HPE DSI 311
Introduction to Machine Learning

Summer 2021

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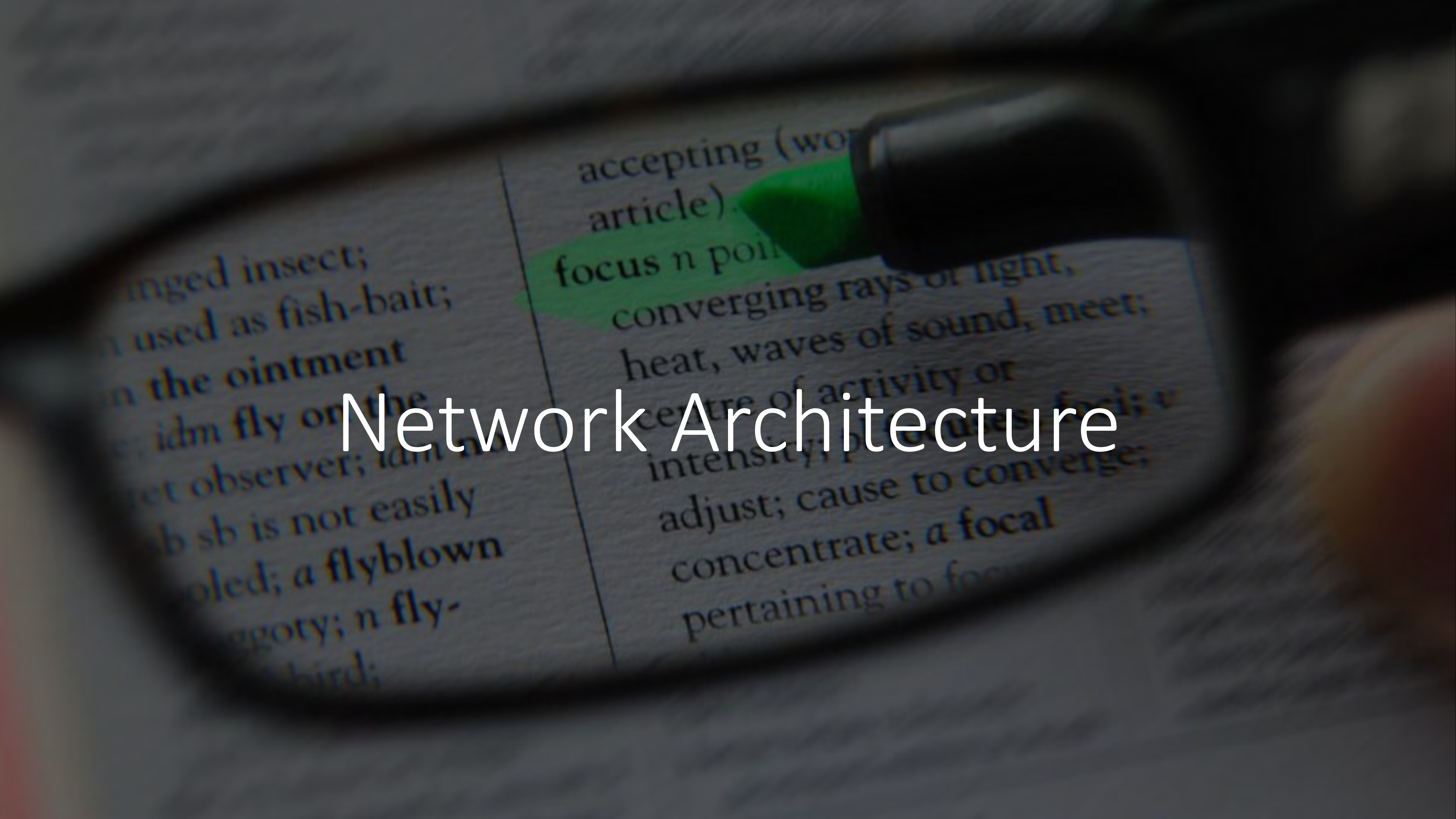
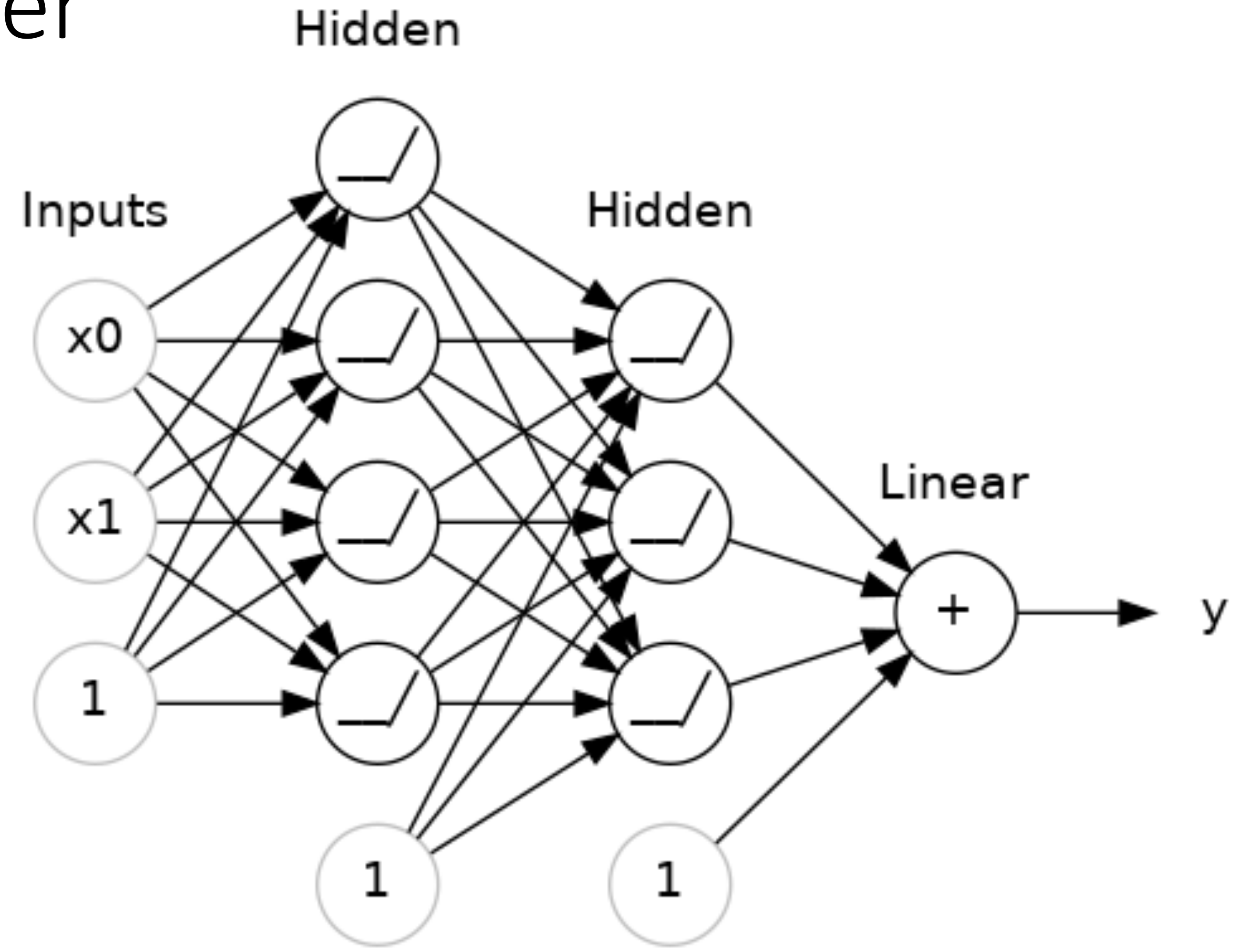
DIVISION OF RESEARCH
HEWLETT PACKARD ENTERPRISE DATA SCIENCE INSTITUTE



Network Architecture

Putting it all together

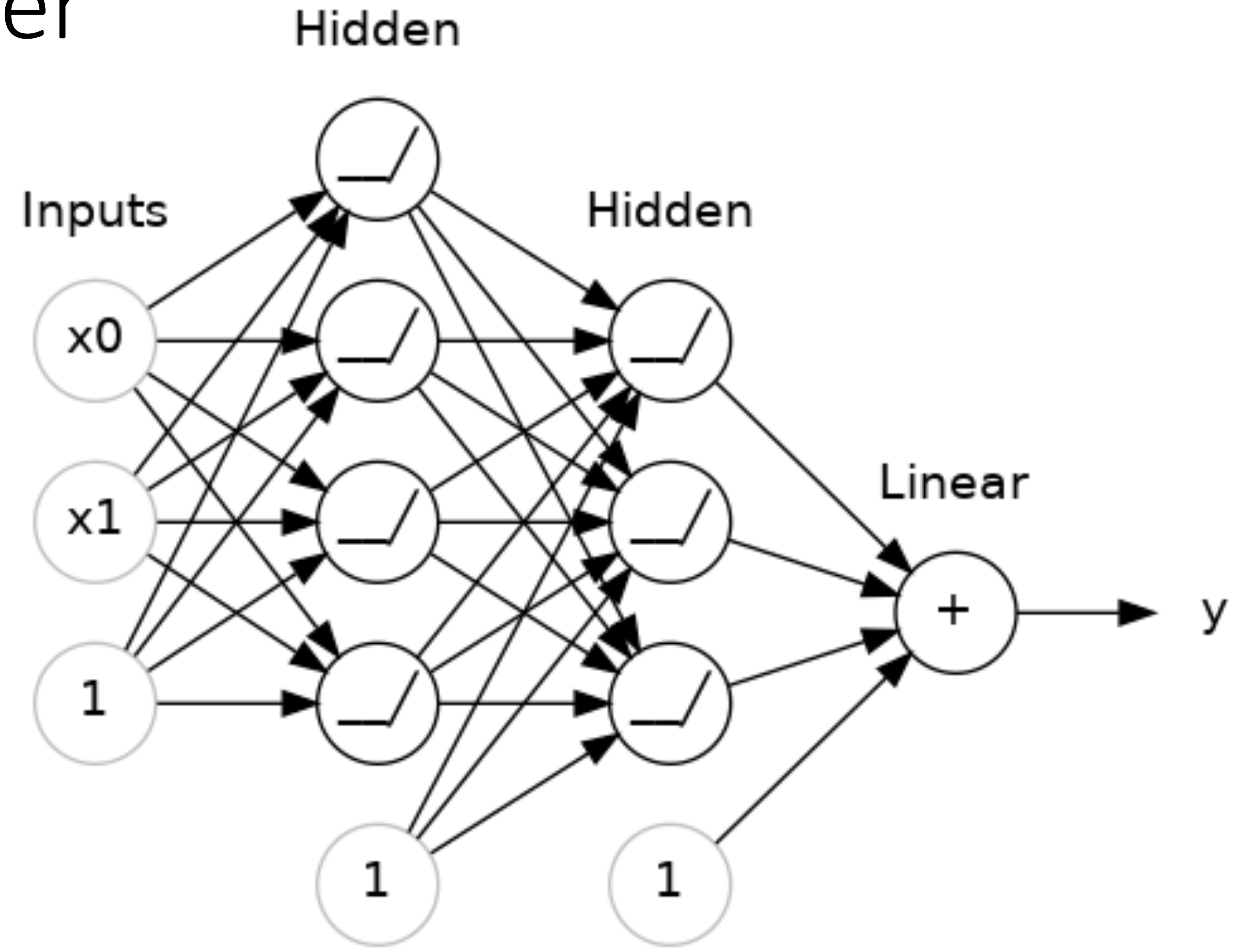
A fully-connected, feed-forward ReLU neural network with two hidden layers

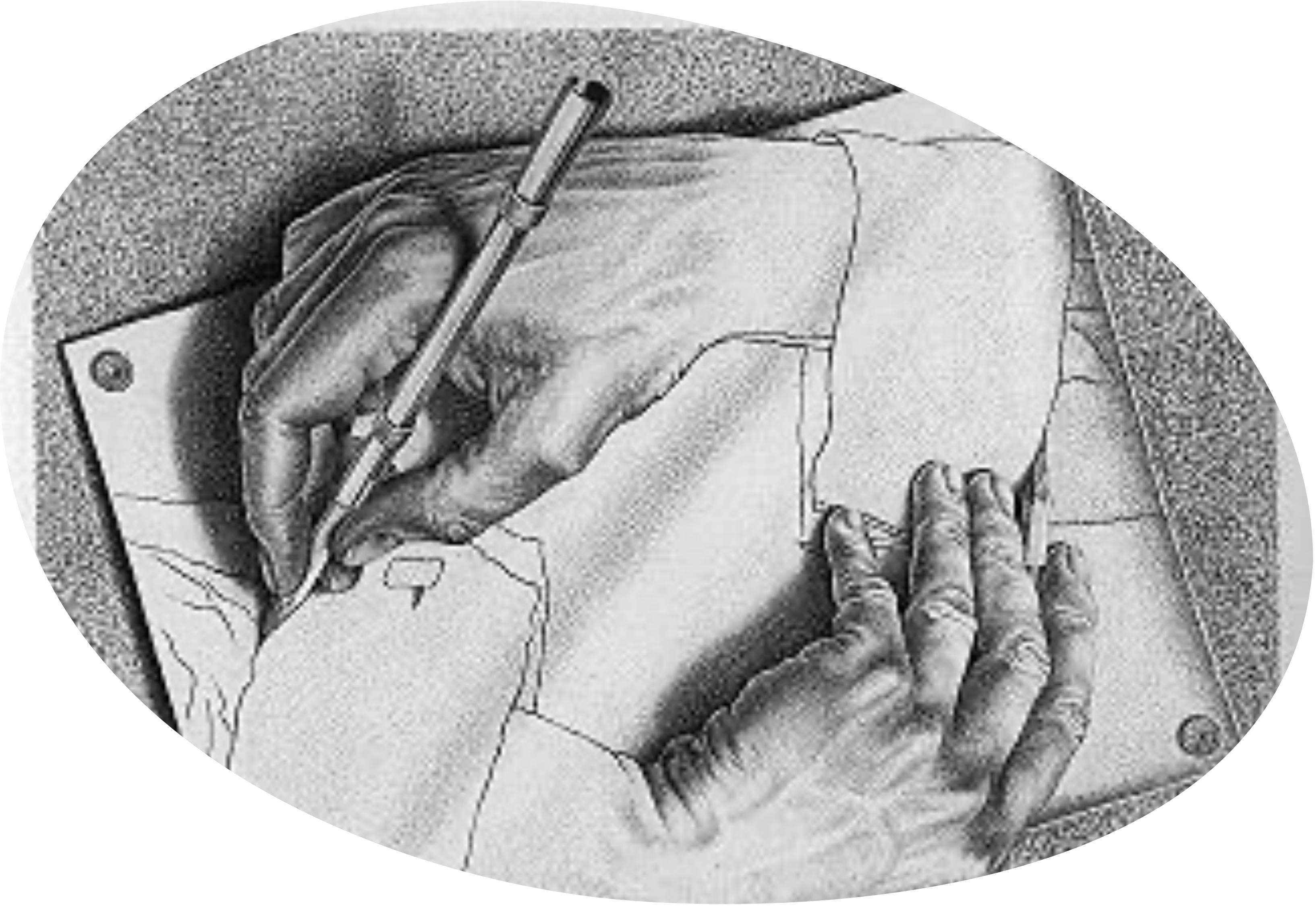


Putting it all together

The architecture of a neural network model is defined by several hyperparameters:

- # of hidden layers
- # of units per layer
- type of activation function

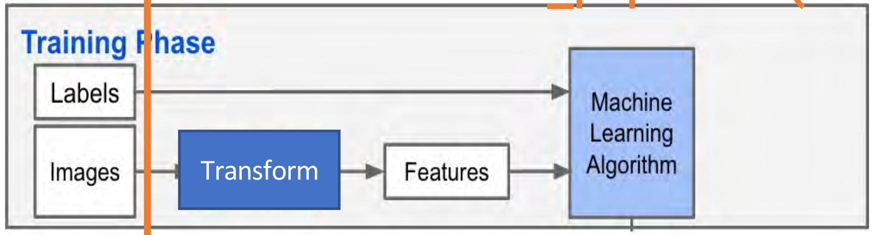




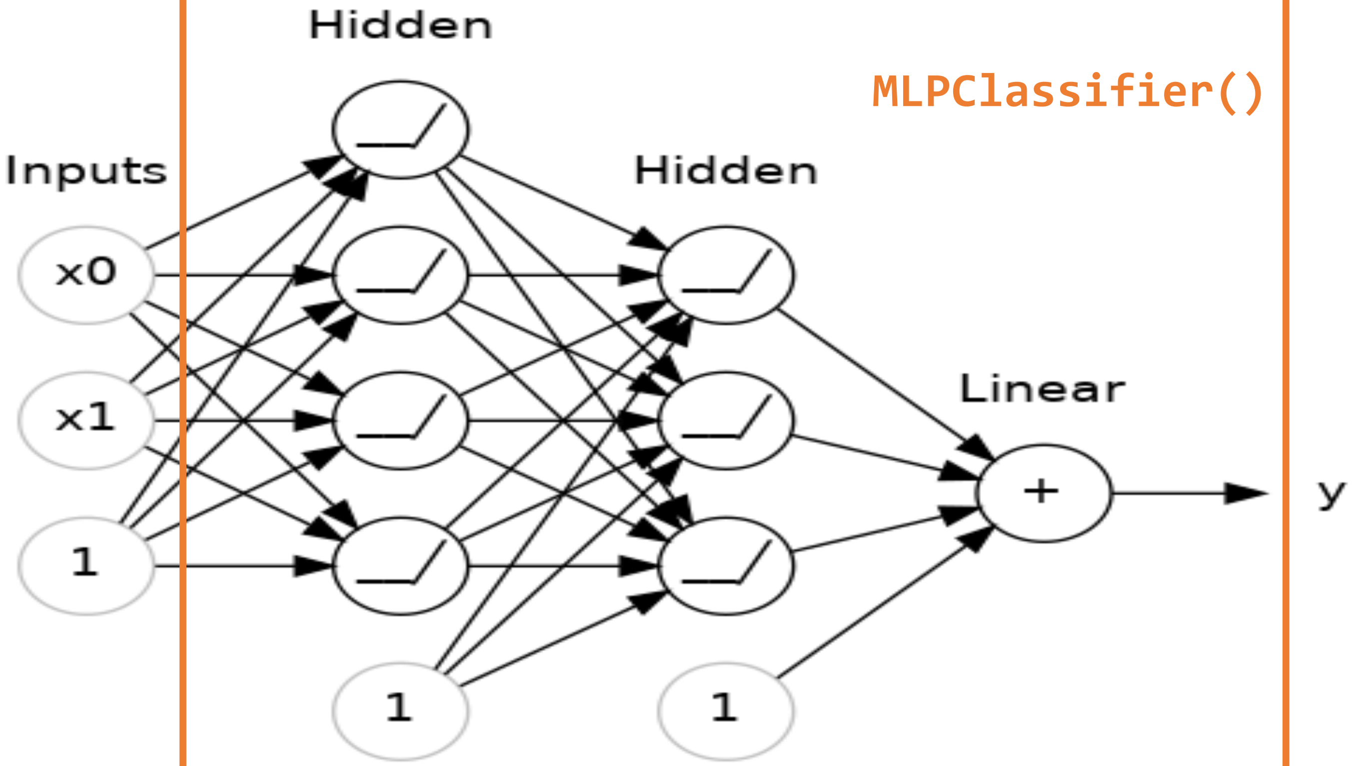
Hands-on Example: MLPClassifier

Multilayer Neural Networks are a complete pipeline

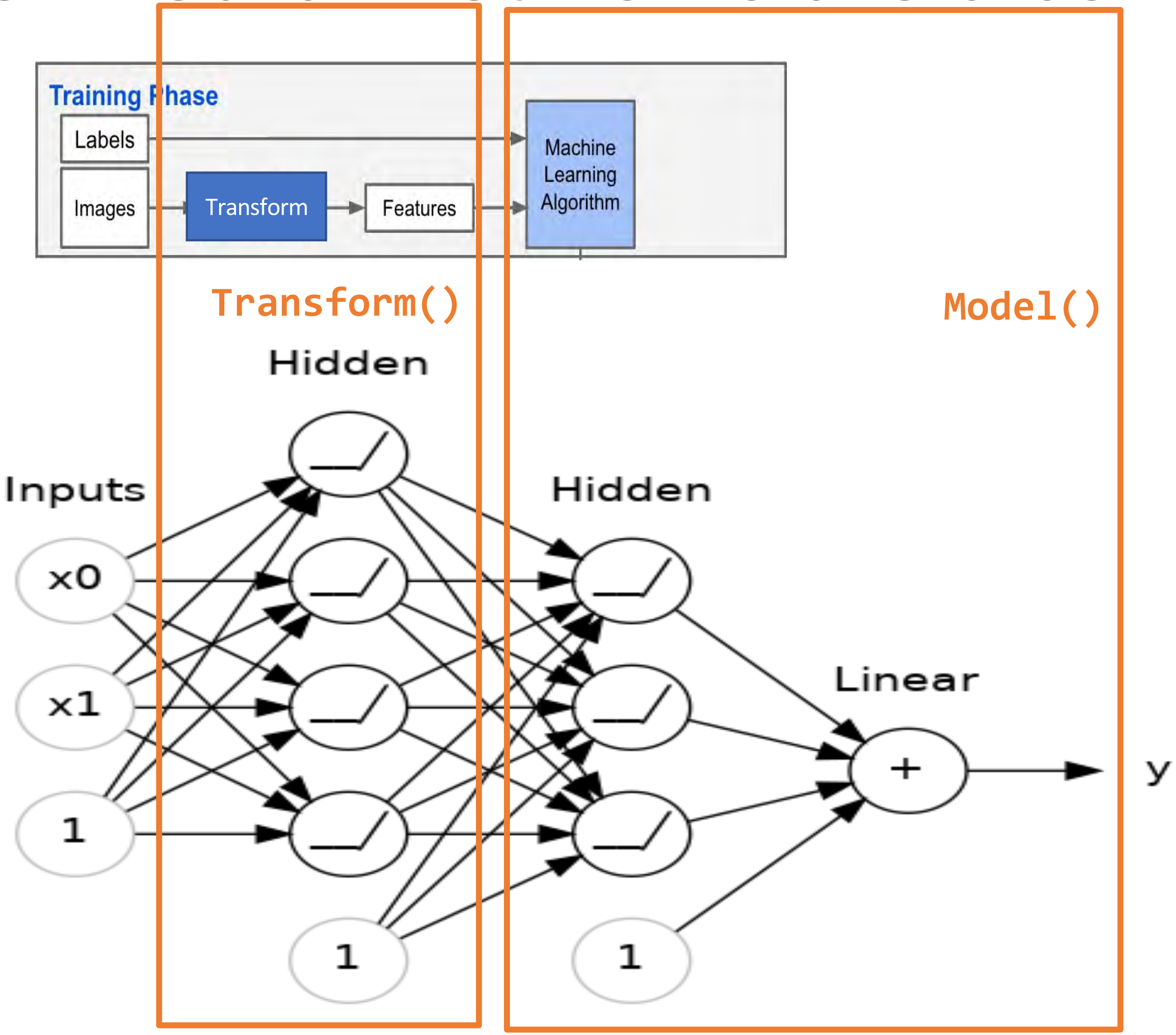
Make_pipeline(Transform,Model)



MLPClassifier()



Multilayer Neural Networks are a complete pipeline



Multilayer Neural Networks are a complete pipeline

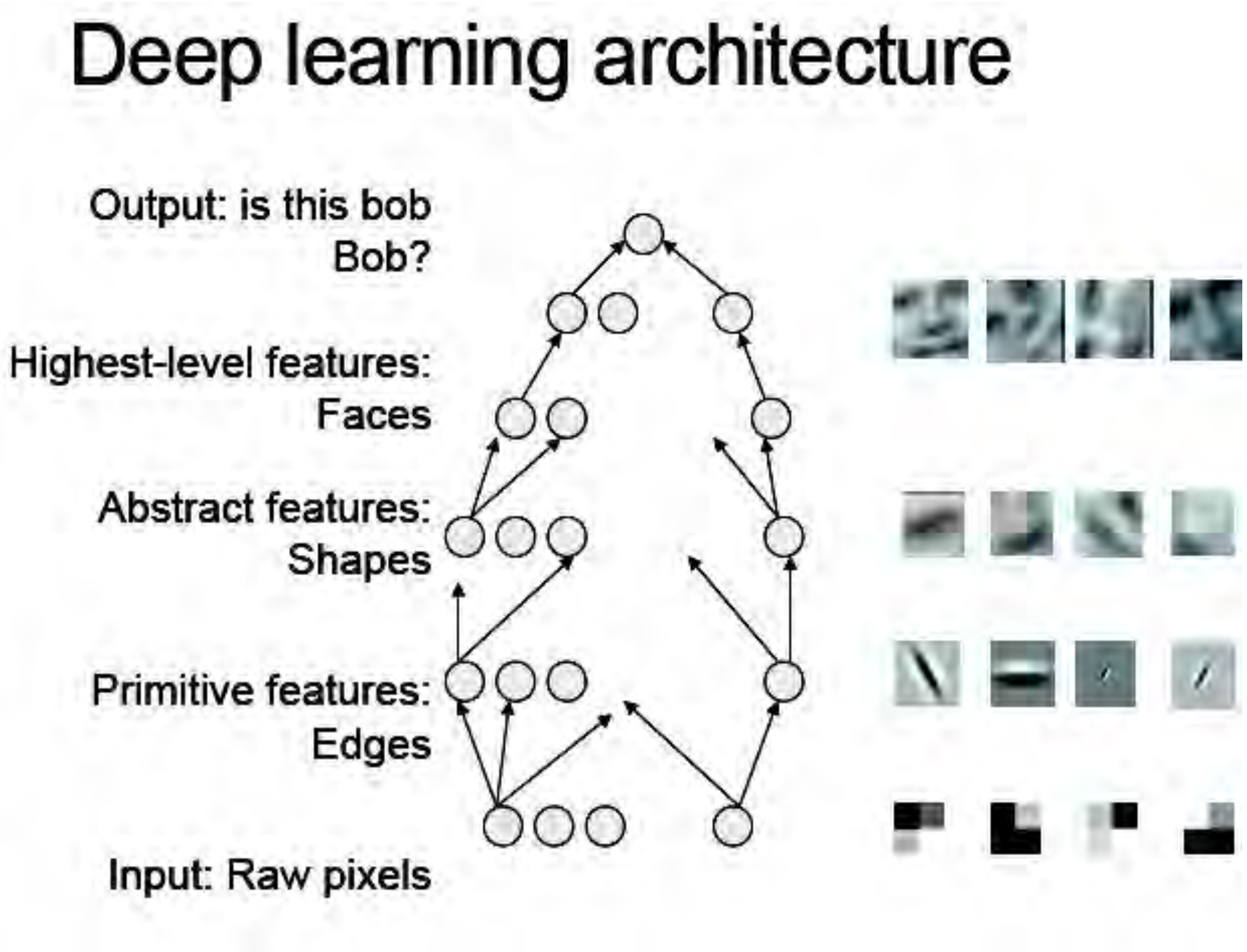
- Feature engineering is automatically “baked into” the process
- Initial layers pick out “low level” features
- Later layers process these transformed data to compute ”higher level” features
- “Top” layers perform classification tasks based on these custom-designed features

Hierarchical representations

“Deep learning methods aim at **learning feature hierarchies** with features from higher levels of the hierarchy formed by the composition of lower level features.

Automatically learning features at multiple levels of abstraction allows a system to learn **complex functions** mapping the input to the output directly from data, without depending completely on human-crafted features.”

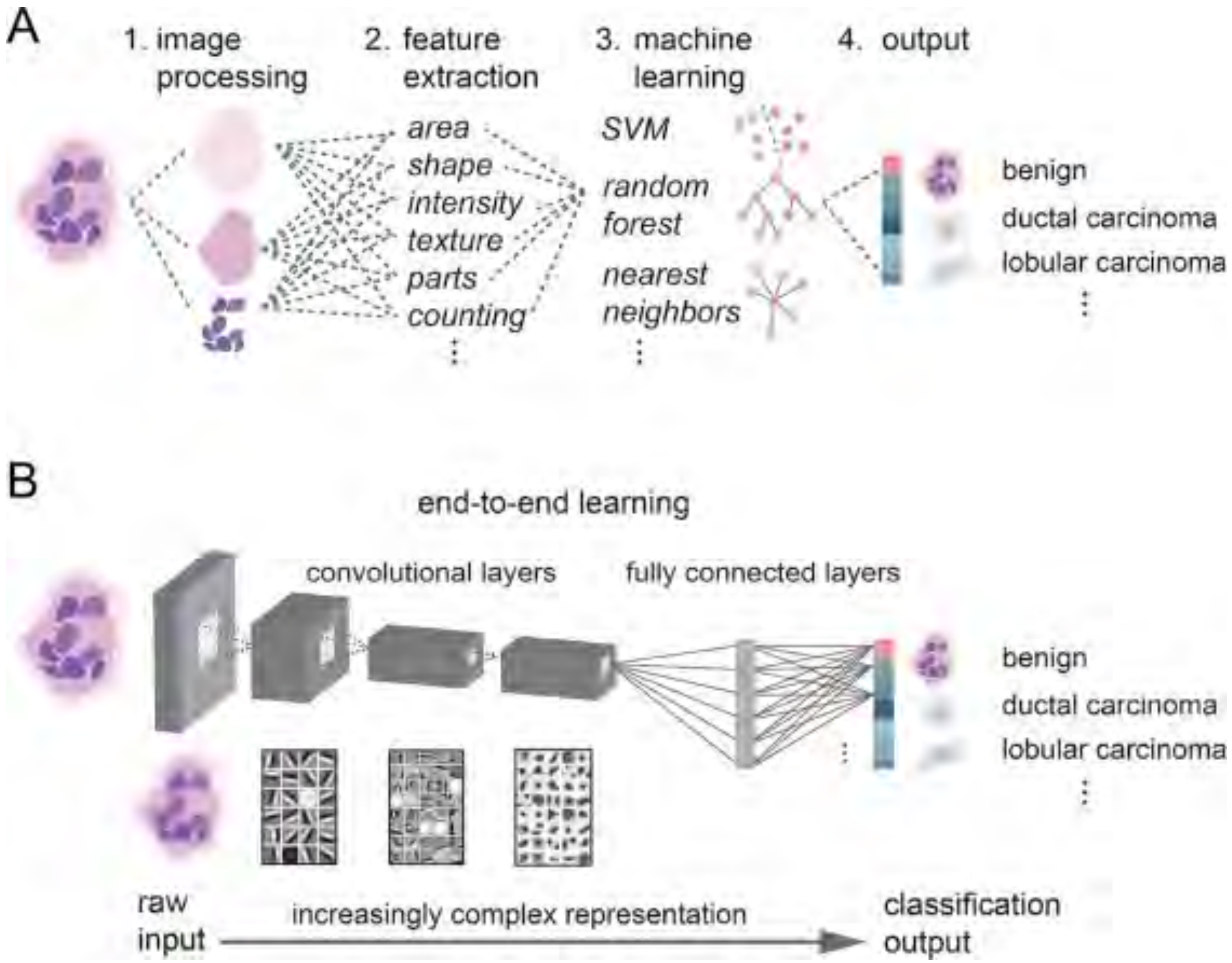
[Bengio, “On the expressive power of deep architectures”, *Talk at ALT*, 2011]
[Bengio, *Learning Deep Architectures for AI*, 2009]

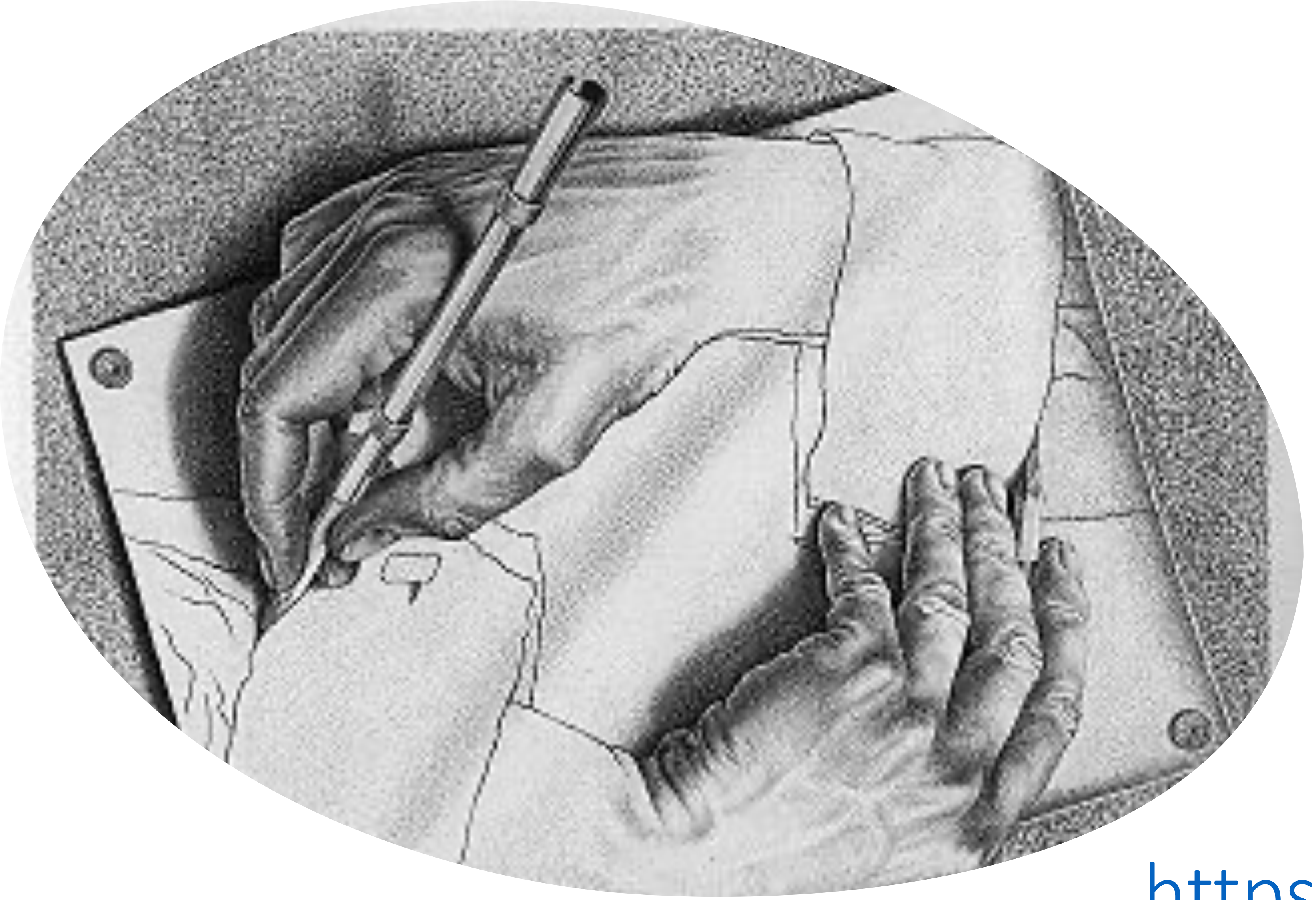


The Deep Learning Revolution

Earlier ML

Deep Learning



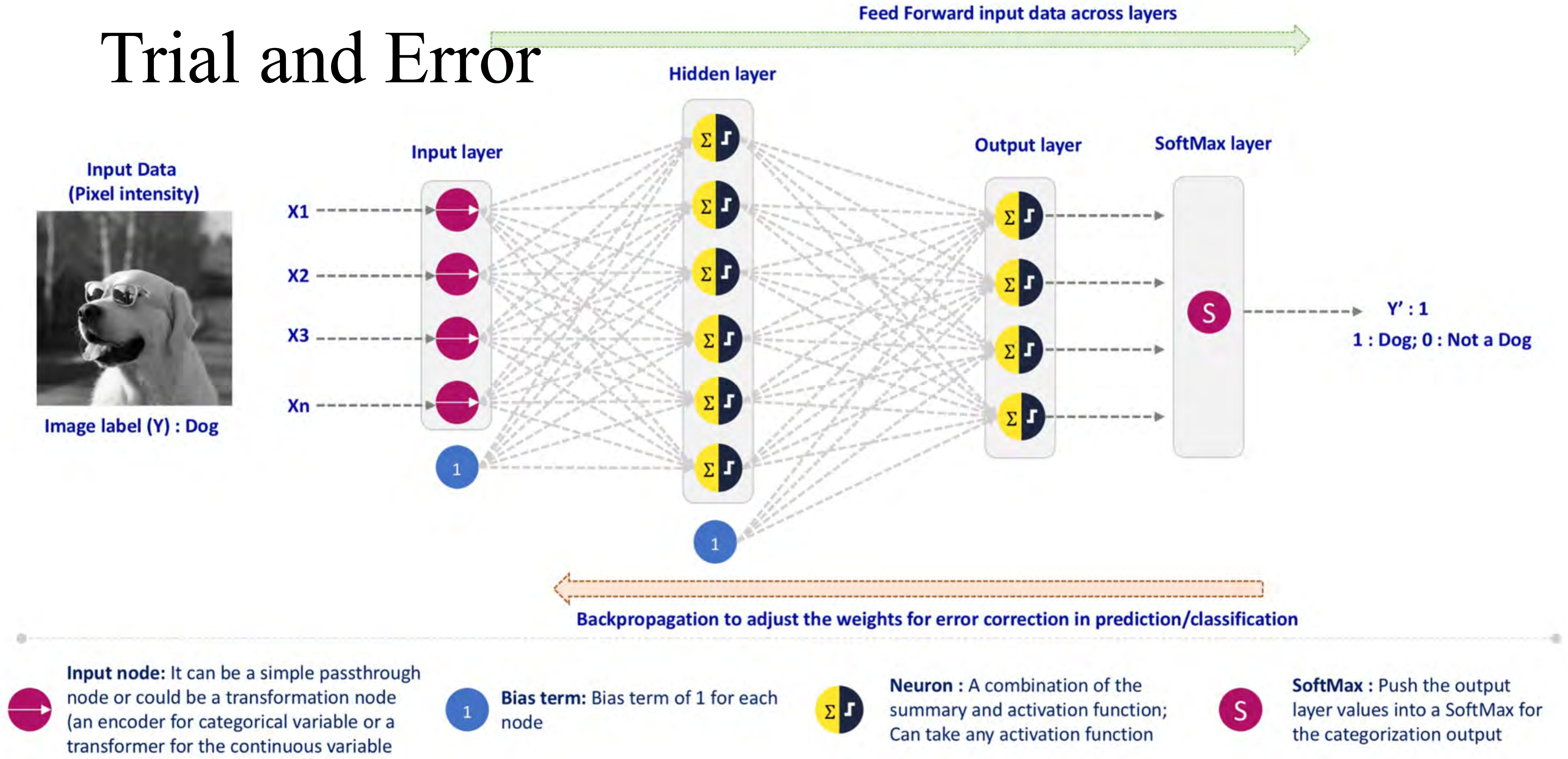


Hands-on Example:

https://playground.tensorflow.org/

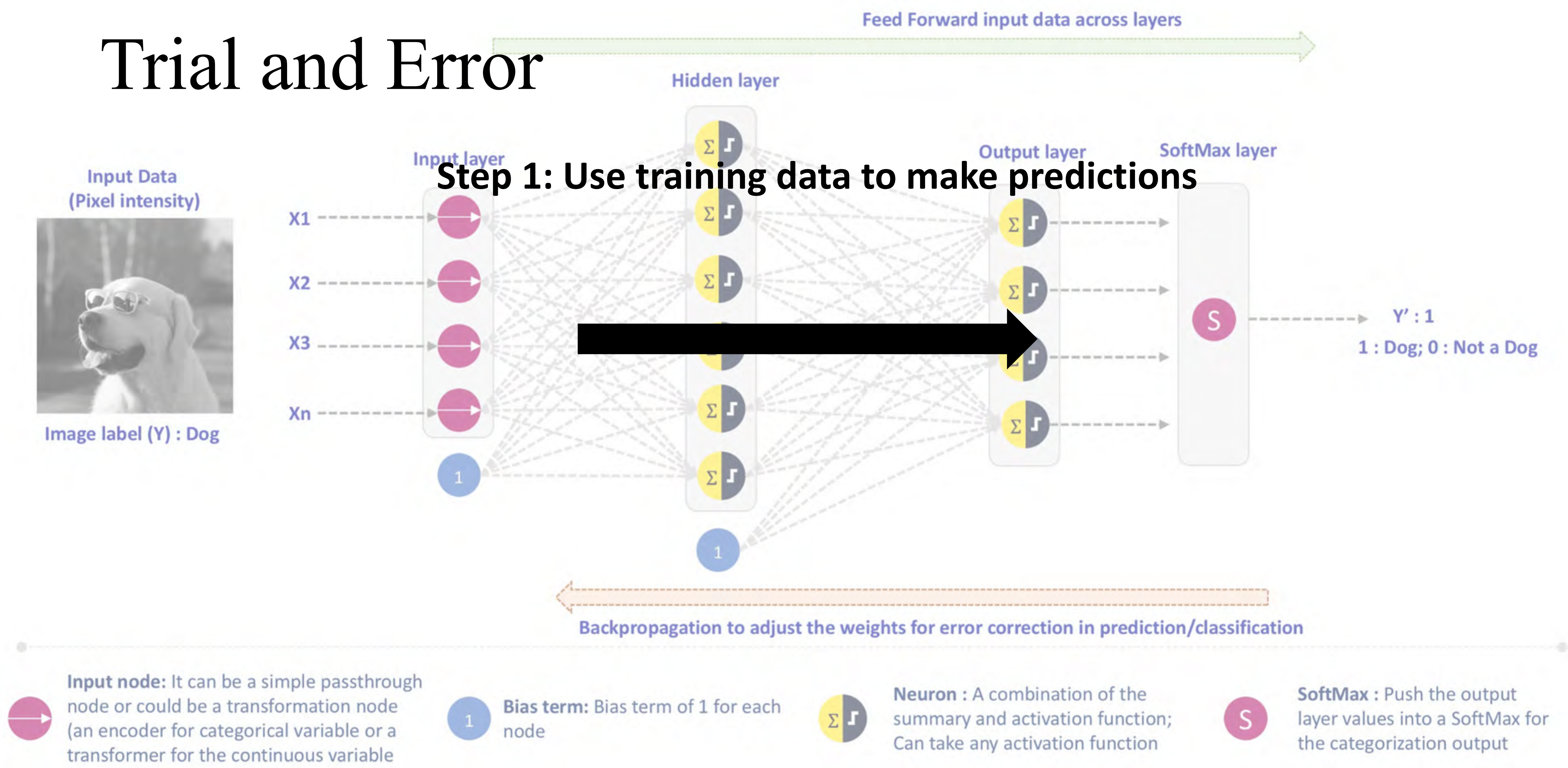
But how does a neural network learn?

Trial and Error

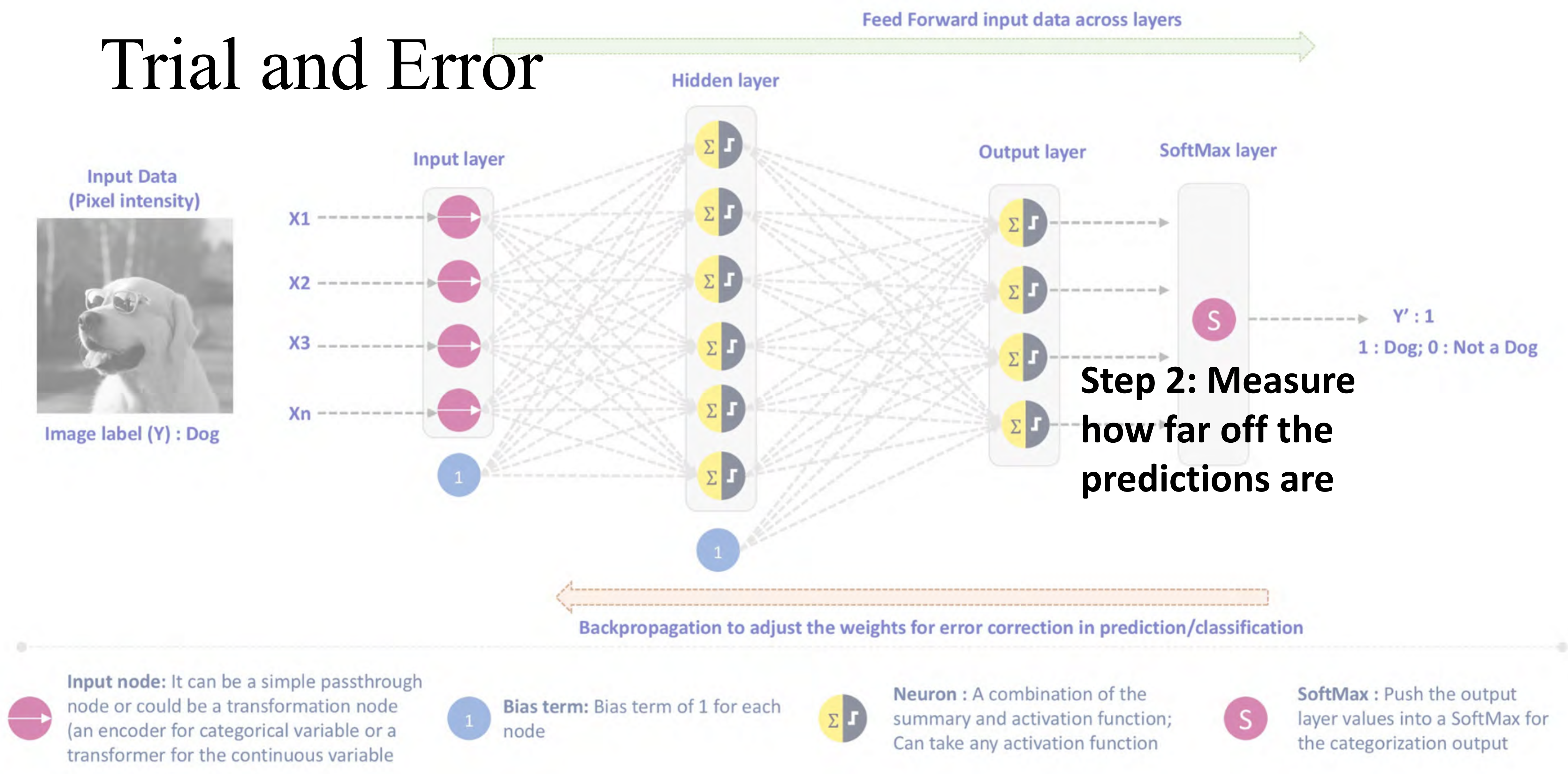


Trial and Error

Step 1: Use training data to make predictions

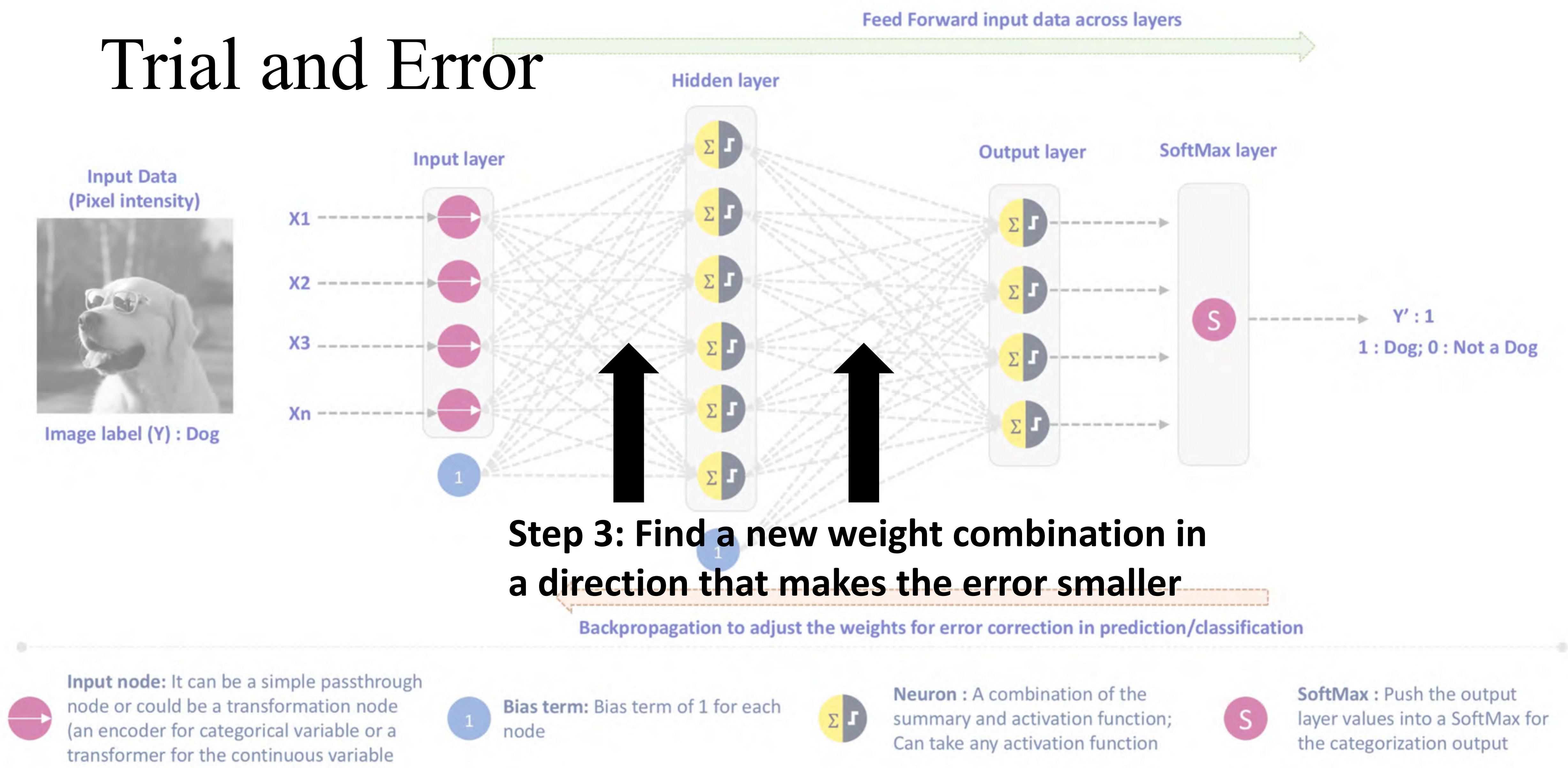


Trial and Error



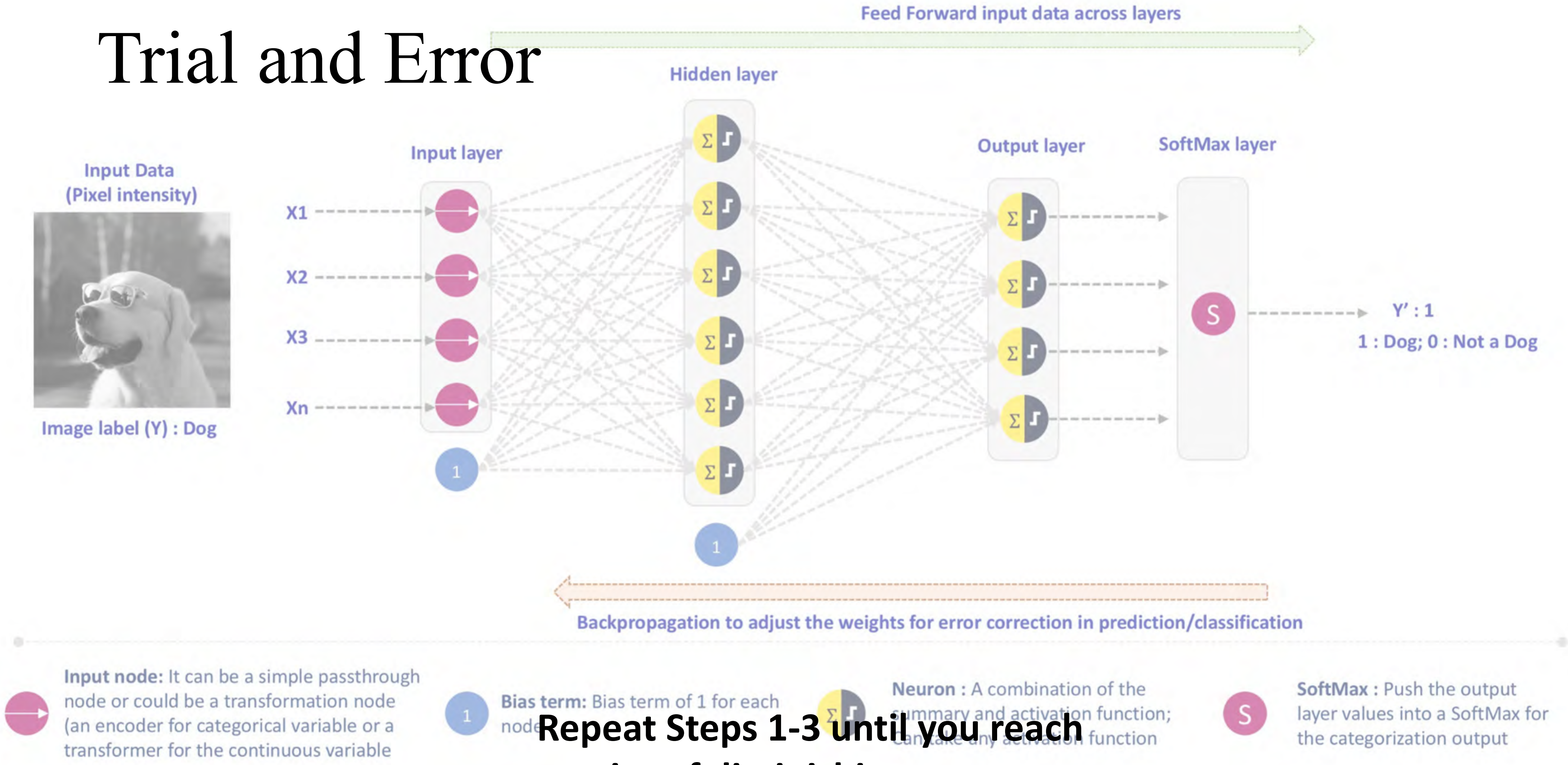
Step 2: Measure how far off the predictions are

Trial and Error



Step 3: Find a new weight combination in a direction that makes the error smaller

Trial and Error



Repeat Steps 1-3 until you reach a point of diminishing returns

Why not exhaustive search?

Curse of dimensionality

- Think of the example with the lost keys; exhaustive search in six million dimensions is prohibitive

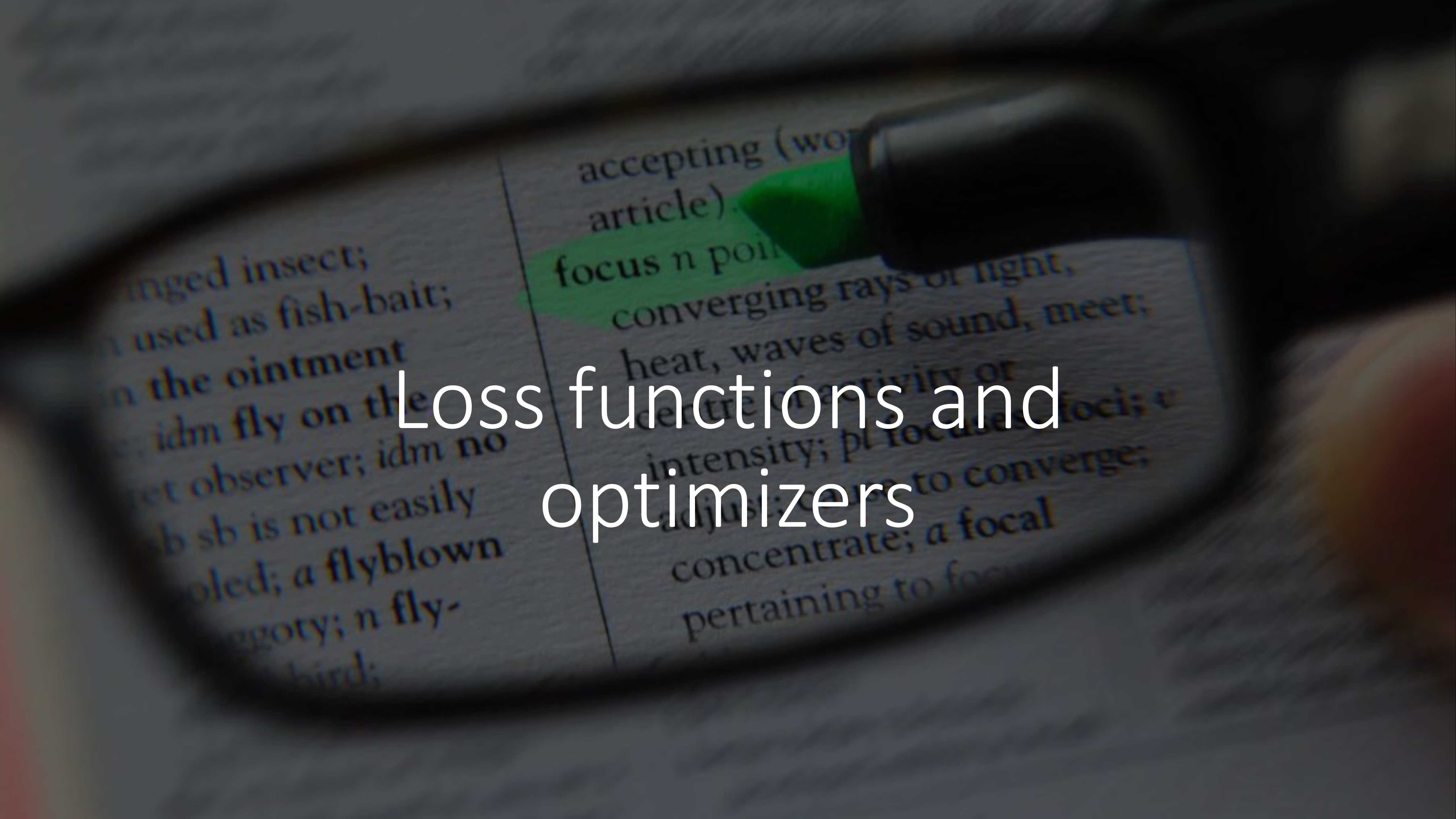
If the loss function is differentiable, the gradient acts like a metal detector

- At any location in the yard, the detector will point you in the direction where the signal *gain* is strongest

Gradient descent allows you to take incremental steps towards the optimal solution

- Walk a step in the direction of the gradient and recalculate

Loss functions and optimizers



Step 2: Measure how far off the predictions are

This is the role of the objective function

- Usually called loss function when applied to Neural Networks

Least squares is a common choice: $C(w,b) = \frac{1}{2N}\sum_n \|y_n - y'_n\|^2$

- All the familiar ones apply (L2, L1, etc.)
- New choice for classification: **Cross-Entropy**

Regularized versions are also used (hyperparameter alpha)

Step 3: Find a new weight combination in a direction that makes the error smaller

This is the role of the optimizer, usually a variation of **stochastic gradient descent (SGD)**

GRADIENT

- Consider each weight in turn (this can be parallelized)
- Compute how much the total error (the loss) would be reduced by if that weight is adjusted by a fixed small amount (the learning rate)
    - The ratio (difference in loss) / (difference in weight) is approximately the partial derivative of the loss function with respect to the weight, i.e., $\frac{\partial C(w,b)}{\partial w_i}$

DESCENT

- Adjust the weight by an amount proportional to $\frac{\partial C(w,b)}{\partial w_i}$
    - Weights that contribute a lot (large derivative) get prioritized

STOCHASTIC

- The partial derivative is only an approximation of the true change in loss
    - Calculate based on a randomly selected subset of the data

Repeat Steps 1-3 until you reach the point of diminishing returns

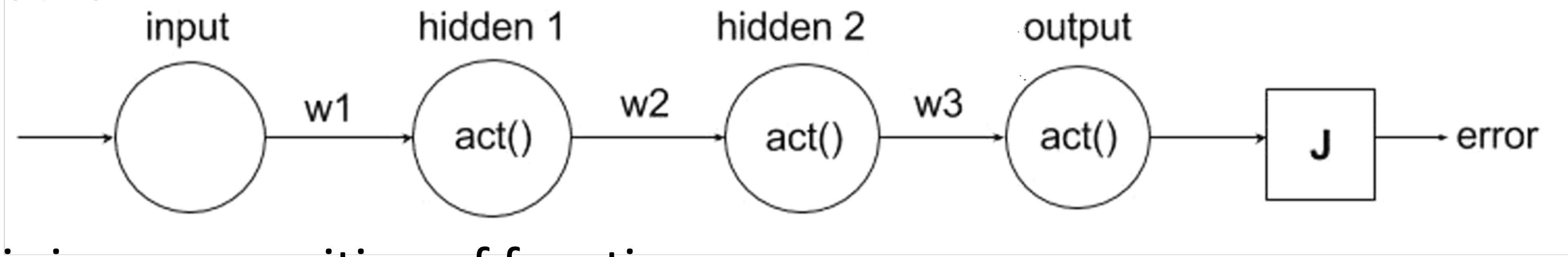
- Each iteration's sample of training data is called a **minibatch** (or often just "batch")

- A complete round of the training data is called an **epoch**.

The number of epochs you train for is how many times the network will see each training example.

Need to compute the gradient $\frac{\partial C(w,b)}{\partial w_i}$

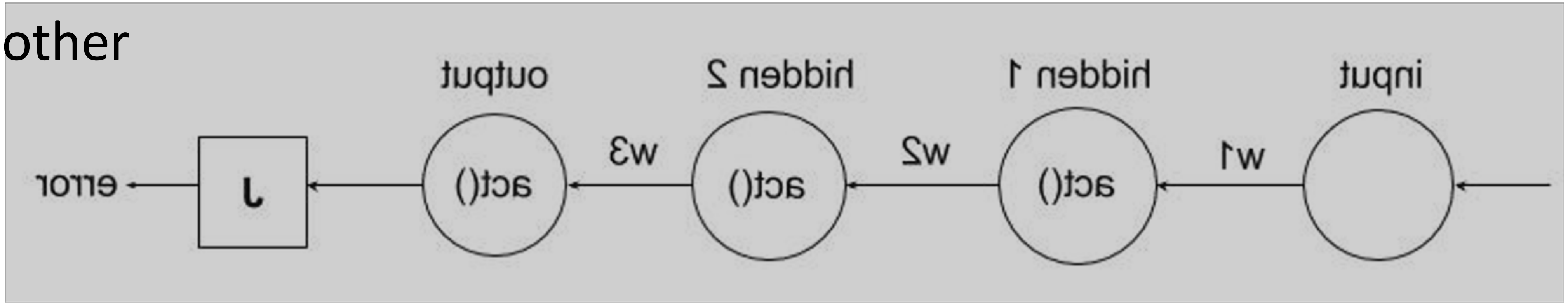
Neural network layers are “stacked”: the input for one is the output of another



This is a composition of functions

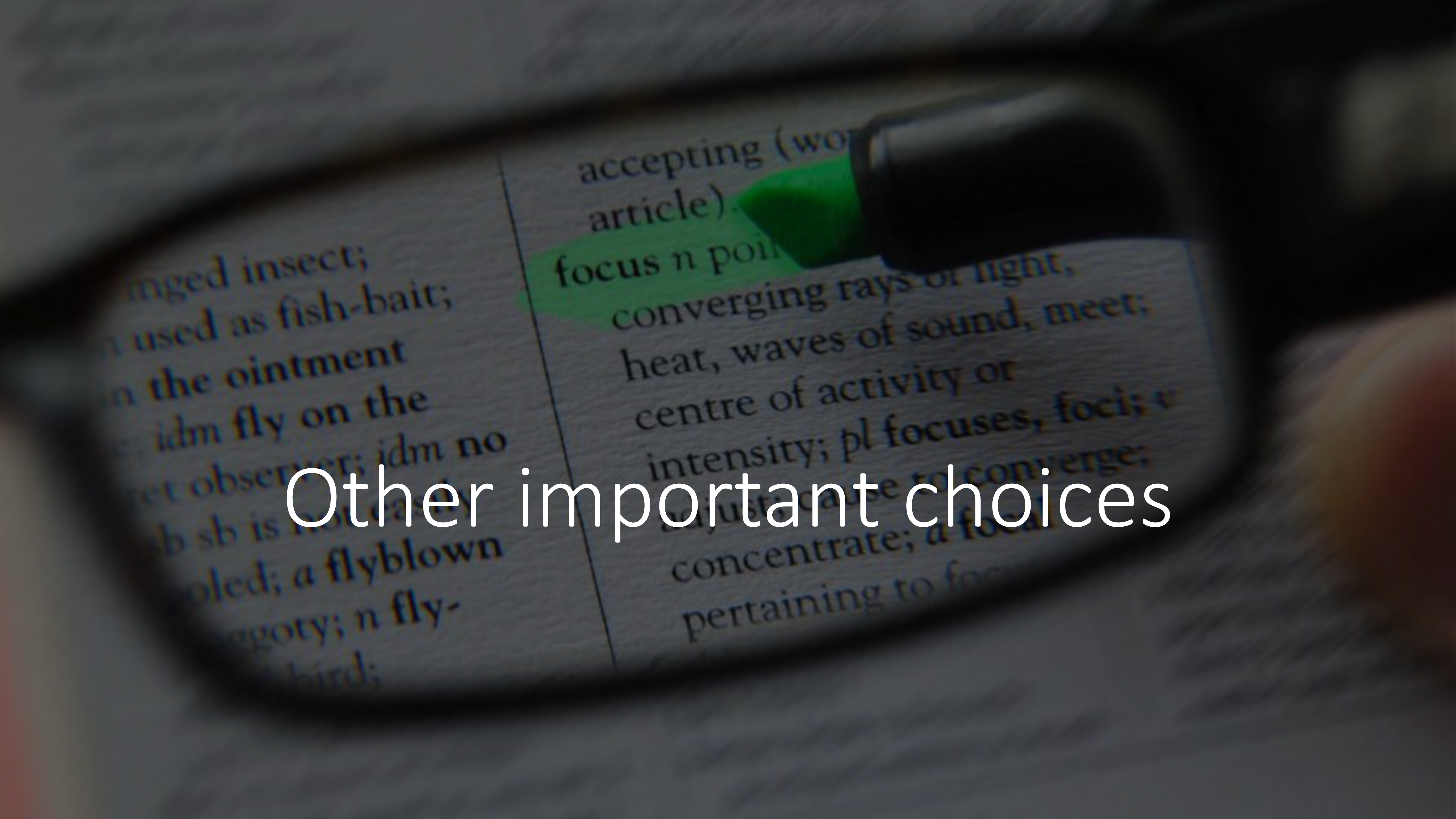
Need to compute the gradient $\frac{\partial C(w,b)}{\partial w_i}$

Neural network layers are "stacked": the input for one is the output of another



This is a composition of functions, so we can use the chain rule from calculus: work backwards from the last (top) layer in:

$$\frac{\partial error}{\partial w1} = \frac{\partial error}{\partial output} * \frac{\partial output}{\partial hidden2} * \frac{\partial hidden2}{\partial hidden1} * \frac{\partial hidden1}{\partial w1}$$



Other important choices

Activation functions

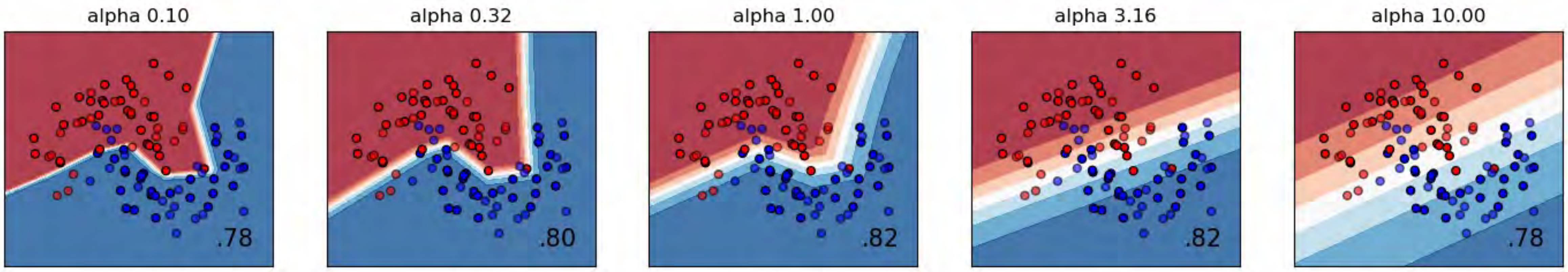
- **Sigmoid function and Hyperbolic Tangent function**: The gradient is very close to zero over a large portion of its domain which makes it slow and harder for the learning algorithm to learn.
- **Rectified Linear Unit (ReLU)**: $g(z) = max\{0, z\}$. Since ReLU shares a lot of the properties of linear functions, it tends to work well on most of the problems. However, this means that for $z \leq 0$ the gradient is zero and again can't learn.

Alpha

Default is close to zero

- Little regularization

Higher alpha means stronger regularization
(less prone to variance/overfitting,
but more prone to bias/underfitting)



Learning rate

The **learning rate** determines how far to go in the direction that makes the error smaller.

- For example, the optimizer may estimate that a change of one in the value of the weight connecting input variable X_{143} to the 54th ReLU of the first hidden layer will reduce the error by 3.72 units
- But this is only an approximation of the true change.
- How big a step to take? How much to change the weight?

Learning rate

The learning rate has a small positive value, often in the range between 0.0 and 1.0

Smaller learning rates mean more conservative changes in weights, taking smaller steps so the approximation will stay valid

- This requires more training epochs; more steps to travel down the optimization path

Larger learning rates can also cause problems; the approximation may no longer hold, and the error is not actually reduced in an optimal way

- The model might converge too quickly to a suboptimal solution (rushing to make hasty decisions)

Learning rate

Instead of a constant learning rate, it is recommended to use a high learning rate during the start and reduce it during training.

Typically optimizers take care of this automatically.

Adam is a type of SGD algorithm that has an adaptive learning rate that makes it suitable for most problems without any parameter tuning (it is "self tuning", in a sense); it is a great general-purpose optimizer

Batches and epoch

Balance between:

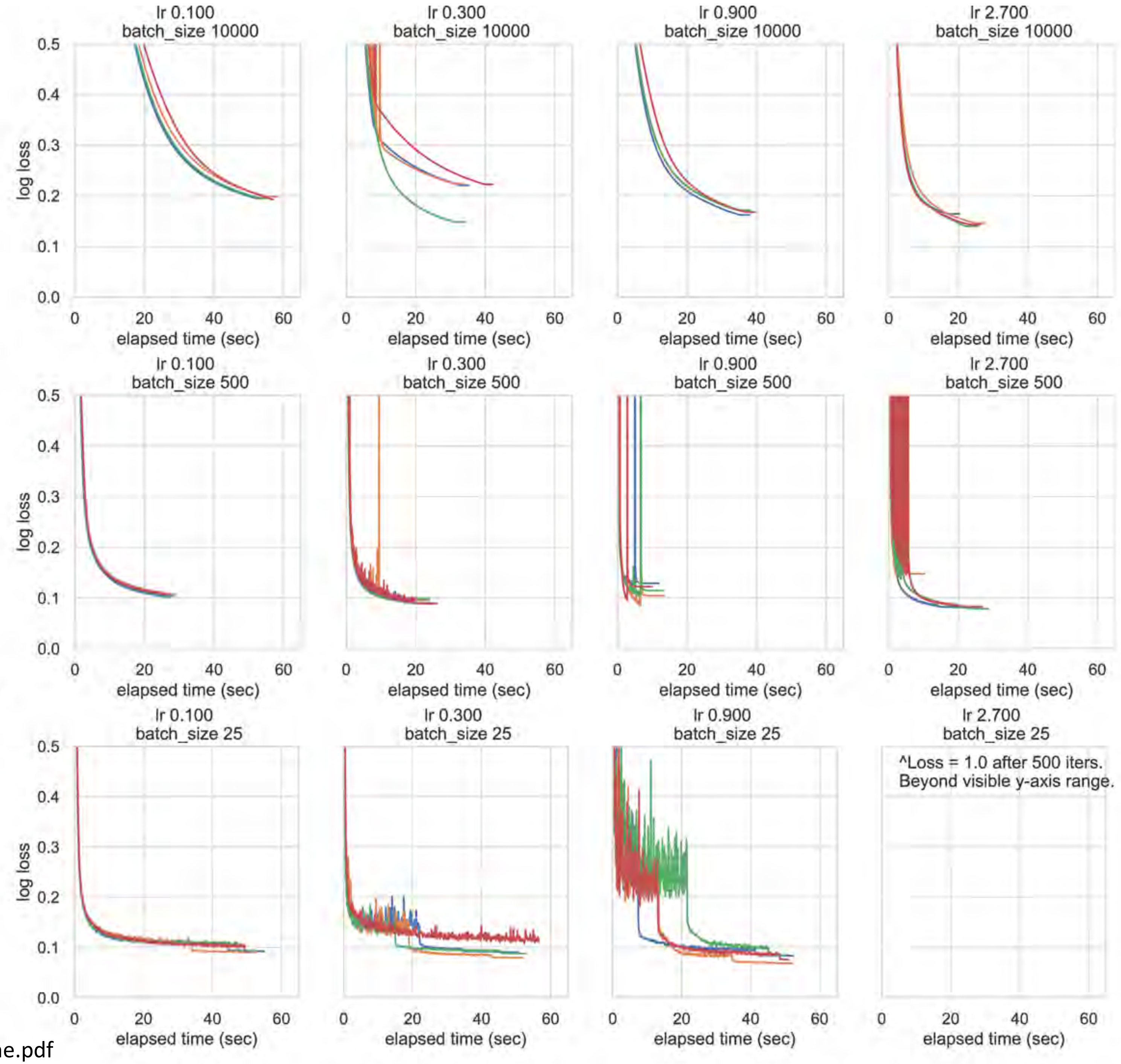
- true stochastic gradient descent (calculate and update separately for each training example)
- true batch gradient descent (calculate and update based on all training examples)

Split the training dataset into small batches of size batch_size

Calculate model error and update model coefficients one batch at a time.

(# of epochs) * (batch_size) = # of training examples

Batch size and learning rate work together



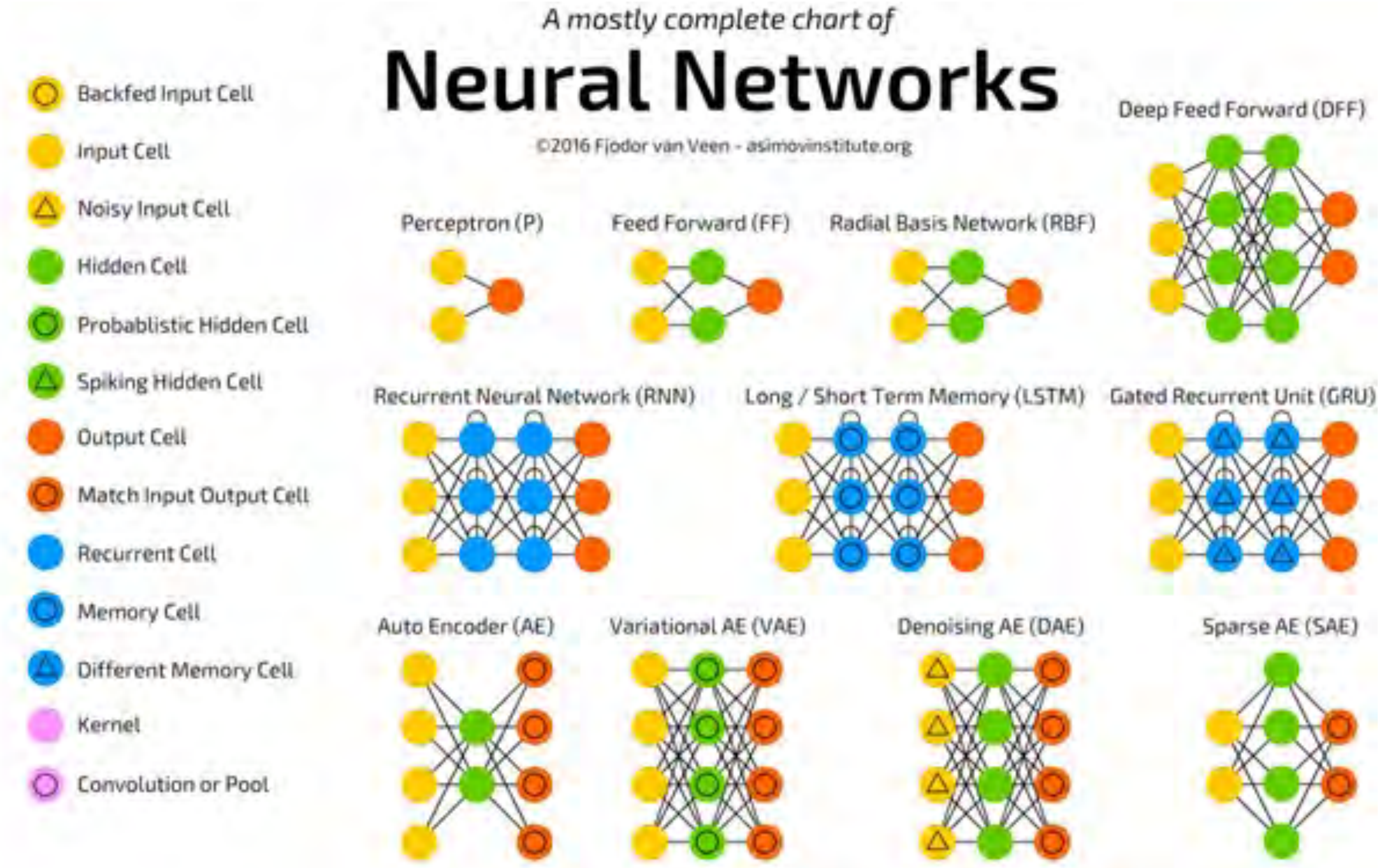
https://www.cs.tufts.edu/comp/135/2020f/images/hw3_fig2_sgd_loss_vs_time.pdf

Homework Assignment #3
Due Tuesday (July 13), 11:59 pm (Central)

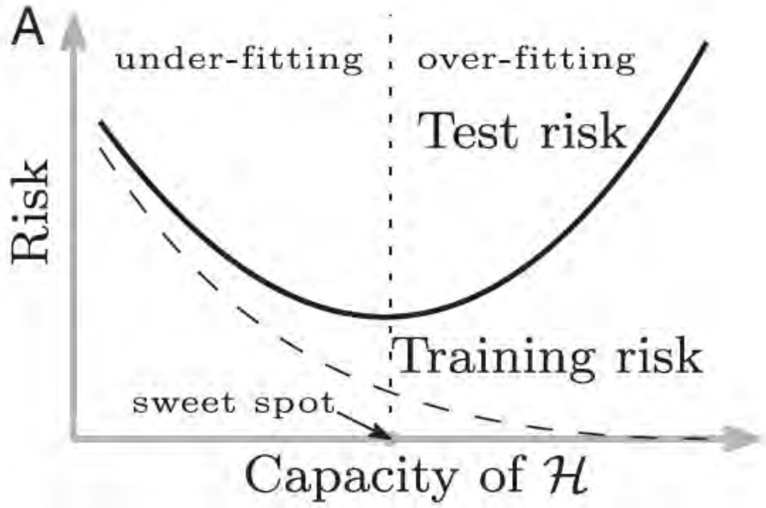
Your assignment is to create a Jupyter notebook that demonstrates how to do the following (use methods discussed in the class materials shared so far):

Load the dataset in the file named winequality_white.csv and set up a classification problem: predicting the quality value (y variable with seven classes labeled 3, 4, 5, …, 9) based on the values of **all** the other eleven variables (acidity, alcohol, pH, etc.).

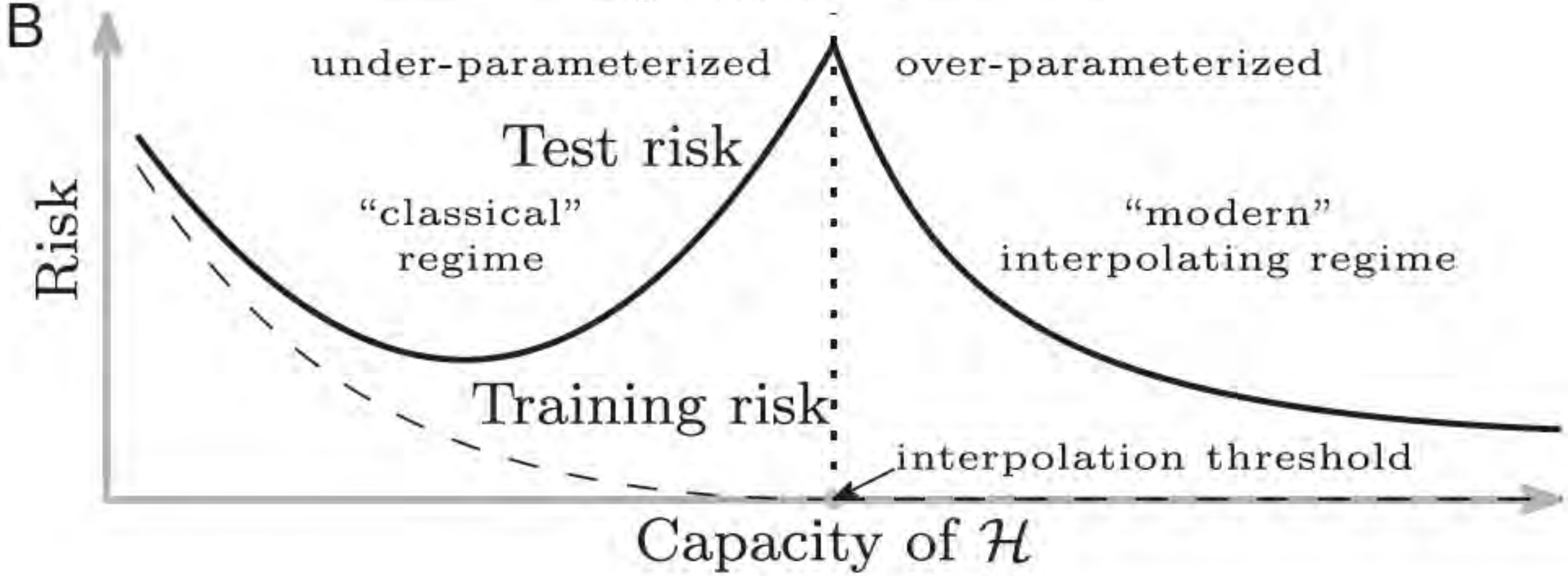
1. Train and tune (via cross-validation) at least three different combinations of MLPClassifier architecture choices (e.g., number of layers, # of neurons per layer, activation function). (6 points)
2. Study and describe the performance impact of varying at least three different combinations of optimizer parameter values (e.g., solver, epoch, learning rate) for one of the architectures in Step 1. (6 points)
3. Test the performance of the best MLPClassifier from Steps 1 and 2, using scoring methods of your choice. Discuss in detail your results. (4 points)
4. Train and tune a different classifier that is not a neural network; compare the MLPClassifier test results from Step 3 to that other classifier. Discuss in detail your results. (4 points)


A mostly complete chart of
Neural Networks
©2016 Fjodor van Veen - asimovinstitute.org
Backfed Input Cell
Input Cell
Noisy Input Cell
Hidden Cell
Probablistic Hidden Cell
Spiking Hidden Cell
Output Cell
Match Input Output Cell
Recurrent Cell
Memory Cell
Different Memory Cell
Kernel
Convolution or Pool
Perceptron (P)
Feed Forward (FF)
Radial Basis Network (RBF)
Deep Feed Forward (DFF)
Recurrent Neural Network (RNN)
Long / Short Term Memory (LSTM)
Gated Recurrent Unit (GRU)
Auto Encoder (AE)
Variational AE (VAE)
Denoising AE (DAE)
Sparse AE (SAE)

Earlier ML

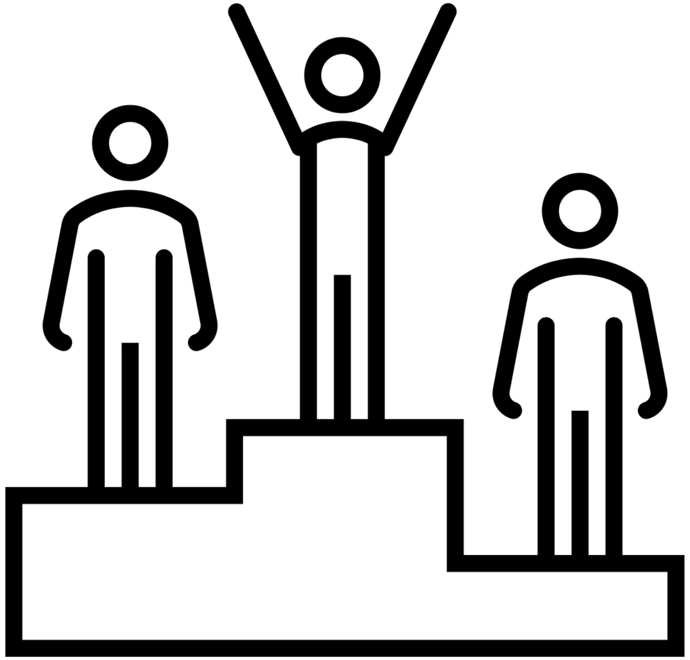


Deep Learning



- Belkin, M., Hsu, D., Ma, S., & Mandal, S. (2019) Reconciling modern machine learning practice and the classical bias-variance trade-off. *PNAS* 116 (32) 15849-15854
- Loog, M., Viering, T., Mey, A., Krijthe, J., & Tax, D. (2020) A brief prehistory of double descent *PNAS* 117 (20) 10625-10626

Can **one** athlete be good at **many** sports?



- If you train for the triathlon,
- you will not outrun a dedicated runner,
- you will not outswim a dedicated swimmer
- you will not cycle faster than a dedicated bicyclist

- But you will finish the triathlon faster than any of them!

What if your model is a superhero?

It could
be **better**
at **all three**
sports!