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Advanced Deep Learning for Physics (IN2298)
Exercise 5
Manual Differentiation

In this exercise you will develop an intuition for the gradient flow through a coupled system consisting of a physics solver and a neural network. Note that you should finish this exercise **manually**, you don't need to write any code.

(1) Backpropagation through one-step control

We study the following discrete system comprised of internal dynamics and a linear controller

$$\mathbf{x}_{n+1} = \begin{bmatrix} x_{n+1,1} \\ x_{n+1,2} \\ x_{n+1,3} \end{bmatrix} = \begin{bmatrix} x_{n,1}^2 + x_{n,2} \\ -x_{n,1} + \frac{x_{n,2}}{2} \\ -x_{n,2}^2 + x_{n,3} \end{bmatrix} + \begin{bmatrix} x_{n,1}\theta_1 \\ x_{n,2}\theta_2 \\ x_{n,3}\theta_3 \end{bmatrix}, \tag{1}$$

where $\mathbf{x}$ represents the system state and $\boldsymbol{\theta}$ represents trainable weights. Suppose that the system state and weights currently are $\mathbf{x}_0 = (2, \text{-}1, 3)^T$ and $\boldsymbol{\theta} = (\text{-}1, 4, 2)^T$. Calculate the back-propagation gradient $\frac{\partial L}{\partial \boldsymbol{\theta}}$ of the trainable parameters when evaluated on the loss function $L = ||\mathbf{x}_1||_1$.

(2) Multi-step control

A new initial state $\mathbf{x}_0 = (\text{-}1, 1, 2)^T$ and weights $\boldsymbol{\theta} = (3, \text{-}1, 1)^T$ are considered. The system is then unrolled for two steps, giving the new state $\mathbf{x}_2$. Calculate the *total* back-propagation gradient for the variables on the loss function $L = ||\mathbf{x}_2||_1$ by accumulating over all appearances of the variables.

(3) Forward propagation

Repeat the one-step calculation using forward-propagation of gradients. Briefly state the differences of forward and backward differentiation and how these relate to their application in deep learning.

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).