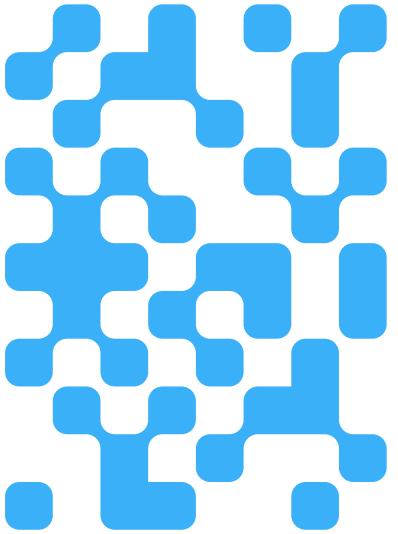


# **Machine Learning**

2024 (ML-2024) Lecture 15. Temporal and spatial signals processing

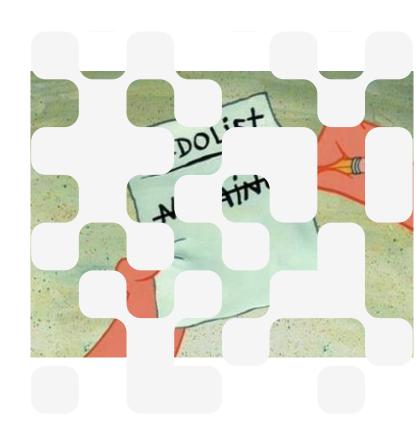
by Alexei Valerievich Kornaev, Dr. habil. in Eng. Sc., Researcher at the RC for AI, Assoc. Prof. of the Robotics and CV Master's Program, Innopolis University Researcher at the RC for AI, National RC for Oncology n.a. NN Blohin Professor at the Dept. of Mechatronics, Mechanics, and Robotics, Orel State University





# **Agenda**

- I. INTRODUCTION TO PHYSICS-INFORMED NEURAL NETWORKS (PINNs)
- II. MODELS WITH ORDINARY DIFFERENTIAL EQUATIONS (ODEs)
- III. MODELS WITH PARTIAL DIFFERENTIAL EQUATIONS (PDEs)
- IV. PROSPECTS IN THE FIELD OF PINNS



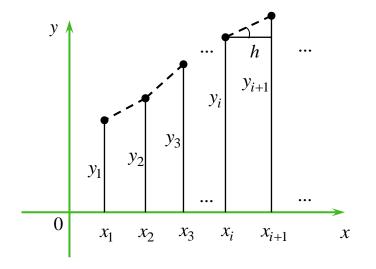


# Recap: what does it mean to solve a differential equation?



### Recap: what does it mean to solve a differential equation numerically?

### Метод Эйлера



$$\frac{y_{i+1} - y_i}{h} = f(x_i, y_i);$$
$$y_{i+1} = y_i + f(x_i, y_i)h;$$

- 1)  $y_1 = y_a$  (начальное условие);
- 2)  $y_2 = y_1 + f(x_1, y_1)h$ ;
- 3)  $y_3 = y_2 + f(x_2, y_2)h;$

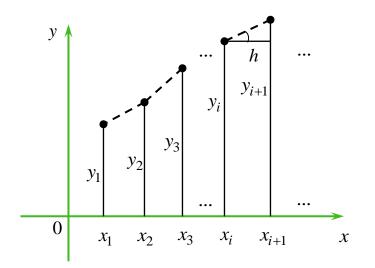
• • •

$$y_n = y_{n-1} + f(x_{n-1}, y_{n-1})h.$$



### Recap: what does it mean to solve a differential equation numerically?

### Методы Рунге-Кутта



$$\frac{dy}{dx} = f(x, y), \ y(0) = y_0, x \in [0; X]$$

Идея: замена искомого решения несколькими членами разложения в ряд Тейлора:

$$y_{i+1} = y(x_i) + \frac{y'(x_i)}{1!}h + \frac{y''(x_i)}{2!}h^2 + \frac{y'''(x_i)}{3!}h^3 + \dots$$

Для нахождения уі+1 необходимо вычислить 4 числа:

$$m_{1} = f(x_{i}, y_{i});$$

$$m_{2} = f\left(x_{i} + \frac{h}{2}, y_{i} + \frac{h}{2}m_{1}\right);$$

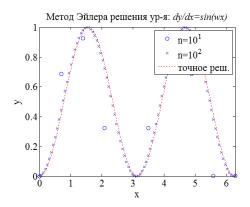
$$m_{3} = f\left(x_{i} + \frac{h}{2}, y_{i} + \frac{h}{2}m_{2}\right);$$

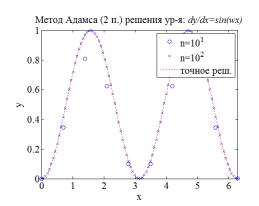
$$m_{4} = f\left(x_{i} + h, y_{i} + hm_{3}\right);$$

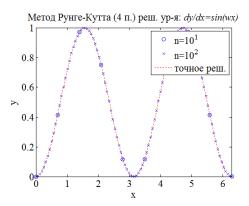
после воспользоваться формулой: 
$$y_{i+1} = y_i + \frac{h}{6}(m_1 + 2m_2 + 2m_3 + m_4).$$



### Recap: what does it mean to solve a differential equation numerically?

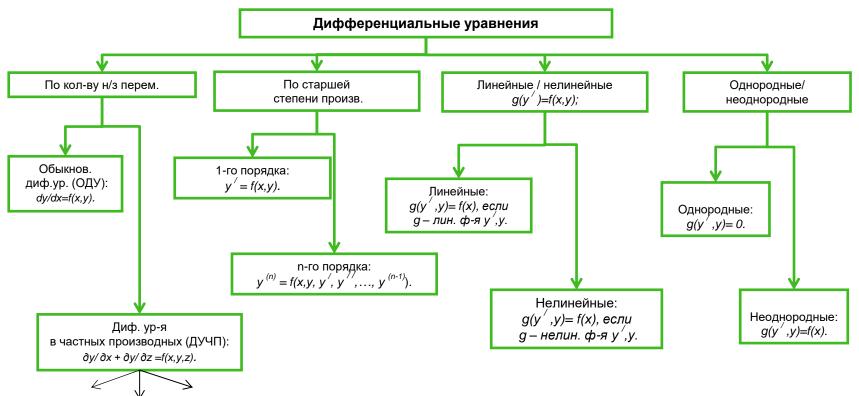








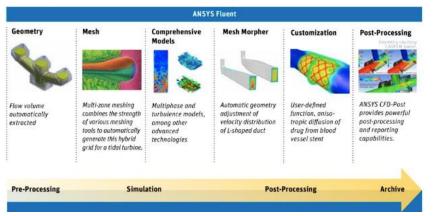
## Recap: classificatioin of differential equations



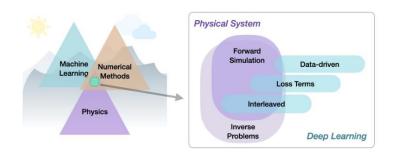


## **CAE-systems vs machine learning**

# Physics and CAE-systems



# Machine learning



+ Prospects:

almost any problem can be solved;

-Limitations:

the software is expensive;

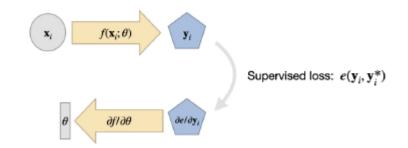
it is hard to use and verify the obtained results.

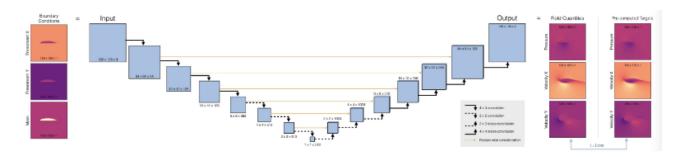


### Physics-informed machine learning: supervised training (diff. eqs. participation level: 0 %)

Given m pairs of data:  $((x_i, y_i^*))$ . In supervised learning we approximate  $y^*$  using function  $f = f(x_i, \theta)$  (i = 1, ..., m) by minimizing loss:

$$\operatorname{arg\,min}_{\theta} \sum_{i} (f(\boldsymbol{x}_{i}, \; \boldsymbol{\theta}) - y_{i}^{*})^{2}.$$







### Physics-informed machine learning: physical loss terms (DEs participation level: up to 100 %)

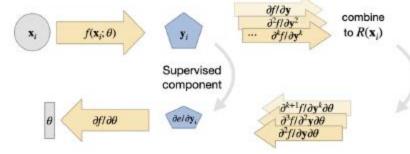
Given PDE:

$$\frac{\partial u}{\partial t} = F\left(\frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \dots, \frac{\partial^n u}{\partial x^n}\right),\,$$

with unknown function: u = u(x, t).

Residual R should be equal to zero:  $R = \frac{\partial u}{\partial t} - F\left(\frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \dots, \frac{\partial^n u}{\partial x^n}\right)$ .

$$\arg \min_{\theta} \alpha_0 \sum_{i} (f(x_i; \theta) - y_i)^2 + \alpha_1 R(x_i),$$



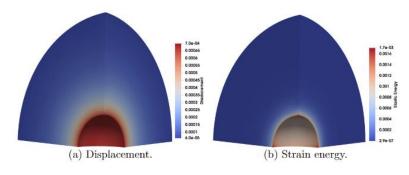


### Physics-informed machine learning: physical loss (a conservation law: 100 %)

#### 4.2. Deep Energy Method

The main idea of the method advocated in this contribution is to take advantage of the variational (energetic) structure of some BVPs. To that end, the energy of the system is used as the loss function for the DNN, as proposed by [14]. Due to its mechanical flavor, we name it the Deep Energy Method (DEM) here. One of the key ingredients is to approximate the energy of the body by a weighted sum of the energy density at integration points. Then, the following form for the loss function,  $\mathcal{L}(p)$  is obtained:

$$\mathcal{E}[u_p] pprox \mathcal{L}(p) = \sum_i \Psi(\epsilon(u_p(x_i)))w_i,$$
 (12)



```
net_uv(self,x,y,vdelta):
X = tf.concat([x,y],1)
uv = self.neural_net(X,self.weights,self.biases)
uNN = uv[:,0:1]
vNN = uv[:,1:2]
u = (1-x)*x*uNN
v = y*(y-1)*vNN
return u, v
```



### Good news: Al libraries (Pytorch, TF) can calculate derivatives very well

Optional Reading - Vector Calculus using autograd

Mathematically, if you have a vector valued function  $ec{y}=f(ec{x})$  , then the gradient of  $ec{y}$  with respect to  $ec{x}$  is a Jacobian matrix J:

$$J = \begin{pmatrix} \frac{\partial \mathbf{y}}{\partial x_1} & \dots & \frac{\partial \mathbf{y}}{\partial x_n} \end{pmatrix} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \dots & \frac{\partial y_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial x_1} & \dots & \frac{\partial y_m}{\partial x_n} \end{pmatrix}$$

Generally speaking, torch autograd is an engine for computing vector-Jacobian product. That is, given any vector  $\vec{v}$ , compute the product  $J^T \cdot \vec{v}$ 

If  $ec{v}$  happens to be the gradient of a scalar function  $l=g\left( ec{y}
ight)$  :

$$ec{v} = \left(egin{array}{ccc} rac{\partial l}{\partial y_1} & \cdots & rac{\partial l}{\partial y_m} \end{array}
ight)^T$$

then by the chain rule, the vector-Jacobian product would be the gradient of l with respect to  $\vec{x}$ :

$$J^T \cdot \vec{v} = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \cdots & \frac{\partial y_m}{\partial x_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_1}{\partial x_n} & \cdots & \frac{\partial y_m}{\partial x_n} \end{pmatrix} \begin{pmatrix} \frac{\partial l}{\partial y_1} \\ \vdots \\ \frac{\partial l}{\partial y_m} \end{pmatrix} = \begin{pmatrix} \frac{\partial l}{\partial x_1} \\ \vdots \\ \frac{\partial l}{\partial x_n} \end{pmatrix}$$

This characteristic of vector-Jacobian product is what we use in the above example; external\_grad represents  $\vec{v}$ .

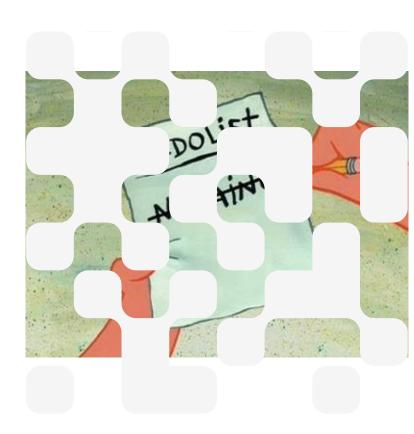
```
python
                                                                                             Copy
import torch
x = torch.tensor([1.0, 2.0, 3.0, 4.0], requires_grad=True)
w = torch.tensor(2.0, requires_grad=True)
b = torch.tensor(1.0, requires_grad=True)
y = w * x + b
target = torch.tensor([3.0, 5.0, 7.0, 9.0])
loss = torch.mean((v - target) ** 2)
loss.backward()
print("Gradient of w:", w.grad)
print("Gradient of b:", b.grad)
```

```
Copy
Gradient of w: tensor(2.5)
Gradient of b: tensor(1.)
```



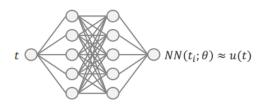
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### **ANNs for ODEs solution intuition**



$$L(\theta) = \frac{1}{N} \sum_{i}^{N} (NN(t_i; \theta) - \underline{u_i})^2$$

We are interested in modelling the displacement of the mass on a spring (green box) over time.

This is a canonical physics problem, where the displacement, u(t), of the oscillator as a function of time can be described by the following differential equation:

$$mrac{d^2u}{dt^2}+\murac{du}{dt}+ku=0 \ ,$$

where m is the mass of the oscillator,  $\mu$  is the coefficient of friction and k is the spring constant.





### PINNs for ODEs solution intuition



$$L(\theta) = \frac{1}{N} \sum_{i}^{N} (NN(t_i; \theta) - \underline{u_i})^2 + \frac{\lambda}{M} \sum_{j}^{M} \left( \left[ m \frac{d^2}{dt^2} + \mu \frac{d}{dt} + k \right] NN(\underline{t_j}; \theta) \right)^2$$



#### From a ML perspective:

 Physics loss is an unsupervised regulariser, which adds prior knowledge

From a mathematical perspective:

- · PINNs provide a way to solve PDEs:
  - Neural network is a mesh-free, functional approximation of PDE solution
  - Physics loss is used to assert solution is consistent with PDE
  - Supervised loss is used to assert boundary/initial conditions, to ensure solution is unique

ML-2024 by Alexei Kornaev



## PINNs training algorithm

#### Training loop:

- 1. Sample boundary/ physics training points
- 2. Compute network outputs
- Compute 1<sup>st</sup> and 2<sup>nd</sup> order gradient of network output with respect to network input <= (recursively) apply autodiff, extending graph
- 4. Compute loss
- Compute gradient of loss function with respect to network parameters <= apply autodiff on extended graph
- 6. Take gradient descent step



## Hadns on session: please join via the <u>link</u>

We are interested in modelling the displacement of the mass on a spring (green box) over time.

This is a canonical physics problem, where the displacement, u(t), of the oscillator as a function of time can be described by the following differential equation:

$$mrac{d^2u}{dt^2}+\murac{du}{dt}+ku=0$$
 ,

where m is the mass of the oscillator,  $\mu$  is the coefficient of friction and k is the spring constant.

We will focus on solving the problem in the **under-damped state**, i.e. where the oscillation is slowly damped by friction (as displayed in the animation above).

Mathematically, this occurs when:

$$\delta < \omega_0 \; , \quad ext{ where } \; \delta = rac{\mu}{2m} \; , \; \omega_0 = \sqrt{rac{k}{m}} \; .$$

Furthermore, we consider the following initial conditions of the system:

$$u(t=0)=1 \;\; , \;\; rac{du}{dt}(t=0)=0 \; .$$

For this particular case, the exact solution is known and given by:

$$u(t) = e^{-\delta t} (2A\cos(\phi + \omega t)) \; , \quad ext{ with } \; \omega = \sqrt{\omega_0^2 - \delta^2} \; .$$

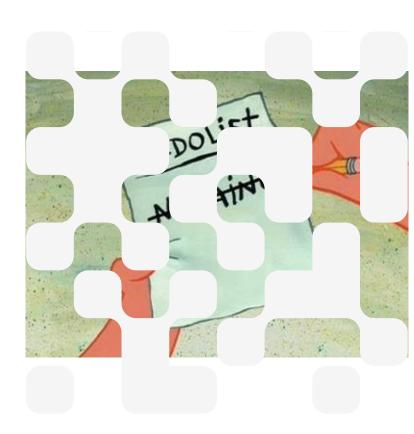
For a more detailed mathematical description of the harmonic oscillator, check out this blog post: <a href="https://beltoforion.de/en/harmonic\_oscillator/">https://beltoforion.de/en/harmonic\_oscillator/</a>.





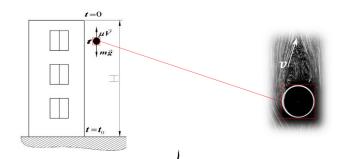
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# Recap: Kinematics -> Dynamics -> Statics



Mechanics studies *motion* of a material point



Mechanics of continua studies *motion* of the media

$$m\frac{d\boldsymbol{v}}{dt} = -b\boldsymbol{v} + m\boldsymbol{g},$$

$$\rho \frac{d\boldsymbol{v}}{dt} = \nabla \cdot \boldsymbol{T}_{\sigma} + \rho \boldsymbol{f},$$

declares the mass conservation law

$$\frac{dm}{dt} = 0.$$

declares the mass conservation law in the form of the *continuity equation* 

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.$$

#### Nomenclature:

$$\nabla = \left[\frac{\partial}{\partial x_i}\right]$$
 is the Hamiltonian;

$$\nabla \cdot \mathbf{y} = \begin{bmatrix} \frac{\partial y_i}{\partial x_i} \\ , \nabla \cdot \mathbf{T}_y = \begin{bmatrix} \frac{\partial y_{ik}}{\partial x_i} \end{bmatrix} \text{ is the divergence;}$$

 $\rho$  is the density;

 $v = [v_i]$  is the velocity;

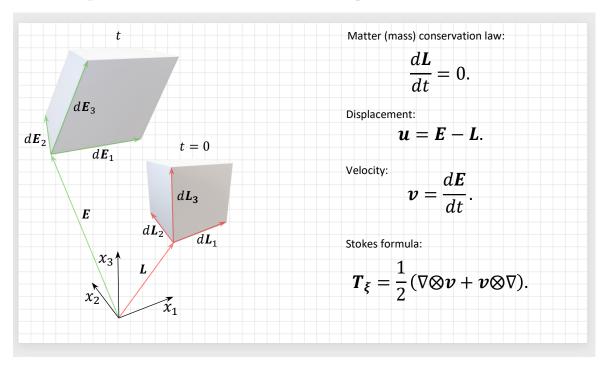
t is time;

 $T_{\sigma} = [\sigma_{ik}]$  is the stress tensor;

**f** is the mass force (e.g. gravity).



# **Recap: Kinematics → Dynamics ← Statics**



#### Nomenclature:

L, E are Lagrangian and Eulerian coord.;

 $T_{\xi} = [\xi_{ik}]$  is the strain rate tensor;

 $T_a = D_a + S_a$  is the decomposition of the tensor into it's deviator and spherical part  $S_a = a_0 T_{\delta}$ ,  $a_0 = a_{ii}/3$ ;

$$\nabla y = \left[\frac{\partial y}{\partial x_i}\right]$$
 is the gradient of a scalar func.

$$\nabla \otimes \mathbf{y} = \begin{bmatrix} \frac{\partial y_k}{\partial x_i} \end{bmatrix}$$
 is the gradient of a vector func.



**Recap: Kinematics → Dynamics ← Statics** 

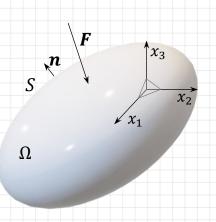
The domain  $\Omega$  with surface S which is characterized by a unit outer normal vector n is under study.

Full stress:

$$\sigma^n = \frac{d\mathbf{F}}{dS}$$
.

Cauchy formula:

$$\sigma^n = \boldsymbol{n} \cdot \boldsymbol{T}_{\sigma}$$



#### Nomenclature:

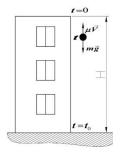
**P** is the total outer force;

 $T_{\sigma} = [\sigma_{ik}]$  is the stress tensor;

 $T_a=D_a+S_a$  is the decomposition of the tensor into it's deviator and spherical part  $S_a=a_0T_\delta$ ,  $a_0=a_{ii}/3$ .



# **Recap: Kinematics → Dynamics ← Statics**



Mechanics studies *motion* of a material point

declares the mass conservation law

$$m = const.$$



Mechanics of continua studies *motion* of the media

$$\rho \frac{d\boldsymbol{v}}{dt} = \nabla \cdot \boldsymbol{T}_{\sigma} + \rho \boldsymbol{f},$$

declares the mass conservation law in the form of the *continuity equation* 

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0.$$

Taking the Newton hypothesis into account  $oldsymbol{D}_{\sigma}=2\muoldsymbol{D}_{oldsymbol{\xi}}$  ,

and the tensor decomposition rule, supposing that the fluid is incompressible  $\rho = \text{const}$ , the motion law transforms into the almost kinematic form – the Navier-Stokes equation

$$\rho \frac{d\boldsymbol{v}}{dt} = \nabla \sigma_0 + \nabla \cdot \left( \mu (\nabla \otimes \boldsymbol{v} + \boldsymbol{v} \otimes \nabla) \right) + \rho \boldsymbol{f},$$

$$\forall \boldsymbol{v} = 0.$$



### PINNs for PDEs solution intuition

Given a PDE and its boundary/initial conditions

$$\mathcal{D}[u(x)] = f(x), \qquad x \in \Omega \subset \mathbb{R}^d$$
  
$$\mathcal{B}_k[u(x)] = g_k(x), \qquad x \in \Gamma_k \subset \partial\Omega$$

Where  $\mathcal{D}$  is some differential operator,  $\mathcal{B}_k$  are a set of boundary operators, and u(x) is the solution to the PDE

PINNs train a neural network to **approximate** the solution to the PDE  $NN(x;\theta) \approx u(x)$  using the following loss function:

$$L(\theta) = L_b(\theta) + L_p(\theta)$$

$$L_b(\theta) = \sum_k \frac{\lambda_k}{N_{bk}} \sum_j^{N_{bk}} \left\| \mathcal{B}_k \left[ NN(x_{kj}; \theta) \right] - g_k(x_{kj}) \right\|^2 \text{ Boundary loss}$$

$$L_p(\theta) = \frac{1}{N_p} \sum_{i}^{N_p} \|\mathcal{D}[NN(x_i; \theta)] - f(x_i)\|^2$$
 Physics loss



### PINNs for PDEs solution intuition

Given a PDE and its boundary/initial conditions

For example, the 1+1D viscous Burgers' equation:

$$\mathcal{D}[u(x)] = f(x), \qquad x \in \Omega \subset \mathbb{R}^d$$
  
$$\mathcal{B}_k[u(x)] = g_k(x), \qquad x \in \Gamma_k \subset \partial\Omega$$

$$[u(x)] = f(x), \qquad x \in \Omega \subset \mathbb{R}^d$$

$$[u(x)] = g_k(x), \qquad x \in \Gamma_k \subset \partial\Omega$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - v \frac{\partial^2 u}{\partial x^2} = 0$$

Where  $\mathcal{D}$  is some differential operator,  $\mathcal{B}_k$  are a set of boundary operators, and u(x) is the solution to the PDE

$$u(x,0) = -\sin(\pi x)$$
  
 
$$u(-1,t) = u(+1,t) = 0$$

PINNs train a neural network to approximate the solution to the PDE  $NN(x; \theta) \approx u(x)$  using the following loss function:

$$NN(x,t;\theta) \approx u(x,t)$$

$$L_b(\theta) = L_b(\theta) + L_p(\theta)$$

$$L_b(\theta) = \frac{\lambda_1}{N_{b1}} \sum_{j}^{N_{b1}} \left( NN(x_j, 0; \theta) + \sin(\pi x_j) \right)^2$$

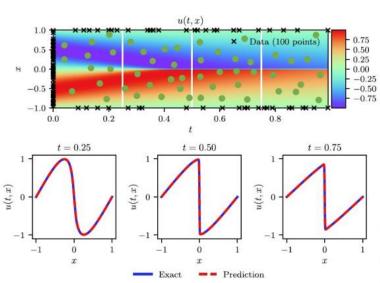
$$L_b(\theta) = \sum_{k} \frac{\lambda_k}{N_{bk}} \sum_{j}^{N_{bk}} \left\| \mathcal{B}_k \left[ NN(x_k; \theta) \right] - g_k(x_{kj}) \right\|^2 \text{ Boundary loss } + \frac{\lambda_2}{N_{b2}} \sum_{k}^{N_{b2}} (NN(-1, t_k; \theta) - 0)^2$$

$$L_p(\theta) = \frac{1}{N_p} \sum_{i}^{N_p} \left\| \mathcal{D}[NN(x_i; \theta)] - f(x_i) \right\|^2 \text{ Physics loss } + \frac{\lambda_3}{N_{b3}} \sum_{l}^{N_{b3}} (NN(+1, t_l; \theta) - 0)^2$$

$$L_p(\theta) = \frac{1}{N_p} \sum_{i}^{N_p} \left( \left( \frac{\partial NN}{\partial t} + NN \frac{\partial NN}{\partial x} - v \frac{\partial^2 NN}{\partial x^2} \right) (x_i, t_i; \theta) \right)^2$$



### PINNs for PDEs solution intuition



Raissi et al, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, JCP (2018)

$$\begin{split} L_b(\theta) &= \frac{\lambda_1}{N_{b1}} \sum_{j}^{N_{b1}} \left( NN\left(\underline{x_j}, 0; \theta\right) + \underline{\sin(\pi x_j)} \right)^2 \\ &+ \frac{\lambda_2}{N_{b2}} \sum_{k}^{N_{b2}} \left( NN(-1, \underline{t_k}; \theta) - \underline{0} \right)^2 \\ &+ \frac{\lambda_3}{N_{b3}} \sum_{l}^{N_{b3}} \left( NN(+1, \underline{t_l}; \theta) - \underline{0} \right)^2 \\ L_p(\theta) &= \frac{1}{N_p} \sum_{l}^{N_p} \left( \left( \frac{\partial NN}{\partial t} + NN \frac{\partial NN}{\partial x} - \nu \frac{\partial^2 NN}{\partial x^2} \right) (\underline{x_i, t_l}; \theta) \right)^2 \end{split}$$

$$\nu = 0.01/\pi$$

 $N_n = 10,000$  (Latin hypercube sampling)

$$N_{h1} + N_{h2} + N_{h3} = 100$$

Fully connected network with 9 layers, 20 hidden units (3021 free parameters)

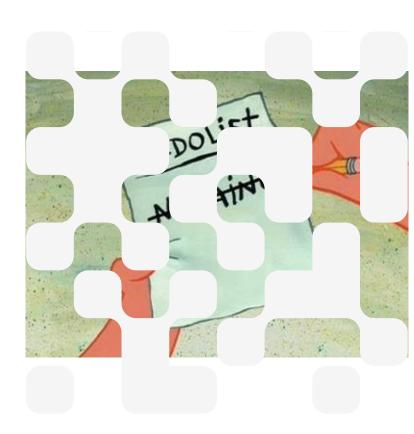
Tanh activation function

L-BFGS optimiser



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## PINNs for equation discovery in a hadns on session: link

How do we learn an **entire** differential operator  $\mathcal{D}$ ?

Build a **library** of *n* operators, such as:

$$\phi = (1, \partial_x, \partial_t, \partial_{xx}, \partial_{tt}, \partial_{xt})^T$$

Then assume the differential operator can be represented as

$$\mathcal{D} = \Lambda \phi$$

Where  $\Lambda$  is a (sparse) matrix of shape  $(d_u, n)$ 

E.g. for 1D damped harmonic oscillator:

$$\mathcal{D} = (k \quad \mu \quad m \quad 0) \begin{pmatrix} 1 \\ d_t \\ d_{tt} \\ d_{ttt} \end{pmatrix}$$
$$= m \frac{d^2}{dt^2} + \mu \frac{d}{dt} + k$$



## PINNs for equation discovery in a hadns on session: link

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$$= m \frac{d^2}{dt^2} + \mu \frac{d}{dt} + k$$

PINNs for equation discovery:

$$L_p(\theta, \mathbf{\Lambda}) = \frac{1}{N_p} \sum_{l}^{N_p} ||\mathbf{\Lambda} \boldsymbol{\phi}[NN(x_l; \theta)]||^2 + ||\mathbf{\Lambda}||^2 \quad \text{Physics loss}$$

$$L_d(\theta) = \frac{\lambda}{N_d} \sum_{l}^{N_d} ||NN(x_l; \theta) - u_l||^2 \quad \text{Data loss}$$

Where 
$$\Lambda$$
 are treated as **learnable** parameters and  $\{x_l,u_l\}$ 

 $L(\theta, \Lambda) = L_n(\theta, \Lambda) + L_d(\theta)$ 

Typically, some regularization / prior on  $\Lambda$  (e.g. sparsity) is needed, as this optimisation problem can be very **ill-posed** 

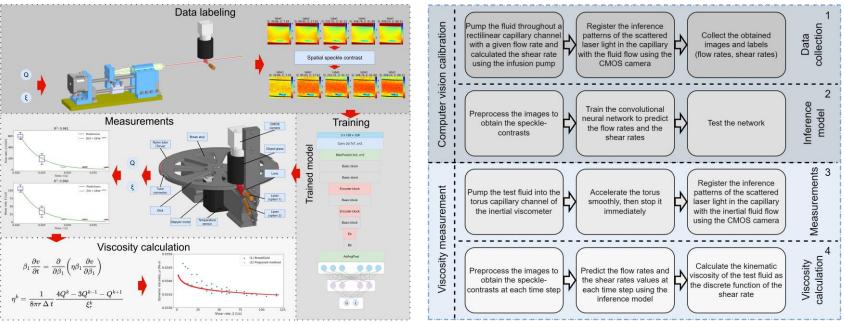
are a set of (potentially noisy) observational data



## PINNs for equation discovery: viscosity measurement

Viscosity measurement method using inertial viscometer with a computer vision system

 $\xi^k$ ,  $Q^k$  are the share rate on the fluid flow and the flow rate at each time  $t^k$ , respectively are obtained by test rig with CV system





## PINNs with energy (power) loss

# Save energy (power)



$$I[?...] = \int f(?,...) \rightarrow min.$$

## Save time

(brachistochrone task)



$$T = I[y(x)] = \int_{a}^{b} f\left(x, y(x), \frac{dy(x)}{dx}\right) \to min.$$

# Save lives (Dido task)

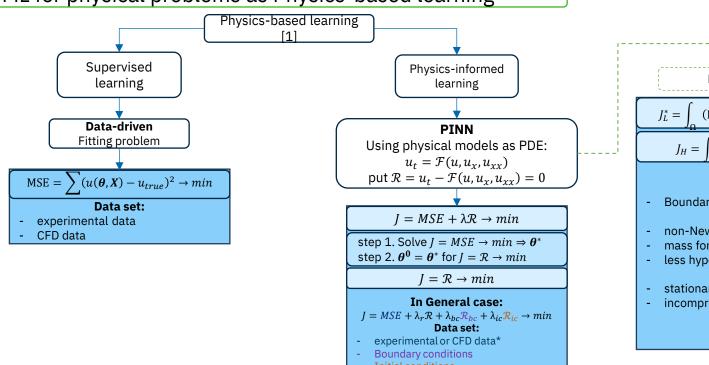


$$S = I[y(x)] \rightarrow max, L = const.$$



## PINNs with energy (power) loss

### ML for physical problems as Physics-based learning



#### **Power loss**

$$J_{L}^{*} = \int_{\Omega} (\Pi_{v} + \rho F(\nabla \times \Psi)) \to min$$

$$J_{H} = \int \mu D_{\mathcal{E}} \cdot D_{\mathcal{E}} d\Omega \to min$$

#### Data set:

Boundary conditions;

#### **Advantages:**

- non-Newtonian fluid:
- mass forces:
- less hyperparameters.

#### **Limitations:**

- stationary or quasi-stationary;
- incompressible



## PINNs with energy (power) loss Step 1: prove that the loss is true

#### Variational problem

$$J[v_1(x_i),v_2(x_i)]=\int_{\varOmega}f\big(x_i,v_1,v_2,r_i^k,q_{ij}^k\big)d\Omega\rightarrow\min(\max)\,,$$
 where  $r_i^k=v_{k_{x_i}}^{'},q_{ij}^k=v_{k_{x_ix_j}}^{''}$ 

The generalized Euler's equations have the following form:

$$f'_{v_k} - \frac{\partial}{\partial x_i} (r_i^k) + \frac{\partial^2}{\partial x_i \partial x_i} (q_{ij}^k) = 0, \qquad i = 1,2; \ k = 1,2^*$$

Boundary conditions for these second order equations:

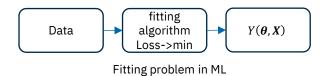
$$v_k(x_i^0) = v_i^0$$
  $v'_k(x_i^0) = u_i^0$   
 $v_k(x_i^1) = v_i^1$   $v'_k(x_i^1) = u_i^1$ ,  $i = 1,2; k = 1,2$ 

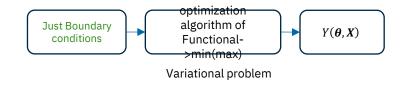
y<sub>1</sub>

1d interpretation

Non-trivial problem: to propose variational problem is equivalent to the partial differential equations (PDEs)

**Task in another way**: To find such functions  $v_1(x_i)$ ,  $v_2(x_i)$  that provide an extremum to the functionality  $J[v_1(x_i), v_2(x_i)]$  looks like a **ML task**:



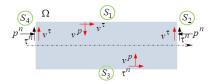


<sup>\*</sup> The Einstein summation notation is used hereinafter



## PINNs with energy (power) loss Step 2: minimize the loss

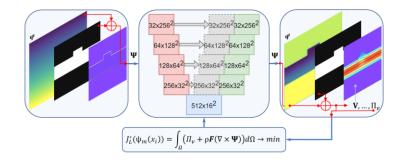
#### Newtonian 2d fluid flow. Convolutional network and image-based flow domain



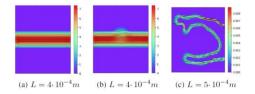
$$\begin{aligned} V &= [ [ v_1 & v_2 & 0 ] ], \Psi = \psi(x_1, x_2), \\ v_1 &= \frac{\partial \psi}{\partial x_2}, v_2 &= -\frac{\partial \psi}{\partial x_1}, \left( \nabla \cdot \pmb{V} = 0 \right) \end{aligned}$$

The unknown  $\Psi$  function can be represented as a three-dimensional image:

- the position of a pixel in the image corresponds to coordinates;
- the pixel intensity corresponds to the value of the  $\psi$  function in the point.



	Maximum velocity, m/s		
Method	parallel plates	parallel plates with notch	nailfold capillary
Analytical solution	7.5	-	-
Ansys Fluent	7.42	7.83	-
UNet with loss (22)	7.35	7.52	$8.8 \cdot 10^{-3}$





## Check the most cited papers on PINNs?

Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations https://www.sciencedirect.com/science/article/abs/pii/S0021999118307125

https://arxiv.org/pdf/1708.07469

https://arxiv.org/pdf/1710.00211

https://arxiv.org/pdf/1910.03193

https://arxiv.org/pdf/2006.10739



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ML-2024 by Alexei Kornaev



# Why PINNs?



# Thank you for your attention!

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Lecture 6. Loss Functions. Uncertainty Estimation Notes



Lecture 6. Loss Functions. Uncertainty Estimation Notes





## PINNs with energy (power) loss

# Save mechanical power

$$O = L_{1} \times 2L_{2} \times L_{3}$$

$$I[v_{1}(x_{2})] = \int_{-L_{2}}^{L_{2}} f\left(x_{2}, v_{1}(x_{2}), \frac{dv_{1}(x_{2})}{dx_{2}}\right) \rightarrow min, \quad flow \ rate = const.$$

$$v_{1}(x_{2}) = \theta_{0} + \theta_{1}x_{2} + \theta_{2}x_{2}^{2},$$

$$v_{1}(x_{2}) = \theta_{0} + \theta_{1}x_{2} + \theta_{2}x_{2}^{2} + \theta_{3}x_{2}^{3} + \theta_{4}x_{2}^{4},$$
...
$$I[v_{1}(x_{2})] = I[\theta_{i}] \rightarrow min.$$

$$v_{1}(x_{2}) = \theta_{0} + \theta_{1}x_{2} + \theta_{2}x_{2}^{2} + \cdots + \theta_{n}x_{2}^{n}.$$