Deep Learning:

Neural Network Architecture & Training

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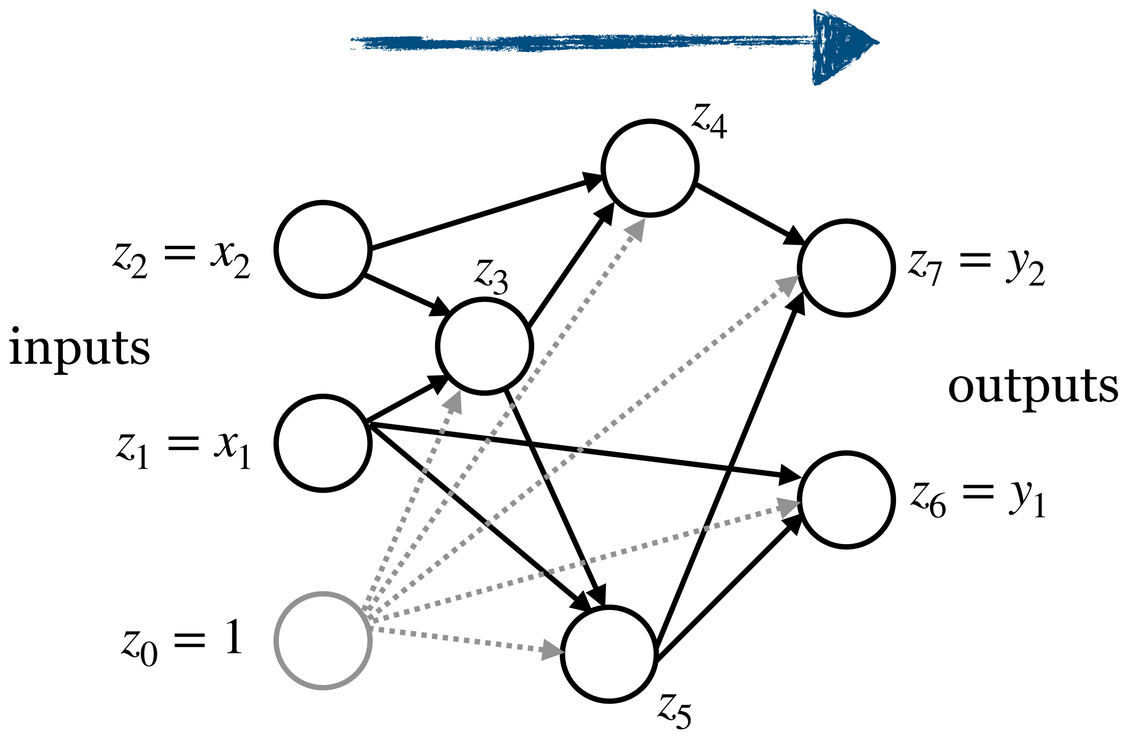
Deep Learning VO - WS 23/24
Lecture 3 - October 16th, 2023

Today

- ☐ Neural Network Architecture
- ☐ Neural Network Training
  - ☐ Error (Loss) Functions
  - ☐ Gradient Descent

General Network Description

- A **neural network** with D inputs and K outputs is defined by a directed graph $G = (V, E)$ with:
  - nodes (neurons and inputs) V
  - edges (connections) E
- a weight w_{ji} for each edge $(i, j) \in E$,
- an activation function h_j for each non-input node j,
- a list $OUT = \langle out_1, \ldots, out_K \rangle$ defining K output nodes.



Network function

- The output of node i is given by:

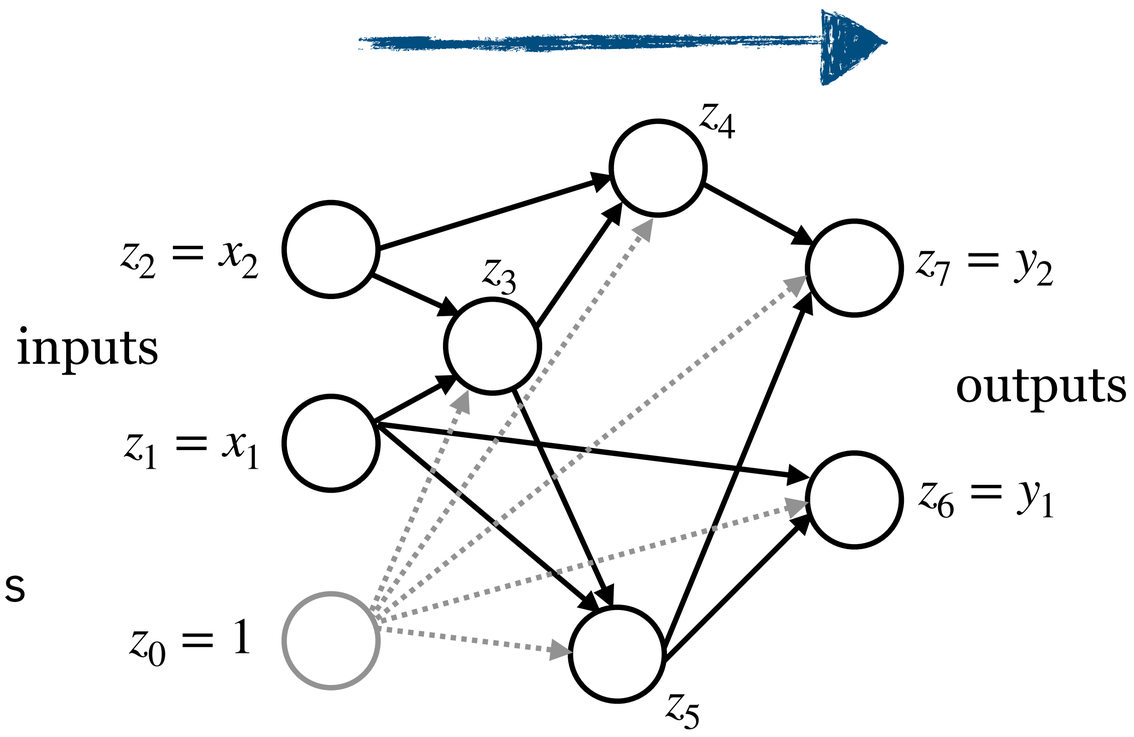
$$z_i = \begin{cases} x_i \,, & \text{if } \; i \in \{0,\ldots,D\} \\ h_i(a_i) \,, & \text{otherwise} \end{cases}$$

with **activations** $a_i = \sum_{j \in pre(i)} w_{ij} z_j$ and mappings:

pre: $pre(i) = \{j \,|\, (j,i) \in E\}$ is the set of neurons which **connect to** neuron i.

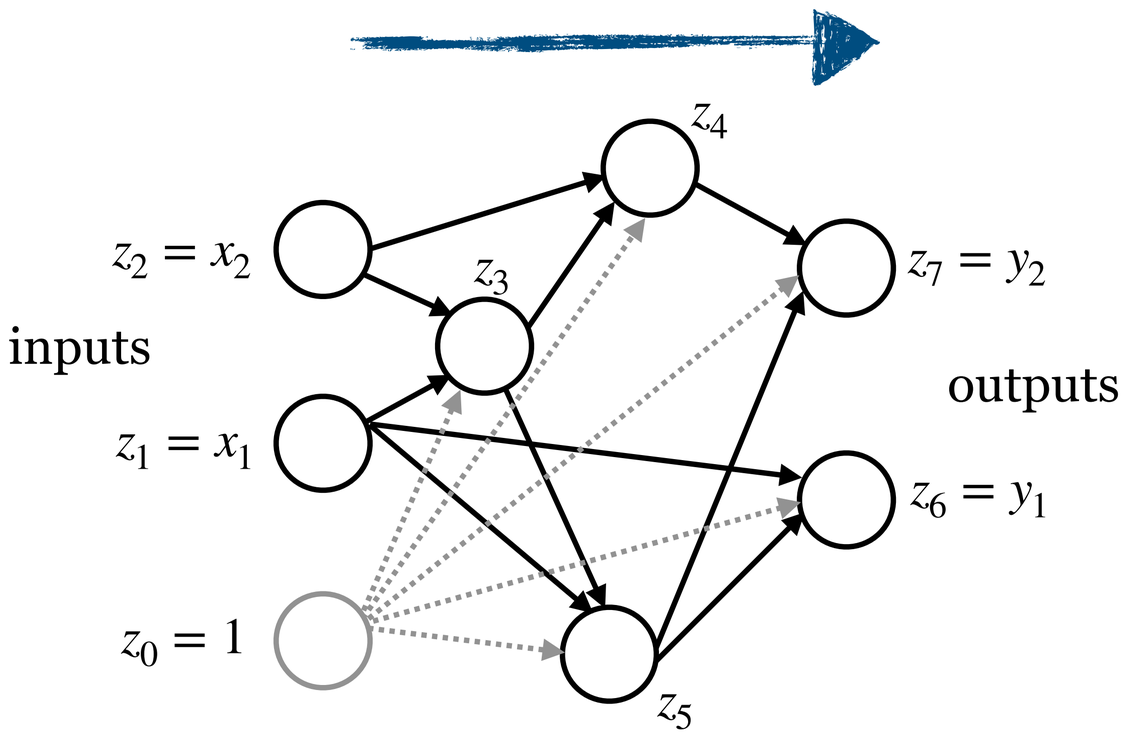
post: $post(i) = \{j \,|\, (i,j) \in E\}$ is the set of neurons which neuron i **connects to**.

Then, the kth output of the network is given by $y_k = z_{out_k}$.



Feedforward networks

- Any network can be described in this way.
- The network function $\mathbf{y}(\mathbf{x}, \mathbf{w})$ can be defined recursively.
- We consider here network graphs without loops, i.e., "**feedforward networks**".
- Such networks are often called **Multilayer Perceptrons** although the neural units are usually **not** perceptrons.



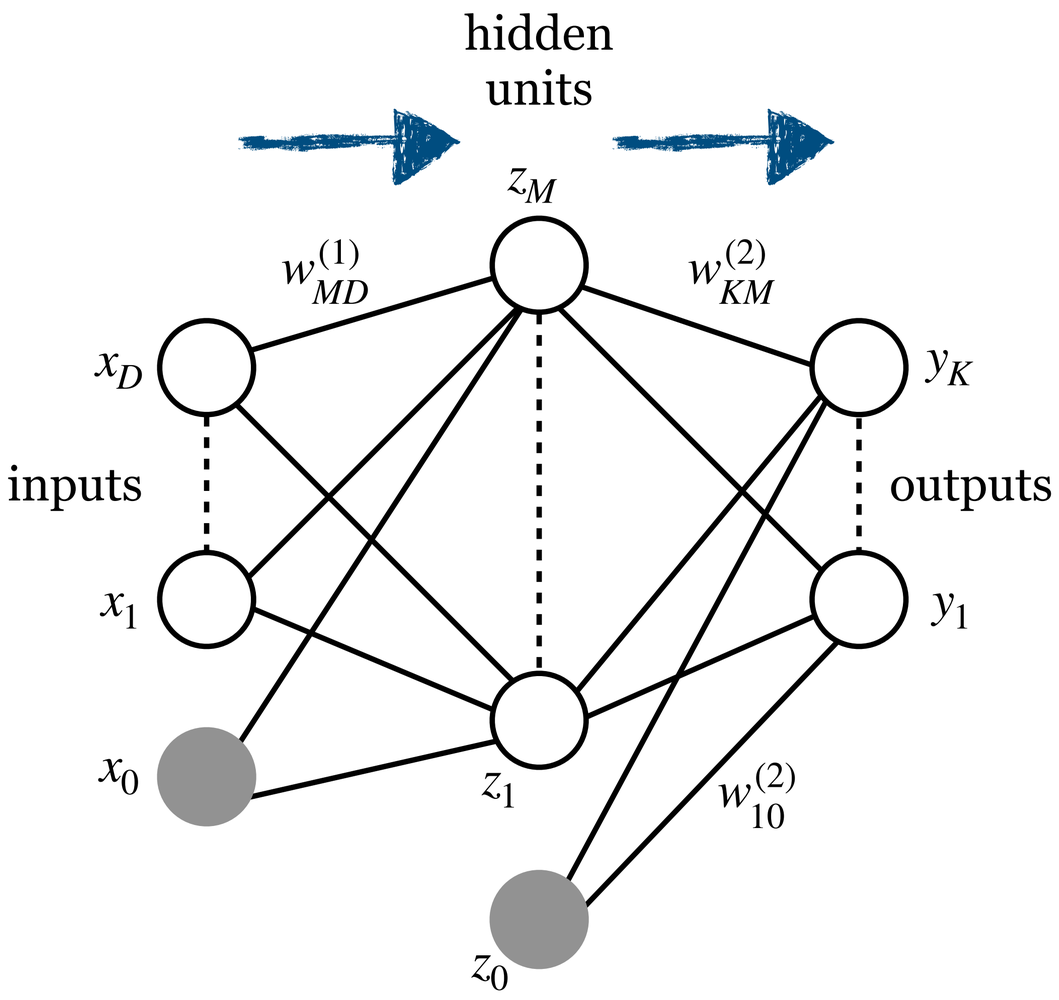
Layered networks

- In a **layered network**, the nodes can be divided into layers, such that:
  - Input nodes are in layer 0 (input layer)
  - A node in layer i has outgoing edges only to nodes in layer $i+1$ for all i.

Network depth: The number of layers of a network excluding the input layer.

Hidden units: Neurons which are neither input nor output units.

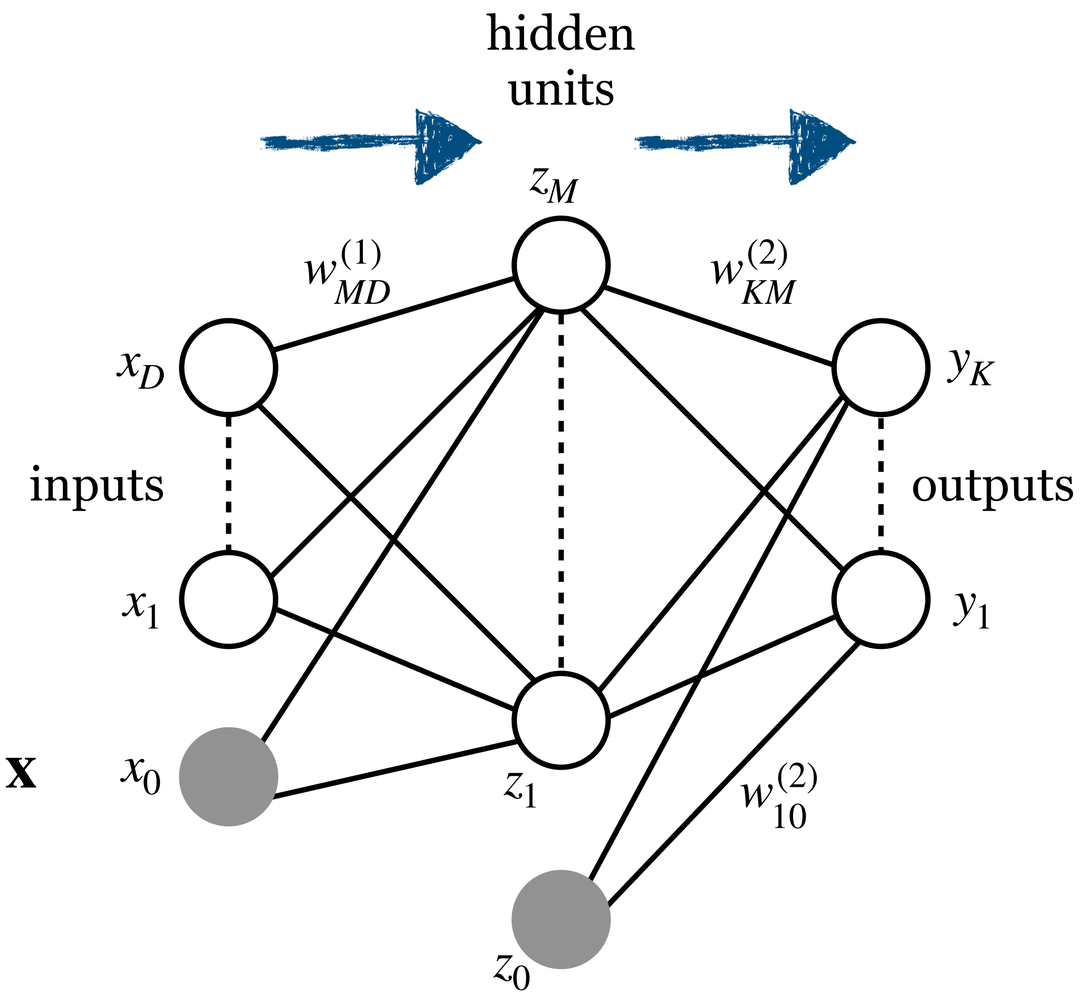
Hidden layers: Layers containing hidden units (for layered network).



Layered networks

- Let M_i be the number of neurons in layer i.
  - $M_0 = D$ (inputs)
  - $M_d = K$ (outputs), d is the network depth.
- In a layered network, each layer $i > 0$ computes a function $f^{(i)} : \mathbb{R}^{M_{i-1}} \to \mathbb{R}^{M_i}$.
- It applies the activation function $h^{(i)}$ component-wise to an affine transformation of the previous layer output:

$$f^{(i)}(\mathbf{x}) = h^{(i)}\left(W^{(i)} f^{(i-1)}(\mathbf{x}) + \mathbf{b}^{(i)}\right) \quad \text{where} \quad f^{(0)}(\mathbf{x}) = \mathbf{x}$$



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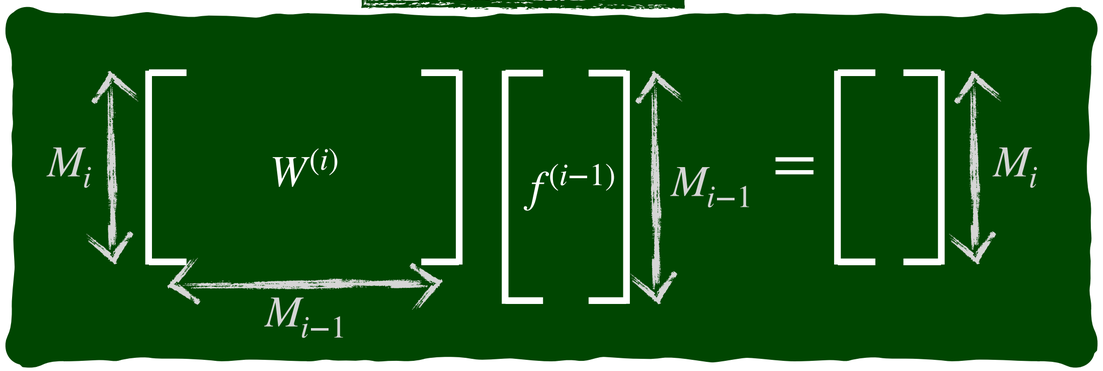

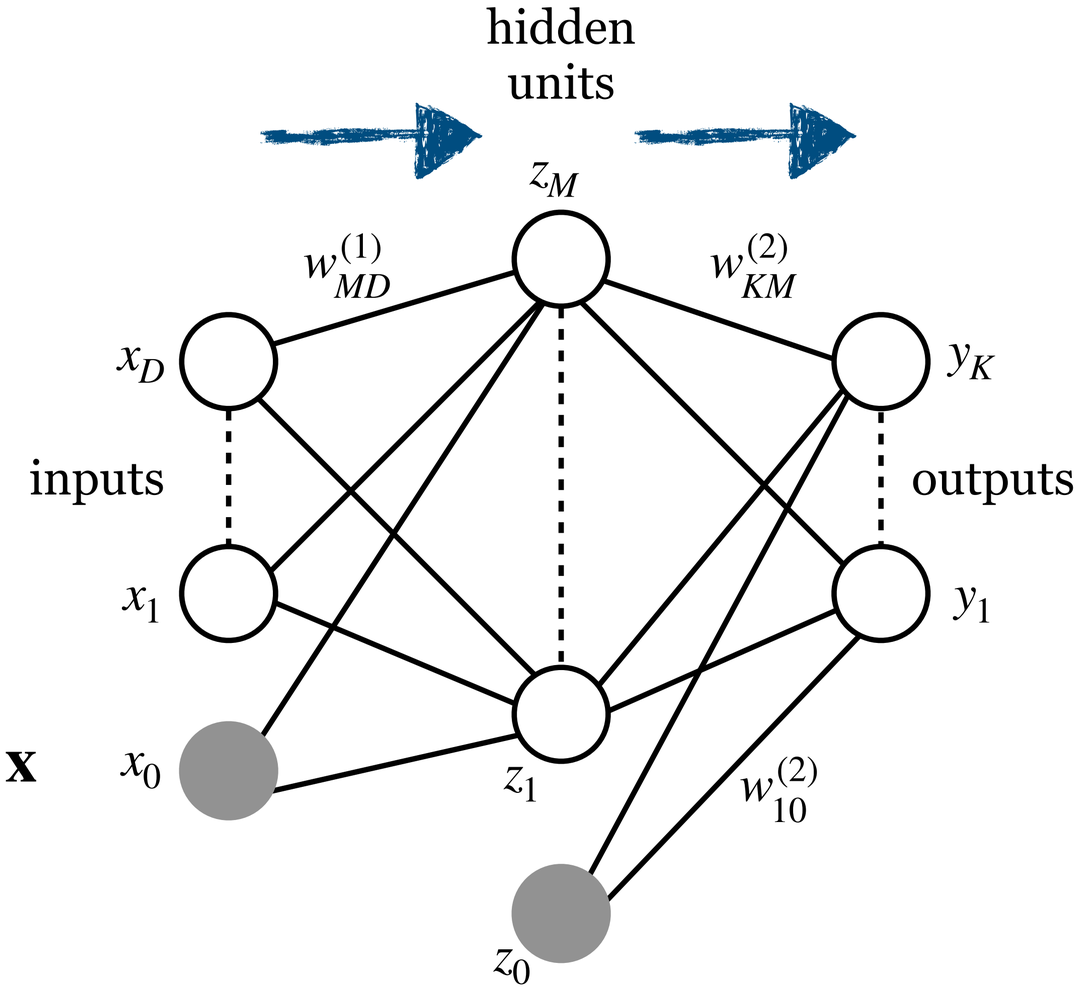

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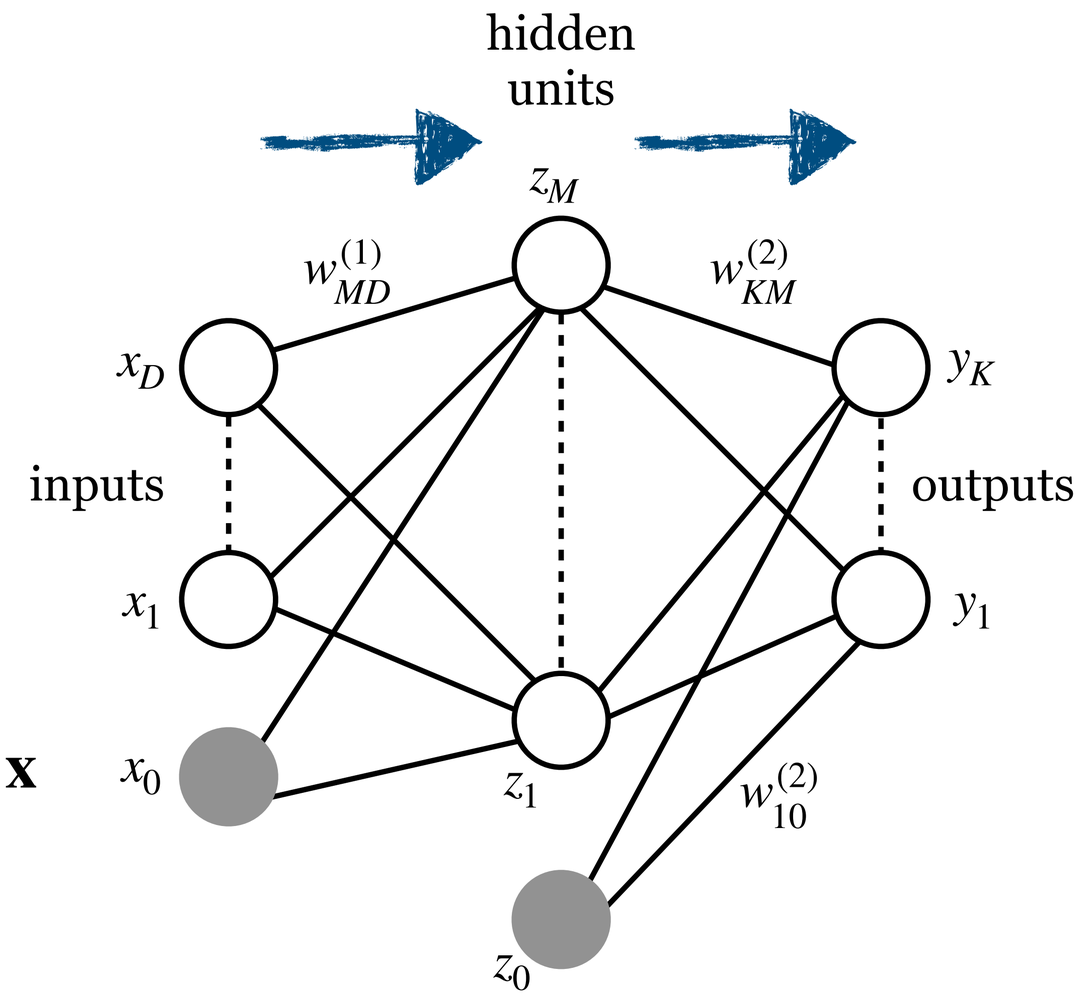


Example: A network with three layers computes:

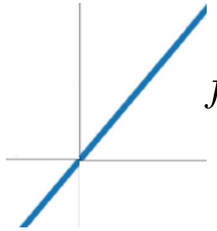
$$y(\mathbf{x}) = f^{(3)}(\mathbf{x}) = h^{(3)}\left(W^{(3)} h^{(2)}\left(W^{(2)} h^{(1)}(W^{(1)}\mathbf{x} + \mathbf{b}^{(1)}) + \mathbf{b}^{(2)}\right) + \mathbf{b}^{(3)}\right)$$

Output Activation functions

The choice of **output activation functions** depends on the nature of the problem:

- **Linear** for regression problems.

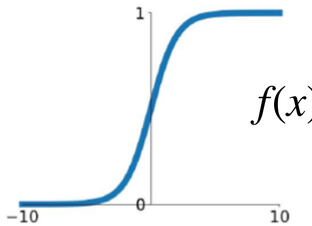
$$h(a) = a$$



$$f(x) = x$$

- **Sigmoid** for (possibly multiple) binary classification problems.

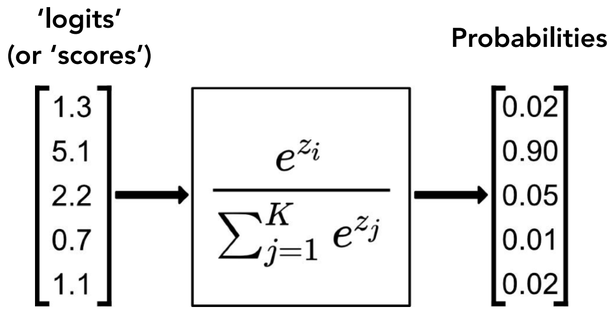
$$h(a) = \frac{1}{1 + \exp(-a)}$$



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

- **Softmax** for multiclass classification problems.

$$h_k(a_1, \ldots, a_K) = \frac{\exp(a_k)}{\sum_j \exp(a_j)}$$



Hidden Unit Activation functions

- **Sigmoidal Units:** Traditional non-linear activations. Discouraged by recent research.

Logsig: $\sigma(x) = \dfrac{1}{1 + e^{-x}}$ or Hyperbolic tangent (tanh): $h(x) = \dfrac{e^x - e^{-x}}{e^x + e^{-x}}$

Note that: $\tanh(x) = 2\sigma(2x) - 1$

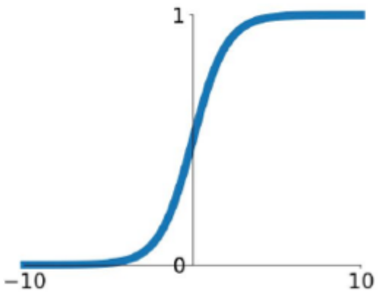
- **Rectified Linear Unit (ReLU):** Excellent default choice. → $h(x) = \max\{0, x\}$

- **Leaky ReLU**: $h(x) = \max\{\alpha x, x\}$ for small α (e.g., $\alpha = 0.1$).

- **Exponential Linear Unit (ELU)**: $h(x) = \begin{cases} x, & x \geq 0 \\ \alpha(e^x - 1), & x < 0 \end{cases}$

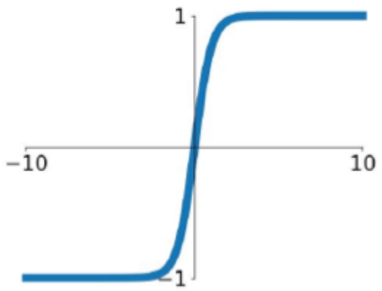
Hidden Unit Activation functions

Sigmoid



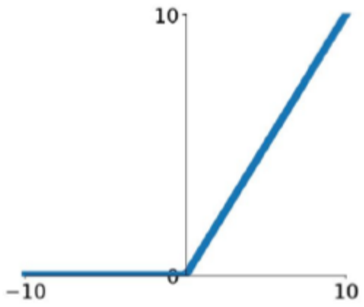
$$\sigma(x) = \frac{1}{1 + \exp(-x)}$$

Hyperbolic Tangent (tanh)



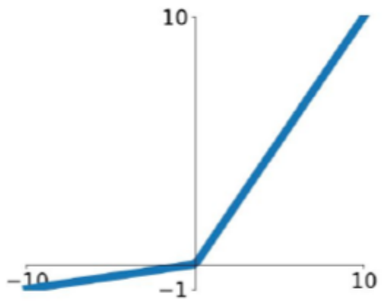
$$h(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

Rectified Linear Unit (ReLU)



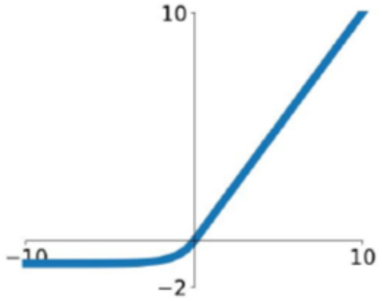
$$h(x) = \max\{0, x\}$$

Leaky ReLU



$$h(x) = \max\{\alpha x, x\}$$

Exponential Linear Unit (ELU)



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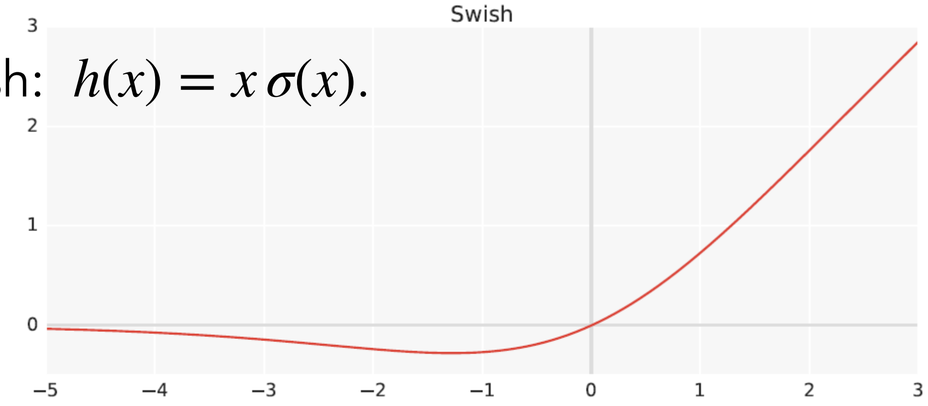
- **Exponential Linear Unit (ELU)**: $h(x) = \begin{cases} x, & x \geq 0 \\ \alpha(e^x - 1), & x < 0 \end{cases}$

- **Others**: Maxout, Hard tanh: $h(x) = \max\{-1, \min\{1, x\}\}$, Swish: $h(x) = x\,\sigma(x)$.



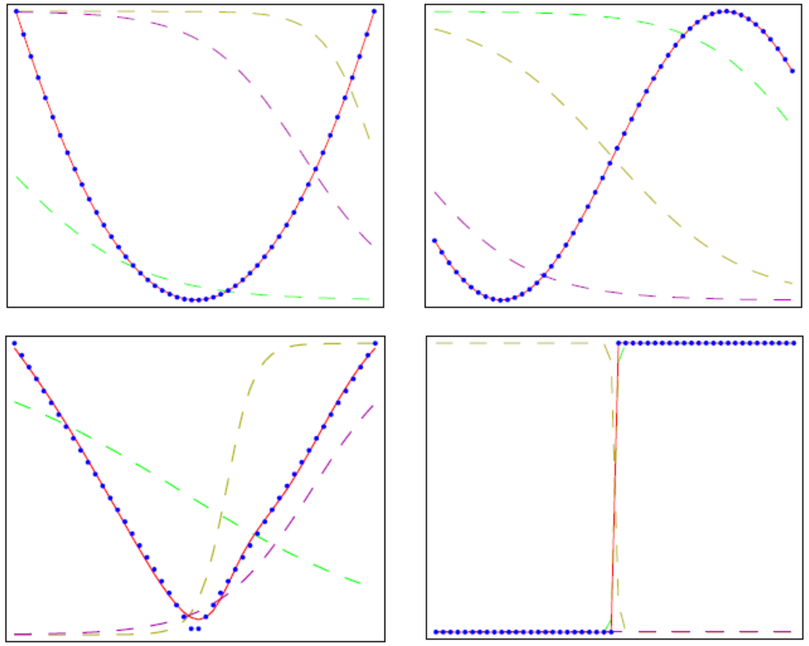
Approximation Properties

- Neural networks define a very general class of functions.
- **Neural networks are universal approximators**:

A two-layer neural network with linear output unit and sigmoidal hidden units can approximate any continuous function on a compact input domain to arbitrary accuracy provided a sufficiently large number of hidden units.

Network with 3 hidden neurons:

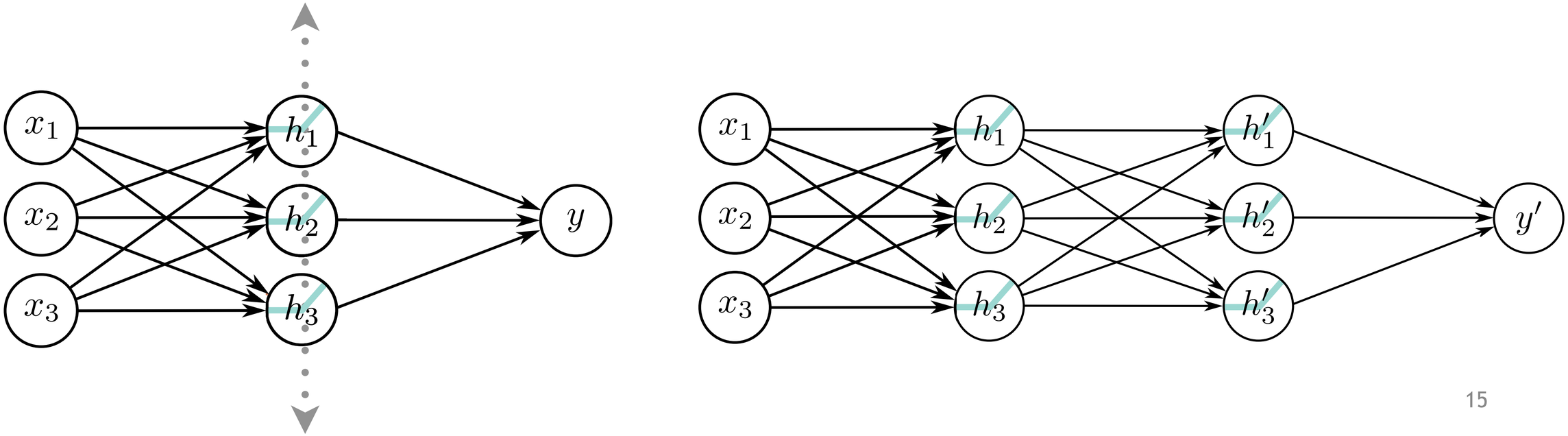
blue target function
red approximation
— — — output of hidden neurons



Hornik, K., Stinchcombe, M., & White, H. (1989)
"Multilayer feedforward networks are universal approximators".

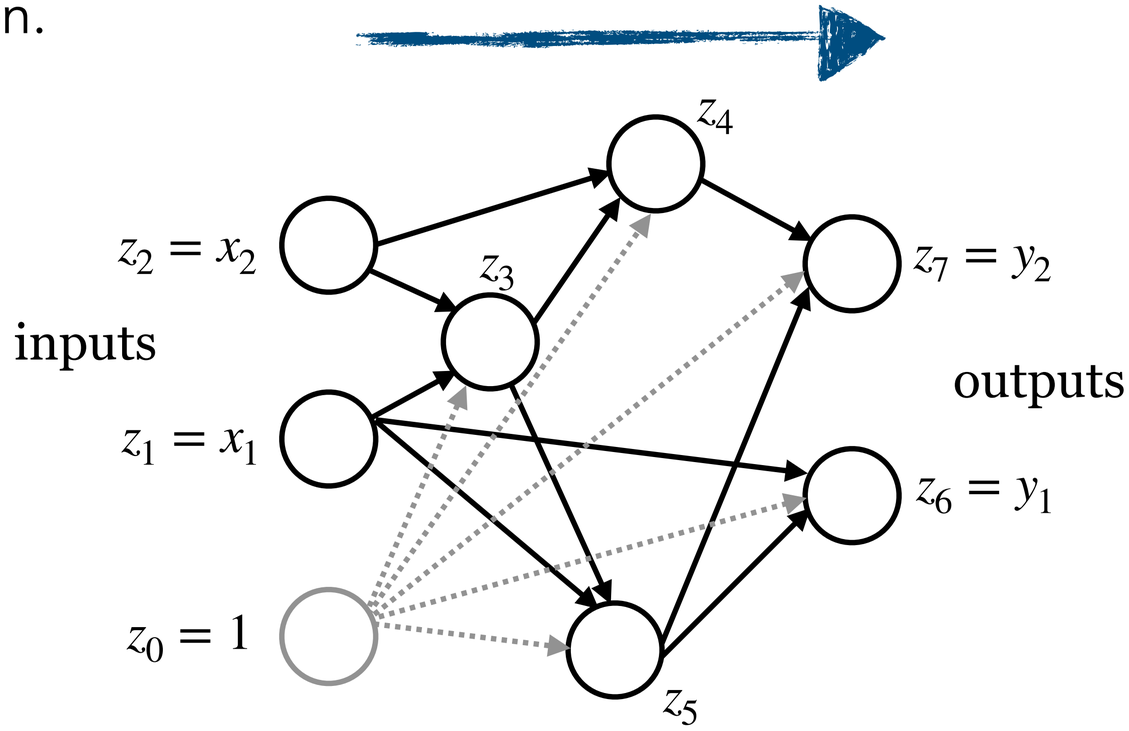
Why deep neural networks are preferable?

- A two-layer neural network can approximate any function.
  - *However, the number of neurons necessary may be extremely large.*
- In many cases, deeper networks can reduce the number of units and improve generalization.
- Using a deep model encodes a general belief that the functions we want to learn involve composition of several simpler functions (multi-step programs).



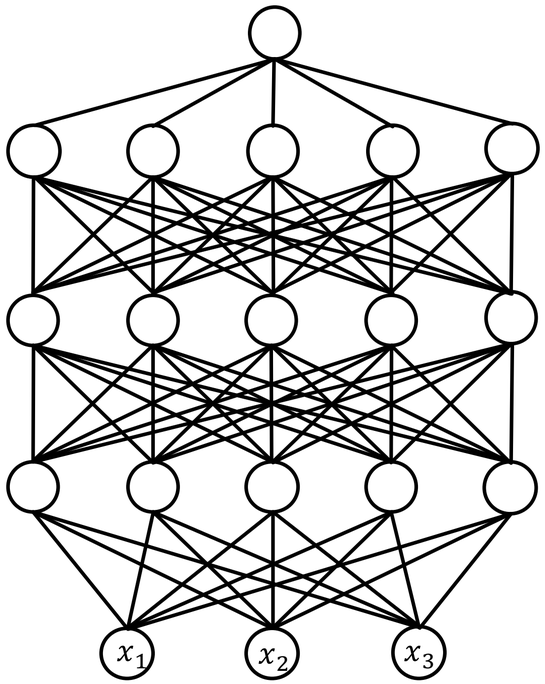
Summary: Neural Network Architectures

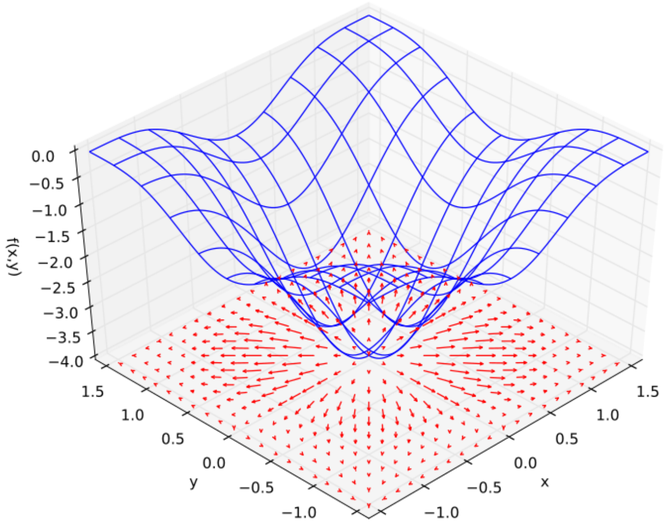
- Neural network architectures can be defined as network graphs.
- For layered networks, we can simplify the definition.
- Many activation functions are possible.
- Neural networks are universal approximators.
- Deep neural networks are preferred.



Today

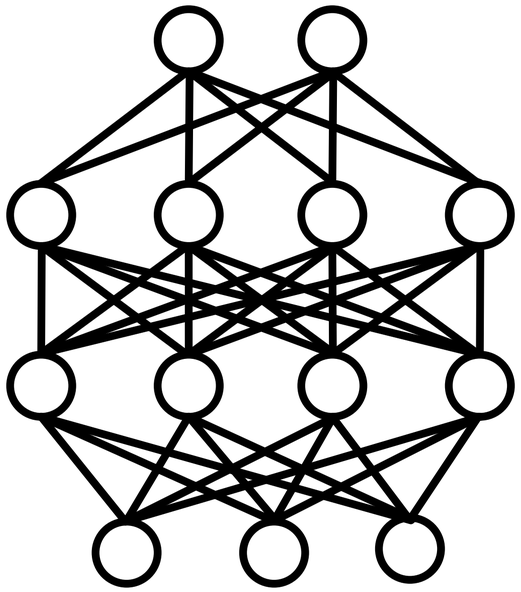
- ☑ Neural Network Architecture
- ☐ Neural Network Training
  - ☐ Error (Loss) Functions
  - ☐ Gradient Descent





Error (Loss) functions

For training we try to minimize a loss function.



- Consider a neural network with D inputs and K outputs.
- We have M training examples.
  - Network inputs: $X = \langle \mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(M)} \rangle$
  - Target vectors: $T = \langle \mathbf{t}^{(1)}, \ldots, \mathbf{t}^{(M)} \rangle$.

- The loss functions for different types of problems can be derived from maximum likelihood and assumptions on the data distribution.
- Corresponding output activation functions arise naturally such that the network output can be interpreted as the (mean of the) posterior distribution.

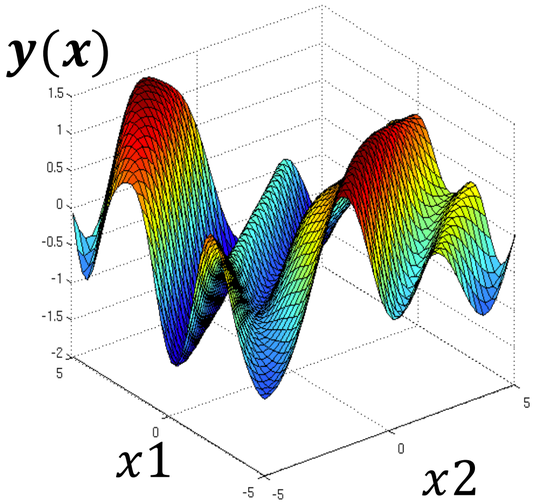
Error (Loss) functions

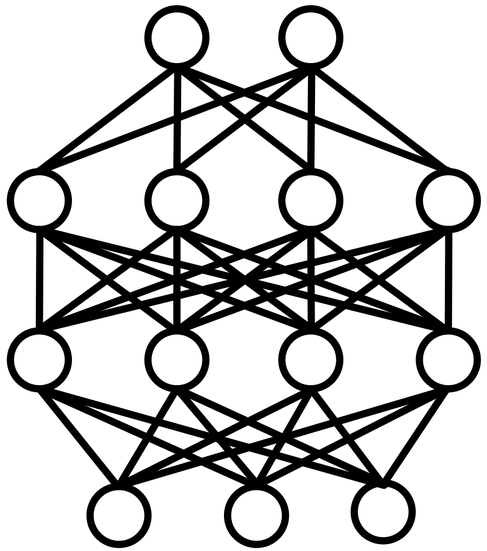
K-dimensional regression

- **Activation function:** identity
- **Data-sample Likelihood:** $N(\mathbf{t}^{(m)} \,|\, \mathbf{y}(\mathbf{x}^{(m)}), \sigma^2\mathbf{I})$
- **Error function:** Sum squared error

$$E(\mathbf{w}) = \frac{1}{2}\sum_m ||\mathbf{y}(\mathbf{x}^{(m)}) - \mathbf{t}^{(m)}||^2$$

$$= \frac{1}{2}\sum_m \sum_k \left(y_k(\mathbf{x}^{(m)}) - t_k^{(m)}\right)^2$$



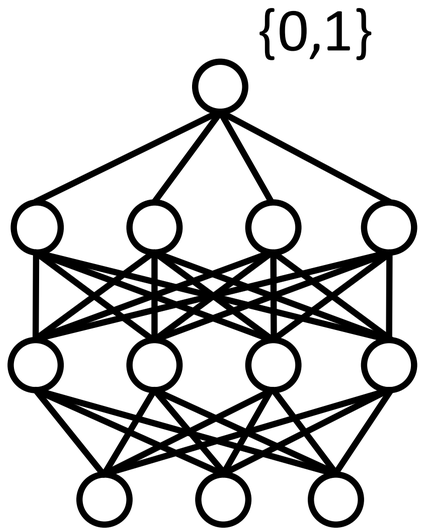


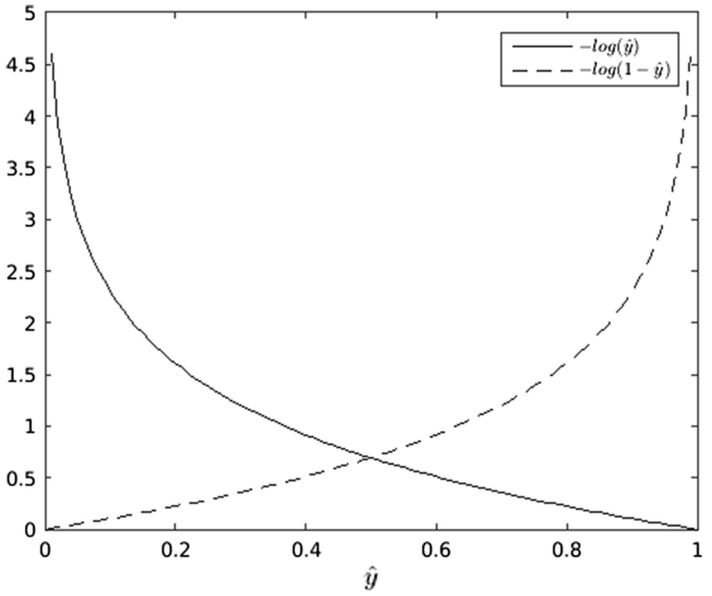
Error (Loss) functions

Binary classification

- **Activation function:** logistic sigmoid
- **Data-sample Likelihood:** $\mathbf{y}(\mathbf{x}^{(m)})^{t^{(m)}}\left(1-\mathbf{y}(\mathbf{x}^{(m)})\right)^{(1-t^{(m)})}$
- **Error function:** Cross-entropy error

$$E(\mathbf{w}) = -\sum_{m}\left[t^{(m)}\log y(\mathbf{x}^{(m)}) + (1-t^{(m)})\log\left(1-y(\mathbf{x}^{(m)})\right)\right]$$





Error (Loss) functions

K-class classification

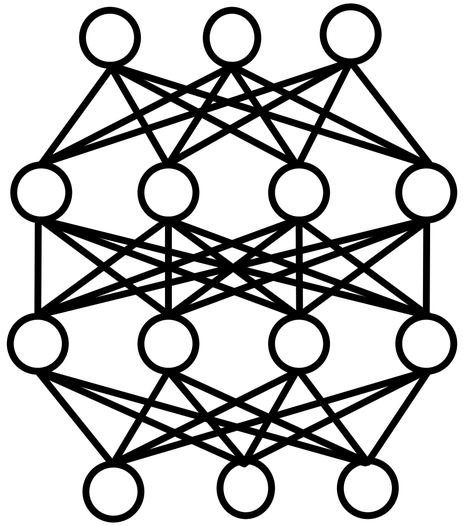
- **Activation function:** softmax
- **Data-sample Likelihood:** $\prod_k y_k(\mathbf{x}^{(m)})^{t_k^{(m)}}$
- **Error function:** Cross-entropy error

$$E(\mathbf{w}) = -\sum_m \sum_k \left[t_k^{(m)} \log y_k(\mathbf{x}^{(m)}) \right]$$

Target vectors are one-hot encodings of the target class:

$$t_k^{(m)} = \begin{cases} 1, & \text{if target class is } k, \\ 0, & \text{otherwise} \end{cases}$$

1	0	0	class 1
0	1	0	class 2
0	0	1	class 3



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The Gradient

- The error is a **scalar field:**

  $E : \mathbb{R}^D \to \mathbb{R}$

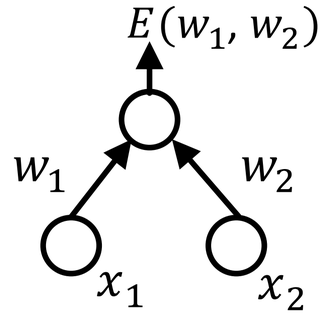
  D : number of parameters

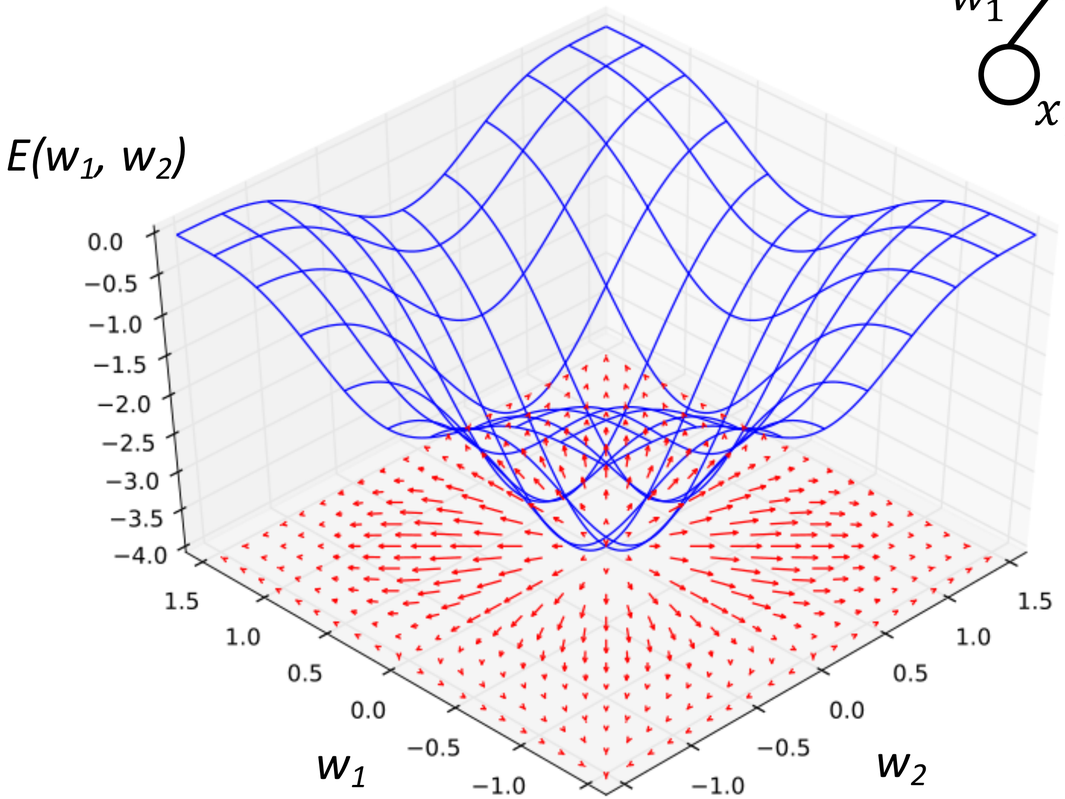
- The gradient is a **vector field:**

$$\nabla_{\mathbf{w}} E : \mathbb{R}^D \to \mathbb{R}^D$$

$$\nabla_{\mathbf{w}} E = \begin{pmatrix} \frac{\partial E}{\partial w_1} \\ \vdots \\ \frac{\partial E}{\partial w_D} \end{pmatrix}$$

- $(\nabla_{\mathbf{w}} E)(\mathbf{w}^*)$ points in the direction of the steepest increase of the error at $\mathbf{w}^*$.





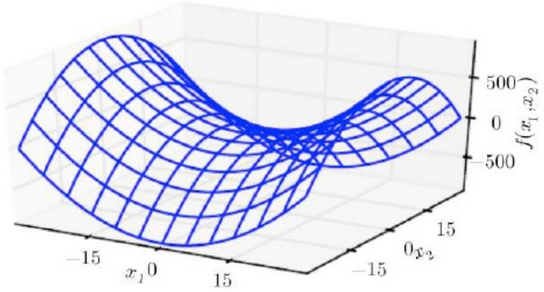
Loss minimization

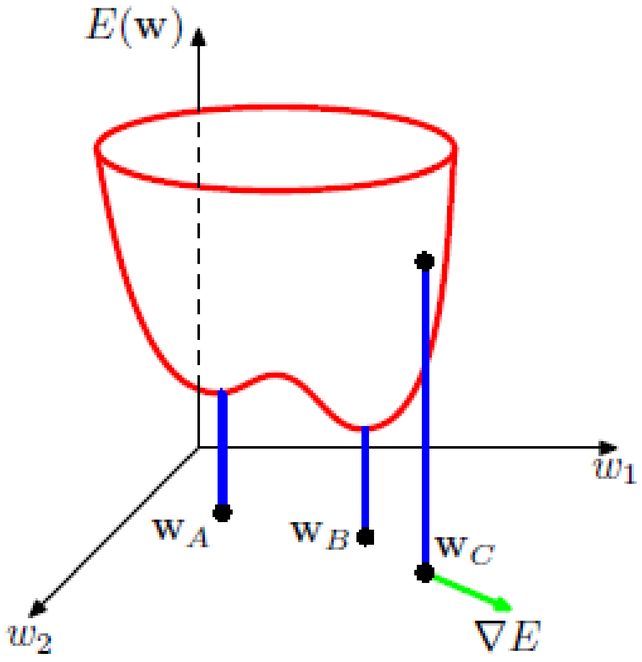
For training we try to minimize the loss function.

The gradient $\nabla_{\mathbf{w}} E$ provides useful information.

Stationary points: Points $\mathbf{w}^*$ where $\nabla_{\mathbf{w}} E(\mathbf{w}^*) = 0$

- Minima:
  - Global minima: $E(\mathbf{w}^*) \leq E(\mathbf{w})$ for all $\mathbf{w}$.
  - Local minima: Smaller errors exist.
- Saddle points:





Our task: Find a good local minimum.

Training: Gradient Descent

- The negative gradient

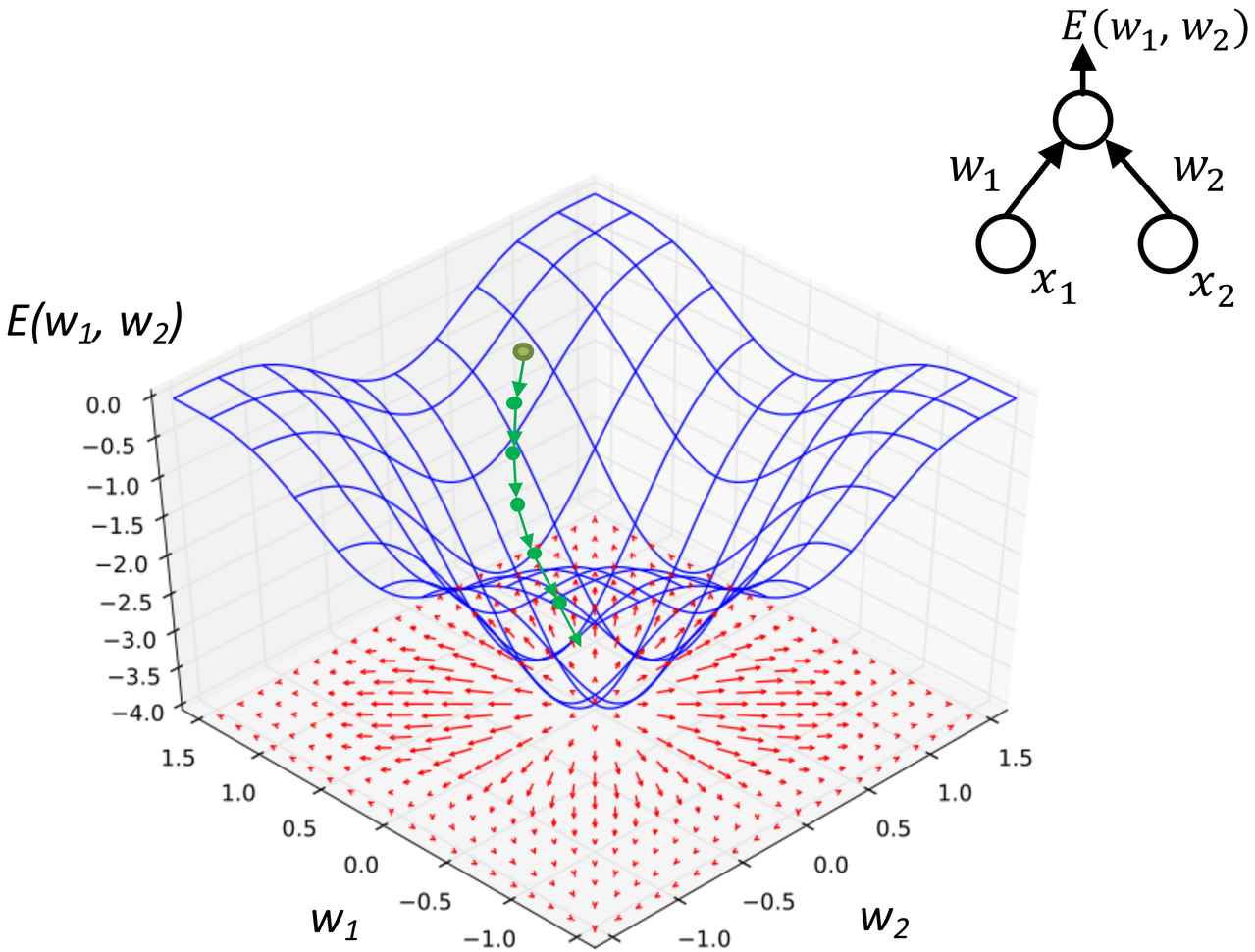
$$-\nabla_{\mathbf{w}} E(\mathbf{w}_{old})$$

at $\mathbf{w}_{old}$ points in the direction where the error **decreases** most strongly.

- We slightly change parameters to reduce error.

$$\mathbf{w}_{new} = \mathbf{w}_{old} - \eta \nabla_{\mathbf{w}} E(\mathbf{w}_{old})$$

$\eta > 0$ is the **learning rate.**



Batch Gradient Descent

```
Choose w randomly
i ← 0
REPEAT
    w ← w − η(i) ∇_w E(w)
    i ← i+1
UNTIL Stopping Criterion met
```

- This follows the true gradient of the error.
- Error function has the form: $E(\mathbf{w}) = \sum_{m=1}^{M} E_m(\mathbf{w})$

$E_m(\mathbf{w})$ is the error for the training sample m

- Hence, we have $\nabla_{\mathbf{w}} E(\mathbf{w}) = \sum_{m} \nabla_{\mathbf{w}} E_m(\mathbf{w})$.

Batch Gradient Descent

```
Choose w randomly
i ← 0
REPEAT
    w ← w − η(i) ∇_w E(w)
    i ← i+1
UNTIL Stopping Criterion met
```

For example in the case of regression with the error function:

$$E(\mathbf{w}) = \sum_m \frac{1}{2} ||\mathbf{y}(\mathbf{x}^{(m)}) - \mathbf{t}^{(m)}||^2$$

- This follows the true gradient of the error.
- Error function has the form: $E(\mathbf{w}) = \sum_{m=1}^{M} E_m(\mathbf{w})$
- Hence, we have $\nabla_{\mathbf{w}} E(\mathbf{w}) = \sum_m \nabla_{\mathbf{w}} E_m(\mathbf{w})$.

$E_m(\mathbf{w})$ is the error for the training sample m

A single descent step has time complexity $O(M)$.

M: number of training examples

Mini-batch (Stochastic) Gradient Descent

```
Choose w randomly
Let B be the set of minibatches
i ← 0
REPEAT
    FOR b in B
        w ← w − η(i) ∇_w E(w, b)
        i ← i+1
UNTIL Stopping Criterion
```

"epoch": one complete pass over the whole training set.

- Divide the training set into **mini-batches** of size M'.
- Approximate the true gradient by the gradient over the mini-batch.
- Here, $E(\mathbf{w}, b)$ denotes the error on mini-batch b.

Mini-batch (Stochastic) Gradient Descent

- Initially, SGD referred to a batch-size of 1.

  i.e., update the weights after every training example.

- Today, mini-batch GD is commonly called SGD.

- For large training sets, batch GD is too slow.

- In SGD, complexity of one update is independent of training set size.

  Instead, depends on the mini-batch size M'.

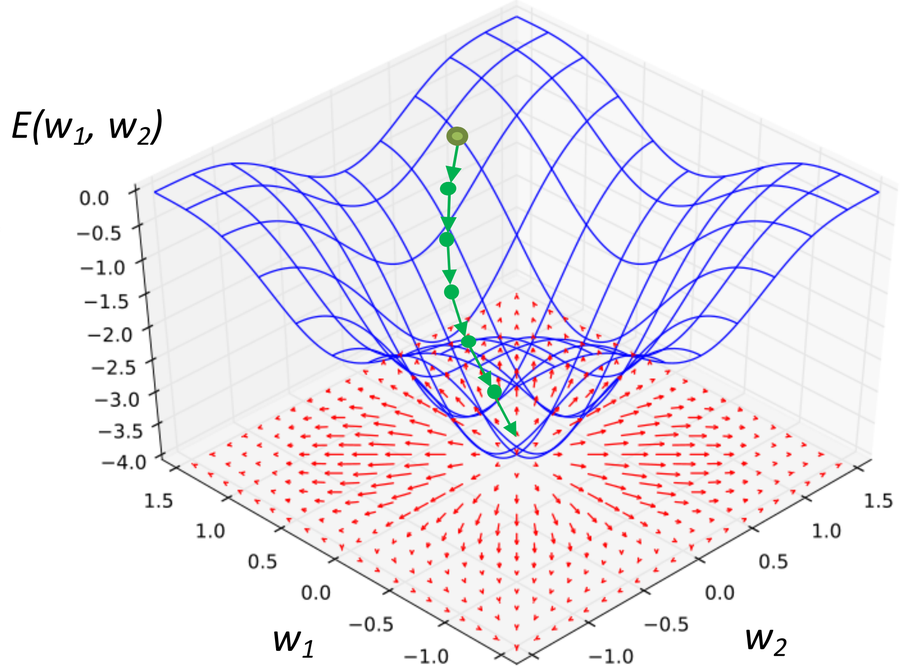
- SGD converges faster.

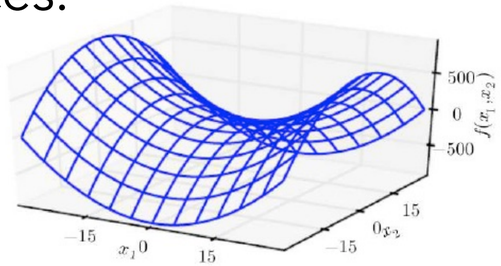
- Gradients within one mini-batch can be computed in parallel (e.g., on GPUs).

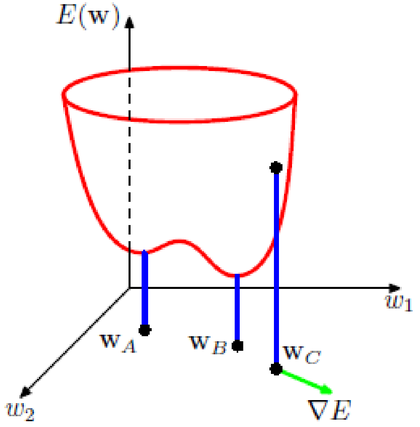
$$\nabla_{\mathbf{w}} E(\mathbf{w}) = \sum_m \underline{\nabla_{\mathbf{w}} E_m(\mathbf{w})}$$

When Gradient Descent struggles

- Local minima: Usually not a problem in neural networks.
  - In high-dimensional spaces, there are many downhill paths.
- Plateaus:
  - Regions of small gradients
  - Gradient scaling techniques help
- Saddle points:
  - They are much more numerous in high-dimensional spaces.
  - Small gradients.
- Ragged error landscapes:
  - Gradients can become very large → unstable training.
  - We can clip/rescale large gradients.







Summary: Gradient Descent

- We want to **minimize a loss function**.
  - But we can only find local minima.
- The loss function is often dictated by the problem-type.
- Training with **gradient descent**

$$\mathbf{w}_{new} = \mathbf{w}_{old} - \eta \nabla_{\mathbf{w}} E(\mathbf{w}_{old})$$

- Mini-batch (stochastic) gradient descent → Much more efficient

Next lecture: How do we compute the gradients in a neural network?

Today

- ☑ Neural Network Architecture
- ☐ Neural Network Training
  - ☑ Error (Loss) Functions
  - ☑ Gradient Descent

Questions?