Intro to Neural Networks

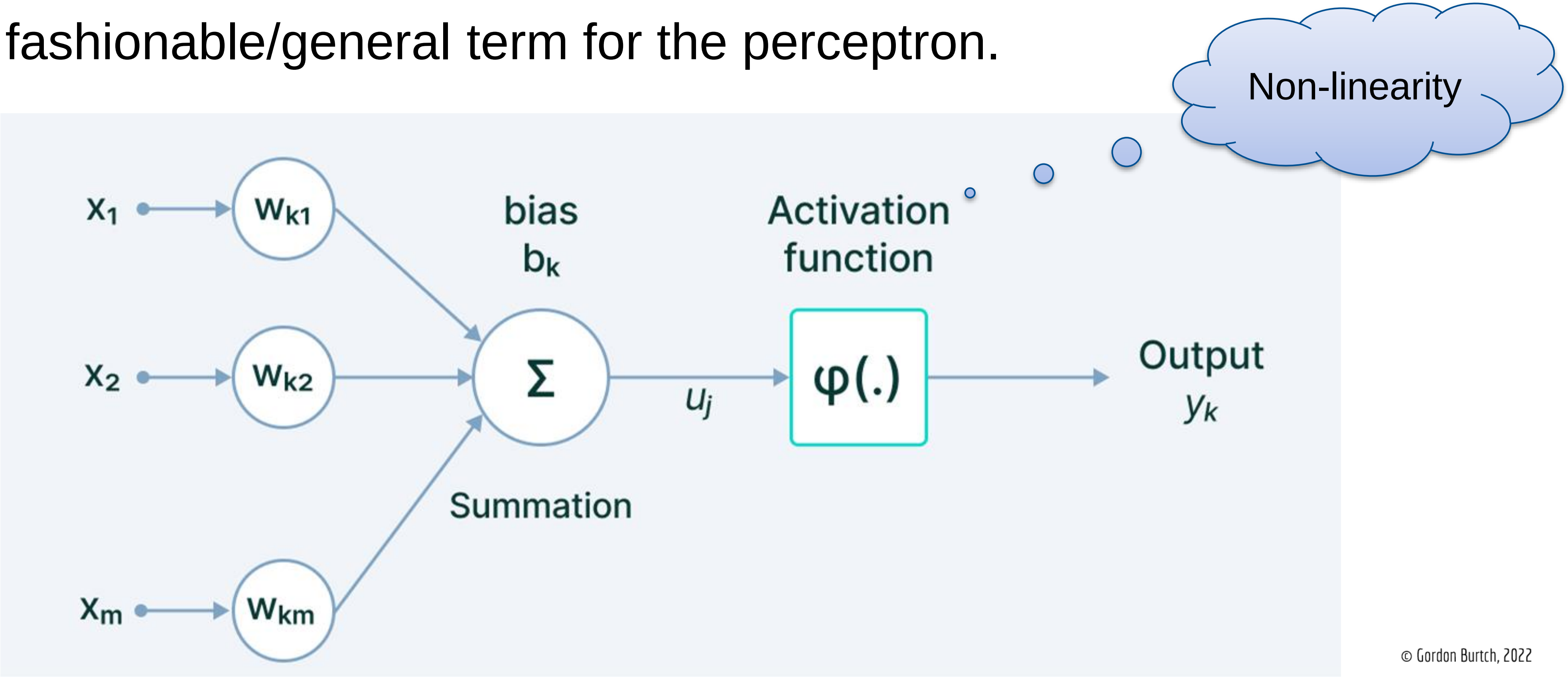
BA865 – Mohannad Elhamod

MLPs

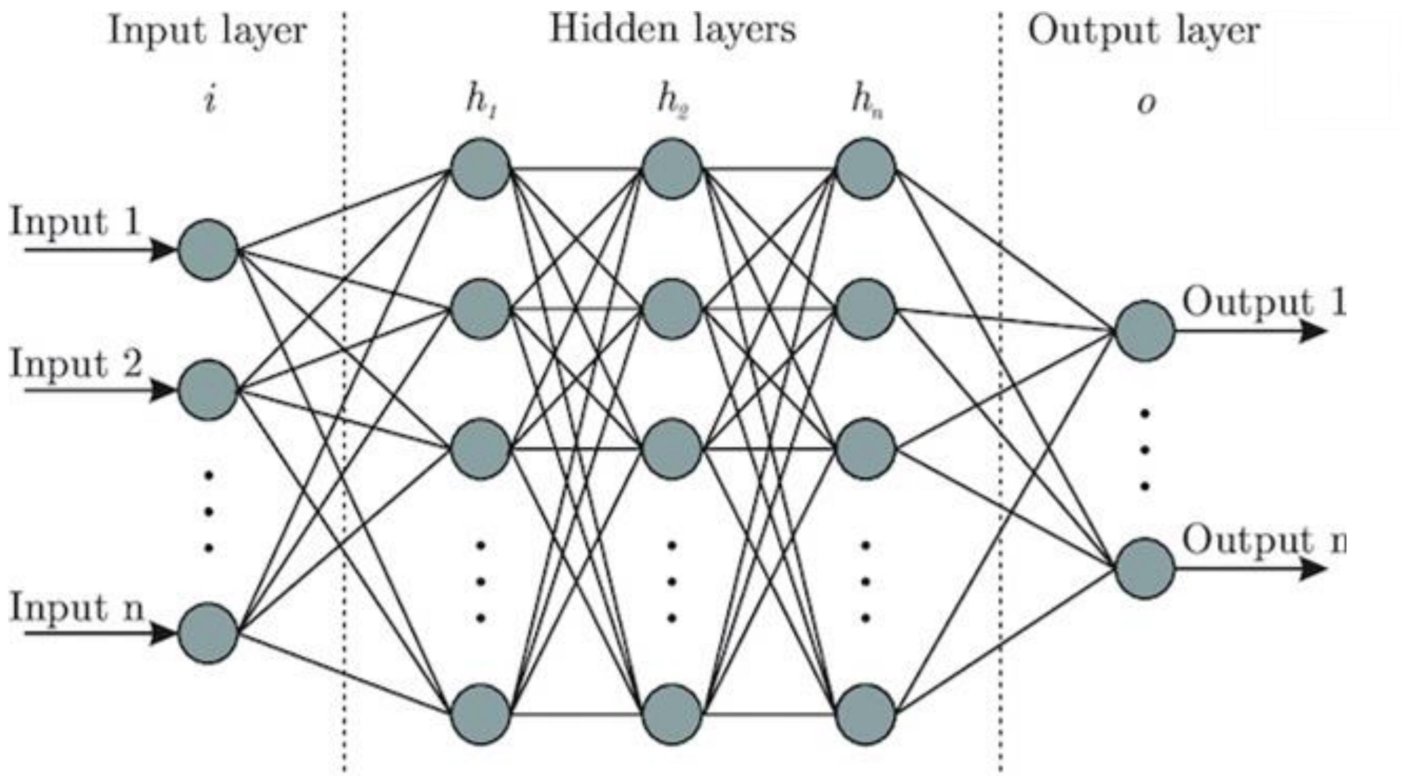
The Multi-Layer Perceptron

A Neuron

- A more fashionable/general term for the perceptron.

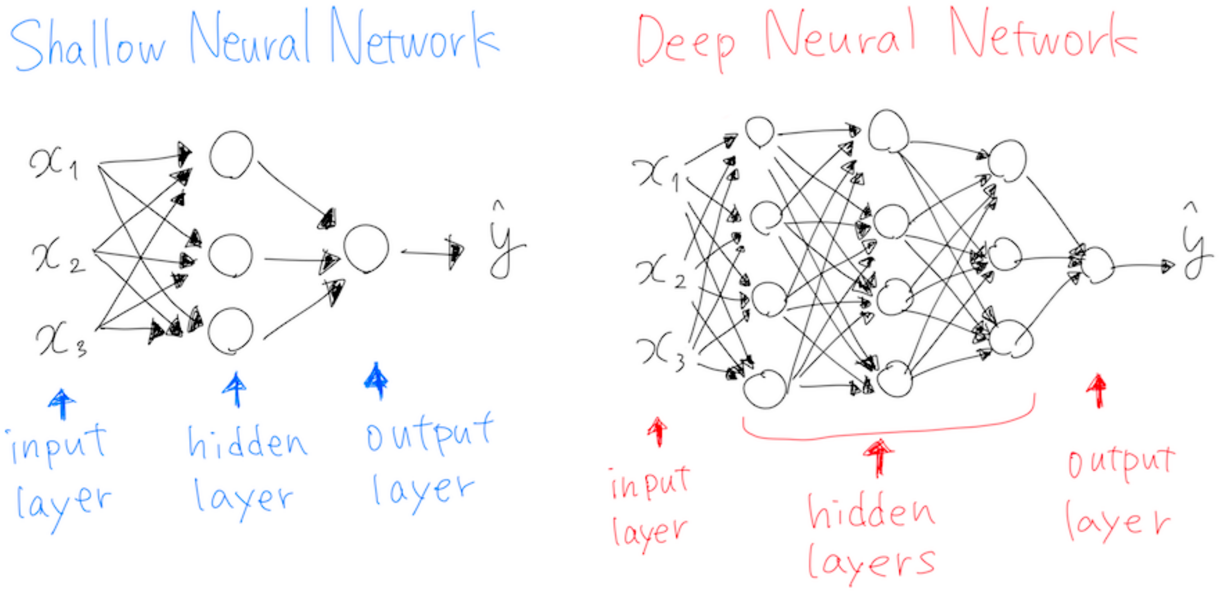


Neural Networks



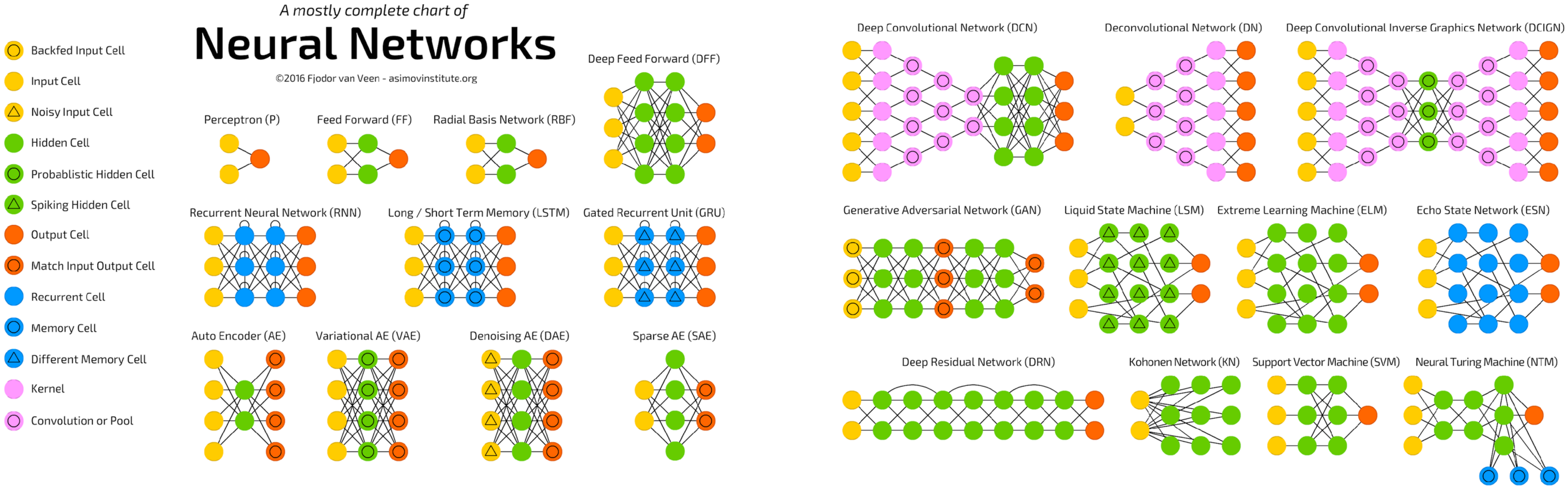
Deep Networks

- Deep = More and more layers…
- leading to more complexity and better capacity for capturing complex phenomena.



MLPs, One of Many Types…

- MLP = FF (Feed Forward) network = FC (Fully-Connected) layers.



Disecting The Neural Network

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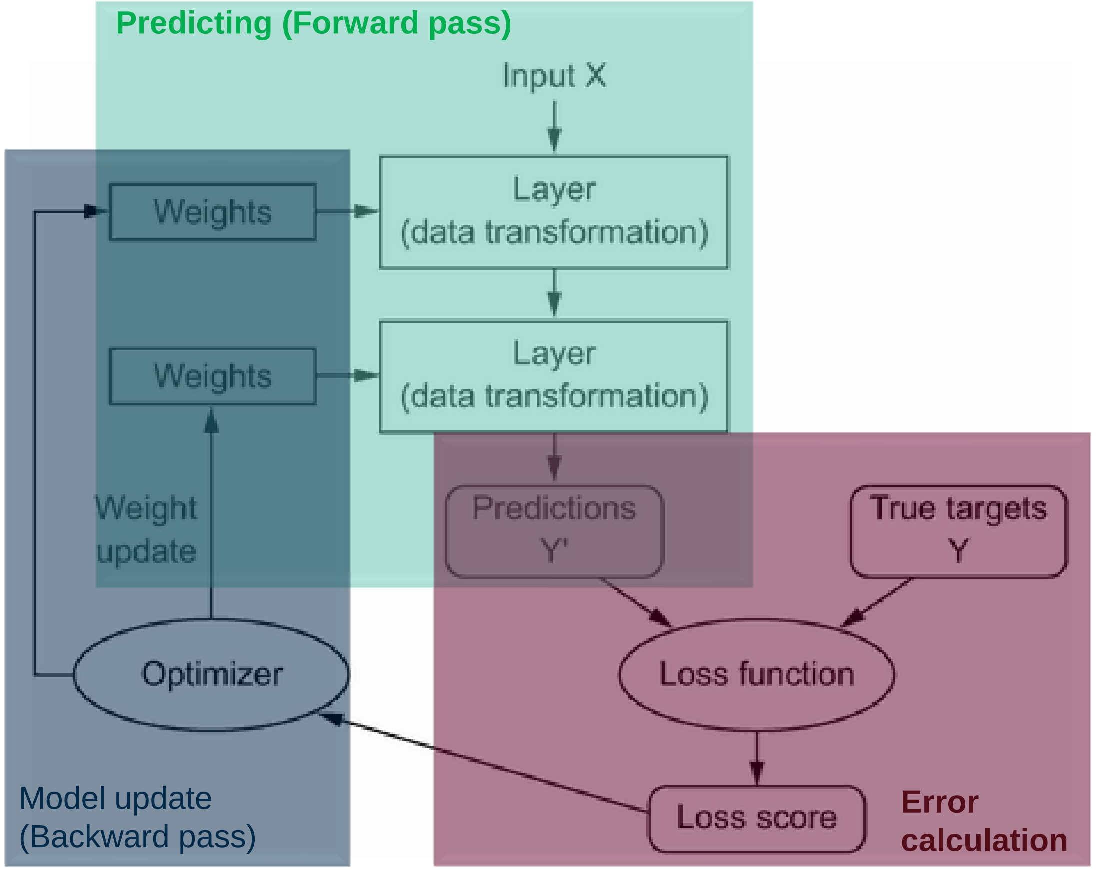
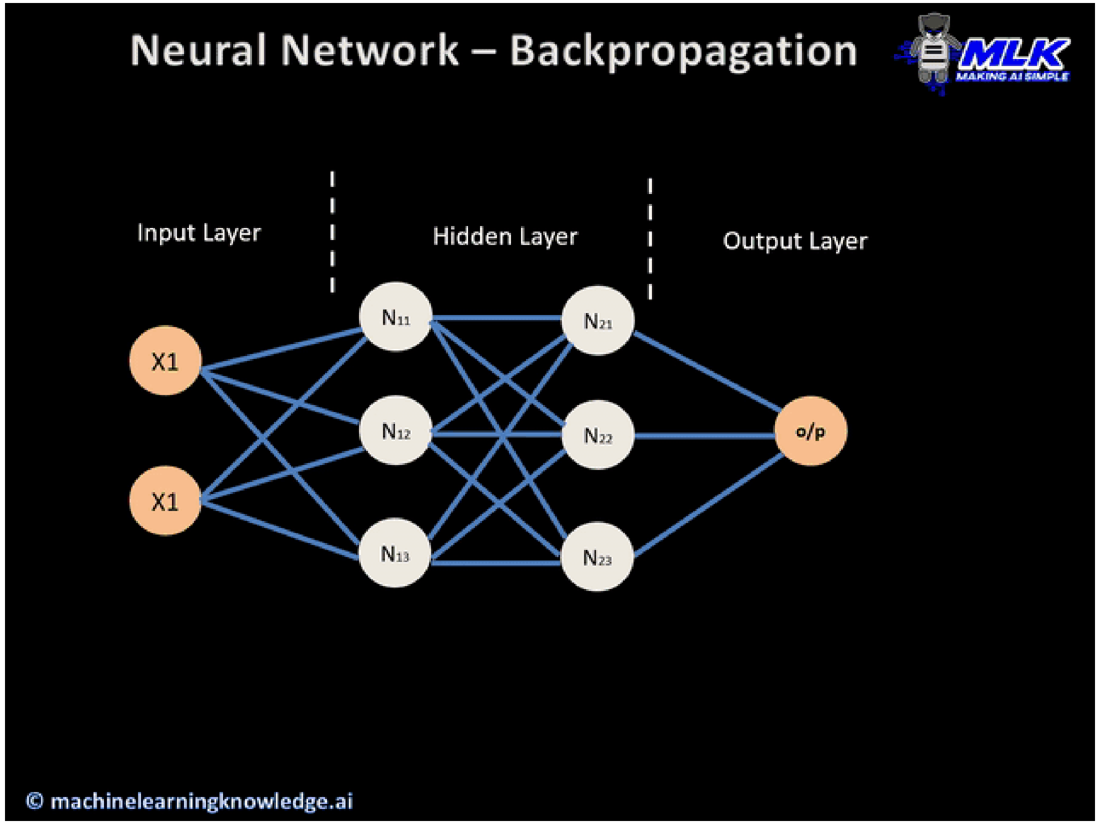
The Framework



The Framework



Predicting

- What is a layer actually doing?
- Each layer is a matrix multiplication followed by a non-linearity!
    - Why bother with the non-linearity?!

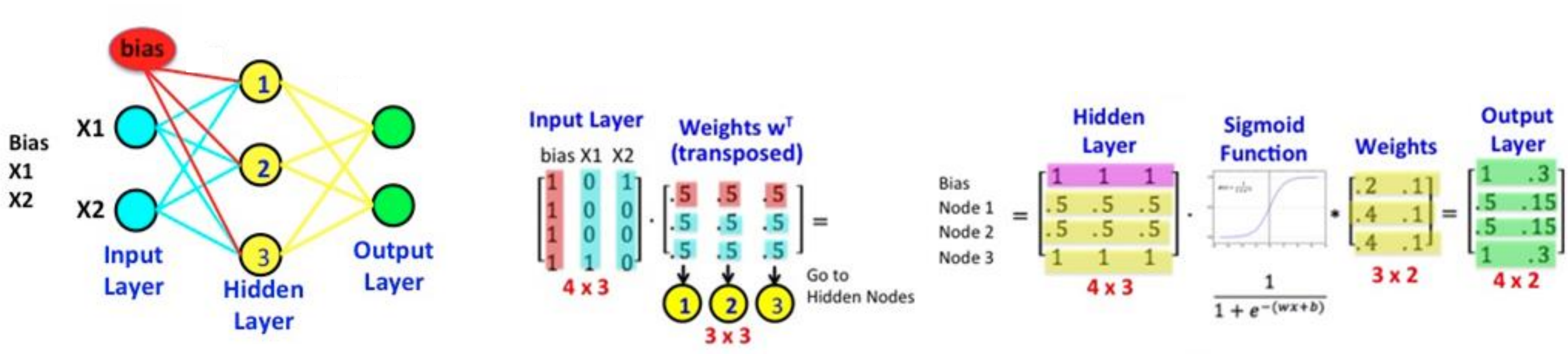


Figure (modified) courtesy of Rubens Zimbres

Predicting

- Demo
- The non-linearities allow the neural net to “warp” a non-linear problem into a linear one!

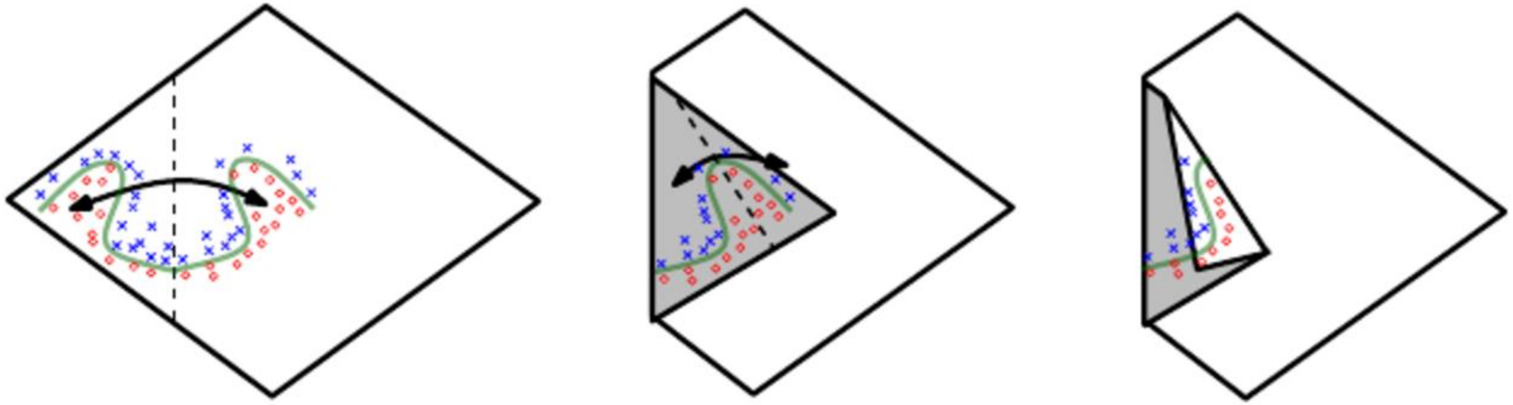


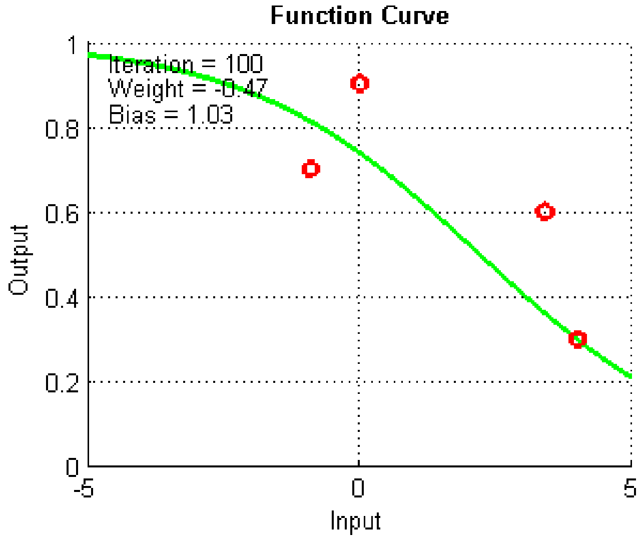
Figure courtesy of Deep Learning Book

Optimization

- Using Gradient Descent (or some other optimizer) to “update the network.”
  - What do we exactly mean by “updating the network”?

Optimization

- Gradient descent is performed *with respect to the weights/biases*.
- Behold…



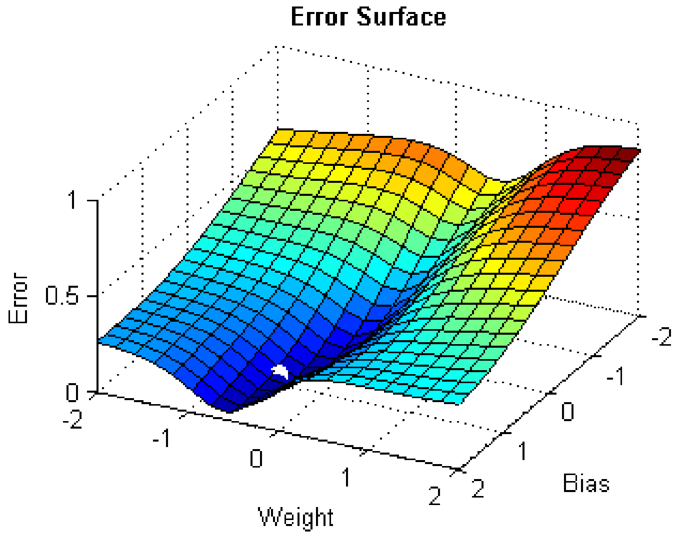
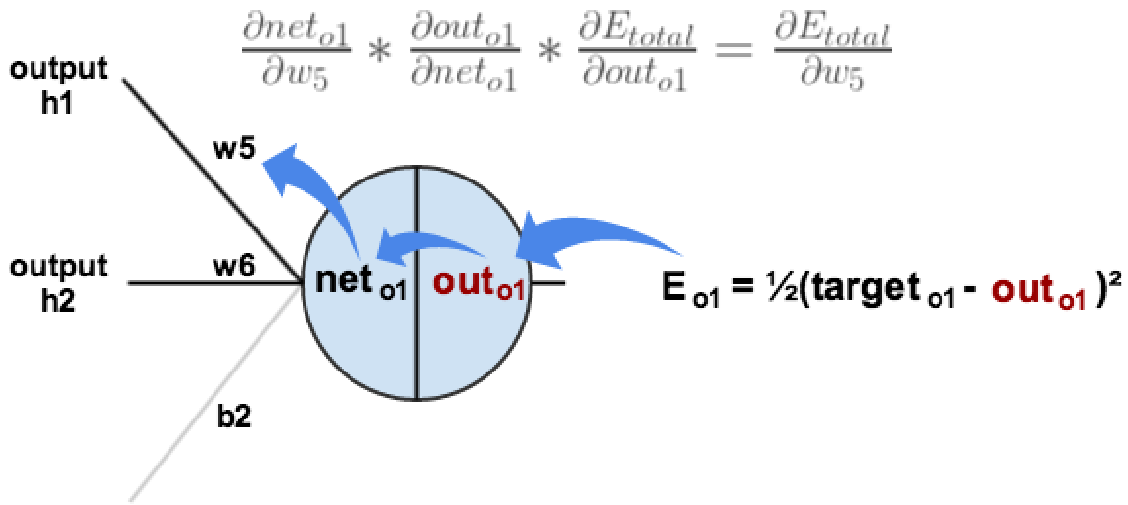


Figure courtesy of Devin Soni

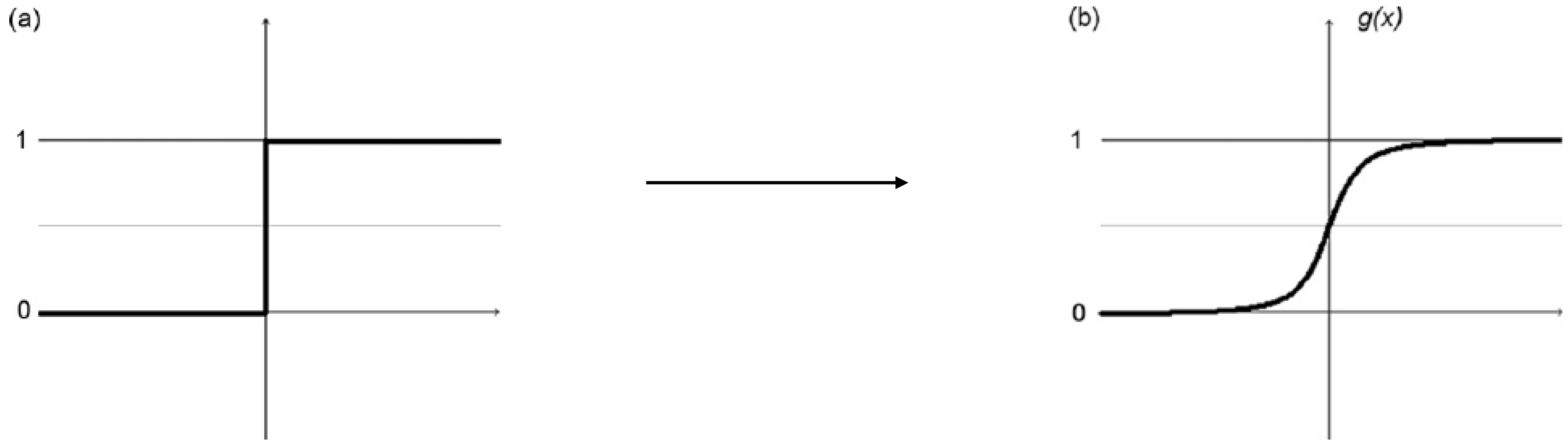
Optimization

- But how does the update get carried all the way back?
  - Chain rule!
  - This is called back-propagation.
- Luckily, these calculations can be automated with *automatic differentiation*.



Optimization

- We need to make sure the gradient is non-zero…
  - Otherwise, the gradient can't "flow"!
- Replace the step function with a continuous one!



Hyper-Parameters

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Learning Rate

- Generally, the most important hyperparameter of them all!
  - Too low: Really slow convergence.
  - Too high: No convergence.

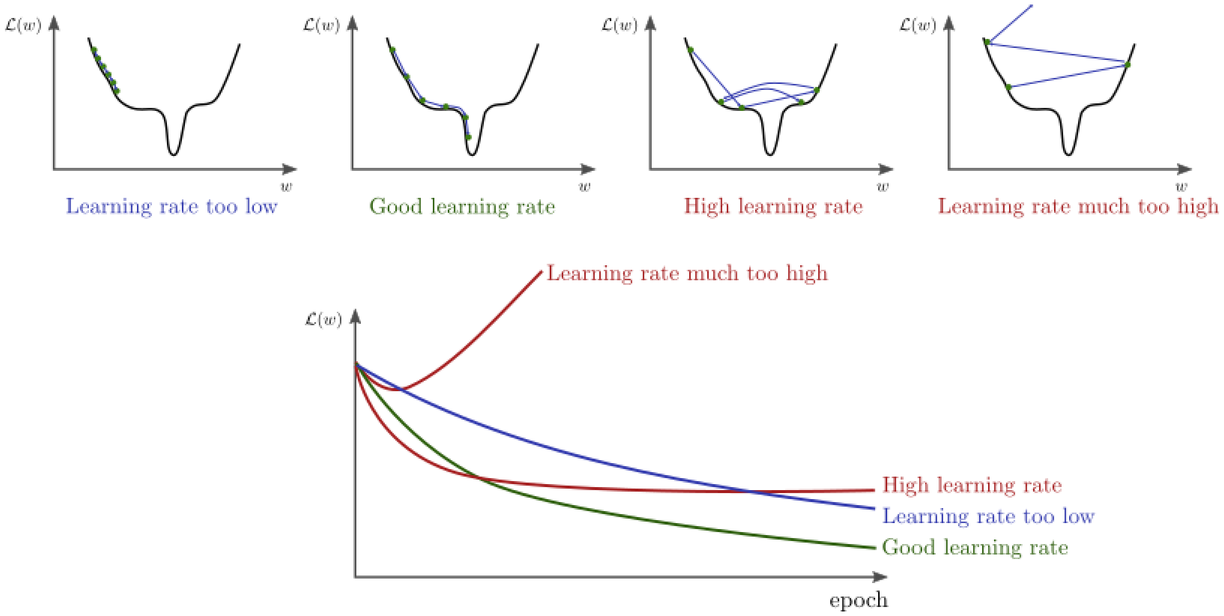


Figure courtesy of Stanford CS class CS231n

Learning Rate: Early Stopping

- The number of epochs impacts the model's fitness.
- Training needs to stop at the "right" epoch.
- How do we achieve that?
    - Better to stop when validation error stops decreasing for a certain number (n) of epochs.
    - Setting n too small or too large will impact convergence.

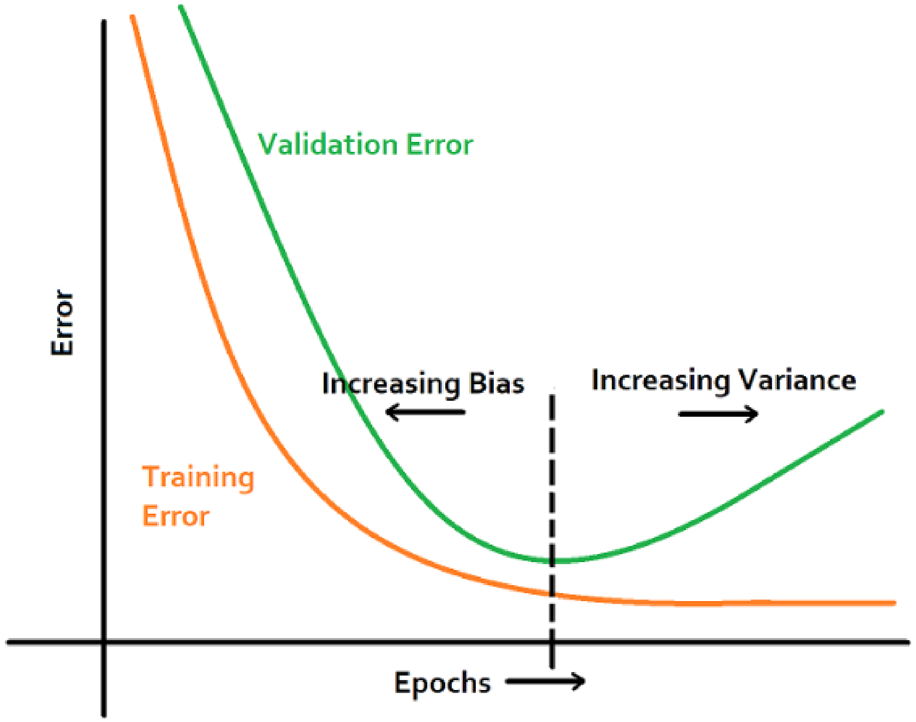


Figure courtesy of RAHUL JAIN

Optimization: Batches

- Datasets are usually huge and won't fit in GPU memory in its entirety.
- So, we split the dataset into *batches*.
  - This is also called *SGD (Stochastic Gradient Descent)* or *mini-batch GD*.
- What is the effect of using batches?
  - Speeds up convergence.

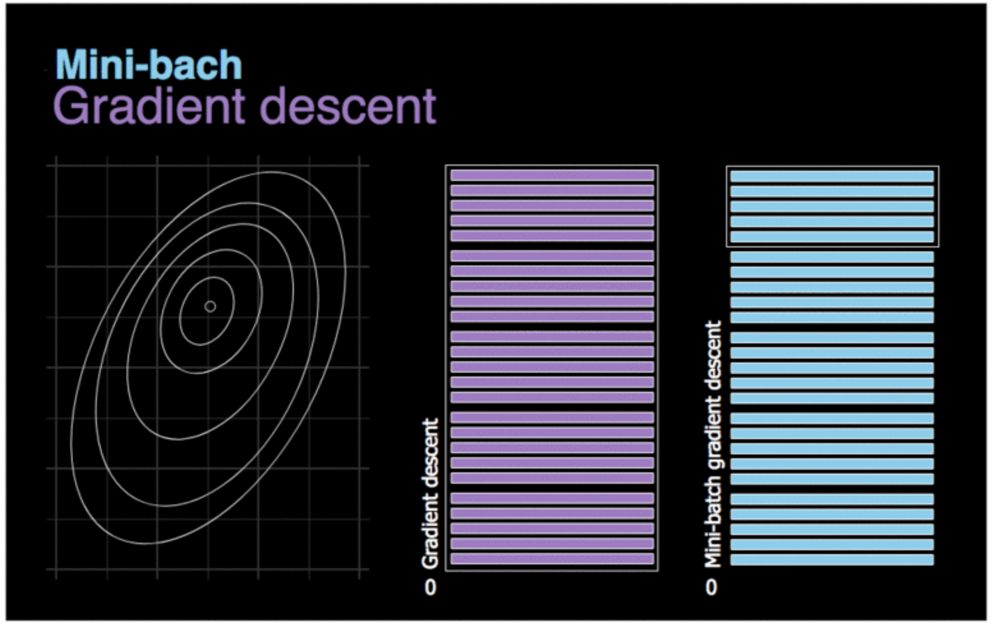
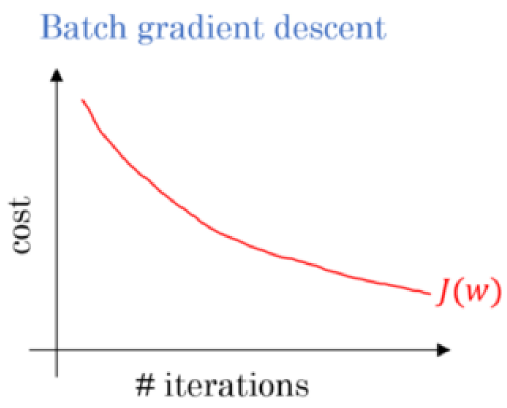
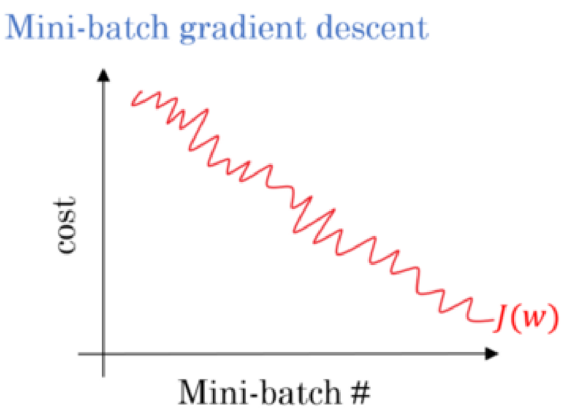


Figure courtesy of Ashish Singhal

Optimization: Batches

- Gradient descent will take the model to the closest minima, not necessarily the global minima.
- By taking batches, we introduce noisiness (randomness) to the loss surface, which may help us avoid local minima.





Optimization: Momentum

- Adding a momentum term (i.e., gradients from previous epochs), helps the convergence process.

$$z^{k+1} = \overbrace{\underbrace{\beta}_{\text{Momentum coefficient}} z^k}^{\text{Momentum}} + \overbrace{\nabla f(w^k)}^{\text{Gradient}}$$

$$w^{k+1} = w^k - \alpha z^{k+1}$$

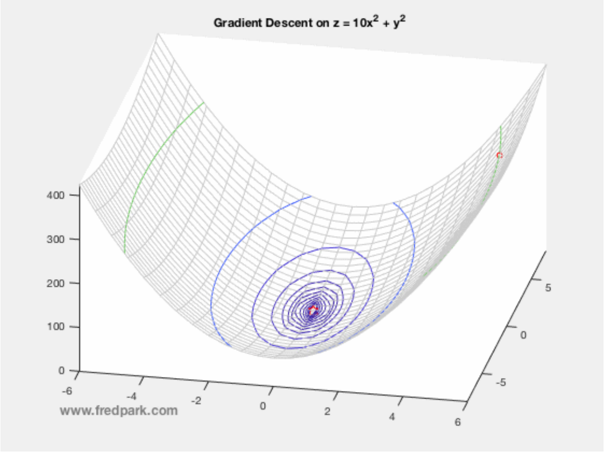
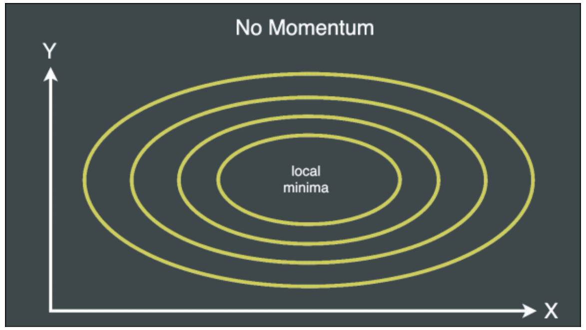


Figure courtesy of Fred Park



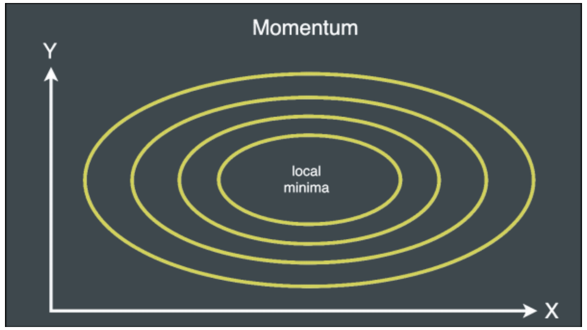
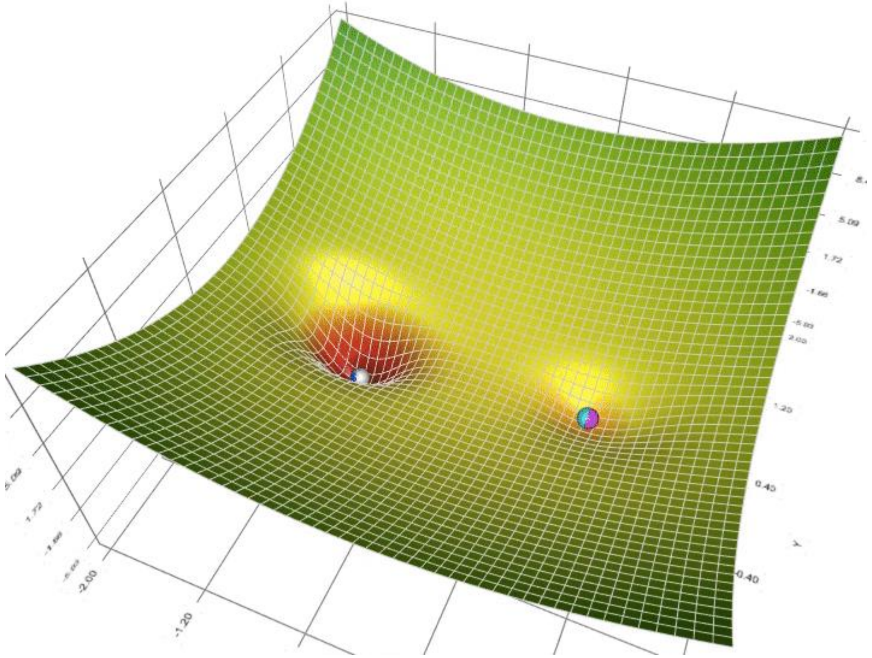


Figure courtesy of Casper Hansen

Optimization: Optimizer

- Optimizers differ in how they scale the gradient differently over epochs and different weights.
- Different optimizers perform differently for different models and datasets.
- More mathematical info can be found here.



Animation of 5 gradient descent methods on a surface: gradient descent (cyan), momentum (magenta), AdaGrad (white), RMSProp (green), Adam (blue). Left well is the global minimum; right well is a local minimum

Figure courtesy of Lili Jiang

Optimization: Regularization

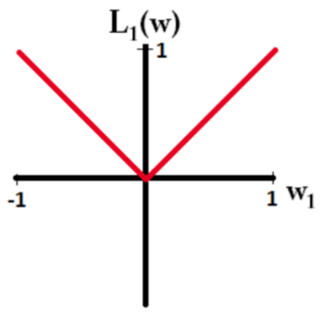
- Large models allow modeling more complex data.
  - However, if too large, they may overfit.
- We need a way to dynamically control the complexity.
- How about we add an additional <u>*loss term*</u> to it?!

$$\nabla_W \left(L_{Error} \right) \longrightarrow \nabla_W \left(L_{Error} + \beta L_{Regularization} \right)$$

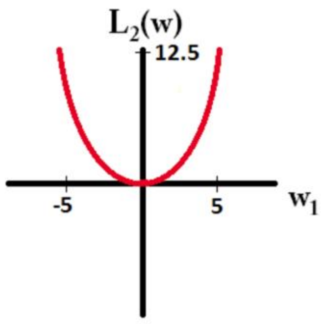
Trade-off coefficient (for control)

Optimization: Regularization

- How about we add a *loss term* for it?!
  - We want to construct a loss term such that, when minimized, the model becomes less complex.
  - We can do that by controlling the magnitudes of the model weights.
- This is also called *weight decay.*
- Demo



$$L_1(w) = \Sigma_i |w_i|$$



$$L_2(w) = \frac{1}{2}\Sigma_i w_i^2$$

Figure courtesy of Prashant Gupta

Weight Initialization

- Has a great impact on optimization.
  - Improper initialization (e.g., all zeros or constants) leads to gradient pathologies.
- Demo

More Hyper-Parameters Later...

MLPs for Regression

- Just like they create decision boundaries in classification problems, neurons can be used to create discrete approximations in regression problems.
- Demo

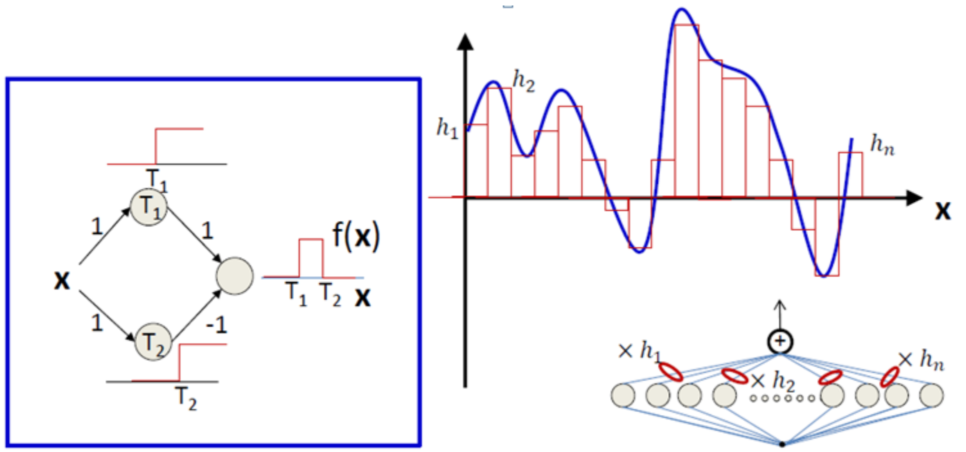


Figure courtesy of Abhisek

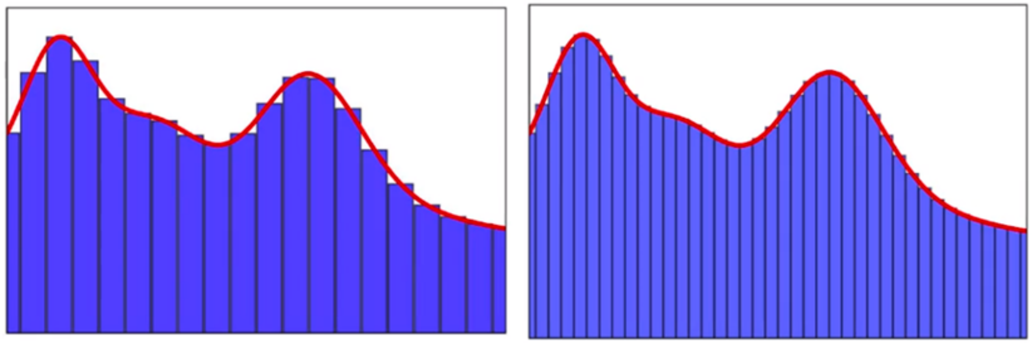


Figure courtesy of Niranjan Kumar