Deep Learning & Applied AI
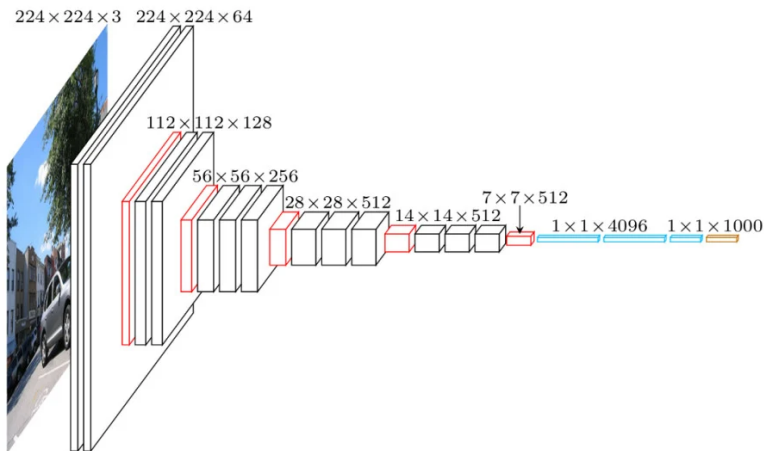
Multi-layer perceptron and back-propagation

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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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More in general, consider other activation functions than logistic:

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

continuous   discontinuous
                    gradient

Multi-layer perceptron

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Remark: The bias can be included in the weight matrix by writing:

$$\mathbf{W} \mapsto \begin{pmatrix} \mathbf{W} & \mathbf{b} \end{pmatrix}, \quad \mathbf{x} \mapsto \begin{pmatrix} \mathbf{x} \\ 1 \end{pmatrix},$$

because each f is linear in the parameters just like in linear regression.

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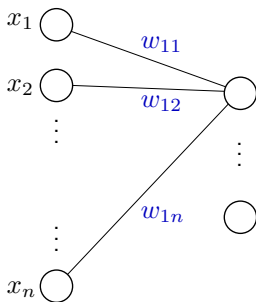
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❷ Each layer has q units acting in parallel.

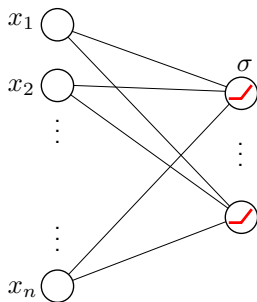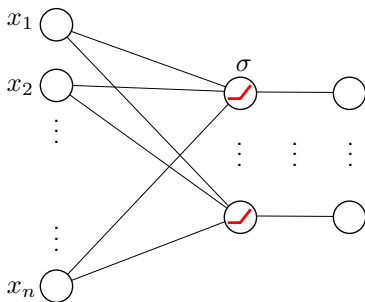Each unit acts as a scalar function $\mathbb{R}^p \to \mathbb{R}$.

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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For generality, it is common to have a linear layer at the output:

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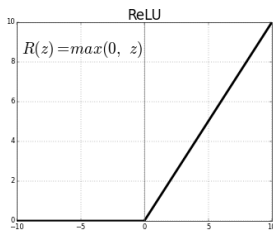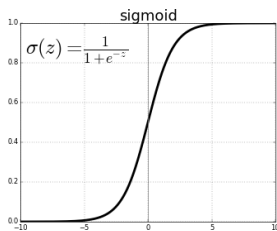
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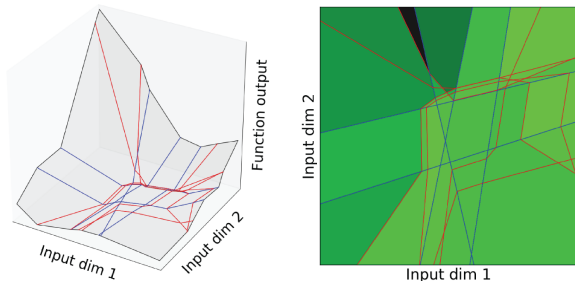
The blue and red edges are produced by the first and second layer.

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> **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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Training

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

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- One layer, sigmoid activation, logistic loss ($\Rightarrow$ logistic regression).

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We want to automatize this computational step efficiently.

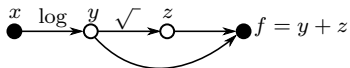# Computational graphs

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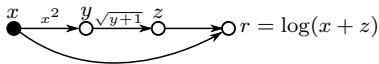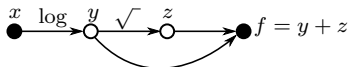
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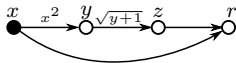A computational graph is a directed acyclic graph representing the computation of $f(x)$ with intermediate variables.

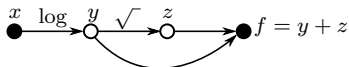**Example:**

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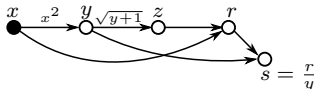A computational graph is a directed acyclic graph representing the computation of $f(x)$ with intermediate variables.

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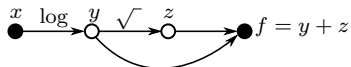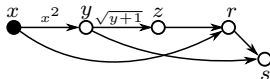$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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Consider a generic function $f : \mathbb{R} \to \mathbb{R}$.

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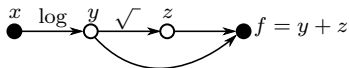$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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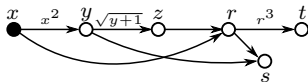
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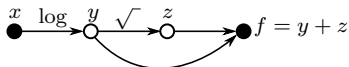$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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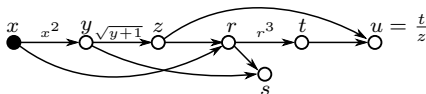
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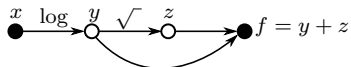$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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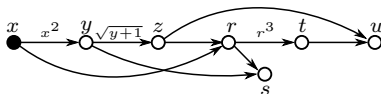
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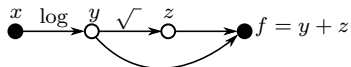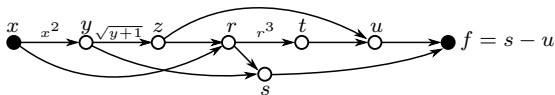$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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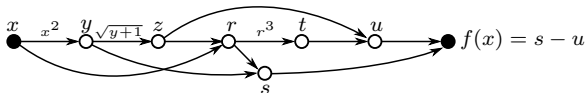
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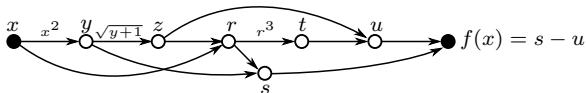
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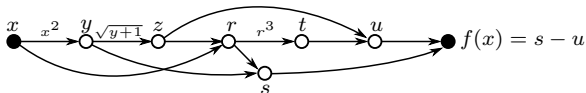
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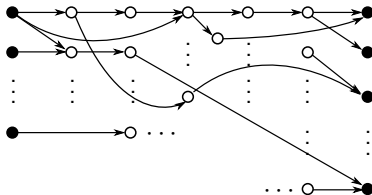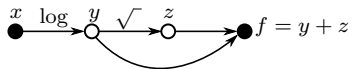
The computational graph gets big quickly.
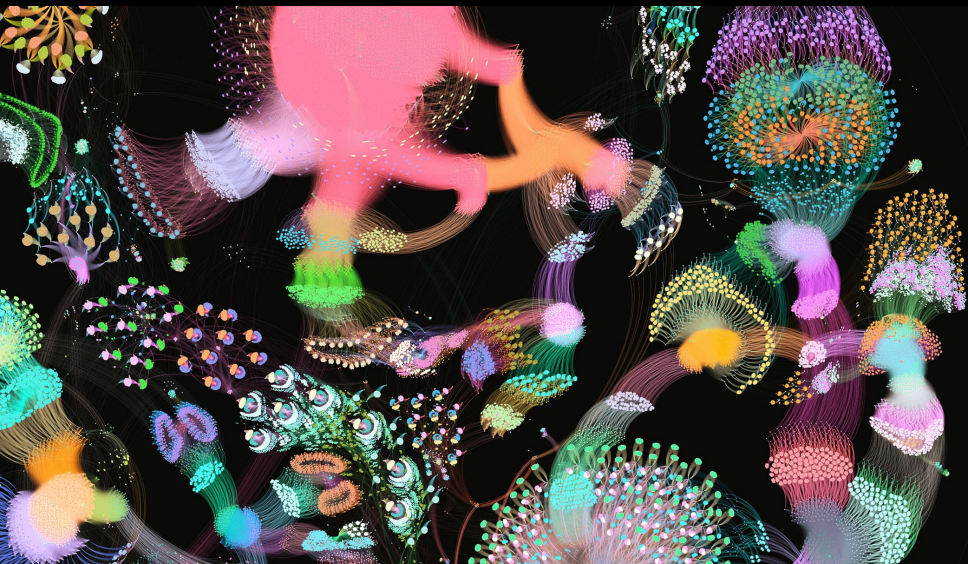
Automatic differentiation: Forward mode
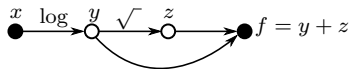
$$f(x) = \log x + \sqrt{\log x}$$

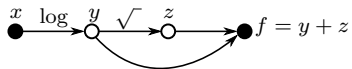# Automatic differentiation: Forward mode

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

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

Automatic differentiation: Forward mode
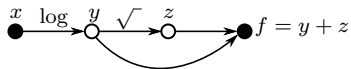
$$f(x) = \log x + \sqrt{\log x}$$

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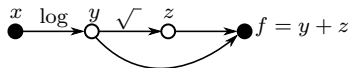
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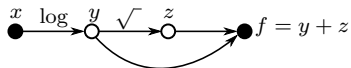
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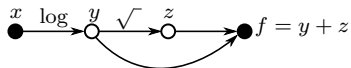
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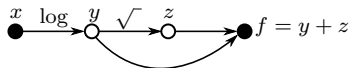
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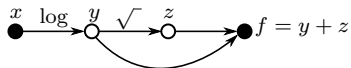Automatic differentiation: Forward mode

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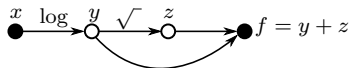$$f(x) = \log x + \sqrt{\log x}$$

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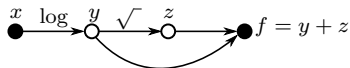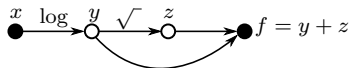$$f(x) = \log x + \sqrt{\log x}$$

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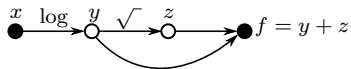$$f(x) = \log x + \sqrt{\log x}$$

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Assumption: Each partial derivative is a "primitive" accessible in closed form and can be computed on the fly.
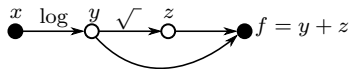
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$$\text{cost of computing } \frac{\partial f}{\partial x}(x) \;=\; \text{cost of computing } f(x)$$

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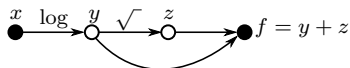$$f(x) = \log x + \sqrt{\log x} \qquad \frac{\partial f}{\partial x} = \frac{1}{2\sqrt{y}}\frac{1}{x} + \frac{1}{x}$$

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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.

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The forward mode computes all the partial derivatives $\frac{\partial y}{\partial x}, \frac{\partial z}{\partial x}, \ldots$ with respect to the input x.

Straightforward application of the chain rule.

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Automatic differentiation $\neq$ Symbolic differentiation
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We accumulate values during code execution to generate numerical derivative evaluations rather than derivative expressions.
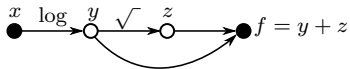
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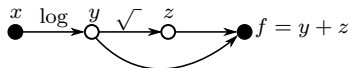$$\text{(e.g. autograd)} \qquad \text{(e.g. Mathematica)}$$

We accumulate values during code execution to generate numerical derivative evaluations rather than derivative expressions.

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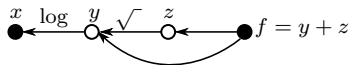
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$$\frac{\partial f}{\partial f} = 1$$

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

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

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

Automatic differentiation: Reverse mode

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

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

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

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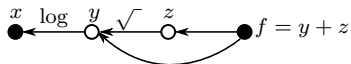
$$\frac{\partial f}{\partial x} =$$

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Automatic differentiation: Reverse mode

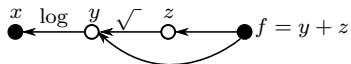$$f(x) = \log x + \sqrt{\log x}$$

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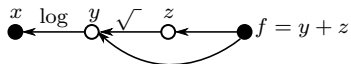$$\frac{\partial f}{\partial f} = 1$$

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Automatic differentiation: Reverse mode

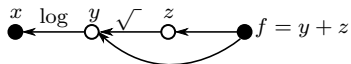$$f(x) = \log x + \sqrt{\log x}$$

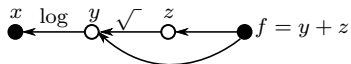$$\frac{\partial f}{\partial f} = 1$$

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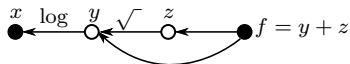$$\frac{\partial f}{\partial f} = 1$$

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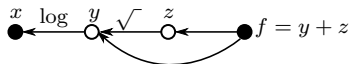$$\frac{\partial f}{\partial f} = 1$$

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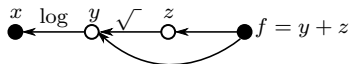$$f(x) = \log x + \sqrt{\log x}$$

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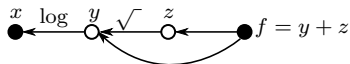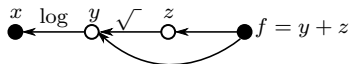$$f(x) = \log x + \sqrt{\log x}$$

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

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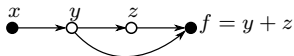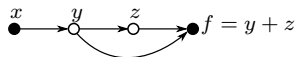
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1. Forward pass to evaluate all the interior nodes $y, z, \ldots$.

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

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2. Backward pass to compute the derivatives.

$$\frac{\partial f}{\partial x} \bullet \longleftarrow \circ \longleftarrow \circ \longleftarrow \bullet f$$

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

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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/pdf/1502.05767