Artificial Neural Networks

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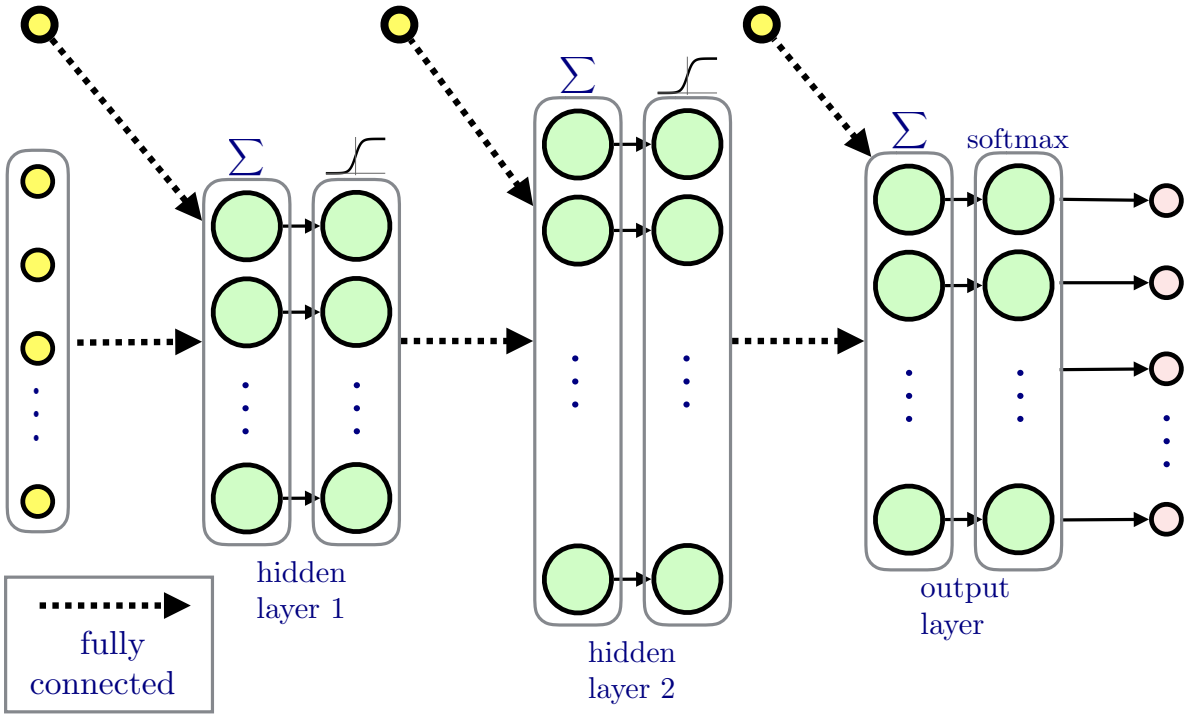
Outline

Topics covered in the lecture:

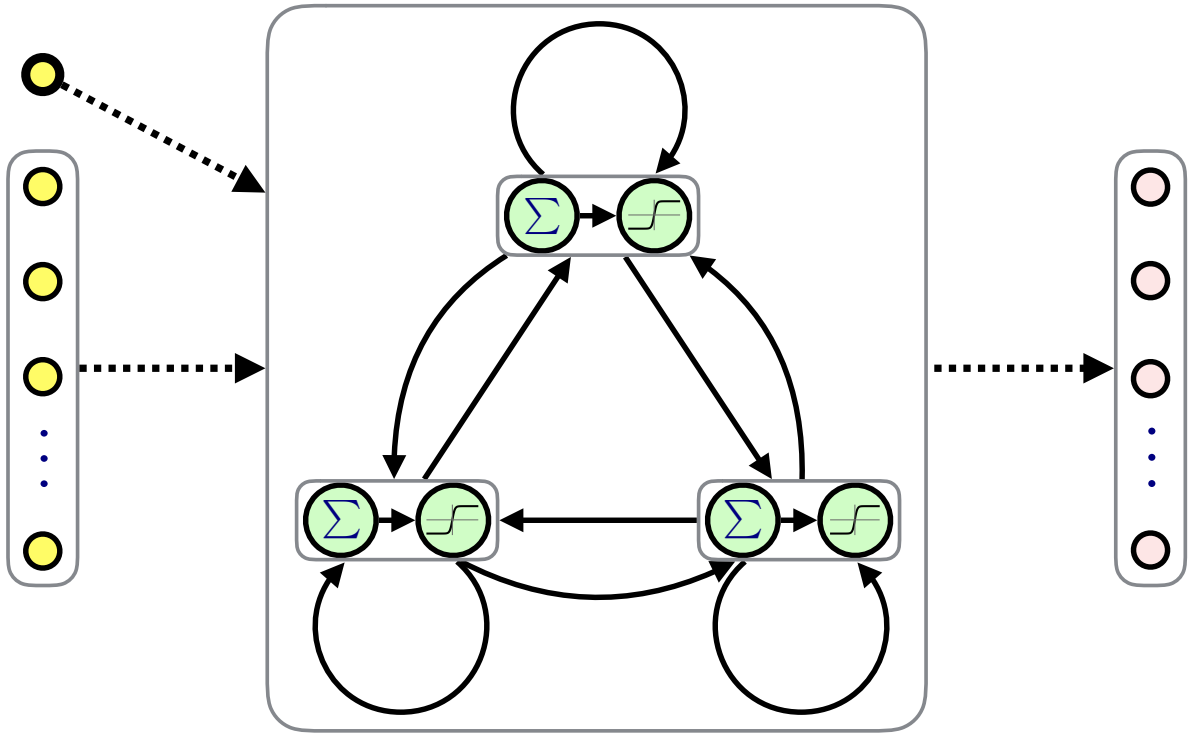
- Neurons
- Layers
- Loss functions
- Backpropagation
- Optimization methods
- Parameter initialization
- Regularization

Multilayer Perceptron (MLP)



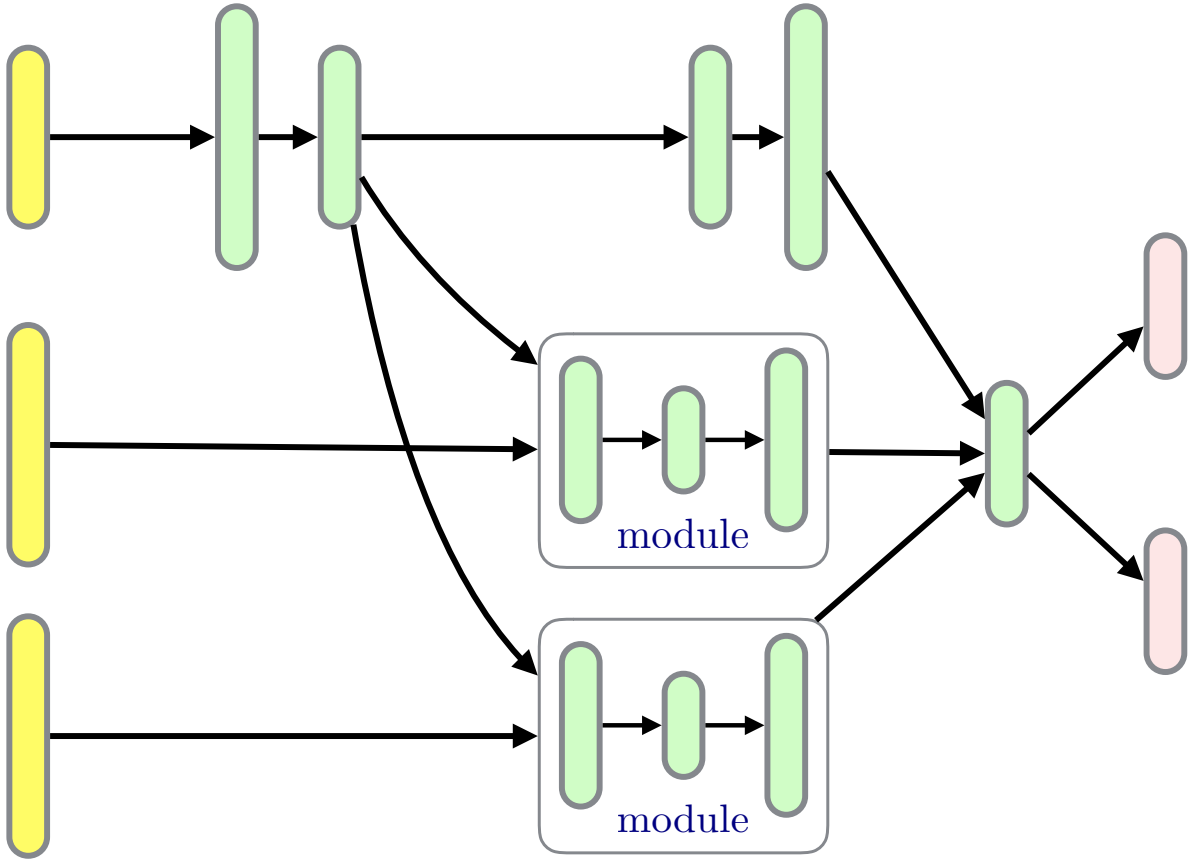
- Feed-forward ANN
- Fully-connected layers

Recurrent Neural Network (RNN)



- Fully-Connected Recurrent Neural Network (FRNN)
- Both inputs and outputs are sequences
- Feedback connections $\rightarrow$ memory (similarly to sequential circuitry)

Modular and Hierarchical Architectures



- Directed Acyclic Graphs (DAGs)
- Layers can be organized in *modules*
- Hierarchies of modules, module reuse

Prediction problem

- $\mathcal{X}$ is a set of input observations (features)
- $\mathcal{Y}$ is a finite set of targets (labels)
- $(x, y) \in \mathcal{X} \times \mathcal{Y}$ is a realization of a random process with p.d.f. $p(x, y)$
- A prediction strategy $h\colon \mathcal{X} \to \mathcal{Y}$
- A loss function $\ell\colon \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$ penalizes a single prediction
- We want to find a precition strategy with the minimal expected risk

$$R(h) = \int_x \int_y \ell(y, h(x))\, p(x, y)\, \mathrm{d}x\mathrm{d}y = \mathbb{E}_{(x,y)\sim p}\Big[\ell(y, h(x))\Big]$$

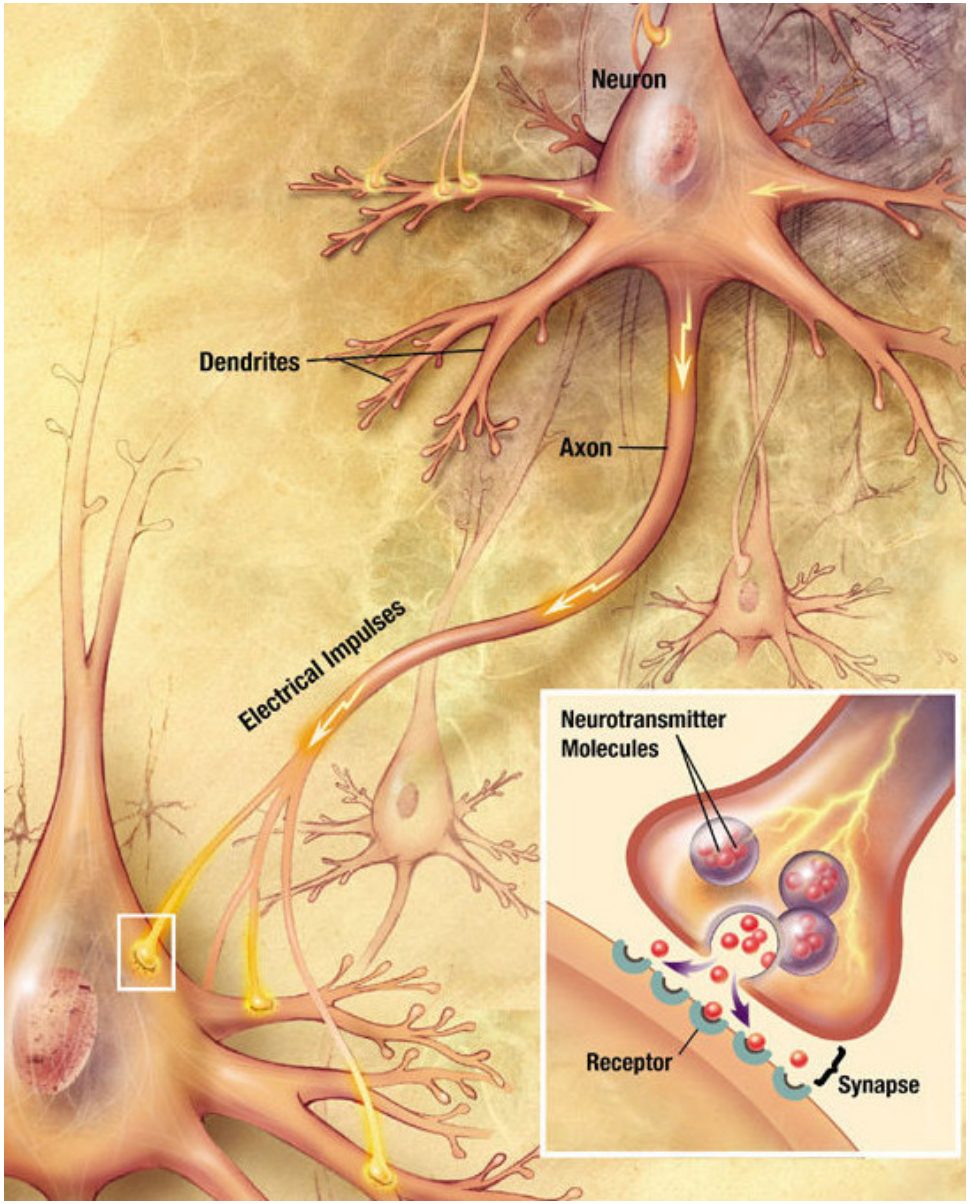
Our Setup

- We have training dataset: $\mathcal{T}^m = \{(x_i, y_i) \in (\mathcal{X} \times \mathcal{Y}) \mid i = 1, \ldots, m\}$, where $\mathcal{X} \subseteq \mathbb{R}^n$ and $\mathcal{Y} \subseteq \mathbb{R}^K$
- We will deal with regression and classification tasks
- Here we consider neural networks $h_{\boldsymbol{\theta}}$ having a fixed architecture, parametrized by $\boldsymbol{\theta}$
- Learning methods are based on minimizing the empirical risk:

$$\mathcal{L}(\boldsymbol{\theta}) = \frac{1}{m} \sum_{i=1}^{m} \ell(y_i, h_{\boldsymbol{\theta}}(x_i))$$

Neurons

Inspiration in Biology



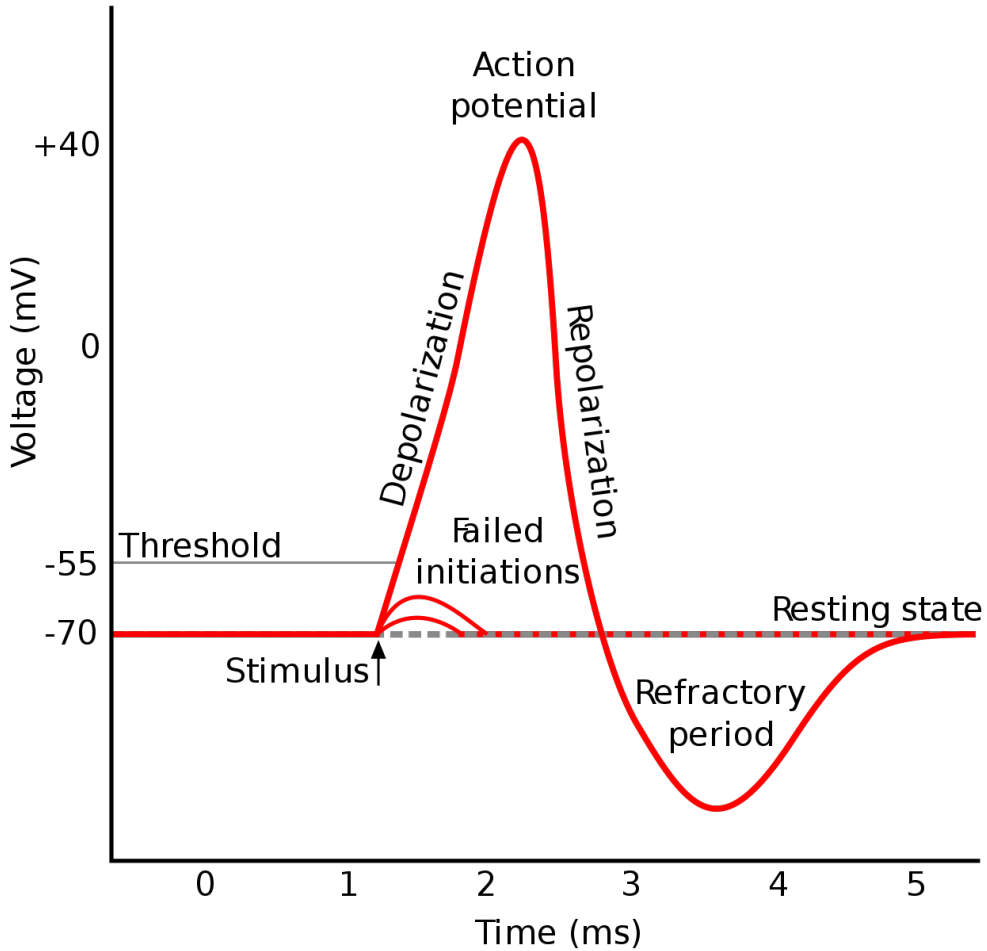
https://en.wikipedia.org/wiki/Synapse

Inspiration in Biology (contd.)

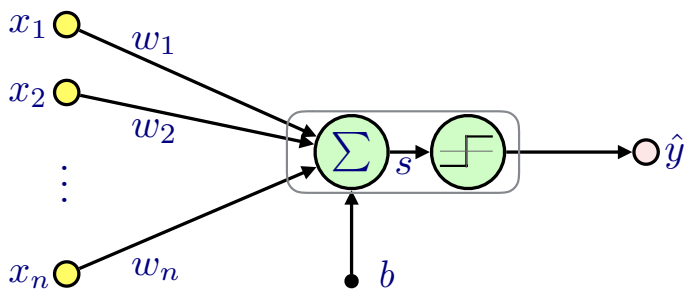
- Neural system of a 1 year old child contains approx. 10^{11} to 10^{12} neurons (loosing 200 000 a day)
- The diameter of soma nucleus ranges from 3 µm to 18 µm
- Dendrite length is 2 mm to 3 mm, there are 10 to 100 000 of dendrites per neuron
- Axon length can be longer than 1 m

Reaction to Stimuli

- After neuron fires through axon, it is unable to fire again for about $10\,\mathrm{ms}$
- The speed of signal propagation ranges from $5\,\mathrm{m\,s^{-1}}$ to $125\,\mathrm{m\,s^{-1}}$



McCulloch-Pitts Perceptron (1943)



$\boldsymbol{x} = \left(x_1, x_2, \ldots, x_n\right)^T \in \mathbb{R}^n$ input (feature vector)

$\boldsymbol{w} = \left(w_1, w_2, \ldots, w_n\right)^T \in \mathbb{R}^n$ weights

$b \in \mathbb{R}$ bias (threshold)

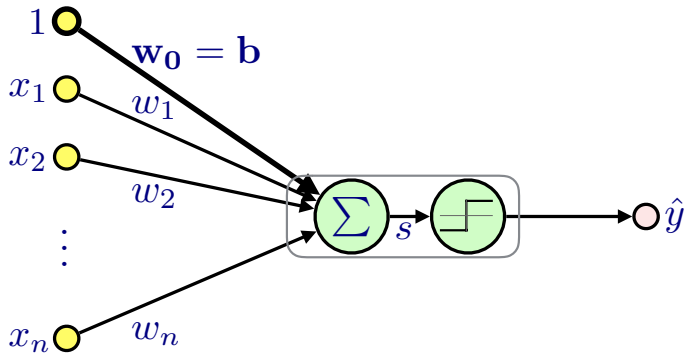
$s = \langle \boldsymbol{w}, \boldsymbol{x} \rangle + b \in \mathbb{R}$ inner potential

$$f(s) = \begin{cases} -1 & \text{if } s < 0 \\ 1 & \text{else} \end{cases}$$ activation function

$\hat{y} = h_{(\boldsymbol{w},\boldsymbol{b})}(\boldsymbol{x}) \in \{-1, 1\}$ output (activity)

$$\hat{y} = f(s) = f\left(\sum_{i=1}^{n} w_i x_i + b\right) = f\left(\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b\right)$$

McCulloch-Pitts Perceptron: Treating Bias

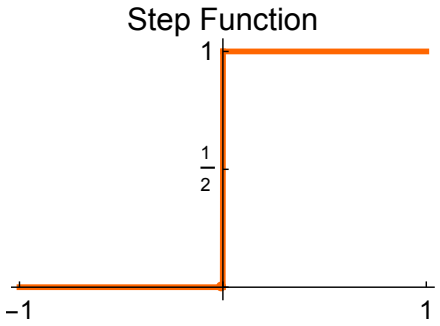


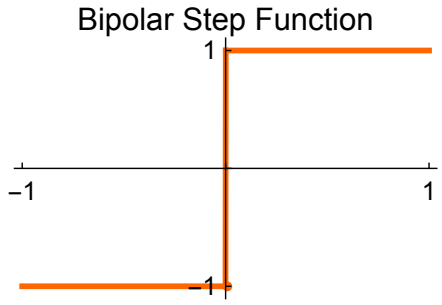
- Treat bias as an extra fixed input $x_0 = 1$ weighted $w_0 = b$:

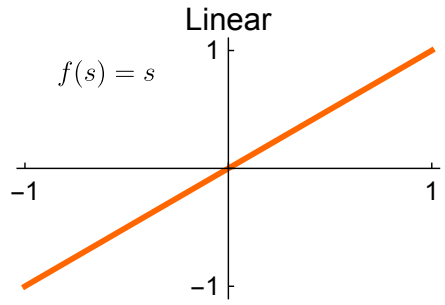
$$\hat{y} = f\left(\langle \boldsymbol{w}, \boldsymbol{x} \rangle + b\right) = f\left(\langle \boldsymbol{w}, \boldsymbol{x} \rangle + w_0 \cdot 1\right) = f\left(\langle \boldsymbol{w}', \boldsymbol{x}' \rangle\right)$$

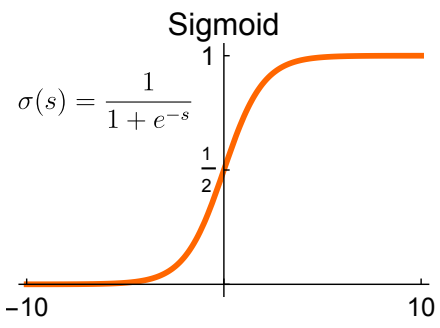
- $\boldsymbol{x}' = \left(1, x_1, \ldots, x_n\right)^T \in \mathbb{R}^{n+1}$
- $\boldsymbol{w}' = \left(w_0, w_1, \ldots, w_n\right)^T \in \mathbb{R}^{n+1}$
- Unless otherwise noted we will use $\boldsymbol{x}$, $\boldsymbol{w}$ instead of $\boldsymbol{x}'$, $\boldsymbol{w}'$

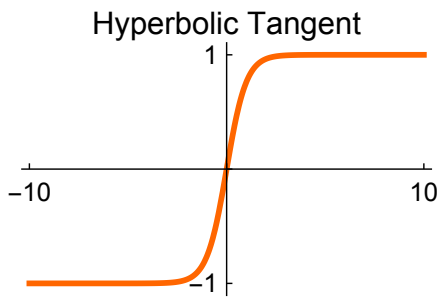
Activation Functions

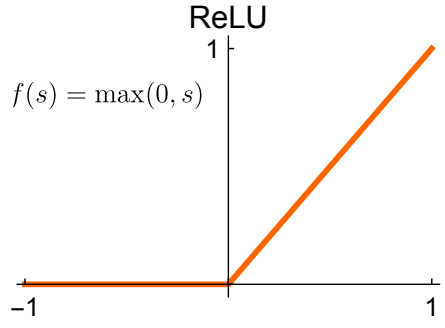












- Logistic sigmoid: $\sigma(s) \triangleq \dfrac{1}{1+e^{-s}} = \dfrac{e^{s}}{e^{s}+1}$
- Note: $\tanh(s) = \dfrac{e^{s}-e^{-s}}{e^{s}+e^{-s}} = 2\,\sigma(s) - 1$

Linear Neuron

- Training examples: $\mathcal{T}^m = \{(\boldsymbol{x}_i, y_i) \in (\mathbb{R}^{n+1} \times \mathbb{R}) \mid i = 1, \ldots, m\}$
- Single neuron with linear activation function $\equiv$ linear regression:

$$\hat{y} = s = \langle \boldsymbol{x}, \boldsymbol{w} \rangle, \quad \hat{y} \in \mathbb{R}$$

- Inputs: $\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \ldots & x_{1n} \\ 1 & \vdots & \ddots & \vdots \\ 1 & x_{m1} & \ldots & x_{mn} \end{pmatrix} = \begin{pmatrix} \boldsymbol{x}_1^T \\ \vdots \\ \boldsymbol{x}_m^T \end{pmatrix}$
- Targets: $\boldsymbol{y} = \begin{pmatrix} y_1, \ldots, y_m \end{pmatrix}^T, \quad y_i \in \mathbb{R}$
- Outputs: $\hat{\boldsymbol{y}} = \begin{pmatrix} \hat{y}_1, \ldots, \hat{y}_m \end{pmatrix}^T, \quad \hat{y}_i \in \mathbb{R}$
- For the whole dataset we get:

$$\hat{\boldsymbol{y}} = \mathbf{X}\boldsymbol{w}, \quad \hat{\boldsymbol{y}} \in \mathbb{R}^m$$

Linear Neuron: Maximum Likelihood Estimation

- Assumption: data are Gaussian distributed with mean $\langle \boldsymbol{x}_i, \boldsymbol{w} \rangle$ and variance σ^2:

$$y_i \sim \mathcal{N}\left(\langle \boldsymbol{x}_i, \boldsymbol{w} \rangle, \sigma^2\right) = \langle \boldsymbol{x}_i, \boldsymbol{w} \rangle + \mathcal{N}\left(0, \sigma^2\right)$$

- Likelihood for i.i.d. data:

$$\begin{aligned} p\left(\boldsymbol{y} | \boldsymbol{w}, \mathbf{X}, \sigma\right) &= \prod_{i=1}^{m} p\left(y_i | \boldsymbol{w}, \boldsymbol{x_i}, \sigma\right) = \prod_{i=1}^{m} \left(2\pi\sigma^2\right)^{-\frac{1}{2}} e^{-\frac{1}{2\sigma^2}\left(y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle\right)^2} = \\ &= \left(2\pi\sigma^2\right)^{-\frac{m}{2}} e^{-\frac{1}{2\sigma^2}\sum_{i=1}^{m}\left(y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle\right)^2} = \\ &= \left(2\pi\sigma^2\right)^{-\frac{m}{2}} e^{-\frac{1}{2\sigma^2}\left(\boldsymbol{y} - \mathbf{X}\boldsymbol{w}\right)^T\left(\boldsymbol{y} - \mathbf{X}\boldsymbol{w}\right)} \end{aligned}$$

- Negative Log Likelihood (switching to minimization):

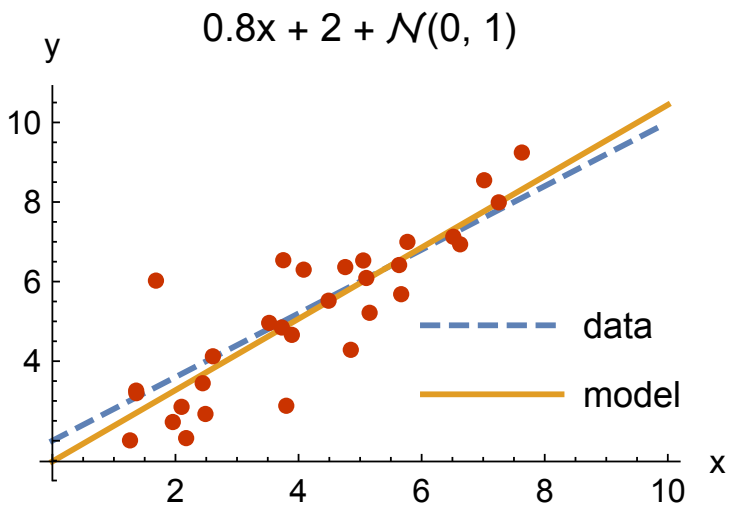
$$\mathcal{L}\left(\boldsymbol{w}\right) = \frac{m}{2}\log\left(2\pi\sigma^2\right) + \frac{1}{2\sigma^2}\left(\boldsymbol{y} - \mathbf{X}\boldsymbol{w}\right)^T\left(\boldsymbol{y} - \mathbf{X}\boldsymbol{w}\right)$$

Linear Neuron: Maximum Likelihood Estimation (contd.)

- Note that

$$\sum_{i=1}^{m} \underbrace{\left(y_i - \langle \boldsymbol{w}, \boldsymbol{x}_i \rangle\right)^2}_{\ell(y_i, \hat{y}_i)} = (\boldsymbol{y} - \mathbf{X}\boldsymbol{w})^T (\boldsymbol{y} - \mathbf{X}\boldsymbol{w})$$

  is the sum-of-squares or squared error (SE)
- Minimization of $\mathcal{L}(\boldsymbol{w}) \equiv$ least squares estimaton
- Solving $\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = 0$ we get $\boldsymbol{w}^* = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\boldsymbol{y}$



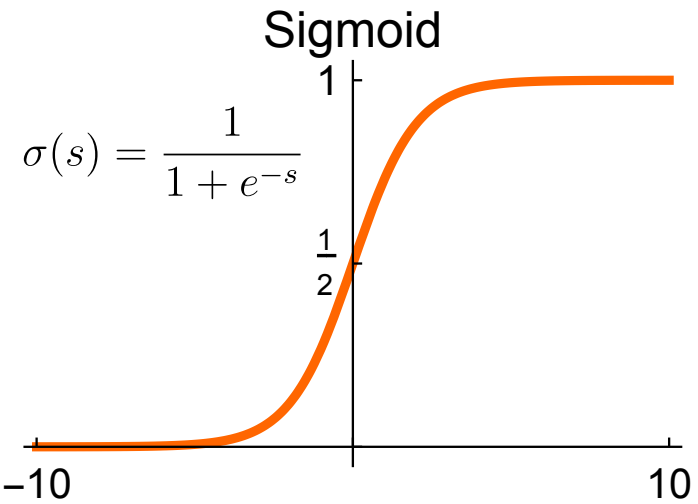
Logistic Sigmoid and Probability

- Denote: $\hat{y} = \sigma(s),\ \hat{y} \in (0, 1)$
- Sigmoid output can represent a parameter of the Bernoulli distribution:

$$p(y|\hat{y}) = \text{Ber}(y|\hat{y}) = \hat{y}^y (1 - \hat{y})^{1-y} = \begin{cases} \hat{y} & \text{for } y = 1 \\ 1 - \hat{y} & \text{for } y = 0 \end{cases}$$

- Models confidence of the positive class $y = 1$
- Binary classifier:

$$h(\hat{y}) = \begin{cases} 1 & \text{if } \hat{y} > \frac{1}{2} \\ 0 & \text{else} \end{cases}$$



Logistic Regression

- MCP neuron using sigmoid activation function $\equiv$ logistic regression:

$$\hat{y} = \sigma(\langle \boldsymbol{w}, \boldsymbol{x} \rangle), \ \hat{y} \in (0, 1)$$

- Inputs: $\mathbf{X} = \begin{pmatrix} 1 & x_{11} & \dots & x_{1n} \\ 1 & \vdots & \ddots & \vdots \\ 1 & x_{m1} & \dots & x_{mn} \end{pmatrix} = \begin{pmatrix} \boldsymbol{x}_1^T \\ \vdots \\ \boldsymbol{x}_m^T \end{pmatrix}$
- Target class: $\boldsymbol{y} = \begin{pmatrix} y_1, \dots, y_m \end{pmatrix}^T, \ y_i \in \{0, 1\}$
- Output class: $\hat{\boldsymbol{y}} = \begin{pmatrix} \hat{y}_1, \dots, \hat{y}_m \end{pmatrix}^T, \ \hat{y}_i \in (0, 1)$
- Note that the logistic regression (including the decision rule) solves actually a classification task

Logistic Regression MLE Leads to the Cross-Entropy

- Likelihood, for the logistic regression:

$$p(\boldsymbol{y}|\boldsymbol{w}, \mathbf{X}) = \prod_{i=1}^{m} \text{Ber}(y_i|\hat{y}_i) = \prod_{i=1}^{m} \hat{y}_i^{y_i} \left(1 - \hat{y}_i\right)^{1-y_i}$$

- Negative Log Likelihood:

$$\mathcal{L}(\boldsymbol{w}) = \sum_{i=1}^{m} \underbrace{-\left[y_i \log \hat{y}_i + (1 - y_i) \log \left(1 - \hat{y}_i\right)\right]}_{\ell(y_i, \hat{y}_i)}$$

- This *loss function* is called the cross-entropy
- The $\ell(y_i, \hat{y}_i)$ is the negative log probability of the correct answer $y_i \in \{0, 1\}$ given by the model output $\hat{y}_i \in (0, 1)$

Maximum Likelihood Estimation

- Maximum Likelihood Estimation: $\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}} \mathcal{L}(\boldsymbol{w})$
- Derivative of the loss w.r.t. to the sigmoid argument:

$$\frac{\partial \mathcal{L}}{\partial s_i} = \hat{y}_i - y_i$$

- Gradient w.r.t. logistic regression parameters:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = \sum_{i=1}^{m} \frac{\partial \mathcal{L}}{\partial s_i} \cdot \frac{\partial s_i}{\partial \boldsymbol{w}} = \sum_{i=1}^{m} \boldsymbol{x}_i (\hat{y}_i - y_i) = \mathbf{X}^T (\hat{\boldsymbol{y}} - \boldsymbol{y})$$

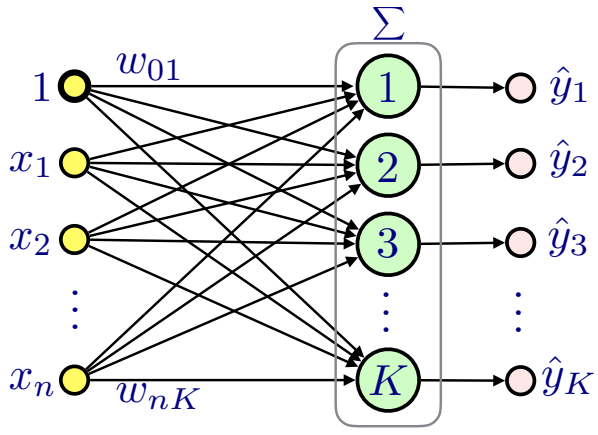
- $\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = \mathbf{0}$ has no analytical solution $\implies$ use numerical methods

Layers

Linear (Dense) Layer

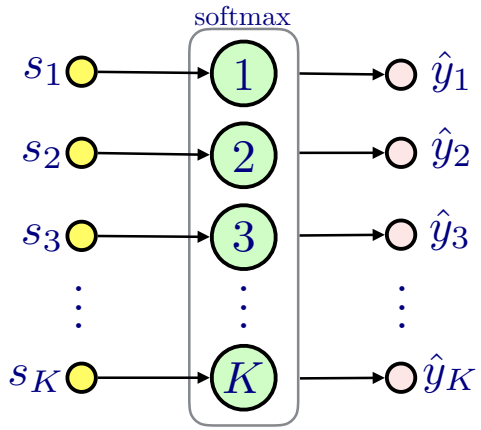
- Output k: $\hat{y}_k = \langle \boldsymbol{x}, \boldsymbol{w}_k \rangle$, $k = 1, 2, \ldots, K$
- All outputs using *weight matrix* $\mathbf{W}$: $\hat{\boldsymbol{y}} = \boldsymbol{x}^T \mathbf{W}$
- Multiple samples: $\hat{\mathbf{Y}} = \mathbf{X}\mathbf{W}$

$$\mathbf{W} = \begin{pmatrix} \boldsymbol{w}_1 \ldots \boldsymbol{w}_K \end{pmatrix} = \begin{pmatrix} w_{01} & \ldots & w_{0K} \\ \vdots & \ddots & \vdots \\ w_{n1} & \ldots & w_{nK} \end{pmatrix}$$



$$\mathbf{X} = \begin{pmatrix} \boldsymbol{x}_1^T \\ \vdots \\ \boldsymbol{x}_m^T \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & \ldots & x_{1n} \\ 1 & \vdots & \ddots & \vdots \\ 1 & x_{m1} & \ldots & x_{mn} \end{pmatrix} \qquad \hat{\mathbf{Y}} = \begin{pmatrix} \hat{\boldsymbol{y}}_1^T \\ \vdots \\ \boldsymbol{y}_m^T \end{pmatrix} = \begin{pmatrix} \hat{y}_{11} & \ldots & \hat{y}_{1K} \\ \vdots & \ddots & \vdots \\ \hat{y}_{m1} & \ldots & \hat{y}_{mK} \end{pmatrix}$$

Softmax Layer



- Multinominal classification, K mutually exclusive classes
- Definition: $\sigma_k(\boldsymbol{s}) \triangleq \frac{e^{s_k}}{\sum_{c=1}^{K} e^{s_c}}$, where K is the number of classes
- Softmax represents a categorical probability distribution: $\sigma_k \in (0, 1)$ for $k \in \{1 \dots K\}$ and $\sum_{k=1}^{K} \sigma_k = 1$
- Describes class membership probabilities: $p(y = k|\boldsymbol{s}) = \sigma_k(\boldsymbol{s})$

Softmax Layer MLE

- Target: $\boldsymbol{y} = \begin{pmatrix} y_1 & \dots & y_m \end{pmatrix}^T$, $y_i \in \{1, 2, \dots, K\}$
- One-hot encoding for sample i and class k: let $y_{ik} = \mathbb{I}\{y_i = k\}$
- Likelihood:

$$p(\boldsymbol{y}|\boldsymbol{w}, \mathbf{X}) = \prod_{i=1}^{m} \prod_{c=1}^{K} \hat{y}_{ic}^{y_{ic}}$$

- Negative Log Likelihood:

$$\mathcal{L}(\boldsymbol{w}) = -\sum_{i=1}^{m} \sum_{c=1}^{K} y_{ic} \log(\hat{y}_{ic})$$

  Again the **cross-entropy**

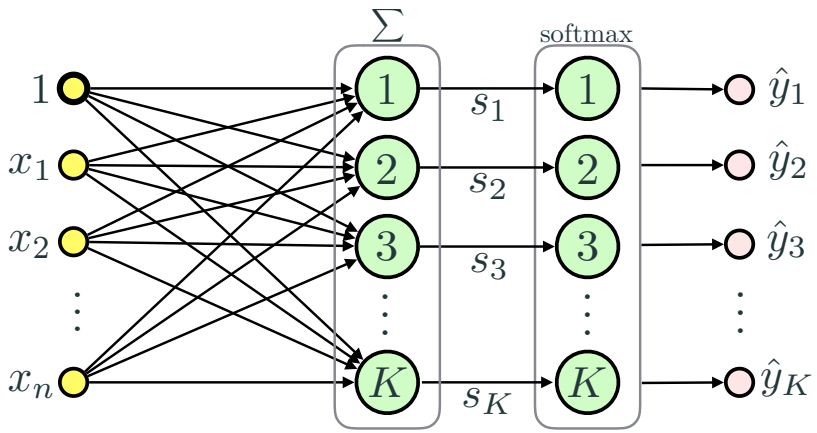
- Gradient:

$$\frac{\partial \mathcal{L}}{\partial s_{ik}} = \sum_{i=1}^{m} (\hat{y}_{ik} - y_{ik})$$

Multinominal Logistic Regression

- linear layer + softmax layer = multinominal logistic regression:

$$\hat{y}_k = \sigma_k(\boldsymbol{x}^T \mathbf{W})$$



- Classifier: $h(\boldsymbol{x}, \mathbf{W}) = \underset{k}{\operatorname{argmax}}\, \hat{y}_k$

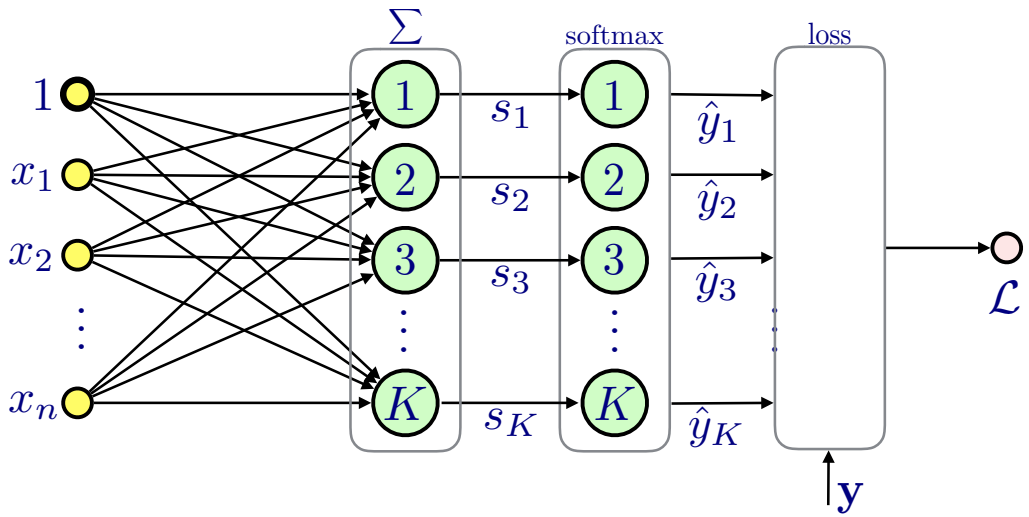
Loss Functions: Summary

problem	**output**	**suggested loss function**
binary classification	sigmoid neuron	cross-entropy $-\frac{1}{m}\sum_{i=1}^{m}\left[y_i \log \hat{y}_i + (1-y_i)\log\left(1-\hat{y}_i\right)\right]$
multinominal classification	softmax	multinominal cross-entropy $-\frac{1}{m}\sum_{i=1}^{m}\sum_{c=1}^{K} y_{ic}\log(\hat{y}_{ic})$
regression	linear neuron	mean squared error $\frac{1}{m}\sum_{i=1}^{m}\left(y_i-\hat{y}_i\right)^2$
multi-output regression	linear layer	mean squared error $\frac{1}{m}\sum_{i=1}^{m}\sum_{c=1}^{K}\left(y_{ic}-\hat{y}_{ic}\right)^2$

Backpropagation

Backpropagation Overview

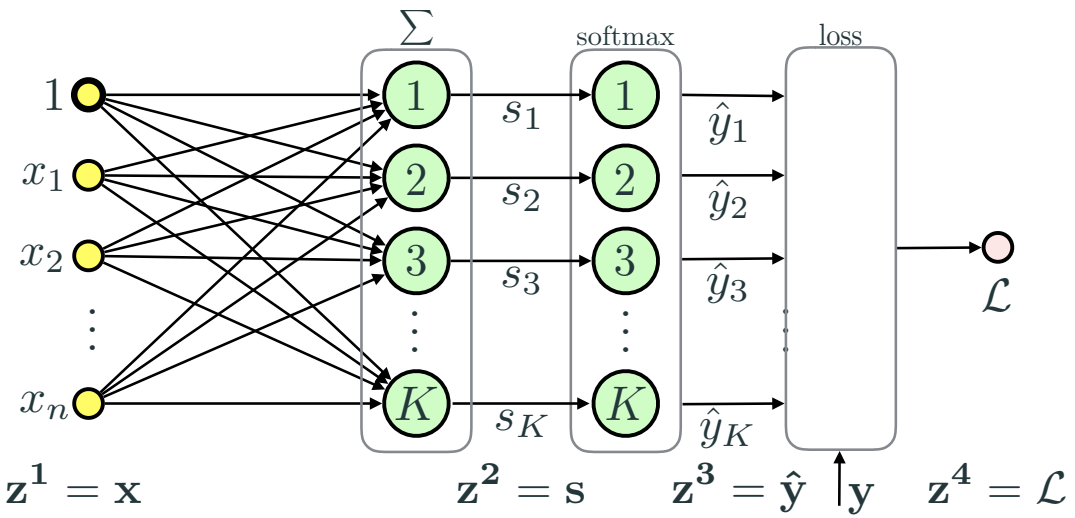
- A method to compute a gradient of the *loss function* with respect to its parameters: $\nabla \mathcal{L}(\boldsymbol{w})$
- $\nabla \mathcal{L}(\boldsymbol{w})$ is in turn used by optimization methods like gradient descent
- Here, we present the "modular" backpropagation (see Nando de Freitas' Machine Learning course: `https://www.cs.ox.ac.uk/people/nando.defreitas/machinelearning/`)
- Let us use multinominal logistic regression as an example



Backpropagation: the Loss Function

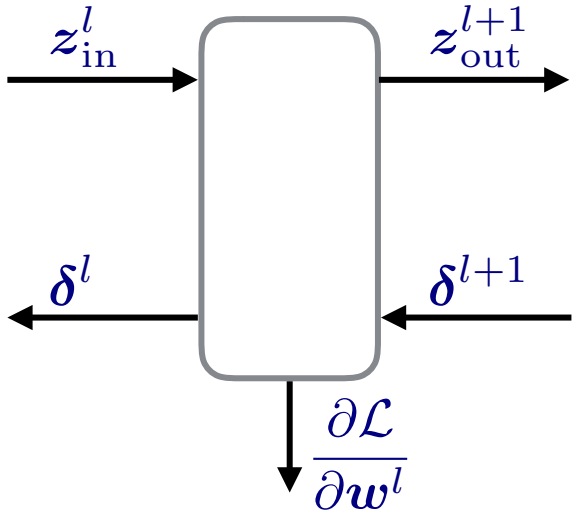
- The loss function is the multinominal cross-entropy in this case:

$$\mathcal{L}(\boldsymbol{w}) = -\frac{1}{m}\sum_{i=1}^{m}\sum_{c=1}^{K}\mathbb{I}\{y_i = c\}\log\left(\frac{\exp\left(\langle \boldsymbol{x}_i, \boldsymbol{w}_c\rangle\right)}{\sum_{k=1}^{K}\exp\left(\langle \boldsymbol{x}_i, \boldsymbol{w}_k\rangle\right)}\right)$$



Backpropagation Based on Modules

- Computation of $\nabla \mathcal{L}(\boldsymbol{w})$ involves repetitive use of the *chain rule*
- We can make things simpler by divide and conquer approach
- Divide to simplest possible modules (these can be later combined into complex networks)
- Represent even the loss function as a module
- Passing messages

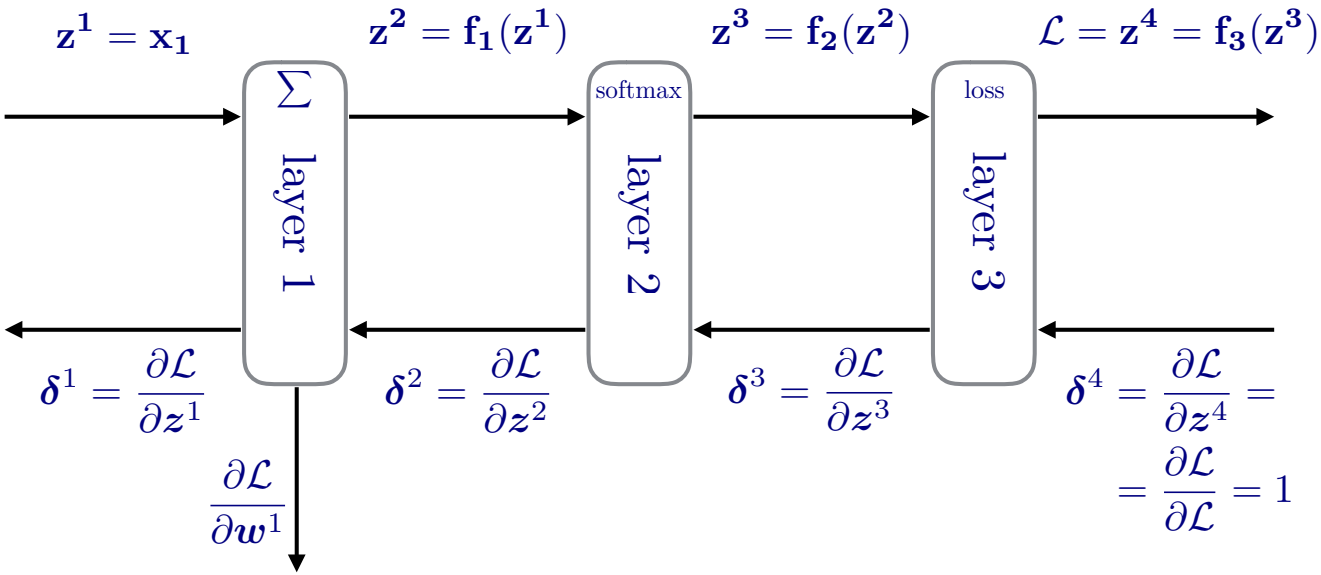


Backpropagation: Backward Pass Message

- Let $\boldsymbol{\delta}^l = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^l}$ be the sensitivity of the loss to the module input for layer l, then:

$$\delta_i^l = \frac{\partial \mathcal{L}}{\partial z_i^l} = \sum_j \frac{\partial \mathcal{L}}{\partial z_j^{l+1}} \cdot \frac{\partial z_j^{l+1}}{\partial z_i^l} = \sum_j \delta_j^{l+1} \frac{\partial z_j^{l+1}}{\partial z_i^l}$$

- We need to know how to compute derivatives of outputs w.r.t. inputs only!

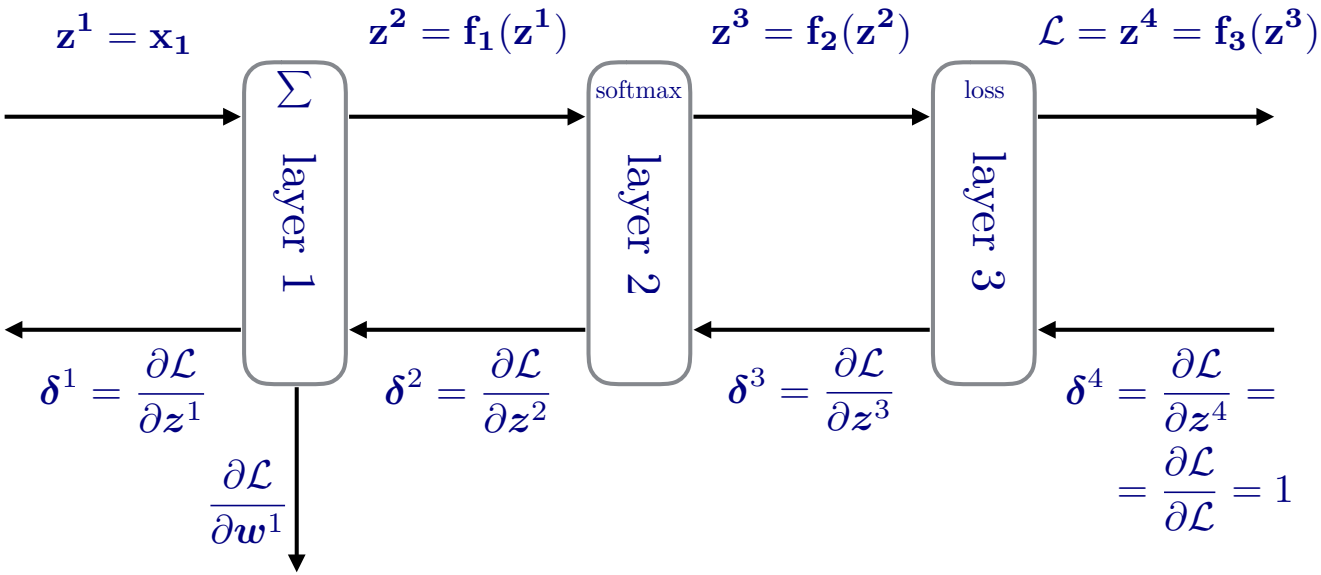


Backpropagation: Parameters

- Similarly if the module has parameters we want to know how the loss changes w.r.t. them:

$$\frac{\partial \mathcal{L}}{\partial w_i^l} = \sum_j \frac{\partial \mathcal{L}}{\partial z_j^{l+1}} \cdot \frac{\partial z_j^{l+1}}{\partial w_i^l} = \sum_j \delta_j^{l+1} \frac{\partial z_j^{l+1}}{\partial w_i^l}$$

- Derivatives of module outputs w.r.t. to the parameters are all we need



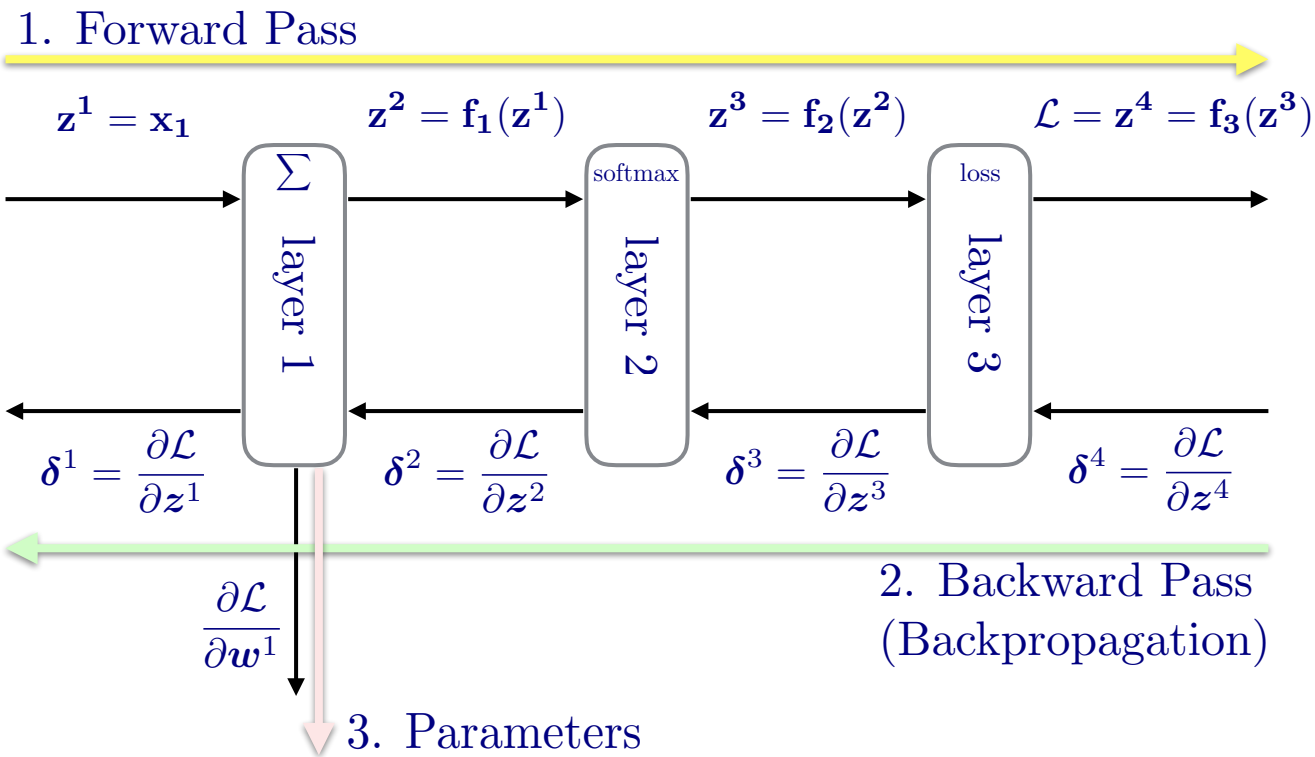
Backpropagation: Steps

- So for each module we need only to specify these three messages:

forward: $z^{l+1} = f(z^l)$

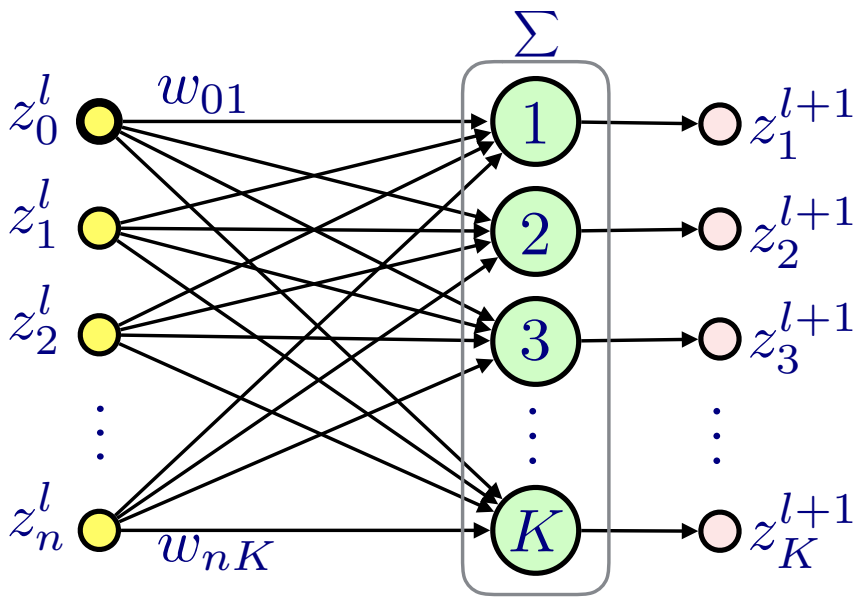
backward: $\dfrac{\partial z^{l+1}}{\partial z^l}$

parameter (optional): $\dfrac{\partial z^{l+1}}{\partial w^l}$



Example: Linear Layer

- **forward**: $z_j^{l+1} = \sum_{i=0}^{n} w_{ij} z_i^l, \quad j = 1, \ldots, K$
- **backward**: $\frac{\partial z_j^{l+1}}{\partial z_i^l} = w_{ij}, \quad i = 0, \ldots, n, \quad j = 1, \ldots, K$
- **parameter**: $\frac{\partial z_j^{l+1}}{\partial w_{ik}} = \mathbb{I}\{j = k\} z_i^l$



Example: Mean Squared Error

- **forward**: $z^{l+1} = \frac{1}{m} \sum_{i=1}^{m} \left(y_i - z_i^l\right)^2$
- **backward**: $\frac{\partial z^{l+1}}{\partial z_i^l} = -\frac{2}{m}(y_i - z_i^l), \quad i \in \{1, \ldots, n\}$

Optimization Methods

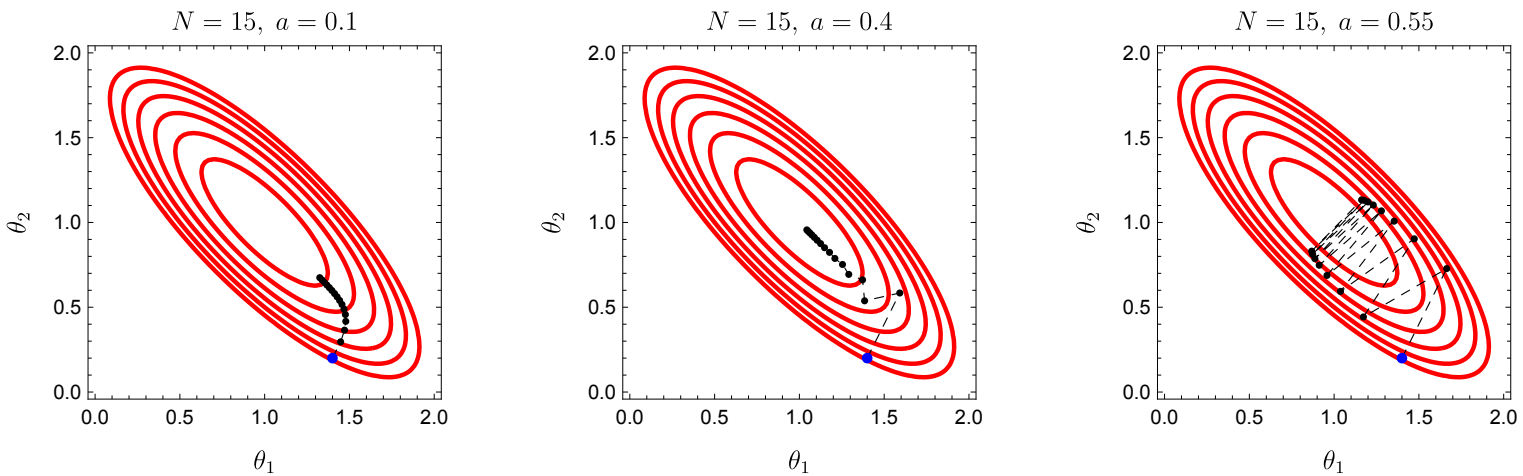
Gradient Descent (GD)

- **Task**: find parameters which minimize loss over the training dataset:

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, \mathcal{L}(\boldsymbol{\theta})$$

  where $\boldsymbol{\theta}$ is a set of all parameters defining the ANN, e.g., all weight matrices and biases

- Gradient descent: $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \alpha_k \nabla \mathcal{L}(\boldsymbol{\theta}_k)$
  where $\alpha_k > 0$ is the **learning rate** or **stepsize** at iteration k



Batch, Online and Mini-Batch Learning

When to update weights?

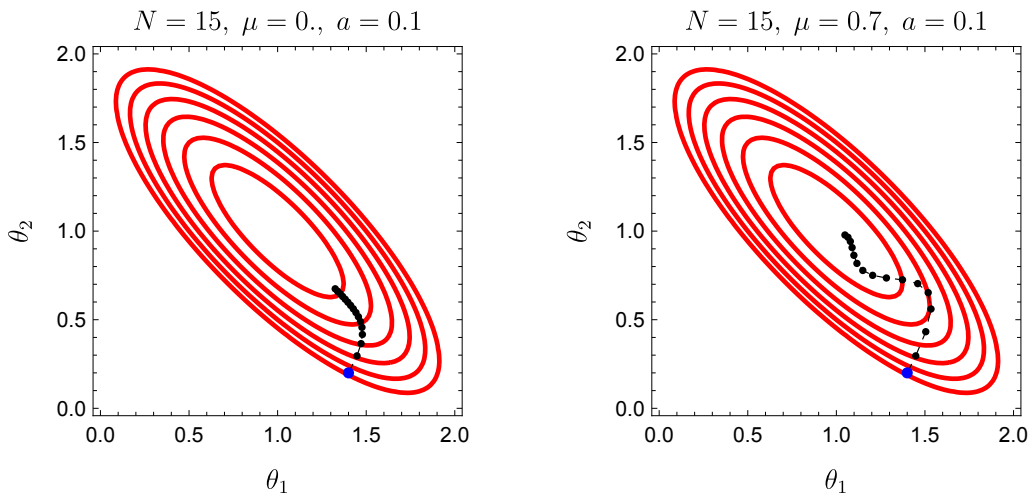
- **(Full) Batch learning**: after all patterns are used (epoch)
  - inefficient for redundant datasets
- **Online learning**: after each training pattern
  - noise can help overcome local minima but can also harm the convergence in the final stages while fine-tuning
  - **Stochastic Gradient Descent (SGD)** does this
  - convergence *almost surely* to local minimum when $\alpha^{(k)}$ decreases *appropriately* in time
- **Mini-batch learning**: after a small sample of training patterns

Momentum

- Simulate inertia to overcome plateaus in the error landscape:

$$\boldsymbol{v}_{k+1} \leftarrow \mu \boldsymbol{v}_k - \alpha_k \, g(\boldsymbol{\theta}_k, s_k)$$
$$\boldsymbol{\theta}_{k+1} \leftarrow \boldsymbol{\theta}_k + \boldsymbol{v}_{k+1}$$

  where $\mu \in [0, 1]$ is the *momentum parameter*
- Momentum damps oscillations in directions of high curvature
- It builds velocity in directions with consistent (possibly small) gradient



Adagrad

- Adaptive Gradient method (Duchi, Hazan and Singer, 2011)
- Motivation: a magnitude of gradient differs a lot for different parameters
- Idea: reduce learning rates for parameters having high values of gradient

$$G_{k+1,i} \leftarrow G_{k,i} + [g(\boldsymbol{\theta}_k, s_k)]_i^2$$
$$\theta_{k+1,i} \leftarrow \theta_{k,i} - \frac{\alpha}{\sqrt{G_{k+1,i}} + \epsilon} \cdot [g(\boldsymbol{\theta}_k, s_k)]_i$$

- $G_{k,i}$ accumulates squared partial derivative approximations w.r.t. to the parameter $\theta_{k,i}$
- ϵ is a small positive number to prevent division by zero
- Weakness: ever increasing G_i leads to slow convergence eventually

RMSProp

- Similar to Adagrad but employs a moving average:

$$G_{k+1,i} = \gamma G_{k,i} + (1 - \gamma) \left[g(\boldsymbol{\theta}_k, s_k) \right]_i^2$$

- γ is a *decay* parameter (typical value $\gamma = 0.9$)
- Unlike for Adagrad updates do not get infinitesimally small

Parameter Initialization

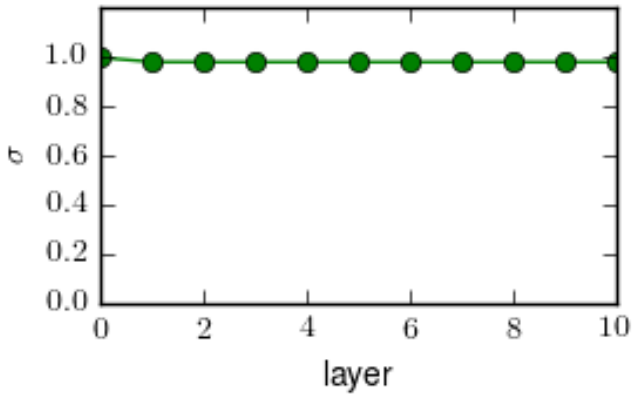
Parameter Initialization

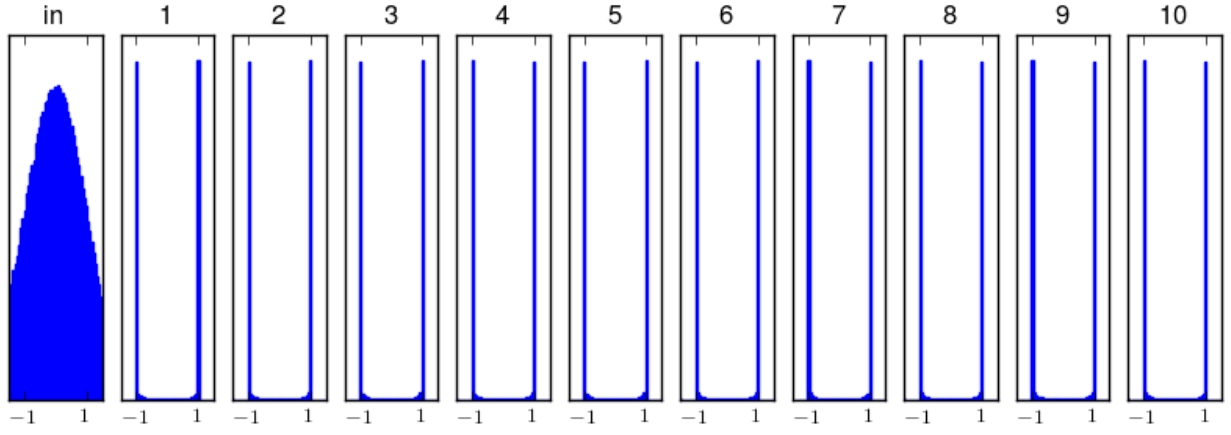
- Is it a good idea to set initially all weights to a constant?
- No. All neurons would behave the same: the same δs are backpropagated. We need to *break the symmetry*
- Use small random numbers, e.g., sample from a Gaussian distribution with zero mean:
  - works well for shallow networks,
  - for deep networks we might get into trouble

Gaussian Initialization Example

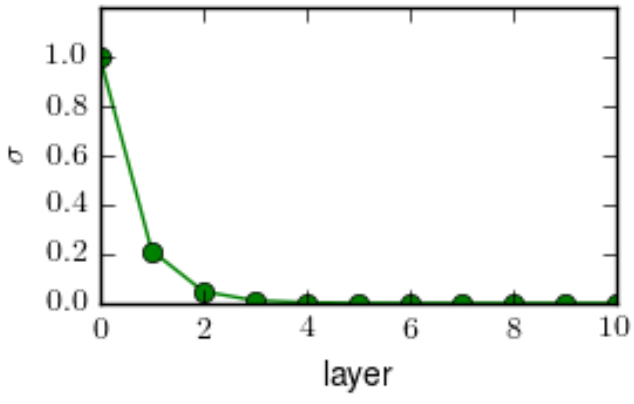
- MLP, ten tanh layers, 500 units each. Each input fed with $\mathcal{N}(0, 1)$
- Weights initialized to $\mathcal{N}(0, \sigma^2)$

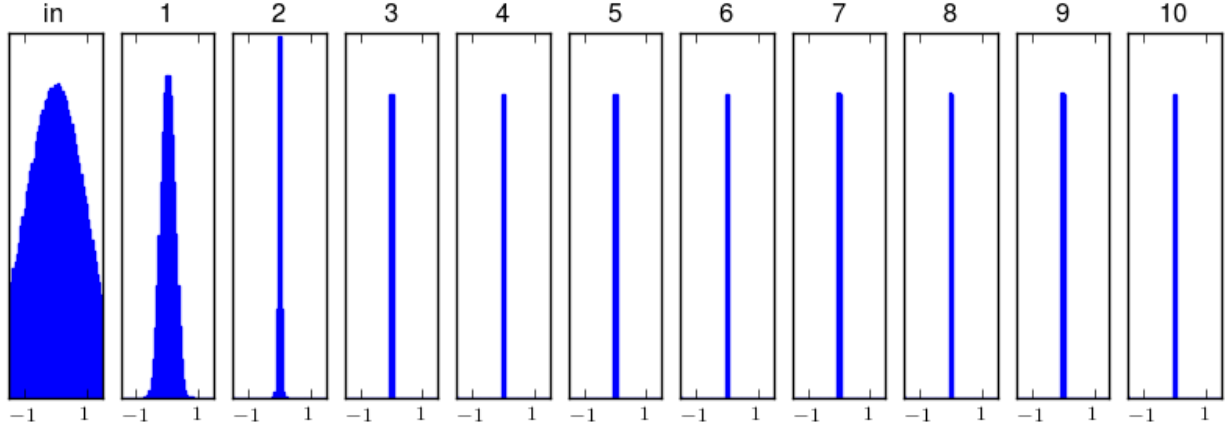
$\sigma = 1$





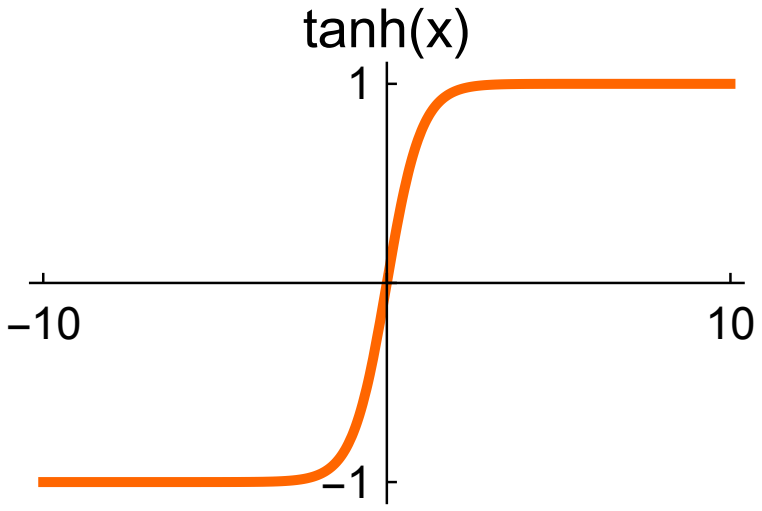
$\sigma = 0.01$

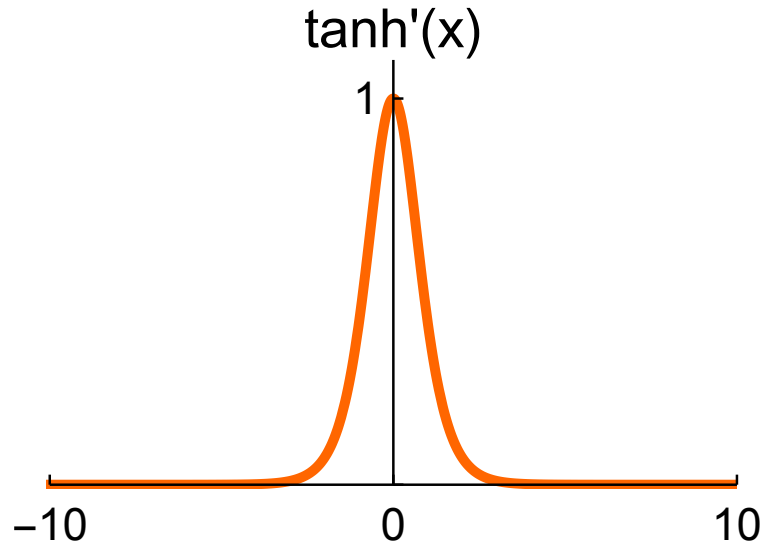




Vanishing Gradient

- For large σ (saturation) the tanh derivative is almost zero
- For small σ (output close to zero):
  - the derivative is at most 1,
  - the weights are very small and $\frac{\partial z_j^{l+1}}{\partial z_i^l} = w_{ij}$ holds for the preceding linear layer
- In both cases: $\delta \to 0$ as the number of layers increases





Xavier Initialization

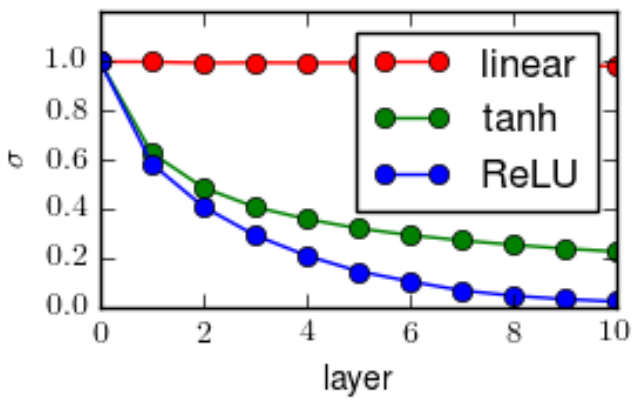
- Glorot and Bengio: *Understanding the difficulty of training deep feedforward neural networks*, 2010
- For the linear neuron $s = \sum_i w_i x_i$, let w_i and x_i be independent random variables, w_i and x_i are i.i.d., $\mathbb{E}(x_i) = \mathbb{E}(w_i) = 0$:

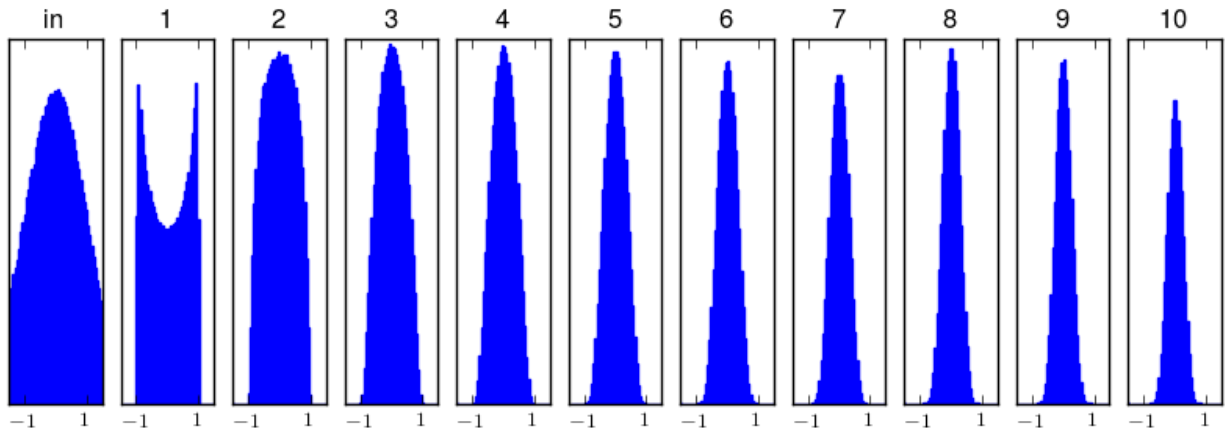
$$\begin{aligned}
\mathrm{Var}(s) &= \mathrm{Var}\left(\sum_i w_i x_i\right) = \sum_i \mathrm{Var}(w_i x_i) = \\
&= \sum_i \mathbb{E}\left([w_i x_i - \mathbb{E}(w_i x_i)]^2\right) = \sum_i \mathbb{E}\left([w_i x_i - \mathbb{E}(w_i)\mathbb{E}(x_i)]^2\right) = \\
&= \sum_i \mathbb{E}(w_i^2 x_i^2) = \sum_i \mathbb{E}(w_i^2)\mathbb{E}(x_i^2) = \\
&= \sum_i \mathbb{E}([w_i - \mathbb{E}(w_i)]^2)\mathbb{E}([x_i - \mathbb{E}(x_i)]^2) = \\
&= \sum_i \mathrm{Var}(x_i)\mathrm{Var}(w_i) = n_{\mathsf{in}}\mathrm{Var}(x)\mathrm{Var}(w)
\end{aligned}$$

Xavier Initialization (contd.)

- We have $\mathrm{Var}(s) = n_{\text{in}}\mathrm{Var}(x)\mathrm{Var}(w)$
- We want $\mathrm{Var}(s) = \mathrm{Var}(x)$
- Choose $\mathrm{Var}(w) = \frac{1}{n_{\text{in}}}$
- Works well for tanh as it is linear near zero
- Do not forget to standardize ANN input data

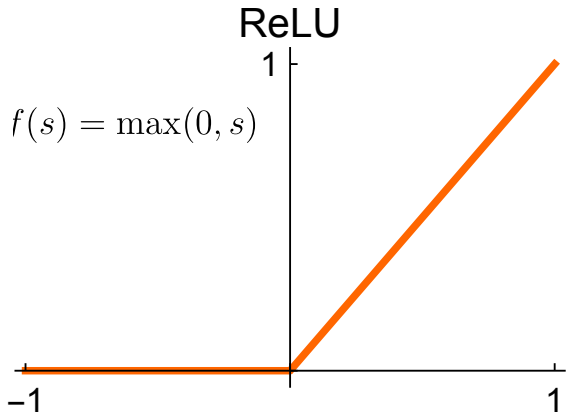
tanh





Rectified Linear Unit (ReLU)

- Definition $f(s) = \max(0, s)$
- Fast to compute
- Helps with *vanishing gradients* problem: the gradient is constant for $s > 0$, while for sigmoid-like activations it becomes increasingly small
- Leads to sparse representations: $s < 0$ turns the neuron completely off
- Might block gradient propagation $\rightarrow$ dead units $\rightarrow$ Leaky ReLU
- Unbounded: use regularization to prevent numerical problems

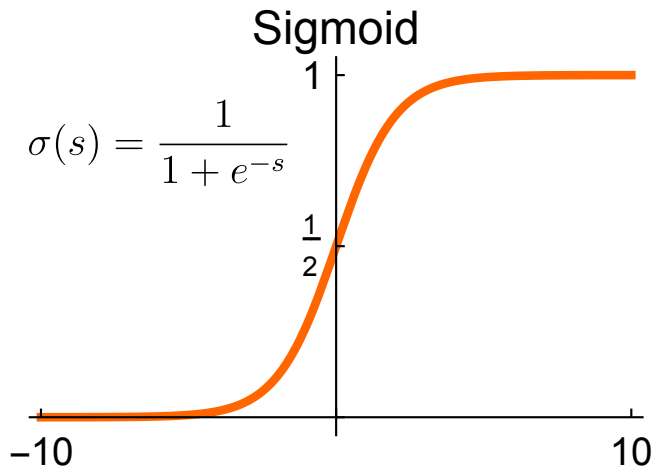


Regularization

- How to deal with overfitting?
  - get more data
  - find simpler model, search for optimal architecture, e.g., number, type and size of layers
  - constrain model by *regularization*
- Most types of regularization are based on constraining the parameter space
- Bayesian point of view: introduce prior distribution on model parameters

L2 Regularization (Weight Decay): Motivation

- Limit hypothesis space by limiting the size of the weight vector
- *Intuition:* sigmoid-like neurons kept near zero potential (via small weights) behave similarly to linear neurons
- L2 regularization (weight decay): zero mean Gaussian prior



Example: L2 Regularization for Linear Regression

- Recall the linear regression likelihood:

$$p\left(\boldsymbol{y}|\boldsymbol{w},\mathbf{X}\right)=\left(2\pi\sigma^{2}\right)^{-\frac{m}{2}}\,e^{-\frac{1}{2\sigma^{2}}(\boldsymbol{y}-\mathbf{X}\boldsymbol{w})^{T}(\boldsymbol{y}-\mathbf{X}\boldsymbol{w})}$$

- Define a Gaussian prior with zero mean and variance σ_0^2 for the parameters:

$$p\left(\boldsymbol{w}\right)=\left(2\pi\sigma_{0}^{2}\right)^{-\frac{1}{2}}\,e^{-\frac{1}{2\sigma_{0}^{2}}\boldsymbol{w}^{T}\boldsymbol{w}}$$

- Then the posterior is:

$$p(\boldsymbol{w}|\boldsymbol{y},\mathbf{X})=\frac{p(\boldsymbol{y}|\boldsymbol{w},\mathbf{X})\cdot p(\boldsymbol{w})}{p(\boldsymbol{y}|\mathbf{X})}$$

  The denominator does not depend on the parameters $\boldsymbol{w}$:

$$p(\boldsymbol{w}|\boldsymbol{y},\mathbf{X})\propto p(\boldsymbol{y}|\boldsymbol{w},\mathbf{X})\cdot p(\boldsymbol{w})$$

MAP Estimate

- Maximizing $p(\boldsymbol{w}|\boldsymbol{y}, \mathbf{X})$ gives us the Maximum a posteriori (MAP) estimate:

$$\boldsymbol{w}_{MAP} = \underset{\boldsymbol{w}}{\operatorname{argmax}}\, p(\boldsymbol{w}|\boldsymbol{y}, \mathbf{X}) = \underset{\boldsymbol{w}}{\operatorname{argmin}}\, (-\log p(\boldsymbol{w}|\boldsymbol{y}, \mathbf{X}))$$

  where

$$-\log p(\boldsymbol{w}|\boldsymbol{y}, \mathbf{X}) = \frac{1}{2\sigma^2} (\boldsymbol{y} - \mathbf{X}\boldsymbol{w})^T (\boldsymbol{y} - \mathbf{X}\boldsymbol{w}) + \frac{1}{2\sigma_0^2} \boldsymbol{w}^T \boldsymbol{w} + C$$

- We can omit C, define $\lambda = \dfrac{\sigma^2}{\sigma_0^2}$ and minimize the loss function:

$$\mathcal{L}(\boldsymbol{w}) = (\boldsymbol{y} - \mathbf{X}\boldsymbol{w})^T (\boldsymbol{y} - \mathbf{X}\boldsymbol{w}) + \lambda \boldsymbol{w}^T \boldsymbol{w}$$

- The term $\lambda \boldsymbol{w}^T \boldsymbol{w} = \lambda \|\boldsymbol{w}\|_2^2$ minimizes the size of the weight vector

L2 Regularization Improves Numerical Stability

- Recall the solution for the linear regression $\boldsymbol{w}^* = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\boldsymbol{y}$
- What if $\mathbf{X}^T\mathbf{X}$ has no inverse?
- We can modify the solution by adding a small element to the diagonal:

$$\boldsymbol{w}^* = \left(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I}\right)^{-1}\mathbf{X}^T\boldsymbol{y}, \quad \lambda > 0$$

- It turns out that the solution is the minimizer of our *regularized* loss function:

$$\mathcal{L}\left(\boldsymbol{w}\right) = \left(\boldsymbol{y} - \mathbf{X}\boldsymbol{w}\right)^T\left(\boldsymbol{y} - \mathbf{X}\boldsymbol{w}\right) + \lambda\boldsymbol{w}^T\boldsymbol{w},$$

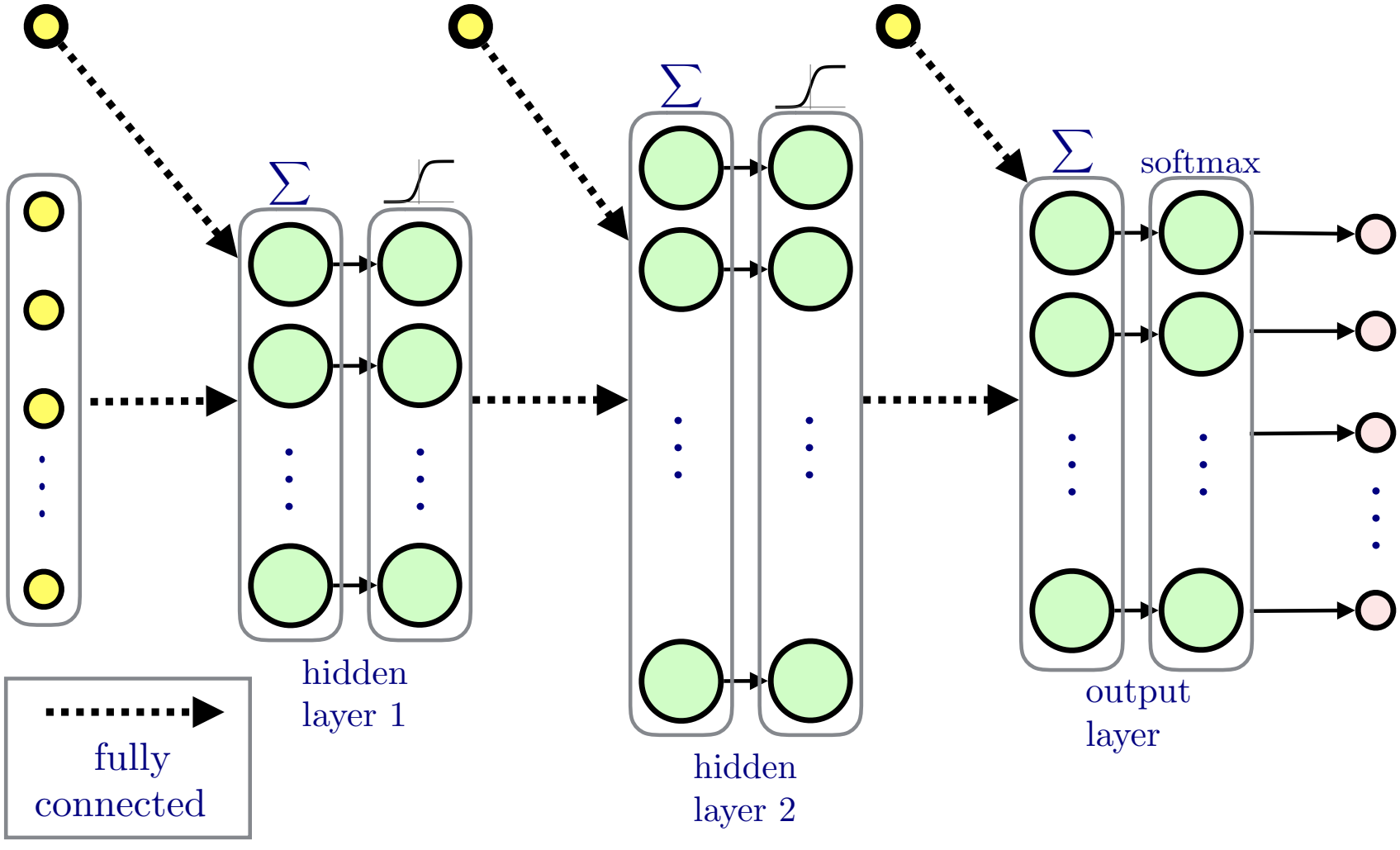
Other Regularization Related Approaches?

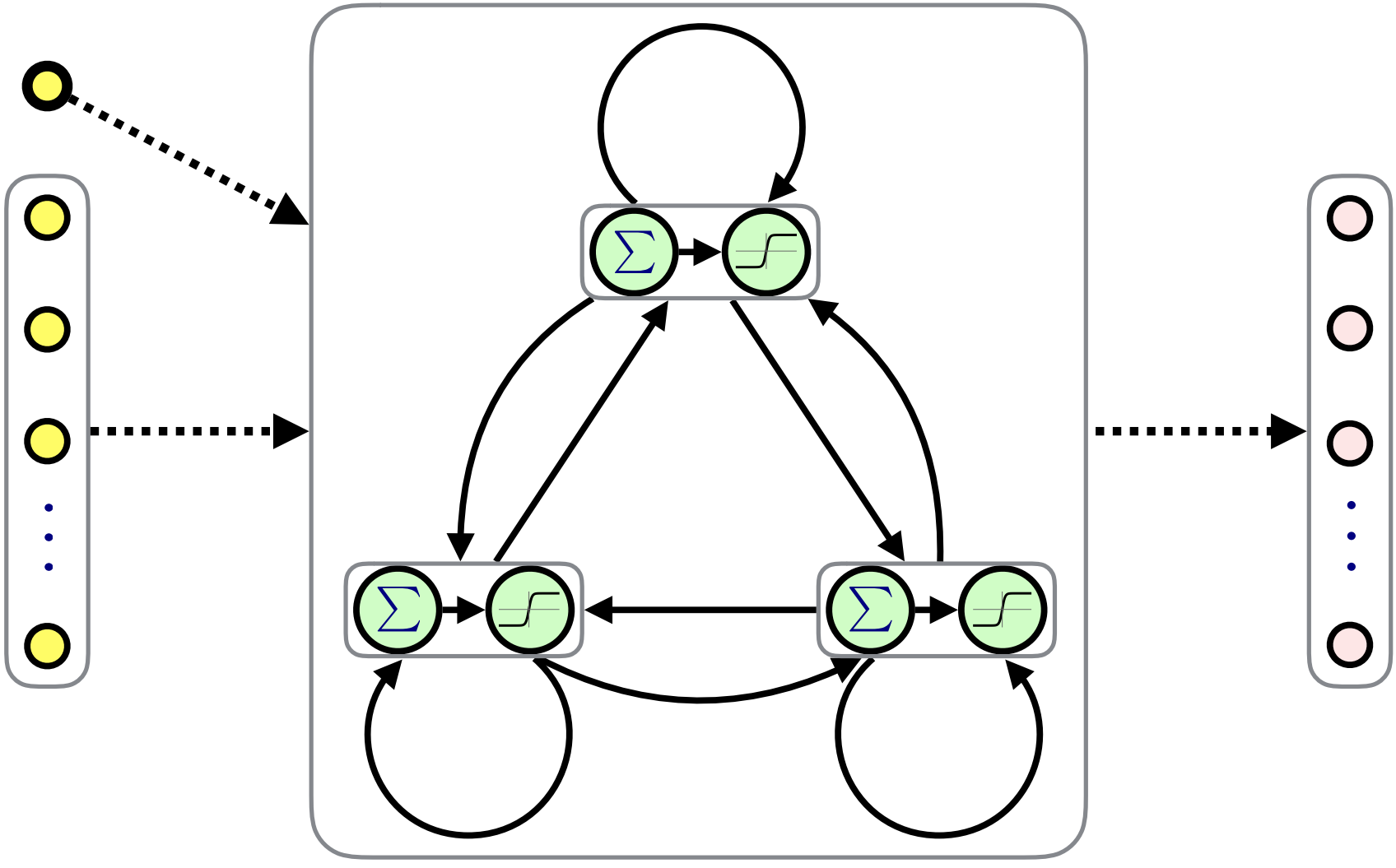
- L1 regularization: sum absolute values, i.e., use $\lambda \|\boldsymbol{w}\|_1$
- Randomize inputs: same as the weight decay for linear neurons
- Dataset augmentation
- Early stopping: start with small weights, stop when validation loss starts to grow, often used for limited time-budget
- Weight sharing and sparse connectivity: Convolutional Neural Networks (next lecture)
- Model averaging (see lectures on Ensembmling)
- Dropout and DropConnect

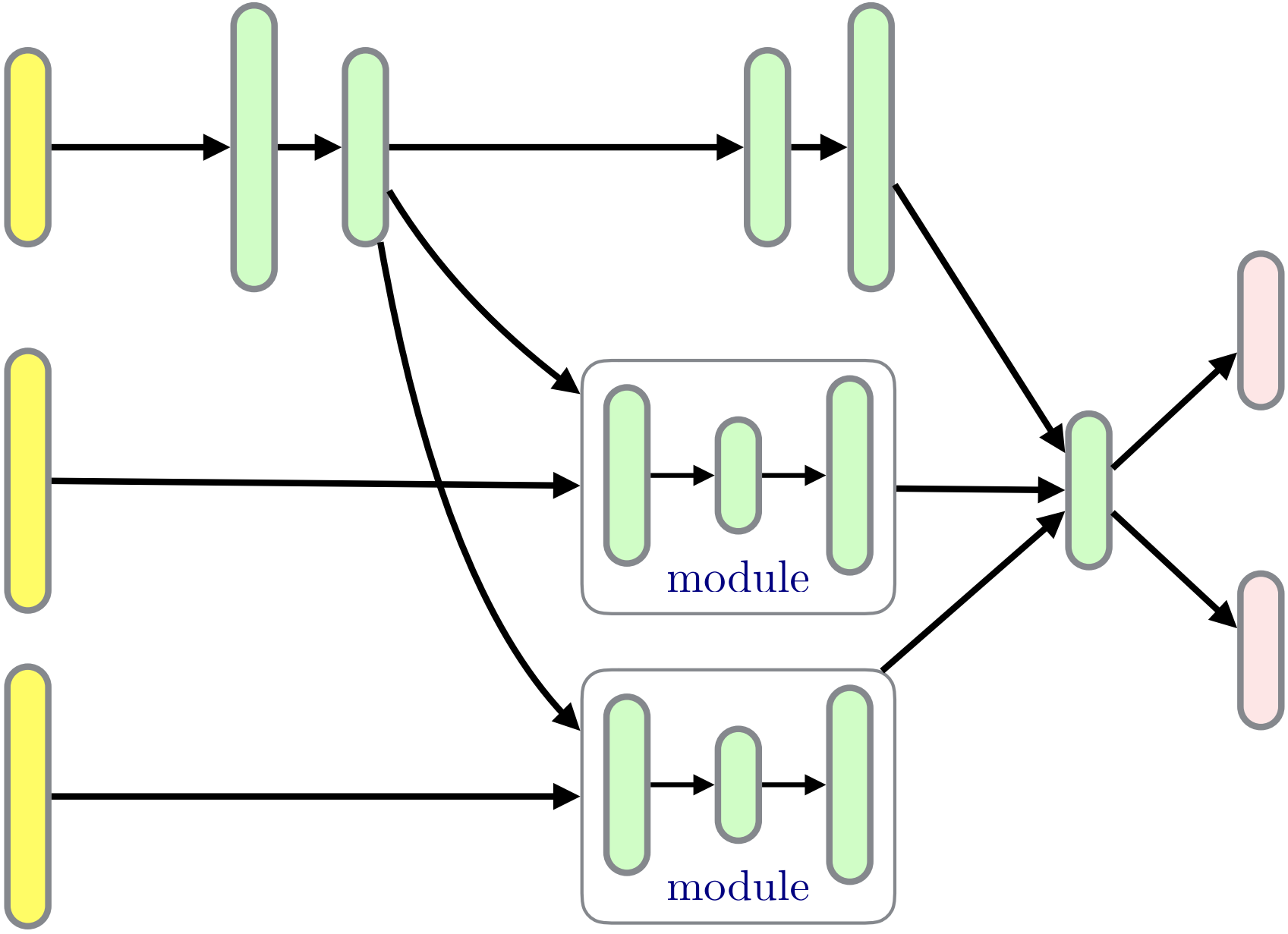
Next Lecture

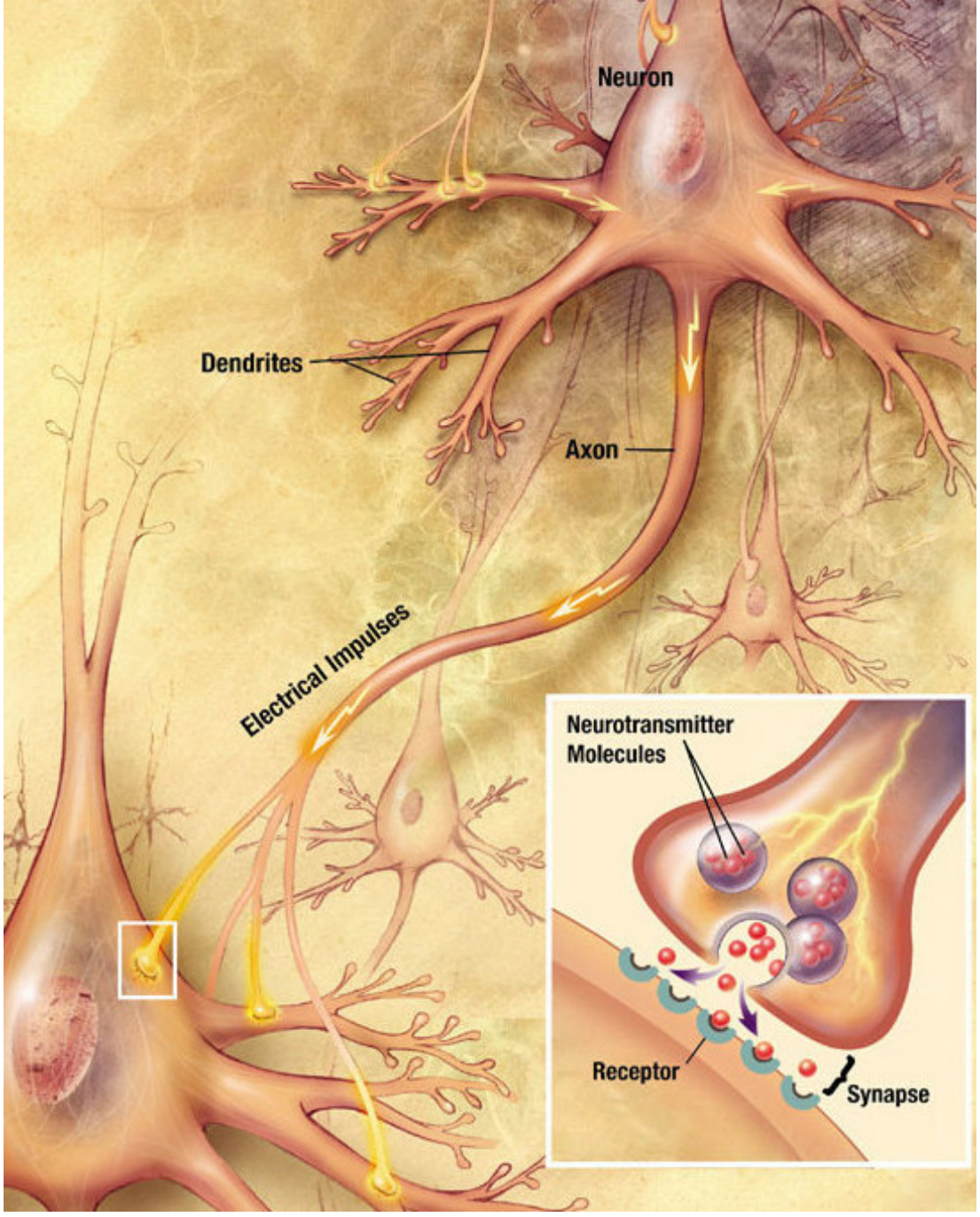
- Deep Neural Networks
- Convolutional Neural Networks
- Transfer learning

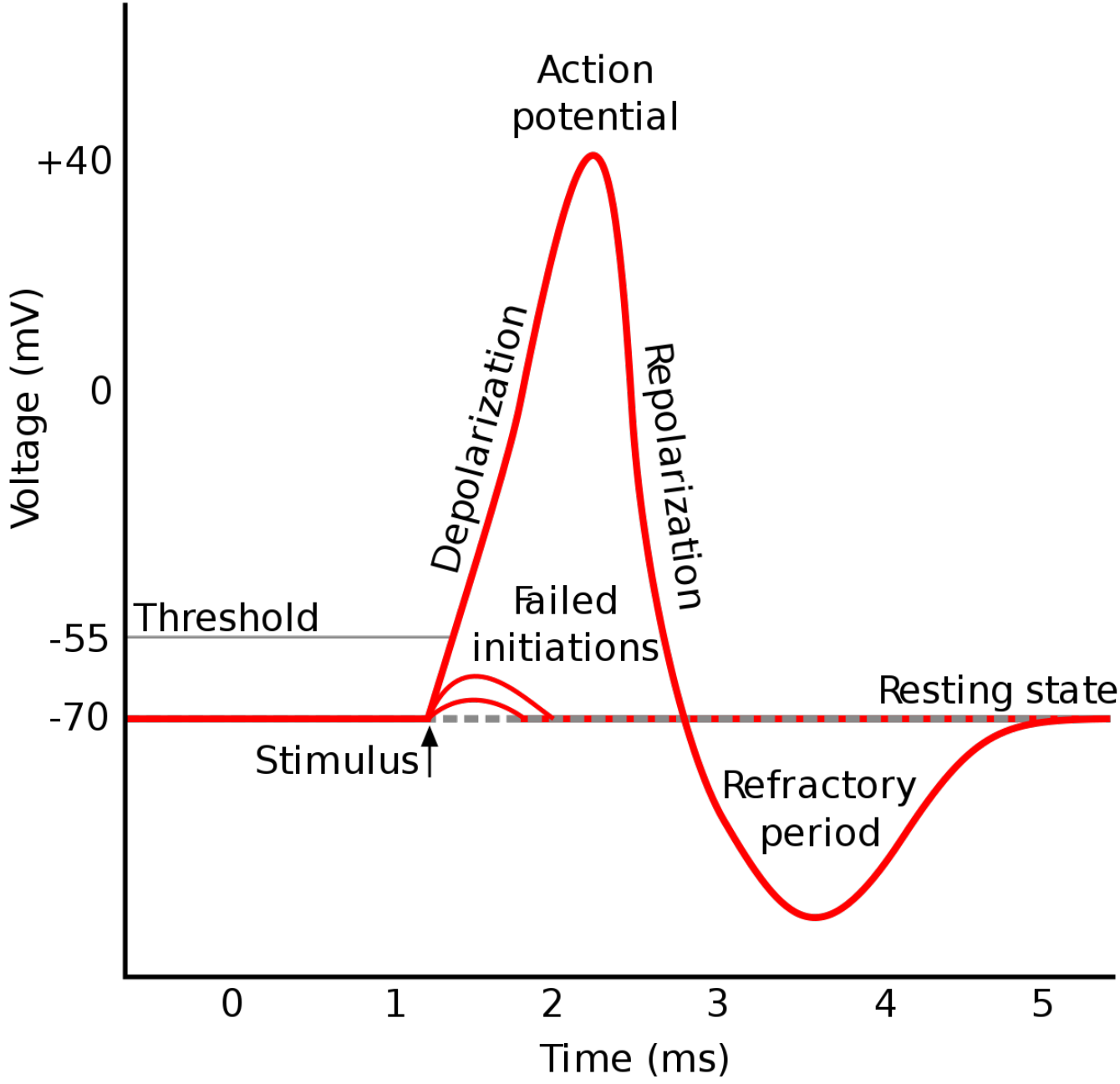

AiCENTER

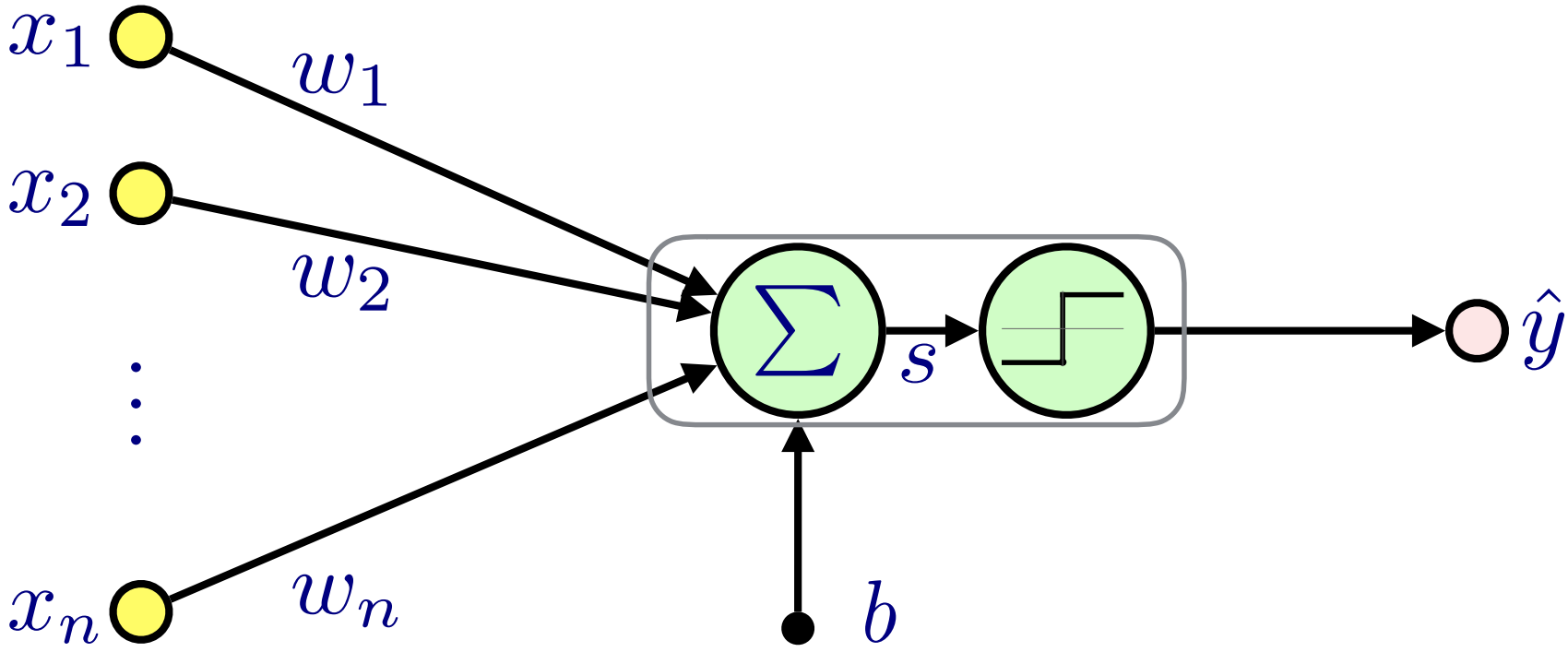

Σ
Σ
Σ
softmax
hidden
layer 1
hidden
layer 2
output
layer
fully
connected

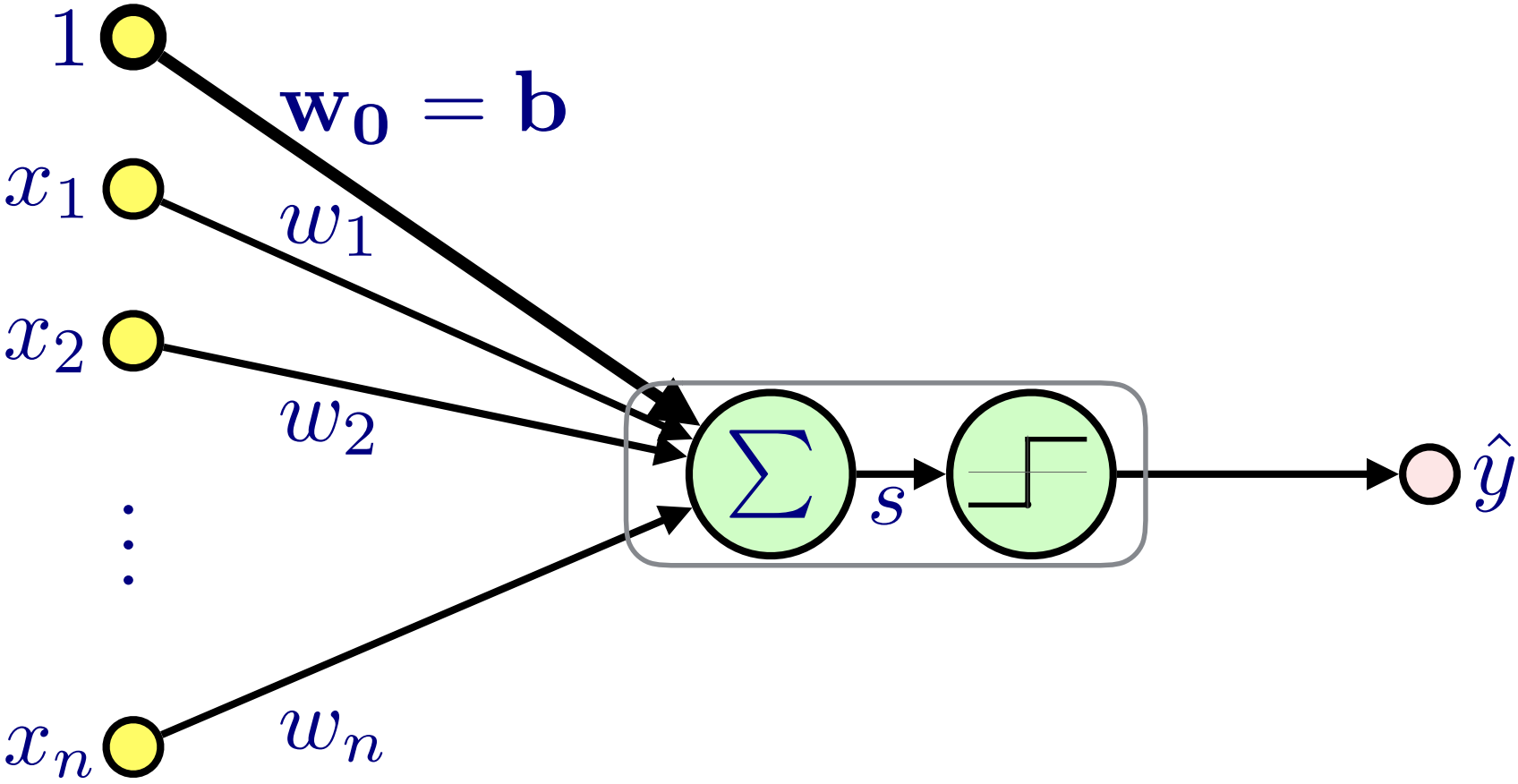


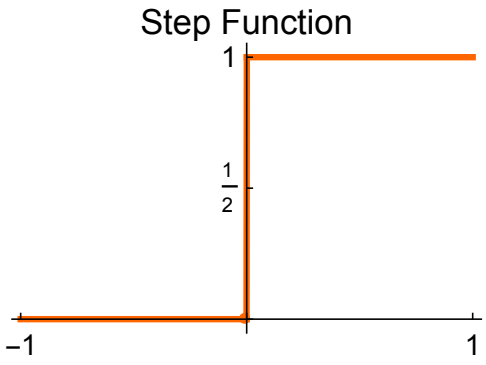

module
module

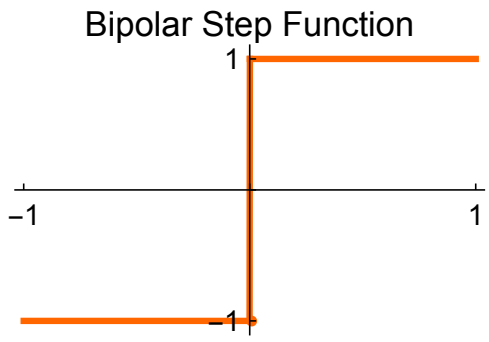

Neuron
Dendrites
Axon
Electrical Impulses
Neurotransmitter Molecules
Receptor
Synapse

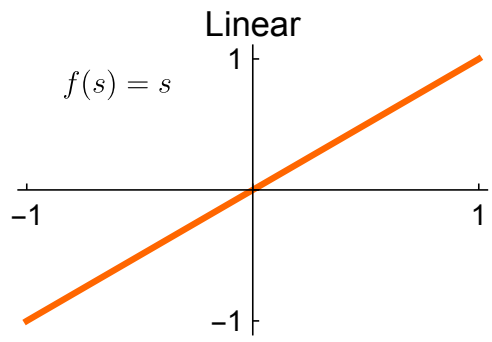

Action
potential
+40
0
Voltage (mV)
Depolarization
Repolarization
Threshold
-55
-70
Failed
initiations
Resting state
Stimulus
Refractory
period
0
1
2
3
4
5
Time (ms)

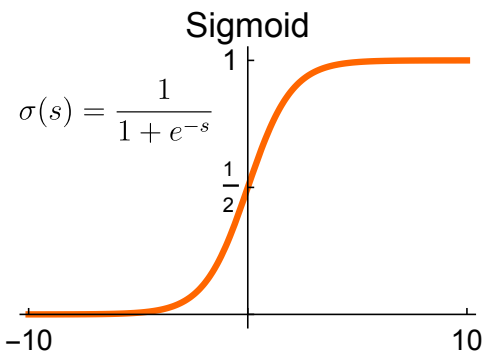

x_1
w_1
x_2
w_2
$\sum$
s
$\hat{y}$
x_n
w_n
b

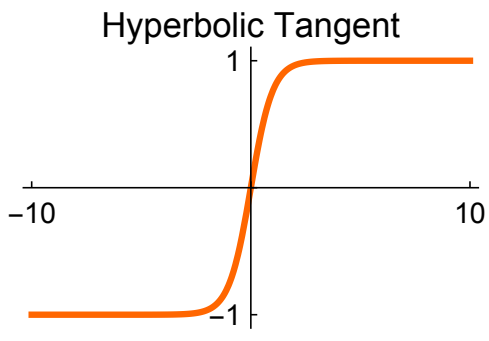

1
$\mathbf{w_0 = b}$
x_1
w_1
x_2
w_2
x_n
w_n
$\sum$
s
$\hat{y}$

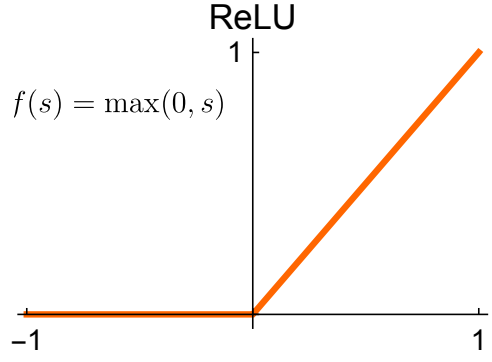

Step Function
1
1/2
−1
1

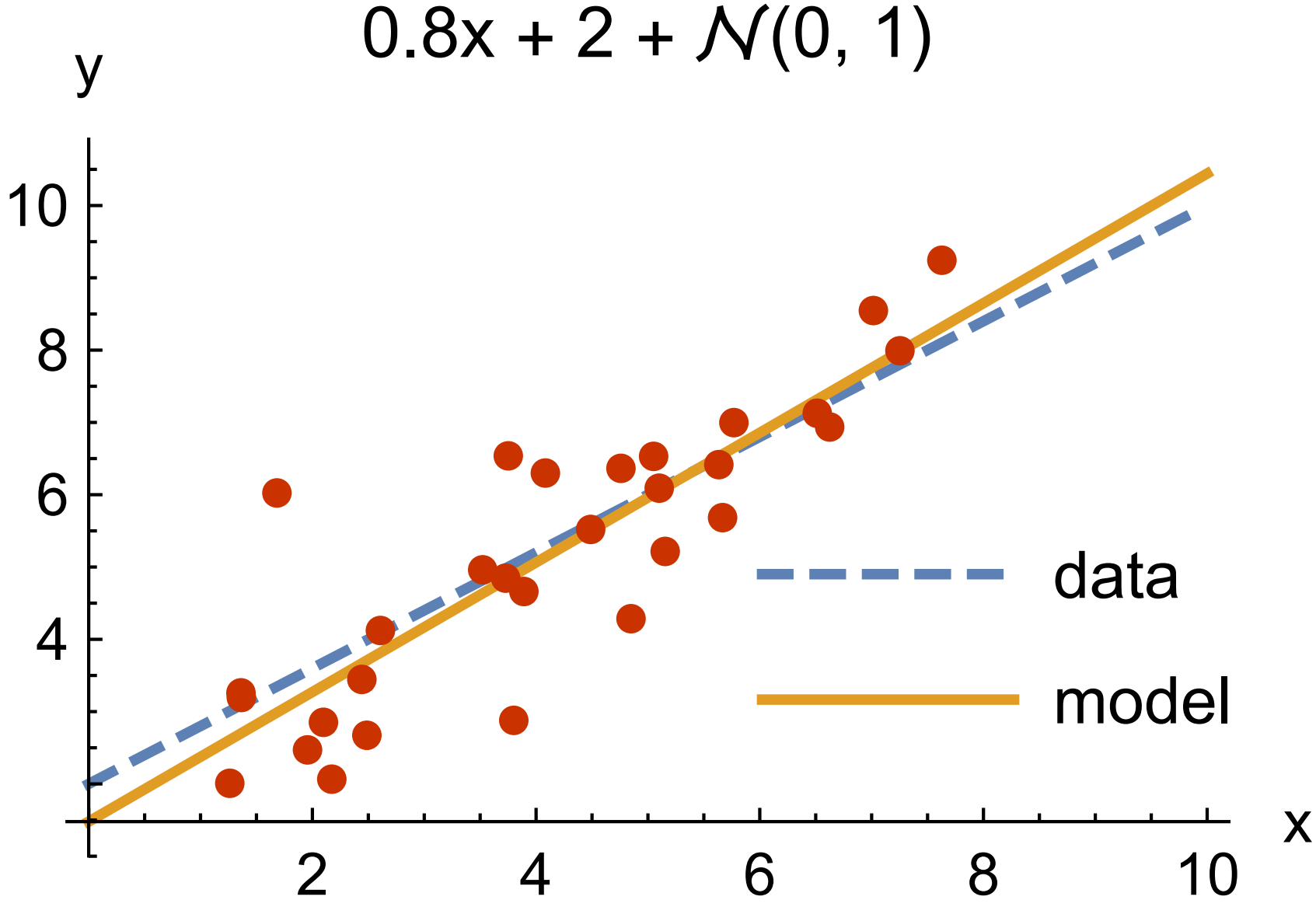

Bipolar Step Function
1
−1
1
−1


Linear
$f(s) = s$
1
−1
1
−1


Sigmoid
$\sigma(s) = \frac{1}{1+e^{-s}}$
1
1/2
−10
10

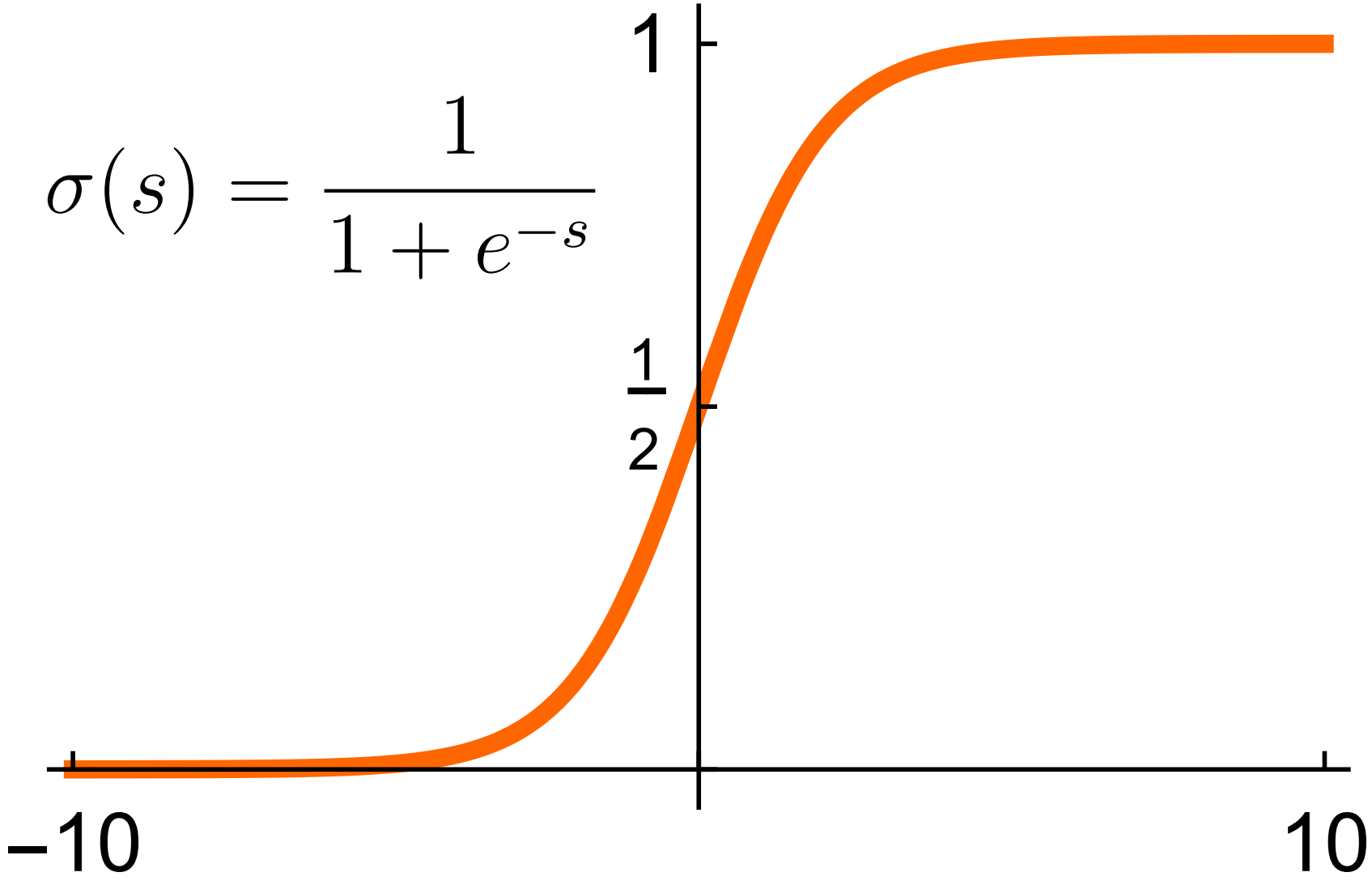

Hyperbolic Tangent
1
−10
10
−1

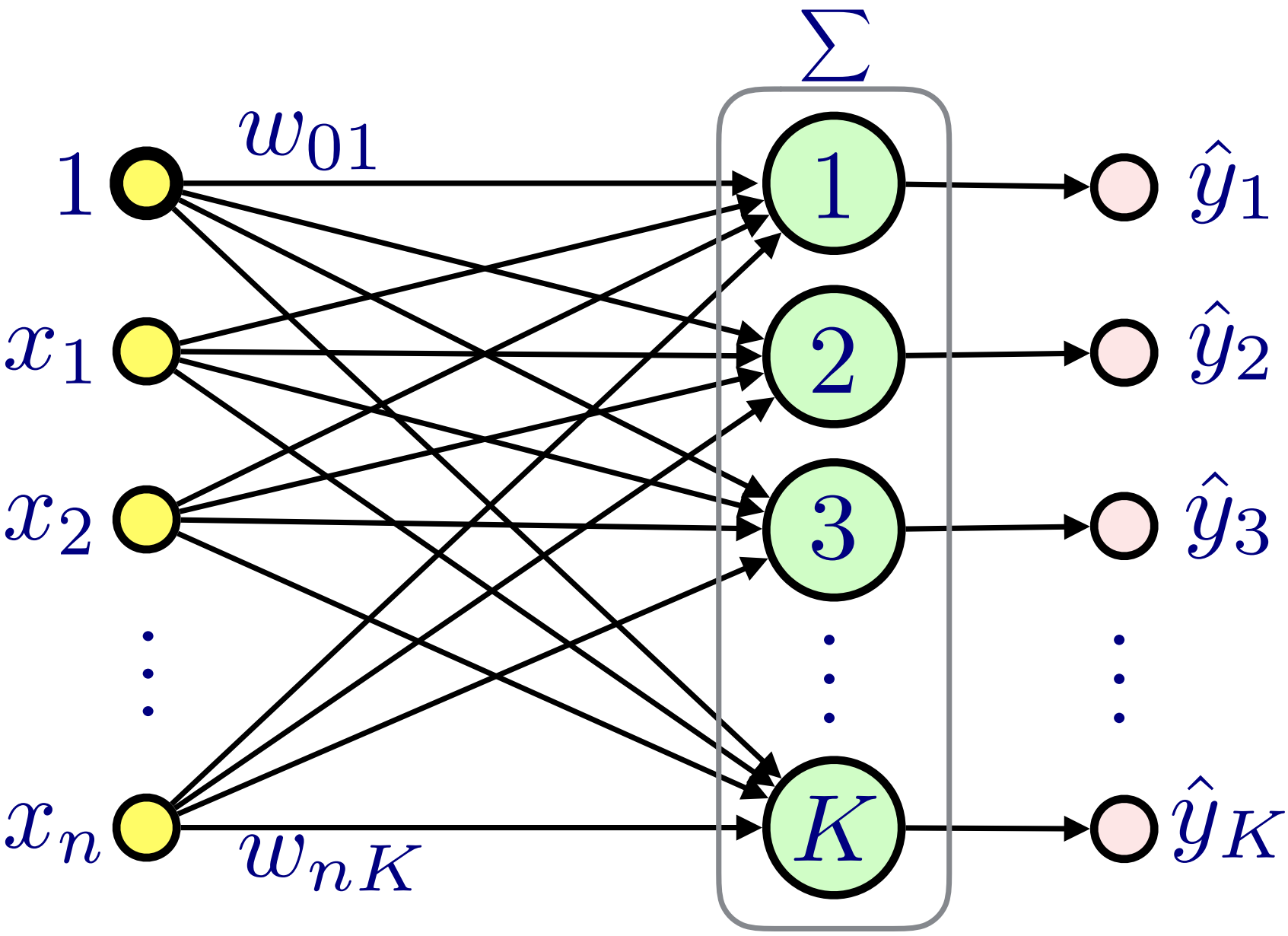

ReLU
$f(s) = \max(0, s)$
1
−1
1

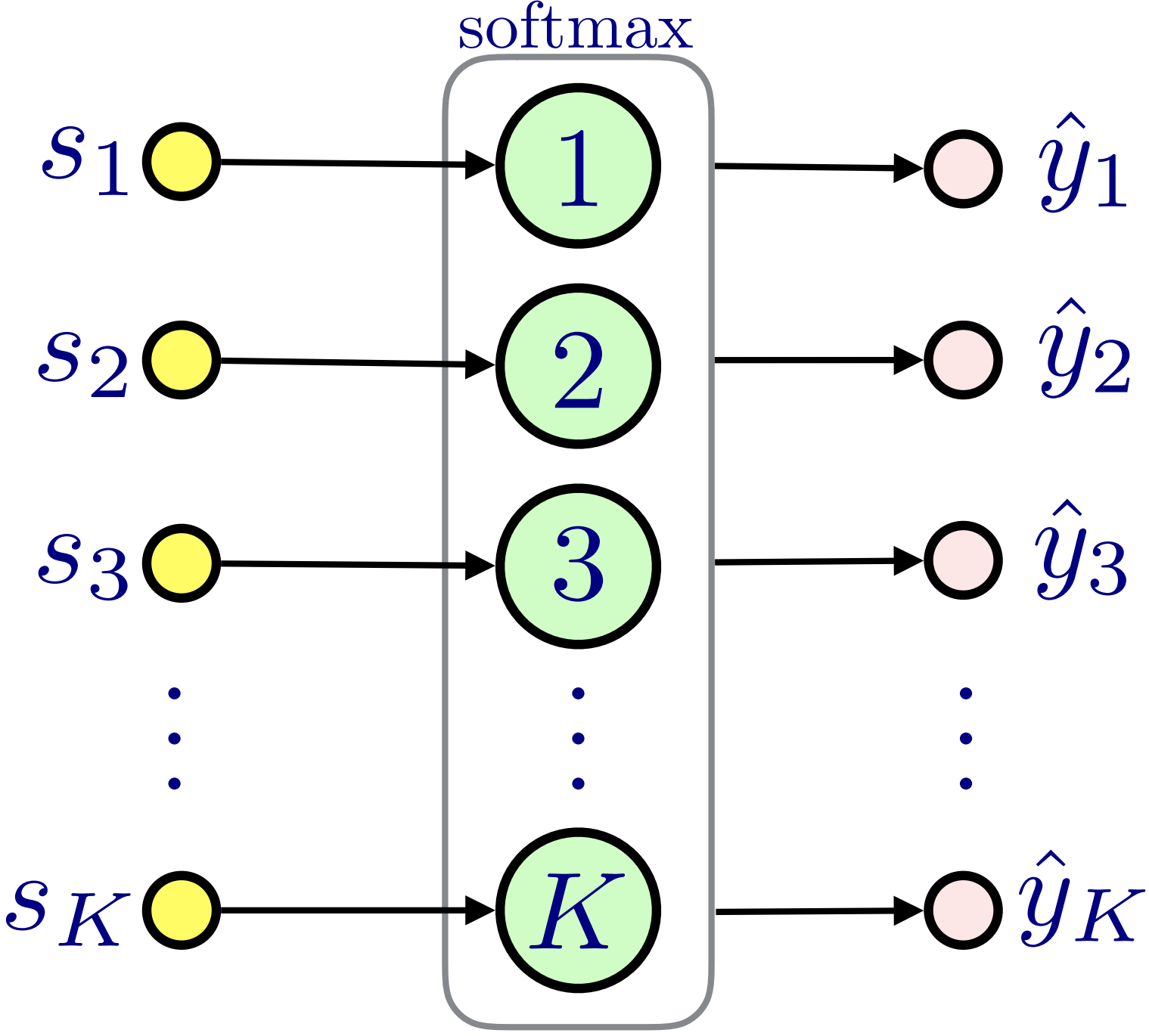

0.8x + 2 + 𝒩(0, 1)
y
10
8
6
4
2
4
6
8
10
x
data
model

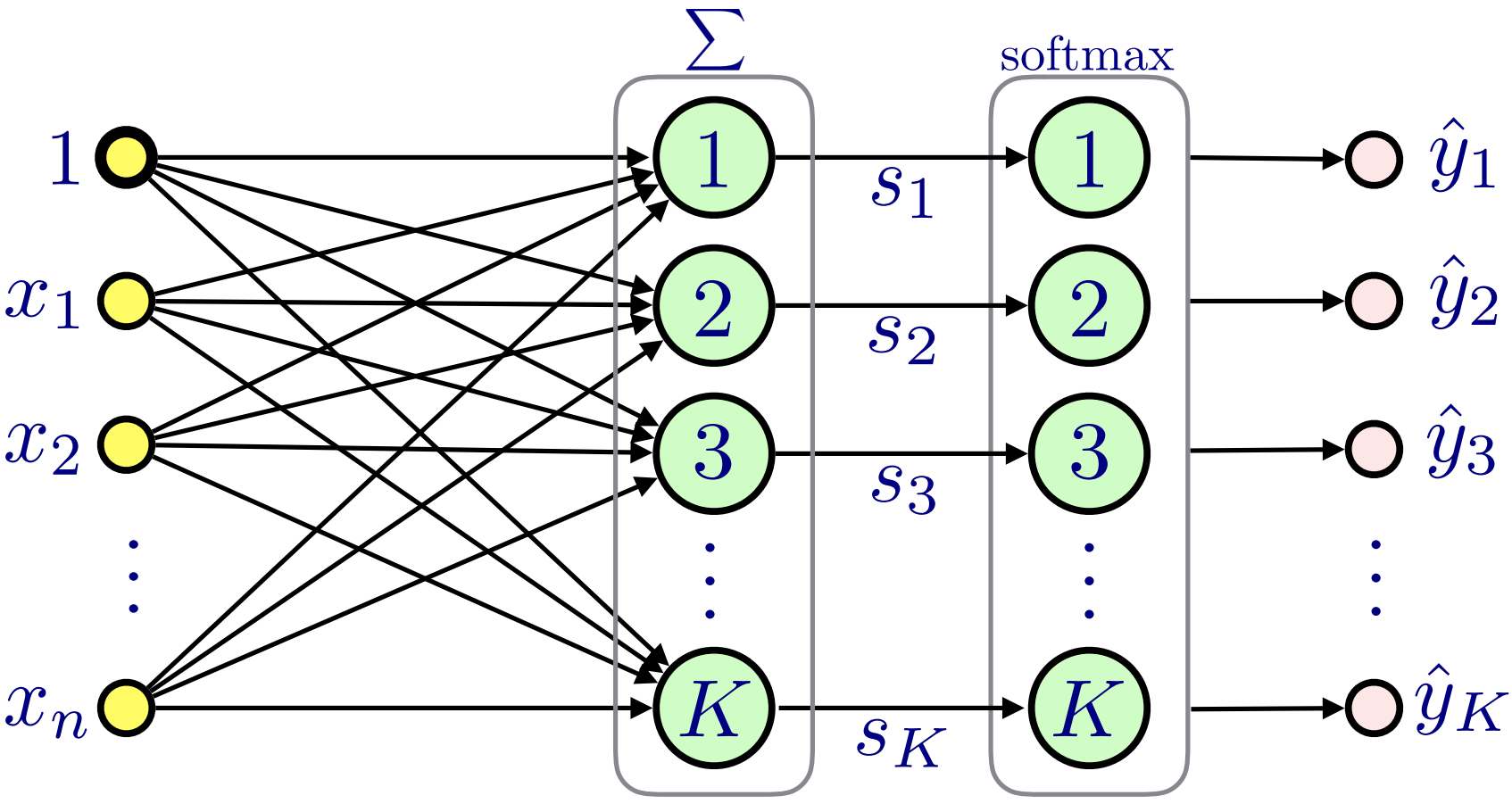
Sigmoid

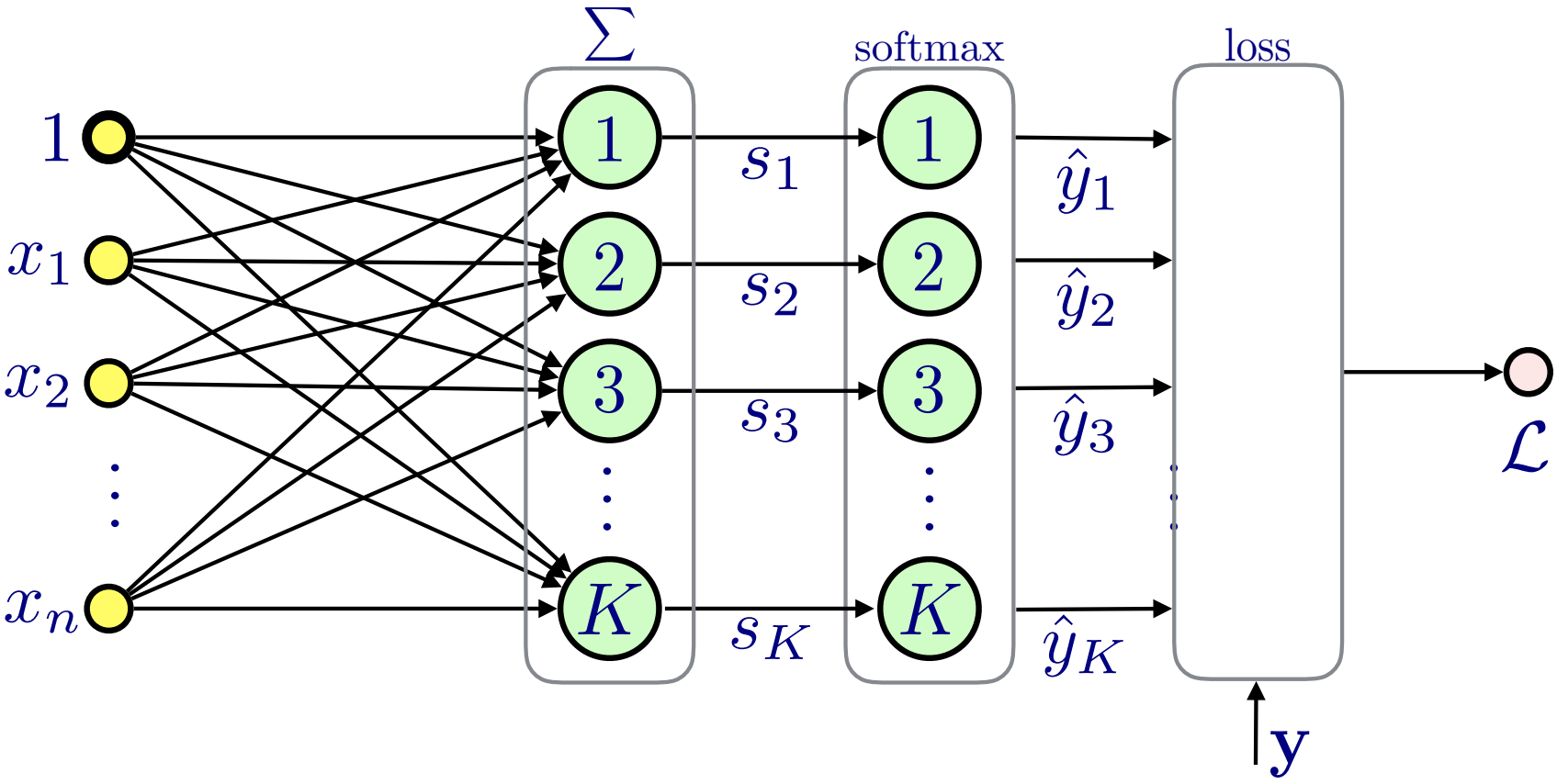
$$\sigma(s) = \frac{1}{1 + e^{-s}}$$

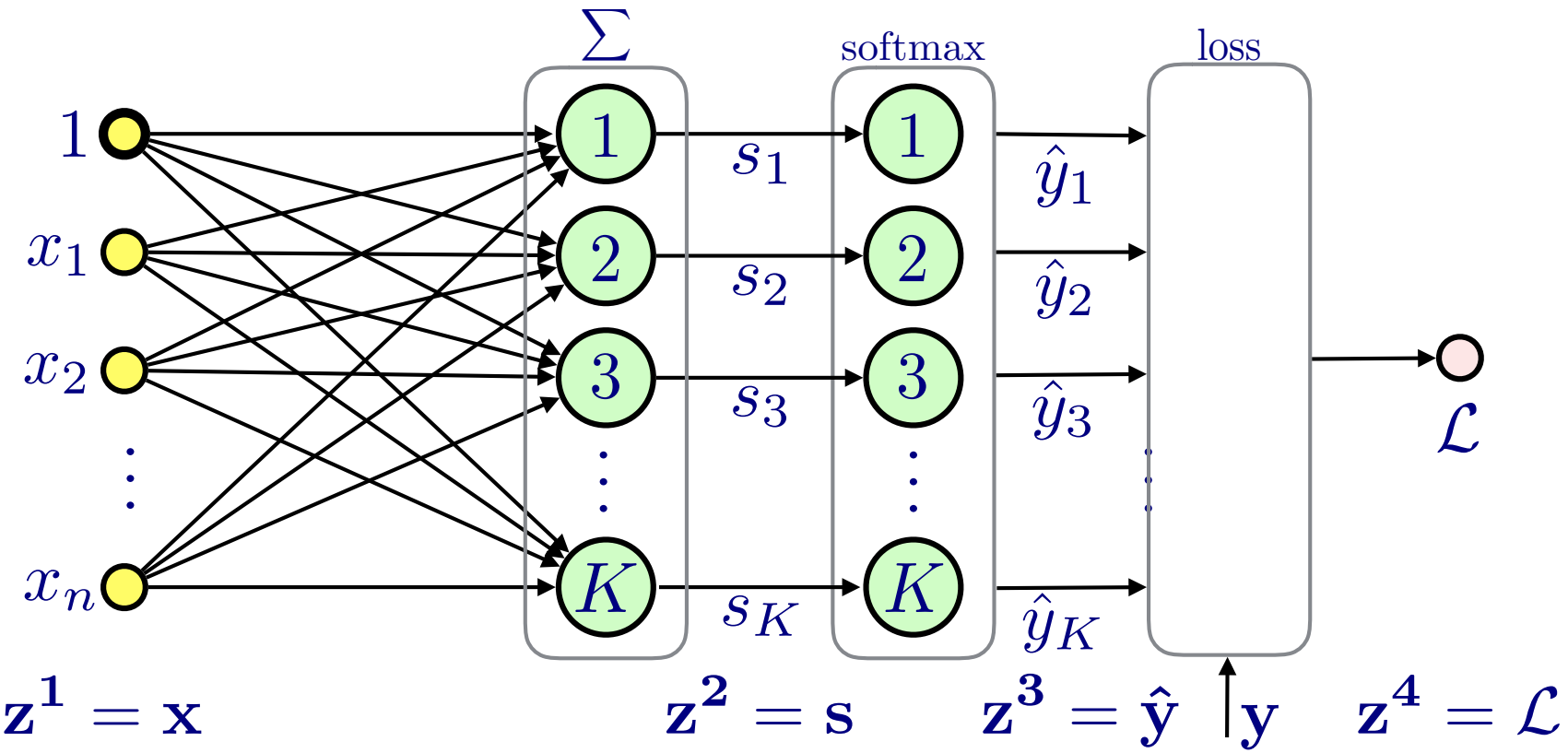


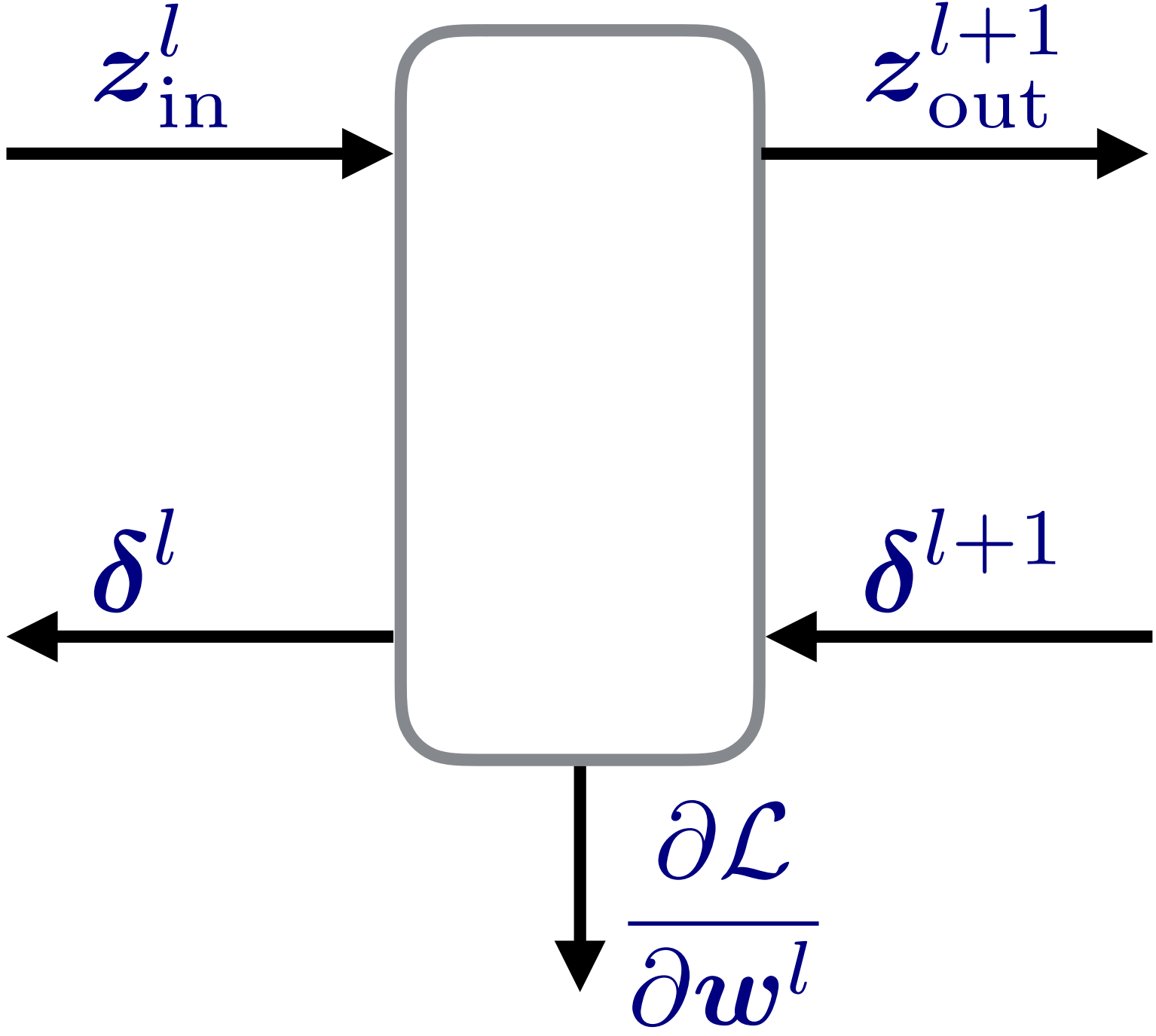

Σ
w_{01}
1
x_1
x_2
x_n
w_{nK}
1
2
3
K
$\hat{y}_1$
$\hat{y}_2$
$\hat{y}_3$
$\hat{y}_K$

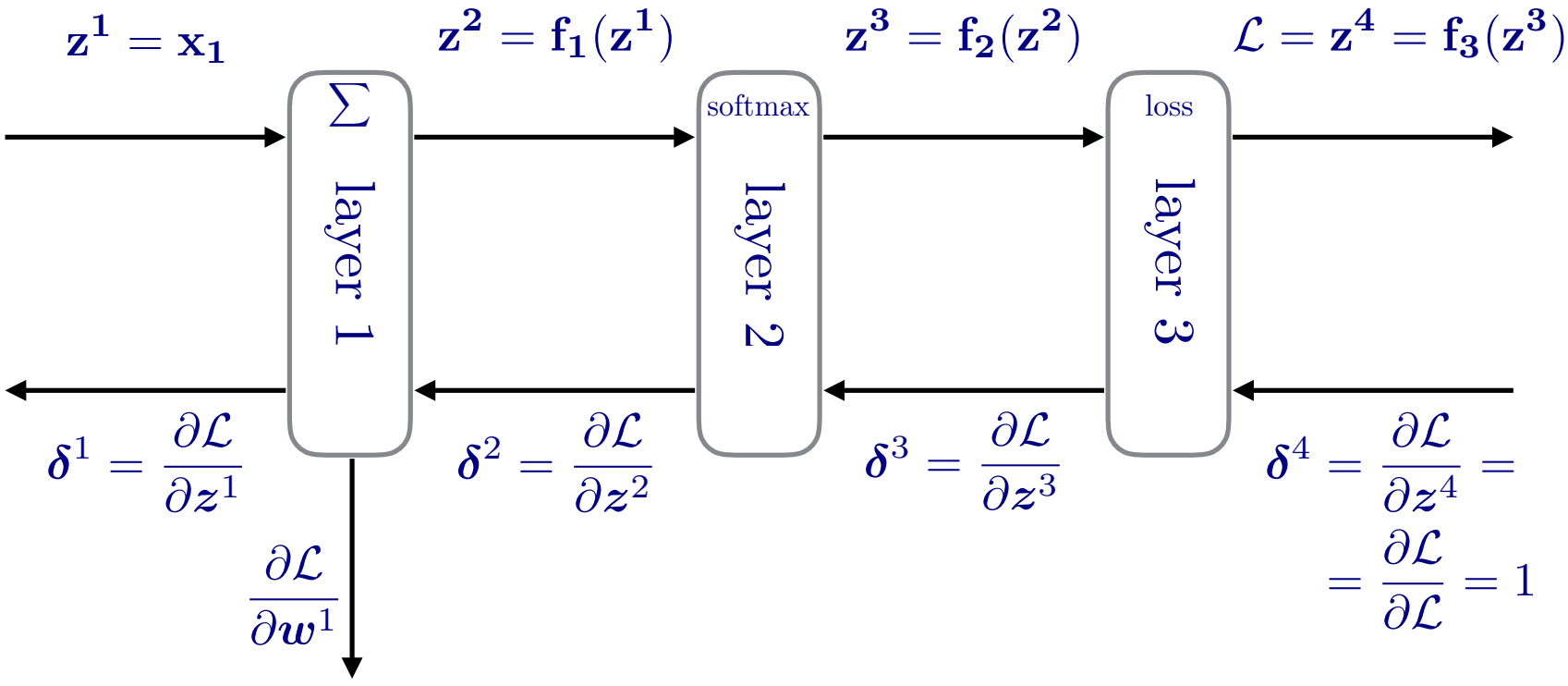

softmax
s_1
s_2
s_3
s_K
1
2
3
K
$\hat{y}_1$
$\hat{y}_2$
$\hat{y}_3$
$\hat{y}_K$

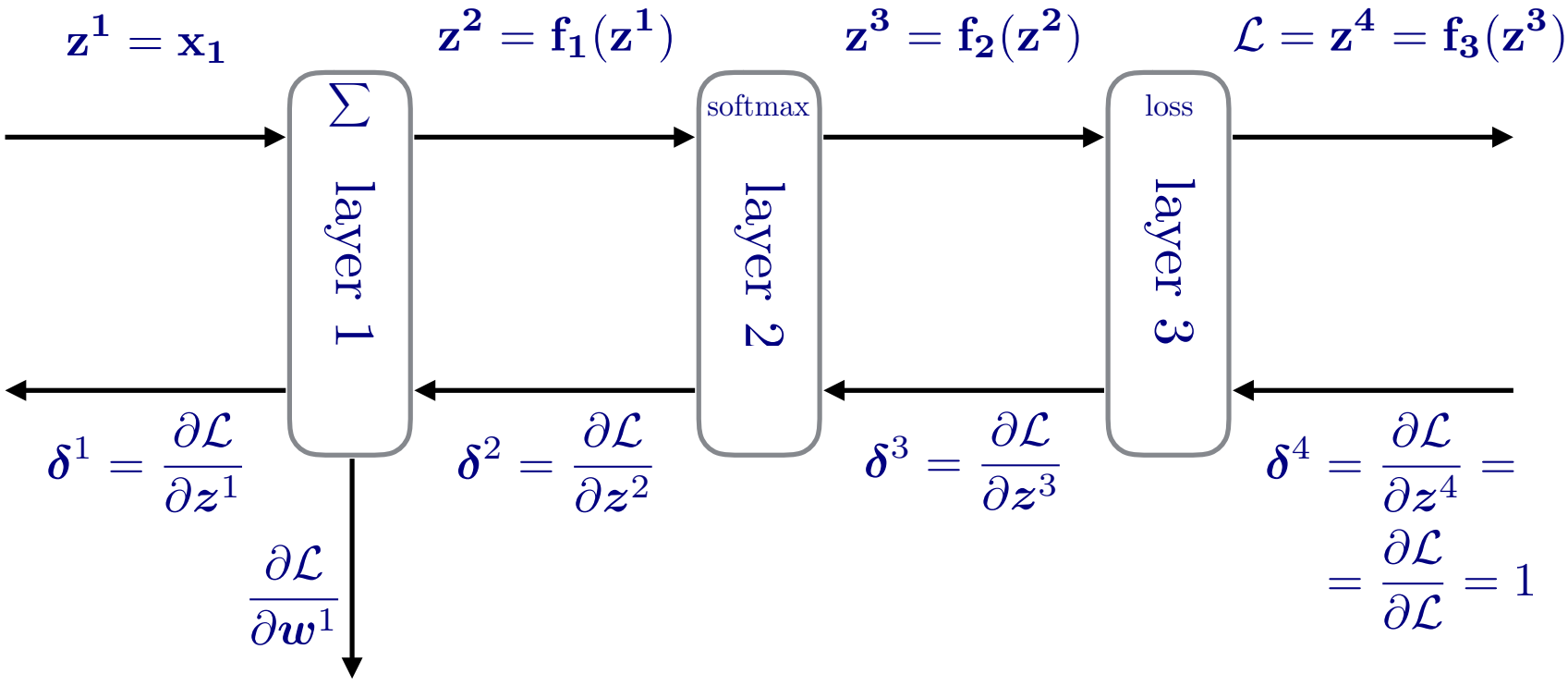

$\sum$
softmax
1
x_1
x_2
x_n
1
2
3
K
s_1
s_2
s_3
s_K
1
2
3
K
$\hat{y}_1$
$\hat{y}_2$
$\hat{y}_3$
$\hat{y}_K$

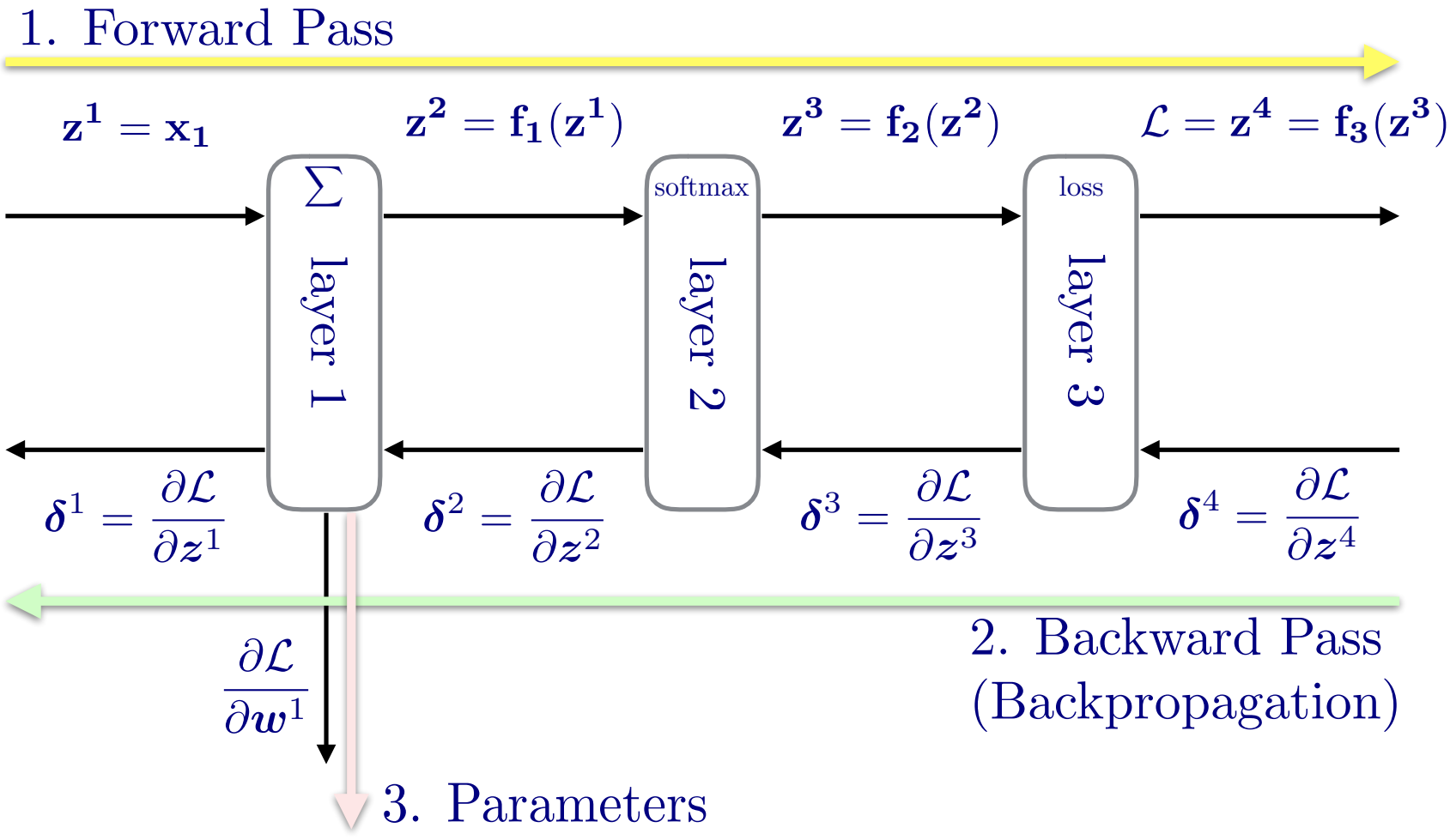

$\sum$
softmax
loss
1
x_1
x_2
x_n
1
2
3
K
s_1
s_2
s_3
s_K
1
2
3
K
$\hat{y}_1$
$\hat{y}_2$
$\hat{y}_3$
$\hat{y}_K$
$\mathcal{L}$
$\mathbf{y}$

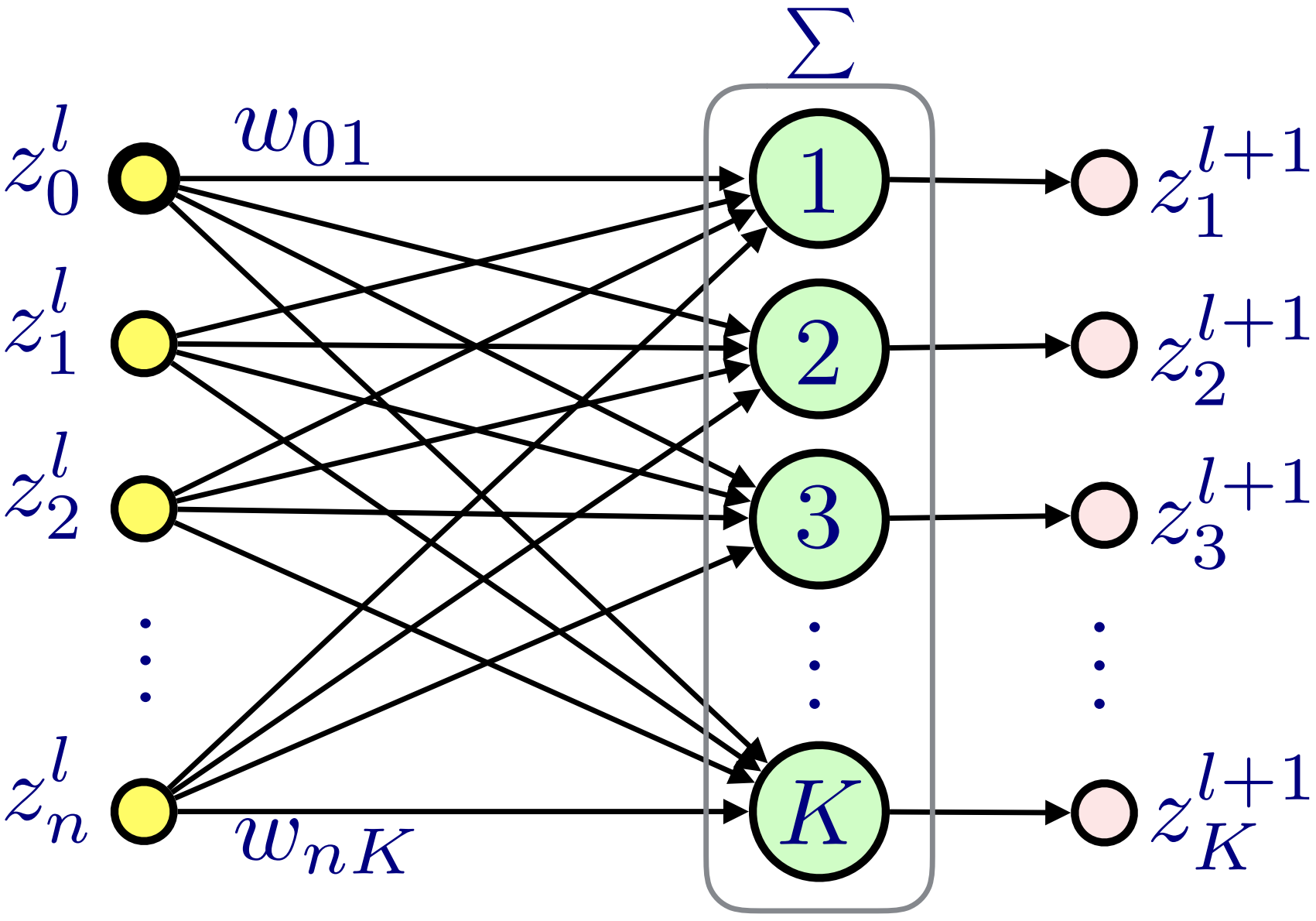

$\sum$
softmax
loss
1
x_1
x_2
x_n
1
2
3
K
s_1
s_2
s_3
s_K
1
2
3
K
$\hat{y}_1$
$\hat{y}_2$
$\hat{y}_3$
$\hat{y}_K$
$\mathcal{L}$
$\mathbf{z^1 = x}$
$\mathbf{z^2 = s}$
$\mathbf{z^3 = \hat{y}}$
$\mathbf{y}$
$\mathbf{z^4 = \mathcal{L}}$

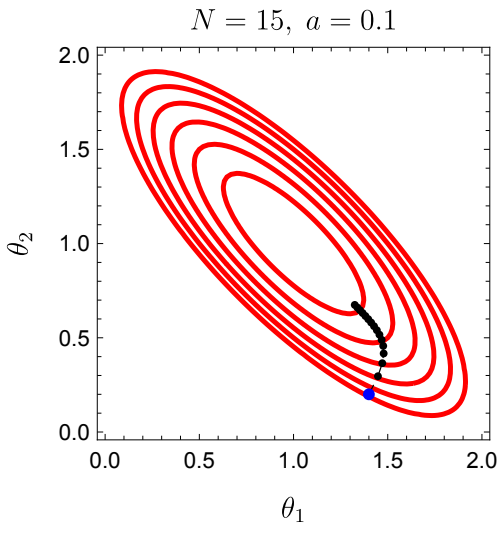

z_{in}^{l}
z_{out}^{l+1}
$\boldsymbol{\delta}^{l}$
$\boldsymbol{\delta}^{l+1}$
$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}^{l}}$

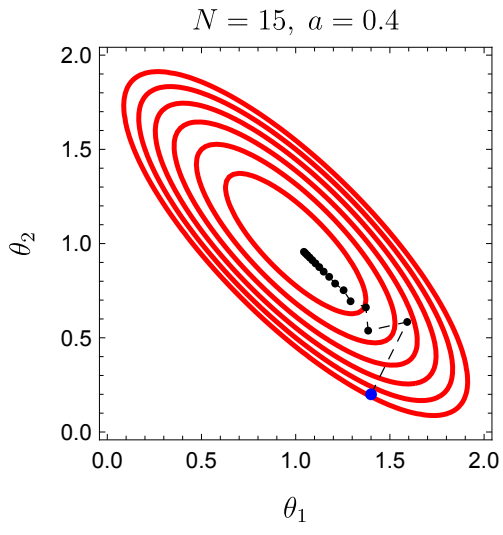

$\mathbf{z^1 = x_1}$
$\mathbf{z^2 = f_1(z^1)}$
$\mathbf{z^3 = f_2(z^2)}$
$\mathcal{L} = \mathbf{z^4 = f_3(z^3)}$
$\sum$ layer 1
softmax layer 2
loss layer 3
$\boldsymbol{\delta}^1 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^1}$
$\boldsymbol{\delta}^2 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^2}$
$\boldsymbol{\delta}^3 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^3}$
$\boldsymbol{\delta}^4 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^4} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} = 1$
$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}^1}$

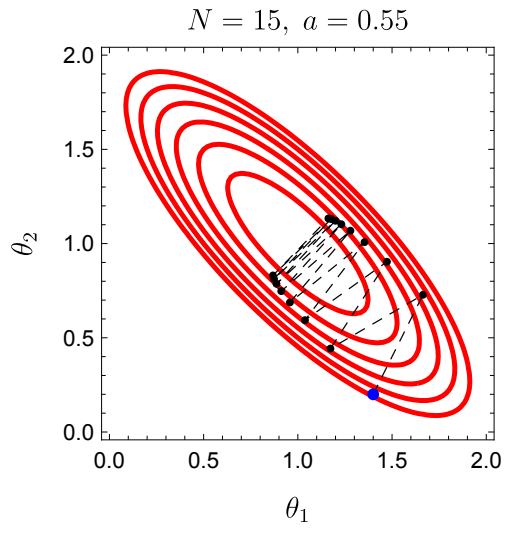

$\mathbf{z^1 = x_1}$
$\mathbf{z^2 = f_1(z^1)}$
$\mathbf{z^3 = f_2(z^2)}$
$\mathcal{L} = \mathbf{z^4 = f_3(z^3)}$
$\sum$ layer 1
softmax layer 2
loss layer 3
$\boldsymbol{\delta}^1 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^1}$
$\boldsymbol{\delta}^2 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^2}$
$\boldsymbol{\delta}^3 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^3}$
$\boldsymbol{\delta}^4 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^4} = \frac{\partial \mathcal{L}}{\partial \mathcal{L}} = 1$
$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}^1}$

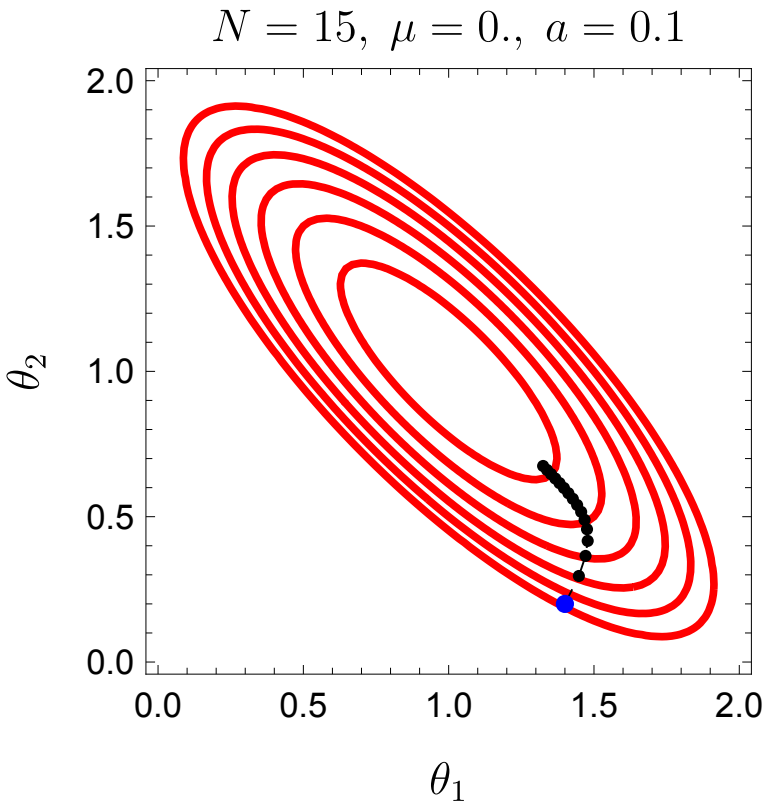

1. Forward Pass
$\mathbf{z^1 = x_1}$
$\mathbf{z^2 = f_1(z^1)}$
$\mathbf{z^3 = f_2(z^2)}$
$\mathcal{L} = \mathbf{z^4 = f_3(z^3)}$
$\sum$ layer 1
softmax layer 2
loss layer 3
$\boldsymbol{\delta}^1 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^1}$
$\boldsymbol{\delta}^2 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^2}$
$\boldsymbol{\delta}^3 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^3}$
$\boldsymbol{\delta}^4 = \frac{\partial \mathcal{L}}{\partial \boldsymbol{z}^4}$
2. Backward Pass
(Backpropagation)
$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}^1}$
3. Parameters

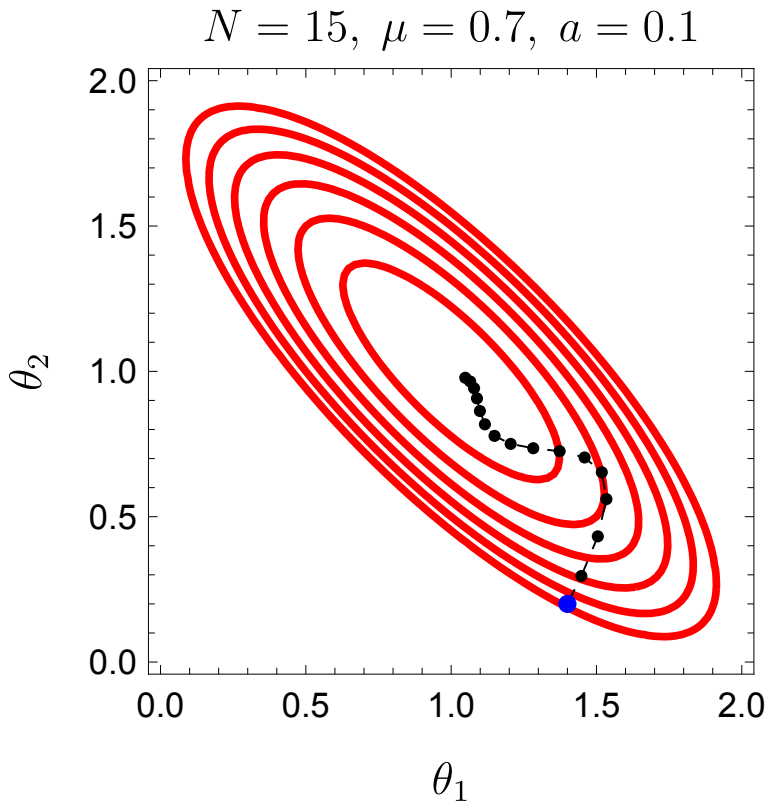

$\sum$
z_0^l
z_1^l
z_2^l
z_n^l
w_{01}
w_{nK}
1
2
3
K
z_1^{l+1}
z_2^{l+1}
z_3^{l+1}
z_K^{l+1}

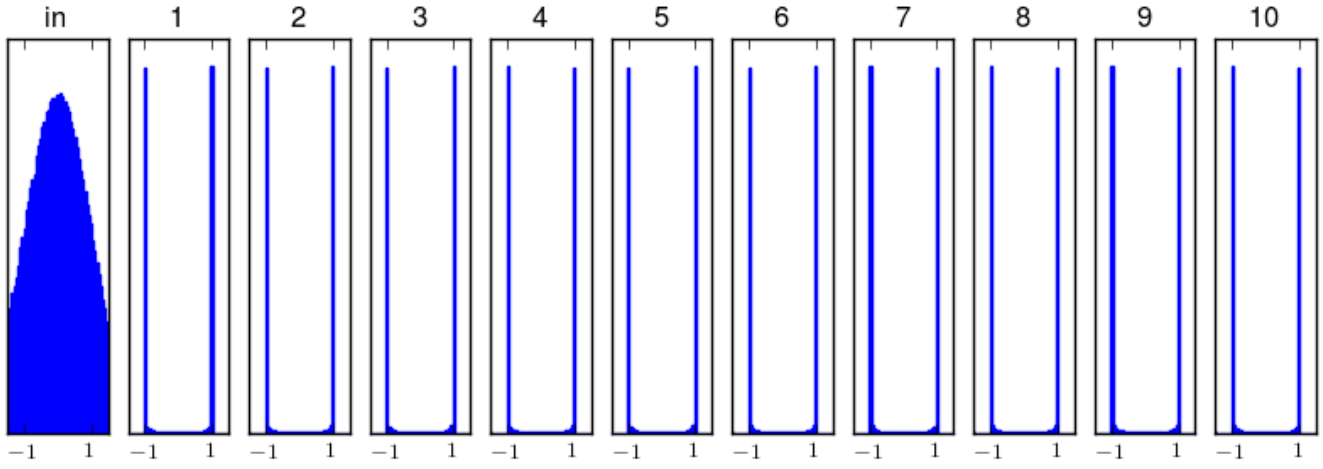

$N = 15,\ a = 0.1$
2.0
1.5
1.0
0.5
0.0
θ_2
0.0
0.5
1.0
1.5
2.0
θ_1

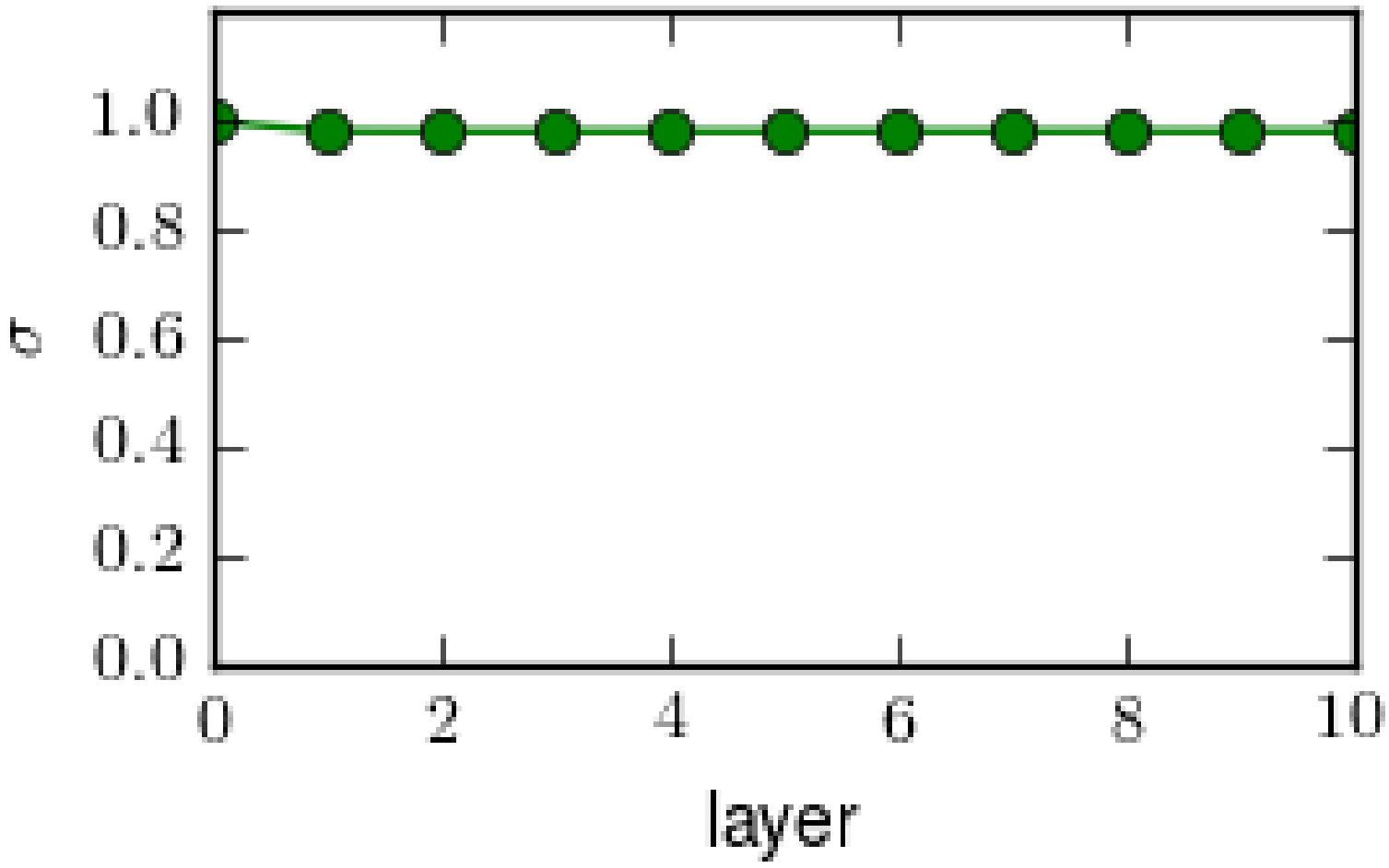

$N = 15,\ a = 0.4$
2.0
1.5
1.0
0.5
0.0
θ_2
0.0
0.5
1.0
1.5
2.0
θ_1

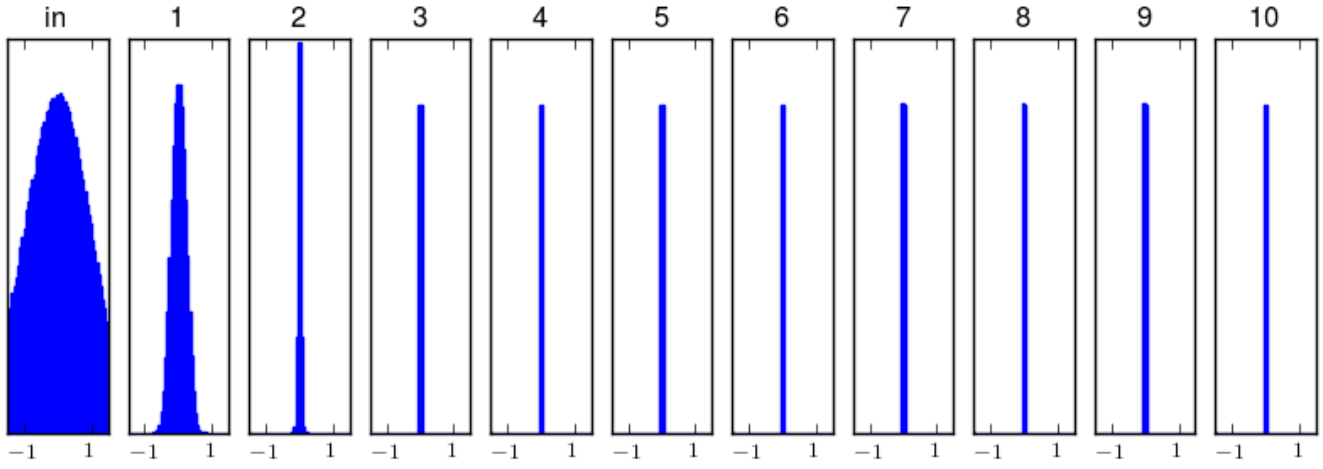

$N = 15,\ a = 0.55$
2.0
1.5
1.0
0.5
0.0
θ_2
0.0
0.5
1.0
1.5
2.0
θ_1

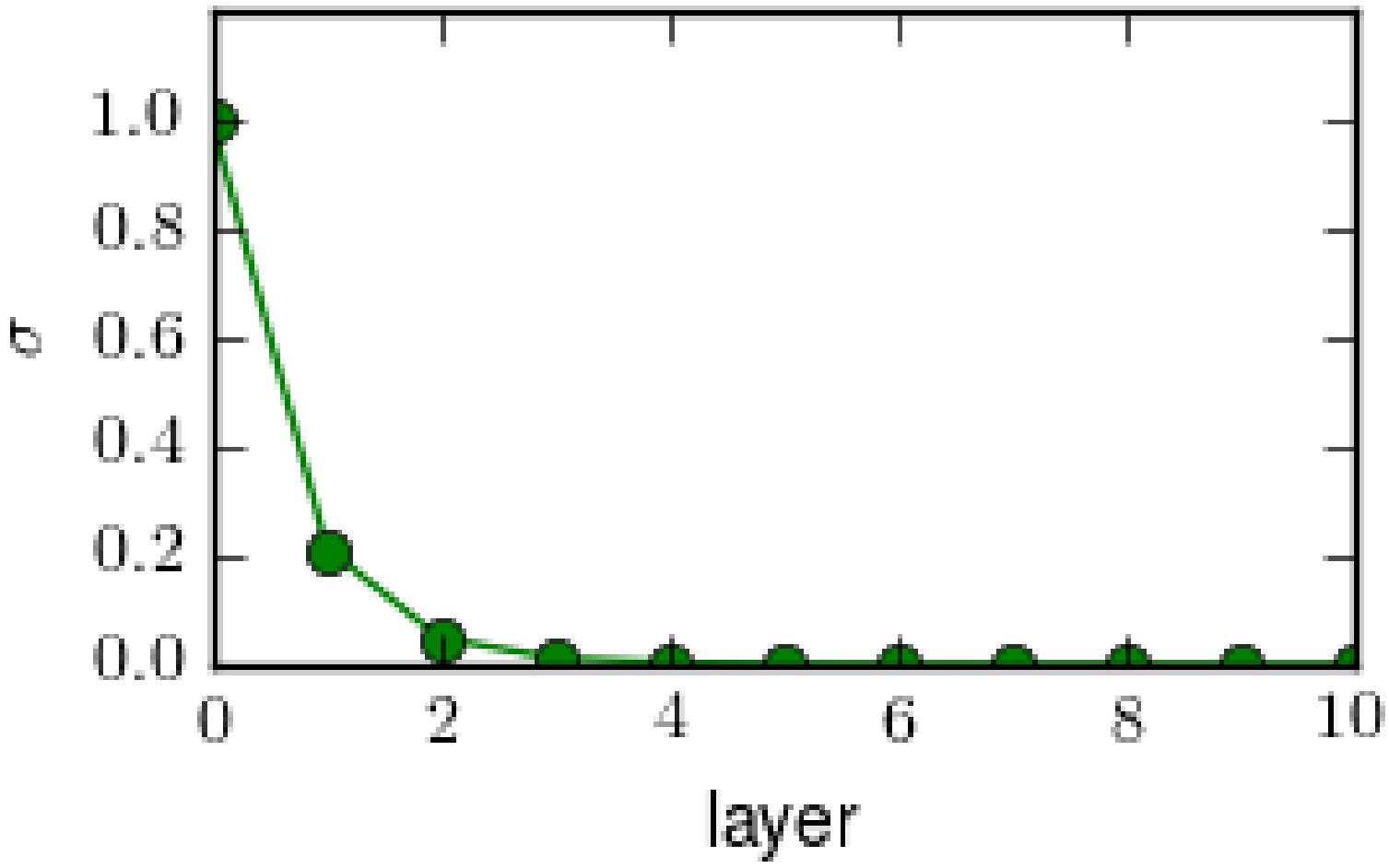

$N = 15,\ \mu = 0.,\ a = 0.1$
2.0
1.5
1.0
0.5
0.0
θ_2
0.0
0.5
1.0
1.5
2.0
θ_1

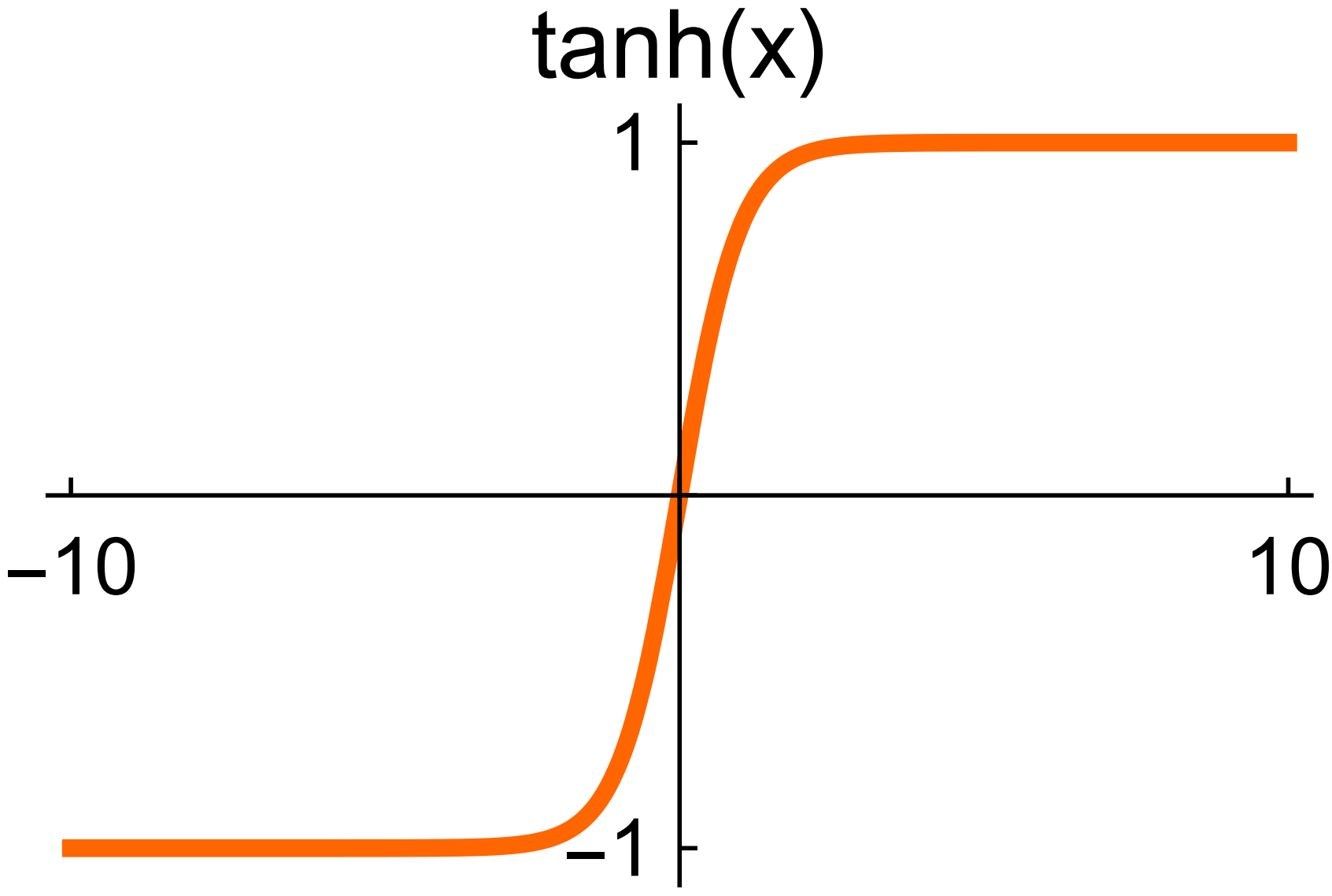

$N = 15,\ \mu = 0.7,\ a = 0.1$
2.0
1.5
1.0
0.5
0.0
θ_2
0.0
0.5
1.0
1.5
2.0
θ_1

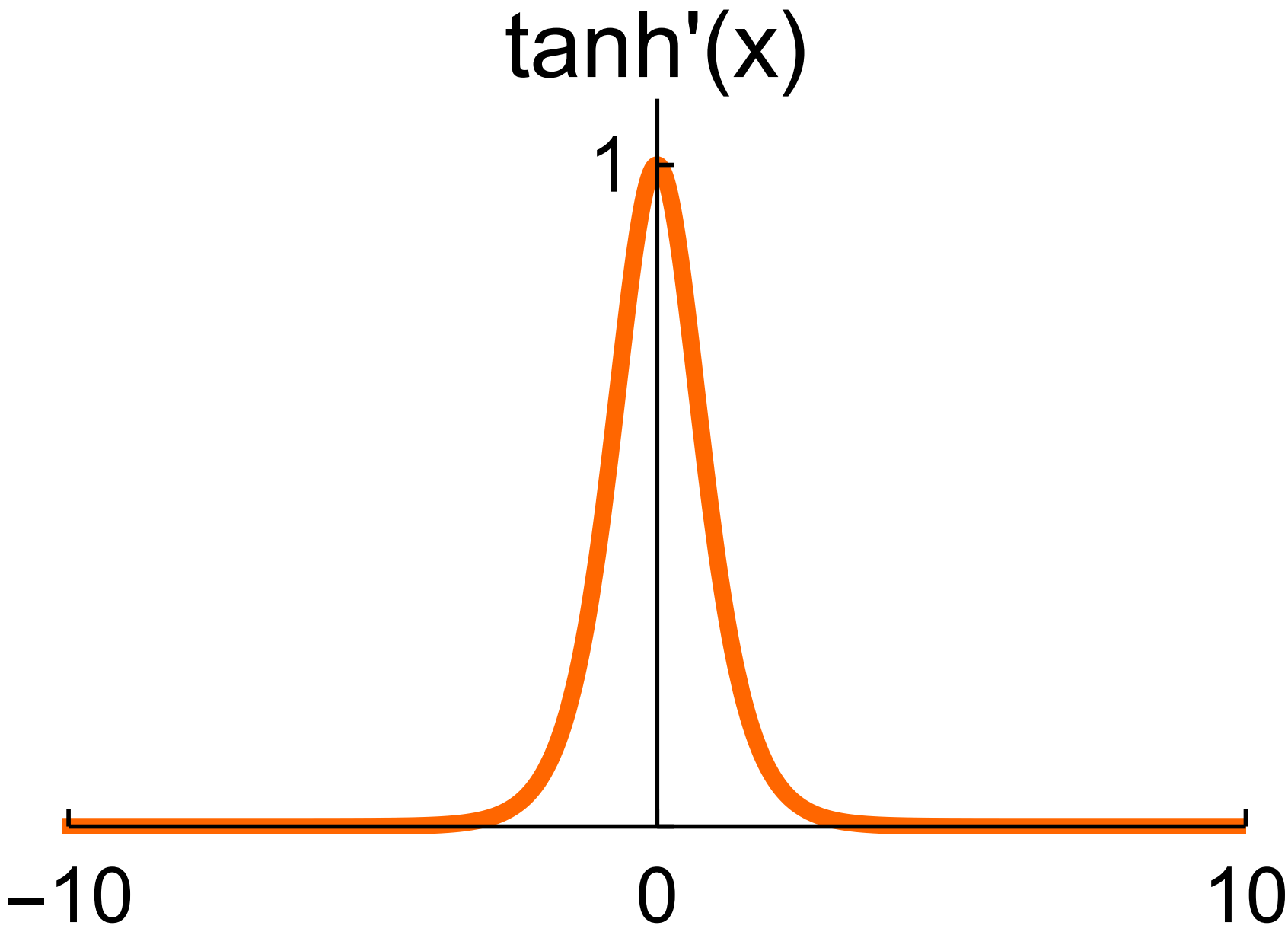

in
1
2
3
4
5
6
7
8
9
10
−1
1

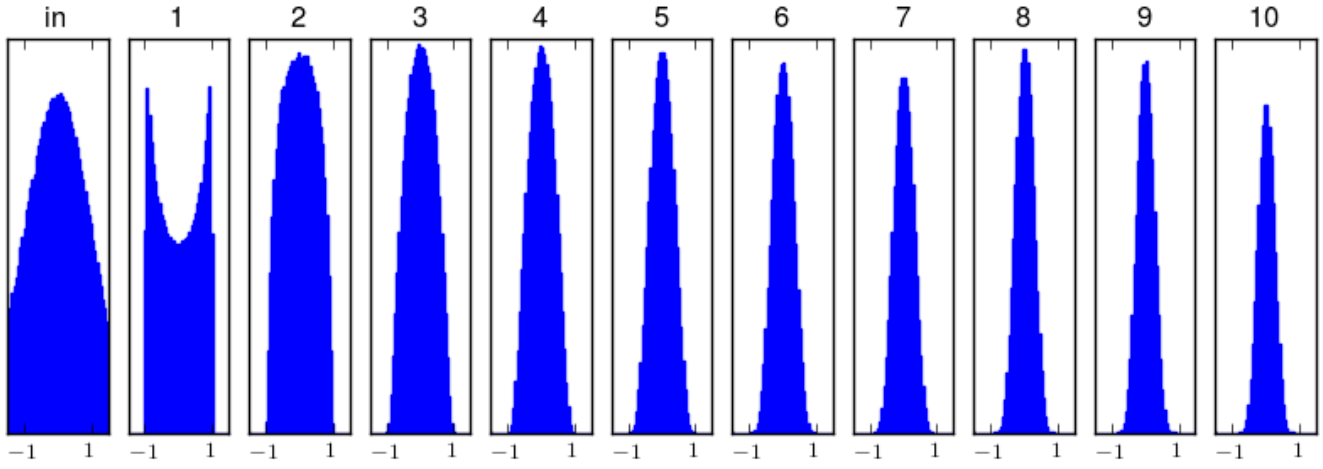

1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
10
layer

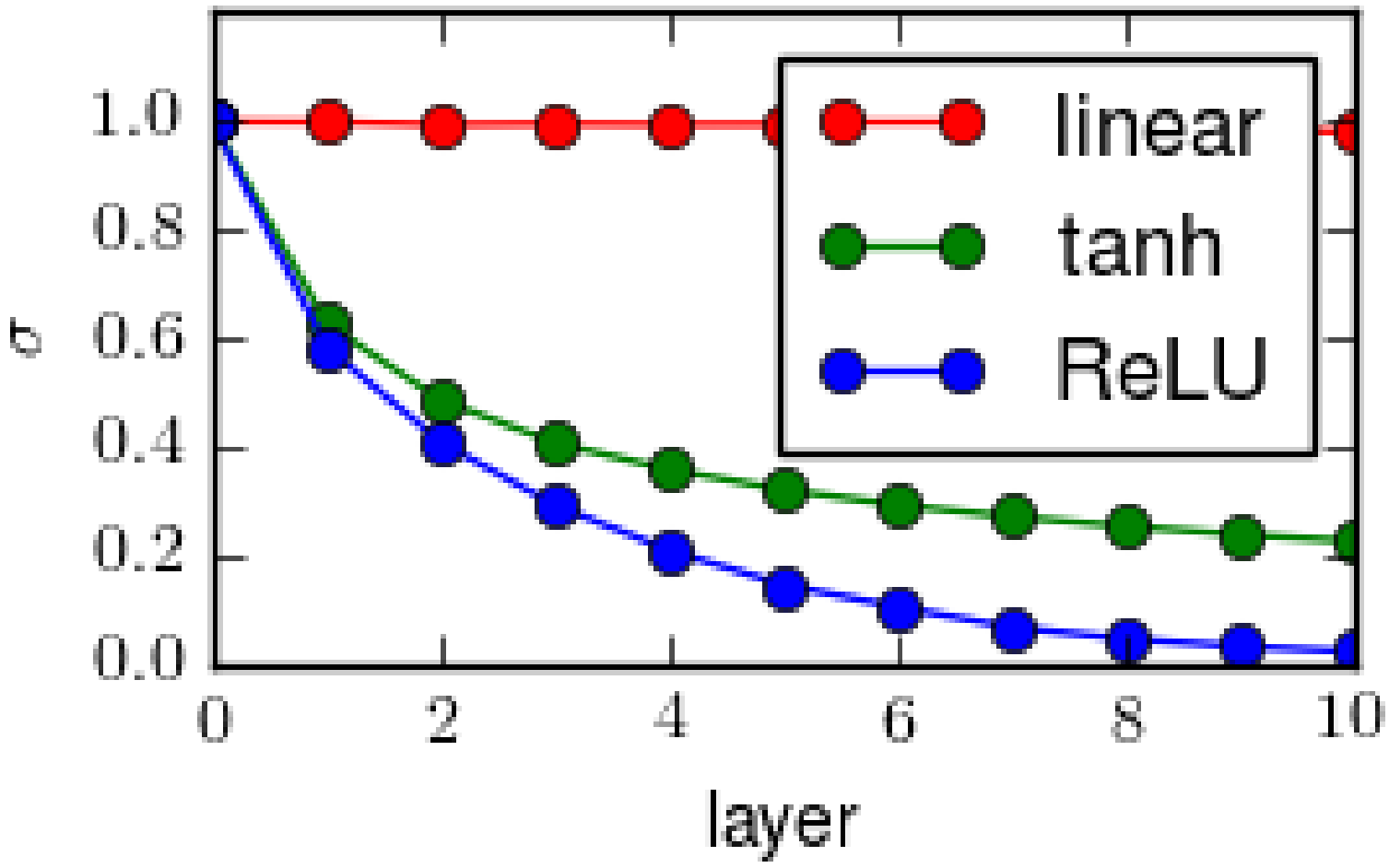

in
1
2
3
4
5
6
7
8
9
10
−1
1


1.0
0.8
0.6
0.4
0.2
0.0
σ
0
2
4
6
8
10
layer


tanh(x)
1
−1
−10
10

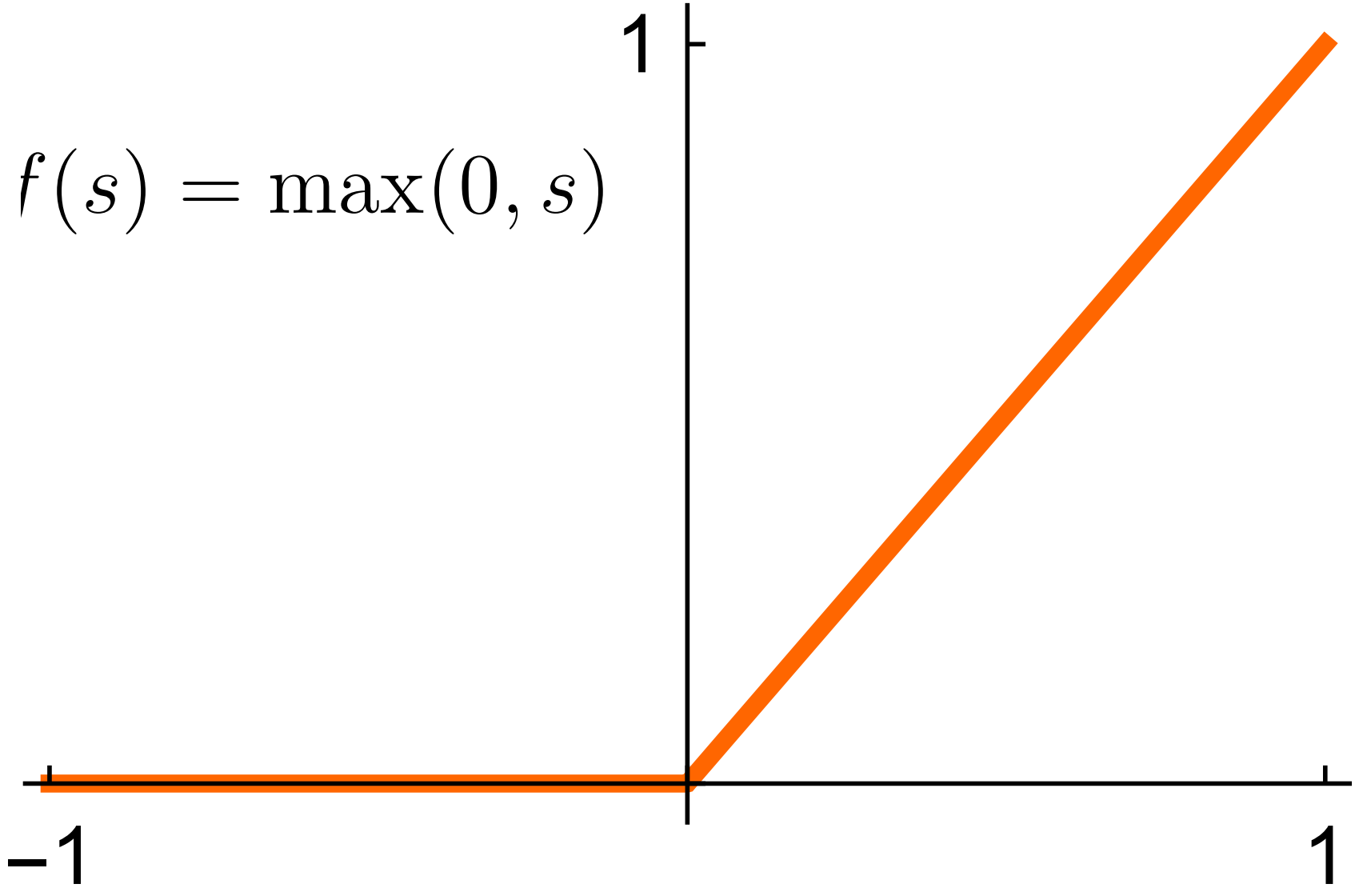

tanh'(x)
1
–10
0
10


in
1
2
3
4
5
6
7
8
9
10
−1
1


linear
tanh
ReLU
1.0
0.8
0.6
0.4
0.2
0.0
σ
0
2
4
6
8
10
layer

ReLU

$$f(s) = \max(0, s)$$



Sigmoid

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