

DEEP NEURAL NETWORK

Deep Learning for Computer Vision

Arthur Douillard



Deep Neural Networks

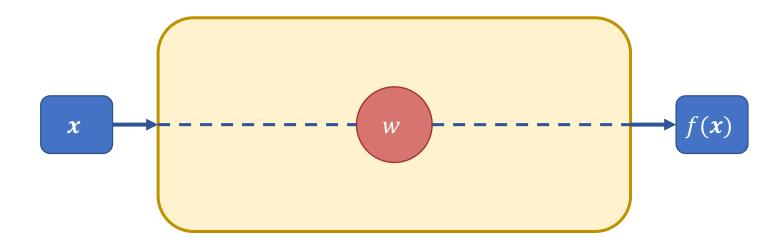


A neural network approximates a function





Linear regression

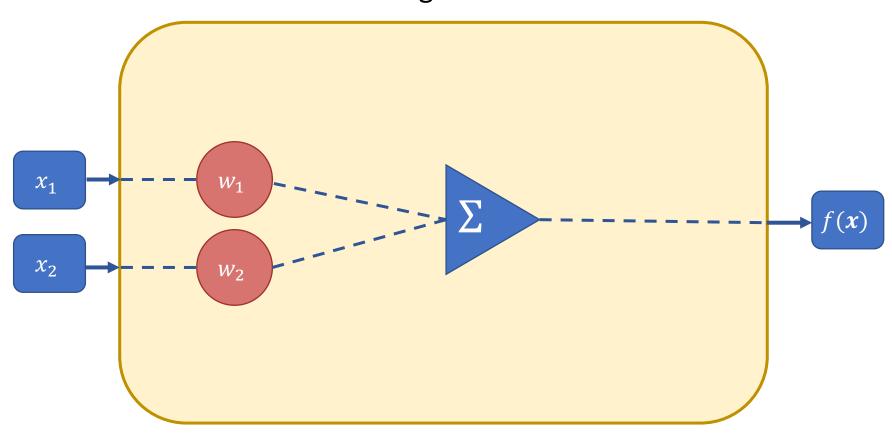


Useful to predict continuous variables

$$f(x) = wx$$



Linear regression

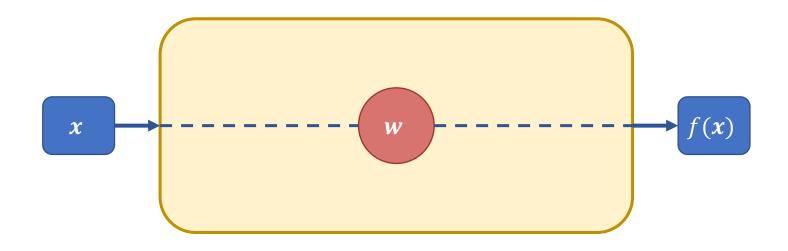


The "connection" often depicted are only multiplications and additions

$$f(\mathbf{x}) = w_1 x_1 + w_2 x_2$$



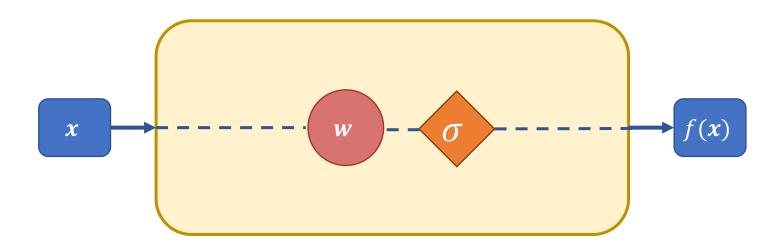
Linear regression



$$f(x) = wx$$



Single Neuron



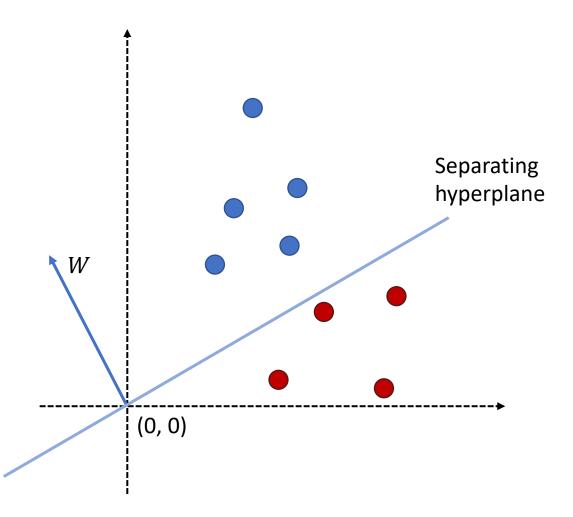
Non-linear activation to determine how much a neuron "fires"

$$f(x) = \sigma(wx)$$

Separating Hyperplane



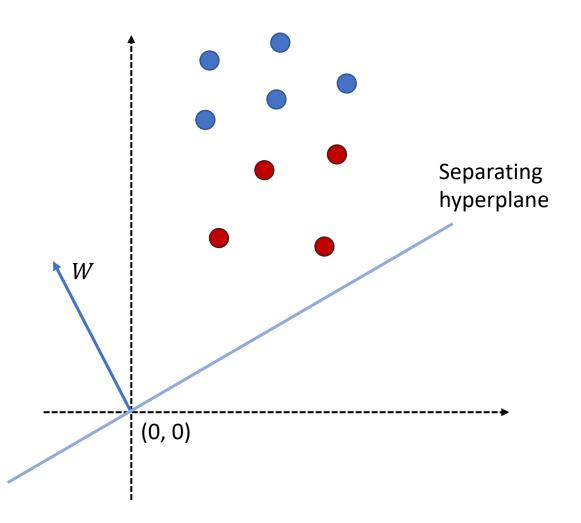
Optimize so that \boldsymbol{W} is orthogonal to the separating hyperplane



Without bias

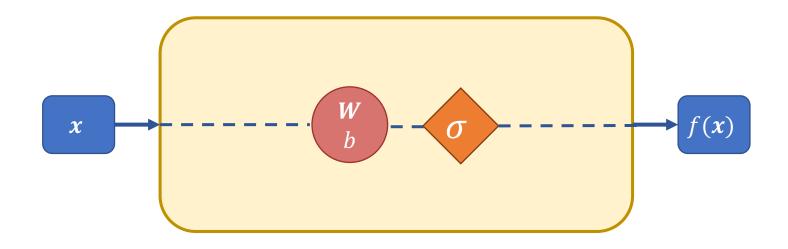


Need bias!





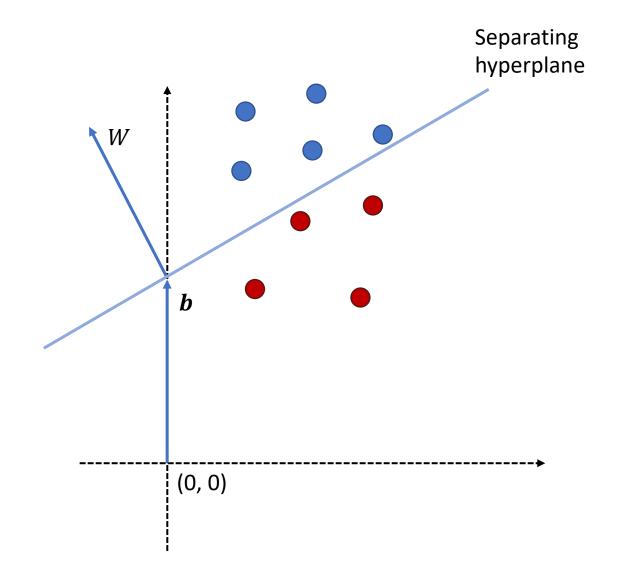
Single Neuron



With a **bias**

$$f(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{w}\mathbf{x} + b)$$

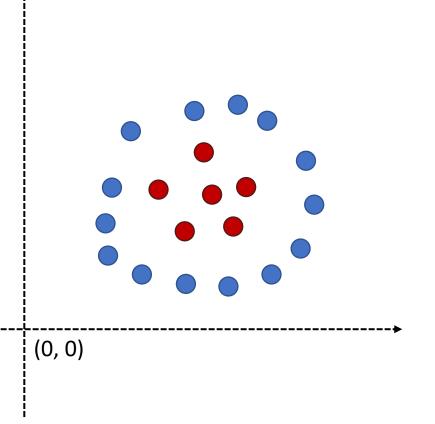




Non-Linear Data



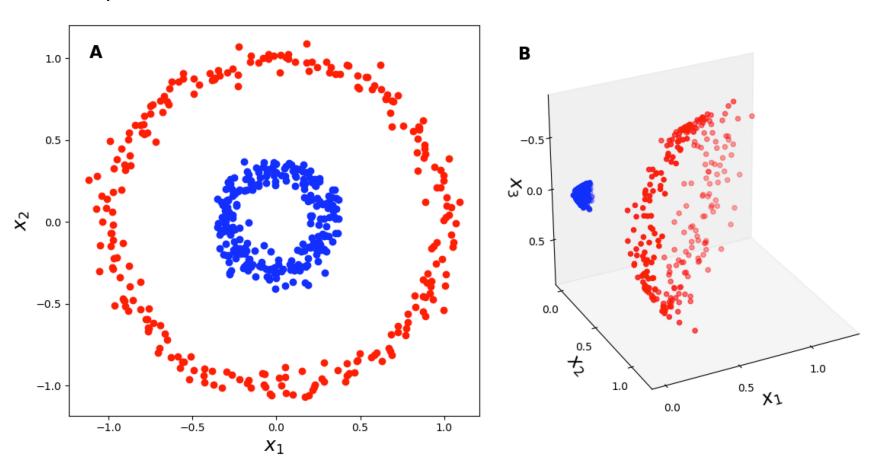
A linear model cannot discriminate blue and red classes!



Features Engineering

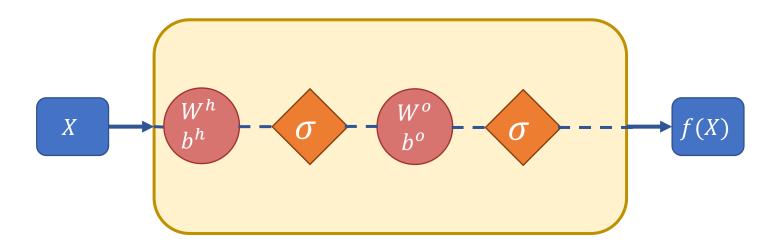


Before, you would have use the **kernel trick**



Excellent blog post on that **Gundersen**



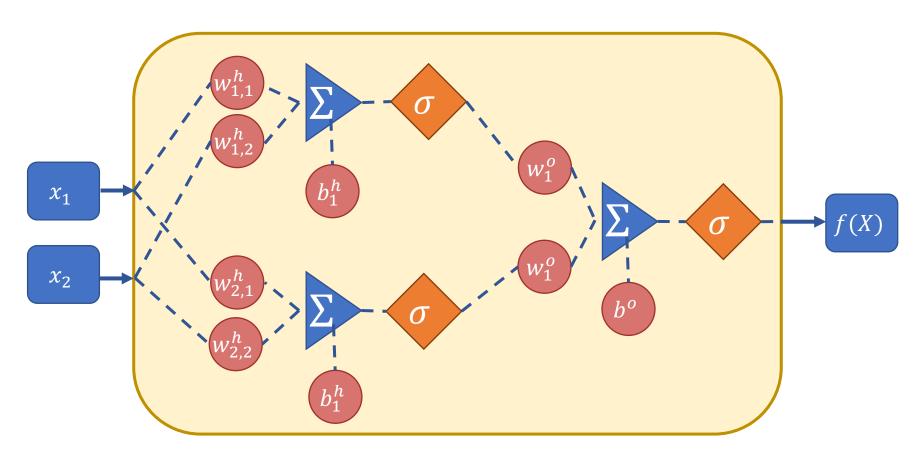


Stack multiple linear transformations and non-linear activation

$$f(\mathbf{x}) = \sigma(\mathbf{w}^o \sigma(\mathbf{W}^h \mathbf{x} + \mathbf{b}^h) + \mathbf{b}^o)$$

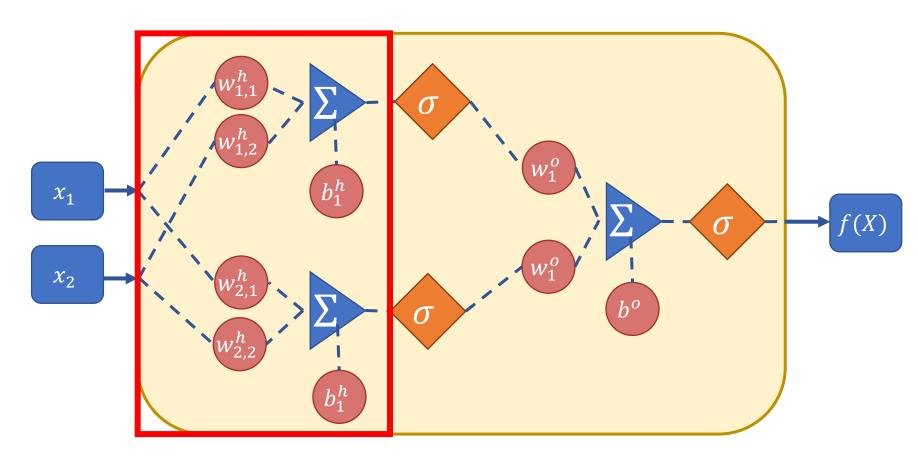


 ${\it W}^h$ is a matrix because it has here 2 output dimensions



$$f(\mathbf{x}) = \sigma(\mathbf{w}^o \sigma(\mathbf{W}^h \mathbf{x} + \mathbf{b}^h) + \mathbf{b}^o)$$

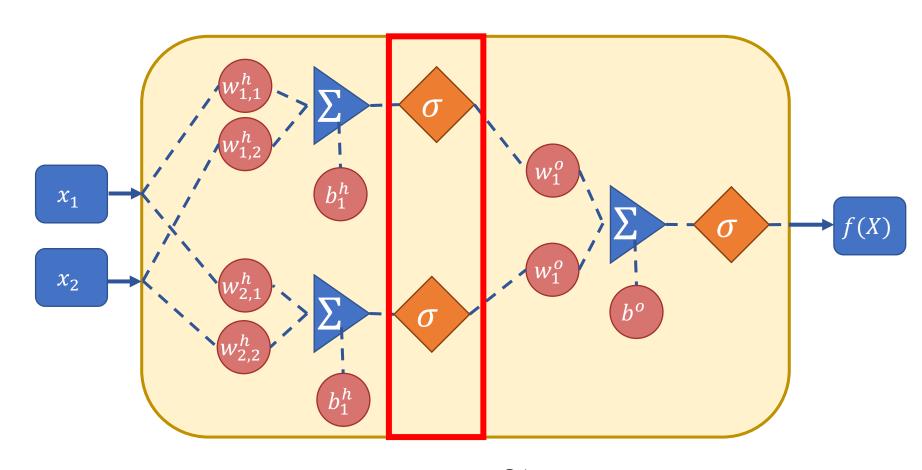




$$\widetilde{\boldsymbol{h}} = \boldsymbol{W}^h \boldsymbol{x} + \boldsymbol{b}^h$$



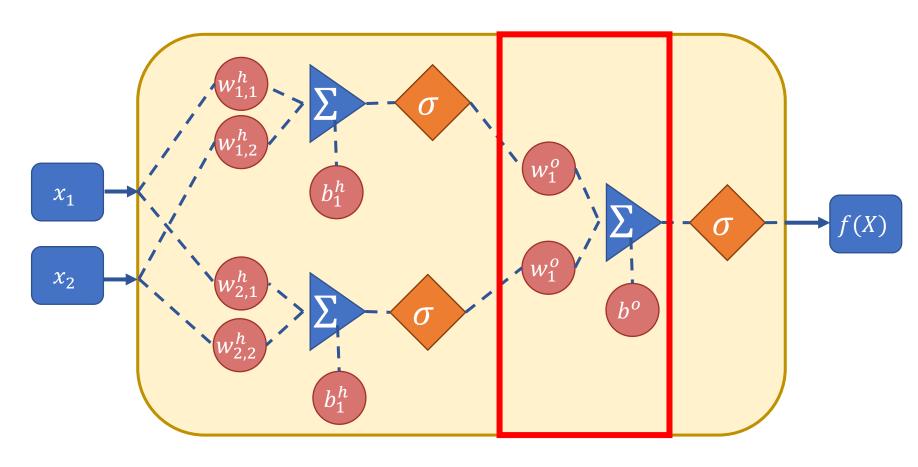
Embeddings/features



$$h = \sigma(\widetilde{h})$$

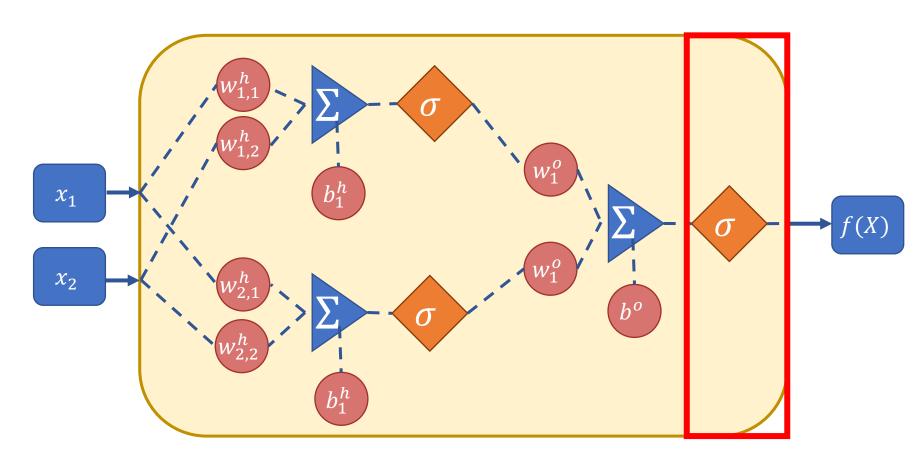


Logits!



$$\widetilde{\mathbf{y}} = \mathbf{w}^{o}\mathbf{h} + b^{o}$$

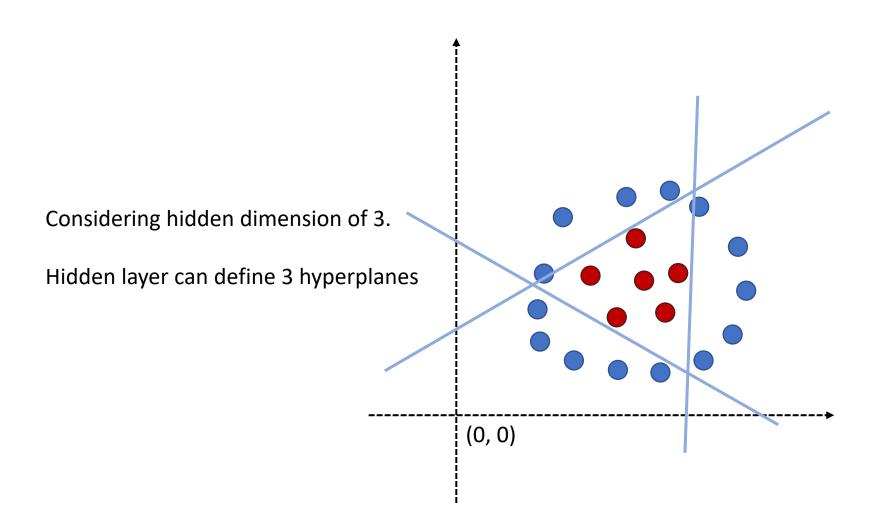




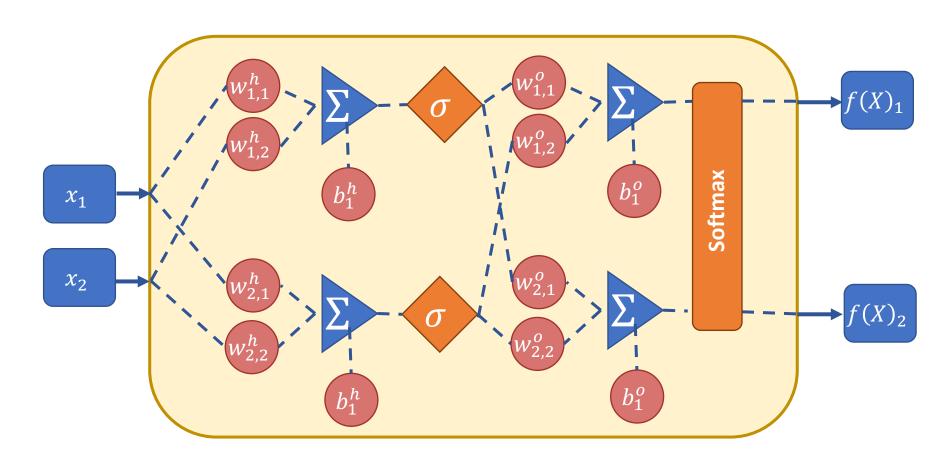
$$\widehat{\mathbf{y}} = \sigma(\widetilde{\mathbf{y}})$$

Non-Linear Data





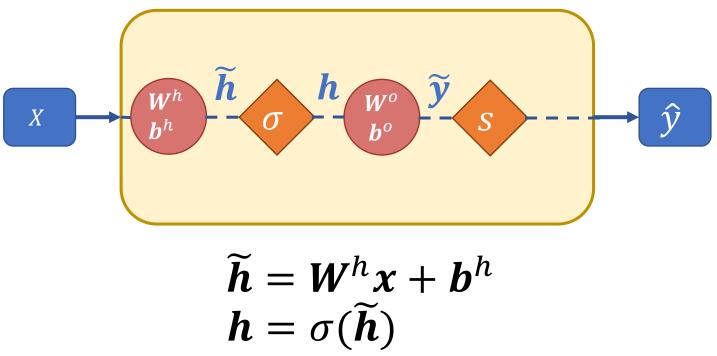




 W^o is a matrix because it has here 2 predicted classes. Can be extended to 3, 4, ..., 1000 classes.



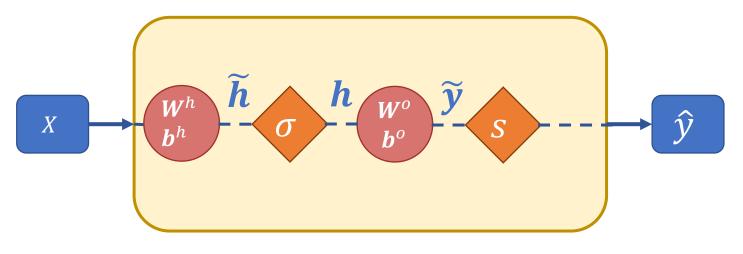
Multi-Layer Perceptron



$$\widetilde{\mathbf{y}} = \mathbf{W}^{o}\mathbf{h} + \mathbf{b}^{o}$$
 $\widehat{\mathbf{y}} = \sigma(\widetilde{\mathbf{y}})$



Multi-Layer Perceptron



$$\widetilde{m{h}} = m{W}^h m{x} + m{b}^h$$
 $m{h} = \sigma(\widetilde{m{h}})$
 $\widetilde{m{y}} = m{W}^o m{h} + m{b}^o$

$$\widehat{\mathbf{y}} = \sigma(\widetilde{\mathbf{y}})$$

→ features / embeddings

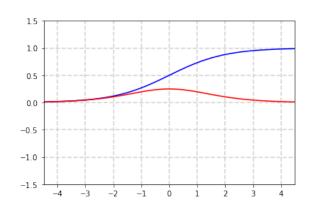
→ logits

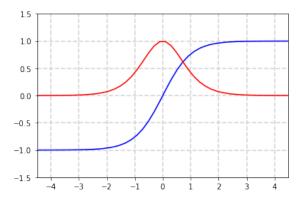
→ Model predictions

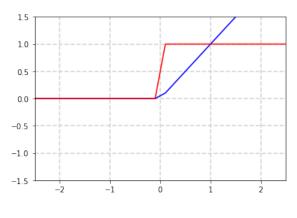
Hidden Activations



Function and their derivative







Sigmoid

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

$$\frac{d}{dx}\sigma(x) = \sigma(x)(1 - \sigma(x))$$

Hyperbolic tangent

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

$$\frac{d}{dx}\tanh(x) = 1 - \tanh(x)^2$$

Rectified Linear Unit

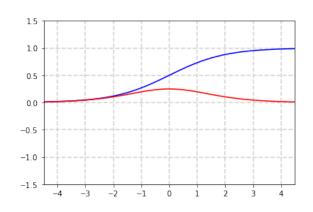
$$ReLU(x) = \max(x, 0)$$

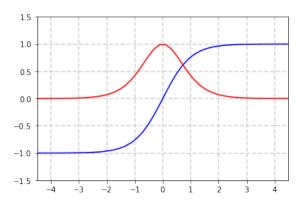
$$\frac{d}{dx}\sigma(x) = \sigma(x)(1 - \sigma(x)) \qquad \frac{d}{dx}\tanh(x) = 1 - \tanh(x)^2 \qquad \frac{d}{dx}ReLU(x) = \begin{cases} 1 & \text{if } x > 0\\ 0 & \text{otherwise} \end{cases}$$

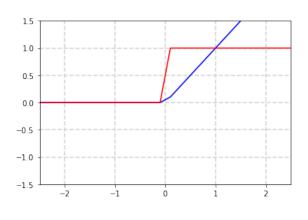
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Rectified Linear Unit

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Without hidden activation, a MLP is equivalent to a single layer!

→ Composition of affine functions is an affine function

Output activations



Binary classification: sigmoid

- → Applied element-wise
- → Range [0, 1]

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

$$\frac{d}{dx}\sigma(x) = \sigma(x)(1 - \sigma(x))$$

Multi-Class classification: softmax

- → Applied over a vector
- → Range [0, 1] per element
- → Sum to 1 for the vector
 - → Probability distribution

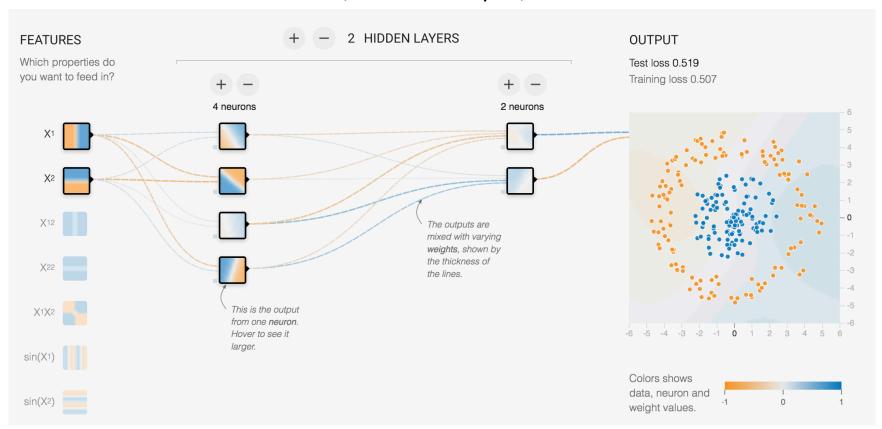
$$softmax(\mathbf{x}) = \frac{1}{\sum_{j} e^{\mathbf{x}_{j}}} \begin{bmatrix} e^{x_{1}} \\ \dots \\ e^{x_{n}} \end{bmatrix}$$

$$softmax(\mathbf{x})_i = \frac{e^{\mathbf{x}_i}}{\sum_j e^{\mathbf{x}_j}}$$

$$\frac{d}{dx_{j}}softmax(\mathbf{x})_{i} = \begin{cases} softmax(\mathbf{x})_{i}(1 - softmax(\mathbf{x})_{i} if i = j \\ -softmax(\mathbf{x})_{i} softmax(\mathbf{x})_{j} if i \neq j \end{cases}$$



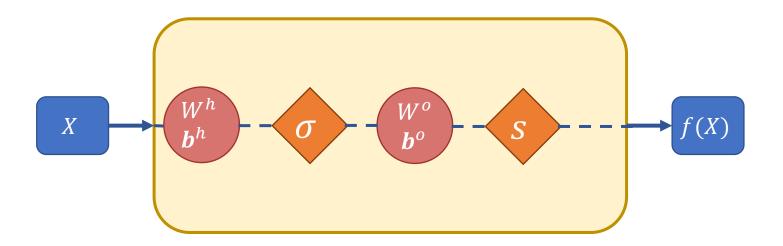
To get an intuition of the effect of hidden dimensions, number of layers, and activations:



playground.tensorflow.org

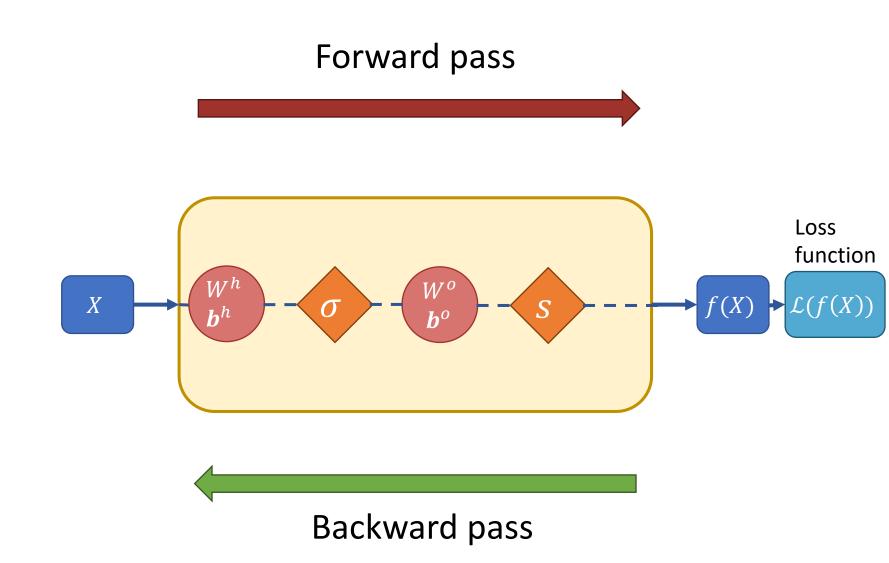
Learning DNNs





1 hidden layer, H hidden dimensions, C output dimensions with a softmax





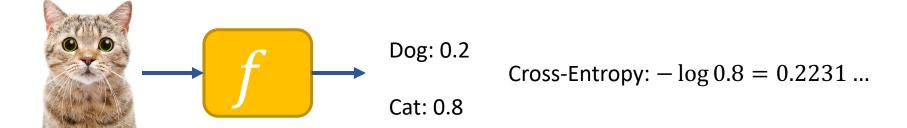


For classification with softmax as final activation:

Cross-entropy (also known as negative log-likelihood):

$$\mathcal{L}_{CE}(\widehat{y}, y) = -\sum_{i} y_{i} \log \widehat{y}_{i}$$

One-hot target



One-Hot



Avoid doing *if* in GPUs, use one-hot in cross-entropy.

Given 5 classes, if the ground-truth class is 3:

0 0 0 1 0

Zero-indexed!

Loss Function



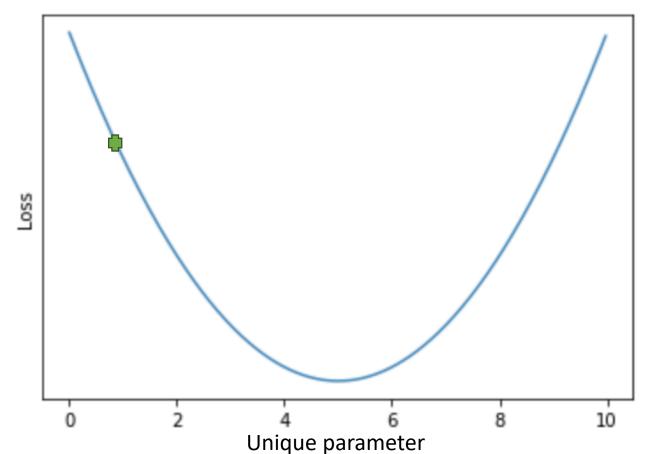
Optimize the network to minimize the loss with respect to all neurons:

$$\mathcal{L}_{CE}(\widehat{y}, y) = -\sum_{i} y_{i} \log \widehat{y}_{i}$$



Optimize the network to minimize the loss with respect to all neurons:

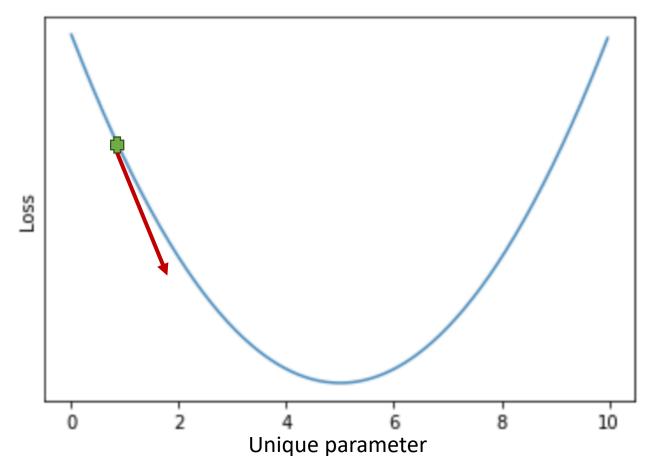
$$\mathcal{L}_{CE}(\widehat{y}, y) = -\sum_{i} y_{i} \log \widehat{y}_{i}$$





Optimize the network to minimize the loss with respect to all neurons θ :

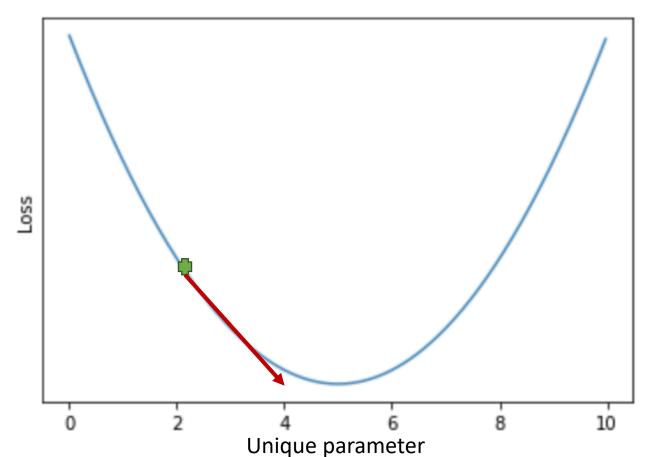
$$\mathcal{L}_{CE}(\widehat{y}, y) \\
-\nabla_{\theta} \mathcal{L}_{CE}(\widehat{y}, y)$$





Optimize the network to minimize the loss with respect to all neurons θ :

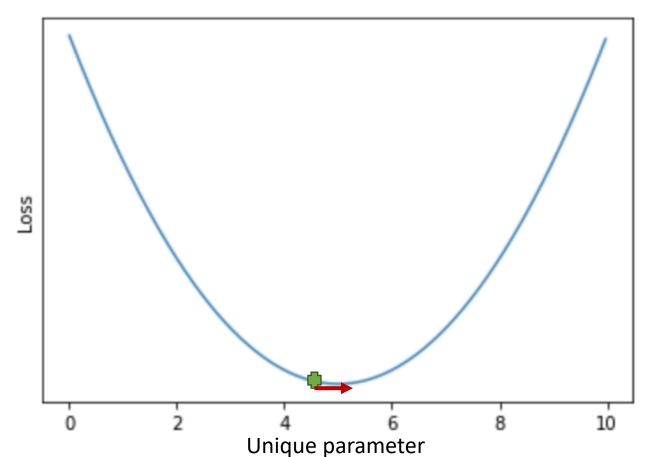
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Optimize the network to minimize the loss with respect to all neurons θ :

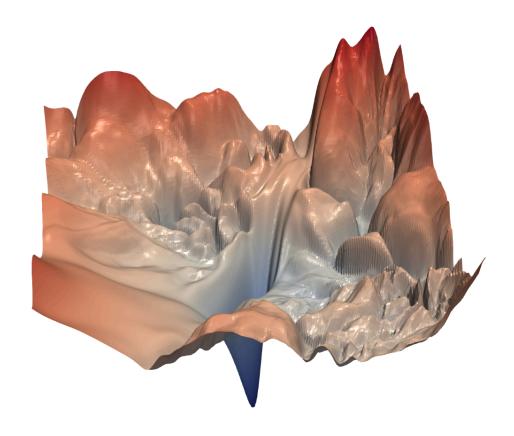
$$\mathcal{L}_{CE}(\widehat{y}, y) \\ -\nabla_{\theta} \mathcal{L}_{CE}(\widehat{y}, y)$$



Minimization of a function



Million of parameters to optimize together! Highly non-convex!

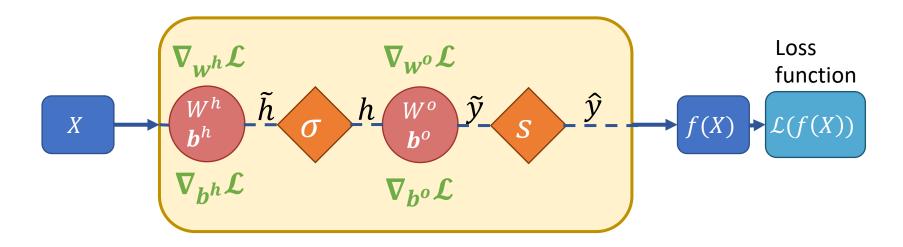


Multiple dimensional derivatives are called gradients

Needed Gradients



We need all parameters gradients in green

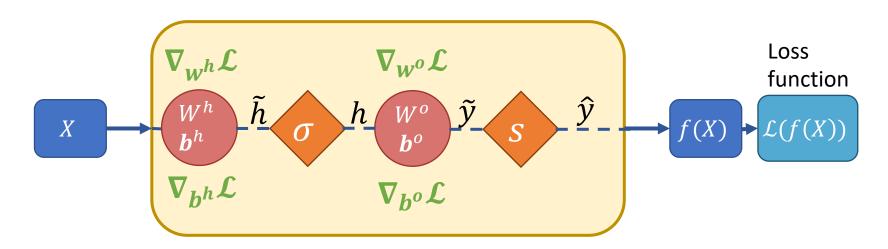


Stochastic Gradient Descent



- 1. Initialize randomly the parameters θ
- 2. For each epoch do
 - 1. Select a random sample of the data
 - 2. Forward
- 3. Compute gradients $\nabla_{\theta} \mathcal{L}$ for each parameter θ
- 4. Update parameters $\theta \leftarrow \theta \eta \nabla_{\theta} \mathcal{L}$

 η is the **learning rate**.



Chain Rule



$$f \circ g(a) = f(b) = c$$

$$\frac{\partial c}{\partial a} = \frac{\partial c}{\partial b} \frac{\partial b}{\partial a}$$

$$\frac{\partial c_i}{\partial a_k} = \sum_i \frac{\partial c_i}{\partial b_j} \frac{\partial b_j}{\partial a_k}$$

$$\nabla_a c = \nabla_b c \nabla_a b^T$$

In denominator layout (\neq numerator layout):

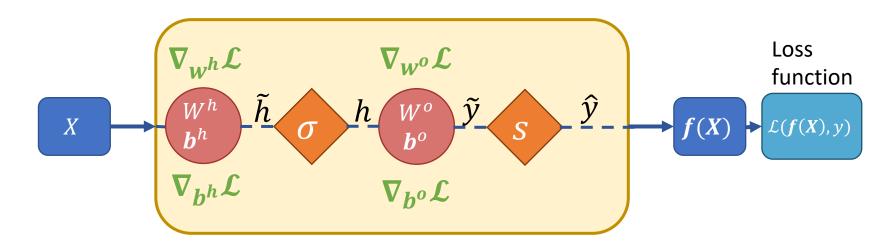
$$\mathbf{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_{n_{\underline{a}}} \end{bmatrix} \quad \mathbf{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_{n_{\underline{b}}} \end{bmatrix} \quad \mathbf{c}$$

$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_{n_a} \end{bmatrix} \quad \boldsymbol{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_{n_b} \end{bmatrix} \quad \boldsymbol{c} = \begin{bmatrix} c_1 \\ \vdots \\ c_{n_c} \end{bmatrix} \qquad \boldsymbol{\nabla_b} \boldsymbol{c} = \begin{bmatrix} \frac{\partial c_1}{\partial b_1} & \dots & \frac{\partial c_{n_c}}{\partial b_1} \\ \vdots & & \vdots \\ \frac{\partial c_1}{\partial b_{n_b}} & \dots & \frac{\partial c_{n_c}}{\partial b_{n_b}} \end{bmatrix}$$



Partial derivative of the cross-entropy loss with respect to (w.r.t.) the probabilities:

$$\frac{\partial \mathcal{L}(f(x),y)}{\partial f(x)_i} = \frac{\partial -\log f(x)_y}{\partial f(x)_i} = \frac{-1_{y=i}}{f(x)_y}, \text{ for simplicity } \frac{\partial \mathcal{L}}{\partial f(x)_i}$$





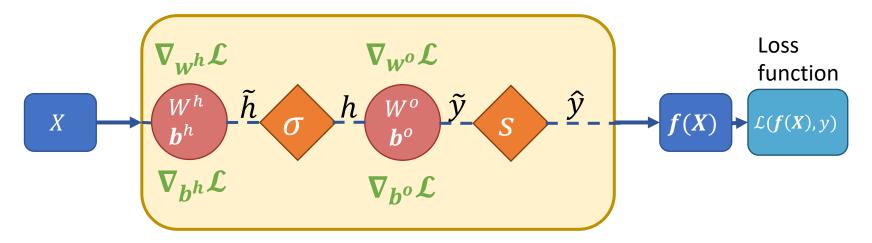
$$\frac{\partial \mathcal{L}}{\partial \tilde{y}_{i}} = \sum_{j} \frac{\partial \mathcal{L}}{\partial f(x)_{j}} \frac{\partial f(x)_{j}}{\partial \tilde{y}_{i}}$$

$$= \sum_{j} \frac{-1_{y=j}}{\partial f(x)_{y}} \frac{\partial softmax(\tilde{y})_{j}}{\partial \tilde{y}_{i}}$$

$$= \begin{cases}
\frac{-1}{f(x)_{y}} softmax(\tilde{y})_{y} (1 - softmax(\tilde{y})_{y}) & \text{if } i = y \\
\frac{1}{f(x)_{y}} softmax(\tilde{y})_{y} softmax(\tilde{y})_{i} & \text{if } i \neq y
\end{cases}$$

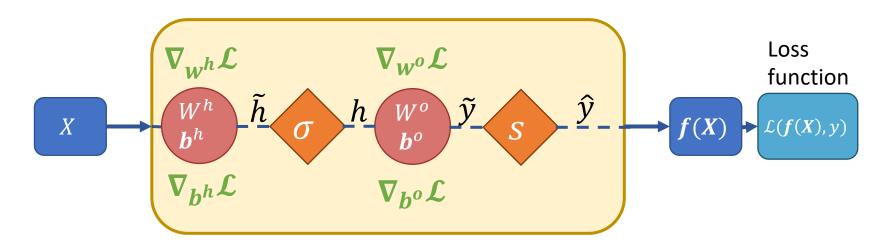
$$= \begin{cases}
-1 + f(x)_{y} & \text{if } i = y \\
f(x)_{i} & \text{if } i \neq y
\end{cases}$$

$$\nabla_{\tilde{y}} \mathcal{L} = f(x) - e(y) \text{ with one-hot encoding of the target}$$





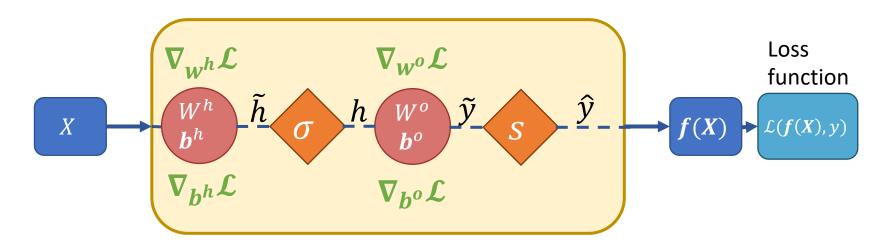
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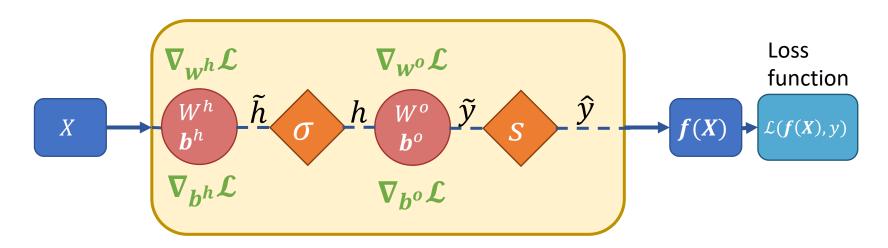




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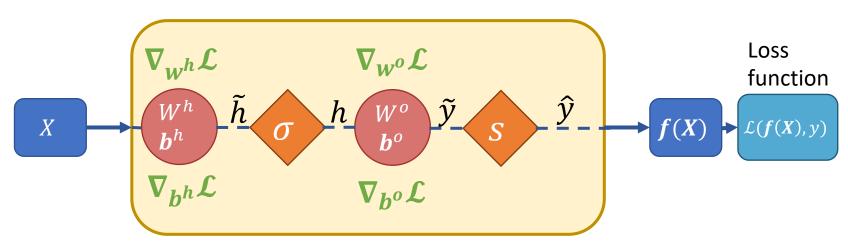


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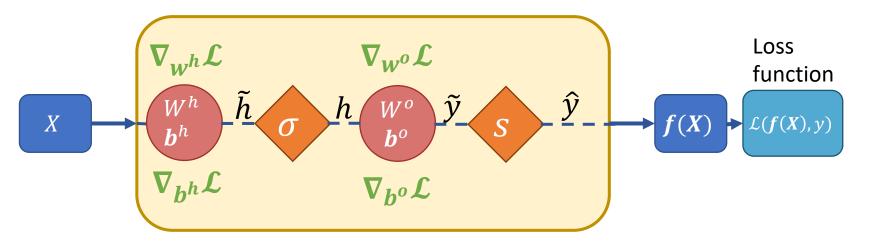
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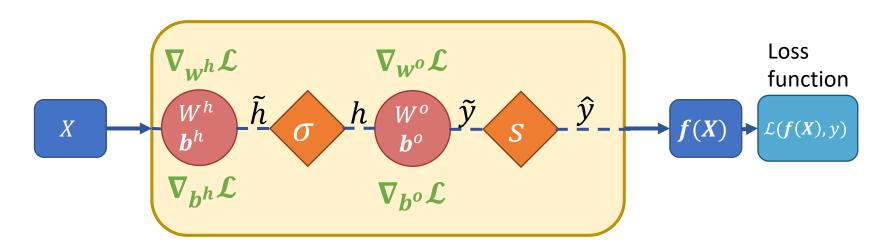


$$abla_{\widetilde{y}}\mathcal{L} = f(x) - e(y)$$

$$abla_{b^o}\mathcal{L} = \nabla_{\widetilde{y}}\mathcal{L}$$

$$abla_{w^o}\mathcal{L} = \nabla_{\widetilde{y}}\mathcal{L} \cdot h^T$$

$$\widetilde{\boldsymbol{y}} = \boldsymbol{W}^o \boldsymbol{h} + \boldsymbol{b}^o$$





$$\nabla_{\tilde{y}} \mathcal{L} = \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{e}(\boldsymbol{y})$$

$$\nabla_{\boldsymbol{b}} \circ \mathcal{L} = \nabla_{\widetilde{\mathcal{V}}} \mathcal{L}$$

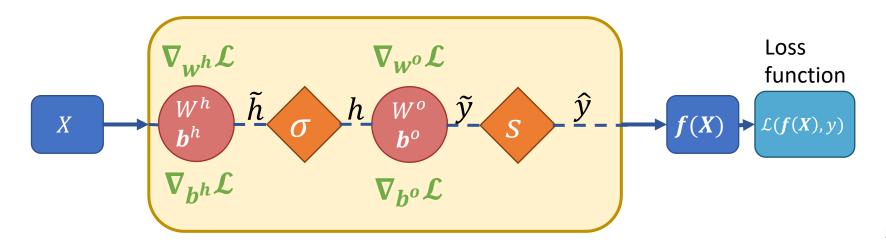
$$\nabla_{\boldsymbol{w}^o} \mathcal{L} = \nabla_{\widetilde{\mathcal{Y}}} \mathcal{L} \cdot \boldsymbol{h}^T$$

$$\nabla_{\boldsymbol{h}} \mathcal{L} = \boldsymbol{W}^{oT} \cdot \boldsymbol{\nabla}_{\widetilde{\boldsymbol{\gamma}}} \mathcal{L}$$

$$\nabla_{\tilde{h}} \mathcal{L} = \nabla_{h} \mathcal{L} \odot \sigma'(\tilde{h})$$

⊙ is the element-wise multiplication (Hadamard product).

Sigmoid is applied element-wise, thus the gradient also.





$$\nabla_{\tilde{y}}\mathcal{L} = f(x) - e(y)$$

$$\nabla_{b^{o}}\mathcal{L} = \nabla_{\tilde{y}}\mathcal{L}$$

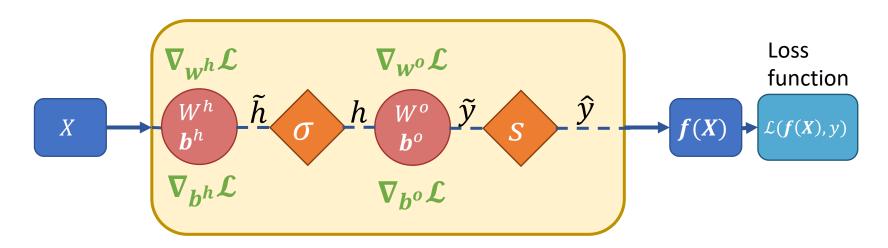
$$\nabla_{w^{o}}\mathcal{L} = \nabla_{\tilde{y}}\mathcal{L} \cdot h^{T}$$

$$\nabla_{h}\mathcal{L} = W^{o^{T}} \cdot \nabla_{\tilde{y}}\mathcal{L}$$

$$\nabla_{\tilde{h}}\mathcal{L} = \nabla_{h}\mathcal{L} \odot \sigma'(\tilde{h})$$

$$\nabla_{b^{h}}\mathcal{L} = ?$$

$$\nabla_{W^{h}}\mathcal{L} = ?$$





$$\nabla_{\tilde{y}}\mathcal{L} = f(x) - e(y)$$

$$\nabla_{b^{o}}\mathcal{L} = \nabla_{\tilde{y}}\mathcal{L}$$

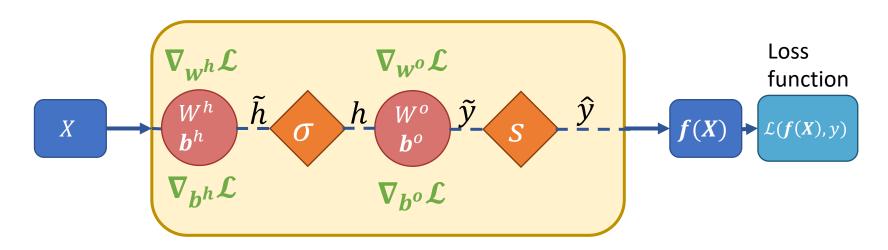
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$$\nabla_{b^{h}}\mathcal{L} = \nabla_{\tilde{h}}\mathcal{L}$$

$$\nabla_{w^{h}}\mathcal{L} = \nabla_{\tilde{h}}\mathcal{L} \cdot x^{T}$$





$$\nabla_{\tilde{y}} \mathcal{L} = \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{e}(\boldsymbol{y})$$

$$\nabla_{\boldsymbol{b}} \circ \mathcal{L} = \nabla_{\widetilde{\mathcal{V}}} \mathcal{L}$$

$$\nabla_{\boldsymbol{w}^o} \mathcal{L} = \nabla_{\widetilde{\boldsymbol{\mathcal{V}}}} \mathcal{L} \cdot \boldsymbol{h}^T$$

$$\nabla_{\boldsymbol{h}} \mathcal{L} = \boldsymbol{W}^{oT} \cdot \boldsymbol{\nabla}_{\widetilde{y}} \mathcal{L}$$

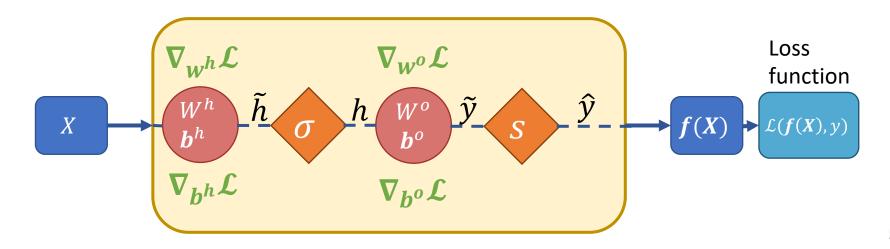
$$\nabla_{\tilde{h}} \mathcal{L} = \nabla_{h} \mathcal{L} \odot \sigma'(\tilde{h})$$

$$\nabla_{\boldsymbol{b}^h} \mathcal{L} = \nabla_{\tilde{h}} \mathcal{L}$$

$$\nabla_{\mathbf{W}^h} \mathcal{L} = \nabla_{\tilde{h}} \mathcal{L} \cdot \mathbf{x}^T$$

When in doubt, look at the shape.

 $\nabla_W \mathcal{L}$ must have the shape of W because of the update rule $W \leftarrow W - \nabla_W \mathcal{L}$





$$\nabla_{\tilde{y}} \mathcal{L} = \boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{e}(\boldsymbol{y})$$

$$\nabla_{\boldsymbol{b}} \circ \mathcal{L} = \nabla_{\widetilde{\mathcal{V}}} \mathcal{L}$$

$$\nabla_{\boldsymbol{w}} \circ \mathcal{L} = \nabla_{\widetilde{\mathcal{V}}} \mathcal{L} \cdot \boldsymbol{h}^T$$

$$\nabla_{\boldsymbol{h}} \mathcal{L} = \boldsymbol{W}^{oT} \cdot \boldsymbol{\nabla}_{\widetilde{y}} \mathcal{L}$$

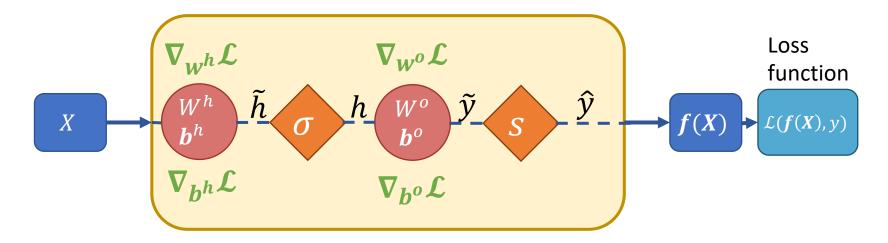
$$\nabla_{\widetilde{h}} \mathcal{L} = \nabla_{h} \mathcal{L} \odot \sigma'(\widetilde{h})$$

$$\nabla_{\boldsymbol{h}^h} \mathcal{L} = \nabla_{\tilde{h}} \mathcal{L}$$

$$\nabla_{\mathbf{W}^h} \mathcal{L} = \nabla_{\tilde{h}} \mathcal{L} \cdot \mathbf{x}^T$$

To have huge speed-up:

- 1. Re-use previous gradients
- 2. Save tensors during forward



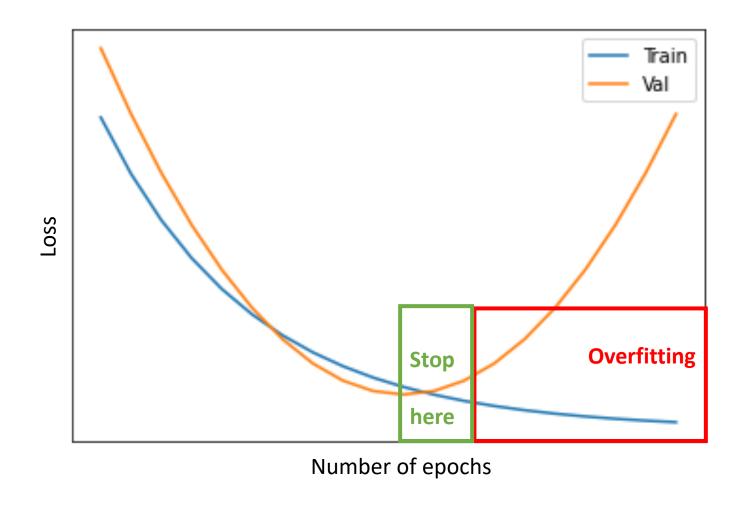
Tips & Tricks

When to Stop?



Split data in train / val / test

Stop when a criterion (loss, accuracy, f1, etc.) stop improving on validation set



(Mini-)Batch Size



Batch Gradient Descent: one forward & backward on the whole dataset

- → Better gradient estimation
- → GPU parallelism
- → Impracticable to fit large dataset in VRAM

Stochastic Gradient Descent: one forward & backward per sample

- → Easy to fit in VRAM
- → Add noise that may improve generalization
- → Add too much noise
- → Slow

Mini-Batch Gradient Descent: one forward & backward per group of samples

- → Trade-off between both
- → Learning rate should be proportional to batch size, e.g. batch size 32->64, lr 0.1->0.2

Learning Rate



$$\theta \leftarrow \theta - \eta \nabla_{\theta} \mathcal{L}$$

Controls the rate of change.

Too high:

→ Cannot converge, but diverge, reduce overfitting

Too low:

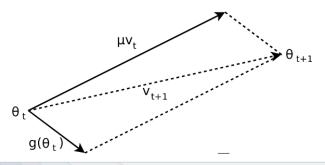
→ Super slow, stuck in bad local minima

Start with high learning rate, and decreases it through time

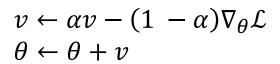
SGD with Momentum

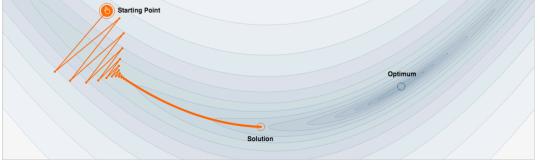
Step-size a = 0.02





Momentum $\beta = 0.0$





We often think of Momentum as a means of dampening oscillations

and speeding up the iterations, leading to faster convergence. But it has other interesting behavior. It allows a larger range of step-sizes

has other interesting behavior. It allows a larger range of step-sizes to be used, and creates its own oscillations. What is going on?

Why Momentum Really works, on distill.pub



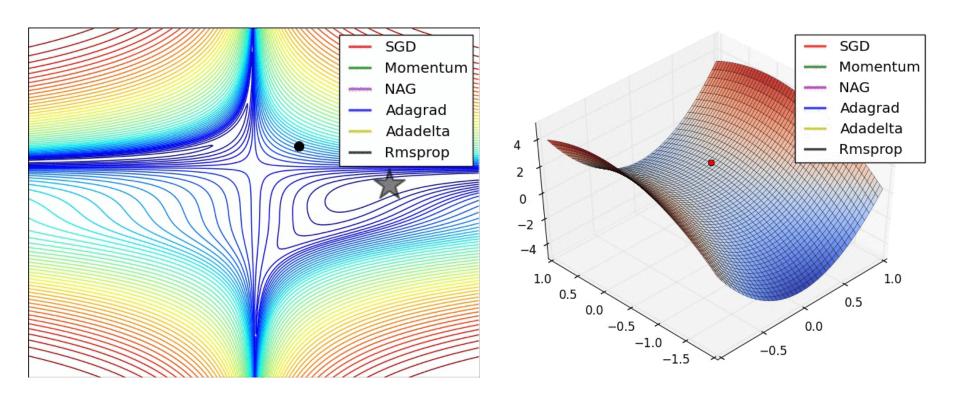
Optimizers



Modern optimizers have an adaptive learning rate per parameter based on gradient statistics.

- → Especially useful on saddle point
- → The most famous is Adam

But a well-tuned SGD with momentum can sometimes be the best.

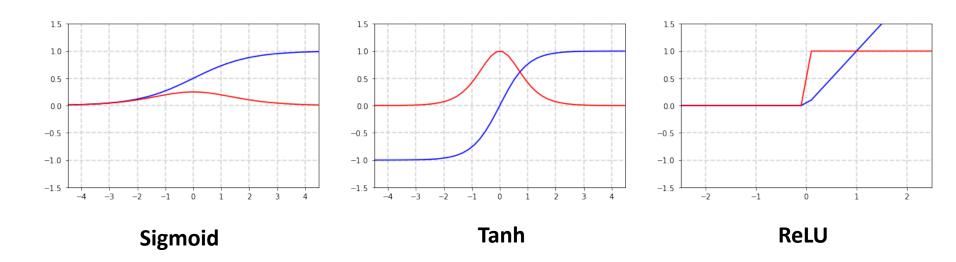


Great overview of gradient-descent based optimizers by Ruder.

Pitfalls of hidden activations



Function and their derivative



Sigmoid and tanh saturates at small and large values.

- → Gradient is zero, no learning
- → Avoid these old-school activations

ReLU is zero if $x \le 0$:

→ **Dying neurons** with zero-output and thus zero-gradient

$$\rightarrow$$
 If it happens, use a **Leaky ReLU** $LReLU(x) = \begin{cases} x & if \ x > 0 \\ \epsilon \ x & otherwise \end{cases}$

Initialization



Initializing the biases \boldsymbol{b}^h and \boldsymbol{b}^o to very small values.

→ Helpful to avoid dying neurons with ReLU

Initializing the weights W^h and W^o to:

- Zero-weights
 - → No learning because gradient w.r.t input is also zero
- Constant weights
 - → Symmetry where two hidden neurons are connected to the same inputs, they learn the same pattern!
- Large values
 - → Risk gradient explosion
- He / Glorot initialization
 - → Normalize weights to avoid explosion with large number of outgoing connections

Small break, then coding session!