Lecture 2 Neural Networks

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E6930 Introduction to Neural Networks

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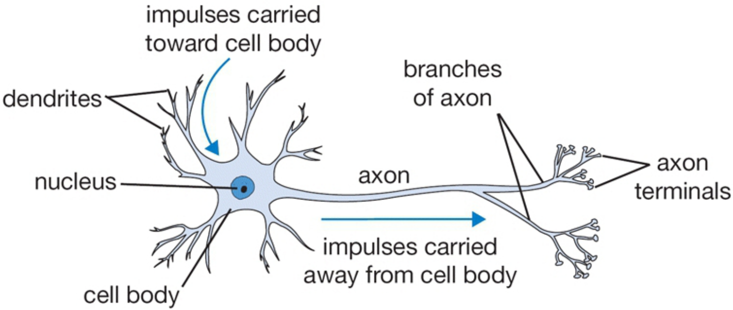
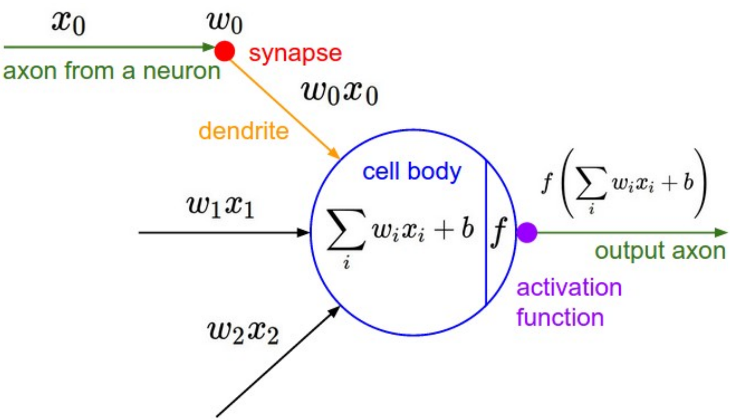
Biological Neuron



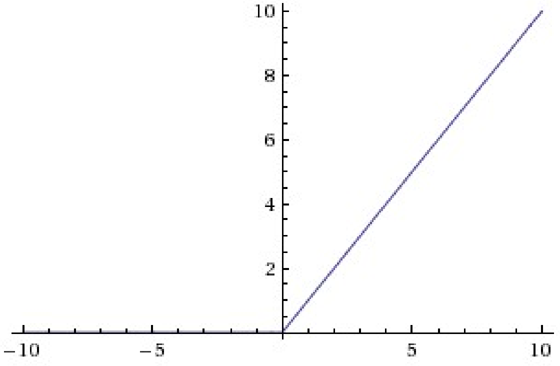
The Road Ahead...

1. Basic Architecture
2. Pre-training Processing
3. Model Training

Mathematical Neuron

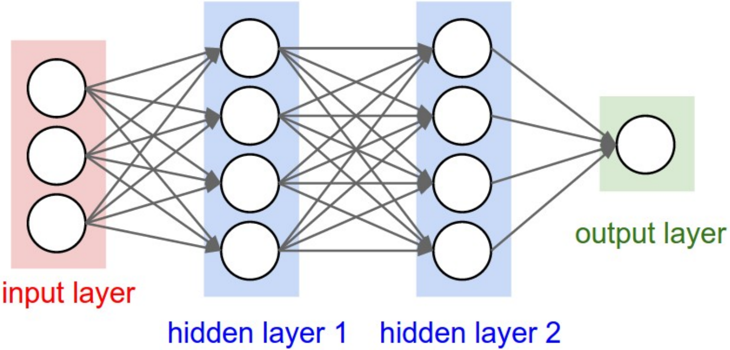


Activation Functions



- 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

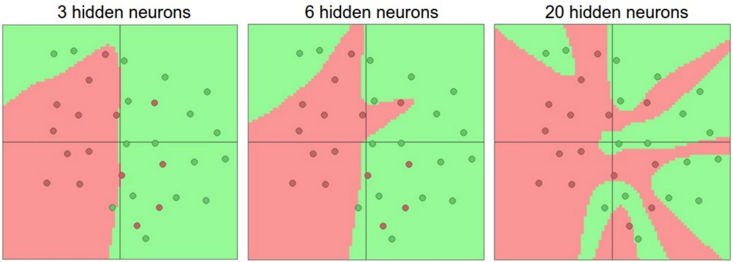


- 3-layer fully connected neural network
- not counting input; no activation in output layer
- Why go 'deep'? (representational power)

Forward Pass

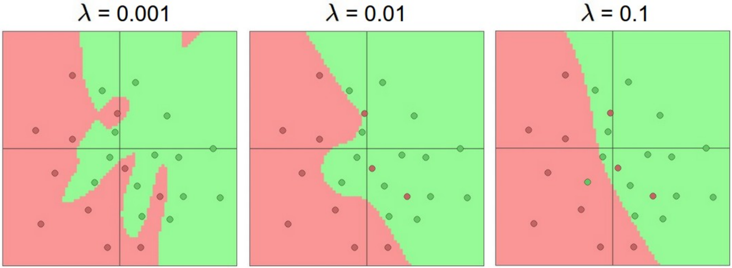
```
import numpy as np

# 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

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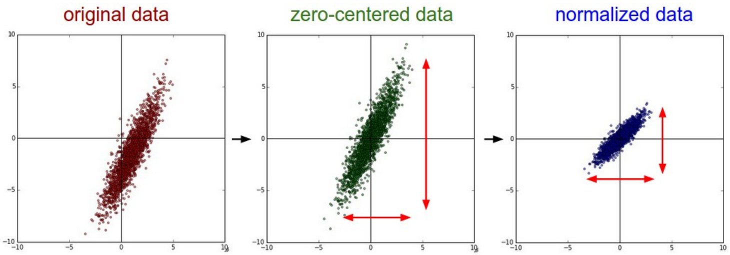
Data Standardization



- 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 normalization to stabilize learning

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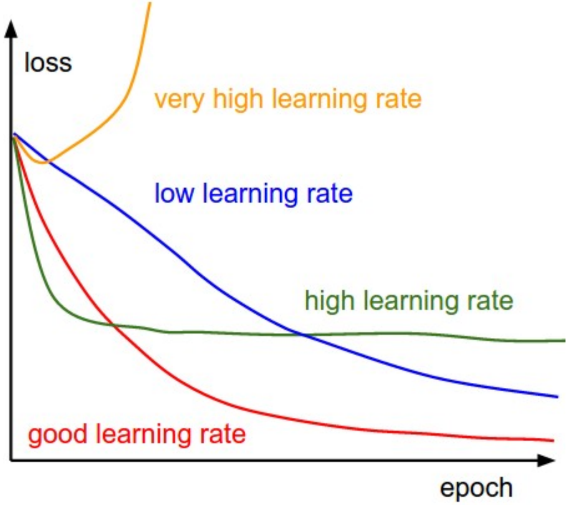
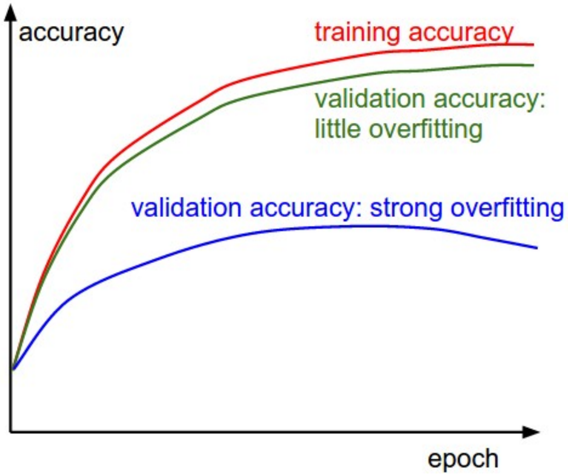
Diagnosis: Loss Function



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

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

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

Adaptive Learning

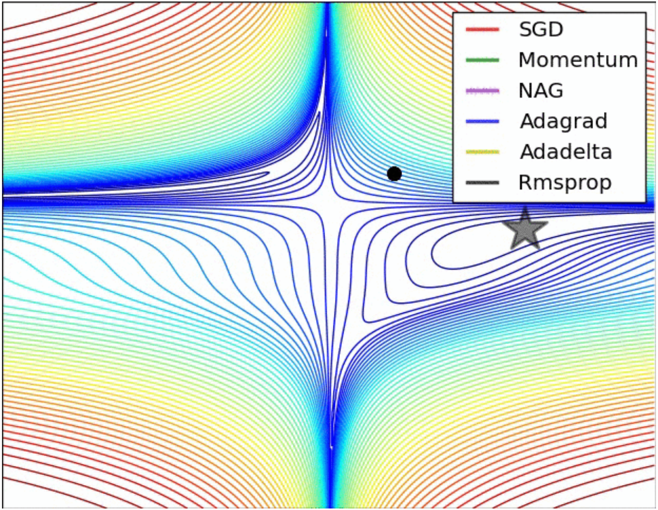
- Adagrad/RMSprop

```
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)
```

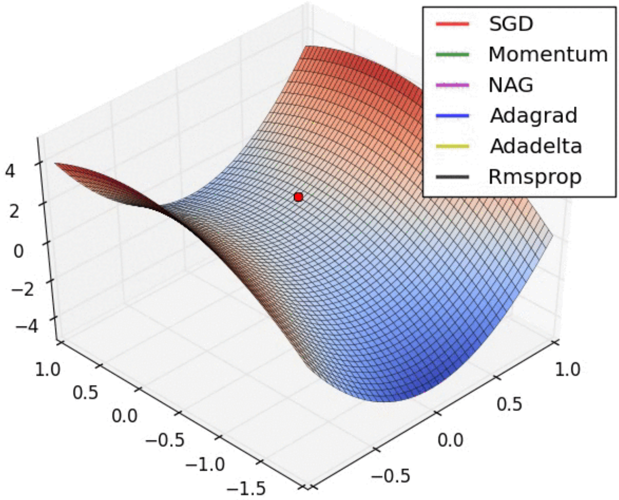
- Adam (recommended)

```
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)



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, by Stanford University
- Goodfellow, Bengio & Courville (2016), "Deep Learning", MIT Press
- Ioffe & Szegedy (2015), "Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift", arXiv:1502.03167
- Goldberg (1991), "What Every Computer Scientist Should Know About Floating-Point Arithmetic", *Computer Surveys*