CS 540 Introduction to Artificial Intelligence
Neural Networks (III)

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Today's outline

- Deep neural networks
  - Computational graph (forward and backward propagation)
- Numerical stability in training
  - Gradient vanishing/exploding
- Generalization and regularization
  - Overfitting, underfitting
  - Weight decay and dropout

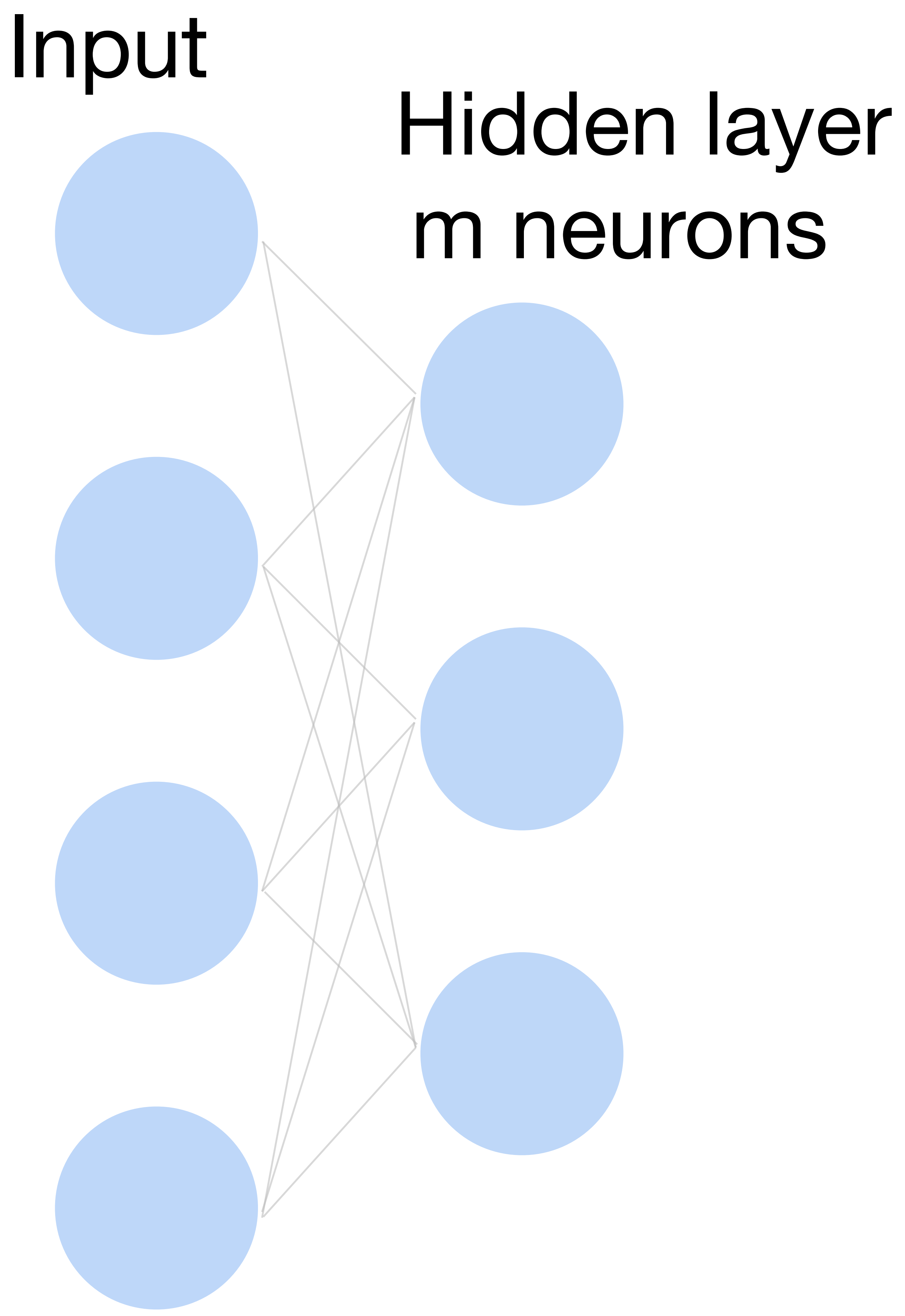
Part I: Neural Networks as a Computational Graph

Review: A single layer in neural networks

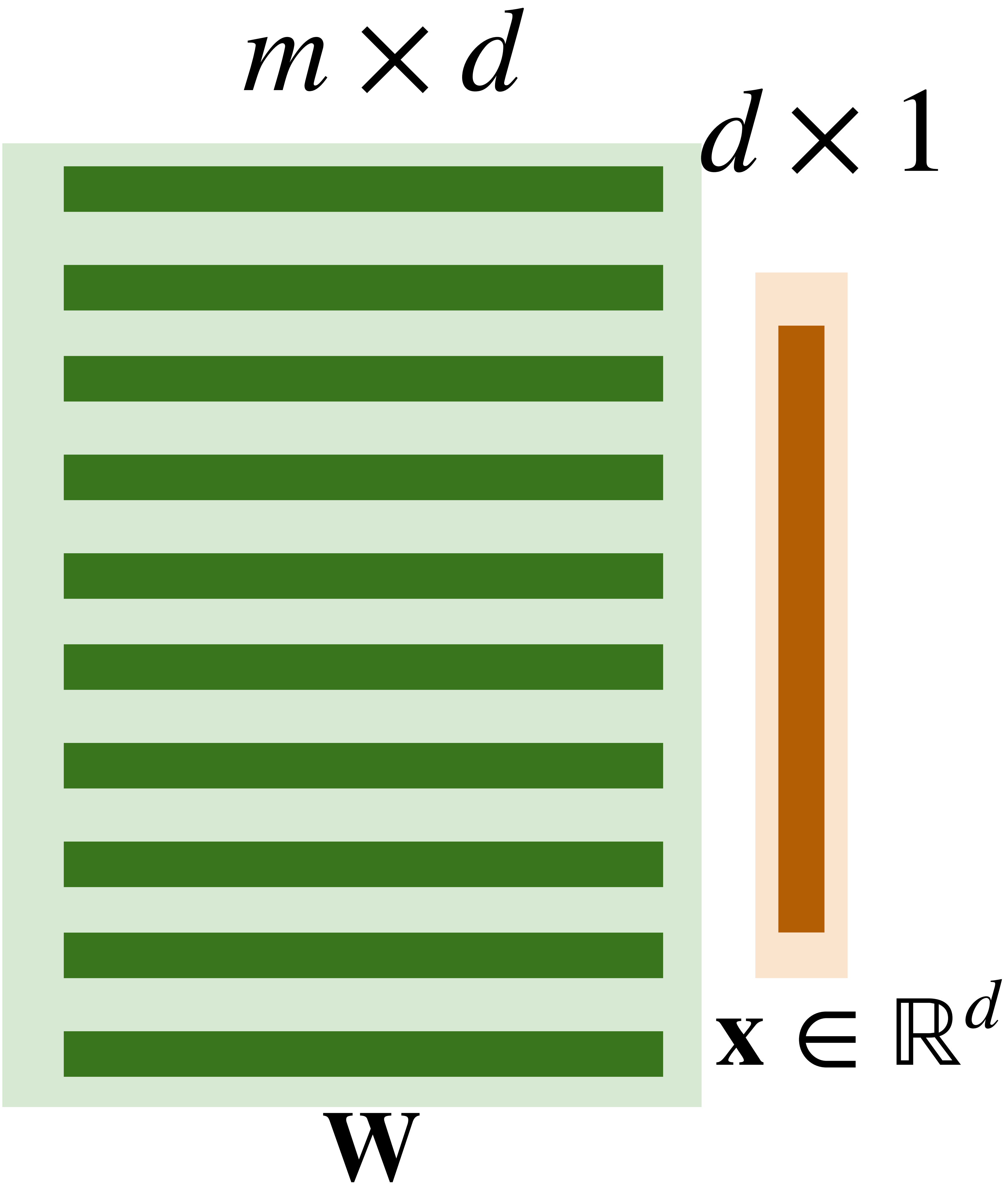
- Input $\mathbf{x} \in \mathbb{R}^d$
- Hidden $\mathbf{W}^{(1)} \in \mathbb{R}^{m \times d}, \mathbf{b} \in \mathbb{R}^m$
- Intermediate output

$$\mathbf{h} = \sigma(\mathbf{W}^{(1)}\mathbf{x} + \mathbf{b})$$

$$\mathbf{h} \in \mathbb{R}^m$$

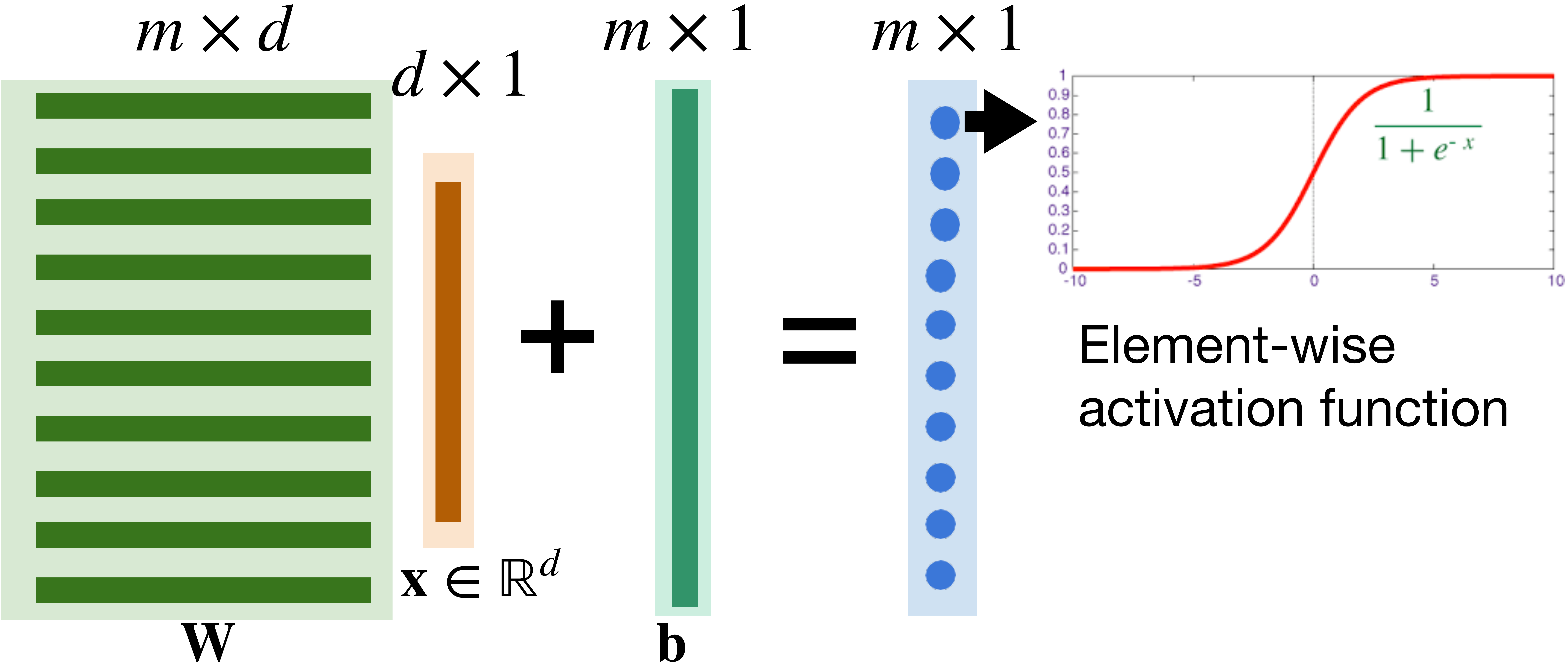


Review: A single layer in neural networks



Review: A single layer in neural networks

Key elements: linear operations + Nonlinear activations



Element-wise activation function

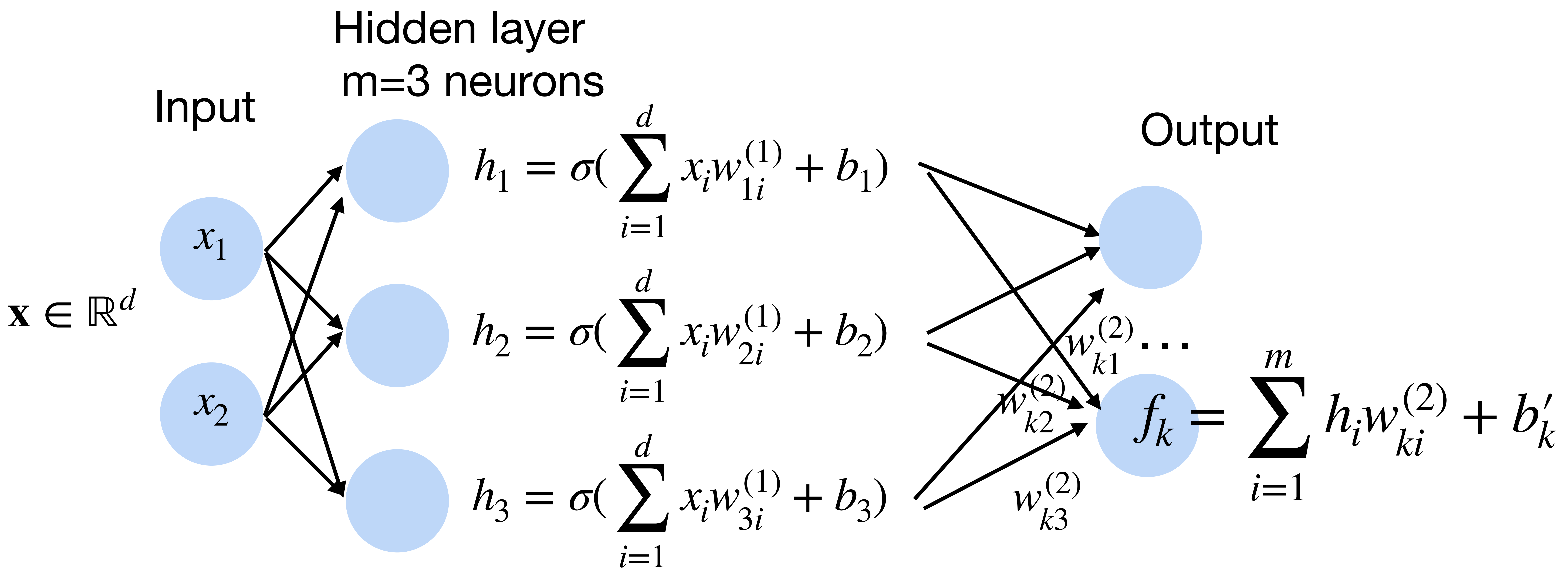
Review: Neural network for k-way classification

- K outputs in the final layer

Review: Neural network for k-way classification

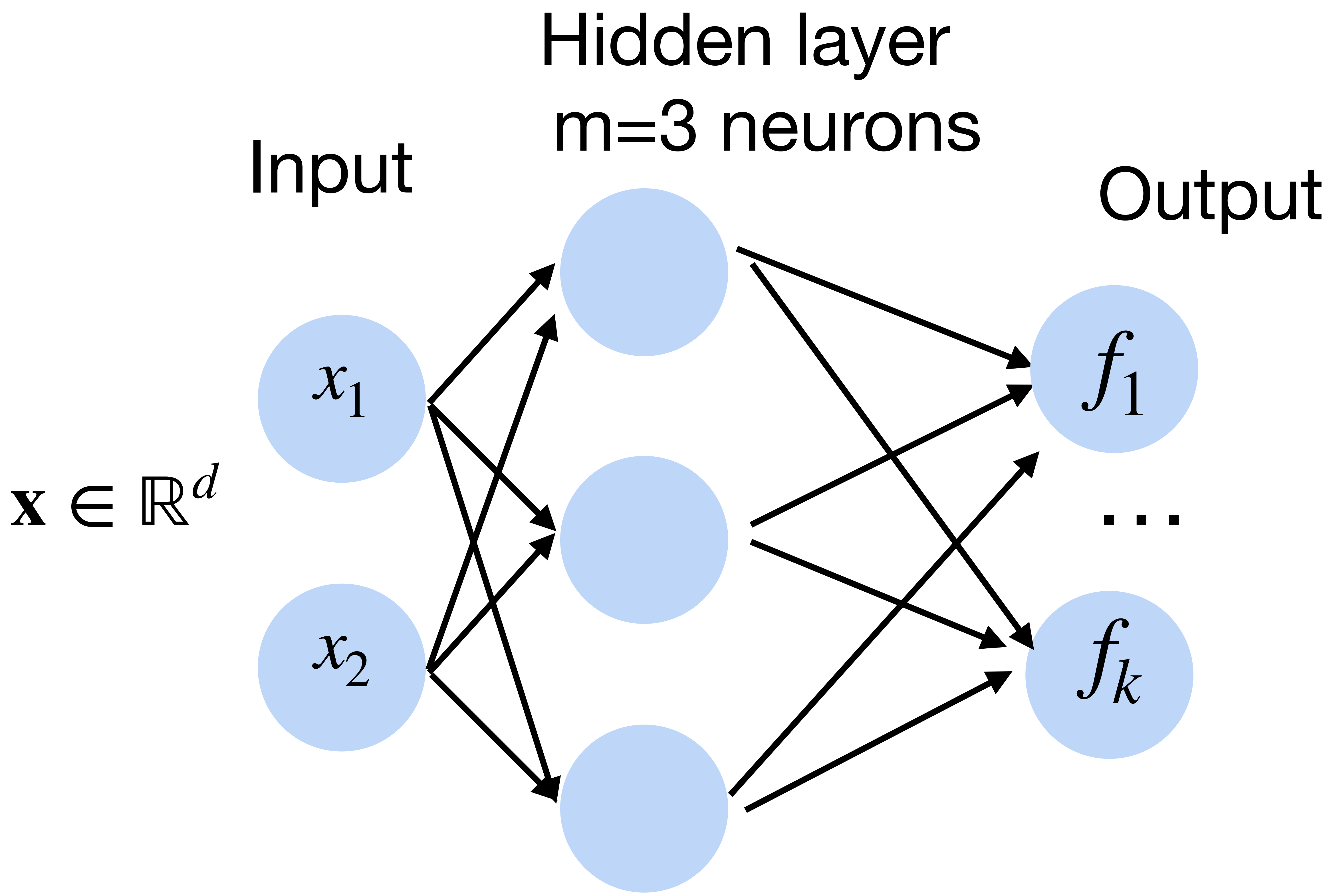
- K outputs units in the final layer

Multi-class classification (e.g., ImageNet with k=1000)



Review: Softmax

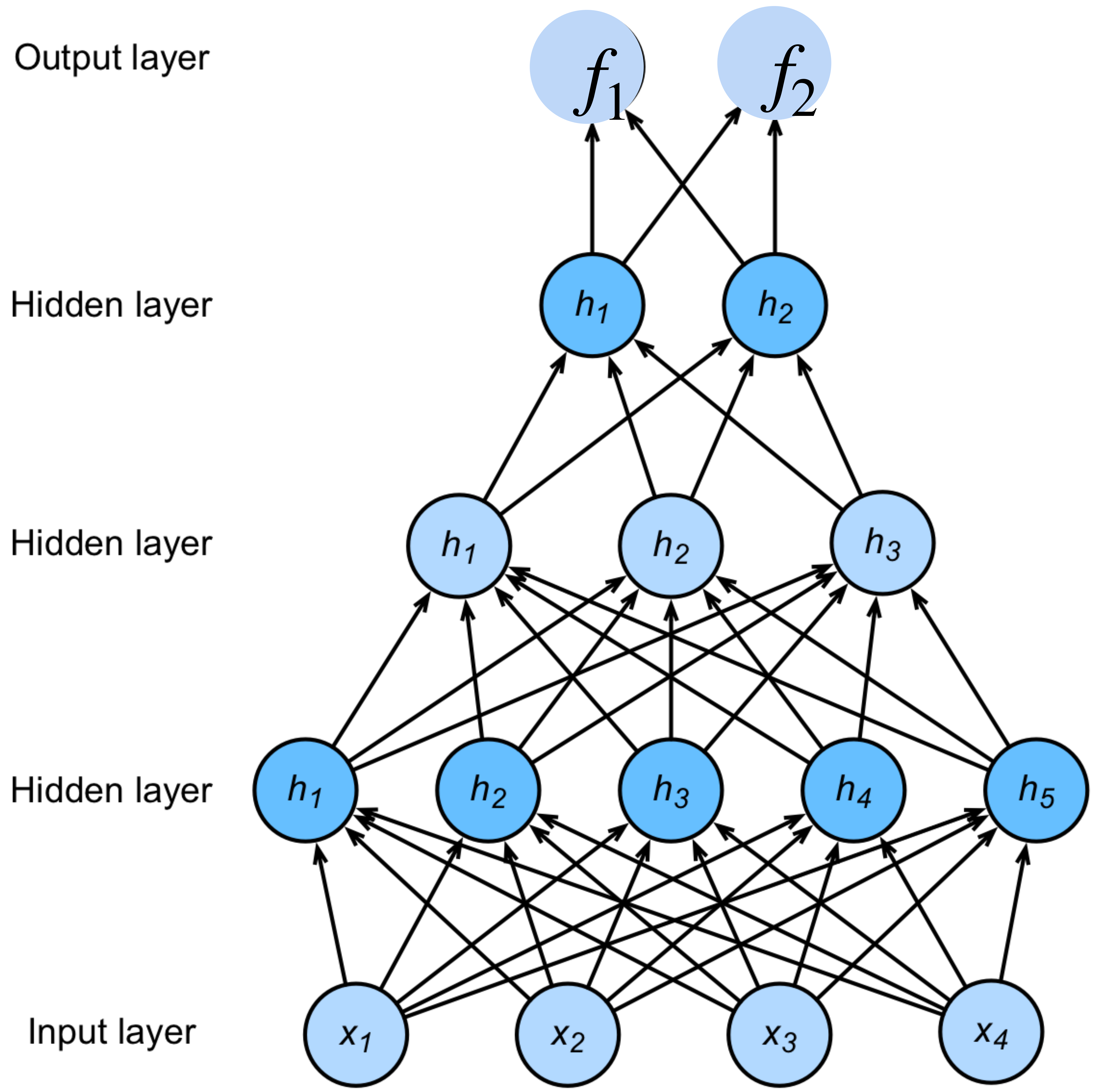
Turns outputs f into probabilities (sum up to 1 across k classes)



$$p(y \mid \mathbf{x}) = \text{softmax}(f)$$

$$= \frac{\exp f_y(x)}{\sum_i^k \exp f_i(x)}$$

Deep neural networks (DNNs)



$$\mathbf{h}_1 = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$

$$\mathbf{h}_2 = \sigma(\mathbf{W}_2\mathbf{h}_1 + \mathbf{b}_2)$$

$$\mathbf{h}_3 = \sigma(\mathbf{W}_3\mathbf{h}_2 + \mathbf{b}_3)$$

$$\mathbf{f} = \mathbf{W}_4\mathbf{h}_3 + \mathbf{b}_4$$

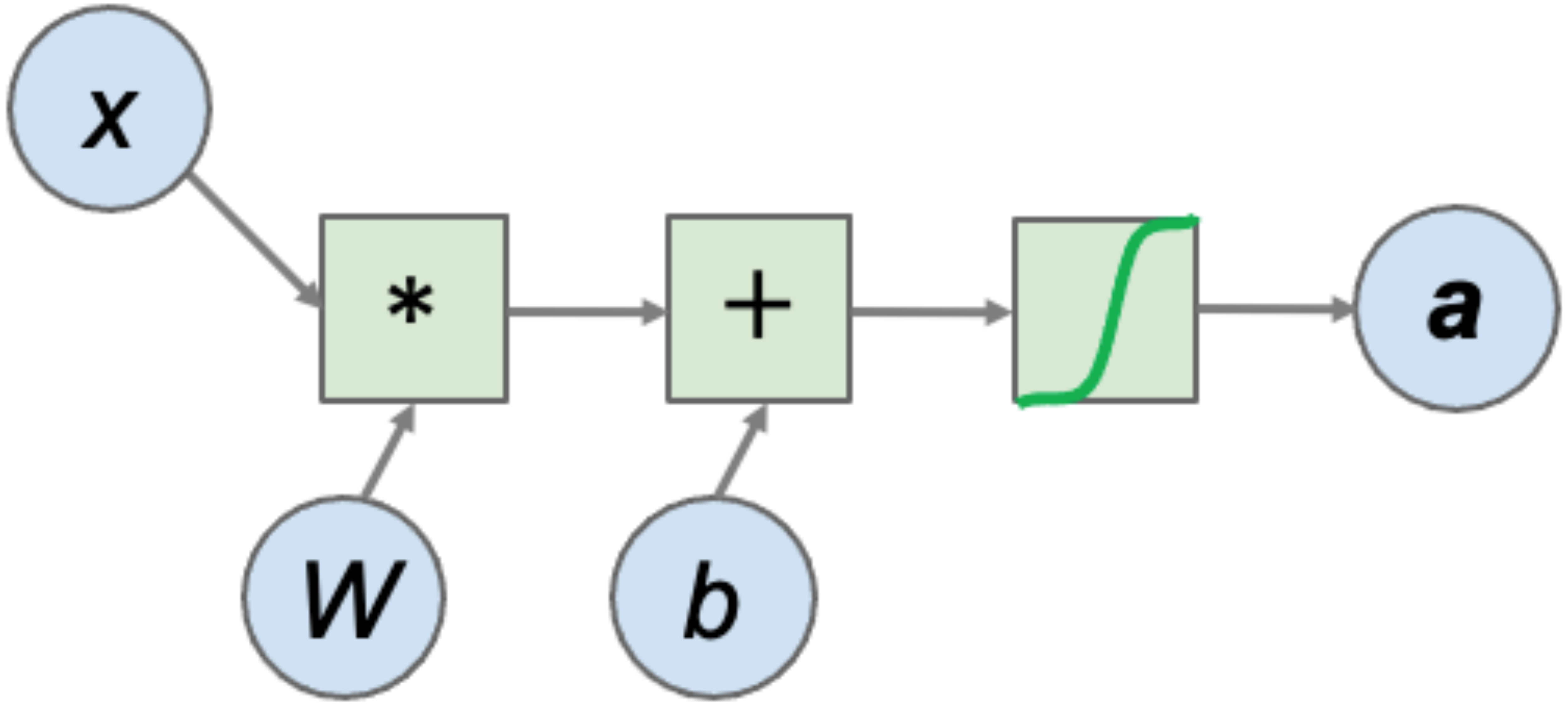
$$\mathbf{y} = \text{softmax}(\mathbf{f})$$

NNs are composition of nonlinear functions

Neural networks as variables + operations

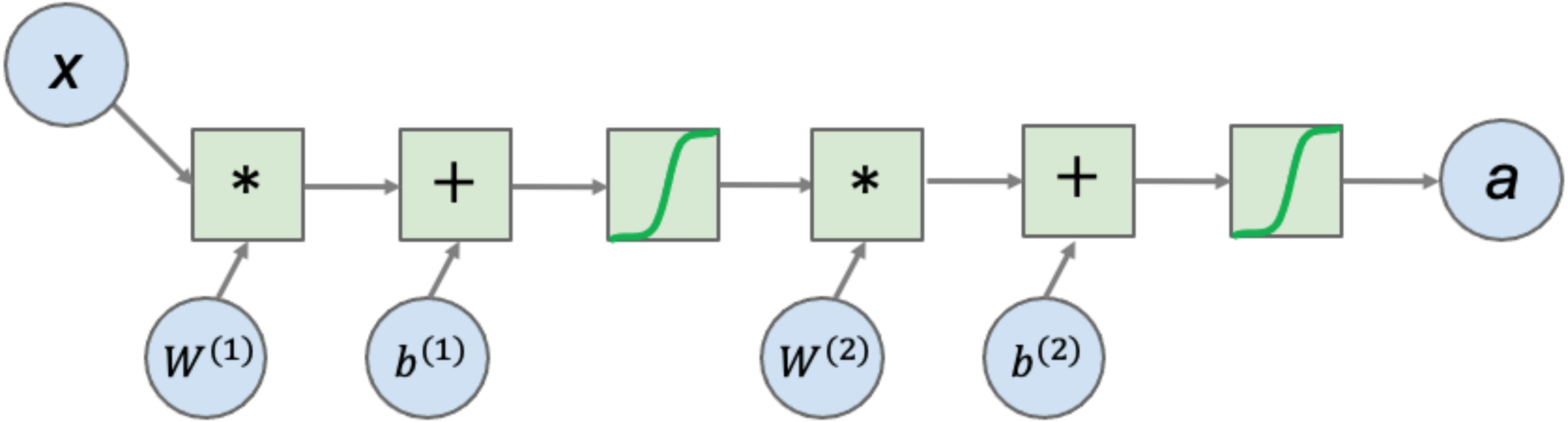
$$\mathbf{a} = \text{sigmoid}(\mathbf{W}\mathbf{x} + \mathbf{b})$$

- Decompose functions into atomic operations
- Separate data (variables) and computing (operations)
- Known as a **computational graph**



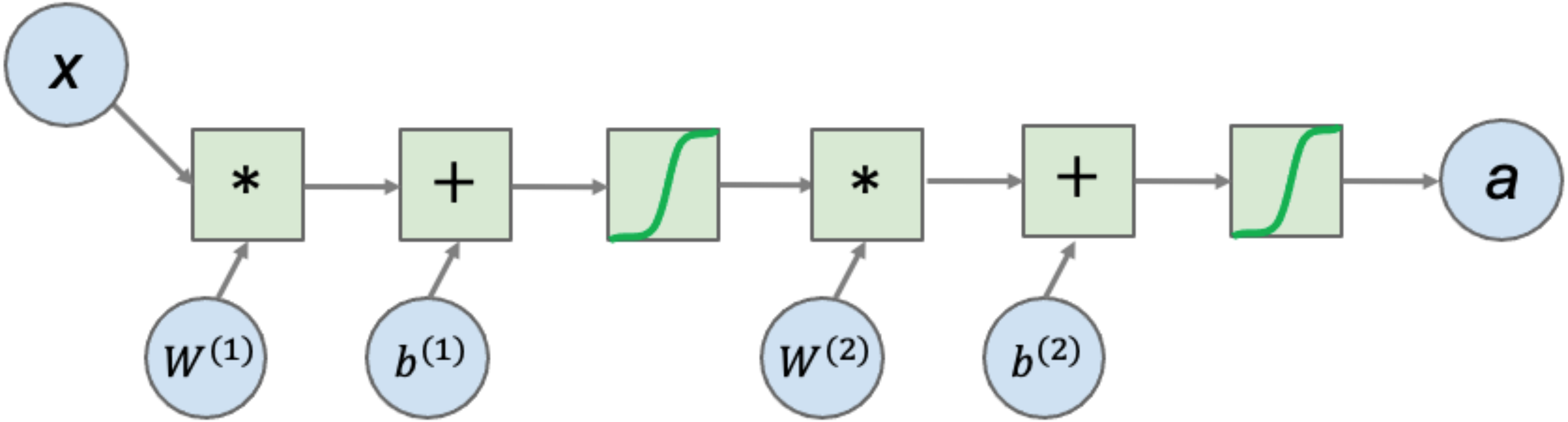
Neural networks as a computational graph

- A two-layer neural network



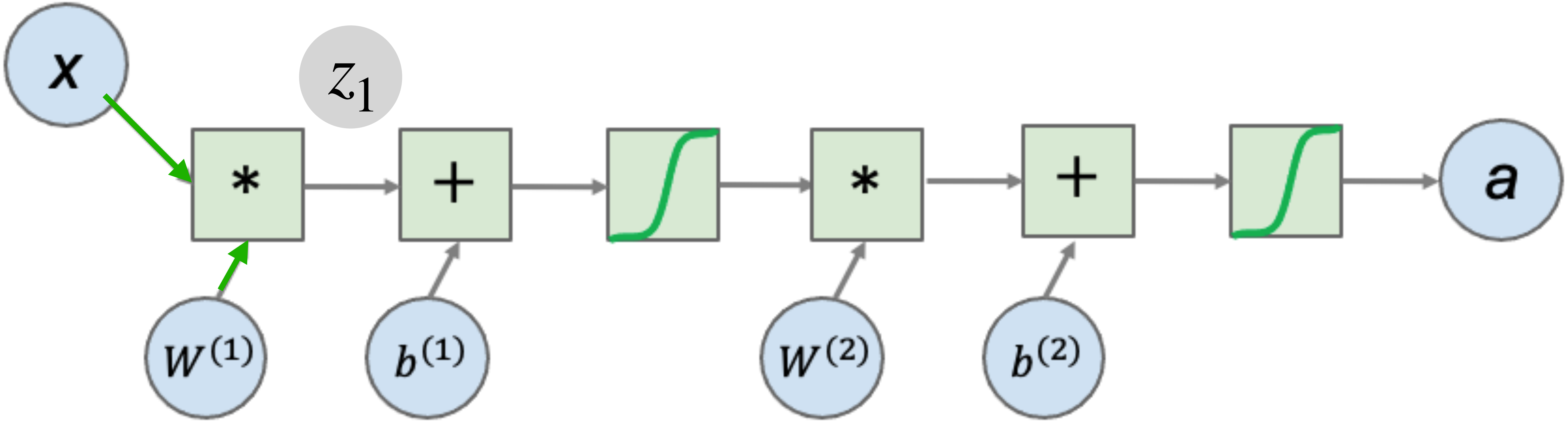
Neural networks as a computational graph

- A two-layer neural network
- Forward propagation vs. backward propagation



Neural networks: forward propagation

- A two-layer neural network
- Intermediate variables Z



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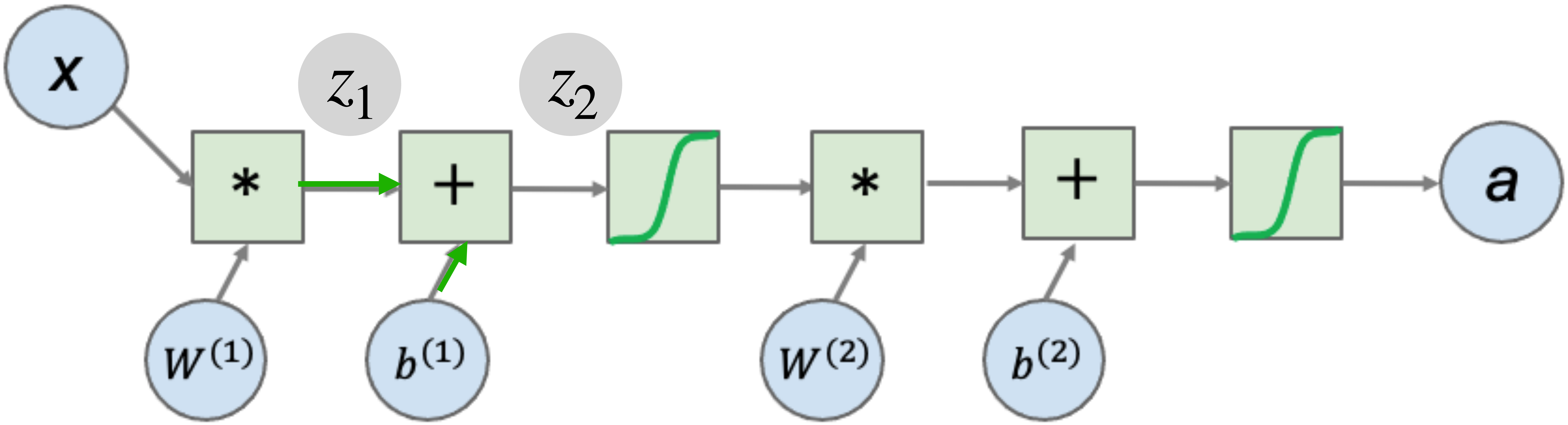

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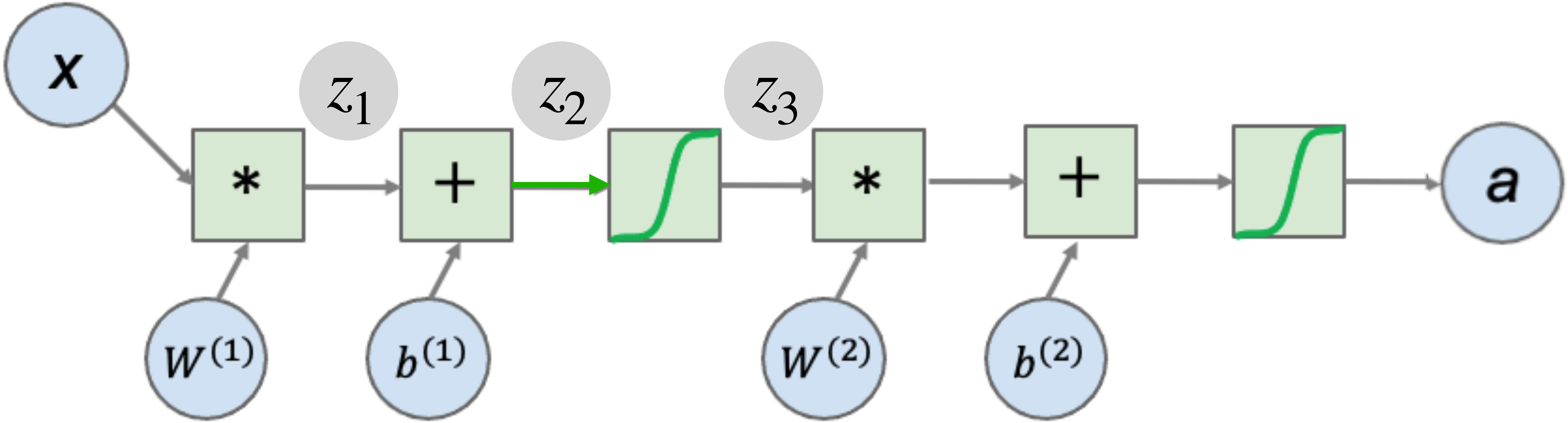

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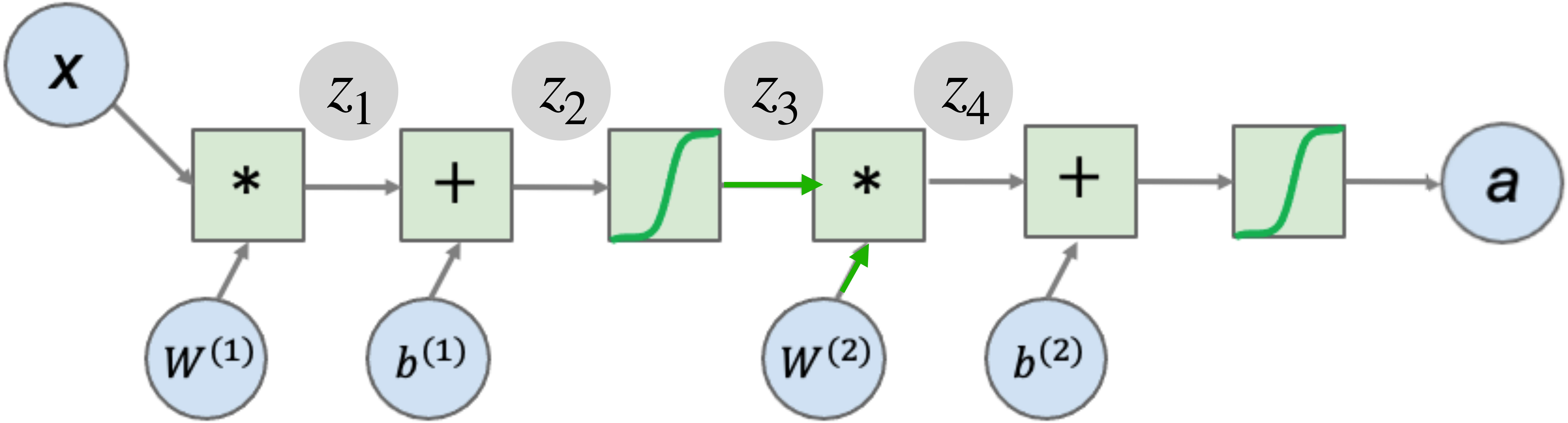

Neural networks: forward propagation

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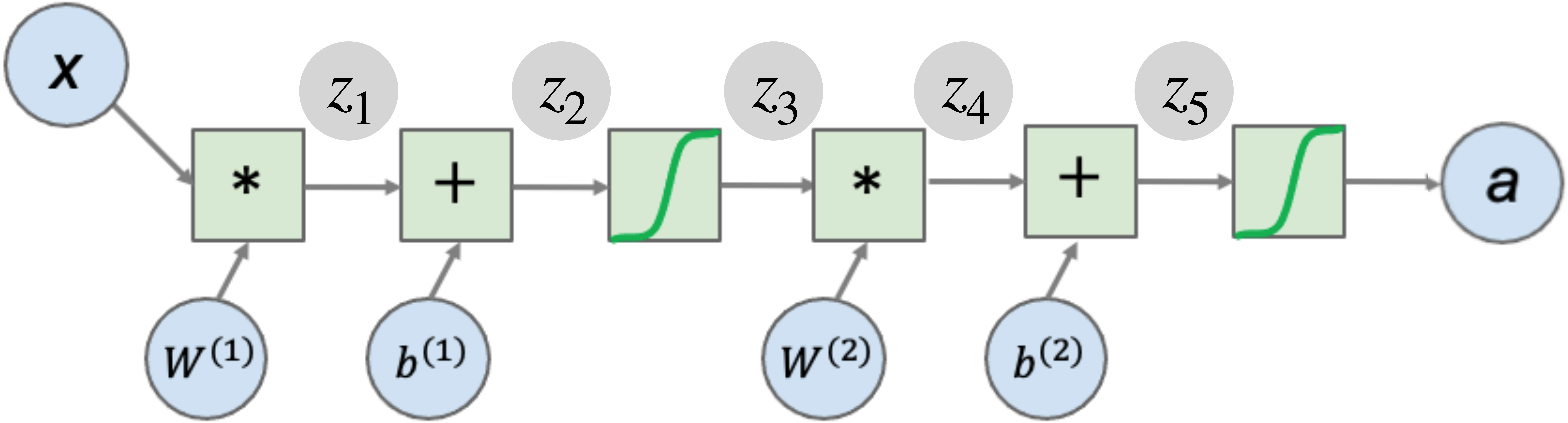
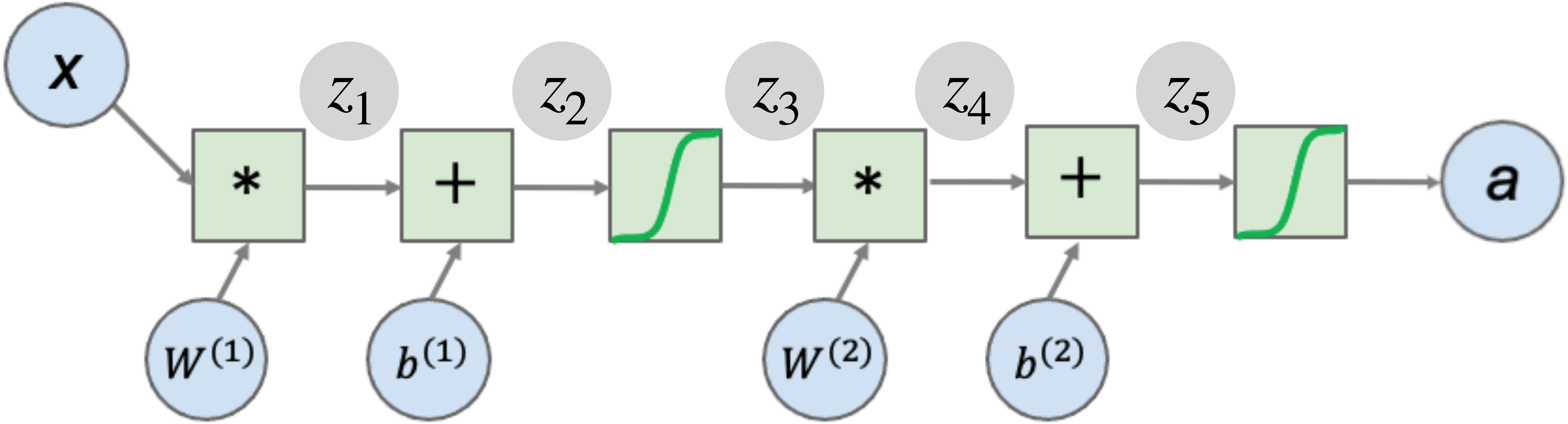


Neural networks: backward propagation

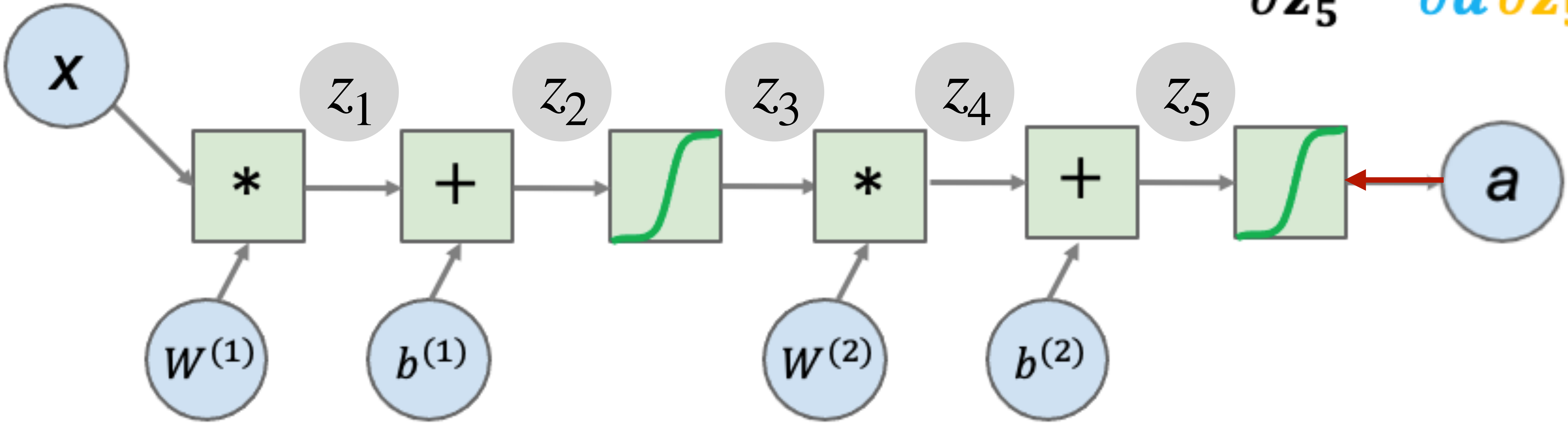
- A two-layer neural network
- Assuming forward propagation is done
- Minimize a **loss function** L



Neural networks: backward propagation

- A two-layer neural network
- Assuming forward propagation is done
- Minimize a **loss function** L

$$\frac{\partial L}{\partial z_5} = \frac{\partial L}{\partial a}\frac{\partial a}{\partial z_5}$$

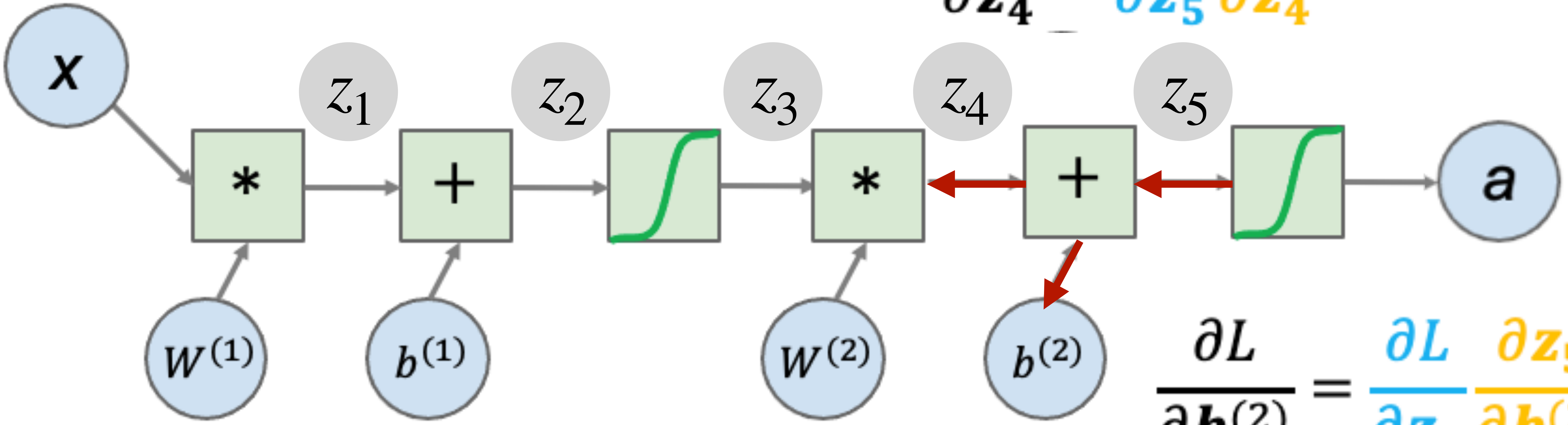


z_1 z_2 z_3 z_4 z_5

Neural networks: backward propagation

- A two-layer neural network
- Assuming forward propagation is done
- Minimize a **loss function** L

$$\frac{\partial L}{\partial \boldsymbol{z_4}} = \frac{\partial L}{\partial \boldsymbol{z_5}} \frac{\partial \boldsymbol{z_5}}{\partial \boldsymbol{z_4}}$$

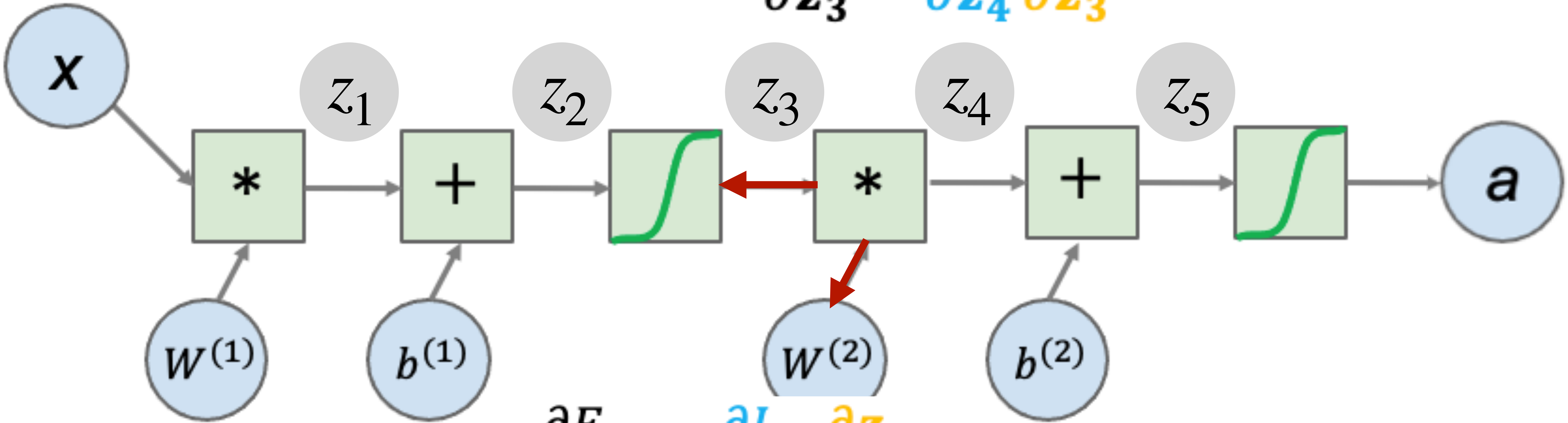


$$\frac{\partial L}{\partial \boldsymbol{b}^{(2)}} = \frac{\partial L}{\partial \boldsymbol{z_5}} \frac{\partial \boldsymbol{z_5}}{\partial \boldsymbol{b}^{(2)}}$$

Neural networks: backward propagation

- A two-layer neural network
- Assuming forward propagation is done

$$\frac{\partial L}{\partial \mathbf{z_3}} = \frac{\partial L}{\partial \mathbf{z_4}} \frac{\partial \mathbf{z_4}}{\partial \mathbf{z_3}}$$



$$\frac{\partial E}{\partial \mathbf{W}^{(2)}} = \frac{\partial L}{\partial \mathbf{z_4}} \frac{\partial \mathbf{z_4}}{\partial \mathbf{W}^{(2)}}$$

Backward propagation: A modern treatment

- Define a neural network as a computational graph
- Must be a directed graph
- Nodes as variables and operations
- All operations must be **differentiable**

Part II: Numerical Stability

Gradients for Neural Networks

- Compute the gradient of the loss ℓ w.r.t. $\mathbf{W}_t$

$$\frac{\partial \ell}{\partial \mathbf{W}^t} = \frac{\partial \ell}{\partial \mathbf{h}^d} \underbrace{\frac{\partial \mathbf{h}^d}{\partial \mathbf{h}^{d-1}} \cdots \frac{\partial \mathbf{h}^{t+1}}{\partial \mathbf{h}^t}}_{\text{Multiplication of } \textit{many} \text{ matrices}} \frac{\partial \mathbf{h}^t}{\partial \mathbf{W}^t}$$

Wikipedia

Two Issues for Deep Neural Networks

$$\prod_{i=t}^{d-1} \frac{\partial \mathbf{h}^{i+1}}{\partial \mathbf{h}^{i}}$$

Gradient Exploding

$$1.5^{100} \approx 4 \times 10^{17}$$

Gradient Vanishing

$$0.8^{100} \approx 2 \times 10^{-10}$$

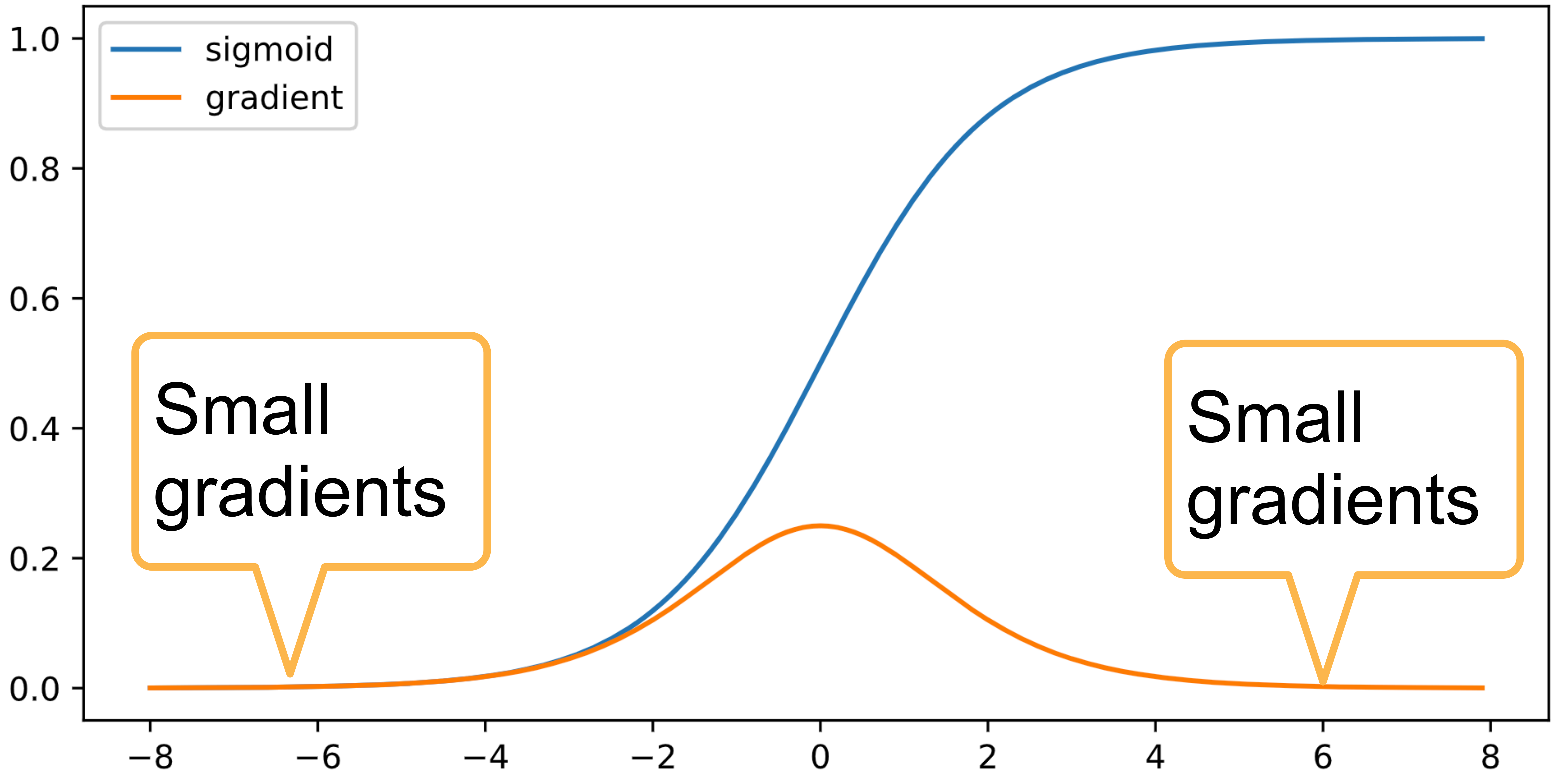
Issues with Gradient Exploding

- Value out of range: infinity value (NaN)
- Sensitive to learning rate (LR)
  - Not small enough LR -> large weights -> larger gradients
  - Too small LR -> No progress
  - May need to change LR dramatically during training

Gradient Vanishing

- Use sigmoid as the activation function

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



Issues with Gradient Vanishing

- Gradients with value 0
- No progress in training
  - No matter how to choose learning rate
- Severe with bottom layers
  - Only top layers are well trained
  - No benefit to make networks deeper

How to stabilize training?

Stabilize Training: Practical Considerations

- Goal: make sure gradient values are in a proper range
  - E.g. in [1e-6, 1e3]
- Multiplication -> plus
  - Architecture change (e.g., ResNet)
- Normalize
  - Batch Normalization, Gradient clipping
- Proper activation functions

Part III: Generalization & Regularization

How good are the models?

Training Error and Generalization Error

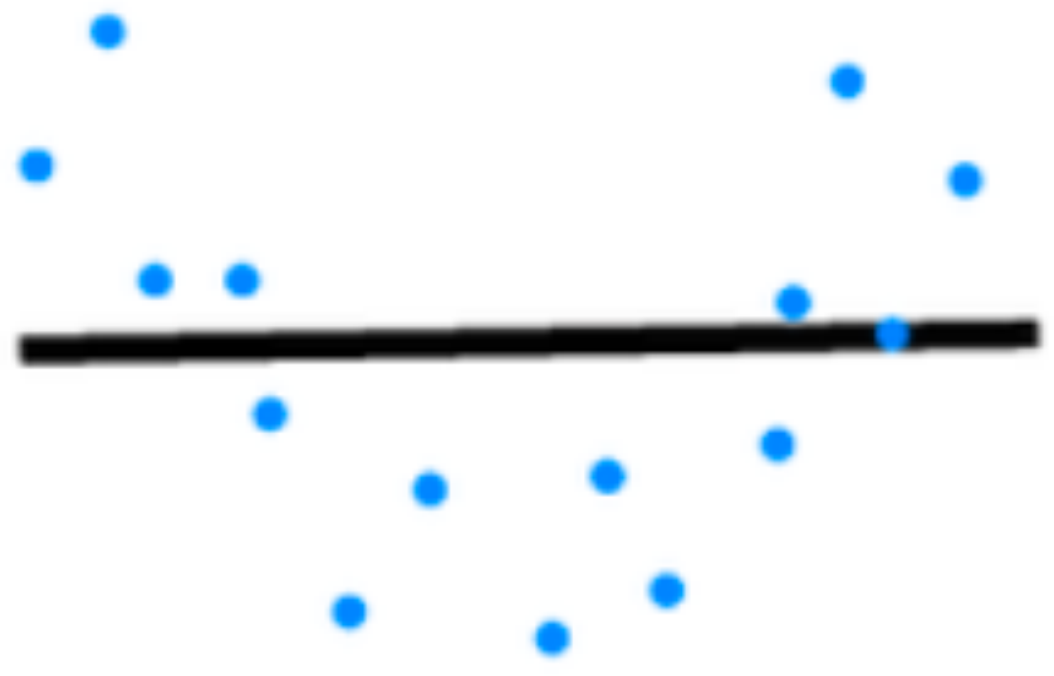
- Training error: model error on the training data
- **Generalization error**: model error on new data
- Example: practice a future exam with past exams
  - Doing well on past exams (training error) doesn’t guarantee a good score on the future exam (generalization error)

Underfitting
Overfitting

Image credit: hackernoon.com

Model Capacity

- The ability to fit variety of functions
- Low capacity models struggles to fit training set
  - Underfitting
- High capacity models can memorize the training set
  - Overfitting



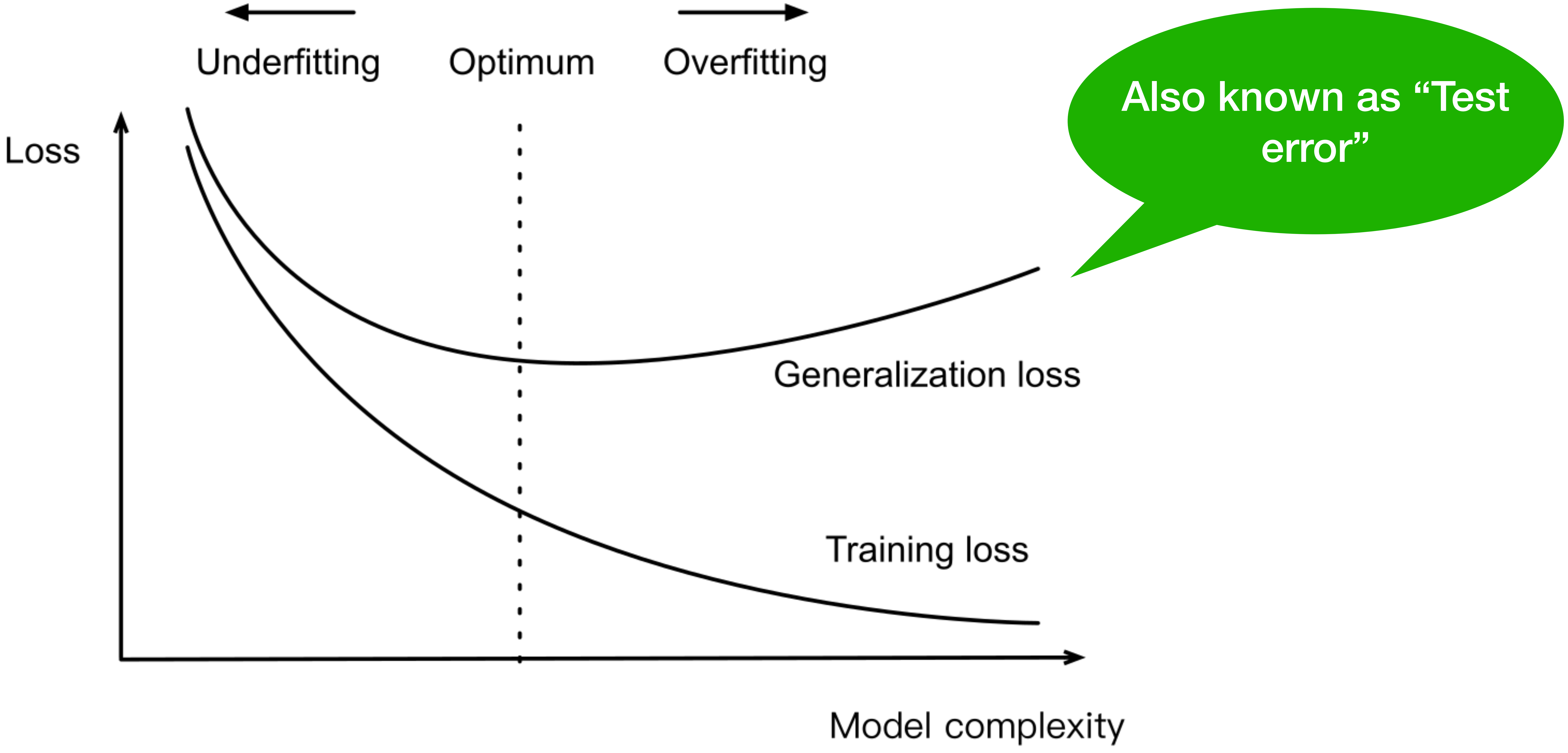
Underfitting and Overfitting

Data complexity

Model capacity

	Simple	Complex
Low	Normal	Underfitting
High	Overfitting	Normal

Influence of Model Complexity



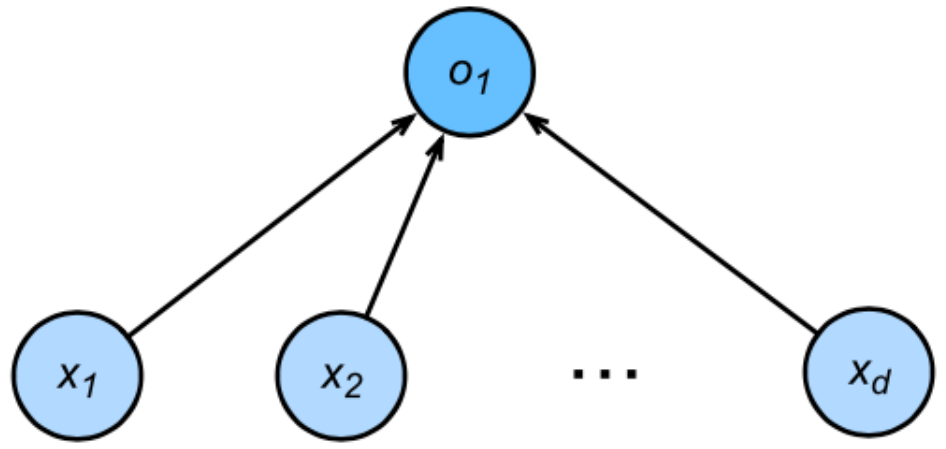
Estimate Neural Network Capacity

- It’s hard to compare complexity between different algorithms
  - e.g. tree vs neural network

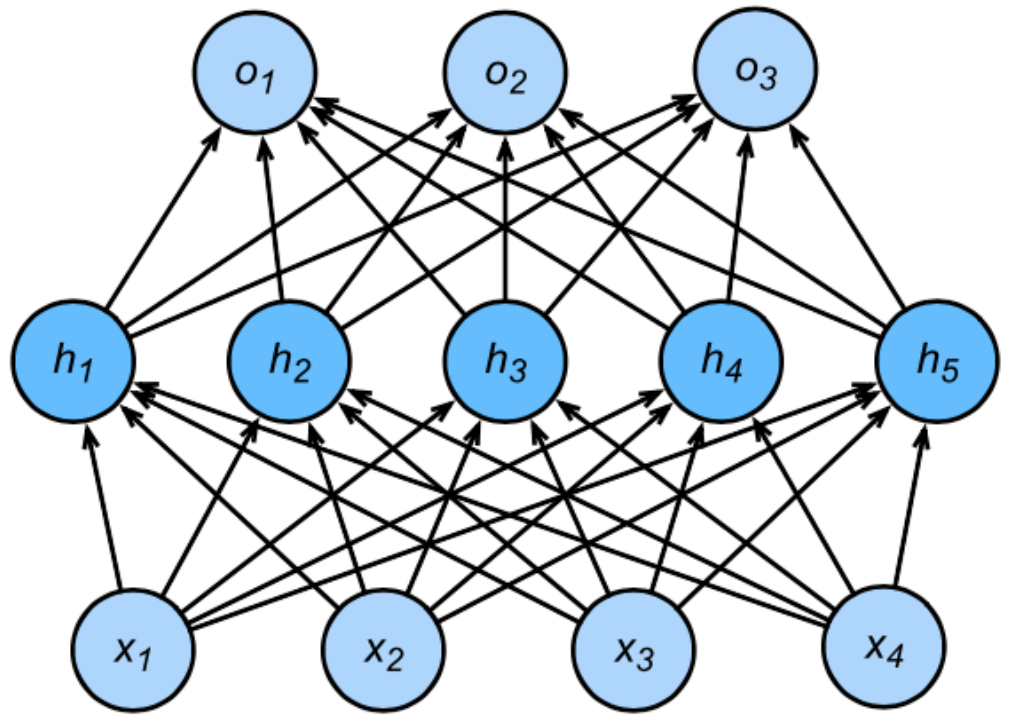
Estimate Neural Network Capacity

- It's hard to compare complexity between different algorithms
  - e.g. tree vs neural network
- Given an algorithm family, two main factors matter:
  - The number of parameters
  - The values taken by each parameter

$$d + 1$$

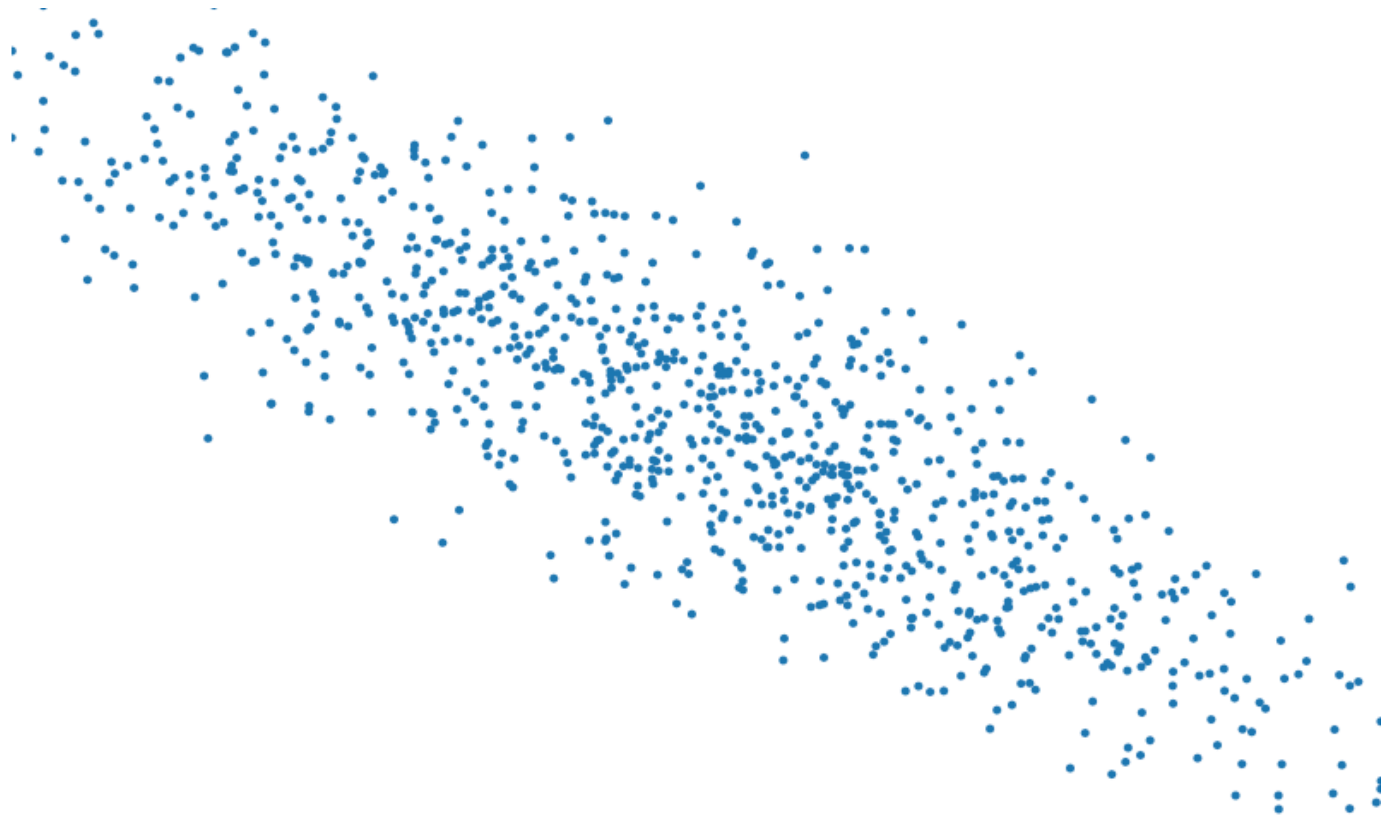


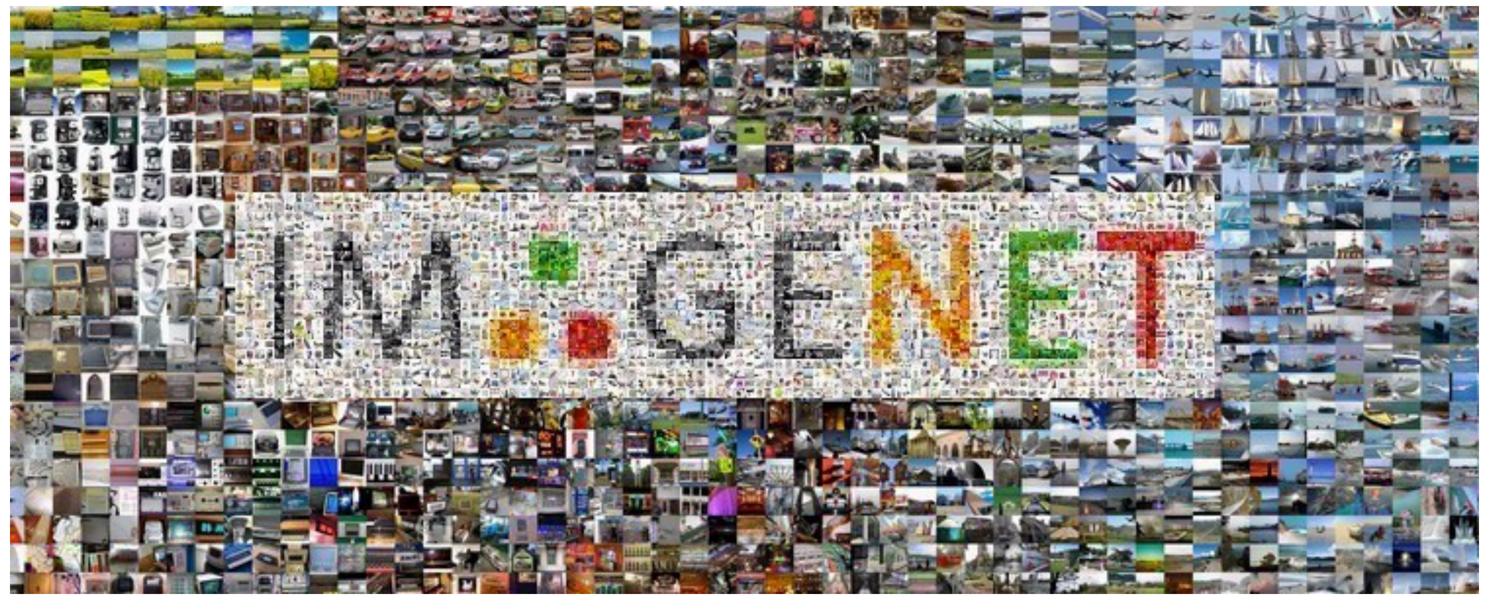
$$(d + 1)m + (m + 1)k$$



Data Complexity

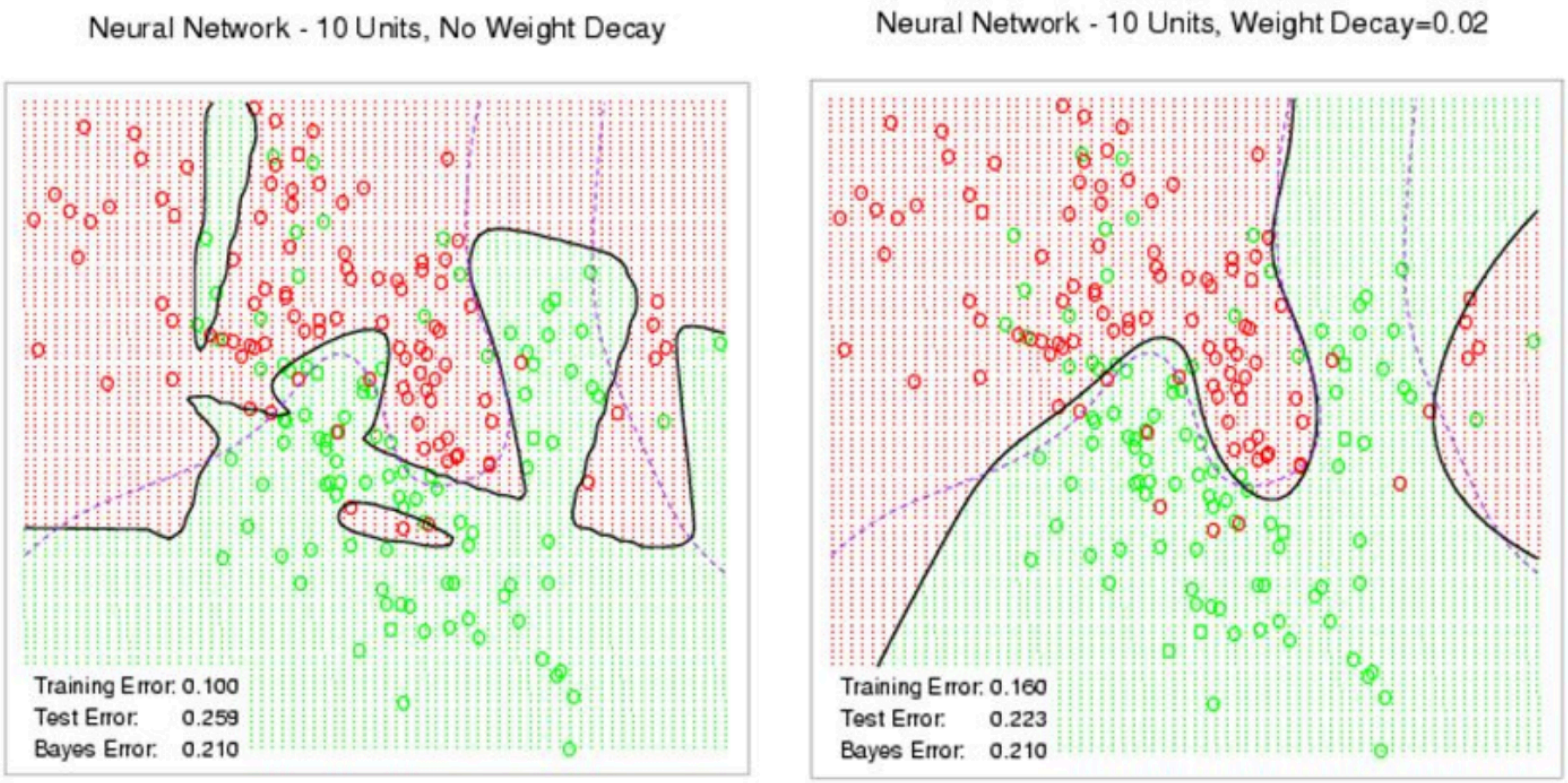
- Multiple factors matters
  - # of examples
  - # of features in each example
  - time/space structure
  - # of labels





How to regularize the model for better generalization?

Weight Decay

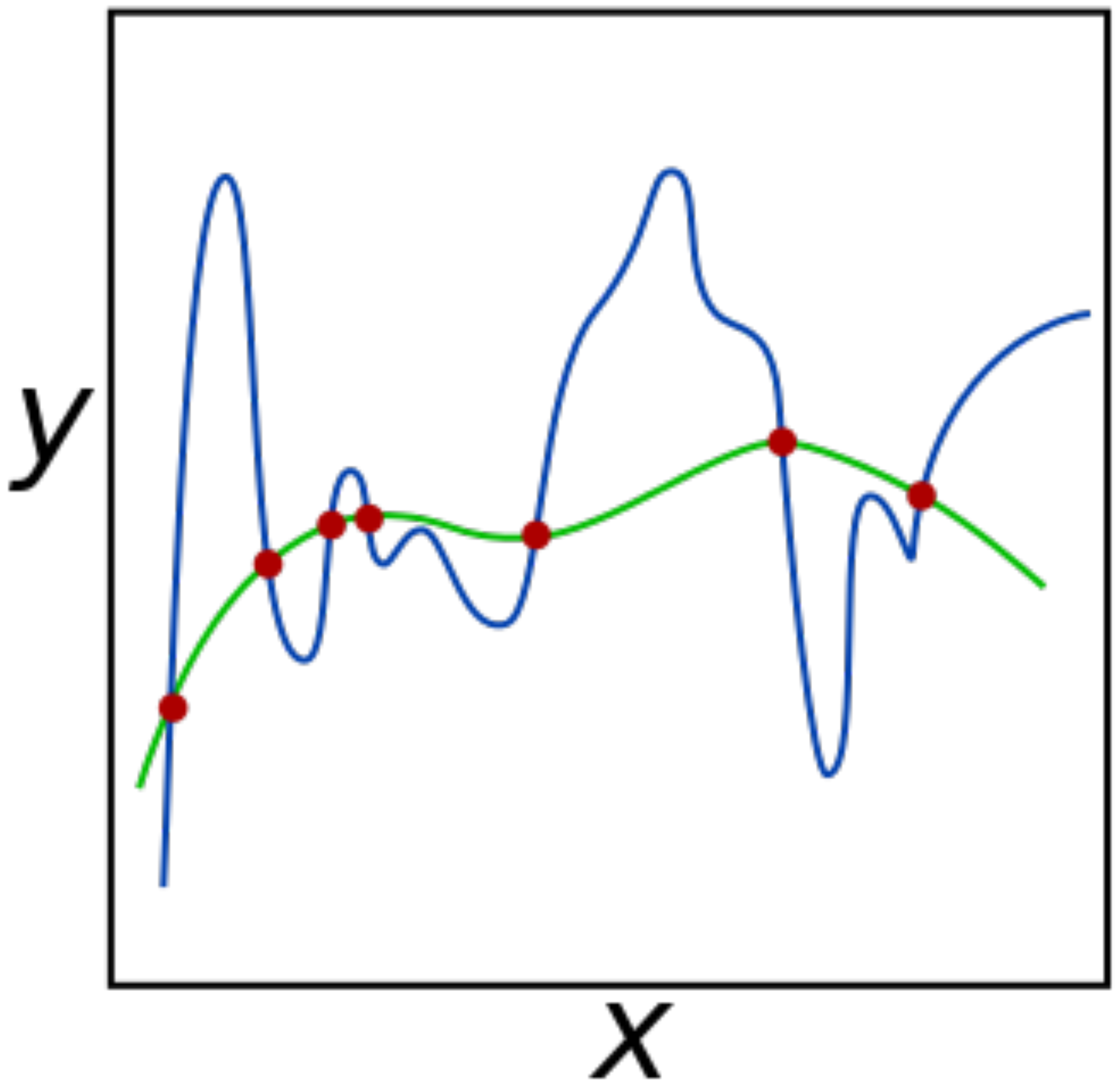


Squared Norm Regularization as Hard Constraint

- Reduce model complexity by limiting value range

$$\min \ \ell(\mathbf{w}, b) \quad \text{subject to} \quad \|\mathbf{w}\|^2 \leq \theta$$

- Often do not regularize bias *b*
  - Doing or not doing has little difference in practice
- A small θ means more regularization



Squared Norm Regularization as Soft Constraint

- We can rewrite the hard constraint version as

$$\min \ \ell(\mathbf{w}, b) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

Squared Norm Regularization as Soft Constraint

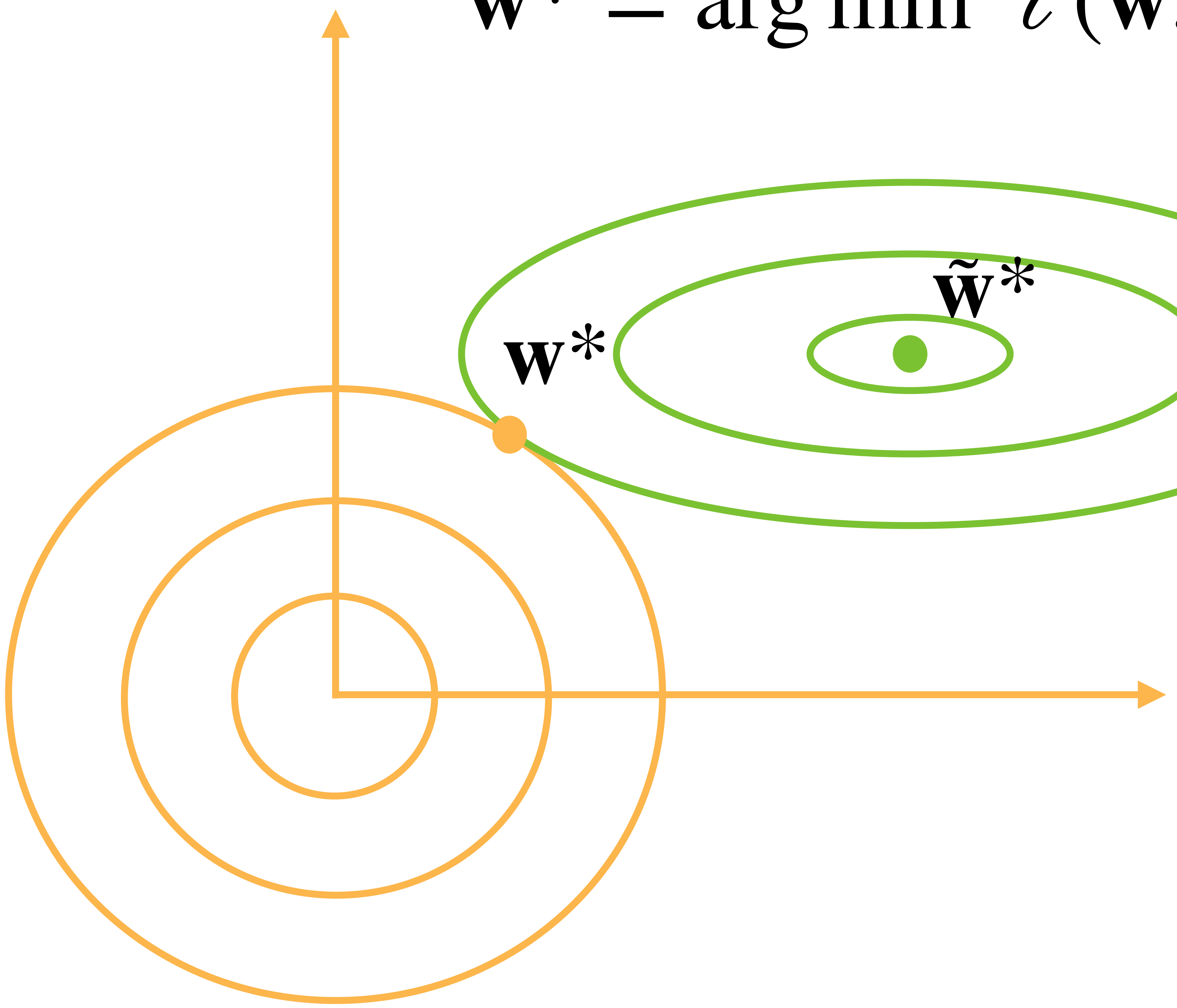
- We can rewrite the hard constraint version as

$$\min \ \ell(\mathbf{w}, b) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

  - Hyper-parameter λ controls regularization importance
  - $\lambda = 0$: no effect
  - $\lambda \to \infty, \mathbf{w}^* \to \mathbf{0}$

Illustrate the Effect on Optimal Solutions

$$\mathbf{w}^* = \arg\min \ \ell(\mathbf{w}, b) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$



$$\tilde{\mathbf{w}}^* = \arg\min \ \ell(\mathbf{w}, b)$$

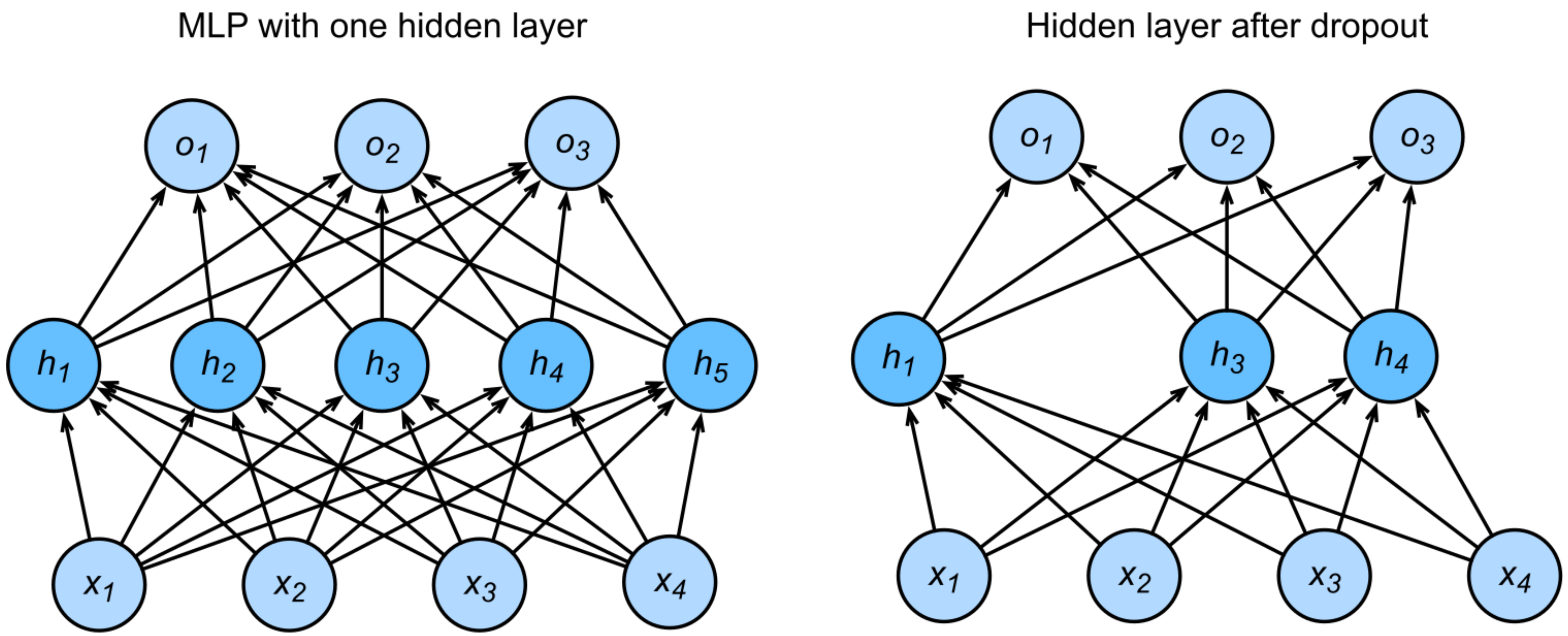
Dropout

Hinton et al.

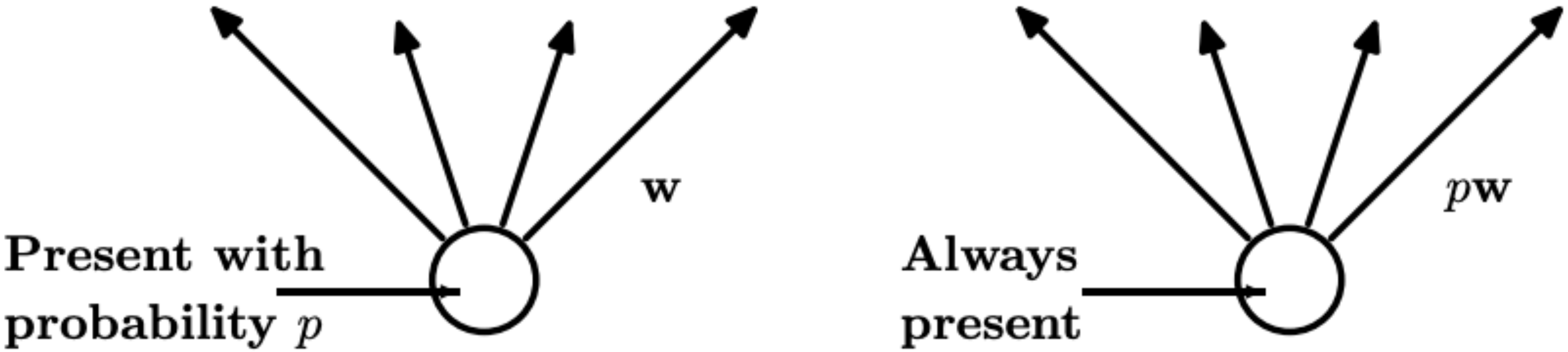
Apply Dropout

- Often apply dropout on the output of hidden fully-connected layers

$$\mathbf{h} = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$
$$\mathbf{h}' = \text{dropout}(\mathbf{h})$$
$$\mathbf{o} = \mathbf{W}_2\mathbf{h}' + \mathbf{b}_2$$
$$\mathbf{y} = \text{softmax}(o)$$



Dropout



(a) At training time

(b) At test time

Figure 2: **Left**: A unit at training time that is present with probability p and is connected to units in the next layer with weights $\mathbf{w}$. **Right**: At test time, the unit is always present and the weights are multiplied by p. The output at test time is same as the expected output at training time.

Dropout

Hinton et al.

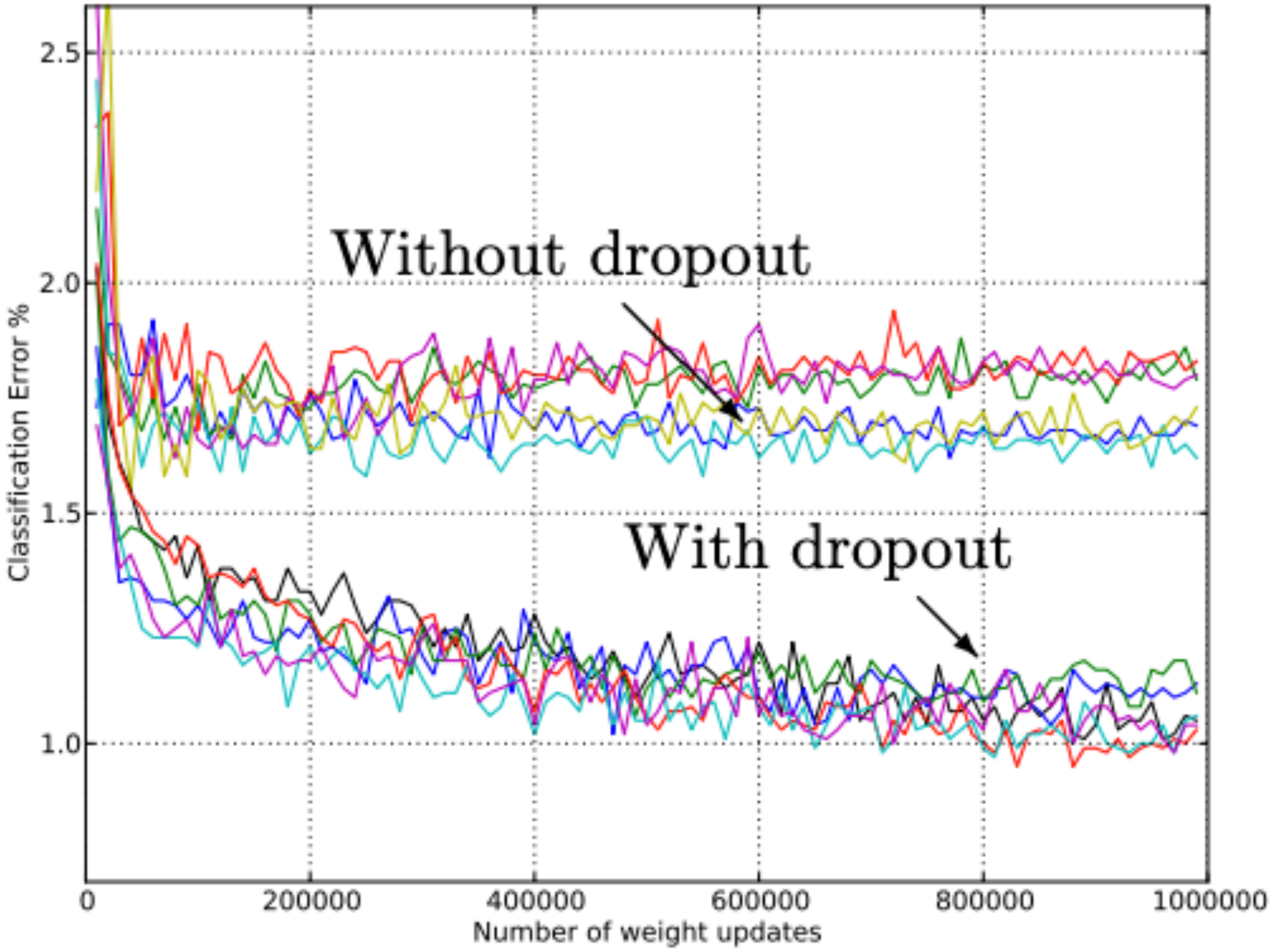


Figure 4: Test error for different architectures with and without dropout. The networks have 2 to 4 hidden layers each with 1024 to 2048 units.

What we’ve learned today…

- Deep neural networks
  - Computational graph (forward and backward propagation)
- Numerical stability in training
  - Gradient vanishing/exploding
- Generalization and regularization
  - Overfitting, underfitting
  - Weight decay and dropout

Thanks!

Based on slides from Xiaojin (Jerry) Zhu, Yingyu Liang, Yin Li (CS540 @ UW-Madison) and Alex Smola:
https://courses.d2l.ai/berkeley-stat-157/units/mlp.html