Machine Learning

Multi-layer perceptron and back-propagation
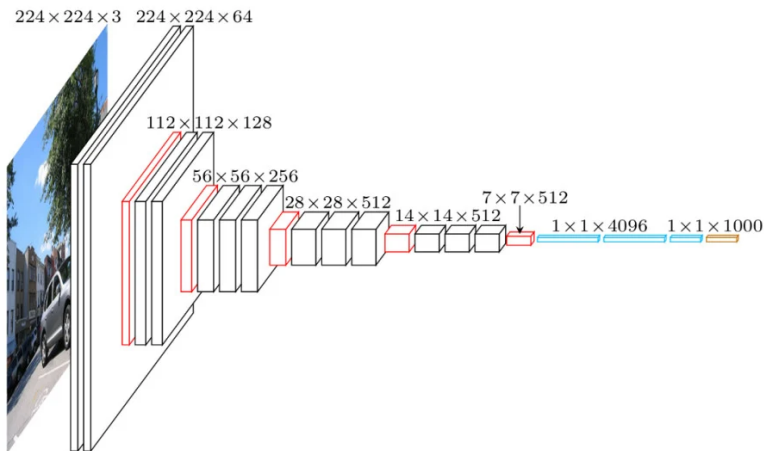
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SAPIENZA
Università di Roma

2nd semester a.y. 2024/2025 · March 25, 2025

A glimpse into neural networks

In deep learning, we deal with highly parametrized models called deep neural networks:

Deep composition

The simplest example of a nonlinear parametric model:

$$f \circ f(\mathbf{x})$$

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The simplest example of a nonlinear parametric model:

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More in general, consider other activation functions:

$$\sigma(x) = \frac{1}{1 + e^{-x}} \qquad \sigma(x) = \max\{0, x\}$$

continuous   discontinuous
                    gradient

Multi-layer perceptron

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where we encode the weights in matrix $\mathbf{W}_\ell$ and bias $\mathbf{b}_\ell$.

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The hidden representations are also called the activations at layer $\ell + 1$.

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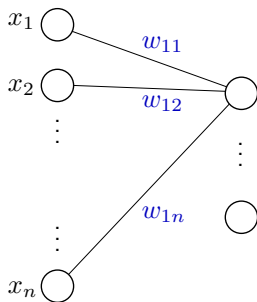
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1. Each layer is a vector-to-vector function $\mathbb{R}^p \to \mathbb{R}^q$.

2. Each layer has q neurons acting in parallel.
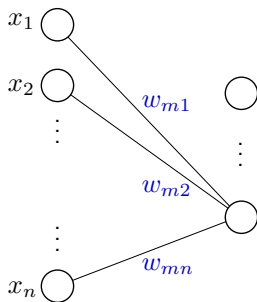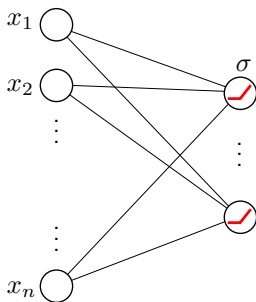   Each neuron acts as a scalar function $\mathbb{R}^p \to \mathbb{R}$.

Single layer illustration

$$\sigma(\mathbf{W}\mathbf{x}) = \sigma \circ \begin{pmatrix} w_{11} & w_{12} & \cdots & w_{1n} \\ w_{21} & w_{22} & \cdots & w_{2n} \\ \vdots & \cdots & \ddots & \vdots \\ w_{m1} & w_{m2} & \cdots & w_{mn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \sigma \circ \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$
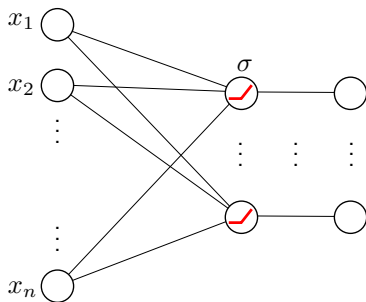
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It is common to have a linear layer at the output:

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which maps:

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Deep ReLU networks

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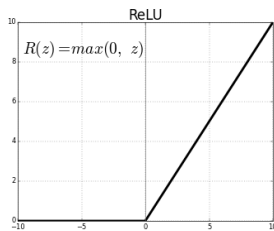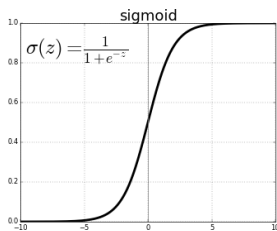
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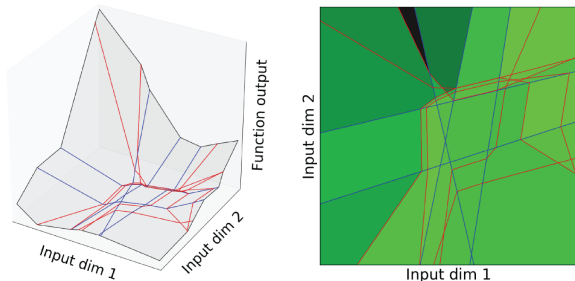
The blue and red edges are produced by the first and second layer.

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Universality

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> **Universal Approximation Theorem** For any compact set $\Omega \subset \mathbb{R}^p$, the space spanned by the functions $\phi(\mathbf{x}) = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b})$ is dense in $\mathcal{C}(\Omega)$ for the uniform convergence.

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For large enough q, the training error can be made arbitrarily small.

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Other UAT theorems for ReLUs and locally bounded non-polynomials.

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In general, we deal with nonconvex functions. Empirical results show that large q + gradient descent leads to very good approximations.

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Training

Given a MLP with training pairs $\{\mathbf{x}_i, \mathbf{y}_i\}$:

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$$\ell_{\boldsymbol{\Theta}}(\{\mathbf{x}_i, \mathbf{y}_i\}) = \frac{1}{n} \sum_{i=1}^{n} \|\mathbf{y}_i - g_{\boldsymbol{\Theta}}(\mathbf{x}_i)\|_2^2$$

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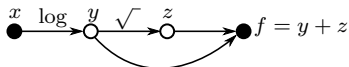
We want to automatize this computational step efficiently.

Computational graphs

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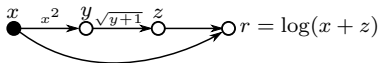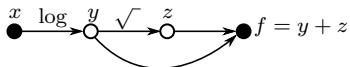A computational graph is a directed acyclic graph representing the computation of $f(x)$ with intermediate variables.

Example:

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x

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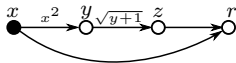A computational graph is a directed acyclic graph representing the computation of $f(x)$ with intermediate variables.

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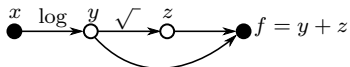# Computational graphs

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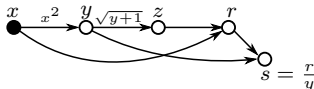
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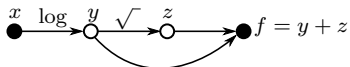$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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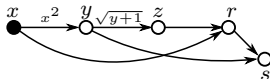
Example:

$$f(x) = \log x + \sqrt{\log x}$$

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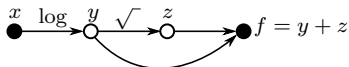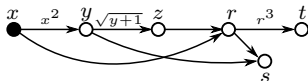$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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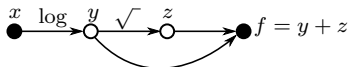$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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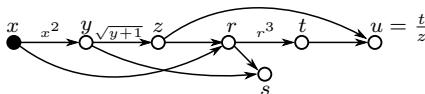
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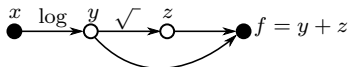$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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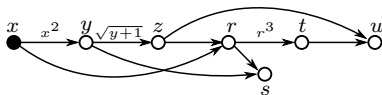
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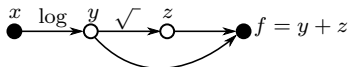$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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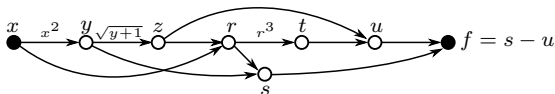
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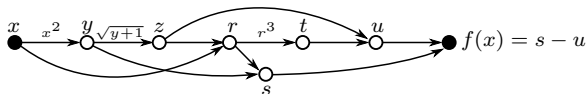
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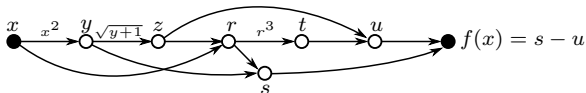
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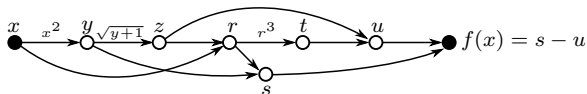
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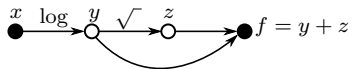
For high-dimensional input/output, the graph may be more complex:
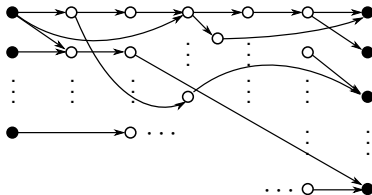
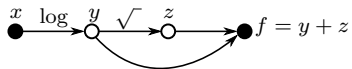The computational graph gets big quickly.
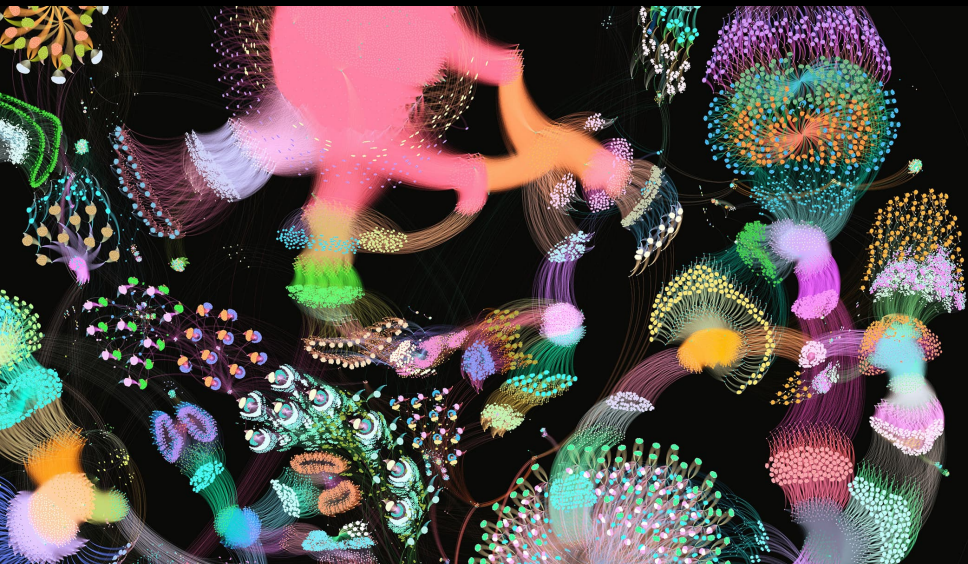
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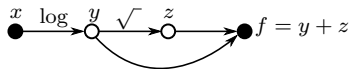
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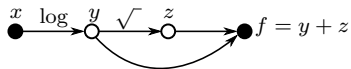$$f(x) = \log x + \sqrt{\log x}$$

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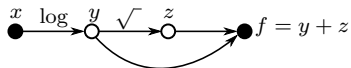
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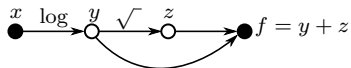
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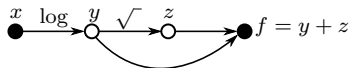
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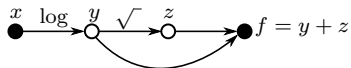
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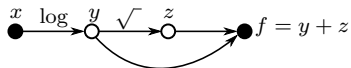
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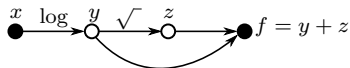$$f(x) = \log x + \sqrt{\log x}$$

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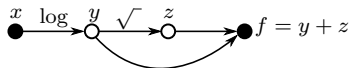$$f(x) = \log x + \sqrt{\log x}$$

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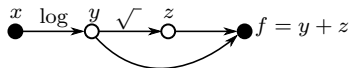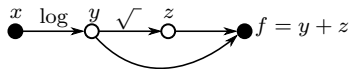$$f(x) = \log x + \sqrt{\log x}$$

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$$f(x) = \log x + \sqrt{\log x} \qquad \frac{\partial f}{\partial x} = \frac{1}{2\sqrt{y}}\frac{1}{x} + \frac{1}{x}$$

Assumption: Each partial derivative is a "primitive" accessible in closed form and can be computed on the fly.

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$$\text{cost of computing } \frac{\partial f}{\partial x}(x) \;=\; \text{cost of computing } f(x)$$

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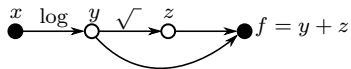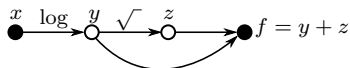$$f(x) = \log x + \sqrt{\log x} \qquad \frac{\partial f}{\partial x} = \frac{1}{2\sqrt{y}}\frac{1}{x} + \frac{1}{x}$$

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However, if the input is high-dimensional, i.e. $f : \mathbb{R}^p \to \mathbb{R}$:

$$\text{cost of computing } \nabla f(\mathbf{x}) \;=\; p \times \text{cost of computing } f(\mathbf{x})$$

since partial derivatives must be computed w.r.t. each input dimension.

Automatic differentiation: Forward mode

Computes all partial derivatives $\frac{\partial y}{\partial x}, \frac{\partial z}{\partial x}, \dots$ with respect to the input x.

Automatic differentiation: Forward mode

Computes all partial derivatives $\frac{\partial y}{\partial x}, \frac{\partial z}{\partial x}, \ldots$ with respect to the input x.

Automatic differentiation $\neq$ Symbolic differentiation
(e.g. autograd)   (e.g. Mathematica)

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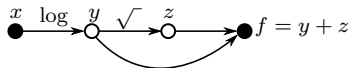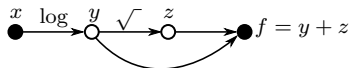(e.g. autograd)   (e.g. Mathematica)

We accumulate values during code execution, to get numerical evaluations rather than expressions for the derivative.

Reverse mode: compute all the partial derivatives $\frac{\partial f}{\partial z}, \ldots, \frac{\partial f}{\partial x}$ with respect to the inner nodes.

Automatic differentiation: Reverse mode

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Automatic differentiation: Reverse mode

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$$\frac{\partial f}{\partial f} = 1$$

Automatic differentiation: Reverse mode

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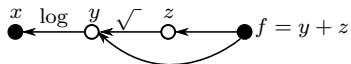
$$\frac{\partial f}{\partial z} =$$

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$$\frac{\partial f}{\partial x} =$$

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$$\frac{\partial f}{\partial f} = 1$$

$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f} \frac{\partial f}{\partial z}$$

$$\frac{\partial f}{\partial y} =$$

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Automatic differentiation: Reverse mode

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x $\log$ y $\sqrt{}$ z $f = y + z$

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Automatic differentiation: Reverse mode

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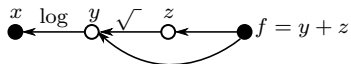$$\frac{\partial f}{\partial f} = 1$$

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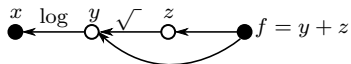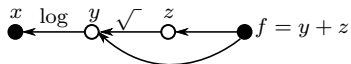$$\frac{\partial f}{\partial f} = 1$$

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$$\frac{\partial f}{\partial x} =$$

Automatic differentiation: Reverse mode

$$f(x) = \log x + \sqrt{\log x}$$

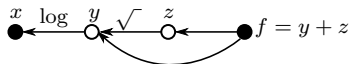$$\frac{\partial f}{\partial f} = 1$$

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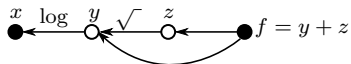

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Automatic differentiation: Reverse mode

$$f(x) = \log x + \sqrt{\log x}$$

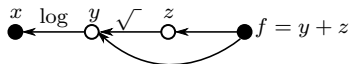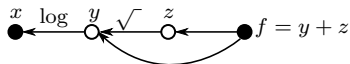$$\frac{\partial f}{\partial f} = 1$$

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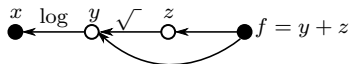$$f(x) = \log x + \sqrt{\log x}$$

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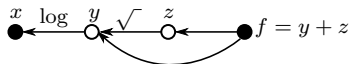$$f(x) = \log x + \sqrt{\log x}$$

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Before computing the derivatives, we must compute the values of the
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❶ Forward pass to evaluate all the interior nodes $y, z, \dots$.

Remark: This is not forward-mode autodiff, since we are only
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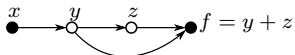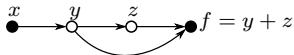Before computing the derivatives, we must compute the values of the internal nodes first:

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1. Forward pass to evaluate all the interior nodes $y, z, \ldots$.

$$\overset{x}{\bullet} \longrightarrow \overset{y}{\circ} \longrightarrow \overset{z}{\circ} \longrightarrow \bullet f = y + z$$

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2. Backward pass to compute the derivatives.
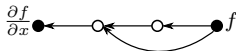
$$\frac{\partial f}{\partial x} \bullet \longleftarrow \circ \longleftarrow \circ \longleftarrow \bullet f$$

Back-propagation

When training NNs, we compute the gradient of a loss

$$\ell : \mathbb{R}^p \to \mathbb{R}$$

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ϵ computes the actual scalar error for the loss.

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Backprop through computational graph of the loss
$\approx$
Backprop "through the network"

Suggested reading

Nice, accessible survey on automatic differentiation:
https://arxiv.org/abs/1502.05767