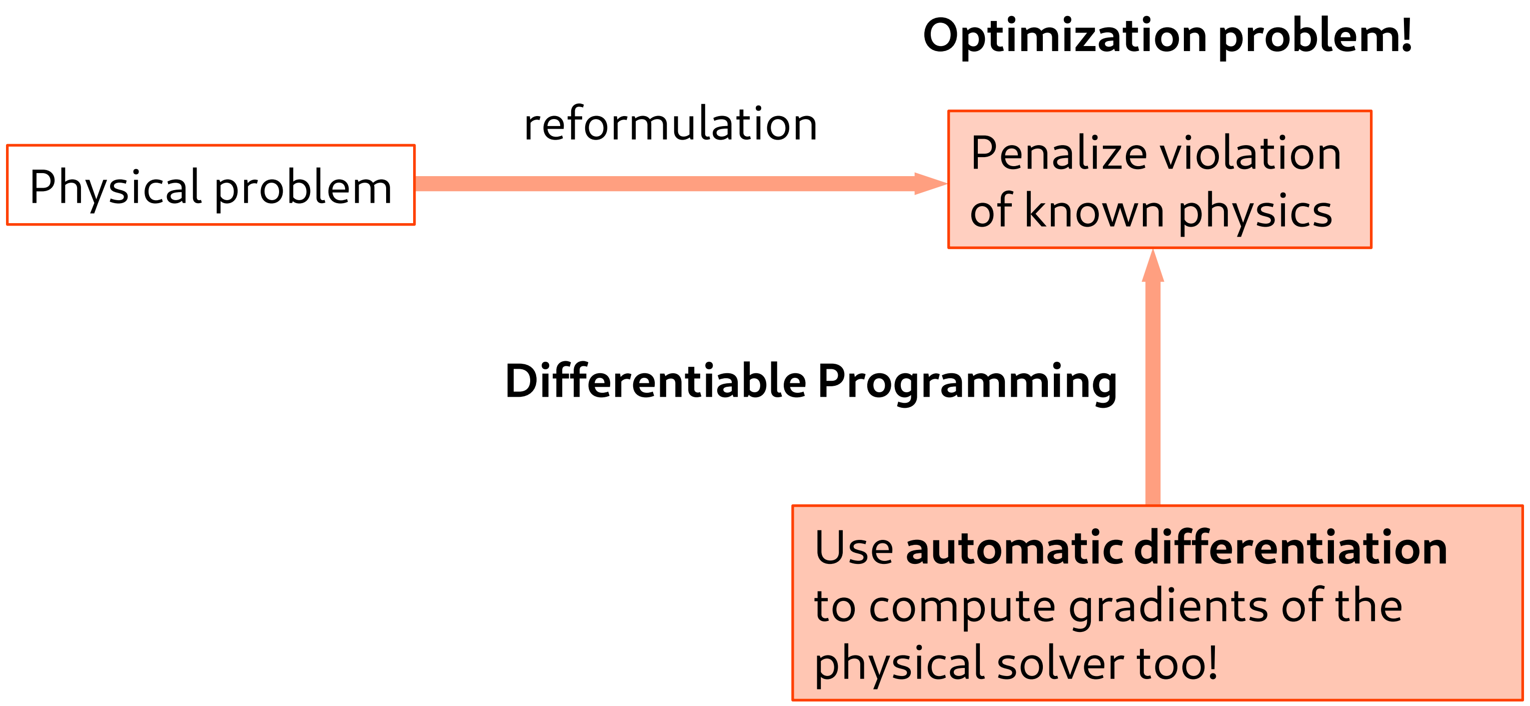


Image source: Mehta (2014): https://people.eng.unimelb.edu.au/imarusic/proceedings/19/10.pdf (+picture on title slide)

Differentiable physics

Differentiable physics enhances data based modeling with known physics prior – **best of both worlds!**



Review of finite dimensional optimization

Unconstrained minimization problem: given **objective function** $f : \mathbb{R}^n \to \mathbb{R}$, find

$$\boxed{x^\star \in \text{argmin}_{x \in \mathbb{R}^n} \; f(x).}$$

First order necessary condition for optimality:

$$\boxed{x^\star \text{ is optimal } \Rightarrow \nabla f(x^\star) = 0.}$$

Second order sufficient condition for minimizer:

$$\boxed{\nabla^2 f(x^\star) \succ 0 \;\Rightarrow\; x^\star \text{ is a local minimizer of } f.}$$

Gradient descent algorithm

Iterative algorithms construct a **minimizing sequence** $(x_1, x_2, \ldots)$ that converge to the true minimizer:

$$\boxed{\lim_{n\to\infty} x_n = x^\star \in \operatorname{argmin}_{x\in\mathbb{R}^n} f(x).}$$

Gradient descent algorithm creates a minimizing sequence by stepping in the direction of the negative gradient of the objective function:

$$\boxed{x_{n+1} = x_n - \alpha_n \nabla f(x_n).}$$

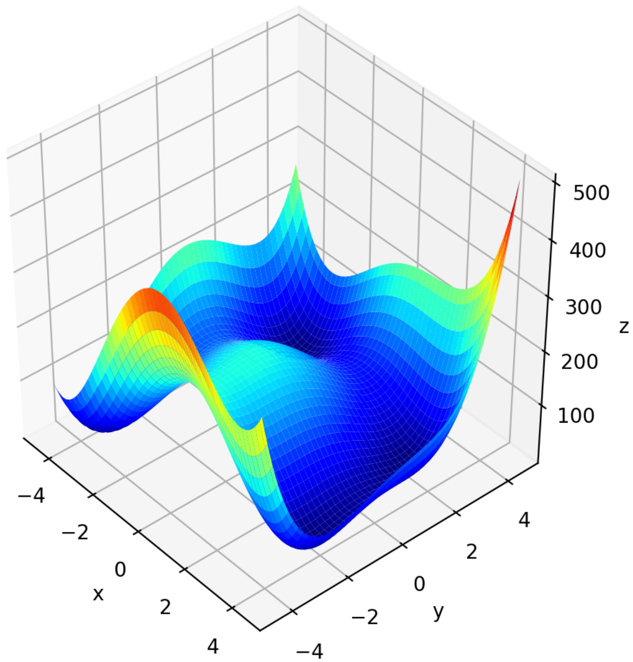
α_n : step size / **learning rate**

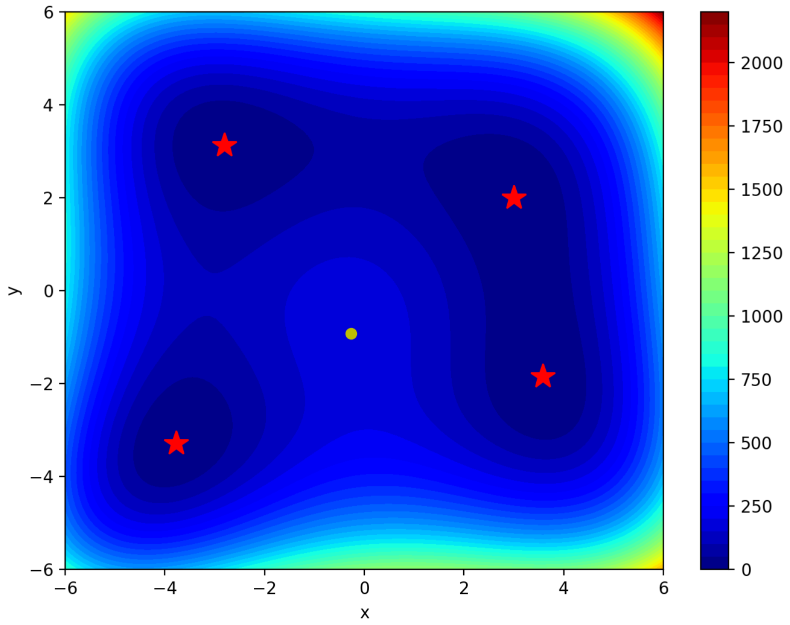
Gradient descent algorithm is **guaranteed to converge** to a local minimizer with appropriate choice of step size!

Example: Himmelblau function

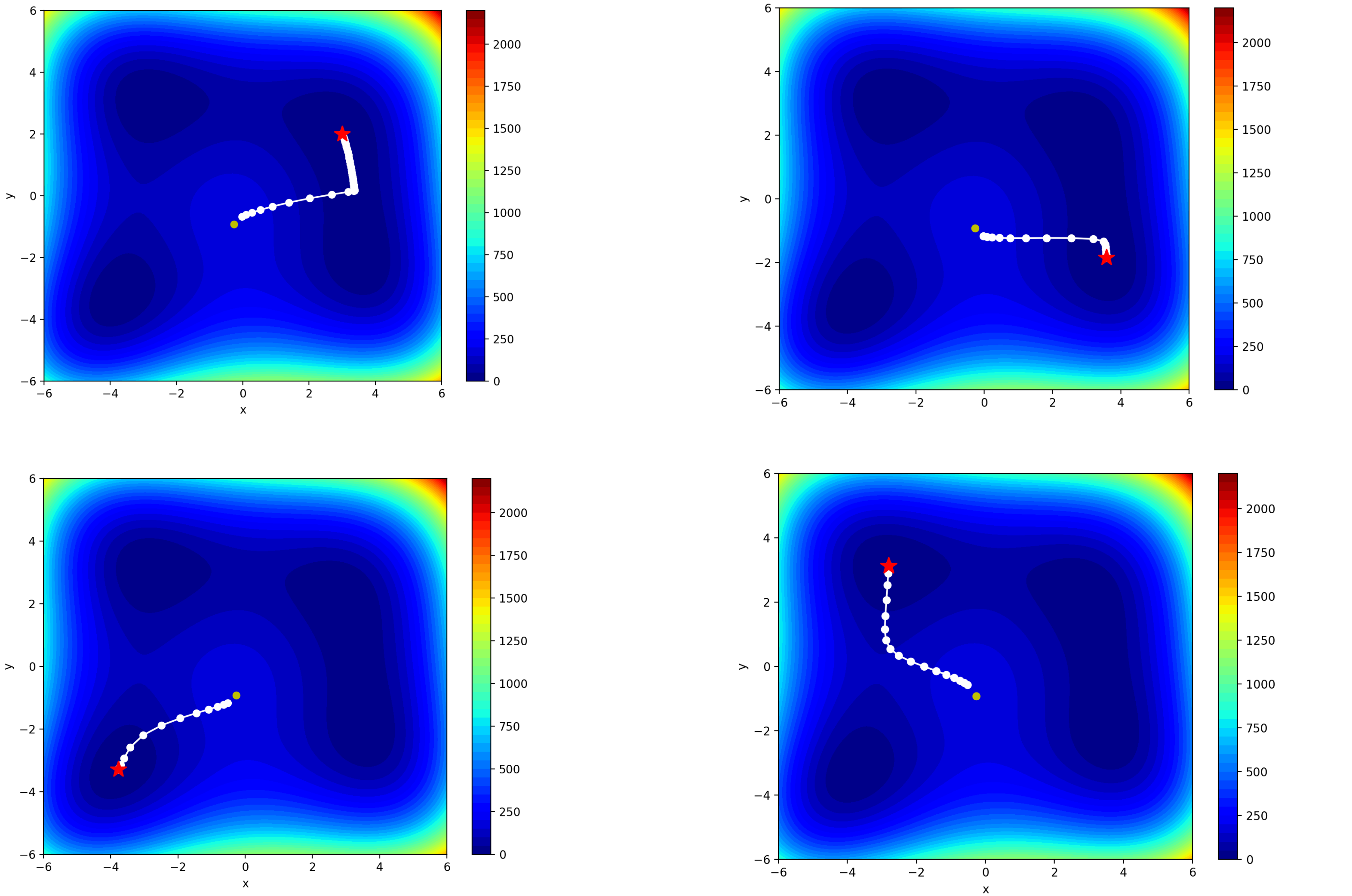
$$f(x, y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2$$

(One local maximum and four global minima)





Gradient descent for Himmelblau function



Equality constrained optimization: Lagrange multipliers

Given objective function $f : \mathbb{R}^n \to \mathbb{R}$, and functions $g_k : \mathbb{R}^n \to \mathbb{R}$, $1 \leq k \leq m(< n)$, find

$$\boxed{\begin{gathered} x^\star \in \operatorname{argmin}_{x \in K} f(x), \\ K = \{x \in \mathbb{R}^n \,|\, g_k(x) = 0,\ 1 \leq k \leq m\}. \end{gathered}}$$

Construct the **Lagrangian** $L : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$, with **Lagrange mutipliers** $\lambda = (\lambda_1, \ldots, \lambda_m)$

$$\boxed{L(x, \lambda) = f(x) + \sum_{k=1}^{m} \lambda_k g_k(x).}$$

If $x^\star \in \mathbb{R}^n$ is a local minimizer, then there exists $\lambda^\star \in \mathbb{R}^m$ such that

$$\boxed{\nabla_x L(x^\star, \lambda^\star) = 0, \quad \nabla_\lambda L(x^\star, \lambda^\star) = 0.}$$

Equality constrained optimization: Penalty method

A simpler approach is to penalize deviations from the constraints and adding it to the objective function:

$$\boxed{x^\star_\epsilon \in \operatorname{argmin}_{x \in \mathbb{R}^n} \; f(x) + \frac{1}{\epsilon}\|g(x)\|^2.}$$

Here $\epsilon > 0$ is a small parameter. In the limit $\epsilon \to 0$ we get the true solution:

$$\boxed{\lim_{\epsilon \to 0} x^\star_\epsilon = x^\star \in \operatorname{argmin}_{x \in K} \; f(x).}$$

Easy to implement, but no simple rationale to choose ϵ !

Automatic differentiation

A key component of gradient based algorithms is **computing the derivatives** of the objective function – this **can be automated**!

Common approaches to computing derivatives:

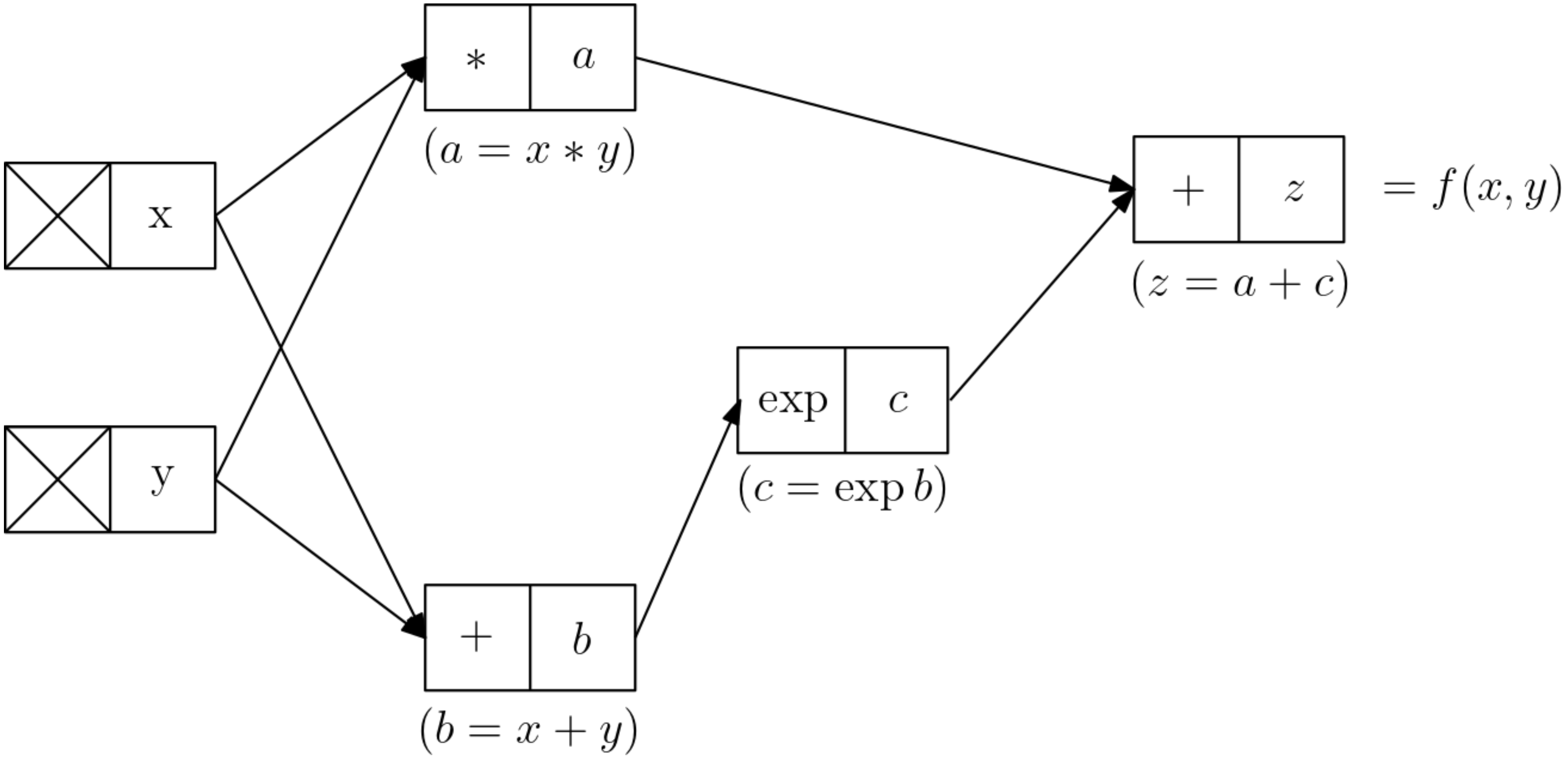
- Numerical differentiation – costly and propagates errors
- Symbolic differentiation – impractical
- **Automatic differentiation (AD)**

AD computes exact derivatives for given inputs. Two major variants:

- Forward mode AD
- Reverse mode AD

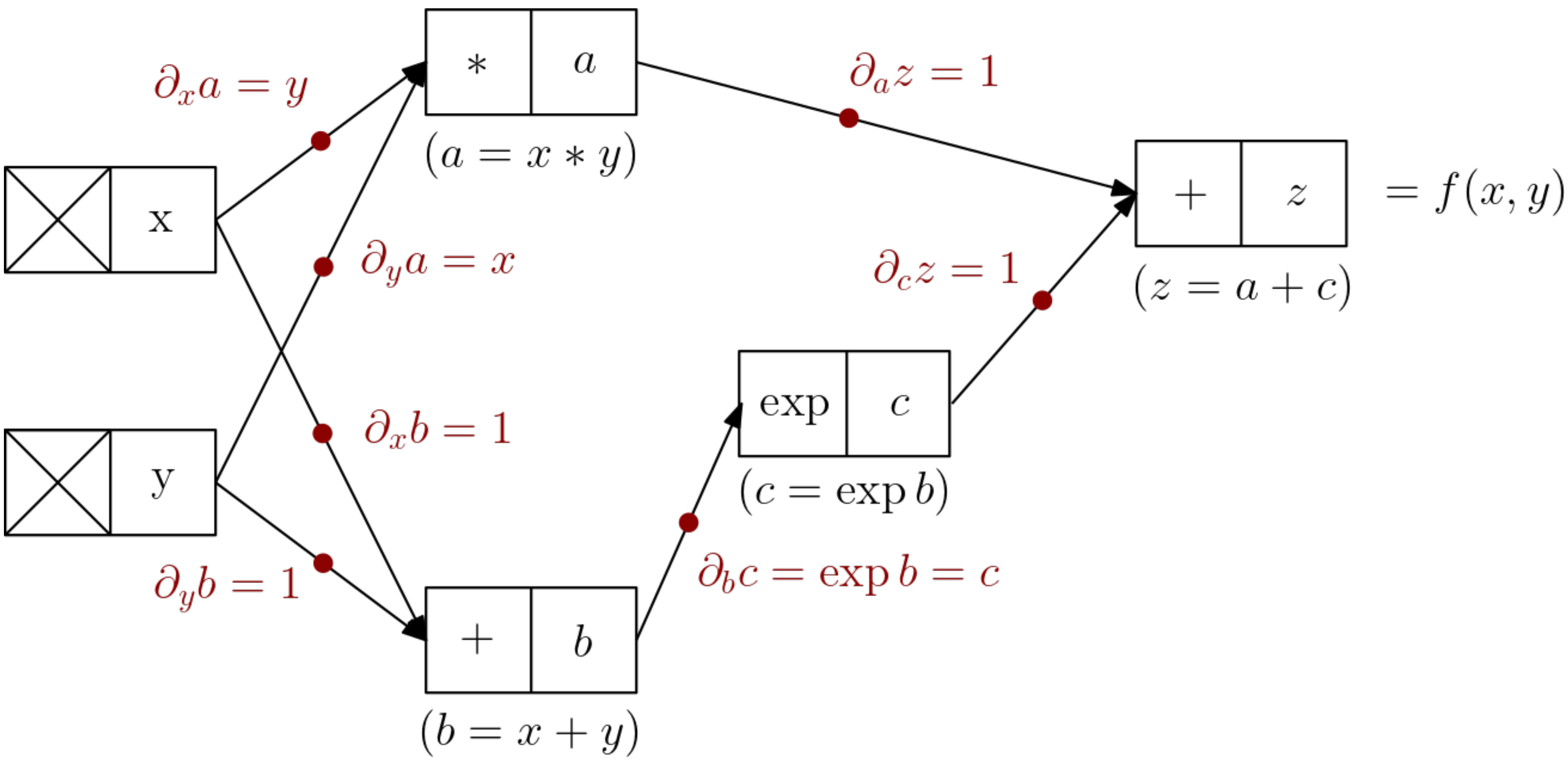
Functions as computational graphs

$$f(x, y) = xy + \exp(x + y)$$



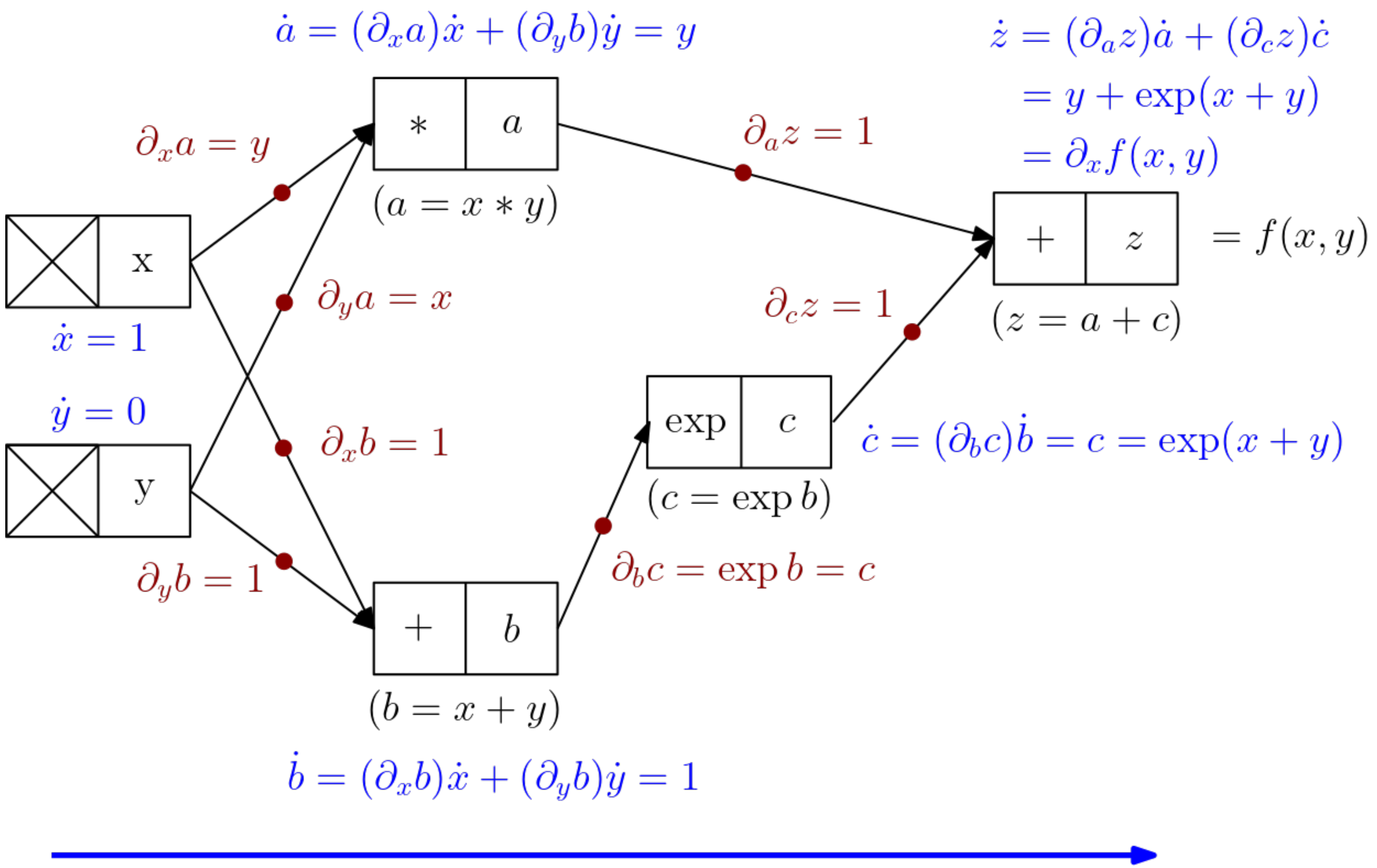
Track derivatives of elementary functions

$$f(x,y) = xy + \exp(x+y)$$



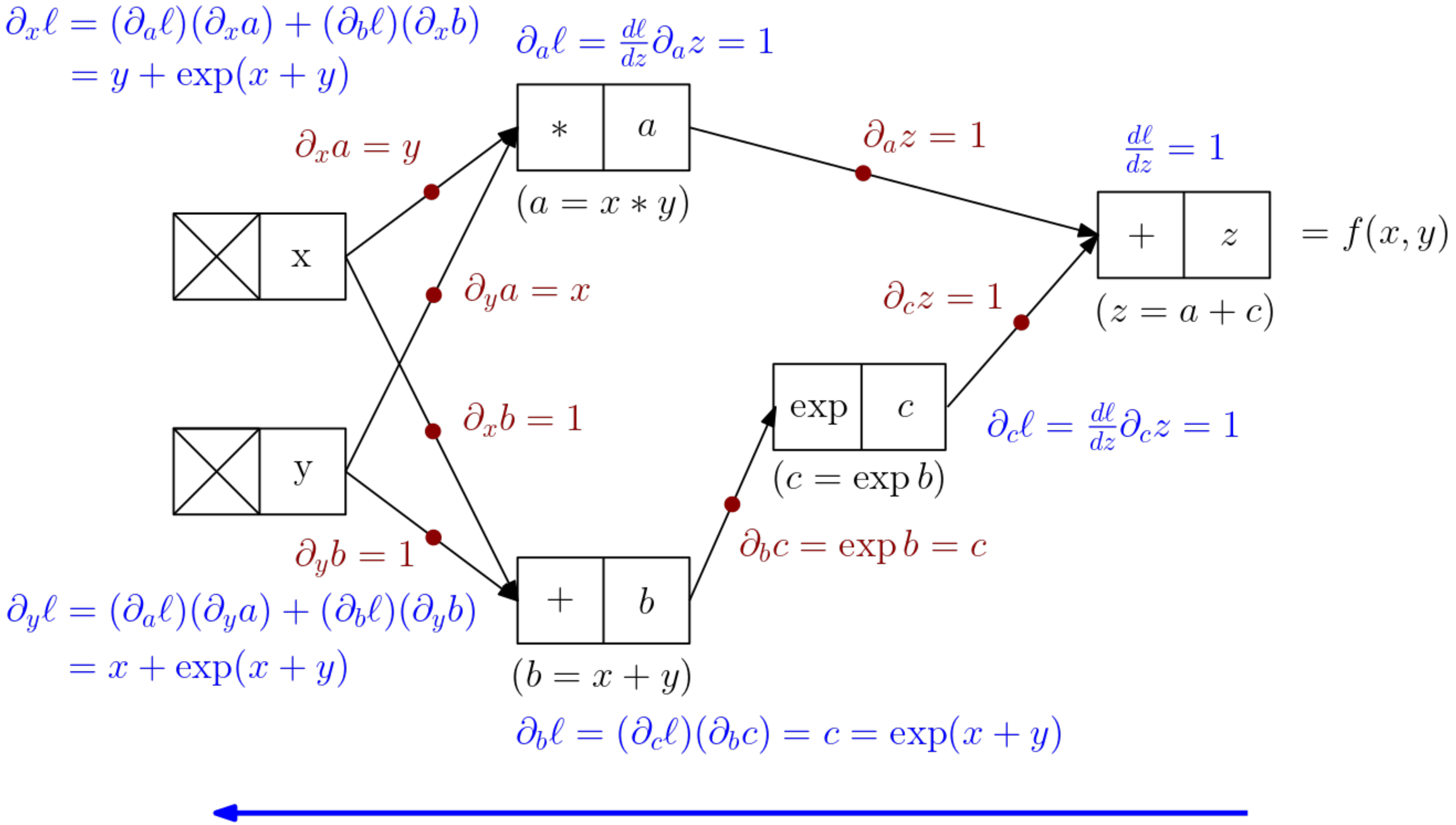
Forward mode AD

$$\partial_x f(x,y) = y + \exp(x+y)$$



Reverse mode AD

$$\partial_x f(x,y) = y + \exp(x+y) \quad \partial_y f(x,y) = x + \exp(x+y)$$



Practical aspects of AD

For computing derivatives of $f : \mathbb{R}^m \rightarrow \mathbb{R}^n$

- Forward mode AD is faster if $m \ll n$
- Reverse mode AD is faster if $m \gg n$

Common AD implementation approaches:

- Source-to-source transformation
- Operator overloading

There are lots of high quality AD packages available now!
Demos in this workshop will use **PyTorch**.

→ **Hands-on session!**

Supervised learning algorithms

Suppose that we are given data of the form

$$D = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\} \subset \mathbb{R}^d \times \mathbb{R}.$$

The goal of **supervised learning** is to find a **function** f in a specified function space $\mathcal{F}$ that **best explains this data**.

$$\boxed{\min_{f \in \mathcal{F}} \sum_{i=1}^{n} \ell(y_i, f(x_i)).}$$

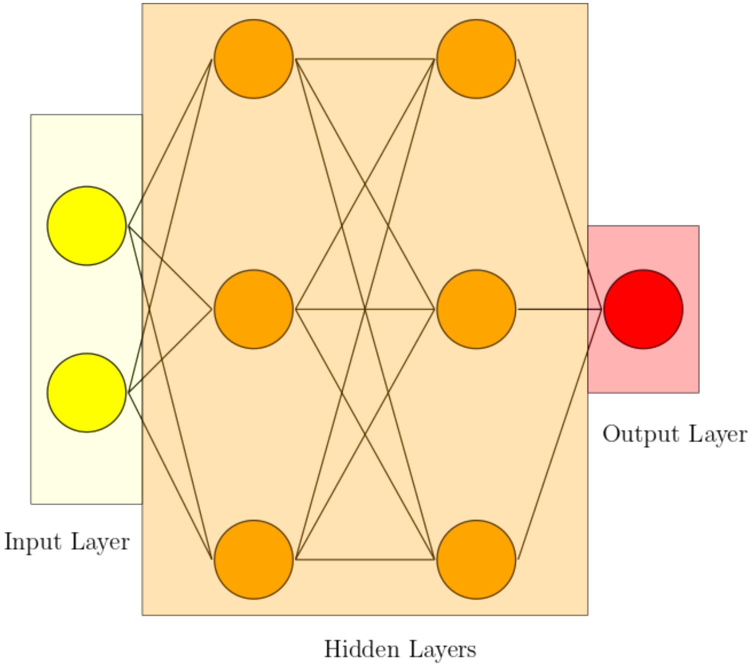
The **loss function** $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is typically chosen as an L^2 distance:

$$\ell(y, z) = \frac{1}{2}|y - z|^2.$$

Deep Neural Networks (DNNs)

A particularly interesting function space is that of **Deep Neural Networks**, which are loosely inspired by biological neural networks.

A DNN is a composition of a finite number of affine transformations and a nonlinear activation function.



Deep Neural Networks (DNNs)

Mathematically, an L layer DNN can be written as

$$\boxed{DNN(x;\theta) = T_L \circ \sigma \odot T_{L-1} \circ \ldots \circ \sigma \odot T_1(x).}$$

Where $\sigma : \mathbb{R} \to \mathbb{R}$ is the activation function, $\odot$ is element-wise function application, and $\{T_l : \mathbb{R}^{n_{l-1}} \to \mathbb{R}^{n_l}\}_{l=1}^{L}$ are the affine functions:

$$T_l(z) = W_l z + b_l, \quad W_l \in \mathbb{R}^{n_l \times n_{l-1}}, b_l \in \mathbb{R}^{n_l}, z \in \mathbb{R}^{n_{l-1}}.$$

$$\sigma\left(\begin{bmatrix} z_1 \\ \vdots \\ z_m \end{bmatrix}\right) = \begin{bmatrix} \sigma(z_1) \\ \vdots \\ \sigma(z_m) \end{bmatrix}.$$

The parameters θ of the DNN are

$$\boxed{\theta = \{(W_1, b_1), \ldots, (W_l, b_l)\}.}$$

Stochastic gradient descent

For loss functions that have an additive structure, the true GD update is

$$\theta \leftarrow \theta - \alpha \nabla_\theta \left(\sum_{i=1}^{n} \ell_i(\theta) \right).$$

When using DNNs, it is convenient to use the **stochastic GD / mini-batch GD** update:

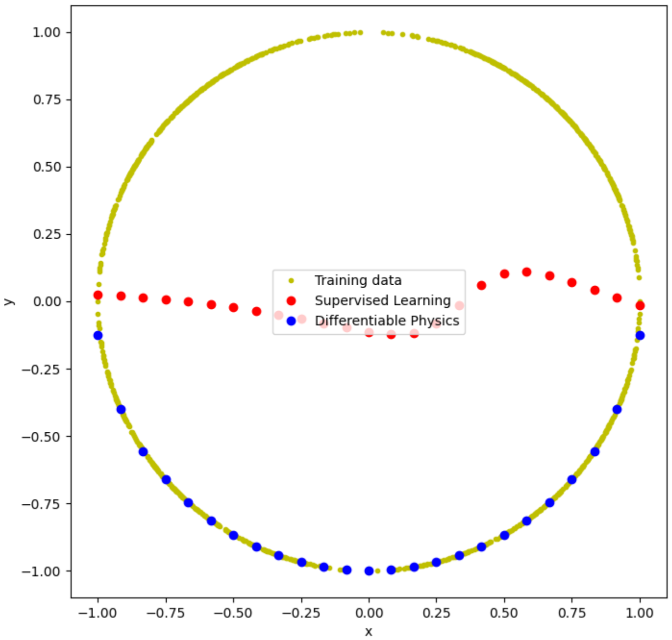
$$\boxed{\theta \leftarrow \theta - \alpha \nabla_\theta \ell_1(\theta), \ldots, \theta \leftarrow \theta - \alpha \nabla_\theta \ell_n(\theta).}$$

The collection of all these partial updates is called an **epoch**.

In practice, a subset of data points defined by a *batch size* are used. This is called **mini-batch SGD**.

Supervised vs physics based learning

Physics based learning is characterized by the choice of a **physically relevant loss function**.



Hands-on session!

Solving ODE with DNNs

Consider the first order ordinary differential equation:

$$\boxed{\frac{dx(t)}{dt} = f(x(t)), \quad x(0) = x_0.}$$

To solve this over $[0, T]$, we approximate the unknown solution as a DNN $\hat{x}(t;\theta)$ and use the following loss function defined as sampling points $\{t_i\}_{i=1}^{N} \subset [0, T]$:

$$\boxed{\ell(\theta) = \sum_{i=1}^{N} \left| \frac{d\hat{x}(t_i;\theta)}{dt} - f(\hat{x}(t_i;\theta)) \right|^2 + \alpha |\hat{x}(0;\theta) - x_0|^2.}$$

Note: The derivatives of the DNN can also be computed using AD!

Original idea: Lagaris et al., *Artificial Neural Networks for solving Ordinary and Partial Differential Equations*, IEEE Transactions on Neural networks, Vol 9 (5), **1998**.
Modern reincarnation: Raissi et al., *Physics-informed neural networs: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations*, Journal of Computational Physics, Vol 378 (1), **2019**.

Review: Forward Euler method for ODEs

The exact solution to the ODE can be written as a **flow map**:

$$\boxed{\Phi_t : x_0 \mapsto x(t).}$$

Here, $x(t)$ is the solution of the ODE at time t with initial condition x_0.

In practice, we can compute only an approximation to this flow map:

$$\boxed{\Phi_t^h : x_0 \mapsto x^h(t).}$$

To keep things simple, we will use the **forward Euler** method for computing the approximate solution to the ODE:

$$\boxed{x_{n+1} = x_n + \Delta t\, f(x_n).}$$

$\longrightarrow$ **Hands-on session!**

Inverse problem: differentiable physics

Consider the same ODE as before:

$$\frac{dx(t)}{dt} = f(x(t)), \quad x(0) = x_0.$$

Given $J : \mathbb{R} \to \mathbb{R}$, the following is an example of an inverse problem:

What should be the value of x_0 such that $J(x(T)) = J_0$?

Strategy: Learn shooting function with a DNN.

- Approximate the function $J_0 \mapsto x_0$ with a DNN.
- Use the discrepancy $\ell = |J(\Phi_T^h(x_0)) - J_0|^2$ as the loss to train the DNN.

Inverse problem: differentiable physics

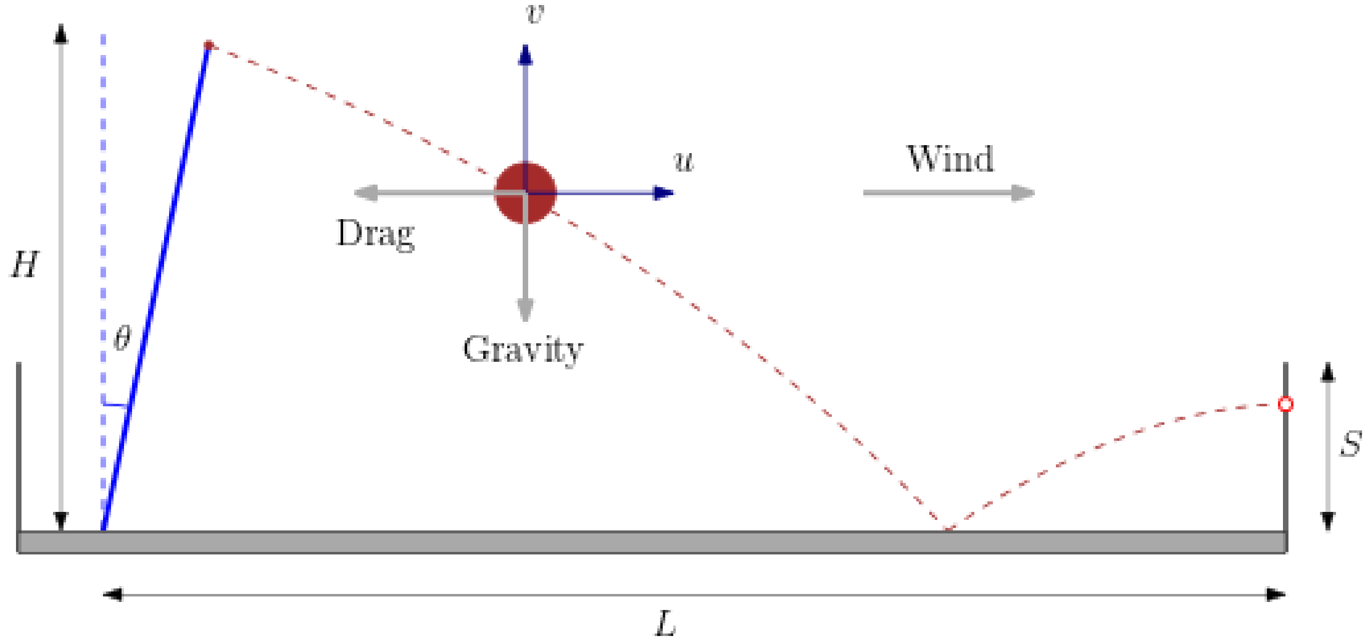
To train the DNN, we need to compute the derivative of the loss function:

$$\frac{d\ell}{d\theta} = (J(\Phi_T^h(x_0)) - J_0)J'(\Phi_T^h(x_0))\nabla_x\Phi_T^h(x_0)\nabla_\theta x_0.$$

- The first term is just an algebraic factor .
- **The second term is the derivative of the solver – differentiable physics!**
- The final term is the gradient of the DNN.

Differentiating solvers is not always easy, and often requires more work.
When developing new software, keep differentiability in mind!

Hands-on session: learning to bowl!



$$m\frac{du}{dt} = -\frac{1}{2}\rho A C_D (u-W)\sqrt{(u-W)^2+v^2}$$

$$m\frac{dv}{dt} = -\frac{1}{2}\rho A C_D v\sqrt{(u-W)^2+v^2} - mg$$

Simplified version of model presented in C.J. Baker, *A calculation of cricket ball trajectories*, Proc. IMechE. Vol 224 Part C: JMES, 2009.

There is more!

- Differentiable physics idea is not new – classic adjoint methods do the same! But **making solvers compatible with AD can provide very interesting new information**!
- The material discussed here can be extended to **PDE**s too. Check out: https://www.physicsbaseddeeplearning.org/intro.html
- **Deep Learning** is all the rage these days, but it is **not interpretable**! Check out our recent work – SPINN – for interpretable neural networks.

Thank you for your attention!
Happy Holidays and Happy New Year!

Amuthan Ramabathiran, Prabhu Ramachandran, **SPINN**: Sparse, Physics-based, and partially Interpretable Neural Networks for PDEs, Journal of Computational Physics, Vol 445 (15), 2021.
Video of my recent talk on SPINN: https://youtu.be/dfGojwG5nU8