University of Idaho
Department of Computer Science
Coeur d'Alene

Lecture #23

Neural Networks

Garrett Wells
revised October 15, 2024

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- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

Review
Machine Learning Paradigms
- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

Review

Perceptrons

- Borrowing from the human biological model for learning

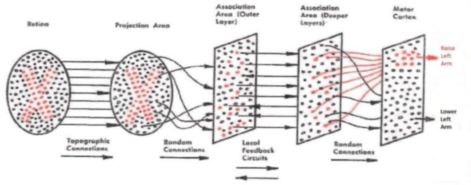

FIG. 1 — Organization of a biological brain. (Red areas indicate active cells, responding to the letter X.)

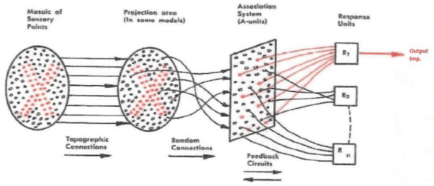

FIG. 2 — Organization of a perceptron.

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└Review
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Review
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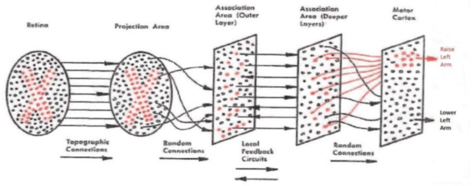
Perceptrons

- Borrowing from the human biological model for learning
- Build a network of connected neurons or nodes



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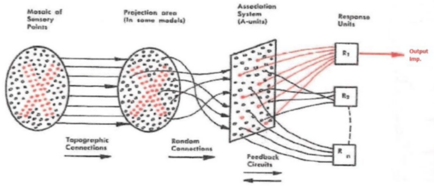

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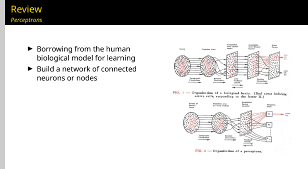

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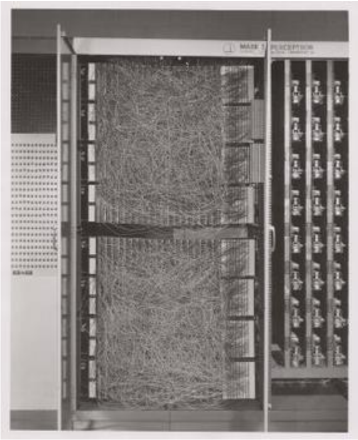

Figure: Mark I Perceptron

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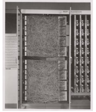

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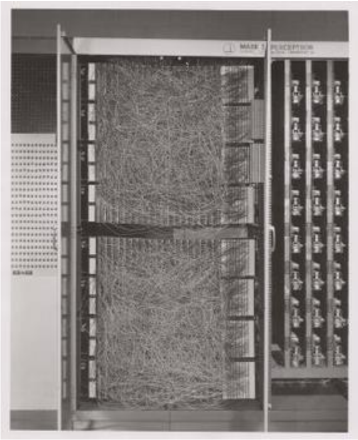

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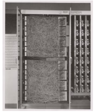

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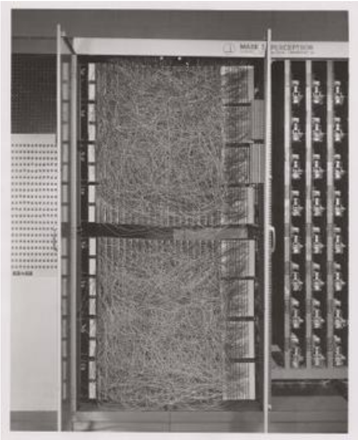

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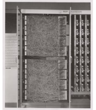

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Neural Network

An artificial mathematical model used to approximate non-linear functions[1].

Remeber. . .

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Remeber...

- Neural Networks a broad class of ML models

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Neural Networks

Characteristics & Parameters. . .

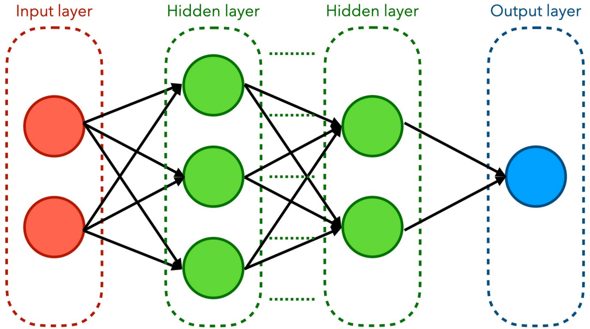
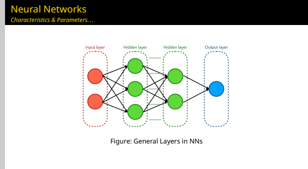


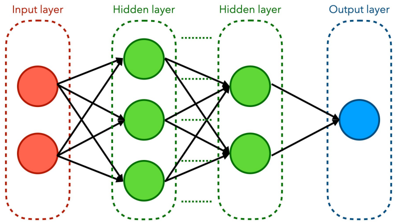
Figure: General Layers in NNs



Neural Networks

Characteristics & Parameters...

Input Layer $\boldsymbol{x}$, input



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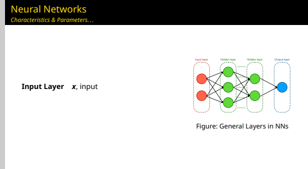
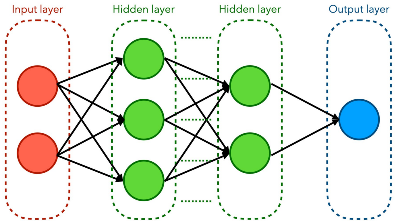
└─Neural Networks



Neural Networks

Characteristics & Parameters...

Hidden Layers Flexible, changes between architectures



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Neural Networks

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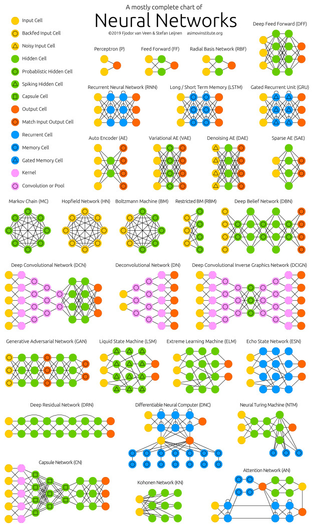
Hidden Layers Flexible, changes between architectures

Network Depth The number of hidden layers



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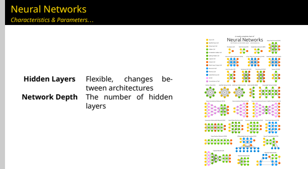
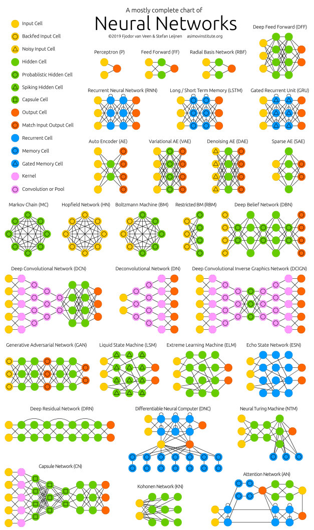

Neural Networks
Characteristics & Parameters…
Hidden Layers Flexible, changes between architectures
Network Depth The number of hidden layers

Neural Networks

Characteristics & Parameters…

Hidden Layers	Flexible, changes between architectures
Network Depth	The number of hidden layers
Layer Breadth/Width	How many nodes per layer



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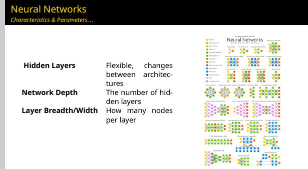
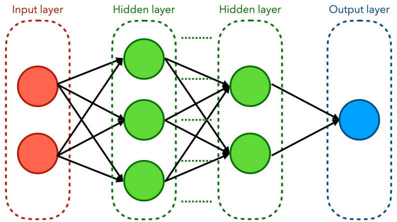
└Neural Networks


Neural Networks
Characteristics & Parameters…

Neural Networks

Characteristics & Parameters...

Output Layer ***y***, Same number of nodes as classes



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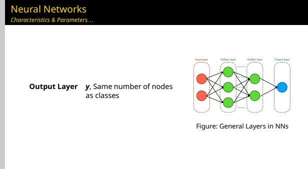

Neural Networks

Setting up a neural network...

1. Specify architecture
   - Number of layers
   - Number of nodes per layer
   - Activation function for nodes in layer
   - Specify output layer & activation function
2. Initialize weight values
3. Initialize bias values

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Neural Network Complexity vs. Human Brain Complexity

Are neural networks equivalent to the human brain?

- Human Brain: 10^{11} [2], $\geq$ 80 billion [3]
- **2018** – 16 million, analagous to frog brain[4]
- **2021** Natural Language Processing(NLP): approx. 110 million
- GPT-3: 125 million – 125 billion

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Neural Network Operation

Resources...

1. Deep Learning – Goodfellow *et. al.* [5]
2. Neural Networks and Deep Learning – [6]
3. Numerous online resources

Neural Network Operation
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Neural Network Operation

Feedforward...

Feedforward

1. Feed input feature vector into the network input layer.
2. Inputs pass through linear function to calculate an activation value.
   - ☞ $a = wx + b$
3. The activation function of each node is run on the activation value producing the output value of the node.
4. Final output values from output layer determine model prediction.

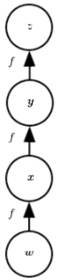

Figure: Minimal NN from [5]

Neural Network Operation
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Neural Network Operation

Feedforward...

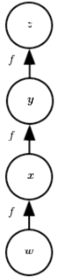
Feedforward

Network prediction, z, expressed as:

$$z = f(y) = f(f(x)) \tag{1}$$

$$y = f(x) = f(f(w)) \tag{2}$$

w	is the input to the network(scalar)
f	is the activation function



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└Feedforward
└Neural Network Operation

Neural Network Operation
Feedforward...
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$z = f(y) = f(f(x))$ (1)
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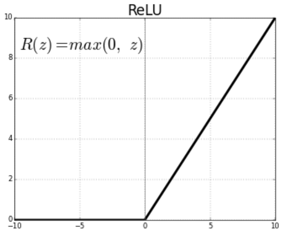
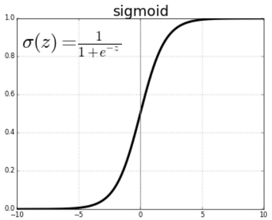
Neural Network Operation

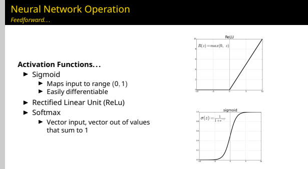
Feedforward…

Activation Functions…

- Sigmoid
  - Maps input to range $(0, 1)$
  - Easily differentiable
- Rectified Linear Unit (ReLu)
- Softmax
  - Vector input, vector out of values that sum to 1







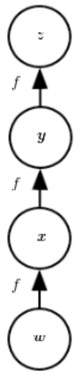
1. Activation function impacts other network functions. For example, with ReLu, bias must be non-zero value when initialized because if zero there is no gradient.
2. Sigmoid is sensitive to change when value is near to zero, however slope means that it is slow to respond to updates when maxed out.
3. Activation functions are not always linear (ReLu) introducing problems when differentiating.

Neural Network Operation

Feedforward…

Implications

1. We can calculate a gradient(partial derivative) between each layer of the network
2. The gradient indicates how much each node contributed to the final prediction



Neural Network Operation
Feedforward…
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Neural Network Operation

Feedforward...

- Iterate through all layers in network
- For each node in current layer calculate $a_i = \sum_i x_i w_i + b$
  - x_i input/output from node i in previous layer
  - w_i the weight associated with the i layer
  - b, bias, which is the same for all nodes in layer
- Output of node, $u_i = f(a_i)$
  - f, activation function

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Neural Network Operation

Feedforward...

- Now we have a prediction, y and a label(ground truth) value $\hat{y}$.
- Multiple nodes contributed to (wrong) prediction.
- How do we blame those nodes and correct behavior?
- Phrased differently, how do we tune our model to fit the input function?

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Neural Network Operation

Feedforward...

1. Need to quantify distance between prediction y and answer $\hat{y}$.

Neural Network Operation
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Neural Network Operation

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Lecture #23
└─Feedforward

└─Neural Network Operation

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   - ☞ *Backpropagation*

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☞ Backpropagation

Backpropagation

Using the prediction from the feedforward algorithm and the ground truth label, calculate the loss/cost/error.

- Loss is distributed among weights and bias, updating them to optimize model performance. This is done by calculating the gradient of the loss w.r.t. each node.

Neural Network Operation
Backpropagation...
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Neural Network Operation

Backpropagation...

Mean Squared Error (MSE)

"MSE...is calculated as teh average of the squared differences between the predicted and actual values." [7]

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y})^2 \quad (1)$$

Cross-Entropy

Penalty is logarithmic, penalizing heavily for large deviance from expected value.

$$H(p, q) = -\sum_{x} p(x)log(q(x)) \quad (2)$$

Neural Network Operation
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Neural Network Operation

Backpropagation...

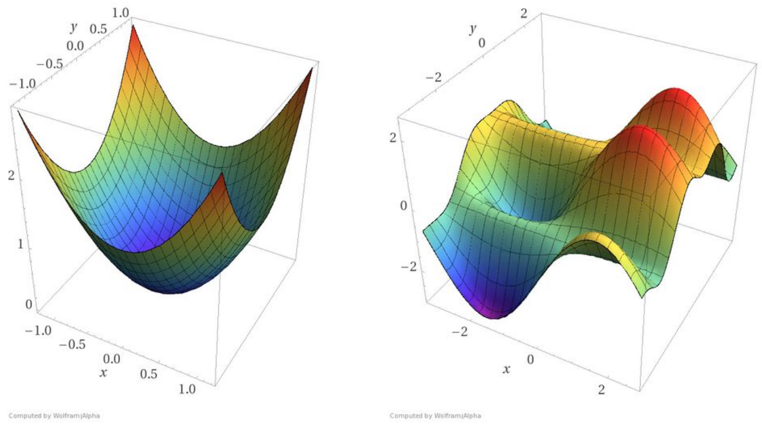
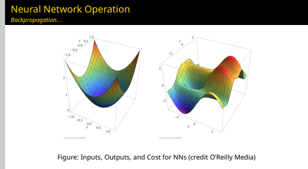


Figure: Inputs, Outputs, and Cost for NNs (credit O'Reilly Media)



1. error function can be thought of as a 3D surface
2. error is *z* axis, with respect to two independent variables *x* and *y*

Neural Network Operation

Backpropagation...

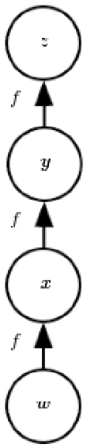
Remember... our prediction as a chain of functions:

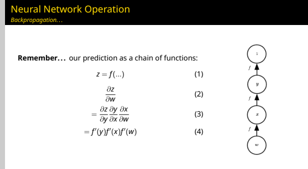
$$z = f(\dots) \tag{1}$$

$$\frac{\partial z}{\partial w} \tag{2}$$

$$= \frac{\partial z}{\partial y}\frac{\partial y}{\partial x}\frac{\partial x}{\partial w} \tag{3}$$

$$= f'(y)f'(x)f'(w) \tag{4}$$





1. We can determine the gradient(change) between each node using the chain rule.
2. This gradient is a quantification of how much each node's output impacts our final prediction.
3. Backpropagation uses this chain to distribute error among participating nodes.
4. All that is missing is our loss calculation.

Neural Network Operation

Backpropagation…

Including Loss[1]**…**

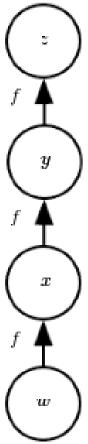
$$\boldsymbol{L}^2 = \frac{1}{2}\sum_i (y - \hat{y})^2 \tag{1}$$

Then, for output node z:

$$\frac{\partial L}{\partial z} = z - \hat{z} \tag{2}$$

Thus…

$$\frac{\partial L}{\partial u} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}\frac{\partial y}{\partial x}\frac{\partial x}{\partial w} \tag{3}$$



[1] Using $\boldsymbol{L}^2$ Norm Loss for simplicity in differentiation

Neural Network Operation
Backpropagation…
Including Loss[1]…
Then, for output node z:
Thus…
[1] Using L² Norm Loss for simplicity in differentiation

1. In equation 4, each partial derivative is taking the derivative of the activation function. For examples with weights and bias, this gradient at the node is then differentiated with respect to the weights and bias.
2. To calculate gradient to x and update parameters, for example, just need to calculate up to $\frac{\partial L}{\partial x}$.

Neural Network Operation

Backpropagation. . .

- Introduced in 1970s, not popular until 1986 [8]

Neural Network Operation
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Neural Network Operation

Backpropagation...

Backpropagation...

1. Calculate loss
2. Calculate derivative of loss
3. Starting with the output layer, iterate over network layers.
4. For each node in layer ☞ calculate $\frac{\partial L}{\partial u_i}$
   - In other words, calculate the gradient of the loss w.r.t. node u_i
   - $\frac{\partial L}{\partial u_i}$ is then used to calculate the loss w.r.t. each weight and bias
5. Update each weight: $w = w - \lambda\frac{\partial L}{\partial w}$ [1]
6. Update the bias $b = b - \lambda\frac{\partial L}{\partial b}$

[1] λ is the learning rate, scaling parameter

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└Backpropagation
└Neural Network Operation

Neural Network Operation
Backpropagation...

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4. For each node in layer ☞ calculate $\frac{\partial L}{\partial u_i}$
   - In other words, calculate the gradient of the loss w.r.t. node u_i
   - $\frac{\partial L}{\partial u_i}$ is then used to calculate the loss w.r.t. each weight and bias
5. Update each weight: $w = w - \lambda\frac{\partial L}{\partial w}$ [1]
6. Update the bias $b = b - \lambda\frac{\partial L}{\partial b}$

[1] λ is the learning rate, scaling parameter

Learning Optimizations

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Stochastic Gradient Descent(SGD)	Update model parameters after every prediction
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1. Gradient descent is enormously expensive computationally. Has higher accuracy.
2. SGD is resource sipping, but can have erratic convergence behavior.
3. Mini-batch considered the cross-over between GD & SGD

Other Topics of Neural Network Design

- Weight Initialization
  - Simplest would be to set all to zero, but then they learn the same thing
  - Setting all weights to same value means they will all be far from a solution
  - So have heuristics for this [9]
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  - Too large → fail to converge
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