Machine Learning

Lecture 7: Deep Learning I

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Section 1

Introduction

Another look at Logistic Regression

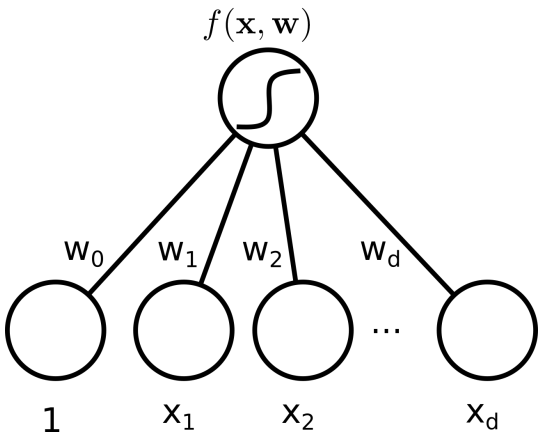
In logistic regression we model posterior distribution as:

$$y \mid \boldsymbol{x} \sim \text{Bernoulli}\Big(\sigma\big(\boldsymbol{w}^T\boldsymbol{x}\big)\Big)$$

with $\boldsymbol{w}^T\boldsymbol{x} := w_0 + w_1 x_1 + ... + w_D x_D$, and $\sigma(a) := \frac{1}{1+\exp(-a)}$.

We can represent this graphically:

- each node is a (scalar) input[1];
- multiply the input with the weight on the edge: $x_j w_j$;
- compute weighted sum of incoming edges: $a_0 = \sum_{j=0}^{D} x_j w_j$;
- apply (activation) function: $p(y = 1 \mid \boldsymbol{x}) = \sigma(a_0) = f(\boldsymbol{x}, \boldsymbol{w})$.



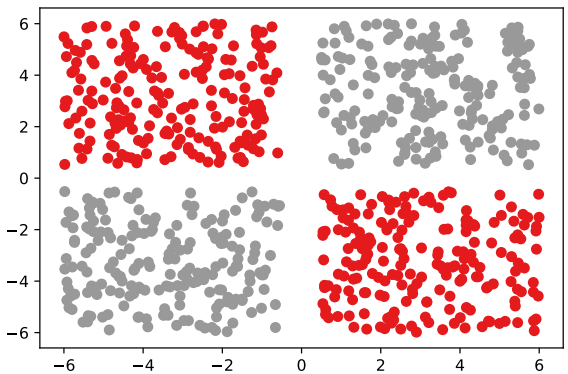
[1] The first node $1 = x_0$ is for the bias term.

The XOR dataset

The XOR dataset is not linearly separable

↓

Logistic regression will fail since it learns a linear decision boundary



How to handle non-linearity? Basis functions

We have input vectors $\boldsymbol{x}$ and associated targets y. We want to describe the underlying functional relation.

We can use the following simple model:

$$f(\boldsymbol{x}, \boldsymbol{w}) = \sigma\left(w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\boldsymbol{x})\right) = \sigma(\boldsymbol{w}^\mathsf{T} \boldsymbol{\phi}(\boldsymbol{x})) \tag{1}$$

where

$\boldsymbol{\phi}$	basis function	—	many choices, can be nonlinear
w_0	bias	—	equivalent to defining $\phi_0 \equiv 1$; or adding constant 1 to every sample

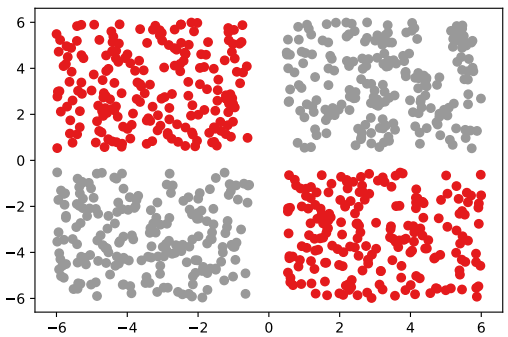
The basis function $\boldsymbol{\phi}$ maps the samples to a new space where the data is linearly separable.

Remember we are linear in $\boldsymbol{w}$!

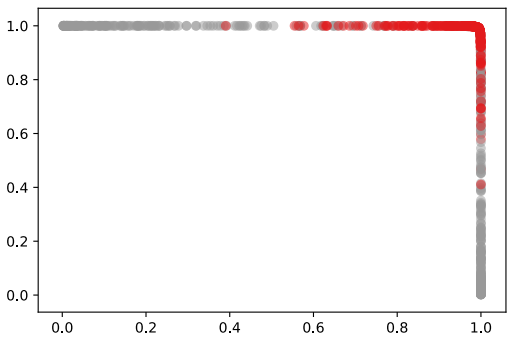
Example: Handling XOR dataset by custom basis functions

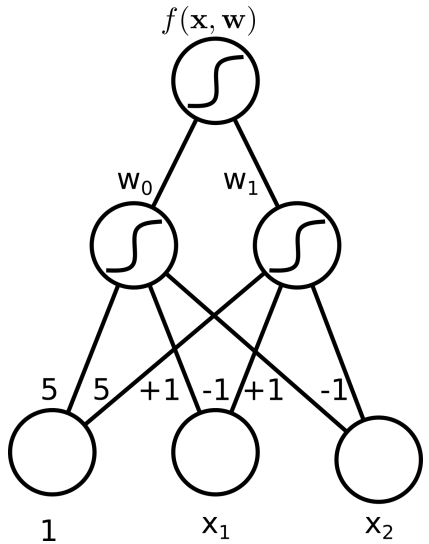
Apply a (nonlinear) transformation ϕ that maps samples to a space where they are linearly separable. For example:

$\mathbb{R}^2$ space



Transformed $\mathbb{R}^2$ space[2]





Here we defined a custom basis function $\boldsymbol{\phi} : \mathbb{R}^3 \to \mathbb{R}^2$

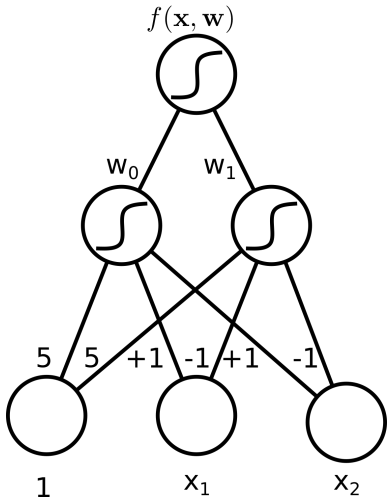
$$\boldsymbol{\phi}(\boldsymbol{x}) = \boldsymbol{\phi}(1, x_1, x_2) = (\ \sigma(5 + x_1 + x_2)\ ,\ \sigma(5 - x_1 - x_2)\ )$$

[2] After applying σ.

Example: Handling XOR dataset by custom basis functions

The overall model is:

$$f(\boldsymbol{x}, \boldsymbol{w}) = \sigma(\boldsymbol{w}^\mathsf{T} \boldsymbol{\phi}(\boldsymbol{x}))$$
$$= \sigma_1 \left(\begin{bmatrix} w_0 & w_1 \end{bmatrix} \cdot \sigma_0 \left(\begin{bmatrix} 5 & 1 & 1 \\ 5 & -1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \right) \right)$$



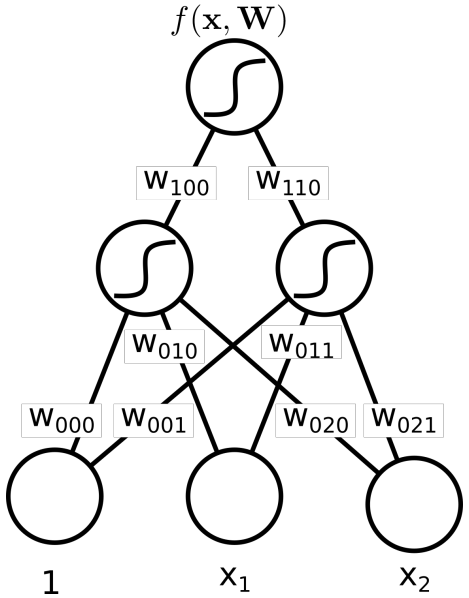
Q: How to find the parameters $\boldsymbol{w}$?
A: Train the model by minimizing a loss function.

This example is a *binary classification problem*, hence we minimize the *binary cross-entropy* loss:

$$\boldsymbol{w}^* = \arg\min_{\boldsymbol{w}} \sum_{n=1}^{N} - \left(y_n \log f(\boldsymbol{x}_n, \boldsymbol{w}) + (1 - y_n) \log \left(1 - f(\boldsymbol{x}_n, \boldsymbol{w}) \right) \right)$$

How to find the basis functions?

Different datasets require different $\boldsymbol{\phi}$ to become (almost) linearly separable.



Idea: learn the basis function and the weights of the logistic regression *jointly* from the data (end-to-end learning).

- *Previously*: only learn w_{100} and w_{110}
- *Now*: learn all w_{ijk}
  where i=layer, j = input node, k = output node

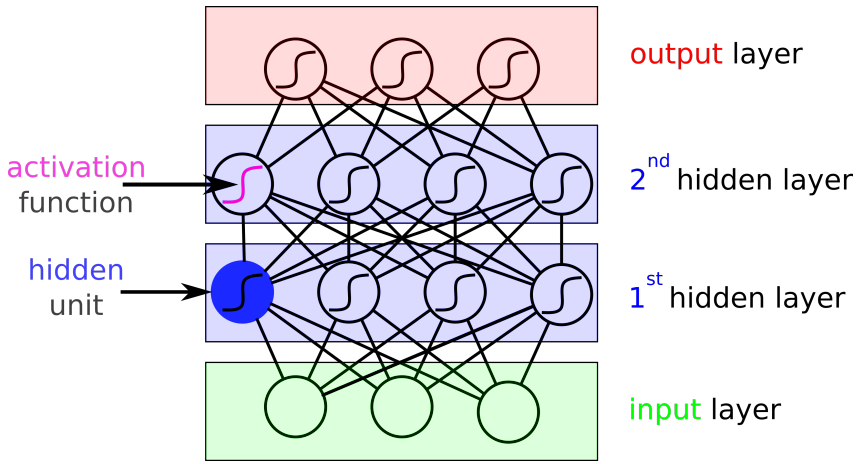
$$f(\boldsymbol{x}, \boldsymbol{W}) = \sigma_1 \left(\begin{bmatrix} w_{100} & w_{110} \end{bmatrix} \cdot \sigma_0 \left(\begin{bmatrix} w_{000} & w_{010} & w_{020} \\ w_{001} & w_{011} & w_{021} \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ x_2 \end{bmatrix} \right) \right)$$

$$\boldsymbol{W}^* = \arg\min_{\boldsymbol{W}} \sum_{n=1}^{N} - \left(y_n \log f(\boldsymbol{x}_n, \boldsymbol{W}) + (1 - y_n) \log \left(1 - f(\boldsymbol{x}_n, \boldsymbol{W}) \right) \right)$$

Feed-Forward Neural Network (FFNN) with 1 hidden layer.
Note: σ_0 and σ_1 can be arbitrary activation functions.

Making the model more complicated

Each basis function can be a more complicated function of the feature vector $\boldsymbol{x}$ (a function of other basis functions rather than a function of $\boldsymbol{x}$).



By adding more hidden layers we get a "deep" neural network[3]:

$$f(\boldsymbol{x}, \boldsymbol{W}, \boldsymbol{b}) = \sigma_2\left(\boldsymbol{W}_2\sigma_1\left(\boldsymbol{W}_1\sigma_0(\boldsymbol{W}_0\,\boldsymbol{x} + \boldsymbol{b}_0) + \boldsymbol{b}_1\right) + \boldsymbol{b}_2\right)$$

where $\boldsymbol{W} = \{\boldsymbol{W}_0, \boldsymbol{W}_1, \boldsymbol{W}_2\}, \boldsymbol{b} = \{\boldsymbol{b}_0, \boldsymbol{b}_1, \boldsymbol{b}_2\}$ are the learnable weights and biases[4].

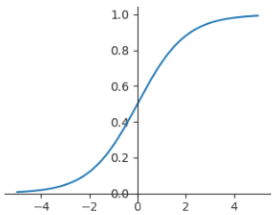
[3] We call this architecture a Multi-layered Perceptron (MLP).

[4] Bias term explicitely added in the equation; not shown in the figure

Activation functions

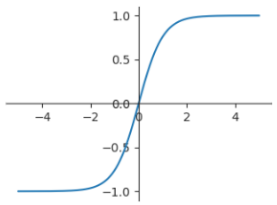
Sigmoid

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



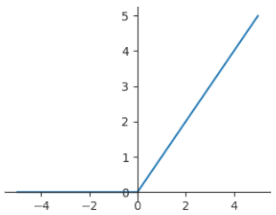
tanh

$$\tanh(x)$$



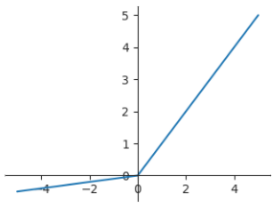
ReLU

$$\max(0, x)$$



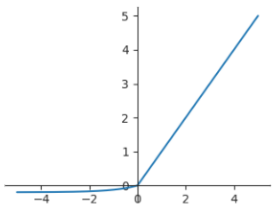
Leaky ReLU

$$\max(0.1x, x)$$



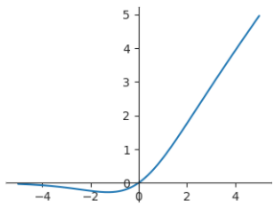
ELU

$$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$$



Swish

$$x \cdot \sigma(x)$$



Most activation functions are applied element-wise when given a *multi-dimensional* input.

Softmax activation is a notable exception!

Why use nonlinear activation functions?

A function composed of multiple *linear* layers can be simplified:

$$\begin{aligned} f(\boldsymbol{x}, \boldsymbol{W}) &= \quad (\boldsymbol{W}_L \quad (\dots \quad (\boldsymbol{W}_0 \boldsymbol{x}) \dots)) \\ &= (\boldsymbol{W}_L \dots \boldsymbol{W}_1 \boldsymbol{W}_0) \boldsymbol{x} \\ &= \boldsymbol{W}' \boldsymbol{x} \end{aligned}$$

hence, resulting in a *linear transformation*!

A function composed of multiple *nonlinear* layers cannot (in general) be simplified:

$$\begin{aligned} f(\boldsymbol{x}, \boldsymbol{W}) &= \sigma_L(\boldsymbol{W}_L \sigma_{L-1}(\dots \sigma_0(\boldsymbol{W}_0 \boldsymbol{x}) \dots)) \\ &\neq \boldsymbol{W}' \boldsymbol{x} \end{aligned}$$

hence, we get a *nonlinear transformation*.

Non-linear transformations allows to learn more complex functions.

Neural networks are universal approximators

Universal approximation theorem

An MLP with a linear output layer and one hidden layer can approximate any continuous function defined over a closed and bounded subset of $\mathbb{R}^D$, under mild assumptions on the activation function ('squashing' activation functions; e.g. sigmoid) and given the number of hidden units is large enough.

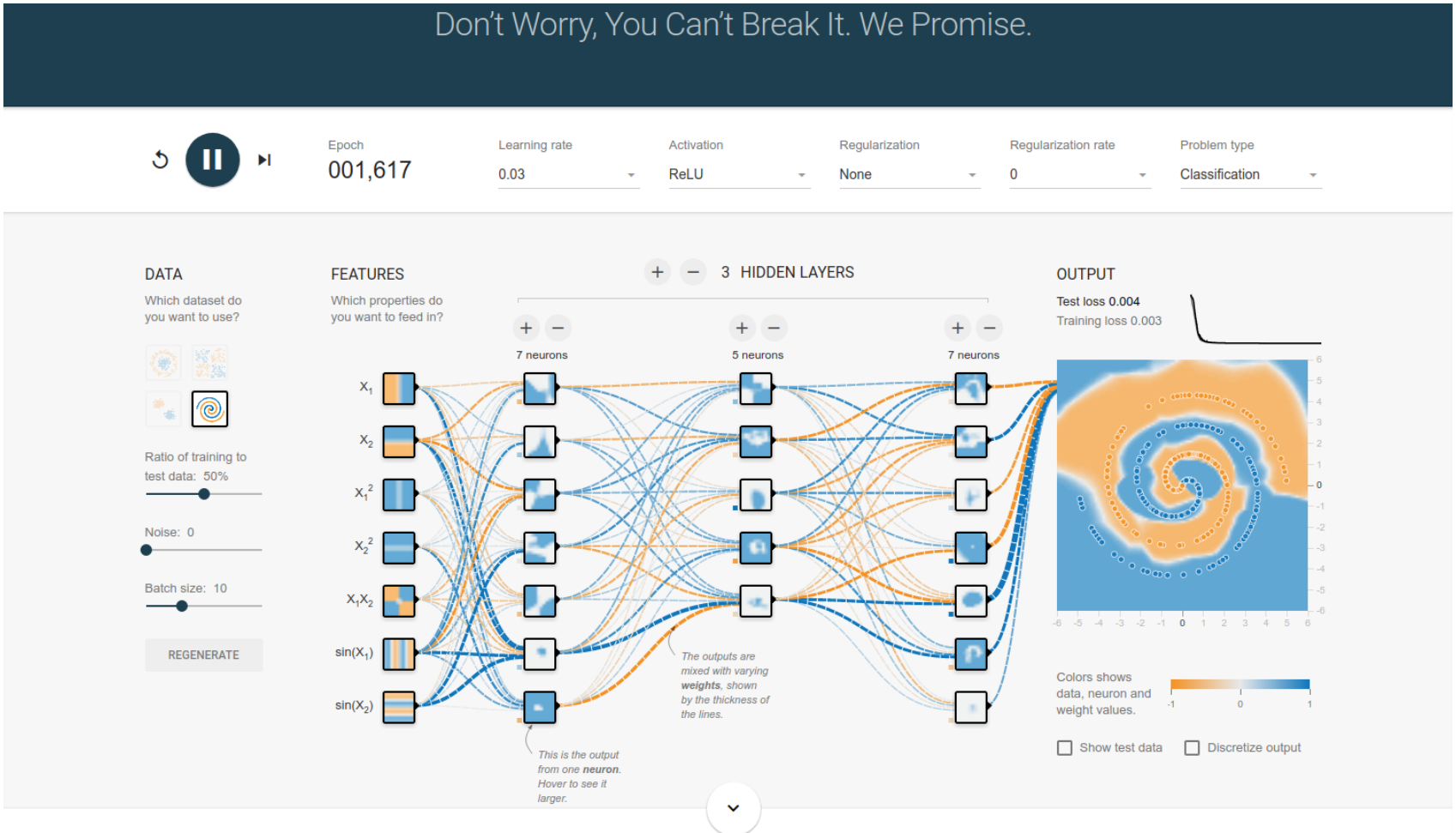
[Cybenko 1989; Funahashi 1989; Hornik et al 1989, 1991; Hartman et al 1990].

Also in the discrete case: a neural network can approximate any function from a discrete space to another.

Good news: Regardless of the function we aim to learn, there exists an MLP that can approximate that function arbitrarily well.

Bad news: Finding the MLP that provides the best approximation is generally a complex and tricky task.

Demo: http://playground.tensorflow.org



Multiple hidden layers

According to the universal approximation theorem, a feed-forward network with 1 hidden layer can represent any function.

Q: Why adding more layers?

Theoretical reason:

- For some families of functions, if we use *a few* layers we would need a large number of hidden units (and therefore parameters). But we can get the same representation power by adding *more layers*, fewer hidden units, and fewer parameters.

Practical reason:

- Deeper networks (with some additional tricks) often train faster and generalize better.

Multiple hidden layers

Functions that can be compactly represented with k layers may require exponentially many hidden units when using only $k-1$ layers.

Deep network can learn a hierarchy of representations.

Different high-level features share lower-level features.

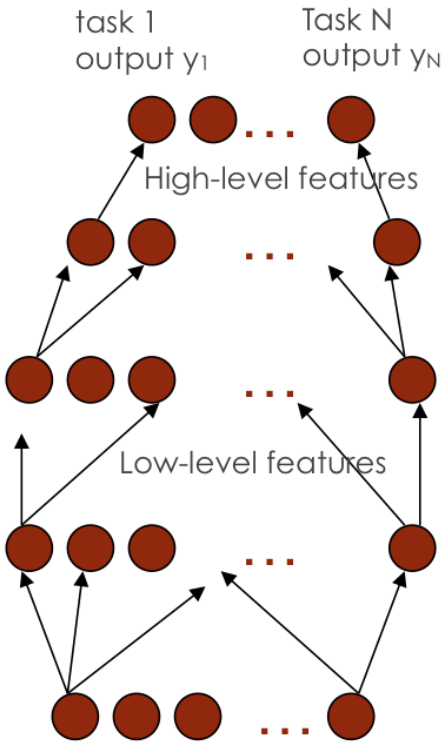


Figure from *Understanding and Improving Deep Learning Algorithms*, Yoshua Bengio, ML Google Distinguished Lecture, 2010

Section 2

Beyond binary classification

Loss function

Neural networks can be used for *various prediction tasks*.

Different tasks require changing

1. the activation function in the *final* layer
2. the loss function

For *supervised learning* common choices are

Prediction target	$p(\boldsymbol{y} \mid \boldsymbol{x})$	**Final layer**	**Loss function**
Binary	Bernoulli	Sigmoid	Binary cross entropy
Discrete	Categorical	Softmax	Cross entropy
Continuous	Gaussian	Identity	Squared error

Example 1: Binary classification

- Data: $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, where $y_n \in \{0, 1\}$.
- Activation in the final layer: sigmoid

$$f(\boldsymbol{x}, \boldsymbol{W}) = \frac{1}{1 + \exp(-a)}$$

  where a is the output of the last layer before activation (*logits*).
- Conditional distribution: Bernoulli

$$p(y \mid \boldsymbol{x}) = \text{Bernoulli}(y \mid f(\boldsymbol{x}, \boldsymbol{W}))$$

- Loss function: binary cross entropy

$$\begin{aligned} E(\boldsymbol{W}) &= -\sum_{n=1}^{N} \log p(y_n \mid \boldsymbol{x}_n) \\ &= -\sum_{n=1}^{N} \Big(y_n \log f(\boldsymbol{x}_n, \boldsymbol{W}) + (1 - y_n) \log \left(1 - f(\boldsymbol{x}_n, \boldsymbol{W})\right) \Big) \end{aligned}$$

Example 2: Multi-class classification

- Data: $\{\boldsymbol{x}_n, \boldsymbol{y}_n\}_{n=1}^N$, where $\boldsymbol{y}_n \in \{0,1\}^K$ (one-hot notation)[5].
- Activation in the final layer: softmax

$$f_k(\boldsymbol{x}, \boldsymbol{W}) = \frac{\exp(a_k)}{\sum_{j=1}^K \exp(a_j)}$$

- Conditional distribution: categorical

$$p(\boldsymbol{y} \mid \boldsymbol{x}) = \text{Categorical}(\boldsymbol{y} \mid f(\boldsymbol{x}, \boldsymbol{W}))$$

- Loss function: categorical cross entropy

$$\begin{aligned} E(\boldsymbol{W}) &= -\sum_{n=1}^N \log p(\boldsymbol{y}_n \mid \boldsymbol{x}_n) \\ &= -\sum_{n=1}^N \sum_{k=1}^K y_{nk} \log f_k(\boldsymbol{x}_n, \boldsymbol{W}) \end{aligned}$$

[5] K is the number of classes.

Example 3: Single-output regression

- Data: $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, where $y_n \in \mathbb{R}$.
- Activation in the final layer: identity (no activation)

$$f(\boldsymbol{x}, \boldsymbol{W}) = a$$

- Conditional distribution: Gaussian

$$p(y \mid \boldsymbol{x}) = \mathcal{N}(y \mid f(\boldsymbol{x}, \boldsymbol{W}), 1)$$

- Loss function: squared error (a.k.a. Gaussian cross-entropy)

$$\begin{aligned} E(\boldsymbol{W}) &= -\sum_{n=1}^{N} \log p(y_n \mid \boldsymbol{x}_n) \\ &= \sum_{n=1}^{N} (y_n - f(\boldsymbol{x}_n, \boldsymbol{W}))^2 + \text{const.} \end{aligned}$$

Unsupervised deep learning

So far we have only considered neural networks for supervised learning.

Unsupervised deep learning is also a very active field of research, with models such as:

- **Autoencoder** (*covered later in this course*)
- **Variational autoencoder** (*covered in our DGM lecture*)
- **Generative adversarial networks** (GAN; *covered in our DGM lecture*)
- **Unsupervised representation learning** (e.g. word or node embeddings; *covered in our MLGS lecture*)

Choosing the loss

We are free to choose any loss that provides a useful gradient for training.

This choice includes both the function and which values to use and compare to. Many model types mainly differ in their choice of loss.

Example loss functions:

- **Cross entropy**: For supervised classification
- **Mean squared error** (MSE)
- **Mean absolute error** (MAE): Useful if we have outliers, but gradient is independent of the distance from the optimum (advanced optimizers handle this surprisingly well, though).
- **Huber loss**, **LogCosh**: MSE at close distances, MAE far away. Combine benefits of MSE and MAE.
- **Wasserstein (earth mover's) distance**, **KL-divergence**: For continuous distributions

Section 3

Parameter learning

Minimizing the loss function

In practice $E(\boldsymbol{W})$ is often non-convex $\rightarrow$ optimization is tricky:

- a local minimum is not necessarily a global minimum;
- potentially there exist several local minima, many of which can be equivalent;
- often it is not possible to find a global minimum nor is it useful.

We may find a few local minima, and pick the one with higher performance on a validation set.

Default approach: Find a local minimum via gradient descent

- Start with some initial parameters $\boldsymbol{W}^{(0)}$
- Update the parameters in the direction of the negative gradient
- Repeat until convergence or stopping criterion is met

$$\boldsymbol{W}^{(new)} = \boldsymbol{W}^{(old)} - \tau \nabla_{\boldsymbol{W}} E(\boldsymbol{W}^{(old)})$$

How can we compute the gradient?

1. **By hand**: manually working out $\nabla_{\boldsymbol{W}} E$ and coding it is tricky and cumbersome (furthermore: see point 3).
2. **Numeric**: can be done as

$$\frac{\partial E}{\partial w_{ijk}} = \frac{E(w_{ijk} + \epsilon) - E(w_{ijk})}{\epsilon} + \mathcal{O}(\epsilon)$$

   - each evaluation of the above equation roughly requires $\mathcal{O}(|\boldsymbol{W}|)$ operations, where $|\boldsymbol{W}|$ is the dimensionality of weight space;
   - the evaluation has to be done for each parameter independently. Therefore computing $\nabla_{\boldsymbol{W}} E$ requires $\mathcal{O}(|\boldsymbol{W}|^2)$ operations!

How can we compute the gradient?

3. **Symbolic differentiation**: automates essentially how you would compute the gradient function by hand.
   But: "writing down" the general expression for the gradient of every parameter is very expensive:
   - potentially exponentially many different cases (e.g., when having multiple layers with ReLUs);
   - many terms reappear in the gradient computation for *different* parameters (since the function f is hierarchically constructed); these terms could be re-used to make computation faster; however symbolic differentiation does not exploit this insight.
4. **Automatic differentiation**: e.g., backpropagation for neural networks (see following slides):
   - evaluate $\nabla_{\boldsymbol{W}} E(\boldsymbol{W})$ at the current point $\boldsymbol{W}$
   - evaluation in $\mathcal{O}(|\boldsymbol{W}|)$ (every "neuron" is visited only twice)

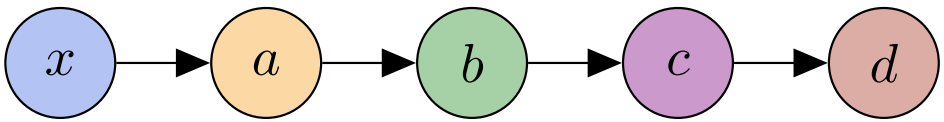
Backpropagation: Toy example

$$f(x) = \frac{2}{\sin(\exp(-x))} \qquad f(x) = d(c(b(a(x))))$$

Modules:

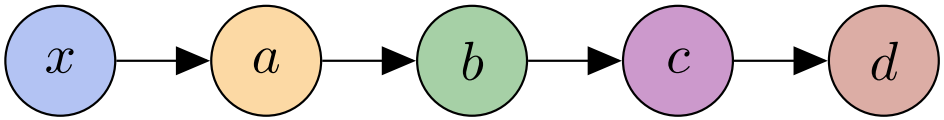
$$a(x) = -x$$
$$b(a) = \exp(a)$$
$$c(b) = \sin b$$
$$d(c) = \frac{2}{c}$$

Computational graph:



Backpropagation: Toy example

$$f(x) = \frac{2}{\sin(\exp(-x))}$$



Modules:

$$a(x) = -x$$
$$b(a) = \exp(a)$$
$$c(b) = \sin b$$
$$d(c) = \frac{2}{c}$$

Chain rule:

$$\frac{\partial f}{\partial x} = \frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial x}$$

$\frac{\partial f}{\partial x}$ is the global derivative

$\frac{\partial d}{\partial c}, \frac{\partial c}{\partial b}, \frac{\partial b}{\partial a}, \frac{\partial a}{\partial x}$ are the local derivatives

Backpropagation in a nutshell

1. Write your function $f(x)$ as a composition of modules
   - the definition of a module depends on the specific task at hand
2. Work out the local derivative of each module symbolically
3. Do a forward pass for a given input x
   - i.e., compute $f(x)$ and remember the intermediate values for each module
4. Compute the local derivatives for x
5. Obtain the global derivative by multiplying the local derivatives

Work out the local derivatives

Compute the local derivative of each module symbolically

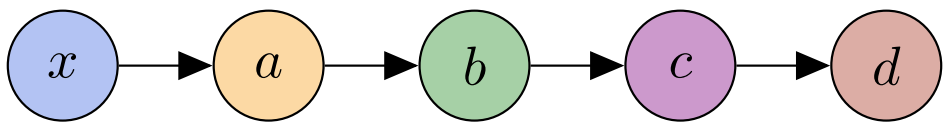
$$a(x) = -x \qquad \frac{\partial a}{\partial x} = -1$$

$$b(a) = \exp(a) \qquad \frac{\partial b}{\partial a} = \exp(a)$$

$$c(b) = \sin b \qquad \frac{\partial c}{\partial b} = \cos b$$

$$d(c) = \frac{2}{c} \qquad \frac{\partial d}{\partial c} = -\frac{2}{c^2}$$

Computational graph:



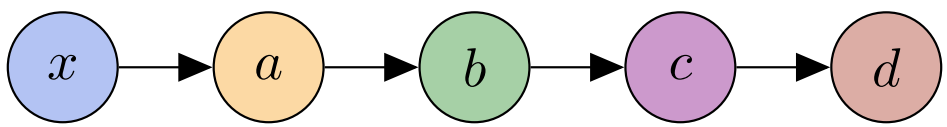
Forward pass

We want to compute the derivative $\frac{\partial f}{\partial x}$ at $x = -4.499$

In the forward pass, we compute f by following the computational graph and cache (memorize) the intermediate values of a, b, c, d

$$a = -x = 4.499$$
$$b = \exp(a) = 90$$
$$c = \sin b = 1$$
$$d = \frac{2}{c} = 2$$

Computational graph:



Backward pass

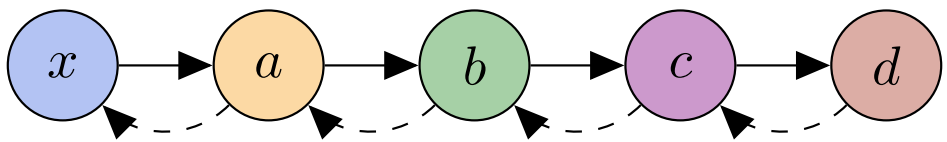
In the backward pass, we use the cached values of a, b, c, d to compute the local derivatives $\frac{\partial d}{\partial c}, \frac{\partial c}{\partial b}, \frac{\partial b}{\partial a}, \frac{\partial a}{\partial x}$

$$\frac{\partial a}{\partial x} = -1 \qquad \frac{\partial b}{\partial a} = \exp(a) = \exp(4.499) = 90$$

$$\frac{\partial c}{\partial b} = \cos b = \cos 90 = 0 \qquad \frac{\partial d}{\partial c} = -\frac{2}{c^2} = -\frac{2}{1^2} = -2$$

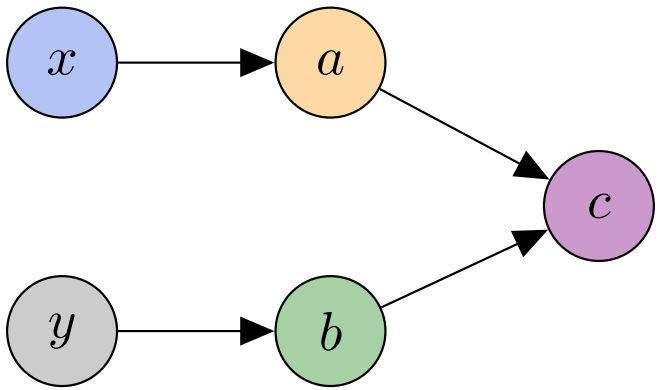
We obtain the global derivative by multiplying the local derivatives

$$\frac{\partial f}{\partial x} = \frac{\partial d}{\partial c}\frac{\partial c}{\partial b}\frac{\partial b}{\partial a}\frac{\partial a}{\partial x} = -2 \cdot 0 \cdot 90 \cdot -1 = 0$$



Multiple inputs

What if a function has multiple inputs?

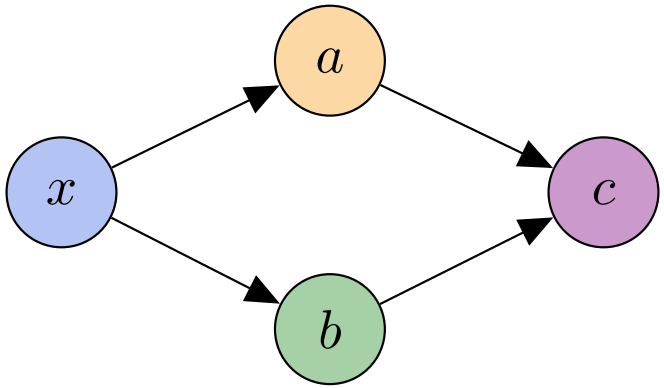


We compute the derivative along each of the paths

$$\frac{\partial c}{\partial x} = \frac{\partial c}{\partial a}\frac{\partial a}{\partial x} \qquad \frac{\partial c}{\partial y} = \frac{\partial c}{\partial b}\frac{\partial b}{\partial y}$$

Multiple paths

What if a computational graph contains multiple paths from x to c?

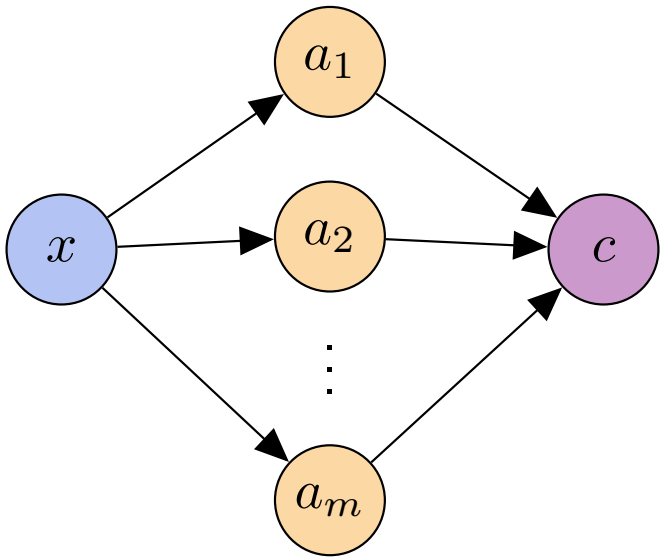


We need to sum the derivatives along each of the paths

$$\frac{\partial c}{\partial x} = \frac{\partial c}{\partial a}\frac{\partial a}{\partial x} + \frac{\partial c}{\partial b}\frac{\partial b}{\partial x}$$

Multivariate chain rule

The generalization to an arbitrary number of paths is given by the multivariate chain rule.



We need to sum the derivatives along all the paths

$$\frac{\partial c}{\partial x} = \sum_{i=1}^{m} \frac{\partial c}{\partial a_i} \frac{\partial a_i}{\partial x}$$

Jacobian and the gradient

Consider a function $f : \mathbb{R}^n \to \mathbb{R}^m$, and let $\boldsymbol{a} = f(\boldsymbol{x})$. The **Jacobian** is an $m \times n$ matrix of partial derivatives:

$$\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} = \begin{bmatrix} \frac{\partial a_1}{\partial x_1} & \cdots & \frac{\partial a_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial a_m}{\partial x_1} & \cdots & \frac{\partial a_m}{\partial x_n} \end{bmatrix} \in \mathbb{R}^{m \times n}$$

Let $g : \mathbb{R}^m \to \mathbb{R}$ and let $c = g(\boldsymbol{a})$.

The gradient $\nabla_{\boldsymbol{a}} c \in \mathbb{R}^m$ is the *transpose* of the Jacobian $\frac{\partial c}{\partial \boldsymbol{a}} \in \mathbb{R}^{1 \times m}$

$$\nabla_{\boldsymbol{a}} c = \left(\frac{\partial c}{\partial \boldsymbol{a}} \right)^T = \begin{bmatrix} \frac{\partial c}{\partial a_1} & \cdots & \frac{\partial c}{\partial a_m} \end{bmatrix}^T$$

Note that the gradient $\nabla_{\boldsymbol{a}} c$ has the same shape as $\boldsymbol{a}$.

We are using the so-called numerator notation. Some other resources use a different (denominator) notation — be careful when using other books or slides.

Chain rule in matrix form

We can compactly represent the chain rule using Jacobian matrices

$$\frac{\partial c}{\partial x_j} = \sum_{i=1}^{m} \frac{\partial c}{\partial a_i} \frac{\partial a_i}{\partial x_j}$$

We can write this in matrix form:

$$\underbrace{\frac{\partial c}{\partial \boldsymbol{x}}}_{\in \mathbb{R}^{1 \times n}} = \underbrace{\frac{\partial c}{\partial \boldsymbol{a}}}_{\in \mathbb{R}^{1 \times m}} \underbrace{\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}}_{\in \mathbb{R}^{m \times n}}, \qquad \text{where } \left[\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}\right]_{ij} = \frac{\partial a_i}{\partial x_j} \in \mathbb{R}$$

or equivalently:

$$\underbrace{\nabla_{\boldsymbol{x}} c}_{\in \mathbb{R}^{n}} = \underbrace{\left(\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}\right)^{T}}_{\in \mathbb{R}^{n \times m}} \underbrace{\nabla_{\boldsymbol{a}} c}_{\in \mathbb{R}^{m}}$$

Computational graph of a neural network

Consider a simple regression problem:

- Data: $\boldsymbol{x} \in \mathbb{R}^D, y \in \mathbb{R}$.
- Loss function: square error

Generate predictions with a feed-forward NN

$$\begin{aligned}\boldsymbol{a} &= \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b} \\ \boldsymbol{h} &= \sigma(\boldsymbol{a}) \\ \hat{y} &= \boldsymbol{V}\boldsymbol{h} + c \\ E &= (\hat{y} - y)^2\end{aligned}$$

In order to optimize $\boldsymbol{W}$ with gradient descent, we need to compute $\frac{\partial E}{\partial \boldsymbol{W}}$.

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In order to optimize $\boldsymbol{W}$ with gradient descent, we need to compute $\frac{\partial E}{\partial \boldsymbol{W}}$.
Does chain rule even make sense in this scenario?

$$\frac{\partial E}{\partial \boldsymbol{W}} = \frac{\partial E}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}}$$

What does it mean to take a derivative of a vector $\boldsymbol{a}$ w.r.t. a matrix $\boldsymbol{W}$?

Digression: matrix calculus

Consider a function having a specific input and output shape (e.g., scalar $\rightarrow$ scalar, vector $\rightarrow$ scalar, matrix $\rightarrow$ scalar, etc.).

		Input is a ...		
		scalar	vector	matrix
Output is a ...	scalar	scalar	vector	matrix
	vector	vector	matrix	3-way tensor
	matrix	matrix	3-way tensor	4-way tensor

Given $\boldsymbol{a} \in \mathbb{R}^H$ and $\boldsymbol{W} \in \mathbb{R}^{H \times D}$, $\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}} \in \mathbb{R}^{H \times H \times D}$ is a 3-way tensor s.t.:

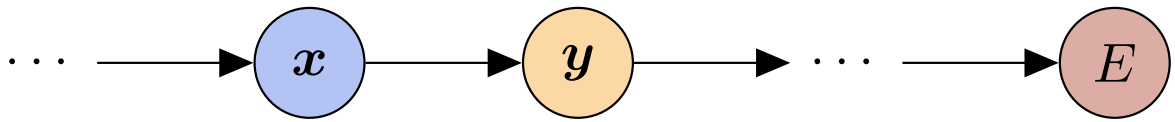
$$\left(\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}} \right)_{ijk} = \frac{\partial a_i}{\partial W_{jk}}$$

Accumulating the gradient

The **local derivatives** (i.e. Jacobians), such as $\frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}}$, are large multidimensional tensors.

Materializing (computing) them is *expensive* and unnecessary.

In reality, we only care about the **global derivative**!



Assume that we know $\frac{\partial E}{\partial \boldsymbol{y}}$, and want to compute $\frac{\partial E}{\partial \boldsymbol{x}}$.

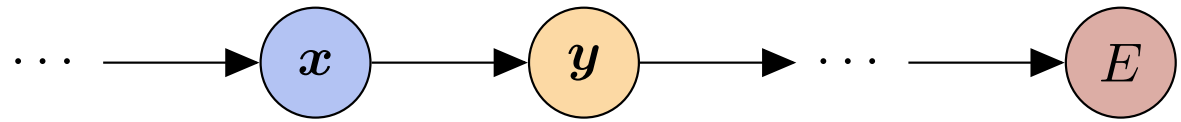
Most of the time, the Jacobian-vector product

$$\frac{\partial E}{\partial \boldsymbol{x}} = \frac{\partial E}{\partial \boldsymbol{y}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}$$

can be computed efficiently without materializing the Jacobian $\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}$!

Accumulating the gradient: Implementation

Backpropagation is typically implemented using the following abstraction.



Each module in the computational graph defines two functions

`forward`$(\boldsymbol{x})$ given input $\boldsymbol{x}$, compute output $\boldsymbol{y}$

`backward`$\left(\frac{\partial E}{\partial \boldsymbol{y}}\right)$ given the incoming global derivative $\frac{\partial E}{\partial \boldsymbol{y}}$

compute the product $\frac{\partial E}{\partial \boldsymbol{x}} = \frac{\partial E}{\partial \boldsymbol{y}} \frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}$

Then, $\frac{\partial E}{\partial \boldsymbol{x}}$ is passed as input to the parent node in the computational graph, etc.

Example: Affine layer

Back to our problem of finding

$$\frac{\partial E}{\partial \boldsymbol{W}} = \frac{\partial E}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \boldsymbol{h}} \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}}$$

An affine layer is defined as

$$\boldsymbol{a} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

where $\boldsymbol{x} \in \mathbb{R}^D, \boldsymbol{W} \in \mathbb{R}^{H \times D}, \boldsymbol{b} \in \mathbb{R}^H, \boldsymbol{a} \in \mathbb{R}^H$

`forward`$(\boldsymbol{W}, \boldsymbol{x}, \boldsymbol{b})$: compute $\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$

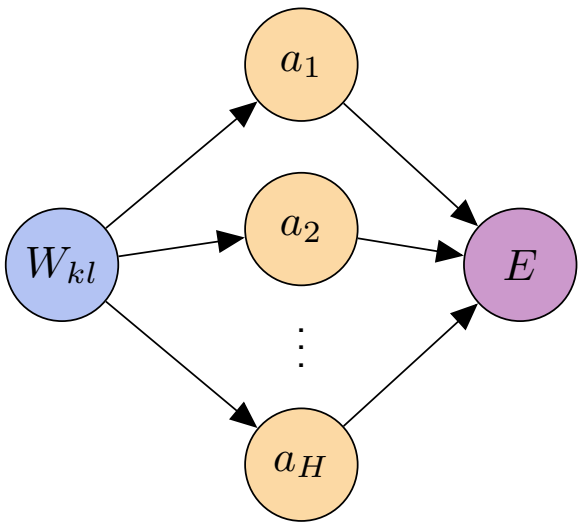
`backward`$\left(\frac{\partial E}{\partial \boldsymbol{a}}\right)$: compute

$$\frac{\partial E}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}}, \qquad \frac{\partial E}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}}, \qquad \frac{\partial E}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{b}}$$

How can we implement this efficiently?

Step 1: work out the scalar derivative

First, let's find $\frac{\partial E}{\partial W_{kl}}$ for some k, l



$$
\begin{aligned}
\frac{\partial E}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial W_{kl}} &= \sum_i \frac{\partial E}{\partial a_i} \frac{\partial a_i}{\partial W_{kl}} \\
&= \sum_i \frac{\partial E}{\partial a_i} \frac{\partial (\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b})_i}{\partial W_{kl}} \\
&= \sum_i \frac{\partial E}{\partial a_i} \frac{\partial (\boldsymbol{W}_{i:}\boldsymbol{x})}{\partial W_{kl}} \\
&= \sum_i \frac{\partial E}{\partial a_i} \frac{\partial (\sum_j W_{ij} x_j)}{\partial W_{kl}} \\
&= \sum_i \sum_j \frac{\partial E}{\partial a_i} \frac{\partial W_{ij} x_j}{\partial W_{kl}} = \frac{\partial E}{\partial a_k} x_l
\end{aligned}
$$

Step 2: backward pass in matrix form

For each element W_{kl} we have

$$\frac{\partial E}{\partial W_{kl}} = \frac{\partial E}{\partial a_k} x_l$$

We can compute $\frac{\partial E}{\partial W_{kl}}$ for all elements k, l in matrix form

$$\times \qquad \begin{bmatrix} x_1 & \cdots & x_D \end{bmatrix}$$

$$\begin{bmatrix} \frac{\partial E}{\partial a_1} \\ \vdots \\ \frac{\partial E}{\partial a_H} \end{bmatrix} \qquad \begin{bmatrix} \frac{\partial E}{\partial W_{11}} & \cdots & \frac{\partial E}{\partial W_{1D}} \\ \vdots & \ddots & \vdots \\ \frac{\partial E}{\partial W_{H1}} & \cdots & \frac{\partial E}{\partial W_{HD}} \end{bmatrix}$$

Or more compactly

$$\frac{\partial E}{\partial \boldsymbol{W}} = \left(\frac{\partial E}{\partial \boldsymbol{a}} \right)^T \boldsymbol{x}^T$$

Matrix operations are much more efficient than `for`-loops thanks to vectorization (especially on GPUs)

Example: Affine layer

An affine layer is defined as

$$\boldsymbol{a} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$$

`forward`$(\boldsymbol{W}, \boldsymbol{x}, \boldsymbol{b})$: compute $\boldsymbol{W}\boldsymbol{x} + \boldsymbol{b}$

`backward`$\left(\frac{\partial E}{\partial \boldsymbol{a}}\right)$: compute

$$\frac{\partial E}{\partial \boldsymbol{W}} = \frac{\partial E}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{W}} = (\boldsymbol{x} \frac{\partial E}{\partial \boldsymbol{a}})^T$$
$$\frac{\partial E}{\partial \boldsymbol{x}} = \frac{\partial E}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{x}} = \frac{\partial E}{\partial \boldsymbol{a}} \boldsymbol{W}$$
$$\frac{\partial E}{\partial \boldsymbol{b}} = \frac{\partial E}{\partial \boldsymbol{a}} \frac{\partial \boldsymbol{a}}{\partial \boldsymbol{b}} = \frac{\partial E}{\partial \boldsymbol{a}}$$

The derivatives for $\boldsymbol{x}$ and $\boldsymbol{b}$ are obtained similarly to $\boldsymbol{W}$.

Backpropagation: Summary

- Define the computation as a composition of modules
- The `forward` function computes the output of the module
- The `backward` function accumulates the total gradient
- We can implement `backward` without materializing the Jacobian
- Backpropagation walks backward through the computational graph, accumulating the product of gradients

Reading material

- Goodfellow, Deep Learning: Chapter 6

Acknowledgements

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- Backpropagation slides are based on the materials from `mlvu.github.io` by Peter Bloem