Deep Learning & Applied AI

Multi-layer perceptron and back-propagation

Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

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A glimpse into neural networks

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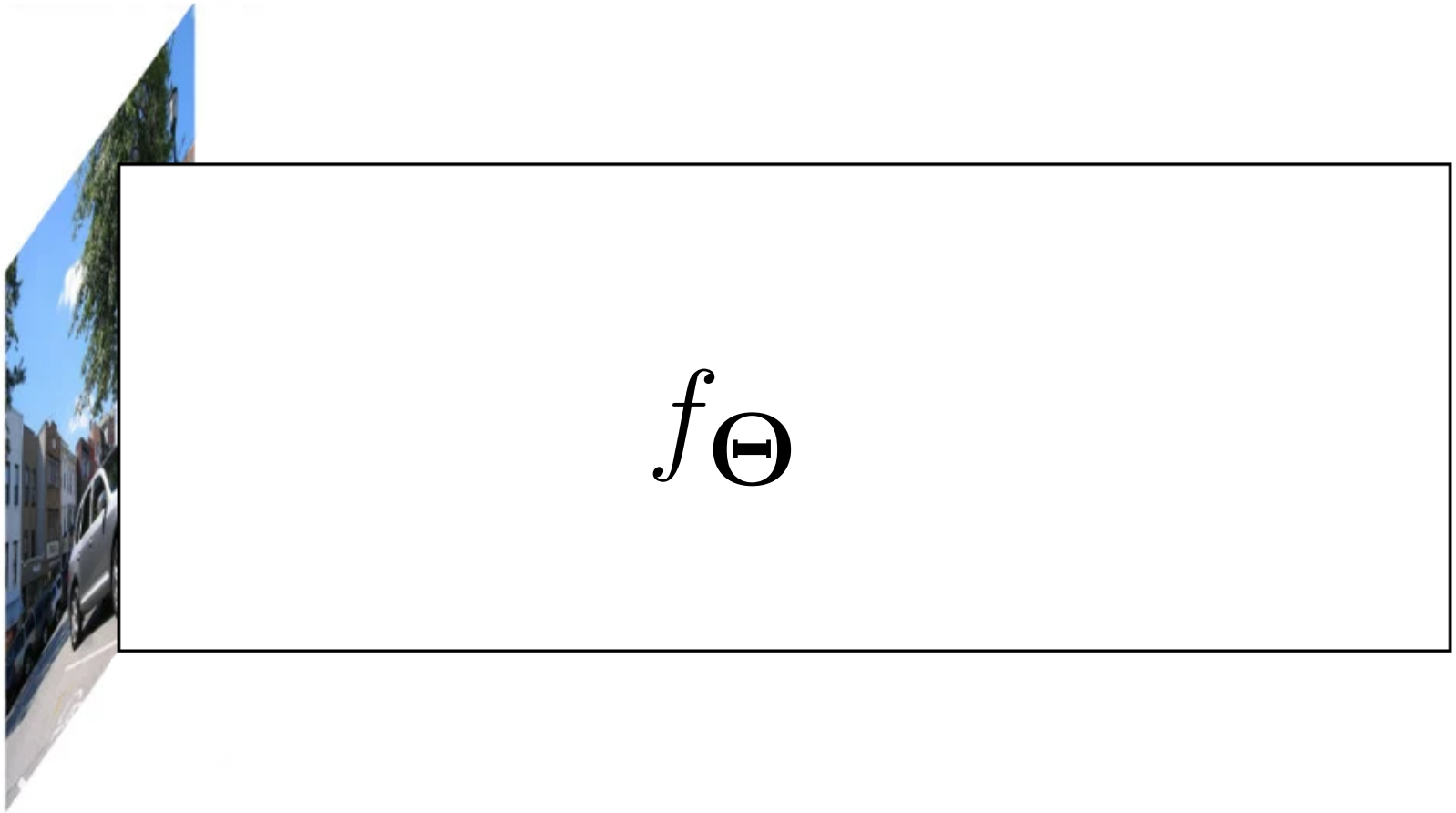

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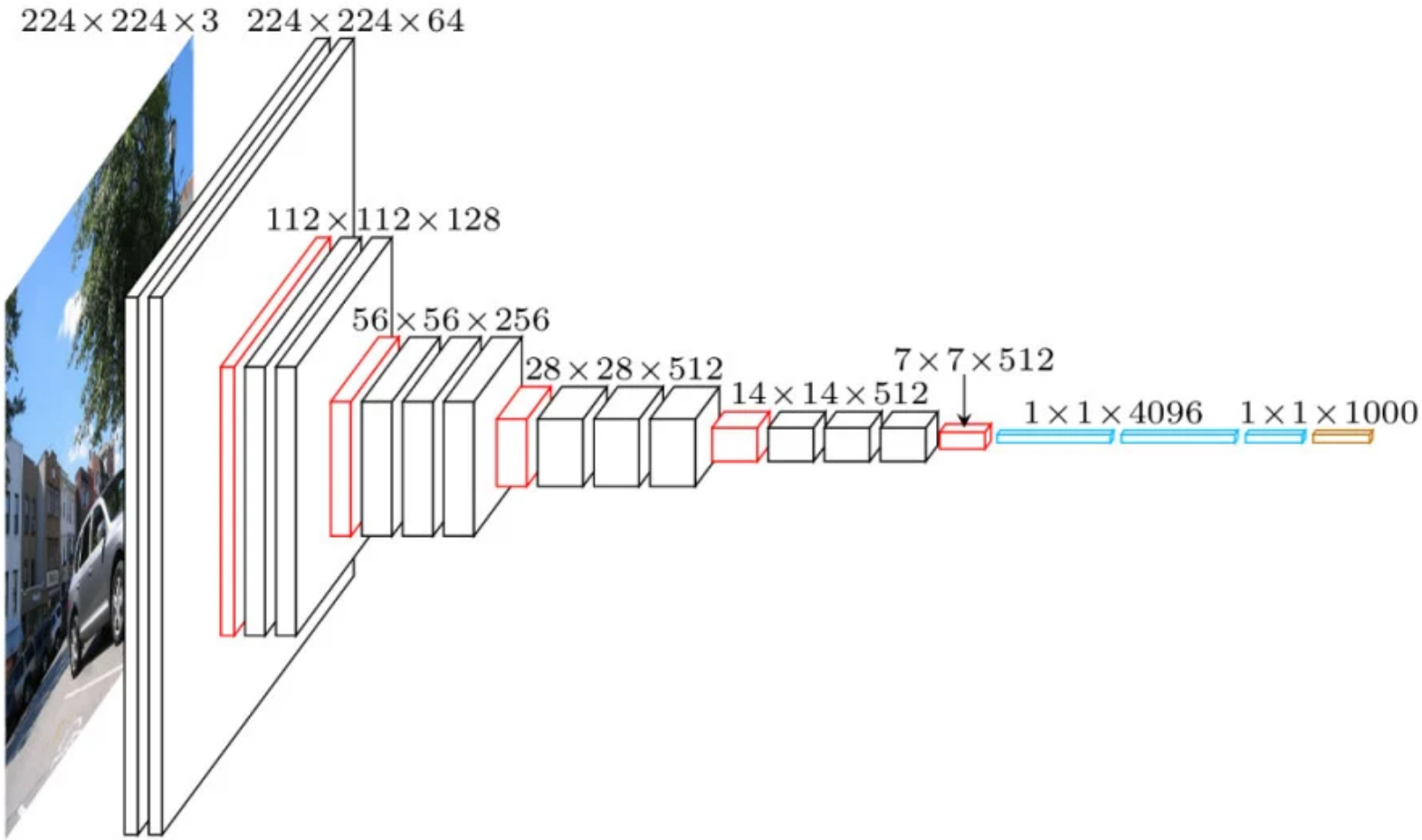

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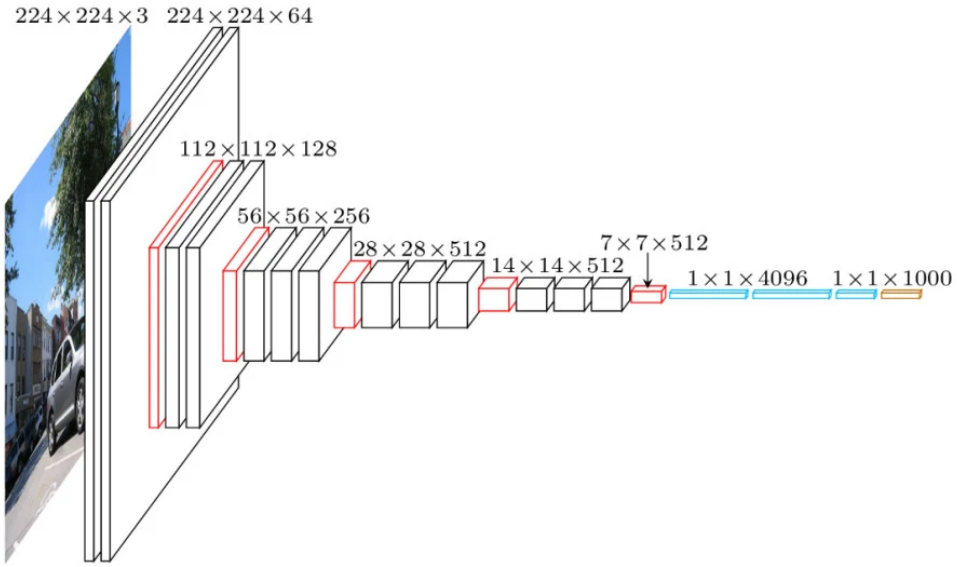

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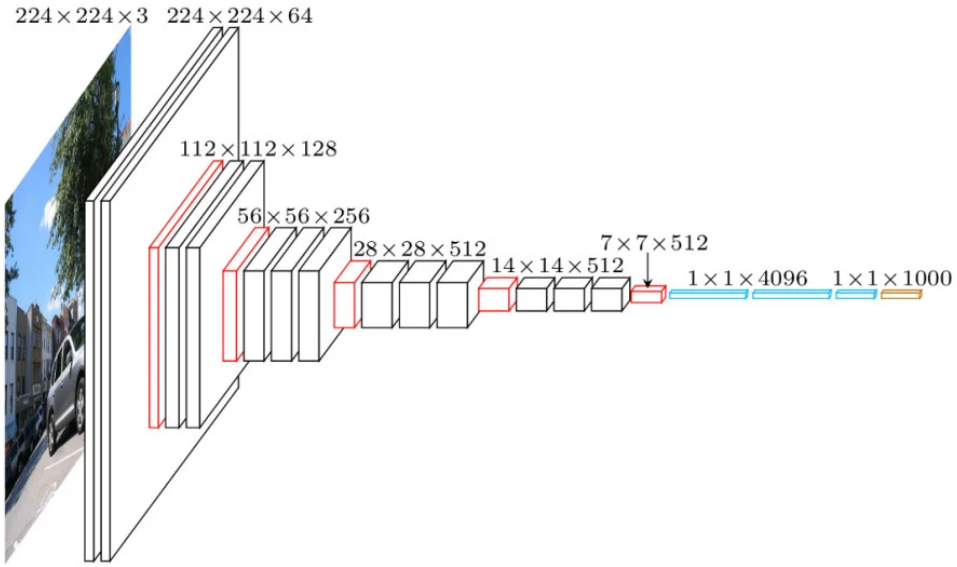

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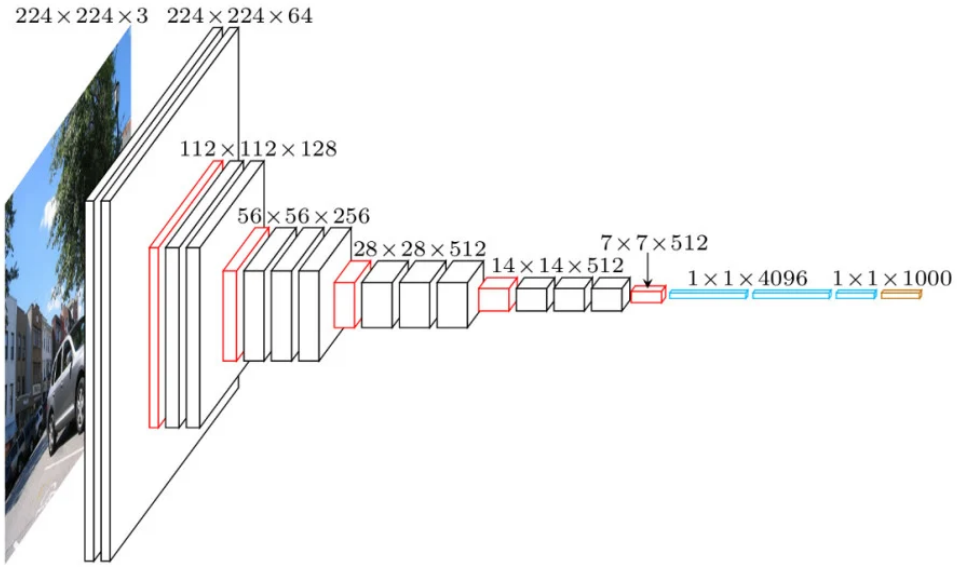

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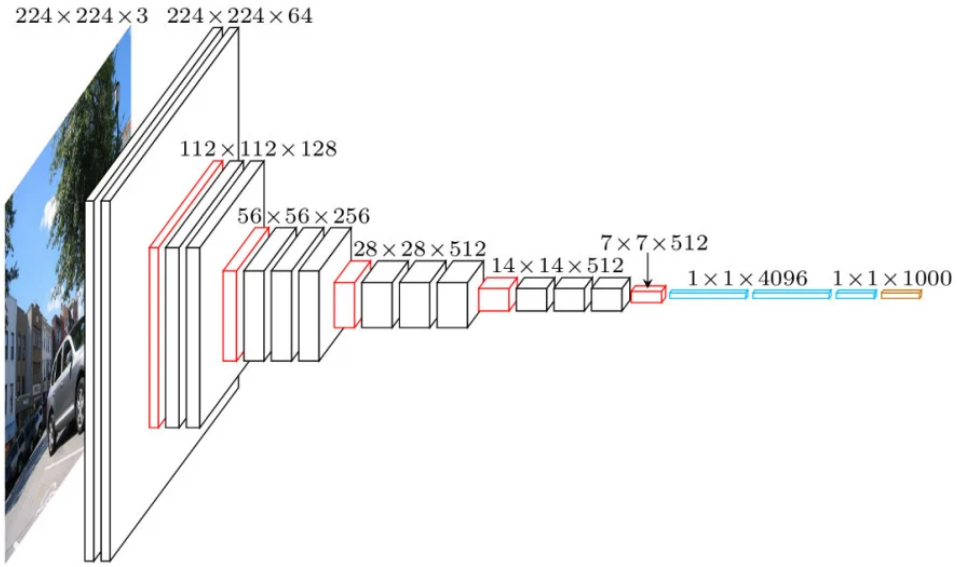

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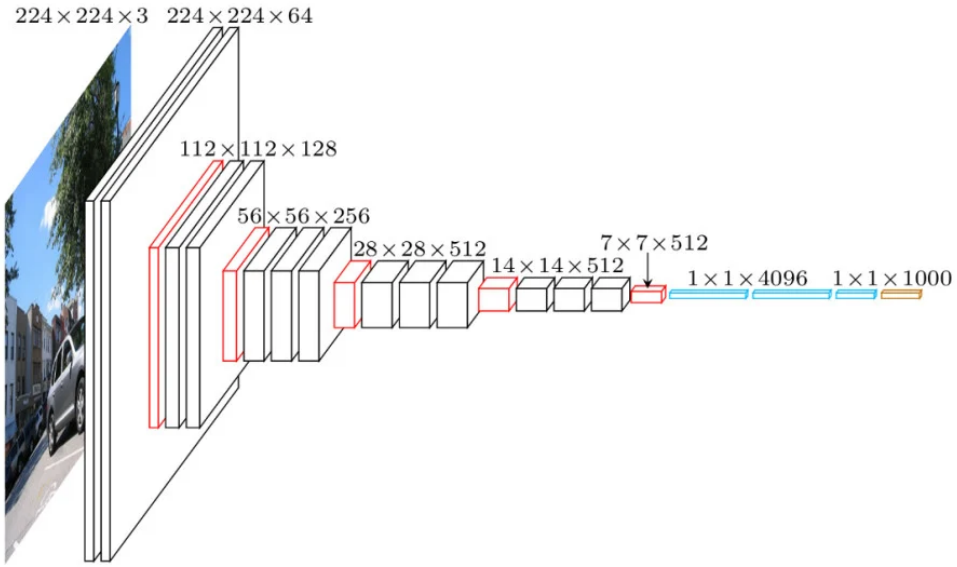

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- Minimization requires computing gradients, called backpropagation

More advanced models

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Bonus:

- The model should be easy to work with.

Deep composition

The simplest example of a nonlinear parametric model:

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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

We call the composition with linear f and nonlinear σ:

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a multi-layer perceptron (MLP) or deep feed-forward neural network.

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Remark: The bias can be integrated inside 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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1. Each layer is a vector-to-vector function $\mathbb{R}^p \to \mathbb{R}^q$.
2. 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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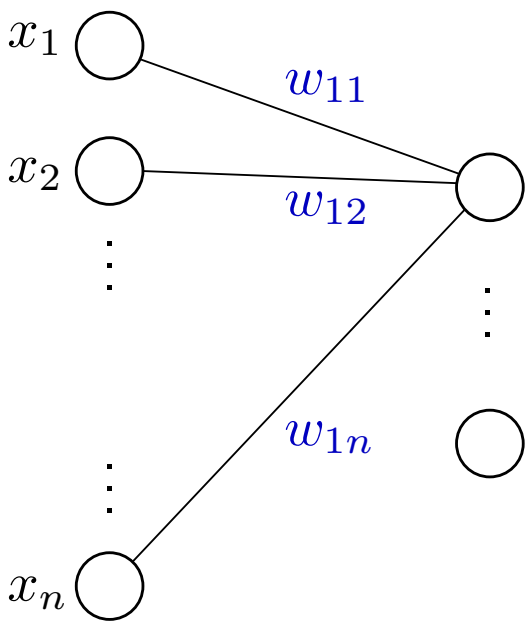

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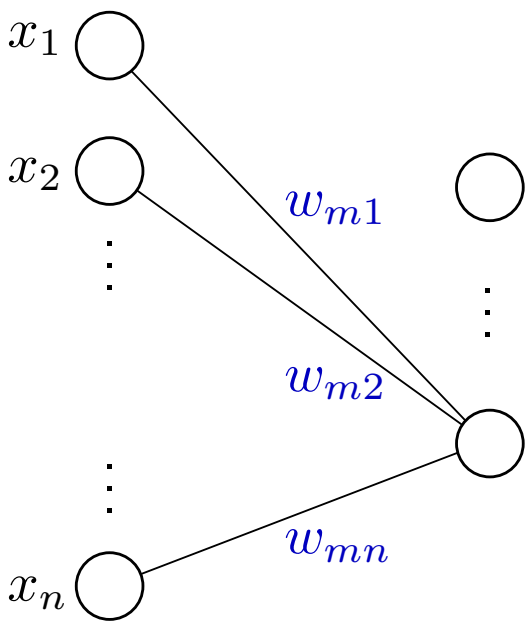

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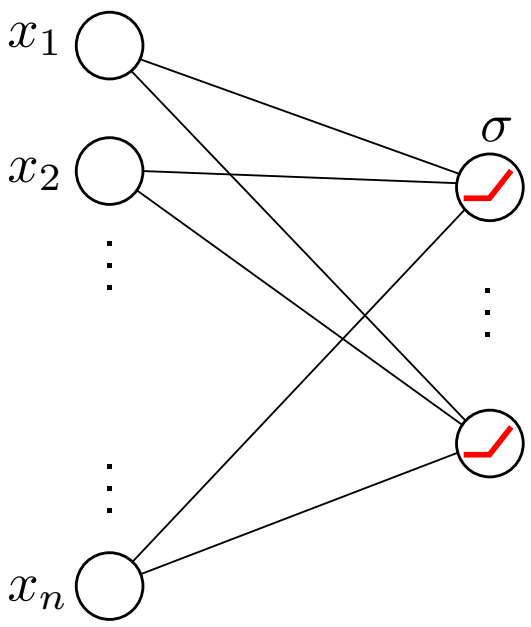

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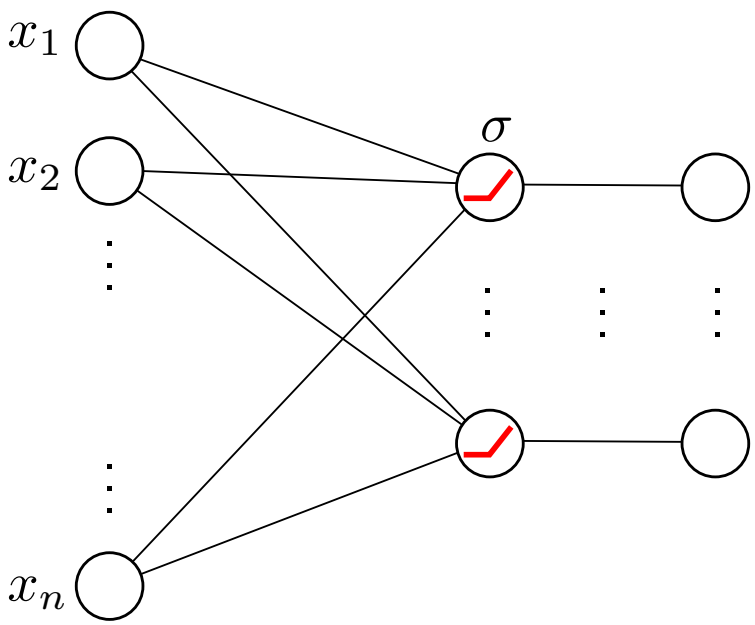

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For generality, it is common to have a linear layer at the output:

$$\mathbf{y} = f \circ (\sigma \circ f) \circ \cdots \circ (\sigma \circ f)(\mathbf{x})$$

mapping:

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Deep ReLU networks

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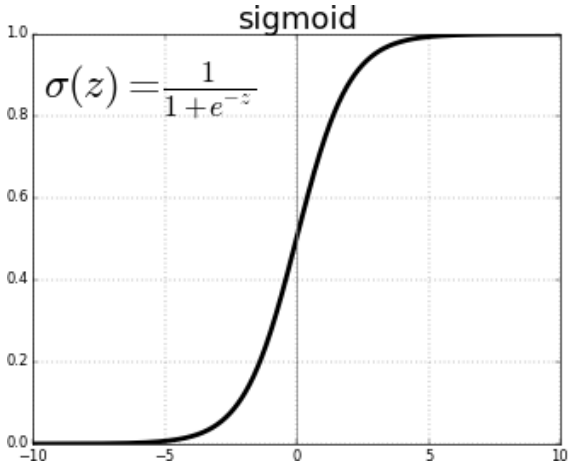

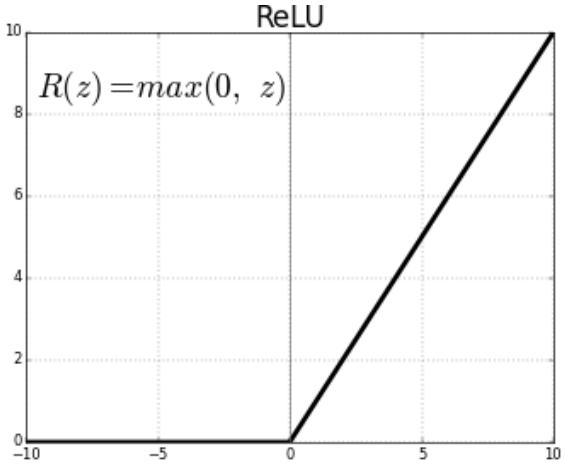

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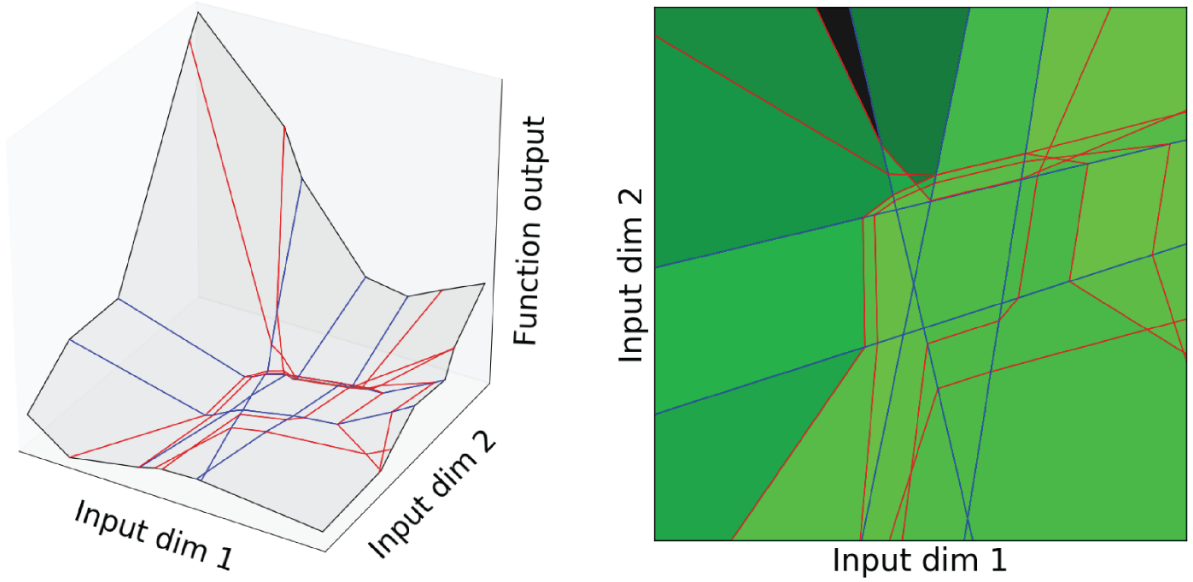

The blue and red edges are produced by the first and second layer.

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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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UAT theorems exist for other activations like 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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In general, the loss is not convex w.r.t. $\boldsymbol{\Theta}$.

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We want to automatize this computational step efficiently.

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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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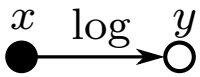

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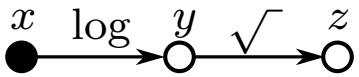

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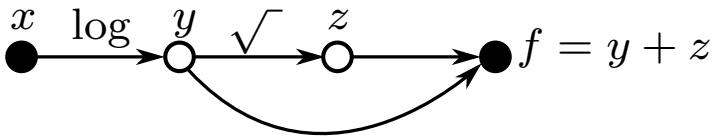

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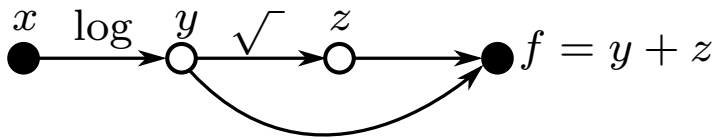

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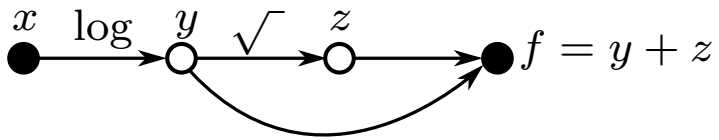

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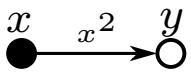

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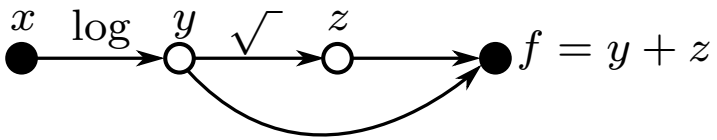

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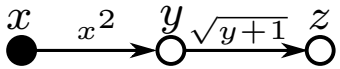

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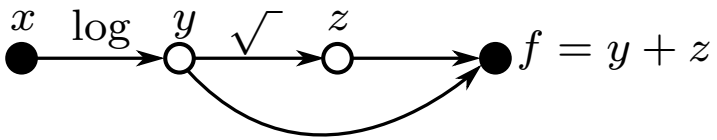

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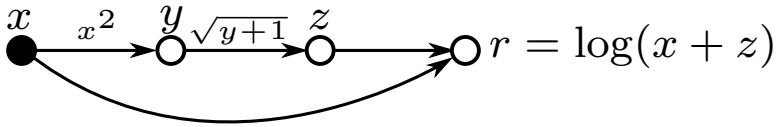

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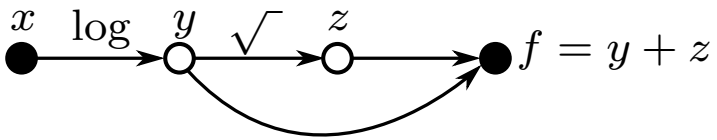

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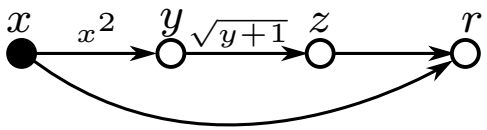

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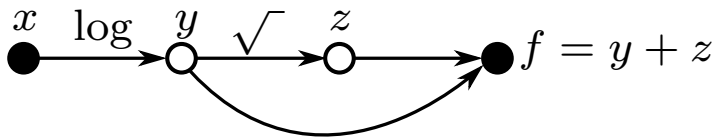

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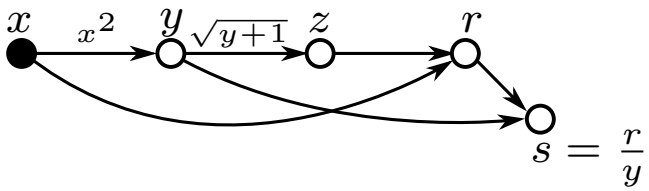

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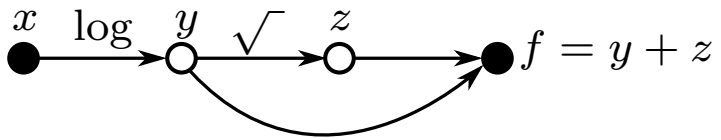

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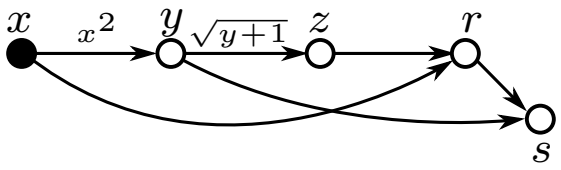

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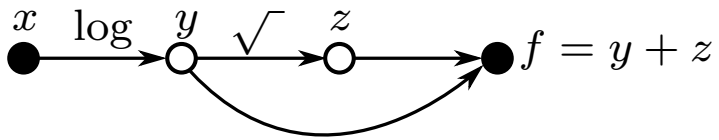

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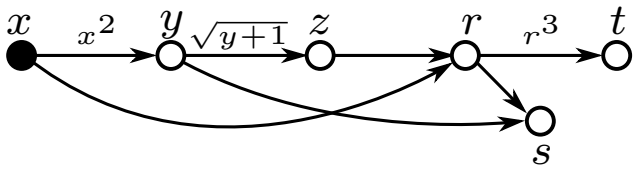

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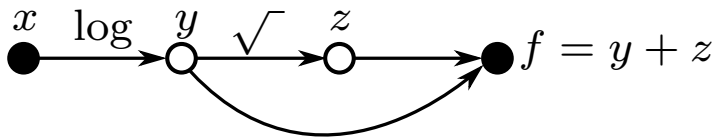

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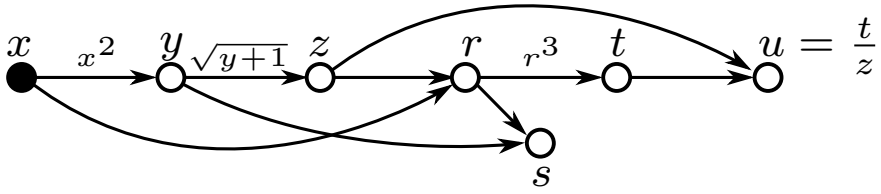

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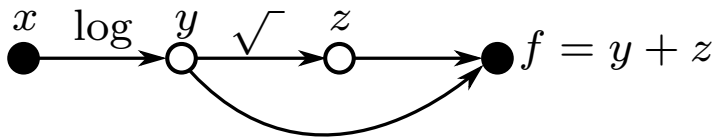

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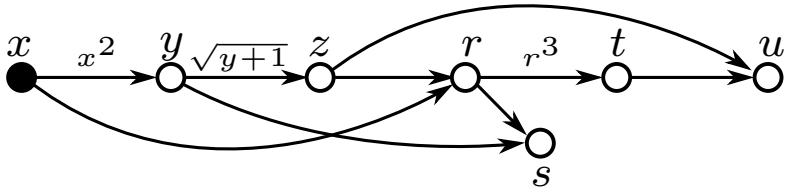

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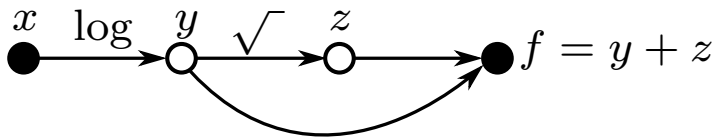

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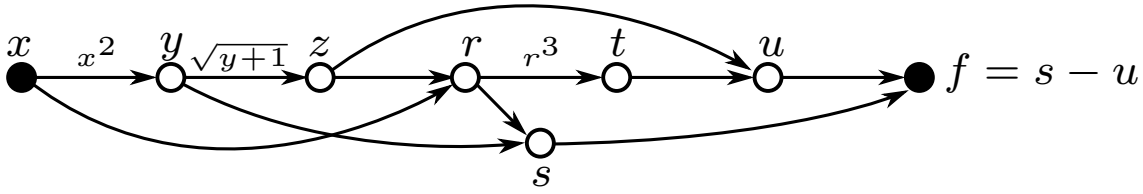
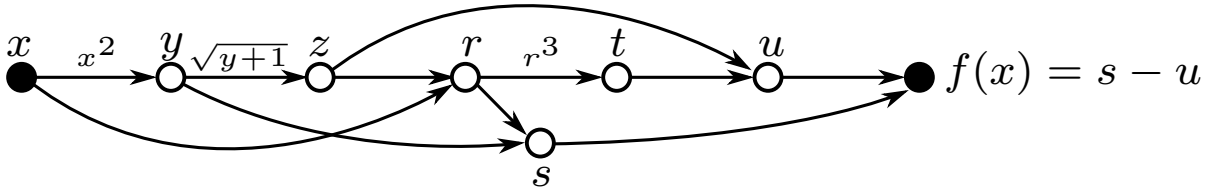


Computational graphs

The evaluation of $f(x)$ corresponds to a forward traversal of the graph:



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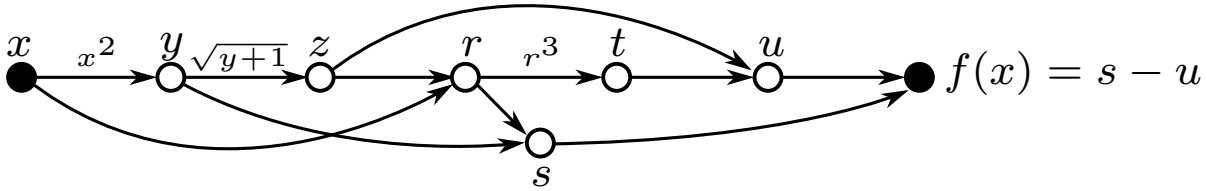

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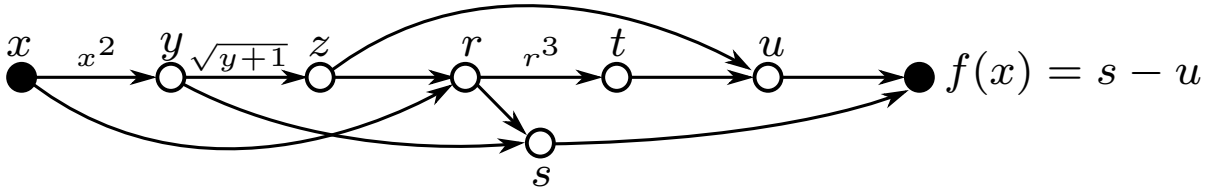

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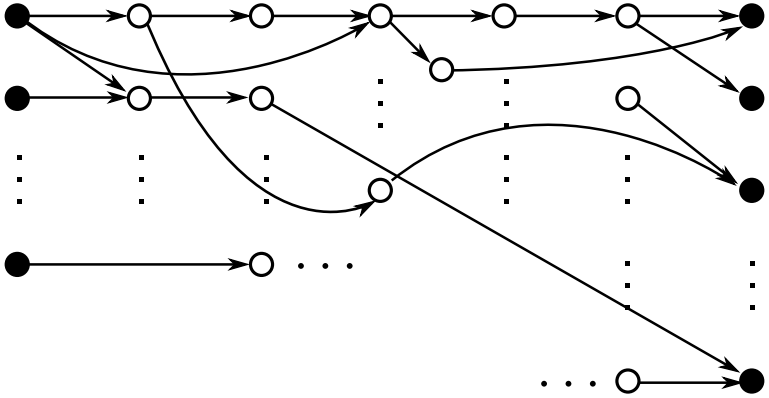
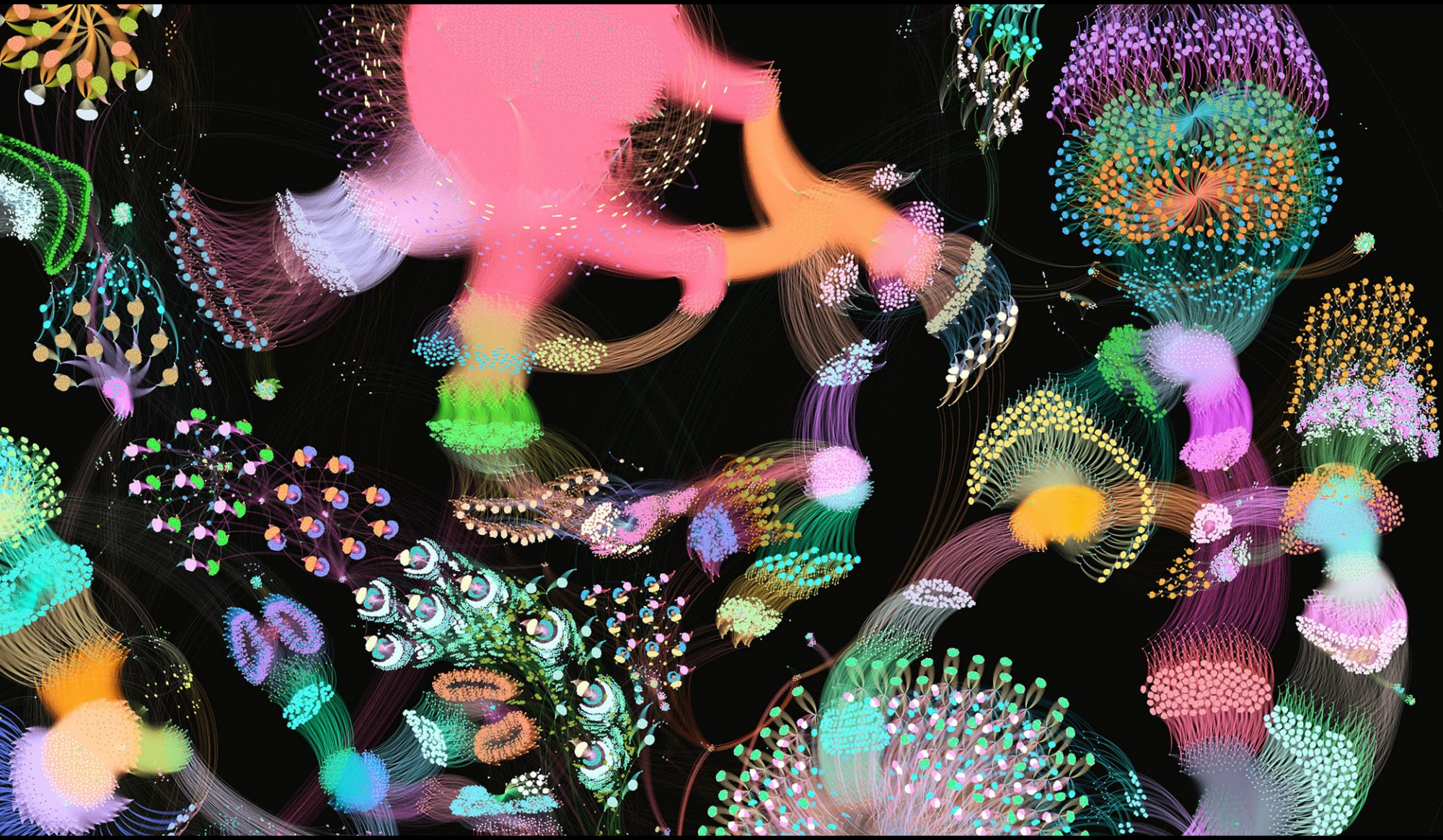
For high-dimensional input/output, the graph may be more complex:



The computational graph gets big quickly.



Poplar visualization, see https://www.graphcore.ai/products/poplar

Automatic differentiation: Forward mode

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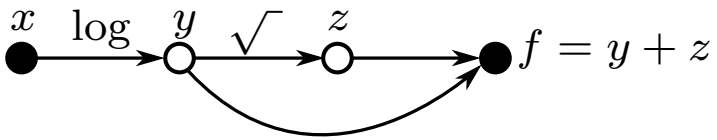

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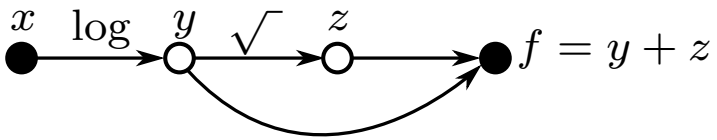

$$\frac{\partial x}{\partial x} = 1$$

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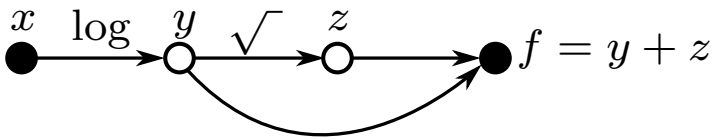

$$\frac{\partial x}{\partial x} = 1$$
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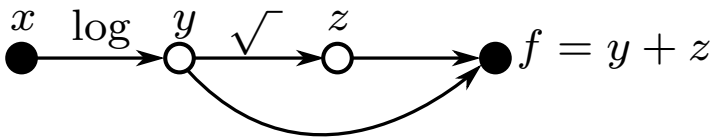

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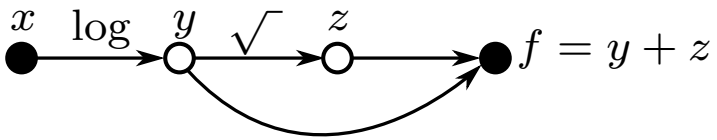

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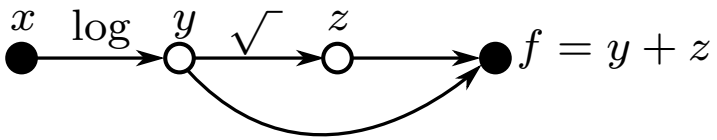

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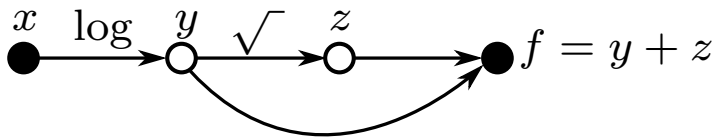

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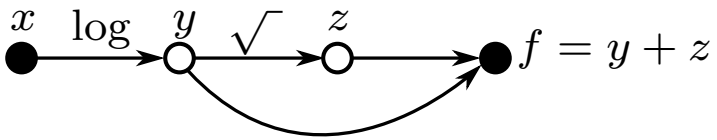

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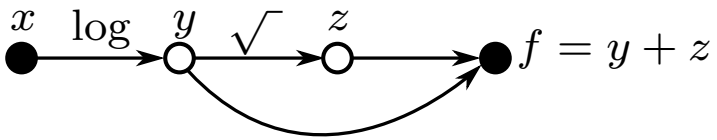

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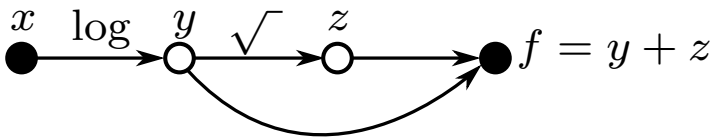

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Automatic differentiation: Forward mode

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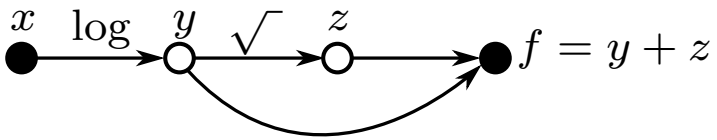

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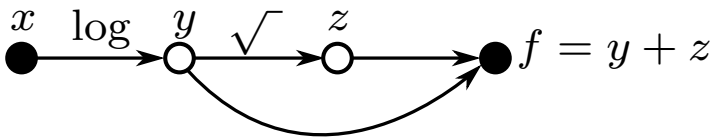

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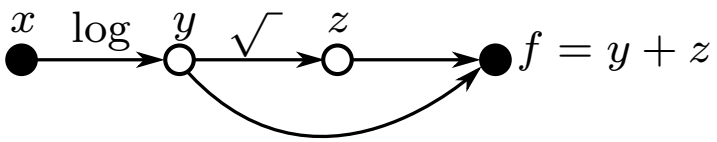

Assumption: Each partial derivative is a "primitive" accessible in closed form and can be computed on the fly.

Automatic differentiation: Forward mode

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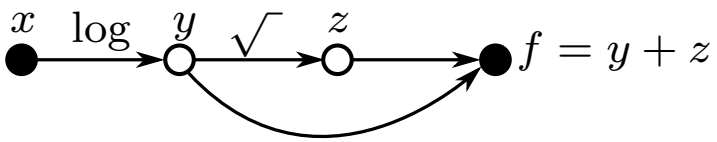

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$$\text{cost of computing } \frac{\partial f}{\partial x}(x) \;=\; \text{cost of computing } f(x)$$

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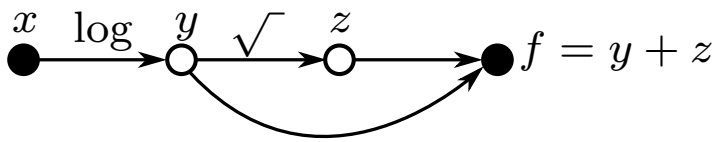

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However, if the input is high-dimensional, i.e. $f : \mathbb{R}^p \to \mathbb{R}$:

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

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

Automatic differentiation: Forward mode

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

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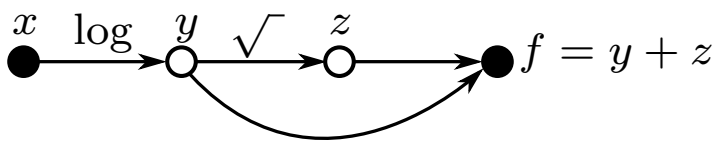
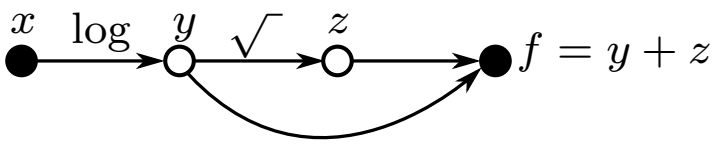


Reverse mode: compute all the partial derivatives $\frac{\partial f}{\partial z}, \ldots, \frac{\partial f}{\partial x}$ with respect to the inner nodes.

Automatic differentiation: Reverse mode

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



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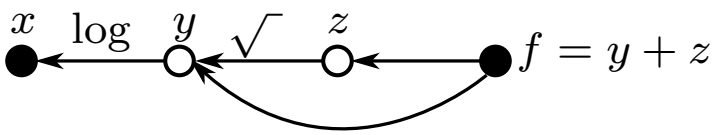

$$\frac{\partial f}{\partial f} = 1$$

Automatic differentiation: Reverse mode

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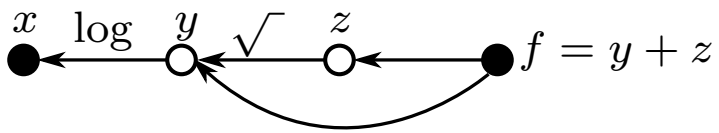

$$\frac{\partial f}{\partial f} = 1$$

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

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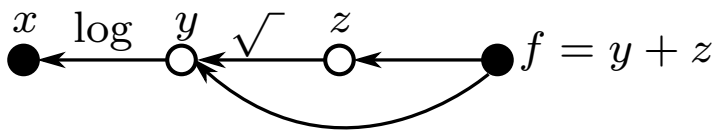

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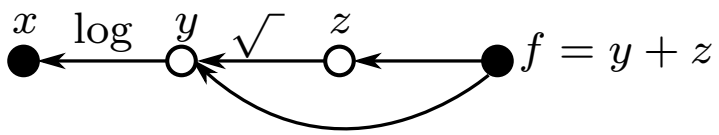

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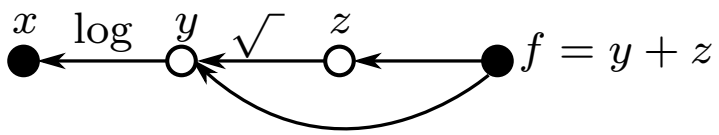

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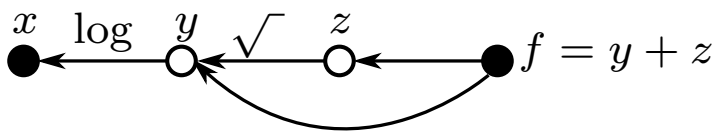

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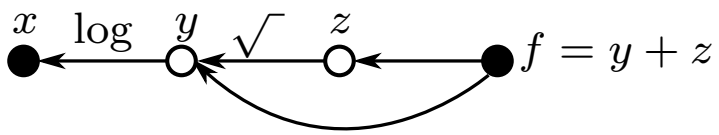

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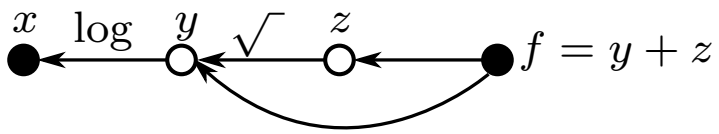

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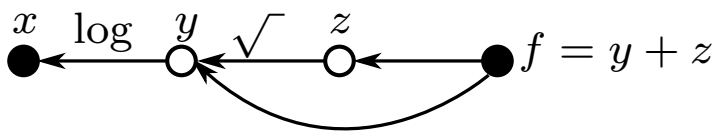

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Automatic differentiation: Reverse mode

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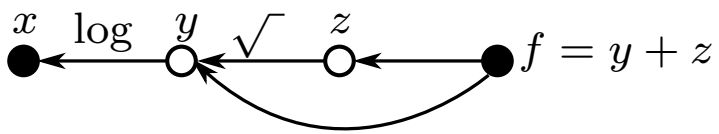

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Automatic differentiation: Reverse mode

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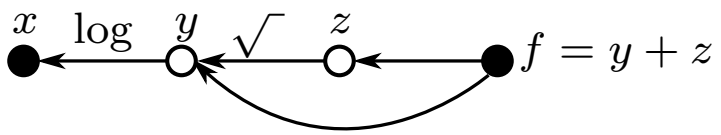

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Automatic differentiation: Reverse mode

Reverse mode requires computing the values of the internal nodes first:

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$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\,\frac{\partial (y+z)}{\partial z} = \frac{\partial f}{\partial f}$$

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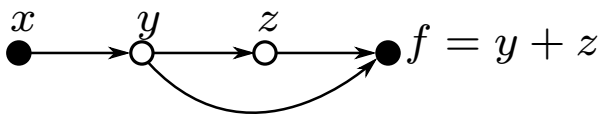
1. Forward pass to evaluate all the interior nodes $y, z, \ldots$.



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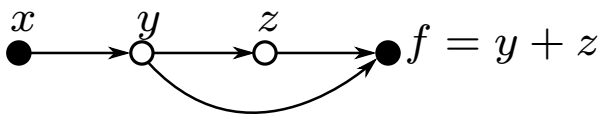

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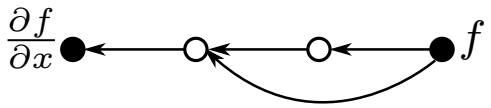
2. Backward pass to compute the derivatives.



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

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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"

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  - Software implementations usually return one of the one-sided derivatives.
  - Numerical issues are always behind the corner.
- Effectively training a deep network is far from a solved problem.

Suggested reading

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