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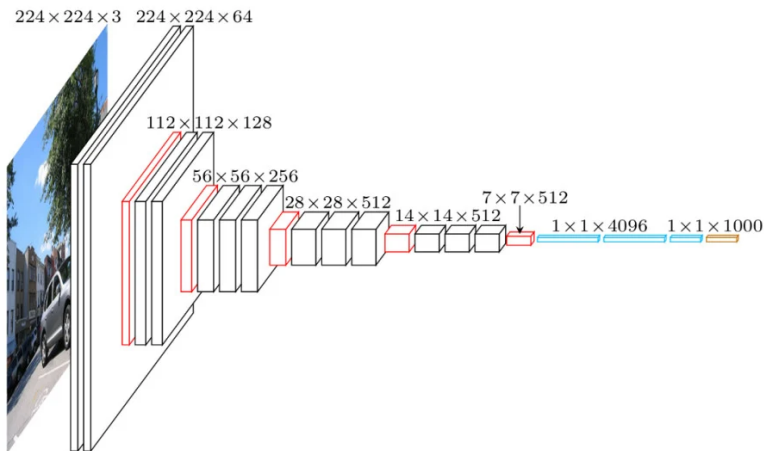
Multi-layer perceptron and back-propagation

Emanuele Rodolà

rodola@di.uniroma1.it

SAPIENZA
Università di Roma

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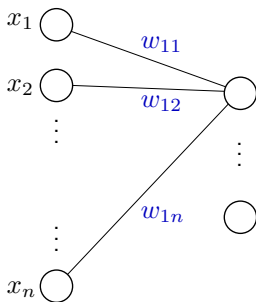
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1. Each layer is a vector-to-vector function $\mathbb{R}^p \to \mathbb{R}^q$.

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

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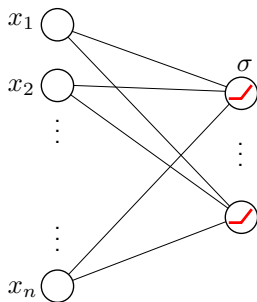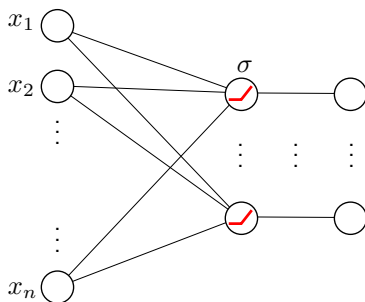
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For generality, it is common to have a linear layer at the output:

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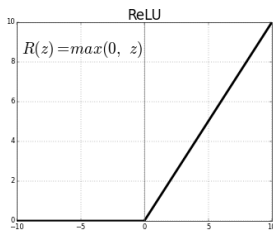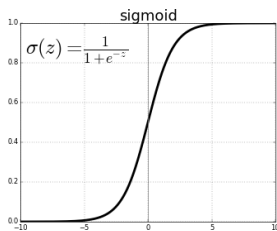
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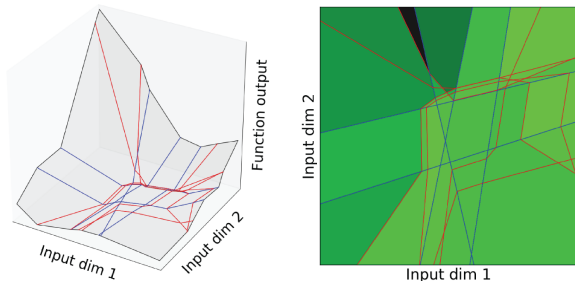
The blue and red edges are produced by the first and second layer.

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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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The network in the theorem has just one hidden layer.

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

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We want to automatize this computational step efficiently.

Computational graphs

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

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

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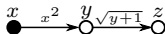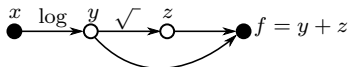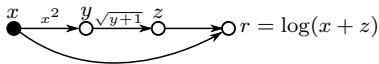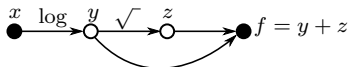
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x
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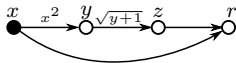A computational graph is a directed acyclic graph representing the computation of $f(x)$ with intermediate variables.

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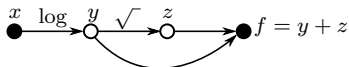# Computational graphs

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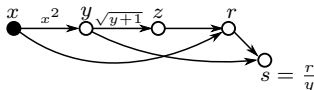A computational graph is a directed acyclic graph representing the computation of $f(x)$ with intermediate variables.

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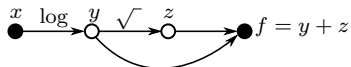# Computational graphs

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

Example:

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

$\overset{x}{\bullet} \xrightarrow{\log} \overset{y}{\circ} \xrightarrow{\sqrt{\;}} \overset{z}{\circ} \longrightarrow \bullet \, f = y + z$

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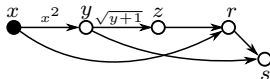A computational graph is a directed acyclic graph representing the computation of $f(x)$ with intermediate variables.

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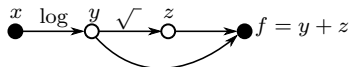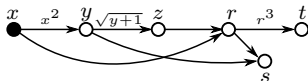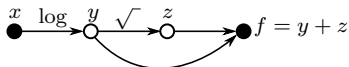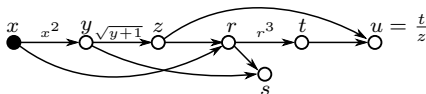$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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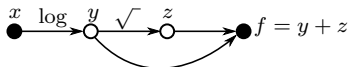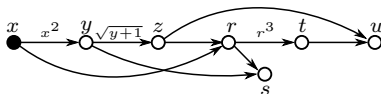$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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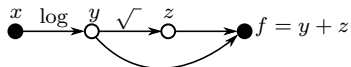$$f(x) = \frac{\log(x + \sqrt{x^2 + 1})}{x^2} - \frac{\log^3(x + \sqrt{x^2 + 1})}{\sqrt{x^2 + 1}}$$

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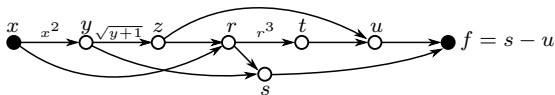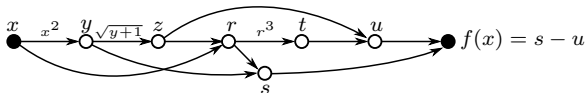
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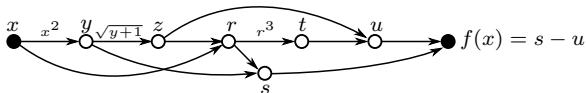
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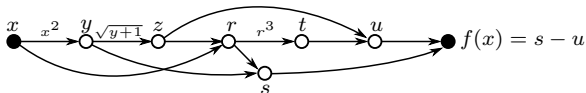
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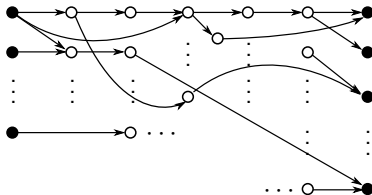
The computational graph gets big quickly.
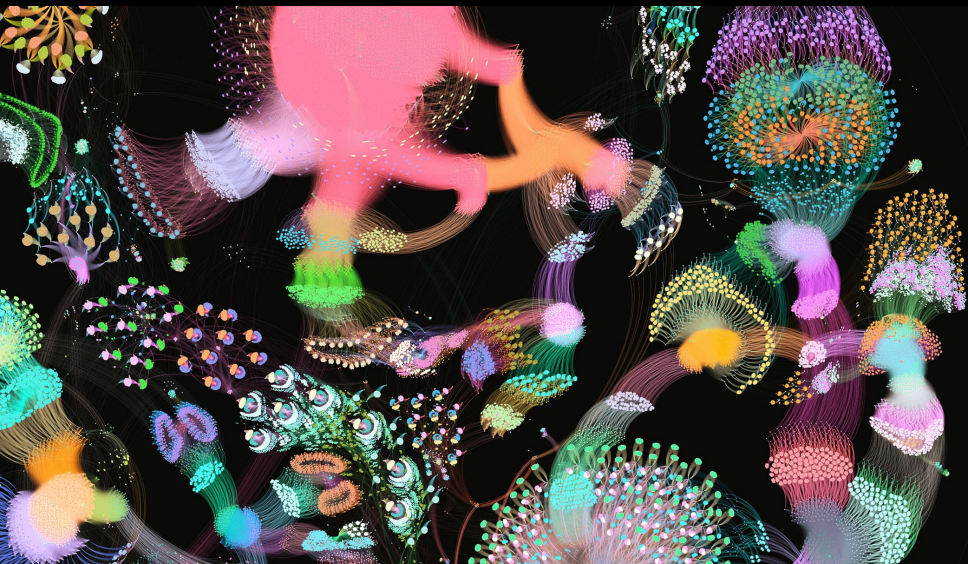
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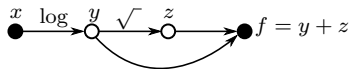
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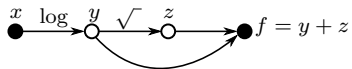
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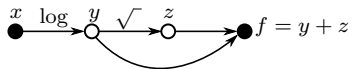
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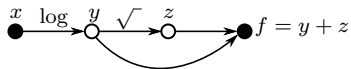
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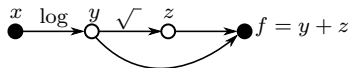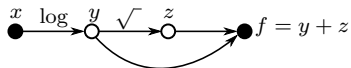
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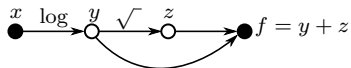
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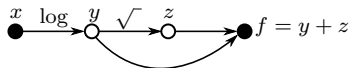
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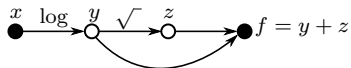
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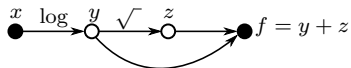$$f(x) = \log x + \sqrt{\log x}$$

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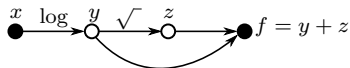$$f(x) = \log x + \sqrt{\log x}$$

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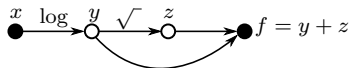$$f(x) = \log x + \sqrt{\log x}$$

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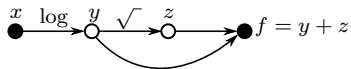$$f(x) = \log x + \sqrt{\log x}$$

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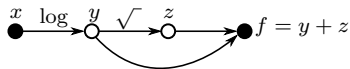
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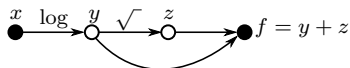

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However, if the input is high-dimensional, i.e. $f : \mathbb{R}^p \to \mathbb{R}$:

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

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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$$\text{(e.g. autograd)} \qquad \text{(e.g. Mathematica)}$$

We accumulate values during code execution to generate numerical derivative evaluations rather than derivative expressions.
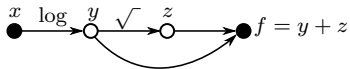
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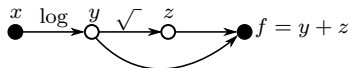
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$$\overset{x}{\bullet} \overset{\log}{\longrightarrow} \overset{y}{\circ} \overset{\sqrt{}}{\longrightarrow} \overset{z}{\circ} \longrightarrow \bullet \, f = y + z$$

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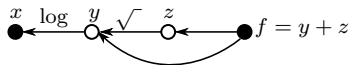
Automatic differentiation: Reverse mode

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

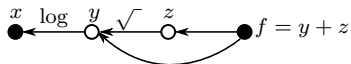# Automatic differentiation: Reverse mode

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

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

Automatic differentiation: Reverse mode

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

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

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

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

Automatic differentiation: Reverse mode

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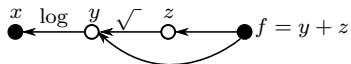$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f} \frac{\partial f}{\partial z}$$

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Automatic differentiation: Reverse mode

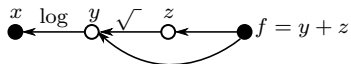$$f(x) = \log x + \sqrt{\log x}$$

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Automatic differentiation: Reverse mode

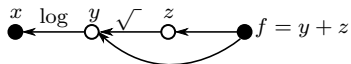$$f(x) = \log x + \sqrt{\log x}$$

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Automatic differentiation: Reverse mode

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

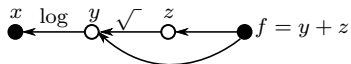$$\frac{\partial f}{\partial f} = 1$$

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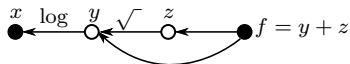

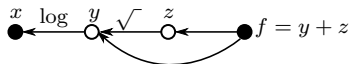$$\frac{\partial f}{\partial f} = 1$$

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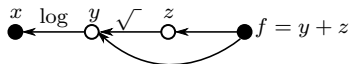$$f(x) = \log x + \sqrt{\log x}$$

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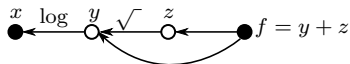$$f(x) = \log x + \sqrt{\log x}$$

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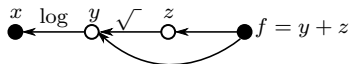$$f(x) = \log x + \sqrt{\log x}$$

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

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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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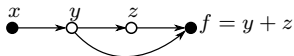Reverse mode requires computing the values of the internal nodes first:
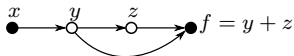
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1. Forward pass to evaluate all the interior nodes $y, z, \ldots$.

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2. Backward pass to compute the derivatives.

Back-propagation

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

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

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

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

ϵ computes the actual scalar error for the loss.

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

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

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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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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