Machine Learning

Multi-layer perceptron and back-propagation

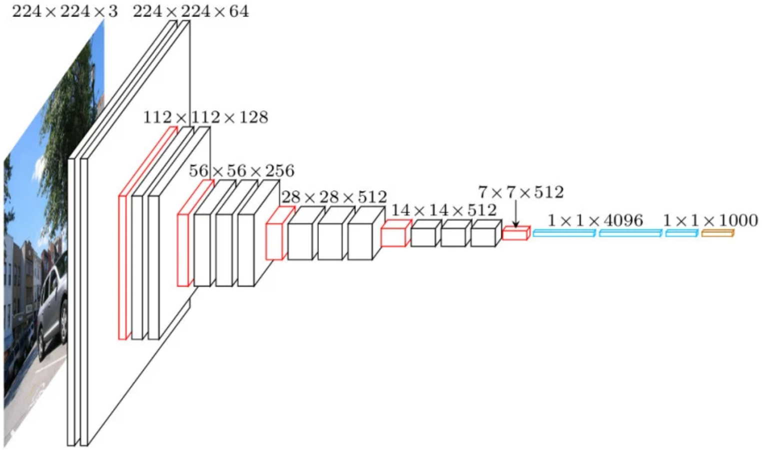
Emanuele Rodolà
rodola@di.uniroma1.it

SAPIENZA
UNIVERSITÀ DI ROMA

2nd semester a.y. 2023/2024 · March 26, 2024

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:

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

Deep composition

The simplest example of a nonlinear parametric model:

$$\underbrace{f}_{\text{linear}} \circ \underbrace{f}_{\text{linear}}(\mathbf{x})$$

Deep composition

The simplest example of a nonlinear parametric model:

$$\underbrace{f \circ f}_{\text{linear}}(\mathbf{x})$$

Deep composition

The simplest example of a nonlinear parametric model:

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

If σ is the logistic function, we have logistic regression.

Deep composition

The simplest example of a nonlinear parametric model:

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

If σ is the logistic function, we have logistic regression.

Consider multiple layers of logistic regression models:

$$\underbrace{(\sigma \circ f)}_{\text{layer}} \circ (\sigma \circ f) \circ \cdots \circ \underbrace{(\sigma \circ f)}_{\text{layer}}(\mathbf{x})$$

Deep composition

The simplest example of a nonlinear parametric model:

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

If σ is the logistic function, we have logistic regression.

Consider multiple layers of logistic regression models:

$$\text{output} \leftarrow \underbrace{(\sigma \circ f)}_{\text{layer } n} \circ (\sigma \circ f) \circ \cdots \circ \underbrace{(\sigma \circ f)}_{\text{layer } 1}(\mathbf{x}) \leftarrow \text{input}$$

Deep composition

The simplest example of a nonlinear parametric model:

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

If σ is the logistic function, we have logistic regression.

Consider multiple layers of logistic regression models:

$$\text{output} \leftarrow \underbrace{(\sigma \circ f)}_{\text{output layer}} \circ (\sigma \circ f) \circ \cdots \circ \underbrace{(\sigma \circ f)}_{\text{input layer}} (\mathbf{x}) \leftarrow \text{input}$$

Deep composition

The simplest example of a nonlinear parametric model:

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

If σ is the logistic function, we have logistic regression.

Consider multiple layers of logistic regression models:

$$\text{output} \leftarrow \underbrace{(\sigma \circ f)}_{\text{output layer}} \circ (\sigma \circ f) \circ \cdots \circ \underbrace{(\sigma \circ f)}_{\text{input layer}} (\mathbf{x}) \leftarrow \text{input}$$

More in general, consider other activation functions:

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

continuous

discontinuous gradient

Multi-layer perceptron

We call the composition:

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

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

Multi-layer perceptron

We call the composition:

$$g_{\mathbf{\Theta}}(\mathbf{x}) = (\sigma \circ f_{\mathbf{\Theta}_n}) \circ (\sigma \circ f_{\mathbf{\Theta}_{n-1}}) \circ \cdots \circ (\sigma \circ f_{\mathbf{\Theta}_1})(\mathbf{x})$$

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

The weights of the MLP are scattered across the layers.

Multi-layer perceptron

We call the composition:

$$g_{\mathbf{\Theta}}(\mathbf{x}) = (\sigma \circ f_{\mathbf{\Theta}_n}) \circ (\sigma \circ f_{\mathbf{\Theta}_{n-1}}) \circ \cdots \circ (\sigma \circ f_{\mathbf{\Theta}_1})(\mathbf{x})$$

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

The weights of the MLP are scattered across the layers.

Each layer outputs an intermediate hidden representation:

$$\mathbf{x}_{\ell+1} = \sigma_\ell(\mathbf{W}_\ell \mathbf{x}_\ell + \mathbf{b}_\ell)$$

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

Multi-layer perceptron

We call the composition:

$$g_{\boldsymbol{\Theta}}(\mathbf{x}) = (\sigma \circ f_{\boldsymbol{\Theta}_n}) \circ (\sigma \circ f_{\boldsymbol{\Theta}_{n-1}}) \circ \cdots \circ (\sigma \circ f_{\boldsymbol{\Theta}_1})(\mathbf{x})$$

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

The weights of the MLP are scattered across the layers.

Each layer outputs an intermediate hidden representation:

$$\mathbf{x}_{\ell+1} = \sigma_\ell(\mathbf{W}_\ell \mathbf{x}_\ell + \mathbf{b}_\ell)$$

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

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

Hidden units

At each hidden layer we have:

$$\mathbf{x}_{\ell+1} = \sigma_\ell(\mathbf{W}_\ell \mathbf{x}_\ell + \mathbf{b}_\ell)$$

Hidden units

At each hidden layer we have:

$$\mathbf{x}_{\ell+1} = \sigma_\ell(\mathbf{W}_\ell \mathbf{x}_\ell + \mathbf{b}_\ell)$$

Each row is called a hidden unit or neuron:

$$\mathbf{W}\mathbf{x} = \begin{pmatrix} \text{--- neuron ---} \\ \vdots \\ \text{--- neuron ---} \end{pmatrix} \begin{pmatrix} | \\ \mathbf{x} \\ | \end{pmatrix}$$

Hidden units

At each hidden layer we have:

$$\mathbf{x}_{\ell+1} = \sigma_\ell(\mathbf{W}_\ell \mathbf{x}_\ell + \mathbf{b}_\ell)$$

Each row is called a hidden unit or neuron:

$$\mathbf{W}\mathbf{x} = \begin{pmatrix} \text{— neuron —} \\ \vdots \\ \text{— neuron —} \end{pmatrix} \begin{pmatrix} | \\ \mathbf{x} \\ | \end{pmatrix}$$

We have two interpretations:

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

Hidden units

At each hidden layer we have:

$$\mathbf{x}_{\ell+1} = \sigma_\ell(\mathbf{W}_\ell \mathbf{x}_\ell + \mathbf{b}_\ell)$$

Each row is called a hidden unit or neuron:

$$\mathbf{W}\mathbf{x} = \begin{pmatrix} \text{— neuron —} \\ \vdots \\ \text{— neuron —} \end{pmatrix} \begin{pmatrix} | \\ \mathbf{x} \\ | \end{pmatrix}$$

We have two interpretations:

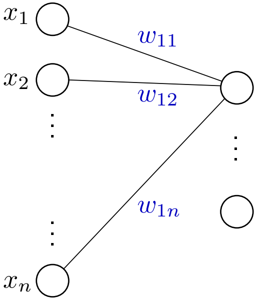
1. Each layer is a vector-to-vector function $\mathbb{R}^p \to \mathbb{R}^q$.
2. Each layer has q neurons acting in parallel.
   Each neuron acts as a scalar function $\mathbb{R}^p \to \mathbb{R}$.

Single layer illustration

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

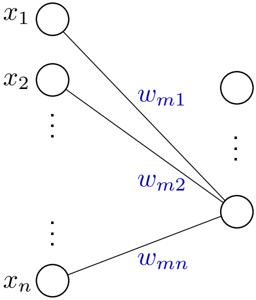
Single layer illustration

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



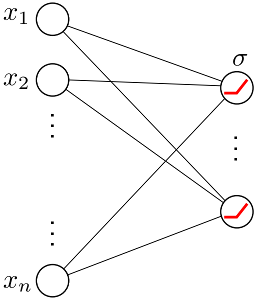
Single layer illustration

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



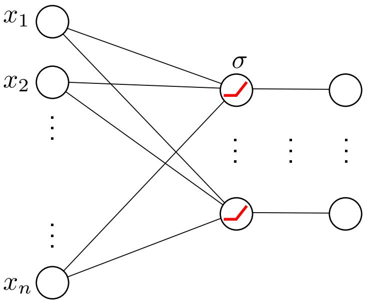
Single layer illustration

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



Single layer illustration

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



Output layer

The output layer determines the co-domain of the network:

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

Output layer

The output layer determines the co-domain of the network:

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

If σ is the logistic sigmoid, the entire network will map:

$$\mathbb{R}^p \to (0,1)^q$$

Output layer

The output layer determines the co-domain of the network:

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

If σ is the logistic sigmoid, the entire network will map:

$$\mathbb{R}^p \to (0,1)^q$$

It is common to have a linear layer at the output:

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

which maps:

$$\mathbb{R}^p \to \mathbb{R}^q$$

Deep ReLU networks

Let's add a linear layer at the output:

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

Deep ReLU networks

Let's add a linear layer at the output:

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

Then, $\mathbf{y}$ is a combination of "ridge functions" $\sigma(\cdots)$.

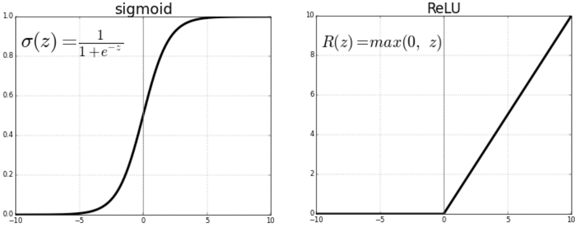
Deep ReLU networks

Let's add a linear layer at the output:

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

Then, $\mathbf{y}$ is a combination of "ridge functions" $\sigma(\cdots)$.

For a 2-layer network with activation $\sigma(x) = \max\{0, x\}$ (rectifier), we get a piecewise-linear function:



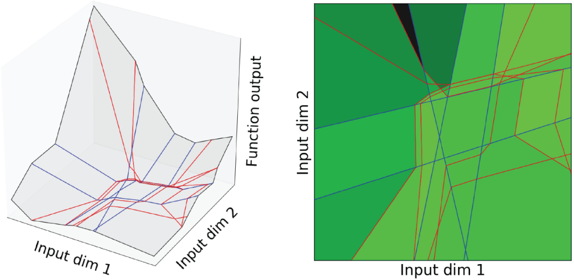
Deep ReLU networks

Let's add a linear layer at the output:

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

Then, $\mathbf{y}$ is a combination of "ridge functions" $\sigma(\cdots)$.

For a 2-layer network with activation $\sigma(x) = \max\{0, x\}$ (rectifier), we get a piecewise-linear function:



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

Universality

What class of functions can we represent with a MLP?

Universality

What class of functions can we represent with a MLP?

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.

Cybenko, "Approximations by superpositions of sigmoidal functions", 1989

Universality

What class of functions can we represent with a MLP?

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. Thus, for any continuous function f and any $\epsilon > 0$, there exists $q \in \mathbb{N}$ and weights s.t.:

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

Cybenko, "Approximations by superpositions of sigmoidal functions", 1989

Universality

What class of functions can we represent with a MLP?

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. Thus, for any continuous function f and any $\epsilon > 0$, there exists $q \in \mathbb{N}$ and weights s.t.:

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

The network in the theorem has just one hidden layer.

Cybenko, "Approximations by superpositions of sigmoidal functions", 1989

Universality

What class of functions can we represent with a MLP?

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. Thus, for any continuous function f and any $\epsilon > 0$, there exists $q \in \mathbb{N}$ and weights s.t.:

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

The network in the theorem has just one hidden layer.

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

Cybenko, "Approximations by superpositions of sigmoidal functions", 1989

Universality

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

Leshno et al, "Multilayer Feedforward Networks With a Nonpolynomial Activation Function Can Approximate Any Function", 1993; Lu et al, "The Expressive Power of Neural Networks: A View from the Width", NIPS 2017

Universality

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

These proofs are not constructive.

They do not say how to compute the weights to reach a desired accuracy.

Leshno et al, “Multilayer Feedforward Networks With a Nonpolynomial Activation Function Can Approximate Any Function”, 1993; Lu et al, “The Expressive Power of Neural Networks: A View from the Width”, NIPS 2017

Universality

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

These proofs are not constructive.

They do not say how to compute the weights to reach a desired accuracy.

Some theorems give bounds for the width q ("# of neurons").

Some theorems show universality for > 1 layers (deep networks).

Leshno et al, "Multilayer Feedforward Networks With a Nonpolynomial Activation Function Can Approximate Any Function", 1993; Lu et al, "The Expressive Power of Neural Networks: A View from the Width", NIPS 2017

Universality

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

These proofs are not constructive.

They do not say how to compute the weights to reach a desired accuracy.

Some theorems give bounds for the width q ("# of neurons").

Some theorems show universality for > 1 layers (deep networks).

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

Leshno et al, "Multilayer Feedforward Networks With a Nonpolynomial Activation Function Can Approximate Any Function", 1993; Lu et al, "The Expressive Power of Neural Networks: A View from the Width", NIPS 2017

Training

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

$$g_{\mathbf{\Theta}}(\mathbf{x}_i) = (\sigma \circ f_{\mathbf{\Theta}_n}) \circ (\sigma \circ f_{\mathbf{\Theta}_{n-1}}) \circ \cdots \circ (\sigma \circ f_{\mathbf{\Theta}_1})(\mathbf{x}_i) = \mathbf{y}_i$$

Training

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

$$g_{\mathbf{\Theta}}(\mathbf{x}_i) = (\sigma \circ f_{\mathbf{\Theta}_n}) \circ (\sigma \circ f_{\mathbf{\Theta}_{n-1}}) \circ \cdots \circ (\sigma \circ f_{\mathbf{\Theta}_1})(\mathbf{x}_i) = \mathbf{y}_i$$

Consider the MSE loss:

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

Solving for the weights $\mathbf{\Theta}$ is referred to as training.

Training

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

$$g_{\boldsymbol{\Theta}}(\mathbf{x}_i) = (\sigma \circ f_{\boldsymbol{\Theta}_n}) \circ (\sigma \circ f_{\boldsymbol{\Theta}_{n-1}}) \circ \cdots \circ (\sigma \circ f_{\boldsymbol{\Theta}_1})(\mathbf{x}_i) = \mathbf{y}_i$$

Consider the MSE loss:

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

Solving for the weights $\boldsymbol{\Theta}$ is referred to as training.

The loss is not convex w.r.t. $\boldsymbol{\Theta}$

Training

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

$$g_{\boldsymbol{\Theta}}(\mathbf{x}_i) = (\sigma \circ f_{\boldsymbol{\Theta}_n}) \circ (\sigma \circ f_{\boldsymbol{\Theta}_{n-1}}) \circ \cdots \circ (\sigma \circ f_{\boldsymbol{\Theta}_1})(\mathbf{x}_i) = \mathbf{y}_i$$

Consider the MSE loss:

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

Solving for the weights $\boldsymbol{\Theta}$ is referred to as training.

The loss is not convex w.r.t. $\boldsymbol{\Theta}$

Only some special cases are convex:

- One layer, no activation, MSE loss ($\Rightarrow$ linear regression).

Training

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

$$g_{\mathbf{\Theta}}(\mathbf{x}_i) = (\sigma \circ f_{\mathbf{\Theta}_n}) \circ (\sigma \circ f_{\mathbf{\Theta}_{n-1}}) \circ \cdots \circ (\sigma \circ f_{\mathbf{\Theta}_1})(\mathbf{x}_i) = \mathbf{y}_i$$

Consider the MSE loss:

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

Solving for the weights $\mathbf{\Theta}$ is referred to as training.

The loss is not convex w.r.t. $\mathbf{\Theta}$

Only some special cases are convex:

- One layer, no activation, MSE loss ($\Rightarrow$ linear regression).
- One layer, sigmoid activation, cross-entropy loss ($\Rightarrow$ logistic regression).

Training

We train using gradient descent-like algorithms.

Bottleneck: Computation of gradients $\nabla \ell_{\boldsymbol{\Theta}}$.

Training

We train using gradient descent-like algorithms.

Bottleneck: Computation of gradients $\nabla \ell_{\mathbf{\Theta}}$.

For the basic MSE, this means:

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

Training

We train using gradient descent-like algorithms.

Bottleneck: Computation of gradients $\nabla \ell_{\mathbf{\Theta}}$.

For the basic MSE, this means:

$$\nabla \ell_{\mathbf{\Theta}}(\{\mathbf{x}_i, \mathbf{y}_i\}) = \frac{1}{n}\sum_{i=1}^{n} \nabla_{\mathbf{\Theta}} \|(\mathbf{y}_i - (\sigma(f_{\mathbf{\Theta}_n}((\sigma(f_{\mathbf{\Theta}_{n-1}}(\cdots(\sigma(f_{\mathbf{\Theta}_1}(\mathbf{x}_i))\cdots))))\|_2^2$$

Training

We train using gradient descent-like algorithms.

Bottleneck: Computation of gradients $\nabla \ell_{\boldsymbol{\Theta}}$.

For the basic MSE, this means:

$$\nabla \ell_{\boldsymbol{\Theta}}(\{\mathbf{x}_i, \mathbf{y}_i\}) = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\boldsymbol{\Theta}} \|(\mathbf{y}_i - (\sigma(f_{\boldsymbol{\Theta}_n}((\sigma(f_{\boldsymbol{\Theta}_{n-1}}(\cdots(\sigma(f_{\boldsymbol{\Theta}_1}(\mathbf{x}_i))\cdots))))\|_2^2$$

- Computing the gradients by hand is infeasible.

Training

We train using gradient descent-like algorithms.

Bottleneck: Computation of gradients $\nabla \ell_{\boldsymbol{\Theta}}$.

For the basic MSE, this means:

$$\nabla \ell_{\boldsymbol{\Theta}}(\{\mathbf{x}_i, \mathbf{y}_i\}) = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\boldsymbol{\Theta}} \|(\mathbf{y}_i - (\sigma(f_{\boldsymbol{\Theta}_n}((\sigma(f_{\boldsymbol{\Theta}_{n-1}}(\cdots(\sigma(f_{\boldsymbol{\Theta}_1}(\mathbf{x}_i))\cdots))))\|_2^2$$

- Computing the gradients by hand is infeasible.
- Finite differences need $O(\#\mathrm{weights})$ evaluations of $\ell_{\boldsymbol{\Theta}}$.

Training

We train using gradient descent-like algorithms.

Bottleneck: Computation of gradients $\nabla \ell_{\boldsymbol{\Theta}}$.

For the basic MSE, this means:

$$\nabla \ell_{\boldsymbol{\Theta}}(\{\mathbf{x}_i, \mathbf{y}_i\}) = \frac{1}{n} \sum_{i=1}^{n} \nabla_{\boldsymbol{\Theta}} \|(\mathbf{y}_i - (\sigma(f_{\boldsymbol{\Theta}_n}((\sigma(f_{\boldsymbol{\Theta}_{n-1}}(\cdots(\sigma(f_{\boldsymbol{\Theta}_1}(\mathbf{x}_i))\cdots))))\|_2^2$$

- Computing the gradients by hand is infeasible.
- Finite differences need $O(\#\text{weights})$ evaluations of $\ell_{\boldsymbol{\Theta}}$.

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

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.

Example:

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

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.

Example:

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

$$x \xrightarrow{\log} y$$

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.

Example:

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

$$x \xrightarrow{\log} y \xrightarrow{\sqrt{\ }} z$$

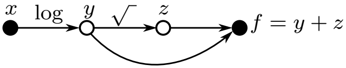
Computational graphs

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.

Example:

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



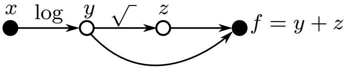
Computational graphs

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.

Example:

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



Example:

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

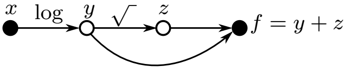
Computational graphs

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.

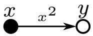
Example:

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



Example:

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



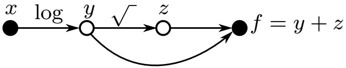
Computational graphs

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.

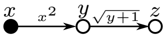
Example:

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



Example:

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



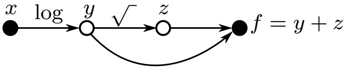
Computational graphs

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.

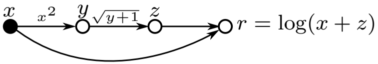
Example:

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



Example:

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



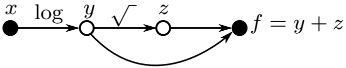
Computational graphs

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.

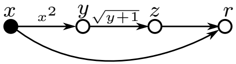
Example:

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



Example:

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



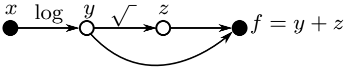
Computational graphs

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.

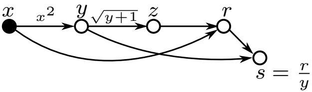
Example:

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



Example:

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



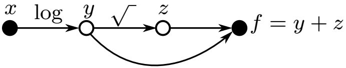
Computational graphs

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.

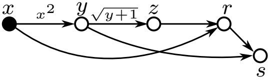
Example:

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



Example:

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



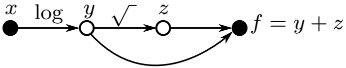
Computational graphs

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.

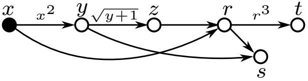
Example:

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



Example:

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



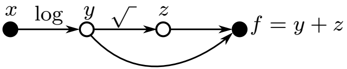
Computational graphs

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.

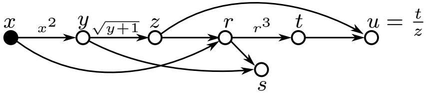
Example:

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



Example:

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



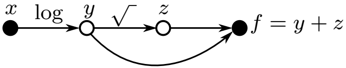
Computational graphs

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.

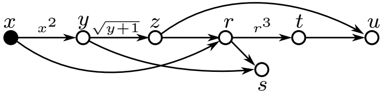
Example:

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



Example:

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



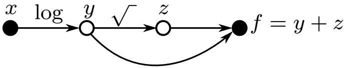
Computational graphs

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.

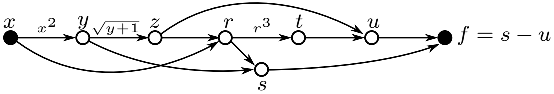
Example:

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



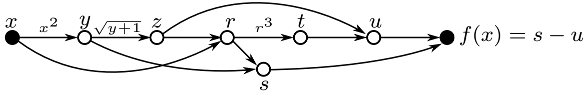
Example:

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



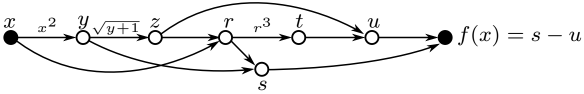
Computational graphs

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



Computational graphs

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

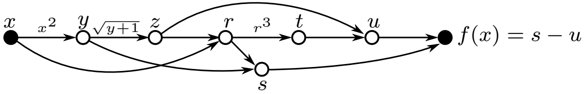


The graph is constructed programmaticaly, for example:

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

Computational graphs

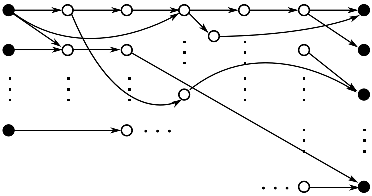
The evaluation of $f(x)$ corresponds to a forward traversal of the graph:



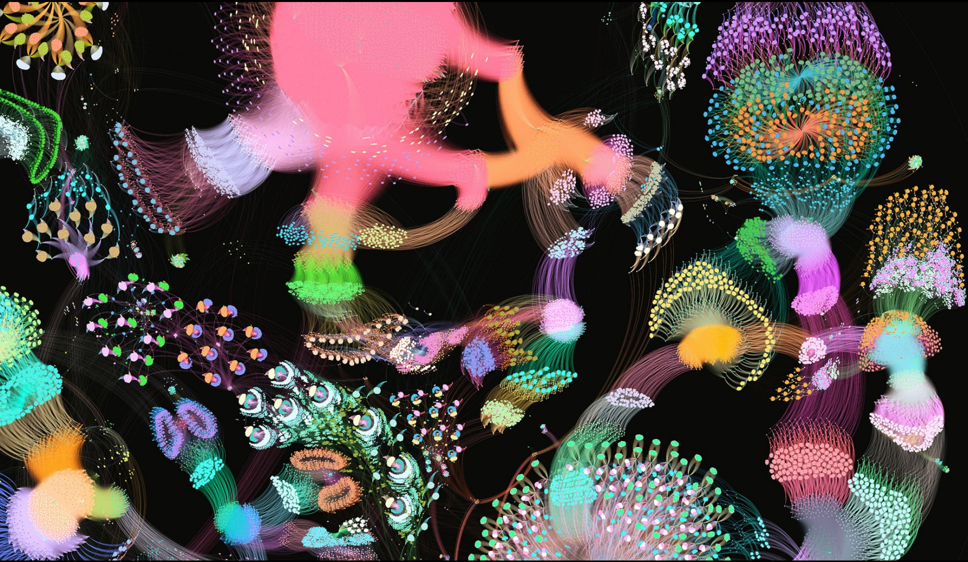
The graph is constructed programmaticaly, for example:

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

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



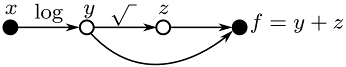
The computational graph gets big quickly.



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

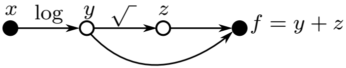
Automatic differentiation: Forward mode

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



Automatic differentiation: Forward mode

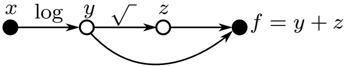
$$f(x) = \log x + \sqrt{\log x}$$



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

Automatic differentiation: Forward mode

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



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

Automatic differentiation: Forward mode

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

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

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

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

Automatic differentiation: Forward mode

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

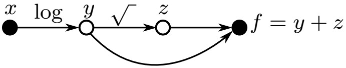
$$\begin{tikzcd}
x \arrow[r, "\log"] & y \arrow[r, "\sqrt{\ }"] \arrow[rr, bend right] & z \arrow[r] & f = y + z
\end{tikzcd}$$

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

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

Automatic differentiation: Forward mode

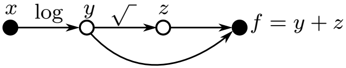
$$f(x) = \log x + \sqrt{\log x}$$



$$\begin{aligned}
\frac{\partial x}{\partial x} &= 1 \\
\frac{\partial y}{\partial x} &= \frac{\partial y}{\partial x}\frac{\partial x}{\partial x} = \frac{\partial \log x}{\partial x}\frac{\partial x}{\partial x} = \frac{1}{x}\frac{\partial x}{\partial x} \\
\frac{\partial z}{\partial x} &= \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}
\end{aligned}$$

Automatic differentiation: Forward mode

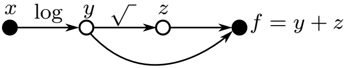
$$f(x) = \log x + \sqrt{\log x}$$



$$\begin{aligned}
\frac{\partial x}{\partial x} &= 1 \\
\frac{\partial y}{\partial x} &= \frac{\partial y}{\partial x}\frac{\partial x}{\partial x} = \frac{\partial \log x}{\partial x}\frac{\partial x}{\partial x} = \frac{1}{x}\frac{\partial x}{\partial x} \\
\frac{\partial z}{\partial x} &= \frac{\partial z}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial \sqrt{y}}{\partial y}\frac{\partial y}{\partial x}
\end{aligned}$$

Automatic differentiation: Forward mode

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



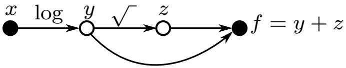
$$\frac{\partial x}{\partial x} = 1$$

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

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial \sqrt{y}}{\partial y}\frac{\partial y}{\partial x} = \frac{1}{2\sqrt{y}}\frac{\partial y}{\partial x}$$

Automatic differentiation: Forward mode

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



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

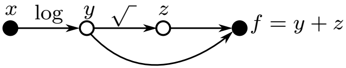
$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial x}\frac{\partial x}{\partial x} = \frac{\partial \log x}{\partial x}\frac{\partial x}{\partial x} = \frac{1}{x}\frac{\partial x}{\partial x}$$

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial \sqrt{y}}{\partial y}\frac{\partial y}{\partial x} = \frac{1}{2\sqrt{y}}\frac{\partial y}{\partial x}$$

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

Automatic differentiation: Forward mode

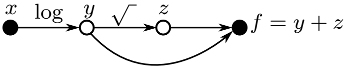
$$f(x) = \log x + \sqrt{\log x}$$



$$
\begin{aligned}
\frac{\partial x}{\partial x} &= 1 \\
\frac{\partial y}{\partial x} &= \frac{\partial y}{\partial x}\frac{\partial x}{\partial x} = \frac{\partial \log x}{\partial x}\frac{\partial x}{\partial x} = \frac{1}{x}\frac{\partial x}{\partial x} \\
\frac{\partial z}{\partial x} &= \frac{\partial z}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial \sqrt{y}}{\partial y}\frac{\partial y}{\partial x} = \frac{1}{2\sqrt{y}}\frac{\partial y}{\partial x} \\
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial y}\frac{\partial y}{\partial x} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial x}
\end{aligned}
$$

Automatic differentiation: Forward mode

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



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

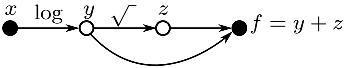
$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial x}\frac{\partial x}{\partial x} = \frac{\partial \log x}{\partial x}\frac{\partial x}{\partial x} = \frac{1}{x}\frac{\partial x}{\partial x}$$

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial \sqrt{y}}{\partial y}\frac{\partial y}{\partial x} = \frac{1}{2\sqrt{y}}\frac{\partial y}{\partial x}$$

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

Automatic differentiation: Forward mode

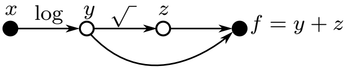
$$f(x) = \log x + \sqrt{\log x}$$



$$\begin{aligned}
\frac{\partial x}{\partial x} &= 1 \\
\frac{\partial y}{\partial x} &= \frac{\partial y}{\partial x}\frac{\partial x}{\partial x} = \frac{\partial \log x}{\partial x}\frac{\partial x}{\partial x} = \frac{1}{x}\frac{\partial x}{\partial x} \\
\frac{\partial z}{\partial x} &= \frac{\partial z}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial \sqrt{y}}{\partial y}\frac{\partial y}{\partial x} = \frac{1}{2\sqrt{y}}\frac{\partial y}{\partial x} \\
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial y}\frac{\partial y}{\partial x} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial x} = \frac{\partial (y+z)}{\partial y}\frac{\partial y}{\partial x} + \frac{\partial (y+z)}{\partial z}\frac{\partial z}{\partial x} = \frac{\partial y}{\partial x} + \frac{\partial z}{\partial x}
\end{aligned}$$

Automatic differentiation: Forward mode

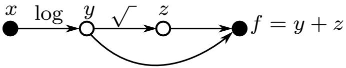
$$f(x) = \log x + \sqrt{\log x} \qquad \frac{\partial f}{\partial x} = \frac{1}{2\sqrt{y}}\frac{1}{x} + \frac{1}{x}$$



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

Automatic differentiation: Forward mode

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

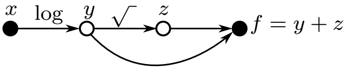


Assumption: Each partial derivative is a "primitive" accessible in closed form and can be computed on the fly.

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

Automatic differentiation: Forward mode

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



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.

Automatic differentiation: Forward mode

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

Automatic differentiation: Forward mode

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

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

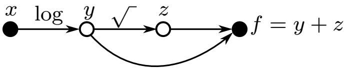
We accumulate values during code execution, to get numerical evaluations rather than expressions for the derivative.

Automatic differentiation: Forward mode

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

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

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



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

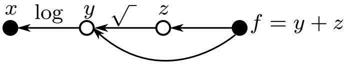
Automatic differentiation: Reverse mode

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

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

Automatic differentiation: Reverse mode

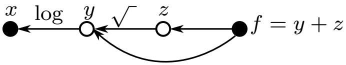
$$f(x) = \log x + \sqrt{\log x}$$



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

Automatic differentiation: Reverse mode

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



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

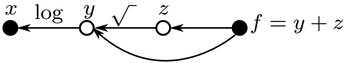
$$\frac{\partial f}{\partial z} =$$

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

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

Automatic differentiation: Reverse mode

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



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

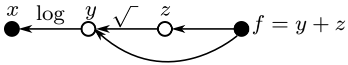
$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial z}$$

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

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

Automatic differentiation: Reverse mode

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



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

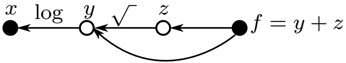
$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial z}$$

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

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

Automatic differentiation: Reverse mode

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



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

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

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

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

Automatic differentiation: Reverse mode

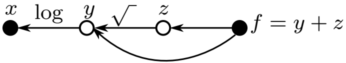
$$f(x) = \log x + \sqrt{\log x}$$

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

$$\begin{aligned}
\frac{\partial f}{\partial f} &= 1 \\
\frac{\partial f}{\partial z} &= \frac{\partial f}{\partial f}\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial z} = \frac{\partial f}{\partial f} \\
\frac{\partial f}{\partial y} &= \frac{\partial f}{\partial z}\frac{\partial z}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial f}{\partial y} \\
\frac{\partial f}{\partial x} &=
\end{aligned}$$

Automatic differentiation: Reverse mode

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



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

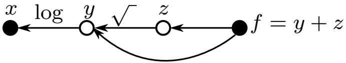
$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial z} = \frac{\partial f}{\partial f}$$

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

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

Automatic differentiation: Reverse mode

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



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

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

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial z}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial \sqrt{y}}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial y} = \frac{\partial f}{\partial z}\frac{1}{2\sqrt{y}} + \frac{\partial f}{\partial f}$$

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

Automatic differentiation: Reverse mode

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

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

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

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

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial z}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial \sqrt{y}}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial y} = \frac{\partial f}{\partial z}\frac{1}{2\sqrt{y}} + \frac{\partial f}{\partial f}$$

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

Automatic differentiation: Reverse mode

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

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

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

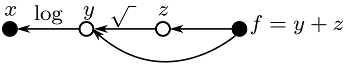
$$\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial f}{\partial z} = \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial z} = \frac{\partial f}{\partial f}$$

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial z}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial \sqrt{y}}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial y} = \frac{\partial f}{\partial z}\frac{1}{2\sqrt{y}} + \frac{\partial f}{\partial f}$$

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

Automatic differentiation: Reverse mode

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



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

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

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial z}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial \sqrt{y}}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial y} = \frac{\partial f}{\partial z}\frac{1}{2\sqrt{y}} + \frac{\partial f}{\partial f}$$

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y}\frac{\partial y}{\partial x} = \frac{\partial f}{\partial y}\frac{\partial \log x}{\partial x} = \frac{\partial f}{\partial y}\frac{1}{x}$$

Automatic differentiation: Reverse mode

Before computing the derivatives, we must compute the values of the internal nodes first:

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

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

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial z}\frac{\partial \sqrt{y}}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial f} = \frac{\partial f}{\partial z}\frac{1}{2\sqrt{\mathbf{y}}} + \frac{\partial f}{\partial f}$$

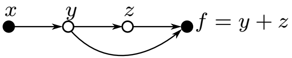
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial y}\frac{\partial \log x}{\partial x} = \frac{\partial f}{\partial y}\frac{1}{\mathbf{x}}$$

Automatic differentiation: Reverse mode

Before computing the derivatives, we must compute the values of the internal nodes first:

$$
\begin{aligned}
\frac{\partial f}{\partial f} &= 1 \\
\frac{\partial f}{\partial z} &= \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial z} = \frac{\partial f}{\partial f} \\
\frac{\partial f}{\partial y} &= \frac{\partial f}{\partial z}\frac{\partial \sqrt{y}}{\partial y} + \frac{\partial f}{\partial f}\frac{\partial (y+z)}{\partial f} = \frac{\partial f}{\partial z}\frac{1}{2\sqrt{\mathbf{y}}} + \frac{\partial f}{\partial f} \\
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial y}\frac{\partial \log x}{\partial x} = \frac{\partial f}{\partial y}\frac{1}{\mathbf{x}}
\end{aligned}
$$

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



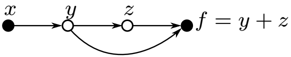
Remark: This is not forward-mode autodiff, since we are only computing function values.

Automatic differentiation: Reverse mode

Before computing the derivatives, we must compute the values of the internal nodes first:

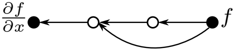
$$
\begin{aligned}
\frac{\partial f}{\partial f} &= 1 \\
\frac{\partial f}{\partial z} &= \frac{\partial f}{\partial f}\,\frac{\partial (y+z)}{\partial z} = \frac{\partial f}{\partial f} \\
\frac{\partial f}{\partial y} &= \frac{\partial f}{\partial z}\,\frac{\partial \sqrt{y}}{\partial y} + \frac{\partial f}{\partial f}\,\frac{\partial (y+z)}{\partial f} = \frac{\partial f}{\partial z}\,\frac{1}{2\sqrt{\mathbf{y}}} + \frac{\partial f}{\partial f} \\
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial y}\,\frac{\partial \log x}{\partial x} = \frac{\partial f}{\partial y}\,\frac{1}{\mathbf{x}}
\end{aligned}
$$

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.

2. Backward pass to compute the derivatives.



Back-propagation

When training NNs, we compute the gradient of a loss

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

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

Back-propagation

When training NNs, we compute the gradient of a loss

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

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

Instead of simple derivatives we must compute gradients and Jacobians.

Back-propagation

When training NNs, we compute the gradient of a loss

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

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

When training NNs, we compute the gradient of a loss

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

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

Instead of simple derivatives we must compute gradients and Jacobians.

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

Back-propagation

When training NNs, we compute the gradient of a loss

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

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

Instead of simple derivatives we must compute gradients and Jacobians.

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

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

- Forward-mode autodiff:

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

Back-propagation

When training NNs, we compute the gradient of a loss

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

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

Instead of simple derivatives we must compute gradients and Jacobians.

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

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

- Forward-mode autodiff:

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

- 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

When training NNs, we compute the gradient of a loss

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

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

Instead of simple derivatives we must compute gradients and Jacobians.

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

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:

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

Back-propagation

When training NNs, 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.

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

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:

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

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.

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.

Back-propagation is not just the chain rule.

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.

Back-propagation is not just the chain rule.

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

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.

Back-propagation is not just the chain rule.

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/abs/1502.05767