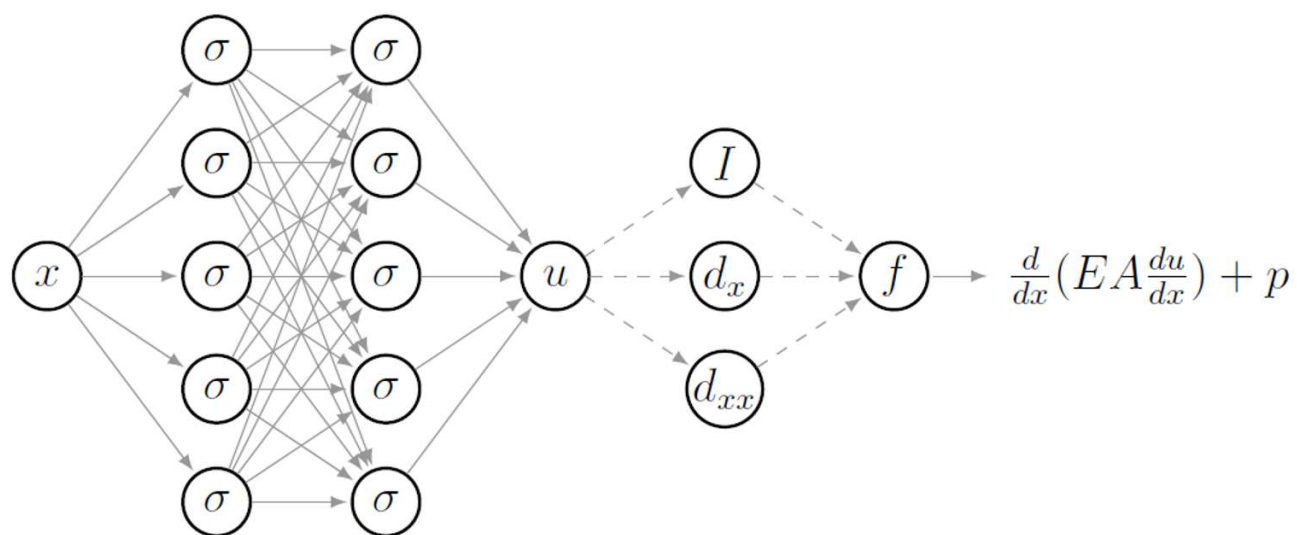


## **Planning of course:**

- Dimensional reduction: singular value decomposition, principal component analysis, model reduction
- Regression, optimization, model selection
- Neural networks
- Physics informed neural networks, model discovery
- Projects



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**Algorithm 4** Training a physics-informed neural network for the static solution of the problem described in Eq. (5.4).

---

**Require:** training data for boundary condition  $\{x_b^i, u_b^i\}_{i=1}^{N_b}$

generate  $N_f$  collocation points with a uniform distribution  $\{x_f^i\}_{i=1}^{N_f}$

define network architecture (input, output, hidden layers, hidden neurons)

initialize network parameters  $\Theta$ : weights  $\{W^l\}_{l=1}^L$  and biases  $\{b^l\}_{l=1}^L$  for all layers  $L$

set hyperparameters for L-BFGS optimizer (*epochs*, learning rate  $\alpha$ , ...)

**for all** *epochs* **do**

$\hat{u}_b \leftarrow u_{NN}(x_b; \Theta)$

$f \leftarrow f_{NN}(x_f; \Theta)$

    compute  $MSE_b, MSE_f$

$\triangleright$  cf. Eqs. (5.12) and (5.13)

    compute cost function:  $C \leftarrow MSE_b + MSE_f$

    update parameters:  $\Theta \leftarrow \Theta - \alpha \frac{\partial C}{\partial \Theta}$

$\triangleright$  L-BFGS

**end for**

---

Continuous time problems , 1D transient heat

$$c \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) - s = 0 \quad \text{on } \mathcal{T} \times \Omega, \quad (5.14)$$

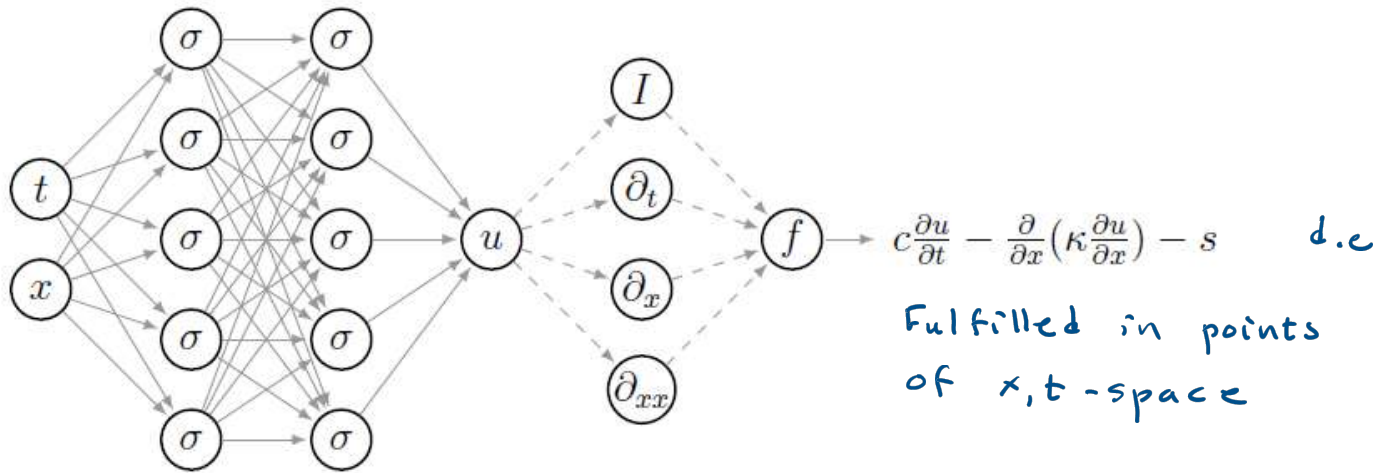
$$\kappa \frac{\partial u}{\partial x} = h \quad \text{on } \mathcal{T} \times \Gamma_N, \quad (5.15)$$

$$u = g \quad \text{on } \mathcal{T} \times \Gamma_D, \quad (5.16)$$

$$u(x, 0) = u_0 \quad \text{on } \Omega. \quad (5.17)$$

$$c(u) = 1/2000 u^2 + 500,$$

$$\kappa(u) = 1/100 u + 7.$$



$$s = \frac{\kappa u}{\sigma^2} + u \frac{x - p}{\sigma^2} \left[ c \frac{\partial p}{\partial t} - \frac{x - p}{\sigma^2} \left( \kappa + u \frac{\partial \kappa}{\partial u} \right) \right]$$

---

**Algorithm 5** Training a physics-informed neural network for the continuous solution of the problem described in Eq. (5.14).

---

**Require:** training data for initial condition  $\{0, x_0^i, u_0^i\}_{i=1}^{N_0}$

**Require:** training data for boundary condition  $\{t_b, x_b^i, u_b^i\}_{i=1}^{N_b}$

generate  $N_f$  collocation points with Latin-hypercube sampling  $\{t_f, x_f^i\}_{i=1}^{N_f}$

define network architecture (input, output, hidden layers, hidden neurons)

initialize network parameters  $\Theta$ : weights  $\{W^l\}_{l=1}^L$  and biases  $\{b^l\}_{l=1}^L$  for all layers  $L$

set hyperparameters for Adam optimizer (Adam-epochs, learning rate  $\alpha, \dots$ )

set hyperparameters for L-BFGS optimizer (L-BFGS-epochs, convergence criterion,  $\dots$ )

**procedure** TRAIN

  compute  $\{u_{NN}(0, x_0^i, \Theta)\}_{i=1}^{N_0}$

  compute  $\{\frac{\partial}{\partial x} u_{NN}(t_b^i, x_b^i; \Theta)\}_{i=1}^{N_b}$

  compute  $\{f_{NN}(t_f^i, x_f^i; \Theta)\}_{i=1}^{N_f}$

  compute  $MSE_0, MSE_b, MSE_f$

  evaluate cost function:  $C \leftarrow MSE_0 + MSE_b + MSE_f$

  update parameters:  $\Theta \leftarrow \Theta - \alpha \frac{\partial C}{\partial \Theta}$

**end procedure**

**for all** Adam-epochs **do**

  run TRAIN with Adam optimizer

**end for**

**for all** L-BFGS-epochs **do**

  run TRAIN with L-BFGS optimizer

**end for**

$$MSE_0 = \frac{1}{N_0} \sum_{i=1}^{N_0} (u_{NN}(0, x_0^i; \Theta) - u_0^i)^2$$

$$MSE_b = \frac{1}{N_b} \sum_{i=1}^{N_b} \left( \frac{\partial}{\partial x} u_{NN}(t_b^i, 0; \Theta) \right)^2 + \frac{1}{N_b} \sum_{i=1}^{N_b} \left( \frac{\partial}{\partial x} u_{NN}(t_b^i, 1; \Theta) \right)^2$$

▷ cf. Eqs. (5.27) to (5.29)

▷ Adam or L-BFGS

$$MSE_f = \frac{1}{N_f} \sum_{i=1}^{N_f} (f_{NN}(t_f^i, x_f^i))^2 \quad f := c \frac{\partial u}{\partial t} - \frac{\partial}{\partial x} \left( \kappa \frac{\partial u}{\partial x} \right) - s$$