# Advanced Prediction Models

Deep Learning, Graphical Models and Reinforcement Learning

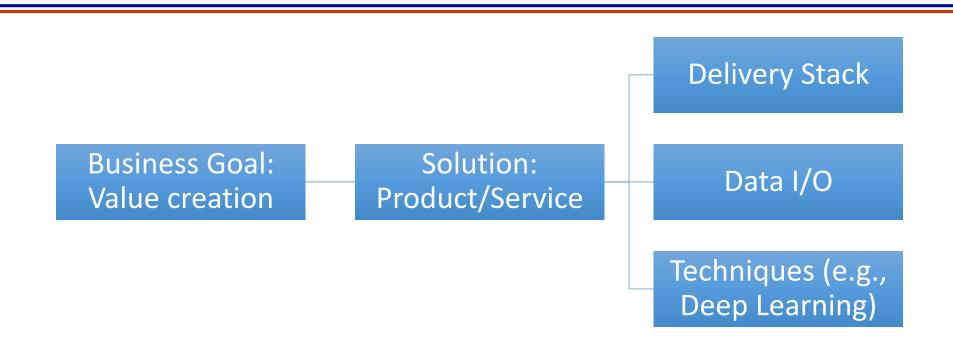
# Today's Outline

- Course Logistics
- Introduction to the Course
- Getting Started with Neural Nets
  - Classification
  - Backpropagation
  - Feedforward Neural Nets

### **Course Topics**

- We will cover several tools under the umbrella of
  - Deep Learning
  - Online and Reinforcement Learning

# Introduction to the Course



- You need a critical understanding of the domain to be successful in shipping solutions
- Before venturing into a complex technique, try a shallow/easy technique

## A Business Analyst's Toolkit

- Techniques
  - Prediction
    - Decision Trees
    - Linear classifiers and logistic regression
    - Naïve Bayes classifier
    - SVMs
    - Neural networks (and deep learning)
    - Online/reinforcement learning
  - Exploration
    - Clustering
    - Market basket analysis

### Example I

- You are an online fashion retailer
- Want to adaptively recommend products
- Cannot measure certain quantities directly
  - Substitution behavior
  - Stock-level sensitivities

### Example I

- You are an online fashion retailer
- Want to adaptively recommend products
- Cannot measure certain quantities directly
  - Substitution behavior
  - Stock-level sensitivities
- Build a personalization system that infers the most likely product that would be bought given censored/partial information
  - Recommend products
  - Tweak prices

### Example II

- You are a home insurance provider
- Want to check houses for risks and opportunities
- Manually checking houses and neighborhood does not scale

### Example II

- You are a home insurance provider
- Want to check houses for risks and opportunities
- Manually checking houses and neighborhood does not scale
- Fly a helicopter/drone and capture video
- Tag objects in the video
  - Classify if a outdoor pool is present or not
  - Classify greenery
  - Segment the house from the background
- Figure out insurance premiums across neighborhoods

### Example III

- Fashion retailing
  - The customer dislikes our recommendation
  - The customer finds the price too high
  - How to update our recommendations and prices?

### Example: Updating our Decisions

- Fashion retailing example
  - The customer dislikes our recommendation
  - The customer finds the price too high
  - How to update our recommendations and prices?
- Home insurance example
  - Prices the premium too low for this year
  - Had to payout a lot
  - How to update the premium for next year?

### Data Variety

- Structured data
  - Examples:
    - Medical/healthcare data
    - Advertising data
  - Have ordinal, integer, binary or categorical fields
  - Among other tools, one can use graphical models

### Data Variety

- Structured data
  - Examples:
    - Medical/healthcare data, advertising data
  - Have ordinal, integer, binary or categorical fields
  - Deep learning allows embedding of categorical features
- Unstructured data
  - Examples:
    - Images (tensor, i.e., typically a 3 dimensional array) and videos (a sequence of images), text strings/documents
  - Deep learning reduces feature engineering effort here

### **Complex Decisions**

- Decisions
  - Examples:
    - which articles to show, how to price products
  - May use many predictions
  - May need to be taken repeatedly for different contexts
  - May have longer term goals
  - Online and reinforcement learning methods address this 'learning on the go' problem

### Two Themes of the Course

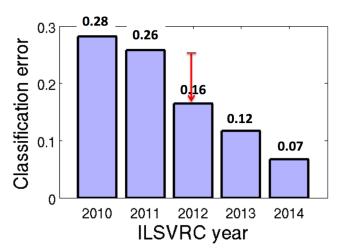
- Data Variety
  - Images and Videos/Audio
  - Text and Language
- Complex Decisions
  - Sequential Decision Making

### Techniques covered in the Course

- To address data variety and complex decision problems, we will look at:
  - Deep Learning
  - Online and Reinforcement Learning + Deep Learning

### **Deep Learning**

- One example (in vision) of its success is at the ILSVRC<sup>1</sup>
- ImageNet dataset has 22000 categories across 14 million images
- ILSVRC Task 1 was a classification challenge
  - Given 1000 categories and 1.5 million images, predict 5 categories for a test image



<sup>1</sup>ImageNet Large Scale Visual Recognition Challenge <sup>2</sup>Figure: Russakovsky et al. arxiv:1409.0575

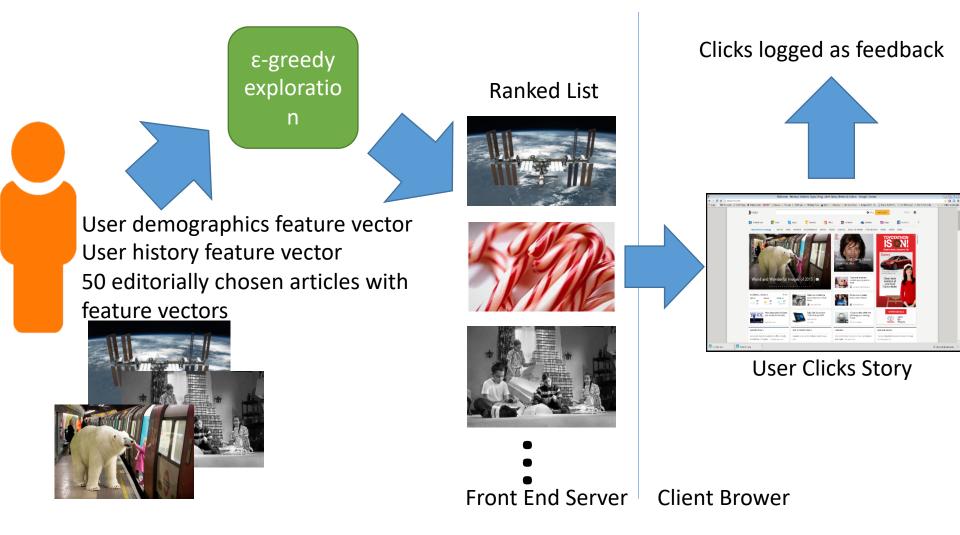
### Deep Learning

- Neural nets are not new (1960s). Applied to handwritten digit recognition back in 1998
- Were not mainstream till around 2010/2012\*
  - What changed? Access to GPUs and Data
- Caveat:
  - Deep learning achieves good performance on some tasks
  - Typically has not worked well beyond classification...
  - There is a lot of scope for improvement, engineering, system building, model building

\*Context-Dependent Pre-trained Deep Neural Networks for Large Vocabulary Speech Recognition, Dahl et al. 2010 Imagenet classification with deep convolutional neural networks, Krizhevsky et al. 2012

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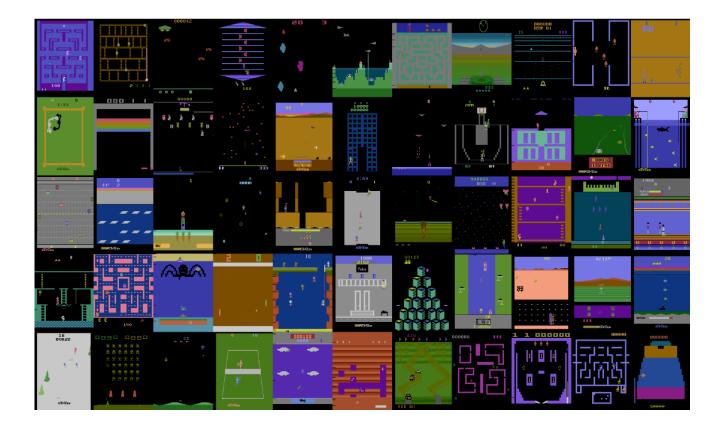
#### <sup>1</sup>Reference: Alekh Agarwal et al., http://arxiv.org/abs/1606.03966



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<sup>1</sup>Reference: DeepMind, March 2016



<sup>1</sup>Figure: Defazio Graepel, Atari Learning Environment

### **Caveat with Any Technique**

- Measurable metrics of business success take priority over technical success metrics
- Need to ask:
  - Does a Y% increase in classification accuracy help in X% increase in sales?
  - Does a Z% increase in classification accuracy due to using a deep learning solution help the bottomline?
  - What is the technical debt incurred? Who will maintain?

# Questions?

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  - Backpropagation

### Classification

- Classification
  - Data
  - Model
  - Loss
  - Optimization

### Classification



- To design the classifier, we need
  - Training data
  - Model specification for the classifier
  - Loss function to define the best model
  - Optimization to get to the best model

# Data (I)

- Lets pick a domain: Vision
- What is an image?
  - A bunch of numbers between 0 to 255
  - A 3 dimensional array
  - The same object can look different based on
    - Location of the camera
    - Location of the light source
    - Rigidity of the object
    - Occluding objects
    - Background
    - Variation across objects of the same category

# Data (II)

- Say we have N training examples  $(x_i, y_i), i = 1, ..., N$ 
  - $x_i$  is the feature vector for the  $i^{\text{th}}$  example
  - $y_i$  is the label for the  $i^{th}$  example
- Before deep learning
  - Carefully designed features
    - Histogram of colors
    - Histogram of Oriented Gradients (HOG)
    - Scale Invariant Feature Transform (SIFT)
    - Various types of filters
- With deep learning
  - Almost no feature engineering (for this type of data)

# Model (I)

- Parametric vs non-parametric
- Example:
  - Logistic classifier is parametric
  - K-Nearest Neighbor is a non-parametric classifier
- We will focus on parametric models
- A fixed set of parameters and hyper-parameters determine a model completely

# Model (II)

- Pick a concrete parametric model f(x, W, b)
  - x is the input ( $d \times 1$  dimensional)
    - Vectorize the image or get features
  - W is a parameter (p imes d dimensional)
  - b is also a parameter ( $p \times 1$  dimensional)
- Let f(x, W, b) = Wx + b
  - This is a linear model
  - We will change this later
  - The output of the linear model is a vector of scores

# Model (III)

- Given a model (i.e., a fixed W, b pair) our classifier can be
  - Pick the index with the highest 'score'
    - $\hat{l} = \operatorname{argmax}_{\{j=1,\dots,p\}} f(x, W, b)$
  - Pick the index with the highest 'probability'
    - Need a map/function from scores to probabilities
- We want to use the best model. How?
  - Define best: Loss function
  - Find the best: Optimization

# Loss functions (I)

- Let the  $j^{\text{th}}$  coordinate of f(x, W, b) be  $s_j$
- Loss  $L_{data}$  is defined over the training data
- Is chosen to be decomposable over  ${\cal N}$  terms, one per example

• 
$$L_{data} = \sum_{i=1}^{N} L_i$$

# Loss functions (I)

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• 
$$L_{data} = \sum_{i=1}^{N} L_i$$

• Logistic loss (Cross-entropy or softmax) for example i

• 
$$L_i = -\log P(Y = y_i | X = x_i)$$
 where  
•  $P(Y = j | X = x_i) = \frac{e^{s_j}}{\sum_k e^{s_k}}$ 

• SVM loss (2 class, W is a row vector) for example i

• 
$$L_i = \max(0, 1 - y_i s_{y_i})$$

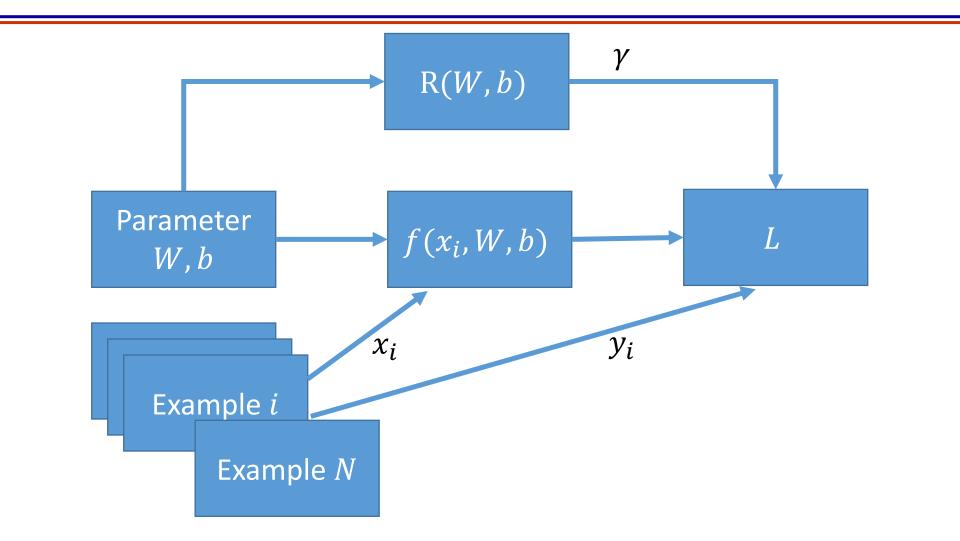
# Loss functions (II)

- Need for regularization
  - Unique model
  - Desired model
  - Control overfitting
- Final loss  $L = L_{data} + \lambda R(W, b)$
- R(W, b) can be just a function of W or b or both

#### Loss functions (III)

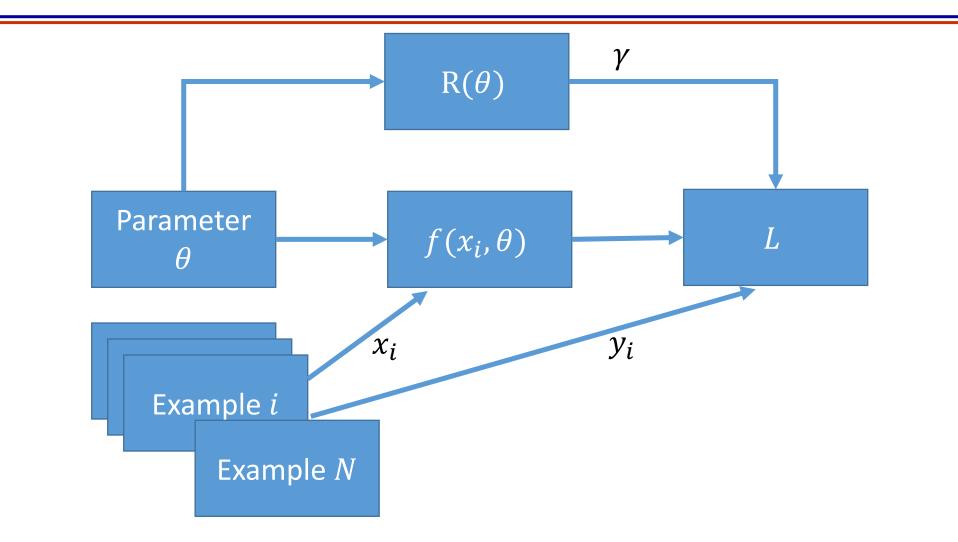
- L2 regularization:  $||W||_2^2 = \sum_i \sum_j W_{ij}^2$
- L1:  $||W||_1 = \sum_i \sum_j |W_{ij}|$
- Elastic net:  $\alpha ||W||_1 + (1-\alpha) ||W||_2^2$
- Regularization may not always be and explicit function of the parameters
  - We will see dropout later

#### **Optimization (I)**



Need to find parameters W, b and hyper-parameter  $\gamma$ 

#### **Optimization (I)**



Need to find parameters  $\theta$  and hyper-parameter  $\gamma$ 

### Optimization (II)

- Many ways to optimize differentiable models
- We will focus on first order methods
  - Key ingredient: Gradient
- Gradient is the vector of partial derivatives of a function
- Can be computed
  - Numerically:  $\lim_{h \to 0} \frac{f(z+h) f(z)}{h}$
  - Analytically: Calculus and chain rule

### Optimization (III)

- Intuition
  - Start with a model (i.e.,  $W_0, b_0$ )
  - Evaluate L for this model on the training data
  - Change  $W_0, b_0$  to  $W_1, b_1$  such that the new L is smaller
  - Repeat

- This intuition is the essence of Gradient Descent methods
  - Gradient of L with respect to the parameters is used to change  $W_0$ ,  $b_0$  to  $W_1$ ,  $b_1$

### **Optimization (IV)**

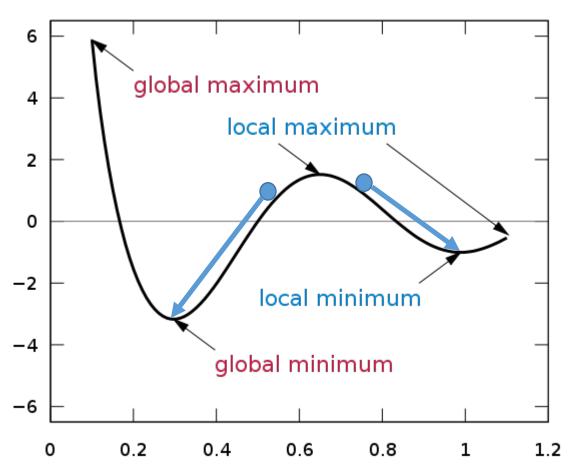
- Example method: Batched Gradient Descent
- Get a sample of training data
  - Example: AlexNet<sup>1</sup> used 256 examples as one batch
- Get gradient of L with respect to parameters W, b
- Update

• 
$$W_{k+1} \leftarrow W_k - \alpha \nabla_W L$$

- $b_{k+1} \leftarrow b_k \beta \nabla_b L$
- Step sizes (learning rates)  $\alpha$ ,  $\beta$  need careful choice

#### **Optimization (IV): Gradient Descent**

Gradient descent can only reach local optima

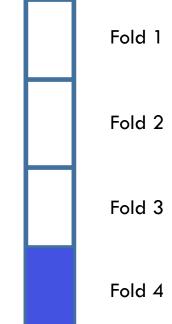


<sup>1</sup>By I, KSmrq, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=2276449

### **Optimization** (V)

- Tuning the hyper-parameter(s)
  - Break dataset into two parts: test and train
  - Remove test data access while you are tuning the parameters of your model
  - With training data, do cross validation to tune parameters and hyper-parameters

Essentially cycle through the choice of validation fold Optimize parameters over the remaining folds



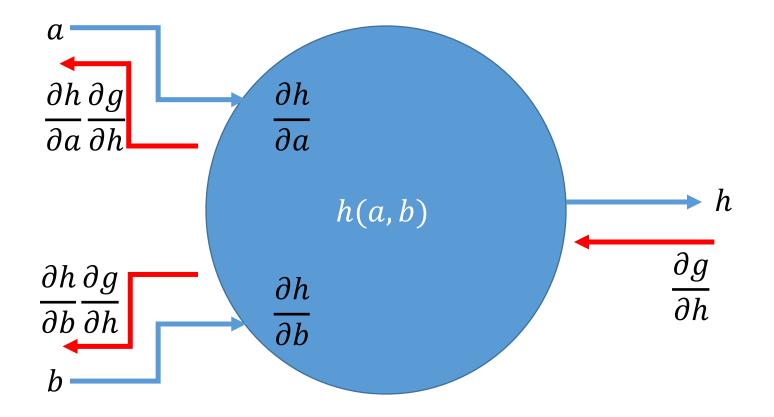
## Questions?

#### Today's Outline

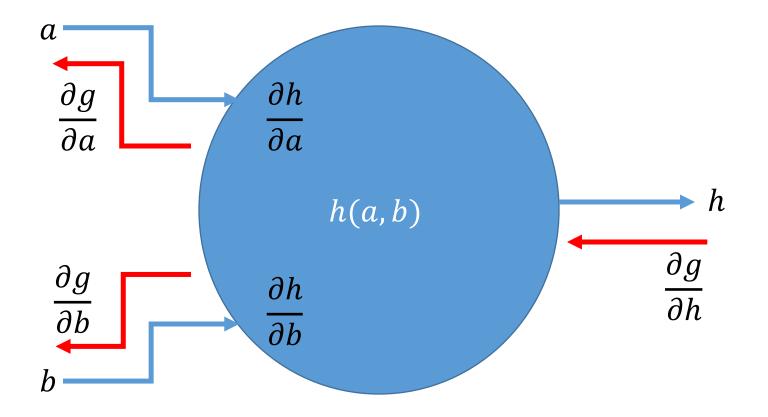
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#### Backpropagation

• An efficient way to get the gradient needed for optimization

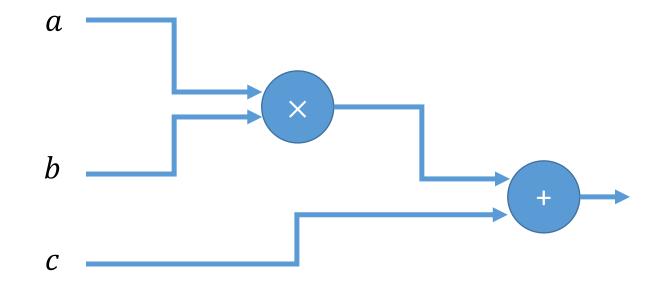


#### Backpropagation

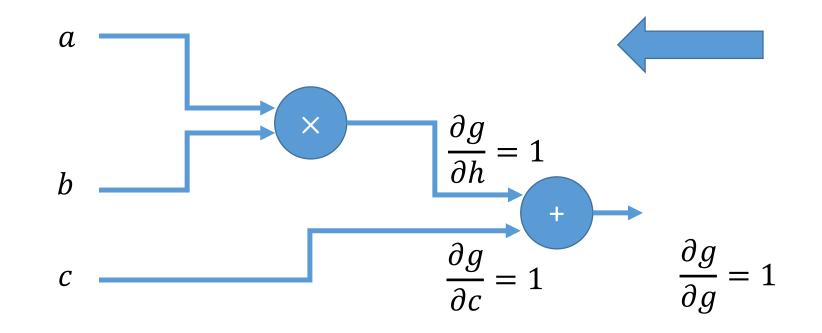


#### Notion of a Computational Graph

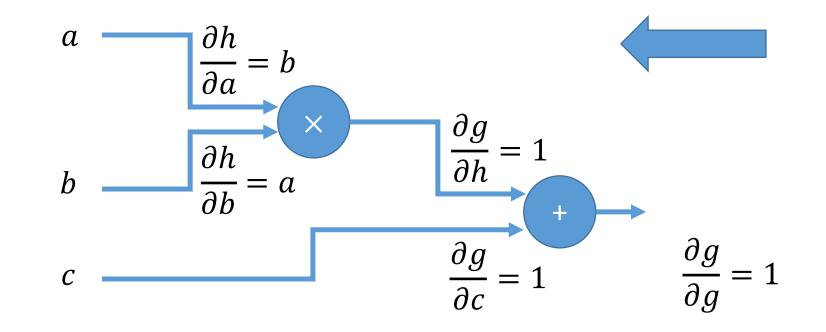
- Consider a function g(a, b, c) = a \* b + c
- Draw a graph



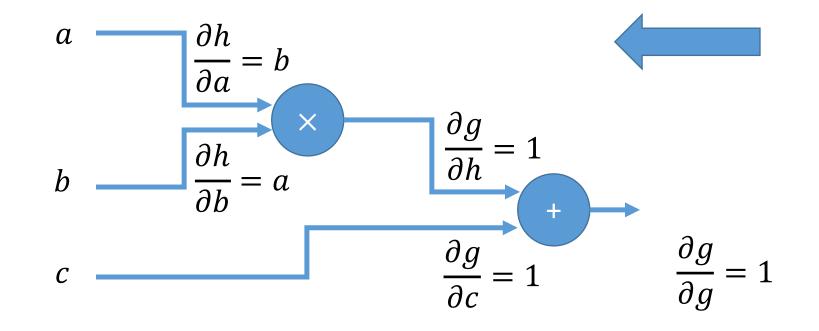
- The circles represent compute nodes
- Let h = a \* b. Then g = h + c



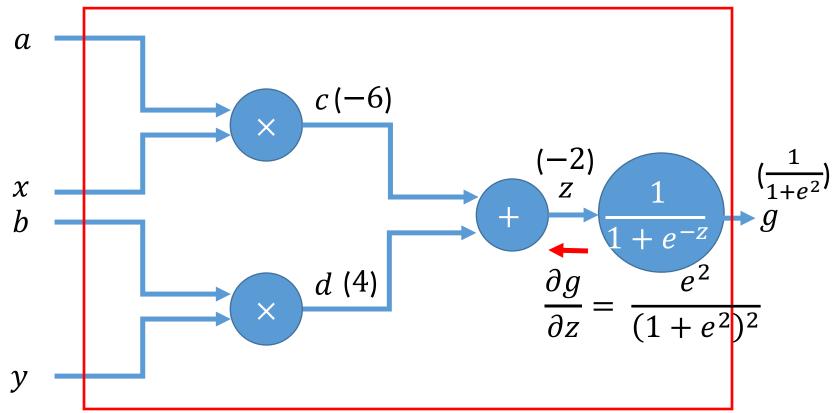
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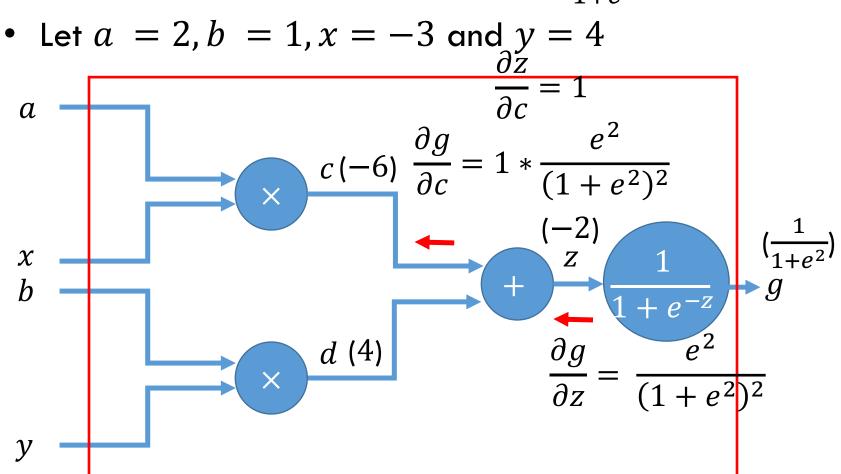
• We can find 
$$\frac{\partial g}{\partial a}$$
,  $\frac{\partial g}{\partial b}$  and  $\frac{\partial g}{\partial c}$  by chain rule!



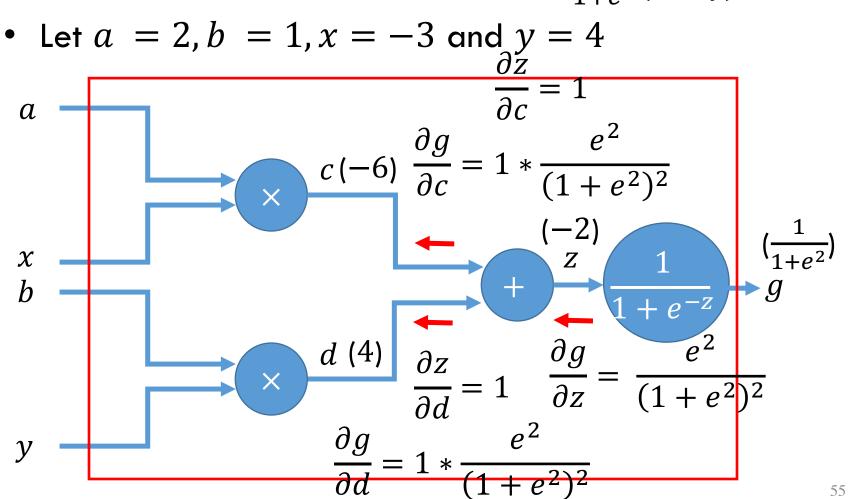
- Consider a function  $g(a, b, x, y) = \frac{1}{1 + e^{-(ax+by)}}$
- Let a = 2, b = 1, x = -3 and y = 4



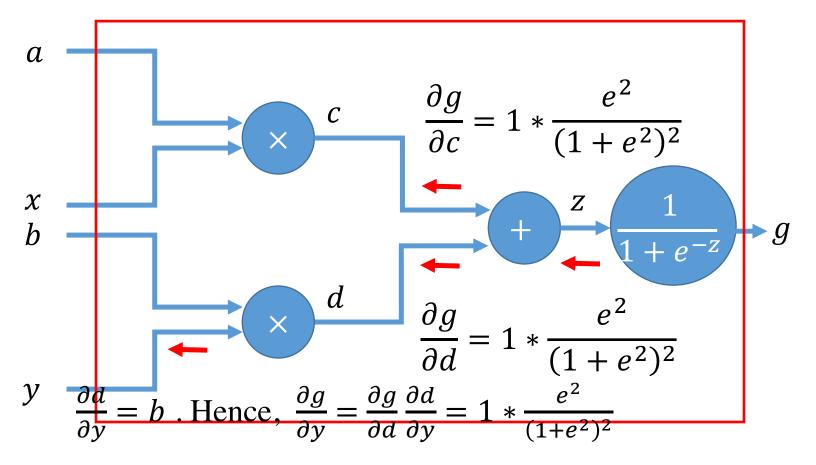
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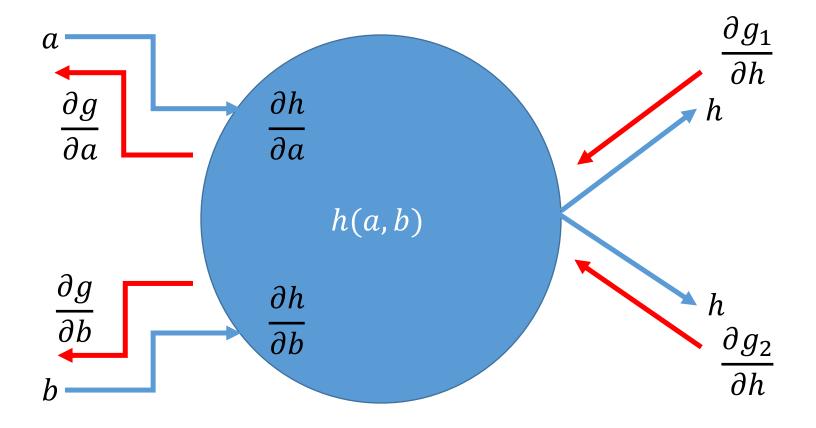


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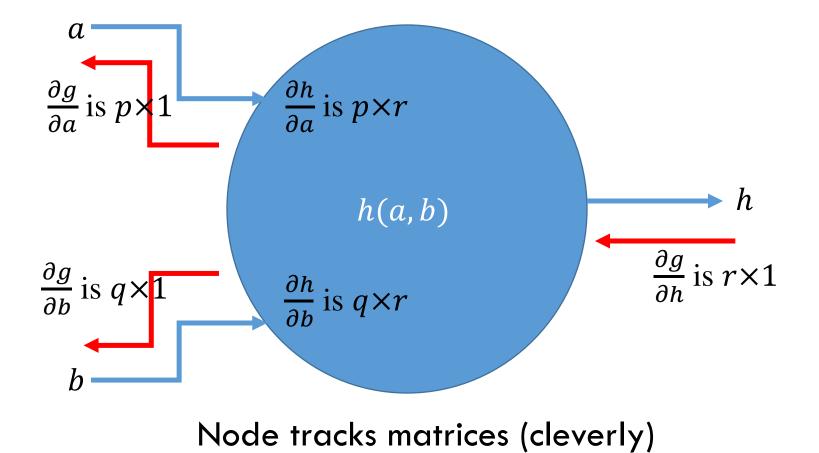
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#### Backprop for multiple outputs



#### **Backprop for vectors**

 Say, a is p×1 dimensional, b is q×1 dimensional and h is r×1 dimensional and g is scalar



#### **Backprop API for a node**

- Implement two functions
  - Forward
  - Backward
- Forward
  - Get input from preceding node(s)
  - Track inputs and local gradients
  - Return computation
- Backward
  - Get gradient from succeeding node(s)
  - Compute gradients (simple multiplication)
  - Return gradients to preceding node(s)

#### **Computational Graph API**

- Data structure a graph (nodes and directed edges)
- Implement two functions for it
  - Forward
  - Backward
- Forward
  - Recursively pass the inputs to the next nodes
  - Return *L*
- Backward
  - Recursively traverse the graph backwards
  - Return gradients

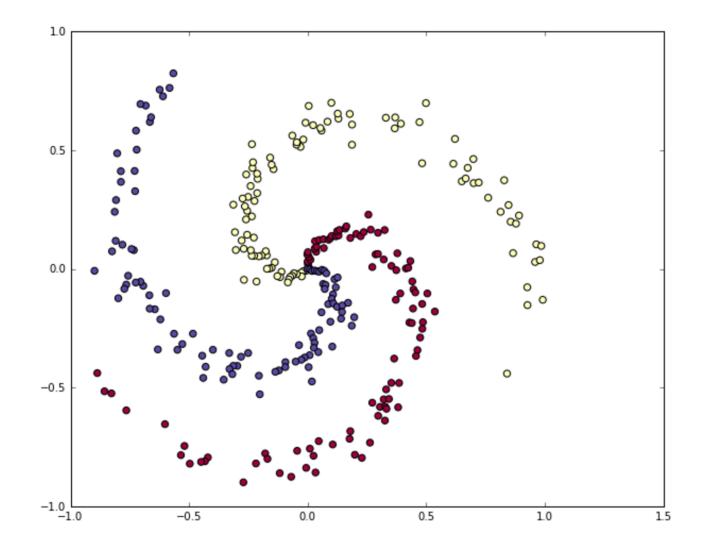
#### **Backprop and batched Gradient Descent**

- Choose a mini-batch (sample) of size B
- Forward propagate through the computation graph
  - Compute losses  $L_{i_1}, L_{i_2}, \dots L_{i_B}$  and R(W, b)
  - Get loss L for the batch
- Backprop to compute gradients with respect to W, b
- Update parameters W, b
  - In the direction of the negative gradient

```
#Example modified from http://cs231n.github.io/neural-networks-case-study/
#Imports
import numpy as np #Represent ndarrays a.k.a. tensors
import matplotlib.pyplot as plt #For plotting
np.random.seed(0) #For repeatability of the experiment
import pickle #To read data for this experiment
#Setup
%matplotlib inline
plt.rcParams['figure.figsize'] = (10.0, 8.0) # set default size of plots
plt.rcParams['image.interpolation'] = 'nearest'
plt.rcParams['image.cmap'] = 'gray'
```

#### Data

```
#Read data
X = pickle.load(open('dataX.pickle','rb'))
y = pickle.load(open('dataY.pickle','rb'))
#Define some local varaibles
D = X.shape[1] #Number of features
K = max(y)+1 #Number of classes assuming class index starts from 0
#Plot the data
fig = plt.figure()
plt.scatter(X[:, 0], X[:, 1], c=y, s=40, cmap=plt.cm.Spectral)
```



#### Model

```
# Linear model
# Start with an initialize parameters randomly
W = 0.01 * np.random.randn(D,K)
b = np.zeros((1,K))
# Initial values from hyperparameter
reg = 1e-3 # regularization strength
#For simplicity, we will not optimize this using grid search here.
```

```
#Perform batch SGD using backprop
```

```
#For simplicity we will take the batch size to be the same as number of examples
num_examples = X.shape[0]
```

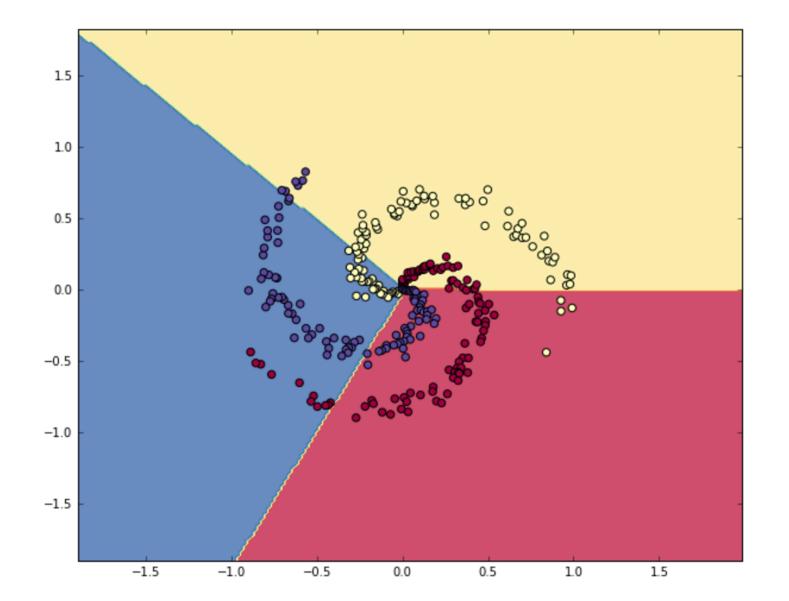
```
#Initial value for the Gradient Descent Parameter
step size = 1e-0 #Also called learning rate
```

#For simplicity, we will not hand tune this algorithm parameter as well.

```
# gradient descent loop
for i in xrange(200):
   # evaluate class scores, [N x K]
   scores = np.dot(X, W) + b
   # compute the class probabilities
   exp scores = np.exp(scores)
   probs = exp scores / np.sum(exp scores, axis=1, keepdims=True) \# [N x K]
   # compute the loss: average cross-entropy loss and regularization
   corect logprobs = -np.log(probs[range(num_examples),y])
   data loss = np.sum(corect logprobs)/num examples
   reg loss = 0.5*reg*np.sum(W*W)
   loss = data loss + reg loss
    if i % 10 == 0:
       print "iteration %d: loss %f" % (i, loss)
    # compute the gradient on scores
   dscores = probs
    dscores[range(num examples),y] -= 1
   dscores /= num examples
   # backpropate the gradient to the parameters (W,b)
   dW = np.dot(X.T, dscores)
   db = np.sum(dscores, axis=0, keepdims=True)
   dW += reg*W # regularization gradient
   # perform a parameter update
   W += -step size * dW
   b += -step size * db
```

#### **Post Training**

```
# Post-training: evaluate test set accuracy
#For simplicity, we will use training data as proxy for test. Do not do this.
X_test = X
y_test = y
scores = np.dot(X_test, W) + b
predicted_class = np.argmax(scores, axis=1)
print 'test accuracy: %.2f' % (np.mean(predicted class == y test))
```



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## Questions?

#### Summary

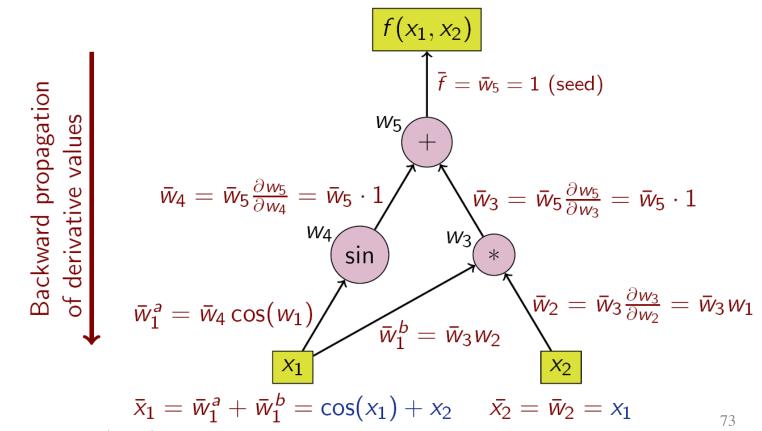
- Data variety poses challenges
  - Missing
  - Noisy
- Complex decisions poses challenges
  - Learning on the go
- We reviewed classification
  - Regression would have similar considerations
- Discussed backpropagation
  - A useful method for optimizing for the best model parameters

# Appendix

#### Reverse mode AutoDiff

 Backpropagation is a case of reverse accumulation automatic differentiation<sup>1</sup>

An example from wikipedia



<sup>1</sup>See <u>https://en.wikipedia.org/wiki/Automatic differentiation</u>