Machine Learning: Part I

UMaine COS 470/570 – Introduction to AI

Spring 2019

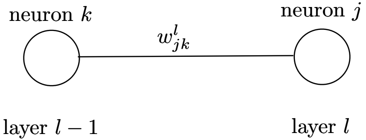
Part 2

From nets to tensors

- Want compact representation of network
- Want representation that can be mapped to parallel processors
- Insight:
  - Inputs can be considered a vector
  - Outputs can be considered a vector
  - Network is completely represented by its weights
  - A weight is between neuron *i* in layer *l* and neuron *j* in layer *l+1*
  - So all weights between two layers can be represented as $i \times j$ or $j \times i$ matrix
- Generalize: Scalars, vectors, matrices, and their *n*-dimensional counterparts: *tensors*
- Can map tensors and tensor operations onto parallel hardware (e.g., GPGPUs)

Notation (from Nielsen)

- Assume a multilayer FF network
- w^l_{jk}: wt from neuron k in layer $l-1$ to neuron j in layer l



- Subscript: *jk* for ease of calculation (later)
- b^l_j: bias of neuron j in layer l

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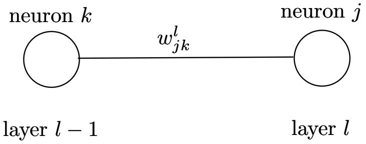
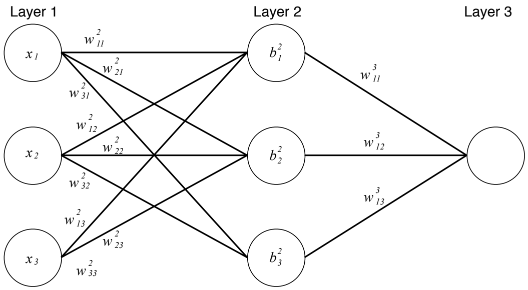


- Subscript: jk for ease of calculation (later)
- b^l_j: bias of neuron j in layer l
- a^l_j: activation (output) of neuron j in layer l

$$a^l_j = \sigma\left(\sum_k w^l_{jk} a^{l-1}_k + b^l_j\right)$$

Matrix form of NN



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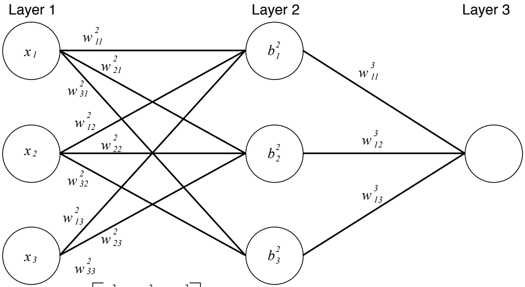

$$\mathbf{w^2} = \begin{bmatrix} w^2_{11} & w^2_{12} & w^2_{13} \\ w^2_{21} & w^2_{22} & w^2_{23} \\ w^2_{31} & w^2_{32} & w^2_{33} \end{bmatrix} \qquad \mathbf{w^3} = \begin{bmatrix} w^3_{11} & w^3_{12} & w^3_{13} \end{bmatrix}$$

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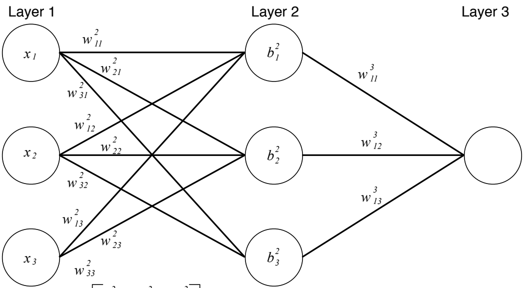

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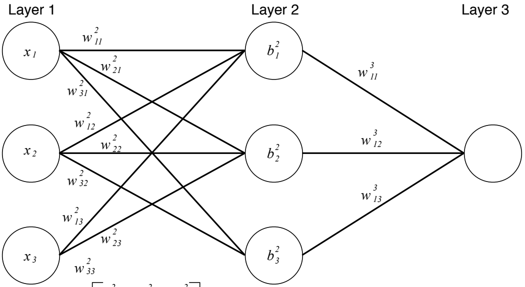

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$$\boxed{\mathbf{a^2} = \sigma(\mathbf{w^2 x + b^2})}$$

Artificial Intelligence

Matrix form

- General equation:

$$a^l = \sigma(w^l a^{l-1} + b^l)$$

- σ is said to be "vectorized"
- Logit (weighted input) vector z^l is important, too

$$z^l = w^l a^{l-1} + b^l$$

- So $a^l = \sigma(z^l)$

Learning in feedforward ANN

- Want to adjust each weight so that NN has less error
- Have to define *error*
- Have to:
    - Determine how change in a each weight $\rightarrow$ change in error
    - Adjust the weight so as to minimize error

What are we learning?

- Network computes function of inputs
- Single output, n inputs $\mathbf{w}$: $h_{\mathbf{w}}(\mathbf{X})$
- What if $m > 1$ outputs?
  - Single layer net: separate into m nets, train separately
  - Multilayer: all outputs depend on hidden layer weights
  - $\Rightarrow$ vector function
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\ldots \\
&= \sigma(\mathbf{w}^L(\sigma(\cdots\sigma(\mathbf{w}^2\mathbf{x} + b^2)\cdots)) + \mathbf{b}^L)
\end{aligned}
$$

Error function

- First, let's eliminate **b** $\Rightarrow$ into **x**
- Error of network:
  - Let **y** = desired output
  - Error on training example **x**:

$$\mathbf{E}_{\mathbf{w}}(\mathbf{x}) = \mathbf{y} - \mathbf{h}_{\mathbf{w}}(\mathbf{x})$$

- But:
  - $\mathbf{E}_{\mathbf{w}}(\mathbf{x})$: positive/negative
  - We don't want any particular error element: want *average* error
  - Want to learn weights, so want a function of weights

Cost (loss) function

- Define a *cost* (loss, objective) function:

$$C_{\mathbf{x}}(\mathbf{w}) = \frac{1}{2}||(\mathbf{E}_{\mathbf{w}}(\mathbf{x}))||^2$$

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- Entire cost function: average over all $\mathbf{x}_i$:

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$$
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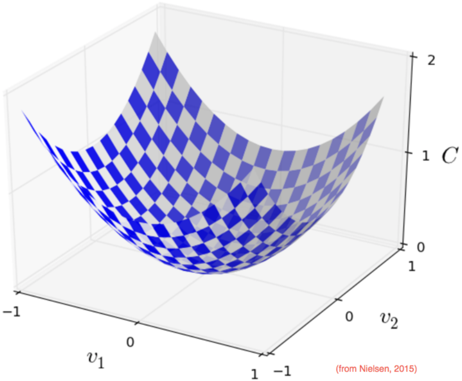
- Always positive, $\to 0$ as output $\to \mathbf{y}$

Minimizing cost function

- If we minimize C, minimize $||\mathbf{E}||$
- Using calculus, can find analytical solution
- But with n weights, $n+1$-dimensional curve
- E.g., two dimension:



- Largest nets: *billions* of weights

Review: Gradient descent search

- *Gradient descent search* instead of analytical solution
- Find *local gradients* wrt weights
- $\Rightarrow$ n *partial derivatives* of C
- Take a small step in direction of decrease in *all* the derivatives
- Repeat until close enough to minimum

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- Thus $\Delta C \approx \nabla C \cdot \Delta \mathbf{v}$

Updating the variables

- Given that:
  - $\Delta C \approx \nabla C \cdot \Delta \mathbf{v}$
  - We want to minimize ΔC
- How shall we choose $\Delta \mathbf{v}$?
- Want any change in $\Delta \mathbf{v}$ to cause ΔC to be negative

Choosing $\Delta\mathbf{v}$

$$\Delta C \approx \nabla C \cdot \Delta\mathbf{v}$$

- Suppose we choose $\Delta\mathbf{v}$ like this:

$$\Delta\mathbf{v} = -\eta\nabla C$$

- The

$$\begin{aligned} \Delta C &\approx \nabla C \cdot -\eta\nabla C \\ &= -\eta(\nabla C \cdot \nabla C) \\ &= -\eta\Sigma_i c_i c_i = -\eta\Sigma_i c_i^2 \end{aligned}$$

- Since $||\mathbf{A}|| = \sqrt{\Sigma_i a_i^2}$,

$$\Delta C \approx -\eta||\nabla C||^2$$

Choosing $\Delta\mathbf{v}$

$$\Delta C \approx -\eta ||\nabla C||^2$$

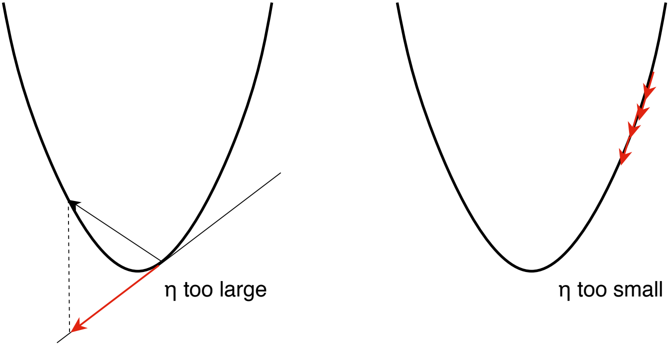
- With $\Delta v = -\eta \nabla C$:
  - Cost function always negative
  - For $||\Delta v|| \leq \epsilon$, minimizes $\nabla C \cdot \Delta v$
- η is learning rate (sometimes α)
- Next value of **v**:

$$\mathbf{v}_{t+1} = \mathbf{v}_t - \eta \nabla C$$

- Now generalize $\mathbf{v} \rightarrow \mathbf{w}$ (including **b**)
- Other gradient descent functions have been tried

Choosing learning rate

- How to choose η?



- If too large $\Rightarrow$ may overshoot minimum
- If too small $\Rightarrow$ will take a very long time to find minimum

Computing gradient

- Difficult
- Cost function: Must compute all C_x then average

$$C = \frac{1}{n}\sum_x C_x = \frac{1}{n}\sum_x \frac{||y(x) - a||^2}{2}$$

- To find overall gradient ∇C:

$$\nabla C = \frac{1}{n}\sum_x \nabla C_x$$

- With many training examples, costly $\Rightarrow$ slow learning

Stochastic gradient descent

- *Stochastic gradient descent*
- Speeds up learning
- Estimate ∇C:
  - Choose small sample of inputs randomly: a *mini-batch*
  - Compute ∇C_x for these to estimate ∇C
- If batch size is large enough, average $\approx \nabla C$
- Idea:
  - Randomly partition training examples into mini-batches
  - Train with each mini-batch
- Doing this: *epoch*
- Repeat until error is satisfactory

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- Problem: Don't know how to calculate ∇C with hidden layers!

Gradient descent

- Computing the gradient ∇C of the cost function:
  - Composed of $\frac{\partial C}{\partial \mathbf{w}}, \frac{\partial C}{\partial \mathbf{b}}$ – where w, b are vectors
  - May be very difficult to compute

Backpropagation

- *Backpropagation* algorithm (Rumelhart, Hinton, & Williams, 1986)
- Rather than trying to adjust all weights at once, do it by layers
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- Propagate by dividing responsibility for error at neuron in l according to contribution from each neuron in $l-1$

Error in output layer

- First define vector δ^{L}, where for element j:

$$\delta_j^L = \frac{\partial C}{\partial a_j^L}\sigma'(z_j^L)$$

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- $\frac{\partial C}{\partial a_j^L}$ for quadratic cost function: $\frac{\partial C}{\partial a_j^L} = (a_j^L - y_j)$

Artificial Intelligence

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- δ^L is a measure of error at L
- z_j^L already computed, $\sigma'(z_j^L)$ easy to compute
- $\frac{\partial C}{\partial a_j^L}$ for quadratic cost function: $\frac{\partial C}{\partial a_j^L} = (a_j^L - y_j)$
- So for quadratic: $\delta_j^L = (a_j^L - y_j)\sigma'(z_j^L)$

Hadamard product

- Need a new operator to simplify expressions
- Define *Hadamard product* as: $\mathbf{s} \odot \mathbf{t} = \mathbf{h}$ s.t. $h_j = s_j \times t_j$
- I.e., elementwise product – e.g.:
  $$\begin{bmatrix} -2 \\ 20 \\ 3 \end{bmatrix} \odot \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix} = \begin{bmatrix} -6 \\ 40 \\ 3 \end{bmatrix}$$

Error in output layer

- $\delta_j^L = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L)$
- Can be rewritten as:

$$\delta^L = \nabla_a C \odot \sigma'(\mathbf{z}^L)$$

- Or

$$\delta^L = (\mathbf{a}^L - \mathbf{y}) \odot \sigma'(\mathbf{z}^L)$$

Finding previous layer's error

- If we know δ^{l+1}, can we find δ^l?
- $(\mathbf{w^{l+1}})^T$ = transpose of weight matrix into $l+1$
- $(\mathbf{w^{l+1}})^T\delta^{l+1}$:
  - Moves error backward
  - Gives measure of error at layer l
- Then
$$\delta^l = ((\mathbf{w}^{l+1})^T\delta^{l+1}) \odot \sigma'(\mathbf{z}^l)$$
- Can now compute the error at any layer

Rate of change for biases, weights

- For any weight in the network:

$$\frac{\partial C}{\partial w^l_{jk}} = a^{l-1}_k \delta^l_j$$

- For any bias in the network:

$$\frac{\partial C}{\partial b^l_j} = \delta^L_j$$

since "activation" for any bias is just 1

Backpropagation & gradient descent

- For each $x \in m$ training examples:

Backpropagation & gradient descent

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Do for some # of epochs, some # mini-batches each.

Backprop algorithm

function BACK-PROP-LEARNING(*examples*, *network*) **returns** a neural network
  inputs: *examples*, a set of examples, each with input vector $\mathbf{x}$ and output vector $\mathbf{y}$
    network, a multilayer network with L layers, weights $w_{i,j}$, activation function g
  local variables: Δ, a vector of errors, indexed by network node

  repeat
    for each weight $w_{i,j}$ in *network* **do**
      $w_{i,j} \leftarrow$ a small random number
    for each example $(\mathbf{x}, \mathbf{y})$ in *examples* **do**
      / Propagate the inputs forward to compute the outputs */*
      for each node i in the input layer **do**
        $a_i \leftarrow x_i$
      for $\ell = 2$ **to** L **do**
        for each node j in layer ℓ **do**
          $in_j \leftarrow \sum_i w_{i,j} a_i$
          $a_j \leftarrow g(in_j)$
      / Propagate deltas backward from output layer to input layer */*
      for each node j in the output layer **do**
        $\Delta[j] \leftarrow g'(in_j) \times (y_j - a_j)$
      for $\ell = L - 1$ **to** 1 **do**
        for each node i in layer ℓ **do**
          $\Delta[i] \leftarrow g'(in_i) \sum_j w_{i,j} \Delta[j]$
      / Update every weight in network using deltas */*
      for each weight $w_{i,j}$ in *network* **do**
        $w_{i,j} \leftarrow w_{i,j} + \alpha \times a_i \times \Delta[j]$
  until some stopping criterion is satisfied
  return *network*

Speed of backprop

- What if we had instead done what we did in HC?
  - For each timestep, look at small changes in the weights
  - Pick set that decreases error
- Could do this for each weight separately, too
- If we have millions of weights, requires *millions* of passes through network
- With backprop: one forward, one backward pass, no matter how many weights

Deep learning

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- Stymied researchers for many years

Deep learning

- So what changed?
  - Faster machines
  - Other activation functions
  - Better versions of backprop-ish algorithms invented
  - Other kinds of networks
- Examples of other networks:
  - Convolutional neural networks
  - LSTM
- Led to tremendous increase in deep learning research, applications

- Front-end to TensorFlow, Theano, MS learning systems
- Static networks (though some dynamic work coming along)
- Use of GPUs automatically
- Choice of back-end
- Easy to use – automates a lot, more declarative

- Dynamic networks
- Easier to play around with, debug
- Very "Python-like" – OO, more imperative

Autoencoders

- Particular kind of neural network for unsupervised learning
- Input layer, ≥ 1 hidden layer, output layer
- Error is computed by comparing output to input
- Goal is to reconstruct the input: i.e., learn the identity function
- Why?

Artificial Intelligence

Autoencoders

- Key is that hidden layer(s) have fewer neurons than input/output
- Network learns a compressed version of input: dimensionality reduction
- Hidden layers: features discovered by network during training
- Useful for:
  - Learning features of input examples
  - Denoising input
  - Information compression
  - Information retrieval:
    - Train to produce reduced low-dimension *binary code* in internal layer(s)
    - Use that code as hash key for information
    - Can $\Rightarrow$ very efficient retrieval

Restricted Boltzmann machines

- Boltzmann machines learn probability distributions over inputs
- Layers of neurons, but undirected links
- Restricted Boltzmann machines [Smolensky, 1986]: no intra-layer links
- First fast deep-learning algorithms [Hinton – mid-2000s]:
  - Treat first hidden layer as RBM – train it.
  - Treat second hidden layer as RBM with inputs from first hidden layer, train it.
  - Etc.
  - Fine-tune with backprop/gradient descent

Neural network training:

"You process a lot of data in a quiet way, don't you, Larry!"

. . . and. . .

You'd like to ask Roy if he's really thought this through.

Preview

- Convolutional NNs: when covering image recognition
- LSTM: when looking at NLP
- GANs: when looking at creativity