ME 536

— Week 12: <u>How deep is your love</u>* — *to learn*?

^{*}old times were very funny... what do you think today will look like in 45 years?

Learning:

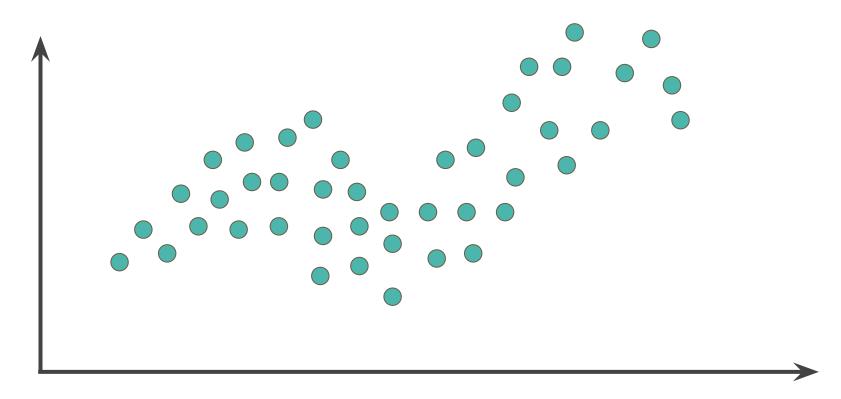
What to learn?

How to learn?

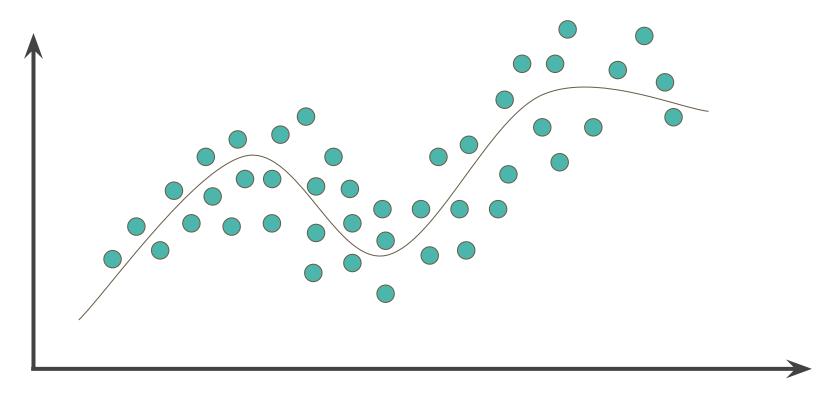
Learn once or life-long learning?

• • •

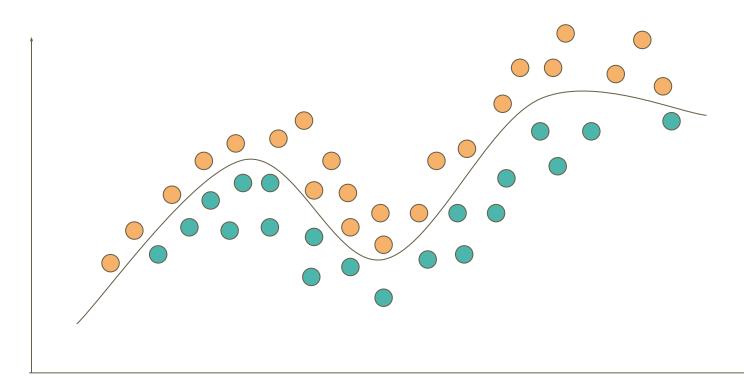
DATA



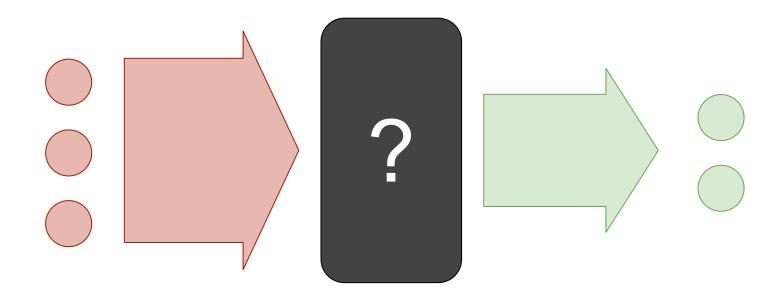
Regression



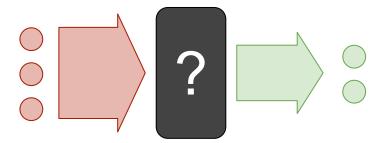
or Classification?



A black box: In general

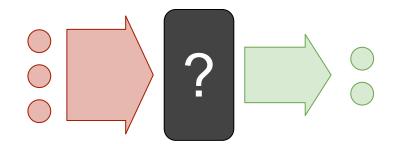


A black box: In general



- Data needed
- Type of model available?
 - What if model is not known at all?
 - What if the model is hard to derive?
- What if all inputs do not propagate at the same speed to output?
- What if data is available?
 - What if whole input spectrum is not covered in data?
- ...
- Does nature help?

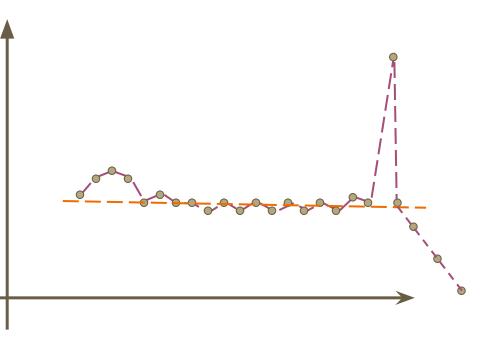
A black box: In general



While blackbox is identified:

- Can it generalize?
- Over- / under-fitting ... /learning

If this is from the step response of a second order system? Why use an ANN?

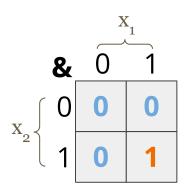


Rules of thumb



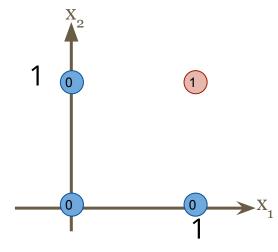
- Do not expect miracles from ANN and do not blindly use them!
- Direct use of ANNs without prior analysis might be **more costly**than expected.
- If you have a good understanding of the model why not identify the parameters and use the model?
- Analysis of why ANNs misbehave is tricky
- Best ANN topology to start with is not necessarily known given the problem.
- If you have partial prior **understanding of your model**, try to inject into the ANN if possible.

A simple case: logic AND

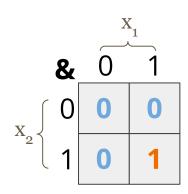


Just a line is enough...

Isn't it?



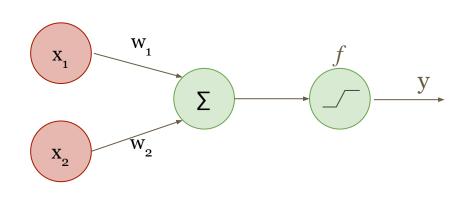
A simple case: perceptron w/o bias

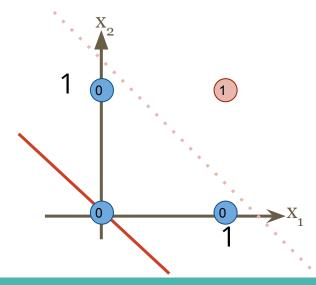


Just a line is enough...

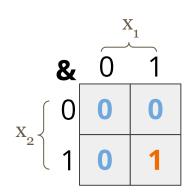
Isn't it? or how about a scalar field?

$$y = f(x_1 w_1 + x_2 w_2)$$





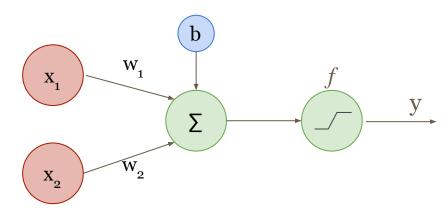
A simple case: perceptron

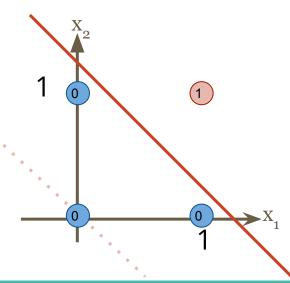


Just a line is enough...

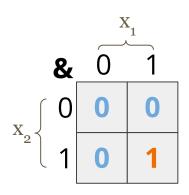
Isn't it? or how about a scalar field?

$$y = f(x_1w_1 + x_2w_2 + b)$$
 where is the y axis?





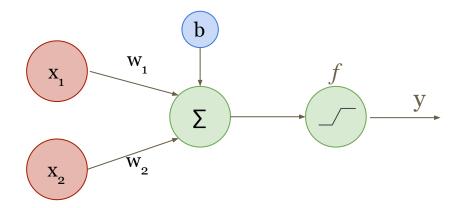
A simple case: More compact form - dimension free

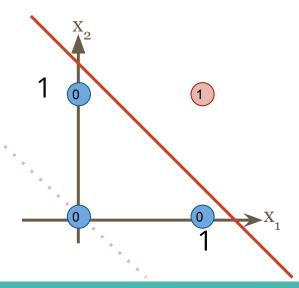


$$y = f(x_1 w_1 + x_2 w_2 + b)$$

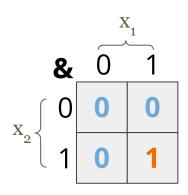
Let $\mathbf{x}^T = [\mathbf{x}_1 \ \mathbf{x}_2], \mathbf{w}^T = [\mathbf{w}_1 \ \mathbf{w}_2]$ - dimension of \mathbf{x}, \mathbf{w} does not matter

$$y = f(\mathbf{x}^{\mathrm{T}} \mathbf{w} + \mathbf{b})$$





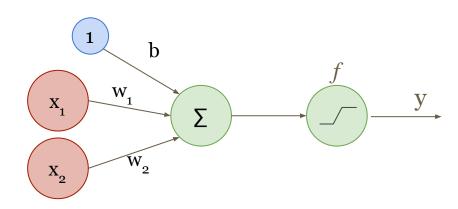
A simple case: Alternative form

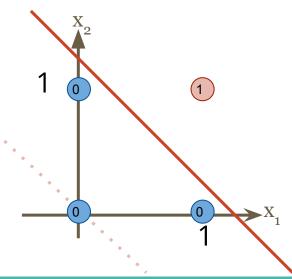


$$y = f(x_1 w_1 + x_2 w_2 + b)$$

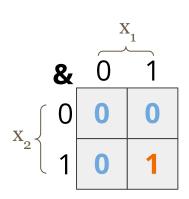
Let
$$\mathbf{x}^{\mathrm{T}} = \begin{bmatrix} 1 \ \mathbf{x}_{1} \ \mathbf{x}_{2} \end{bmatrix}$$
, $\mathbf{w}^{\mathrm{T}} = \begin{bmatrix} \mathbf{b} \ \mathbf{w}_{1} \ \mathbf{w}_{2} \end{bmatrix}$

$$y = f(\mathbf{x}^T \mathbf{w})$$





A simple case: How to initialize w_i ?



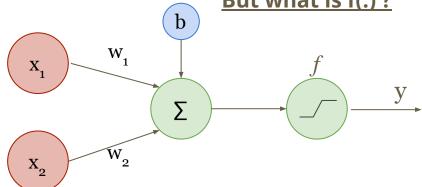
Random sounds good in general,

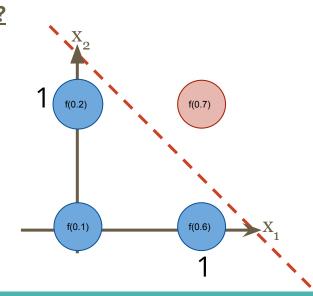
so let:
$$\mathbf{w}^{T} = [0.5 \ 0.1], b = 0.1$$

$$y = f(x^T w + b) = f(0.5x_1 + 0.1x_2 + 0.1)$$

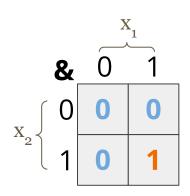
What should f(.) return?

But what is f(.)?





A simple case: How lucky can we get?



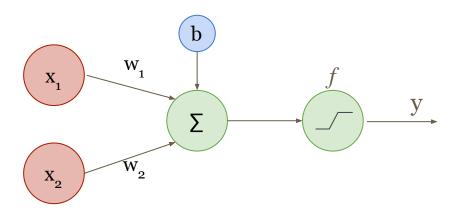
Random sounds good in general, so let: $\mathbf{w}^{T} = [0.5 \ 0.1], b = 0.1$

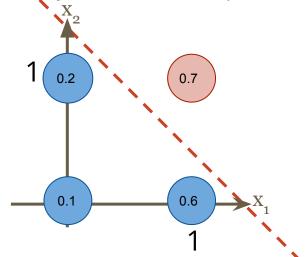
$$y = f(x^T w + b) = f(0.5x_1 + 0.1x_2 + 0.1)$$

What if
$$f(x) = x$$

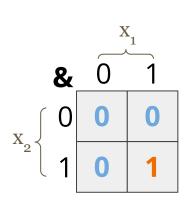
$$y = 0.5 x_1 + 0.1 x_2 + 0.1$$

Will simple case work here? May be with a bit of post-work?





A simple case: Which *f*?



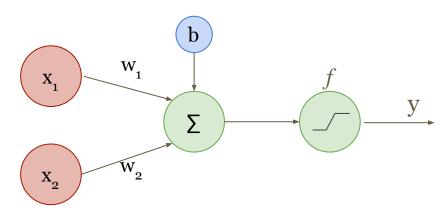
Let:
$$\mathbf{w}^{T} = [0.5 \ 0.1], b = 0.1$$

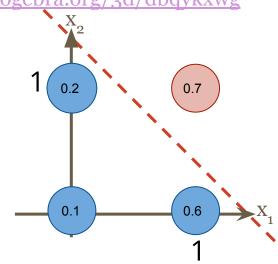
$$y = f(x^T w + b) = f(0.5x_1 + 0.1 x_2 + 0.1),$$

simple case
$$f(x) = x$$
,

simple case
$$f(x) = x$$
, $y = 0.5 x_1 + 0.1 x_2 + 0.1$

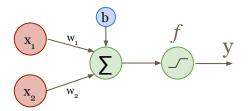
Check out https://www.geogebra.org/3d/dbgykxwg





In general: Which *f*?

Check out: https://www.geogebra.org/calculator/kzexwpwz



Sigmoid

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

$$f'(x) = f(x)(1 - f(x))$$

Tangent Hyperbolic

Tanh and its derivative

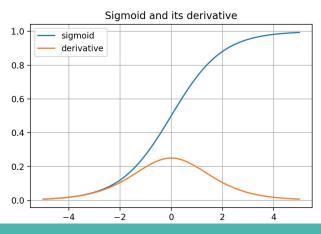
$$f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

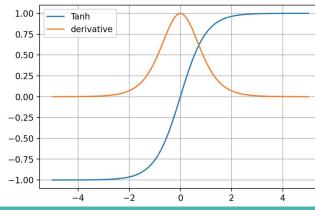
$$f'(x) = 1 - f(x)^2$$

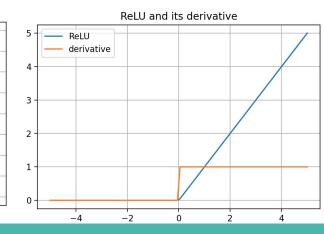
Rectified Linear Unit: a.k.a ReLU

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

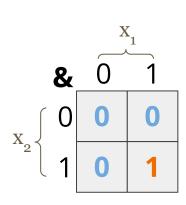
$$f'(x) = \begin{cases} 1, & for x > 0 \\ 0, & otherwise \end{cases}$$







A simple case: Which f is?

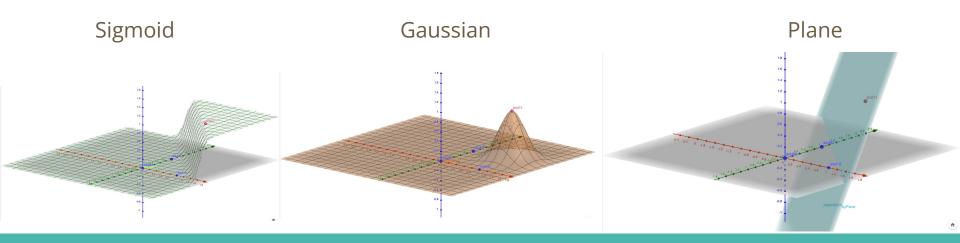


Let:
$$\mathbf{w}^{T} = [0.5 \ 0.1], b = 0.1$$

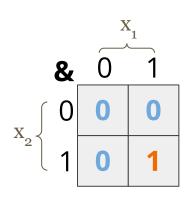
$$y = f(\mathbf{x}^T \mathbf{w} + \mathbf{b}) = f(0.5x_1 + 0.1x_2 + 0.1),$$

sigmoid case
$$f(x) = (1+e^{-x})^{-1}$$
,

Check out https://www.geogebra.org/3d/dbqykxwg



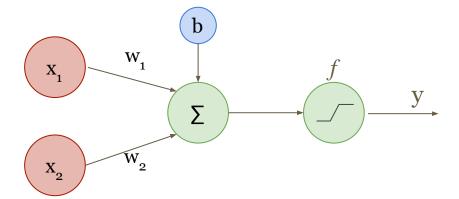
A simple case: How to generate training data?

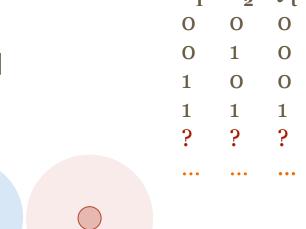


$$y = f(x_1 w_1 + x_2 w_2 + b)$$

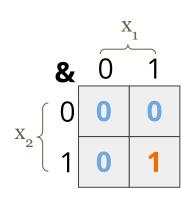
Let
$$\mathbf{x}^{\mathrm{T}} = [\mathbf{x}_{1} \ \mathbf{x}_{2}], \mathbf{w}^{\mathrm{T}} = [\mathbf{w}_{1} \ \mathbf{w}_{2}]$$

$$y = f(\mathbf{x}^{\mathrm{T}} \mathbf{w} + \mathbf{b})$$





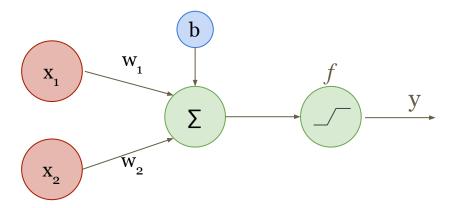
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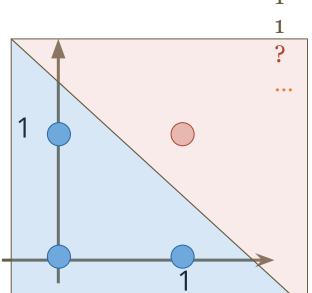


$$y = f(x_1 w_1 + x_2 w_2 + b)$$

Let
$$\mathbf{x}^{T} = [\mathbf{x}_{1} \ \mathbf{x}_{2}], \mathbf{w}^{T} = [\mathbf{w}_{1} \ \mathbf{w}_{2}]$$

$$y = f(\mathbf{x}^{\mathrm{T}} \mathbf{w} + \mathbf{b})$$





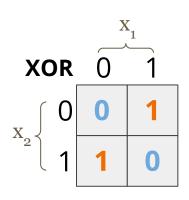
 $\mathbf{X_1}$ $\mathbf{X_2}$ $\mathbf{y_1}$ $\mathbf{0}$ $\mathbf{0}$ $\mathbf{0}$

1 0 0

 $\begin{array}{ccc} 1 & 1 \\ \hline \end{array}$?

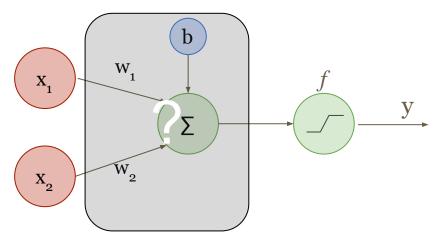
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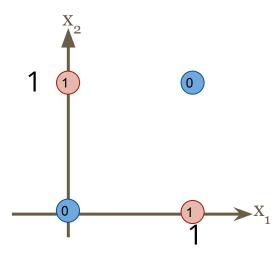
A not so simple case: when one line ain't enough



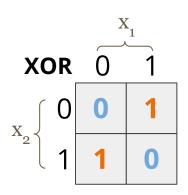
$$y = f(x_1 w_1 + x_2 w_2 + b)$$
Let $\mathbf{x}^T = [x_1 \ x_2], \mathbf{w}^T = [w_1 \ w_2]$

$$y = f(\mathbf{x}^T \mathbf{w} + b)$$



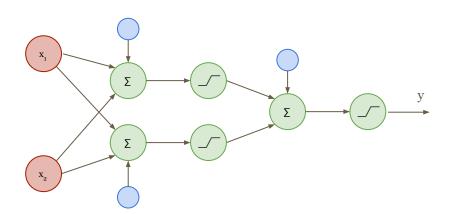


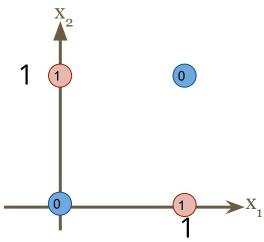
A not so simple case: when one line ain't enough



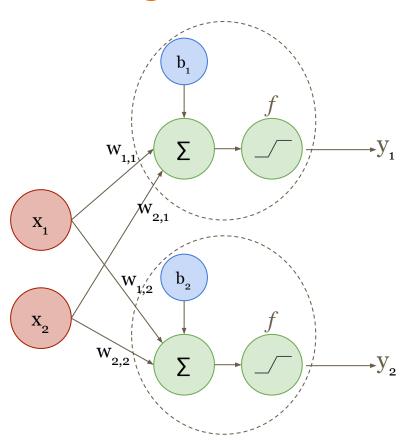
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Let $\mathbf{x}^T = [x_1 \ x_2], \mathbf{w}^T = [w_1 \ w_2]$

$$y = f(\mathbf{x}^T \mathbf{w} + b)$$





A more general case: MIMO - 2x2



Let:

$$\mathbf{x}^{\mathrm{T}} = [\mathbf{x}_{1} \ \mathbf{x}_{2}]$$

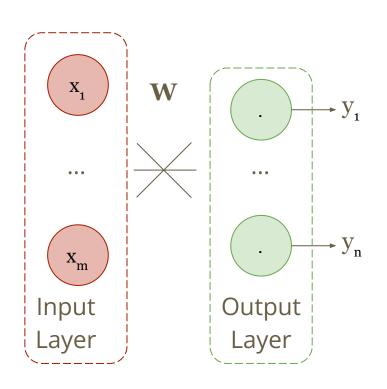
$$\mathbf{W} = \left[\begin{array}{c} \mathbf{W}_{1,1} & \mathbf{W}_{1,2} \\ \mathbf{W}_{2,1} & \mathbf{W}_{2,2} \end{array} \right]$$

$$\mathbf{b} = [b_1 \ b_2]$$

$$\mathbf{y} = [\mathbf{y}_1 \ \mathbf{y}_2]$$

$$\mathbf{y} = f(\mathbf{x}^{\mathrm{T}} \mathbf{W} + \mathbf{b})$$

A more general case: Input & Output Layers - MIMO



Let:

$$\mathbf{x}^{\mathrm{T}} = [\mathbf{x}_{1} \dots \mathbf{x}_{m}]$$

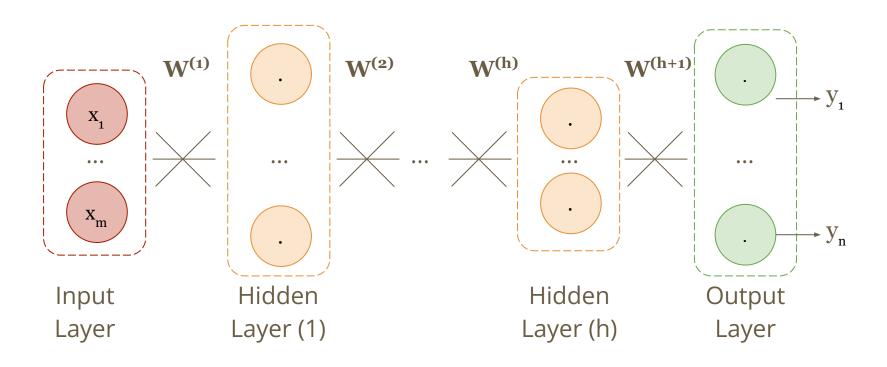
$$\mathbf{W} = \begin{bmatrix} \mathbf{w}_{1,1} & \dots & \mathbf{w}_{1,n} \\ \dots & \dots & \\ \mathbf{w}_{m,1} & \dots & \mathbf{w}_{m,n} \end{bmatrix}$$

$$\mathbf{b} = [b_1 \dots b_n]$$

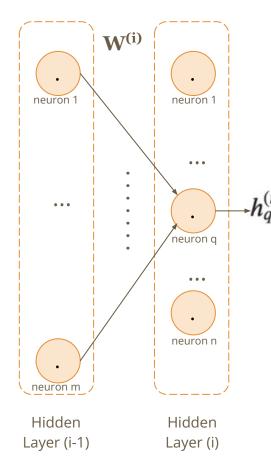
$$\mathbf{y} = [\mathbf{y}_1 \dots \mathbf{y}_n]$$

$$\mathbf{y} = f(\mathbf{x}^{\mathrm{T}} \mathbf{W} + \mathbf{b})$$

Most general case: Shallow & Deep & Deeper



Most general case: Output of any neuron



Let hidden layers (i-1), i have m, n neurons respectively.

 $\boldsymbol{h}_{q}^{(i)}$ is the output of the \boldsymbol{q}^{th} neuron at the i^{th} hidden layer.

Weight $w_{p,q}^{(i)}$ is between the q^{th} neuron at hidden layer i and p^{th} neuron at the previous layer.

Bias for neuron q at hidden layer i is $b_q^{(i)}$.

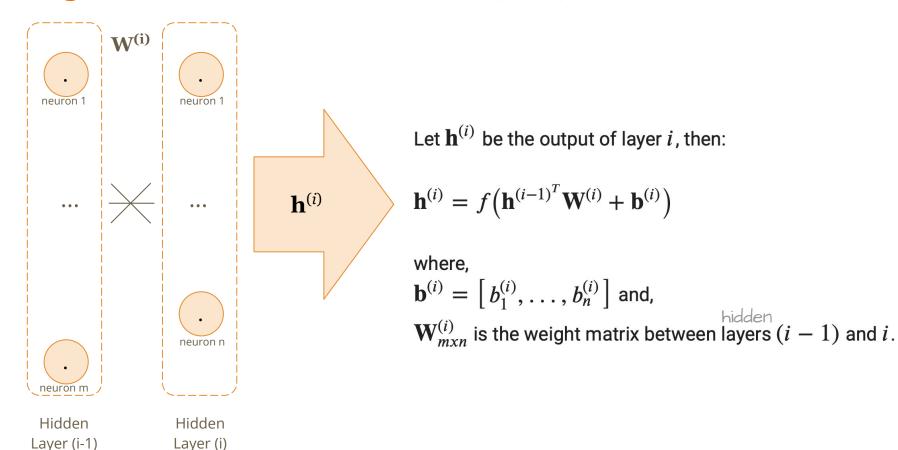
Then $h_q^{(i)}$ can be written as:

$$h_q^{(i)} = f\left(\sum_{i=1}^m \left[h_j^{(i-1)} w_{j,q}^{(i)} + b_q^{(i)}\right]\right)$$

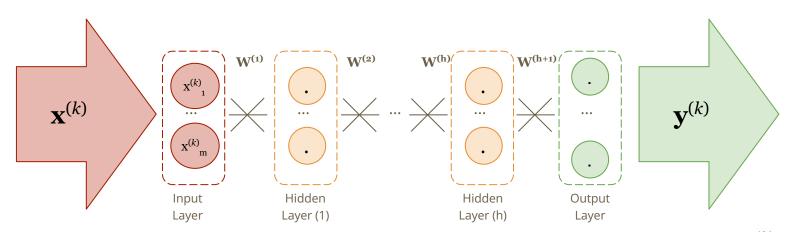
where,

 $f(\cdot)$ is the activation function.

Most general case: Output of any layer



Most general case: Output of the network



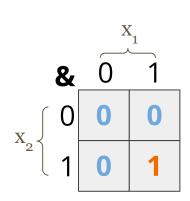
Note that, in general there will be several inputs, so let there be d many data points $\mathbf{x}^{(k)}$ as input and $\mathbf{y}^{(k)}$ is the corresponding network *prediction*/output, where $k=1,\ldots,d$.

$$\mathbf{y}^{(k)} = f(f(\dots f(f(\mathbf{x}^{(k)^T}\mathbf{W}^{(1)} + \mathbf{b}^{(1)})^T\mathbf{W}^{(2)} + \mathbf{b}^{(2)})^T \dots)^T\mathbf{W}^{(h+1)} + \mathbf{b}^{(h+1)})$$

In more general terms,

$$\mathbf{y}^{(k)} = F(\mathbf{x}^{(k)}, \mathbf{W})$$
, where $\mathbf{W} = \left\{\mathbf{W}^{(1)}, \dots, \mathbf{W}^{(h+1)}\right\}$ i.e. it represents the set of all $\mathbf{W}^{(i)}$ s.

A sample case: How to train? When to train?



Initialize: $\mathbf{w}^{T} = [0.5 \ 0.1], b = 0.1$

$$y = f(x^T w + b) = f(0.5x_1 + 0.1x_2 + 0.1)$$
, simple case $\rightarrow f(x) = x$

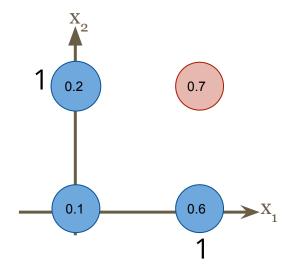
$$y = 0.5 x_1 + 0.1 x_2 + 0.1,$$

where y_t is the **true value**, i.e. ground truth

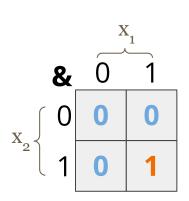
How and **when** to update w_i ?

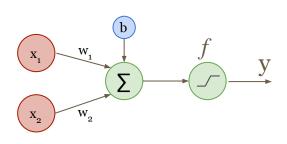
| (b) | X_{1} | X |
|--|---------|---|
| $v \rightarrow w$ | 0 | C |
| X_1 W_1 Y | O | 1 |
| 2 | 1 | C |
| $\left(\begin{array}{c} X_2 \\ \end{array}\right)$ | 1 | 1 |

| X_{1} | X_2 | \mathbf{y}_{t} | y | error |
|---------|-------|------------------|-----|-------|
| 0 | O | (O | 0.1 | 0.1 |
| O | 1 | O | 0.2 | 0.2 |
| 1 | 0 | 0 | 0.6 | 0.6 |
| 1 | 1 | 1 | 0.7 | 0.3 |
| | | | | |



A sample case: What to minimize at the end? J?





Initialize: $\mathbf{w}^{T} = [0.5 \ 0.1], b = 0.1$

$$y = f(x^T w + b) = f(0.5x_1 + 0.1x_2 + 0.1)$$
, simple case $f(x) = x$

$$y = 0.5 x_1 + 0.1 x_2 + 0.1$$

| X_{1} | X_2 | \mathbf{y}_{t} | y | err |
|---------|-------|------------------|-----|--------------------|
| O | O | O | 0.1 | $\left[0.1\right]$ |
| 0 | 1 | O | 0.2 | 0.2 |
| 1 | O | O | 0.6 | 0.6 |
| 1 | 1 | 1 | 0.7 | 0.3 |
| | | | | $\sim \sim$ |

Loss function: $L(\mathbf{y}_t, \mathbf{y})$ $L_i(\mathbf{y}_t, \mathbf{y})$ Loss for *input i*

Total loss in this case:

$$J = L_1 + ... + L_4$$

Where J is the cost function

where \mathbf{y}_{t} , \mathbf{y} are the vectors representing the **ground truth** and the **network output**, *i.e. network prediction* respectively.

Tensor Flow: Loss functions...

```
class BinaryCrossentropy: Computes the cross-entropy loss between true labels and predicted labels.
class CategoricalCrossentropy: Computes the crossentropy loss between the labels and predictions.
class CategoricalHinge: Computes the categorical hinge loss between y_true and y_pred.
class CosineSimilarity: Computes the cosine similarity between labels and predictions.
class Hinge: Computes the hinge loss between y_true and y_pred.
class Huber: Computes the Huber loss between y_true and y_pred.
class KLDivergence: Computes Kullback-Leibler divergence loss between y_true and y_pred.
class LogCosh: Computes the logarithm of the hyperbolic cosine of the prediction error.
class Loss Loss base class.
class MeanAbsoluteError: Computes the mean of absolute difference between labels and predictions.
class MeanAbsolutePercentageError: Computes the mean absolute percentage error between v_true and v_pred.
class MeanSquaredError: Computes the mean of squares of errors between labels and predictions.
class MeanSquaredLogarithmicError: Computes the mean squared logarithmic error between y_true and y_pred.
class Poisson: Computes the Poisson loss between y_true and y_pred.
class Reduction: Types of loss reduction.
class SparseCategoricalCrossentropy: Computes the crossentropy loss between the labels and predictions.
class SquaredHinge: Computes the squared hinge loss between y_true and y_pred.
```

Check out: https://www.tensorflow.org/api_docs/python/tf/keras/losses

pyTorch Flow: Loss functions...

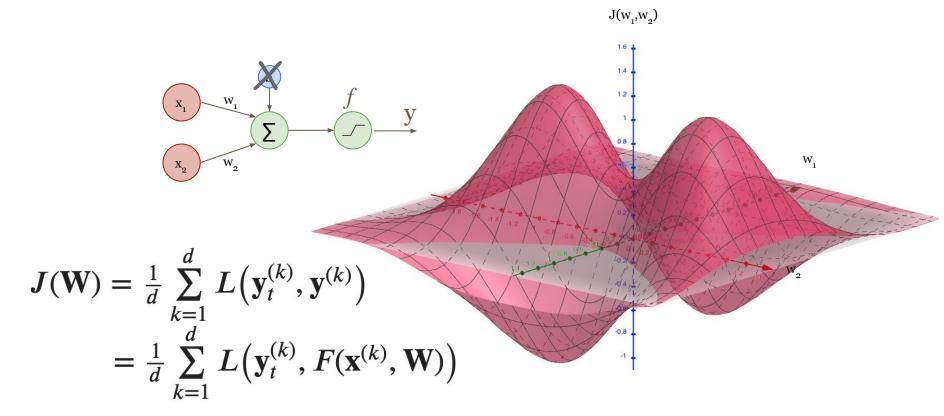
| nn.L1Loss | Creates a criterion that measures the mean absolute error (MAE) between each element in the input \boldsymbol{x} and target \boldsymbol{y} . |
|----------------------|---|
| nn.MSELoss | Creates a criterion that measures the mean squared error (squared L2 norm) between each element in the input x and target y . |
| nn.CrossEntropyLoss | This criterion computes the cross entropy loss between input and target. |
| nn.CTCLoss | The Connectionist Temporal Classification loss. |
| nn .NLLLoss | The negative log likelihood loss. |
| nn.PoissonNLLLoss | Negative log likelihood loss with Poisson distribution of target. |
| nn.GaussianNLLLoss | Gaussian negative log likelihood loss. |
| nn.KLDivLoss | The Kullback-Leibler divergence loss measure |
| nn.BCELoss | Creates a criterion that measures the Binary Cross Entropy between the target and the input probabilities: |
| nn.BCEWithLogitsLoss | This loss combines a <i>Sigmoid</i> layer and the <i>BCELoss</i> in one single class. |
| nn.MarginRankingLoss | Creates a criterion that measures the loss given inputs $x1$, $x2$, two 1D mini-batch <i>Tensors</i> , and a label 1D mini-batch tensor y (containing 1 or -1). |

| n.HingeEmbeddingLoss | Measures the loss given an input tensor \boldsymbol{x} and a labels tensor \boldsymbol{y} (containing 1 or -1). |
|---------------------------------|--|
| n.MultiLabelMarginLoss | Creates a criterion that optimizes a multi-class multi-class filtration hinge loss (margin-based loss) between input x (a 2D mini-batch $Tensor$) and output y (which is a 2D $Tensor$ of target class indices). |
| n.HuberLoss | Creates a criterion that uses a squared term if the absolute element-wise error falls below delta and a delta-scaled L1 term otherwise. |
| n.SmoothLiloss | Creates a criterion that uses a squared term if the absolute element-wise error falls below beta and an L1 term otherwise. |
| n.SoftMarginLoss | Creates a criterion that optimizes a two-class classification logistic loss between input tensor x and target tensor y (containing 1 or -1). |
| n.MultiLabelSoftMarginLoss | Creates a criterion that optimizes a multi-label one-versus-all loss based on max-entropy, between input x and target y of size $(N,C).$ |
| n.CosineEmbeddingLoss | Creates a criterion that measures the loss given input tensors x_1,x_2 and a \textit{Tensor} label y with values 1 or -1. |
| n.MultiMarginLoss | Creates a criterion that optimizes a multi-class classification hinge loss (margin-based loss) between input x (a 2D mini-batch <i>Tensor</i>) and output y (which is a 1D tensor of target class indices, $0 \leq y \leq x.size(1)-1$): |
| n.TripletMarginloss | Creates a criterion that measures the triplet loss given an input tensors $x1,x2,x3$ and a margin with a value greater than $0.$ |
| n.TripletMarginWithDistanceLoss | Creates a criterion that measures the triplet loss given input tensors $a, p,$ and n (representing anchor, positive, and negative examples, respectively), and a nonnegative, real-valued function ("distance function") used to compute the relationship between the anchor and positive example ("positive distance") and the anchor and negative example ("negative distance"). |
| | |

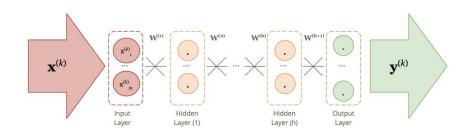
Measures the loss given an input tensor x and a labels

Check out: https://pytorch.org/docs/stable/nn.html#loss-functions

Simple Loss Surface & Cost Function: A hypothetical case



Loss Surface Minima: A search problem



For d data points, cost function can be written as:

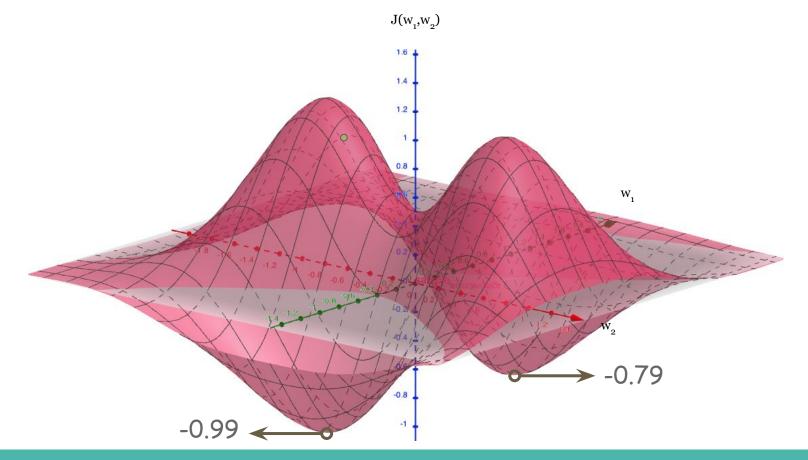
$$J(\mathbf{W}) = \frac{1}{d} \sum_{k=1}^{d} L(\mathbf{y}_{t}^{(k)}, \mathbf{y}^{(k)}) = \frac{1}{d} \sum_{k=1}^{d} L(\mathbf{y}_{t}^{(k)}, F(\mathbf{x}^{(k)}, \mathbf{W}))$$

 $J(w_1, w_2)$

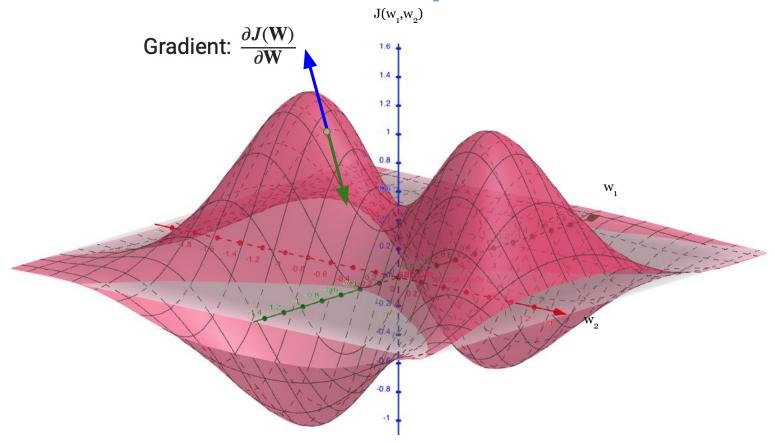
Best set of weight matrices given the selected cost function:

$$W^* = \arg\min_{\mathbf{W}} J(\mathbf{W})$$

Loss Surface Gradient: Slide to Minima but which?



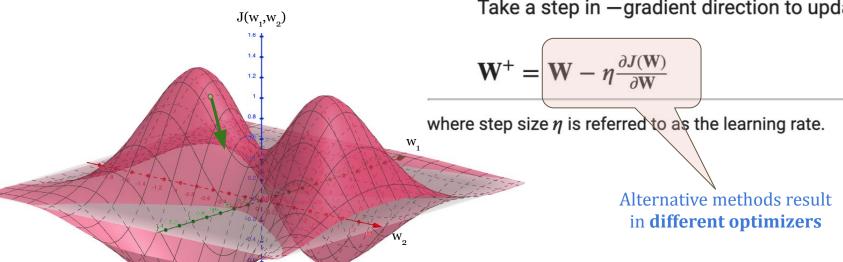
Loss Surface Gradient: Steepest Descent to Minima



Loss Surface Gradient: Steepest Descent to Minima

Gradient Descent Algorithm:

- ullet Initialize network: ${f W}$, random is a good choice
- Loop until not worth it:
 Take a step in —gradient direction to update W as:



$$(\mathbf{W}) = \frac{1}{d} \sum_{t=0}^{d} L(\mathbf{y}_{t}^{(k)}, \mathbf{y}^{(k)})$$

$$\frac{1}{d} \sum_{k=1}^{k-1} L(\mathbf{y}_t^{(k)}, F(\mathbf{x}^{(k)}, \mathbf{W}))$$

What is the effect of w_1 on **J**:

$$X_1$$
 W_1 Y X_2 W_2

$$\frac{\partial J(\mathbf{W})}{\partial w_1} = \frac{\partial J(\mathbf{W})}{\partial y} \cdot \frac{\partial y}{\partial w_1}$$

$$\frac{\partial J(\mathbf{W})}{\partial w_1} = \frac{\partial J(\mathbf{W})}{\partial y} \cdot \frac{\partial y}{\partial h} \cdot \frac{\partial h}{\partial w_1}$$

Tensor Flow: Optimizers... Gradient Descent

```
class Adadelta: Optimizer that implements the Adadelta algorithm.
class Adagrad: Optimizer that implements the Adagrad algorithm.
class Adam: Optimizer that implements the Adam algorithm.
class Adamax: Optimizer that implements the Adamax algorithm.
class Ftrl: Optimizer that implements the FTRL algorithm.
class Nadam: Optimizer that implements the NAdam algorithm.
class Optimizer: Base class for Keras optimizers.
class RMSprop: Optimizer that implements the RMSprop algorithm.
class SGD: Gradient descent (with momentum) optimizer.
```

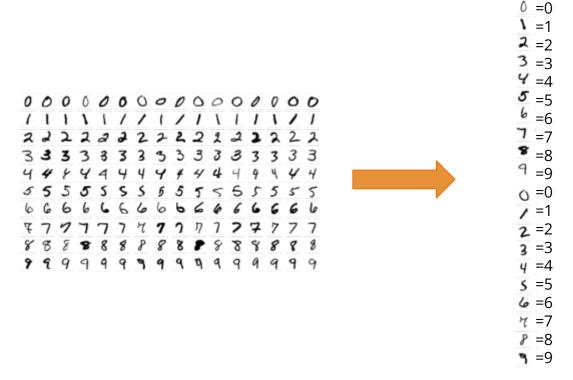
Check out: https://www.tensorflow.org/api docs/python/tf/keras/optimizers

pyTorch Flow: Optimizers... Gradient Descent

| Adadelta | Implements Adadelta algorithm. |
|------------|---|
| Adagrad | Implements Adagrad algorithm. |
| Adam | Implements Adam algorithm. |
| AdamW | Implements AdamW algorithm. |
| SparseAdam | Implements lazy version of Adam algorithm suitable for sparse tensors. |
| Adamax | Implements Adamax algorithm (a variant of Adam based on infinity norm). |
| ASGD | Implements Averaged Stochastic Gradient Descent. |

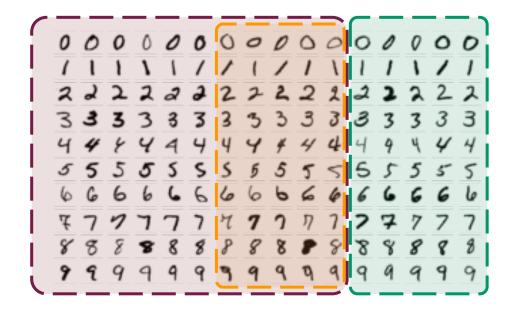
| LBFGS | Implements L-BFGS algorithm, heavily inspired by minFunc. |
|---------|--|
| NAdam | Implements NAdam algorithm. |
| RAdam | Implements RAdam algorithm. |
| RMSprop | Implements RMSprop algorithm. |
| Rprop | Implements the resilient backpropagation algorithm. |
| SGD | Implements stochastic gradient descent (optionally with momentum). |

Big Picture: Getting started - Labelled Data



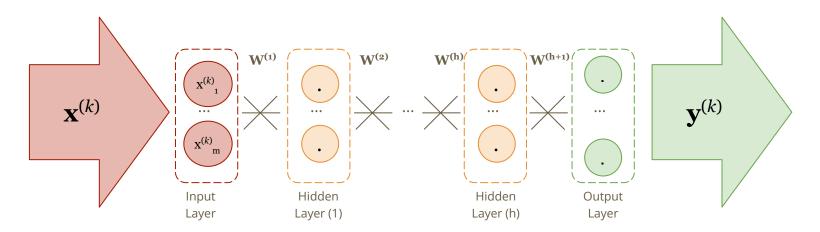
Labelled data: If not available you get the honor to label 70K of them! Enjoy...

Big Picture: Getting started - Divide Data



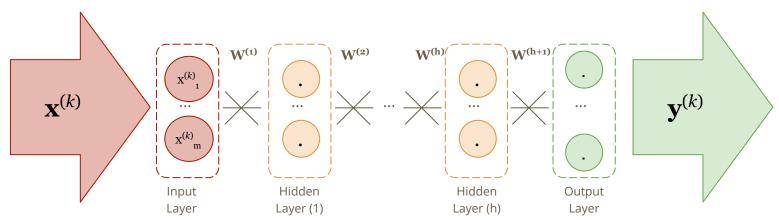
Data → **Training** data, **Validation** data, **Test** data

Big Picture: Getting started - Train where?



Hyperparameters: network topology, number of layers, number of neurons etc, *regularization* (dropout, early stopping, data augmentation, etc), optimizer, activation function, ...

Big Picture: Regularization...



Fight against: complex solutions lead to overfitting / overlearning / memorizing data

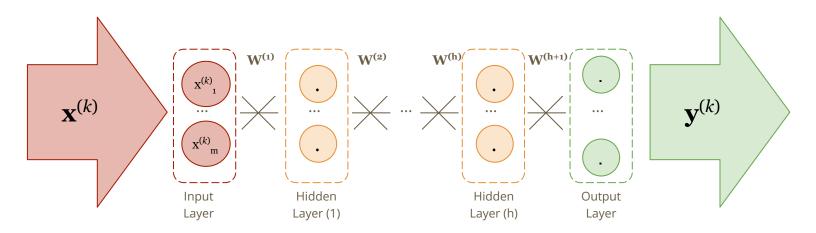
Dropout: Probabilistically pop some of the neurons in each iteration

Data Augmentation: shift, scale, rotate, add noise, etc. to generate variations

Regularization term: add a term to the cost function

Early Stopping: Stop when validation error stops improving

Big Picture: When to update?

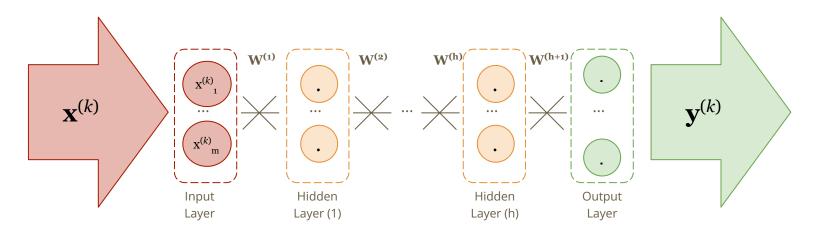


Epoch / Batch: Pass all the data through the network, calculate loss, update weights.

After every data point: Randomly select one - <u>SGD - check this video out</u>

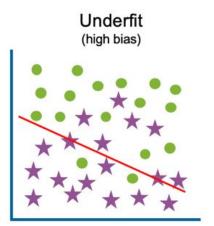
Mini-Batch: Data passed in subsets and weights updated after each batch

Big Picture: Loop until not worth it?

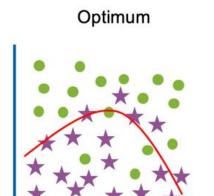


- Error is low enough i.e. error is below a preset threshold
- Got bored i.e. maximum epoch limit is reached
- Validation error started to increase while training decreases how is this even possible?
- ???

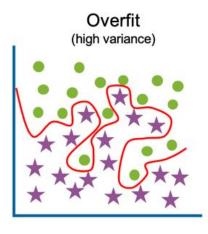
Big Picture: Try not to over- or under-fit



High training error High test error

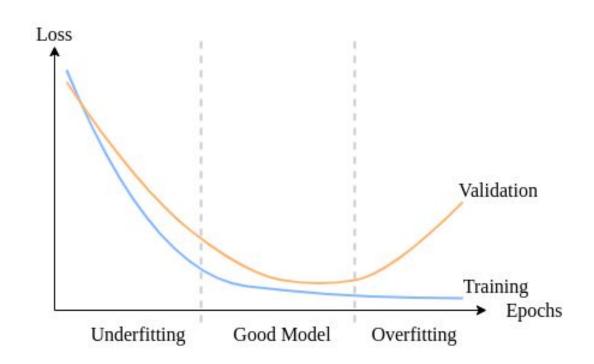


Low training error Low test error

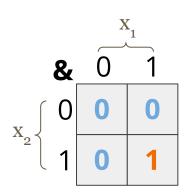


Low training error High test error

Big Picture: How to avoid overfit?



A simple case: Try backpropagation manually

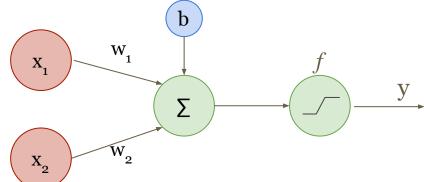


Initialize w, b as you like

choose f(.), loss function and learning rate

Given
$$y = f(\mathbf{x}^T \mathbf{w} + \mathbf{b})$$

Run gradient descent



By the way, you can implement this in numpy

Good news

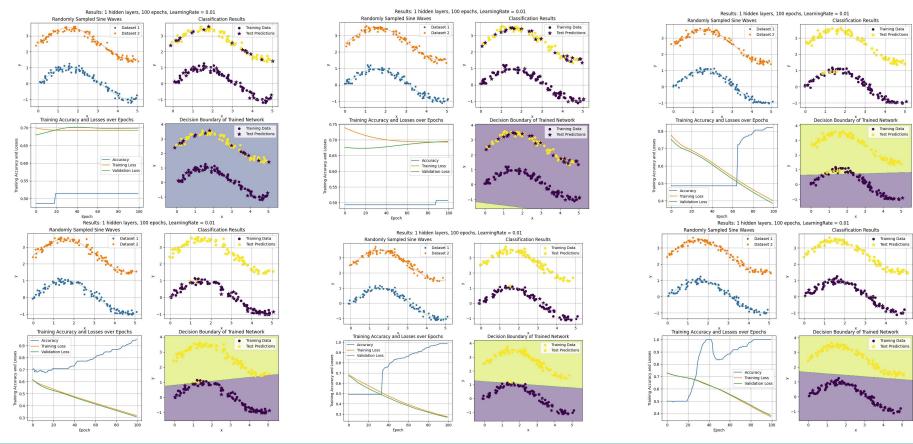
<u>13 lines of code</u> → A Neural Network: A good read, a good practice

You won't need to code a ANN from scratch:

- TF, pyTorch, etc. exit
- LLMs assist

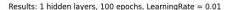
Check out: <u>Tensorflow playground</u>

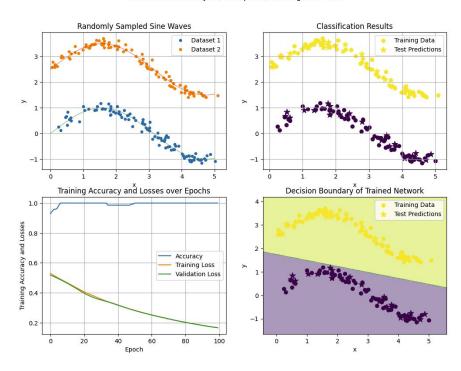
Same conditions, Just re-runs from scratch



Let's try together

Check this colab notebook





to be continued...