Introduction to Deep Learning

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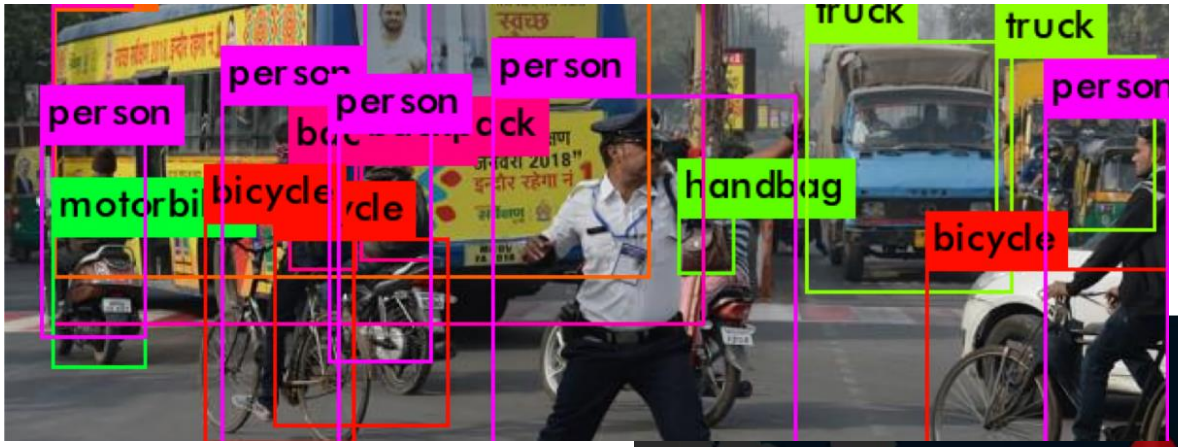
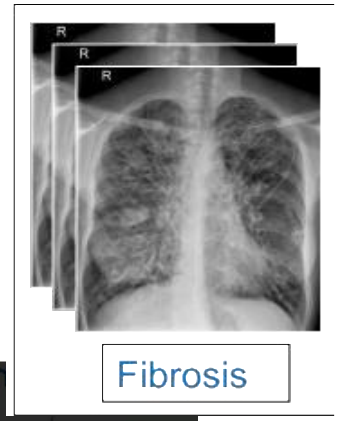
Introduction & Outline

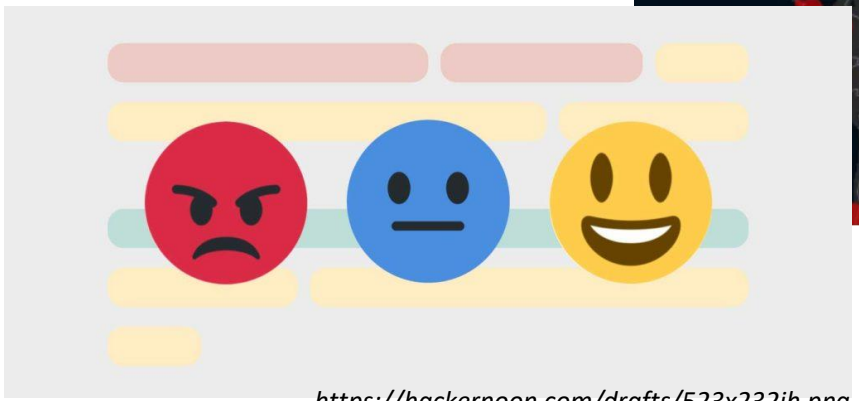
http://people.csail.mit.edu/stefje/

- **Today: Feedforward neural networks**
  - How do neural networks represent data?
  - How can we “train” a neural network?
  - Example: Fashion MNIST
- **Wed:** Neural networks for images: convolutional neural networks
- **Fri:** Transfer learning and Neural networks for graphs

Predictions from “everything”







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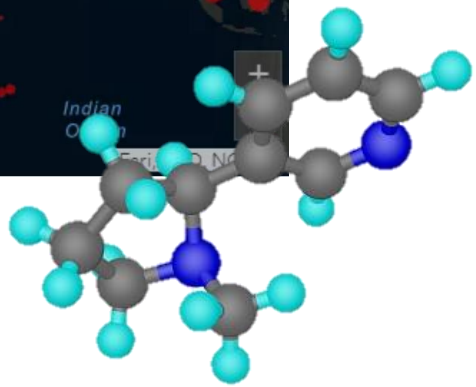
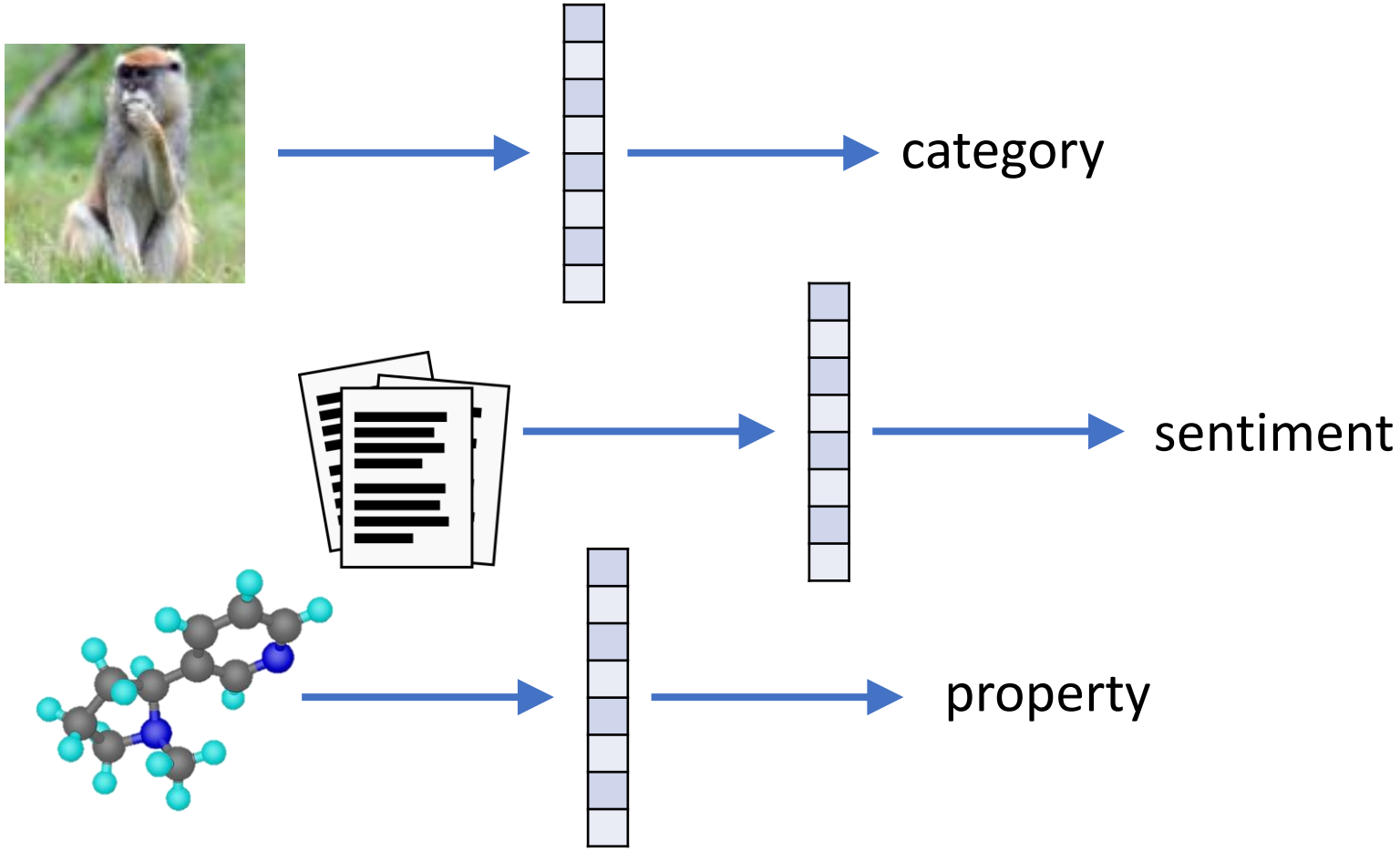
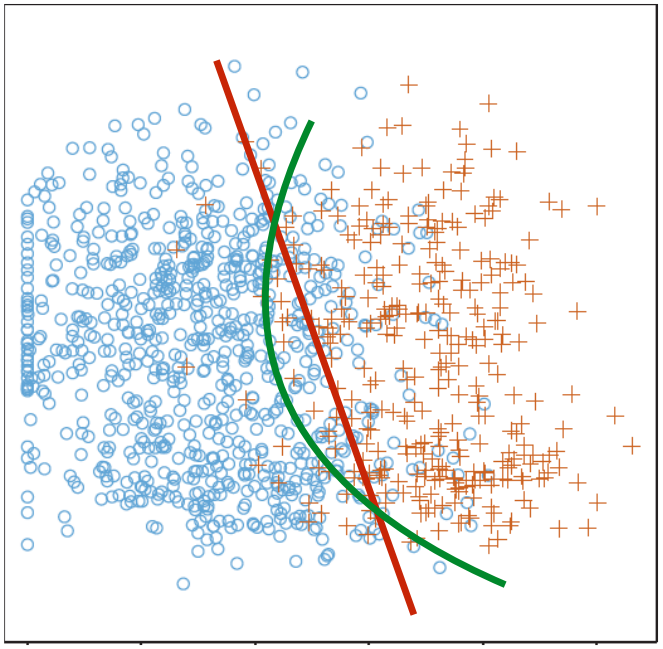


A general strategy

- Encode data as useful, informative feature vectors



Feature encodings: we've seen them before

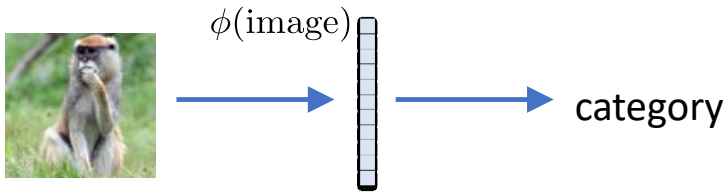


- Linear classifiers: compare $\checkmark^T X$ to a threshold
  - learn "good" vector $\checkmark$ and threshold
- Nonlinear classifiers: compare $h(X)$ to a threshold
  - learn "good" function h and threshold

- Nonlinear classifier $\checkmark_1 X_1 + \checkmark_2 X_2 + \checkmark_{12} X_1 X_2$ is actually linear if we redefine $X = (X_1, X_2, X_1 X_2)$
- Feature-based linear classifier: compare $\checkmark^T \varphi(X)$ to a threshold

A general strategy

- Encode data as useful, informative feature vectors



- But, what is a good encoding?
- **Neural Networks: learn it from the data!**
- Challenge: learn encoding and prediction *simultaneously*

Specialized methods to encode

$\phi(\text{image})$

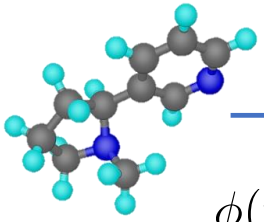
category

CNN (Wed)

RNN

$\phi(\text{text})$

sentiment



$\phi(\text{molecule})$

property

GNN (Fri)

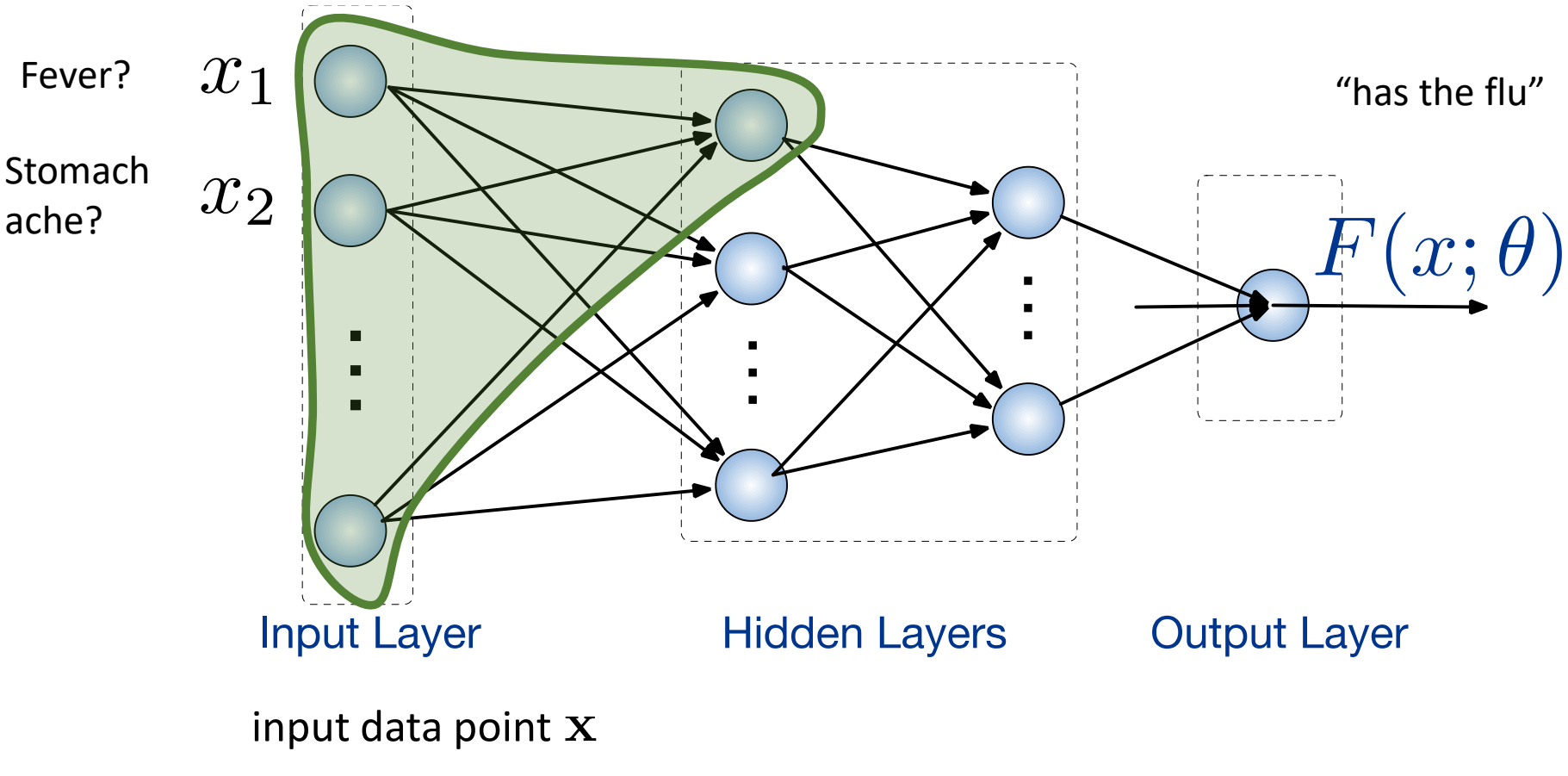
Deep Learning: reasons for success

- **Lots of data**
  - many problems can only be solved at scale
- **Computational resources** (e.g. GPUs)
  - systems that support running deep ML algorithms at scale
- **Large models are easier to train**
  - can be successfully estimated with simple gradient based algorithms
- **Flexible neural "lego pieces"**
  - common representations, diversity of architecture choices

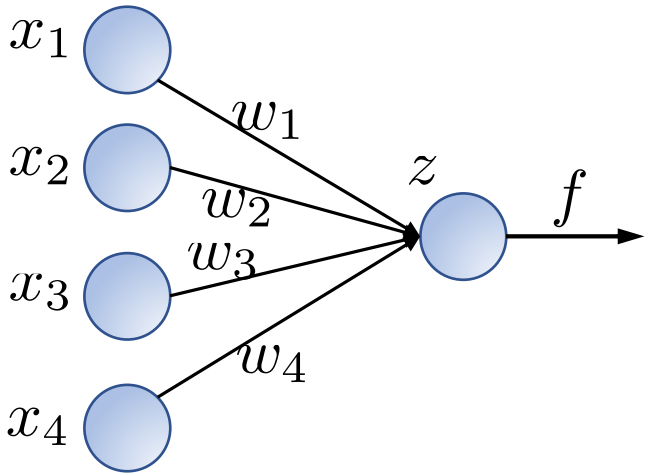
Outline

- **How do neural networks represent data?**
- How can we “train” a neural network?
- Example: Fashion MNIST

Feedforward neural networks



A unit in a neural network



1. Weighted sum of inputs:

$$\sum_{j=1}^{d} w_j x_j = \mathbf{w}^\top \mathbf{x}$$

2. Compare to threshold.

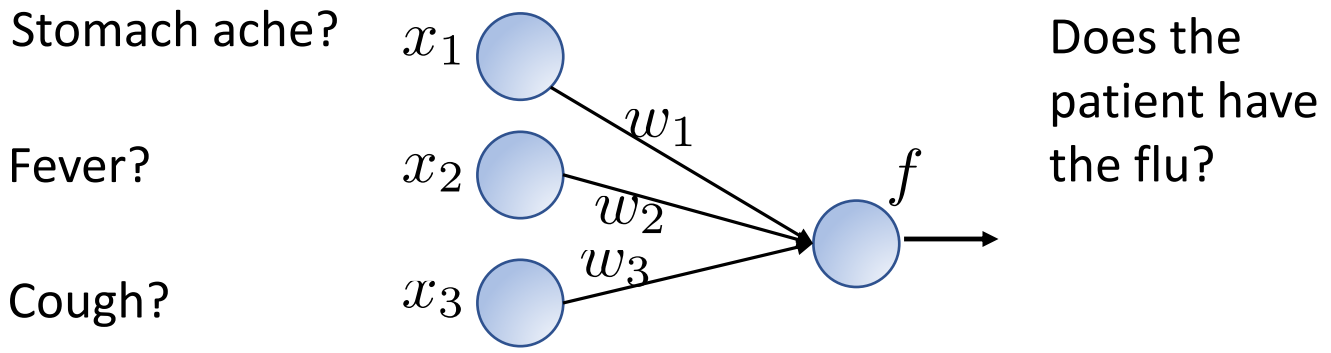
$$z = \mathbf{w}^\top \mathbf{x} + b$$

$$F(\mathbf{x}; \theta) = f(z)$$

$$f(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{otherwise} \end{cases}$$

just a linear classifier with parameters $\theta = (w_1, \ldots, w_d, b)$

More intuition: a simple example

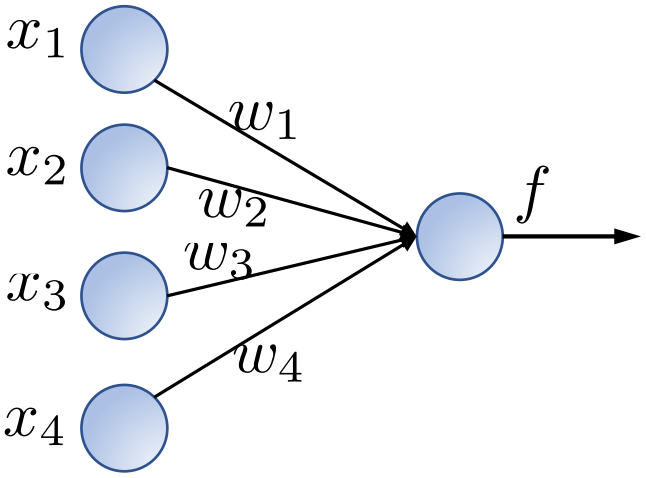


$$w_1 x_1 + w_2 x_2 + w_3 x_3 > 5 \quad ?$$

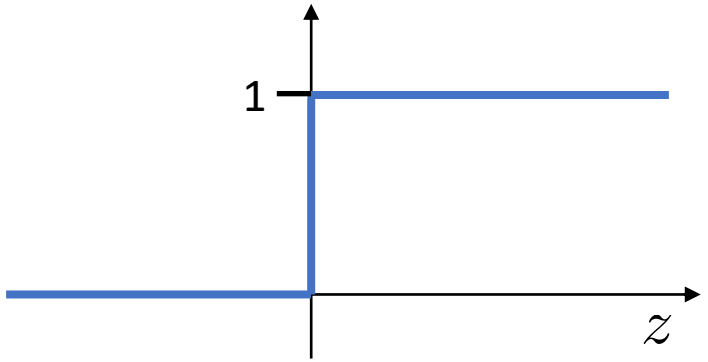
$$-1 \cdot x_1 + 3 \cdot x_2 + 3 \cdot x_3 > 5$$

Intuition:
sum of pieces of evidence, weigh them by trust/importance

Activation functions: threshold

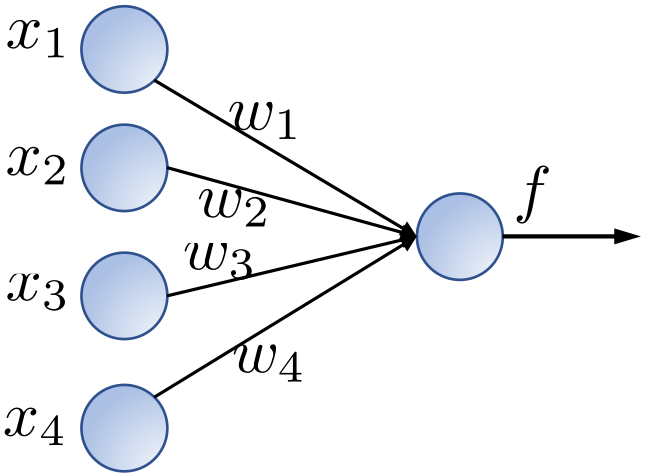


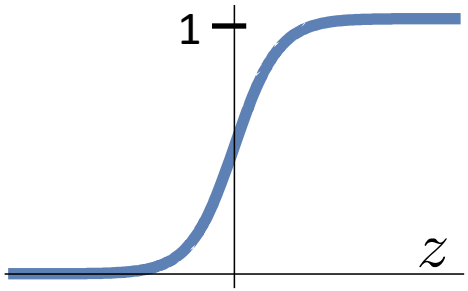
$$f(z) = \begin{cases} 1 & \text{if } z > 0 \\ 0 & \text{otherwise} \end{cases}$$



Small change in weights can cause big change in output
Not good for “learning”!

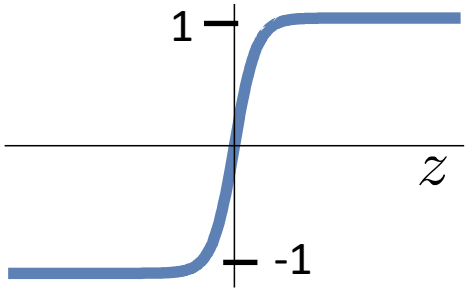
Common activation functions





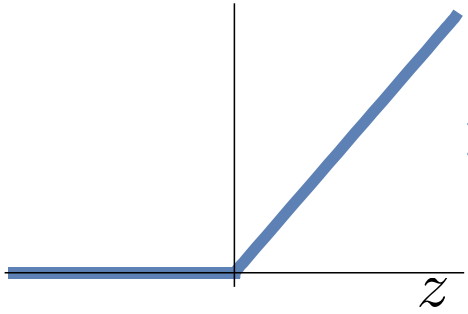
$$\frac{e^z}{1+e^z}$$

sigmoid



$$\tanh(z)$$

tanh



$$\max(0, z)$$

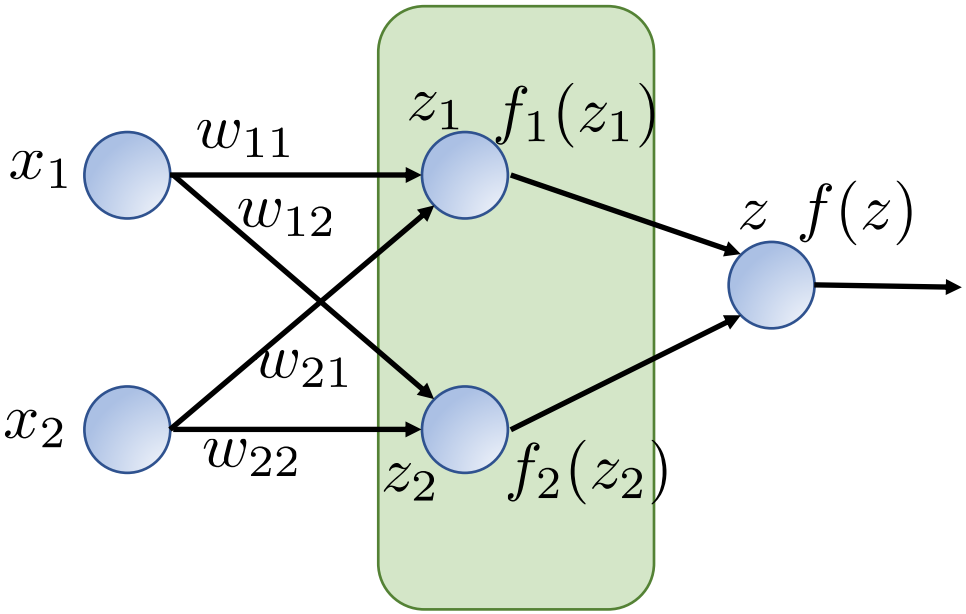
rectifier: Rectified Linear Unit (ReLu)

In summary: one neuron in a neural network…

- is just a linear classifier
- can be a simple pattern detector
- sums up weighted “evidence”

Putting things together: 1 hidden layer

- New encoding of the data: z_1, z_2

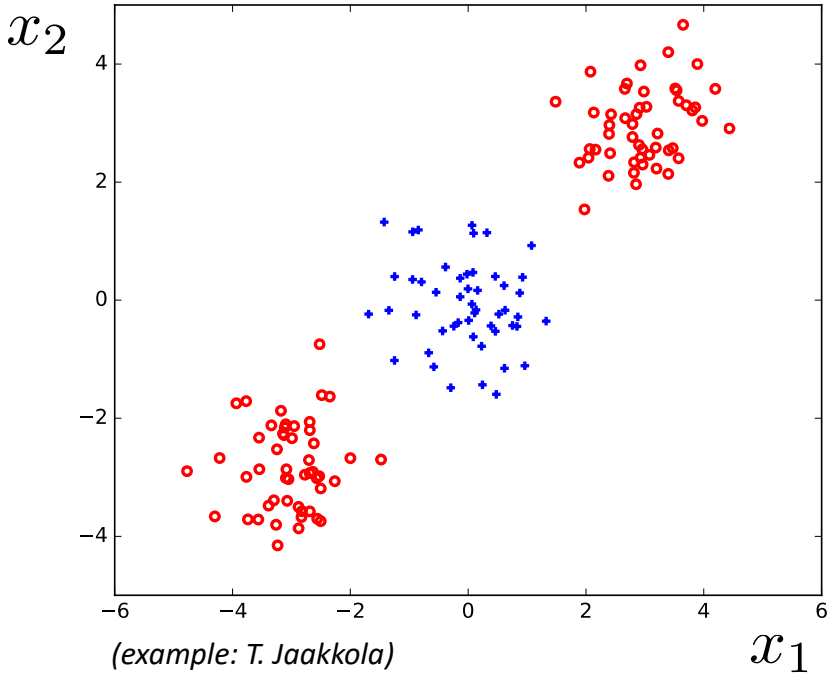


input layer

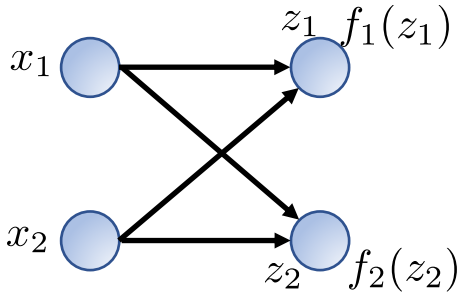
hidden layer: new encoding (representation)

output layer

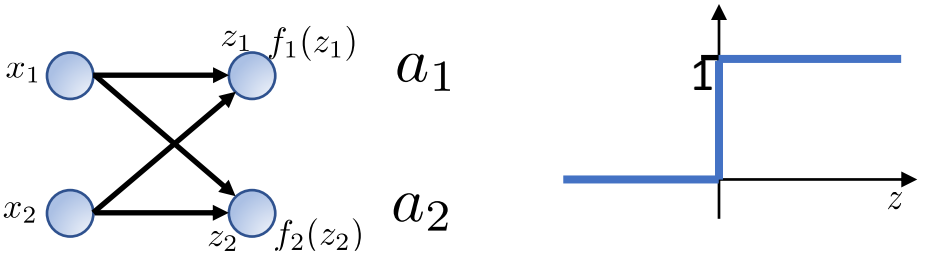
New encoding: example

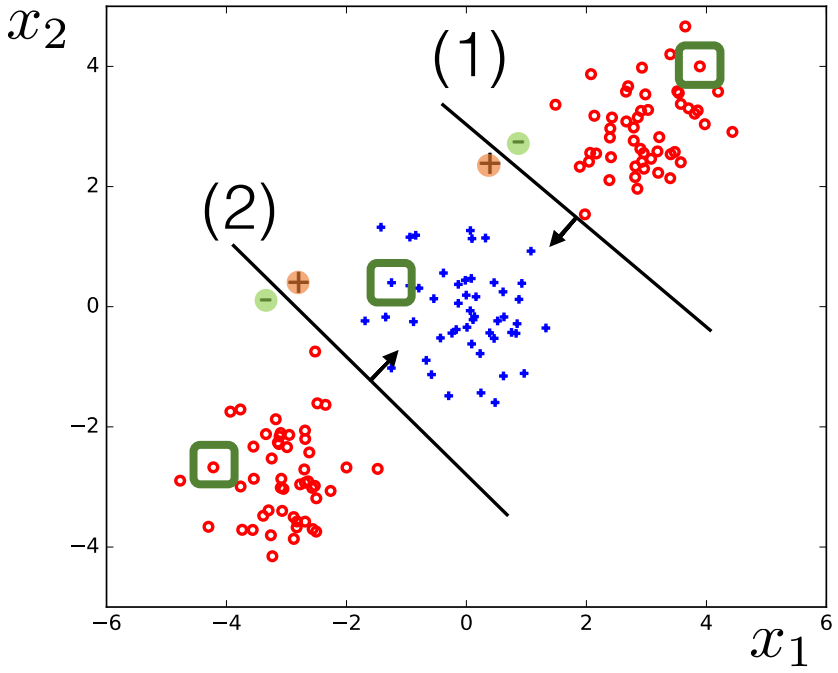


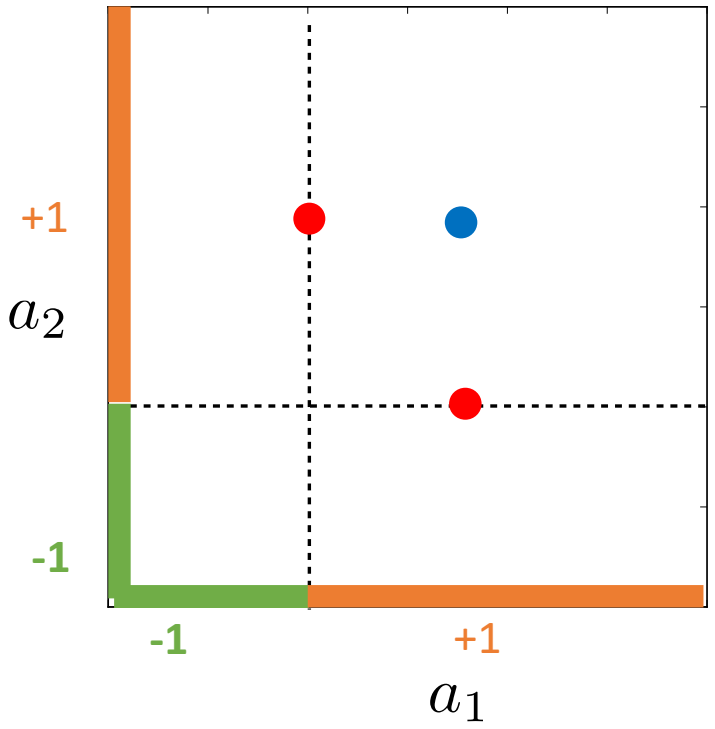
(example: T. Jaakkola)



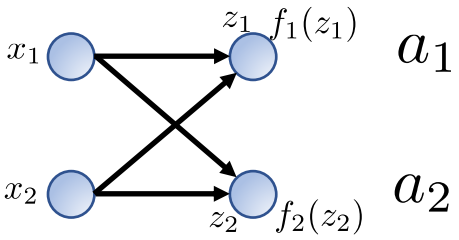
Example: step function activations

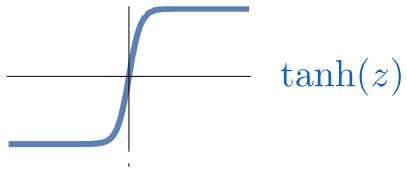


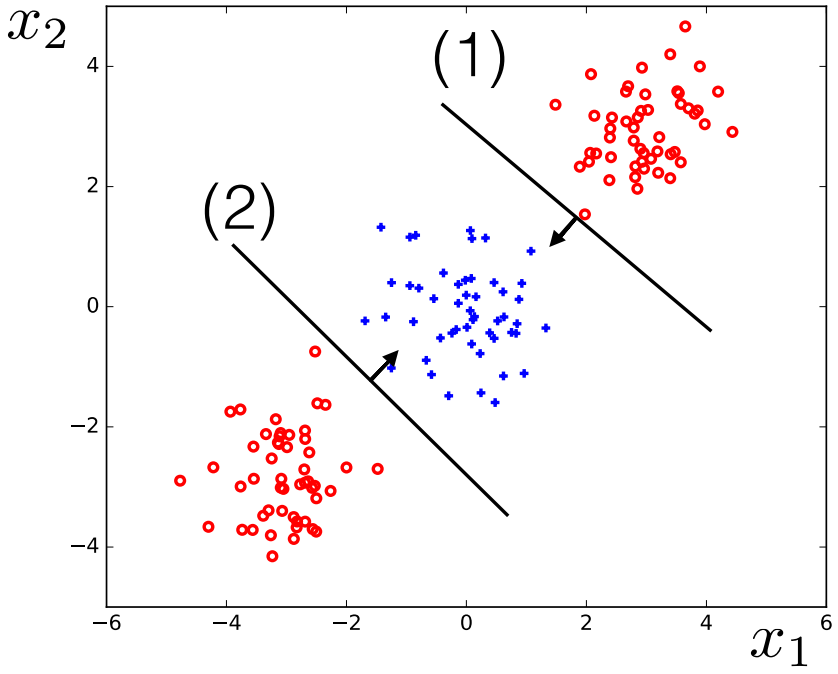


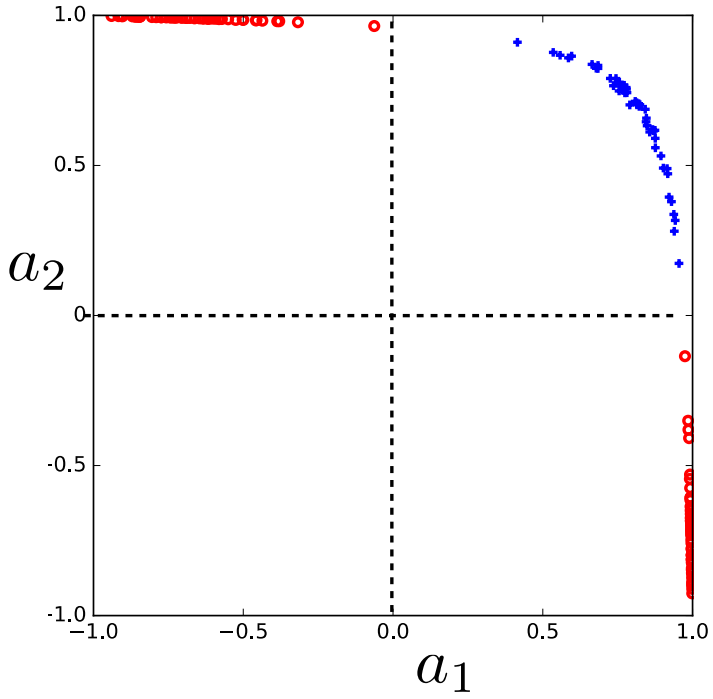


Example: tanh activations

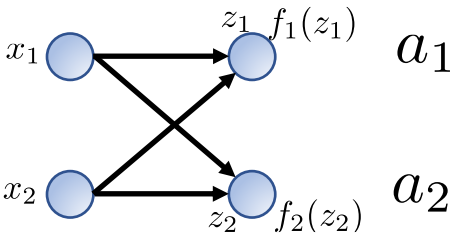


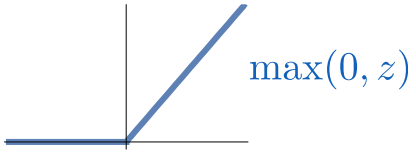


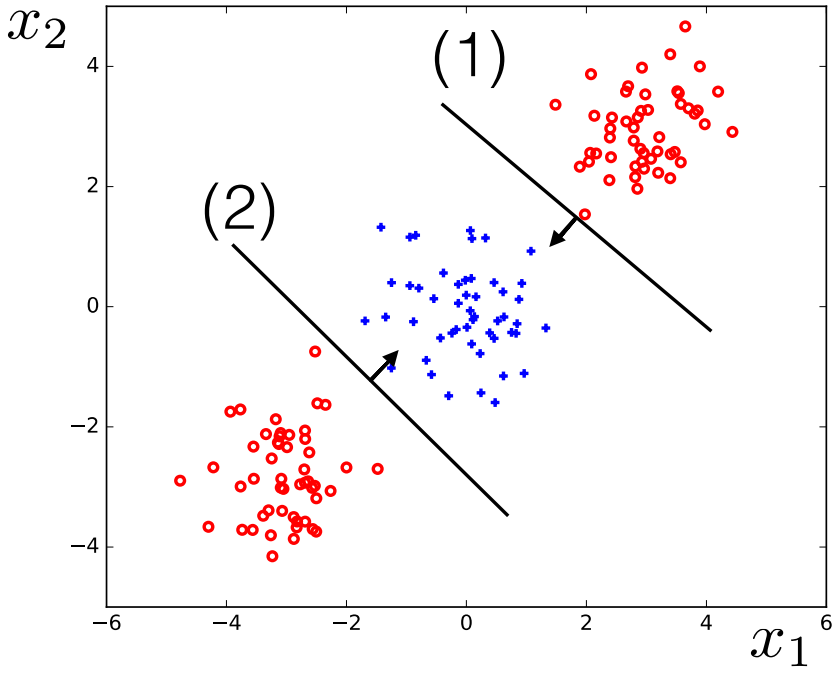


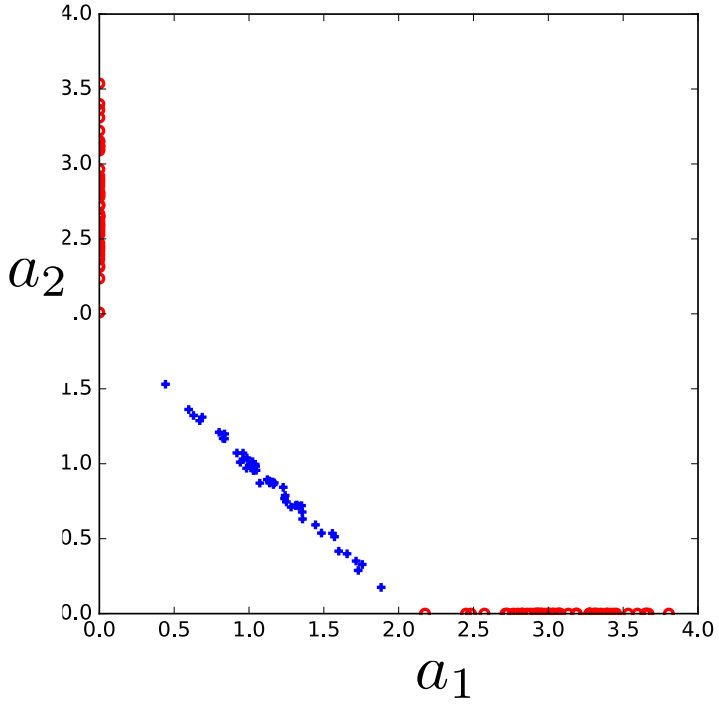


Example: ReLu activations

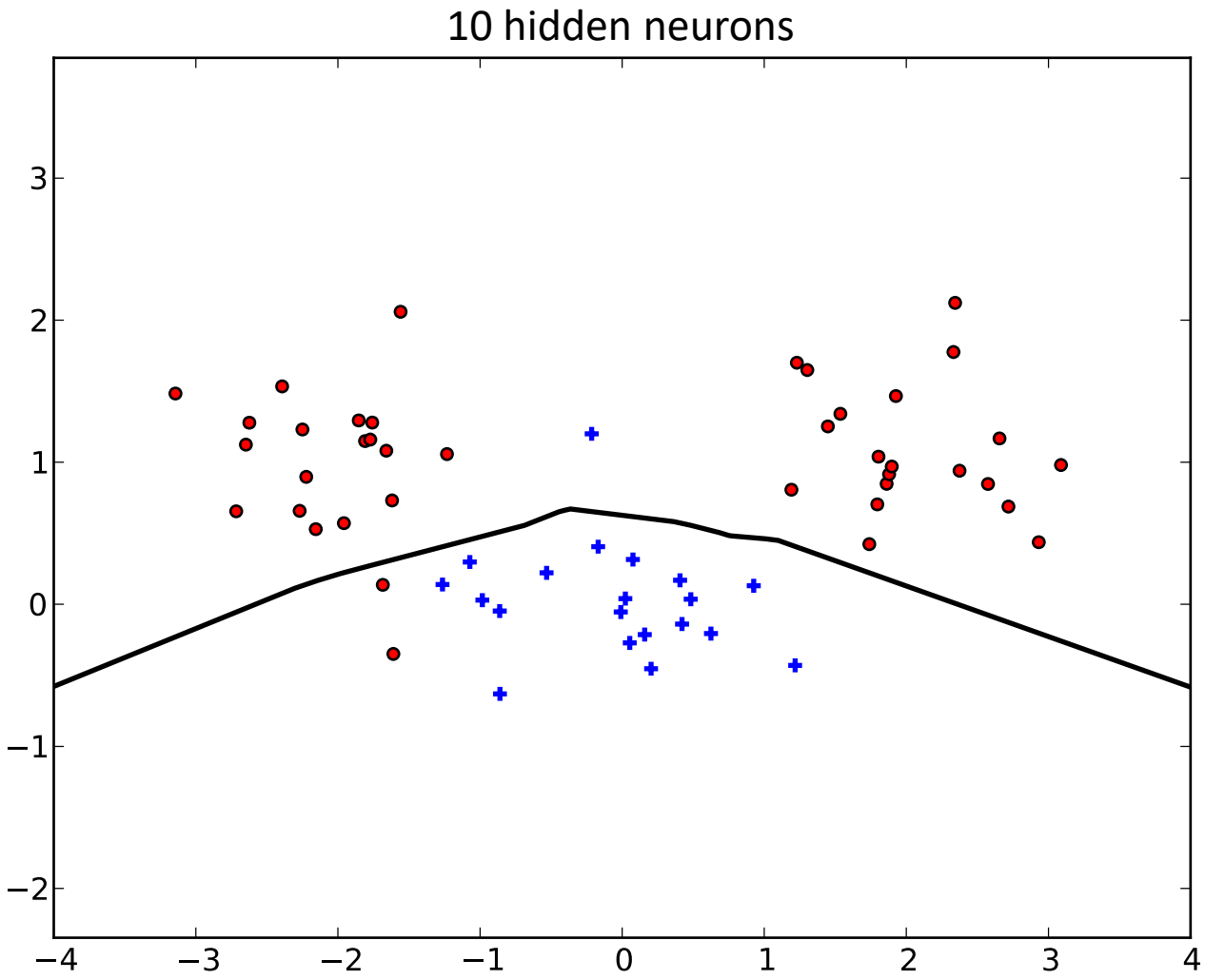






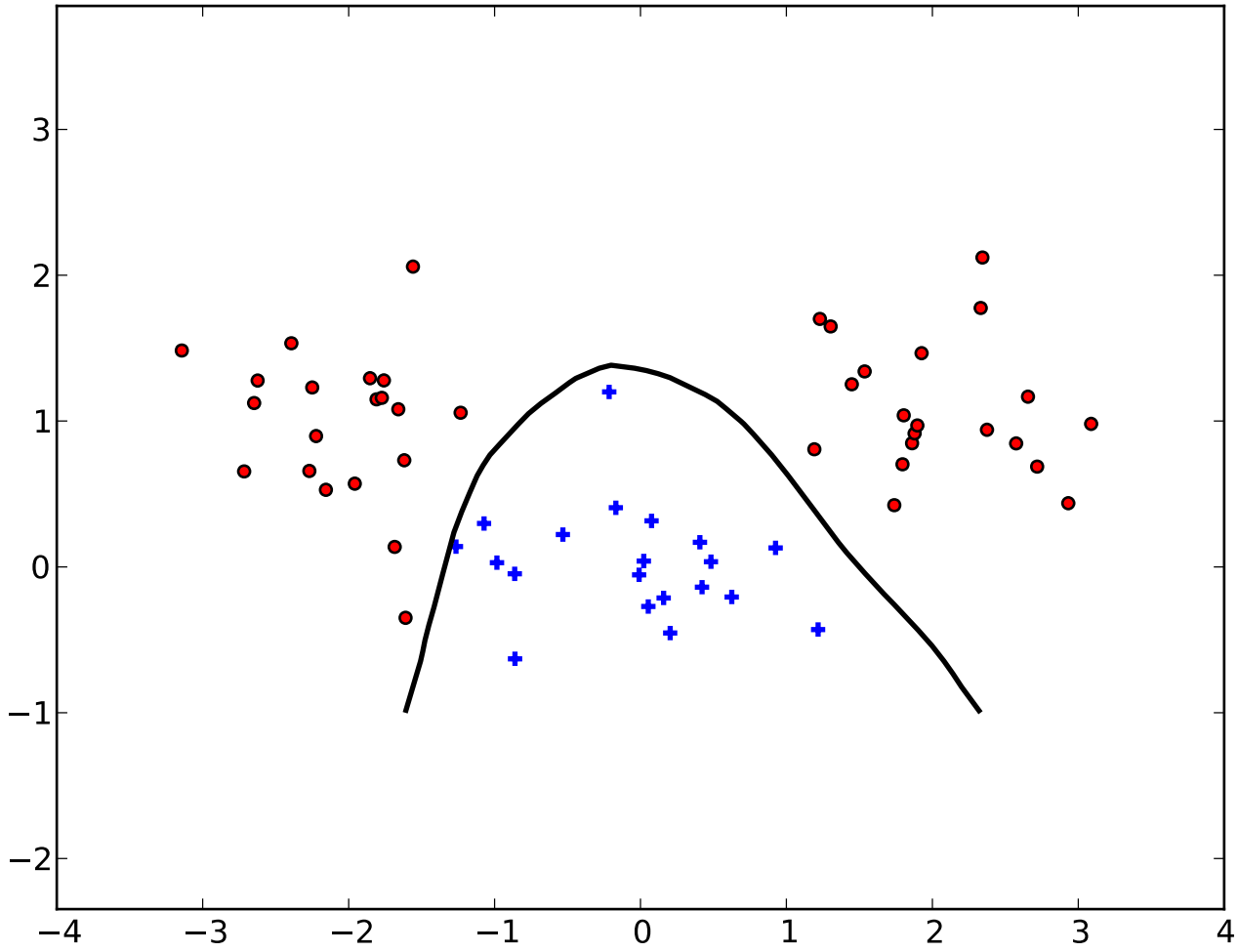


What happens with more hidden neurons?

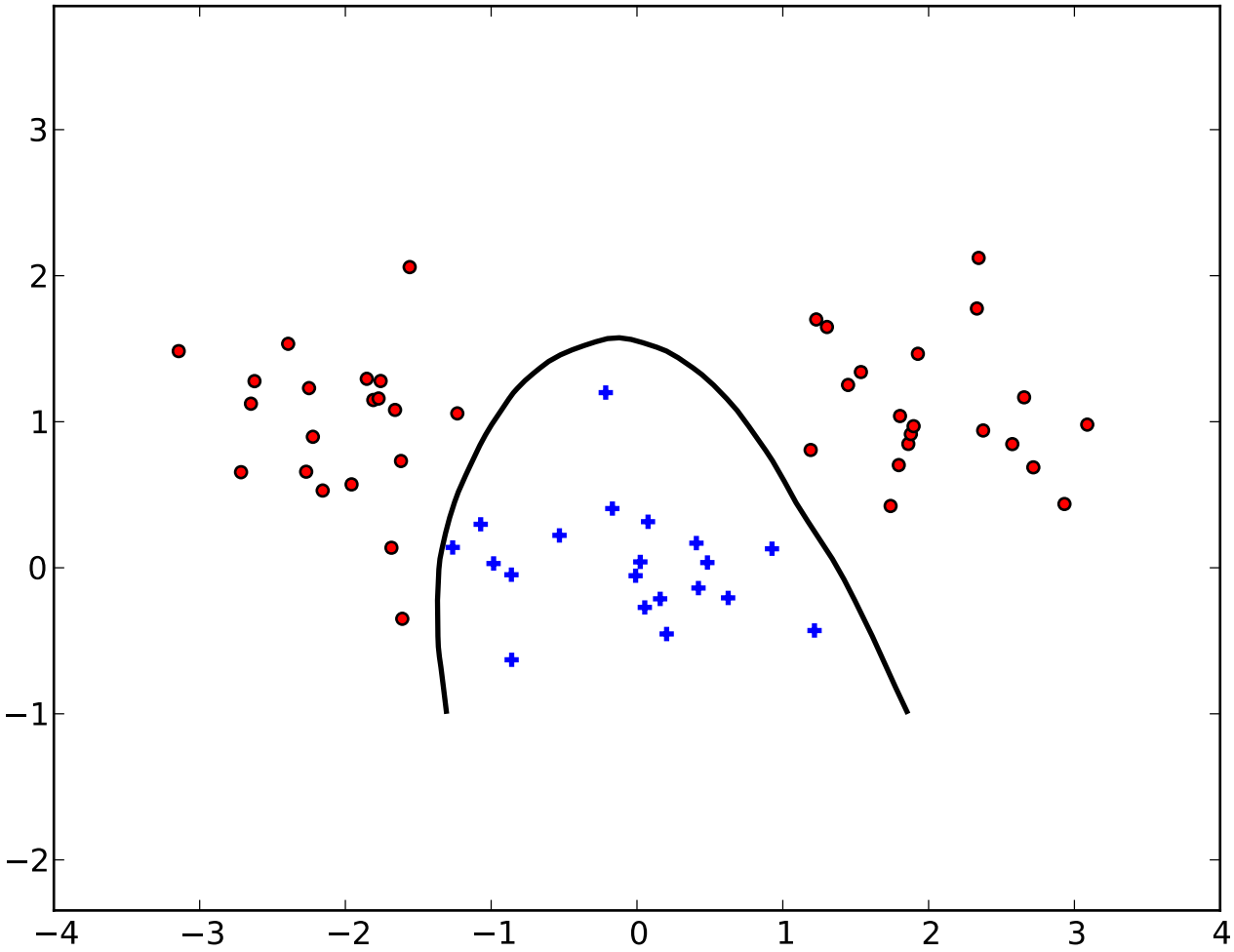


How many neurons would we need at least to separate the 2 classes?

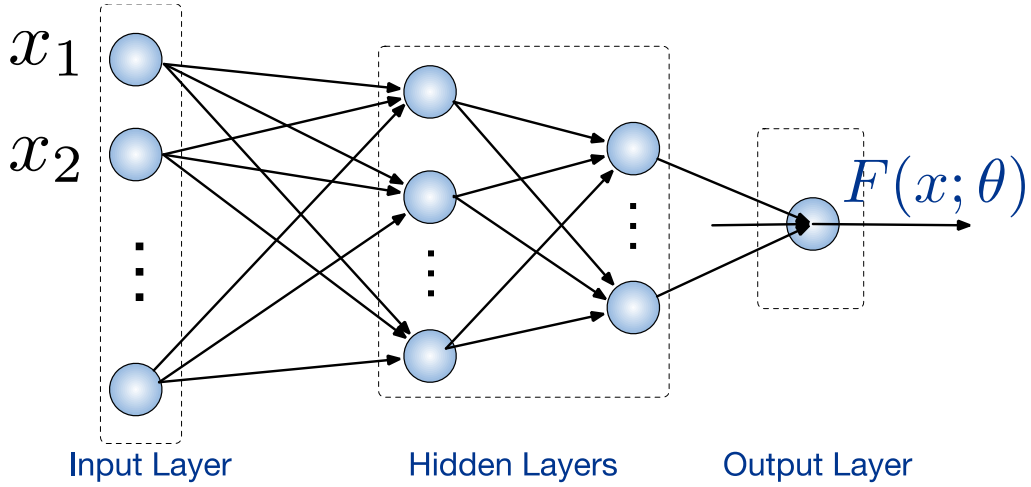
100 hidden neurons



500 hidden neurons



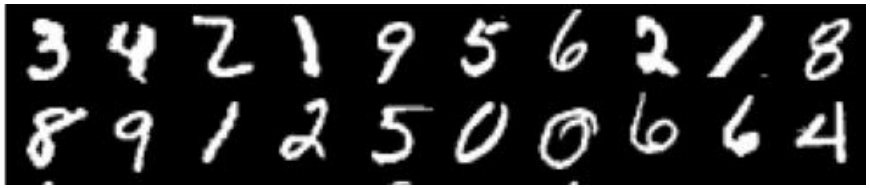
Hierarchical representations: multiple layers



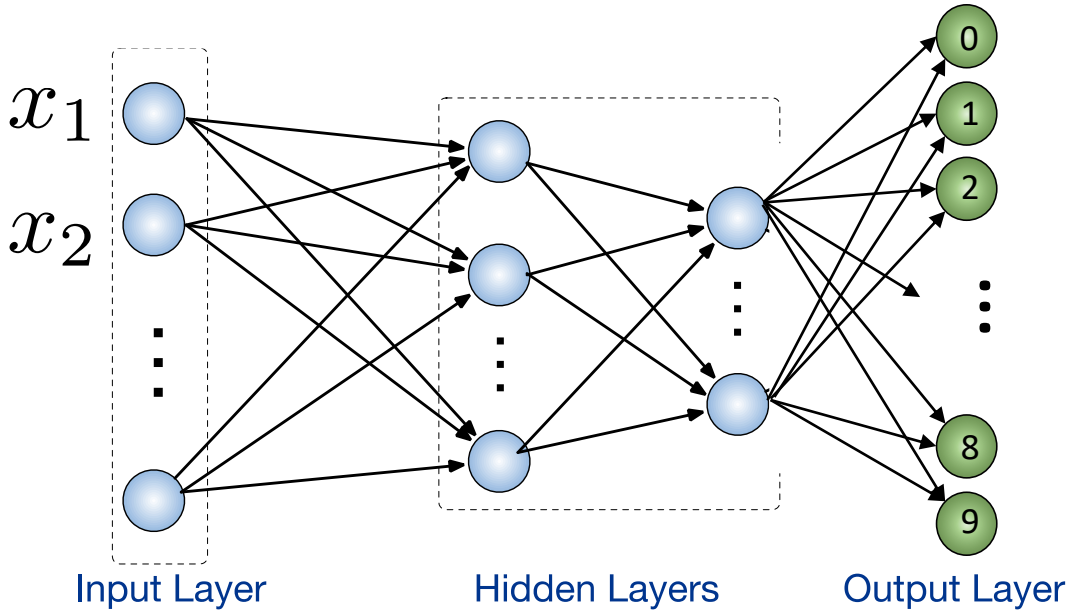
Complicated decisions by breaking them down into simpler ones, e.g.:

Input → edges → simple parts → parts → objects → scenes

Multi-class predictions



- What will the output of the network be? How encode 0—9?
- 10 output units (= 10 classifiers):
  e.g. “ideal”: 2 = [0,0,1,0,0,0,0,0,0,0]



for probabilities:
use *softmax*
(cf logistic regression)

$$a_j = \frac{\exp(z_j)}{\sum_k \exp(z_k)}$$

Summary: neural representations

- Multiple simple units arranged in layers
- Each unit is a linear “classifier”
- Complicated decision by breaking it up into simpler questions
- More units often learn more easily
- Can have multiple outputs

Outline

- How do neural networks represent data?
- **How can we “train” a neural network?**
- Example: Fashion MNIST

Learning Neural Networks

- Small adjustment to weights to minimize a loss function

Common loss functions:

- Regression: squared loss

$$\mathcal{L}(\text{data}, \theta) = \frac{1}{n} \sum_{i=1}^{n} (y^i - F(\mathbf{x}^i; \theta))^2$$

- Classification: negative log-likelihood / cross-entropy
  (like logistic regression)
  for 2 classes:

$$\mathcal{L}(\text{data}, \theta) = -\frac{1}{n} \left[\sum_{i:y^i=1} \log \underbrace{F(\mathbf{x}^i; \theta)}_{\mathbb{P}(y=1 \mid \mathbf{x}^j)} + \sum_{j:y^j=0} \log(1 - \underbrace{F(\mathbf{x}^j; \theta)}_{\mathbb{P}(y=0 \mid \mathbf{x}^i)}) \right]$$

Gradient Descent: main idea

- **Main idea:**
  small adjustments to weights w_{ij} to decrease the loss.
- Decrease or increase w_{ij} ?
- How does a small change Δw_{ij} of weight w_{ij} change the loss?

$$\approx \frac{\partial \mathcal{L}}{\partial w_{ij}} \Delta w_{ij}$$

Partial derivative

- Hence: if $\frac{\partial \mathcal{L}}{\partial w_{ij}}$ is >0, then decrease weight
  otherwise increase weight

Gradient Descent: main idea

- **Main idea:**
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- Decrease or increase w_{ij} ?
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$$\approx \frac{\partial \mathcal{L}}{\partial w_{ij}} \Delta w_{ij}$$

Partial derivative

- Starting with some w_{ij}^0 iterate:

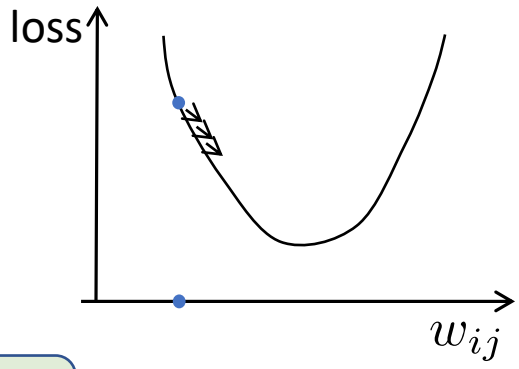
$$w_{ij}^{t+1} \leftarrow w_{ij}^t - \eta \frac{\partial \mathcal{L}}{\partial w_{ij}}$$

new weight

current weight

step size

"direction"



Stochastic gradient descent (SGD)

- Initialize all weights w_{jk}^0

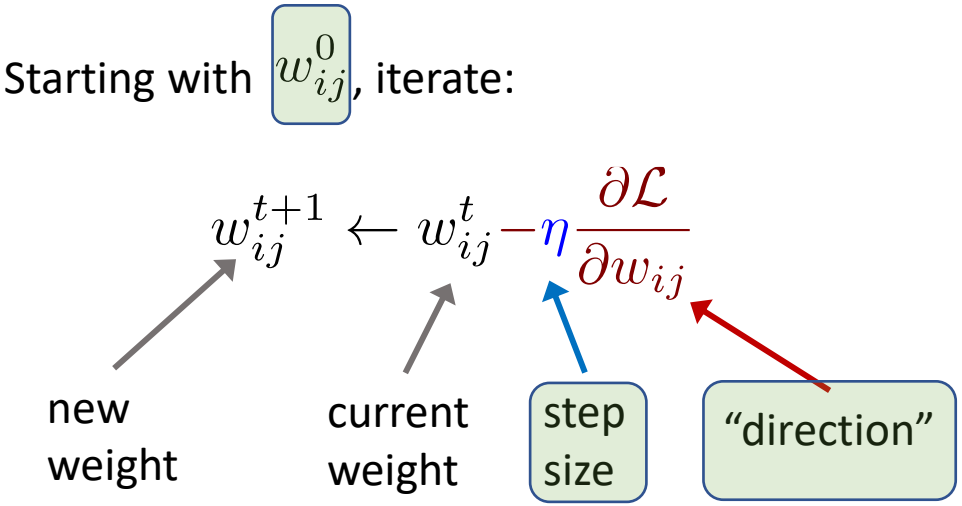
- For iteration $t = 1, \ldots.$:

  Pick a data point $\mathbf{x}^i$ randomly
  and make the prediction for that point a bit better:

  Update weights $w_{jk}^{t+1} \leftarrow w_{jk}^t - \eta \frac{\partial}{\partial w_{jk}} \mathcal{L}(\mathbf{x}^i, y^i, \theta)$

Variation: **Batch SGD:** use *B* instead of 1 data point and average the derivatives

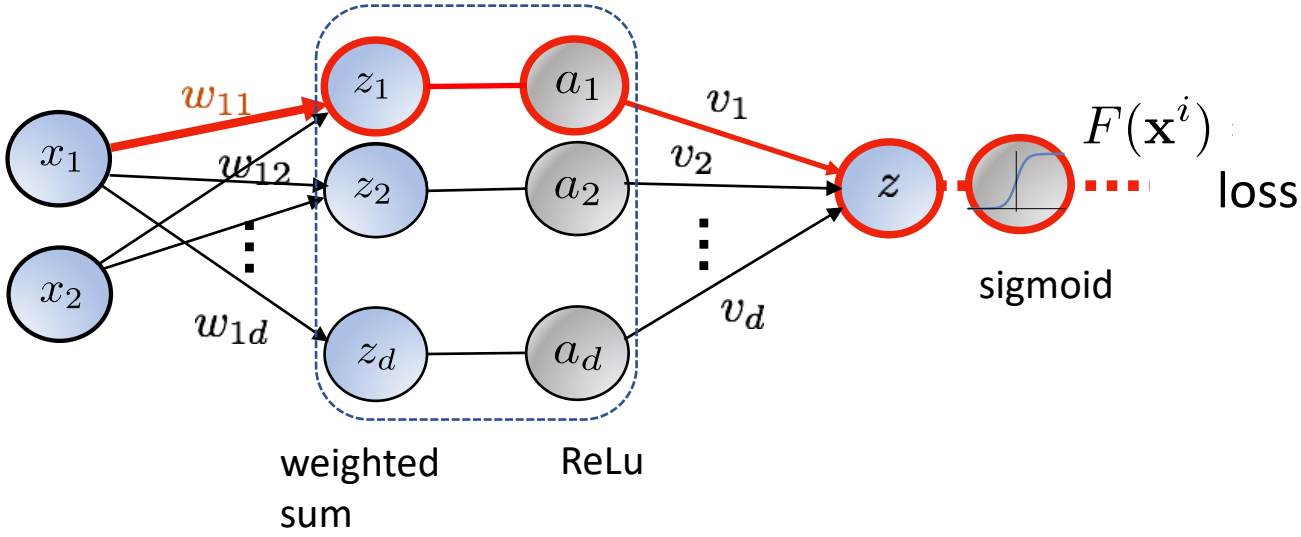
Challenges



- How compute the derivatives (gradient)?
- What is a good initialization?
- What is a good step size?

Gradients for 1 hidden layer

Want to update w_{11}



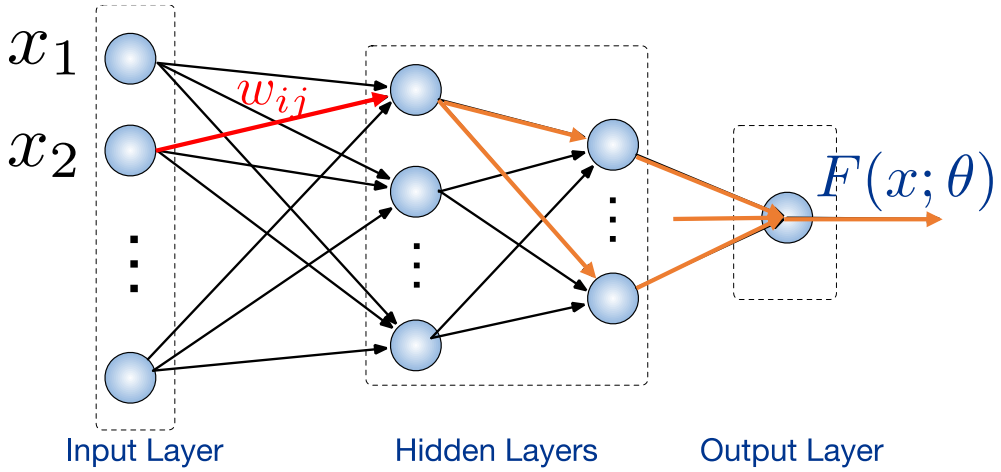
$$\frac{\partial}{\partial w_{11}}\mathcal{L}(\mathbf{x}^i, y^i, \theta) = \frac{\partial z_1}{\partial w_{11}} \cdot \frac{\partial a_1}{\partial z_1} \cdot \frac{\partial z}{\partial a_1} \cdot \frac{\partial}{\partial z}\mathcal{L}$$

Chain rule of calculus

$$= x_1^i \cdot \mathbf{1}[z_1 > 0] \cdot v_1 \cdot \left[F(\mathbf{x}^i) - y^i\right]$$

activation — subsequent weight — prediction — desired

Chain rule for multiple layers



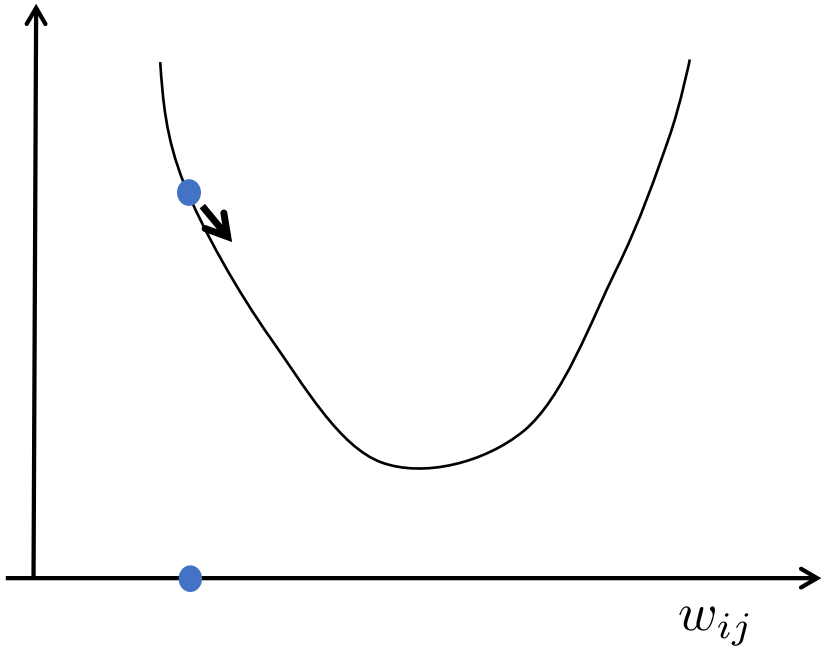
Updates scaled by:
error,
subsequent weights,
activations

- w_{ij} affects many activations downstream!
- Still possible to compute the gradient efficiently: memorization
- **Backpropagation** *(60s,70s; popularized by Rumelhart, Hinton, Williams 1986)*
  forward pass: compute activations
  backward pass: compute gradients, store & reuse
- Problem: **vanishing / exploding** gradients

→ **Initialization** matters

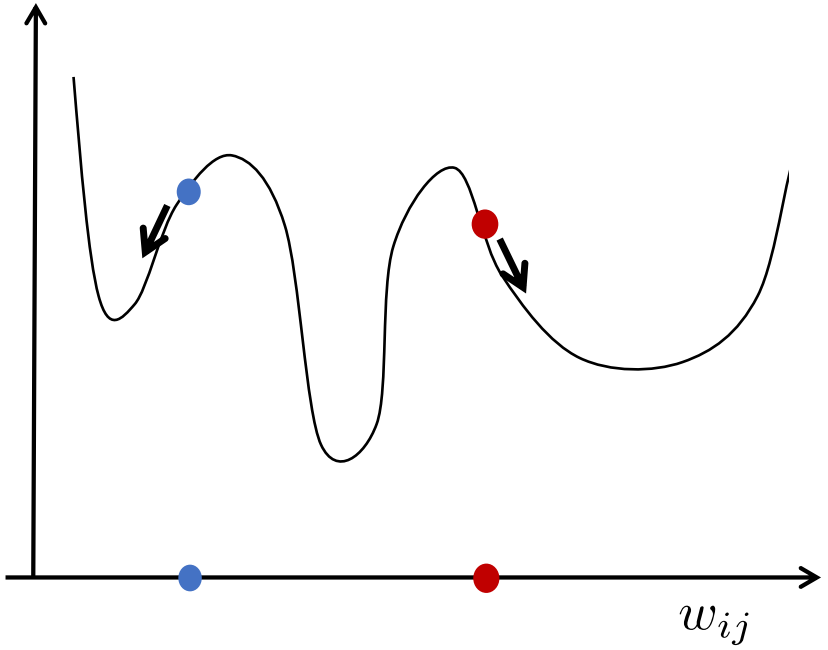
Convexity and Initialization

Convex function



- "one valley": global minimum
- with the right step size, will always reach minimum

Nonconvex function (neural networks)

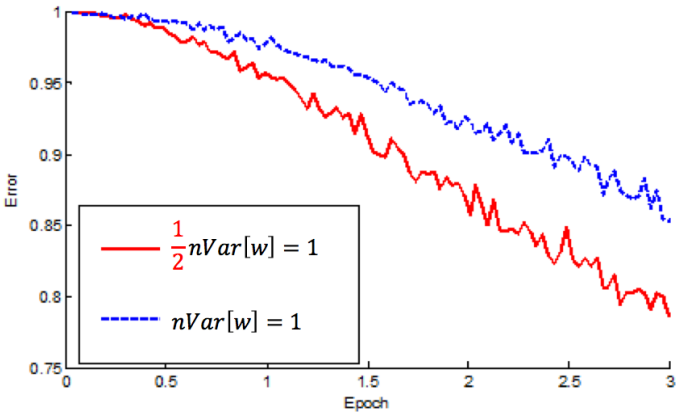


- multiple minima
- Different initializations can lead to different outcomes!
- may not even reach a local minimum

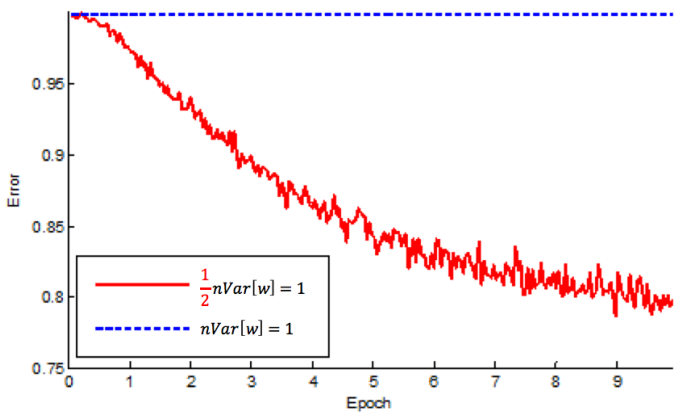
Initialization

- Typically: random, with Gaussian distribution, zero mean. Variance depends on #units in a layer.
  E.g. variance 2/#units
- Initialization can have a big impact!

22-layer ReLU net:
good init converges faster



30-layer ReLU net:
good init is able to converge

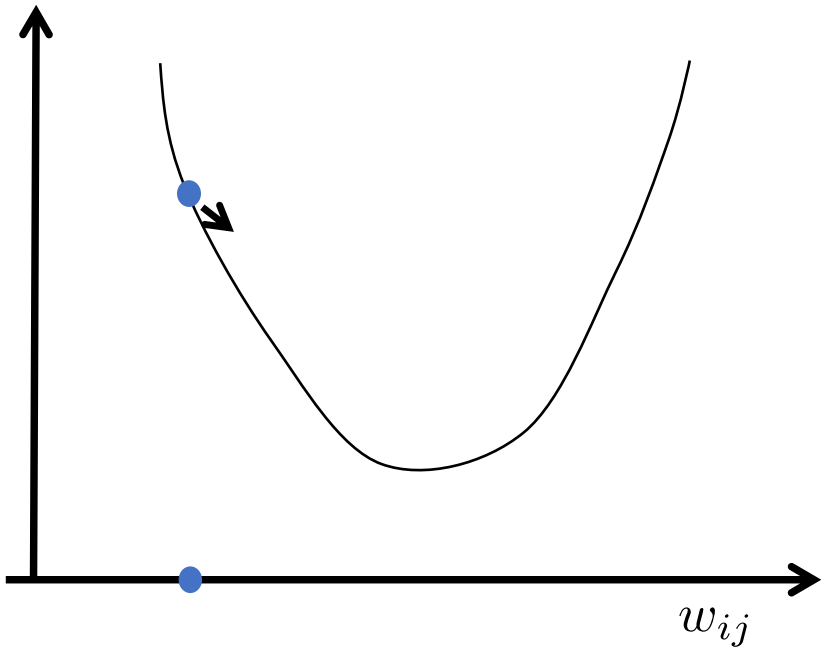


*Figures show the beginning of training

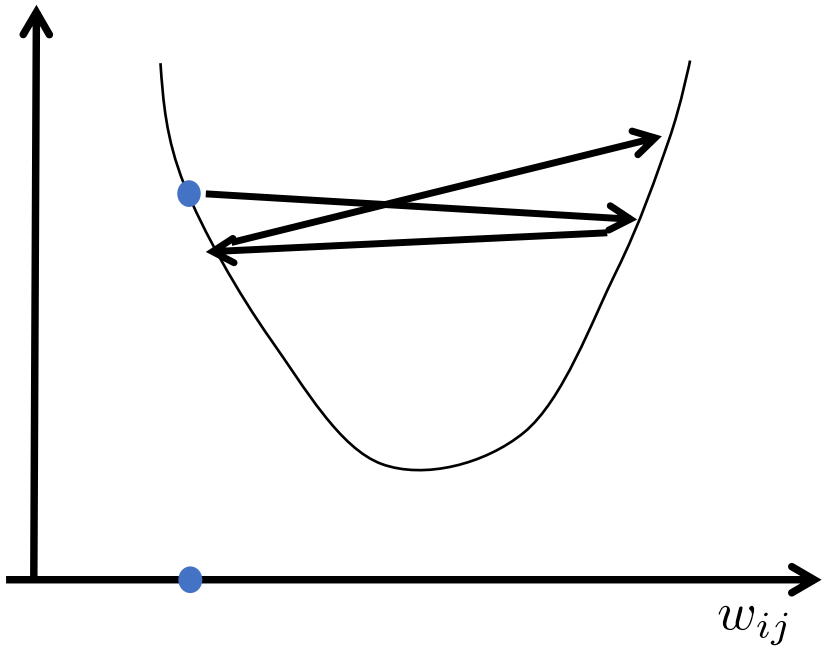
Kaiming He, Xiangyu Zhang, Shaoqing Ren, & Jian Sun. "Delving Deep into Rectifiers: Surpassing Human-Level Performance on ImageNet Classification". ICCV 2015.

Step sizes

$$w_{ij}^{t+1} \leftarrow w_{ij}^{t} - \eta \frac{\partial \mathcal{L}}{\partial w_{ij}}$$



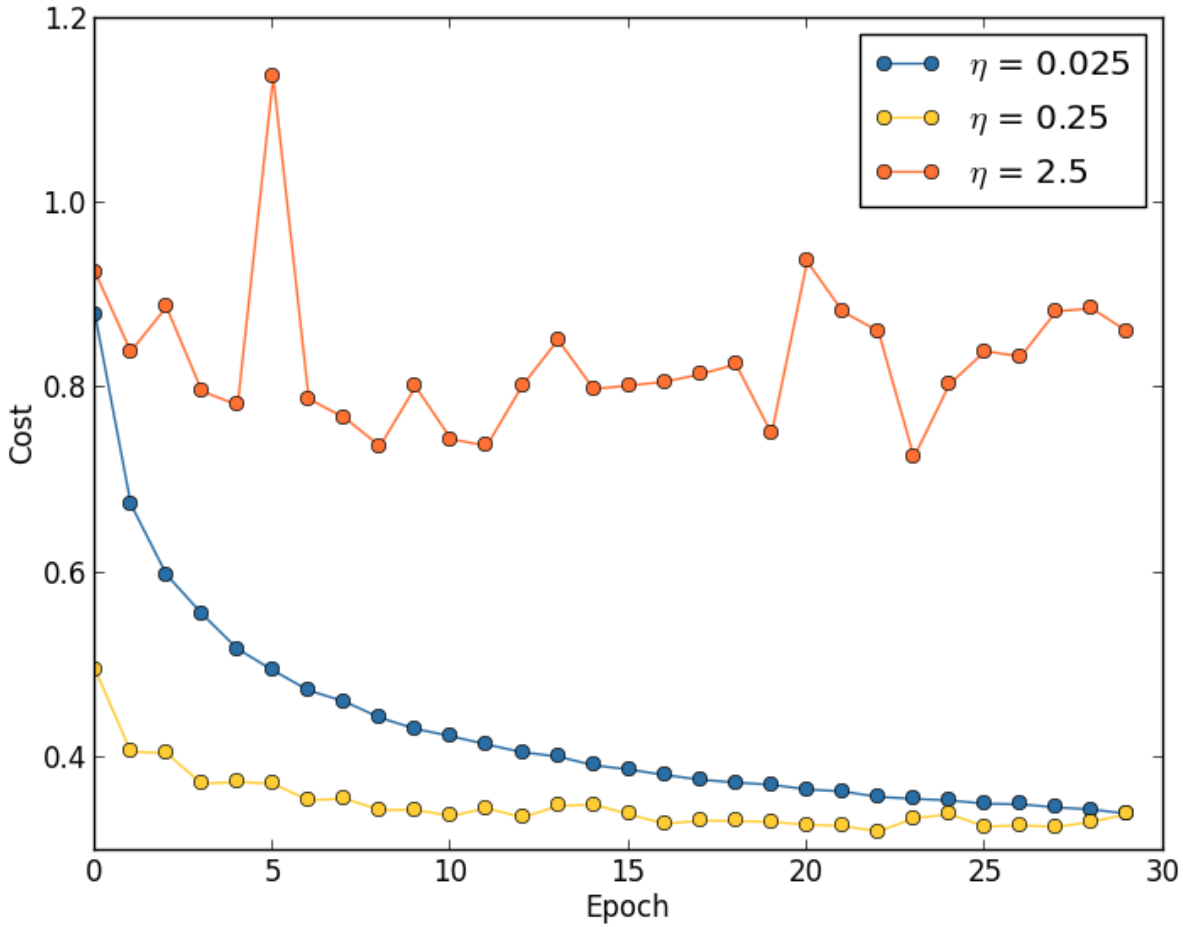
Too small: very slow progress

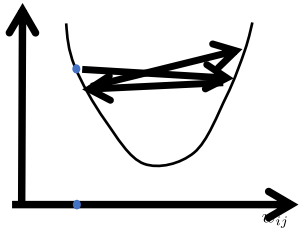


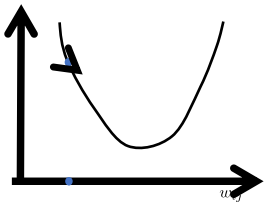
Too large: “overshoot”, loss can increase again, will not converge

- Typically small, decreasing. Tune…

Step sizes







http://neuralnetworksanddeeplearning.com/chap3.html

Widely used improvements of SGD

- Adaptive Methods (e.g. AdaGrad)
  adaptively set step size for each network weight
- Momentum
  use weighted sum of current gradient with past gradients to be less erratic
- Adam
  combines Momentum & AdaGrad

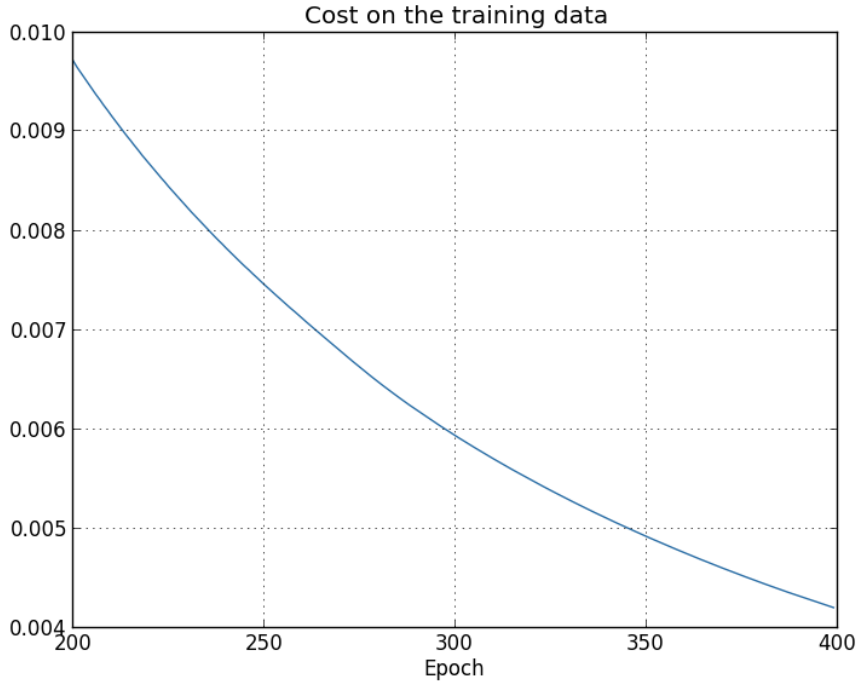
Summary: Neural Network training

- "Training": minimize a loss function over training data
- Iterative, small adjustments of network weights: stochastic gradient descent
- Gradients can be computed with backpropagation (a special case of auto-differentiation)
- Step sizes and initialization matter!

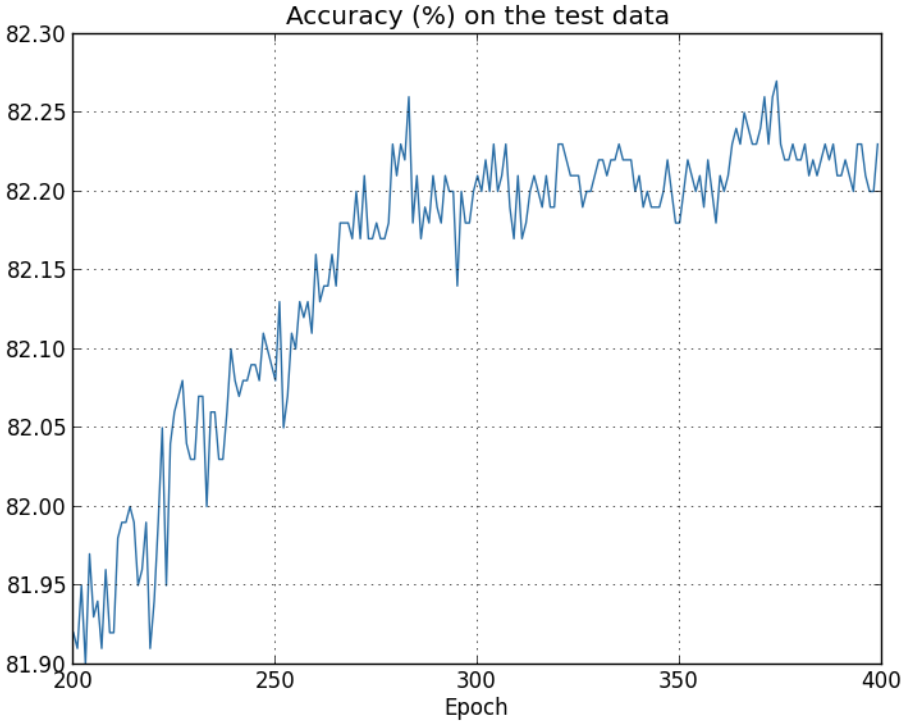
- *More practical hints for training: e.g.*
  Y. Bengio. Practical Recommendations for Gradient-Based Training of Deep Architectures.
  https://arxiv.org/pdf/1206.5533v2.pdf

Regularization

Loss on the training data



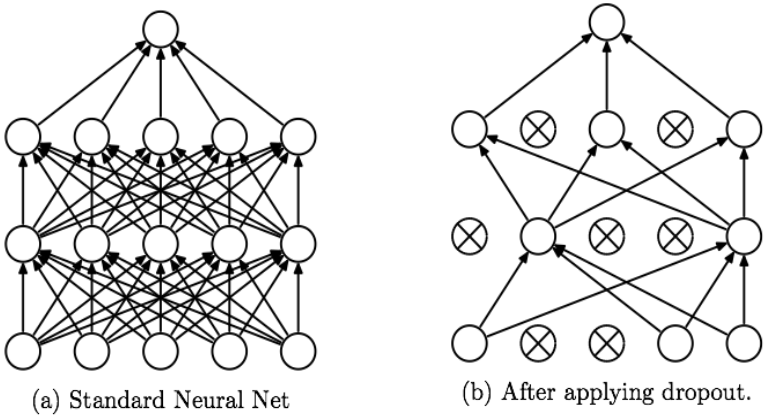
Accuracy on the test data



http://neuralnetworksanddeeplearning.com/chap3.html

Regularization

- **Squared norm / weight decay**
  add $+\frac{\lambda}{2}\|\theta\|^2$ to training loss
- **Early stopping**
  Check error on validation set after each epoch
- **Data augmentation**
  Perturbations (rotation, noise,…), averaging
- **Dropout**
  for each training data point, randomly switch off ½ of the units, don't update them either;
  at test time, scale weights by ½
- **Batch normalization**
  normalize inputs of each layer

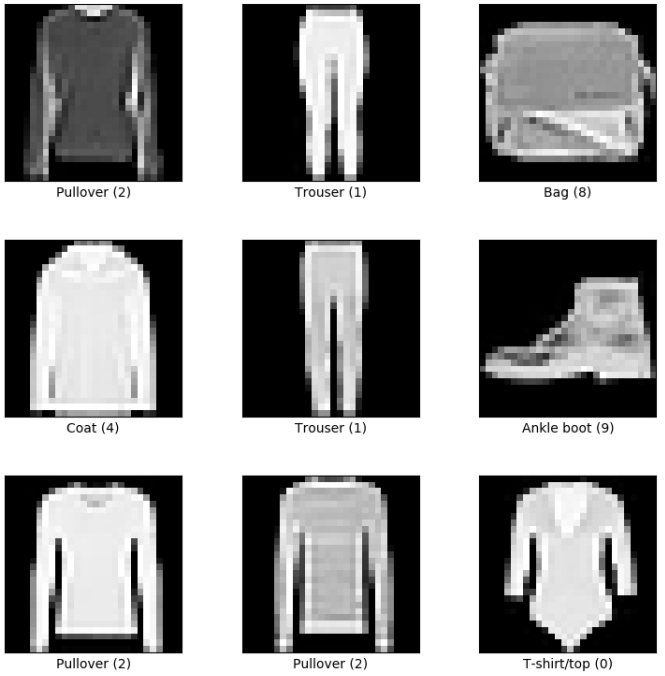


(a) Standard Neural Net (b) After applying dropout.

Figure: (Srivastava et al. Dropout: A Simple Way to Prevent Neural Networks from Overfitting. JMLR, 2014)

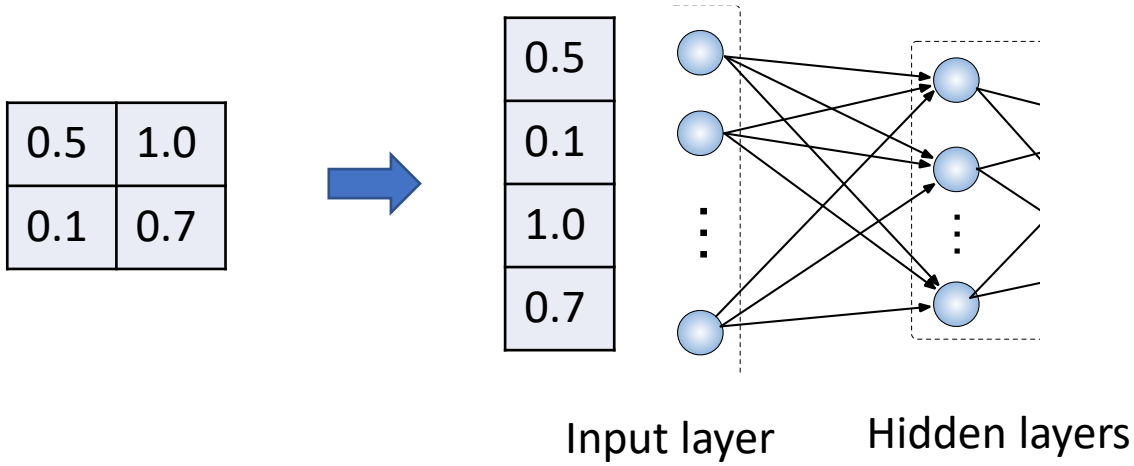
Example: Fashion MNIST

- 60,000 (train) + 10,000 (test) article images from Zalando
- 28x28 images
- 10 classes:
  T-shirt/top, Trouser, Pullover, Dress, Coat, Sandal, Shirt, Sneaker, Bag, Ankle Boot



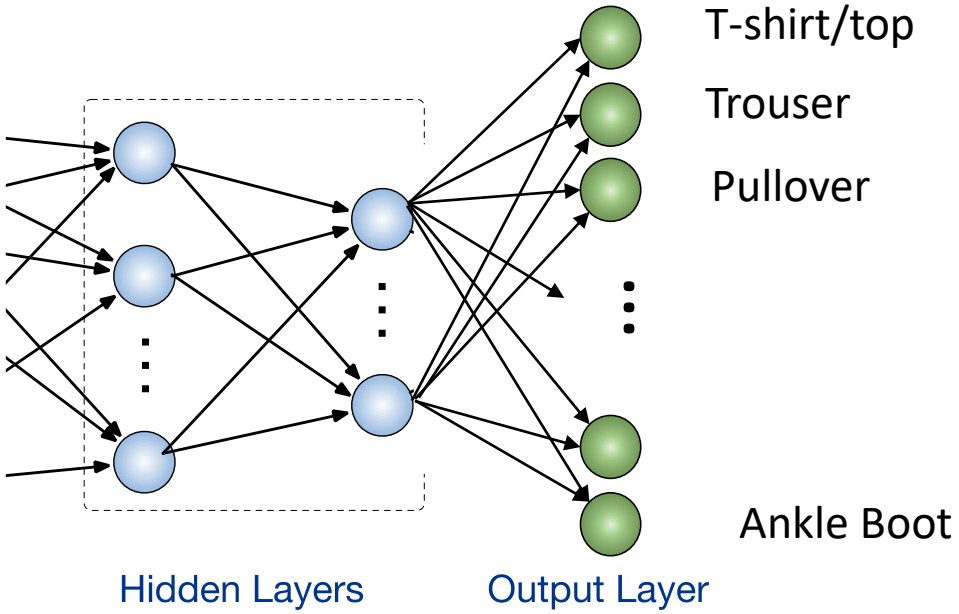
A neural network for Fashion-MNIST

- What are the inputs?
- Grayscale images = matrices



A neural network for Fashion-MNIST

- What are the outputs? Loss function?
- 10 classes



- Classification → Cross-entropy

Summary: Neural Networks

- Multiple simple units arranged in layers
- Complicated decision by breaking it up into simpler questions
- Modular structure: “lego pieces”
- Trainable by Stochastic gradient descent
- Compute gradients via Backpropagation
- Several hyperparameters to tune: step size, regularization/stopping, width, depth