Deep Learning & Applied AI

Multi-layer perceptron and back-propagation

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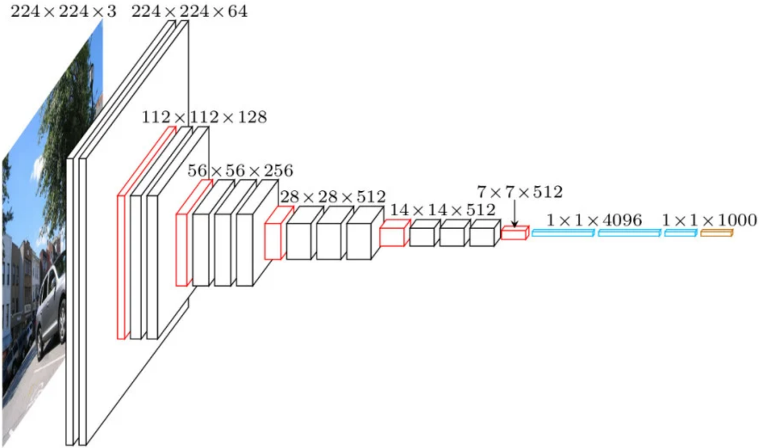
A glimpse into neural networks

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



Deep composition

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(Function composition is associative, so parentheses are not necessary.)

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quindi una linear map seguita da una funzione non lineare (**activation function**)

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More in general, consider other activation functions than logistic:

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

ReLu

continuous

discontinuous gradient

Multi-layer perceptron

We call the composition with linear f and nonlinear σ:

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

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

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

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

viene aggiunta una nuova
dimensione (parametro)

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. perché le unità sono indipendenti tra di loro
   Each unit acts as a scalar function $\mathbb{R}^p \to \mathbb{R}$.

Single layer illustration

$$\sigma(\mathbf{W}\mathbf{x}) = \sigma \circ \begin{pmatrix} w_{11} & w_{12} & \cdots & w_{1n} \\ w_{21} & w_{22} & \cdots & w_{2n} \\ \vdots & \ldots & \ddots & \vdots \\ w_{m1} & w_{m2} & \cdots & w_{mn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \sigma \circ \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

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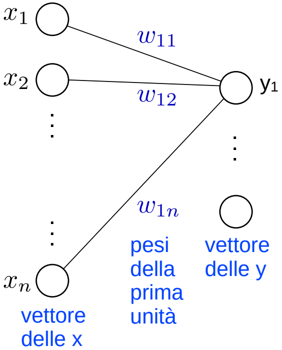
questo è un modo di scrivere le moltiplicazioni tra vettori di sopra (spoiler: è la struttura del MLP)



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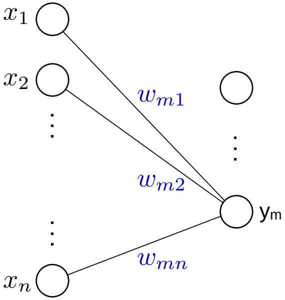

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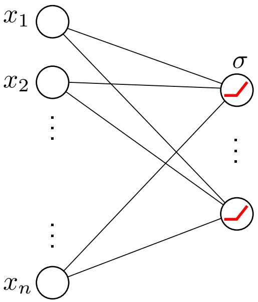

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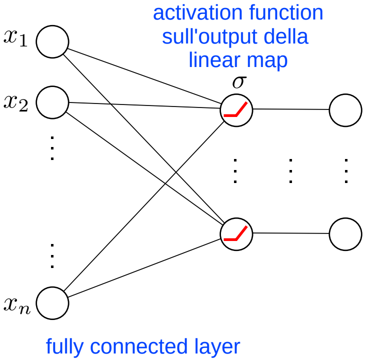

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indica un vettore di dimensione q dove ogni dimensione può assumere valore (0, 1) con 0 e 1 esclusi (classification)

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

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

tranne nel caso di classificazione binaria

mapping:

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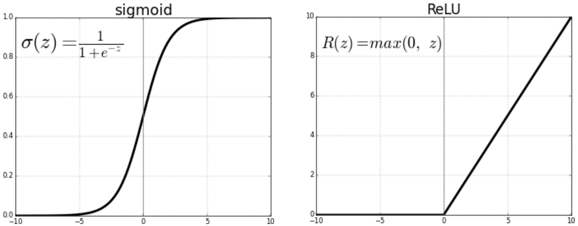

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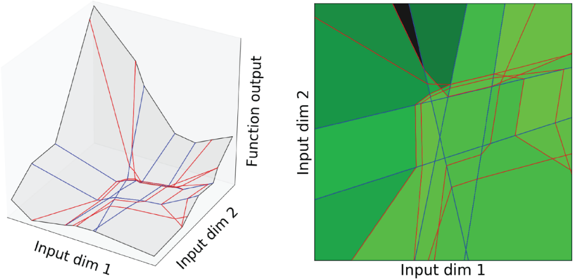

The blue and red edges are produced by the first and second layer.

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If σ is sigmoidal, we have the following:

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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$$|f(\mathbf{x}) - \sum_{k=1}^{q} u_k \phi(\mathbf{x})| \leq \epsilon \qquad \text{for all } \mathbf{x} \in \Omega$$

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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.

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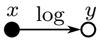

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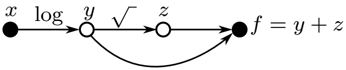

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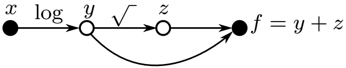

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Consider a generic function $f : \mathbb{R} \to \mathbb{R}$.

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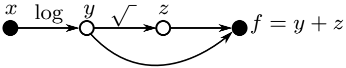

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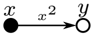

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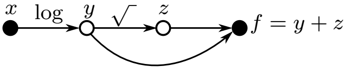

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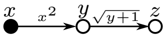

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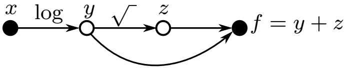

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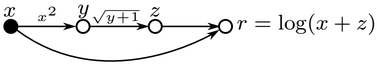

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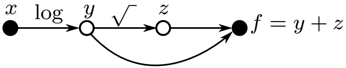

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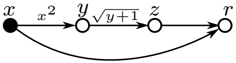

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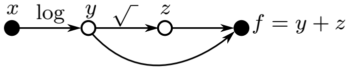

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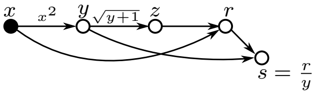

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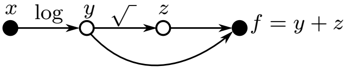

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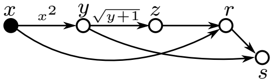

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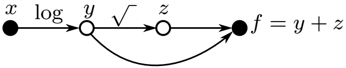

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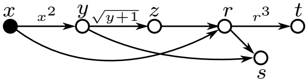

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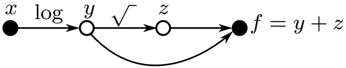

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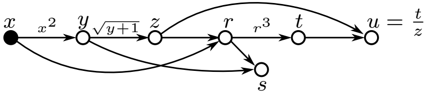

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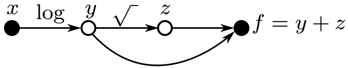

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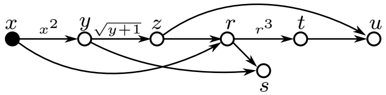

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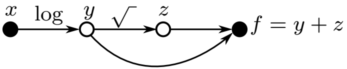
le variabili intermedie sono i pallini bianchi, quelli neri sono l'input e l'output

Example:

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

le frecce indicano che l'operazione è salvata nella variabile successiva



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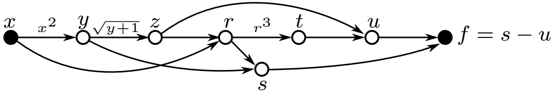
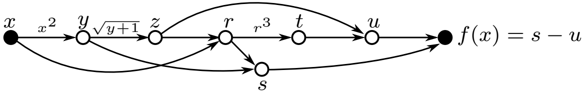


Computational graphs

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



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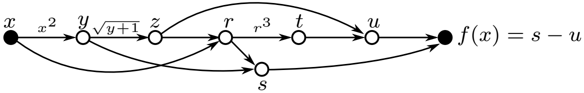

The graph is constructed programmaticaly, for example:

z = sqrt(sum(square(x), 1));

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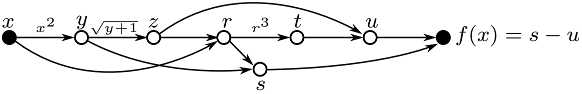

The graph is constructed programmaticaly, for example:

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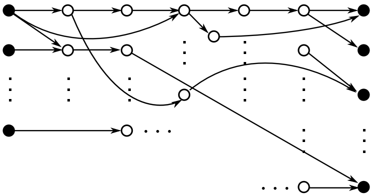
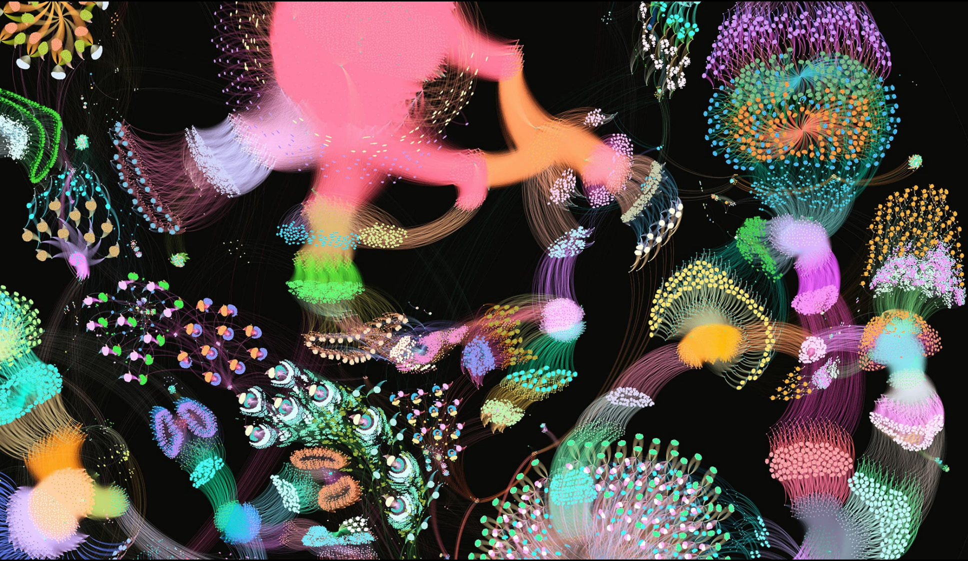
For high-dimensional input/output, the graph may be more complex:



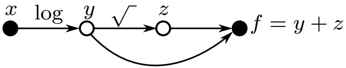
The computational graph gets big quickly.



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

Automatic differentiation: Forward mode

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



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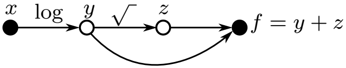

$$\frac{\partial x}{\partial x} = 1$$

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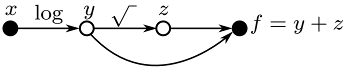

$$\frac{\partial x}{\partial x} = 1$$
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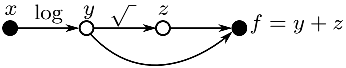

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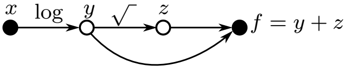

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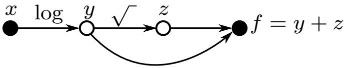

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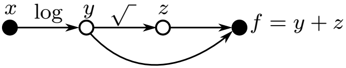

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Automatic differentiation: Forward mode

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$$\begin{tikzcd} x \arrow[r, "\log"] & y \arrow[r, "\sqrt{\ }"] \arrow[rr, bend right] & z \arrow[r] & f = y + z \end{tikzcd}$$

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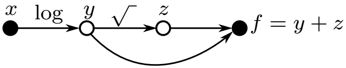

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Automatic differentiation: Forward mode

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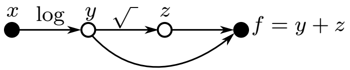
Automatic differentiation: Forward mode

PRIMO METODO PER FARE
AUTOMATIC DIFFERENTATION

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



in pratica, calcola la derivata parziale
per ogni nodo (variabile intermedia e output)
SULLA BASE DI X (l'input) applicando la
chain rule e poi somma tutto. Questo è il
significato di "forward mode"

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

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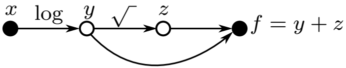
Automatic differentiation: Forward mode

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



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

Automatic differentiation: Forward mode

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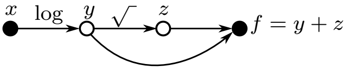

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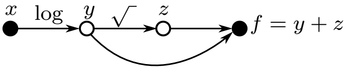
$$\text{cost of computing } \tfrac{\partial f}{\partial x}(x) \;\; = \;\; \text{cost of computing } f(x)$$

Automatic differentiation: Forward mode

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

era il risultato
della slide precedente



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

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

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.

In pratica, è efficiente per funzioni con un piccolo numero di input

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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$$\begin{array}{ccc} \text{Automatic differentiation} & \neq & \text{Symbolic differentiation} \\ \text{(e.g. autograd)} & & \text{(e.g. Mathematica)} \end{array}$$

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

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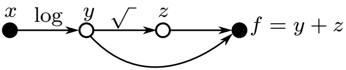
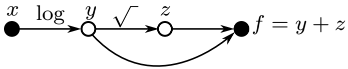


Reverse mode: compute all the partial derivatives $\frac{\partial f}{\partial z}, \ldots, \frac{\partial f}{\partial x}$ with respect to the inner nodes.

Automatic differentiation: Reverse mode

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



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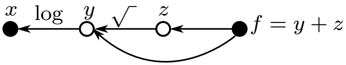
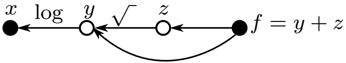


$$\frac{\partial f}{\partial f} = 1$$

Automatic differentiation: Reverse mode

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



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

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

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

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Automatic differentiation: Reverse mode

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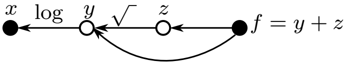

$$\frac{\partial f}{\partial f} = 1$$

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

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

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

Automatic differentiation: Reverse mode

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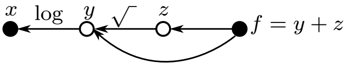

$$\frac{\partial f}{\partial f} = 1$$

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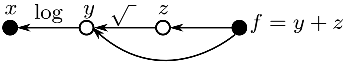

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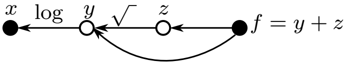

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\frac{\partial f}{\partial y} &= \frac{\partial f}{\partial z}\frac{\partial z}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial f}{\partial y} \\
\frac{\partial f}{\partial x} &=
\end{aligned}
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Automatic differentiation: Reverse mode

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

$$\begin{tikzcd} x & y \arrow[l, "\log"] & z \arrow[l, "\sqrt{\ }"] & f = y + z \arrow[l] \arrow[ll, bend left] \end{tikzcd}$$

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

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

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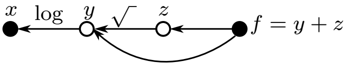

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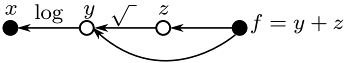

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$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y}\frac{\partial y}{\partial x}$$

Automatic differentiation: Reverse mode

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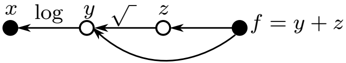

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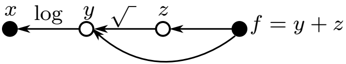
\end{aligned}
$$

Automatic differentiation: Reverse mode

SECONDO METODO PER FARE
AUTOMATIC DIFFERENTATION

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



viene ripetuto lo stesso procedimento di prima, ma inversamente (sulla base dei nodi intermedi partendo da f)

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

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

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Automatic differentiation: Reverse mode

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

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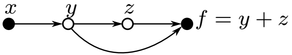
\end{aligned}
$$

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



Remark: This is not forward-mode autodiff, since we are only computing function values.

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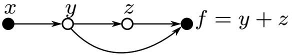
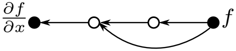


Remark: This is not forward-mode autodiff, since we are only computing function values.

2. Backward pass to compute the derivatives.



La reverse mode è più efficiente per funzioni con un grande numero di parametri (come nelle reti neurali)

Back-propagation

When training neural nets, we compute the gradient of a loss

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

il codominio di una loss function
sarà sempre unidimensionale

where $p \gg 1$ is the number of weights.

Back-propagation

When training neural nets, we compute the gradient of a loss

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matrici di gradienti

Instead of simple derivatives we must compute gradients and Jacobians.

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

where $p \gg 1$ is the number of weights.

Instead of simple derivatives we must compute gradients and Jacobians.

$$\ell = \epsilon(\sigma \circ f \circ \sigma \circ f \circ \cdots \circ f)$$

ϵ computes the actual scalar error for the loss.

Back-propagation

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$$\ell = \epsilon(f_{t-1} \circ f_{t-2} \circ \cdots \circ f_2 \circ f_1)$$

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Denote by $\mathbf{J}_k$ the Jacobian at layer k.

- Forward-mode autodiff:

$$\nabla \ell = \mathbf{J}_{t-1}(\mathbf{J}_{t-2}(\cdots(\mathbf{J}_3(\mathbf{J}_2\mathbf{J}_1))))$$

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- Reverse-mode autodiff:

$$\nabla \ell = ((((\mathbf{J}_{t-1}\mathbf{J}_{t-2})\mathbf{J}_{t-3})\cdots)\mathbf{J}_2)\mathbf{J}_1$$

Back-propagation ridenominazione della reverse mode

When training neural nets, we compute the gradient of a loss

$$\ell : \mathbb{R}^{p} \to \mathbb{R}^{1}$$

where $p \gg 1$ is the number of weights.

Instead of simple derivatives we must compute gradients and Jacobians.

le derivate allo step k

$$\ell = \epsilon(f_{t-1} \circ f_{t-2} \circ \cdots \circ f_2 \circ f_1)$$

Denote by $\mathbf{J}_k$ the Jacobian at layer k.

- Forward-mode autodiff:

$$\nabla \ell = \mathbf{J}_{t-1}(\mathbf{J}_{t-2}(\cdots(\mathbf{J}_3(\mathbf{J}_2\mathbf{J}_1)))) \qquad \#\text{ ops: } \; p\sum_{k=2}^{t-1} d_k d_{k+1}$$

- Reverse-mode autodiff:

$$\nabla \ell = ((((\mathbf{J}_{t-1}\mathbf{J}_{t-2})\mathbf{J}_{t-3})\cdots)\mathbf{J}_2)\mathbf{J}_1 \qquad \#\text{ ops: } \; 1\sum_{k=1}^{t-2} d_k d_{k+1}$$

le parentesi indicano che
il risultato di quella chain rule
è salvato in qualche modo

Back-propagation

We call back-propagation the reverse mode automatic differentiation applied to deep neural networks.

Evaluating $\nabla \ell$ with backprop is as fast as evaluating ℓ.

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In fact, not even the costly forward mode is just the chain rule. There are intermediate variables. Backprop is a computational technique.

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