Content

1 Introduction

Artificial neural networks (ANNs) are a family of models inspired by biological neural networks. Usually, ANNs have an *input layer* and an *output layer*. Deep learning consists of ANNs with multiple *hidden layers,* that perform intermediate computations.

Embeddings are learned dense, continuous, low-dimensional vector representations of objects. They are useful to represent complex objects (image data, graph data, tabular data, textual data).

In practice, neural networks are usually trained using deep learning frameworks such as *PyTorch*. When using training data, the framework collects operations and their outputs to build a *computation graph*. This allows automatic gradient computation from this graph using *backpropagation*. The optimizer uses this gradient to update the model parameters in order to minimize some cost function.

Common Problems

We have large and complex models with many parameters. Training takes time and is costly.

We may face limited training data as large, labeled datasets are generally not available. The supervision signal alone may be insufficient to achieve reasonable performance.

Overfitting is a severe concern. Universal approximation theorem states that with sufficiently many hidden neurons, FNNs can perform arbitrarily well on the *training* set.

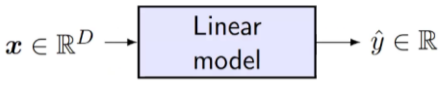
2 Feed-Forward Neural Networks

2.1 Embeddings

2.1.1 Linear Models

Consider a prediction task with inputs $x \in \mathcal{X}$ and outputs $y \in \mathcal{Y}$. The goal is to learn a function from $\mathcal{X}$ to $\mathcal{Y}$. Perhaps the simplest approach is to use a (generalized) linear model.

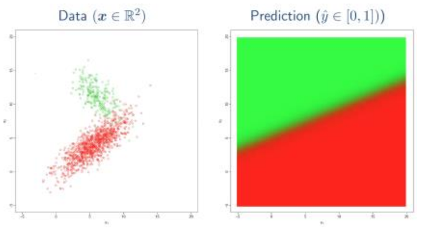
- Inputs must be real-valued feature vectors $\boldsymbol{x} \in \mathbb{R}^D$
- Outputs are a real value (e.g. lin./log. regression)



A linear model computes a weighted sum (inner product) of the feature vector $\boldsymbol{x}$ with the model weights $\boldsymbol{w}$:

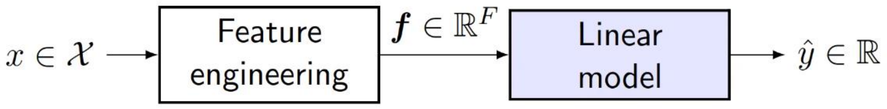
$$\hat{y} = \phi(\boldsymbol{w}^\top \boldsymbol{x} + b)$$

where $\boldsymbol{w} \in \mathbb{R}^D$ is a weight vector (one weight per feature), $b \in \mathbb{R}$ is a bias term and ϕ is a mean function.



❗ The problem of these models is the *low representational capacity* due to the linearity assumption. This means that the decision boundary is a linear hyperplane.

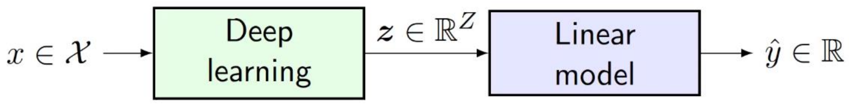
One approach to solve this problem is to perform *feature engineering*. Design some form of function that maps arbitrary input spaces to real-valued vectors $f: \mathcal{X} \to \mathbb{R}^F$



But this is hard to get right, usually requires expert domain knowledge and extensive experimentation.

2.1.2 Use of Deep Learning

📝 Deep Learning methods can be interpreted as an approach to learning features. Input objects $x \in \mathcal{X}$ are transformed into dense, low-dimensional representations called *embeddings* $\boldsymbol{z} \in \mathbb{R}^Z$.

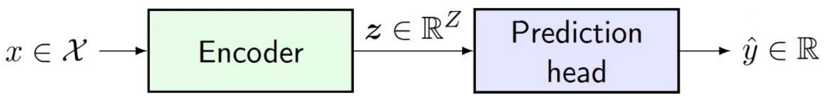


Instead of engineering features manually, embeddings are learned from data. They are also called latent code or distributed representations. The *embedding space* is also called *latent space*.

💡 Functions that transform objects $x \in \mathcal{X}$ to embeddings $\boldsymbol{z} \in \mathbb{R}^Z$ are known as *encoders*.

2.1.3 Terminology

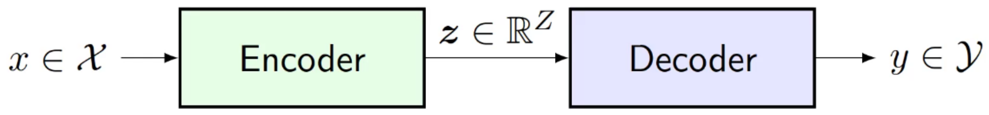
📝 Functions that transform embeddings $\boldsymbol{z} \in \mathbb{R}^Z$ to predictions $y \in \mathcal{Y}$ are known as *prediction heads*. They can be arbitrary simple/linear or complex.



Both encoder and prediction head are learned neural (sub-) networks.

2.1.4 Encoder-Decoder

Functions that decompress embeddings $\boldsymbol{z} \in \mathbb{R}^Z$ to obtain (complex) outputs $y \in \mathcal{Y}$ (or reconstructions $\hat{\boldsymbol{x}}$) are known as *decoders*. They generate a structured output.



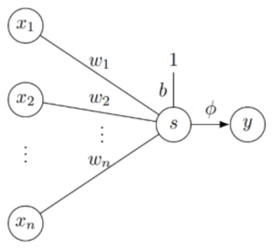
Decoders may be a reversed architecture of the encoder, but not necessarily.

2.2 Artificial Neurons

An artificial neuron (AN) is a function $f: \mathbb{R}^n \to \mathbb{R}$ that takes as some real-valued vector $\boldsymbol{x} \in \mathbb{R}^n$ an input and produces a single real value $y \in \mathbb{R}$ as an output, called *activation*.

$$y = \phi(\boldsymbol{w}^\top \boldsymbol{x} + b)$$

There are many types of neurons that only differ in their *activation* (*transfer*) function ϕ.

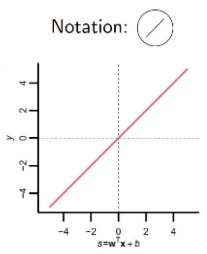


The simplest type of neuron is a **constant neuron**

- No inputs; output fixed value $x \in \mathbb{R}$
- Notation (from now on): $\textcircled{x}$

2.2.1 Linear Neuron / Identity

The linear neuron uses $\phi(s) = s$ as an activation function. This is very simple but computationally limited. We often (not always) want non-linear transfer functions

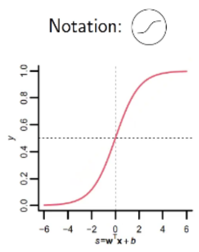


2.2.2 Logistic Neuron

The logistic neuron uses $\phi(s) = \sigma(s) \overset{\text{def}}{=} \frac{1}{1+\exp(-s)}$ as an activation function. This gives a real-valued output that is smooth and bounded in [0,1].

- negative activations mapped to $\phi(s) < 0.5$
- 0 activation mapped to $\phi(s) = 0.5$
- positive activations mapped to $\phi(s) > 0.5$

This gives us non-linearity and is often used in the output layer!

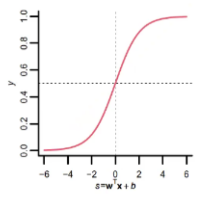


2.2.3 Stochastic Binary Neuron

Also uses the logistic function, but the output is treated as a probability of producing a spike:

$$\phi(s) = \begin{cases} 1 & \text{with probability } \sigma(s) \\ 0 & \text{otherwise} \end{cases}$$

This defines a probability distribution over outputs.



2.3 Artificial Neural Networks

A network of artificial neurons has a set of ANs with (directed or undirected) connections between these neurons. There are many architectural choices to be made:

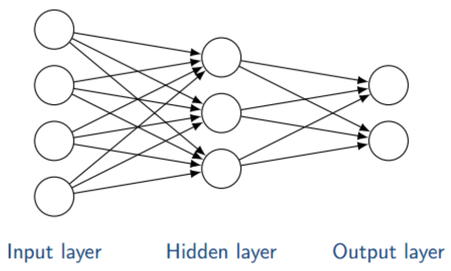
- How many neurons, which type?
- Output neurons? Hidden Neurons?
- Which are connected?
- Directed or undirected connections?

Picking the right architecture for the problem at hand is important → *architecture engineering*.

2.3.1 Feedforward Neural Network (FNN)

A feedforward neural network (FNN) is an ANN in which

- all connections are directed
- there are no cycles (i.e., forms a DAG)



Neurons usually grouped in layers

- Input neurons: no incoming edges (first layer)
- Output neurons: no outgoing edges (last layer)
- Hidden neurons: all others (layer = maximum distance from input)

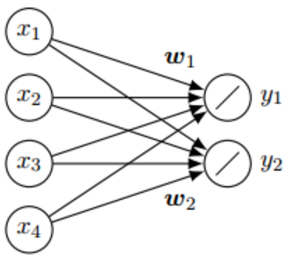
Layers do not need to be fully connected. Traditionally edges are only between subsequent layers (but: edges that skip layers are allowed, too)

💡 FFNs are discriminative models; given an input they compute an output but don’t allow going from out- to inputs.

💡 As hidden layers outputs are the inputs of the next layer, we may think of hidden layers as intermediate features for the next layer. These are not provided upfront but learned.

2.3.2 Linear Layers

📄 Layers in which all layer inputs are connected with all layer’s outputs are called *dense* or *fully connected layers*. A dense *linear layer* is a layer consisting of only linear neurons: n layer inputs ($\boldsymbol{x} \in \mathbb{R}^n$) and m layer outputs ($\boldsymbol{y} \in \mathbb{R}^m$).



Example:
$n = 4, m = 2$, no bias

They are parameterized by weight vectors $\boldsymbol{w}_1, \dots, \boldsymbol{w}_m \in \mathbb{R}^n$ and optionally: biases $b_1, \dots, b_m \in \mathbb{R}$. Neuron outputs are given by:

$$y_j = \sum_i [\boldsymbol{w}_j]_i x_i + b_j = \langle \boldsymbol{w}_j, \boldsymbol{x} \rangle + b$$

💡 Let $\boldsymbol{W} \in \mathbb{R}^{n \times m}$ be a *weight matrix* in which the j-th column equals the weights $\boldsymbol{w}_j$ of the j-th layer output:

$$\boldsymbol{W} = (\boldsymbol{w}_1 \quad \boldsymbol{w}_2 \quad \dots \quad \boldsymbol{w}_m)$$

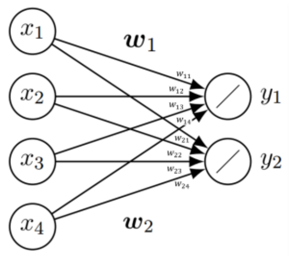
Linear layers compute a matrix-vector product:

$$\boldsymbol{y} = \boldsymbol{W}^\top \boldsymbol{x}$$

For our example $\boldsymbol{W} = (\boldsymbol{w}_1 \quad \boldsymbol{w}_2)$, and:

$$\boldsymbol{W}^\top \boldsymbol{x} = \begin{pmatrix} \boldsymbol{w}_1^\top \\ \boldsymbol{w}_2^\top \end{pmatrix} \boldsymbol{x} = \begin{pmatrix} \langle \boldsymbol{w}_1, \boldsymbol{x} \rangle \\ \langle \boldsymbol{w}_2, \boldsymbol{x} \rangle \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \boldsymbol{y}$$

Example



$$\boldsymbol{W} = (\boldsymbol{w_1} \quad \boldsymbol{w_2}) = \begin{pmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \\ w_{13} & w_{23} \\ w_{14} & w_{24} \end{pmatrix}$$

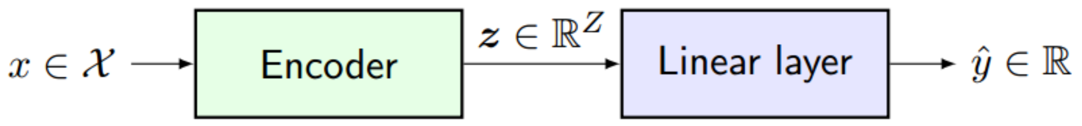
$$\boldsymbol{x}^\top = (x_1 \quad x_2 \quad x_3 \quad x_4)$$

$$\boldsymbol{y} = \boldsymbol{W}^\top \boldsymbol{x} = \overset{\in \mathbb{R}^{2\times4}}{\begin{pmatrix} w_{11} & w_{12} & w_{13} & w_{14} \\ w_{21} & w_{22} & w_{23} & w_{24} \end{pmatrix}} \overset{\in \mathbb{R}^{4\times1}}{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}} = \overset{\in \mathbb{R}^{2\times1}}{\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}}$$

TODO Refer to batch processing.

Linear layers are typically used as:

- an output layer for regression tasks

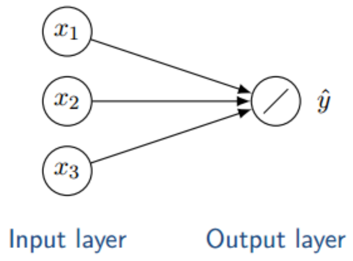


- a hidden layers to perform dimensionality reduction ($m < n$)
- a hidden layer to increase dimensionality ($m > n$)

2.3.3 Linear Regression as FNN

In a linear FNN, all neurons/layers are linear. The simplest linear FNN has a single linear layer with one output. Its output is:

$$\hat{y} = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b$$

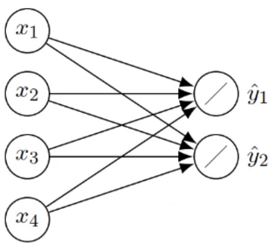


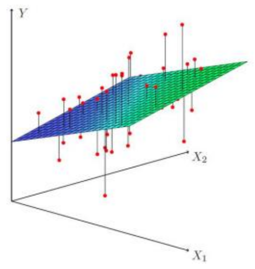
Suppose we train this network using ERM with squared loss:

$$\frac{1}{N}\sum_i (y_i - \hat{y}_i)^2$$

Then we obtain the ordinary least squares (OLS) estimate for linear regression. With multiple outputs, we obtain *multiple linear regression*.

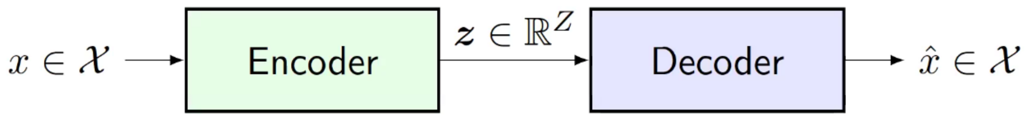
The output of a linear FFN remains linear even when adding hidden layers. That’s why we often want non-linear transfer functions.





2.3.4 Autoencoders

FNNs are useful for unsupervised learning as well. Given an unlabeled dataset $\mathcal{D} = \{\boldsymbol{x}_i\}_{i=1}^N$ we want to find structure, patterns or reduce dimensionality. The way autoencoders do this, is by training the FNN to predict its input, i.e., set $\boldsymbol{y}_i = \boldsymbol{x}_i$.



Autoencoders are a technique to learn embeddings. We don’t really care about the decoder.

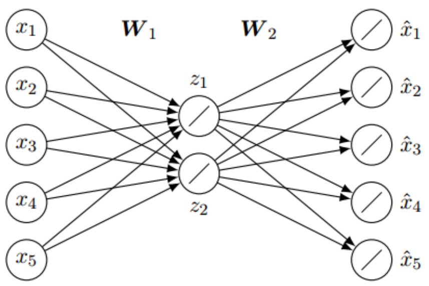
💡 Further, e.g. in semi-supervised learning, we can train the autoencoder on all inputs (unsupervised) and can then only train the prediction head in a supervised fashion using the labeled data. This allows the model to benefit from both, especially when labeled data is scarce.

Other uses are:

- Clustering: use embeddings as inputs to, say, K-means
- Denoising: use $\hat{x}$ (noisy input) instead of x but still try to predict x
- Visualization: visualize $\boldsymbol{z}$ (e.g., using Z=2 as in SVD)

2.3.5 Linear Autoencoders

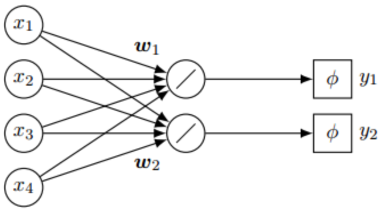
📝 A linear autoencoder uses only linear layers (in both encoder and decoder). Consider a linear autoencoder with $\boldsymbol{x} \in \mathbb{R}^D$ and one hidden layer with $Z < D$ hidden neurons.



💡 A layer with few neurons is referred to as a *bottleneck, i*.e., fewer neurons than the surrounding layers. This forces FNN to compress information → *dimensionality reduction*

Since autoencoders need to reconstruct all inputs well, the optimal "compression" depends on all training inputs. E.g., above: 5D data ($\boldsymbol{x}$) compressed into a 2D representation ($\boldsymbol{z}$).

2.4 Non-Linear Layers

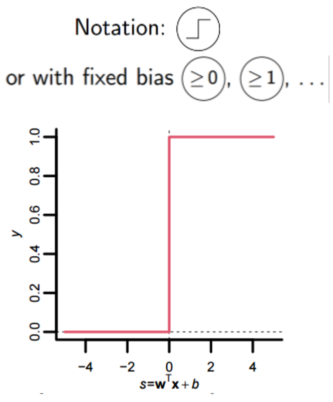


We can also interpret a fully connected layer as a (learned) linear layer followed by a (fixed) non-linearity. The action of the layer (without bias) is:

$$\boldsymbol{y} = \phi(\boldsymbol{W}^\top \boldsymbol{x})$$

where we take the convection that ϕ is applied elementwise on vector inputs.

2.4.1 Binary Threshold Neuron

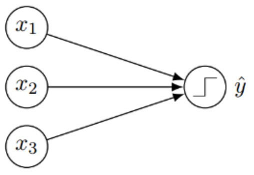


📝 One of the (seemingly) simplest non-linear neurons is the binary threshold neuron (also called *McCulloch-Pitts neuron*). It uses the binary threshold function as transfer function:

$$\phi(s) = \mathbb{I}(s \geq 0) = \begin{cases} 1 & \text{if s} \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

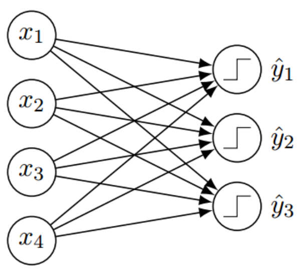
outputs fixed "spike" if input s is non-negative, else "nothing".

2.4.2 Perceptron



Corresponds to an FNN without hidden layers and binary threshold units for outputs (*single-layer perceptron*). Perceptrons can classify perfectly if there exists an *affine hyperplane* that separates the classes, i.e., when the data is *linearly separable*. Otherwise, the perceptron must make errors on some inputs. This is quite limited; e.g., perceptrons cannot learn the XOR function.

2.4.3 Perceptron's with multiple output units



💡 Consider a perceptron with m binary outputs for classification tasks.

There are mutliple ways to interpret/use the output of such a network for classification.

1. **multi-label classification** → works.

- Each input is associated with m binary class labels
- Goal is to predict each of them:
  E.g.: height (small/tall), hair color (light/dark), ...

m = 3 class labels

$$\begin{array}{c|cccccccc|c}
\text{Output} & & & & & & & & & \text{Classes} \\
\hat{y}_1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & \text{A} \\
\hat{y}_2 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 & \text{B} \\
\hat{y}_3 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 & \text{C}
\end{array}$$

2. **multi-class classification** → problematic

- Each input is associated with one out of 2^m class labels
- We associate each label (A-H) with one output vector $(\hat{y}_1 \quad \hat{y}_2 \quad \hat{y}_3)^\top$ of the perceptron
- ❗ Problem: Which class label corresponds to which output vector? → choice matters!

$m = 3$, $2^3 = 8$ class labels

$$\begin{array}{c|cccccccc}
\text{Output} & & & & & & & & \\
\hat{y}_1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\
\hat{y}_2 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\
\hat{y}_3 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \\
\hline
\text{Classes} & \text{A} & \text{B} & \text{C} & \text{D} & \text{E} & \text{F} & \text{G} & \text{H}
\end{array}$$

3. **multi-class classification** → problematic

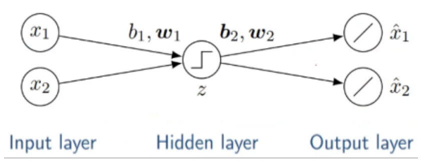
- Each input is associated with one out of m class labels
- We associate each label with its indicator vector (one-hot encoding)
- ❗ Problem: What if the network outputs less/more than a single 1?

m = 3 class labels

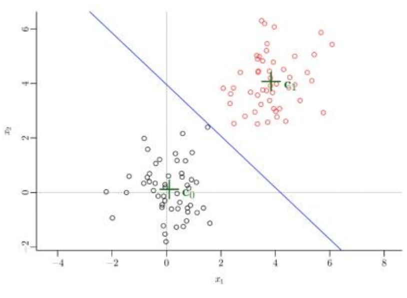
$$\begin{array}{c|ccc}
\text{Output} & & & \\
\hat{y}_1 & 1 & 0 & 0 \\
\hat{y}_2 & 0 & 1 & 0 \\
\hat{y}_3 & 0 & 0 & 1 \\
\hline
\text{Classes} & \text{A} & \text{B} & \text{C}
\end{array}$$

2.4.4 Autoencoders with Binary Threshold Unit

Consider the following autoencoder (image on the right). Here, the output z is constrained to be binary, taking values from the set $\{0,1\}$, creating a binary embedding.



💡 When minimizing the squared error over the training data, the autoencoder effectively computes the centroids of *"K=2"* clusters as embeddings.

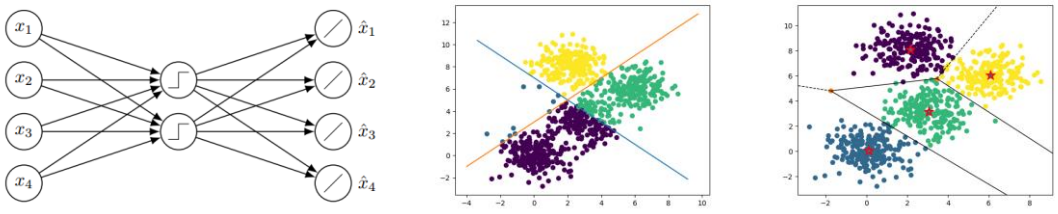


This happens as the binary threshold unit acts as a linear classifier. The input x is either mapped to $z = 0$ or to $z = 1$.

The weights b_1 and $\boldsymbol{w}_1$ will define a hyperplane separating the two possible outputs.

This is due to the binary threshold unit acting as a lin. classifier. Input $\boldsymbol{x}$ is mapped either to $z = 0$ or $z = 1$, depending on the weights b_1 and $\boldsymbol{w}_1$, effectively defining a hyperplane separating the two potential outputs. This is akin to the decision boundary in traditional linear classification.

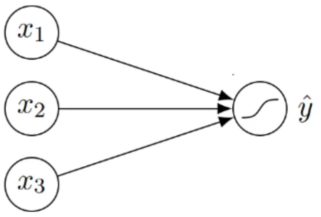
What happens if we have multiple binary threshold units?



Output produced from the autoencoder (left) vs. the K-Means counterpart (right).

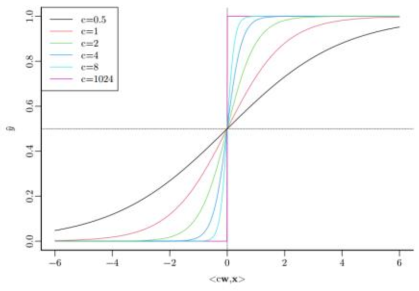
2.4.5 FNN with single Logistic Neuron

Recall the logistic neuron, *cf. 2.2.2*, and consider the FNN to the right.



If the output of the logistic unit $\hat{y} = \sigma(\langle \boldsymbol{w}, \boldsymbol{x} \rangle)$ is rounded to the nearest integer ($\in \{0,1\}$), we obtain the output of the corresponding perceptron (has binary threshold unit). Hence, we can see the logistic unit as a smooth version of a binary threshold unit.

If we scale the weights $\boldsymbol{w}$ by some constant $c > 0$, we change the degree of smoothing. This means that the norm of the weight vector $||\boldsymbol{w}||$, essentially determines the behavior of the logistic neuron.



Now suppose we use the network for a binary classification task, given a labeled set $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^N$ of input-output pairs.

We can minimize the misclassification error (0-1 loss):

$$\sum_i |y_i - \text{round}(\hat{y}_i)|$$

which is *equivalent to the perceptron*. While the outputs $\hat{y}$ are related to the distance from decision boundary, there is no probabilistic interpretation possible.

We can also maximize the log-likelihood of the provided labels:

$$\ln \mathcal{L} = \sum_i [y_i \ln \hat{y}_i + (1 - y_i) \ln(1 - \hat{y}_i)]$$

which is *equivalent to logistic regression*. Inputs $\langle \boldsymbol{w}, \boldsymbol{x} \rangle$ to logistic transfer function can be interpreted as estimate of the log odds of positive class. The output $\hat{y}_i$ can be interpreted as confidence for positive class.

Hence, the output layer of FNNs for binary classification tasks is typically a logistic neuron.

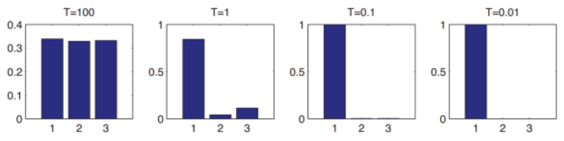
2.4.6 Softmax Function

The *Softmax function* takes as input a vector $\boldsymbol{\eta} = (\eta_1, \dots, \eta_C)^\mathrm{T} \in \mathbb{R}^C$ consisting of C real numbers and transforms these real values into a *probability vector* $S(\boldsymbol{\eta})$.

$$S(\boldsymbol{\eta})_c = \frac{\exp(\eta_c)}{\sum_{c'=1}^{C} \exp(\eta_{c'})}$$

It exaggerates differences in the input vector. Below is the result for $\boldsymbol{\eta} = (3, 0, 1)^{\mathrm{T}}$ with $S\left(\frac{\boldsymbol{\eta}}{T}\right)$ at different *temperatures* T.

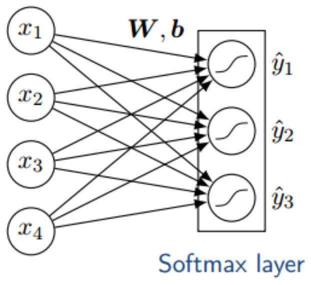
When the temperature T is high (left), the distribution is rather uniform, whereas when the temperature T is low (right), the distribution is "spiky", with all its mass on the largest element.



2.4.7 Softmax Layer

A *softmax layer* computes $\hat{\boldsymbol{y}} = S\left(\frac{\boldsymbol{W}^{\mathrm{T}}\boldsymbol{x}+\boldsymbol{b}}{T}\right)$, where $\hat{\boldsymbol{y}} \in \mathcal{S}_C$ is a probability vector, T is the temperature hyperparameter that controls smoothness of distribution (assume T = 1 for now).

A FNN with single softmax layer, trained with MLE / ERM + log loss, allows us to interpret $\hat{y}_c$ as the model's confidence in label c. This is *equivalent to multinomial logistic regression* (Softmax regression).



The output of a softmax layer with C neurons is an element of the *probability simplex* $\mathcal{S}_C$, with the following properties:

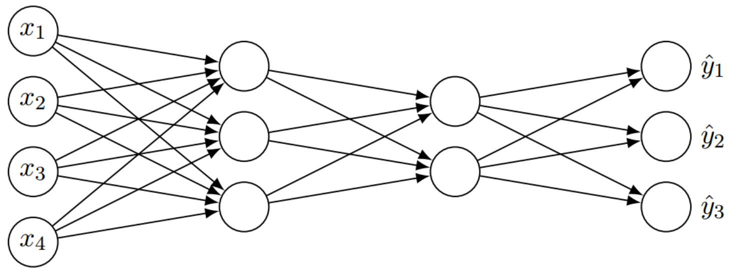
$$\mathcal{S}_C = \left\{ \boldsymbol{y}_c \in \mathbb{R}^C, \qquad 0 < y_c \leq 1, \qquad \sum_c y_c = 1 \right\}$$

this simply is the set of all vectors of size C, such that they are probability vectors.

2.4.8 Multi-Layer FNN / Perceptron (MLP)

💡 We can improve performance by engineering better features: by including *hidden layers*, we let the network perform feature engineering (we can interpret them as features for the next layers).

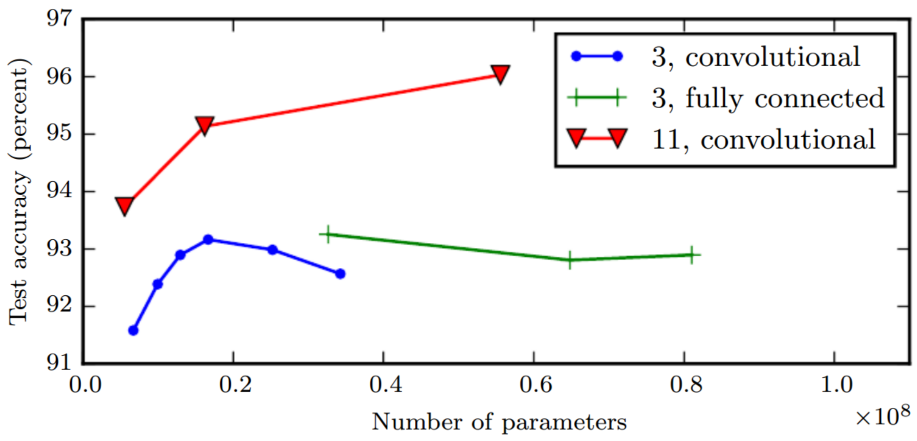
📝 If there is at least one hidden layer ($L \geq 1$) , the network is called a *multi-layer FNN* (or also *multi-layer perceptron: MLP*). If $L > 1$, we call this network *deep*.



❗ The *Universal Approximation Theorem* states that "any" function (on $[0,1]^D$) can be represented either via sufficient *width* or sufficient *depth* -- but that doesn't mean that we can learn it!

- Training methods may fail to find good parameterization
- Overfitting may occur
- Number of required units can be exponential in the input dimensionality

In general, empirical evidence shows that deep models tend to show better generalization performance than wide models.



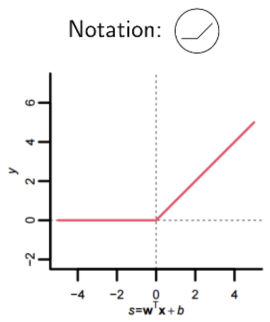
The legend indicates the *depth* of network used to make each curve. Increasing the number of parameters in layers of convolutional networks *without increasing their depth* is not nearly as effective at increasing test set performance.

2.4.9 Rectified Linear Unit (ReLU)

📝 Also called *linear threshold neuron* or *rectifier*. It outputs the weighted sum s if s is non-negative, else "nothing".

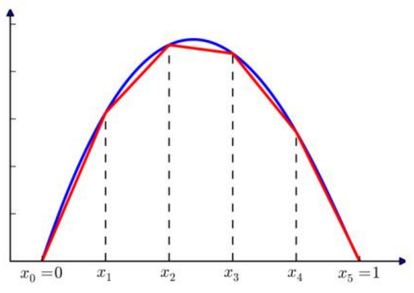
$$\phi(s) = \max\{0, s\} = \begin{cases} s & \text{if } s \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

💡 Common non-linearity for intermediate layers in deep NNs.

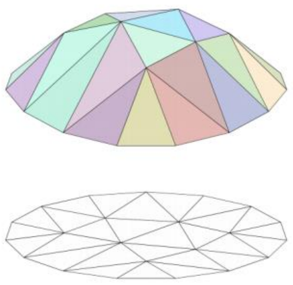


2.4.10 Rectifier Networks

Rectifier networks are MLPs with only ReLU in hidden and output layers. The function computed by rectifier network is *piecewise linear it* → approximates a function by decomposing it into linear regions. The more linear regions, the more flexible/expressive (roughly).



1D example


2D example

Consider rectifier networks of form:

- D = input dimensionality (assumed constant)
- H = total number of hidden units
- L = total number of hidden layers, each of width $Z \geq D$ (→ *wide*)

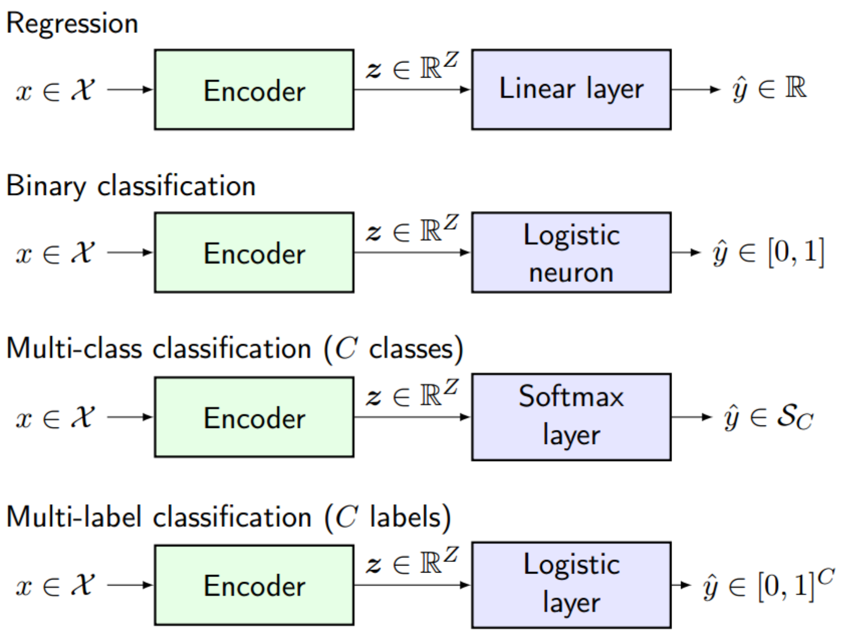
Then, the number of linear regions is *at most* 2^H → not more than exponentially many linear regions are possible! ("bounded from above")

The number of *attainable* linear regions *at least* $\Omega\left(\left(\frac{Z}{D}\right)^{(L-1)D} Z^D\right)$ → "bounded from below", with *attainable* meaning: assuming an optimal parameterization for a given architecture/form.

- Polynomial in Z (width)
- Exponential in L (depth)

Exponentially many linear regions are indeed possible!

2.5 Summary



3 Gradient-Based Training

Training FNNs in a supervised fashion involves minimizing a chosen *cost function*, typically through techniques like gradient descent or its variants. *Empirical risk minimization* (ERM) is a common approach in machine learning, with the goal to *minimize the average loss over the training data* $\{(\boldsymbol{x}_i, \boldsymbol{y}_i)_{i=1}^{N}\}$. *Also see* *3.4.2 Effect of Batch Size*:

$$R_{emp}(\boldsymbol{\theta}) = \frac{1}{N}\sum_i L(\hat{\boldsymbol{y}}_i, \boldsymbol{y}_i) \qquad \text{where} \quad \hat{\boldsymbol{y}}_i = f(\boldsymbol{x}_i; \boldsymbol{\theta})$$

where $\boldsymbol{\theta}$ refers to the FNN's parameters. In the context of FNNs, this often involves minimizing the difference between the network's predictions $\hat{\boldsymbol{y}}_i = f(\boldsymbol{x}_i; \boldsymbol{\theta})$ and the true labels $\boldsymbol{y}_i$ of the training examples. The choice of cost function is crucial in determining the behavior and performance of the trained model. It defines what the network is trying to optimize during the training process.

💡 Loss vs. Cost

A *cost function* typically refers to the objective function that the model aims to minimize during training. It encompasses not only the loss incurred on the training data but also potentially other regularization terms that penalize complex models or encourage certain properties. It is with respect to a single training example.

A *loss function* specifically refers to the part of the cost function that quantifies the discrepancy between the model's predictions and the actual targets on the training data. Its is with respect to the entire training set.

Some common loss functions include:

- Squared error (for regression)
- Log loss / binary cross entropy (for binary / multi-label classification)
- Cross entropy / KL divergence (for multi-class classification)
- Hinge loss (for margin-based classification)
- 0-1 loss / misclassification rate (for classification)

3.1 Backpropagation

📝 Backpropagation is an algorithm to compute gradients. Given a compute graph CG, it performs:

1. Forward pass to compute (all) outputs → *forward propagation*
2. Backward pass to compute (all) gradients → *backward propagation*

For us the *comp. graph* typically represents:

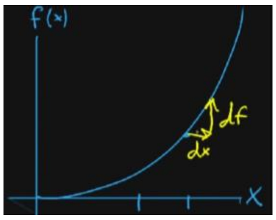
- Output $\hat{y}$ of an FNN, given $\boldsymbol{x}, \boldsymbol{\theta}$
- Loss L of an FNN, given $(\boldsymbol{x}, y), \boldsymbol{\theta}$
- Cost function J for an FNN, given $\{(\boldsymbol{x}_i, y_i)\}, \boldsymbol{\theta}$

We are also interested in gradients ∇:

- w.r.t. weights ($\nabla_{\boldsymbol{\theta}} J$) for gradient-based training
- w.r.t. intermediate outputs ($\nabla_{\boldsymbol{z}} L$) for model debugging
- w.r.t. inputs ($\nabla_{\boldsymbol{x}} L$ of $\nabla_{\boldsymbol{x}} \hat{y}$) for sensitivity analysis or adversarial training

3.2 Recap: Basics

3.2.1 Ordinary Derivatives



Ordinary derivatives are notated like this: $\frac{df}{dx}$ or simply $\frac{d}{dx}f$

They measure how a function $f(x)$ changes with respect to changes in x.

3.2.2 Partial Derivatives

The notation $\frac{\partial f}{\partial x}$ or $\frac{\partial}{\partial x}f$ is used for partial (∂) derivatives, where f is a function of several variables. Here we're finding the derivative with respect to one of those variables (e.g.: ∂x) while holding the others constant. For functions with multiple inputs, there are multiple partial derivatives.

$$f(x_1, x_2) = x_1^2 + 5x_1x_2 \qquad \frac{\partial}{\partial x_1}f = 2x_1 + 5x_2 \qquad \frac{\partial}{\partial x_2}f = 5x_1$$

3.2.3 Gradient

📝 The gradient $\nabla_{x^\top}$ of any function f gathers all its partial derivatives in a (row) vector:

$$\nabla_{x^\top} f \overset{\text{def}}{=} \begin{pmatrix} \frac{\partial}{\partial x_1}f & \frac{\partial}{\partial x_2}f & \cdots & \frac{\partial}{\partial x_n}f \end{pmatrix}$$

For the example in 3.2.2, we obtain:

$$\nabla_{x^\top} f = \begin{pmatrix} 2x_1 + 5x_2 & 5x_1 \end{pmatrix} \qquad \nabla_x f = \begin{pmatrix} 2x_1 + 5x_2 \\ 5x_1 \end{pmatrix}$$

Numerator layout (row) Denominator layout (column)

3.2.4 Chain Rule

The chain rule tells us how to differentiate composite functions; it states:

$$\frac{d}{dv} f\big(g(v)\big) = \frac{df}{dg} \cdot \frac{dg}{dv} = f'\big(g(v)\big) * g'(v)$$

A function is composite if you can write it as $f\big(g(v)\big)$. In other words, it is a function within a function. For example, $f = \cos(v^2)$ is composite and $\frac{\partial}{\partial v} f = -\sin(v^2) * 2v$.

This can be generalized to any number of composite functions, for example:

$$\frac{d}{dx} f\Big(g\big(h(x)\big)\Big) = \frac{df}{dg} \cdot \frac{dg}{dh} \cdot \frac{dh}{dx} = f'\Big(g\big(h(x)\big)\Big) * g'\big(h(x)\big) * h'(x)$$

3.2.5 Product Rule

In calculus, the product rule is a formula used to find the derivatives of *products of two or more functions*. For two functions $u(x)$ and $v(x)$, it states:

$$(u * v)' = u' * v + u * v'$$

in Lagrange's notation

$$\frac{d}{dx}(u * v) = \frac{du}{dx} * v + \frac{dv}{dx} * u$$

in Leibniz's notation

The product rule can be generalized to products of more than two factors, e.g., for three factors:

$$\frac{d}{dx}(u * v * w) = \frac{du}{dx}vw + u\frac{dv}{dx}w + uv\frac{dw}{dx}$$

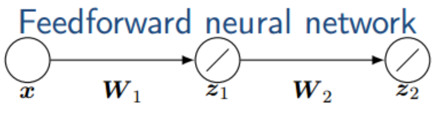
3.2.6 Multivariate Chain Rule

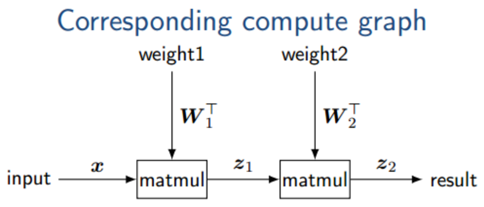
Consider a composite multivariable function $f\big(x(t), y(t)\big)$, its ordinary derivate is:

$$\frac{d}{dt}f\big(x(t), y(t)\big) = \frac{\partial f}{\partial x}\cdot\frac{dx}{dt} + \frac{\partial f}{\partial y}\cdot\frac{dy}{dt}$$

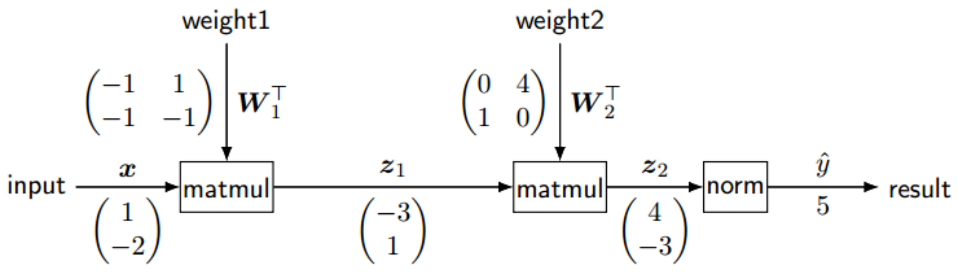
3.3 Compute Graphs

Backpropagation generally operates on a *compute graph*; a directed, acyclic graph that models a computation. Vertices (□) correspond to operations and edges (→) correspond to data passed between operations.





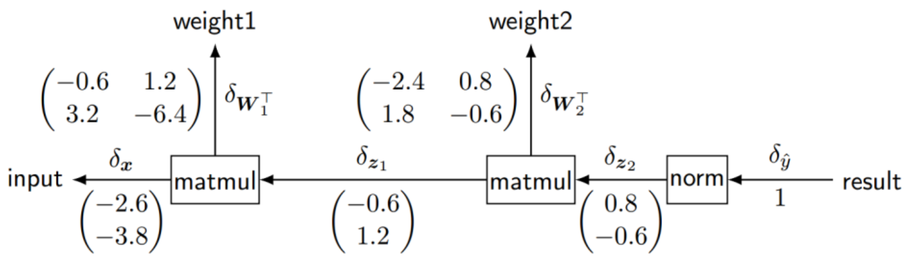
Example: Forward Pass


weight1
$\begin{pmatrix}-1 & 1\\ -1 & -1\end{pmatrix}$
$\boldsymbol{W}_1^\top$
weight2
$\begin{pmatrix}0 & 4\\ 1 & 0\end{pmatrix}$
$\boldsymbol{W}_2^\top$
input
$\boldsymbol{x}$
$\begin{pmatrix}1\\ -2\end{pmatrix}$
matmul
z_1
$\begin{pmatrix}-3\\ 1\end{pmatrix}$
matmul
z_2
$\begin{pmatrix}4\\ -3\end{pmatrix}$
norm
$\hat{y}$
5
result

Operators are evaluated in topological order ("forwards"). Whenever an operator is evaluated, all its inputs must be available. Furthermore, the computation is *local*: only input values are required (the remainder of the compute graph does not matter). Inputs and/or outputs are generally tensor valued. E.g., $matmul(\boldsymbol{A}, \boldsymbol{B}) = \boldsymbol{AB}$ takes two 2D tensors and produces a 2D tensor.

💡 Intermediate results may need to be kept in order to evaluate subsequent operators and to enable gradient computation with backpropagation. Parallel processing is possible → transformer encoders.

Example: Backward Pass


weight1
weight2
$\begin{pmatrix}-0.6 & 1.2\\ 3.2 & -6.4\end{pmatrix}$
$\delta_{W_1^\top}$
$\begin{pmatrix}-2.4 & 0.8\\ 1.8 & -0.6\end{pmatrix}$
$\delta_{W_2^\top}$
input
δ_x
matmul
δ_{z_1}
matmul
δ_{z_2}
norm
$\delta_{\hat{y}}$
result
1
$\begin{pmatrix}-2.6\\ -3.8\end{pmatrix}$
$\begin{pmatrix}-0.6\\ 1.2\end{pmatrix}$
$\begin{pmatrix}0.8\\ -0.6\end{pmatrix}$

We now want to compute gradients of the result for every edge in the compute graph.

$\delta_e \overset{\text{def}}{=}$ **gradient of result $\hat{y}$ wrt. values on edge e**

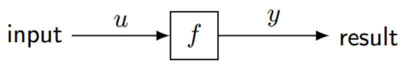
Example: $\delta_{\mathbf{z}_2} = \nabla_{\mathbf{z}_2}\hat{y} = \begin{pmatrix}0.8\\ -0.6\end{pmatrix}$. This gradient tells us, that increasing the first value in $\mathbf{z}_2$ causes the result to *increase*; similarly, increasing the second value in $\mathbf{z}_2$ causes the result to *decrease*.

Note that the shape of each gradient in the backward pass is exactly the same as the shape of the respective inputs in the forward pass; generally: tensor valued.

Gradients δ_e can be computed incrementally akin to forward pass. Operators are evaluated in reverse topological order ("backwards"). When an operator is evaluated, its output gradient(s) must be available Computation is *local*: only input values and output gradient(s) are required (the remainder of the compute graph does not matter). Intermediate outputs of forward pass are required → memory consumption (or re-computation). Parallel Processing is possible.

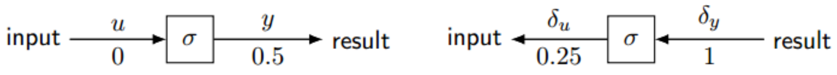
3.3.1 Gradient: Single Univariate Function

- Output $y = f(u)$
- Gradient $\delta_y \overset{\text{def}}{=} \nabla_y y = 1$
- Gradient $\delta_u \overset{\text{def}}{=} \nabla_u y = \nabla_u f(u) = \frac{\partial}{\partial u} f(u) = f'(u)$



Take-away: The gradient depends on the input u from the forward pass → we need to keep it!

Example: Consider the logistic function $y = \sigma(u)$ with input $u = 0$.



Forward pass Backward pass

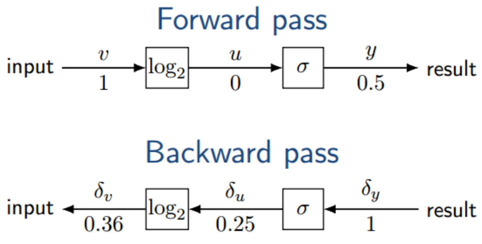
Gradient $\delta_u = \sigma'(u) = \sigma(u)\big(1 - \sigma(u)\big)$, evaluated at input $u = 0$ from forward pass:

$$\sigma(0)\big(1 - \sigma(0)\big) = 0.5 * (1 - 0.5) = 0.25 = \delta_u$$

3.3.2 Gradient: Composition of Two Univariate Functions

Output $y = f(u) = f(g(v)) \rightarrow$ function composition

Gradients can be obtained:

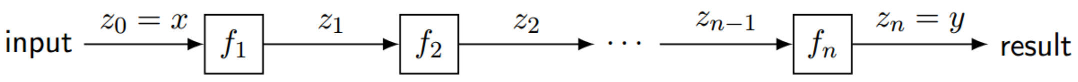


$$\delta_u \overset{\text{def}}{=} \nabla_u y = \frac{\partial}{\partial u} f(u) = f'(u) = f'(g(v))$$

$$\delta_v \overset{\text{def}}{=} \nabla_v y = \underbrace{\frac{\partial}{\partial v} f(g(v)) = g'(v) * f'(g(v))}_{\text{Chain Rule}}$$

$$= g'(v) * \delta_u$$

This generalizes, e.g., consider n operators:



We have: $y = f_n\left(f_{n-1}(\ldots(f_1(x))\ldots)\right)$

At each operator f_i, the required gradient can be computed as follows:

$$\delta_{z_{i-1}} \overset{\text{def}}{=} \nabla_{z_{i-1}} y = \frac{\partial y}{\partial z_{i-1}} = \frac{\partial y}{\partial z_i} \cdot \frac{\partial z_i}{\partial z_{i-1}}$$

$$= f_i'(z_{i-1}) \cdot \delta_{z_i}$$

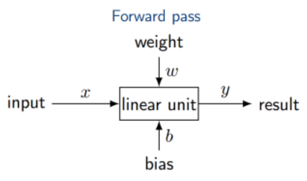
Let's derive an expression for the gradients individually:

$$\begin{aligned}
\delta_{z_n} &= 1 \\
\delta_{z_{n-1}} &= f_n'(z_{n-1}) \cdot \delta_{z_n} &&= f_n'(z_{n-1}) \\
\delta_{z_{n-2}} &= f_n'(z_{n-2}) \cdot \delta_{z_{n-1}} &&= f_{n-1}'(z_{n-2}) \cdot f_n'(z_{n-1}) \\
\delta_{z_{n-3}} &= f_n'(z_{n-3}) \cdot \delta_{z_{n-2}} &&= f_{n-2}'(z_{n-3}) \cdot f_{n-1}'(z_{n-2}) \cdot f_n'(z_{n-1}) \\
&\ldots
\end{aligned}$$

💡 The gradient is a product of local gradients along the path from the result to the resp. edge.

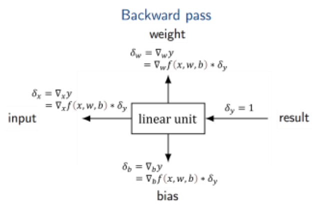
3.3.3 Gradient: Multiple Inputs

Operators often have multiple inputs, e.g., a simple linear unit. In the forward pass, the operator computes: $f(x, w, b) = wx + b = y$



In the backward pass, we simply compute gradients of result w.r.t. each edge using the chain rule:

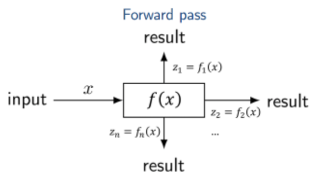
- $\delta_y = 1$
- $\delta_x = \nabla_x y = \nabla_x f(x, w, b) * \delta_y = x * 1$
- $\delta_w = \nabla_w y = \nabla_w f(x, w, b) * \delta_y = w * 1$
- $\delta_b = \nabla_b y = \nabla_b f(x, w, b) * \delta_y = 1 * 1$



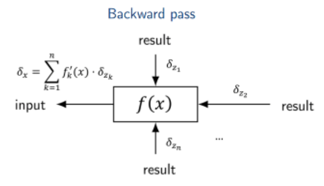
💡 We consider each input separately and reuse the δ-value.

3.3.4 Gradient: Multiple Outputs

Operators may have multiple outputs: multivariate operator $f(x)$ (single input) may output n values, say, $z_1 = f_1(x), \dots, z_n = f_n(x)$. During backpropagation, we obtain $\delta_{z_1}, \dots, \delta_{z_n}$. We are interested in:



$$\delta_x = \nabla_x y = \frac{\partial y}{\partial x} = \sum_{k=1}^{n} \frac{\partial y}{\partial z_k} \cdot \frac{\partial z_k}{\partial x} = \sum_{k=1}^{n} f_k'(x) \cdot \delta_{z_k}$$



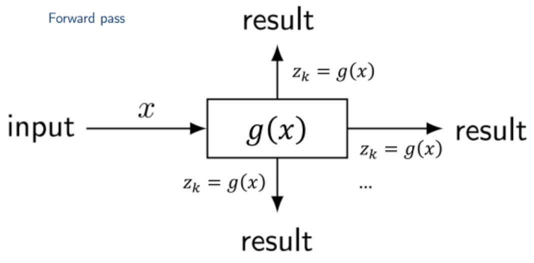
💡 We consider each output independently and sum up.

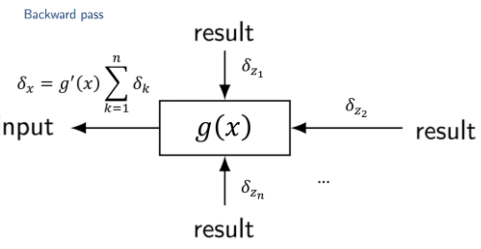
3.3.5 Gradient: Multiple Use

Sometimes an operator's output is "used" multiple times. E.g., the output of an operator $g(x)$ is used n times. That's equivalent to a single operator f with n identical outputs (i.e., $z_k = f_k(x) = g(x)$), each being used once.

$$\delta_x = \nabla_x y = \sum_{k=1}^{n} f_k'(x) \cdot \delta_{z_k} = \sum_{k=1}^{n} g'(x) \cdot \delta_{z_k} = g'(x) \sum_{k=1}^{n} \delta_k$$

💡 We sum up all incoming δ-values and proceed as before.



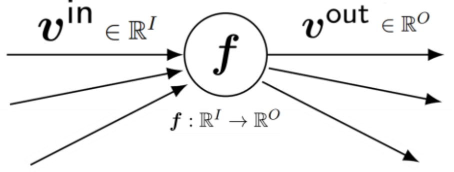


3.3.6 Gradient Computation with Tensors

📝 In practice, we usually pass along *tensors* along the edges of the compute graph. Consider an arbitrary operator $\boldsymbol{f}: \mathbb{R}^I \to \mathbb{R}^O$ that performs on multiple inputs and outputs multiple values.

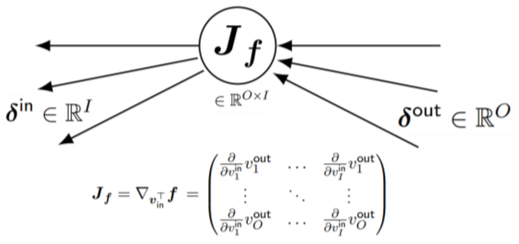
Forward pass

$$\boldsymbol{v}^{out} = \boldsymbol{f}(\boldsymbol{v}^{in})$$


$\boldsymbol{v}^{\text{in}} \in \mathbb{R}^I$
$\boldsymbol{f}$
$\boldsymbol{v}^{\text{out}} \in \mathbb{R}^O$
$\boldsymbol{f}: \mathbb{R}^I \to \mathbb{R}^O$

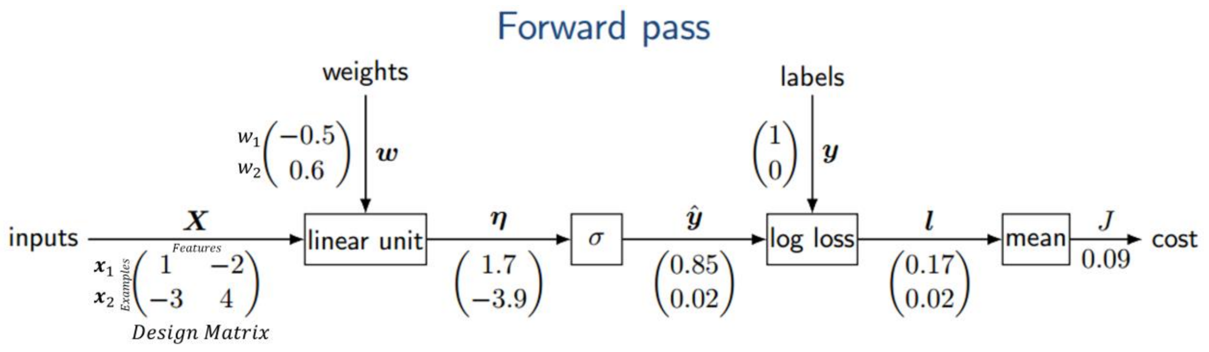
Backward pass

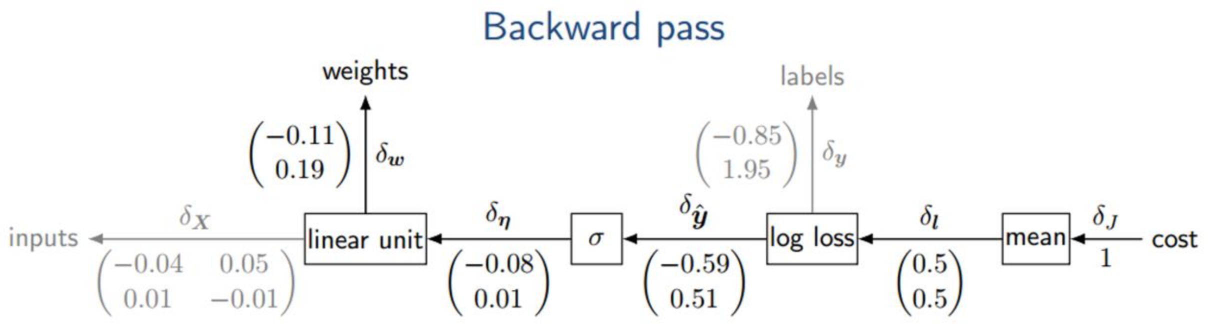
$$\boldsymbol{\delta}^{in} = \boldsymbol{J_f}(\boldsymbol{v}^{in})^\top \cdot \boldsymbol{\delta}^{out}$$


$\boldsymbol{J_f}$
$\in \mathbb{R}^{O \times I}$
$\boldsymbol{\delta}^{\text{in}} \in \mathbb{R}^I$
$\boldsymbol{\delta}^{\text{out}} \in \mathbb{R}^O$
$\boldsymbol{J_f} = \nabla_{\boldsymbol{v}_{\text{in}}^\top} \boldsymbol{f} = \begin{pmatrix} \frac{\partial}{\partial v_1^{\text{in}}} v_1^{\text{out}} & \cdots & \frac{\partial}{\partial v_I^{\text{in}}} v_1^{\text{out}} \\ \vdots & \ddots & \vdots \\ \frac{\partial}{\partial v_1^{\text{in}}} v_O^{\text{out}} & \cdots & \frac{\partial}{\partial v_I^{\text{in}}} v_O^{\text{out}} \end{pmatrix}$

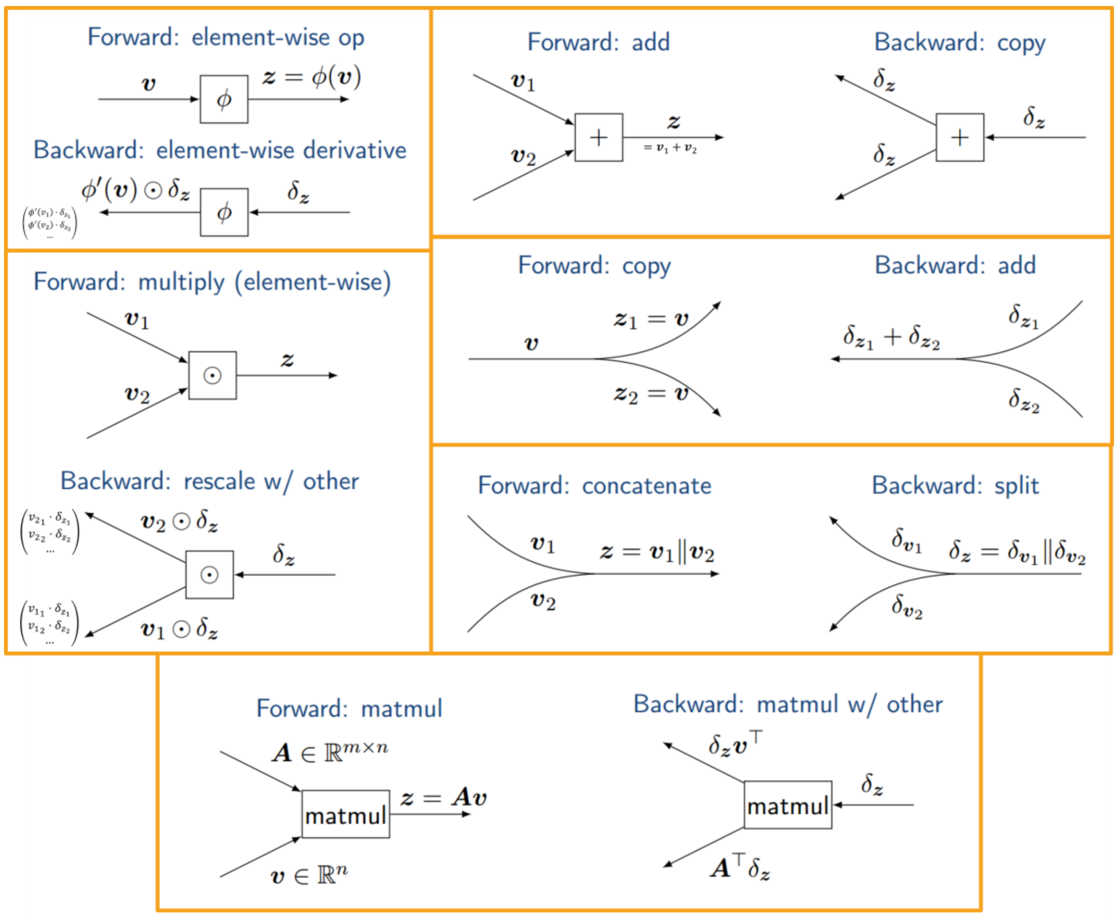
💡 The *Jacobian Matrix* $\boldsymbol{J_f}$ contains all partial derivatives of each output (columns) of $\boldsymbol{f}$ with respect to each input of $\boldsymbol{f}$ (rows). In the backward pass, these will be evaluated at the respective input value v^{in} from the forward pass, to obtain the real-valued matrix $\boldsymbol{J_f}(\boldsymbol{v}^{in})^\top$.

3.3.7 Example: Logistic Regression (2D), *N=2*


Forward pass
weights
w_1 w_2 $\begin{pmatrix}-0.5\\0.6\end{pmatrix}$ $\boldsymbol{w}$
labels
$\begin{pmatrix}1\\0\end{pmatrix}$ $\boldsymbol{y}$
inputs
$\boldsymbol{X}$
Features
Examples
$\boldsymbol{x}_1$ $\boldsymbol{x}_2$ $\begin{pmatrix}1 & -2\\-3 & 4\end{pmatrix}$
Design Matrix
linear unit
$\boldsymbol{\eta}$ $\begin{pmatrix}1.7\\-3.9\end{pmatrix}$
σ
$\hat{\boldsymbol{y}}$ $\begin{pmatrix}0.85\\0.02\end{pmatrix}$
log loss
$\boldsymbol{l}$ $\begin{pmatrix}0.17\\0.02\end{pmatrix}$
mean
J 0.09
cost


Backward pass
weights
$\begin{pmatrix}-0.11\\0.19\end{pmatrix}$ $\delta_{\boldsymbol{w}}$
labels
$\begin{pmatrix}-0.85\\1.95\end{pmatrix}$ $\delta_{\boldsymbol{y}}$
inputs
$\delta_{\boldsymbol{X}}$ $\begin{pmatrix}-0.04 & 0.05\\0.01 & -0.01\end{pmatrix}$
linear unit
$\delta_{\boldsymbol{\eta}}$ $\begin{pmatrix}-0.08\\0.01\end{pmatrix}$
σ
$\delta_{\hat{\boldsymbol{y}}}$ $\begin{pmatrix}-0.59\\0.51\end{pmatrix}$
log loss
$\delta_{\boldsymbol{l}}$ $\begin{pmatrix}0.5\\0.5\end{pmatrix}$
mean
δ_J 1
cost

3.3.8 Backpropagation for Selected Operators


Forward: element-wise op
$\boldsymbol{v}$ ϕ $\boldsymbol{z} = \phi(\boldsymbol{v})$
Backward: element-wise derivative
$\phi'(\boldsymbol{v}) \odot \delta_{\boldsymbol{z}}$ ϕ $\delta_{\boldsymbol{z}}$
Forward: add
$\boldsymbol{v}_1$ $\boldsymbol{v}_2$ $+$ $\boldsymbol{z}$ $= v_1 + v_2$
Backward: copy
$\delta_{\boldsymbol{z}}$ $\delta_{\boldsymbol{z}}$ $+$ $\delta_{\boldsymbol{z}}$
Forward: multiply (element-wise)
$\boldsymbol{v}_1$ $\boldsymbol{v}_2$ $\odot$ $\boldsymbol{z}$
Forward: copy
$\boldsymbol{v}$ $\boldsymbol{z}_1 = \boldsymbol{v}$ $\boldsymbol{z}_2 = \boldsymbol{v}$
Backward: add
$\delta_{\boldsymbol{z}_1} + \delta_{\boldsymbol{z}_2}$ $\delta_{\boldsymbol{z}_1}$ $\delta_{\boldsymbol{z}_2}$
Backward: rescale w/ other
$\boldsymbol{v}_2 \odot \delta_{\boldsymbol{z}}$ $\odot$ $\delta_{\boldsymbol{z}}$ $\boldsymbol{v}_1 \odot \delta_{\boldsymbol{z}}$
Forward: concatenate
$\boldsymbol{v}_1$ $\boldsymbol{v}_2$ $\boldsymbol{z} = \boldsymbol{v}_1 \| \boldsymbol{v}_2$
Backward: split
$\delta_{\boldsymbol{v}_1}$ $\delta_{\boldsymbol{v}_2}$ $\delta_{\boldsymbol{z}} = \delta_{\boldsymbol{v}_1} \| \delta_{\boldsymbol{v}_2}$
Forward: matmul
$\boldsymbol{A} \in \mathbb{R}^{m \times n}$ matmul $\boldsymbol{z} = \boldsymbol{A}\boldsymbol{v}$ $\boldsymbol{v} \in \mathbb{R}^n$
Backward: matmul w/ other
$\delta_{\boldsymbol{z}} \boldsymbol{v}^\top$ matmul $\delta_{\boldsymbol{z}}$ $\boldsymbol{A}^\top \delta_{\boldsymbol{z}}$

3.4 Optimizers

3.4.1 Gradient Descent

📝 Recall *vanilla gradient descent*. This optimizer aims to minimize an objective function. It iteratively updates the current estimate $\boldsymbol{\theta}_t$ until some stopping criterion is met.

$$\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t - \epsilon \cdot \boldsymbol{g}_t$$

where $\boldsymbol{g}_t$ is the gradient (estimate) of the *objective* wrt. parameters $\boldsymbol{\theta}$ at time t (e.g., $\boldsymbol{g}_t = \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_t)$).

💡 There are multiple variants for supervised learning:

- **Batch** gradient descent: computes exact gradient using *all training examples*
  - high cost - easy to parallelize - exact gradient
- **Stochastic** gradient descent: estimates gradient using *a single random training example*
  - low cost - noisy gradient - hard to parallelize
- **Mini-batch** gradient descent: estimates gradient using *some training examples*
  - middle ground between cost and parallelizability
  - number of examples called batch size

❗ GD is suitable for large datasets/models but can converge slowly and gets stuck in local minima.

During training, we aim to minimize a potentially highly non-convex cost function $J(\boldsymbol{\theta}) \rightarrow$ difficult!

3.4.2 Effect of Batch Size

💡 Empirical Risk Minimization is a theoretic principle that guides the design of a variety of learning algorithms. Core idea:we cannot know exactly how well a predictive algorithm will work in practice (true "risk") because we do not know the true data distribution. We can instead *estimate* and optimize the performance of the algorithm on a known set of training data → minimize the *empirical risk* $R_{emp}(h)$. *Also see 3 Gradient-Based Training.*

Consider a *cost function* $J(\boldsymbol{\theta})$ over training examples $\mathcal{D}$ in the form of *empirical risk* $R_{emp}(h)$:

$$J(\boldsymbol{\theta}) = \frac{1}{|\mathcal{D}|} \sum_{i \in \mathcal{D}} L_i(\boldsymbol{\theta})$$

where $L_i(\boldsymbol{\theta}) = L(\hat{y}_i, y_i)$ is the loss on example i. Suppose we construct each batch $\mathcal{B}$ by sampling a fixed number of examples (uniformly & iid) and average losses:

$$J_{\mathcal{B}}(\boldsymbol{\theta}) = \frac{1}{|\mathcal{B}|} \sum_{z \in \mathcal{B}} L_z(\boldsymbol{\theta})$$

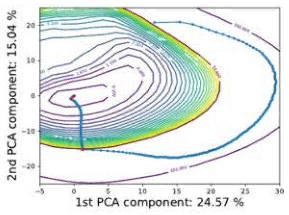
Then, since $E[L_z] = \sum_{i \in \mathcal{D}} p_i \cdot L_i(\boldsymbol{\theta})$ with $p_i = \frac{1}{|\mathcal{D}|}$ (uniformly sampled) $E[L_z] = J$ follows; and:

$$E[J_{\mathcal{B}}(\boldsymbol{\theta})] = J(\boldsymbol{\theta})$$
$$E[\nabla_{\boldsymbol{\theta}} J_{\mathcal{B}}(\boldsymbol{\theta})] = \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$$
$$\operatorname{var}[\nabla_{\boldsymbol{\theta}} J_{\mathcal{B}}(\boldsymbol{\theta})] = \frac{1}{|\mathcal{B}|} \operatorname{var}[\nabla_{\boldsymbol{\theta}} L_z(\boldsymbol{\theta})]$$

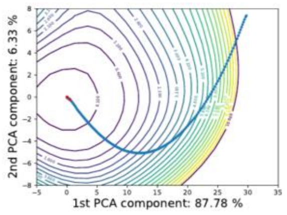
💡 **Conclusion**: gradient is correct in expectation; variance decreases with increasing batch size.
(this holds for this type of cost function)

3.4.3 Learning Rate ϵ and Batch Size $|\mathcal{B}|$

Red dot → learning rate reduced



Batch size 128



Batch size 8192

For small batch sizes $|\mathcal{B}| \rightarrow$ high variance gradients
- trajectory takes "detours"
- **regularizing effect** (escapes local minima)

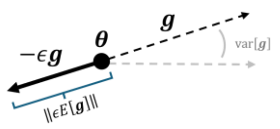
For large batch sizes $|\mathcal{B}| \rightarrow$ low variance gradients
- trajectory attracted by local minima
- empirically often lower generalization performance

For low learning rates $\epsilon \rightarrow$ small steps (slow trajectory)
- high variance gradient estimates average out

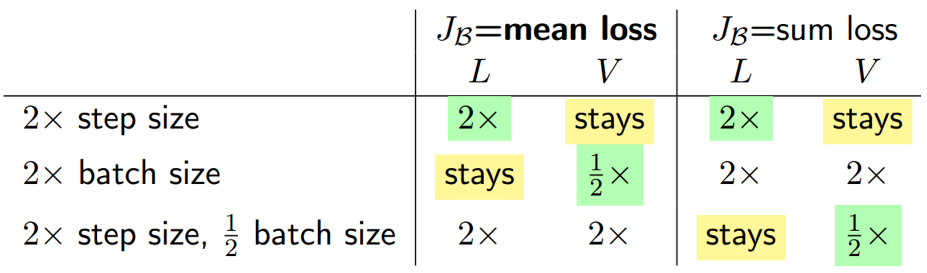
For high learning rates $\epsilon \rightarrow$ large steps (fast trajectory)
- noisy gradient may be problematic

Consider $\boldsymbol{\theta}$ and the update to $\boldsymbol{\theta} - \epsilon \boldsymbol{g}$ during a mini-batch GD step.

- Step length $L = \|\epsilon E[\boldsymbol{g}]\|$
- Gradient variance $V = \text{var}[\hat{\boldsymbol{g}}]$



Both are affected by learning rate ϵ, batch size $|\mathcal{B}|$ and cost function J.

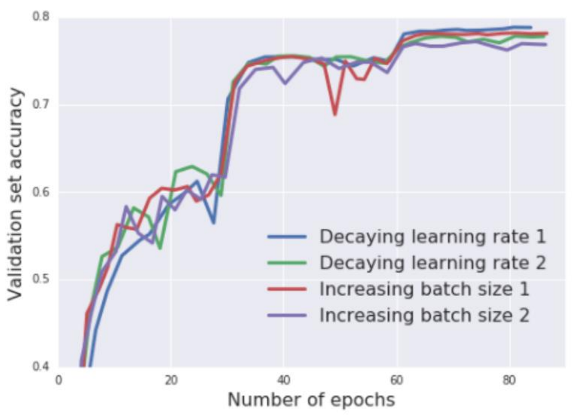


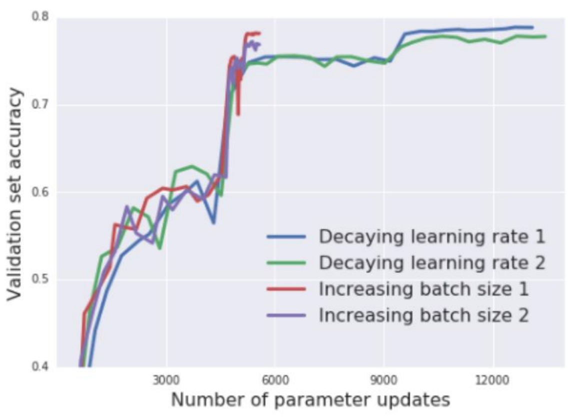
	$J_\mathcal{B}$=mean loss		$J_\mathcal{B}$=sum loss	
	L	V	L	V
2× step size	2×	stays	2×	stays
2× batch size	stays	$\frac{1}{2}$×	2×	2×
2× step size, $\frac{1}{2}$ batch size	2×	2×	stays	$\frac{1}{2}$×

Sum-Loss does not average examples in batch but sums them up.

💡 Learning rate and batch size are selected during hyperparameter tuning. Often a le*arning rate scheduler* is used to decrease an initially large ϵ to slowly approach the optimum once in vicinity.

Similarly, a *batch size scheduler* can also be used to increase the batch size later during the training to slowly approach the optimum. This also eases parallelization.

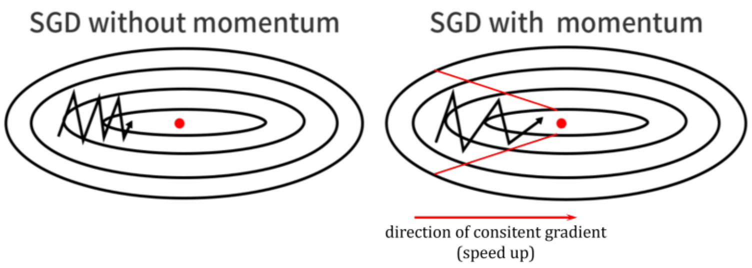




Increasing the batch size during training achieves similar results to decaying the learning rate, but it reduces the number of parameter updates from just over 14000 to below 6000. Each experiment ran twice to illustrate the variance.

3.4.4 Momentum

A key idea to accelerate the GD algorithm is to build up velocity in directions that have consistent gradient.



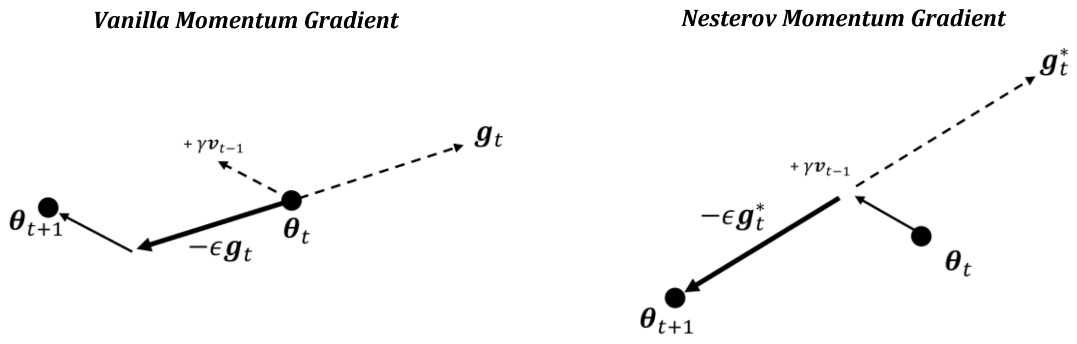
This solves two problems: poor conditioning of the Hessian matrix (narrow valleys, see figure) and variance in the stochastic gradient.

Vanilla/Basic *Momentum* (also: *heavy-ball method*) uses an exponentially-decaying moving average of the negative gradient.

$$\boldsymbol{v}_t \leftarrow \gamma \boldsymbol{v}_{t-1} - \epsilon \boldsymbol{g}_t$$
$$\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t + \boldsymbol{v}_t$$

where we can think of $\boldsymbol{v}$ as *velocity*; hyperparameter $\gamma \in [0, 1)$ is referred to as *momentum.*

- The speed (norm of update) increased up to $\frac{1}{1-\gamma} \times$ w.r.t. GD step.
- $\frac{\epsilon}{1-\gamma}$ is called the *effective learning rate*, in the direction of a consistent gradient


Vanilla Momentum Gradient
$+\gamma\boldsymbol{v}_{t-1}$
$\boldsymbol{g}_t$
$\boldsymbol{\theta}_{t+1}$
$-\epsilon\boldsymbol{g}_t$
$\boldsymbol{\theta}_t$
Nesterov Momentum Gradient
$\boldsymbol{g}_t^*$
$+\gamma\boldsymbol{v}_{t-1}$
$-\epsilon\boldsymbol{g}_t^*$
$\boldsymbol{\theta}_t$
$\boldsymbol{\theta}_{t+1}$

Another variant is the *Nesterov momentum*, where the momentum update is applied *before* computing the gradient:

$$\boldsymbol{v}_t \leftarrow \gamma \boldsymbol{v}_{t-1} - \epsilon \boldsymbol{g}_t \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta} + \gamma \boldsymbol{v}_{t-1})$$
$$\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t + \boldsymbol{v}_t$$

For convex functions (unique global optimum) and batch gradients, convergence rate improves from $O(1/t)$ to $O(1/t^2)$. Note that:

- this does not apply to SGD
- cost functions in DL are generally not convex
- but, in practice leads to much better performance

❗ Requires additional memory to store velocity $\boldsymbol{v}$ (same size as model parameters $\boldsymbol{\theta}$).

3.4.5 Adaptive Learning Rates

The idea of adaptive learning rates is to use individual, per-parameter learning rates

- smaller learning rate for sensitive parameters (large derivative)
- larger learning rate for insensitive parameters (small derivative)

Example: Adagrad

Computes the sum of squared gradients to quantify parameter sensitivity:

$$\boldsymbol{r}_t \leftarrow \boldsymbol{r}_{t-1} + \boldsymbol{g}_t \odot \boldsymbol{g}_t$$

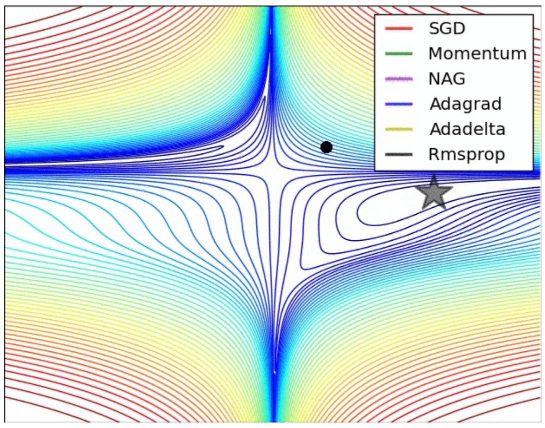
Note: operator $\odot$ is the elementwise multiplication.

$$\boldsymbol{\theta}_{t+1} \leftarrow \boldsymbol{\theta}_t - \frac{\epsilon}{\delta + \sqrt{\boldsymbol{r}_t}} \odot \boldsymbol{g}_t$$

Learning rate gets reduced over time, more so for parameters with larger derivatives.

- Good theoretical properties for convex functions
- For deep learning the learning rate reduction can happen too quick initially

Requires additional memory to store $\boldsymbol{r}$ (same size as model parameters $\boldsymbol{\theta}$).



Adadelta and *RMSProp* are variants that use an exponentially-decaying moving average of squared derivatives.

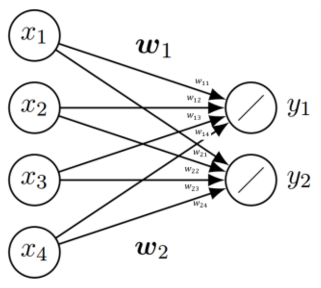
3.4.6 Discussion

- Optimizers that use adaptive learning rates are popular
- Momentum and adaptive learning rates can also be combined
  - E.g., Adagrad or RMSProp with momentum, Adam, NAdam, AMSGrad, AdamX, ...
  - Yet higher memory consumption (velocity and per-parameter LR)
- No consensus on best optimizer → hyperparameter tuning

3.5 Forward Pass: Batch Processing

While we often use $\boldsymbol{y} = \boldsymbol{W}^\top \boldsymbol{x} + \boldsymbol{b}$ to describe the operation of a single layer during the forward pass, this is not quite accurate in practice. The reason why this notation is so common is to follow the existing notation of the rest of the models in the literature.

As we often want to pass batches (multiple $\boldsymbol{x}$'s), we'd like to make use of a design-matrix-like input structure. Consider the following example (omitting bias):

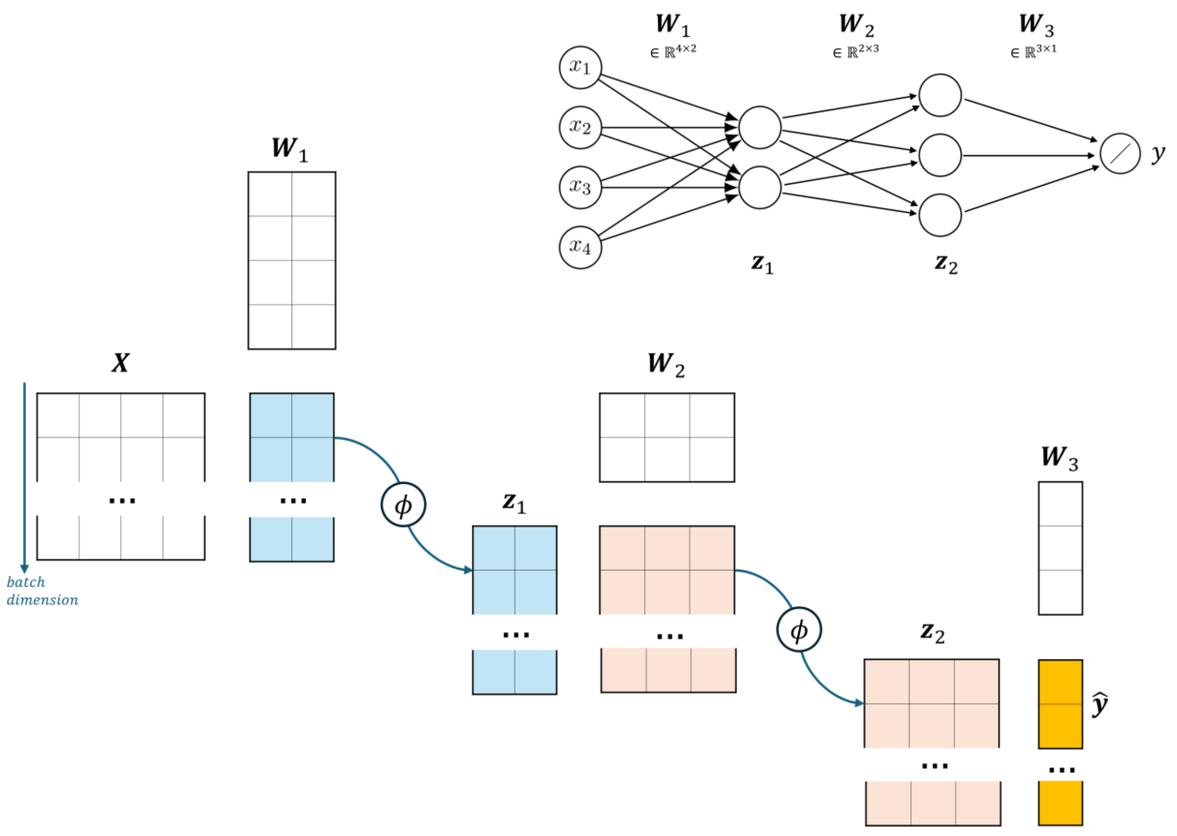


$$\boldsymbol{W} = (\boldsymbol{w}_1 \quad \boldsymbol{w}_2) = \begin{pmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \\ w_{13} & w_{23} \\ w_{14} & w_{24} \end{pmatrix} \qquad \boldsymbol{X} = \begin{pmatrix} \boldsymbol{x}_1^\top \\ \boldsymbol{x}_2^\top \\ \boldsymbol{x}_3^\top \\ \boldsymbol{x}_4^\top \end{pmatrix} = \begin{pmatrix} x_1 & x_2 & x_3 & x_4 \\ & \dots & & \\ & \dots & & \\ & \dots & & \end{pmatrix}$$

$$\boldsymbol{y} = \boldsymbol{X} * \boldsymbol{W} = \underbrace{\overset{\text{feature dimension (4)}}{\begin{pmatrix} x_1 & x_2 & x_3 & x_4 \\ & \dots & & \\ & \dots & & \\ & \dots & & \end{pmatrix}}}_{\in \mathbb{R}^{N\times 4}} * \underbrace{\begin{pmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \\ w_{13} & w_{23} \\ w_{14} & w_{24} \end{pmatrix}}_{\in \mathbb{R}^{4\times 2}} = \begin{pmatrix} \boldsymbol{y} \\ \dots \\ \dots \\ \dots \end{pmatrix} = \underbrace{\begin{pmatrix} y_1 & y_2 \\ \dots & \dots \\ \dots & \dots \\ \dots & \dots \end{pmatrix}}_{\in \mathbb{R}^{N\times 2}}$$

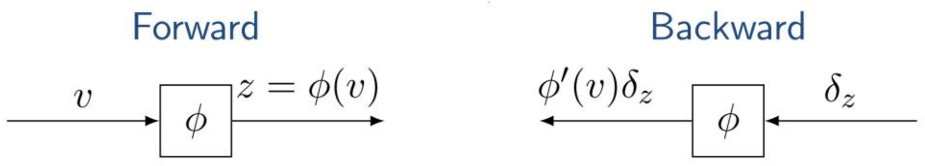
batch dimension N

💡 Here we instead perform $\boldsymbol{y} = \boldsymbol{X} * \boldsymbol{W} + \boldsymbol{b}$ as the structure of our input has changed:



3.6 Vanishing/Exploding Gradient Problem

Consider an activation function ϕ and recall the gradient computation in the backwards pass:



❗ If $\phi' < 1$, then the gradient becomes smaller. If this happens in consecutive layers, the gradient *vanishes* exponentially fast with depth, since local gradients multiply.

- If $\phi' \approx 0$, the gradient barely passes through → *saturated unit*
- If $\phi' = 0$, the gradient is gone right away → *dead unit*

This is problematic since prior layers do not receive a useful gradient signal. For $\nabla_{\boldsymbol{w}} J \approx 0$, gradient-based learning fails as weights are not updated in prior layers. For $\nabla_{\boldsymbol{x}}\, \hat{y} \approx 0$, model output becomes insensitive to input changes.

❗ Similarly, if $\phi' > 1$, then the gradient becomes larger. If this happens in consecutive layers, the gradient *explodes* exponentially fast with depth, since local gradients multiply.

This is problematic since the output is extremely sensitive to prior layers. For very large $\nabla_{\boldsymbol{w}} J$, gradient-based learning fails as weights diverge. For large $\nabla_{\boldsymbol{x}}\hat{y}$, model predictions are unstable.

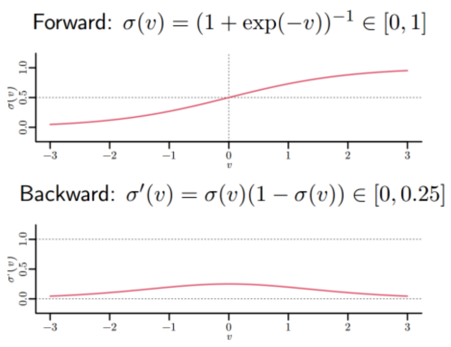
Note that this does not occur because of the activation functions, but rather due to other layers!

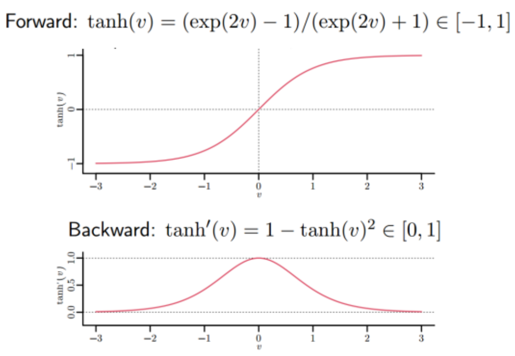
Example: Logistic Unit

The logistic unit is not well suited as a hidden layer unit:

- $\sigma(0) = 0.5$ → zeros not passed through
- $\sigma'(v) \leq 0.25$ → gradients reduce by at least ¼
- The unit becomes saturated when $|v| \geq 5$.

💡 For these reasons we typically do not use logistic units as hidden neurons.





Example: *tanh*( ) activation function

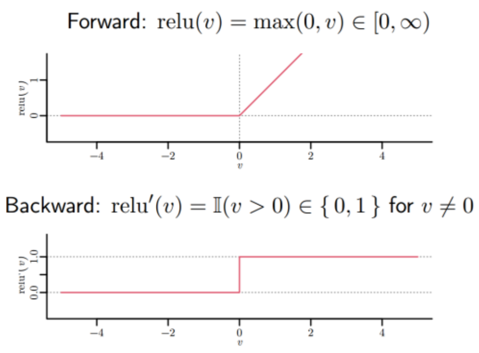
The *tanh*()is a good alternative:

- $tanh(0) = 0$ → zeros passed through
- $tanh'(0) = 1$ → gradients are retained for small inputs
- The unit becomes saturated when $|v| \geq 3$.

Example: $ReLU(\,)$ function

The $relu(\,)$ function is a good alternative:

- $relu(0) = 0 \rightarrow$ zeros passed through
- $relu'(v > 0) = 1 \rightarrow$ gradients passed through
- $relu'(v < 0) = 0 \rightarrow$ gradients gone right away



Desirable Properties of Activation Functions

Non-Linearity → needed for expressiveness	**Differentiability** → enables gradient-based learning	**Zero's pass through** $\phi(0) = 0$ → avoids need to learn zero-outputs
Approximates linear unit around 0 → mitigates vanishing gradient ∇	**Gradients bounded from above** → stability, mitigates expl. grad. ∇	**Low computational cost** → (Leaky) ReLU wins $

3.7 Architecture Design

Degradation problem: performance of plain MLPs tends to deteriorate beyond certain depth.

- Due to complicated optimization landscape
- Gradients may vanish/explode exponentially fast with increasing depth in MLP

This can be mildened by choice of suitable activation function, but not by much. Instead, we can modify the *network architecture* to mitigate training challenges → better empirical performance.

Goals include

- Improve gradient flow through network
- Facilitate training and effectiveness of deep networks → mitigate the degradation problem
- Simplify the optimization landscape

3.7.1 Representation View

Consider a parameterized layer $\boldsymbol{f}: \mathbb{R}^Z \rightarrow \mathbb{R}^Z$ somewhere in an FNN, e.g.: $\boldsymbol{f} = \phi\left(\boldsymbol{W}_l^\top \cdot \boldsymbol{v}^{in} + \boldsymbol{b}_l\right)$ for a layer l:

$$\begin{tikzcd} {} \arrow[r, dash, "\boldsymbol{v}^{\text{in}}"] & \boldsymbol{f} \arrow[r, "\boldsymbol{v}^{\text{out}}"] & {} \end{tikzcd}$$

❓ How can we interpret what a layer is doing in an FNN? → *Representation view:*

• $\boldsymbol{v}^{in}$ is representation/embedding of input	(obtained from previous layer)
• $\boldsymbol{v}^{out}$ is updated representation of input	(for next layer)

💡 Each layer is considered a “step” in a multi-step computation

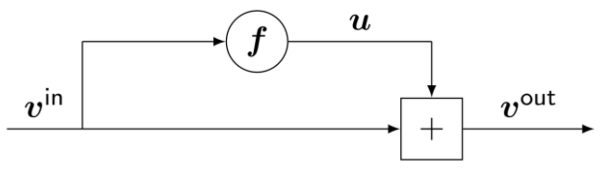
- How many steps? ≈ *network depth* (L)
- How much memory? ≈ *network width* (Z)

❗ If $\boldsymbol{v}^{in}$is already a good representation, the model needs to learn to preserve it. The deeper the network is, the more this matters → one reason for the degradation problem.

3.7.2 Residual Connections

Residual Connections are an architectural design pattern that change the layer:

$$\boldsymbol{v}^{out} = \boldsymbol{v}^{in} + \boldsymbol{f}(\boldsymbol{v}^{in})$$



We think of $\boldsymbol{f}(\boldsymbol{v}^{in})$ not as a representation that should be used downstream but rather as an *update* or *residual*. How much should the representation change – not how should it be.

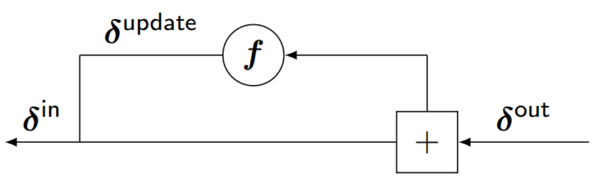
If $\boldsymbol{v}^{in}$ already is a good representation, then learning to preserve this is now easier to do. This reduced degradation of performance that would happen due to "too many" layers.

In the backward pass we obtain (cf. *3.3.8*):

$$\boldsymbol{\delta}^{in} = \boldsymbol{\delta}^{out} + \boldsymbol{\delta}^{update}$$

After L of such layers, the gradient is:

$$\boldsymbol{\delta}^{in} = \boldsymbol{\delta}^{out} + \boldsymbol{\delta}_L^{update} + \cdots + \boldsymbol{\delta}_1^{update}$$

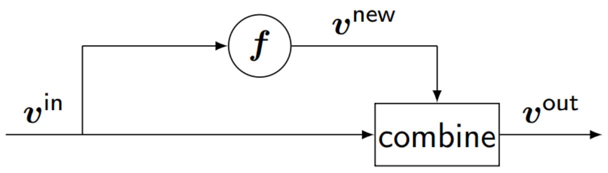


Therefore, the original gradient $\boldsymbol{\delta}^{out}$ passes through → addresses vanishing gradient problem.

3.7.3 Skip Connections

More generally, *skip connections* (also: *shortcut connections*) skip one or more layers. Residual Connections are just one example of these.

The original representation $\boldsymbol{v}^{in}$ and the new representation $\boldsymbol{v}^{new}$ are ultimately combined in some form.



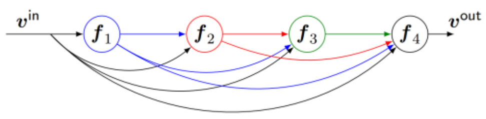
Common combine-options include:

- Concatenation
- Averaging
- Max-Pooling
- Attention
- Addition (→ *3.7.2*Residual Connections)

Concatenation

In an extreme case, we concatenate *all* representations of previous layers. This makes preservation of information across layers trivial. Each layer merely enhances the current representation (increases effective dimensionality). Note that:

- Input size per layer increases linearly
- Amount of weight matrices increases linearly
- Total number of weights increases quadratically



But we can get away with a much smaller output size Z per layer, reducing cost.

After L of such layers, the gradient is:

$$\boldsymbol{\delta}^{in} = \boldsymbol{\delta}_L + \cdots + \boldsymbol{\delta}_1$$

In a similar manner, the gradient from later layers $\boldsymbol{\delta}_L$ passes through.

3.7.4 Batch Normalization

Batch normalization (BN) is a layer that mitigates two problems:

1. *Covariate shift*: when parameters of one layer change, the (training distribution of) inputs to the next layer changes too → ignored by gradient-based methods
2. Gradient magnitudes may vary wildly across layers → complicates gradient-based learning

For BN we need to run batch or mini-batch gradient descent. It normalizes the input features to zero mean and unit variance within each batch. I.e., input $\boldsymbol{z} \in \mathbb{R}^Z$ is normalized to:

$$\tilde{\boldsymbol{z}} = \frac{(\boldsymbol{z} - \boldsymbol{\mu})}{\sqrt{\boldsymbol{\sigma}^2}}$$

where $\boldsymbol{\mu}, \boldsymbol{\sigma}^2 \in \mathbb{R}^Z$ are computed from the entire batch. This normalization is part of the layer, and the gradient is backpropagated through these operations. At test time, we use running average of $\boldsymbol{\mu}$ and $\boldsymbol{\sigma}^2$ that we kept from training.

Variant: normalize to mean β and variance γ, where β and γ are learned parameters

Sometimes BN is problematic:

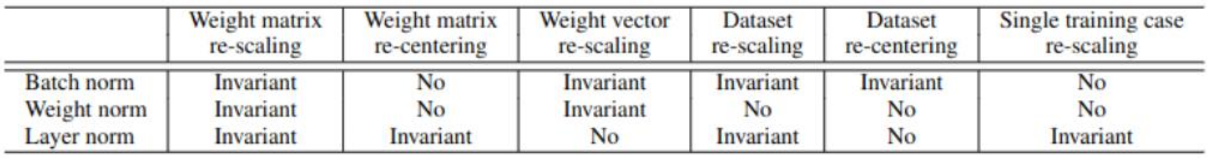
- During training, batch size must be sufficiently large (e.g., no online learning possible).
- When the number of layers is not fixed but depends on input (e.g., RNN, Transformer), where the number of required mean/variance statistics varies with input lengths.

3.7.5 Layer Normalization

Layer normalization (LN) is an alternative, where we normalize each input vector individually:

$$norm(\boldsymbol{z}) = \frac{\boldsymbol{z} - mean(\boldsymbol{z})}{\sqrt{std(\boldsymbol{z})}}$$

Mean/Standard deviation are computed across the elements of $\boldsymbol{z}$.



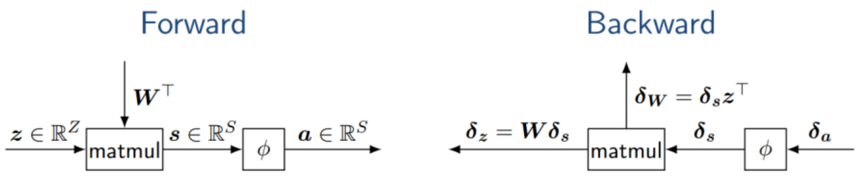
	Weight matrix re-scaling	Weight matrix re-centering	Weight vector re-scaling	Dataset re-scaling	Dataset re-centering	Single training case re-scaling
Batch norm	Invariant	No	Invariant	Invariant	Invariant	No
Weight norm	Invariant	No	Invariant	No	No	No
Layer norm	Invariant	Invariant	No	Invariant	No	Invariant

3.8 Initialization

Initialization refers to choosing starting values for all parameters of a NN. This is important since it affects the *performance* as well as *solutions found* by gradient-based optimizers.

3.8.1 Zero Initialization

Initializing weight matrices with zeros ($\boldsymbol{W} = \boldsymbol{0}$) is problematic as $\boldsymbol{\delta_z}$ in turn also is zero.


Forward
$\boldsymbol{W}^\top$
$\boldsymbol{z} \in \mathbb{R}^Z$
matmul
$\boldsymbol{s} \in \mathbb{R}^S$
ϕ
$\boldsymbol{a} \in \mathbb{R}^S$
Backward
$\boldsymbol{\delta}_W = \boldsymbol{\delta}_s \boldsymbol{z}^\top$
$\boldsymbol{\delta}_z = \boldsymbol{W}\boldsymbol{\delta}_s$
matmul
$\boldsymbol{\delta}_s$
ϕ
$\boldsymbol{\delta}_a$

If $\boldsymbol{\delta_a} = c \cdot \boldsymbol{1}$ (only constant values), all vectors receive the same gradients. As a consequence, all units at each layer always have the same output and learning fails no matter for how long we train (→ *co-adaptation*: output neurons are highly correlated no matter the output).

3.8.2 Normal Initialization

When initializing $\boldsymbol{W}$ using iid. samples from a normal distribution $\mathcal{N}(0, \boldsymbol{\sigma}^2)$, the variance of the first layer output increases with increased *input* dimensionality Z. Depending on activation function ϕ this can lead to vanishing/exploding gradients. A solution is to initialize with samples from $\mathcal{N}(0, \boldsymbol{\sigma}^2/Z)$ → variance retained.

Similarly in the backward pass, when sampling from a standard normal distribution, the variance increases with increased *output* dimensionality S. Depending on activation function ϕ this can lead to exploding gradients. A solution is to initialize with samples from $\mathcal{N}(0, \boldsymbol{\sigma}^2/S)$ → variance retained.

❗ If input and output dimensionality differ ($S \neq Z$) a tradeoff is necessary. Generally, for MLPs, vanishing/exploding gradients can be mitigated at the start when variances are retained across layers. As forward and backward pass are affected differently, we need a compromise.

3.8.3 Xavier/Kaiming Initialization

For $\phi = \tanh(\,)$ or linear( ) we can select *Xavier initialization* (also: *Glorot init.*). Samples from:

$$\mathcal{N}(0, 1/D) \qquad \text{or} \qquad \mathcal{U}\left(-\sqrt{3/D}, \sqrt{3/D}\right)$$

where $D = mean(Z, S)$.

💡 For other activation functions, can multiply by gain, e.g., for relu: $\sqrt{2}$ (*Kaiming/He initialization*)

3.8.4 Discussion

- Suitable scale matters for standard MLPs and depends on dimensionality
- Initialization differs based on architecture,
  - e.g., residual layers typically need a small weight matrix
  - scaling is less influential if layer/batch/weight normalization is used

4 Layers for Categorical Data

One-hot encoding for categorical inputs, e.g.:

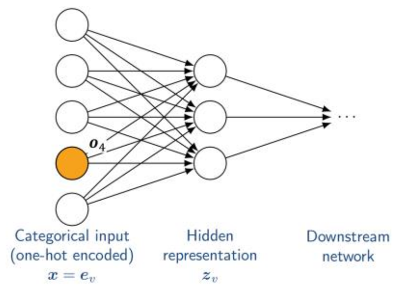
$$x \in \{\text{red}, \text{green}, \text{blue}\} \text{ then for } x = \text{green, we encode it as } x = (0 \quad 1 \quad 0)^\top$$

is not efficient regarding compute cost and limited in parameter sharing.

4.1 Embedding Layers

Consider an FNN with a single categorical input.

- The set of categories (i.e. {red, green, blue}) is referred to as *vocabulary* $\mathcal{V} = \{1, \dots, V\}$.
- The input $v \in \mathcal{V}$ is one-hot encoded to $\boldsymbol{e}_v \in \{0,1\}^V$, e.g. $v = (0 \quad 1 \quad \dots \quad 0)^\top \to$ vth standard basis vector


$\boldsymbol{o}_4$
Categorical input (one-hot encoded) $\boldsymbol{x} = \boldsymbol{e}_v$
Hidden representation $\boldsymbol{z}_v$
Downstream network
...

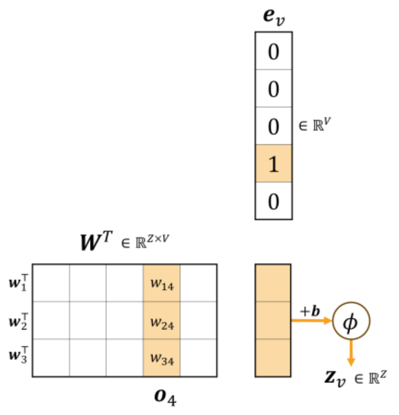
The downstream network only sees $\boldsymbol{z}_v$ and not $\boldsymbol{e}_v$.

If we view the weight matrix $\boldsymbol{W}$ as

$$\boldsymbol{W} \in \mathbb{R}^{V \times Z} = (\boldsymbol{w}_1 \quad \boldsymbol{w}_2 \quad \dots \quad \boldsymbol{w}_Z) = \begin{pmatrix} \boldsymbol{o}_1^\top \\ \boldsymbol{o}_2^\top \\ \dots \\ \boldsymbol{o}_V^\top \end{pmatrix}$$

where $\boldsymbol{o}_V^\top = (w_{1V} \quad w_{2V} \quad \dots \quad w_{ZV})$ are the weights coming from input neuron V to hidden neuron Z. Then we can express the output of the first layer in the following way:

$$\begin{aligned} v \in \mathcal{V} \to \boldsymbol{z}_v \in \mathbb{R}^Z &= \phi(\boldsymbol{W}^\top \boldsymbol{e}_v + \boldsymbol{b}) \\ &= \phi(\boldsymbol{o}_v + \boldsymbol{b}) \\ &\overset{\text{def}}{=} \text{emb}(v) \end{aligned}$$



An *embedding layer* stores a representation of each category (*embeddings*) → no computation. It maps each category $v \in \mathcal{V}$ to a vector $\text{emb}(v) \in \mathbb{R}^Z$, the *embedding* of v. Such a layer is parameterized an *embedding matrix* $\boldsymbol{E} \in \mathbb{R}^{V \times Z}$ with categories as rows. This is more efficient than modelling via a fully connected layer. When training such a network, we can use the obtained gradient to update the embedding matrix and learn representations.

Embedding layers are used for *non-divisible* objects (i.e. words, atomic objects); for divisible objects an encoder is used such that exploiting the structure of the object is possible (e.g., document embeddings, image embeddings, ...)

Discussion

- Embedding layers may use large vocabularies $V \gg Z \to$ dimensionality reduction
- Two categories should be similar in embedding space when they have similar impact on final output → Embeddings expose similarities
- When multiple inputs use the same categories (e.g. RNNs) the embedding layer is typically shared → this is an example of *parameter sharing.*

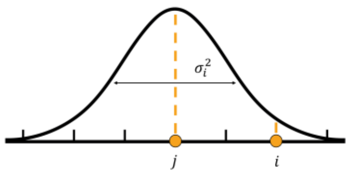
4.2 t-SNE

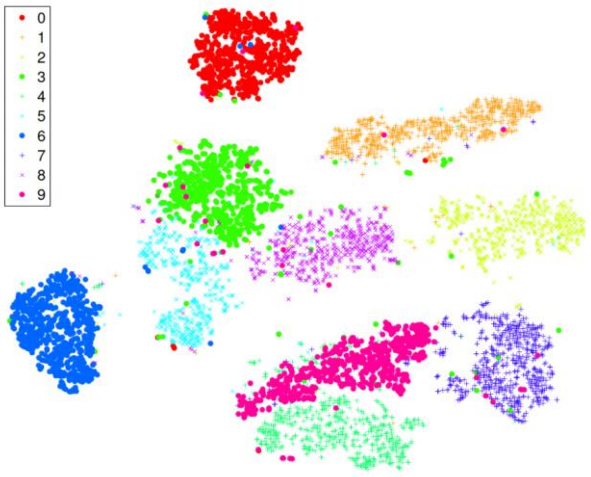
t-SNE (*t-distributed Stochastic Neighbor Embedding*) is a popular approach to visualize embedding spaces. It approximates the neighborhood of data points in the embedding space, or any other high-dimensional space, and outputs these neighborhoods in 2D/3D space.

High-Level-Idea: Data points close in the embedding space should also be close in the low-dimensional space → *small distances matter*

The similarity in the embedding space is measured with an isotropic Gaussian distribution with data-point-specific variance:

$$p(\boldsymbol{z}_j|\boldsymbol{z}_i) = \mathcal{N}(\boldsymbol{z}_j|\boldsymbol{z}_i, \sigma_i^2\boldsymbol{I})$$



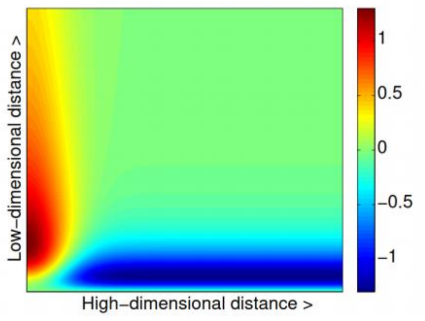


6000 MNIST handwritten digits; 28 × 28 → 784D

The data-point-specific variance σ_i^2 controls the number of effective neighbors. t-SNE sets this automatically such that we have small variance in dense areas and wide variance in sparsely populated areas (→ in embedding space).

In the low-dimensional space, t-SNE uses the Cauchy distribution s.t. the model accepts (*green area in plot*) data points with moderate similarity in the original data space to be far away in the low-dimensional space and vice-versa.

This makes *large* distances and cluster sizes in the t-SNE plot meaningless, i.e., the distance between number zero (**red**) and number one (**orange**) cannot be compared to the distance between number zero (**red**) and number four (**mint**). As they are far away in low-dimensional space we cannot reason about distance in the embedding space.



Gradient of t-SNE

4.3 Softmax Layers for Similarity

Softmax layers also compute similarity. By computing the inner product between weight vector for each class and input to obtain the softmax score telling us the class probability p_c.

$$p(y = c|\boldsymbol{z}) = S(\boldsymbol{W}^\top \boldsymbol{z})_c = \frac{\exp(\langle \boldsymbol{w}_c, \boldsymbol{z}\rangle)}{\sum_{c'} \exp(\langle \boldsymbol{w}_{c'}, \boldsymbol{z}\rangle)} = p_c$$

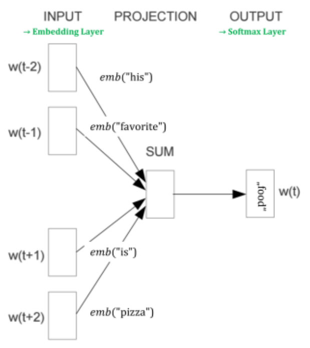
Class probabilities are implicitly determined by softmax scores: $\eta_c = \langle \boldsymbol{w}_c, \boldsymbol{z}\rangle$. Using the geometric interpretation of the inner product: being proportional to the cosine similarity, the softmax layer normalizes these similarity scores to produce probabilities. We may thus think of a softmax layer as measuring the similarity between input $\boldsymbol{z}$ and each class vector $\boldsymbol{w}_c$. *Also see 2.4.6 and 2.4.7*.

Cosine similarity only cares about angle difference, while the inner product cares about angle and magnitude. If you normalize your data to have the same magnitude, the two are indistinguishable.

4.4 Word Vectors

Word vectors, a type of word embeddings, use embedding layers and softmax layers to represent words in NLP tasks. While less relevant in current research, they are instructive. These vectors map words to continuous representations, aiming to *capture semantic similarity* and *compositionality*. By using word vectors, downstream models require fewer parameters to train and can handle unseen words in the training data by focusing on the meaning rather than the words themselves.

They are guided by the *distributional hypothesis* (linguistics), which posits that words with similar meanings tend to occur in similar contexts. Thus, word vectors are trained to ensure that words with similar contexts have similar representations, thereby encoding similar meanings.



Example: *continuous bag-of-words* model (*CBOW*)

Predicts the missing word given a set of surrounding words (→ *context*).

- Hyperparameter Z: Size of the word vector.
- Hyperparameter W: Size of the left/right context.

The input layer maps words to word vectors (each of the $2W$ words separately) via an embedding layer. The embedding matrix $\boldsymbol{E} \in \mathbb{R}^{V \times Z}$ is shared across context words → *parameter sharing*

The sum layer takes $2W$ embeddings and sums them elementwise $\sum_i \text{emb}(w_i)$ (*composition*) producing a Z-dimensional *continuous* representation of the context.

The output layer (Softmax, trained to predict w_t with $C = V$ classes) will be ignored for downstream models, i.e., only $\boldsymbol{E}$ used).

The standard BOW model would simply sum the word counts $\boldsymbol{e}_{w_i}$ (one-hot encoded).

"This"	0	1	0	0
"is"	0	0	1	0
$\sum_i \boldsymbol{e}_{w_i}$	0	1	1	0

4.5 Extreme Classification

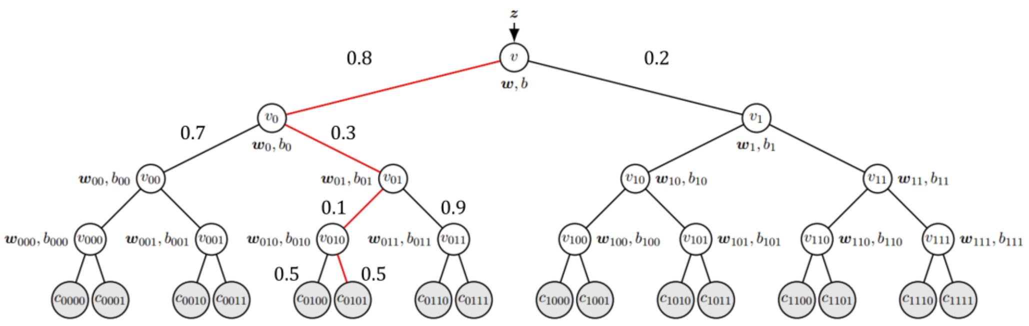
❗ Training with a softmax layers is very costly due to computing the normalization term $\exp(\langle \boldsymbol{w}_{c'}, \boldsymbol{z}\rangle)$ for every class (cf. *2.4.6*, *2.4.7 and 4.3*). Hence, the *plain softmax* is commonly avoided.

4.5.1 Hierarchical Softmax

The hierarchical softmax computes it in multiple steps instead of a single one with the goal of reducing cost. For this, we arrange classes in a decision tree like manner.

- Input is $\boldsymbol{z}$, the ouput of the layer before the softmax
- Output is $\boldsymbol{p}$, the probability for each class

The leaves of our trees are classes, interior vertices are decision points, and each possible choice is associated with a probability. The probability of each class is obtained by computing the product along the corresponding path.



To model the probability distribution over the children of each interior vertex v_i, we still use a plain softmax. We have to store one weight matrix $\boldsymbol{w}$ and bias vector $\boldsymbol{b}$ per v_i. The probability distribution over the children of any v_i is $S(\boldsymbol{W}_i^\top \boldsymbol{z} + \boldsymbol{b}_i)$. Note that $\boldsymbol{z}$ is used at each v_i → influences all decisions. For example, the probability p_y of leaf $y = 0101$ is:

$$S(0, \mathbf{w}^\top \boldsymbol{z} + \boldsymbol{b})_0 \cdot S(0, \mathbf{w}_0^\top \boldsymbol{z} + b_0)_1 \cdot S(0, \mathbf{w}_{01}^\top \boldsymbol{z} + b_{01})_0 \cdot S(0, \mathbf{w}_{010}^\top \boldsymbol{z} + b_{010})_1$$

→ only depends on 4 (out of 15) weight vectors and bias terms! All other weight vectors / biases have zero gradient during backprop.

💡 For balanced binary trees with C classes, we generally access $\log_2 C$ weight vectors & biases.

Discussion

- The choice of tree matters for prediction performance. Hierarchical softmax is able to produce good predictions if the classes in the "right" subtree are easy to discriminate from the classes of the "wrong" subtrees, i.e. similar classes are close together.
- The choice of tree matters for training speed
  - Flat: as slow as softmax
  - Balanced: logarithmic cost
  - Fastest: *Huffman* tree based on class frequencies → minimizes expected path lengths (frequent classes get short path)
- No/limited runtime improvement during prediction as we still need to compute all probabilities to get distribution over labels

4.6 Next lecture (9.4.)

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