Deep Learning

Lecture 02: Neural Network

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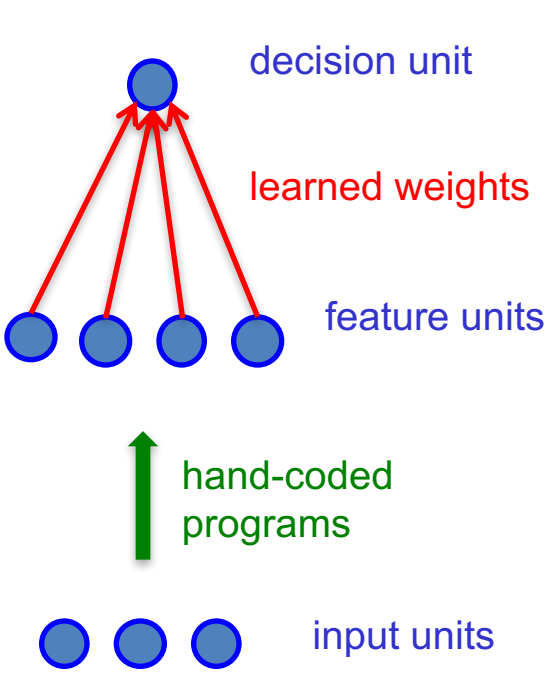
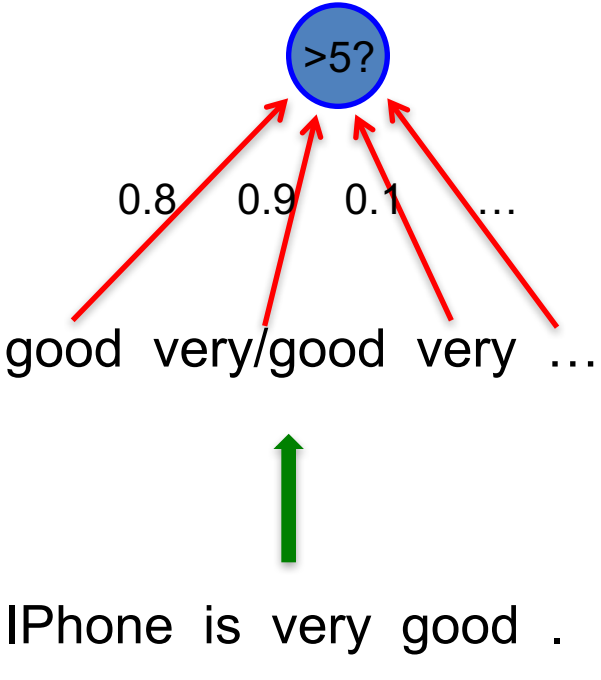
The Standard Paradigm (范式) for ML

1. Convert the raw input vector into a vector of feature activations
   - Use hand-written programs based on common-sense to define the features
2. Learn how to weight each of the feature activations to get a single scalar quantity
3. If this quantity is above some threshold, decide that the input vector is a positive example of the target class

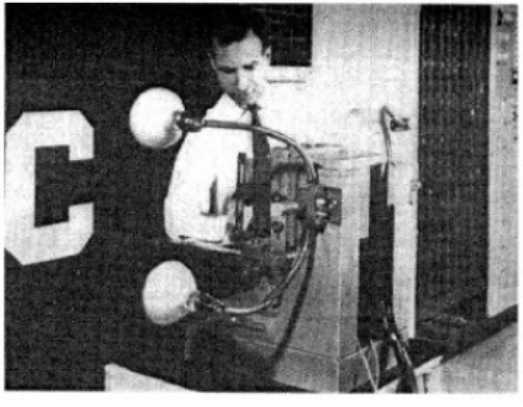
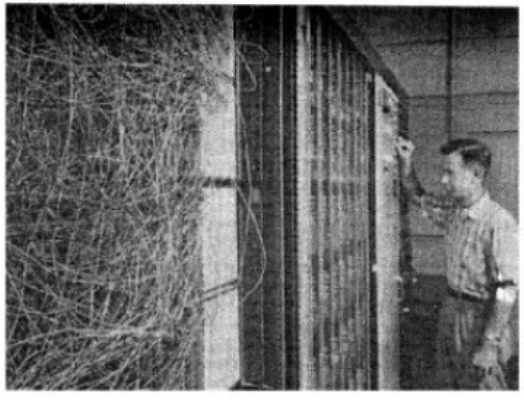
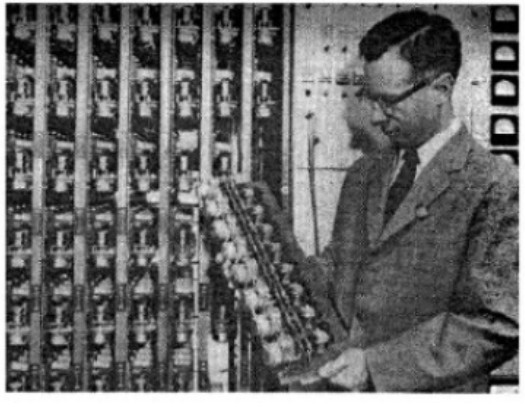
The Standard Perceptron (感知器) Architecture





The History of Perceptrons

- Invented in 1957 by Frank Rosenblatt
- In 1969, Minsky and Papert published a book called “Perceptrons” that analysed what they could do and showed their limitations (XOR function)
- Still **widely used today** for tasks with enormous feature vectors, such as NLP

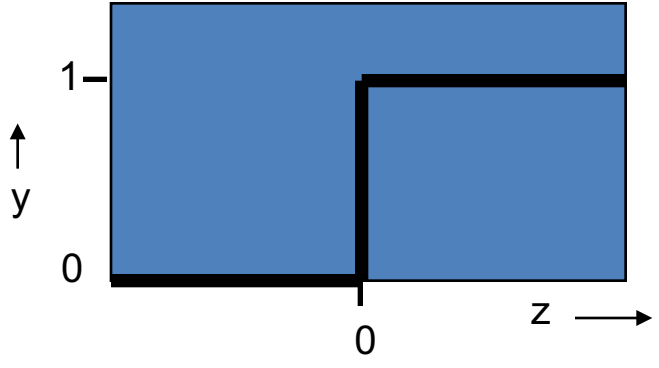
Binary Neurons (Decision Units)

- McCulloch-Pitts (1943)
  - First compute a weighted sum of the inputs from other neurons (plus a bias)
  - Then output a 1 if the weighted sum exceeds 0

Negative threshold

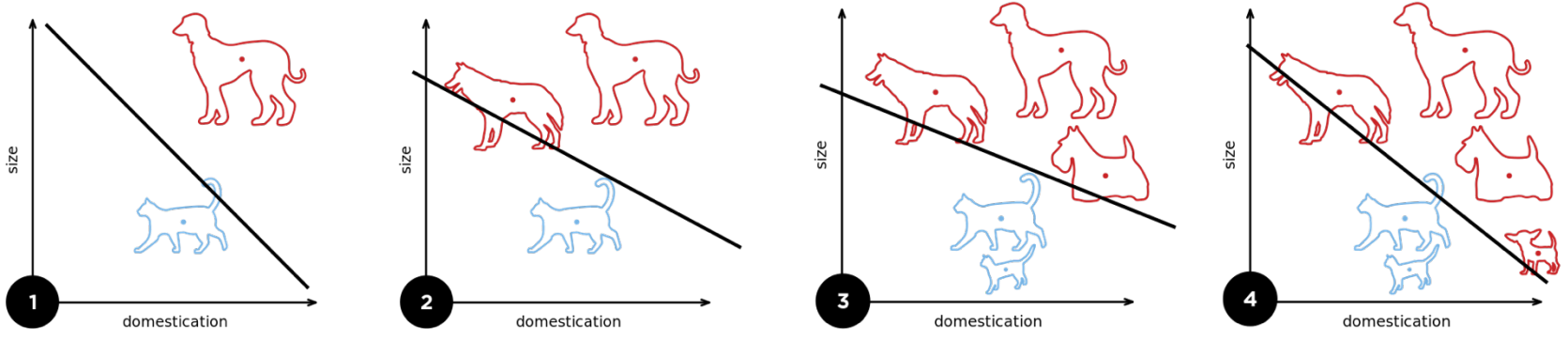
$$z = b + \sum_i x_i w_i$$

$$y = \begin{cases} 1 \text{ if } z \geq 0 \\ 0 \text{ otherwise} \end{cases}$$



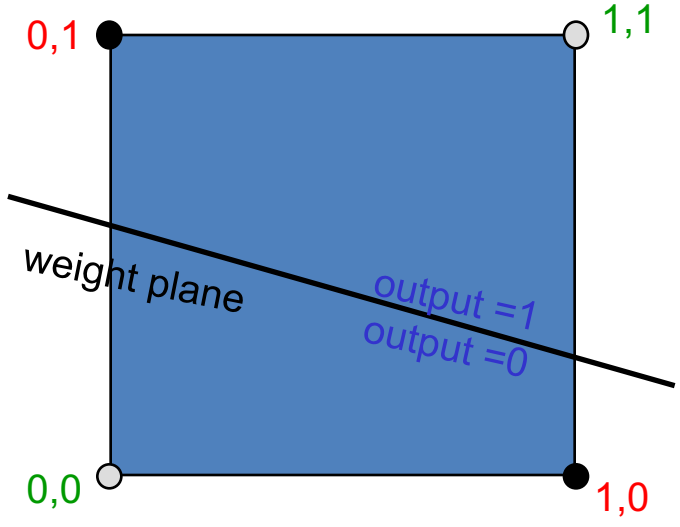
The Perceptron Training Algorithm

1. Initialize the weights $\boldsymbol{w}$
2. For each example n in training set, perform the following steps over the input $\boldsymbol{x}^n$ and desired output t^n
   a. Calculate the output: $y^n = f(\boldsymbol{w} \bullet \boldsymbol{x}^n)$
   b. Update the weights: $\boldsymbol{w} = \boldsymbol{w} + (t^n - y^n)\boldsymbol{x}_i$



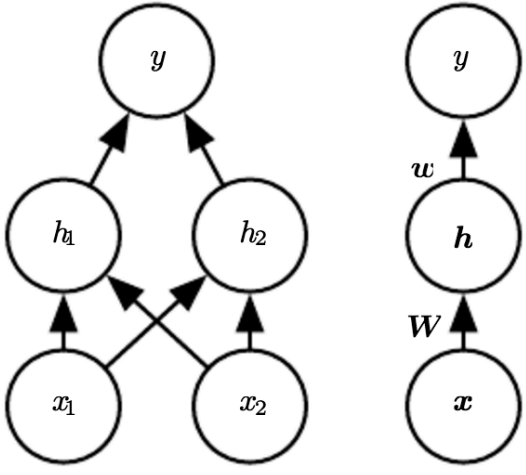
The Limitations of Perceptrons

- The **hand-coded features**
  - Great influence on the performance
  - Need lots of cost to find suitable features
- A **linear classifier** with a hyperplane
  - Cannot separate non-linear data, such as XOR function cannot be learned by a single-layer perceptron



The positive and negative cases cannot be separated by a plane

Learning with Non-linear Hidden Layers

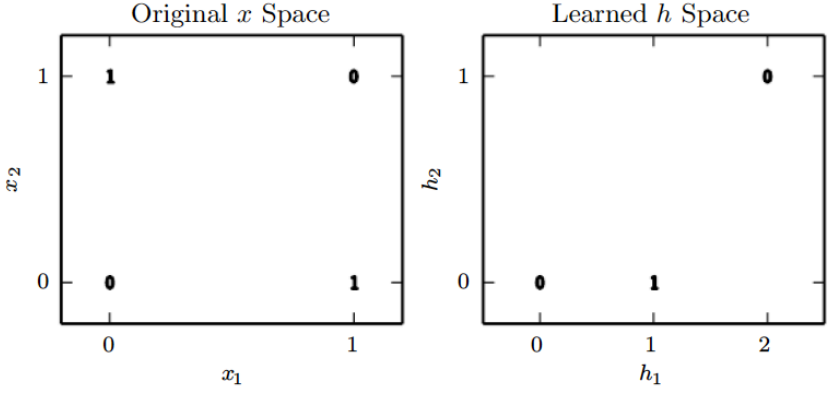


$$\boldsymbol{W} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix},$$

$$\boldsymbol{c} = \begin{bmatrix} 0 \\ -1 \end{bmatrix},$$

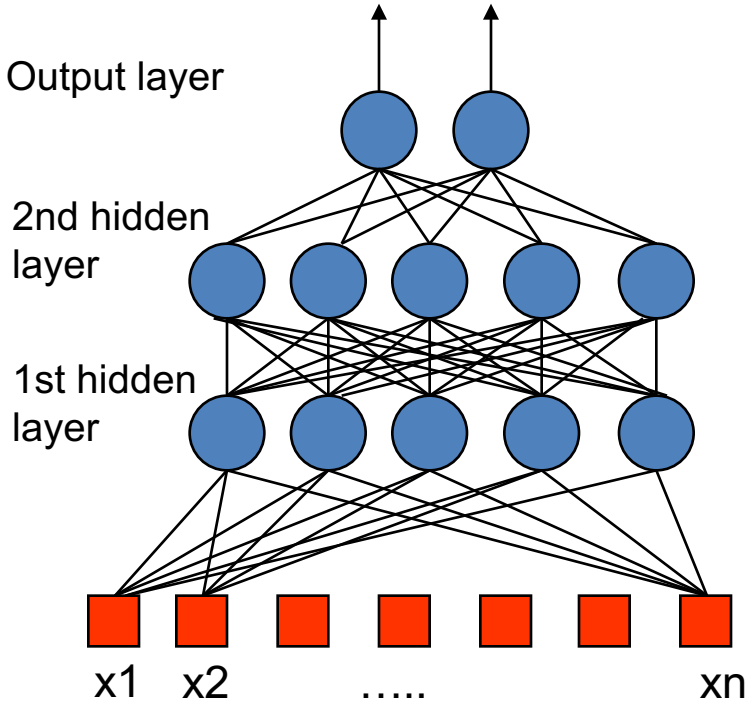
$$\boldsymbol{w} = \begin{bmatrix} 1 \\ -2 \end{bmatrix},$$

$$b = 0.$$



$$f(\boldsymbol{x}; \boldsymbol{W}, \boldsymbol{c}, \boldsymbol{w}, b) = \boldsymbol{w}^\top \max\{0, \boldsymbol{W}^\top \boldsymbol{x} + \boldsymbol{c}\} + b.$$

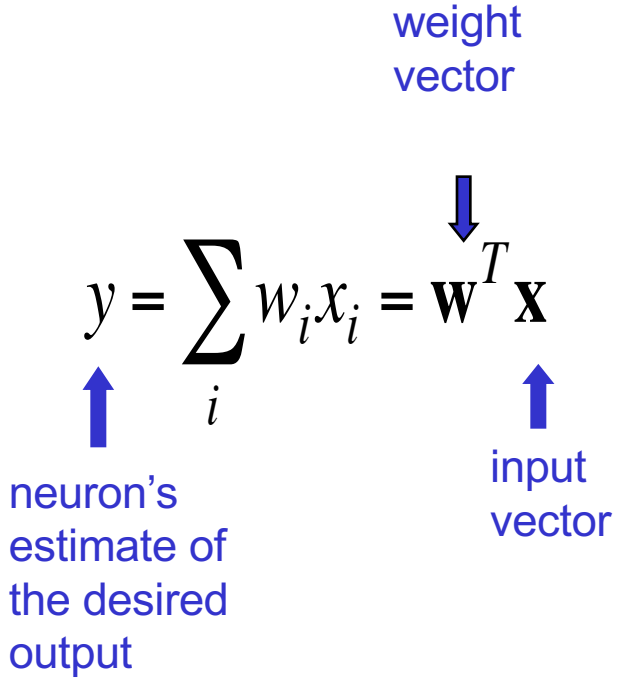
Feed Forward Neural Networks (前馈神经网络)



- The information is propagated from the inputs to the outputs
- Time has no role (NO cycle between outputs and inputs)
- Multi-layer Perceptron (MLP)?
- Learning the weights of hidden units is equivalent to **learning features**
- Networks without hidden layers are very limited in the input-output mappings
  - More layers of linear units do not help. Its still linear
  - Fixed output non-linearities are not enough

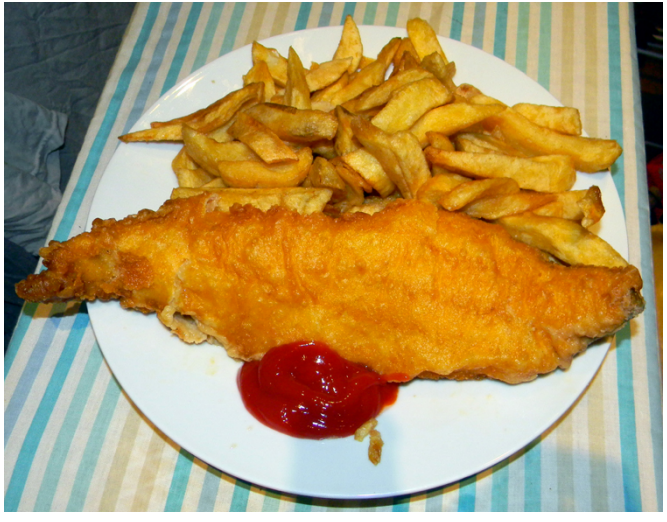
Linear Neurons (linear regression)

- The neuron has a **real-valued** output which is a weighted sum of its inputs
- The aim of learning is to minimize the error summed over all training cases
  - The error is the squared difference between the desired output and the actual output.



A Toy Example

- Each day you get lunch at the cafeteria
  - Your diet consists of fish, chips, and ketchup
  - You get several portions of each
- The cashier only tells you the total price of the meal
  - After several days, you should be able to figure out the price of each portion



Solving the Equations Iteratively (迭代)

- Each meal price gives a linear constraint on the prices of the portions

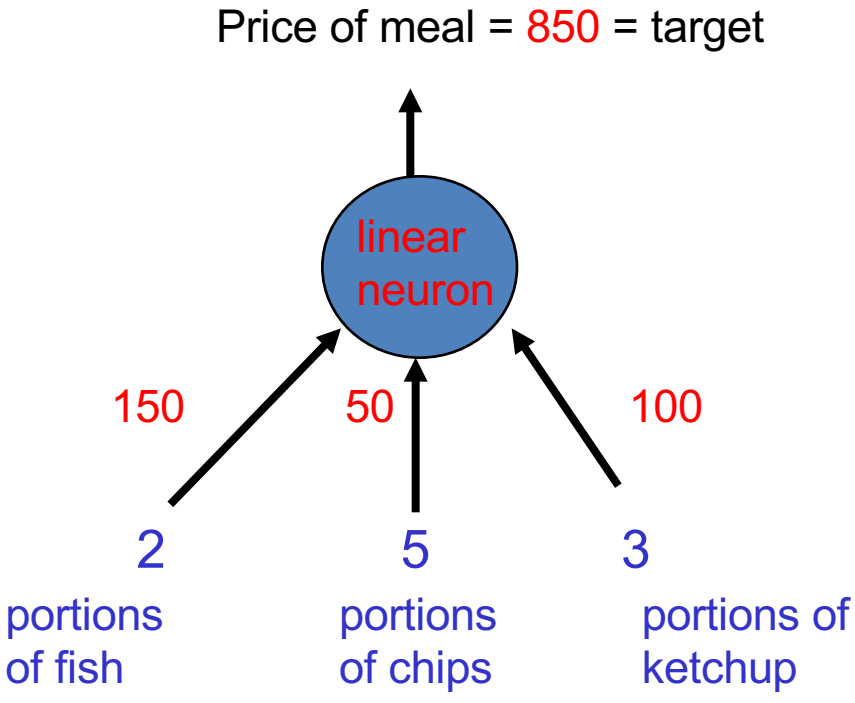
$$price = x_{fish} w_{fish} + x_{chips} w_{chips} + x_{ketchup} w_{ketchup}$$

- The prices of the portions are like the weights in of a linear neuron

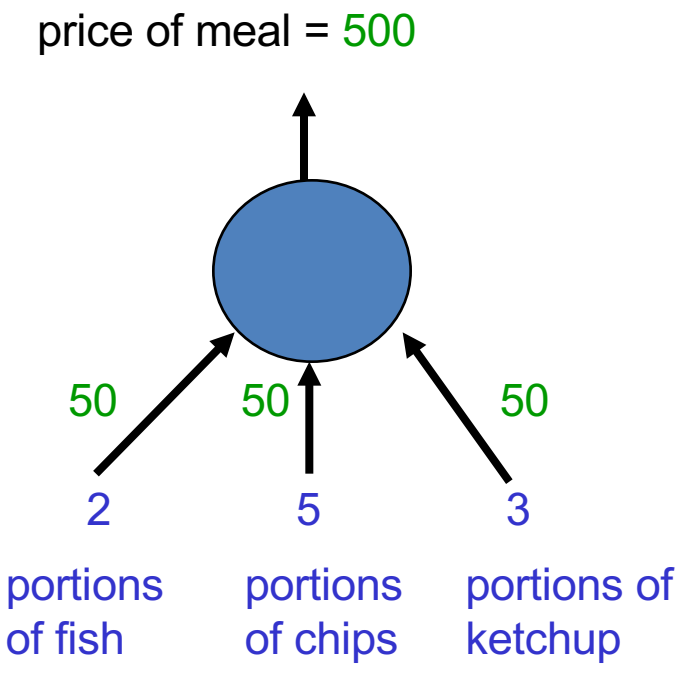
$$\mathbf{w} = (w_{fish}, w_{chips}, w_{ketchup})$$

- The iterative approach
  - Start with **guesses** for the weights and then adjust the guesses slightly to give a **better** fit to the prices given by the cashier

The True Weights Used by the Cashier



With an Random Initial Weights



- Residual error = 850 – 500 = 350
- The "delta-rule" for learning

$$\Delta w_i = \varepsilon \, x_i (t - y)$$

- With a learning rate: 1/35, the weight changes are +20, +50, +30
- New weights of 70, 100, 80.
  - Notice that the weight for chips got worse!

Implementation in Python

- ```
  eta = 1 / 35.0
  ws = [50, 50, 50]

  train = (
    ((2, 5, 3), 850), ((1, 4, 7), 1050), ((2, 3, 5), 950), ((3, 6, 9), 1650), ((7, 4, 1), 1350),
    )

  for _ in range(100):
    for xs, t in train:
      y = sum([w * x for w, x in zip(ws, xs)])
      delta_ws = [eta * x * (t - y) for x in xs]
      ws = [w + delta_w for w, delta_w in zip(ws, delta_ws)]

  print ws
  ```

- [149.9999854696171, 50.00004609118093, 99.99997795027406]
  ```

Deriving the delta rule

- Define the error (loss/cost) as the squared residuals summed over all training cases (损失/代价函数)
- Now differentiate to get error derivatives (导数) for weights
- The batch delta rule changes the weights in proportion to their error derivatives summed over all training cases

$$E = \frac{1}{2} \sum_{n \in training} (t^n - y^n)^2$$

$$\frac{\partial E}{\partial w_i} = \frac{1}{2} \sum_n \frac{\partial y^n}{\partial w_i} \frac{dE^n}{dy^n}$$

$$= -\sum_n x_i^n (t^n - y^n)$$

$$\Delta w_i = -\varepsilon \frac{\partial E}{\partial w_i} = \sum_n \varepsilon \, x_i^n (t^n - y^n)$$

General Optimizing (Learning) Algorithms

- Gradient Descent (梯度下降)

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \epsilon \nabla_{\boldsymbol{\theta}} \sum_t L(f(\boldsymbol{x}^{(t)}; \boldsymbol{\theta}), \boldsymbol{y}^{(t)}; \boldsymbol{\theta})$$

- Stochastic Gradient Descent (SGD, 随机梯度下降)
  - Minibatch SGD (m > 1), Online GD (m = 1)

Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

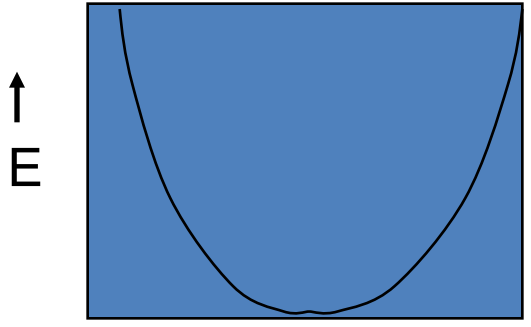
Require: Learning rate ϵ_k.
Require: Initial parameter $\boldsymbol{\theta}$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow +\frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \hat{\boldsymbol{g}}$
  end while

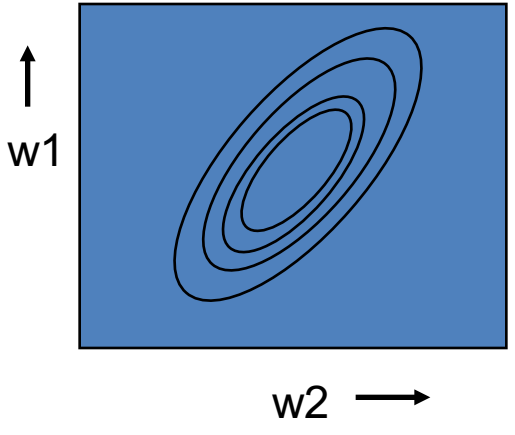
Behavior of the Iterative Learning Procedure

- Does the learning procedure eventually get the right answer?
  - There **may be no perfect** answer
  - By making the learning rate small enough we can get as close as we desire to the best answer
- How quickly do the weights converge to their correct values?
  - It can be very slow if two input dimensions are **highly correlated**. If you almost always have the same number of portions of ketchup and chips, it is hard to decide how to divide the price between ketchup and chips.

The Error Surface

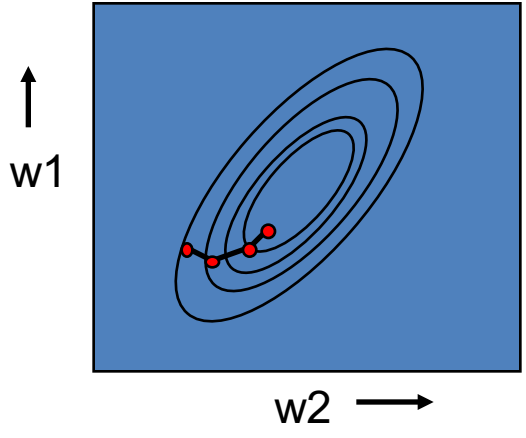
- The error surface lies in a space with a horizontal axis for each weight and one vertical axis for the error
  - For a linear neuron with a squared error, it is a quadratic bowl
  - Vertical cross-sections are parabolas
  - Horizontal cross-sections are ellipses
- For multi-layer, non-linear nets the error surface is much more complicated.



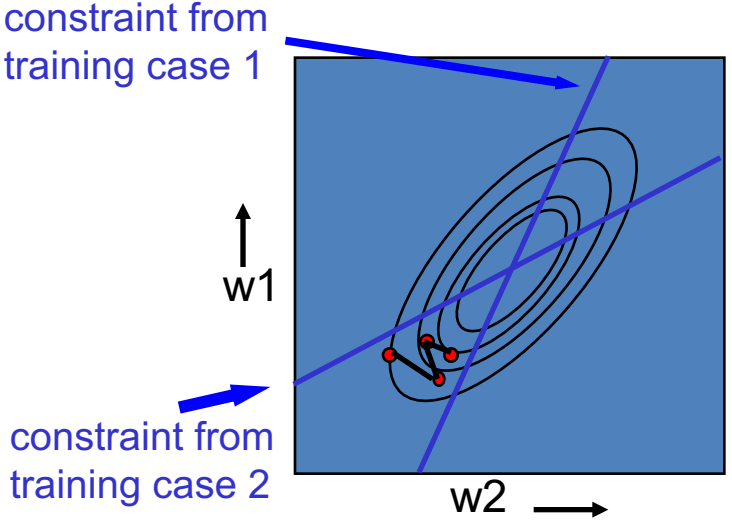


Online versus batch learning

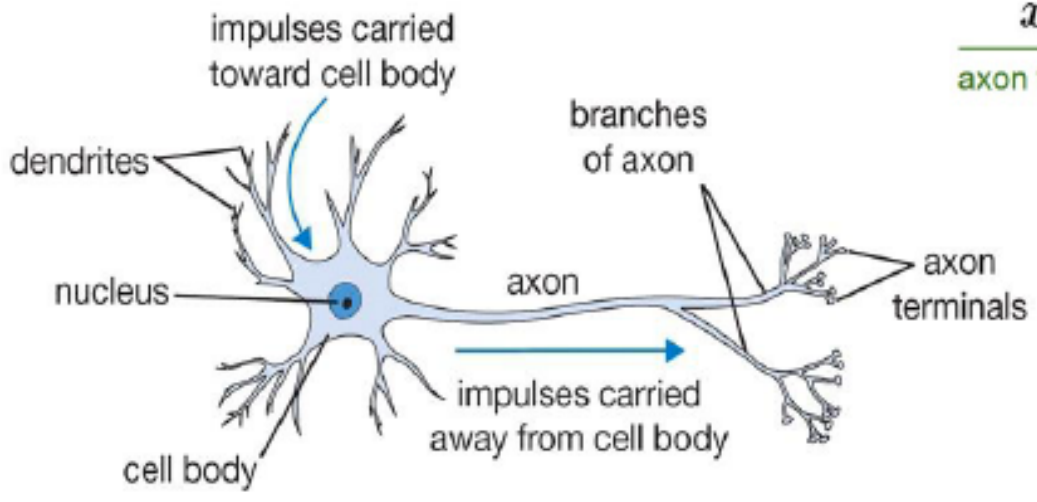
- The simplest kind of batch learning does steepest descent on the error surface.
  - This travels perpendicular to the contour lines.

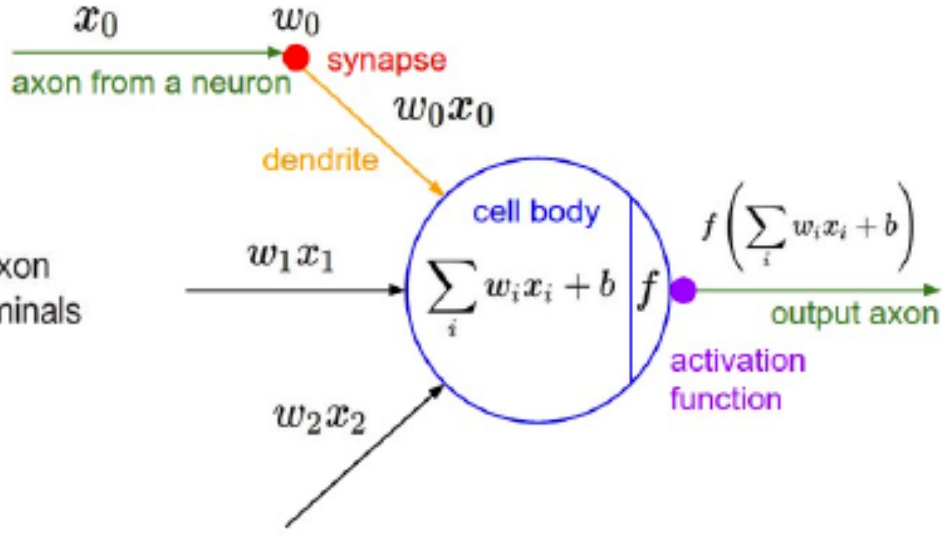


- The simplest kind of online learning zig-zags around the direction of steepest descent:



Non-linear Neurons

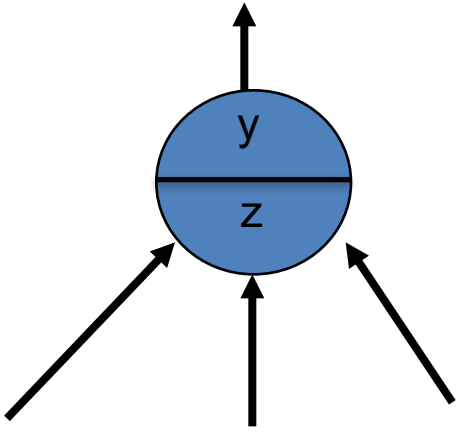


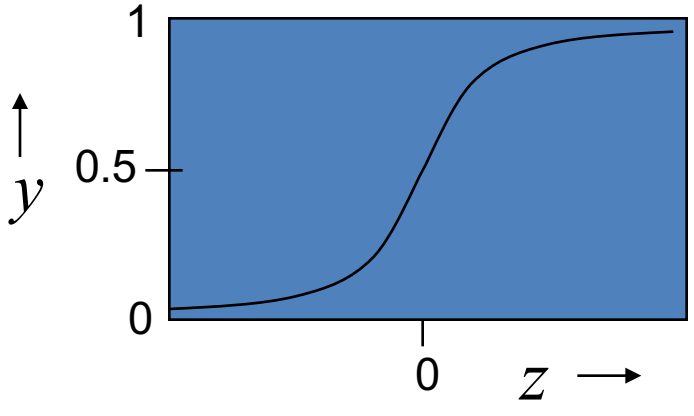


Logistic Regression (sigmoid function)

- These give a real-valued output that is a **smooth and bounded** function of their total input
  - They have nice derivatives which make learning easy.

$$z = b + \sum_i x_i w_i \qquad y = \frac{1}{1 + e^{-z}}$$





The Derivatives of a Logistic Regression

- The derivatives of the logit, z, with respect to the inputs and the weights are very simple:

$$z = b + \sum_i x_i w_i$$

$$\frac{\partial z}{\partial w_i} = x_i \qquad \frac{\partial z}{\partial x_i} = w_i$$

- The derivative of the output with respect to the logit is simple if you express it in terms of the output:

$$y = \frac{1}{1 + e^{-z}}$$

$$\frac{dy}{dz} = y\,(1 - y)$$

The Derivatives of a Logistic Regression

$$y = \frac{1}{1+e^{-z}} = (1+e^{-z})^{-1}$$

$$\frac{dy}{dz} = \frac{-1(-e^{-z})}{(1+e^{-z})^2} = \left(\frac{1}{1+e^{-z}}\right)\left(\frac{e^{-z}}{1+e^{-z}}\right) = y(1-y)$$

because $\frac{e^{-z}}{1+e^{-z}} = \frac{(1+e^{-z})-1}{1+e^{-z}} = \frac{(1+e^{-z})}{1+e^{-z}} - \frac{1}{1+e^{-z}} = 1-y$

The Derivatives of a Logistic Neuron

- Using the chain rule to get the derivatives needed for learning the weights of a logistic unit
- To learn the weights we need the derivative of the output with respect to each weight:

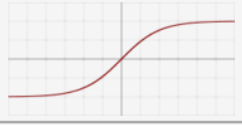
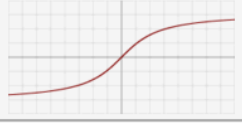
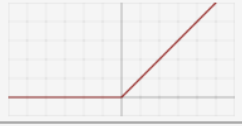
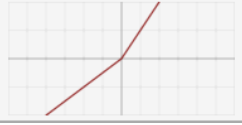
$$\frac{\partial y}{\partial w_i} = \frac{\partial z}{\partial w_i}\frac{dy}{dz} = x_i\, y\,(1-y)$$

$$\frac{\partial E}{\partial w_i} = \sum_n \frac{\partial y^n}{\partial w_i}\frac{\partial E}{\partial y^n} = -\sum_n x_i^n \, y^n\,(1-y^n)\,(t^n - y^n)$$

delta-rule

extra term = derivative of logistic

More Activation Functions

Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1+e^{-x}}$	$f'(x) = f(x)(1-f(x))$
TanH		$f(x) = \tanh(x) = \frac{2}{1+e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2+1}$
Rectified Linear Unit (ReLU)[7]		$f(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU)[8]		$f(x) = \begin{cases} \alpha x & \text{for} \quad x < 0 \\ x & \text{for} \quad x \geq 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for} \quad x < 0 \\ 1 & \text{for} \quad x \geq 0 \end{cases}$

Learning with Hidden Units -- Backpropagation

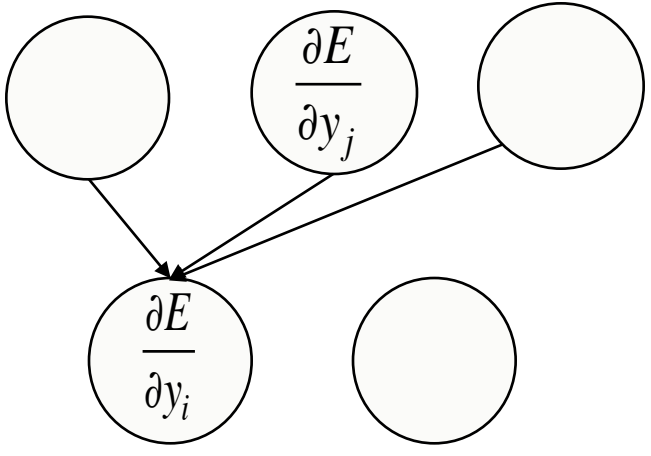
- Don't know what the hidden units' errors, but we can compute **how fast the error changes** as we change a hidden activity
  - Instead of using desired activities to train the hidden units, use error derivatives w.r.t. hidden activities
  - Each hidden activity can affect many output units and can therefore have many separate effects on the error. These effects must be combined
  - Once we have the error derivatives for the hidden activities, its easy to get the error derivatives for the weights going into a hidden unit.

Backpropagation on a Single Case

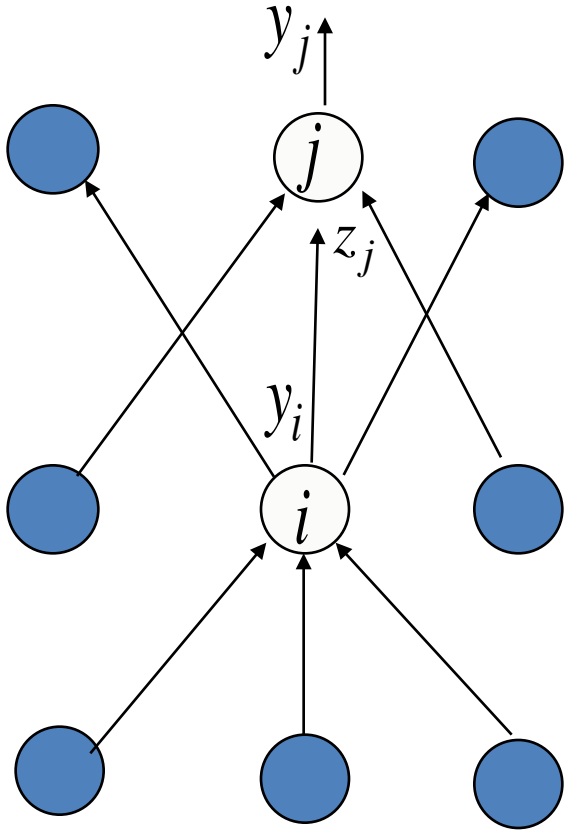
- First convert the discrepancy between each output and its target value into an **error derivative**
- Then compute **error derivatives** in each hidden layer from error derivatives in the layer above
- Then use error derivatives *w.r.t.* activities to get error derivatives *w.r.t.* the incoming **weights**

$$E = \frac{1}{2} \sum_{j \in output} (t_j - y_j)^2$$

$$\frac{\partial E}{\partial y_j} = -(t_j - y_j)$$



Backpropagating dE/dy



$$\frac{\partial E}{\partial z_j} = \frac{dy_j}{dz_j}\frac{\partial E}{\partial y_j} = y_j(1-y_j)\frac{\partial E}{\partial y_j}$$

$$\frac{\partial E}{\partial w_{ij}} = \frac{\partial z_j}{\partial w_{ij}}\frac{\partial E}{\partial z_j} = y_i\frac{\partial E}{\partial z_j}$$

$$\frac{\partial E}{\partial y_i} = \sum_j \frac{dz_j}{dy_i}\frac{\partial E}{\partial z_j} = \sum_j w_{ij}\frac{\partial E}{\partial z_j}$$

Backpropagation (vector version)

- Define the error of neurons in layer l: $\delta^l = \frac{\partial E}{\partial z^l}$
- The 4 Equations of Backpropagation
  - $\delta^L = \nabla_y E \odot f'(z^L)$
  - $\delta^l = ((w^{l+1})\delta^{l+1}) \odot f'(z^l)$
  - $\frac{\partial E}{\partial b^l} = \delta^l$
  - $\frac{\partial E}{\partial w^l} = y^{l-1}\delta^l$

Backpropagation Algorithm

1. **Input *x***: Set the corresponding activation y^1 for the input layer
2. **Feedforward**: For each $l = 2,3,\cdots,L$ compute $z^l = w^l y^{l-1} + b^l$ and $y^l = f(z^l)$
3. **Output error** δ^L: Compute the vector $\delta^L = \nabla_y E \odot f'(z^L)$
4. **Backpropgrate the error**: For each $l = L-1, L-2, \cdots, 2$ compute $\delta^l = ((w^{l+1})\delta^{l+1}) \odot f'(z^l)$
5. **Output**: The gradient of the cost function is given by $\frac{\partial E}{\partial b^l} = \delta^l$ and $\frac{\partial E}{\partial w^l} = y^{l-1}\delta^l$

Gradient Checks

- Allow you to know that there are no bugs in your neural network implementation!
- Steps
  - Implement your gradient
  - Implement a finite difference computation by looping through the parameters of your network, adding and subtracting a small epsilon (~10^-5) and estimate derivative

$$f'(\theta) \approx \frac{J\left(\theta^{(i+)}\right) - J\left(\theta^{(i-)}\right)}{2\epsilon} \qquad \theta^{(i+)} = \theta + \epsilon \times e_i$$

  - Compare the two and make sure they are **almost the same**

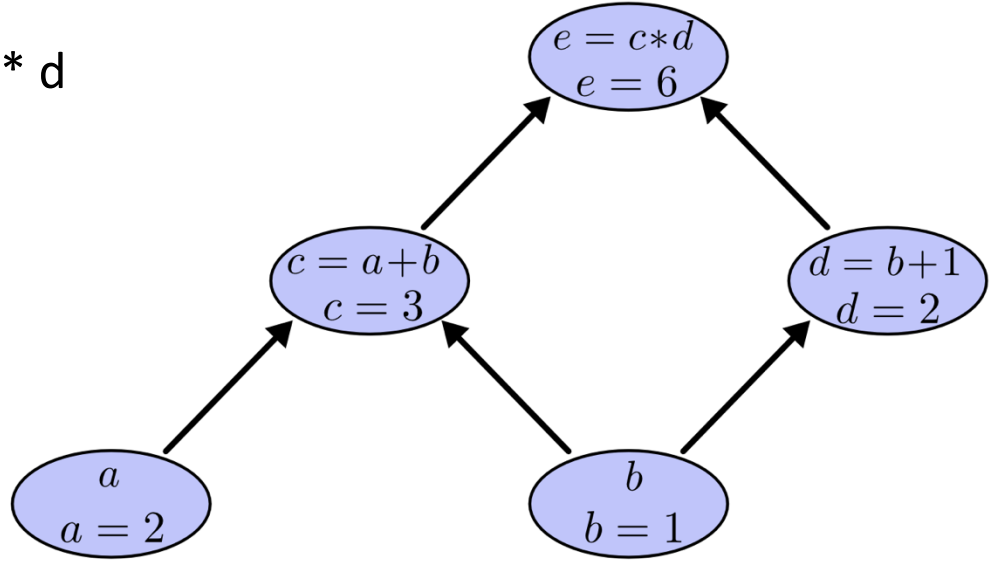
$$\frac{|f_a' - f_n'|}{\max(|f_a'|, |f_n'|)}$$

Gradient Computation in DL Libraries

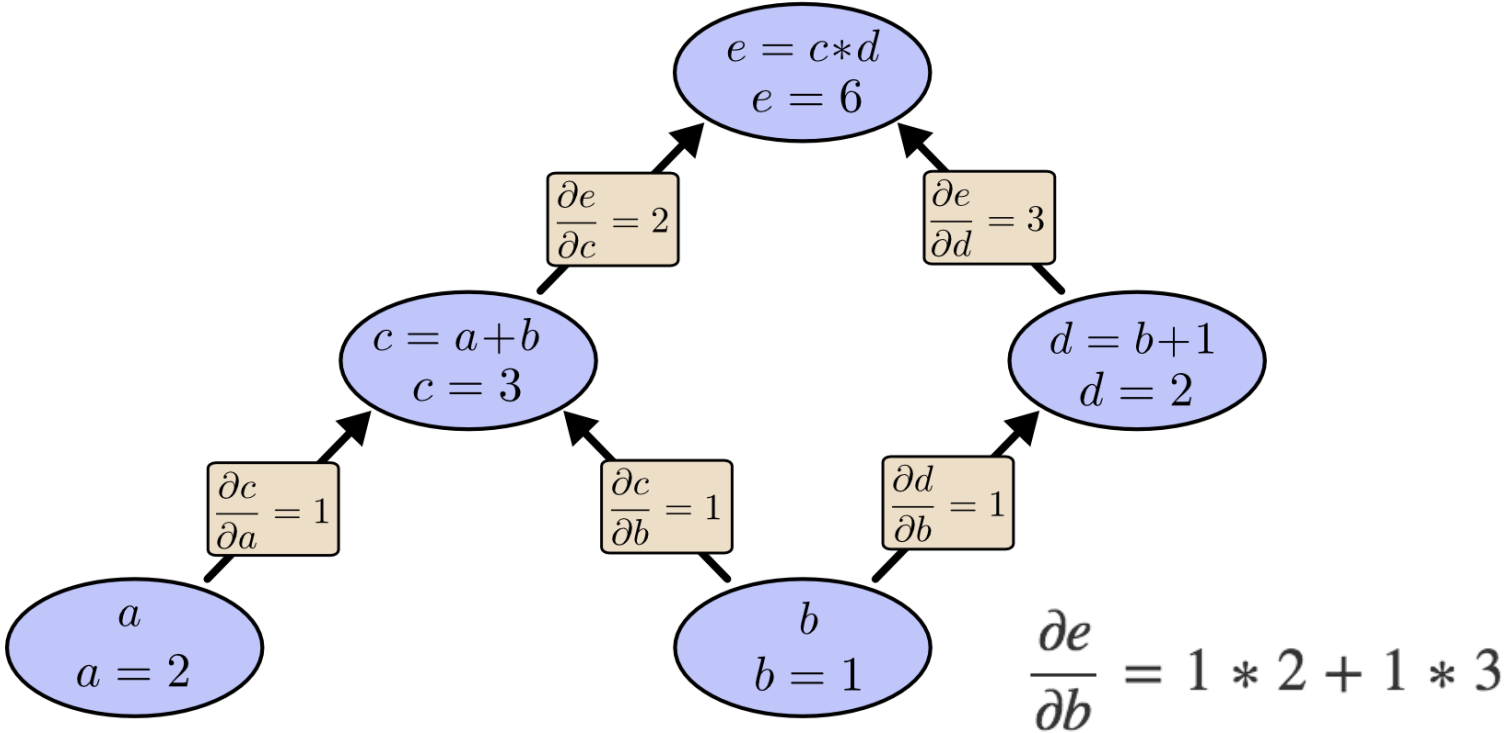
- TensorFlow
  - tf.gradients(ys, xs)
- Theano
  - theano.tensor.grad(y, x)

Computational Graphs

- Describing Mathematical Expressions
- For example
  - e = (a + b) * (b + 1)
    - c = a + b, d = b + 1, e = c * d
  - If a = 2, b = 1

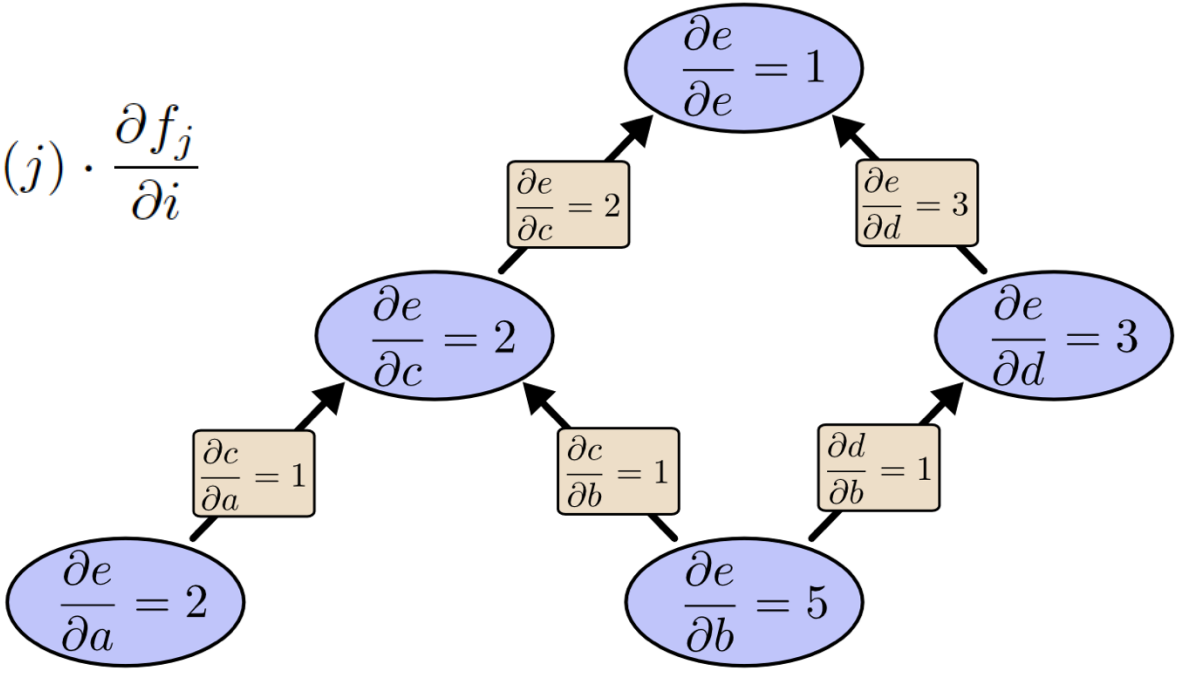


Derivatives on Computational Graphs



Computational Graph Backward Pass (Backpropagation)

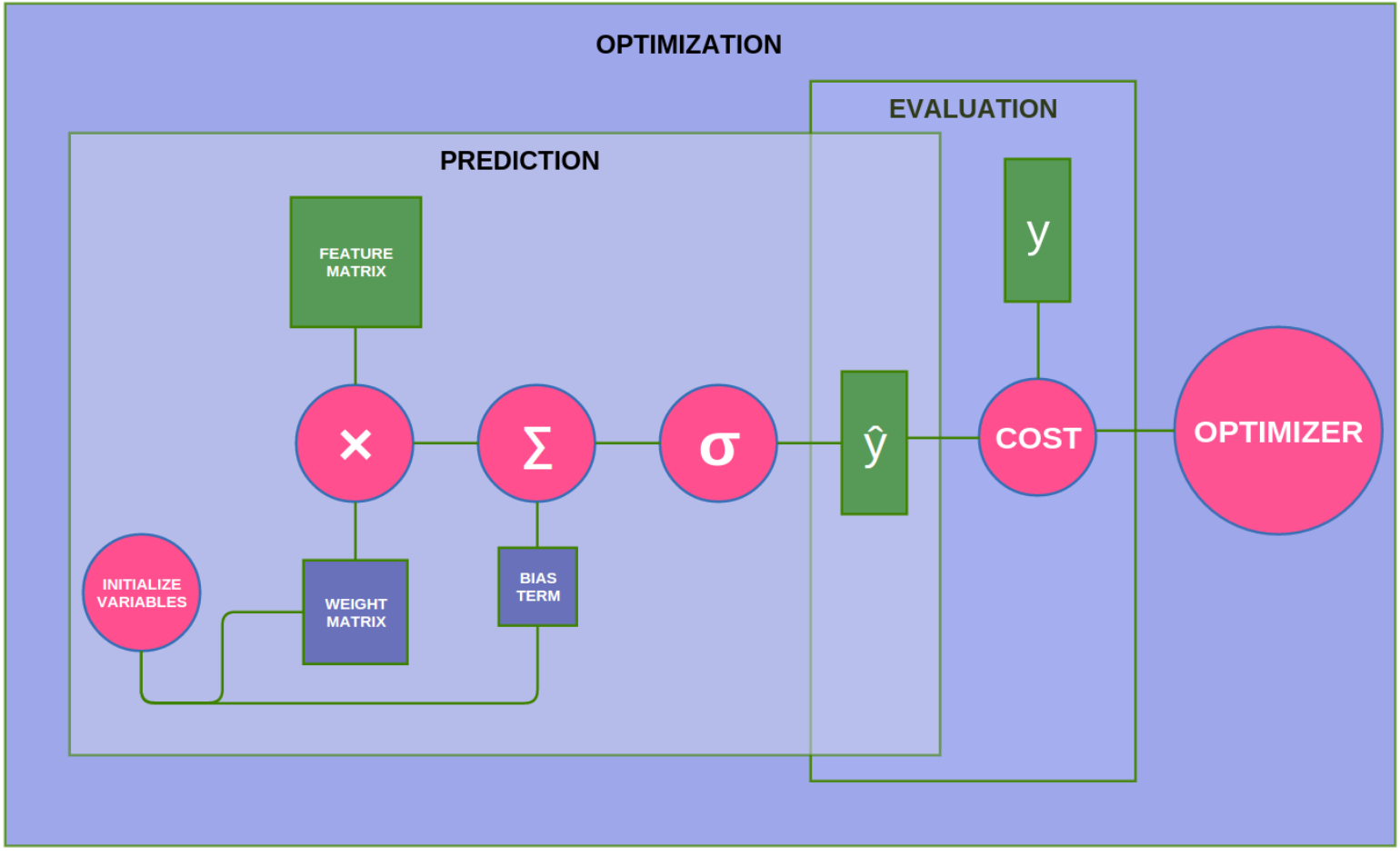
1: $d(N) \leftarrow 1$
2: **for** i = N-1 to 1 **do**
3: $\quad d(i) \leftarrow \sum_{j \in \pi(i)} d(j) \cdot \frac{\partial f_j}{\partial i}$



Quiz

- Draw the cg of:
  - f = (a * b + 1) * (a * b + 2)
  - a = 1, b = 2
- Backpropagate on the cg

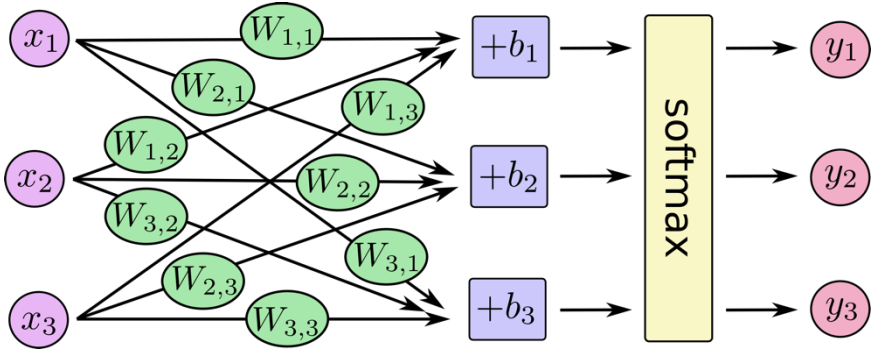
Computational Graph of Sigmoid Function



MNIST Example

- 10 digit OCR (Multi-class classification)
- Input layer
  - 28 by 28 pixel, 784 neurons
- Output layer
  - 10 neurons, digits 0, 1, …, 9

Softmax Regression (Multinomial Logistic Regression)

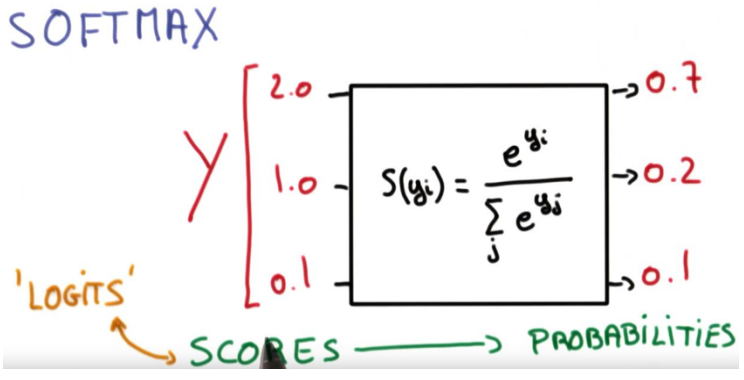


$$y = \text{softmax}(Wx + b)$$

$$\sigma(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{K} e^{z_k}} \quad \text{for } j = 1, \ldots, K.$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \text{softmax} \left(\begin{matrix} W_{1,1}x_1 + W_{1,2}x_2 + W_{1,3}x_3 + b_1 \\ W_{2,1}x_1 + W_{2,2}x_2 + W_{2,3}x_3 + b_2 \\ W_{3,1}x_1 + W_{3,2}x_2 + W_{3,3}x_3 + b_3 \end{matrix} \right)$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \text{softmax} \left(\begin{bmatrix} W_{1,1} & W_{1,2} & W_{1,3} \\ W_{2,1} & W_{2,2} & W_{2,3} \\ W_{3,1} & W_{3,2} & W_{3,3} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix} \right)$$



Cross-entropy Loss/Cost Function (交叉熵损失函数)

- A better (faster) loss function
- Also referred to as *negative log likelihood*

$$L_{cross-entropy}(\hat{\mathbf{y}}, \mathbf{y}) = -\sum_i y_i \log(\hat{y}_i)$$

  - $\boldsymbol{y} = y_1, \ldots, y_K$ is a vector representing the true multinomial distribution
  - $\hat{\boldsymbol{y}} = \hat{y}_1, \ldots, \hat{y}_k$ is the network's output by softmax function

$$L_{cross-entropy(\text{hard classification})}(\hat{\mathbf{y}}, \mathbf{y}) = -\log(\hat{y}_t)$$

Implementation with TensorFlow

```
# Create the model
x = tf.placeholder(tf.float32, [None, 784])
W = tf.Variable(tf.zeros([784, 10]))
b = tf.Variable(tf.zeros([10]))
y = tf.nn.softmax(tf.matmul(x, W) + b)

# Define loss and optimizer
y_ = tf.placeholder(tf.float32, [None, 10])
cross_entropy = tf.reduce_mean(-tf.reduce_sum(y_ * tf.log(y), reduction_indices=[1]))
train_step = tf.train.GradientDescentOptimizer(0.5).minimize(cross_entropy)
```

https://github.com/tensorflow/tensorflow/blob/master/tensorflow/examples/tutorials/mnist/mnist_softmax.py

Implementation with TensorFlow

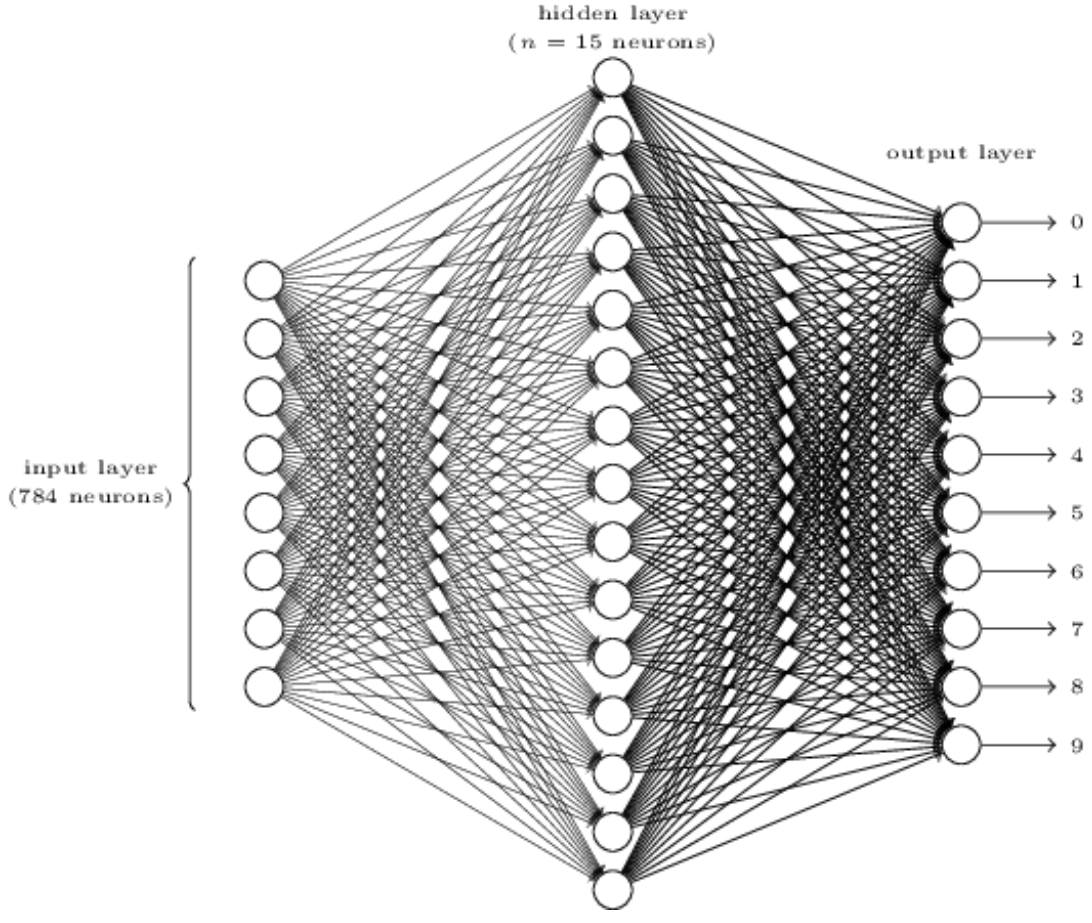
```
# Train
tf.initialize_all_variables().run()
for i in range(1000):
  batch_xs, batch_ys = mnist.train.next_batch(100)
  train_step.run({x: batch_xs, y_: batch_ys})

# Test trained model
correct_prediction = tf.equal(tf.argmax(y, 1), tf.argmax(y_, 1))
accuracy = tf.reduce_mean(tf.cast(correct_prediction, tf.float32))
print(accuracy.eval({x: mnist.test.images, y_: mnist.test.labels}))
```

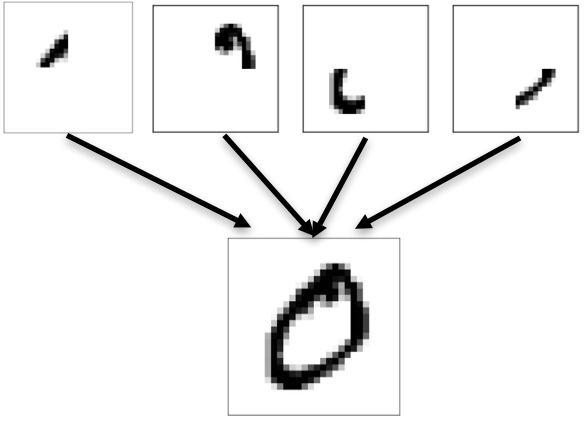
Acc: ~92%

https://github.com/tensorflow/tensorflow/blob/master/tensorflow/examples/tutorials/mnist/mnist_softmax.py

Multiple Layer Neural Networks



- What are those hidden neurons doing?
  - Maybe represent outlines

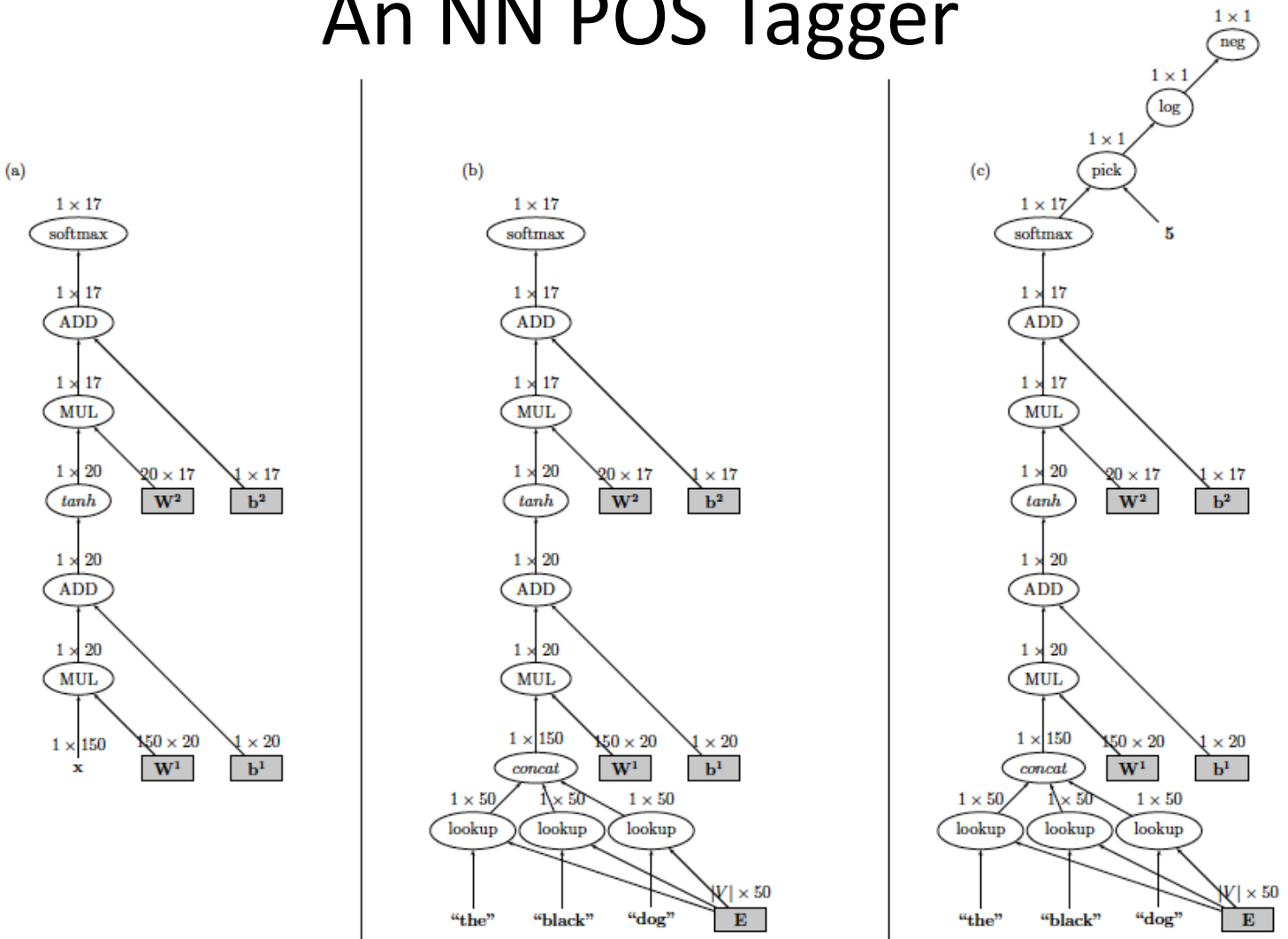


Multiple Layer Neural Networks

```
# Create the model
x = tf.placeholder(tf.float32, [None, 784])
W1 = tf.Variable(tf.truncated_normal([784, 100]))
b1 = tf.Variable(tf.truncated_normal([100]))
W2 = tf.Variable(tf.truncated_normal([100, 10]))
b2 = tf.Variable(tf.truncated_normal([10]))
y = tf.nn.softmax(tf.matmul(tf.sigmoid(tf.matmul(x, W1) + b1), W2) + b2)
```

Acc: >**96%** with tuning some hyper-parameters

An NN POS Tagger



Converting error derivatives into a learning procedure

- The backpropagation algorithm is an efficient way of computing the error derivative dE/dw for every weight on a single training case.
- To get a fully specified learning procedure, we still need to make a lot of other decisions about how to use these error derivatives:
  - Optimization issues: How do we use the error derivatives on individual cases to discover a good set of weights?
  - Generalization issues: How do we ensure that the learned weights work well for cases we did not see during training?