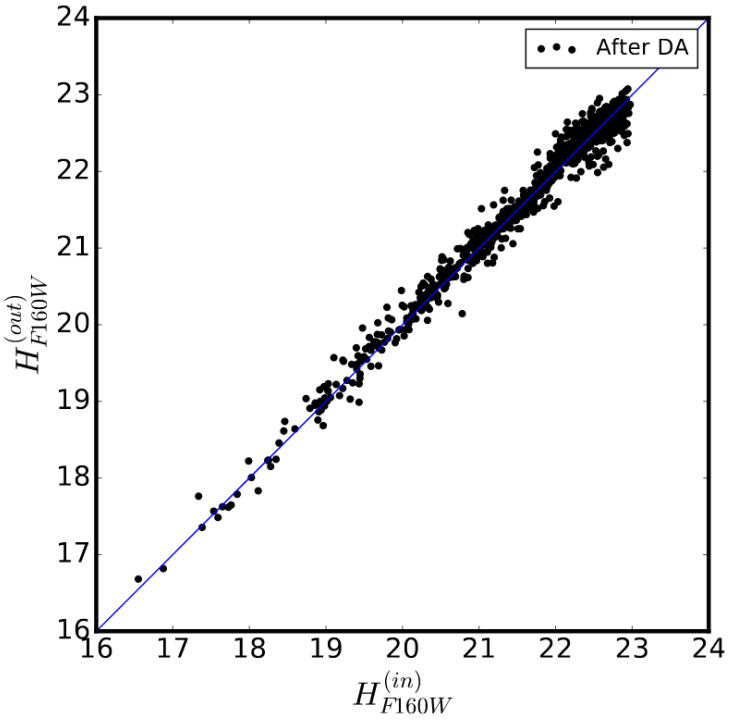
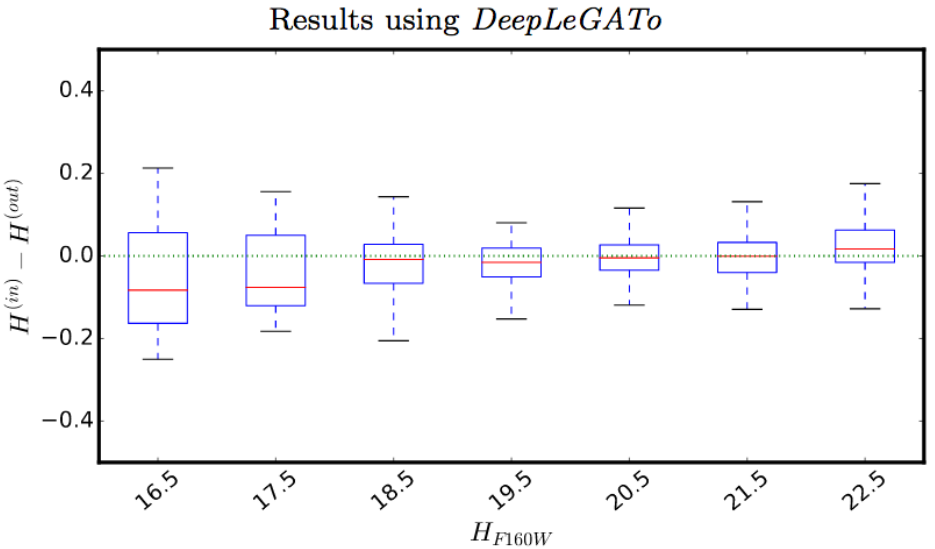
Evaluation of results [regression]



FOR REGRESSIONS, SIMPLY USE
“STANDARD ACCURACY MEASUREMENTS

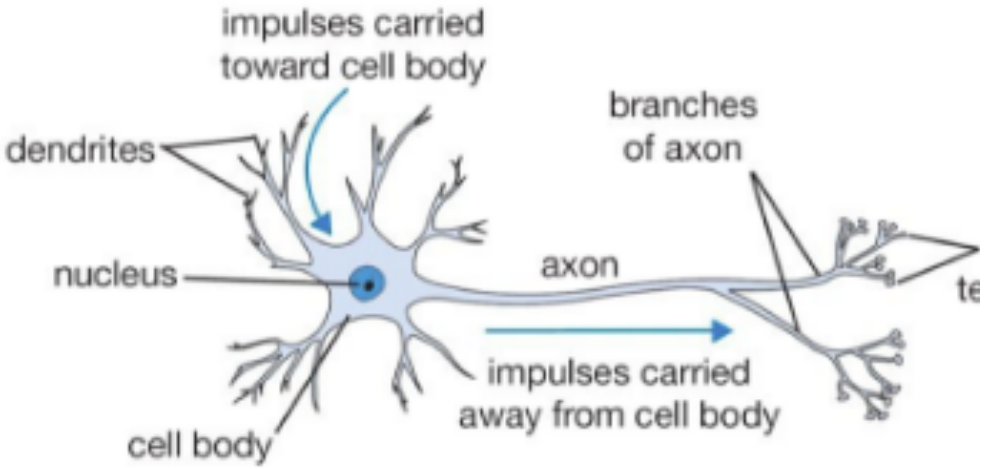
BIAS, SCATTER …YOU KNOW!



Tuccillo+18

PART II: A FOCUS ON "SHALLOW" NEURAL NETWORKS

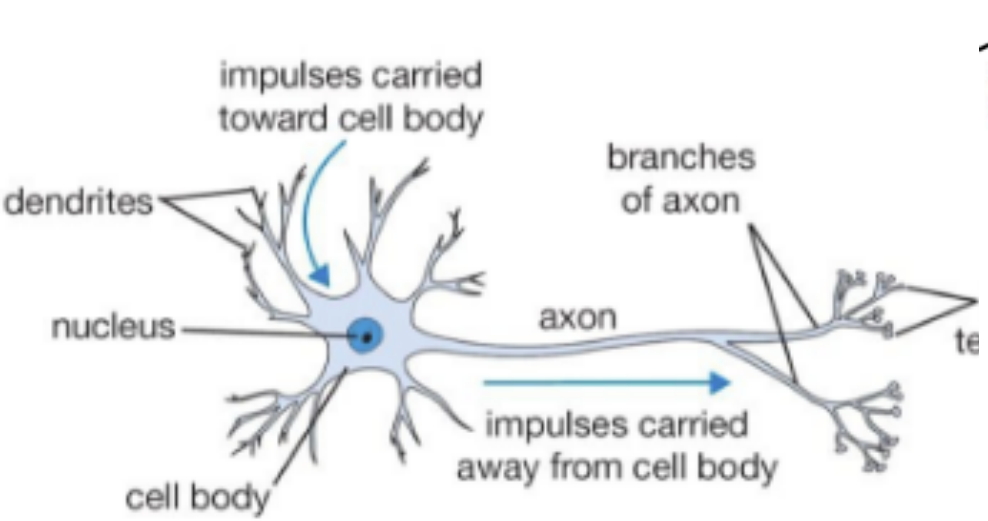
THE NEURON

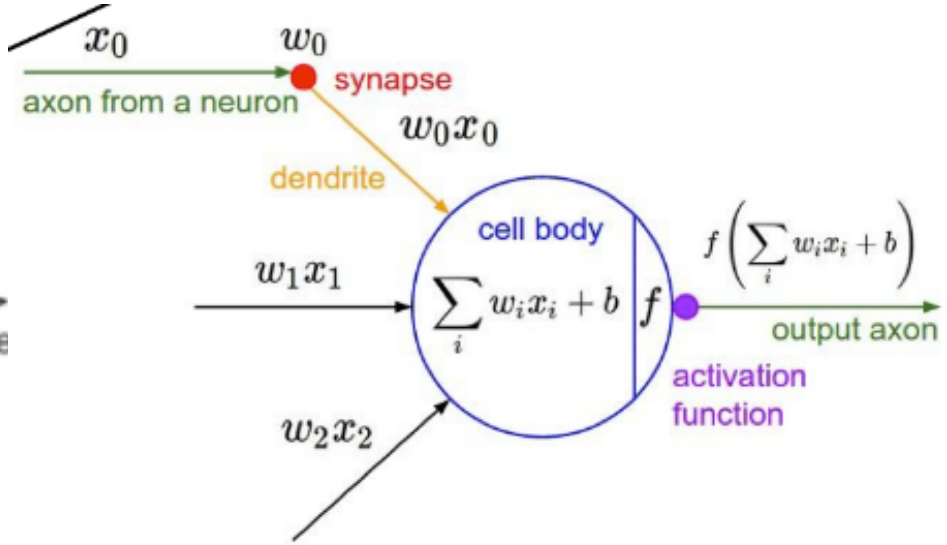


INSPIRED BY NEURO - SCIENCE?

Credit: Karpathy

THE NEURON





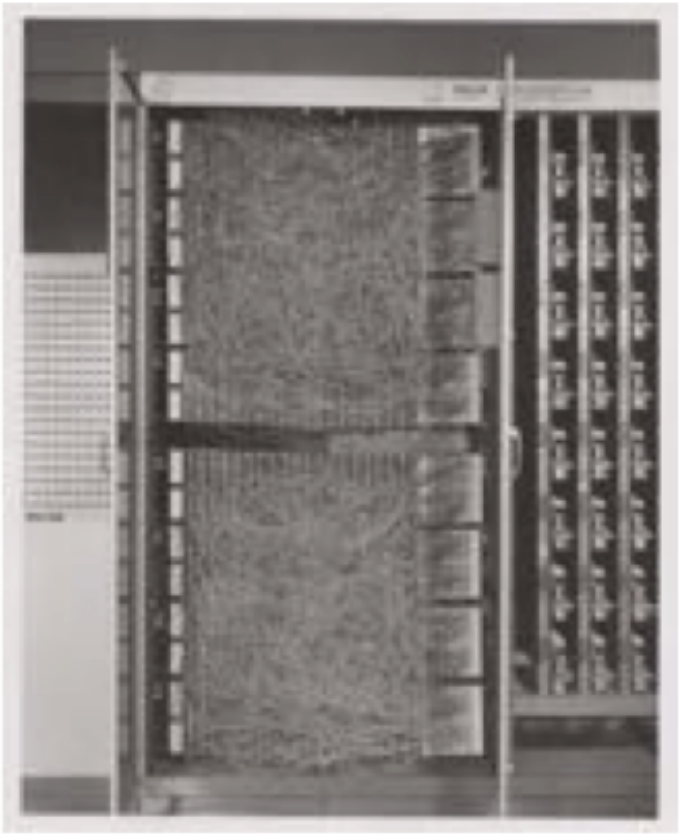
INSPIRED BY NEURO - SCIENCE?

Credit: Karpathy

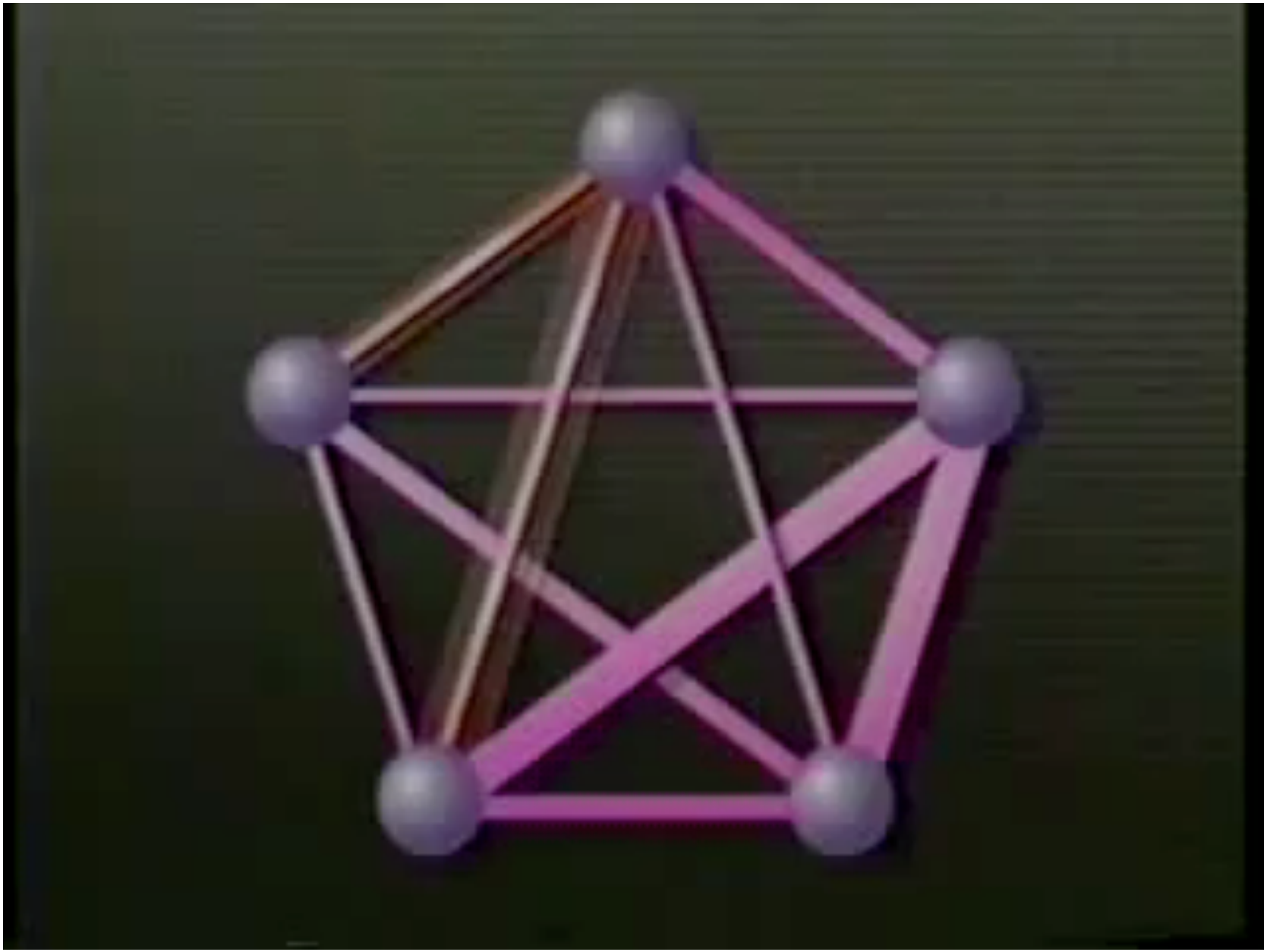
Rosenblatt Perceptron

FIRST IMPLEMENTATION OF NEURAL NETWORK [Rosenblatt, **1957!**]

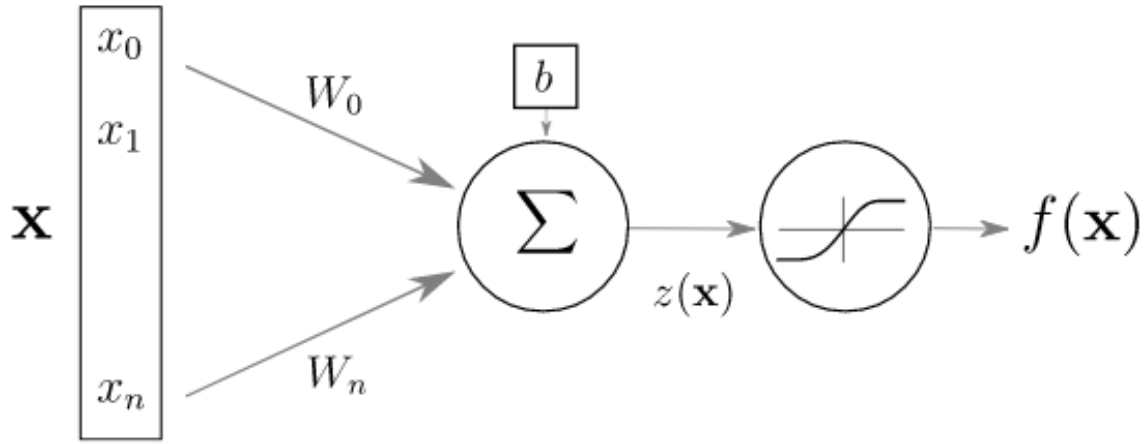
INTENDED TO BE A MACHINE (NOT AN ALGORITHM)



it had an array of 400 photocells, randomly connected to the "neurons". Weights were encoded in potentiometers, and weight updates during learning were performed by electric motors



TODAY'S ARTIFICIAL NEURON



$$z(\vec{x}) = \vec{W}.\vec{x} + b \qquad f(\vec{x}) = g(\vec{W}.\vec{x} + b)$$

Pre-Activation

Weights

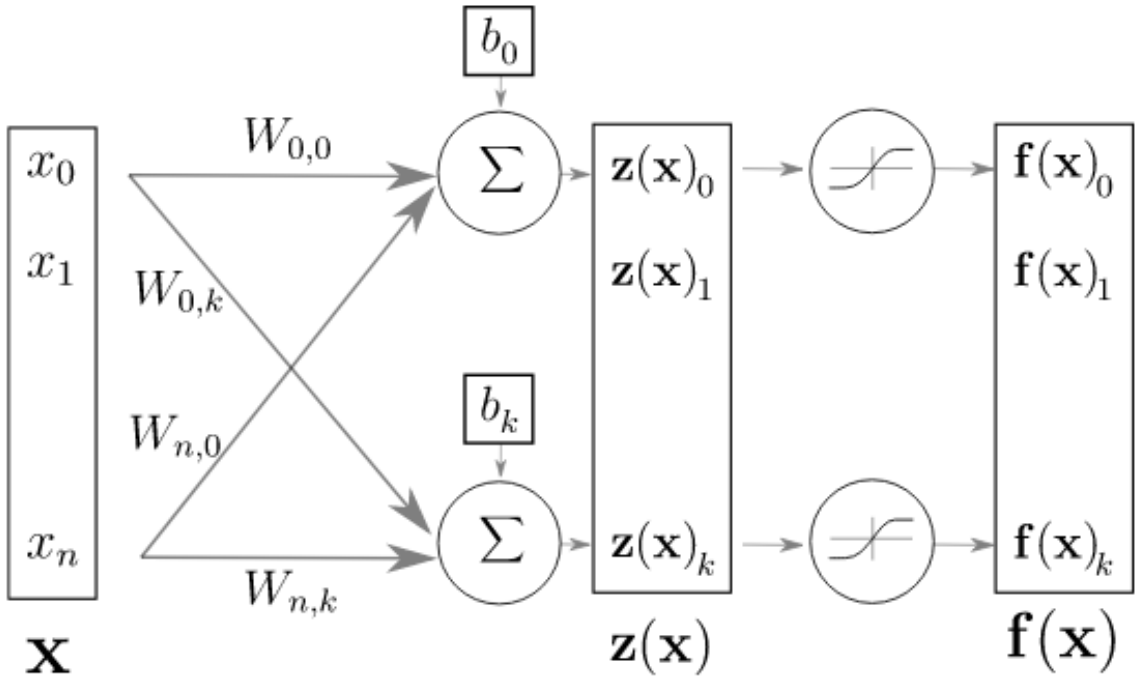
Input

Bias

Output

Activation Function

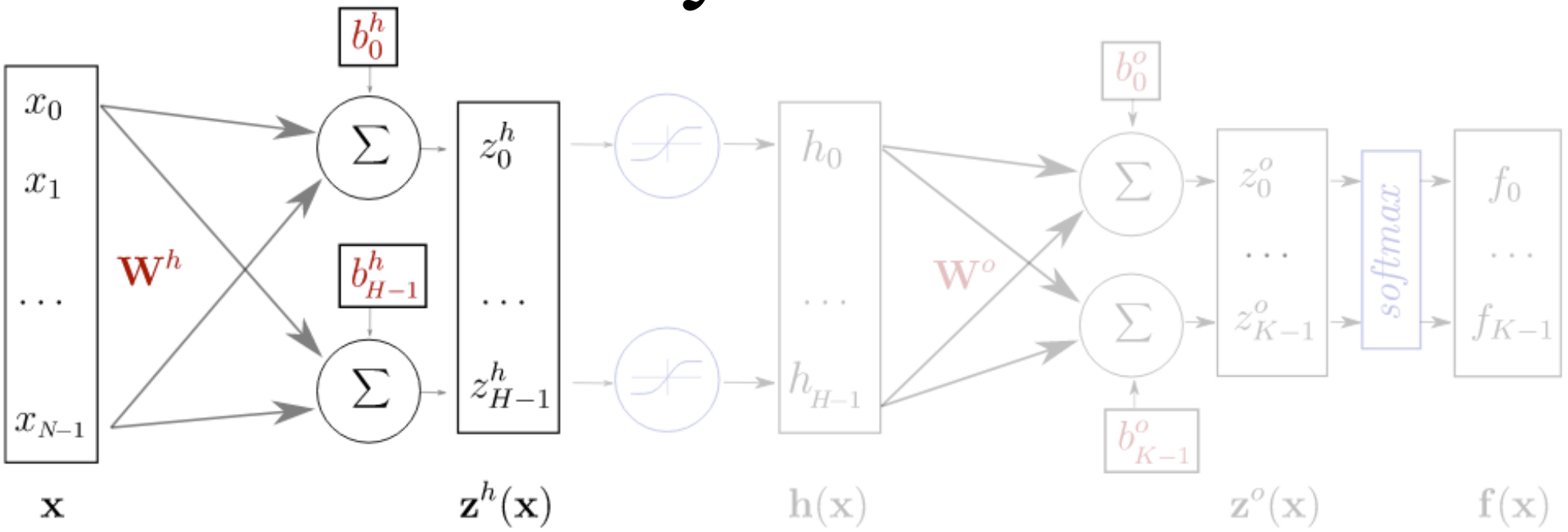
LAYER OF NEURONS



$$f(\vec{x}) = g(\mathbf{W}.\vec{x} + \vec{b})$$

SAME IDEA. NOW **W** becomes a matrix and **b** a vector

Hidden Layers of Neurons

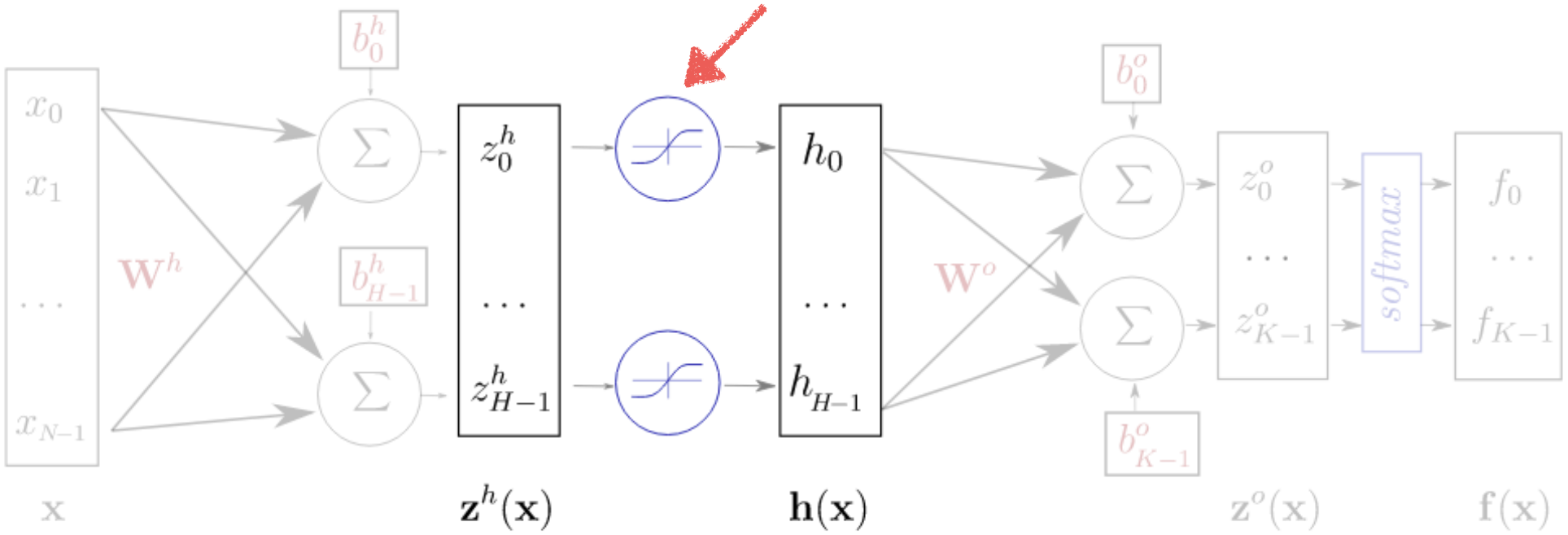


FIRST LAYER

INPUT

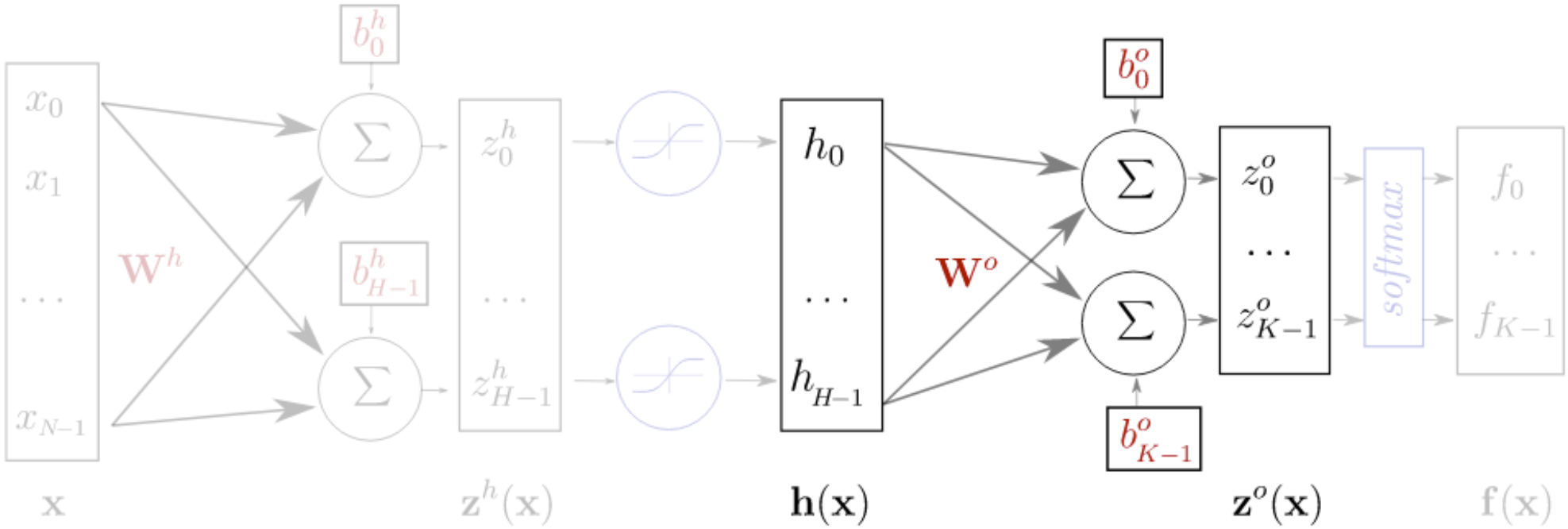
$$z^h(x) = W^h x + b^h$$

ACTIVATION FUNCTION



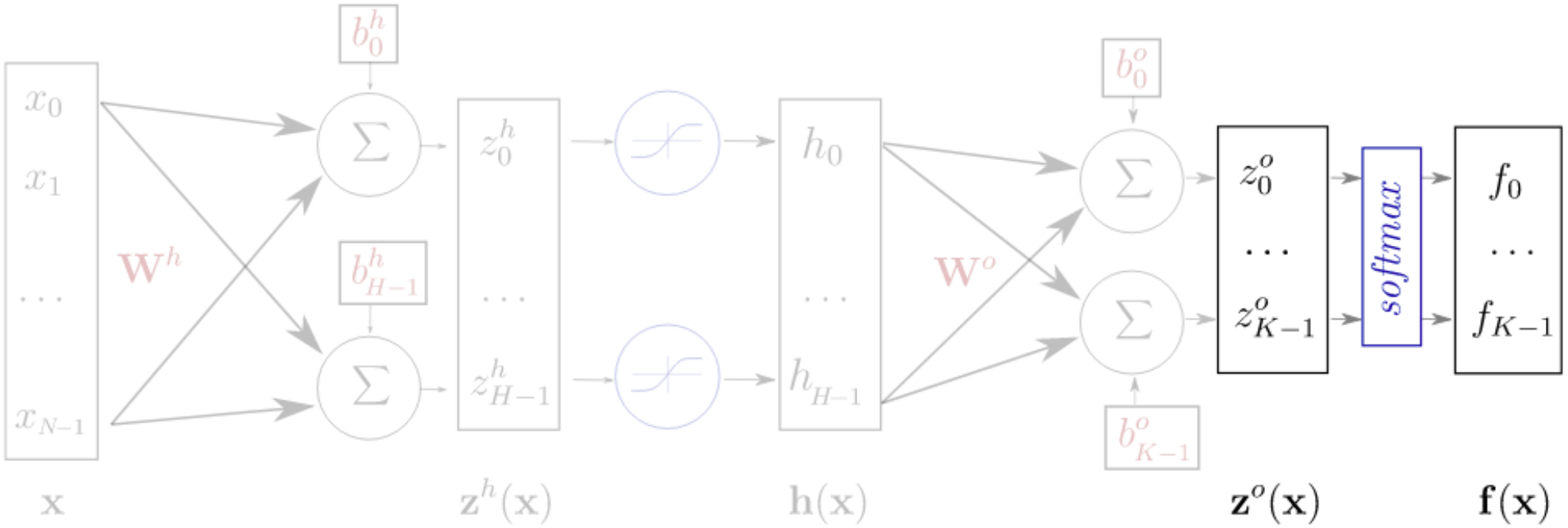
HIDDEN LAYER

$$h(x) = g(z^h(x)) = g(W^h x + b^h)$$



OUTPUT LAYER

$$z^0(\mathbf{x}) = W^0 h(\mathbf{x}) + b^0$$



PREDICTION LAYER

$$f(\mathbf{x}) = softmax(\mathbf{z^0})$$

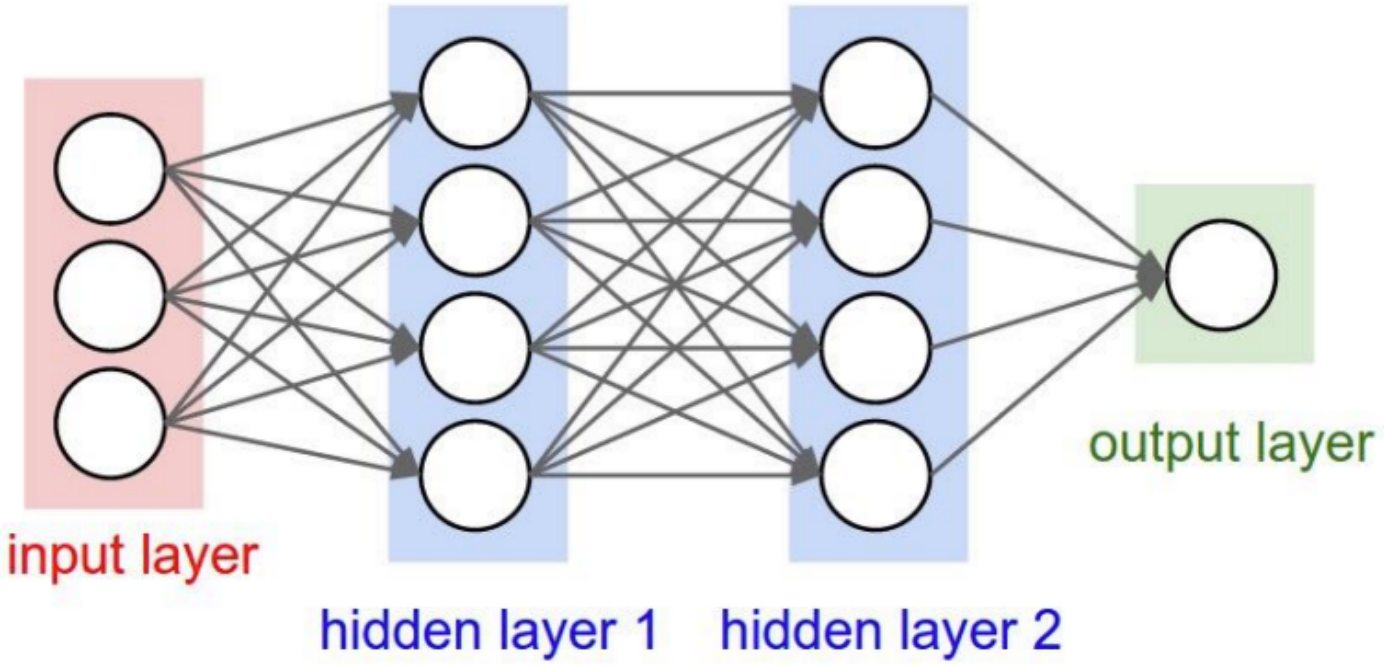
“CLASSICAL” MACHINE LEARNING

$$f_{\vec{W}}(\vec{x}) = \vec{y}$$

LABEL

Q , SF

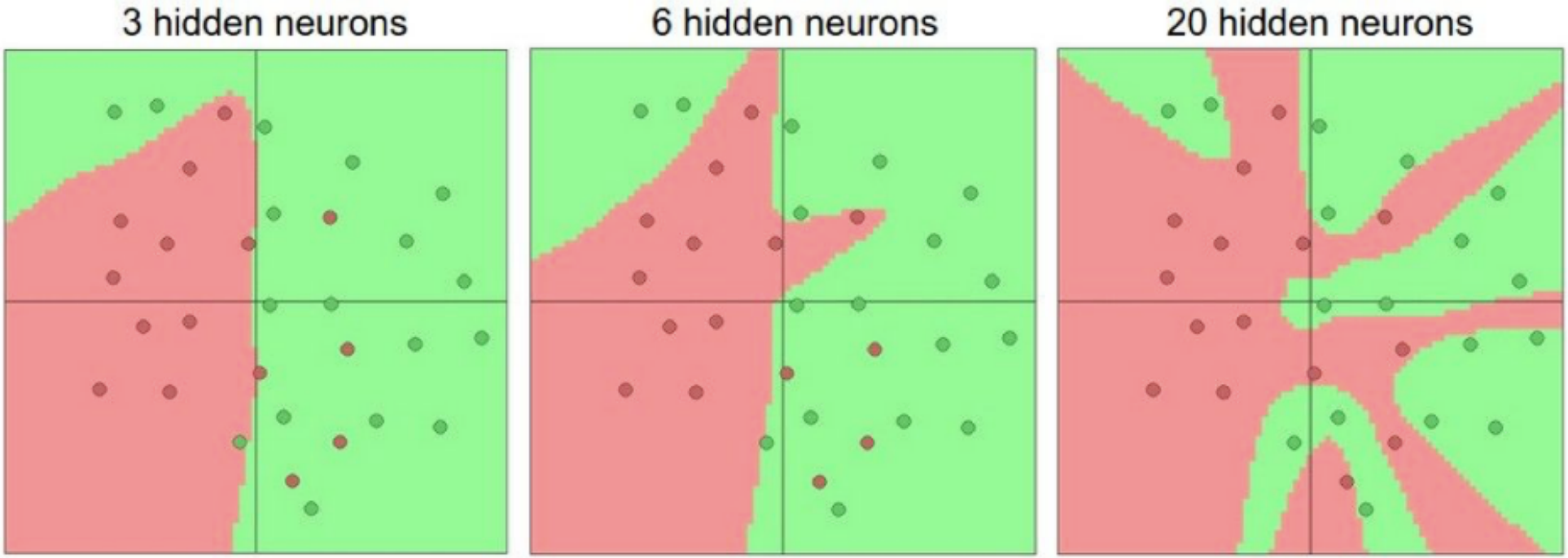
REPLACE THIS BY A GENERAL NON LINEAR FUNCTION WITH SOME PARAMETERS W



$$p = g_3(W_3 g_2(W_2 g_1(W_1 \vec{x_0})))$$

NETWORK FUNCTION

WHY HIDDEN LAYERS?



More complex functions allow increasing complexity

Credit: Karpathy

SO LET’S GO DEEPER AND DEEPER!

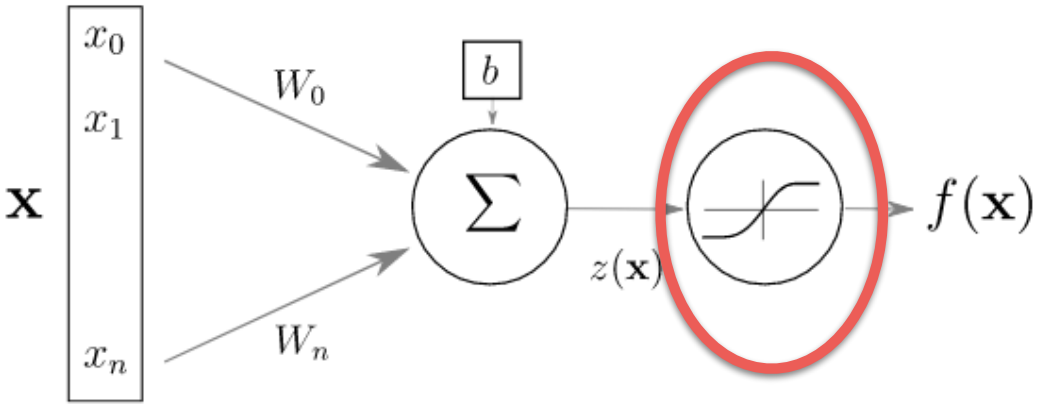
SO LET’S GO DEEPER AND DEEPER!

YES BUT…

NOT SO STRAIGHTFORWARD, DEEPER MEANS MORE WEIGHTS, MORE DIFFICULT OPTIMIZATION, RISK OF OVERFITTING…

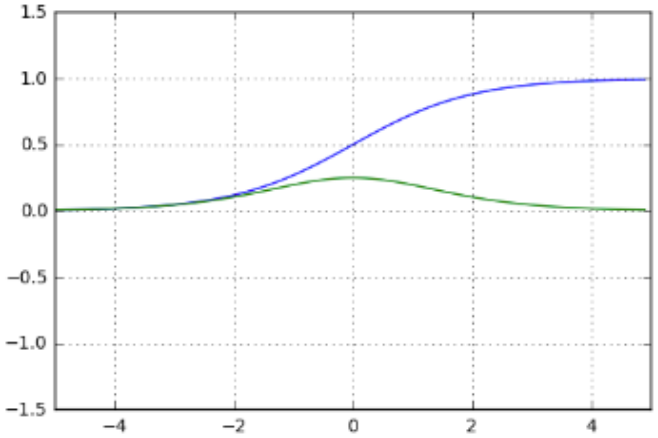
LET’S FIRST EXAMINE IN MORE DETAIL HOW SIMPLE “SHALLOW” NETWORKS WORK

ACTIVATION FUNCTIONS?



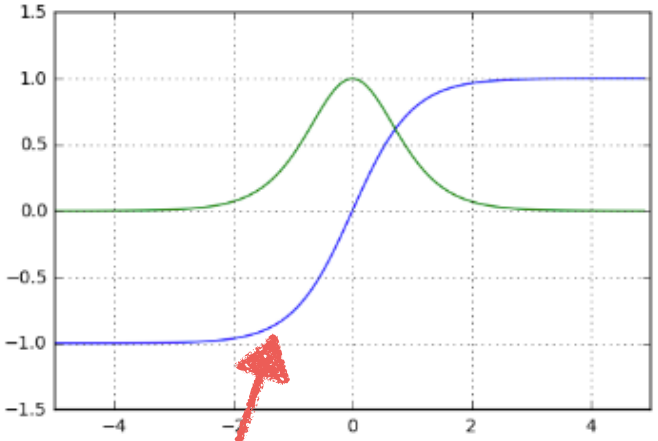
ADD NON LINEARITIES TO THE PROCESS

ACTIVATION FUNCTIONS



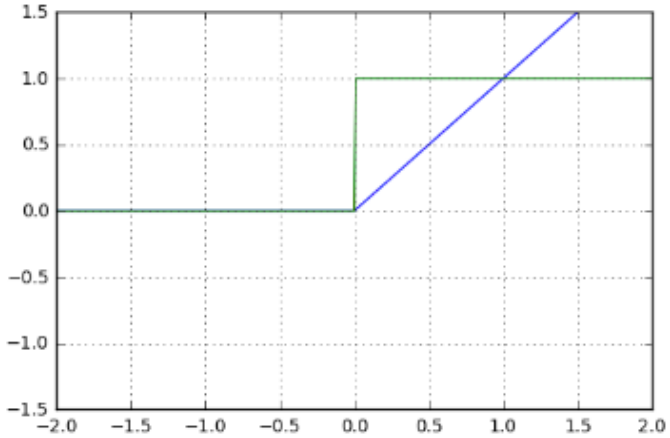
$$\text{sigm}(x) = \frac{1}{1+e^{-x}}$$

$$\text{sigm}'(x) = \text{sigm}(x)(1-\text{sigm}(x))$$



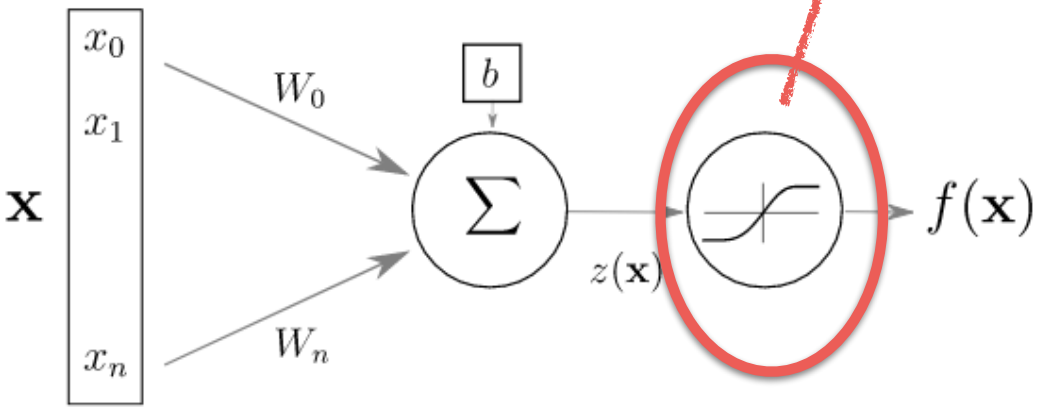
$$\tanh(x) = \frac{e^{2x}-1}{e^{2x}+1}$$

$$\tanh'(x) = 1-\tanh(x)^2$$



$$\text{relu}(x) = \max(0,x)$$

$$\text{relu}'(x) = 1_{x>0}$$



SOFTMAX

A generalization of the SIGMOID ACTIVATION

$$softmax(\mathbf{x}) = \frac{e^{\mathbf{x}}}{\sum_{i=1}^{n} e^{x_i}}$$

THE OUTPUT IS NORMALIZED BETWEEN 0 AND 1

THE COMPONENTS ADD TO 1

CAN BE INTERPRETED AS A PROBABILITY

$$p(Y = c|X = \mathbf{x}) = softmax(z(\mathbf{x}))_c$$

SOFTMAX

A generalization of the SIGMOID ACTIVATION

GENERALLY
USED AS ACTIVATION
OF LAST LAYER

(will come back later)

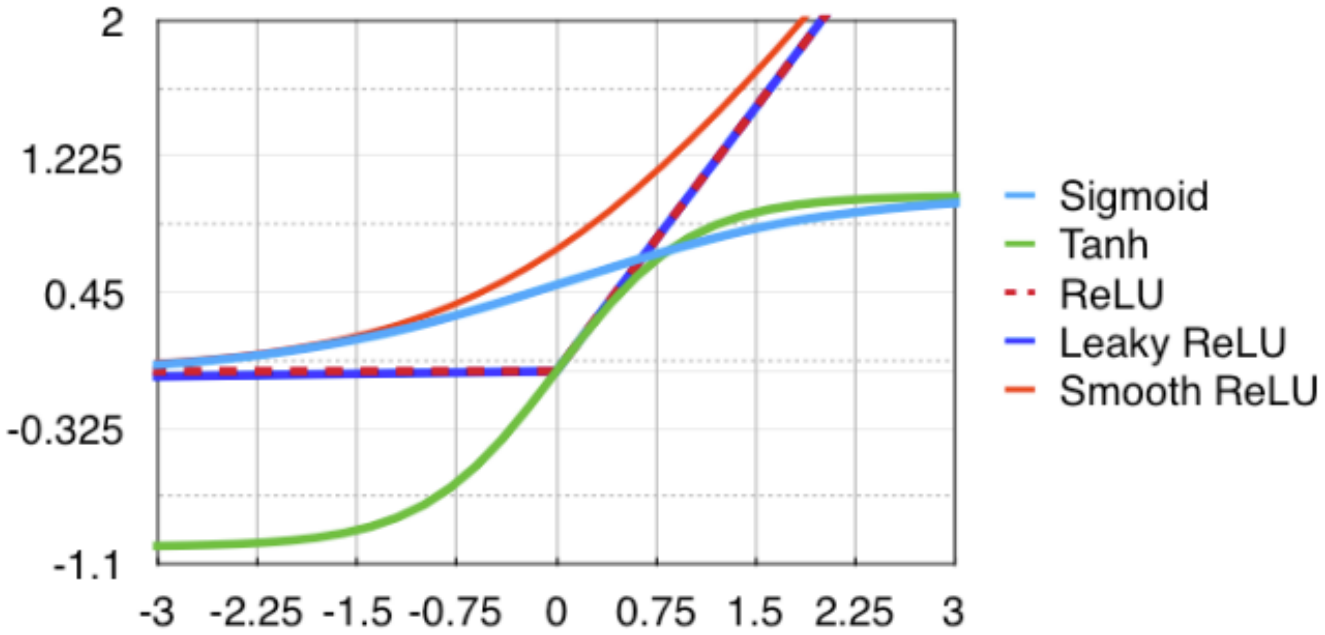
THE OUTP AND 1

THE COMPONENTS ADD TO 1

CAN BE INTERPRETED AS A PROBABILITY

$$p(Y = c|X = \mathbf{x}) = softmax(z(\mathbf{x}))_c$$

ACTIVATION FUNCTIONS



Sigmoid: $f(x) = \frac{1}{1+e^{-x}}$

Tanh: $f(x) = tanh(x)$

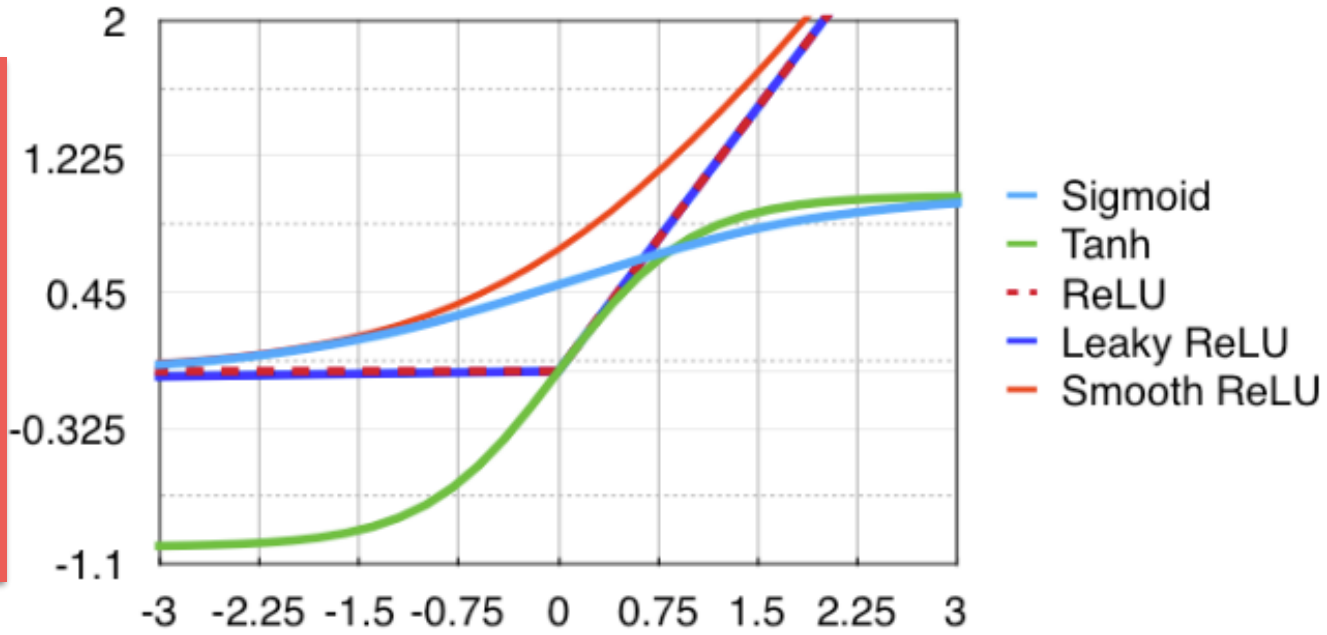
ReLu: $f(x) = max(0, x)$

Soft ReLu: $f(x) = log(1+e^{x})$

Leaky ReLu: $f(x) = \epsilon x + (1-\epsilon)max(0, x)$

ACTIVATION FUNCTIONS

+ MANY OTHERS!



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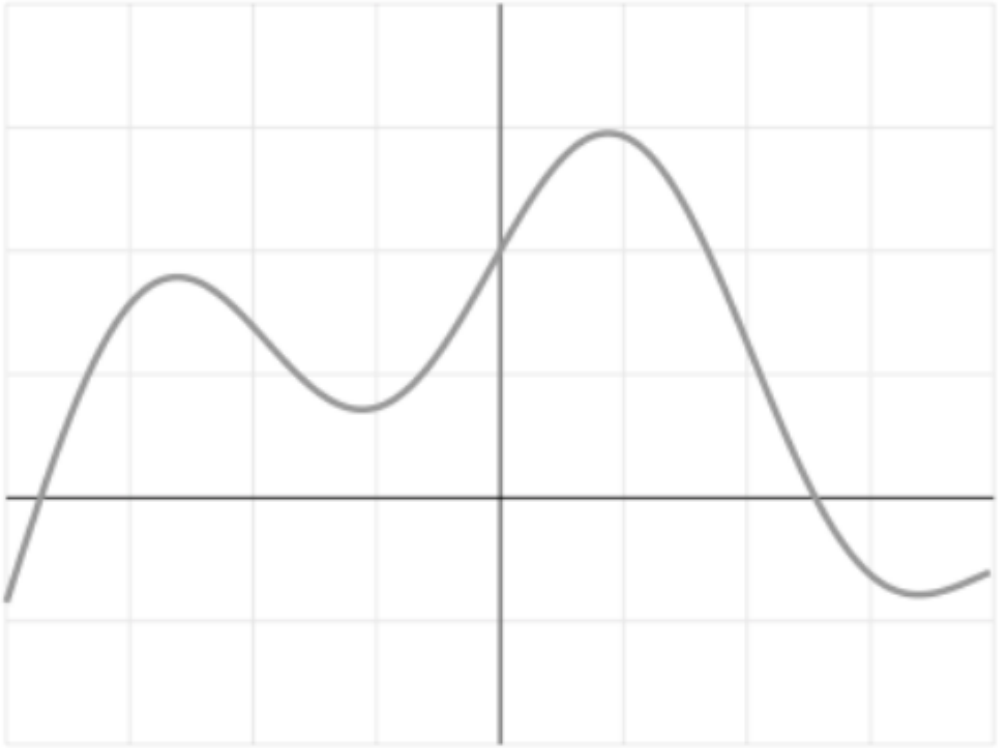
WHAT IS THE MEANING OF THE ACTIVATION FUNCTION?



Any real function in a interval (a,b) can be approximated with a linear combination of translated and scaled ReLu functions

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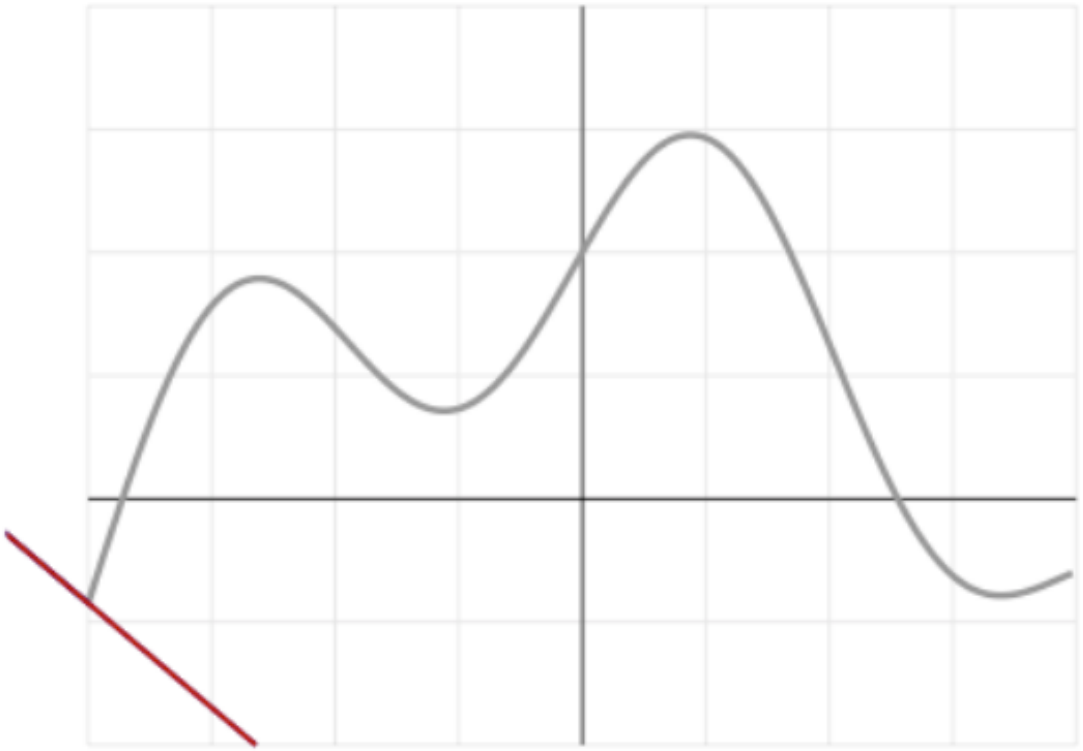

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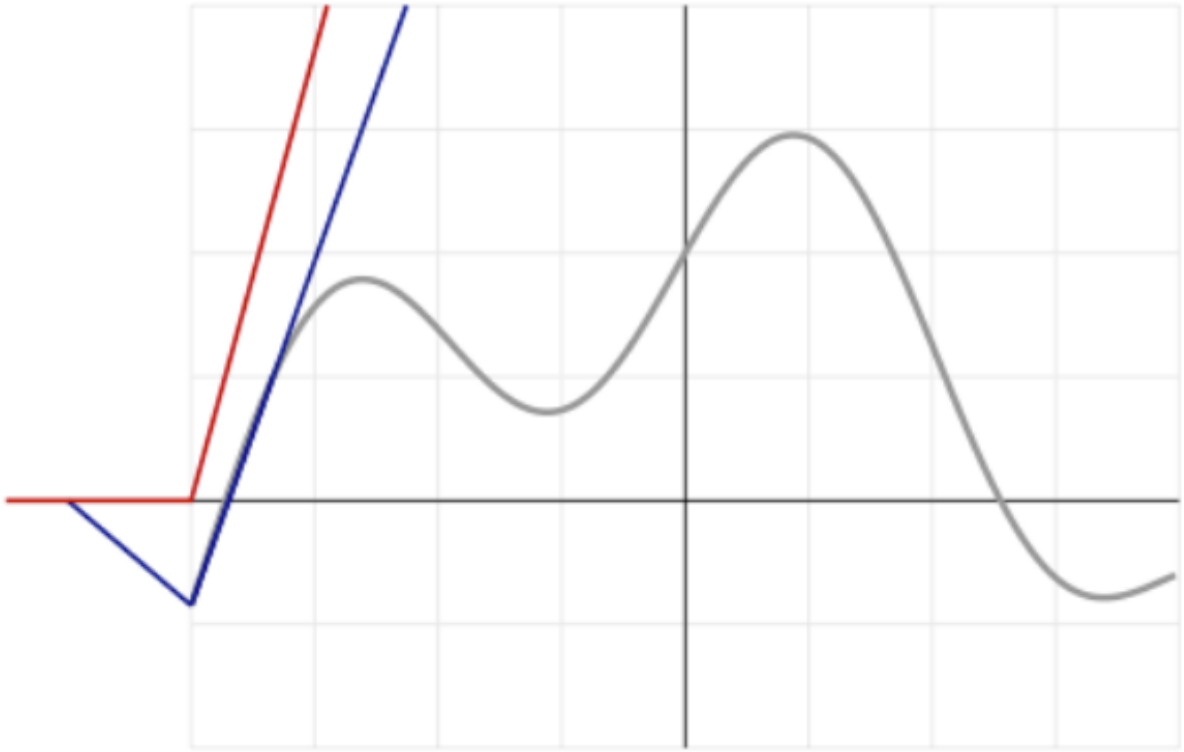

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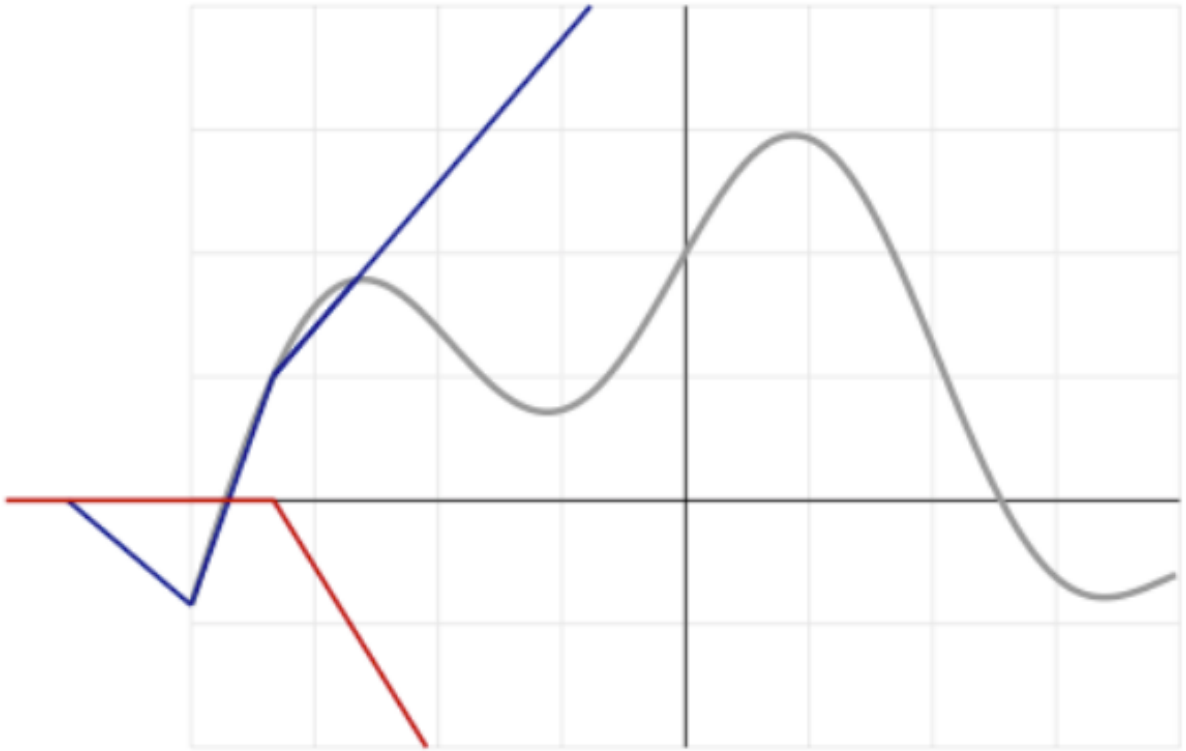

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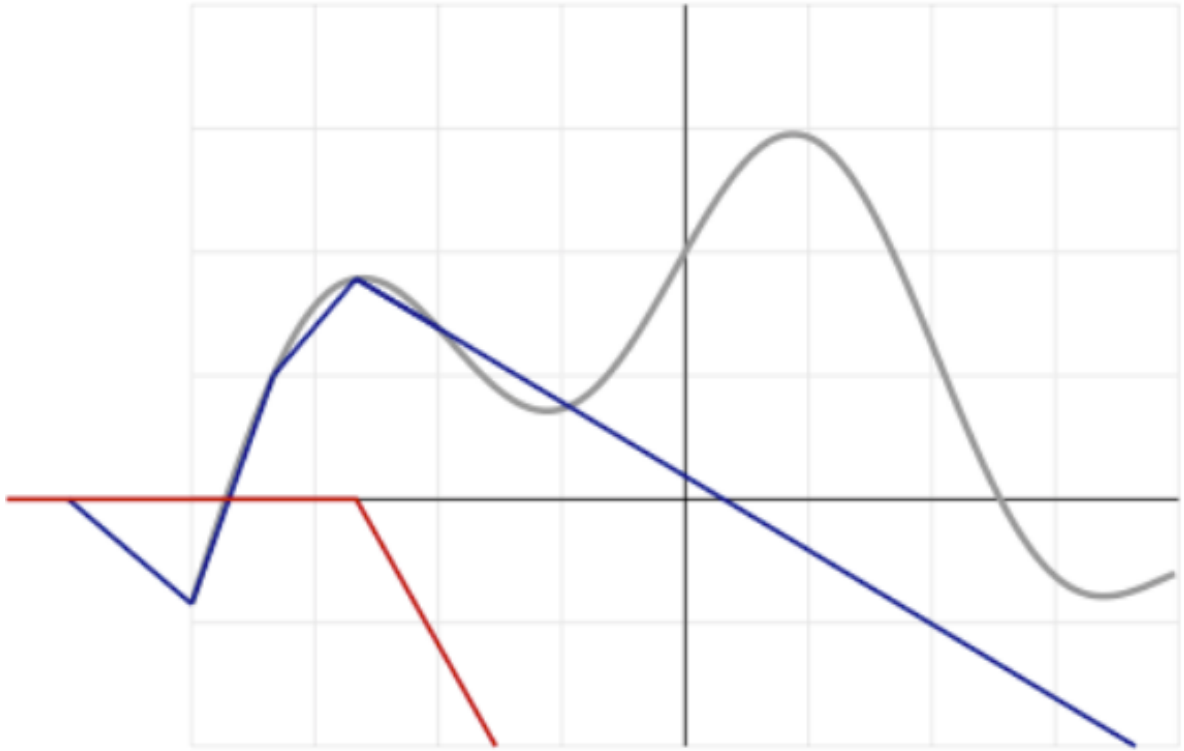

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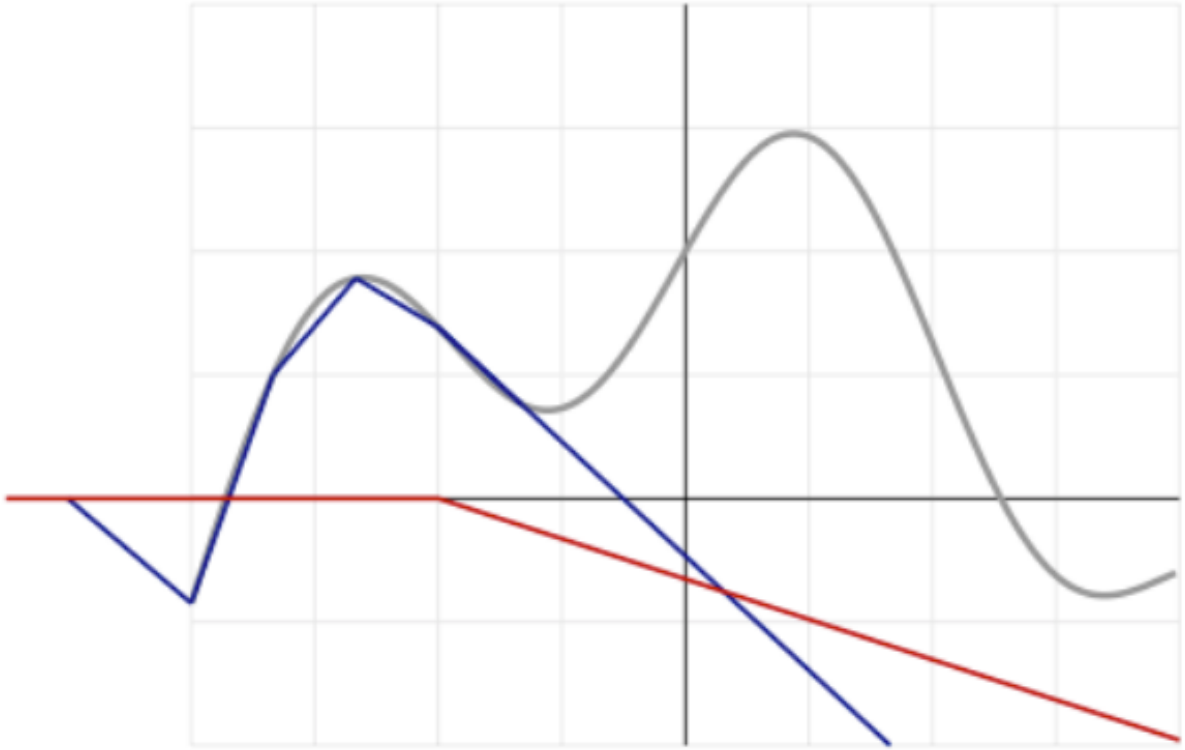

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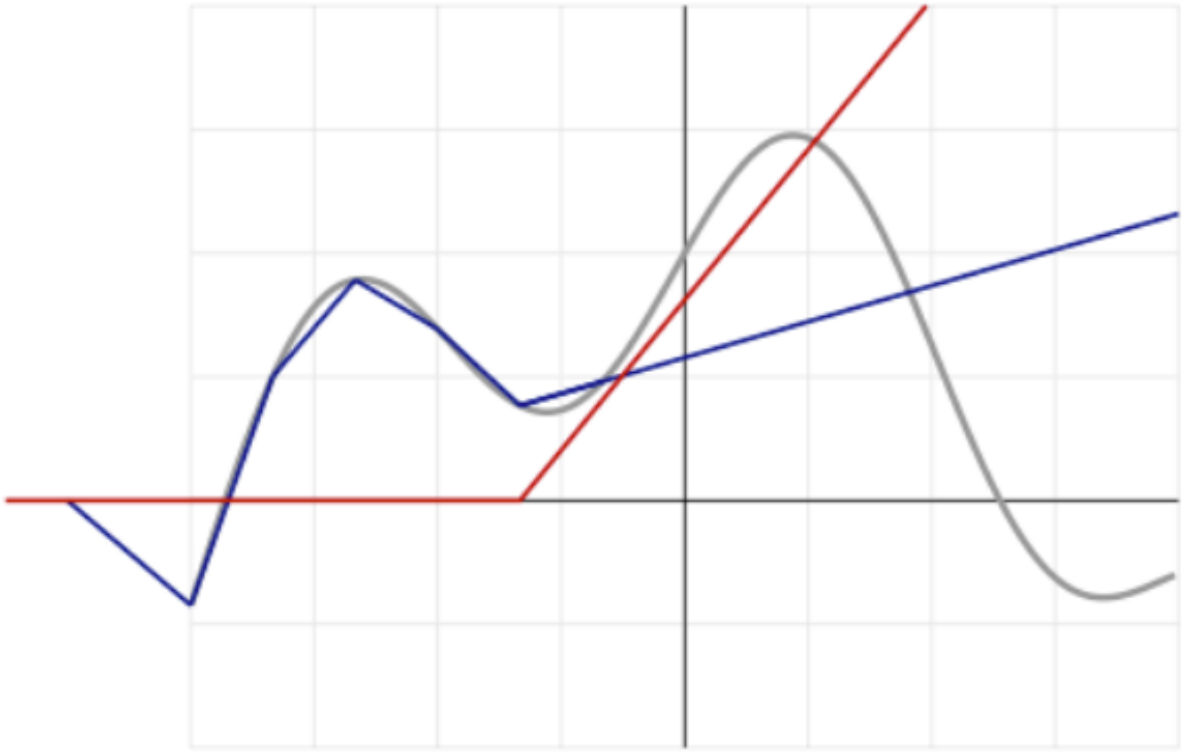

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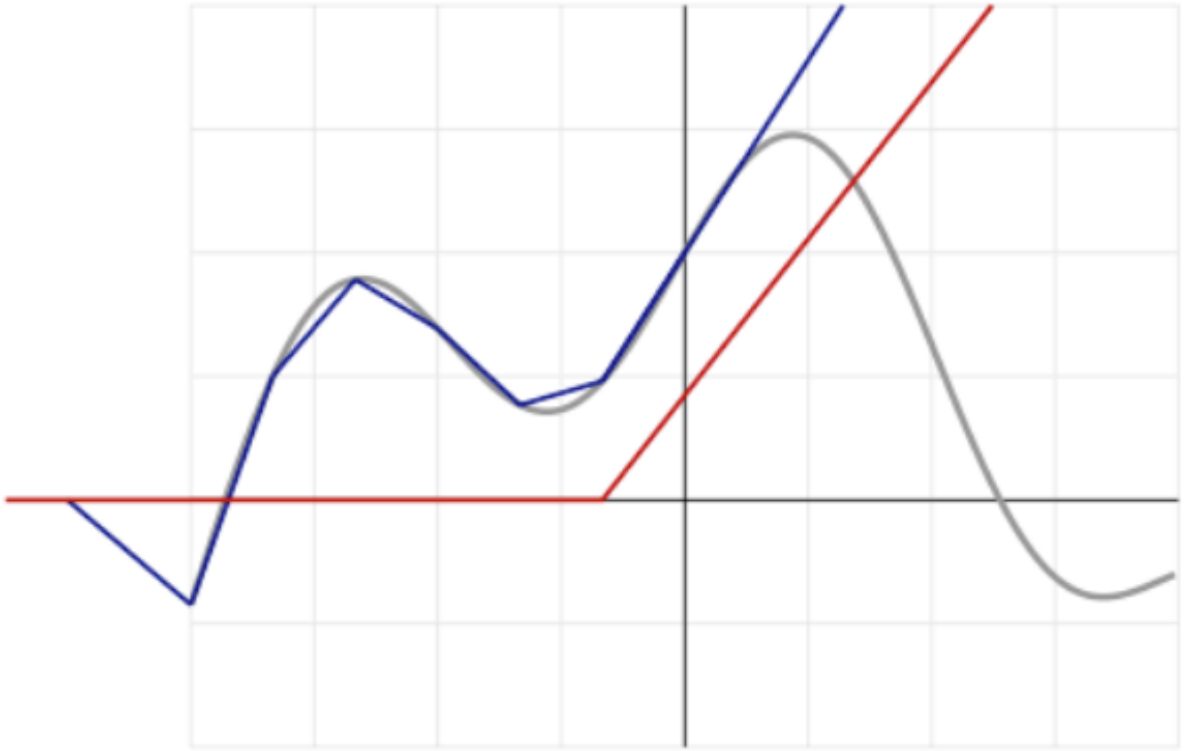

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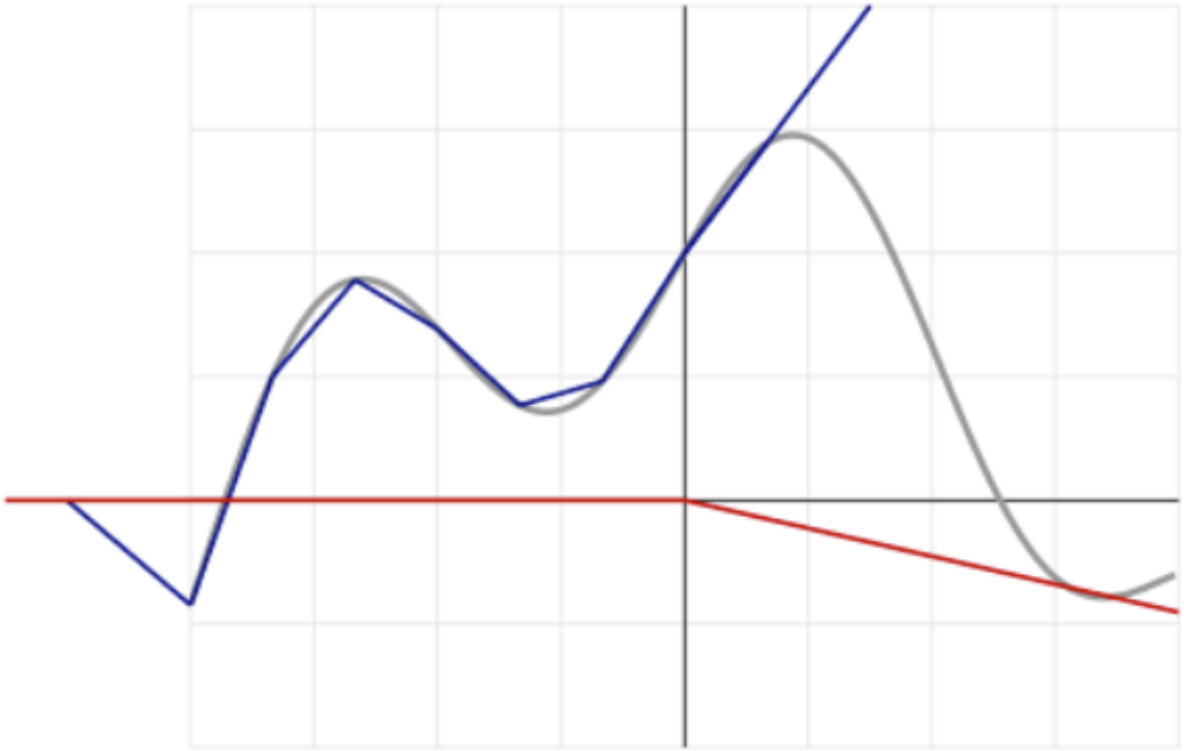

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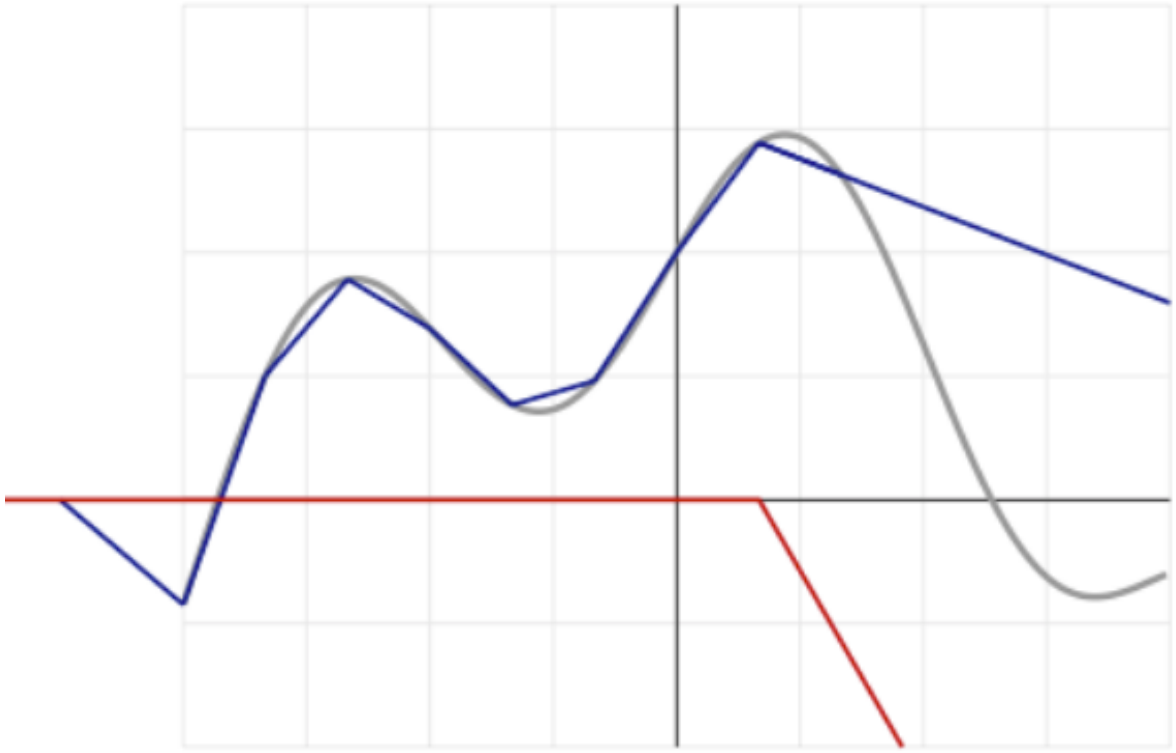

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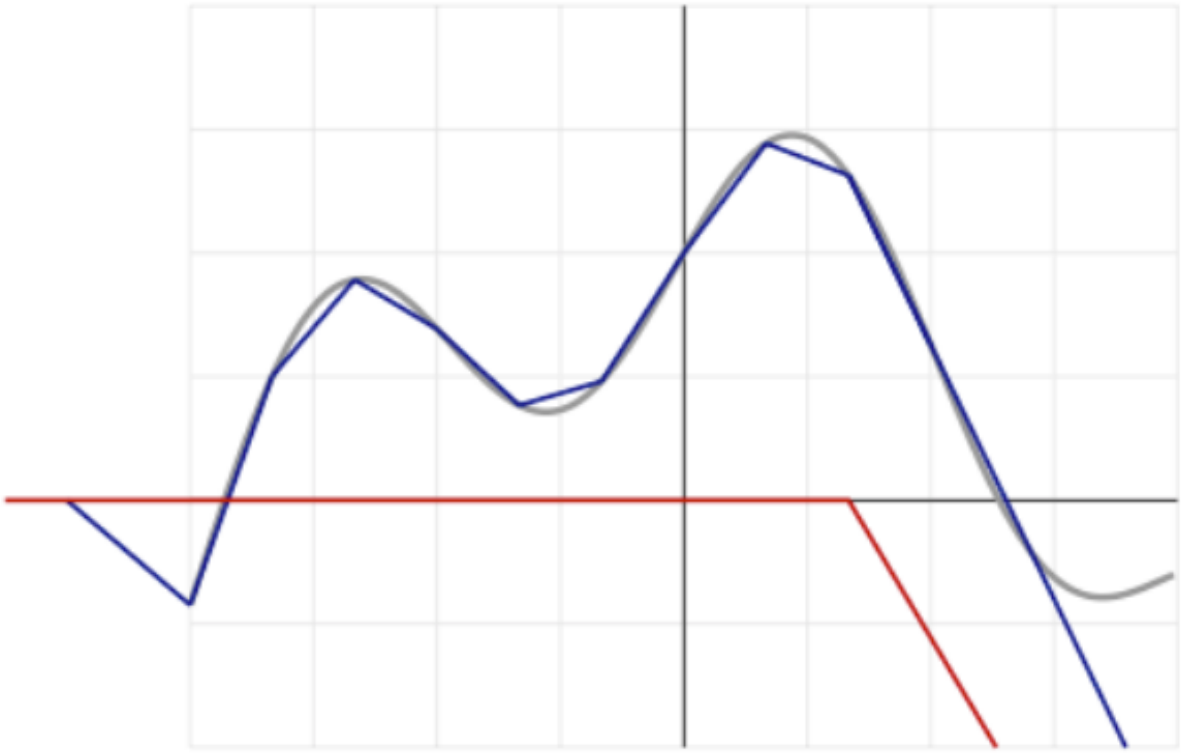

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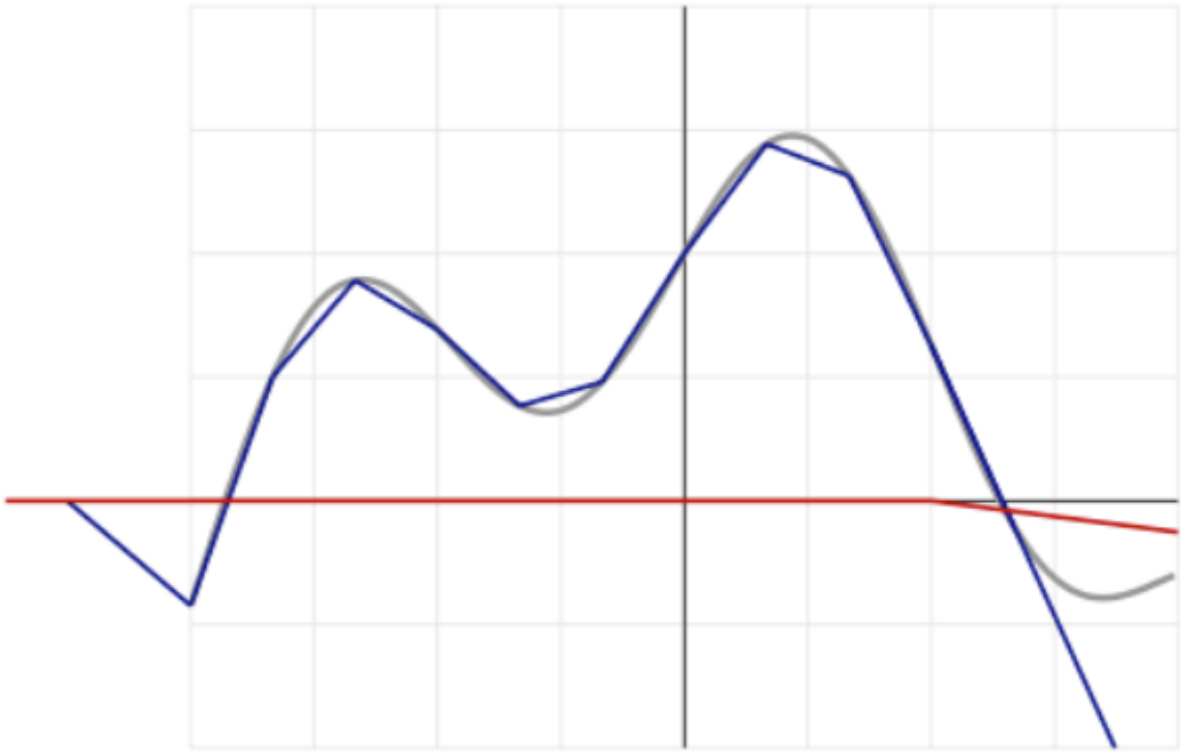

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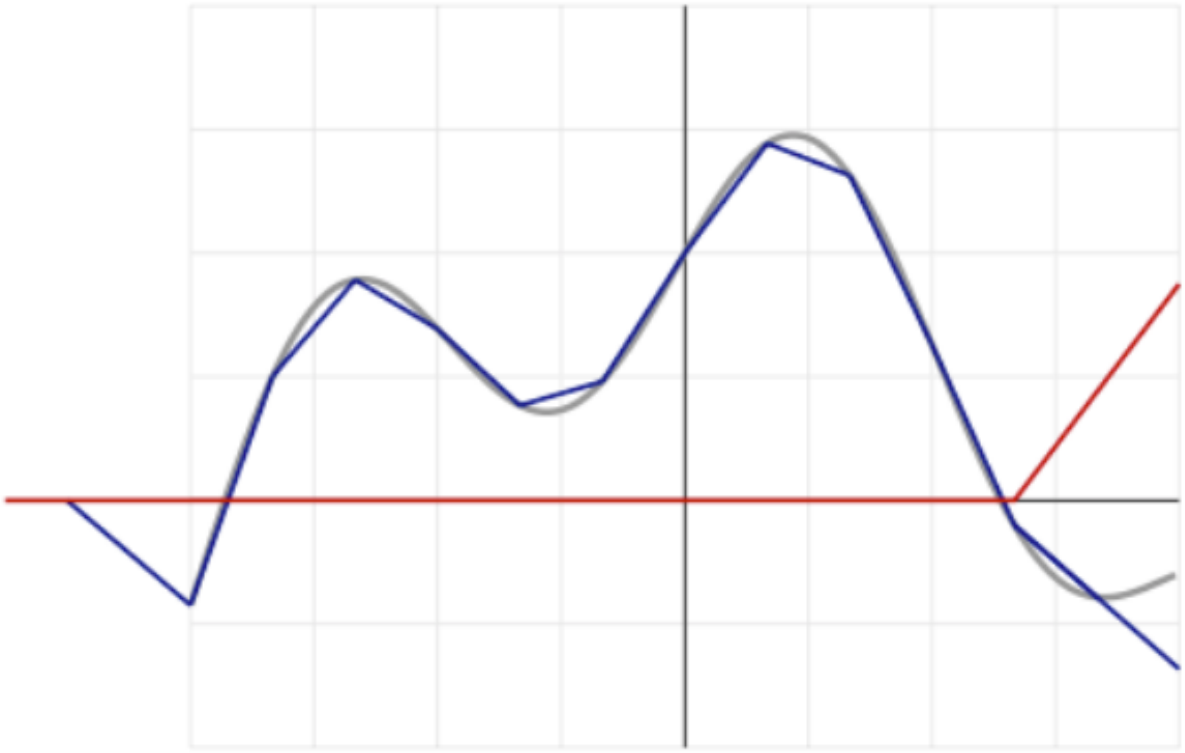

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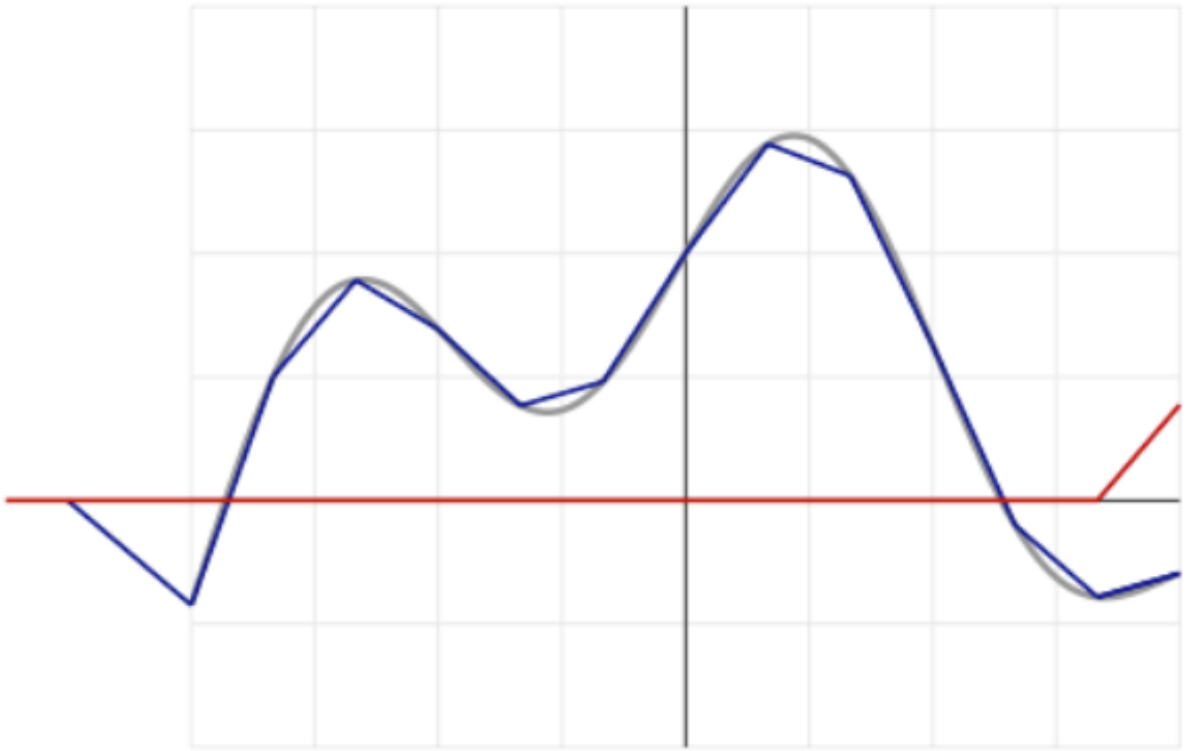

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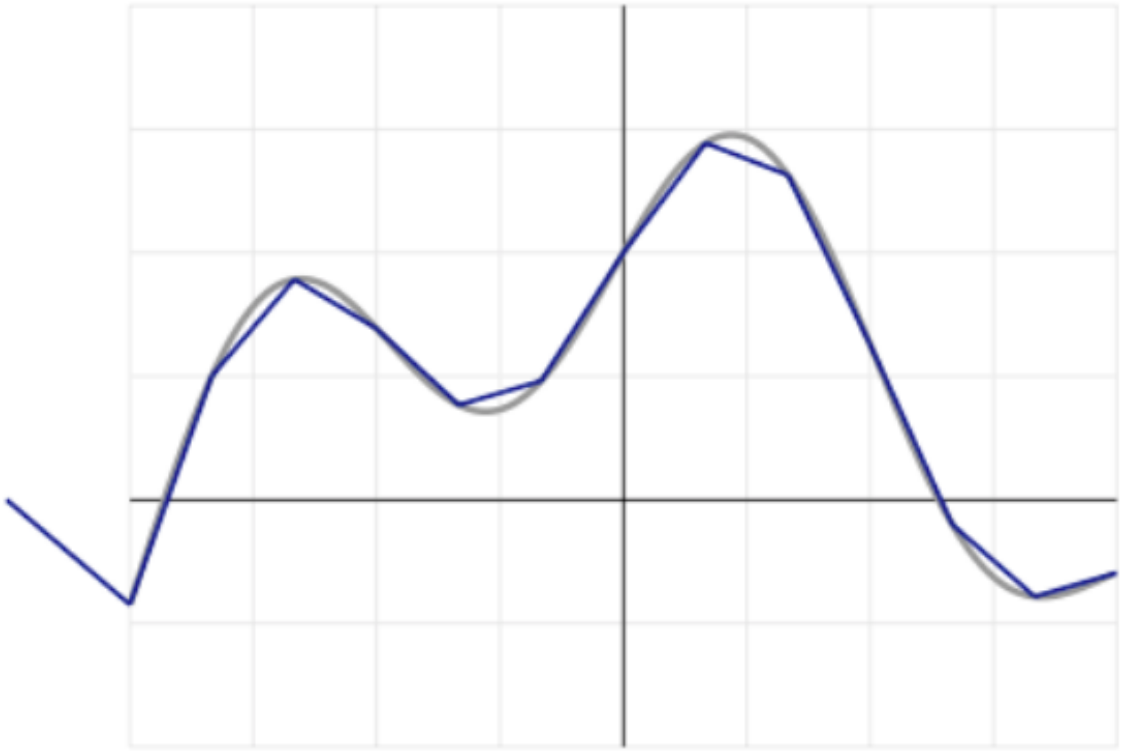

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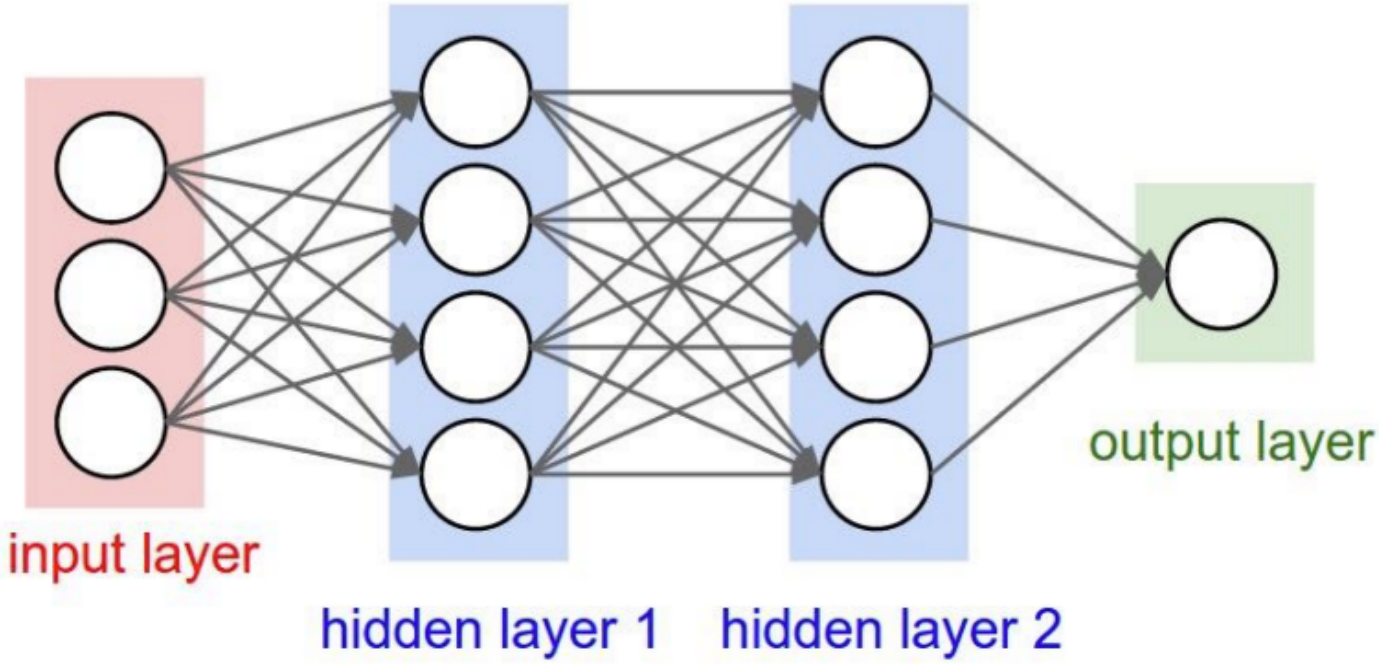
OK, SO NOW LET'S FIND THE WEIGHTS

OPTIMIZATION

[OR HOW TO FIND THE WEIGHTS?]

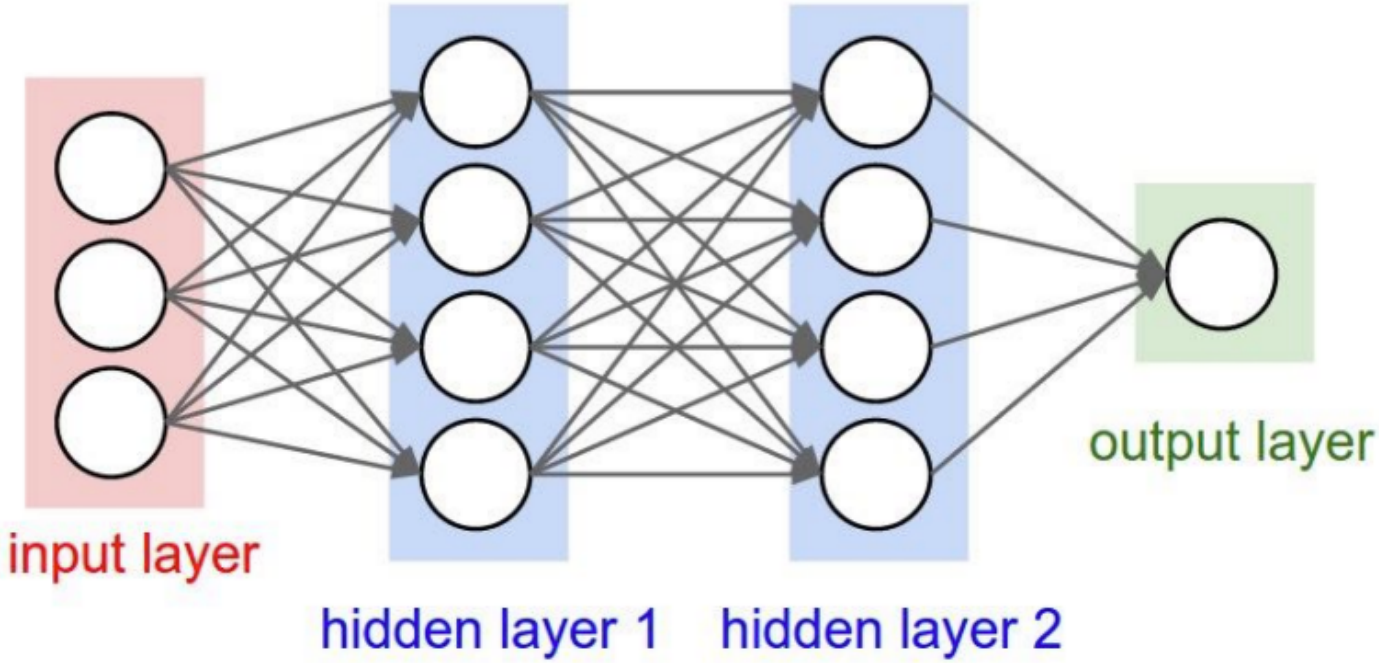


$$p = g_3(W_3 g_2(W_2 g_1(W_1 \vec{x_0})))$$

NETWORK FUNCTION

OPTIMIZATION

[OR HOW TO FIND THE WEIGHTS?]



$$p = g_3(W_3 g_2(W_2 g_1(W_1 \vec{x_0})))$$

$$\frac{1}{N}\sum_{i=1}^{N}(y_i - p_i)^2$$

LOSS FUNCTION

WE SIMPLY WANT TO MINIMIZE THE LOSS FUNCTION WITH RESPECT TO THE WEIGHTS, i.e. FIND THE WEIGHTS THAT GENERATE THE MINIMUM LOSS

WE SIMPLY WANT TO MINIMIZE THE LOSS FUNCTION WITH RESPECT TO THE WEIGHTS, i.e. FIND THE WEIGHTS THAT GENERATE THE MINIMUM LOSS

WE THEN USE STANDARD MINIMIZATION ALGORITHMS THAT YOU ALL KNOW…

FOR EXAMPLE….

Gradient Descent

$$W_{t+1} = W_t - \lambda_t \nabla f(W_t)$$

[gradient]

Newton

$$W_{t+1} = W_t - \lambda [Hf(W_t)]^{-1} \nabla f(W_t)$$

[hessian]

NEWTON CONVERGES FASTER…

FOR EXAMPLE….

Gradient Descent

$$W_{t+1} = W_t - \lambda_t \nabla f(W_t)$$

[gradient]

Newton

$$W_{t+1} = W_t - \lambda [Hf(W_t)]^{-1} \nabla f(W_t)$$

[hessian]

NEWTON CONVERGES FASTER…

BUT NEEDS THE HESSIAN

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial W_1^2} & \frac{\partial^2 f}{\partial W_1 \, \partial W_2} & \cdots & \frac{\partial^2 f}{\partial W_1 \, \partial W_n} \\ \frac{\partial^2 f}{\partial W_2 \, \partial W_1} & \frac{\partial^2 f}{\partial W_2^2} & \cdots & \frac{\partial^2 f}{\partial W_2 \, \partial W_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial W_n \, \partial W_1} & \frac{\partial^2 f}{\partial W_n \, \partial W_2} & \cdots & \frac{\partial^2 f}{\partial W_n^2} \end{bmatrix}$$

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MOST USED BY FAR….

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FOR EXAMPLE….

Gradient Descent

$$W_{t+1} = W_t - \lambda_t \nabla f(W_t)$$

[gradient]

EVERYTHING RELIES
ON COMPUTING THE GRADIENT

MOST USED BY FAR….

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[hessian]

NEWTON CONVERGES FASTER…

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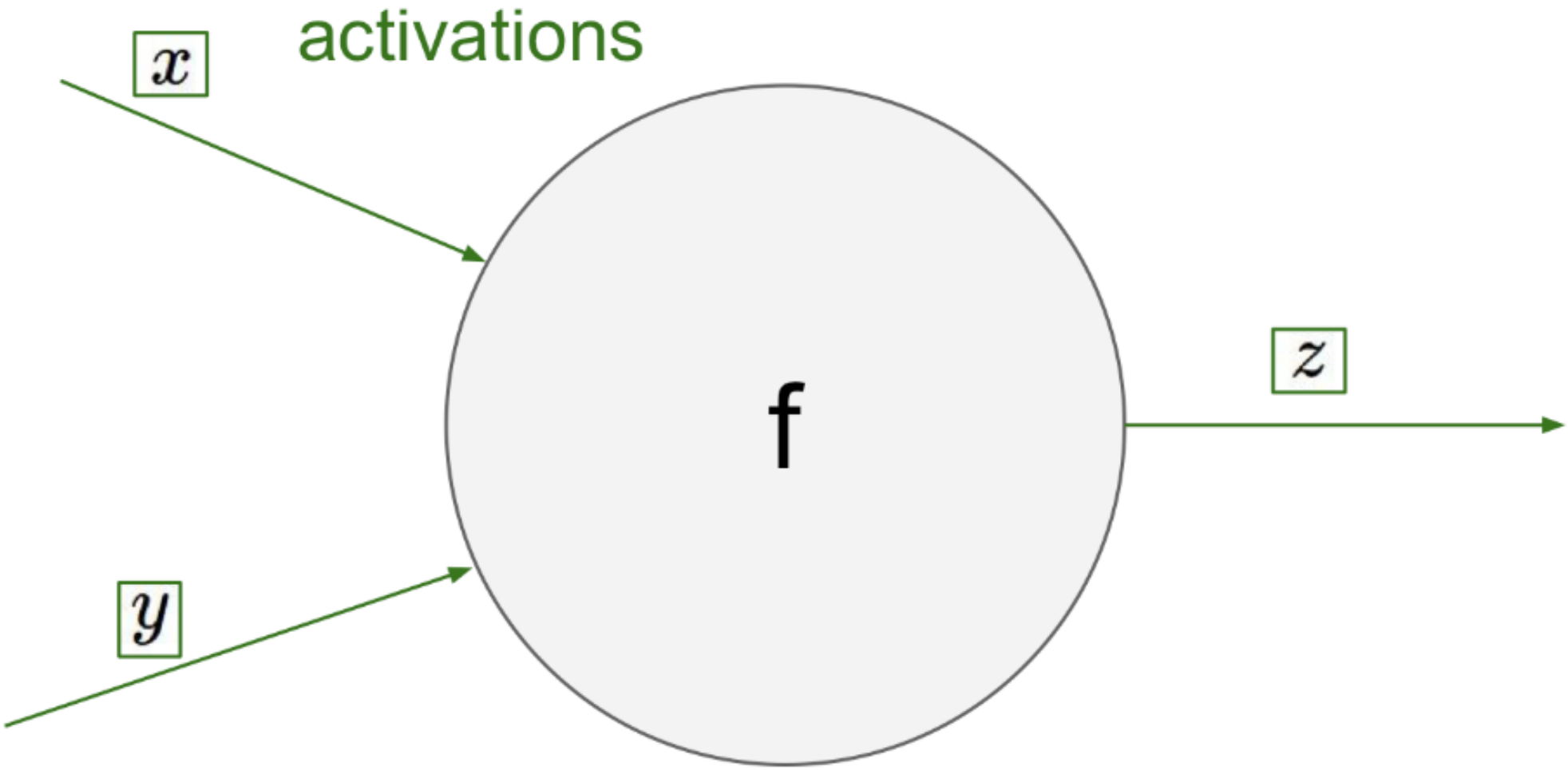
NICE, BUT I NEED TO COMPUTE TE GRADIENT AT EVERY ITERATION OF AN ARBITRARY COMPLEX FUNCTION!

BACKPROPAGATION

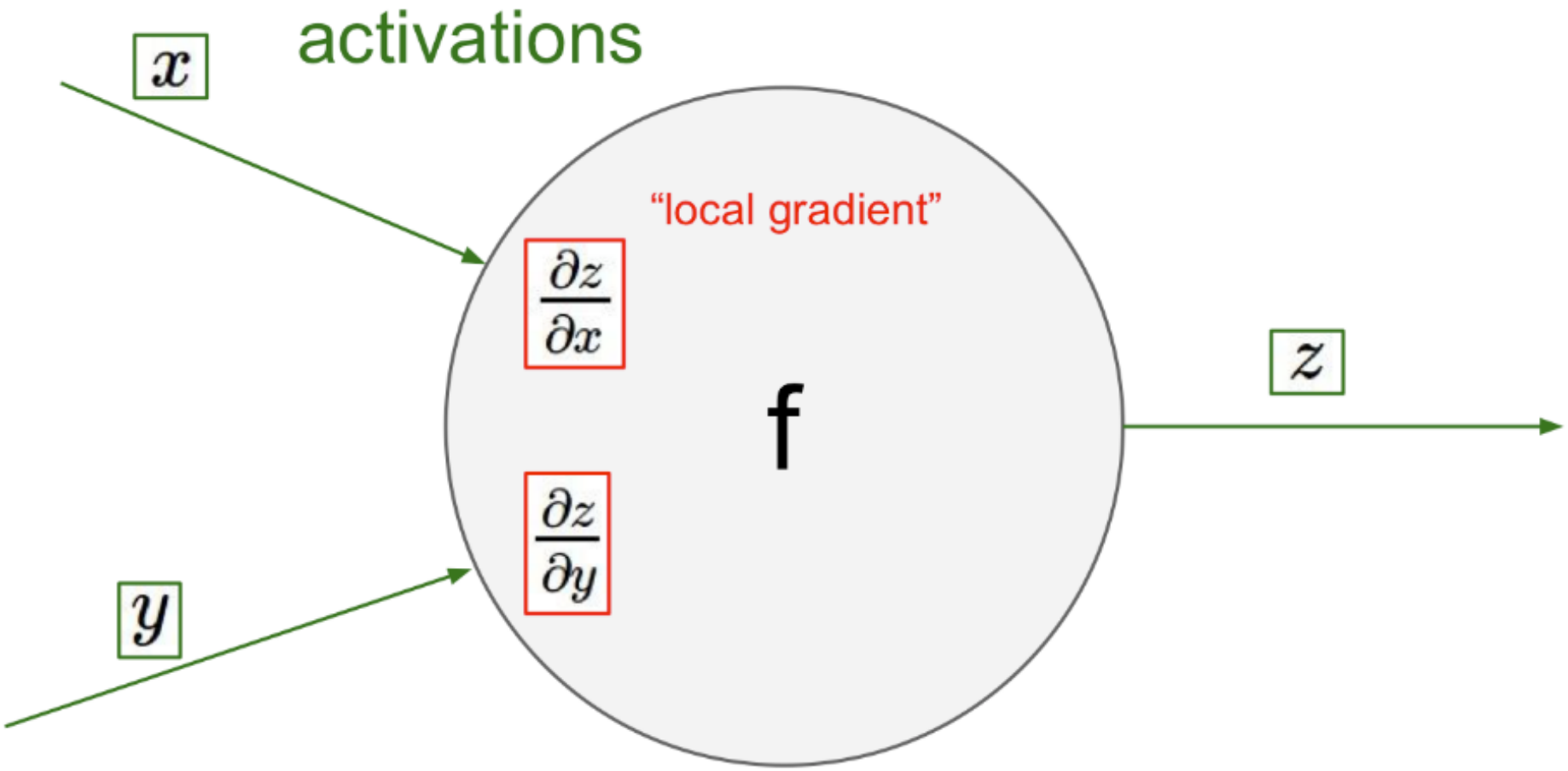
[AT THE NEURON LEVEL]



Credit: A. Karpathy

BACKPROPAGATION

[AT THE NEURON LEVEL]



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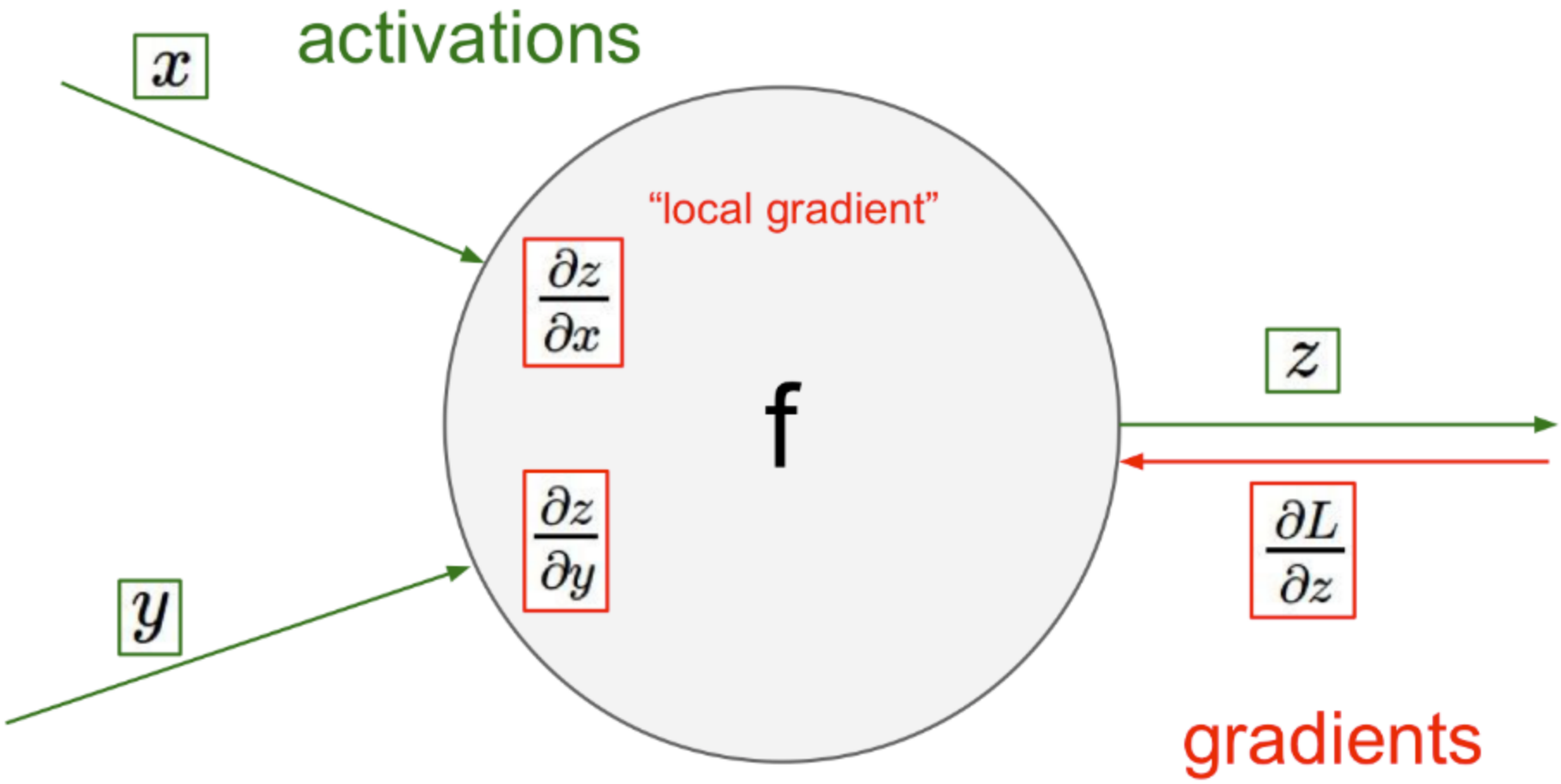
BACKPROPAGATION

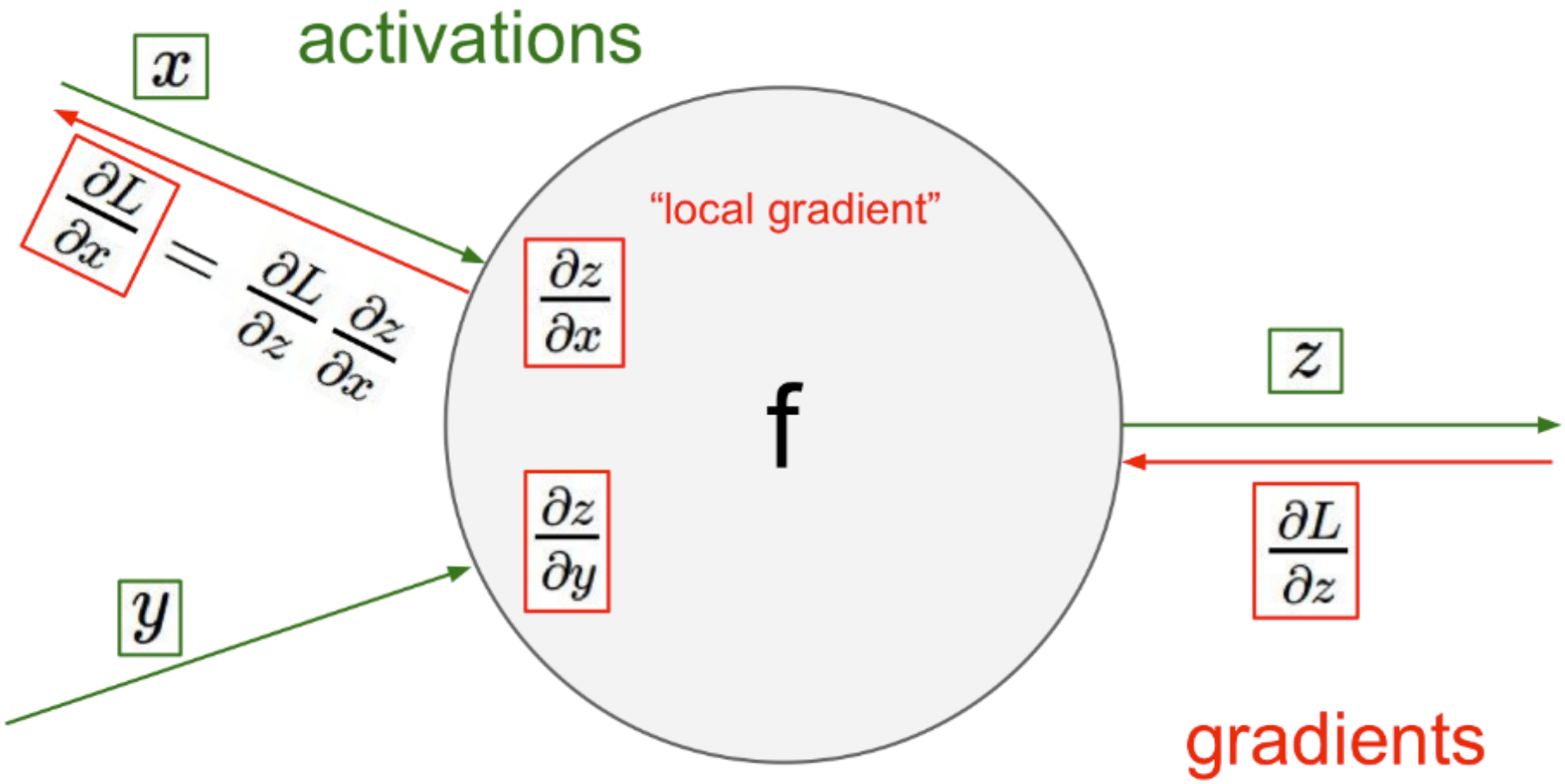
[AT THE NEURON LEVEL]



Credit: A. Karpathy

BACKPROPAGATION

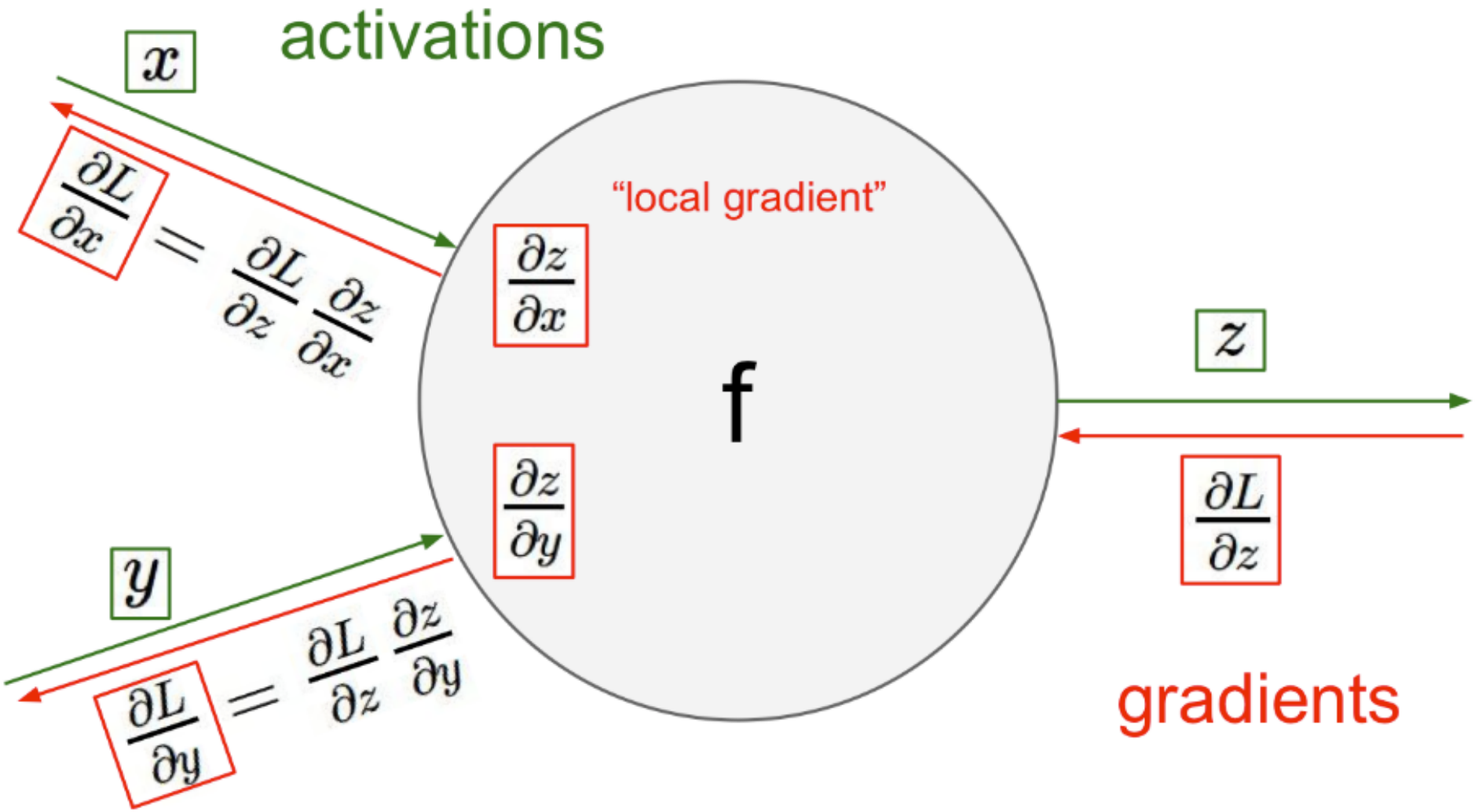
[AT THE NEURON LEVEL]



Credit: A. Karpathy

BACKPROPAGATION

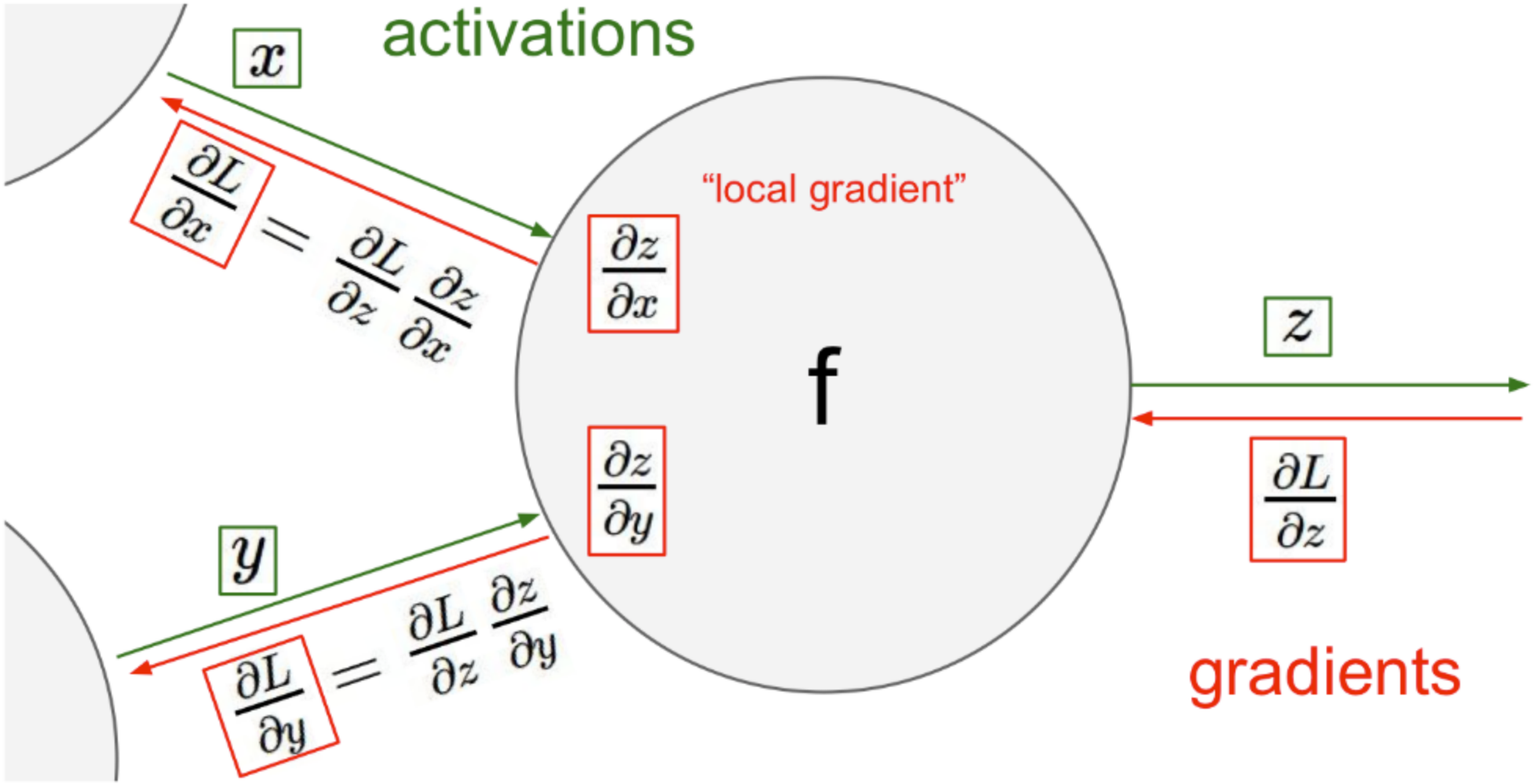
[AT THE NEURON LEVEL]



Credit: A. Karpathy

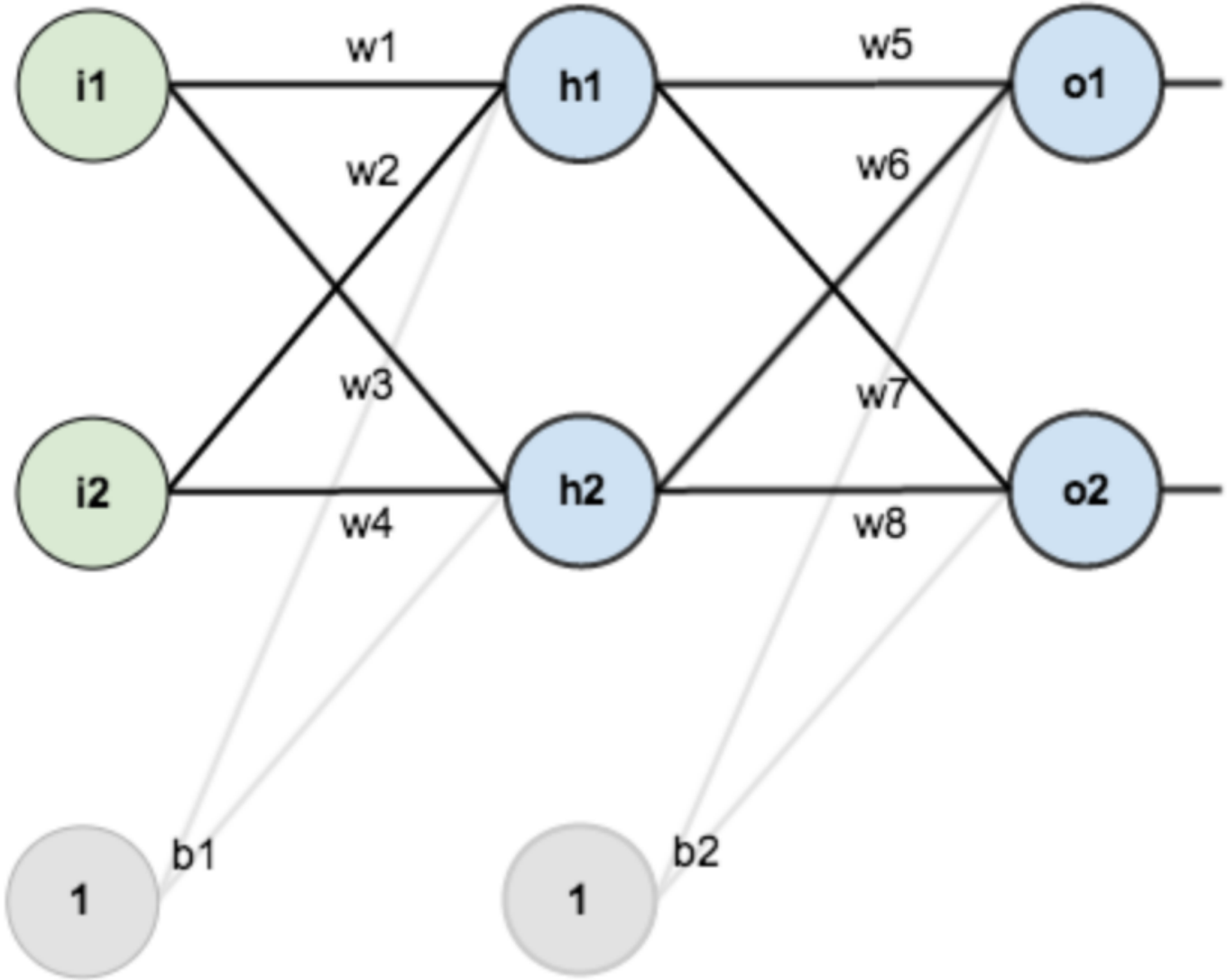
BACKPROPAGATION

[AT THE NEURON LEVEL]

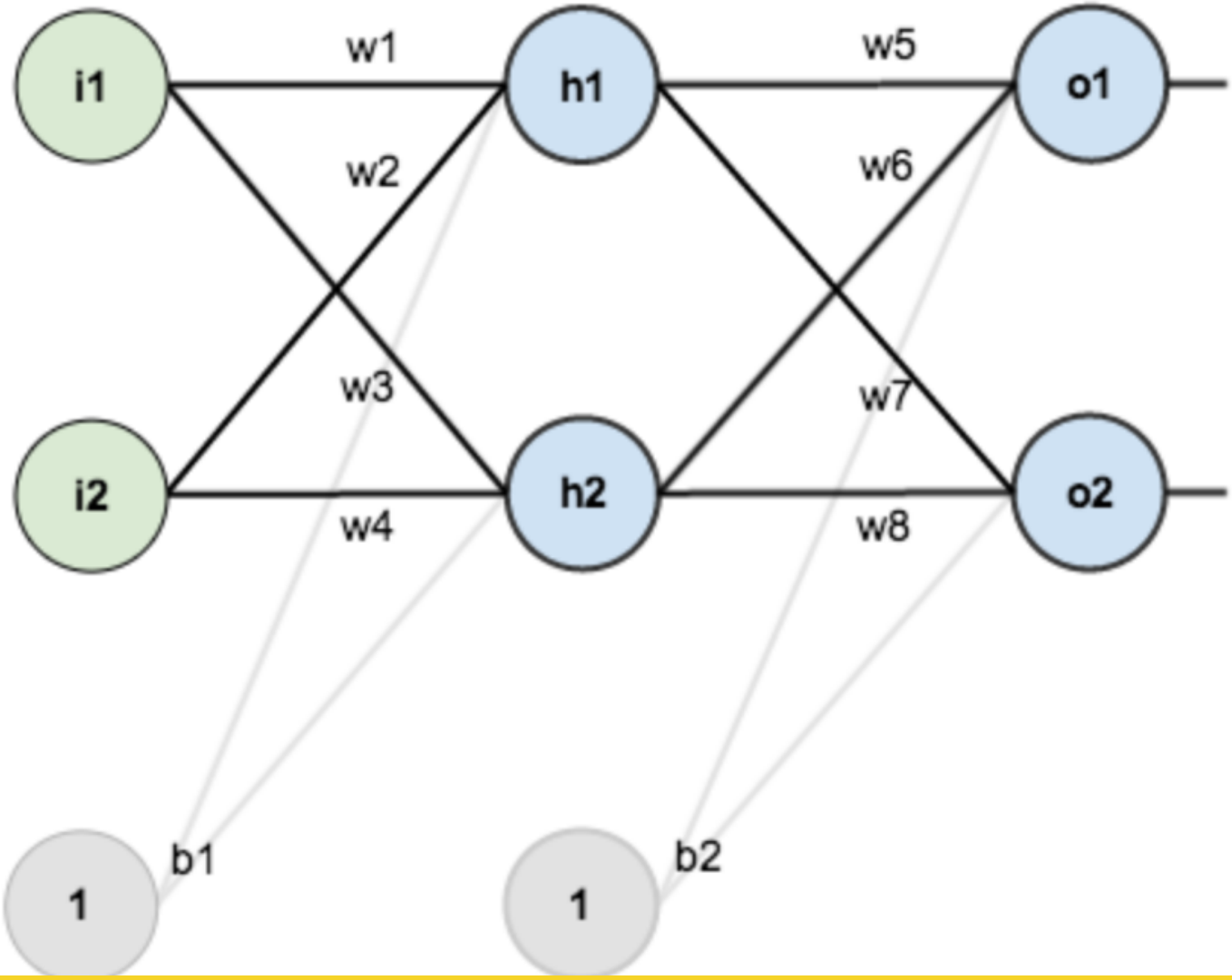


Credit: A. Karpathy

LET’S FOLLOW A NETWORK WHILE IT LEARNS…

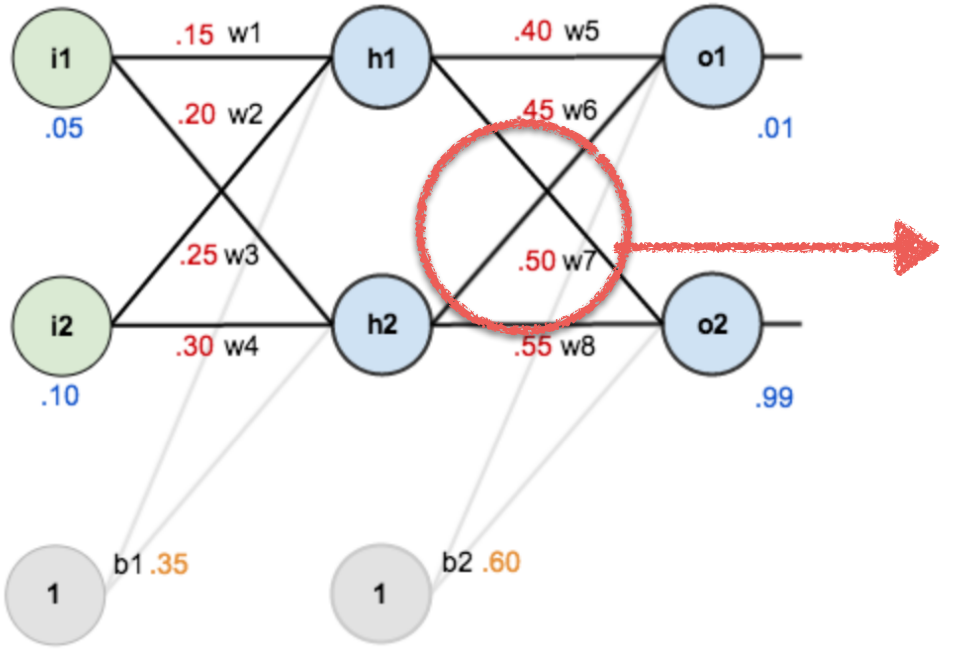


EXAMPLE TAKEN FROM HERE



LET'S ASSUME A VERY SIMPLE TRAINING SET:
X=(0.05, 0.10) —> Y=(0.01,0.99)

EXAMPLE TAKEN FROM HERE



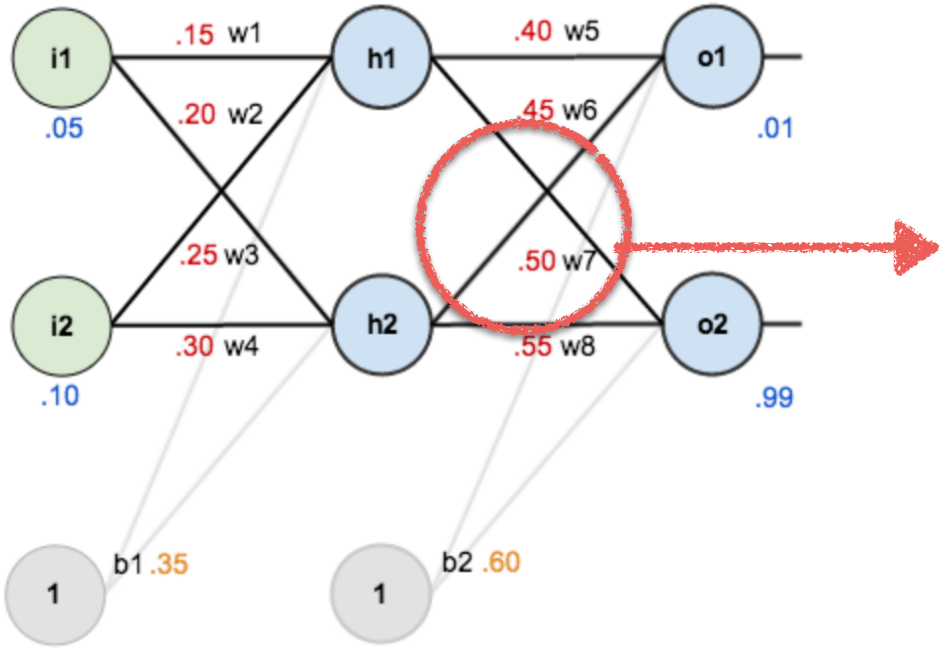
initial weights

1. THE FORWARD PASS

$$in_{h1} = w_1 i_1 + w_2 i_2 + b_1$$

$$in_{h1} = 0.15 \times 0.05 + 0.2 \times 0.1 + 0.35 = 0.3775$$

[with initial weights]



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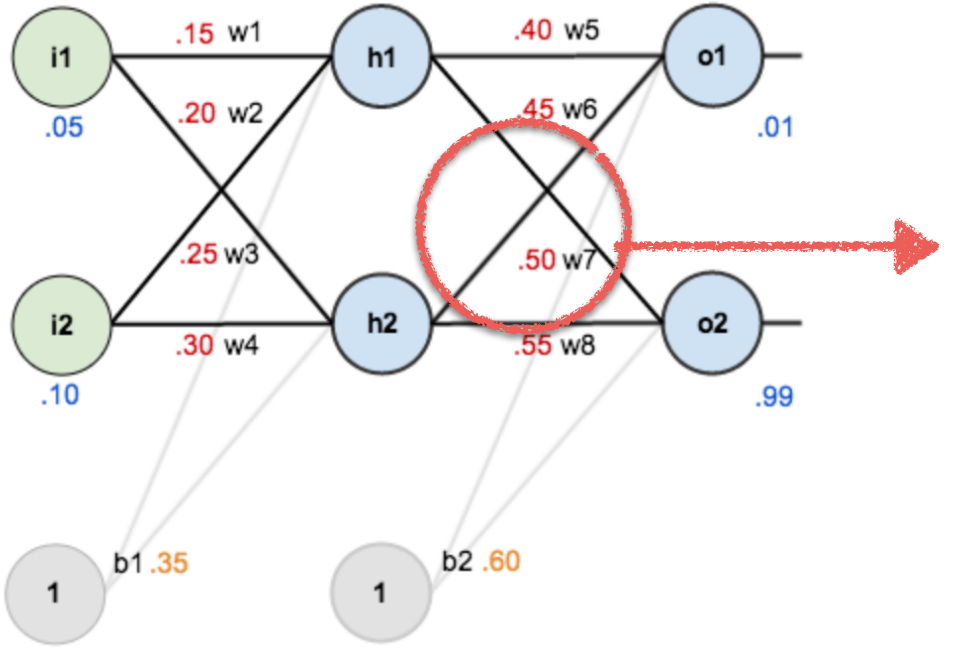
$$in_{h1} = 0.15 \times 0.05 + 0.2 \times 0.1 + 0.35 = 0.3775$$

[with initial weights]

$$out_{h1} = \frac{1}{1 + e^{-in_{h1}}} = 0.5932$$

[after the activation function]



initial weights

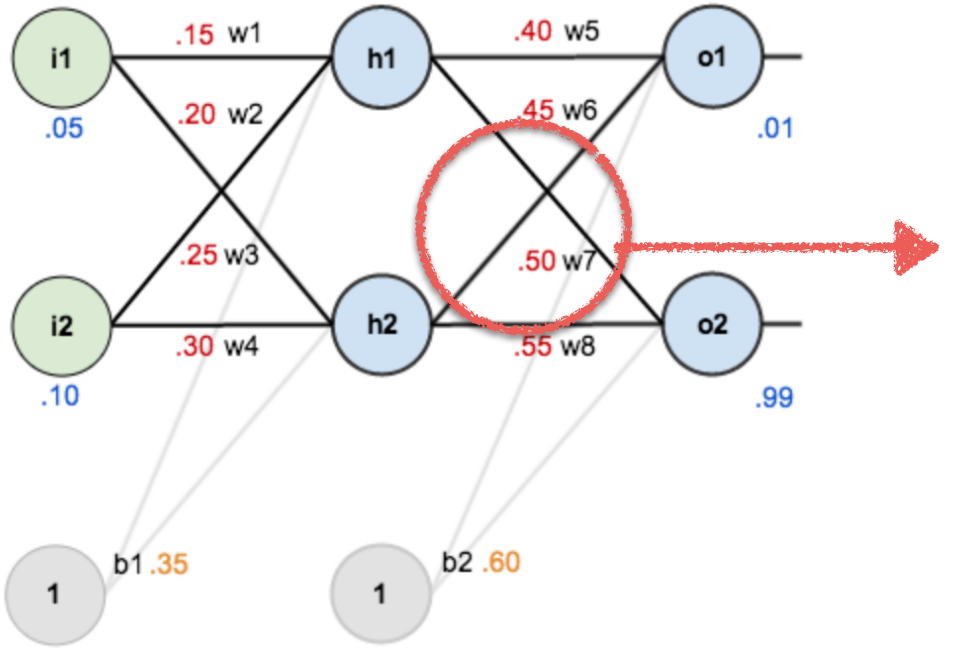
1. THE FORWARD PASS

WE CONTINUE TO o1

$$in_{o1} = w_5 out_{h1} + w_6 out_{h2} + b_2$$

$$in_{o1} = 0.4 \times 0.593 + 0.45 \times 0.596 + 0.6 = 1.105$$

$$out_{o1} = \frac{1}{1 + e^{-1.105}} = 0.751$$

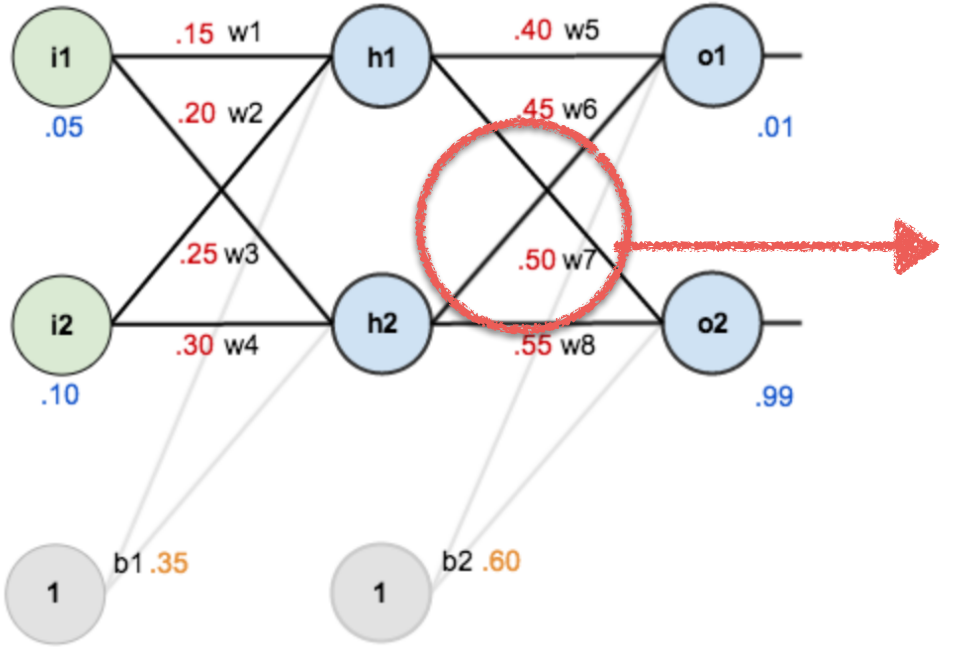


initial weights

1. THE FORWARD PASS

AND THE SAME FOR o2

$$out_{o2} = 0.7729$$



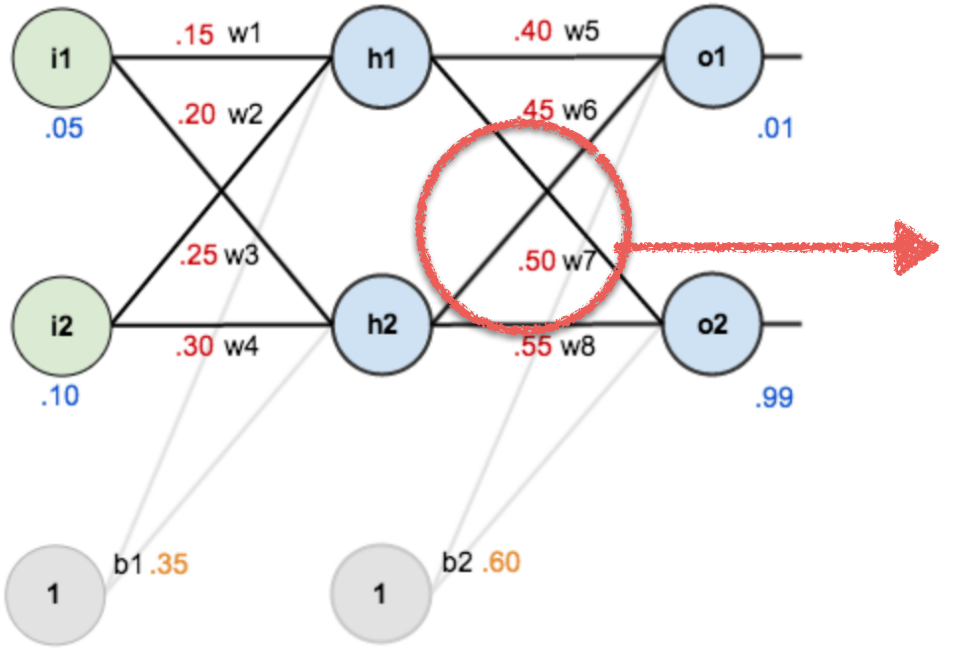
initial weights

2. THE LOSS FUNCTION

$$L_{total} = \sum 0.5(target - output)^2$$

$$L_{o1} = 0.5(target_{o1} - output_{01})^2 = 0.5 \times (0.01 - 0.751)^2 = 0.274$$

$$L_{o2} = 0.023$$



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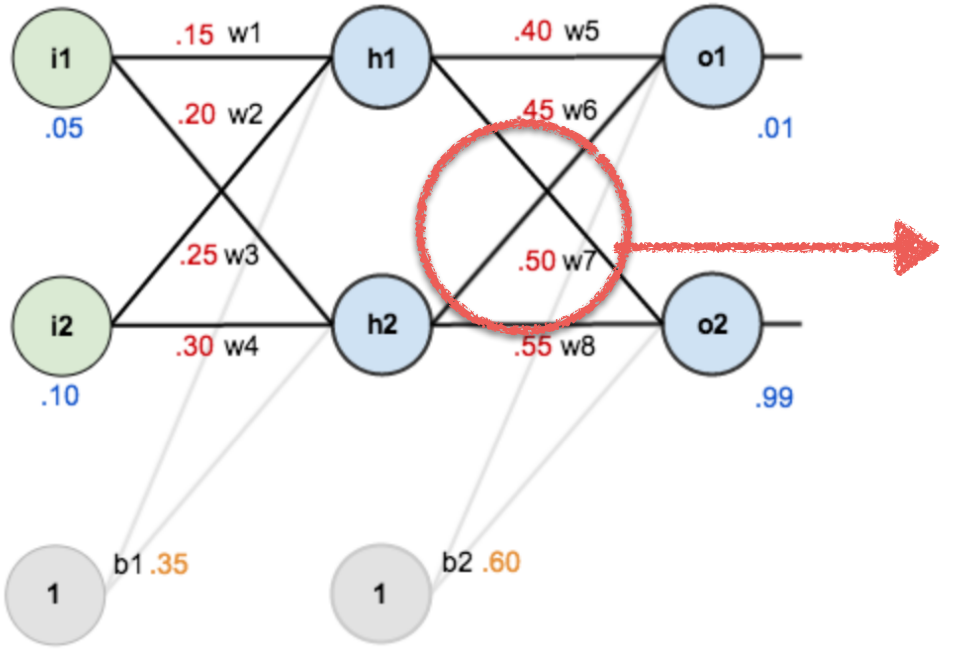
$$L_{o2} = 0.023$$

$$L_{total} = L_{o1} + L_{o2} = 0.298$$



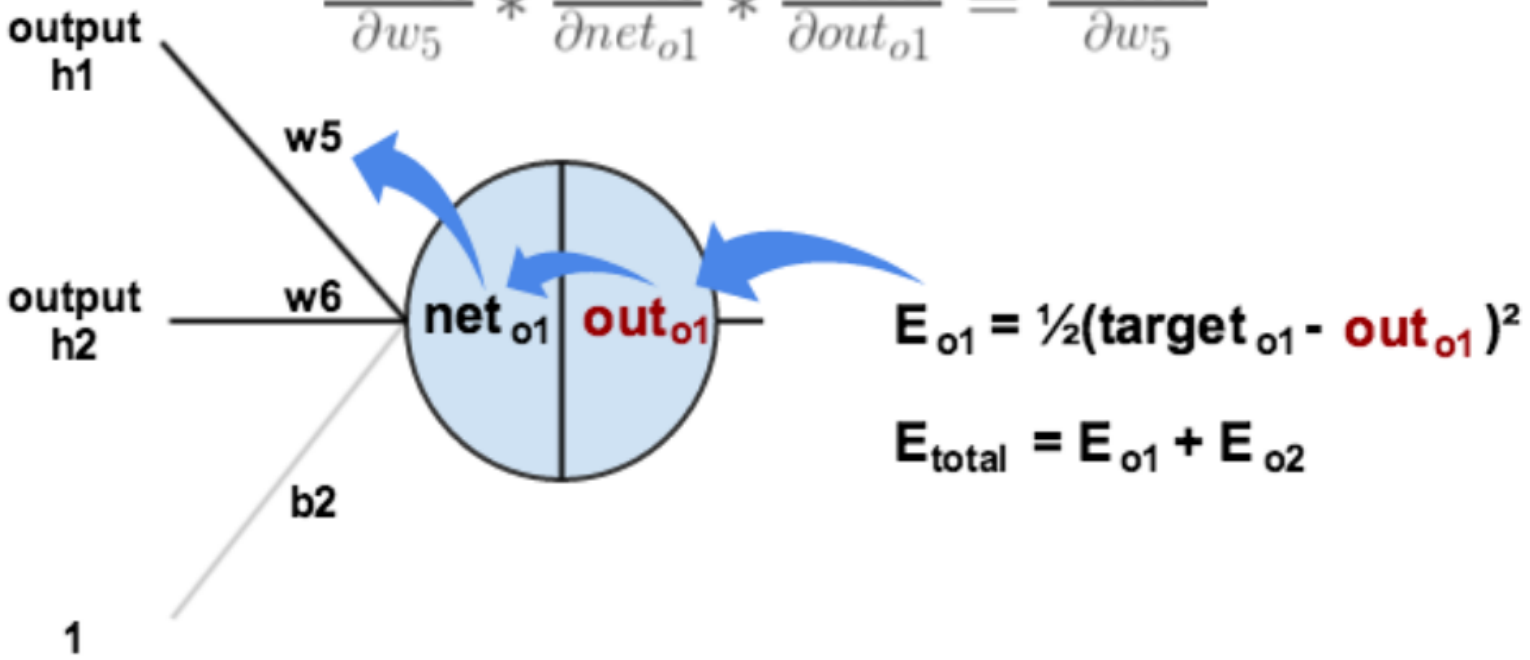
initial weights

3. THE BACKWARD PASS

FOR W5

WE WANT: $\frac{\partial L_{total}}{\partial w_5}$ [gradient of loss function]

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



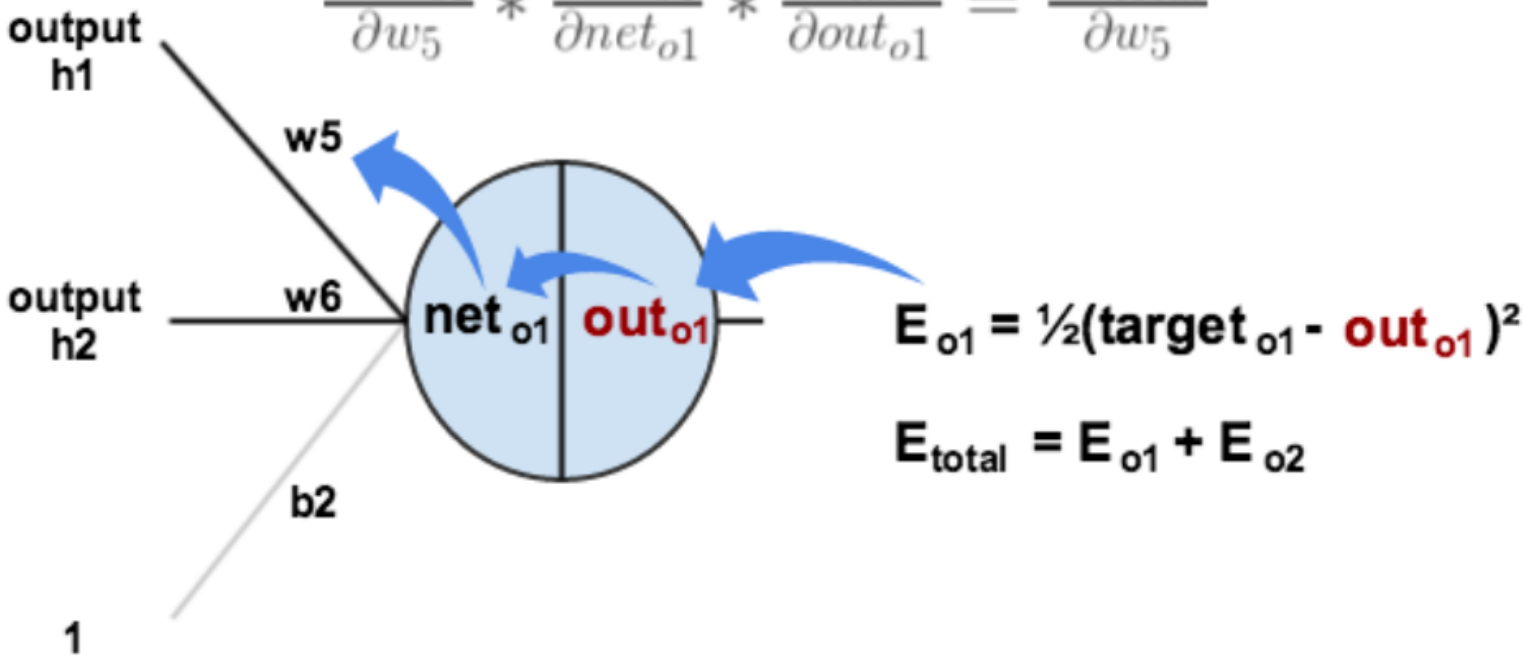
3. THE BACKWARD PASS

FOR W5 WE WANT: $\frac{\partial L_{total}}{\partial w_5}$ [gradient of loss function]

WE APPLY THE CHAIN RULE:

$$\frac{\partial L_{total}}{\partial w_5} = \frac{\partial L_{total}}{\partial out_{o1}} \times \frac{\partial out_{o1}}{\partial in_{o1}} \times \frac{\partial in_{o1}}{\partial w_5}$$

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



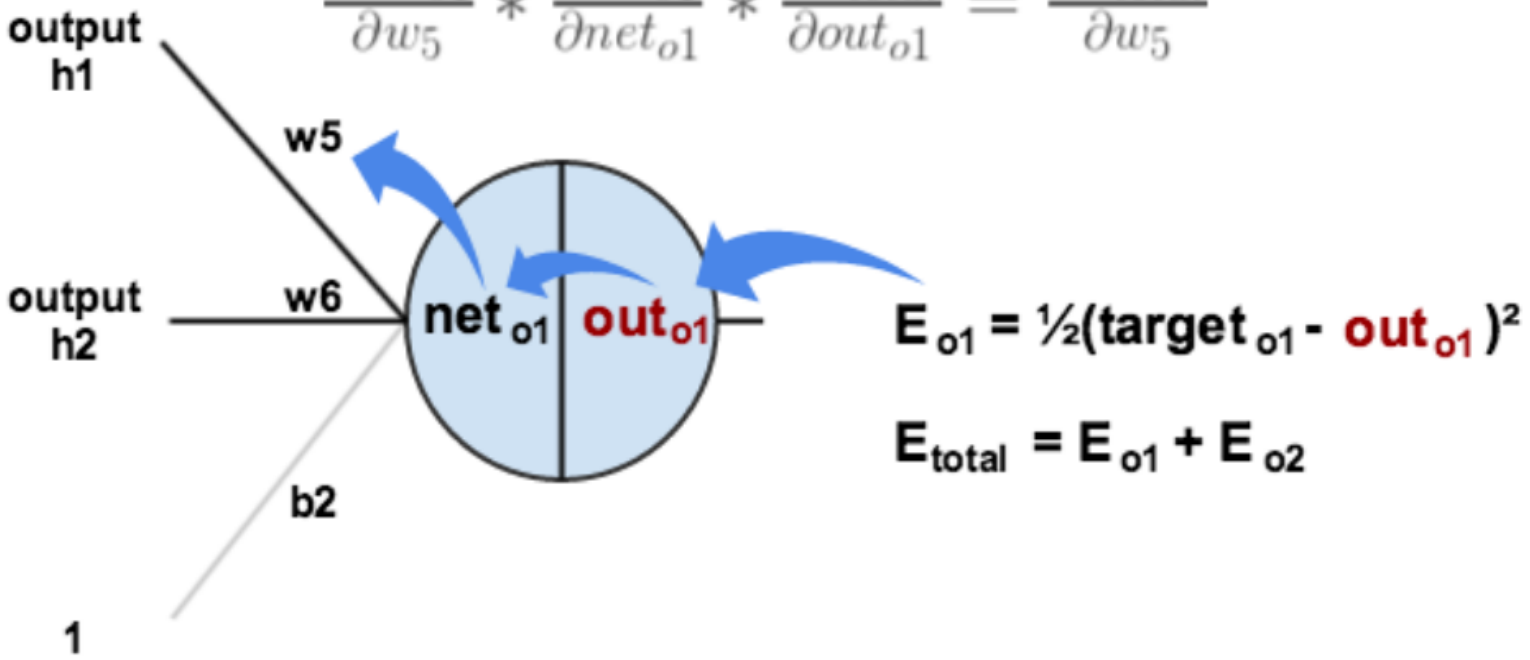
3. THE BACKWARD PASS

$$\frac{\partial L_{total}}{\partial w_5} = \frac{\partial L_{total}}{\partial out_{o1}} \times \frac{\partial out_{o1}}{\partial in_{o1}} \times \frac{\partial in_{o1}}{\partial w_5}$$

$$L_{total} = 0.5(target_{o1} - out_{o1})^2 + 0.5(target_{o2} - out_{o2})^2$$

$$\frac{\partial L_{total}}{\partial out_{o1}} = 2 \times 0.5(target_{o1} - out_{o1}) \times (-1) = 0.741$$

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



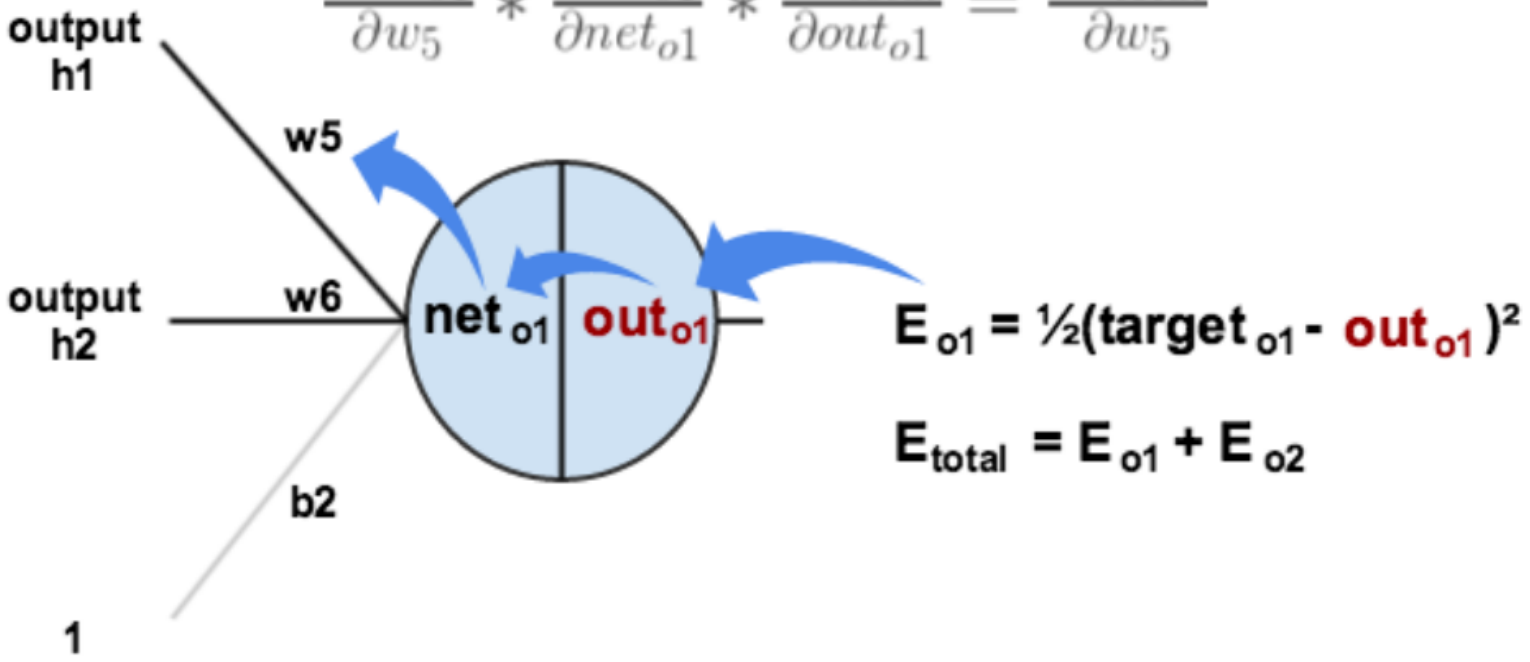
3. THE BACKWARD PASS

$$\frac{\partial L_{total}}{\partial w_5} = \frac{\partial L_{total}}{\partial out_{o1}} \times \frac{\partial out_{o1}}{\partial in_{o1}} \times \frac{\partial in_{o1}}{\partial w_5}$$

$$out_{o1} = \frac{1}{1 + e^{-in_{o1}}}$$

$$\frac{\partial out_{o1}}{\partial in_{o1}} = out_{o1} \times (1 - out_{o1}) = 0.186$$

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



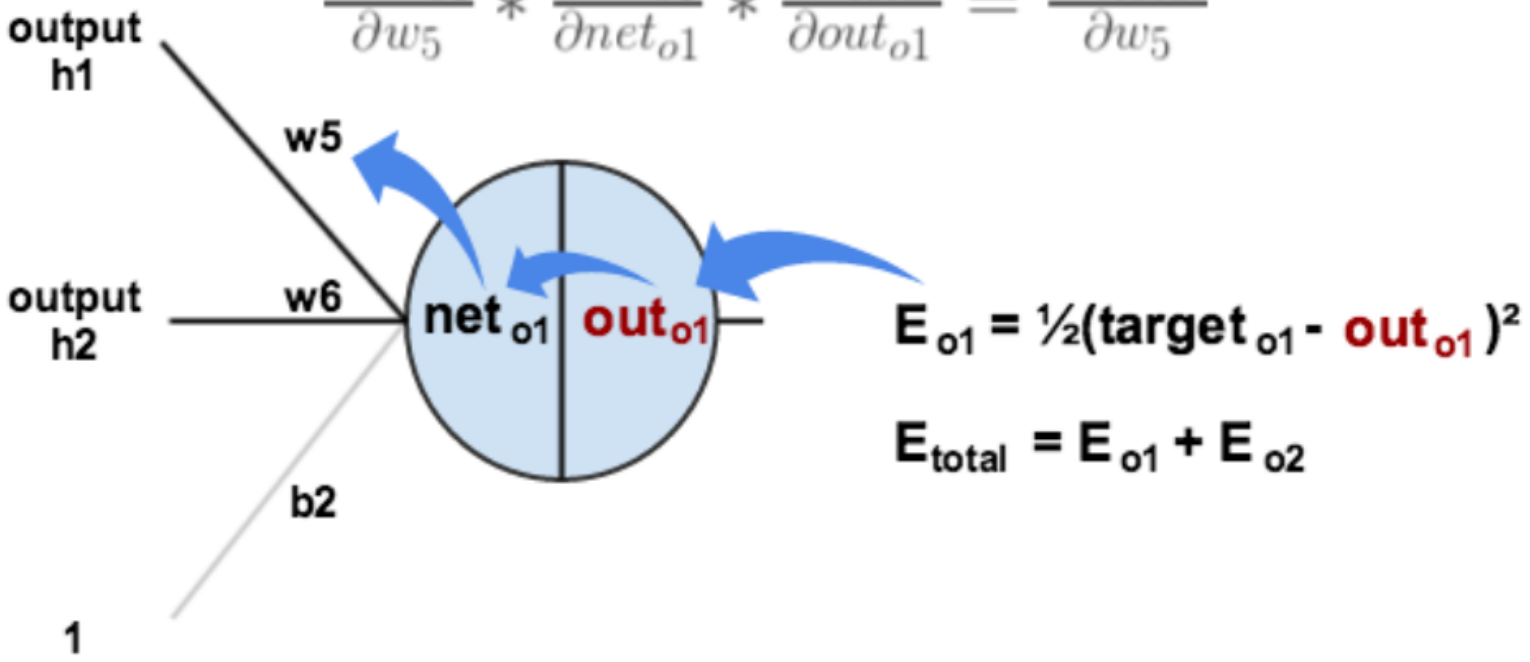
3. THE BACKWARD PASS

$$\frac{\partial L_{total}}{\partial w_5} = \frac{\partial L_{total}}{\partial out_{o1}} \times \frac{\partial out_{o1}}{\partial in_{o1}} \times \frac{\partial in_{o1}}{\partial w_5}$$

$$in_{o1} = w_5 \times out_{h1} + w_6 \times out_{h2} + b_2$$

$$\frac{\partial in_{o1}}{\partial w_5} = out_{h1} \times w_5^{1-1} = out_{h1} = 0.593$$

$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



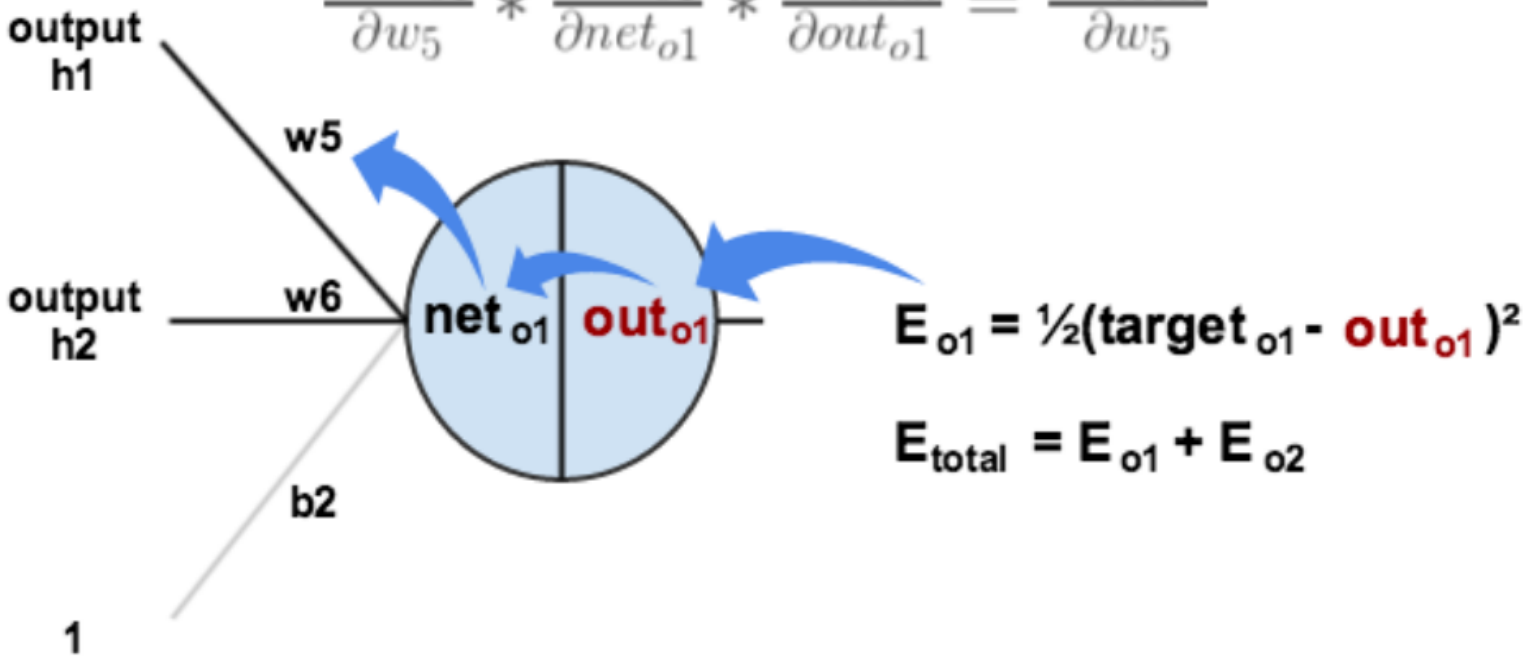
3. THE BACKWARD PASS

ALL TOGETHER:

$$\frac{\partial L_{total}}{\partial w_5} = \frac{\partial L_{total}}{\partial out_{o1}} \times \frac{\partial out_{o1}}{\partial in_{o1}} \times \frac{\partial in_{o1}}{\partial w_5}$$

$$\frac{\partial L_{total}}{\partial w_5} = 0.741 \times 0.186 \times 0.593 = 0.082$$

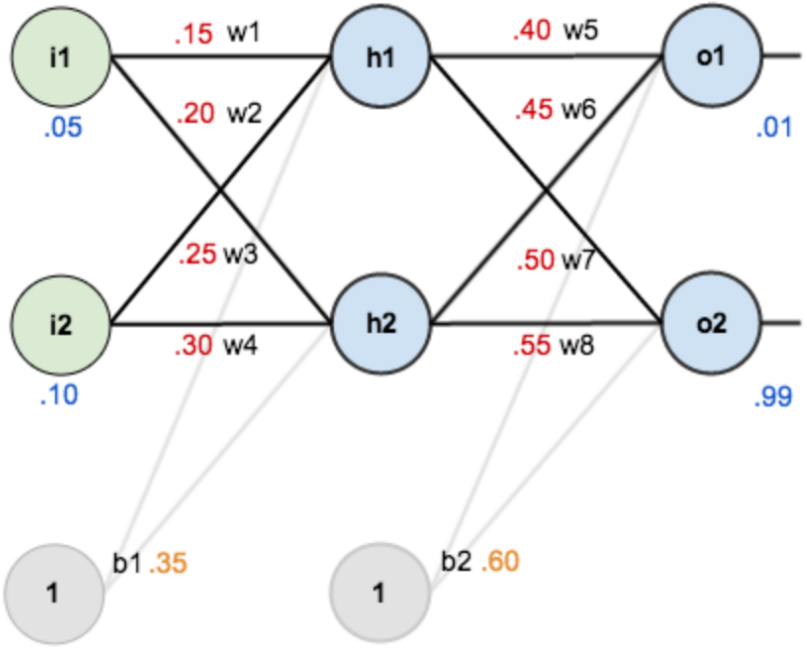
$$\frac{\partial net_{o1}}{\partial w_5} * \frac{\partial out_{o1}}{\partial net_{o1}} * \frac{\partial E_{total}}{\partial out_{o1}} = \frac{\partial E_{total}}{\partial w_5}$$



4. UPDATE WEIGHTS WITH GRADIENT AND LEARNING RATE

$$w_5^{t+1} = w_5 - \lambda \times \frac{\partial L_{total}}{\partial w_5}$$

$$w_5^{t+1} = 0.4 - 0.5 \times 0.082 = 0.358$$

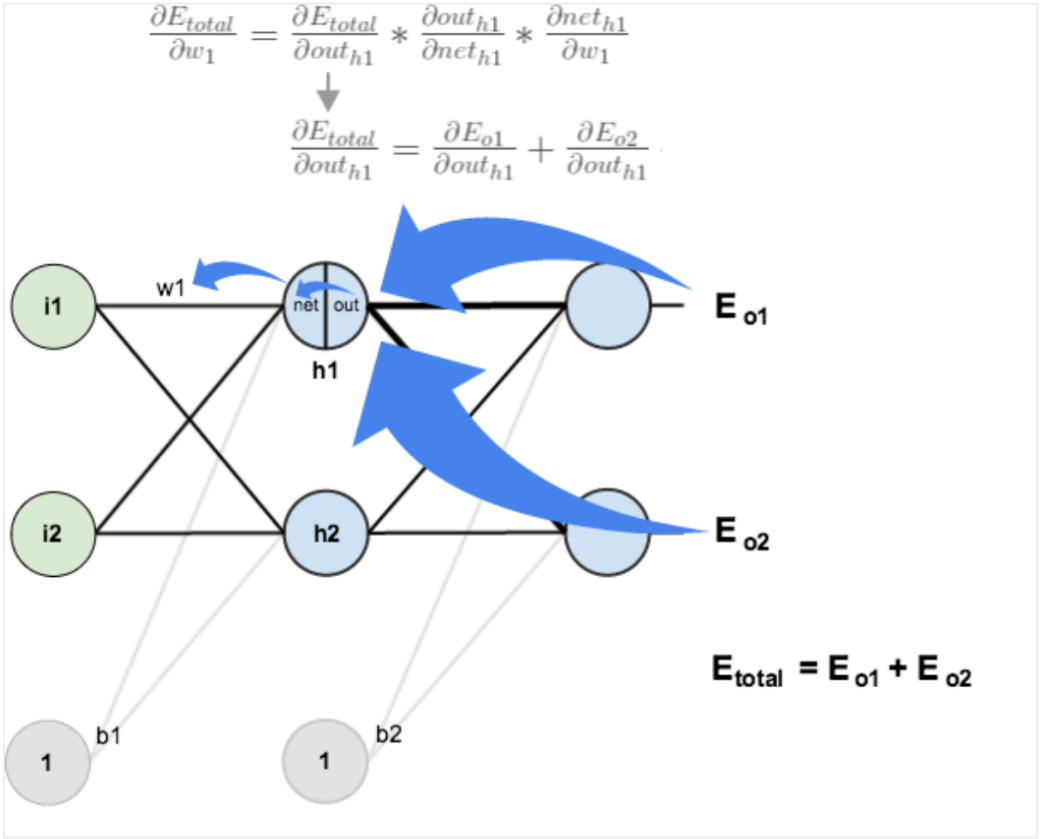


THIS IS REPEATED FOR THE OTHER WEIGHTS OF THE OUTPUT LAYER

$$w_6^{t+1} = 0.408$$

$$w_7^{t+1} = 0.511$$

$$w_8^{t+1} = 0.561$$



AND BACK-PROPAGATED TO THE HIDDEN LAYERS

VISUALIZE SIMPLE NETWORK LEARNING

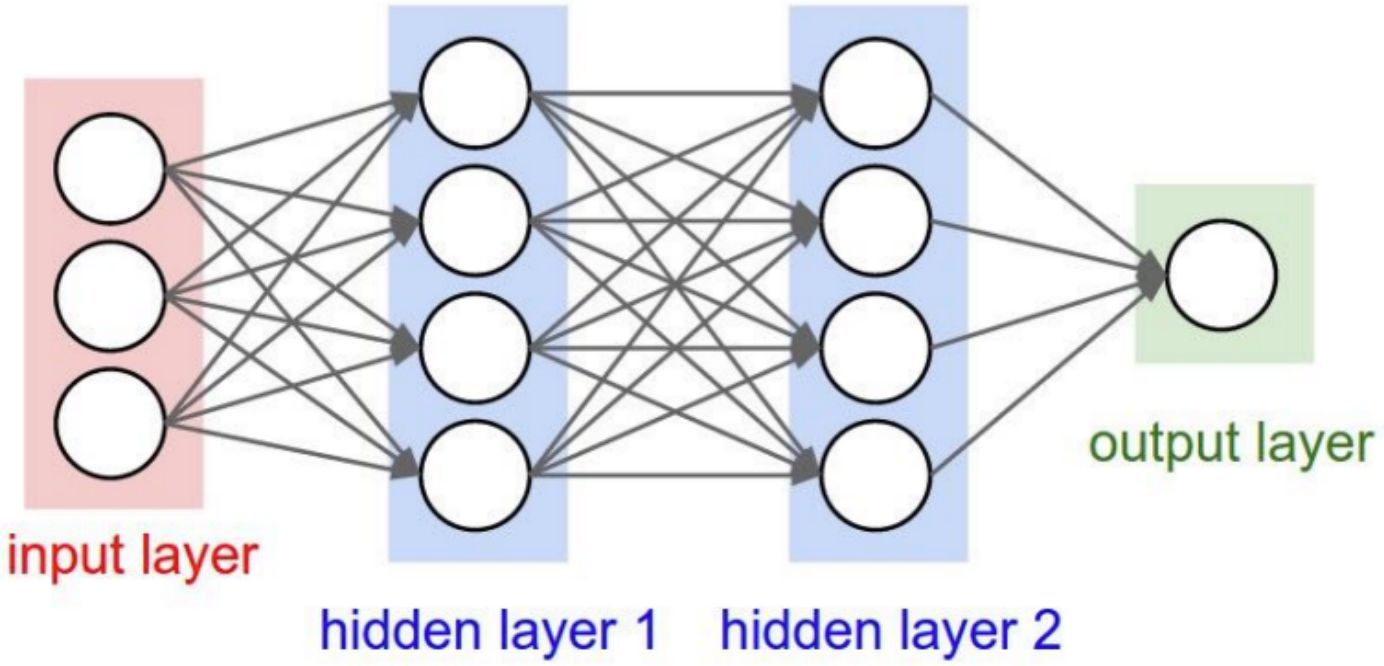
“CLASSICAL” MACHINE LEARNING

$$f_{\vec{W}}(\vec{x}) = \vec{y}$$

LABEL

Q , SF

REPLACE THIS BY A GENERAL NON LINEAR FUNCTION WITH SOME PARAMETERS W



$$p = g_3(W_3 g_2(W_2 g_1(W_1 \vec{x_0})))$$

NETWORK FUNCTION

ONE KEY PROBLEM WITH GRADIENT DESCENT IS THAT IT EASILY CONVERGES TO LOCAL MINIMA BY FOLLOWING THE STEEPEST DESCENT

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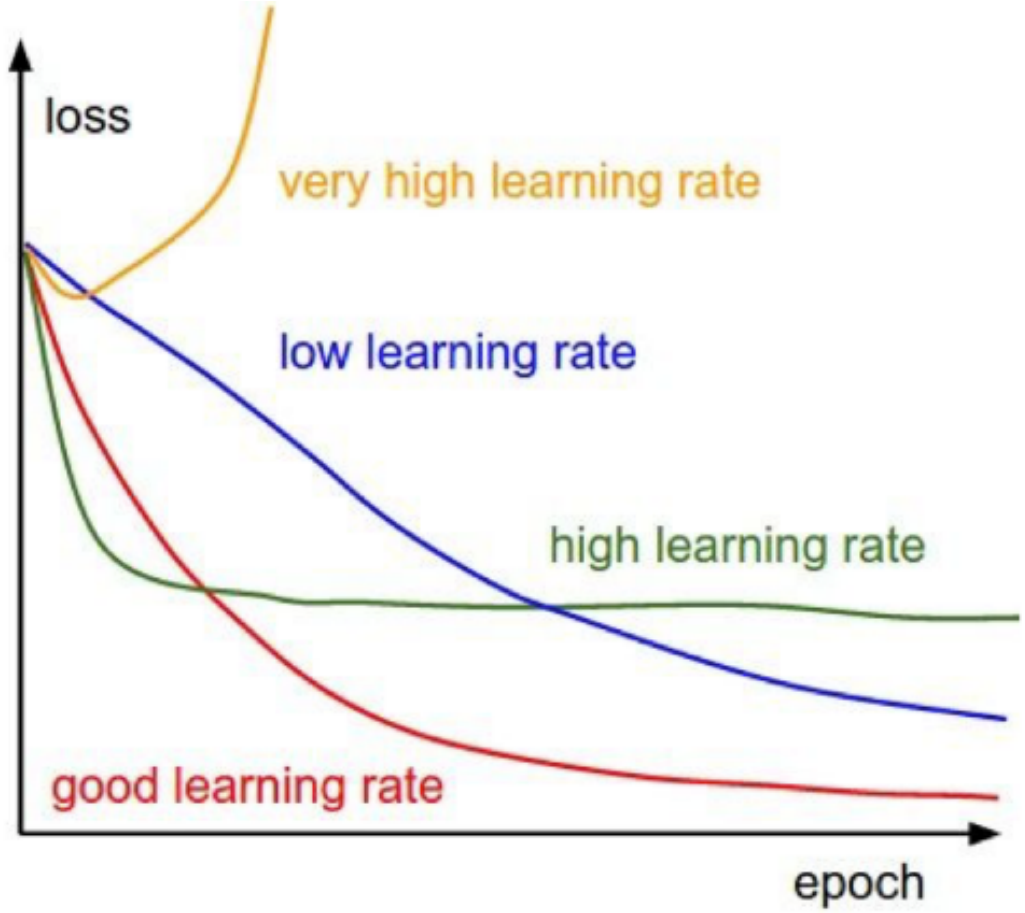
THE CHOICES OF THE INITIAL WEIGHTS AND THE LEARNING RATES ARE IMPORTANT

ONE KEY PROBLEM WITH GRADIENT DESCENT IS THAT IT EASILY CONVERGES TO LOCAL MINIMA BY FOLLOWING THE STEEPEST DESCENT

THE CHOICES OF THE INITIAL WEIGHTS AND THE LEARNING RATES ARE IMPORTANT

WE WILL TALK ABOUT THIS LATER

LEARNING RATES



Credit:

LEARNING RATES

$$W_{t+1} = W_t - \lambda \nabla f(W_t)$$

THERE ARE DIFFERENT WAYS
TO UPDATE THE LEARNING RATE

Credit:

LEARNING RATES

$$W_{t+1} = W_t - \lambda \nabla f(W_t)$$

THERE ARE DIFFERENT WAYS
TO UPDATE THE LEARNING RATE

ADAGRAD:

THE LEARNING RATE IS SCALED DEPENDING ON THE HISTORY OF PREVIOUS GRADIENTS

$$W_{t+1} = W_t - \frac{\lambda}{\sqrt{G_t + \epsilon}} \nabla f(W_t)$$

G IS A MATRIX CONTAINING ALL PREVIOUS GRADIENTS. WHEN THE GRADIENT BECOMES LARGE THE LEARNING RATE IS DECREASED AND VICE VERSA.

$$G_{t+1} = G_t + (\nabla f)^2$$

Credit:

LEARNING RATES

$$W_{t+1} = W_t - \lambda \nabla f(W_t)$$

THERE ARE DIFFERENT WAYS
TO UPDATE THE LEARNING RATE

RMSPROP:

THE LEARNING RATE IS SCALED DEPENDING ON THE HISTORY OF PREVIOUS GRADIENTS

$$W_{t+1} = W_t - \frac{\lambda}{\sqrt{G_t + \epsilon}} \nabla f(W_t)$$

SAME AS **ADAGRAD** BUT G IS CALCULATED BY EXPONENTIALLY DECAYING AVERAGE

$$G_{t+1} = \lambda G_t + (1 - \lambda)(\nabla f)^2$$

Credit:

ADAM [Adaptive moment estimator]:

SAME IDEA, USING FIRST AND SECOND ORDER MOMENTUMS

$$G_{t+1} = \beta_2 G_t + (1-\beta_2)(\nabla f)^2 \quad M_{t+1} = \beta_1 M_t + (1-\beta_1)(\nabla f)$$

$$W_{t+1} = W_t - \frac{\lambda}{\sqrt{\hat{G}_t + \epsilon}} \hat{M}_t$$

with: $\hat{M}_{t+1} = \frac{M_t}{1-\beta_1}$ $\hat{G}_{t+1} = \frac{G_t}{1-\beta_2}$

ADAM [Adaptive moment estimator]:

SAME IDEA, USING FIRST AND SECOND ORDER MOMENTUMS

$$G_{t+1} = \beta_2 G_t + (1-\beta_2)(\nabla f)^2 \qquad M_{t+1} = \beta_1 M_t + (1-\beta_1)(\nabla f)$$

ONLY FOR YOUR RECORDS

$$\sqrt{G_t + \epsilon}$$

with: $\hat{M}_{t+1} = \dfrac{M_t}{1-\beta_1}$ $\hat{G}_{t+1} = \dfrac{G_t}{1-\beta_2}$

IN KERAS:

RMSprop [source]

```
keras.optimizers.RMSprop(lr=0.001, rho=0.9, epsilon=None, decay=0.0)
```

RMSProp optimizer.

It is recommended to leave the parameters of this optimizer at their default values (except the learning rate, which can be freely tuned).

This optimizer is usually a good choice for recurrent neural networks.

Arguments

- **lr**: float >= 0. Learning rate.
- **rho**: float >= 0.
- **epsilon**: float >= 0. Fuzz factor. If `None`, defaults to `K.epsilon()`.
- **decay**: float >= 0. Learning rate decay over each update.

References

- rmsprop: Divide the gradient by a running average of its recent magnitude

IN KERAS:

Adam [source]

```
keras.optimizers.Adam(lr=0.001, beta_1=0.9, beta_2=0.999, epsilon=None, decay=0.0, amsgrad=False)
```

Adam optimizer.

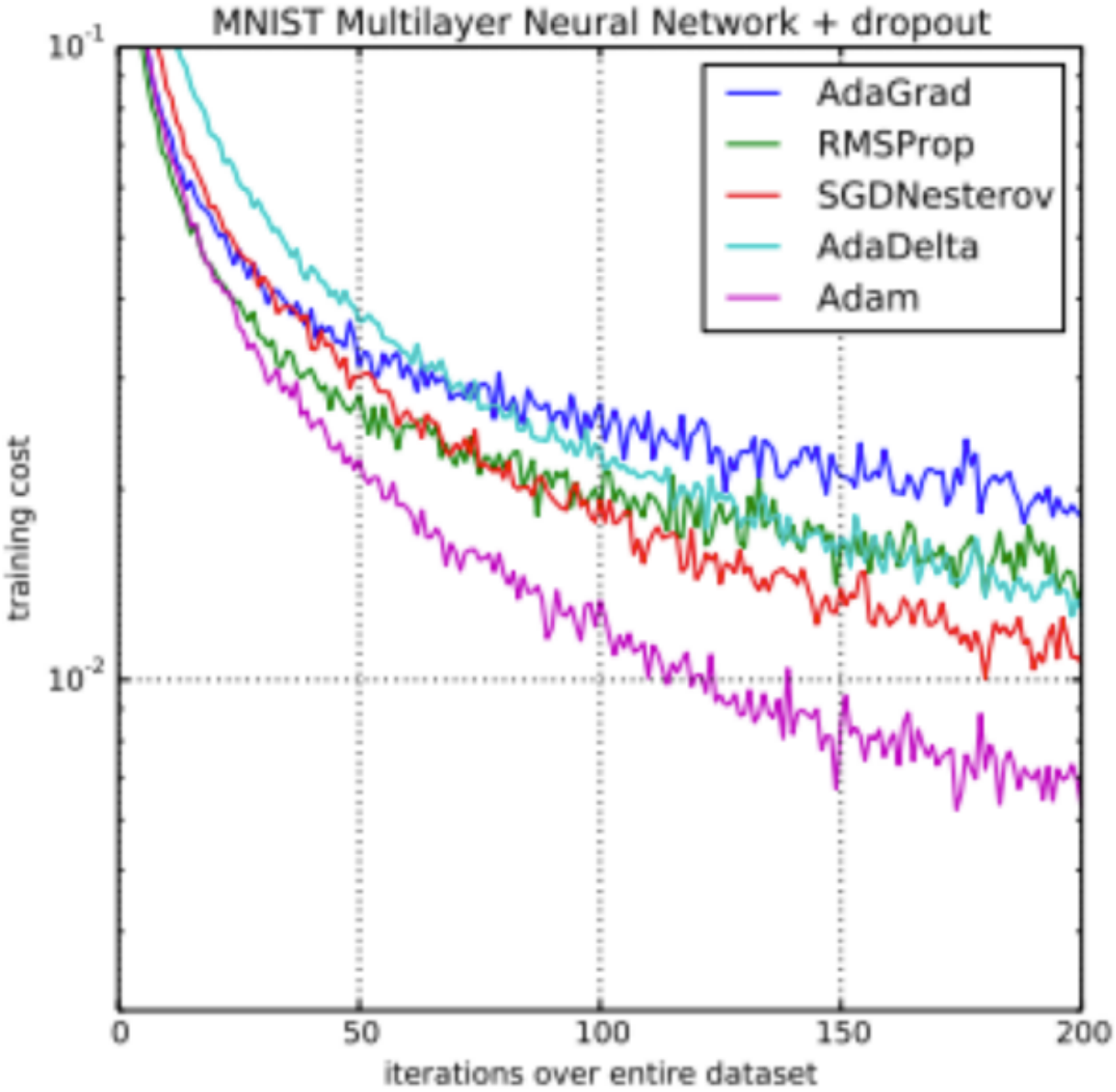
Default parameters follow those provided in the original paper.

Arguments

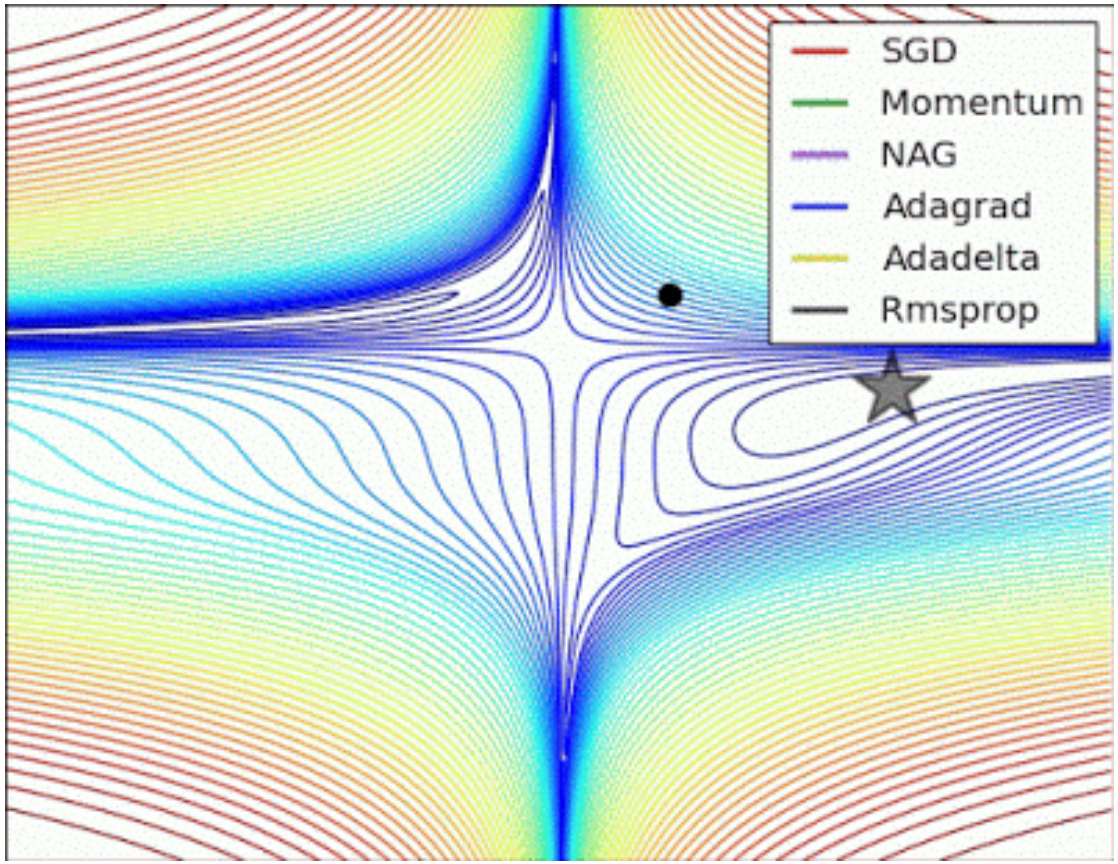
- **lr**: float >= 0. Learning rate.
- **beta_1**: float, 0 < beta < 1. Generally close to 1.
- **beta_2**: float, 0 < beta < 1. Generally close to 1.
- **epsilon**: float >= 0. Fuzz factor. If `None`, defaults to `K.epsilon()`.
- **decay**: float >= 0. Learning rate decay over each update.
- **amsgrad**: boolean. Whether to apply the AMSGrad variant of this algorithm from the paper "On the Convergence of Adam and Beyond".

References

- Adam - A Method for Stochastic Optimization
- On the Convergence of Adam and Beyond


MNIST Multilayer Neural Network + dropout
AdaGrad
RMSProp
SGDNesterov
AdaDelta
Adam
training cost
10^{-1}
10^{-2}
0
50
100
150
200
iterations over entire dataset

Credit



Credit

BATCH GRADIENT DESCENT

LOCAL MINIMA CAN ALSO BE AVOIDED BY COMPUTING THE GRADIENT IN SMALL BATCHES INSTEAD OF OVER THE FULL DATASET

BATCH GRADIENT DESCENT

LOCAL MINIMA CAN ALSO BE AVOIDED BY COMPUTING THE GRADIENT IN SMALL BATCHES INSTEAD OF OVER THE FULL DATASET

MINI-BATCH GRADIENT DESCENT

$$V_{t+1/num} = W_t - \lambda_t \nabla f(W_t; x^{(i,i+b)}, y^{(i,i+b)})$$

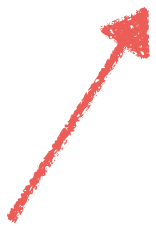
THE GRADIENT IS COMPUTED OVER A BATCH OF SIZE B

STOCHASTIC GRADIENT DESCENT

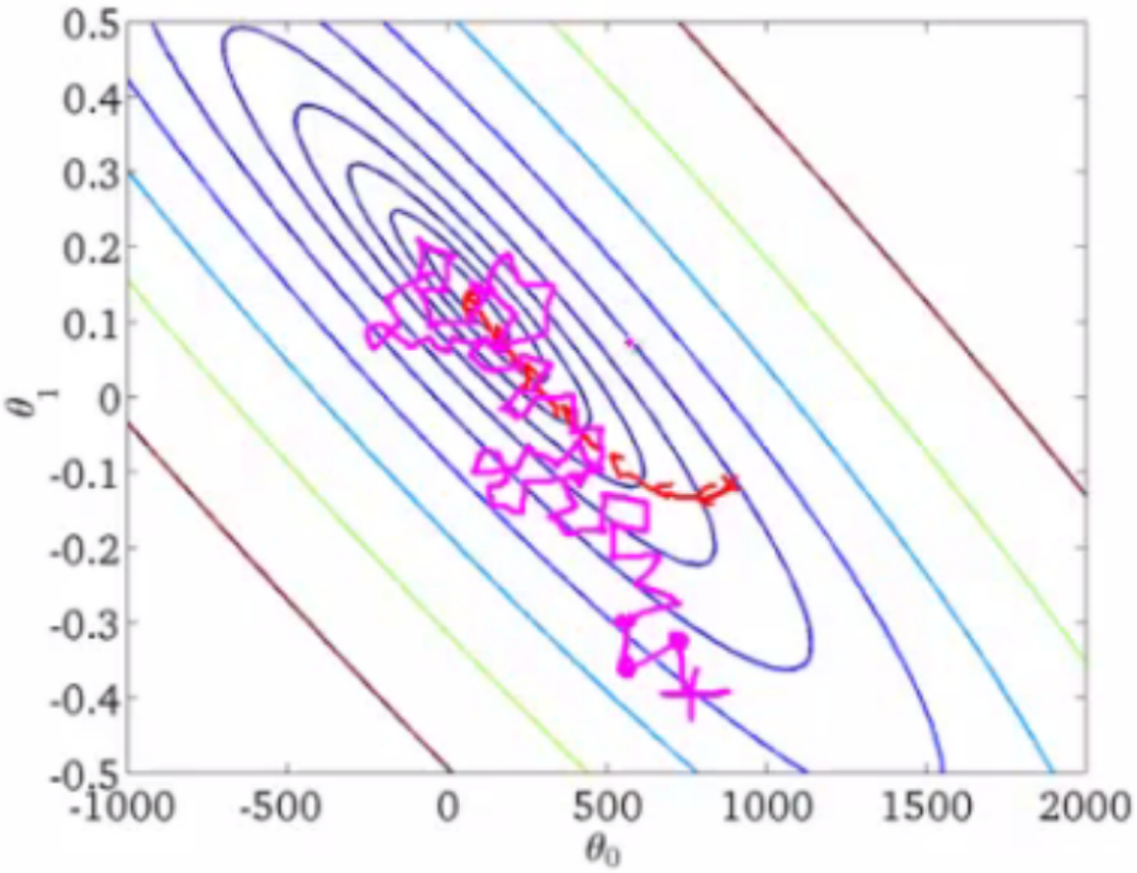
THE EXTREME CASE IS TO COMPUTE THE GRADIENT ON EVERY TRAINING EXAMPLE.

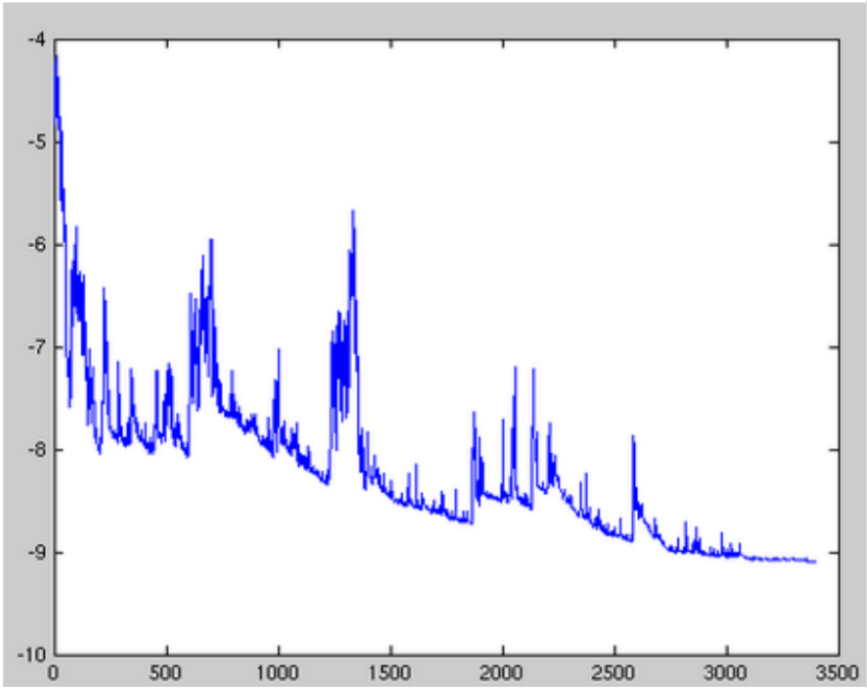
STOCHASTIC GRADIENT DESCENT

$$V_{t+1/num} = W_t - \lambda_t \nabla f(W_t; x^{(i,i+b)}, y^{(i,i+b)})$$



b=1





Fluctuations in the total objective function as gradient steps with respect to mini-batches are taken.

Credit

LET'S TALK LOSS FUNCTIONS….

THE CHOICE OF THE LOSS FUNCTION IS CRITICAL AND WILL DETERMINE THE BEHAVIOR OF THE ALGORITHM (*REMEMBER: LOSS IS WHAT IS MINIMIZED BY THE OPTIMIZATION ALGORITHM*)

SOME ALGORITHMS SUCH AS RFs HAVE LESS FLEXIBILITY. ONE ADVANTAGE OF NNs IS THAT THE LOSS FUNCTION CAN BE CHANGED VERY EASILY.

(BINARY) CLASSIFICATION

WE TYPICALLY USE THE BINARY CROSS-ENTROPY LOSS:

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} y_i.log(p(y_i)) + (1-y_i).log(1-p(y_i))$$

GROUND TRUTH

NETWORK OUTPUT (SOFTMAX)

GROUND TRUTH

NETWORK OUTPUT (SOFTMAX)

(BINARY) CLASSIFICATION

WE MINIMIZE THE CROSS ENTROPY BETWEEN THE TRUE (q(y)) AND PREDICTED (p(y)) DISTRIBUTIONS

$$H_p(q) = -\frac{1}{N}\sum_{i=1}^{N} q(y_i).log(p(y_i)) + (1 - q(y_i)).log(1 - p(y_i))$$

GROUND TRUTH

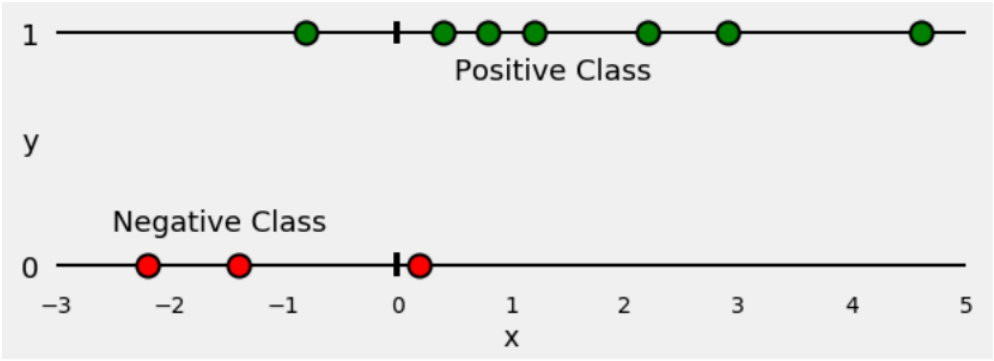
GROUND TRUTH

NETWORK OUTPUT (SOFTMAX)

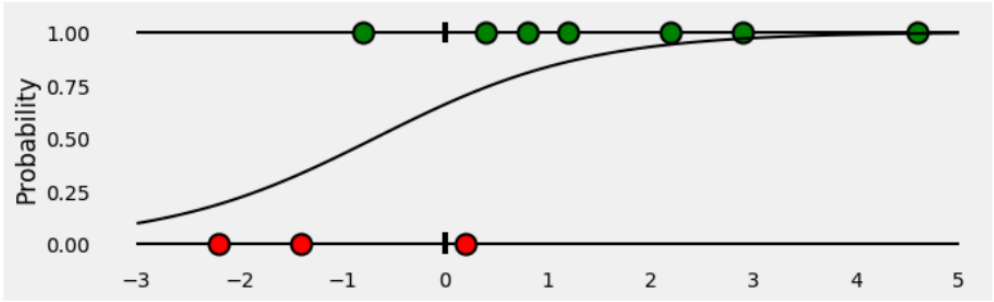
NETWORK OUTPUT (SOFTMAX)

EXAMPLE:

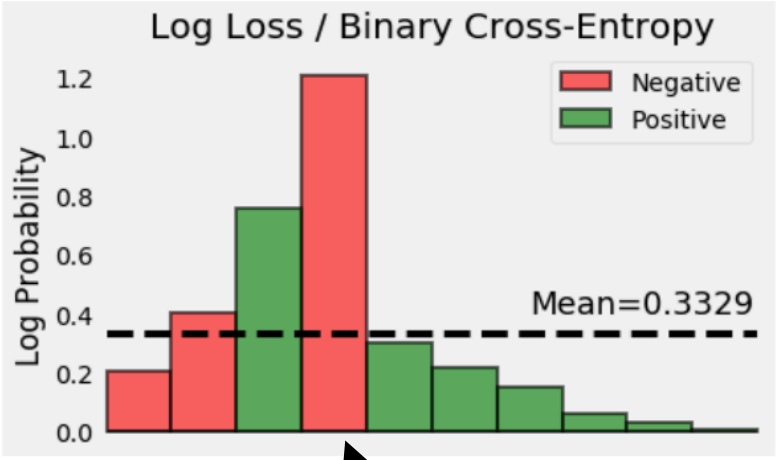
1. LAST LAYER OF NN:



2. FIT LOGISTIC REGRESSION:

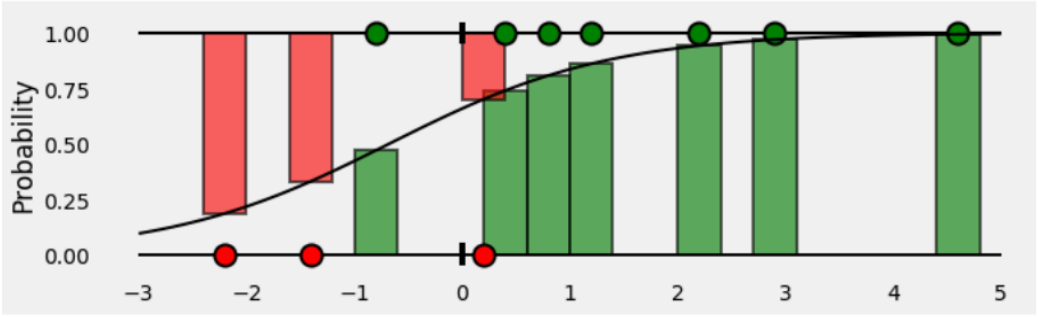


2. COMPUTE THE -LOG AND AVERAGE:



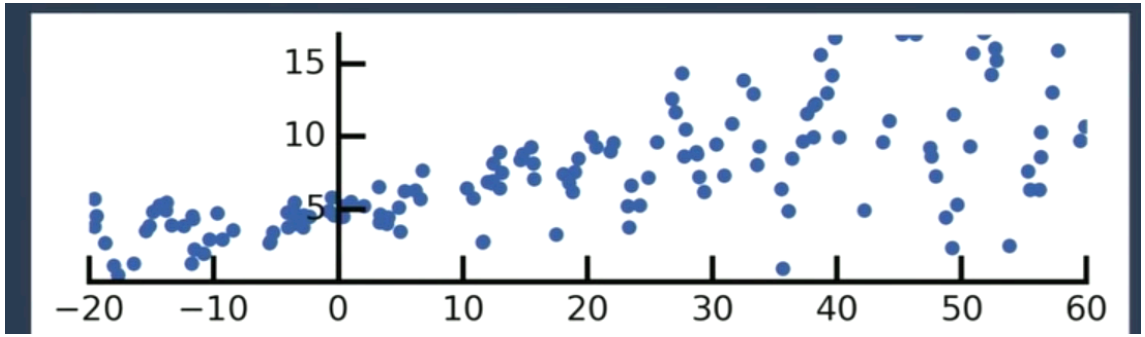
THE LOWER IS P, THE LARGER THE CONTRIBUTION TO TO THE LOSS

3. COMPUTE SOFTMAX FOR EVERY POINT IN TRAINING:



TAKEN FROM HERE

WHAT ABOUT REGRESSIONS?




```
model = tf.keras.Sequential([
  tf.keras.layers.Dense(hidden_units, ...),
  tf.keras.layers.Dense(1),
])
model.compile(loss=tf.keras.mean_squared_error)
```

WE CAN USE THE STANDARD MSE,
BUT THIS PROVIDES A SINGLE POINT ESTIMATE
AND DOESN'T KNOW ANYTHING ABOUT ERRORS

TensorFlow
DEV SUMMIT 2019

SEE THIS GREAT TALK: https://www.youtube.com/watch?v=BrwKURU-wpk

TURNING YOUR MODEL BAYESIAN…

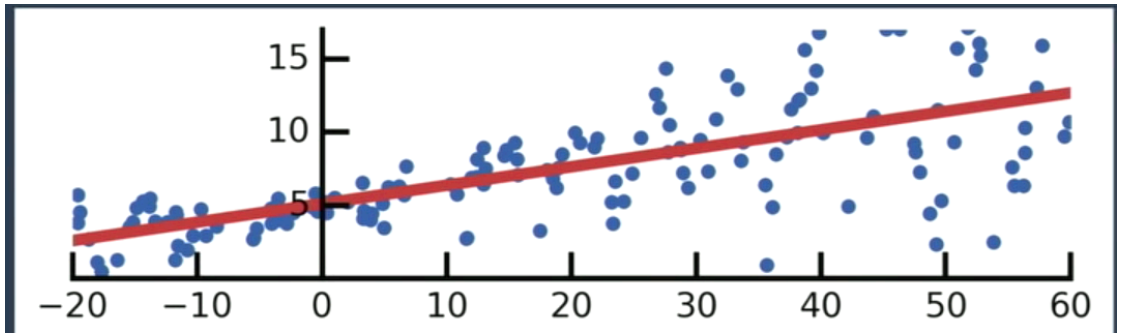
```
model = tf.keras.Sequential([
  tf.keras.layers.Dense(hidden_units, ...),
  tf.keras.layers.Dense(1),
])
model.compile(loss=lambda y, rv_y: -rv_y.log_prob(y))
yhat = model(x_tst) # A Distribution, not a Tensor!
```

Our wish.

Guess what! *You* can.

```
model = tf.keras.Sequential([
  tf.keras.layers.Dense(hidden_units, ...),
  tf.keras.layers.Dense(1),
  tfp.layers.DistributionLambda(lambda t:
    tfd.Normal(loc=t[..., 0],
               scale=1)),
```

TURNING YOUR MODEL BAYESIAN…



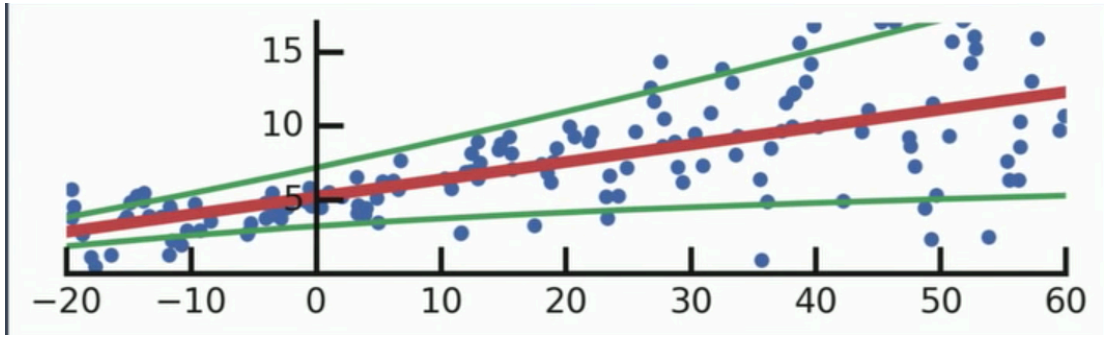
PARAMETRIZE THE POSTERIOR WITH A GAUSSIAN PDF

AND LEARN THE PARAMETERS OF THE NORMAL DISTRIBUTION

Guess what! *You can*.

```
model = tf.keras.Sequential([
  tf.keras.layers.Dense(hidden_units, ...),
  tf.keras.layers.Dense(1),
  tfp.layers.DistributionLambda(lambda t:
    tfd.Normal(loc=t[..., 0],
               scale=1)),
```

TURNING YOUR MODEL BAYESIAN…



PARAMETRIZE THE POSTERIOR WITH A GAUSSIAN PDF

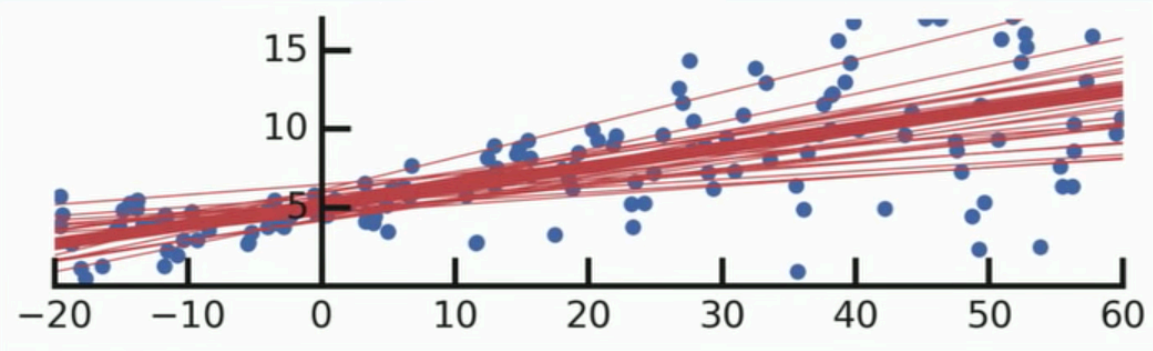
THE VARIANCE CAN ALSO BE LEARNED

CAPTURING “DATA UNCERTAINTY”

Learn known unknowns.

```
model = tf.keras.Sequential([
  tf.keras.layers.Dense(hidden_units, ...),
  tf.keras.layers.Dense(1+1),
  tfp.layers.DistributionLambda(lambda t:
    tfd.Normal(loc=t[..., 0],
               scale=tf.softplus(t[..., 1]))),
])
```

TURNING YOUR MODEL BAYESIAN…



CAPTURING “MODEL UNCERTAINTY”

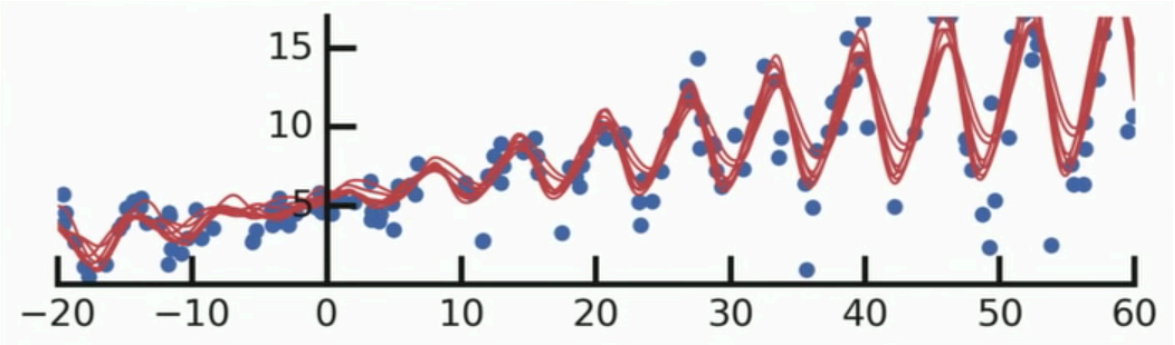
WEIGHTS ARE ALSO DISTRIBUTIONS

```
model = tf.keras.Sequential([
  tfp.layers.DenseVariational(hidden_units, ...),
  tfp.layers.DenseVariational(1),
  tfp.layers.DistributionLambda(lambda t:
    tfd.Normal(loc=t[..., 0],
               scale=1)),
])
```

"Bayesian Weights"

Linear Regressio

TURNING YOUR MODEL BAYESIAN…



CAPTURING “MODEL UNCERTAINTY”

NO NEED TO RESTRICT TO GAUSSIAN FUNCTIONS…

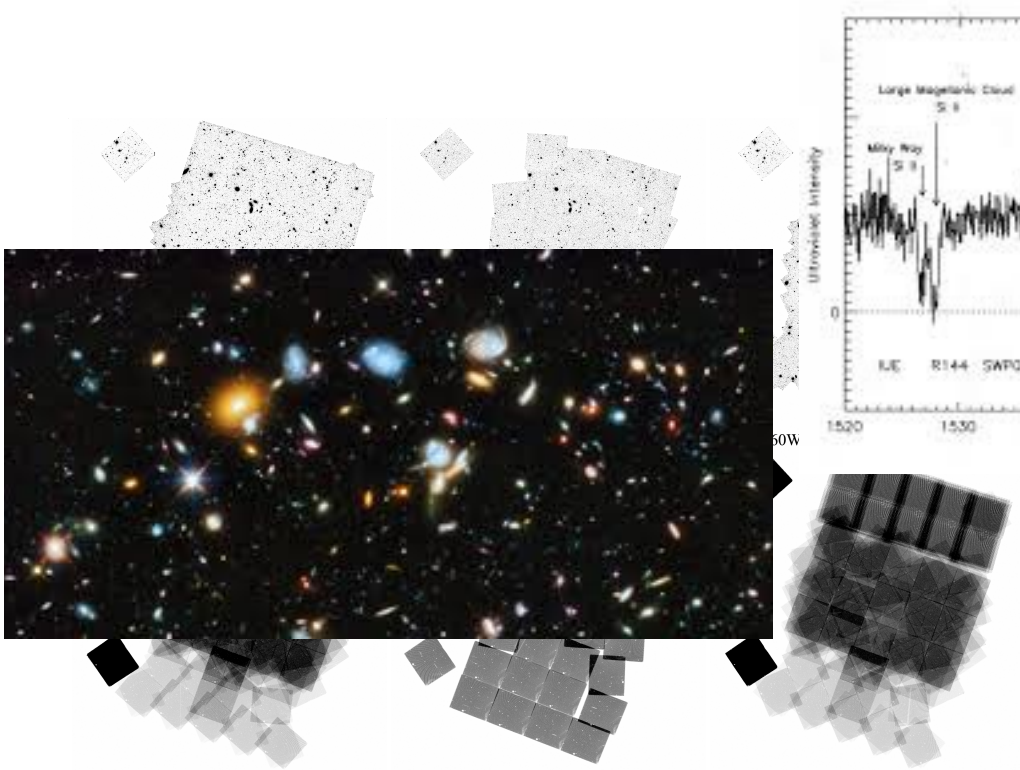
```
model = tf.keras.Sequential([
  tf.keras.layers.Dense(hidden_units, ...),
  tf.keras.layers.Dense(1),
  tfp.layers.VariationalGaussianProcess(
    num_inducing_points, kernel_provider),
])
```

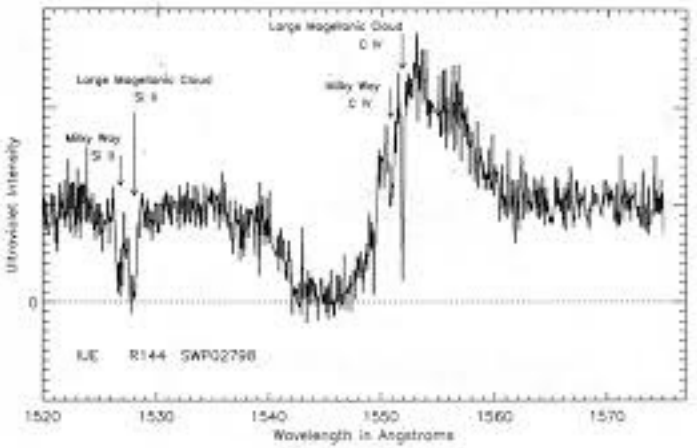
CAN WE GO DEEP NOW?

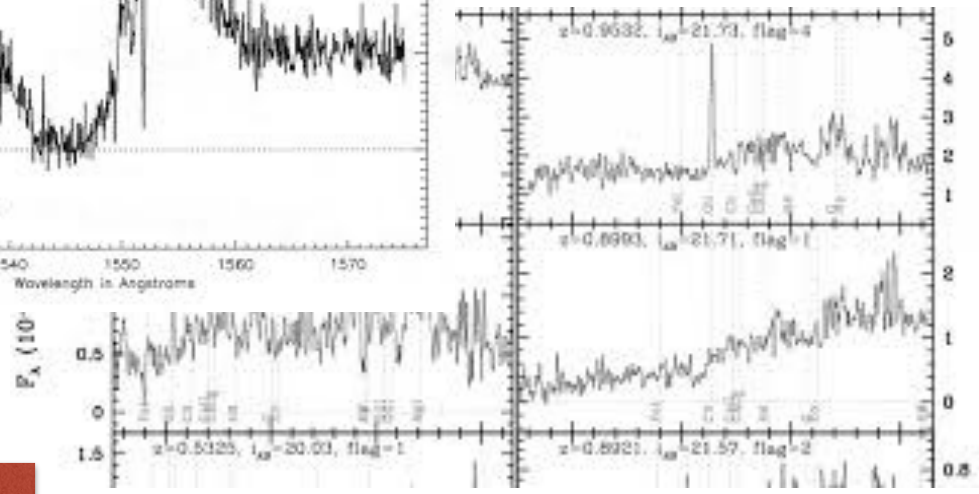
CAN WE GO DEEP NOW?

ALMOST THERE…LET'S THINK FOR A MOMENT ABOUT WHAT WE PUT AS INPUT…

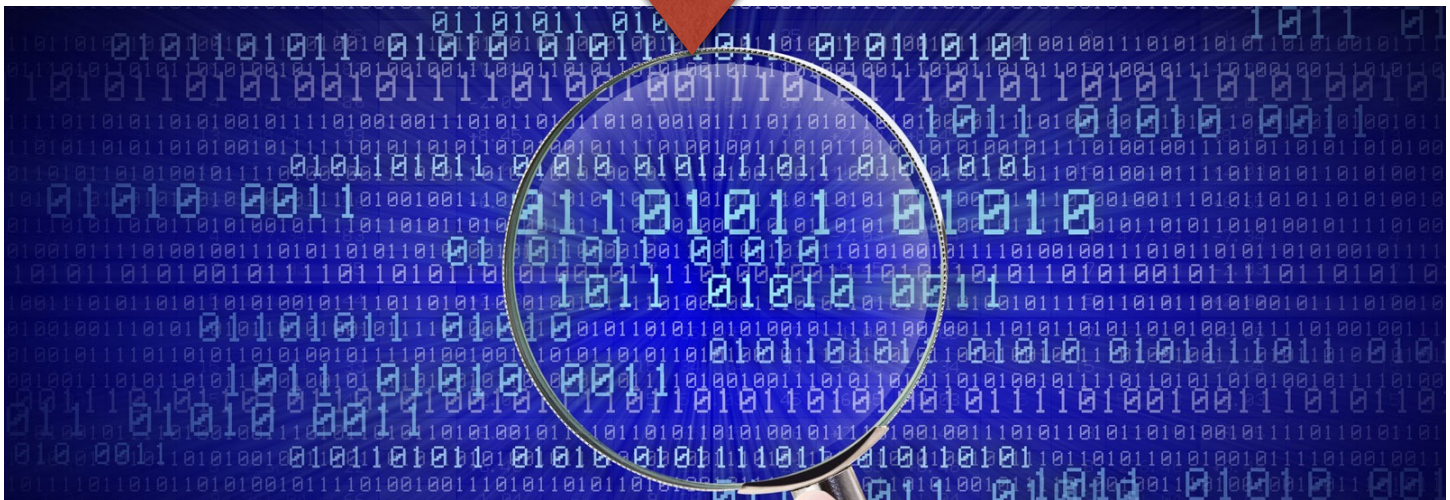
What do we put as input?



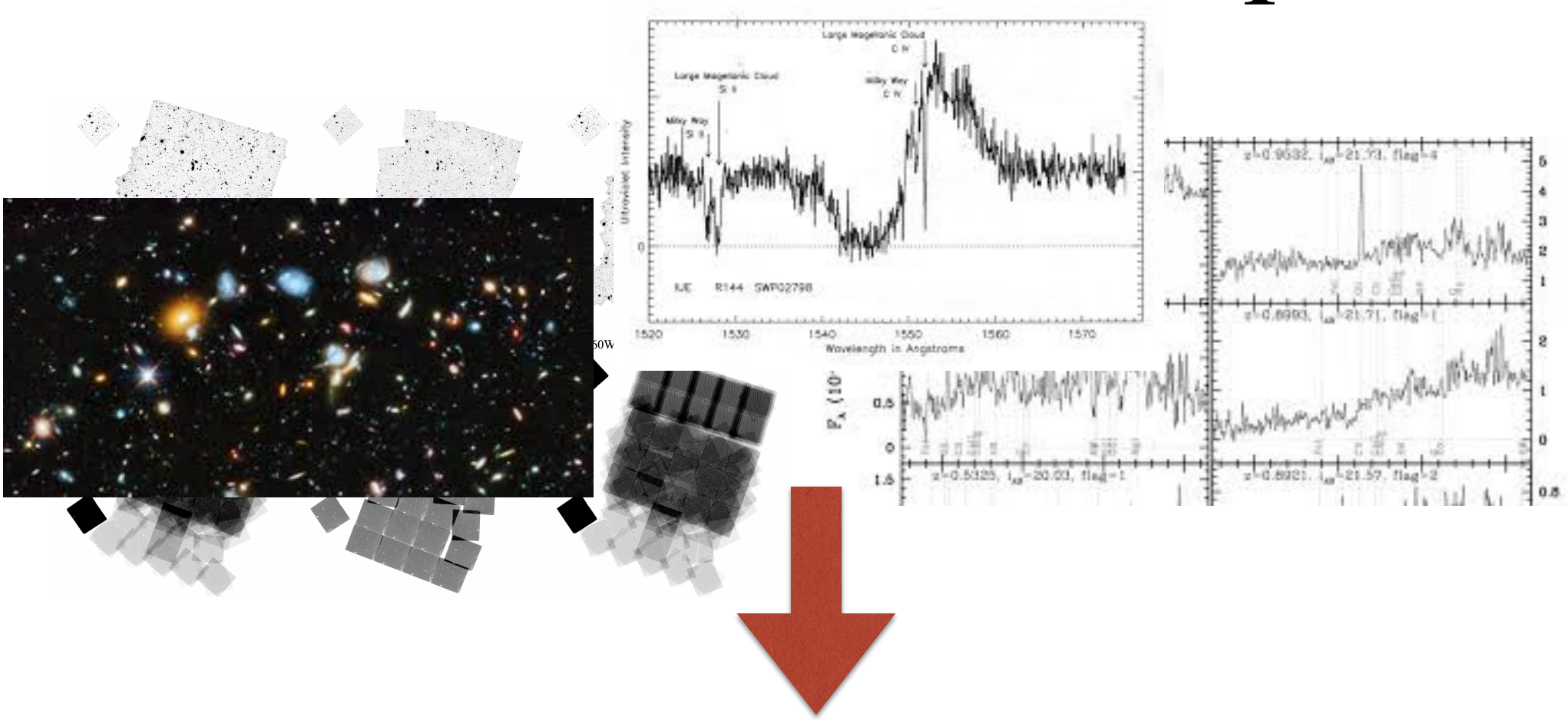




THIS IS WHAT MACHINES SEE

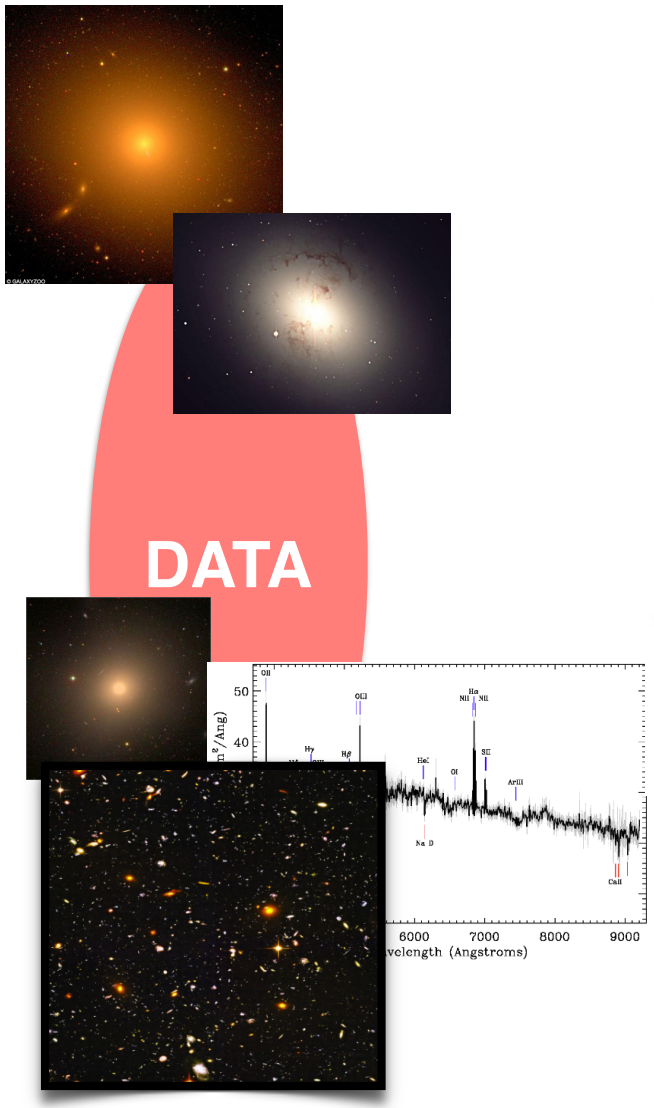


What do we put as input?



PRE-PROCESS DATA TO EXTRACT MEANINGFUL INFORMATION

THIS IS GENERALLY CALLED **FEATURE EXTRACTION**



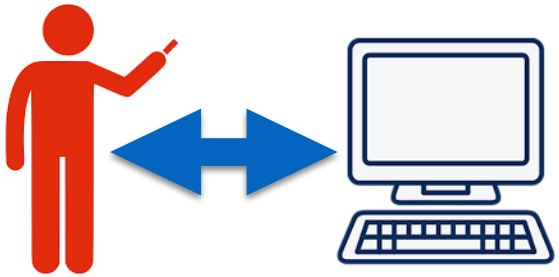
Spiral!

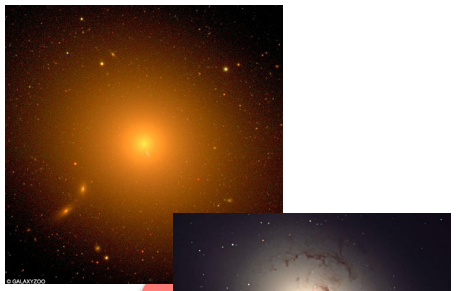
Emission line!

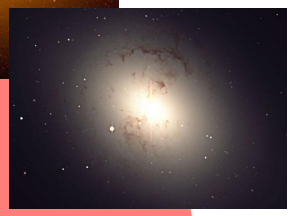
Merger!

Clump!

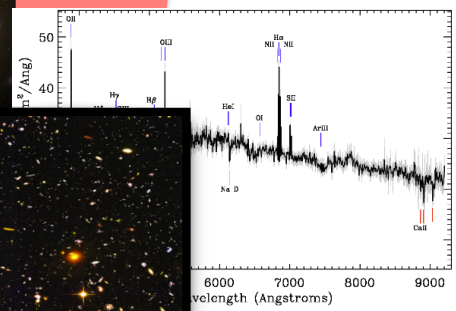
AGN!







DATA



Spiral!

Emission line!

Merger!

Clump!

AGN!

$$f_{\vec{W}}(\vec{x}) = \vec{y}$$

LABEL

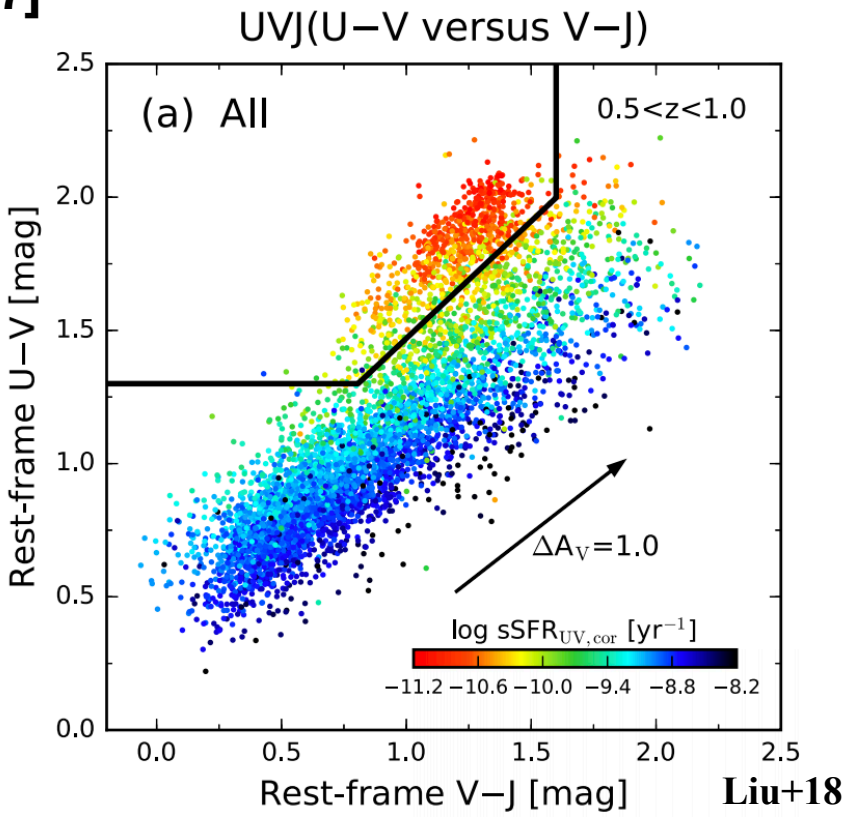
Q(0) , SF(1)

NETWORK FUNCTION

(U-V, V-J) FEATURES

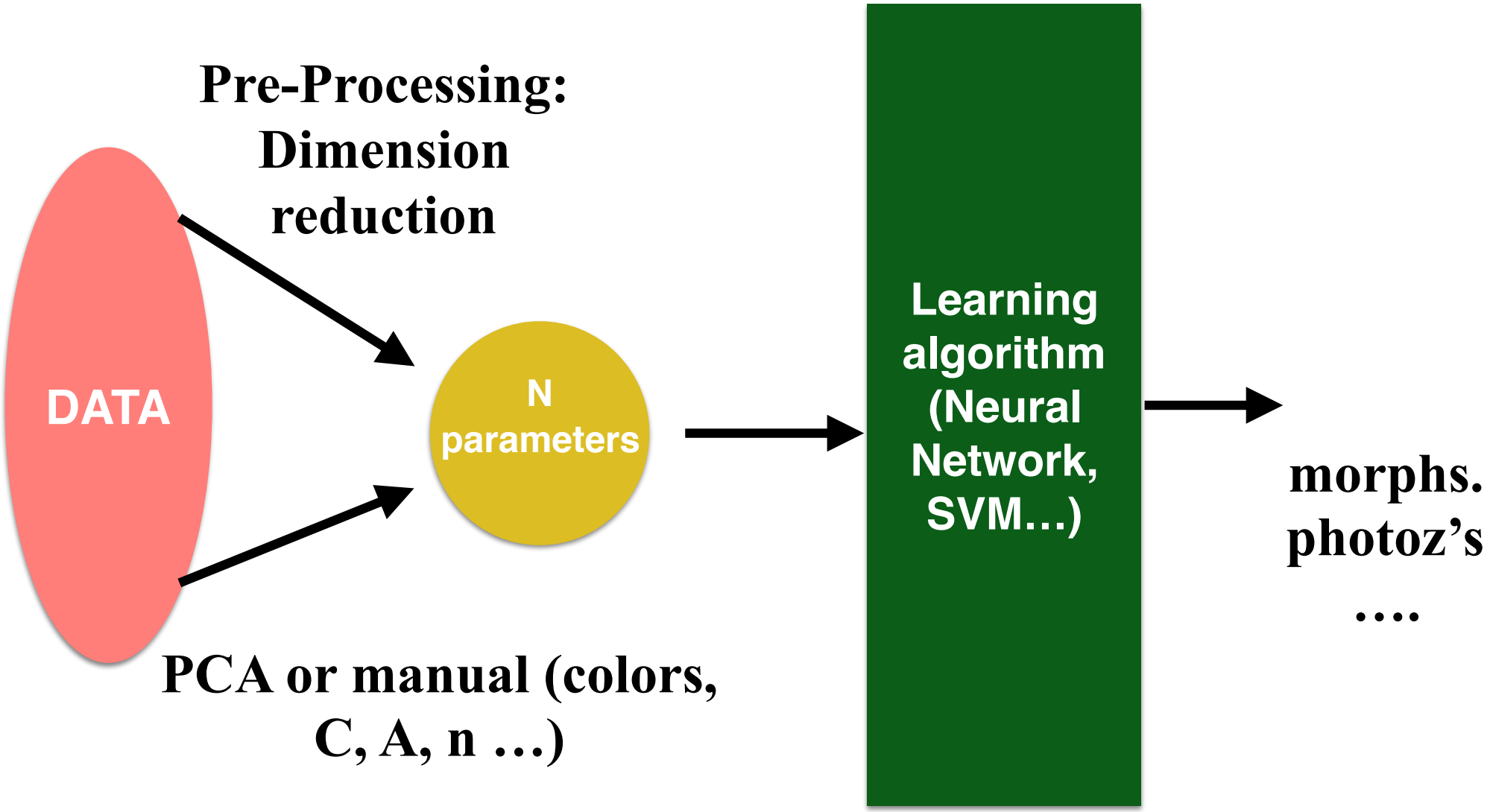
sgn[(u-v)-0.8*(v-j)-0.7]

WEIGHTS

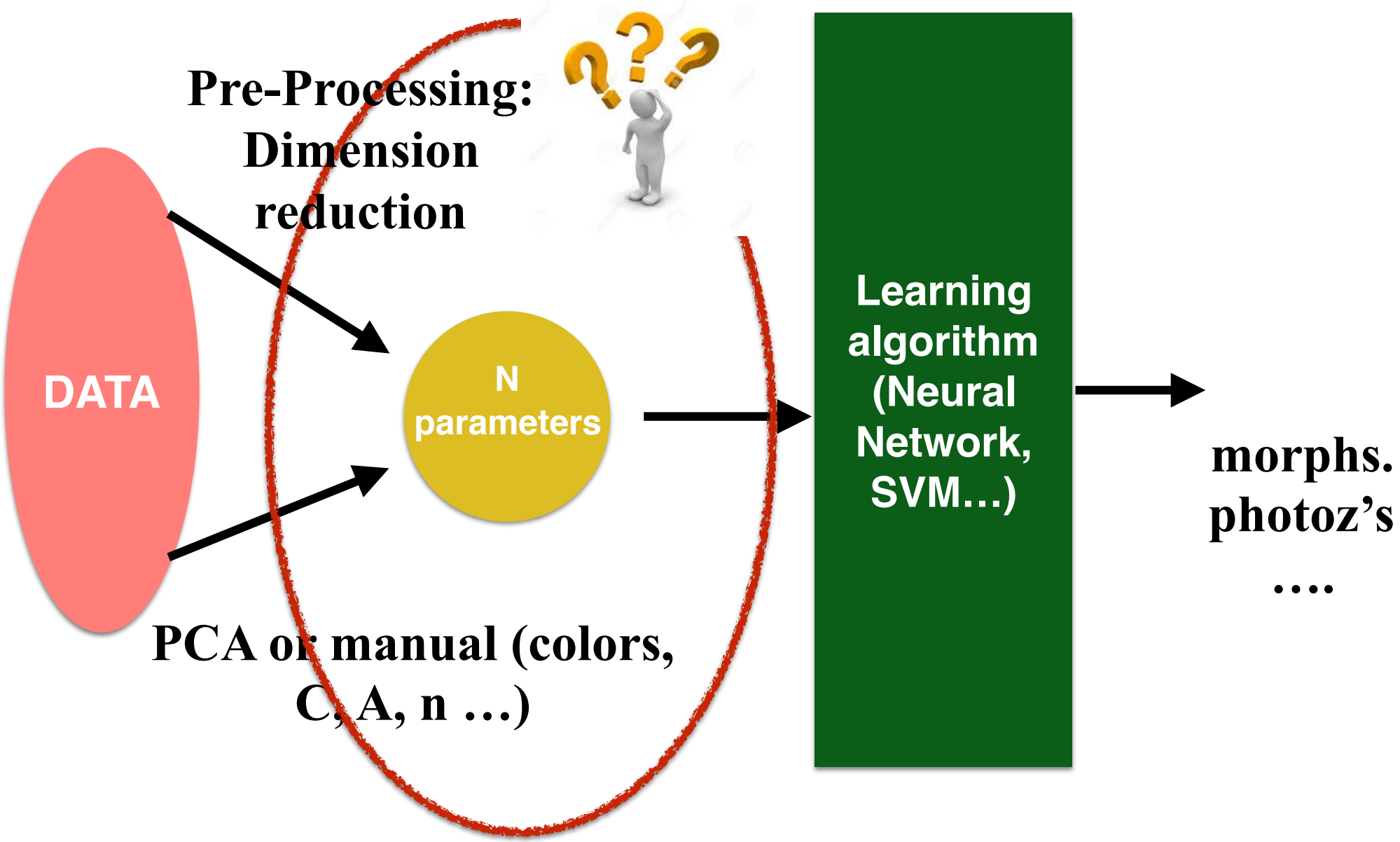


Liu+18

THE "CLASSICAL" APPROACH

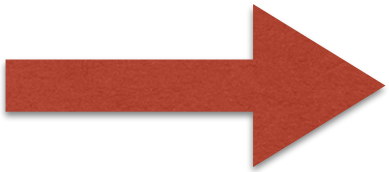


“CLASSICAL” MACHINE LEARNING



In Astronomy

- Colors, Fluxes
- Shape indicators
- Line ratios, spectral features
- Stellar Masses, Velocity Dispersions



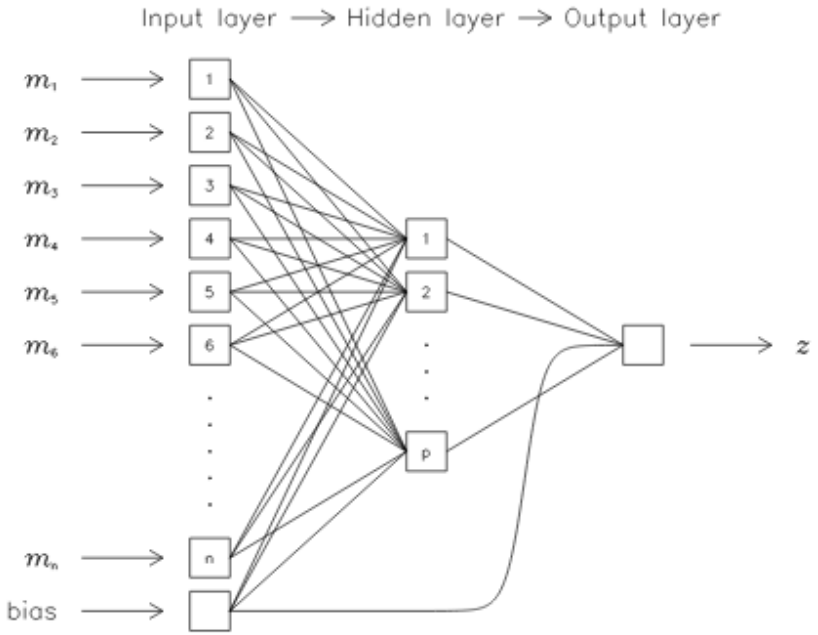
Requires specialized software before feeding the machine learning algorithm

IT IMPLIES A DIMENSIONALITY REDUCTION!

PHOTOMETRIC REDSHIFTS

SDSS

g
r
i
z



Collister+08

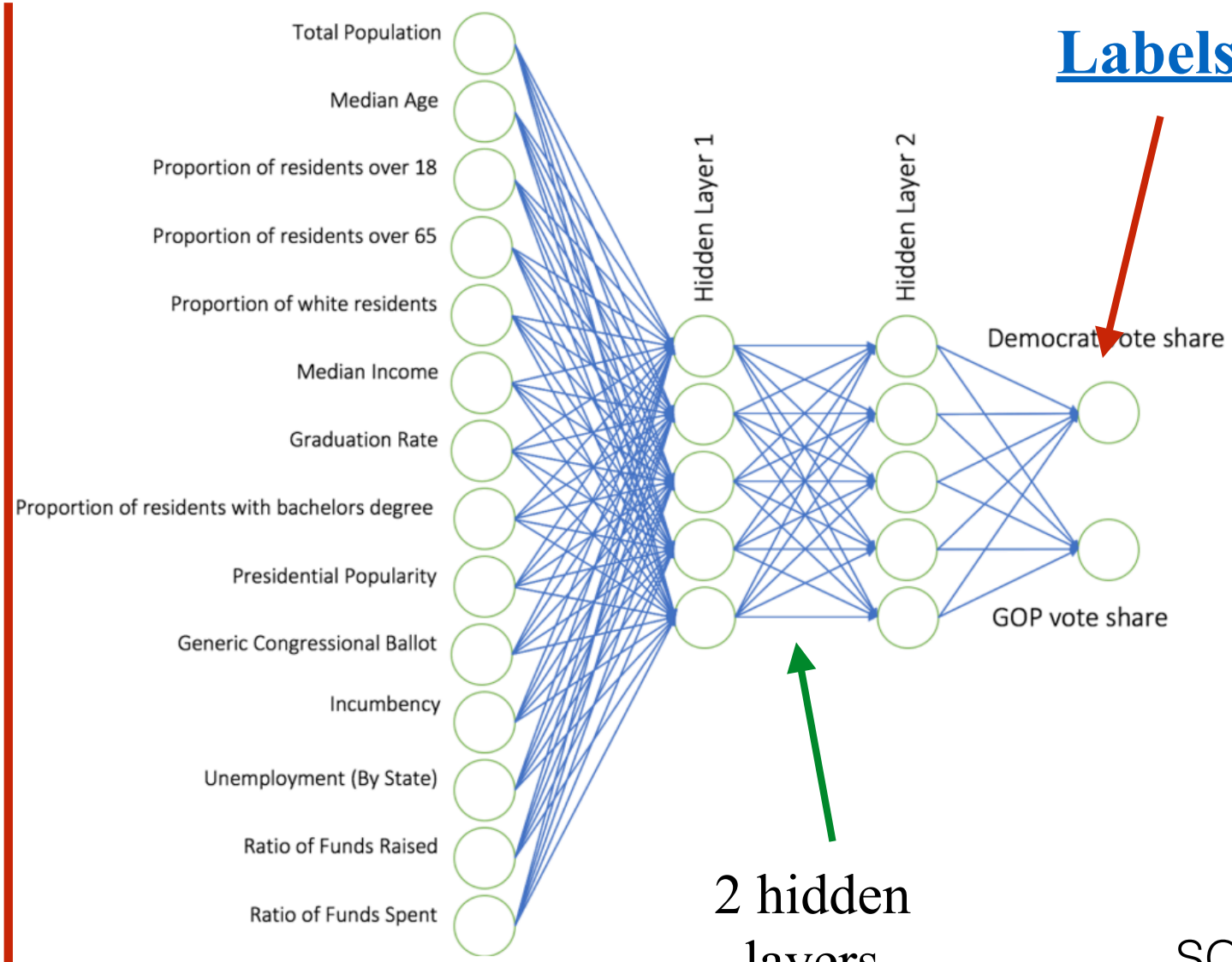
EVERYTHING IS IN THE FEATURES….WHAT IF I IGNORED SOME IMPORTANT FEATURES?

EVERYTHING IS IN THE FEATURES….WHAT IF I IGNORED SOME IMPORTANT FEATURES?

NEURAL NETWORK TO PREDICT RESULTS OF MIDTERM ELECTIONS

$$p = g_3(W_3 g_2(W_2 g_1(W_1 \vec{x_0})))$$

Features (x)



Labels (y)

2 hidden layers

SOURCE

NEURAL NETWORK TO PREDICT RESULTS OF MIDTERM ELECTIONS

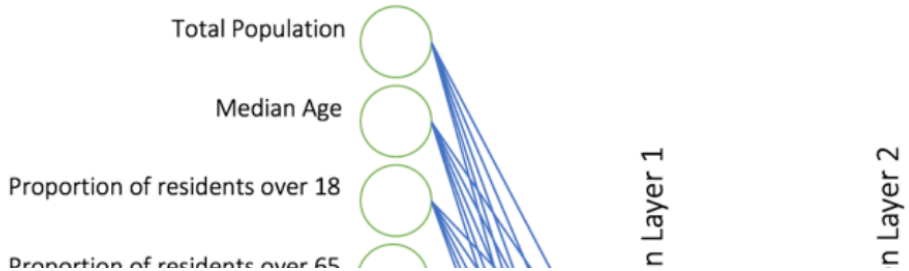
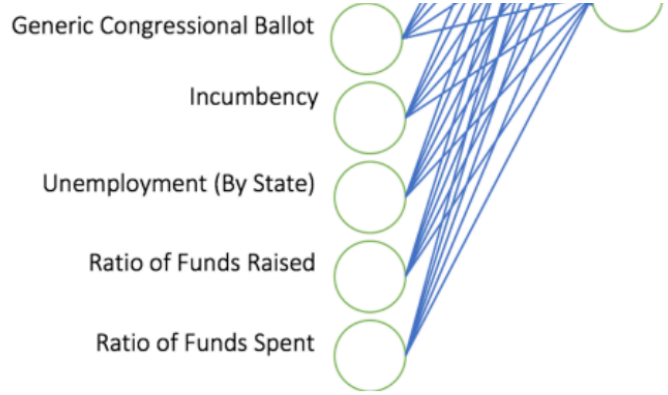


Table 2 – Results of both Models:

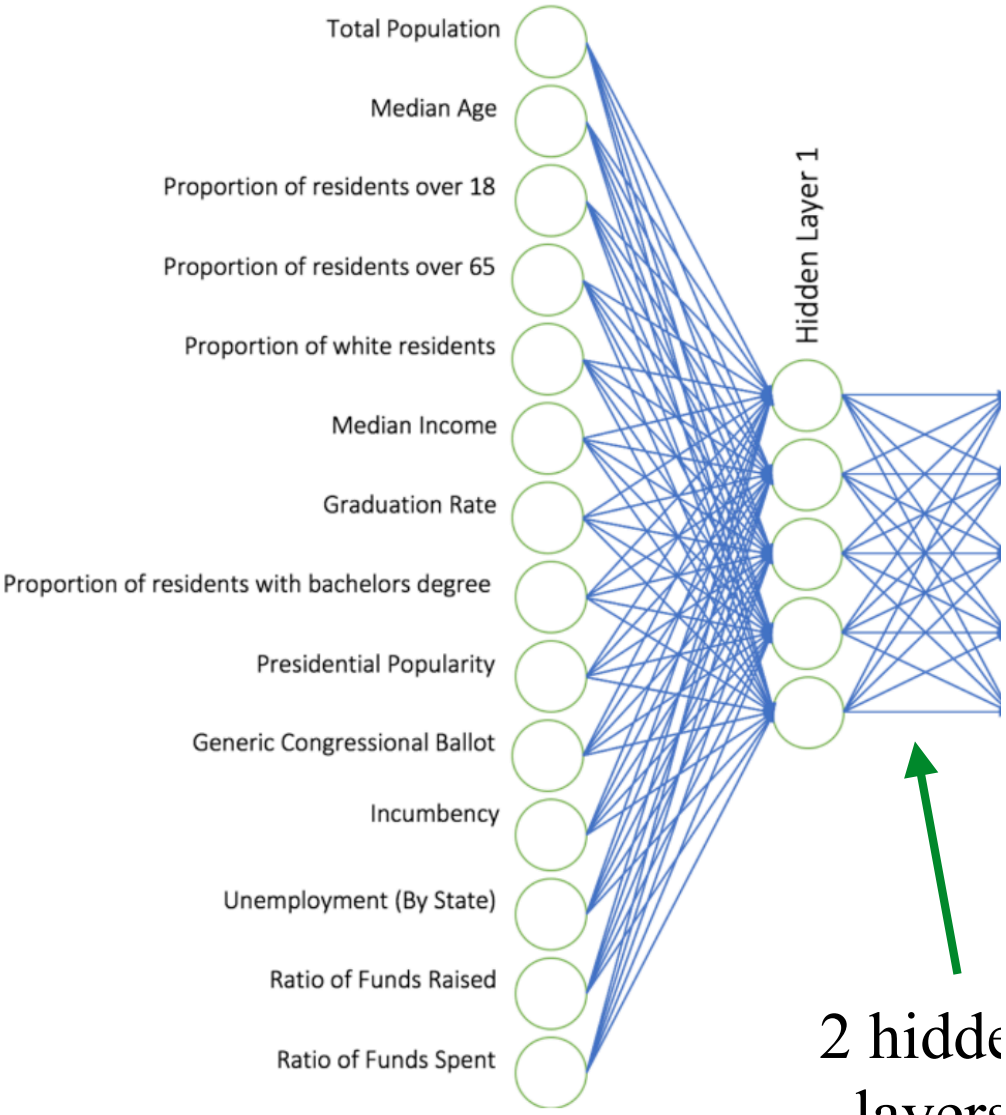
Model not including past elections (Model A)	***Model including past elections (Model B)***
D +3	***D +17***
Democrat Seats: 219	***Democrat Seats: 226***
Republican Seats: 216	***Republican Seats: 209***
33% chance of Republicans keeping house*	**0.3% chance of Republicans keeping house***



232+198

NEURAL NETWORK TO PREDICT RESULTS OF MIDTERM ELECTIONS

Features (x)



Bad Weather, Known to Lower Turnout, Will Greet Many Voters

Rain can decrease voter numbers, which studies show tends to help Republicans. “I hope it rains hard tomorrow,” one Republican candidate said.

10h ago

Other general computer vision features [for images!]

- Pixel Concatenation
- Color histograms
- Texture Features
- Histogram of Gradients
- SIFT

FOR MANY YEARS COMPUTER VISION RESEARCHERS HAVE BEEN TRYING TO FIND THE MOST GENERAL FEATURES

Other general computer vision features [for images!]

- Pixel Concatenation
- Color histograms
- Texture Features
- Histogram of Gradients
- SIFT

FOR MANY YEARS COMPUTER VISION RESEARCHERS HAVE BEEN TRYING TO FIND THE MOST GENERAL FEATURES

THE BEST CLASSICAL SOLUTION [BEFORE 2012] WHERE BASED **ON LOCAL FEATURES**

WHAT ABOUT USING RAW DATA?

ALL INFORMATION IS IN THE INPUT DATA

WHY REDUCING ?

LET THE NETWORK FIND THE INFO

WHAT ABOUT USING RAW DATA?

ALL INFORMATION IS IN THE INPUT DATA

WHY REDUCING ?

LET THE NETWORK FIND THE INFO

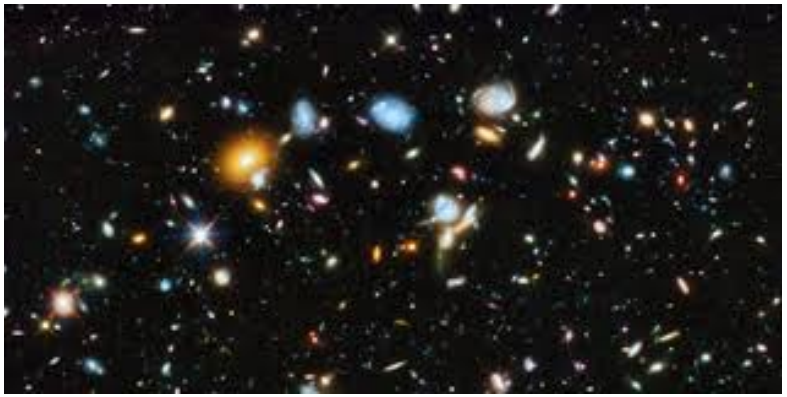
LARGE DIMENSION SIGNALS SUCH AS IMAGES OR SPECTRA WOULD REQUIRE TREMENDOUSLY LARGE MODELS

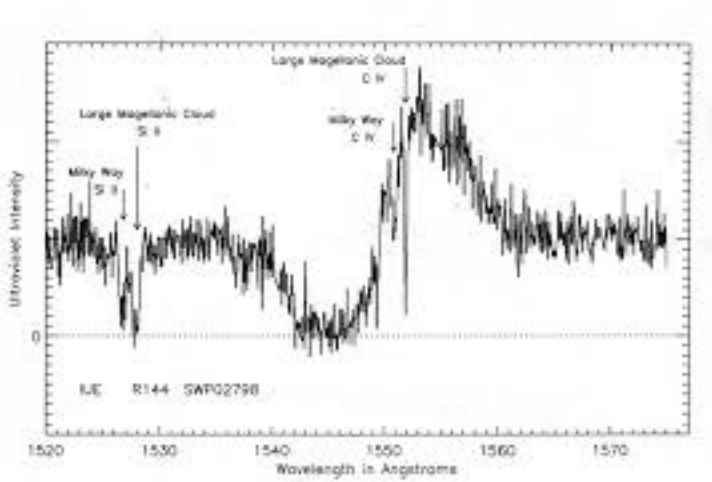
A 512x512 image as input of a fully connected layer producing output of same size:

$$(512 \times 512)^2 = 7e10$$

BUT

FEEDING INDIVIDUAL RESOLUTION ELEMENTS IS NOT VERY EFFICIENT SINCE IT LOOSES ALL INVARIANCE TO TRANSLATION AND IGNORES CORRELATION IN THE DATA AT ALL SCALES





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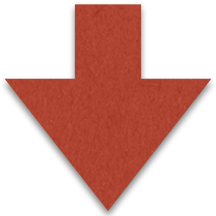
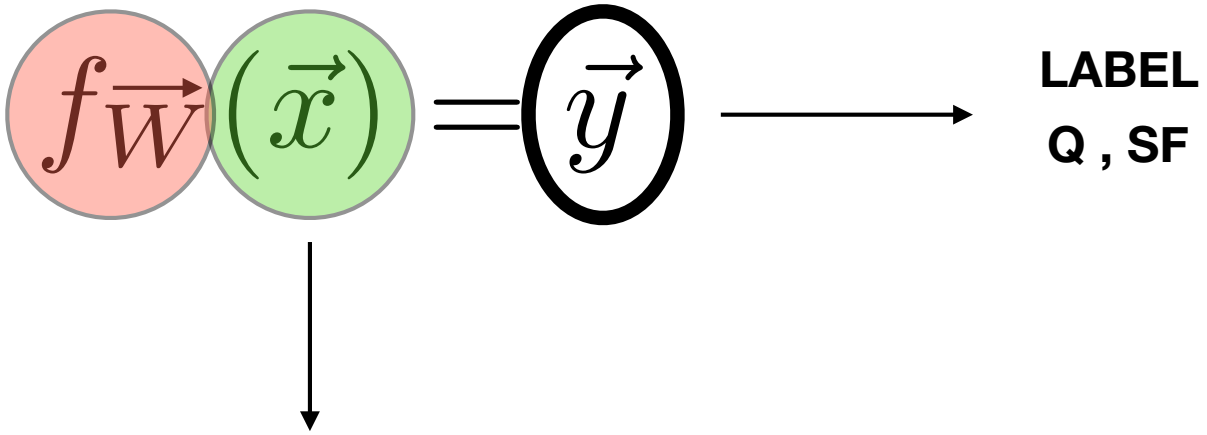


SO?

DEEP LEARNING



LET THE MACHINE FIGURE THIS OUT ("unsupervised feature extraction")

LET'S GO A STEP FORWARD INTO LOOSING CONTROL….