

Lecture 2 Neural Networks

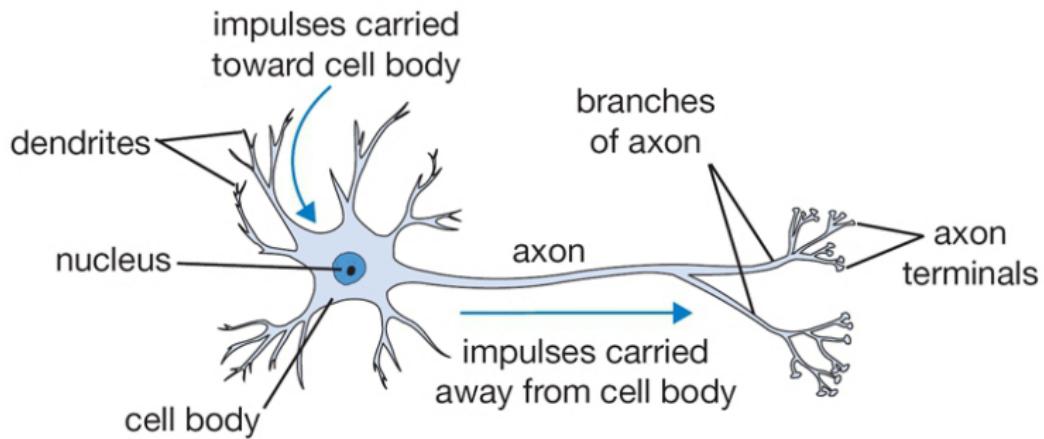
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E6930 Introduction to Neural Networks

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Biological Neuron



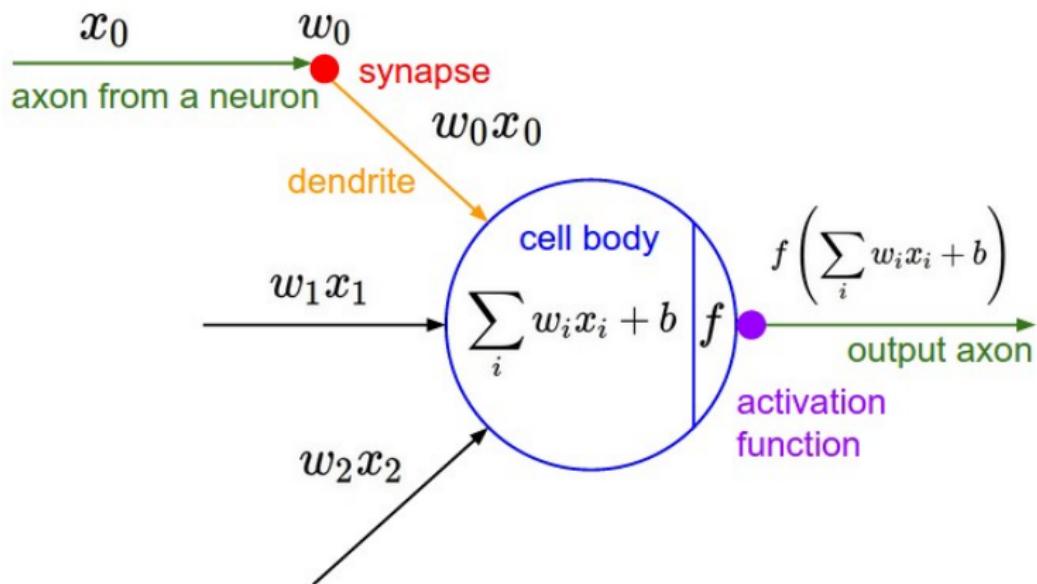
The Road Ahead...

① Basic Architecture

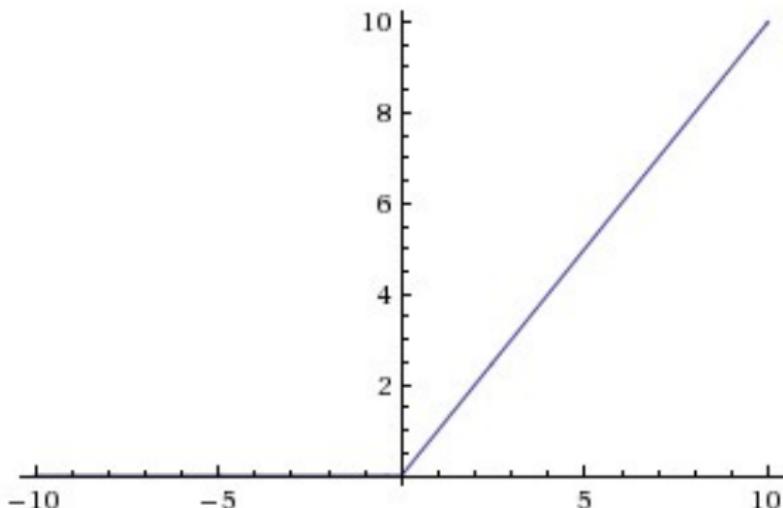
② Pre-training Processing

③ Model Training

Mathematical Neuron

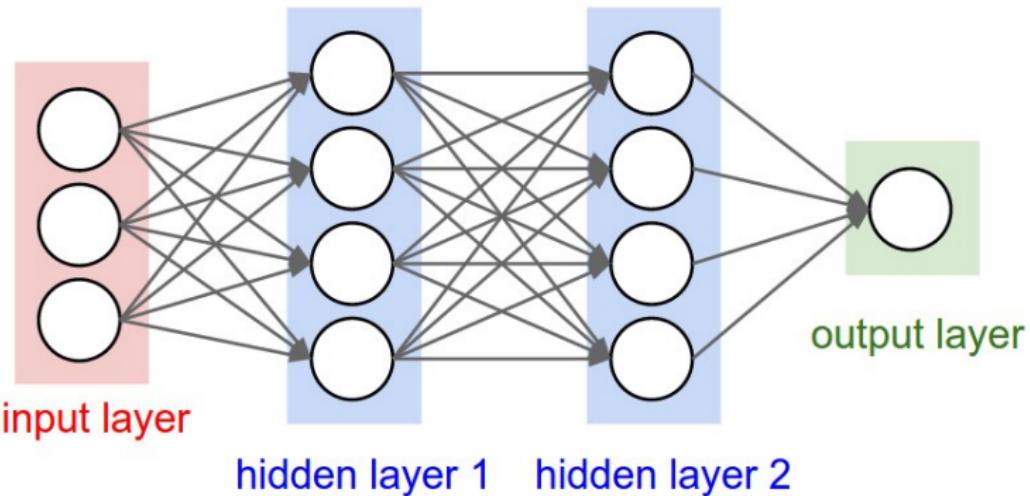


Activation Functions



- ▶ Rectified linear unit (ReLU): $f(x) = \max(0, x)$
- ▶ Leaky ReLU: $f(x) = \max(0.01x, x)$ (avoid dying ReLU)
- ▶ Historically, sigmoid or tanh (vanishing/exploding gradient)

Multilayer Perceptron



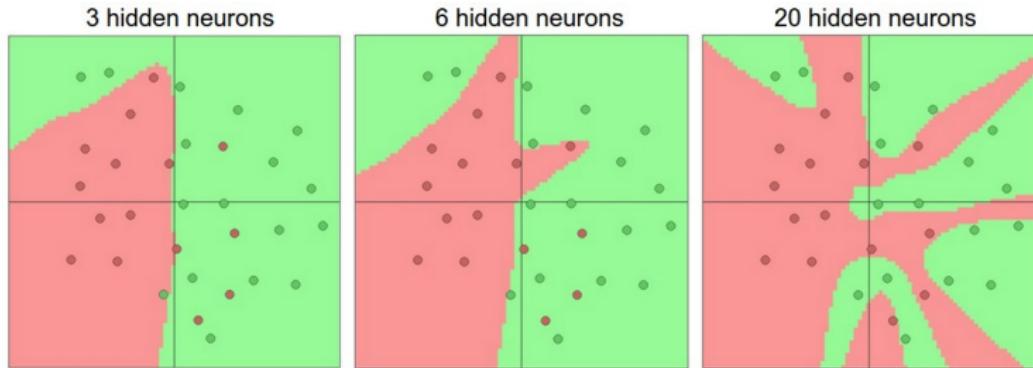
- ▶ 3-layer fully connected neural network
- ▶ not counting input; no activation in output layer
- ▶ Why go ‘deep’? (representational power)

Forward Pass

```
import numpy as np

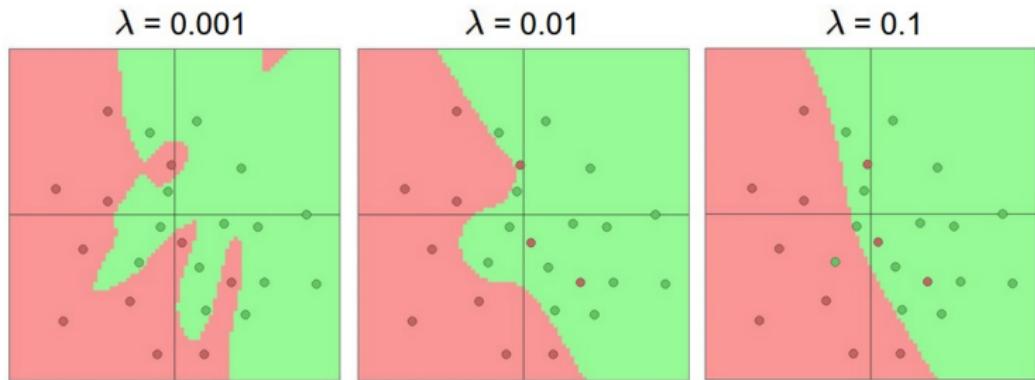
# Forward pass
f = lambda x: 1.0/(1.0 + np.exp(-x)) # sigmoid
activation
x = np.random.randn(3, 1)      # random input vector
(3x1)
h1 = f(np.dot(W1, x) + b1)    # first hidden layer
activations (4x1)
h2 = f(np.dot(W2, h1) + b2)    # second hidden layer
activations (4x1)
out = np.dot(W3, h2) + b3      # output neuron (1x1)
```

Overfitting



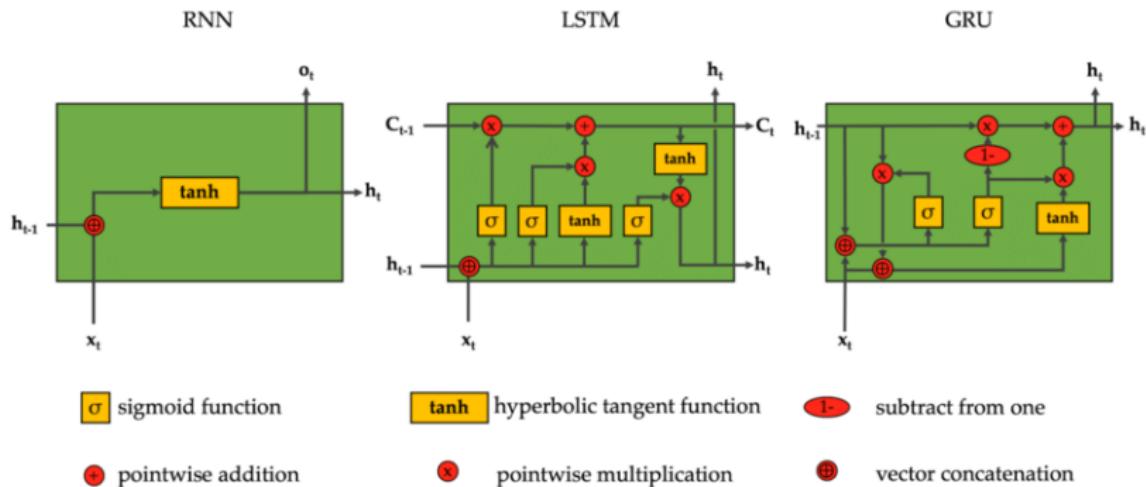
- ▶ In-sample fitting vs. out-of-sample generalization
- ▶ How to control overfitting?

Regularization

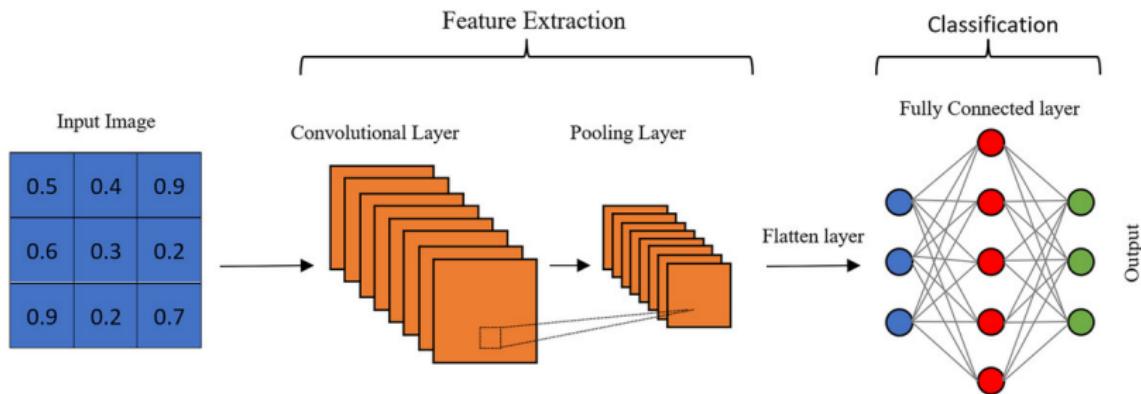


- ▶ L^1 , L^2 , max-norm, and dropout to control overfitting
- ▶ Regularization/prior from structural models

Variant: Recurrent Neural Net



Variant: Convolutional Neural Net



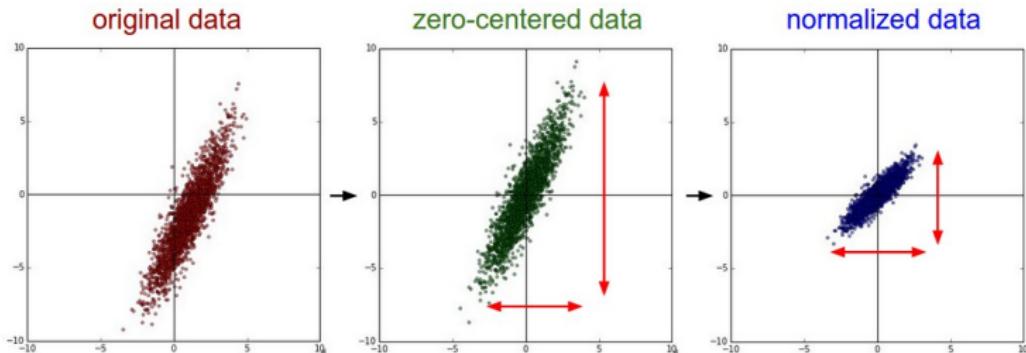
The Road Ahead...

① Basic Architecture

② Pre-training Processing

③ Model Training

Data Standardization



- ▶ Mean subtraction + normalization by s.d. (or principal component, whitening)
- ▶ *Only* on training set, then on validation/test set

Weight Initialization

- ▶ Avoid all-zero initialization, use small random numbers to break symmetry

```
W = 0.01 * np.random.randn(D,H)          # randn
    samples from standard Gaussian
b = np.zeros((1,H))                      # bias
w = np.random.randn(n) / sqrt(n)          #
    normalization; n = number of inputs
w = np.random.randn(n) * sqrt(2.0/n)      # ReLU
    neurons
```

- ▶ Batch/layer normalization + residual connection to stabilize learning

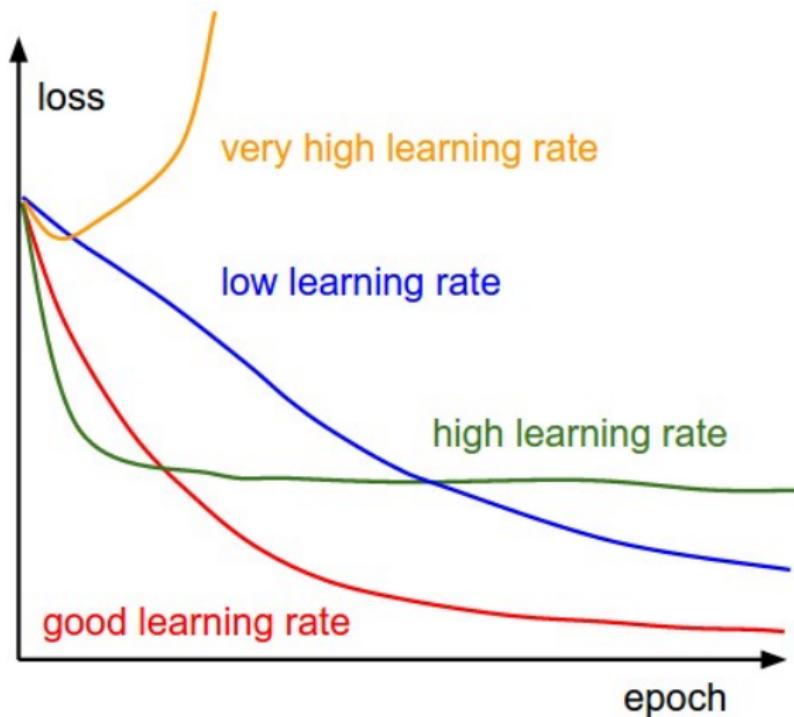
The Road Ahead...

① Basic Architecture

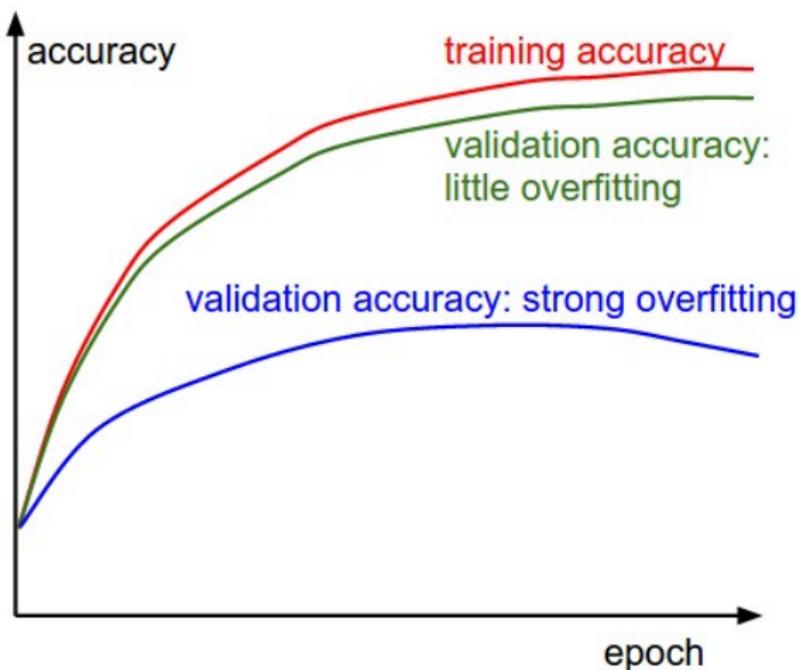
② Pre-training Processing

③ Model Training

Diagnosis: Loss Function



Diagnosis: Accuracy



Other Diagnoses

- ▶ Ratio of update to weight magnitudes ($\sim 10^{-3}$)

```
# Parameter vector W and gradient vector dW
param_scale = np.linalg.norm(W.ravel())
update = -learning_rate*dW          # SGD update
update_scale = np.linalg.norm(update.ravel())
W += update
print update_scale / param_scale # about 1e-3
```

- ▶ Activation/gradient distribution per layer

Non-adaptive Learning

- ▶ Nesterov momentum update

```
v_prev = v                      # back up
v = mu * v - learning_rate * dx  # velocity
    update; mu = 0.9
x += -mu * v_prev + (1 + mu) * v # position
    update
```

- ▶ Anneal learning rate over time
- ▶ Newton's second-order method

$$x_{k+1} = x_k - (\nabla^2 f(x_k))^{-1} \nabla f(x_k)$$

- ▶ expensive to compute and inverse Hessian $\nabla^2 f(x)$
- ▶ Quasi-Newton method, e.g. L-BFGS

Adaptive Learning

- ▶ Adagrad/RMSprop

```
cache += dx**2 # Adagrad
cache = decay_rate * cache + (1 - decay_rate)
    * dx**2      # RMSprop; decay_rate = 0.99
x += - learning_rate * dx / (np.sqrt(cache) +
    eps)
```

- ▶ Adam (recommended)

```
m = beta1*m + (1-beta1)*dx # beta1 = 0.9
mt = m / (1-beta1**t)       # bias correction;
    t = iter counter
v = beta2*v + (1-beta2)*(dx**2) # beta2 =
    0.999
vt = v / (1-beta2**t)
x += -learning_rate * mt / (np.sqrt(vt) + eps)
```

Learning Dynamics

Learning Dynamics (Cont'd)

Need for Speed

- ▶ Choosing right device
 - ▶ central processing unit (CPU)
 - ▶ graphics processing unit (GPU) (NVIDIA's CUDA, AMD's ROCm, Apple's MPS)
- ▶ Mixed precision training
 - ▶ half-precision floating point (FP16)
 - ▶ brain floating point (BF16)
 - ▶ quarter-precision floating point (FP8)
- ▶ PyTorch distributed data parallel (DDP)

Miscellaneous Pointers

- ▶ Gradient check with small batch of data
- ▶ Prefer larger networks with proper regularization
- ▶ For continuous and multivariate outcome space, *discretize* and train *independently* for each attribute
- ▶ Random search for good hyperparameters
- ▶ Form model ensemble for extra performance

References

- ▶ cs231n.stanford.edu – CS231n: Deep Learning for Computer Vision
- ▶ Ioffe & Szegedy (2015), “Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift”, [arXiv:1502.03167](https://arxiv.org/abs/1502.03167)
- ▶ Ba, Kiros & Hinton (2016), “Layer Normalization”, [arXiv:1607.06450](https://arxiv.org/abs/1607.06450)
- ▶ He et al. (2015), “Deep Residual Learning for Image Recognition”, [arXiv:1512.03385](https://arxiv.org/abs/1512.03385)
- ▶ Srivastava et al. (2014), “Dropout: A Simple Way to Prevent Neural Networks from Overfitting”, *Journal of Machine Learning Research*