Technical University of Munich
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Advanced Deep Learning for Physics (IN2298)
Exercise 7
Optimal Path Simulator

(1) Optimal Path: Physics-Based Optimization

We explore a classical optimization problem: Given a potential landscape and a starting point, how can we reach a target point with minimal effort?

Define a scalar-valued potential function in two dimensions (x, y):

$$f(x, y) = (x^2 + y^2 - 1)^2 \tag{1}$$

A movement on the landscape is defined repeating the following update step:

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} x_0 \\ y_0 \end{pmatrix} + \begin{pmatrix} \Delta x \\ F_0 \end{pmatrix} \tag{2}$$

Here, (x_0, y_0) is the current position, Δx is a fixed horizontal step, and F_0 is a variable vertical force. Repeat this step N times to generate a trajectory from (x_0, y_0) to (x_N, y_N). The full trajectory is defined by the starting point and a force vector $\mathbf{F} = [F_0, F_1, ..., F_{N-1}]$. Viewing the potential as a mountain landscape, our goal is to move on the landscape while staying minimal total potential energy, which is defined as

$$L = \sum_{i=1}^{N} f(x_i, y_i) \tag{3}$$

This defines an optimization problem with loss L and optimization variables $\mathbf{F}$. Solve this using Gradient Descent and plot the potential landscape with the optimized trajectory. Run the optimization multiple times and identify the different types of solutions obtained.

Parameters:

- Initial position: $(x_0, y_0) = (-1, 0)$
- Number of steps: $N = 20$
- Horizontal step size: $\Delta x = 0.1$
- Initialization: Sample each F_i from Uniform$[-0.1, 0.1]$
- Optimizer: Gradient Descent with learning rate 0.001, momentum 0.95, and 500 iterations

(2) Optimal Path: Supervised Learning Approach

Now consider a variable initial position of the form $(x_0, y_0) = (-1, \epsilon)$, where $\epsilon \sim$ Uniform$[-0.01, 0.01]$. Train a neural network to predict the optimal force vector $\mathbf{F}$ for each starting point.

(a) **Dataset Generation**
Generate 100 values of y_0 sampled from Uniform$[-0.01, 0.01]$. For each, compute the corresponding optimal force vector $\mathbf{F}$ using the previous optimization procedure.

(b) **Network Training**
Train a feedforward neural network with:

- One hidden layer with 10 ReLU units
- Linear output layer
- Loss: Mean Squared Error
- Optimizer: Adam with learning rate 0.01

- Training: Full-batch, 1500 steps

(c) **Evaluation**
Generate 25 new initial y_0 values and use the trained network to predict corresponding force vectors. Simulate the resulting paths and visualize them in the potential landscape.

(3) Optimal Path: Differentiable Physics Training

Instead of using supervised labels, train the network end-to-end using differentiable physics.

(a) **Network Training**
Initialize the network and input samples as before. Replace the supervised loss with the physics-based loss that directly computes total potential energy from simulated trajectories. Use the same optimizer and training parameters.

(b) **Evaluation**
Visualize the predicted paths from the new model. Compare with the supervised case. Why is better performance expected?

Submission instruction

Please upload a single PDF file containing your results along with your code for implementation tasks or your derivation for non-implementation tasks (LaTex typesetting). The uploaded PDF should only include the final code, so please trim empty spaces and your intermediate work before submitting.

The easiest way to generate such a PDF is by using Jupyter notebooks and LaTex (we recommend MiKTeX for Windows users). With Jupyter and LaTeX installed, you can create a PDF from your notebook by running *jupyter nbconvert –to pdf your-notebook.ipynb*

Additional information

This is an individual assignment. Plagiarism will result in the loss of eligibility for the bonus this semester.

If you have any questions about the exercises, please contact us via the forum on Moodle. If you need further face-to-face discussion, please join our weekly online Q&A session (every Monday at 15:00 and 16:00 via BBB).