Workshop

eman ta zabal zazu

Universidad del País Vasco   Euskal Herriko Unibertsitatea

Taller

Coding Deep Neural Networks for PDEs
Session I: Introduction

Professors: Carlos Uriarte*, Ángel Javier Omella*, David Pardo*

Organizers: Ignacio Muga†, Paulina Sepúlveda†

*Research Group on Applied Mathematical Modelling, Statistics, and Optimization (MATHMODE) at UPV/EHU

†IMA Numerics Research Group at PUCV

Follow us on: @mathmode.science, @ima.numerics.pucv†*

Biosfera Lodge, Olmué. January 19-24, 2025

Motivation: Partial Differential Equations

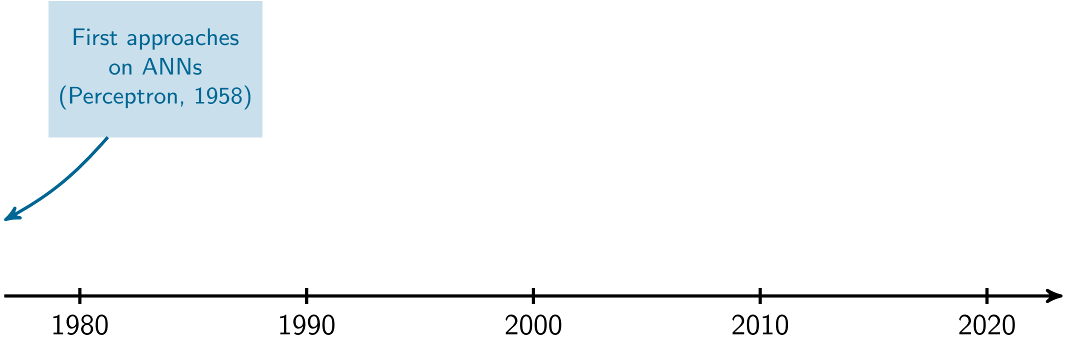
- Partial Differential Equations (PDEs) **model** multiple phenomena.
- **For example:**
  - Steady-state heat distribution in heterogeneous media via diffusion equation:
  $$-\nabla \cdot \sigma \nabla u = f.$$
  - Electromagnetic fields via Maxwell's equations (in the frequency domain):
  $$\begin{cases} \nabla \times \mathbf{E} = -j\omega\boldsymbol{\mu}\mathbf{H} - \mathbf{M}, & \text{Faraday's Law.} \\ \nabla \times \mathbf{H} = (\boldsymbol{\sigma} + j\omega\boldsymbol{\varepsilon})\mathbf{E} + \mathbf{J}, & \text{Amperè's Law.} \\ \nabla \cdot (\boldsymbol{\varepsilon}\mathbf{E}) = \rho_f, & \text{Gauss' Law of Electricity.} \\ \nabla \cdot (\boldsymbol{\mu}\mathbf{H}) = 0, & \text{Gauss' Law of Magnetism.} \end{cases}$$

Parameters, Solution, Equation structure and source terms.

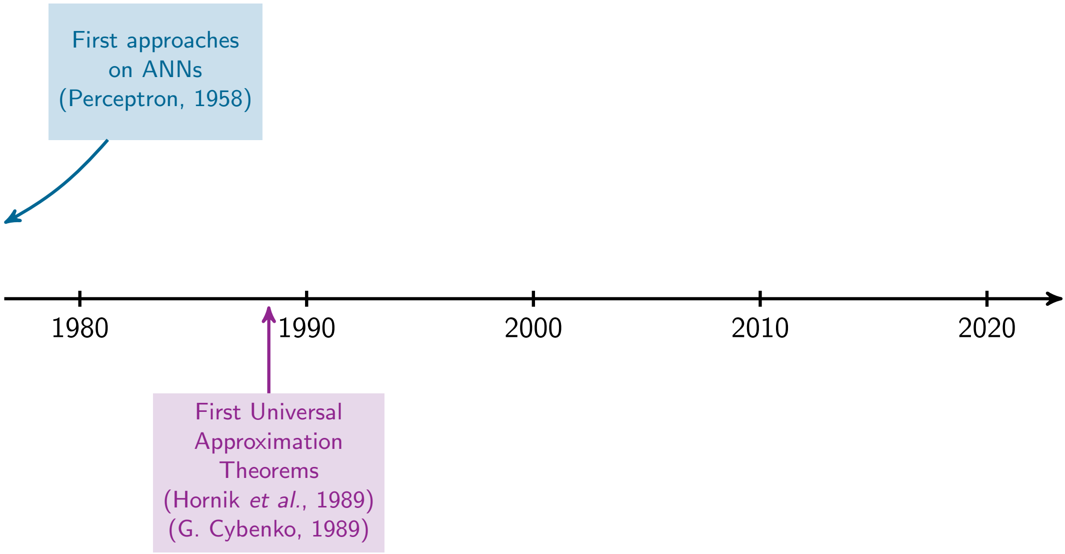
Motivation: Methods for solving linear PDEs

Numerical methods	**Advantages and limitations**
• Finite Difference Method (FDM) • Finite Element Method (FEM) • Spectral Methods (e.g., Fourier)	✓ Converts the PDE into a system of linear equations (for a chosen finite basis) ! Basis choice is critical ✗ Curse of dimensionality
• Feed-Forward Neural Networks • Convolutional Neural Networks • Recurrent Neural Networks	✓ Universal approximation property ✓ Overcome the curse of dimensionality ✗ Non-convex optimization ✗ Integration is challenging

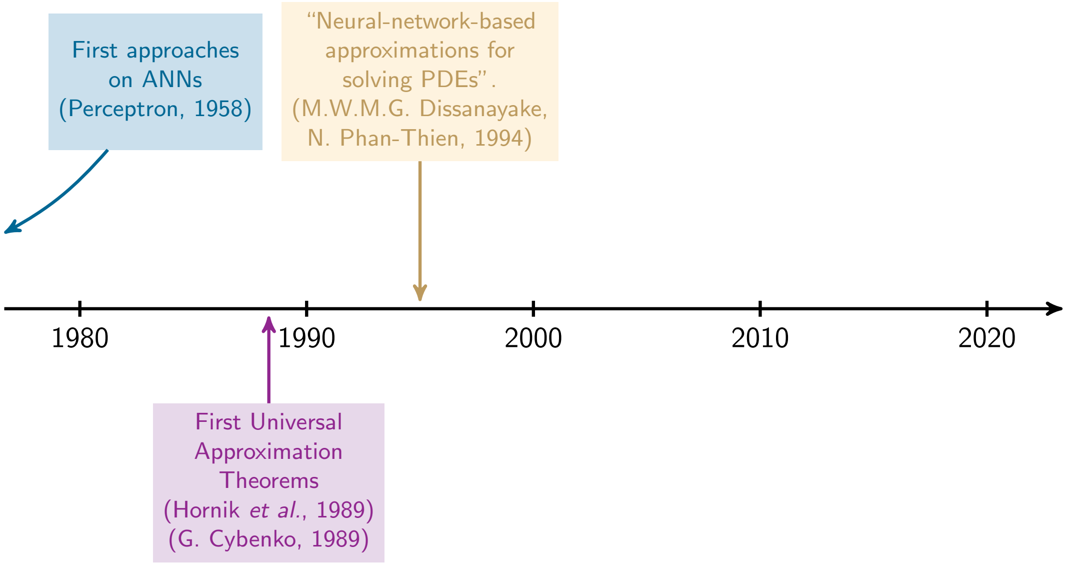
Timeline


First approaches on ANNs (Perceptron, 1958)
1980
1990
2000
2010
2020

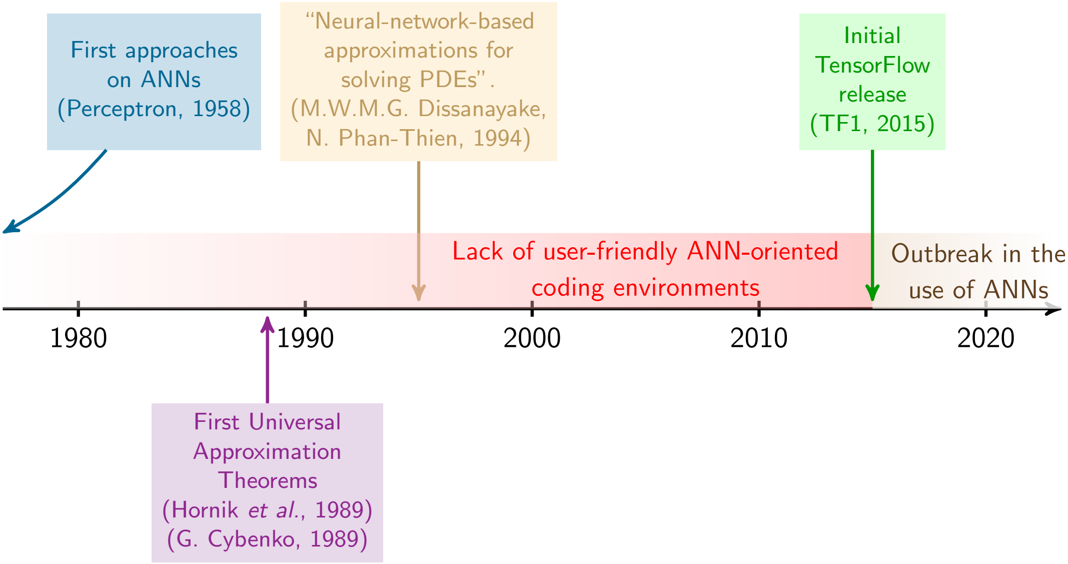
Timeline


First approaches on ANNs (Perceptron, 1958)
1980
1990
2000
2010
2020
First Universal Approximation Theorems
(Hornik *et al.*, 1989)
(G. Cybenko, 1989)

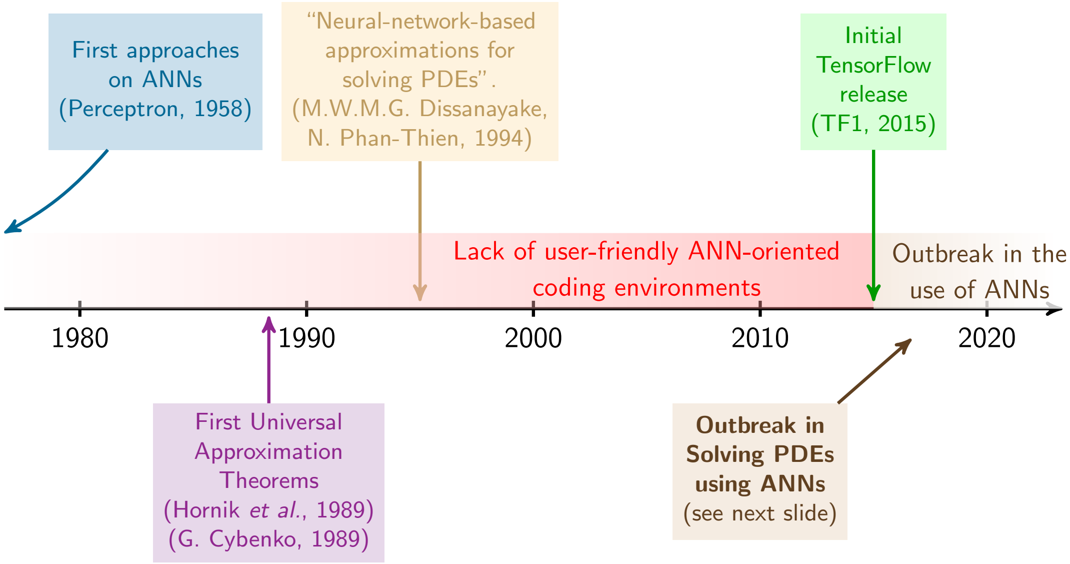
Timeline


First approaches on ANNs (Perceptron, 1958)
“Neural-network-based approximations for solving PDEs”. (M.W.M.G. Dissanayake, N. Phan-Thien, 1994)
1980
1990
2000
2010
2020
First Universal Approximation Theorems (Hornik *et al.*, 1989) (G. Cybenko, 1989)

Timeline


First approaches on ANNs (Perceptron, 1958)
"Neural-network-based approximations for solving PDEs". (M.W.M.G. Dissanayake, N. Phan-Thien, 1994)
Initial TensorFlow release (TF1, 2015)
Lack of user-friendly ANN-oriented coding environments
Outbreak in the use of ANNs
1980
1990
2000
2010
2020
First Universal Approximation Theorems (Hornik *et al.*, 1989) (G. Cybenko, 1989)

Timeline


First approaches on ANNs (Perceptron, 1958)
"Neural-network-based approximations for solving PDEs". (M.W.M.G. Dissanayake, N. Phan-Thien, 1994)
Initial TensorFlow release (TF1, 2015)
Lack of user-friendly ANN-oriented coding environments
Outbreak in the use of ANNs
1980
1990
2000
2010
2020
First Universal Approximation Theorems (Hornik *et al.*, 1989) (G. Cybenko, 1989)
Outbreak in Solving PDEs using ANNs (see next slide)

Literature review

- Yu, B. (2018). The Deep Ritz method: A deep learning-based numerical algorithm for solving variational problems. *Communications in Mathematics and Statistics*, 6(1), 1-12.
- Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, 378, 686-707.
- Kharazmi, E., Zhang, Z., & Karniadakis, G. E. (2021). hp-VPINNs: Variational physics-informed neural networks with domain decomposition. *Computer Methods in Applied Mechanics and Engineering*, 374, 113547.

⋮

- Uriarte, C. (2024). Solving Partial Differential Equations Using Artificial Neural Networks. *arXiv preprint arXiv:2403.09001*. PhD Dissertation (Section 1.4). `https://arxiv.org/pdf/2403.09001`.

Minimization problem

- Assume that our problem of interest reformulates as

$$u^* := \arg\min_{u\in\mathbb{U}} \mathcal{L}(u), \qquad \mathcal{L}: \ \textbf{loss/objective function}, \qquad \mathbb{U}: \ \text{space of functions.}$$

E.g., To find u^* solving $Au^* = f$, we might consider $\mathcal{L}(u) = \|Au - f\|$.

- To approximate $u^* \in \mathbb{U}$, we proceed as follows:

1. Consider a **discretization** θ for $\mathbb{U}$, denoted $\theta \longmapsto u(\theta) \in \mathbb{U}$.
2. "Seek" θ^* such that $\mathcal{L}(u(\theta^*)) = \inf_\theta \mathcal{L}(u(\theta))$. For simplicity, we will write:

$$\theta^* = \arg\inf_\theta \mathcal{L}(u(\theta)),$$

where "arg inf" should be read *loosely*.

By abuse of notation, θ denotes both the discretization mapping and the set of variables.

Discretization

Linear (Traditional) Approach

$$\theta \longmapsto u(\theta)(x) := \sum_{j=1}^{n} \theta_j \, \psi_j(x),$$

$$\theta = (\theta_1, \theta_2, \cdots, \theta_n)$$

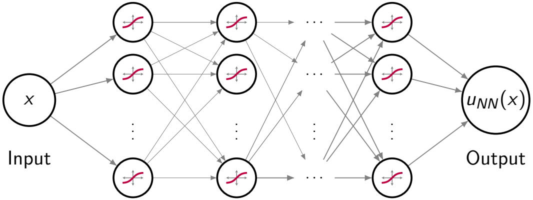
where $\psi_j \in \mathbb{U}$ and $\theta_j \in \Theta = \mathbb{R}^n$.

Typically:

- ψ_j is easy to implement (e.g., a polynomial).
- $\{\psi_j\}_{j=1}^n$ is linearly indep.

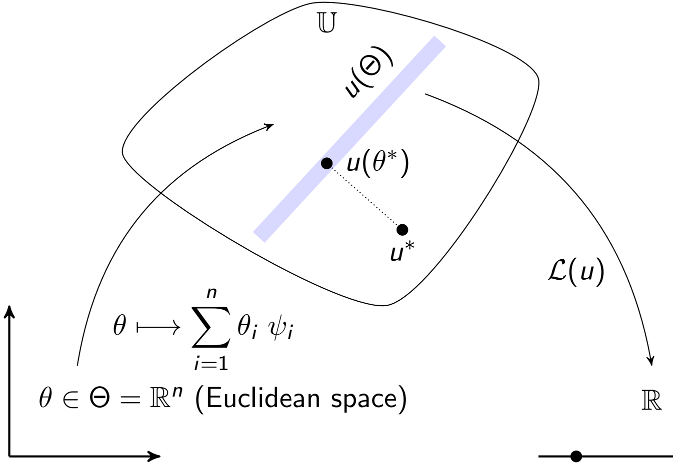
Artificial Neural Networks (ANNs)

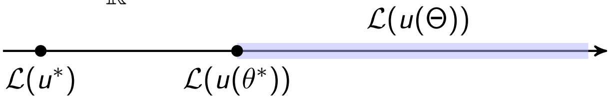
$$\theta \longmapsto u(\theta)(x) := u_{NN}(x),$$
$$\theta = \{\mathbf{W}_j, \mathbf{b}_j\}_{j=1}^k \cup \{\mathbf{W}\} \in \Theta = \mathbb{R}^n.$$



$$\mathbf{y}_0(x) := x \in \mathbb{R}^{n_0},$$
$$\mathbf{y}_j(x) := \varphi(\mathbf{W}_j \mathbf{y}_{j-1} + \mathbf{b}_j) \in \mathbb{R}^{n_j}, \quad 1 \le j \le k,$$
$$u_{NN}(x) := \mathbf{W}\mathbf{y}_k \in \mathbb{R}^{n_{k+1}},$$

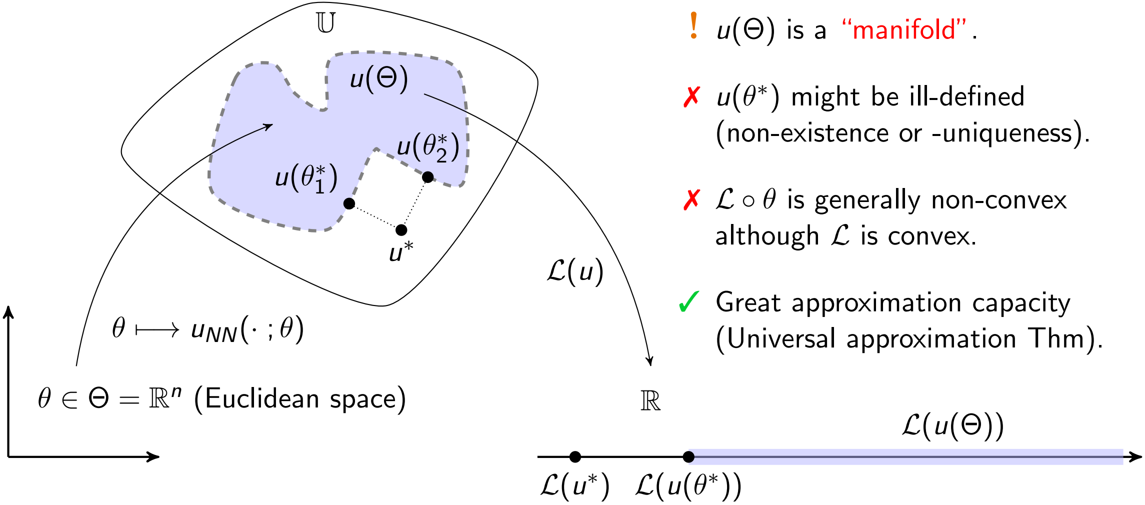
Linear-combination approach





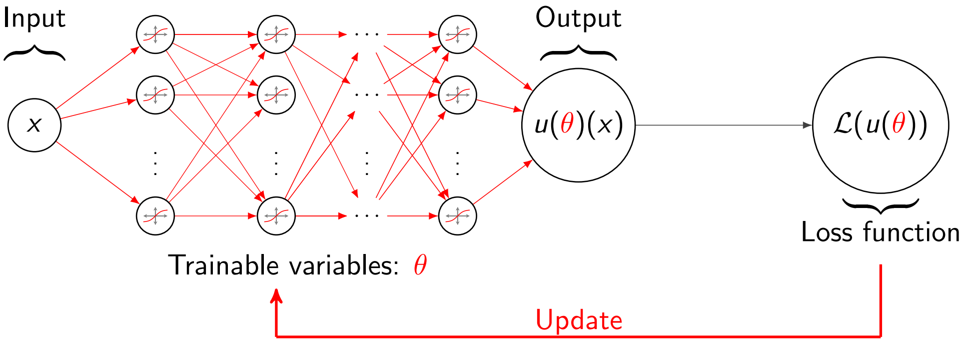
- ✓ $u(\Theta)$ is a finite subspace of $\mathbb{U}$.
- ✓ Typically, $u(\theta^*)$ is well-defined.
- ✓ If $\mathcal{L}$ convex $\implies$ $\mathcal{L} \circ \theta$ convex.
- ! Approximation capacity is sensitive to the choice of $\{\psi_i\}_{i=1}^n$.

ANN approach



- ! $u(\Theta)$ is a "manifold".
- ✗ $u(\theta^*)$ might be ill-defined (non-existence or -uniqueness).
- ✗ $\mathcal{L} \circ \theta$ is generally non-convex although $\mathcal{L}$ is convex.
- ✓ Great approximation capacity (Universal approximation Thm).

Optimization



Optimization

- Tipically performed in the form of a **first-order gradient-descent-based** methods.

✓ **Automatic differentiation** computes $\nabla_\theta \mathcal{L}(u(\theta))$ with a cost similar to evaluating $\mathcal{L}(u(\theta))$.

✗ Second-order methods (e.g., Newton methods) involve $\mathcal{H}_\theta(\mathcal{L}) := \nabla_\theta^2 \mathcal{L}(u(\theta))$. Computing $\mathcal{H}_\theta(\mathcal{L})$ employing automatic differentiation is $\#\theta$ times more expensive than computing $\nabla_\theta \mathcal{L}(u(\theta))$. In ANN approaches, $\#\theta$ is huge!

- Continuum-level descriptions of gradient-descent and Newton optimization schemes,

$$\theta_t' = -\overbrace{\mathcal{H}_\theta(\mathcal{L})^{-1} \underbrace{\nabla_\theta \mathcal{L}(u(\theta_t))}_{\text{Gradient Desc.}}}^{\text{Newton step}}, \qquad \begin{cases} \theta_t = \theta(t), \\ \theta_0 = \theta(0). \end{cases}$$

Optimization

- Iterative gradient-descent optimization:

$$\begin{cases} \theta_t' \approx \frac{\theta_{t+1}-\theta_t}{\eta} \\ \theta_t' = -\nabla_\theta \mathcal{L}(u(\theta_t)) \end{cases} \qquad \Longrightarrow \qquad \theta_{t+1} = \theta_t - \eta \nabla_\theta \mathcal{L}(u(\theta_t))$$

- Adding momentum:
  - At the continuum level:

$$\theta_t'' + \gamma \theta_t' = -\nabla_\theta \mathcal{L}(u(\theta_t)) \iff \begin{cases} \theta_t' & = v_t, \\ v_t' + \gamma v_t & = -\nabla_\theta \mathcal{L}(u(\theta_t)), \end{cases} \quad .$$

  - At the iterative level:

$$\begin{cases} v_{t+1} = \beta v_{t-1} - \eta \nabla_\theta \mathcal{L}(u(\theta_t)), \\ \theta_{t+1} = \theta_t + v_{t+1}, \end{cases} \qquad 0 < \beta := 1 - \gamma\eta < 1.$$

  - There exist multiple gradient-descent variants of this: with Nesterov acceleration, Adagrad, Adadelta, RMSprop, Adam/AdaMax, Nadam, etc.

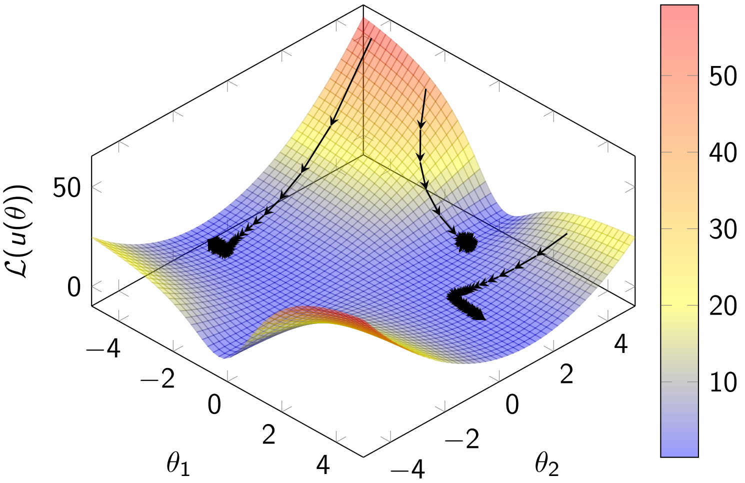
Optimization

Let $\theta = (\theta_1, \theta_2)$,

- $u(\theta)(x) = \theta_2 \tanh(\theta_1 x)$,
- $u^*(x) = \begin{cases} 1, & x > 0, \\ 0, & x = 0, \\ -1, & x < 0, \end{cases}$
- $\mathcal{L}(u) = \|u - u^*\|^2_{L^2(-1,1)}$.

Infimizer: $(\theta_1^*, \theta_2^*) = (\pm\infty, \pm 1)$.

We perform 200 gradient-descent iterations with $\eta = 0.05$.



Integration: General Comments

- **Exact integration** is typically **unavailable** due to the nonlinearity of activation functions.

- When our loss function has an integral form, we employ **numerical integration**:

$$\mathcal{L}(u(\theta)) = \int_\Omega \mathcal{I}_{u(\theta)}(x)dx \approx \sum_{k=1}^{K} \omega_k \mathcal{I}_{u(\theta)}(x_k).$$

- To avoid overfitting, **stochastic** quadrature is a must! (e.g., Monte Carlo integration)

- **Unbiasedness** of the chosen stochastic quadrature is another must! (e.g., MC is unbiased)

$$\mathbb{E}\left[\sum_{k=1}^{K} \omega_k I(u(\theta))(X_k)\right] = \mathcal{L}(u(\theta)).$$

- Big **variance** entails big integration errors! (in MC, variance is of order $\mathcal{O}\left(\frac{1}{N}\right)$).