# Multi-Layer Perceptrons

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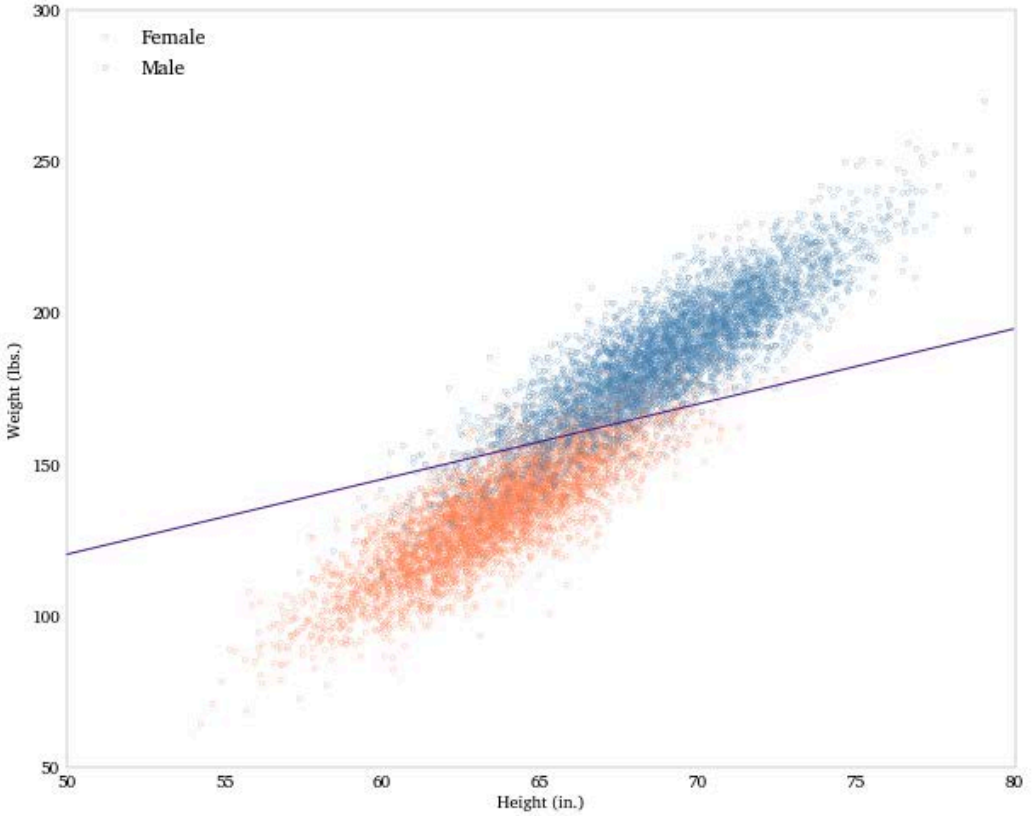
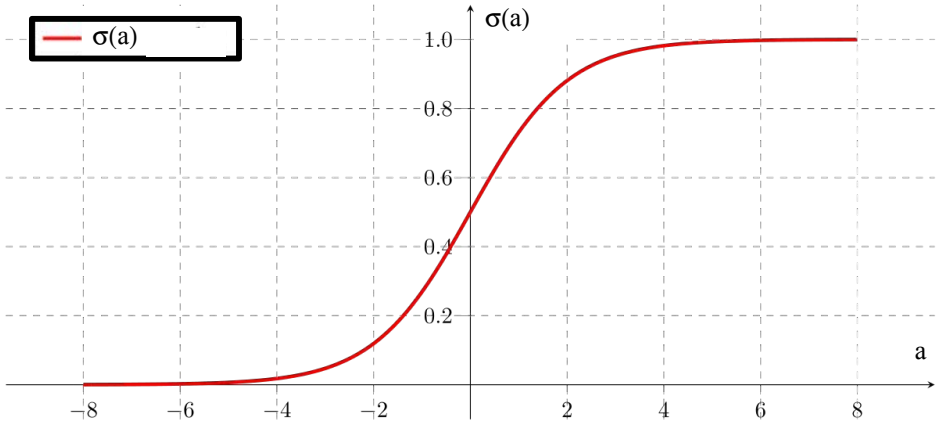
IC-CVLab

# Reminder: Logistic Regression




$$y(\mathbf{x}; \tilde{\mathbf{w}}) = \sigma(\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}})$$

$$= \frac{1}{1 + \exp(-\tilde{\mathbf{w}} \cdot \tilde{\mathbf{x}})}$$

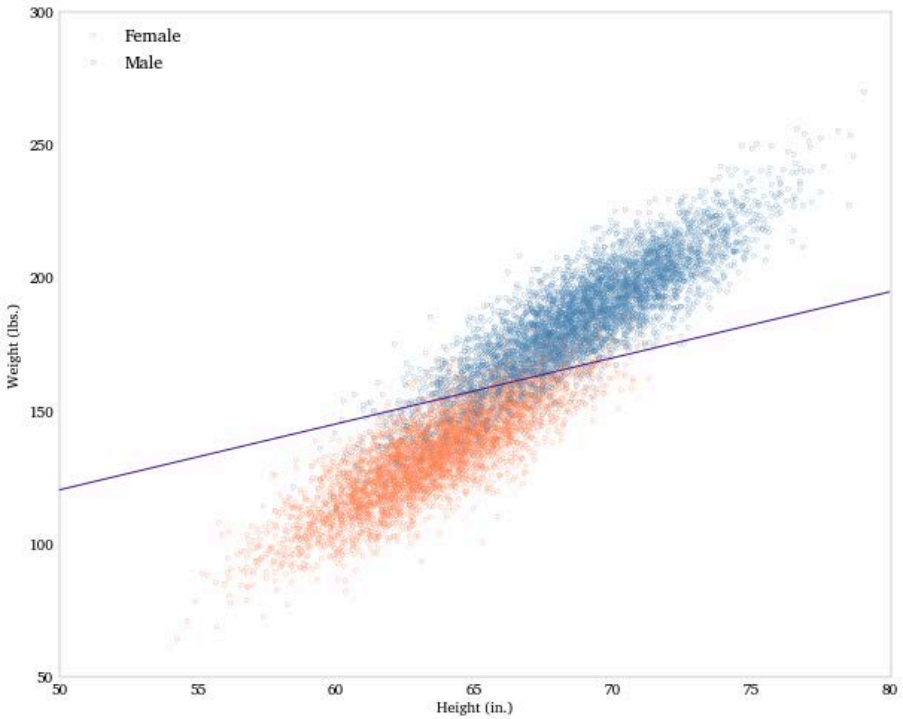


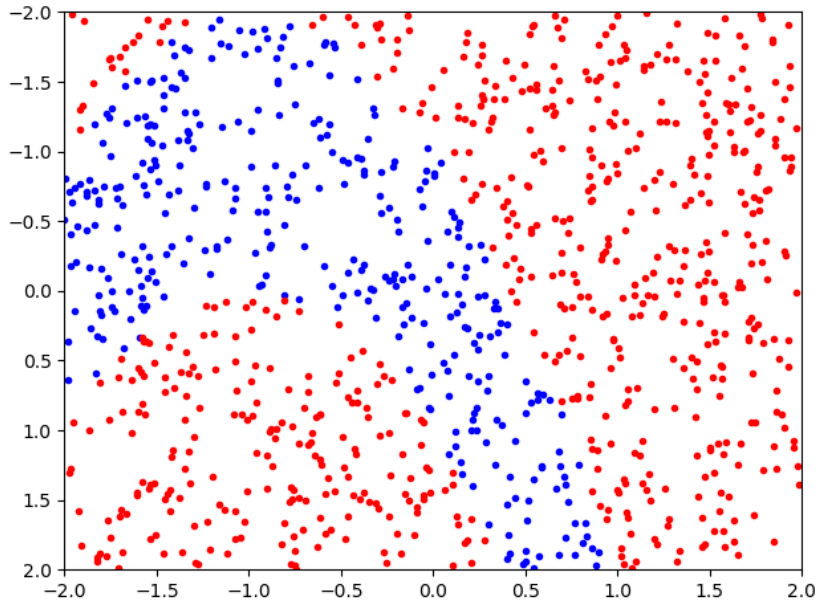

Given a **training** set $\{(\mathbf{x}_n, t_n)_{1 \leq n \leq N}\}$ minimize

$$-\sum_n (t_n \ln y(\mathbf{x}_n) + (1 - t_n) \ln(1 - y(\mathbf{x}_n))$$

with respect to $\tilde{\mathbf{w}}$.

# Reminder: Non Separable Distribution



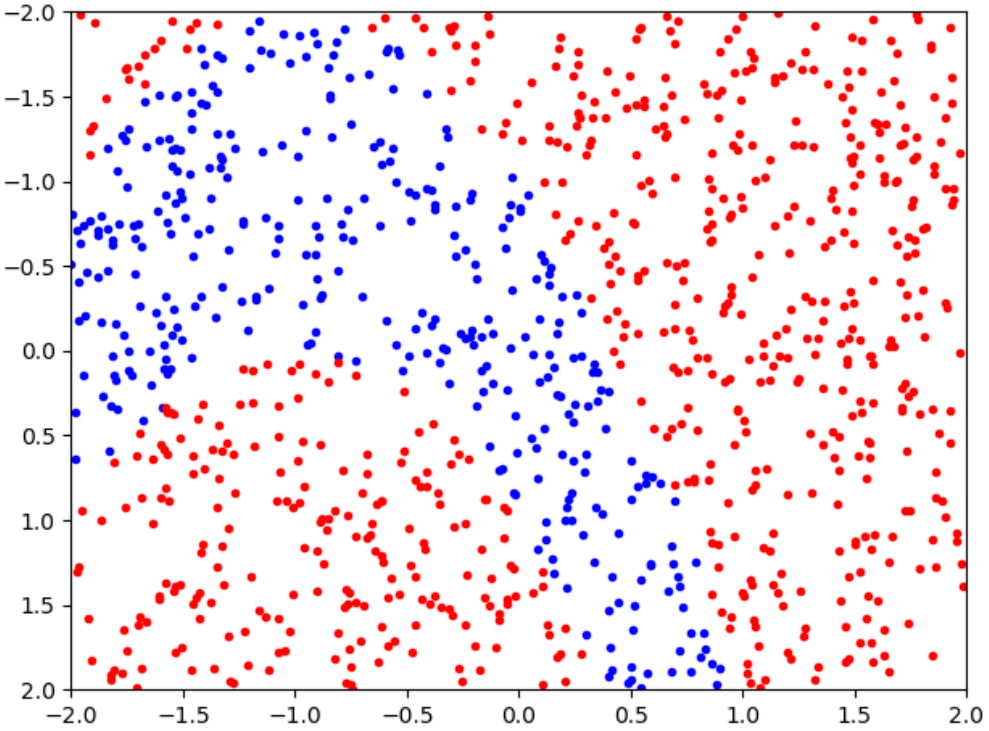



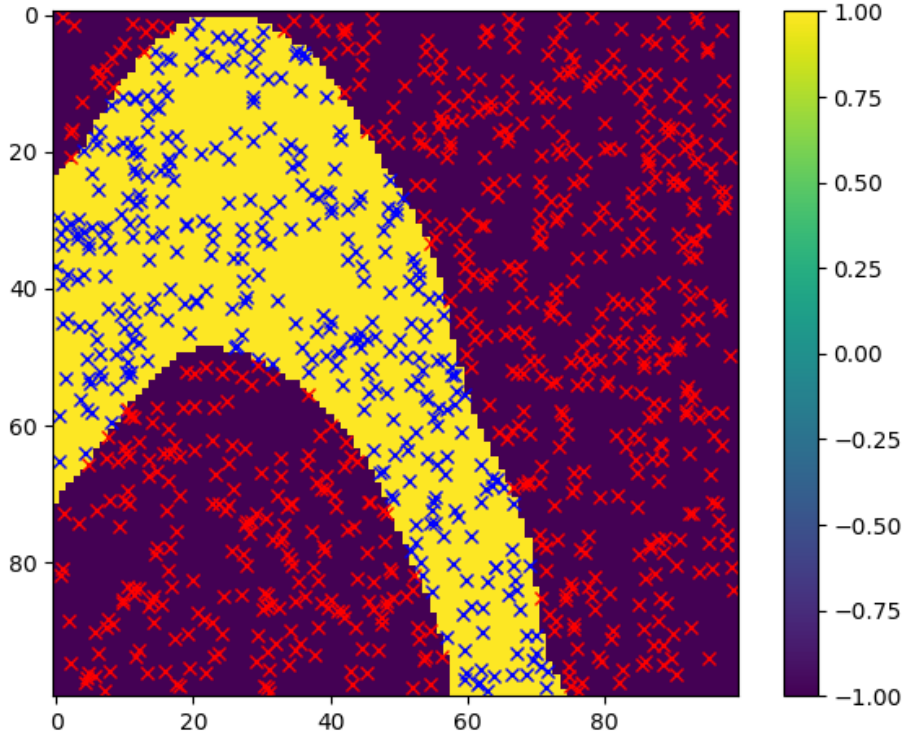

Positive: $100(x_2 - x_1^2)^2 + (1 - x_1)^2 < 0.5$

Negative: Otherwise

- Logistic regression can handle a few outliers.
- But but not a complex non-linear boundary.

# Reminder: Non Separable Distribution




Positive: $100(x_2 - x_1^2)^2 + (1 - x_1)^2 < 0.5$

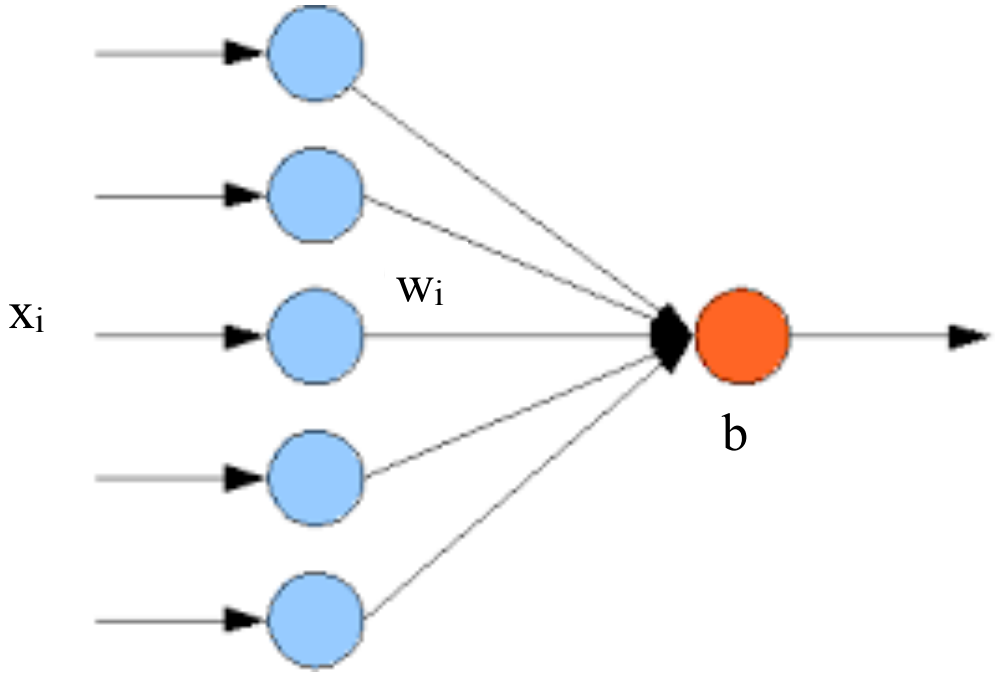
Negative: Otherwise

$y(\mathbf{x}; \tilde{\mathbf{w}})$

How can we learn a function y such that $y(\mathbf{x}; \tilde{\mathbf{w}})$ is close to 1 for positive samples and close to 0 or -1 for negative ones:

- AdaBoost: Use several hyperplanes.
- SVMs: Map to a higher dimension.
- Neural Nets: Map to a higher dimension and use lots of hyperplanes.

# Reformulating Logistic Regression

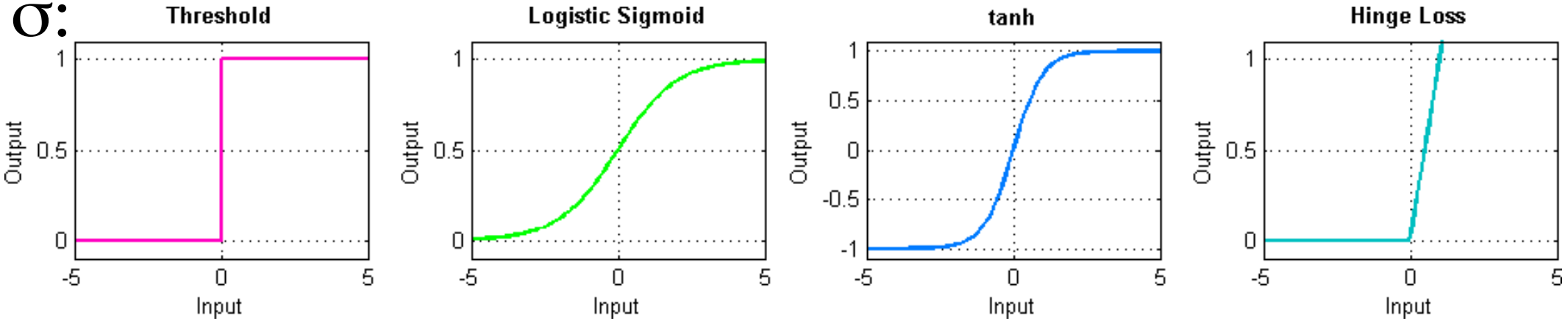



$$y(\mathbf{x}) = \sigma(\mathbf{w} \cdot \mathbf{x} + b)$$

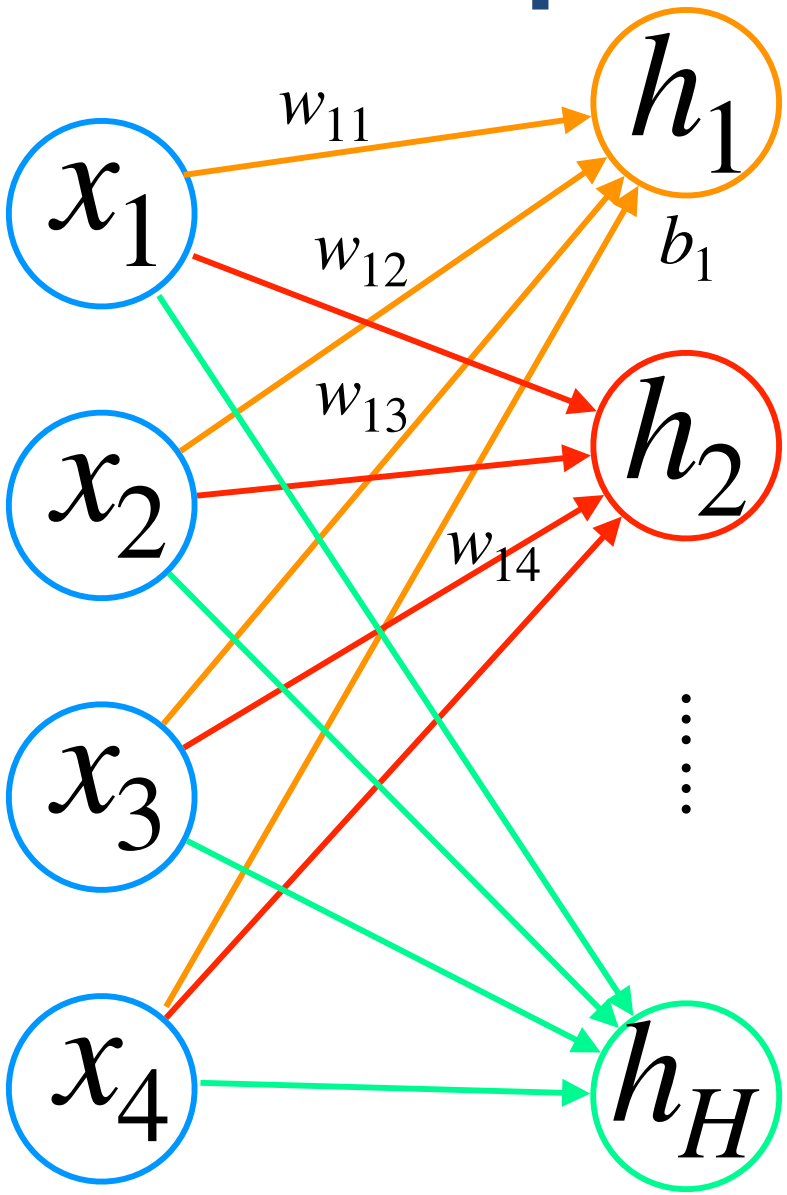
$$\mathbf{x} = \left[x_1, x_2, \ldots, x_n\right]^T$$

$$\mathbf{w} = \left[w_1, w_2, \ldots, w_n\right]^T$$

$\sigma$:



# Repeating the Process

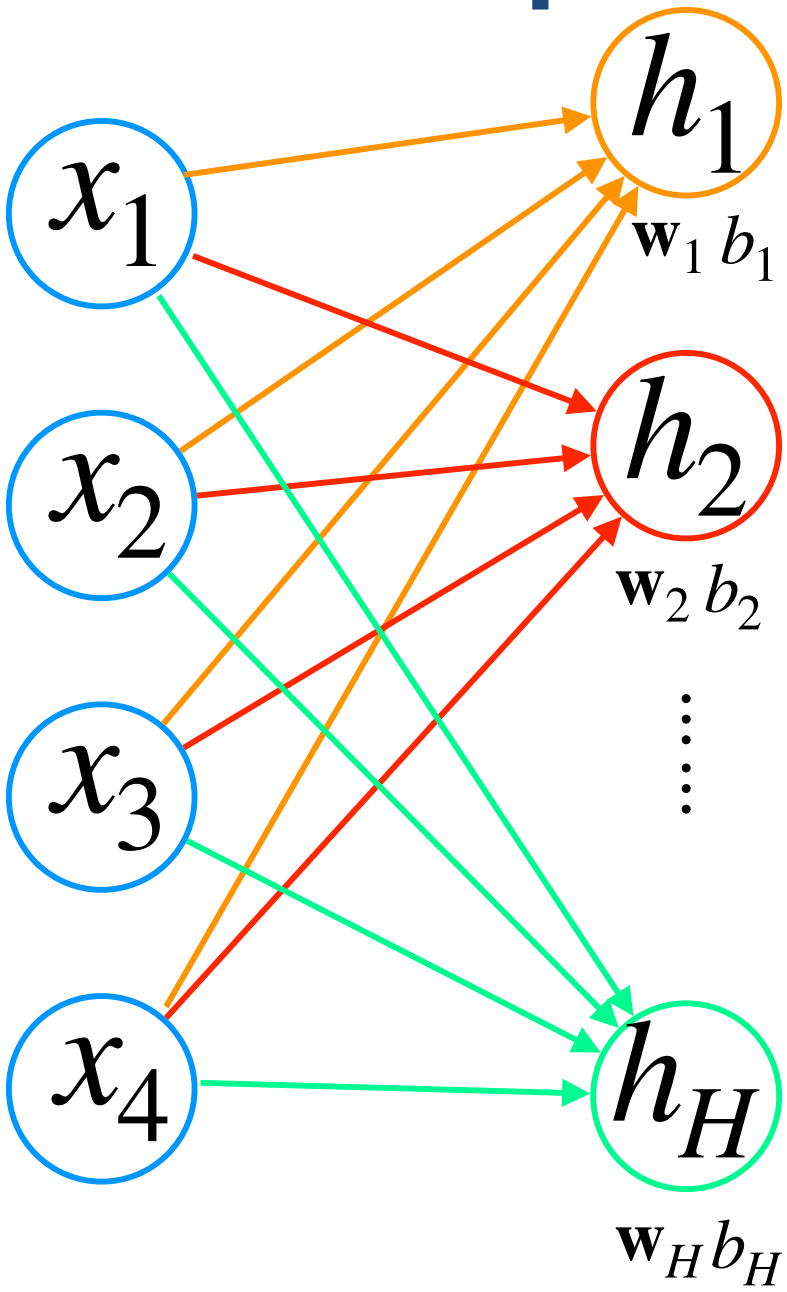



$$h_1 = \sigma(\mathbf{w}_1 \cdot \mathbf{x} + b_1)$$
$$\mathbf{w}_1 = \left[w_{11}, w_{12}, w_{13}, w_{14}\right]^T$$

$$h_2 = \sigma(\mathbf{w}_2 \cdot \mathbf{x} + b_2)$$
$$\mathbf{w}_2 = \left[w_{21}, w_{22}, w_{23}, w_{24}\right]^T$$

$$h_H = \sigma(\mathbf{w}_H \cdot \mathbf{x} + b_H)$$
$$\mathbf{w}_H = \left[w_{H1}, w_{H2}, w_{H3}, w_{H4}\right]^T$$

# Repeating the Process

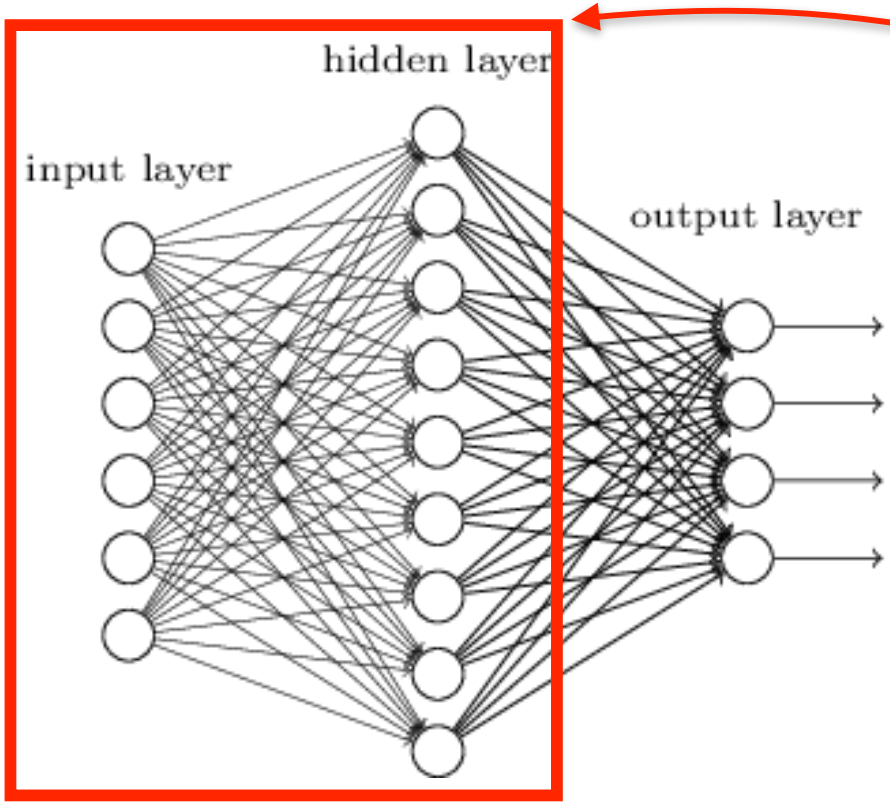



$$\mathbf{h} = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b}) \ ,$$

$$\text{with } \mathbf{W} = \begin{bmatrix} \mathbf{w}_1 \\ \mathbf{w}_2 \\ \vdots \\ \mathbf{w}_H \end{bmatrix}$$

$$\text{and } \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_H \end{bmatrix} \ .$$

# Multi-Layer Perceptron (MLP)

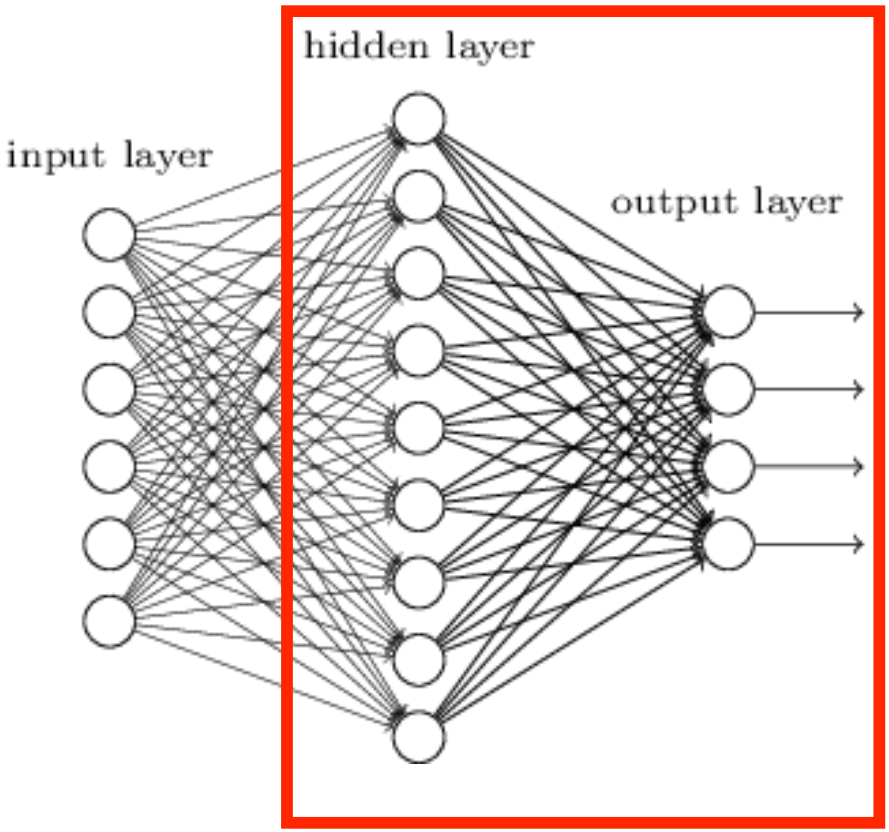



$$\mathbf{h} = \sigma_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$

$$\mathbf{y} = \sigma_2(\mathbf{W}_2\mathbf{h} + \mathbf{b}_2)$$

- The process can be repeated several times to create a vector **h**.

# Multi-Layer Perceptron (MLP)



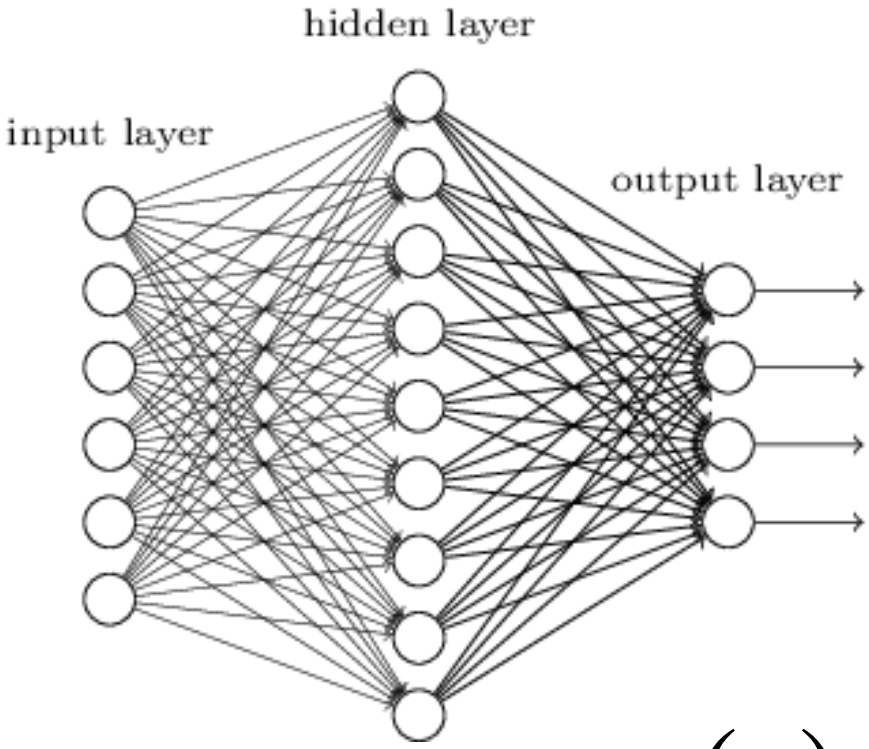

$$\mathbf{h} = \sigma_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$

$$\mathbf{y} = \sigma_2(\mathbf{W}_2\mathbf{h} + \mathbf{b}_2)$$

- The process can be repeated several times to create a vector **h**.
- It can then be done again to produce an output **y**.

—> This output is a **differentiable** function of the weights.

# MLP with ReLU



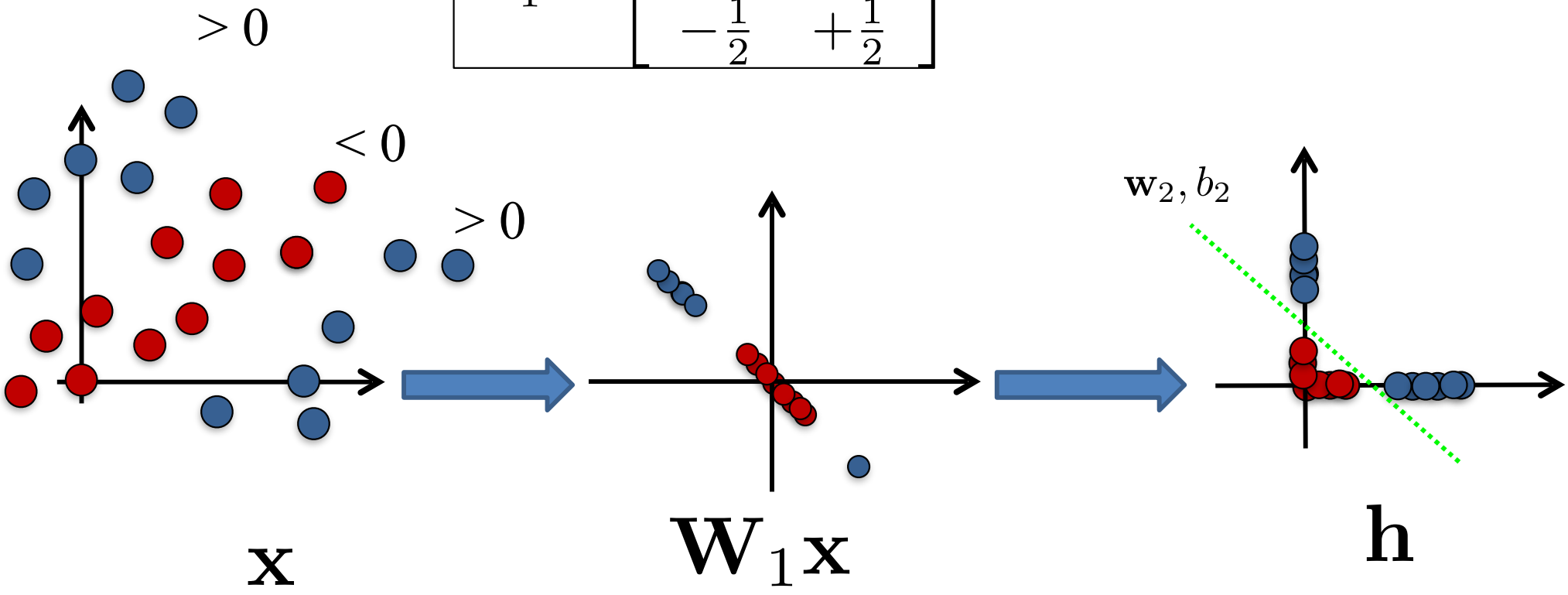

$$\mathbf{h} = \sigma_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$
$$\mathbf{y} = \sigma_2(\mathbf{W}_2\mathbf{h} + \mathbf{b}_2)$$

$$\sigma_1(\mathbf{x}) = \max(\mathbf{0}, \mathbf{x})$$

- Each node defines a hyperplane.
- The resulting function is piecewise linear affine and continuous.

# ReLu Behavior

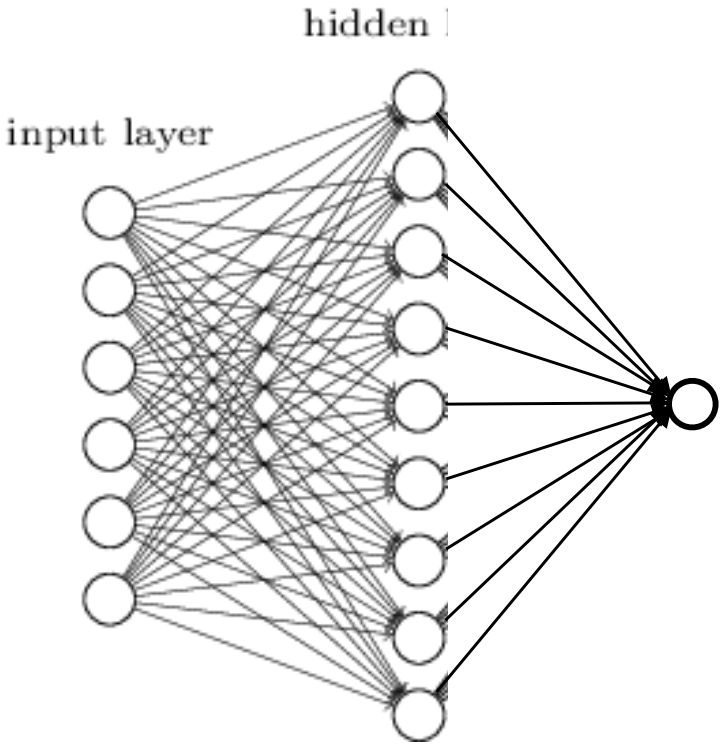
$$\mathbf{W}_1 = \begin{bmatrix} +\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & +\frac{1}{2} \end{bmatrix}$$




$$\mathbf{h} = \mathrm{ReLu}(\mathbf{W}_1\mathbf{x})$$

$$\mathbf{y} = \mathbf{w}_2^T\mathbf{h} + b_2$$

# Binary Case




$$\mathbf{h} = \sigma_1(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)$$

$$y = \sigma_2(\mathbf{w}_2\mathbf{h} + b_2)$$

In this case $w_2$ is vector.

# Binary Case

- Let the training set be $\{(\mathbf{x}_n, t_n)_{1 \leq n \leq N}\}$ where $t_n \in \{0,1\}$ is the class label and let us consider a neural net with a 1D output.

- We write

$$y_n = \sigma(\mathbf{w}_2(\sigma(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)) + \mathbf{b}_2) \in [0.1]$$

- We want to minimize the binary cross entropy

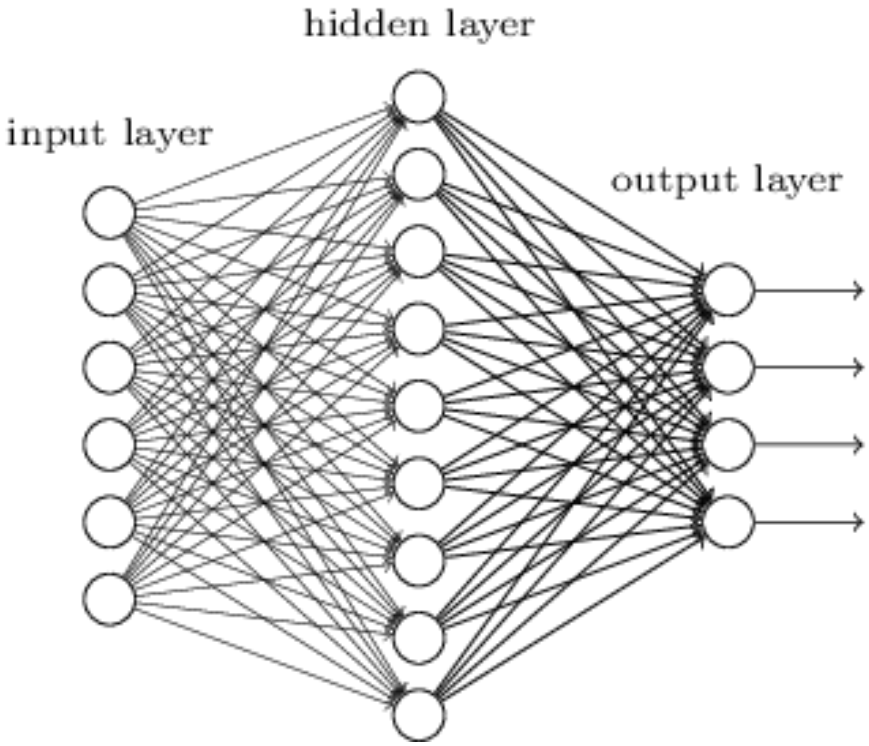
$$E(\mathbf{W}_1, \mathbf{w}_2, \mathbf{b}_1, \mathbf{b}_2) = \frac{1}{N}\sum_{n=1}^{N} E_n(\mathbf{W}_1, \mathbf{w}_2, \mathbf{b}_1, \mathbf{b}_2) \ ,$$

$$E_n(\mathbf{W}_1, \mathbf{w}_2, \mathbf{b}_1, \mathbf{b}_2) = -\left(t_n \ln(y_n) + (1 - t_n)\ln(1 - y_n)\right) \ ,$$

  with respect to the coefficients of $\mathbf{W}_1$, $\mathbf{w}_2$, $\mathbf{b}_1$, and $\mathbf{b}_2$.

- E is a differentiable function and this can be done using a gradient-based technique.

# Multi-Class Case




$$\mathbf{h} = \sigma(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)$$

$$y = \sigma(\mathbf{W}_2\mathbf{h} + \mathbf{b}_2)$$

In this case $\mathbf{W}_2$ is a matrix.

# Multi-Class Case

Let the training set be $\{(\mathbf{x}_n, [t_n^1, \ldots, t_n^K])_{1 \leq n \leq N}\}$ where $t_n^k \in \{0,1\}$ is the probability that sample $\mathbf{x}_n$ belongs to class k.

- We write

$$\mathbf{y}_n = \sigma(\mathbf{W}_2(\sigma(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)) + \mathbf{b}_2) \in R^K$$

$$p_n^k = \frac{\exp(\mathbf{y}_n[k])}{\sum_j \exp(\mathbf{y}_n[j])}$$

- We want to minimize the cross entropy

$$E(\mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2) = \frac{1}{N} \sum_{n=1}^{N} E_n(\mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2) \ ,$$

$$E_n(\mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2) = -\sum t_n^k \ln(p_n^k) \ ,$$

with respect to the coefficients of $\mathbf{W}_1$, $\mathbf{W}_2$, $\mathbf{b}_1$, and $\mathbf{b}_2$.

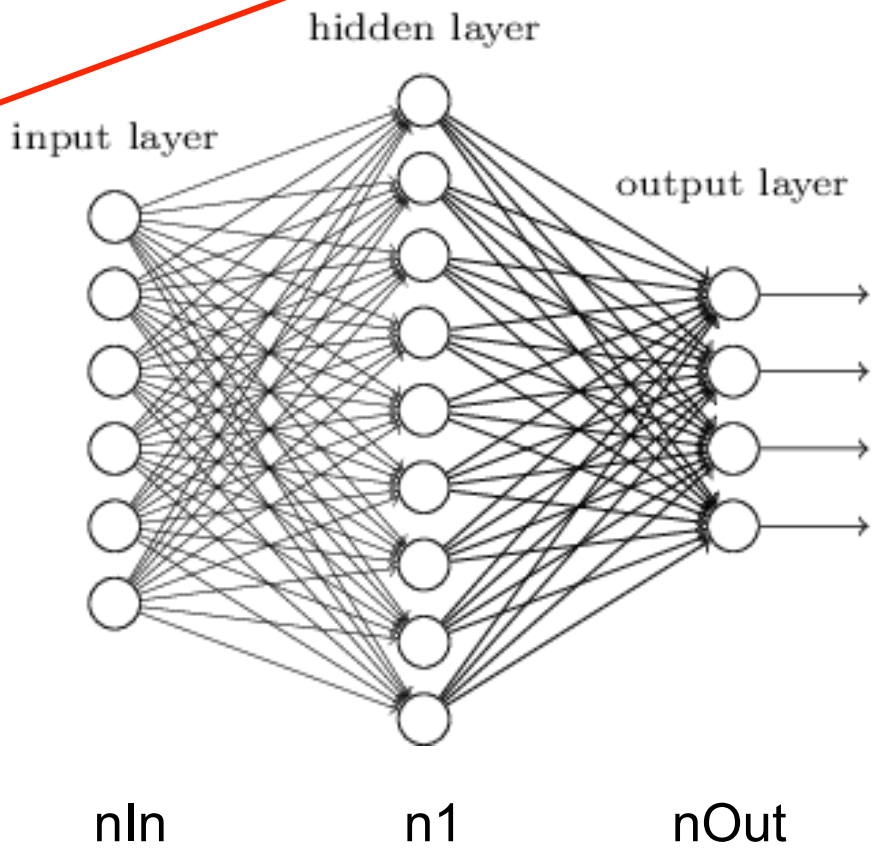
# Optional: PyTorch Translation (1)

```
class MLP(nn.Module):

    def __init__(self,n1=10,nIn=2,nOut=1):
        self.l1 = nn.Linear(nIn,n1)
        self.l2 = nn.Linear(n1,nOut)

    def forward(self,x):
        h = sigm(self.l1(x))
        return sigm(self.l2(h))
```

$\mathbf{W}_1$ is an nIn x $n_1$ matrix.

$\mathbf{W}_2$ is an n1 x nOut matrix.

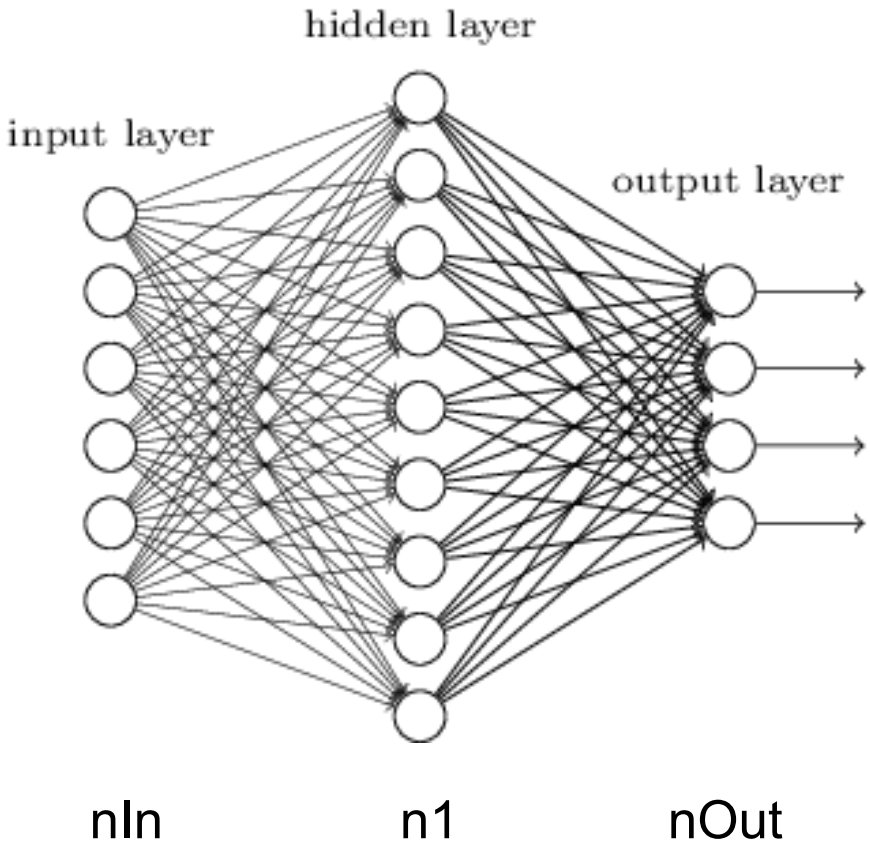
Return $\sigma(\mathbf{W}_2(\sigma(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)) + \mathbf{b}_2)$



# Optional: PyTorch Translation (2)

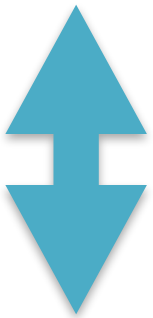
```
class MLP(nn.Module):

    def __init__(self,n1=10,nIn=2,nOut=1):
        self.l1 = nn.Linear(nIn,n1)
        self.l2 = nn.Linear(n1,nOut)

    def forward(self,x):
        h = sigm(self.l1(x))
        return self.l2(h)

    def loss(self,x,target):
        loss_fn = torch.nn.CrossEntropyLoss()
        output = self(x)
        return loss_fn(output,target)
```

Return $-\sum t_n^k \ln(p_n^k)$



# More Compact Notation

$$\begin{aligned}\mathbf{h} &= \sigma_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1) \\ \mathbf{y} &= \sigma_2(\mathbf{W}_2\mathbf{h} + \mathbf{b}_2)\end{aligned}$$



$$\begin{aligned}\mathbf{h} &= \sigma_1([\mathbf{W}_1|\mathbf{b}_1]\begin{bmatrix}\mathbf{x}\\1\end{bmatrix}) \\ \mathbf{y} &= \sigma_2([\mathbf{W}_2|\mathbf{b}_2]\begin{bmatrix}\mathbf{h}\\1\end{bmatrix})\end{aligned}$$

$$\begin{aligned}\mathbf{w} &= [\mathbf{w}_1|\mathbf{b}_1|\mathbf{w}_2|\mathbf{b}_2] \\ E(\mathbf{w}) &= \sum_{n=1}^{N} E_n(\mathbf{w})\end{aligned}$$

$\mathbf{w}_n$: Matrix $\mathbf{W}_n$ represented by a 1D vector.

# More Compact Formulation

- Given a training set be $\{(\mathbf{x}_n, [t_n^1, \ldots, t_n^K])_{1 \le n \le N}\}$ where $t_n^k \in \{0,1\}$ is the probability that sample $\mathbf{x}_n$ belongs to class k, we write:

$$\mathbf{y}_n = f_{\mathbf{w}}(\mathbf{x}_n) \in R^K$$

$$p_n^k = \frac{\exp(\mathbf{y}_n[k])}{\sum_j \exp(\mathbf{y}_n[j])}$$

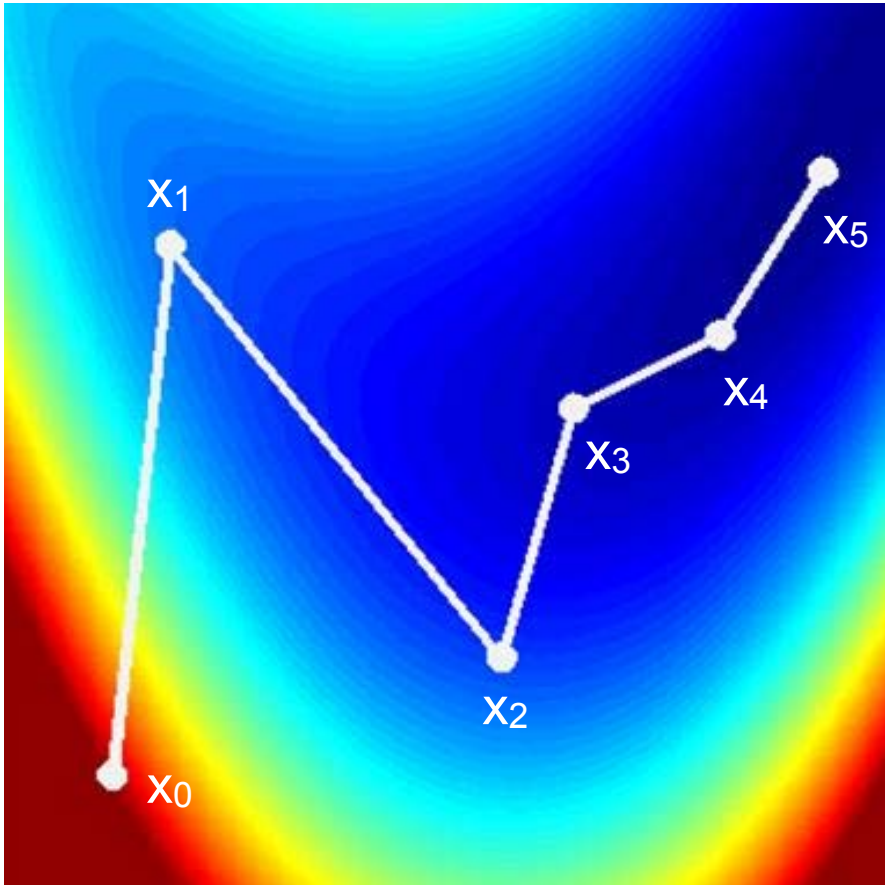
- We want to minimize the cross entropy

$$E(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} E_n(\mathbf{w}) \ ,$$

$$E_n(\mathbf{w}) = - \sum_{k=1}^{K} t_n^k \ln(p_n^k) \ ,$$

with respect to the coefficients of $\mathbf{w}$.

# Reminder: Gradient Descent




$$f(\mathbf{x} + d\mathbf{x}) \approx f(\mathbf{x}) + \nabla f \cdot d\mathbf{x}$$

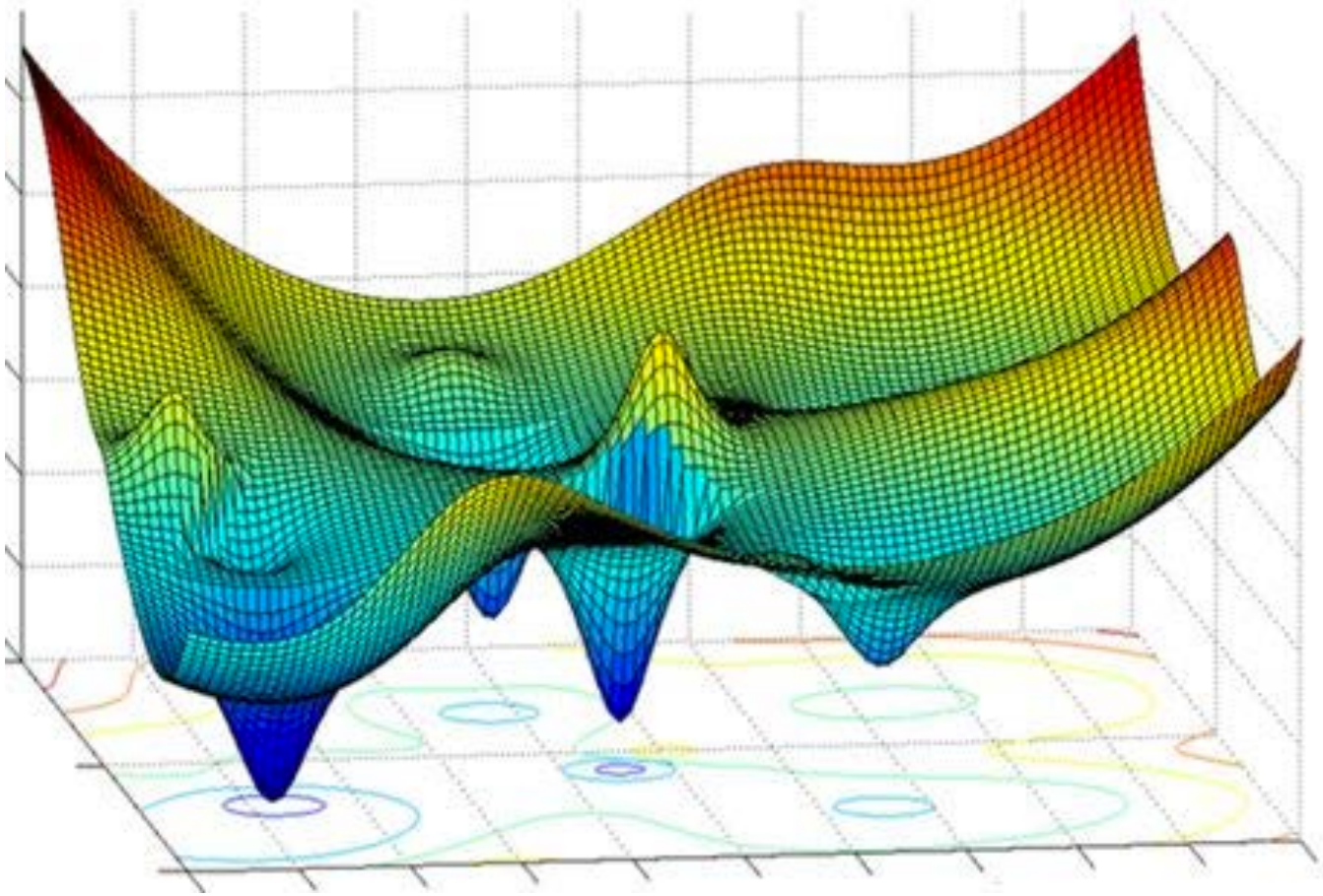
$$d\mathbf{x} = -\eta \nabla f$$

$$\Rightarrow f(\mathbf{x} + d\mathbf{x}) \approx f(\mathbf{x}) - \eta \|\nabla f\|^2 < f(\mathbf{x})$$

$$\mathbf{x}^{\tau+1} = \mathbf{x}^{\tau} - \eta \nabla f(\mathbf{x}^{\tau})$$

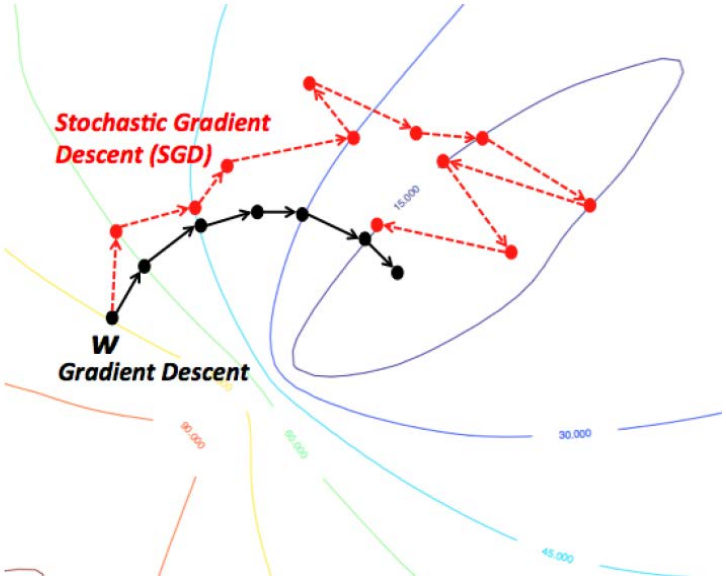
—> $\eta$ is known as the learning rate and must be carefully chosen.

# Reminder: Local Minima



The result depends critically on the starting point and is very likely to be closest local minimum, which is not usually the global one.

# Stochastic Gradient Descent




$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

Gradient descent: $\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \sum_{n=1}^{N} \nabla E_n(\mathbf{w}^{\tau})$ .

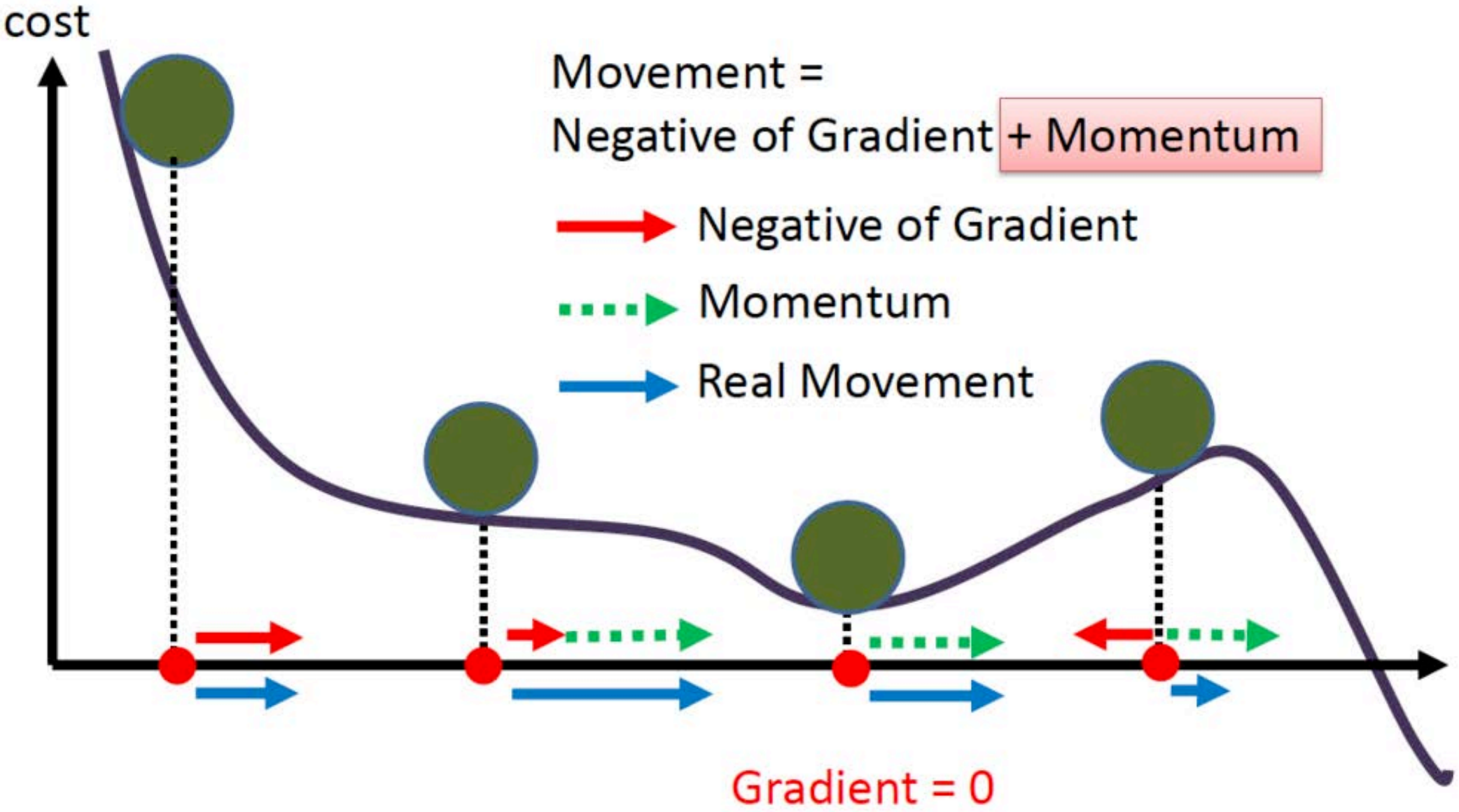
Stochastic descent: $\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \sum_{n \in B^{\tau}} \nabla E_n(\mathbf{w}^{\tau})$ ,

where $B^{\tau}$ represents a different randomly chosen set of indices at each iteration, also known as a mini-batch.

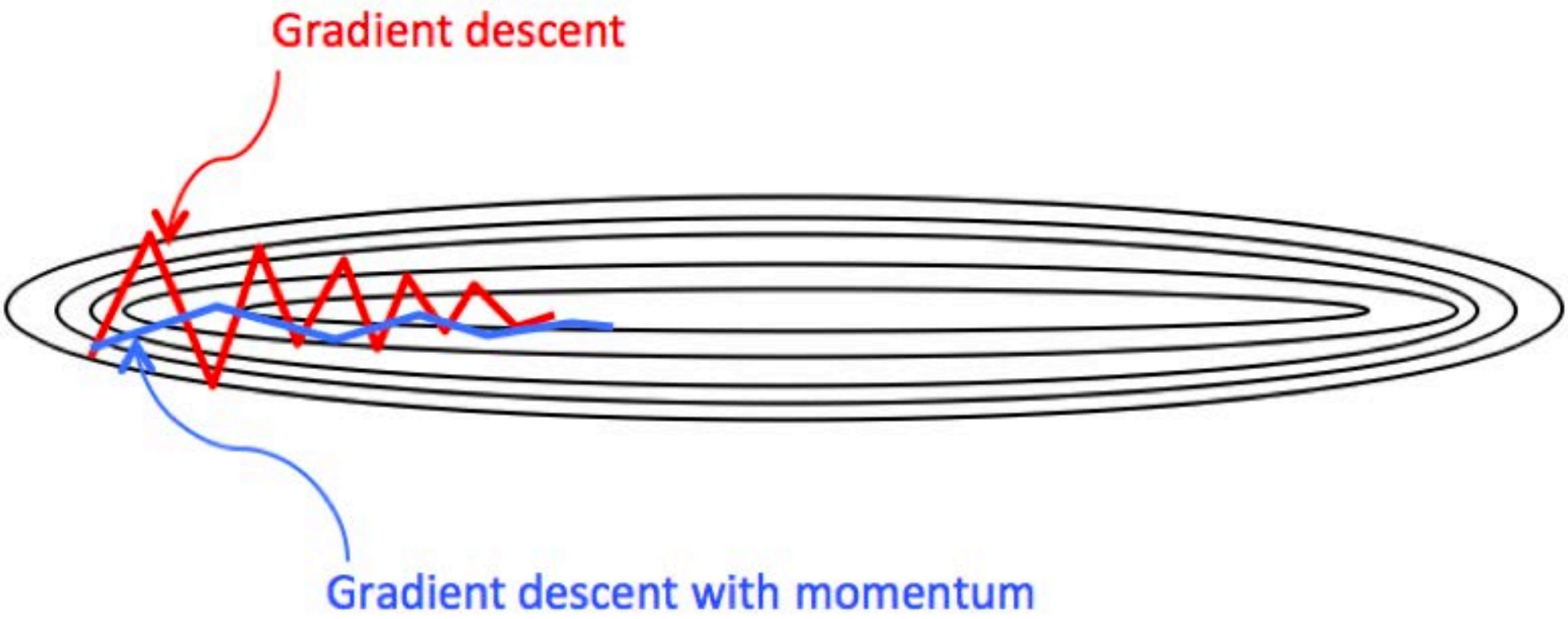
Randomly choosing batches

- helps reduce the chances of falling into local minima,
- makes the computation possible on GPUs even when dealing with LARGE databases.

# Escaping Local Minima



# Improved Gradient Descent



# Adaptive Moment Estimation

$$\mathbf{g}_{\tau+1} = \sum_{n \in B^\tau} \nabla E_n(\mathbf{w}^\tau)$$ Minibatch gradient.

$$\mathbf{m}_{\tau+1} = \beta_1 \mathbf{m}_\tau + (1-\beta_1)\mathbf{g}_{\tau+1}$$ Mean gradient.

$$\mathbf{v}_{\tau+1} = \beta_2 \mathbf{v}_\tau + (1-\beta_2)\mathbf{g}^2_{\tau+1}$$ Mean gradient squared.

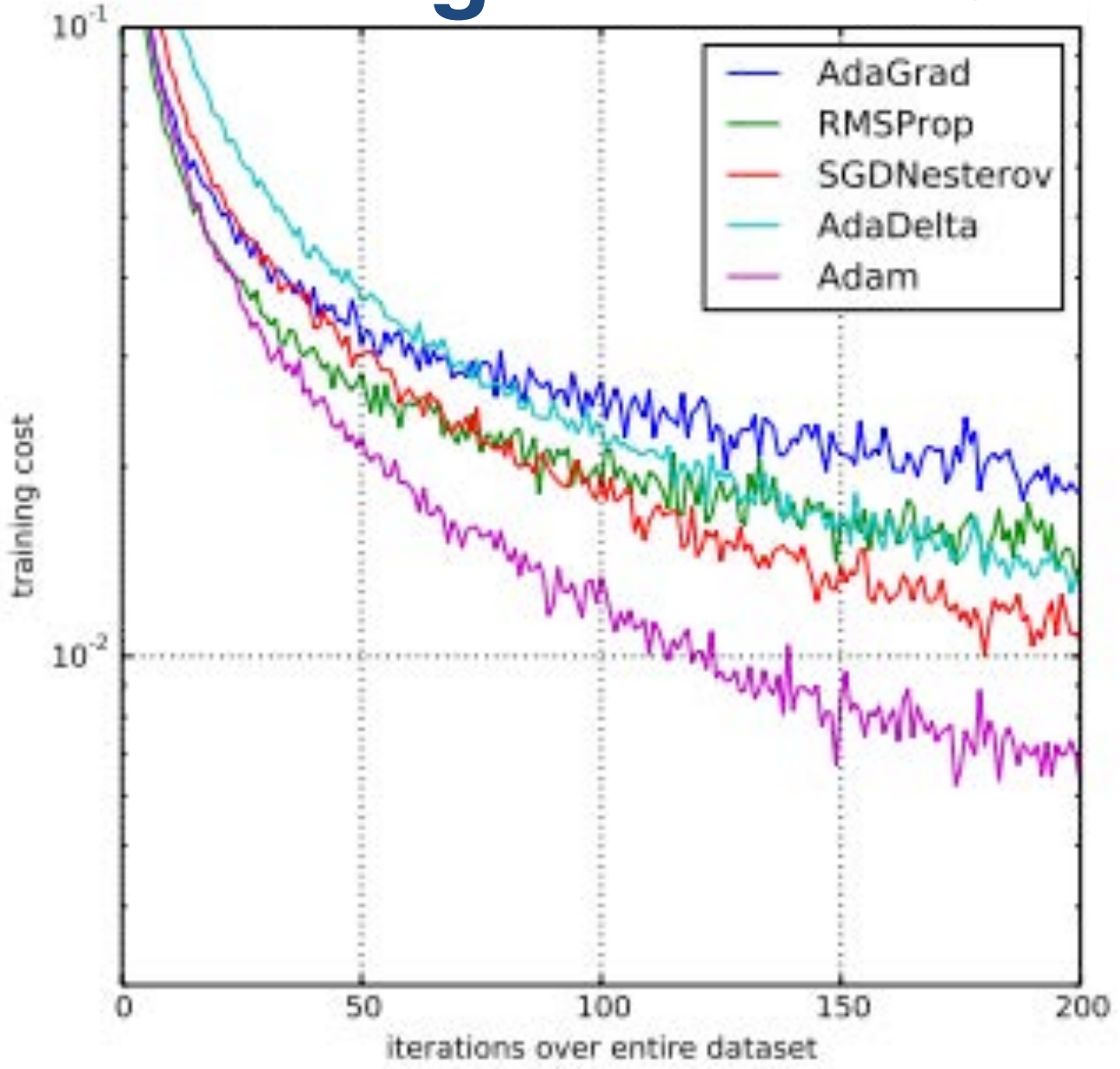
$$\hat{\mathbf{m}}_{\tau+1} = \frac{\mathbf{m}_{\tau+1}}{1-\beta_1^t}$$ Corrective factor.

$$\hat{\mathbf{v}}_{\tau+1} = \frac{\mathbf{v}_{\tau+1}}{1-\beta_2^t}$$ Corrective factor.

$$\mathbf{w}_{\tau+1} = \mathbf{w}_\tau - \alpha \frac{\hat{\mathbf{m}}_{\tau+1}}{\sqrt{\hat{\mathbf{v}}_{\tau+1} + \epsilon}}$$ Gradient step.

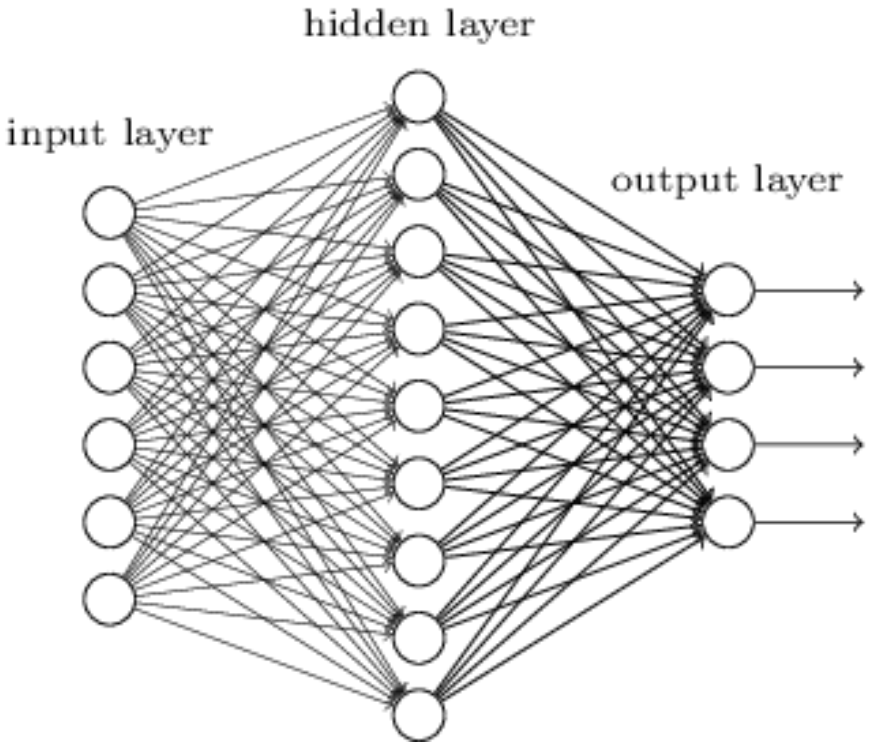
$$\mathbf{m}_0 = \mathbf{v}_0 = 0,$$
$$\beta_1 = 0.9,$$
$$\beta_2 = 0.999,$$
$$\alpha = 0.001,$$
$$\epsilon = 10^{-8}$$

# Training the Network




- The loss decreases over time but not monotonically.
- It can take a very long time to converge.

# Reminder: MLP with ReLU

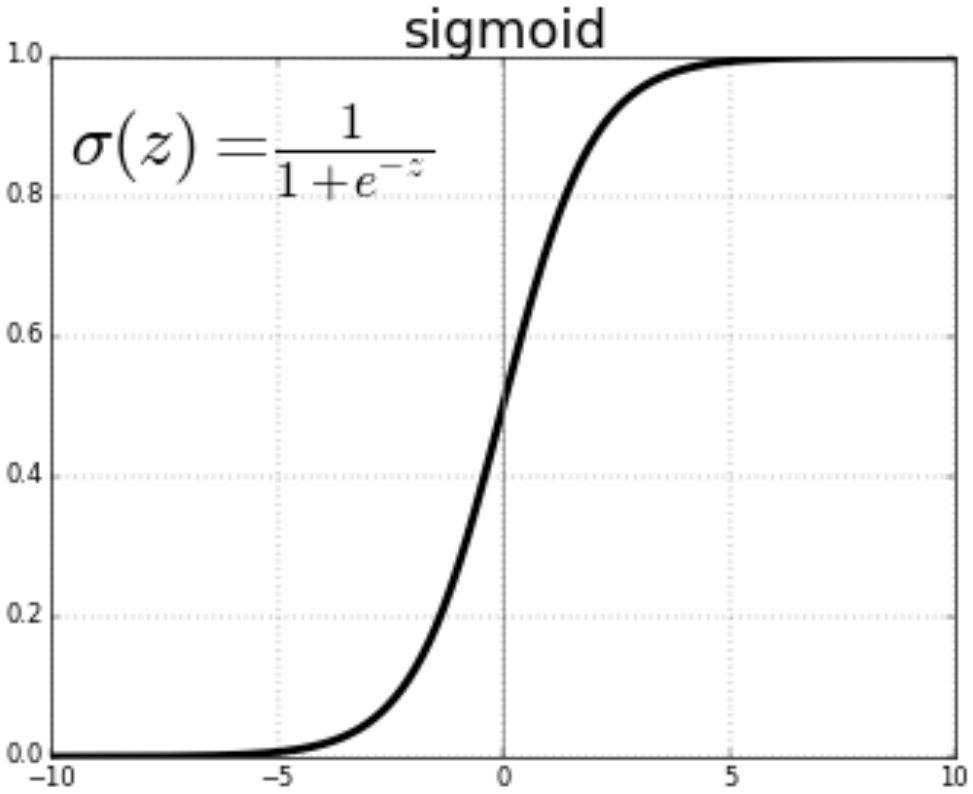


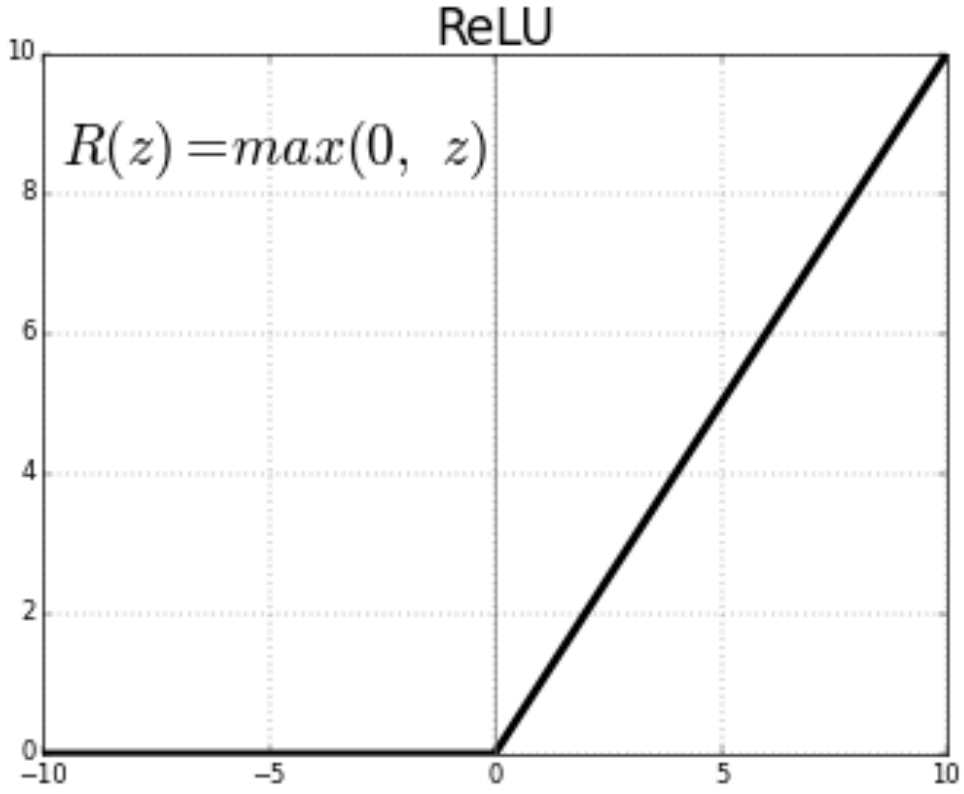

$$\mathbf{h} = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$
$$\mathbf{y} = \sigma(\mathbf{W}_2\mathbf{h} + \mathbf{b}_2)$$

$\sigma(\mathbf{x}) = \max(0,\mathbf{x})$.

- Each node defines a hyperplane.
- The resulting function is piecewise linear affine and continuous.

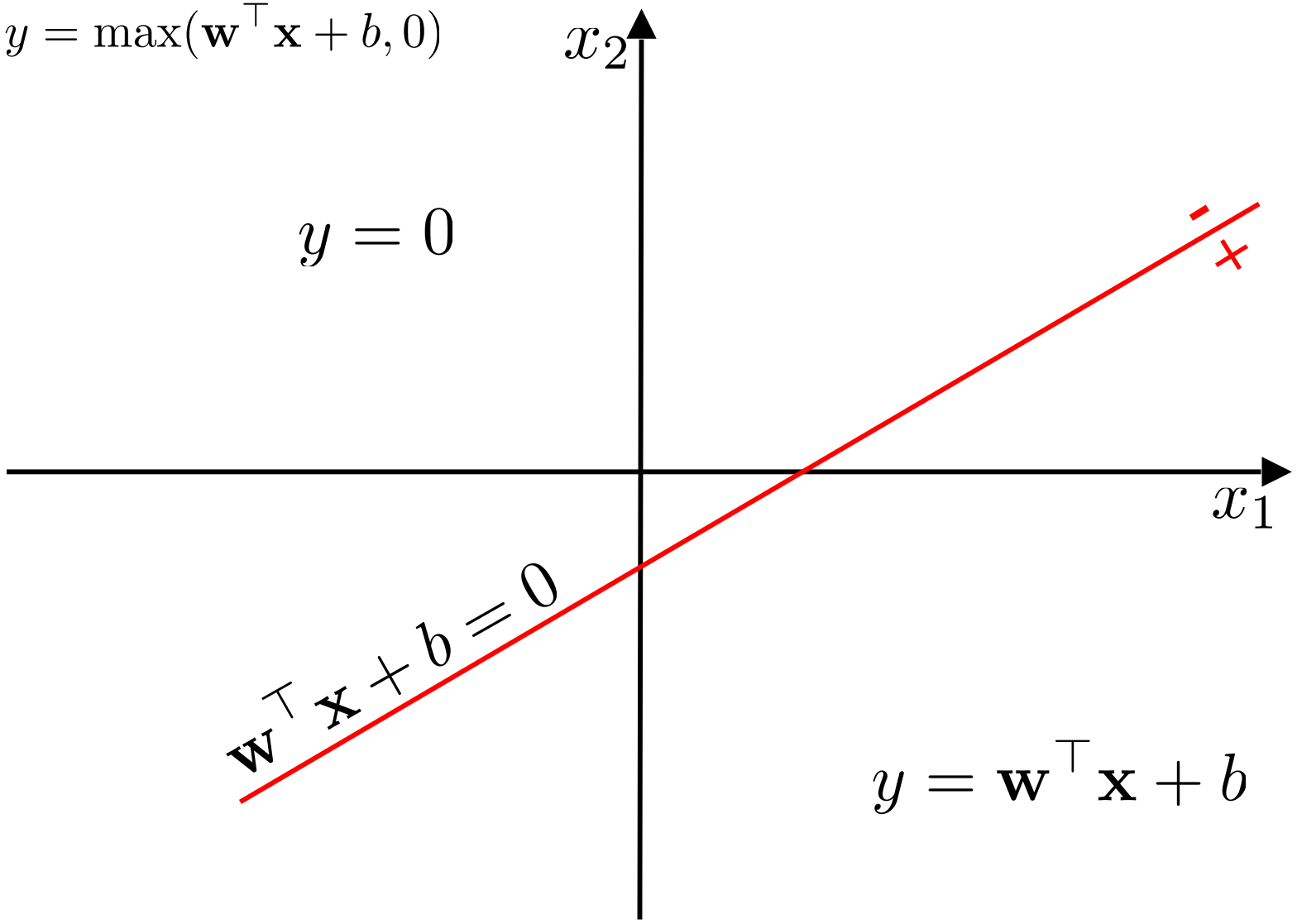
# Sigmoid vs ReLu




- One problem with the sigmoid function is that when the argument is not close to zero the gradients vanish.
- Empirically, replacing the Sigmoid by ReLu has significantly boosted performance in many cases.

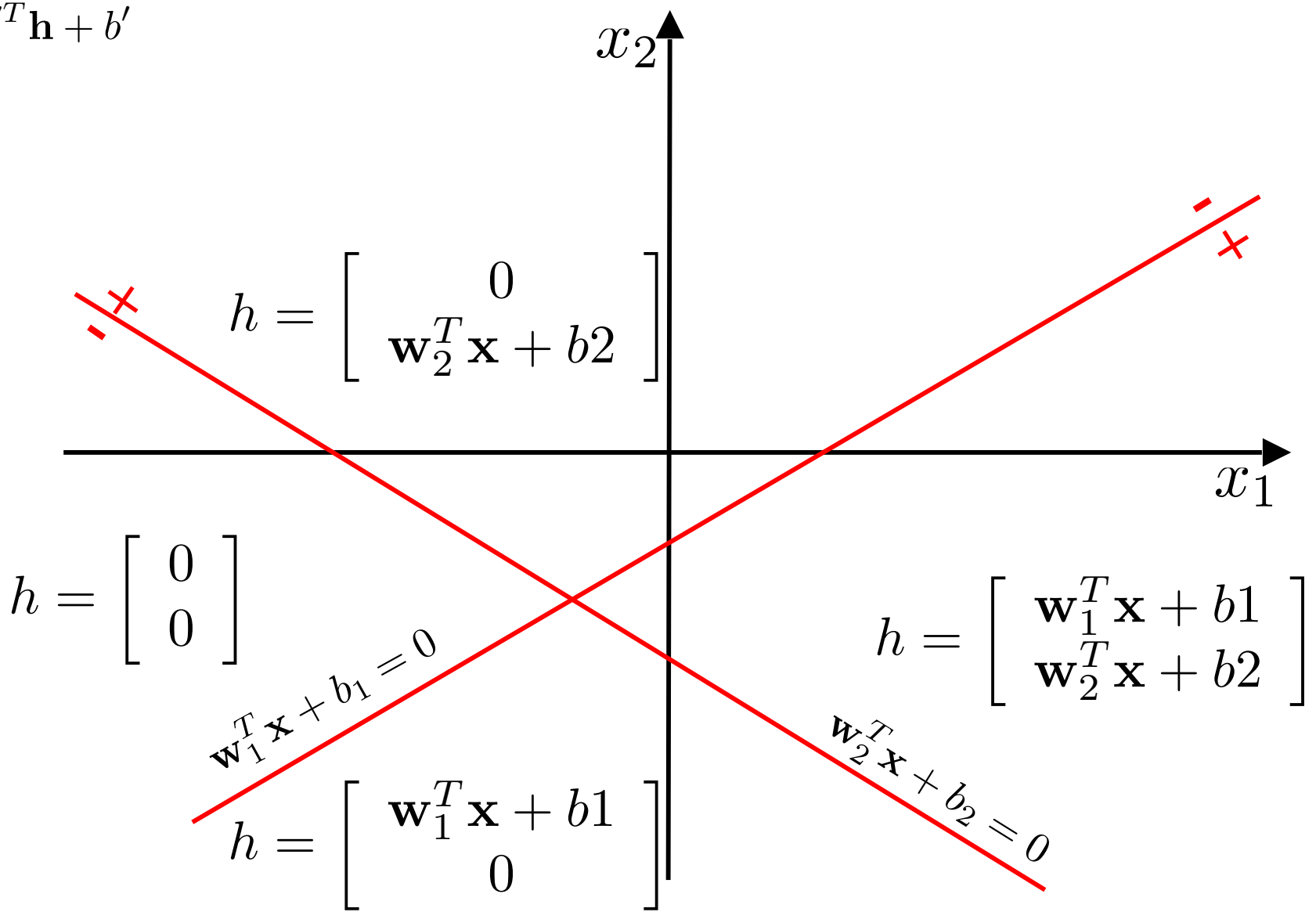
# One Single Hyperplane



# Two Hyperplanes

$$\mathbf{h} = \max(\mathbf{W}\mathbf{x} + \mathbf{b}, 0) \text{ with } \mathbf{W} = \begin{bmatrix} \mathbf{w}_1^T \\ \mathbf{w}_2^T \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

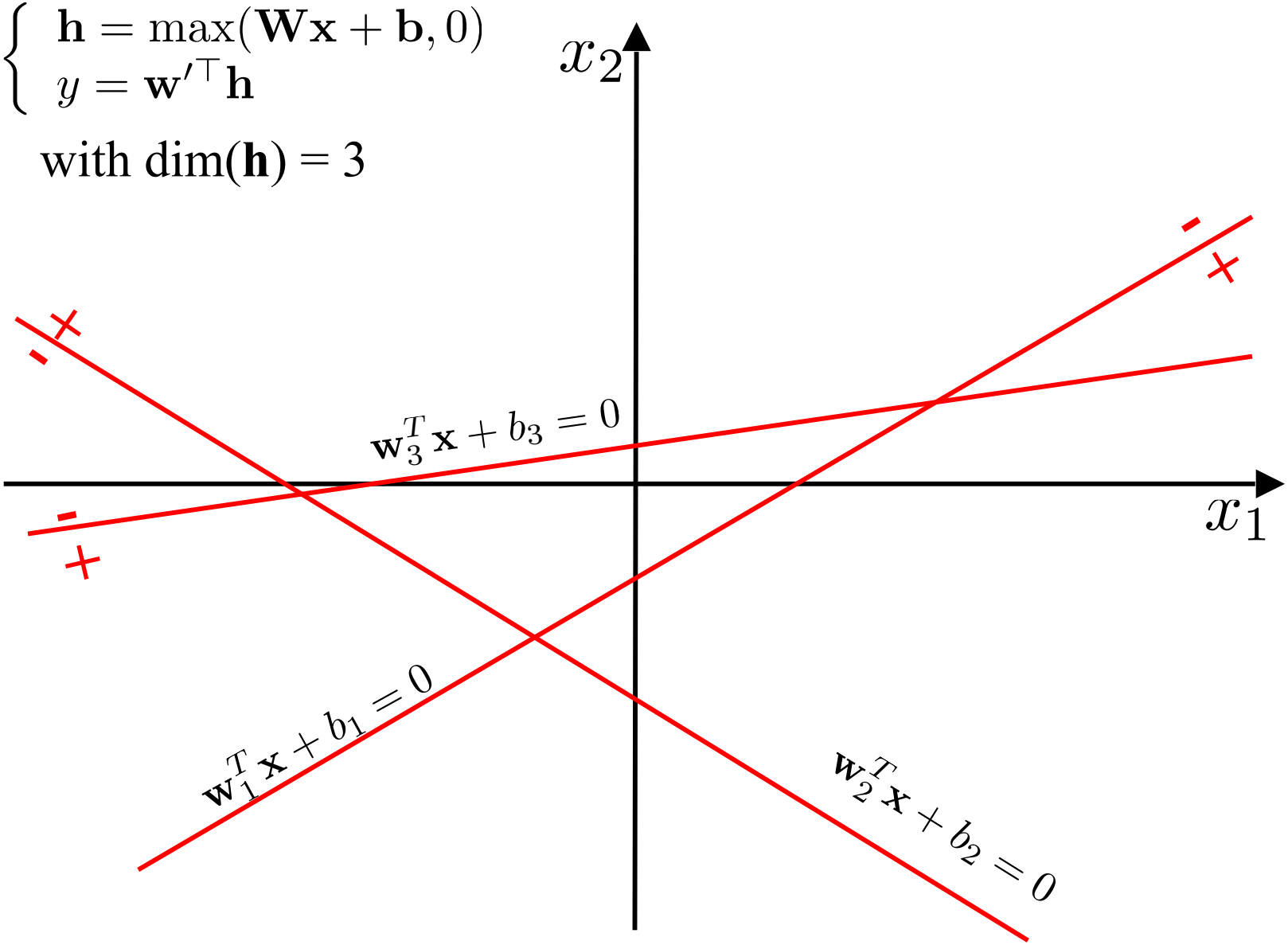
$$y = \mathbf{w}'^T \mathbf{h} + b'$$



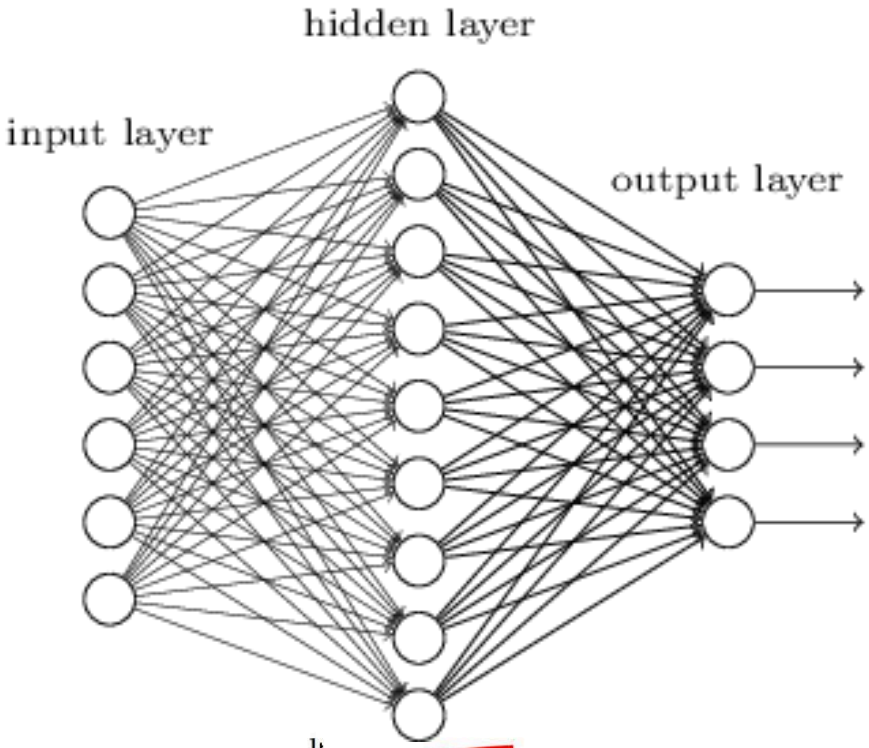
# Three Hyperplanes

$$\begin{cases} \mathbf{h} = \max(\mathbf{W}\mathbf{x} + \mathbf{b}, 0) \\ y = \mathbf{w}'^{\top}\mathbf{h} \end{cases}$$

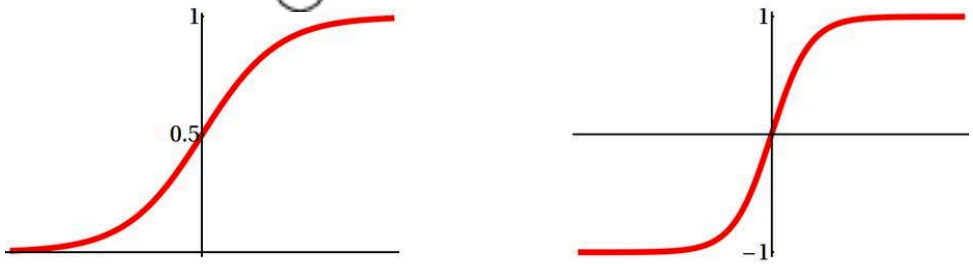
with $\dim(\mathbf{h}) = 3$



# MLP with Sigmoid or Tanh




$$\mathbf{h} = \sigma(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$
$$\mathbf{y} = \sigma(\mathbf{W}_2\mathbf{h} + \mathbf{b}_2)$$

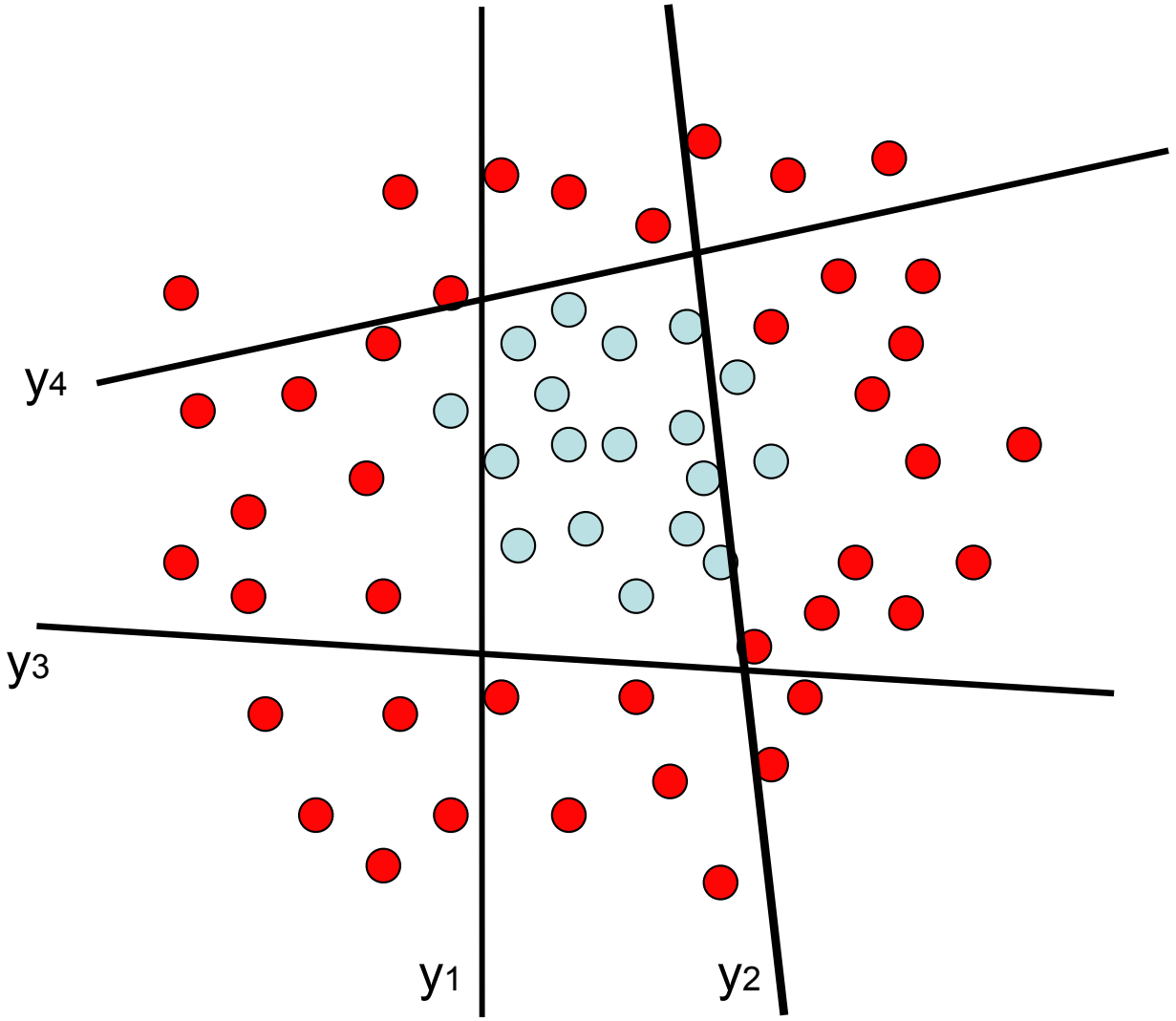



$$\text{sigm:} \quad \sigma(x) = \frac{1}{1+\exp(-x)}$$
$$\tanh: \quad \sigma(x) = \frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)}$$

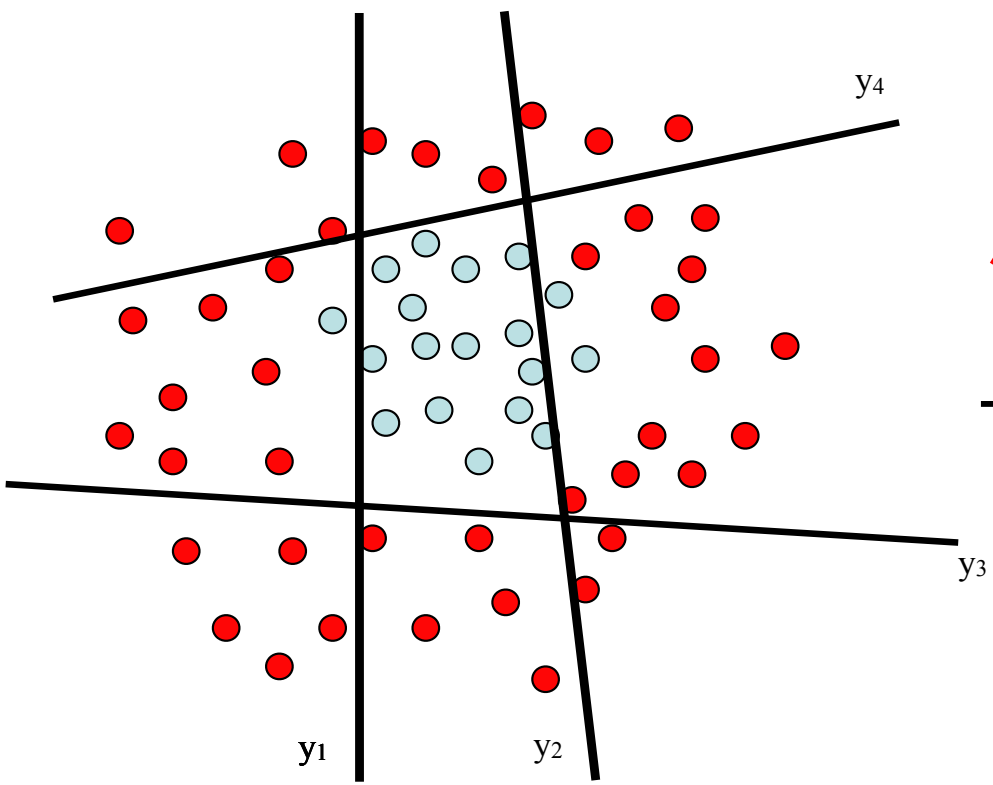
- Each node defines a hyperplane.
- The resulting function is continuously differentiable.

# Reminder: AdaBoost

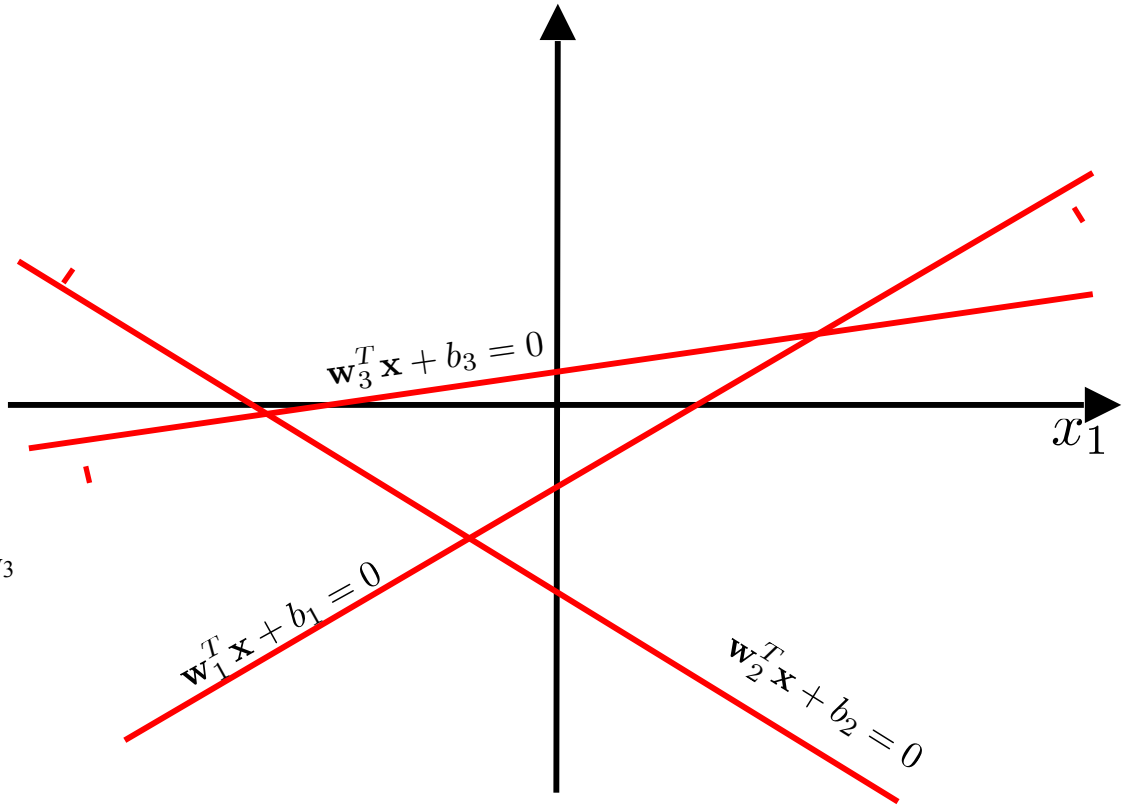
$$y(\mathbf{x}) = \alpha_1 y_1(\mathbf{x}) + \alpha_2 y_2(\mathbf{x}) + \alpha_3 y_3(\mathbf{x}) + \alpha_4 y_4(\mathbf{x})$$



# AdaBoost vs MLP




AdaBoost

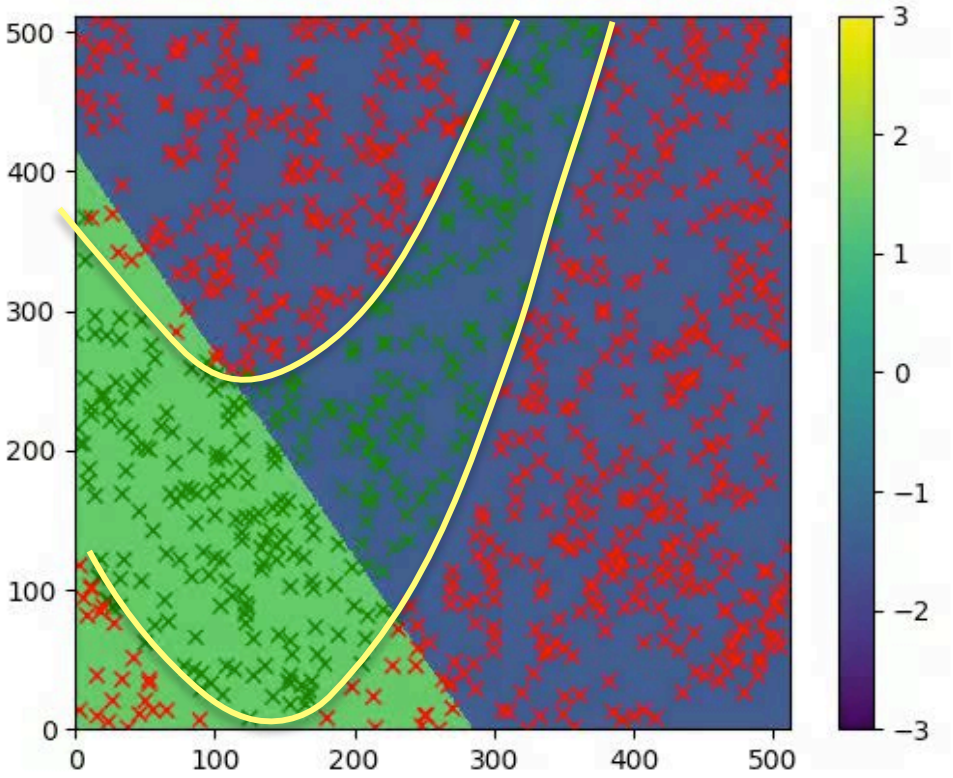



MLP

Both methods find a set of hyperplanes:

- One at a time for a AdaBoost.
- All together for MLPs.

# Rosenbrock using Adaboost



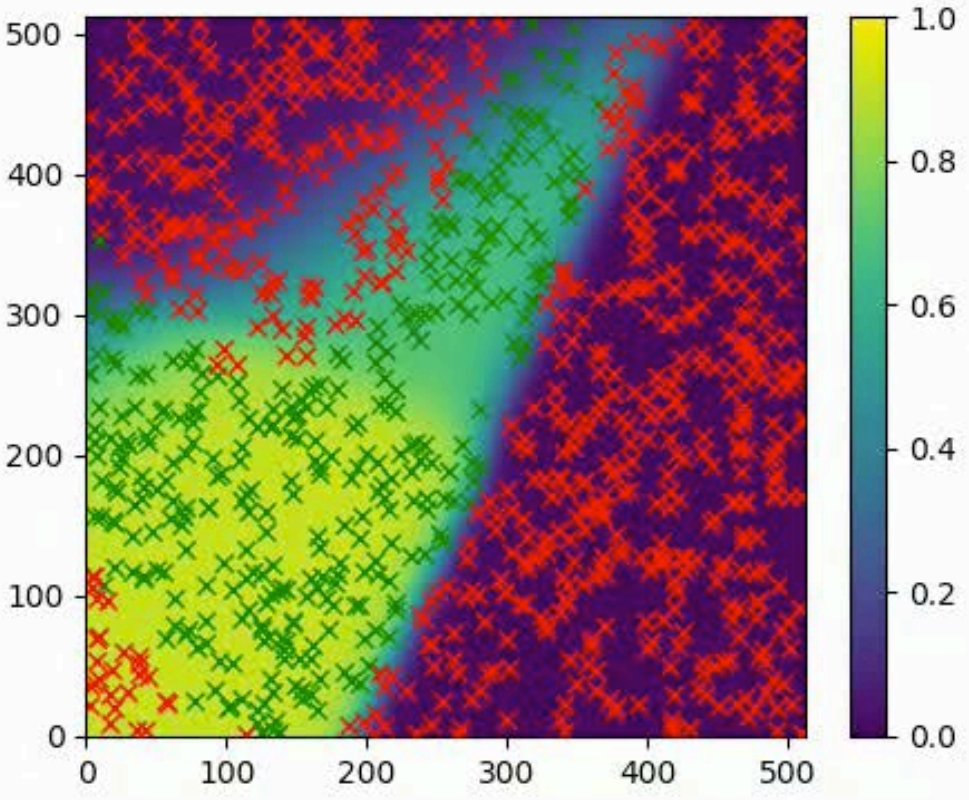

Training (100 iterations)

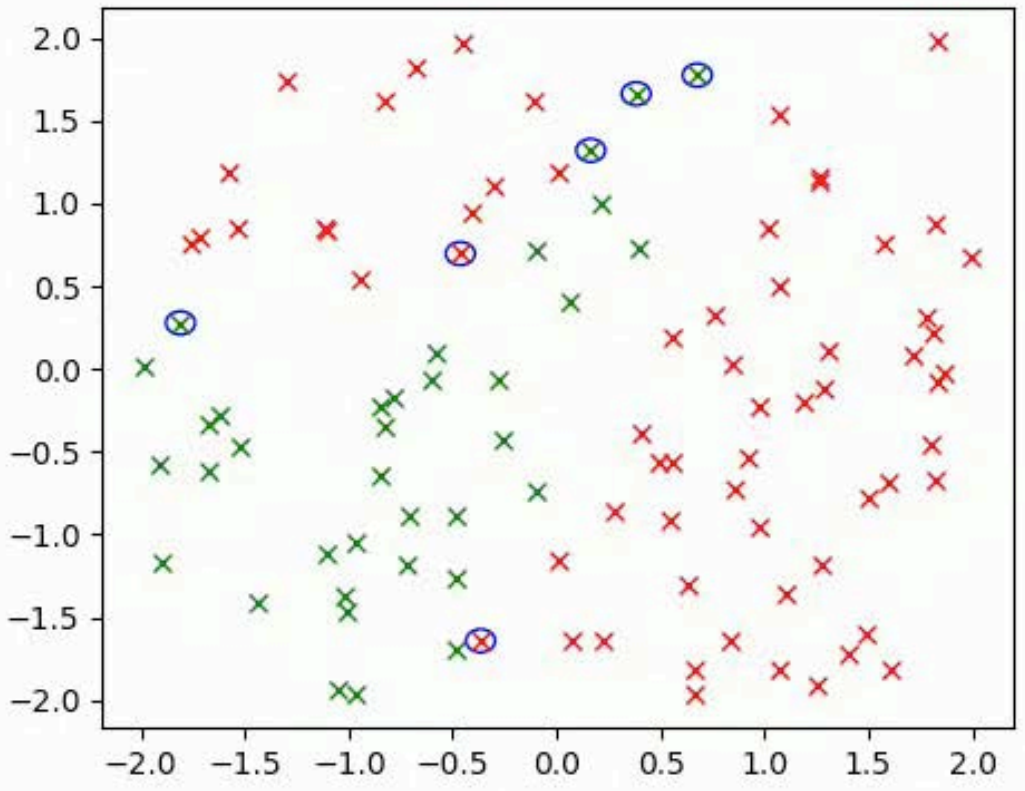
$$r(x,y) = 100 * (y - x^2)^2 + (1 - x)^2$$

$$f(x,y) = \begin{cases} \text{-1} & \text{if } r(x,y) < \text{T} \\ 1 & \text{otherwise} \end{cases}$$

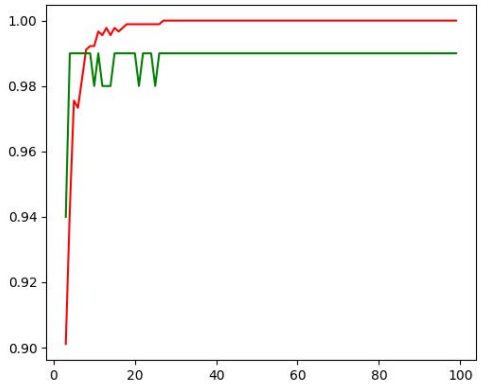
- Adaboost adds one linear classifier at a time.
- MLP works with a fixed number of classifiers and optimizes them all at the same time.

# Rosenbrock using a MLP



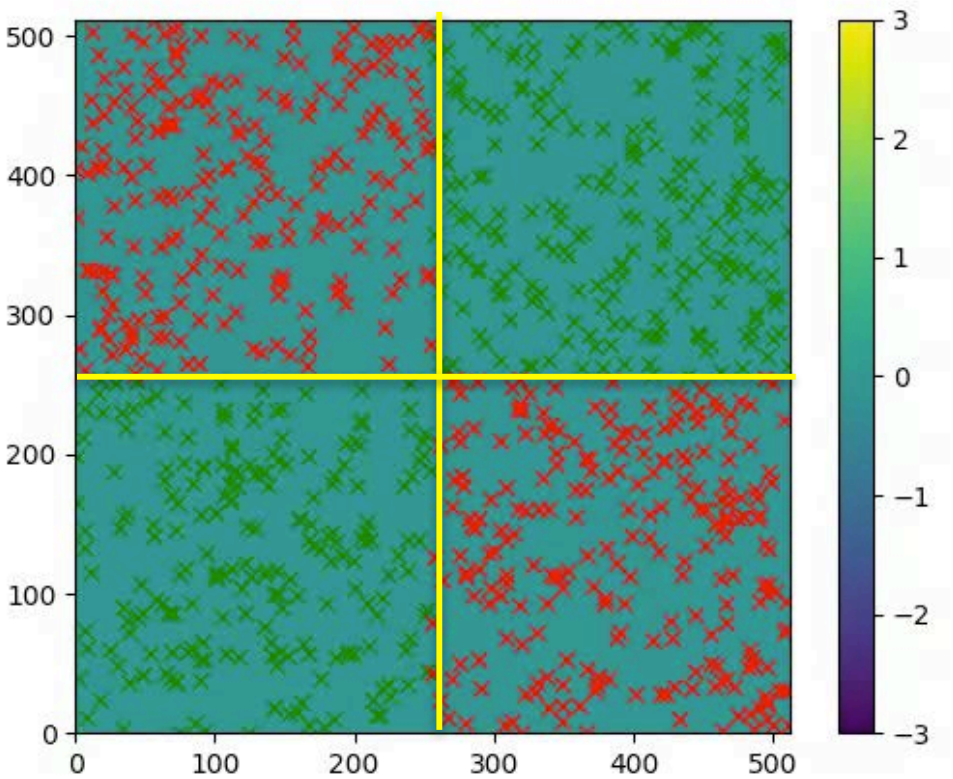




One hidden layer: 3 < n < 100

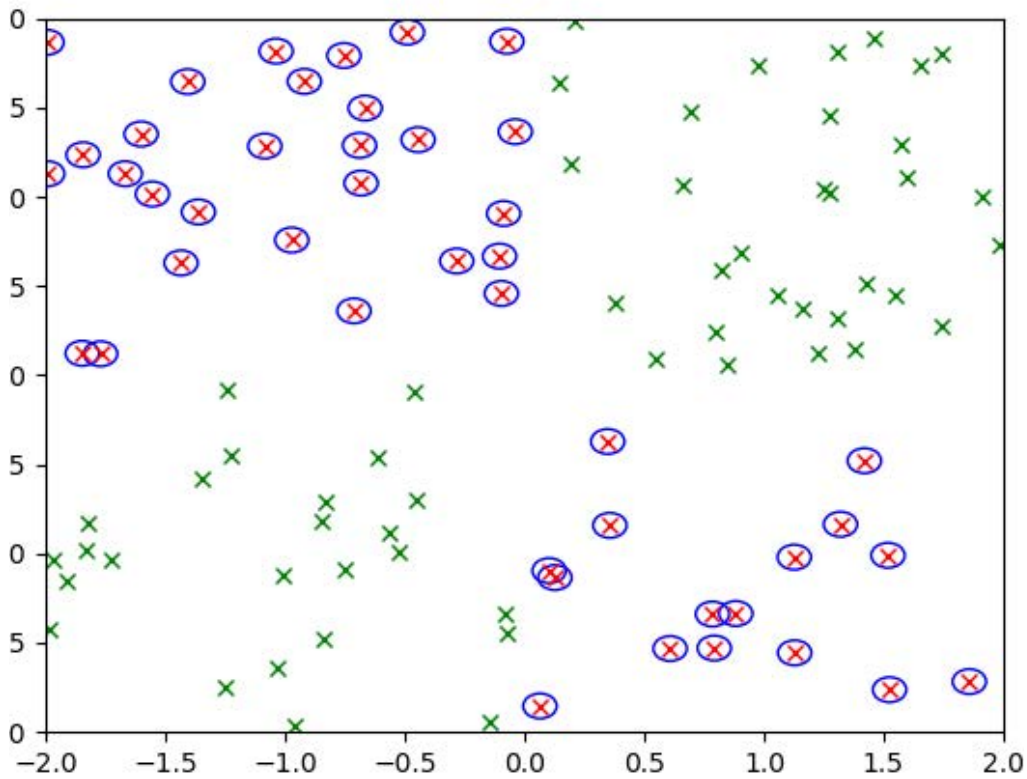



Accuracy as a function of n:
— Adaboost
— MLP

# Checker Board using Adaboost



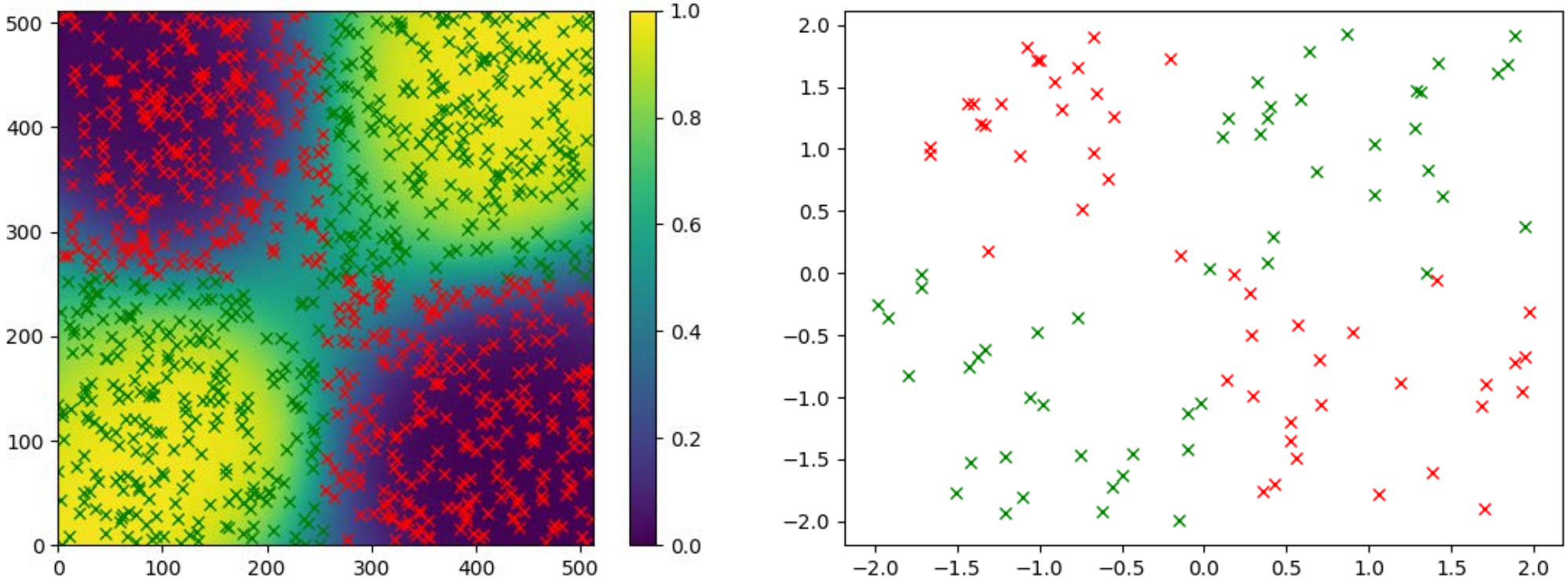

Training (100 iterations)




Validation (56% accuracy)

Individual weak classifiers cannot do better than chance.
—> AdaBoost with linear weak classifiers fails in this example.

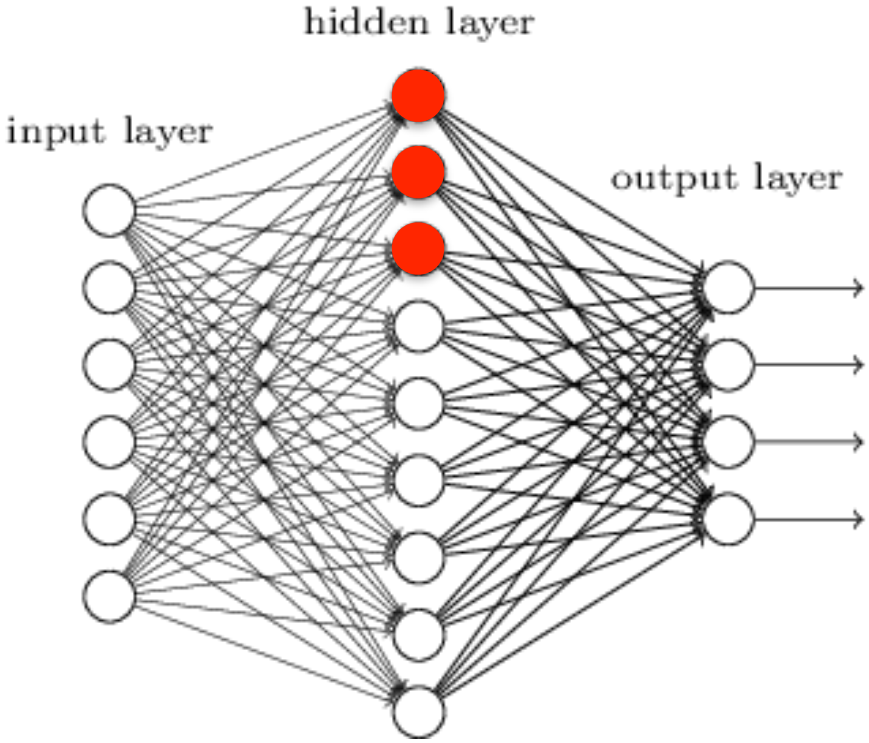
# Checkerboard using a MLP



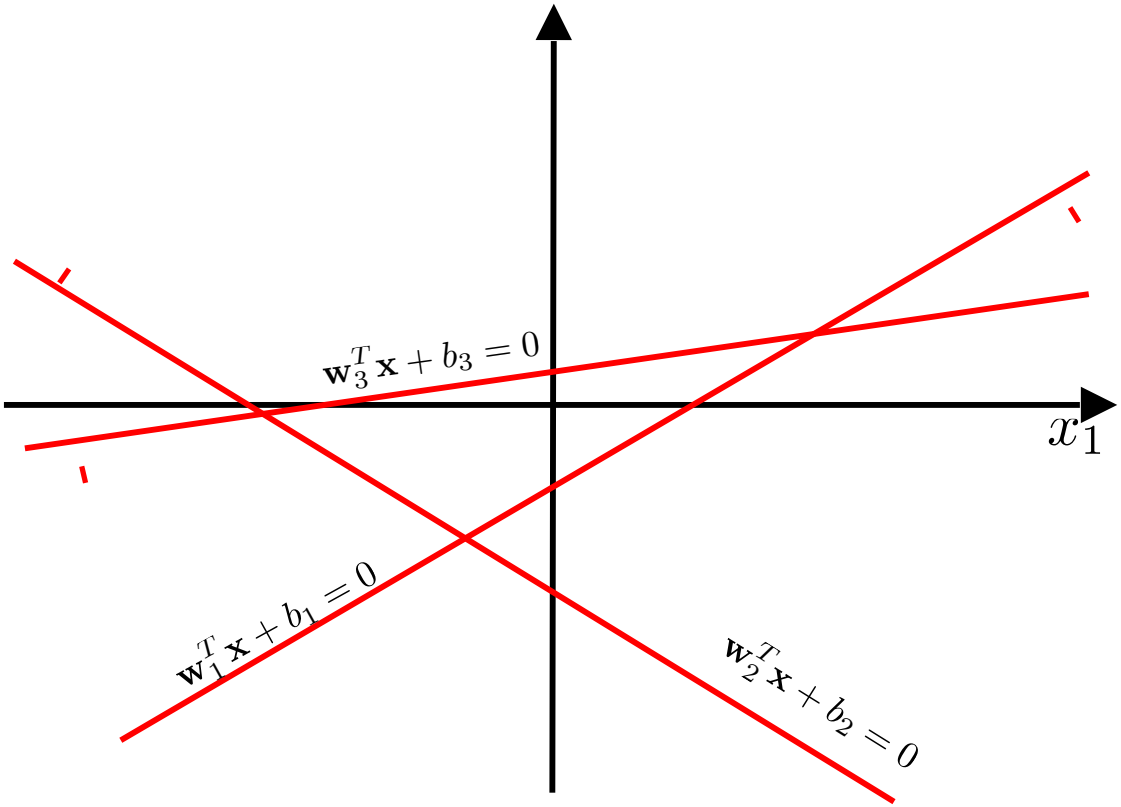

One hidden layer: n=10

MLPs solve the problem by using several hyperplanes at the same time.
—> They succeed in this example.

# SVM vs MLP




$\mathbf{x}$ $\phi(\mathbf{x})$ $\mathbf{W}\phi(\mathbf{x})+\mathbf{b}$

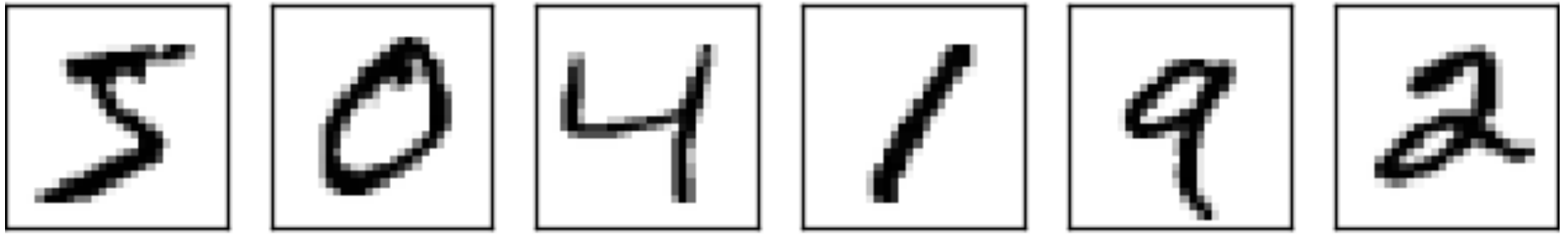



Both methods

- create a high-dimensional feature vector,
- define a classifier on that feature vector.

But the form of $\phi$ is not defined a priori in a MLP.

# Reminder: MNIST



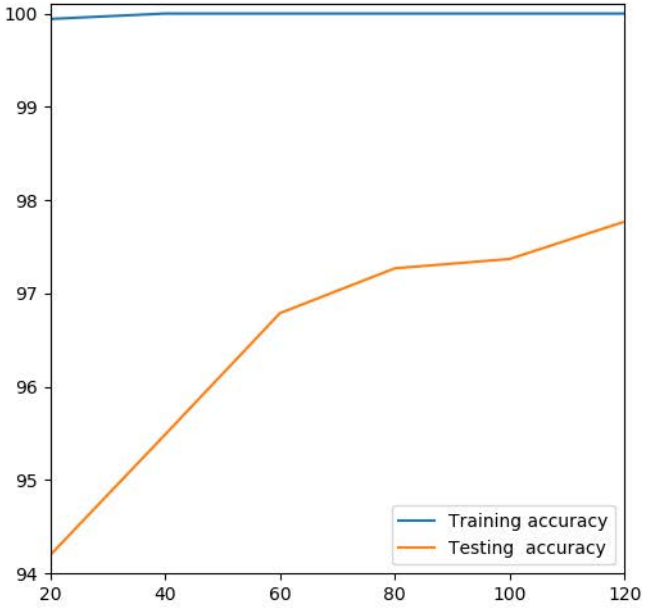
- The network takes as input 28x28 images represented as 784D vectors.
- The output is a 10D vector giving the probability of the image representing any of the 10 digits.
- There are 50'000 training pairs of images and the corresponding label, 10'000 validation pairs, and 5'000 testing pairs.

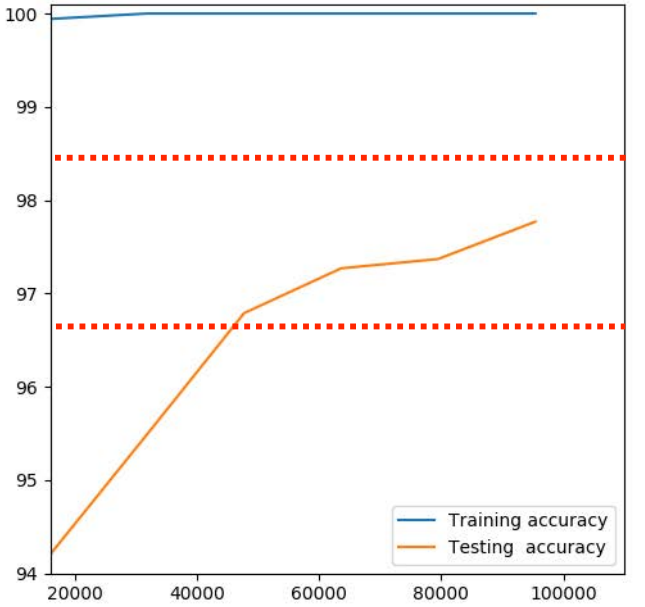
# MNIST Results

nIn =784

nOut = 10

20 < n1 < 120




- Deep nets have **many** parameters.
- This has long been a major problem.

—> Was eventually solved by using GPUs.

SVM: 98.6

Knn: 96.8

- Around 2005, SVMs were often felt to be superior to neural nets.
- This is no longer the case ….

# Optional: Converting Words to Vectors

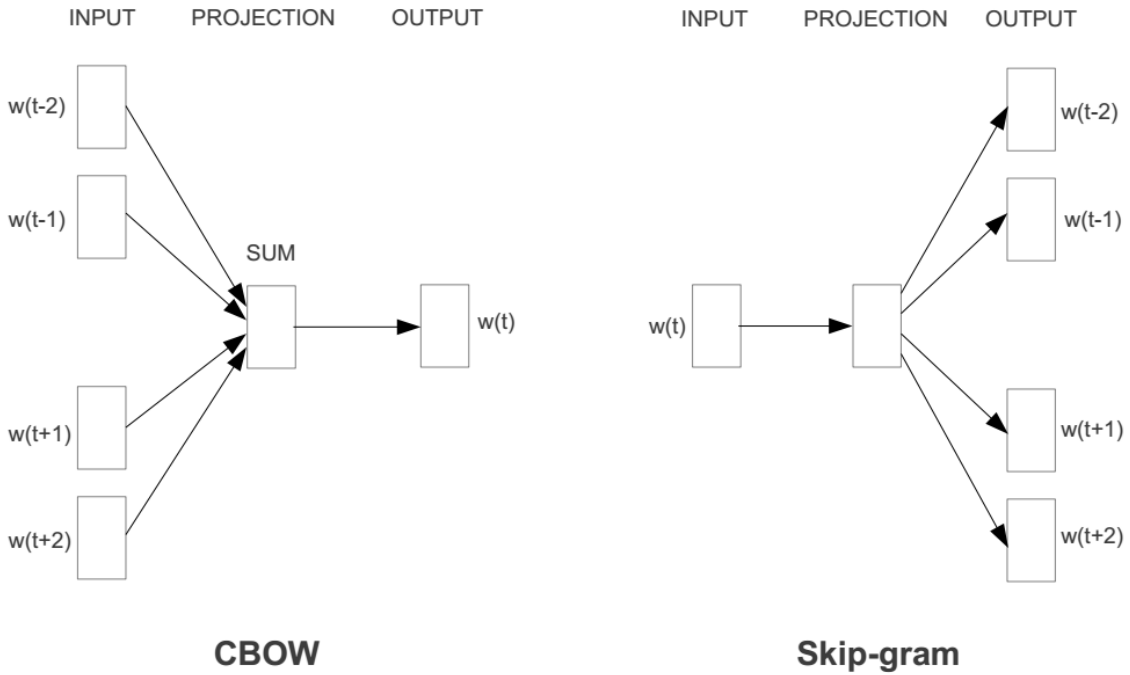
- How similar is **pizza** to **pasta**?
- How related is **pizza** to **Italy**?

- Representing words as vectors allows for easy computation of similarity.
- Makes it possible to use the Machine Learning techniques we have discussed.
- Exploit the theory that similar words tend to occur in similar context.



Harris'54, Firth'57

# Optional: Words in Context (*word2vec*)

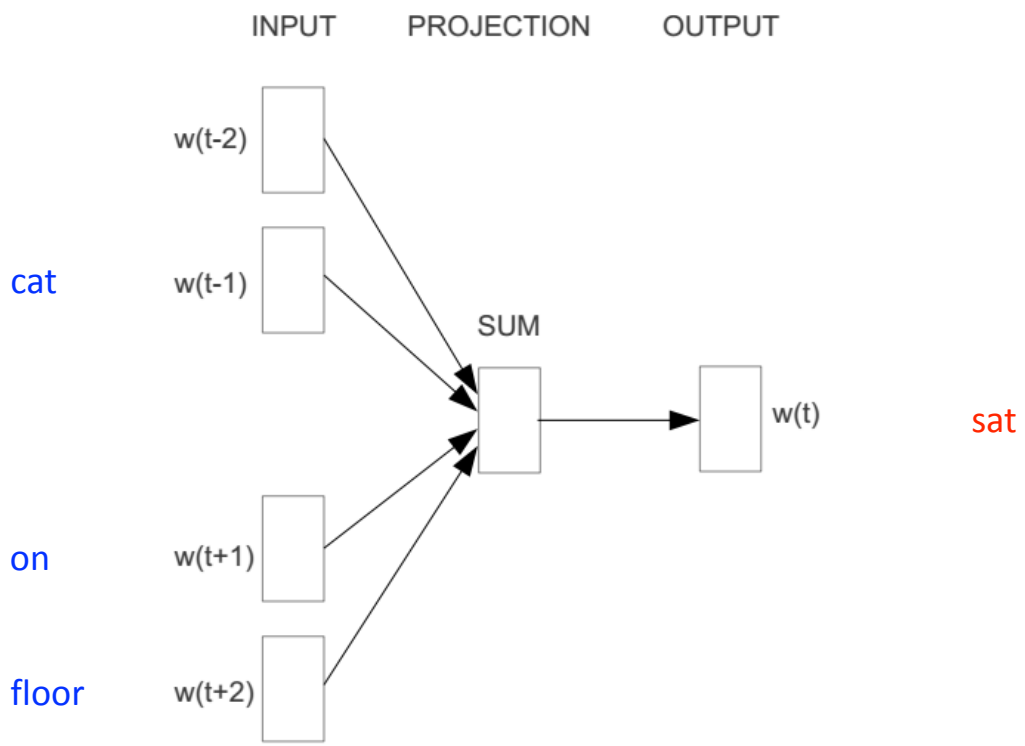



Two basic neural network models:

- Continuous Bag of Word (CBOW). Use a window of words to predict the middle one.
- Skip-gram (SG). Use a word to predict the surrounding ones in a window.

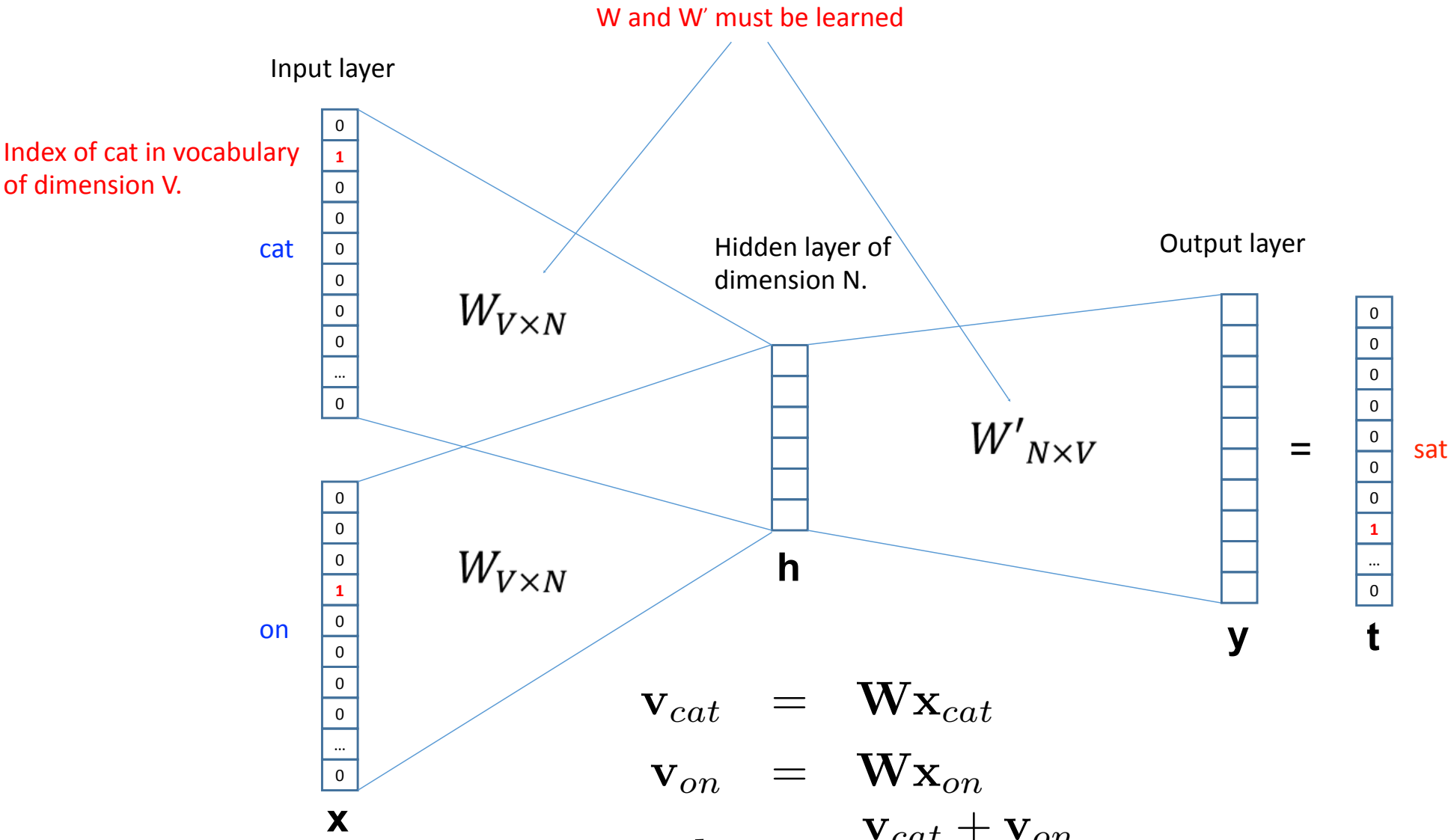
# Optional: Continuous Bag of Words

The cat sat on the floor.




sat should be predicted from the words around it.

# Optional: Window of Size 2



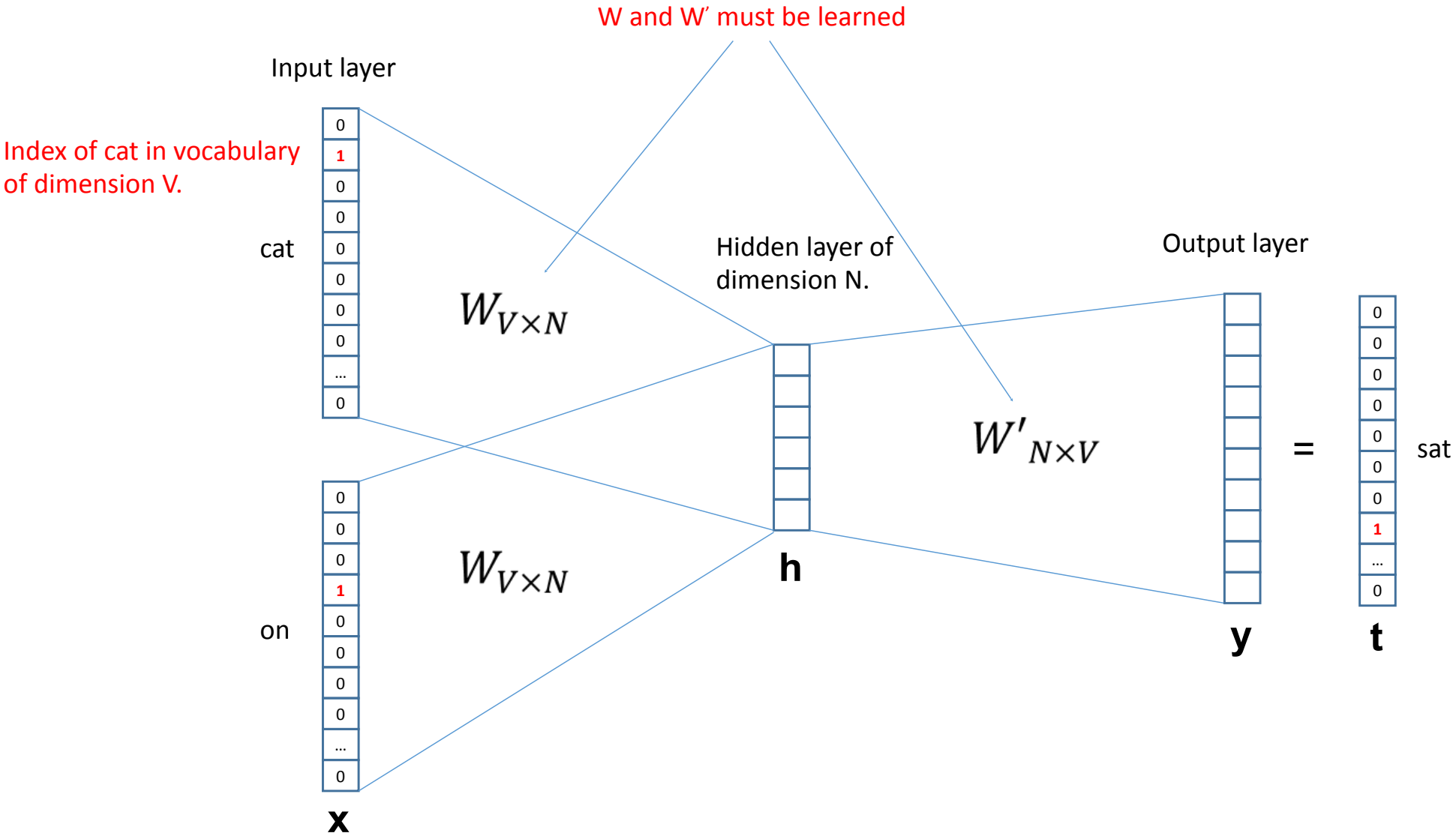

$$\mathbf{v}_{cat} = \mathbf{W}\mathbf{x}_{cat}$$

$$\mathbf{v}_{on} = \mathbf{W}\mathbf{x}_{on}$$

$$\mathbf{h} = \frac{\mathbf{v}_{cat} + \mathbf{v}_{on}}{2}$$

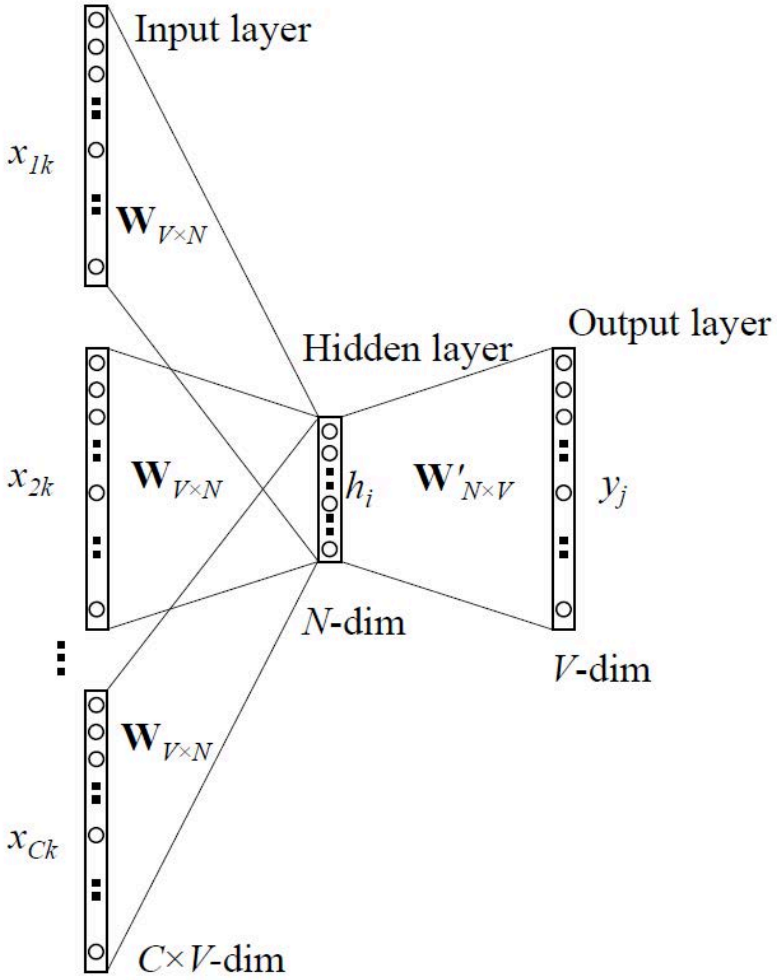
$$\mathbf{y} = \text{softmax}(\mathbf{W}'\mathbf{h})$$

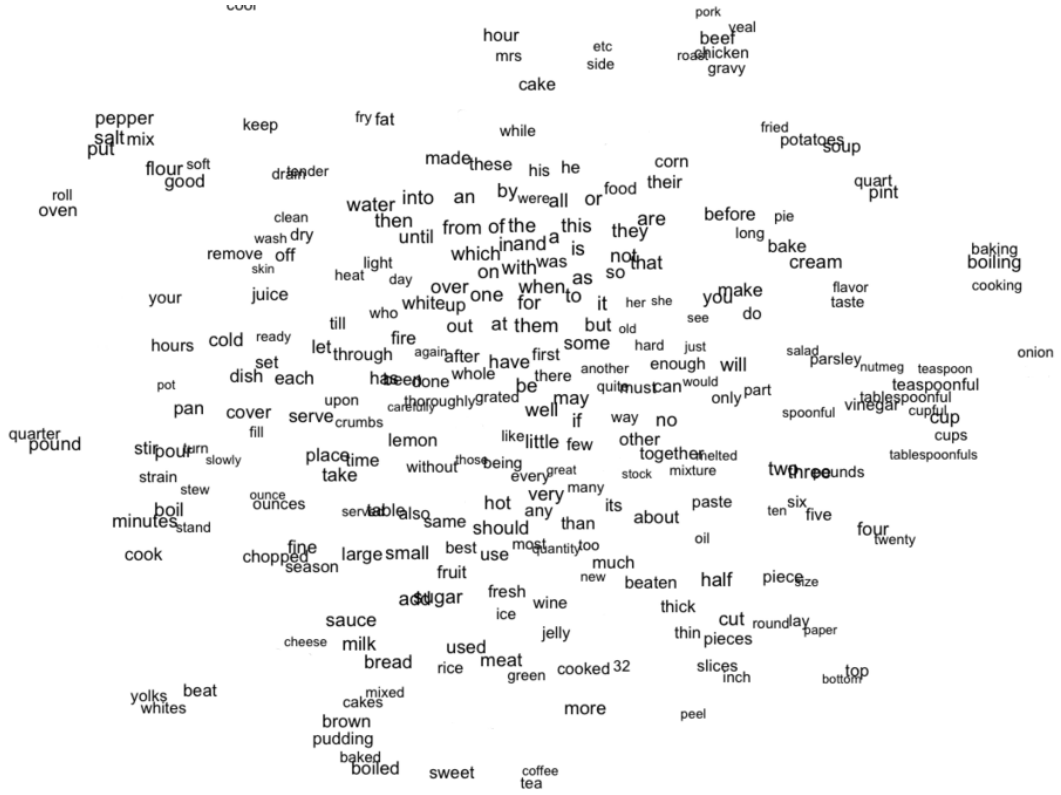
# Optional: Window of Size 2




Once the training is complete, the W matrices associate to each word a vector of dimension N.

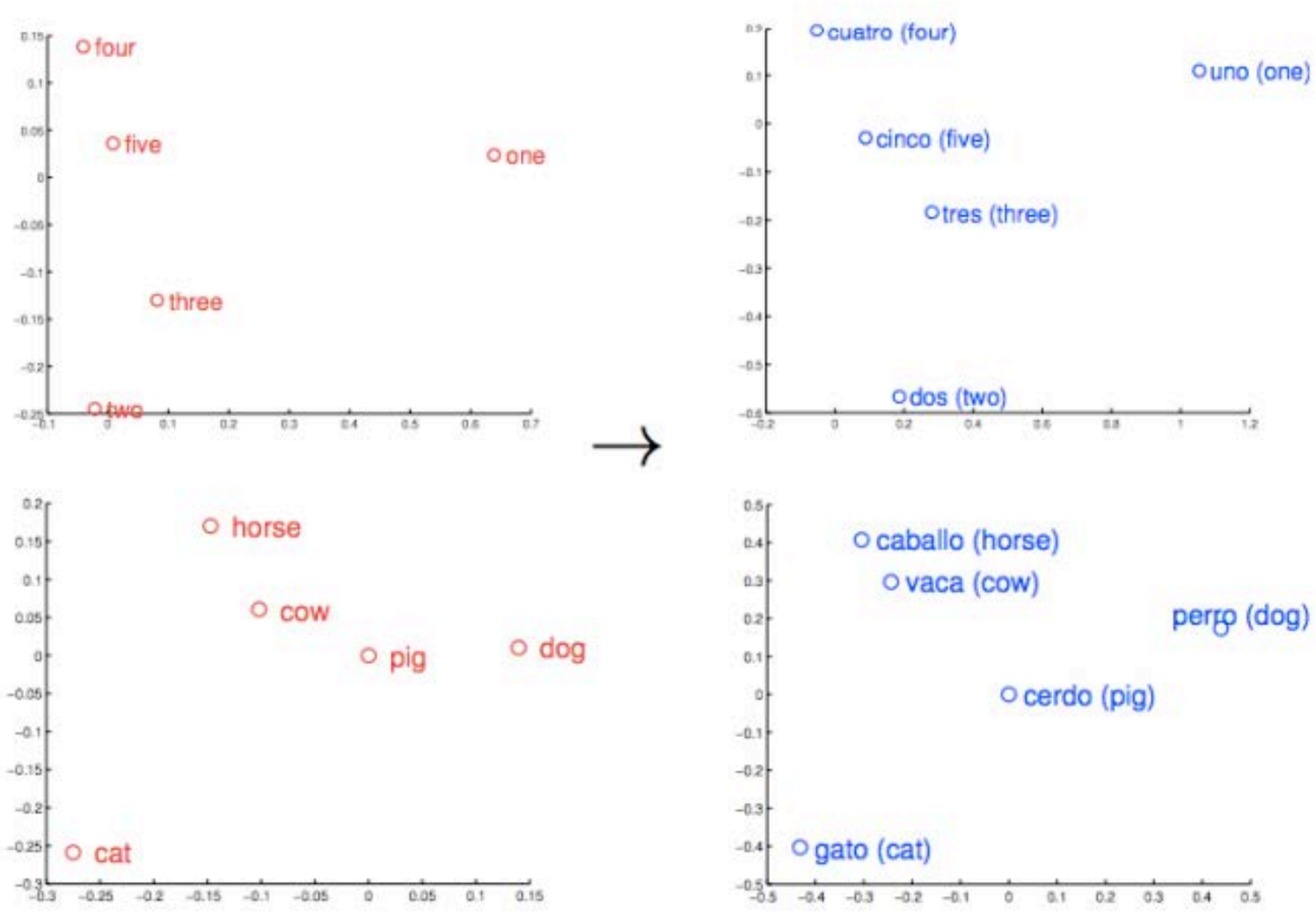
# Optional: Larger Windows




- Once the training is complete, the W matrices associate to each word a vector of dimension N.
- The distances of between these vectors is highly correlated to the similarity of the corresponding words.

# Optional: Geometry of Words




English Spanish

https://skymind.ai/wiki/word2vec

# Optional: Some Results

Training on Google News Vocab:

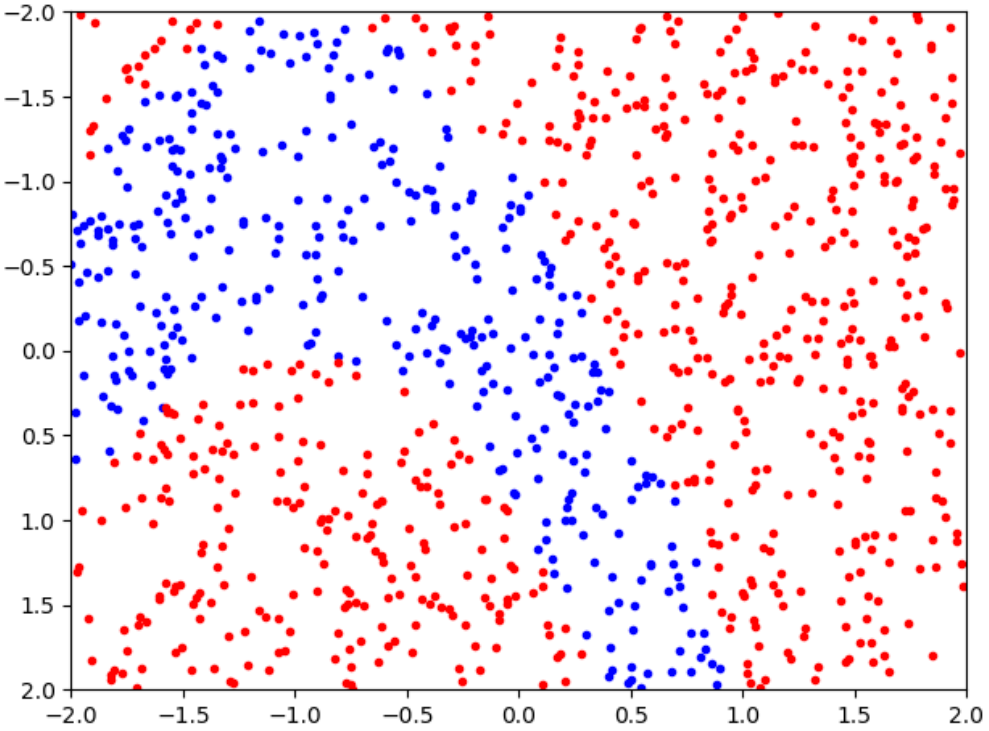
- Beijing is to China what Bern is to Switzerland

Testing:

- king:queen man:[woman,attempted,abduction,girl]
- knee:leg elbow:[forearm,arm,ulna_bone]
- love:indifference fear:[apathy,callousmess,timidity,helplessness]

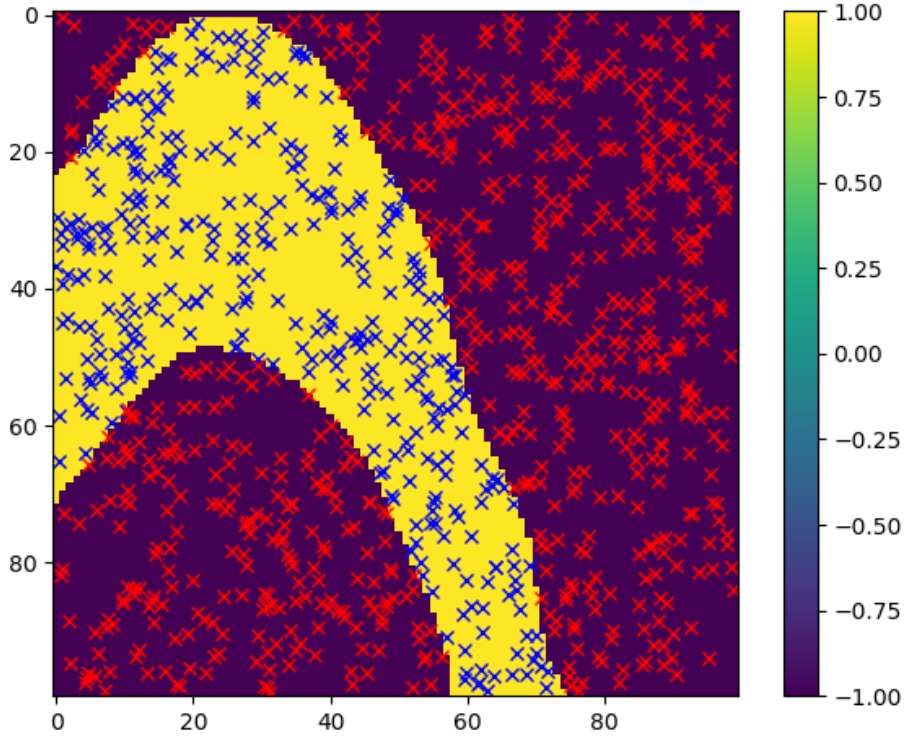
Not bad given that word2vec knows **nothing** about syntax, about the world, or even about logic!!

# From Classification to Regression




Positive: $100(x_2 - x_1^2)^2 + (1 - x_1)^2 < 0.5$

Negative: Otherwise

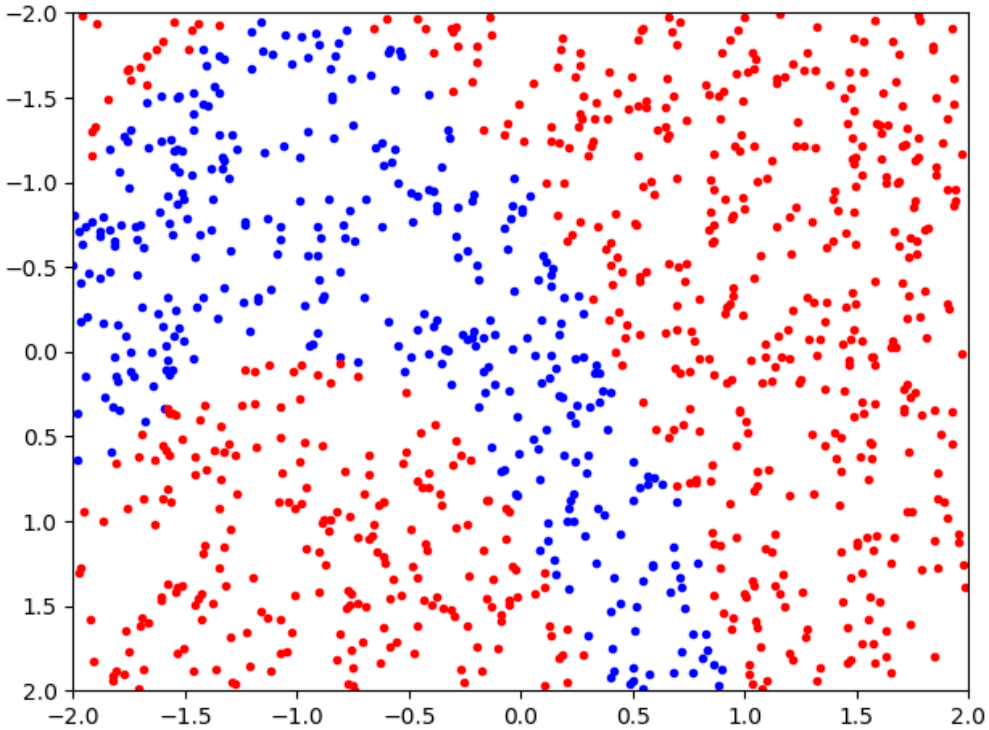



$y(\mathbf{x}; \tilde{\mathbf{w}})$

- The deep network implements the function $f_{\tilde{\mathbf{w}}} = y(\,\cdot\,; \tilde{\mathbf{w}})$.
- Ideally, we would like $f_{\tilde{\mathbf{w}}}(\mathbf{x})$ to be approximately equal to the probability that $\mathbf{x}$ belongs to the positive class.

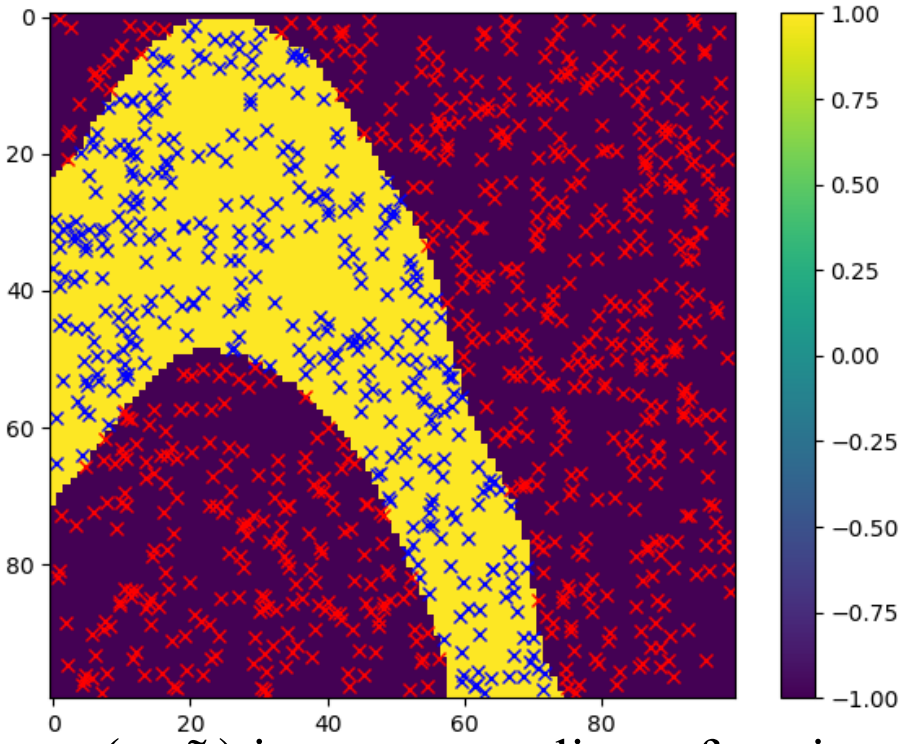
—> This raises a theoretical question: If $f_{\tilde{\mathbf{w}}}$ were known, how well could a network approximate it?

# Rosenbrock Regression




Positive: $100(x_2 - x_1^2)^2 + (1 - x_1)^2 < 0.5$

Negative: Otherwise

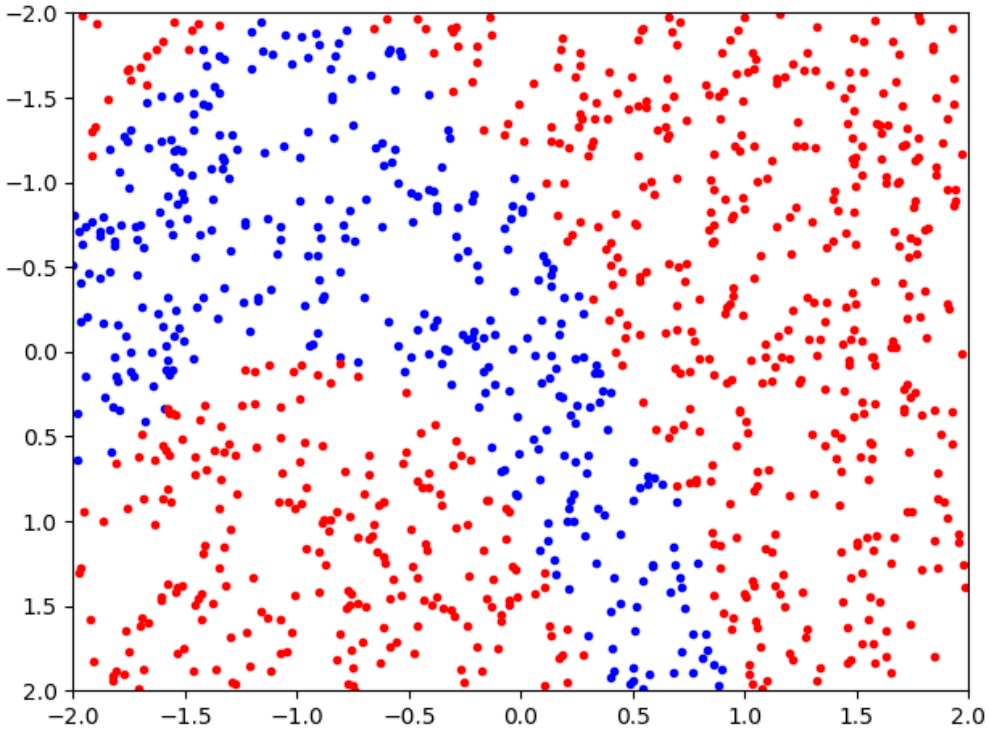



$y(\mathbf{x}; \tilde{\mathbf{w}})$ is now a non-linear function implemented by the network.

**Problem statement:** Find $\tilde{\mathbf{w}}$ such that

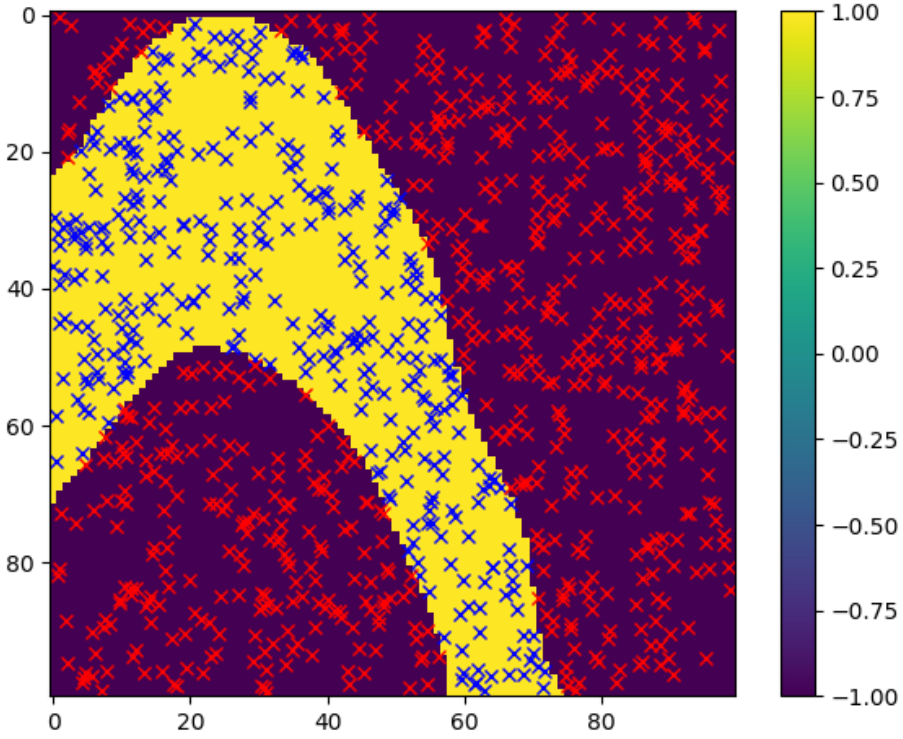
$$y(\mathbf{x}; \tilde{\mathbf{w}}) \approx 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$

# Classification / Regression




Positive: $f(\mathbf{x}) < 0.5$

Negative: Otherwise



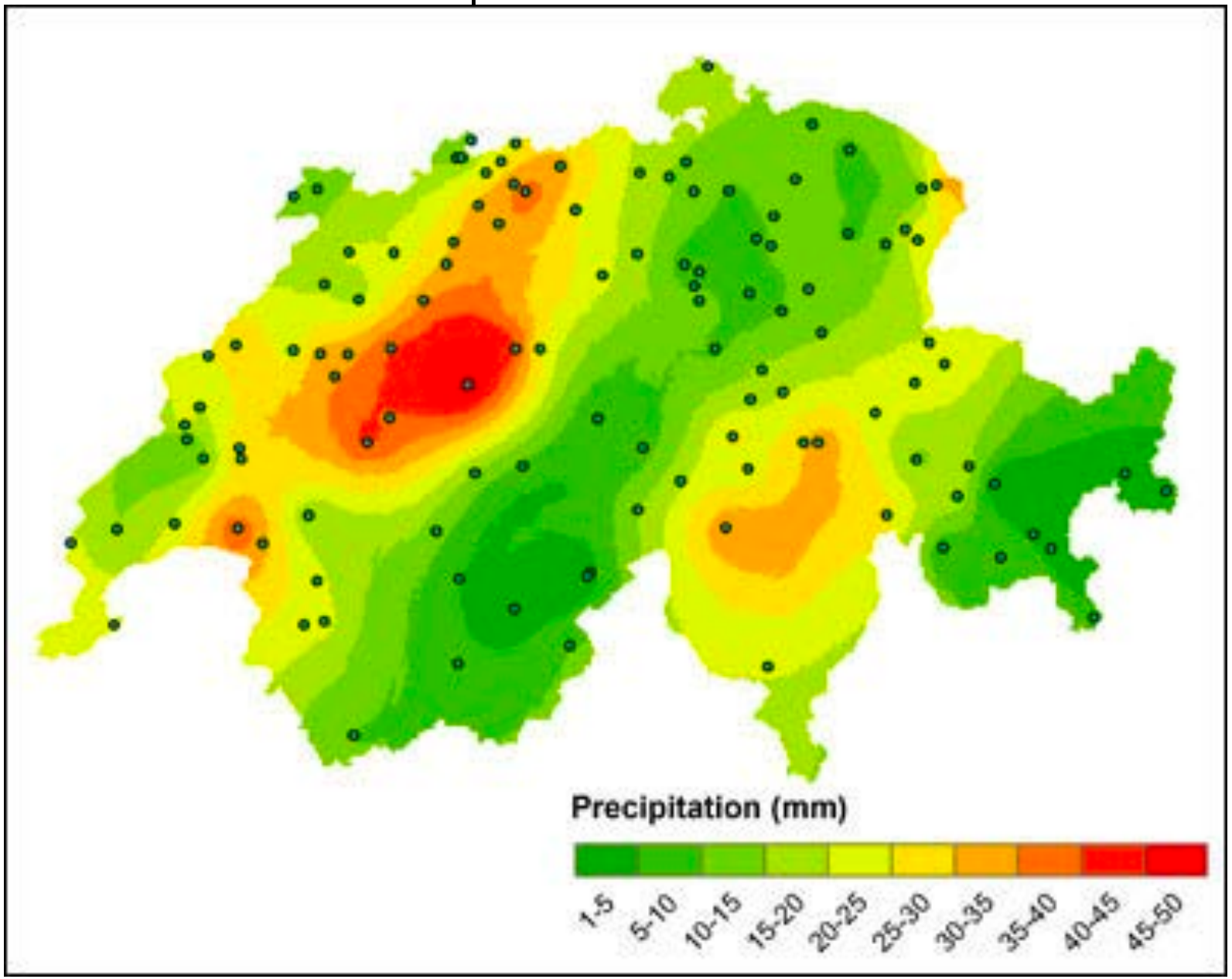

$y(\mathbf{x}; \tilde{\mathbf{w}})$ is now a non-linear function implemented by the network.

Classification can be understood as finding $\tilde{\mathbf{w}}$ such that

$$y(\mathbf{x}; \tilde{\mathbf{w}}) \approx f(x)$$

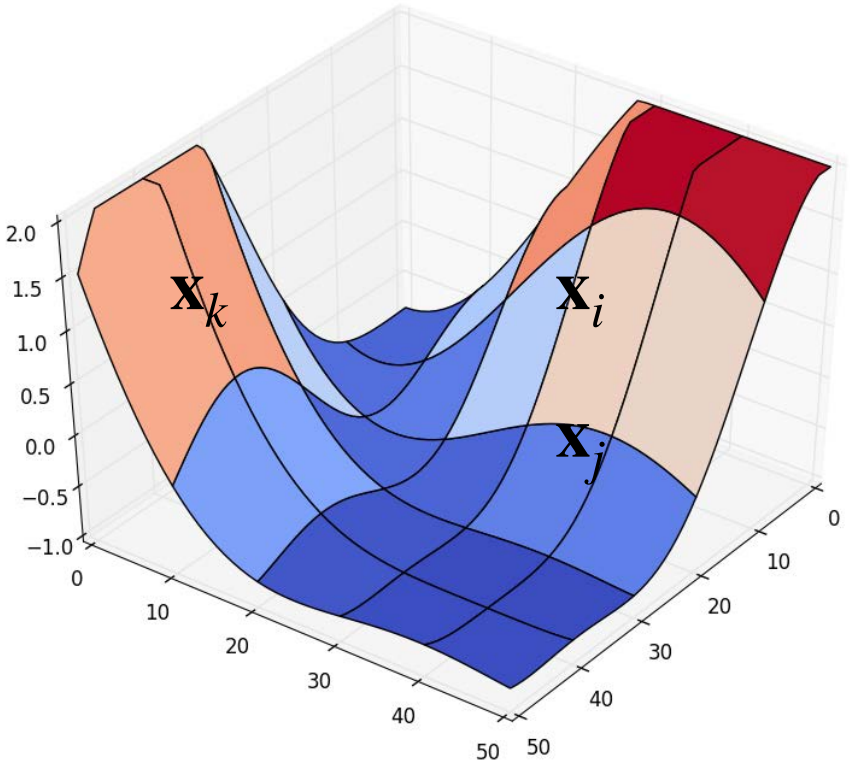
# Regression in Everyday Life

The circles represent actual measurements




The map has been regressed from them

# Non-Linear Regression



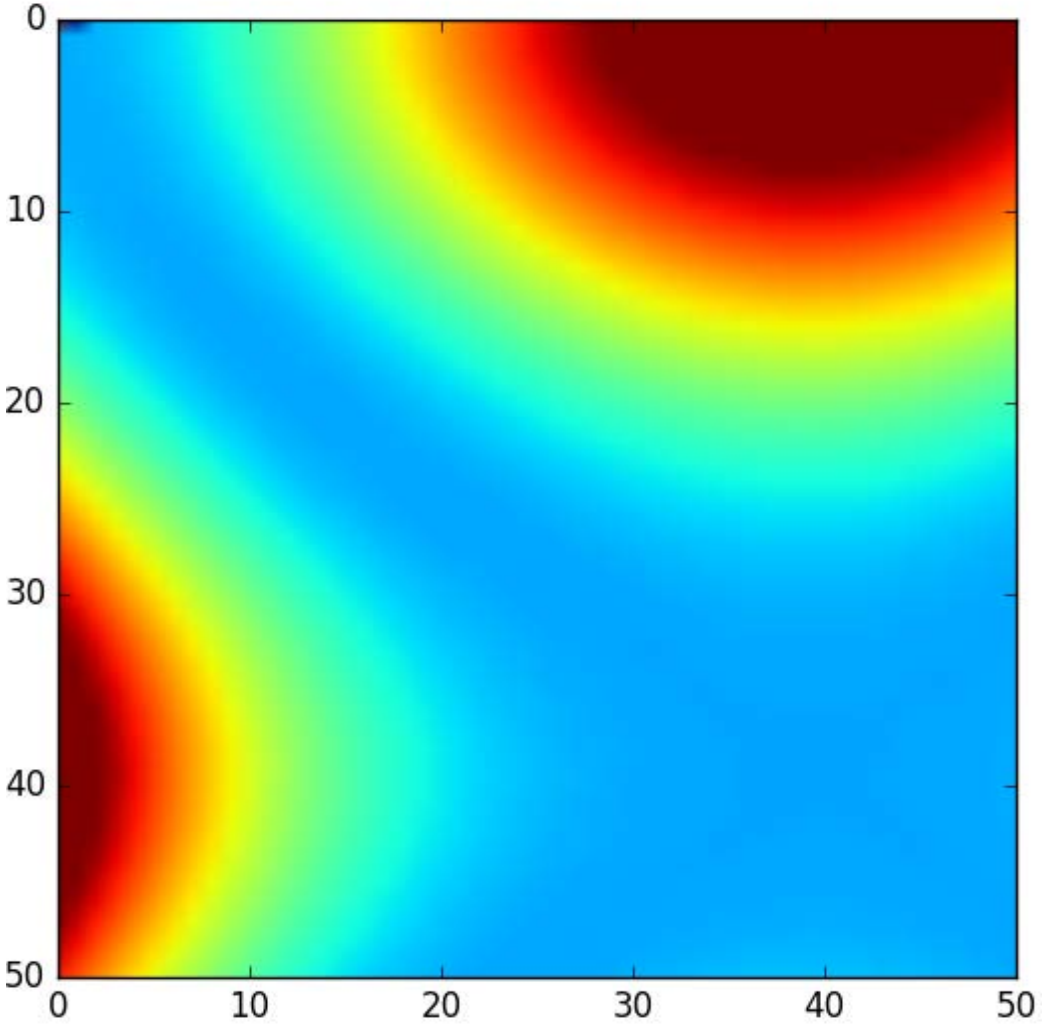

$$z = f(\mathbf{x})$$

**Problem statement:** Given $(\{\mathbf{x}_1, z_1\}, \ldots, \{\mathbf{x}_n, z_n\})$, minimize

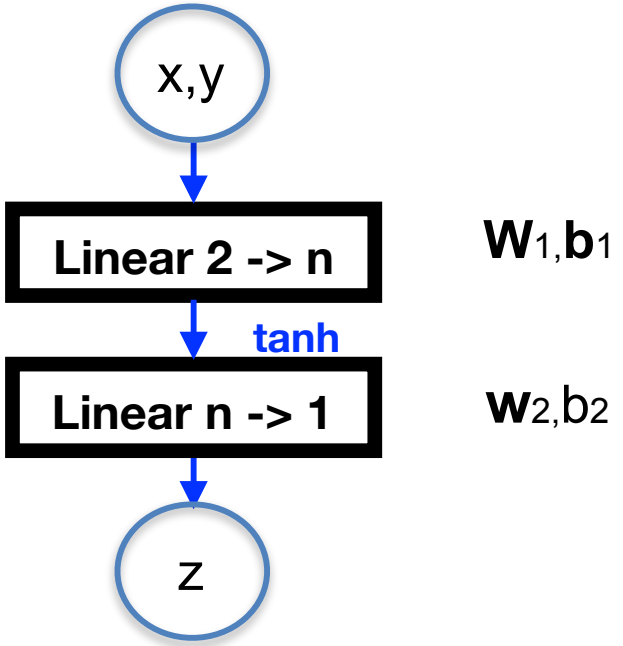
$$\sum_i (z_i - f(\mathbf{x}_i, \tilde{\mathbf{w}}))^2$$

w.r.t. $\tilde{\mathbf{w}}$.

# Regressing the Rosenbrock Function



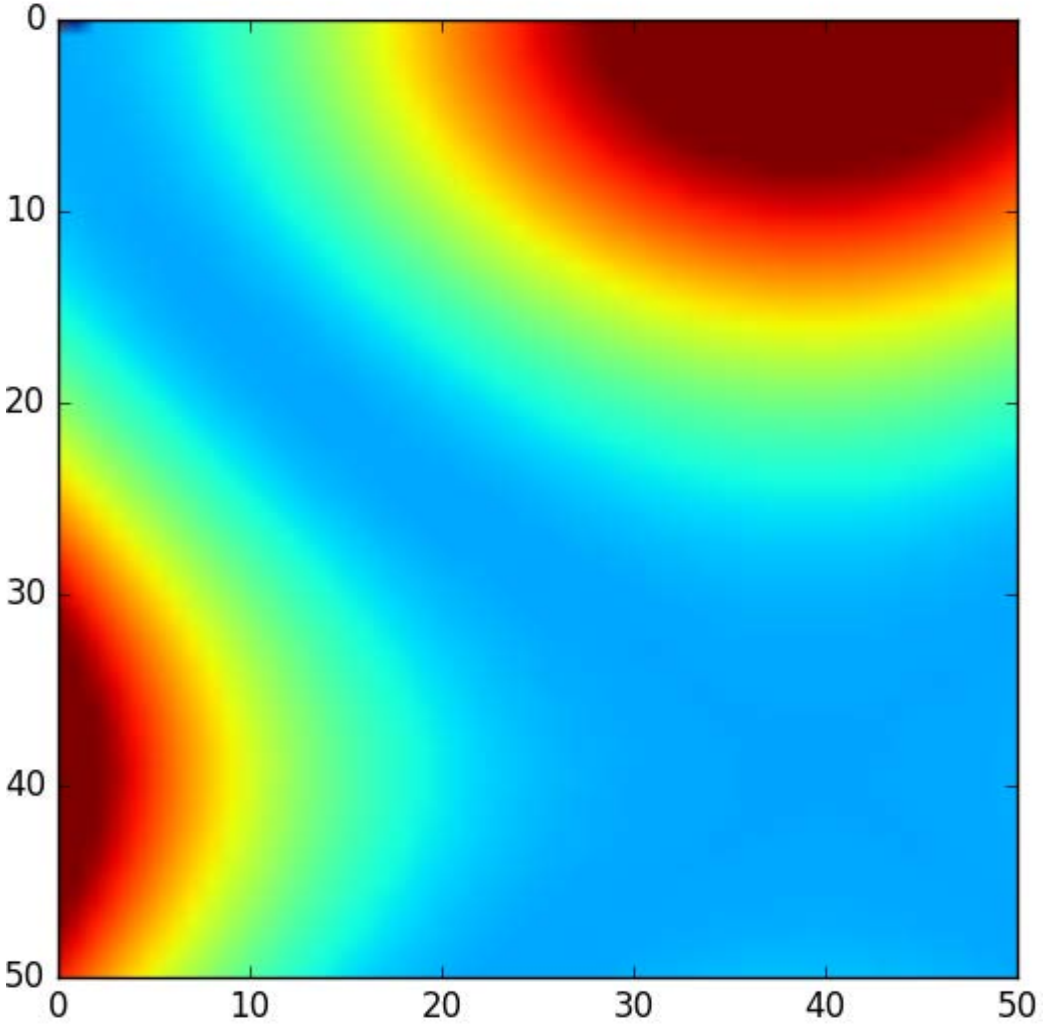

$$z = f(\mathbf{x}) = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



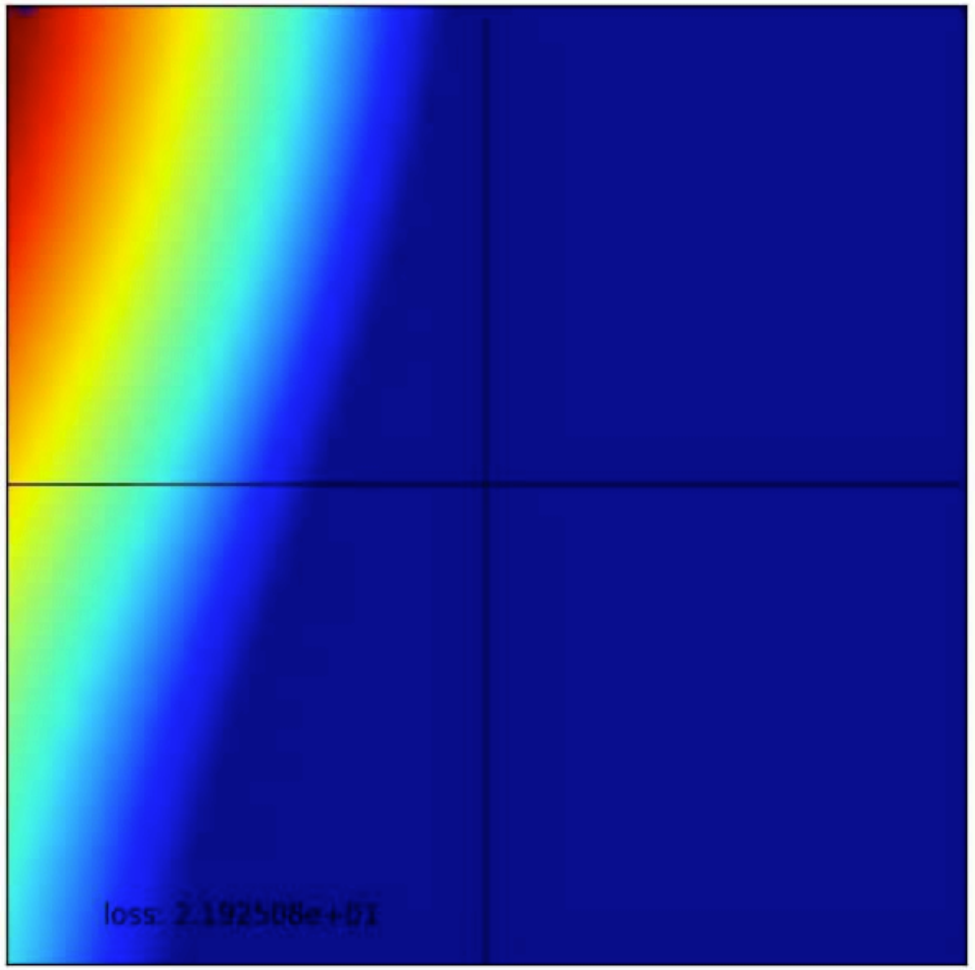

$$\begin{aligned} z &= f(x, y) \\ &= \mathbf{w}_2 \sigma(\mathbf{W}_1 \begin{bmatrix} x \\ y \end{bmatrix} + \mathbf{b}_1) + b_2 \end{aligned}$$

Minimize $\sum_i (z_i - f(x_i, y_i))^2$,
with respect to $\mathbf{W}_1, \mathbf{w}_2, b_x, b_y, b_z$.

# Regressing the Rosenbrock Function



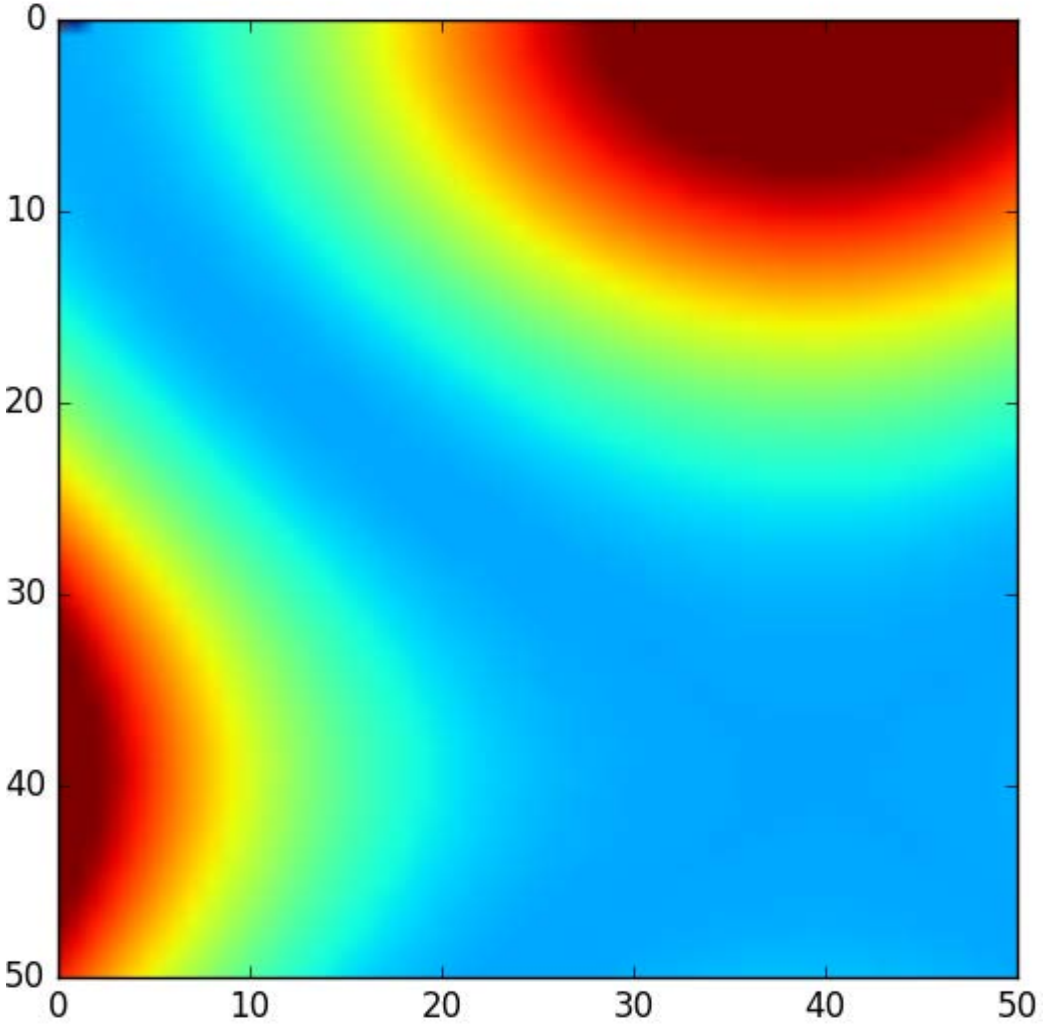

$$z = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



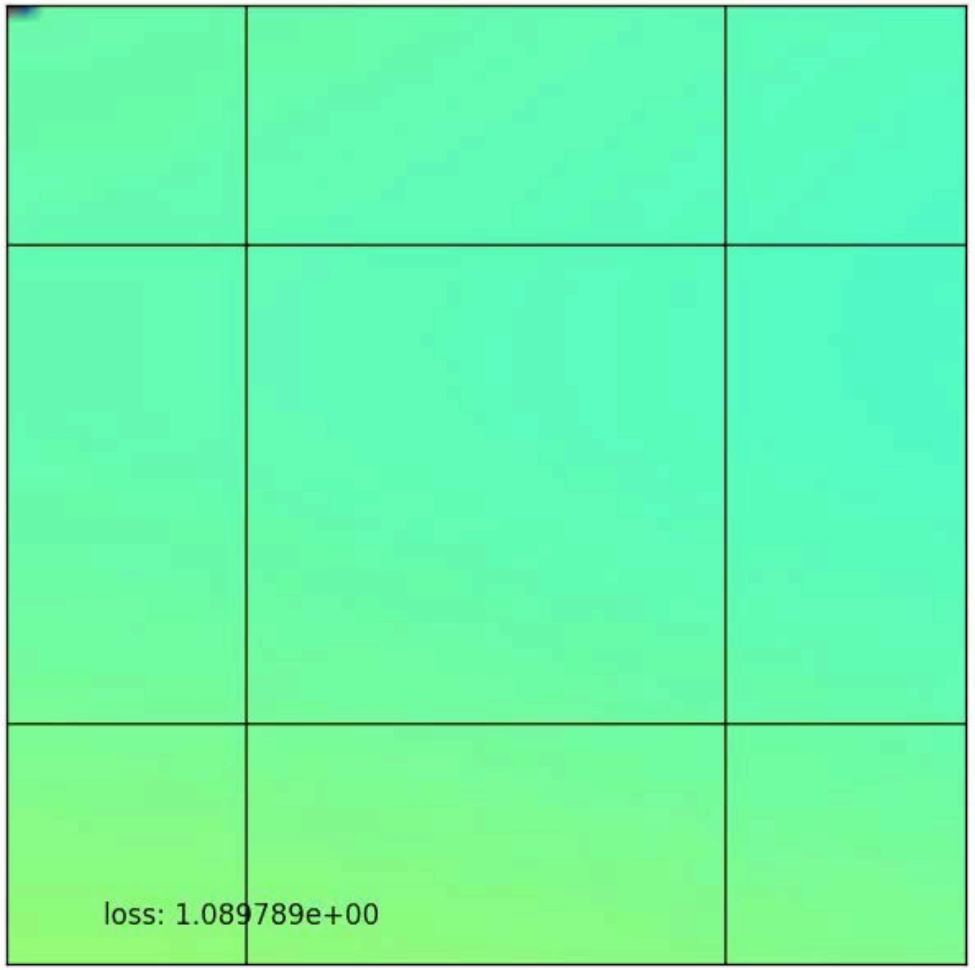

3-node hidden layer

—> 3 nodes is not quite enough.

# Regressing the Rosenbrock Function



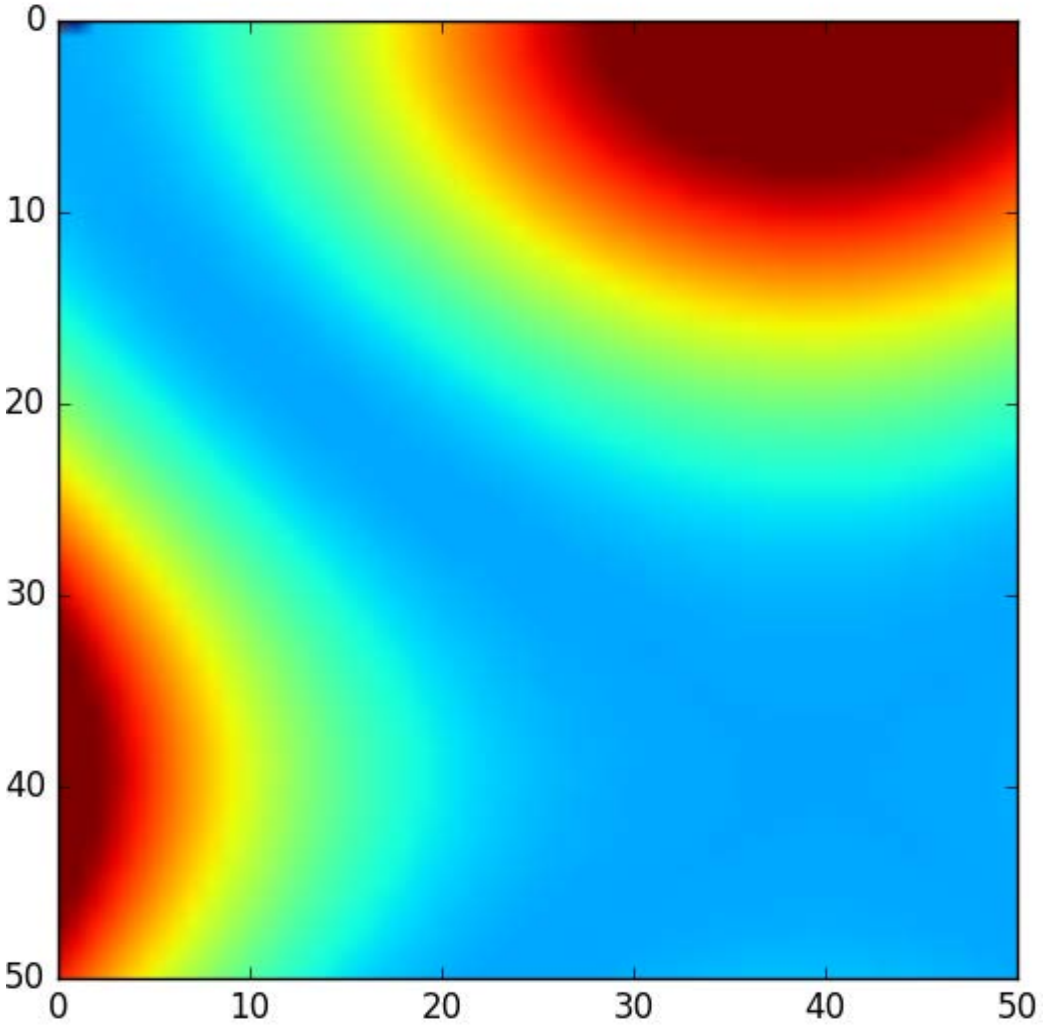

$$z = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



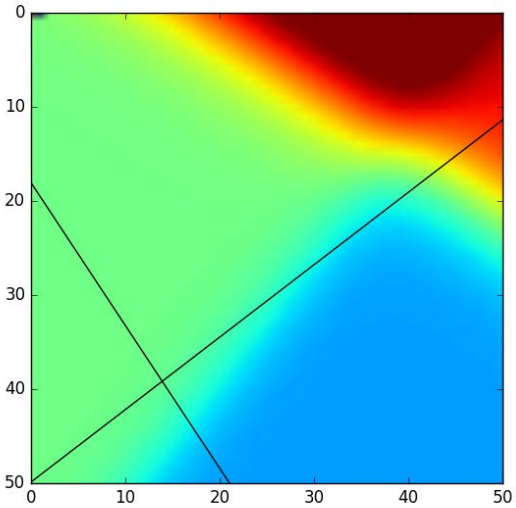

4-node hidden layer

—> 4 nodes is better.

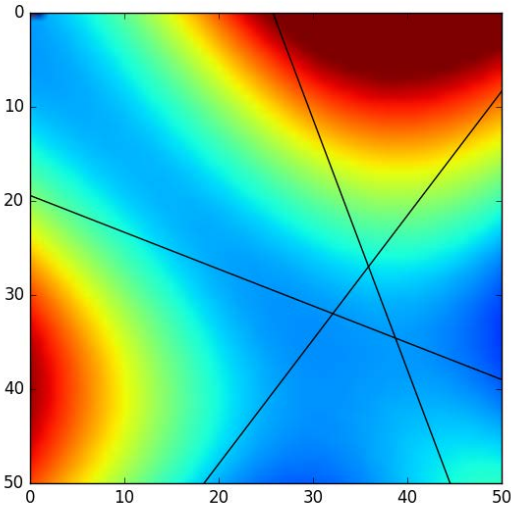
# Accuracy as a Function of the Number of Nodes



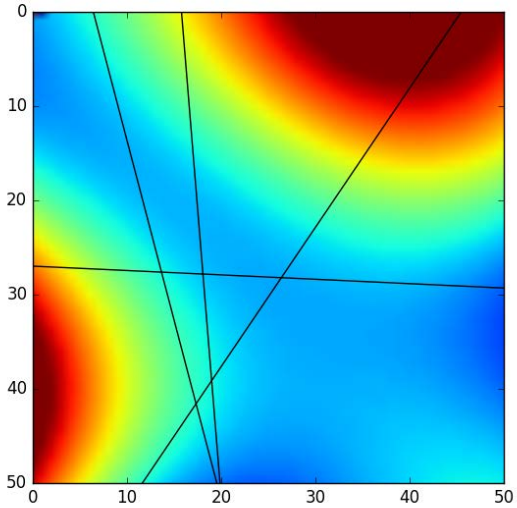

$$z = 100 * (y - x^2)^2 + (1 - x)^2$$




2 nodes -> loss 3.02e-01



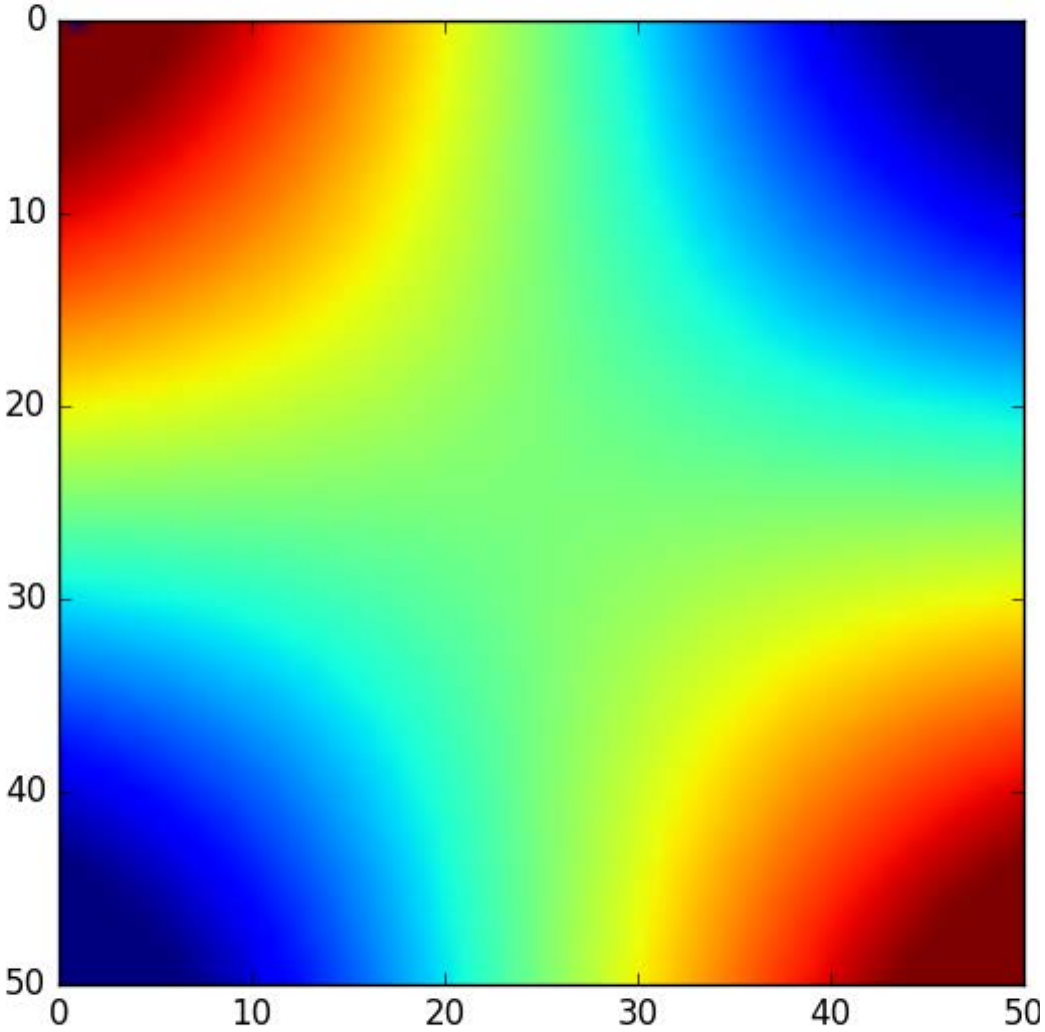

3 nodes -> loss 2.08e-02



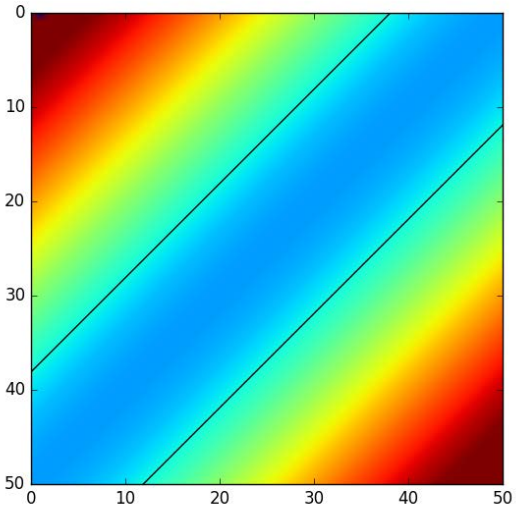

4 nodes -> loss 8.27e-03

—> The more nodes the more accurate the approximation.

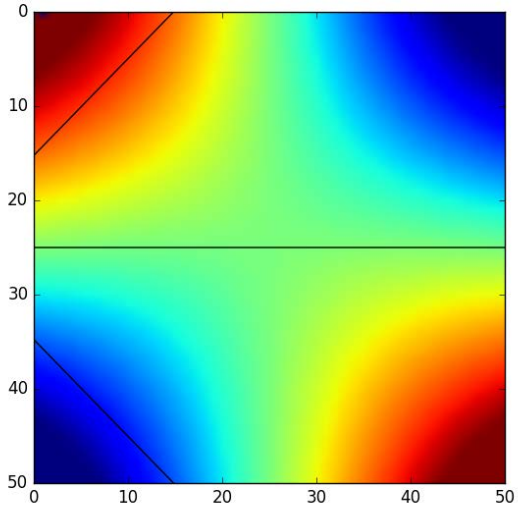
# Accuracy as a Function of the Number of Nodes



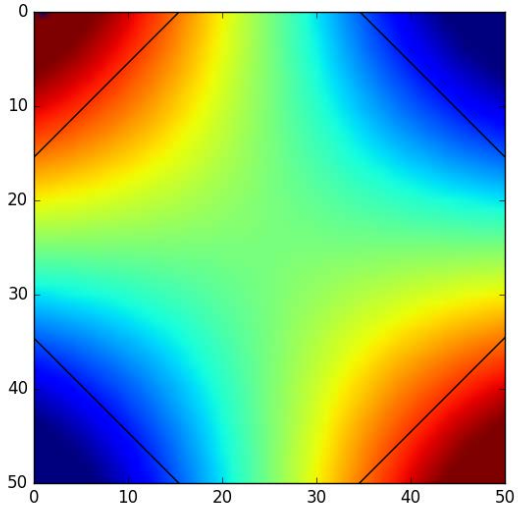
$z = sin(x)sin(y)$



2 nodes -> loss 2.61e-01



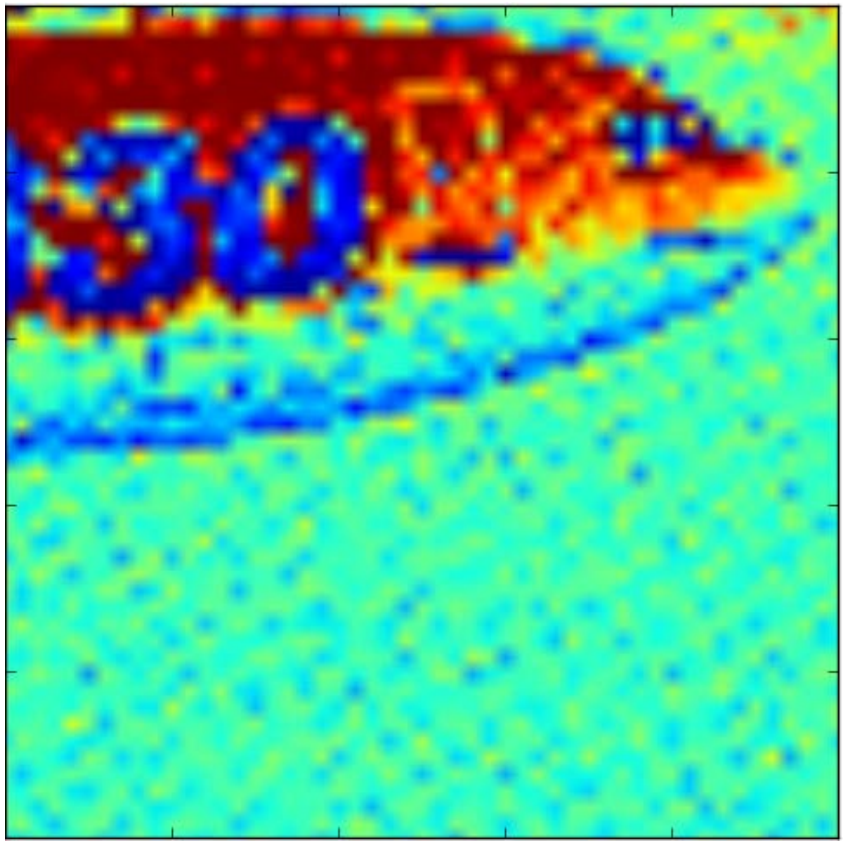
3 nodes -> loss 2.51e-04

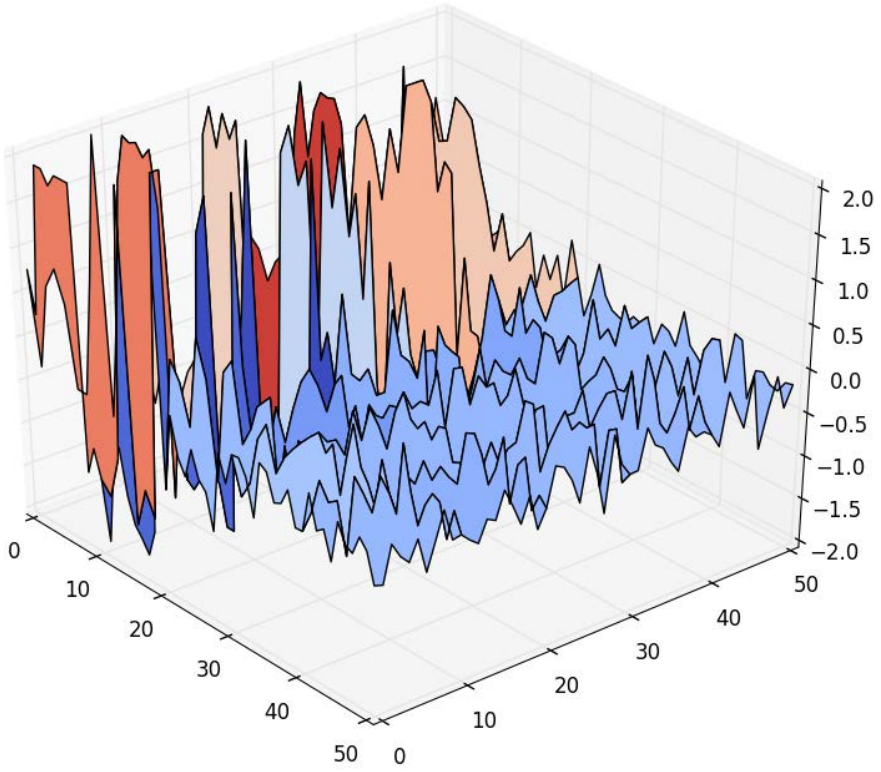


4 nodes -> loss 3.07e-07

—> The more nodes the more accurate the approximation.

# Image as a 3D Surface



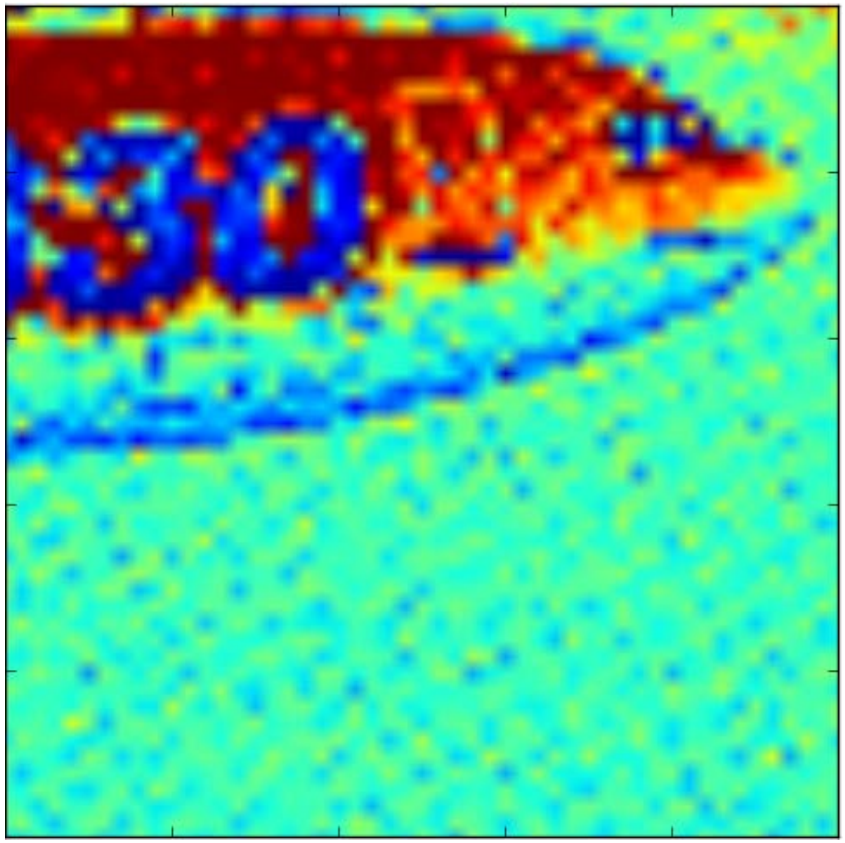



$$I = f(x, y)$$

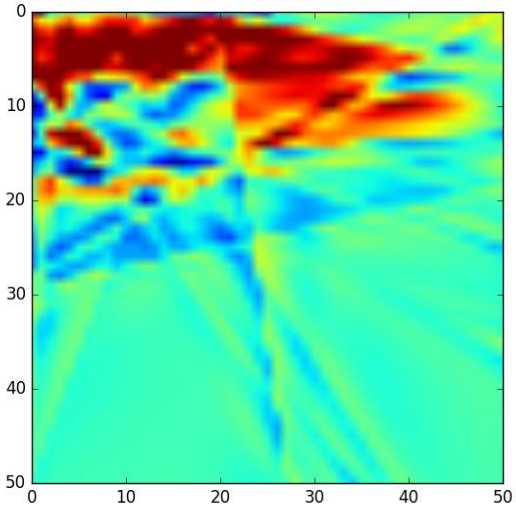
We treat the image as a surface:

- The intensity is the z coordinate.
- It is shown in false color on the left.
- The corresponding surface is complex.

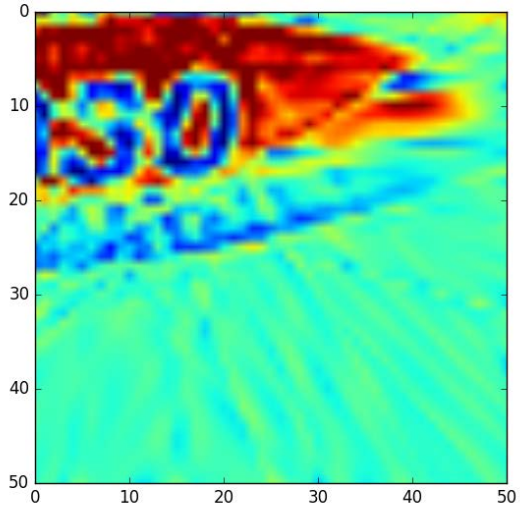
# More Complex Surface



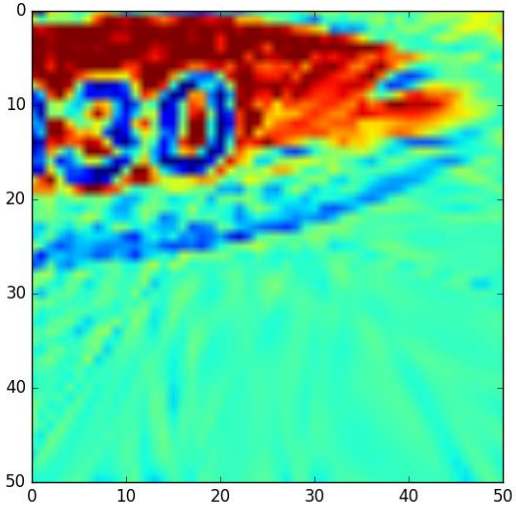
$$I = f(x, y)$$



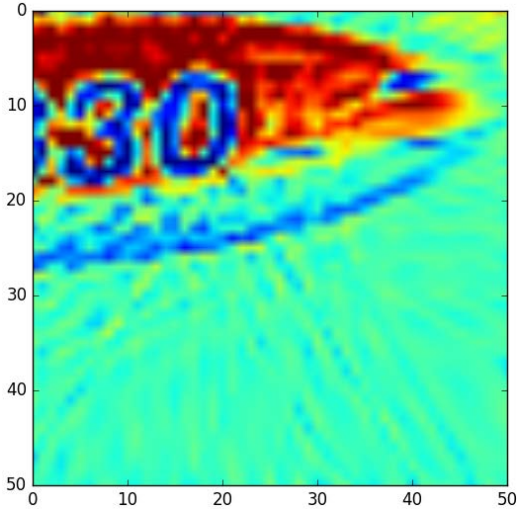
50 nodes -> loss 3.65e-01



100 nodes -> loss 2.50e-01



125 nodes -> loss 2.40e-01



300 nodes -> loss 1.92e-01

—> The more nodes the more accurate the approximation.

# Universal Approximation Theorem

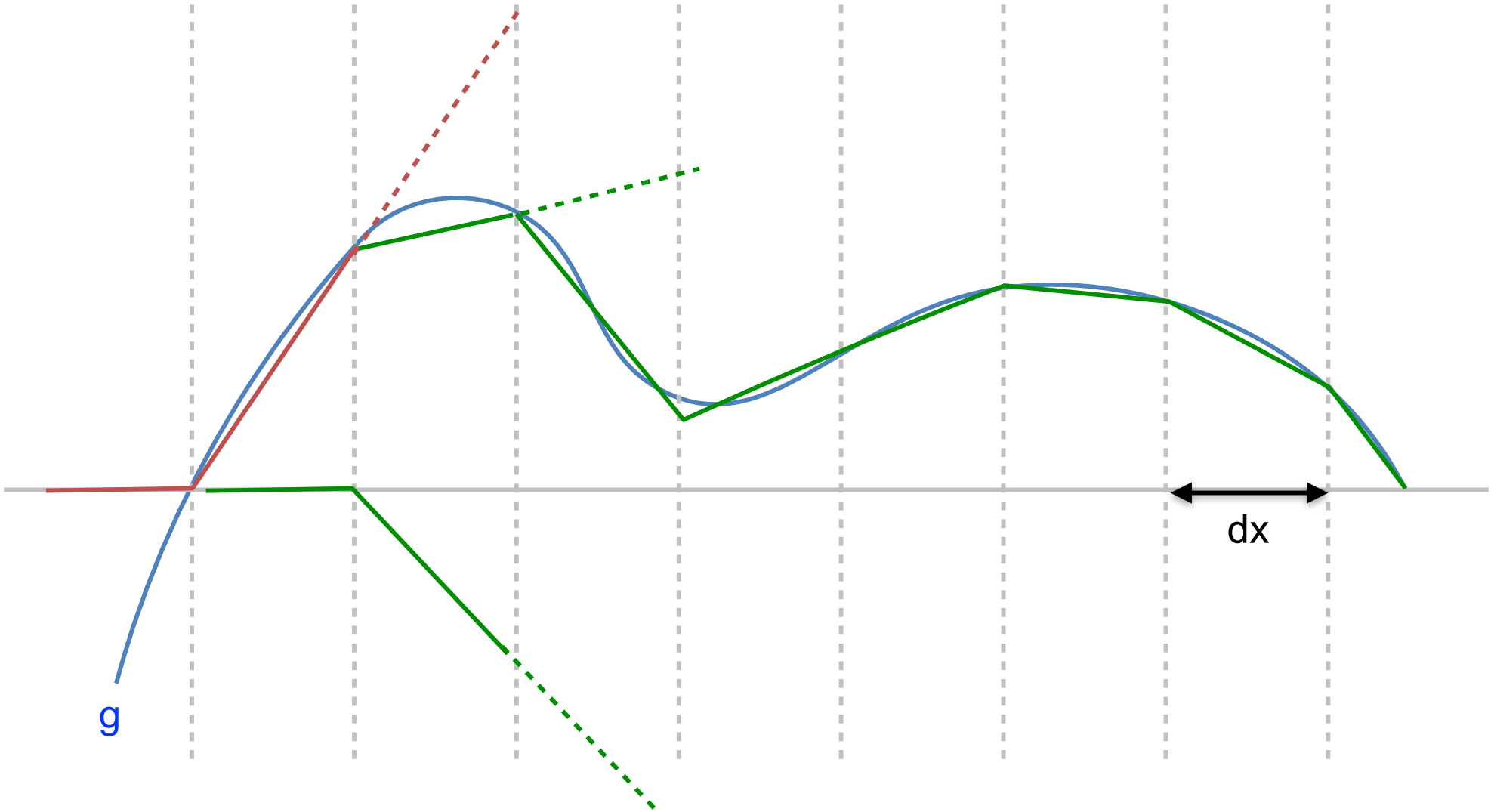
A feedforward network with a linear output layer and at least one hidden layer with any 'squashing' activation function (e.g. logistic sigmoid) can approximate any Borel measurable function (from one finite-dimensional space to another) with any desired nonzero error.

Any continuous function on a closed and bounded set of $R^n$ is Borel-measurable.

—> In theory, any reasonable function can be approximated by a one-hidden layer network as long as it is continuous.

[Hornik et al, 1989; Cybenko, 1989]

# Universal Approximation Theorem in 1D



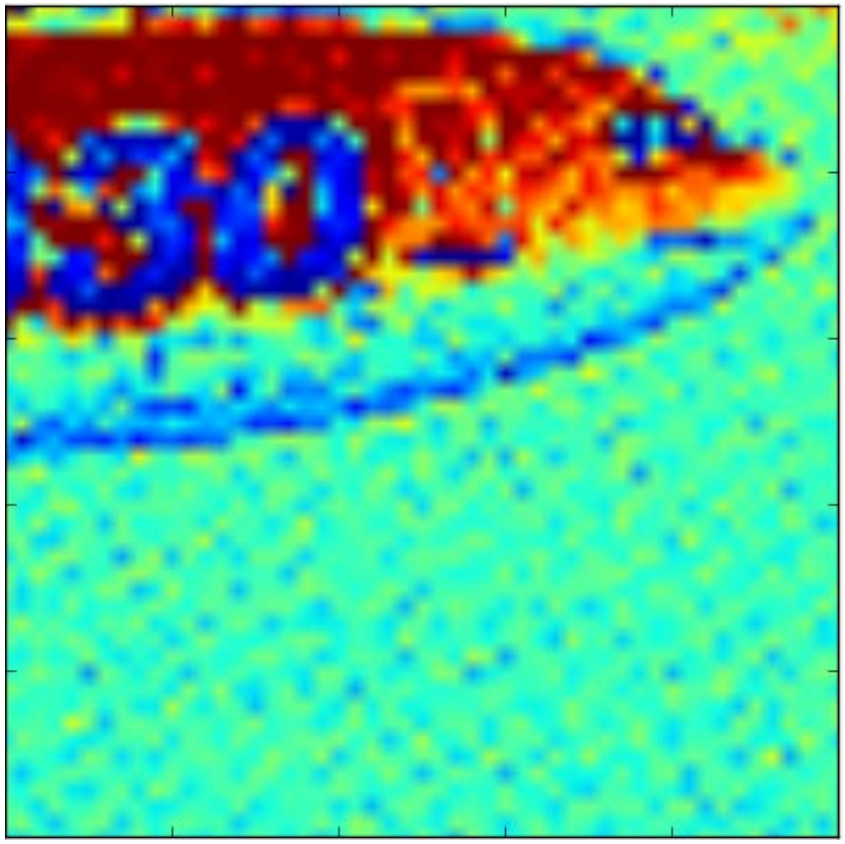

$$f(x) = \sigma(w_1 x + b_1) + \sigma(w_2 x + b_2) + \ldots + \sigma(w_n x + b_n)$$

When dx —> 0, f —> g.

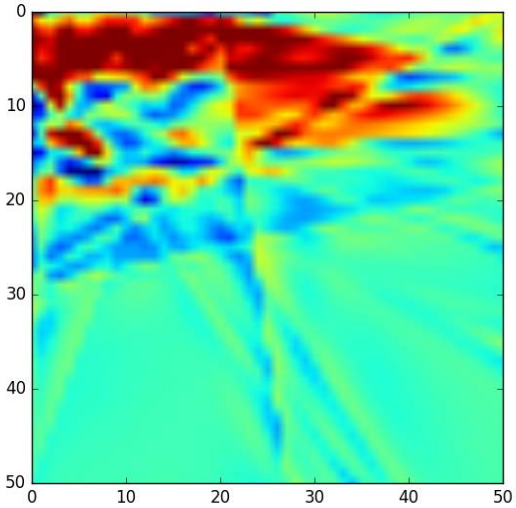
# Universal Approximation Theorem in nD

- The sine function can be approximated arbitrarily well.
- According to Fourier analysis, continuous functions from $R^N$ into R can be approximated arbitrarily well by a weighted sum of sine functions.

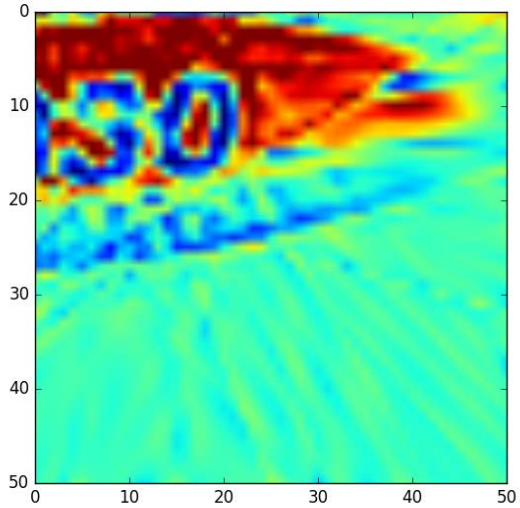
# More Complex Surface



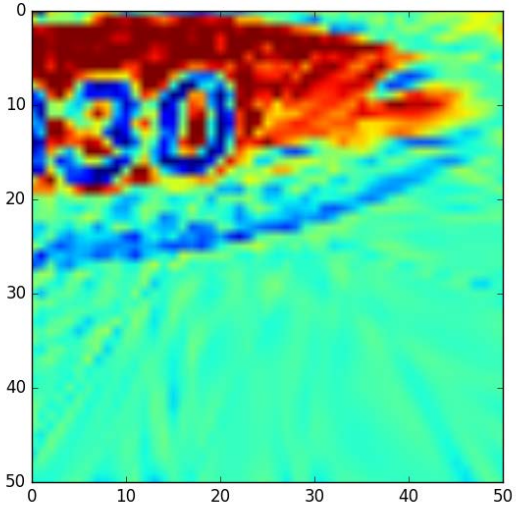
$$I = f(x, y)$$



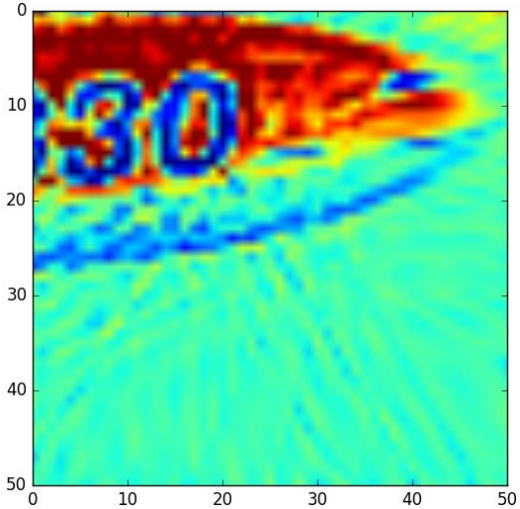
50 nodes -> loss 3.65e-01



100 nodes -> loss 2.50e-01



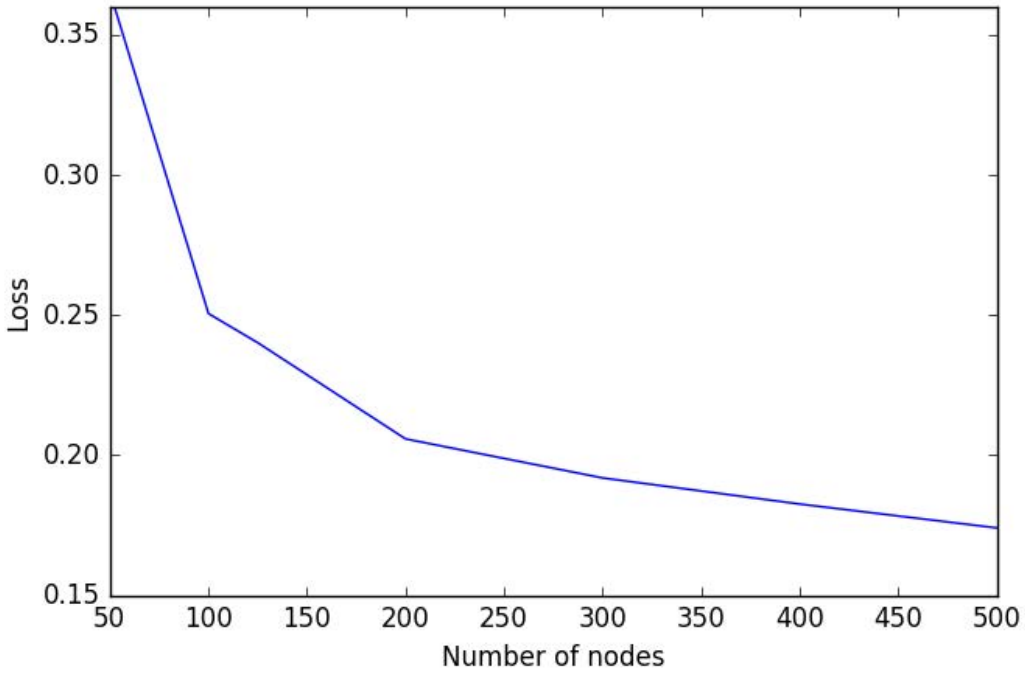
125 nodes -> loss 2.40e-01

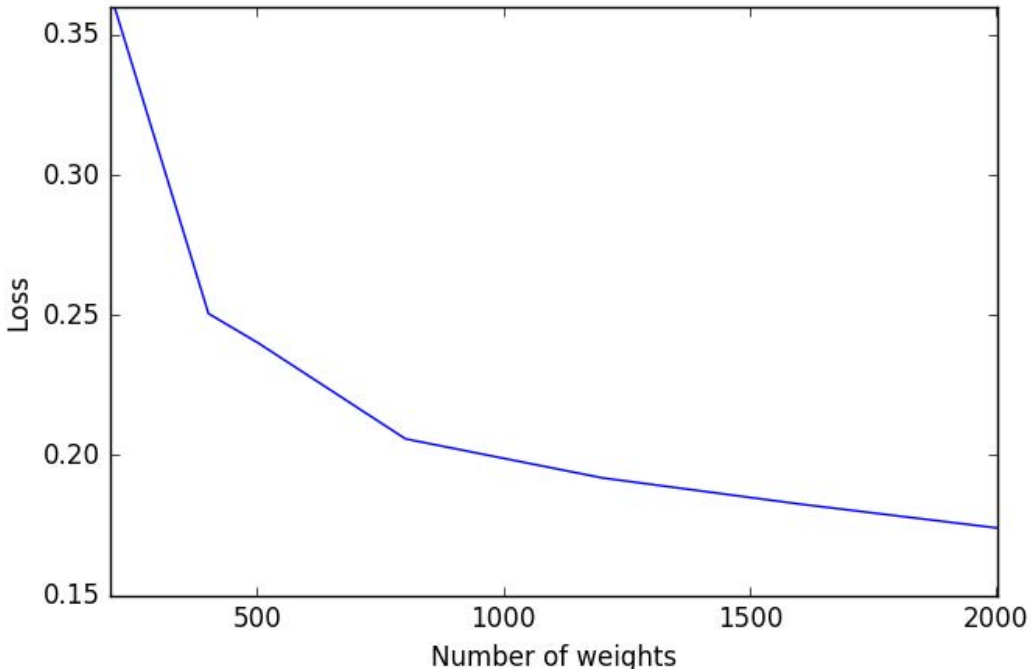


300 nodes -> loss 1.92e-01

—> The more nodes the more accurate the approximation.

# In Practice

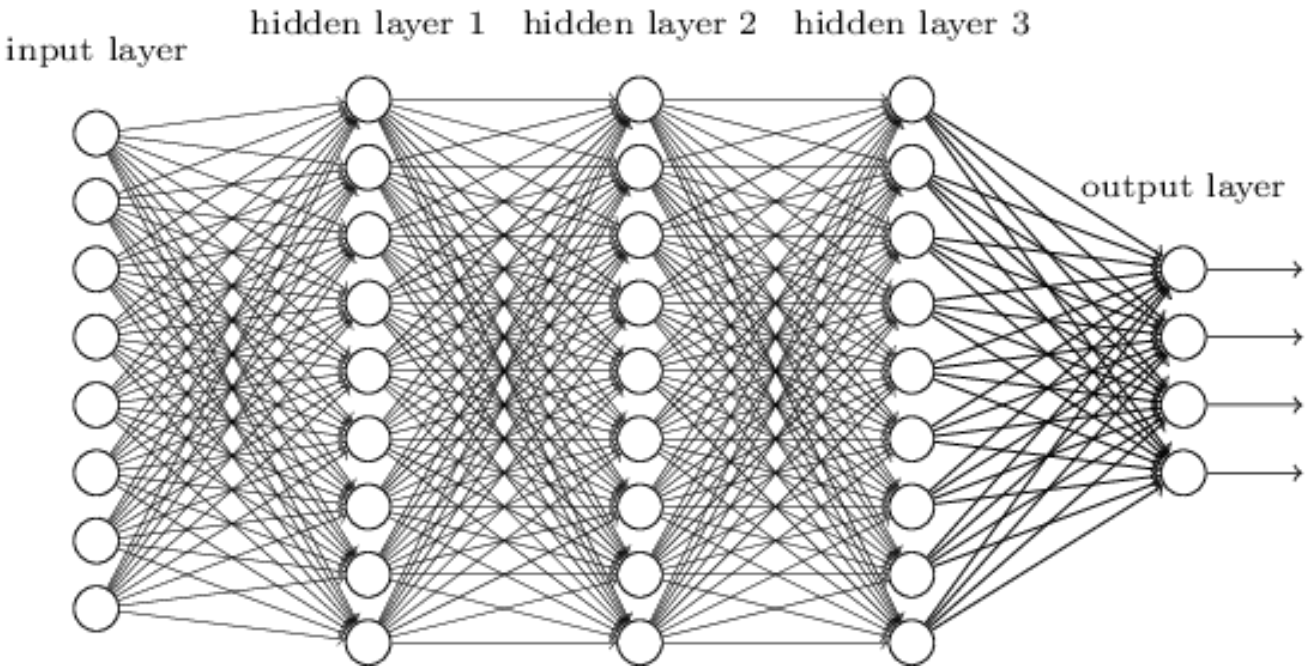



- It may take an exponentially large number of parameters for a good approximation.
- The optimization problem becomes increasingly difficult.

—> The one hidden layer perceptron may not converge to the best solution!

# From MLP to Deep Learning

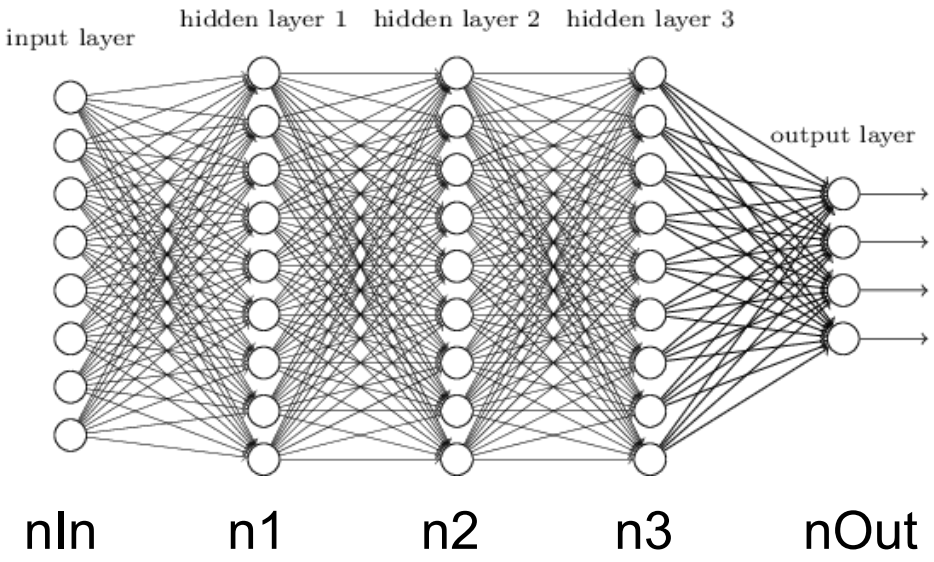



$$
\begin{aligned}
\mathbf{h}_1 &= \sigma_1(\mathbf{W}_1\mathbf{x}_1 + \mathbf{b}_1) \\
\mathbf{h}_2 &= \sigma_2(\mathbf{W}_2\mathbf{h}_1 + \mathbf{b}_2) \\
&\cdots \\
\mathbf{y} &= \sigma_n(\mathbf{W}_n\mathbf{h}_n + \mathbf{b}_n)
\end{aligned}
$$

- MLPs can have more than one hidden layer.
- Their descriptive power increases with the number of layers.

# PyTorch Translation

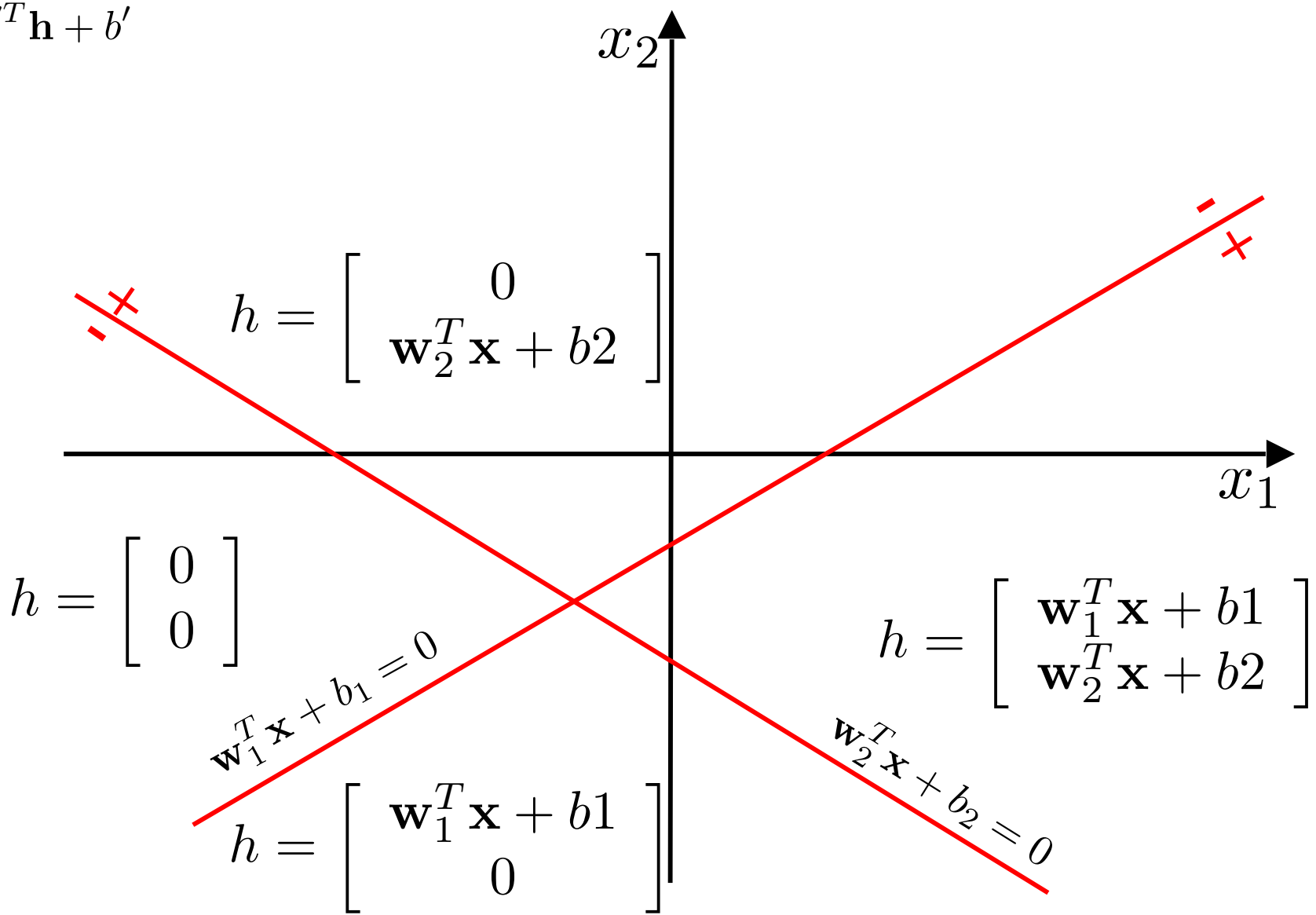
```
class MLP(nn.Module):

    def __init__(self,n1=10,n2=10,n3=10,nIn=2,nOut=1):
        self.l1 = nn.Linear(nIn,n1)
        self.l2 = nn.Linear(n1,n2)
        self.l3 = nn.Linear(n2,n3)
        self.l4 = nn.Linear(n3,nOut)

    def forward(self,x):
        h1 = sigm(self.l1(x))
        h2 = sigm(self.l2(h1))
        h3 = sigm(self.l3(h2))
        return(self.l4(h3))

    def loss(self,x,target):
        loss_fn = torch.nn.CrossEntropyLoss()
        output = self(x)
        return loss_fn(output,target)
```



# One Layer: Two Hyperplanes

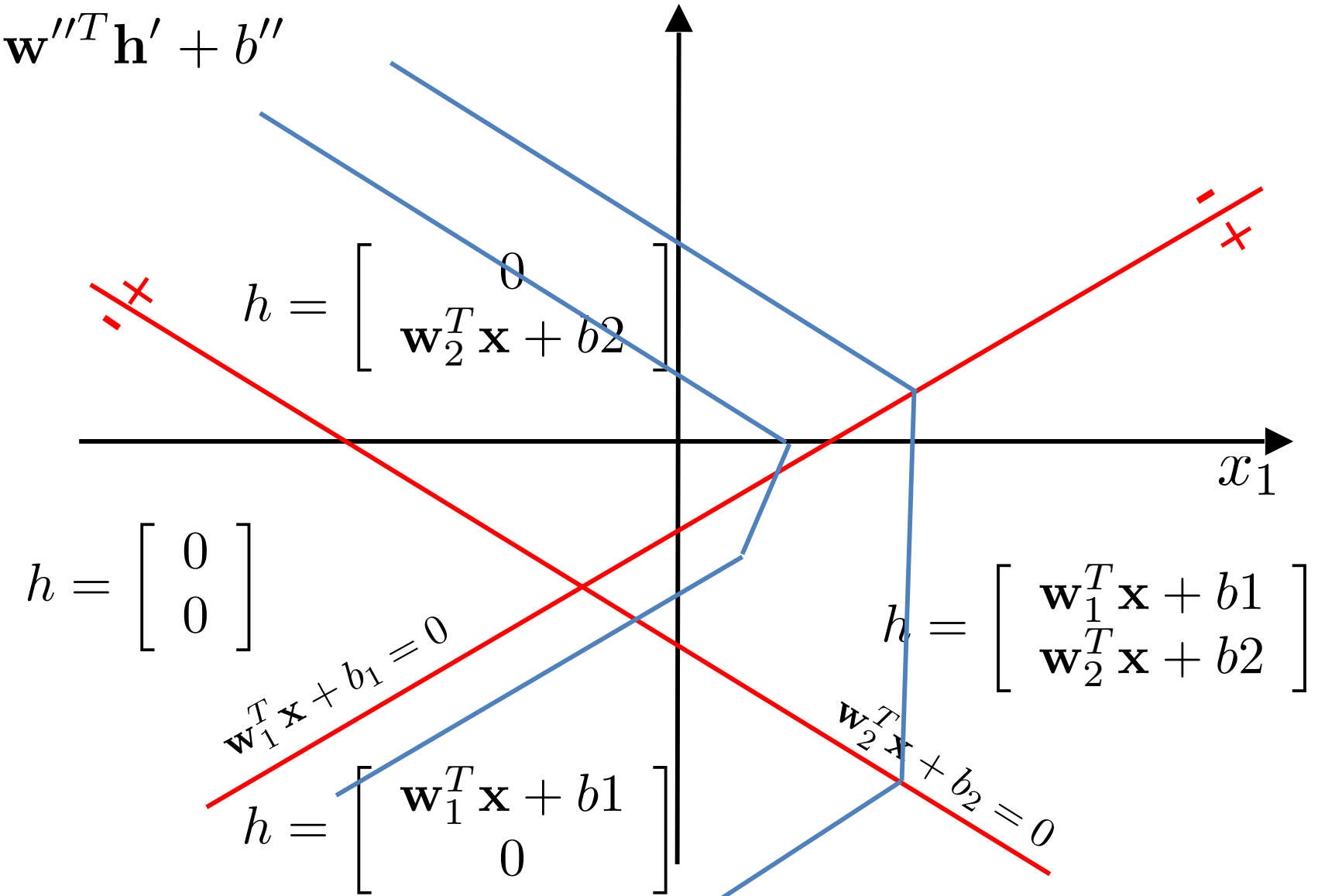
$$\mathbf{h} = \max(\mathbf{W}\mathbf{x} + \mathbf{b}, 0) \text{ with } \mathbf{W} = \begin{bmatrix} \mathbf{w}_1^T \\ \mathbf{w}_2^T \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

$$y = \mathbf{w}'^T \mathbf{h} + b'$$



# Two Layers: Two Hyperplanes

$$\mathbf{h} = \max(\mathbf{W}\mathbf{x} + \mathbf{b}, 0)$$
$$\mathbf{h}' = \max(\mathbf{W}'\mathbf{h} + \mathbf{b}', 0)$$
$$y = \mathbf{w}''^T\mathbf{h}' + b''$$



# Multi Layer Perceptrons

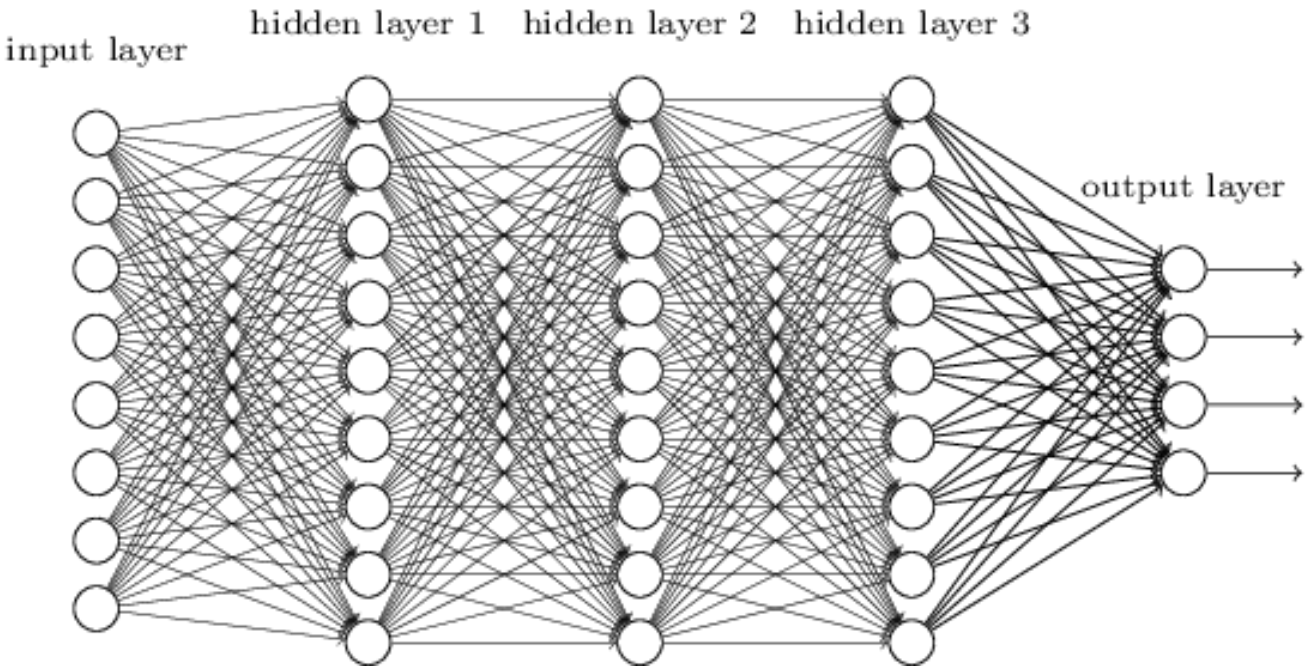
The function learned by a DNN using either ReLU, Sigmoid, or Tanh operators is:

- piecewise affine or smooth;
- continuous because it is a composition of continuous functions.

Each region created by a layer is split into smaller regions:

- Their boundaries are correlated in a complex way.
- Their descriptive power is **larger** than that of shallow networks for the **same number** of parameters.

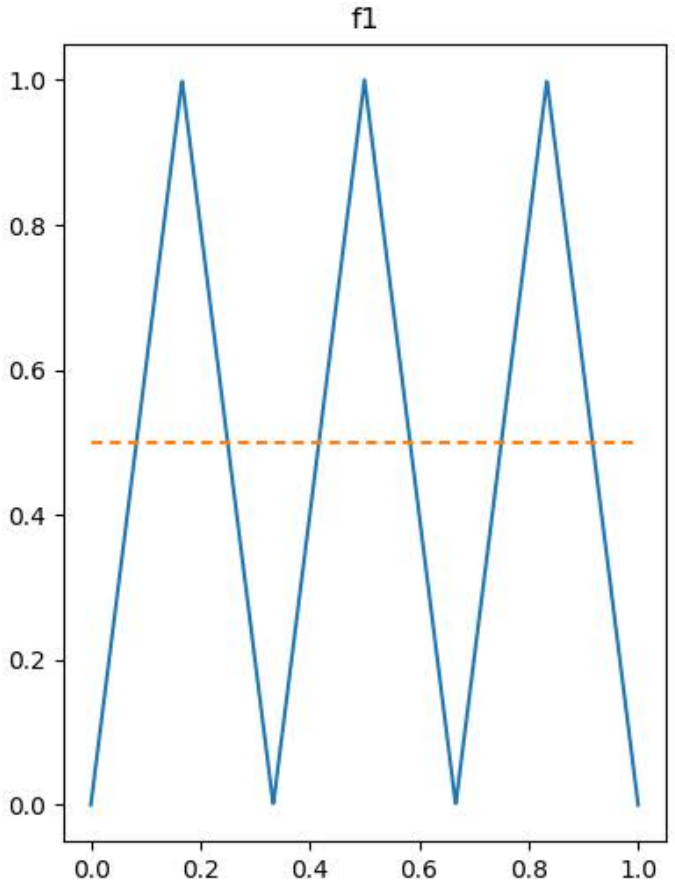
# Deep Learning

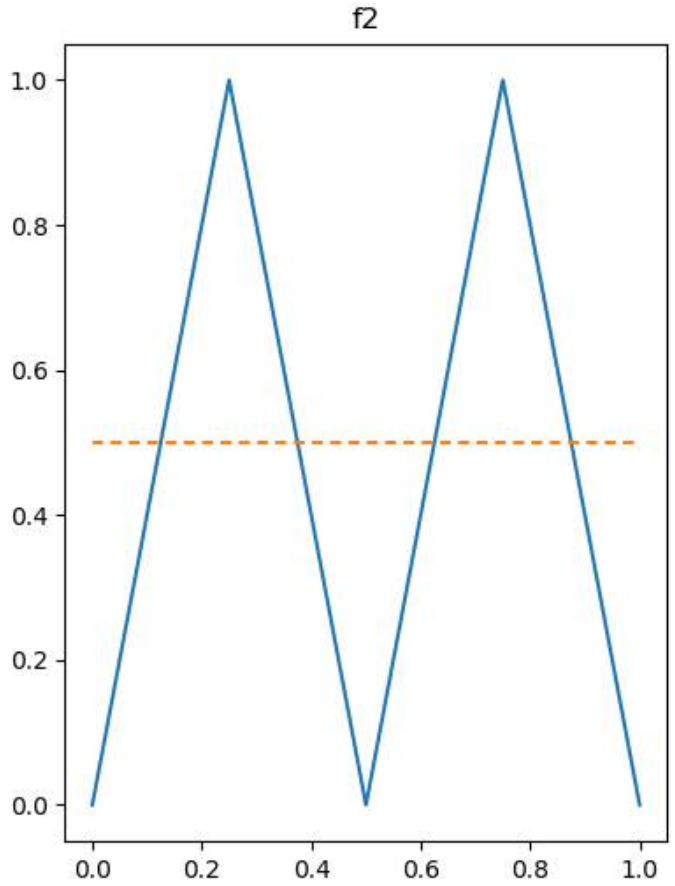


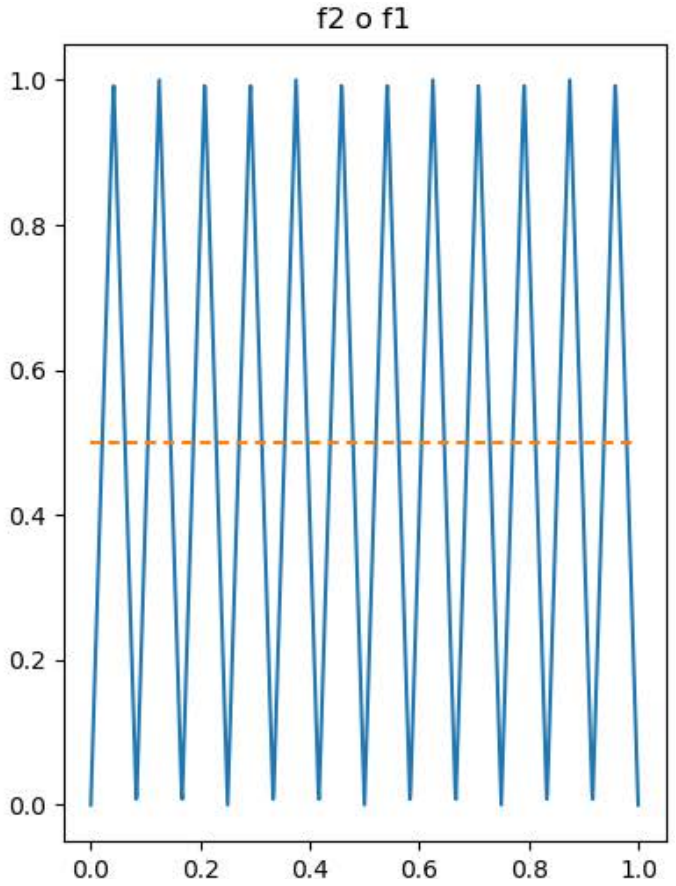

$$\begin{aligned} \mathbf{h}_1 &= \sigma_1(\mathbf{W}_1\mathbf{x}_1 + \mathbf{b}_1) \\ \mathbf{h}_2 &= \sigma_2(\mathbf{W}_2\mathbf{h}_2 + \mathbf{b}_2) \\ &\dots \\ \mathbf{y} &= \sigma_n(\mathbf{W}_n\mathbf{h}_n + \mathbf{b}_n) \end{aligned}$$

- MLPs can have more than one hidden layer.
- Their descriptive power increases with the number of layers.
- In the case of a 1D signal, it is roughly proportional to $\prod_n W_n$ where $w_n$ is the width of layer n.

# The Power of Composition

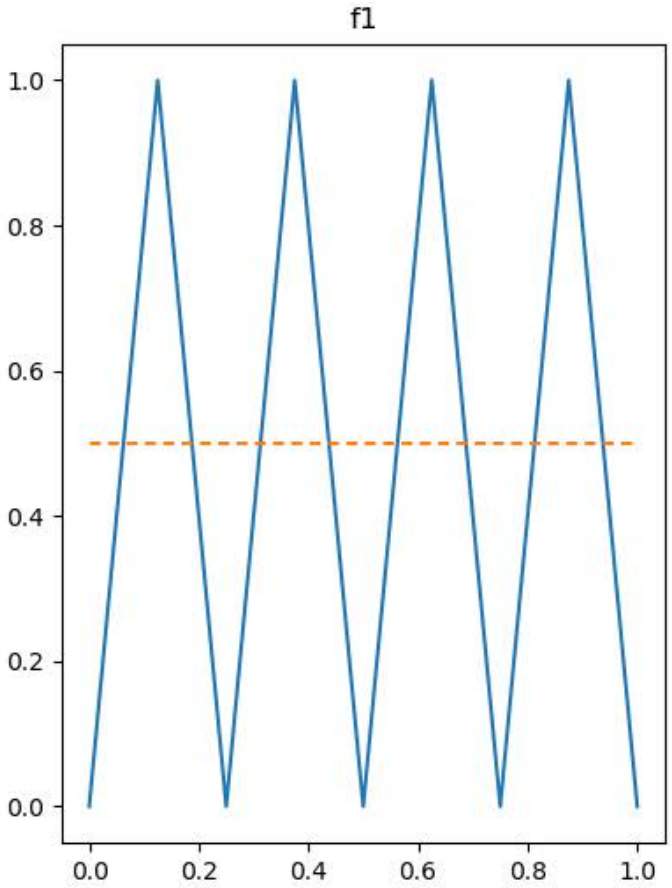


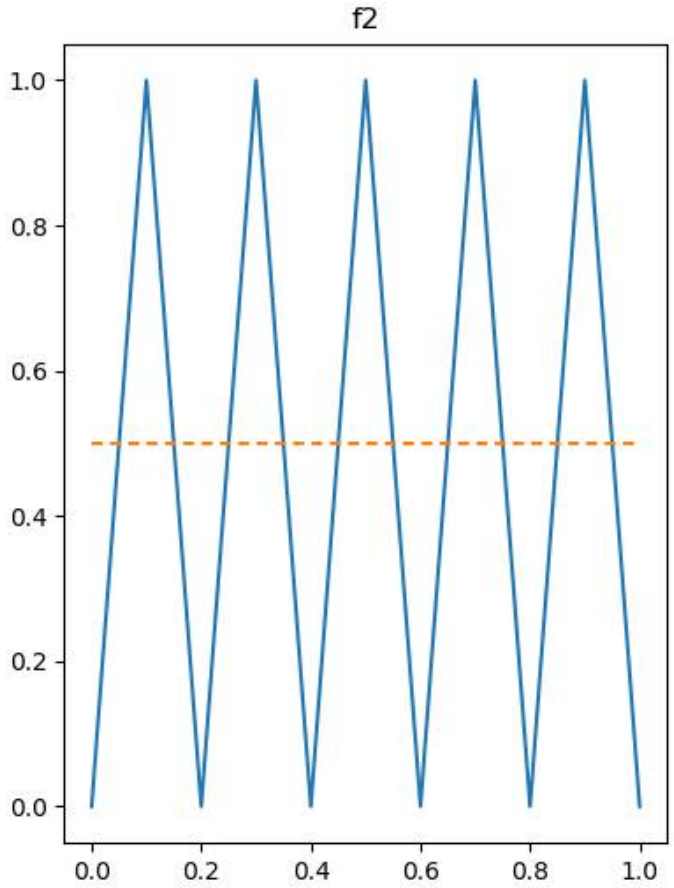



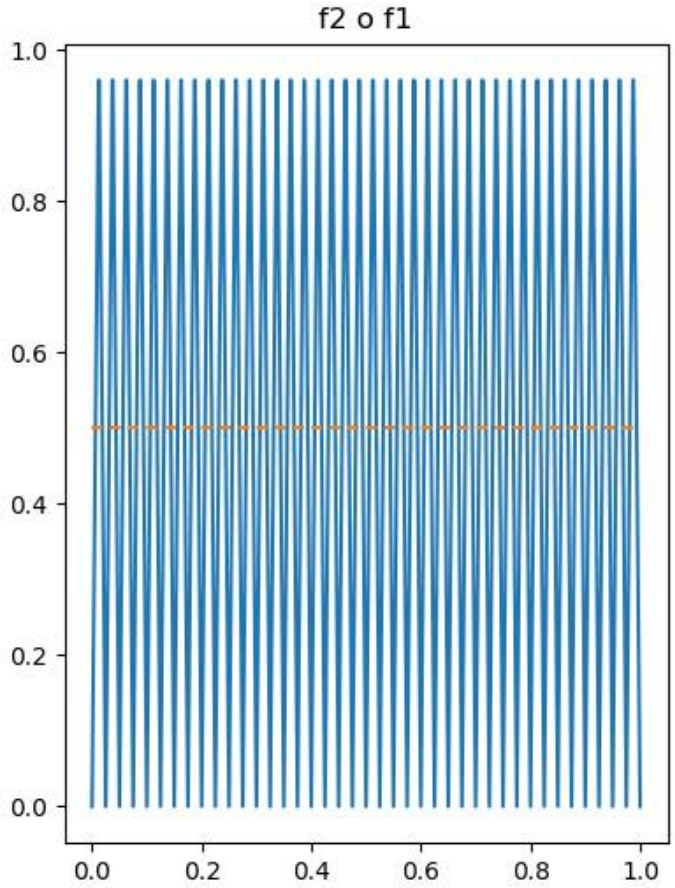




- $f_1(.)$ has $n_1=3$ peaks.
- $f_2(.)$ has $n_2=2$ peaks.
- $f_2(f_1(.))$ has $2n_1n_2=12$ peaks.

# The Power of Composition



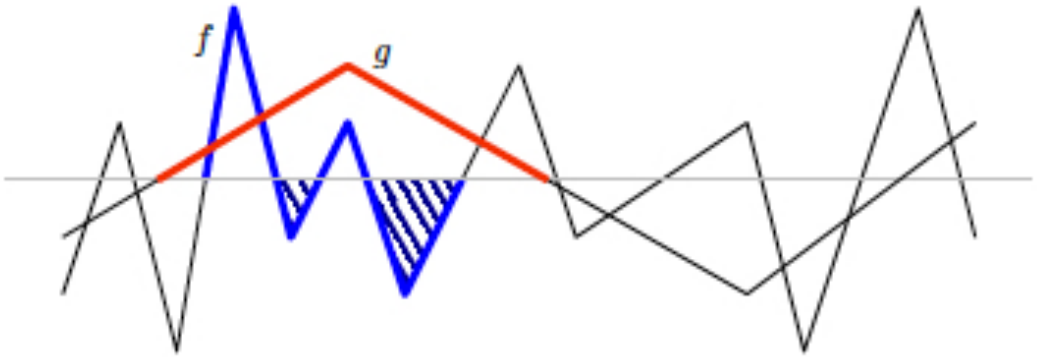




- $f_1(.)$ has $n_1=4$ peaks.
- $f_2(.)$ has $n_2=5$ peaks.
- $f_2(f_1(.))$ has $2n_1n_2=40$ peaks.

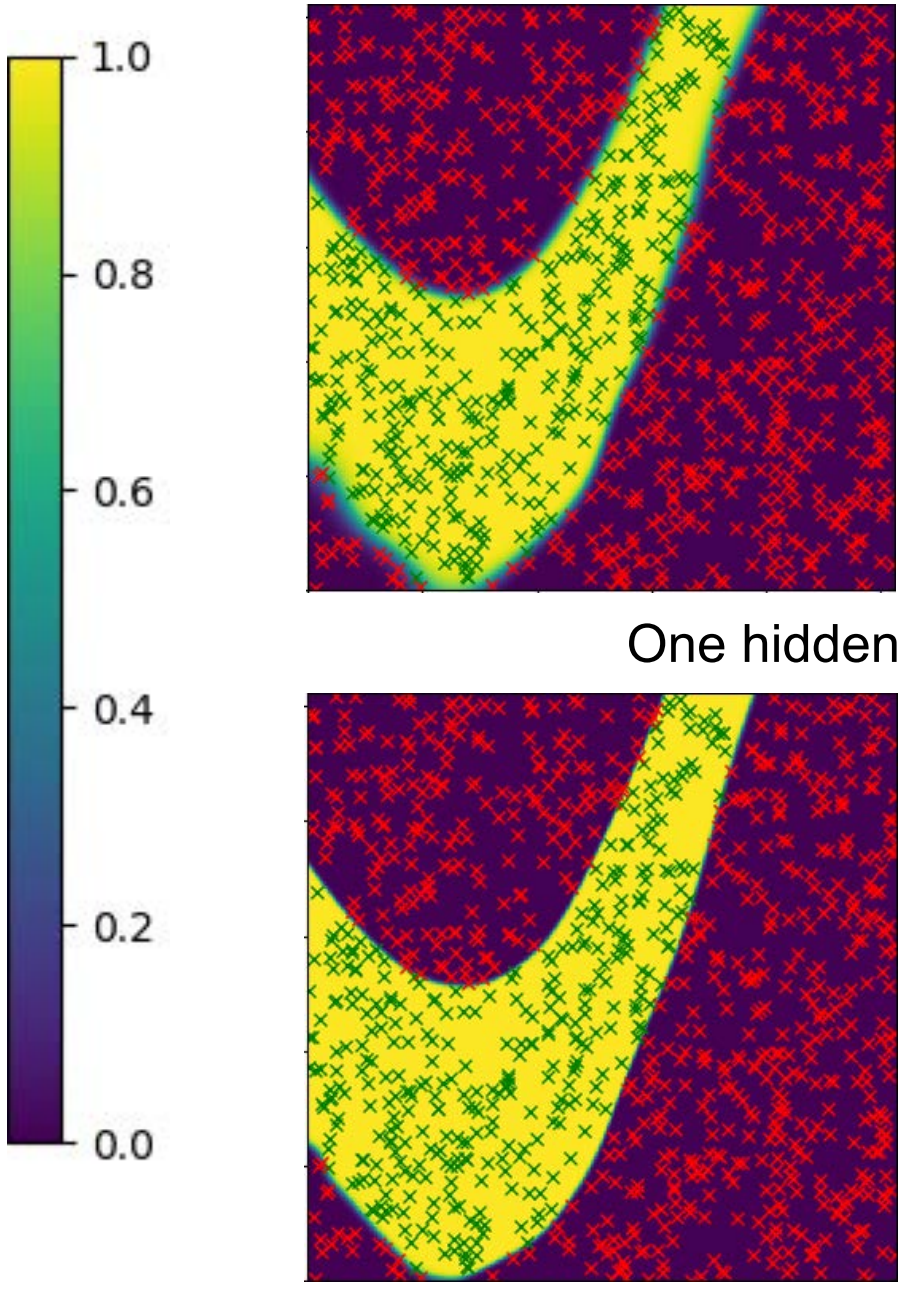
—> Descriptive power is proportional to $n_1n_2$

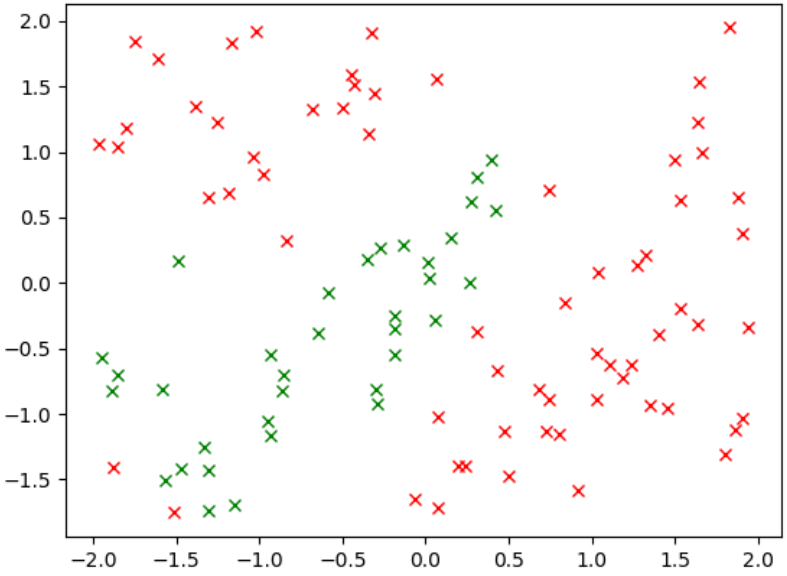
# Optional: Proof Sketch



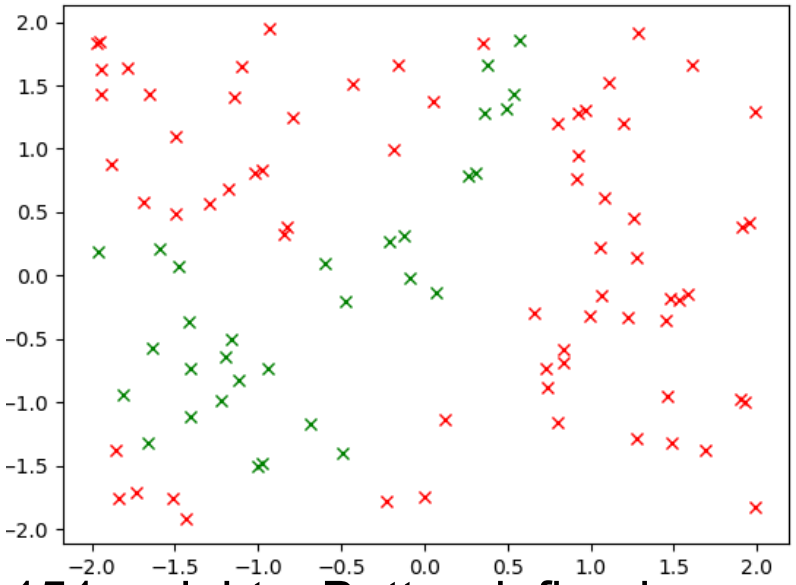

- Functions with few oscillations do not approximate well functions that have many.
- Networks can depict functions that have as many as $\prod_n W_n$ oscillations, where $w_n$ is the width of layer n.
  - Functions computed by networks with few layers have few oscillations.
  - Functions computed by deeper networks have many more oscillations.

# Back to Non-Linear Classification



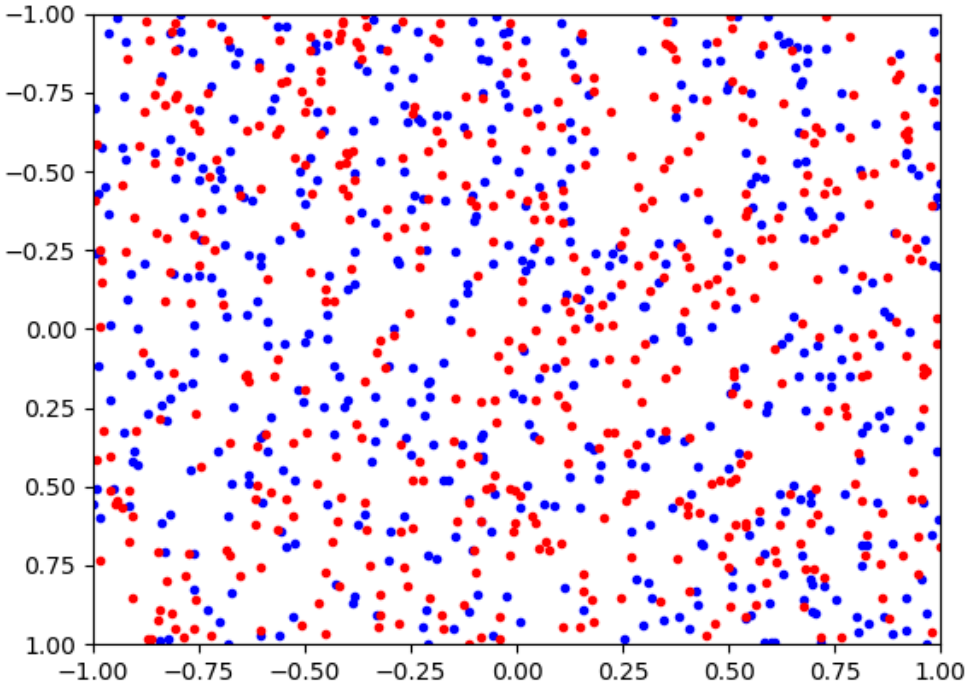



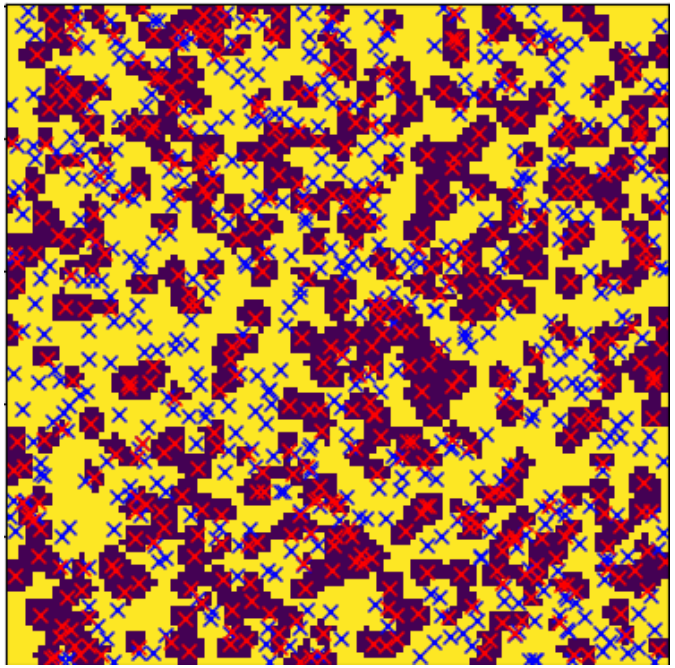

One hidden layer: n=100, 401 weights.




Two hidden layers: n1=10, n2=10, 151 weights: Better defined boundaries with far fewer weights.

# Randomly Distributed Points and RBF Kernels



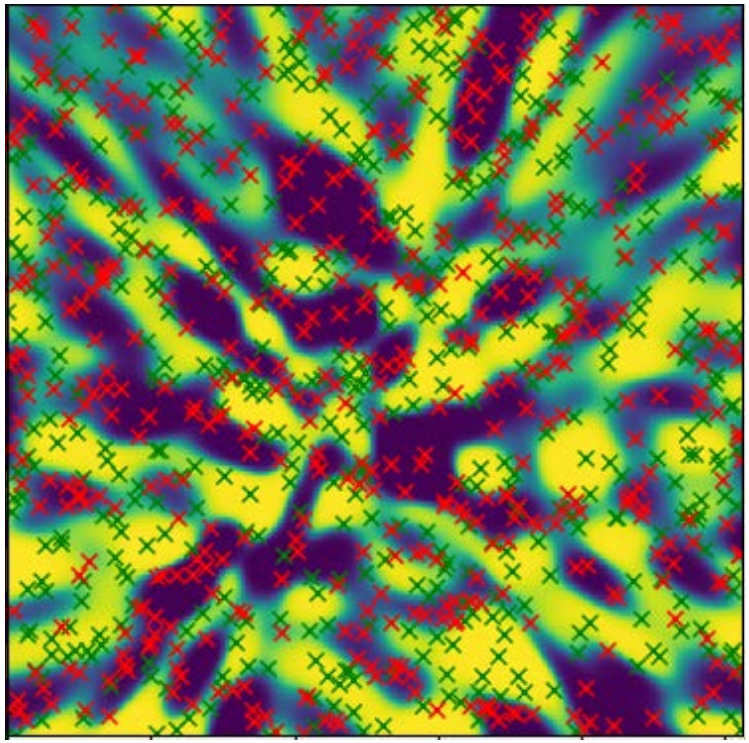



Rbf, $\gamma = 200$

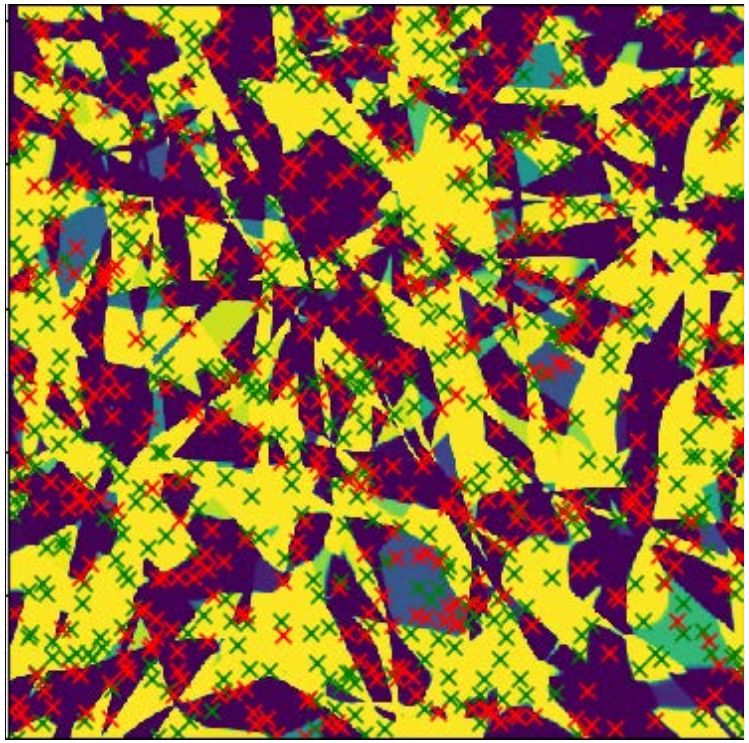
n=100, 72%

n=400, 77%

n=1600,79%



One hidden layer



Two hidden layers

n=10, 70%

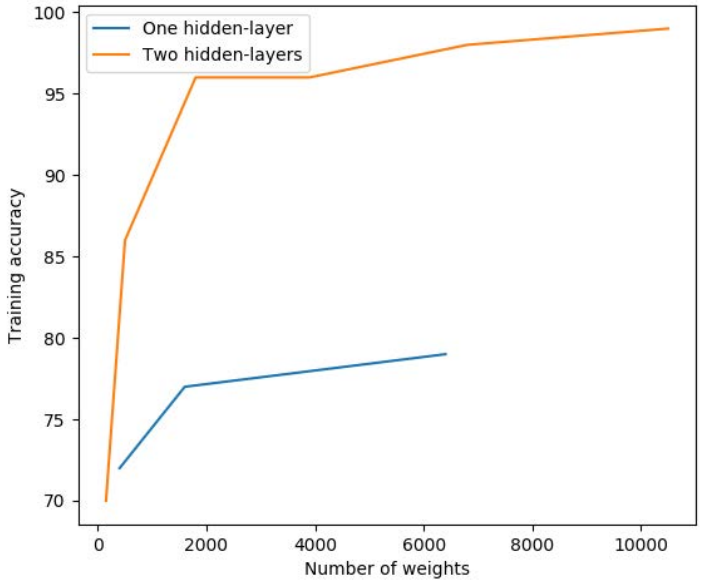
n=20, 86%

n=40, 96%

n=60, 96%

n=80, 98%

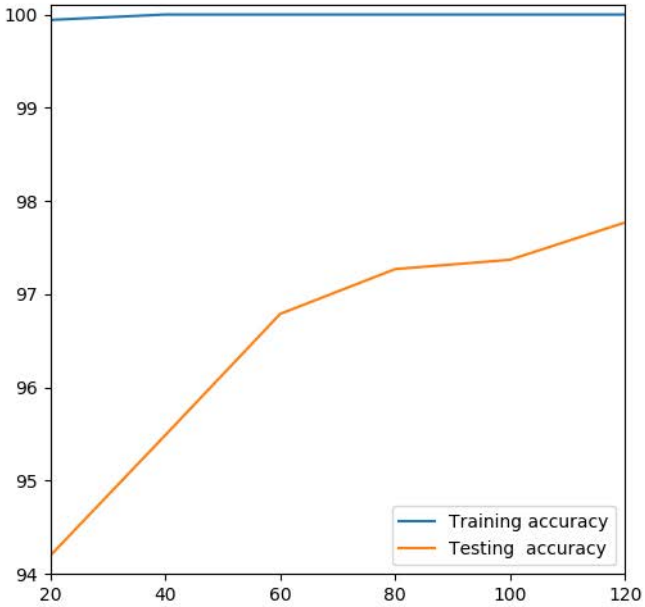
n=100, 99%

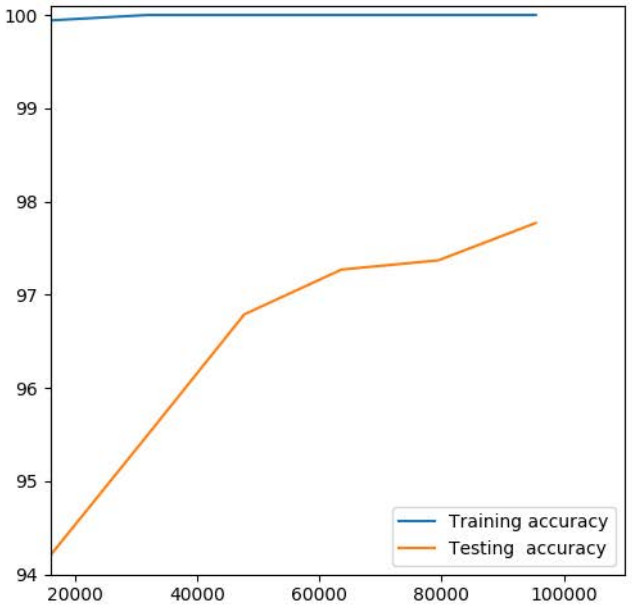



Empirical observation: The two layer networks converge faster and better.

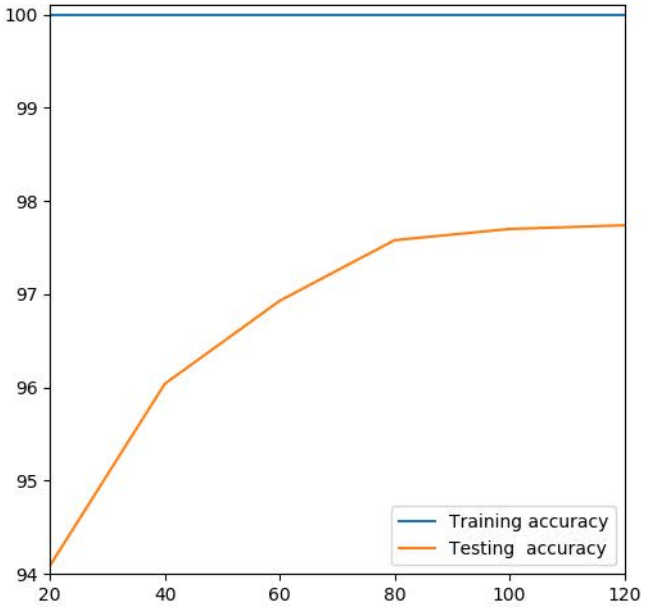
# MNIST Results

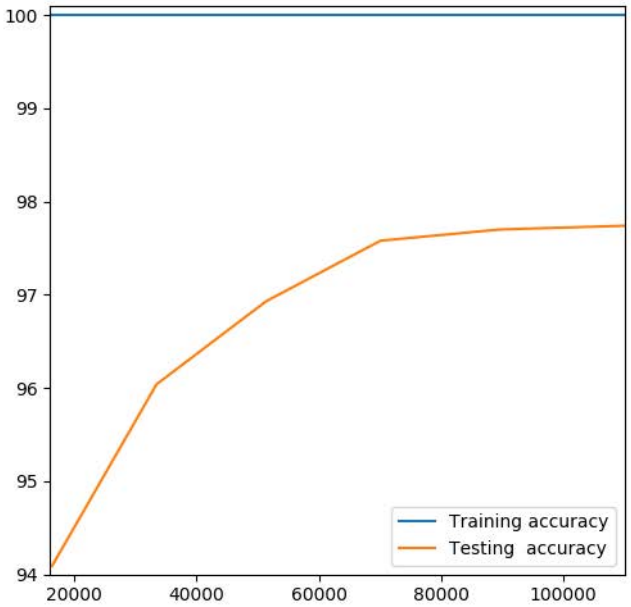
nIn =784
nOut = 10
20 < n1 < 120




One Layer MLP

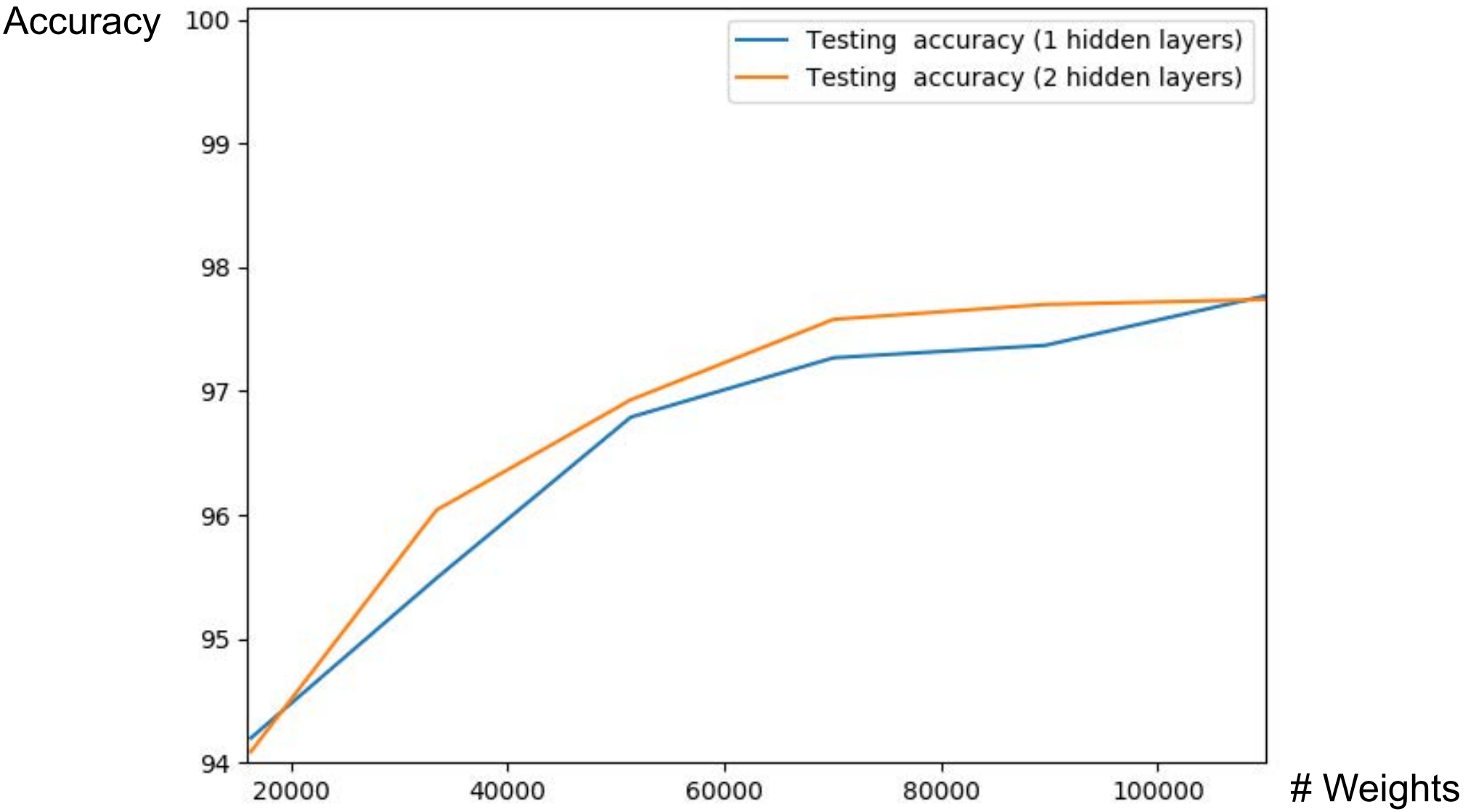



Two-Layer MLP

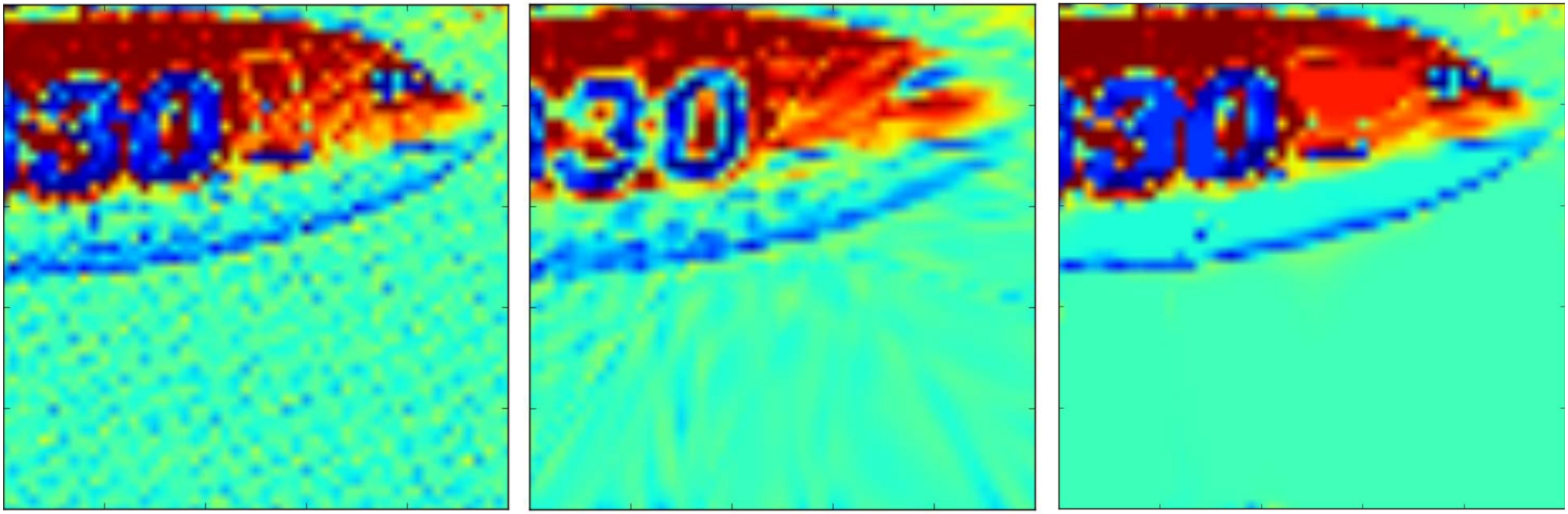
nIn =784
nOut = 10
20 < n1=n2 < 120

# Testing Accuracy on MNIST




- Two-layer MLP yield better accuracy with fewer weights initially.
- One-layer MLP eventually catches up in this simple case.

# Second Layer for Regression



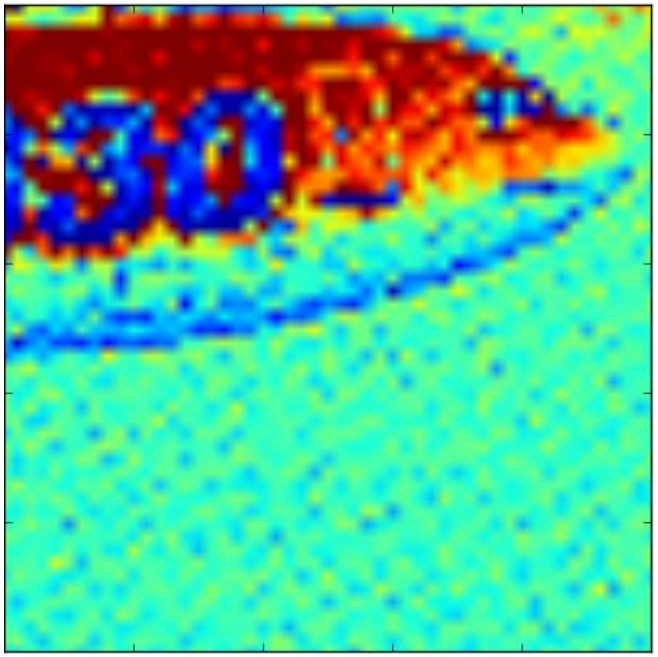
$$I = f(x, y)$$

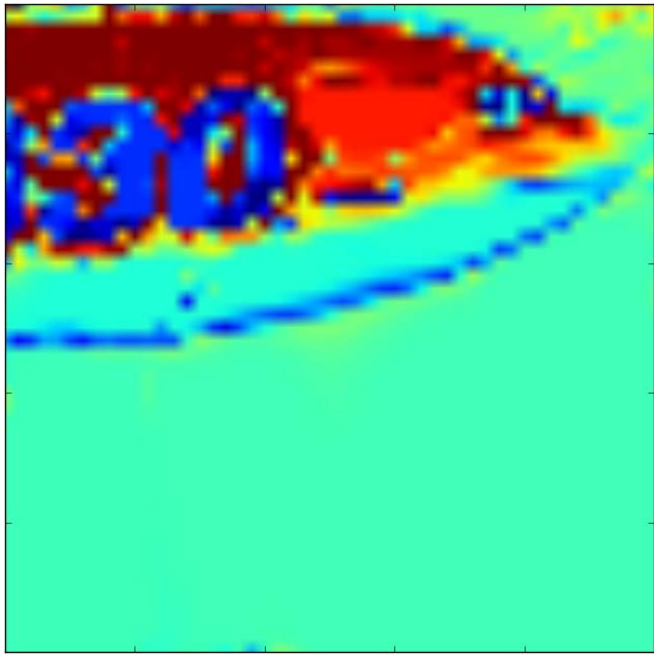
1 Layer: 125 nodes -> loss 2.40e-01  2 Layers: 20 nodes -> loss 8.31e-02

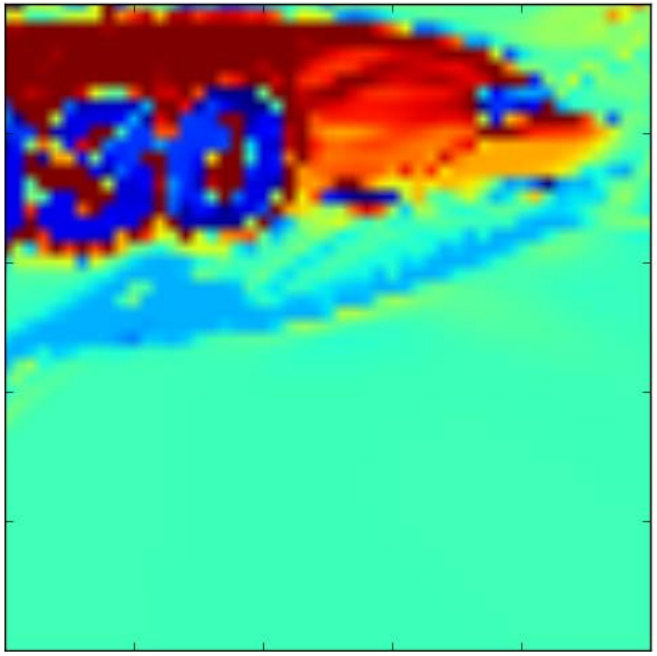
501 weights in both cases

—> The two-layer MLP yields a better approximation with the same number of weights.

# Adding a Third Layer







$$I = f(x, y)$$

2 Layers: 20 nodes -> loss 8.31e-02

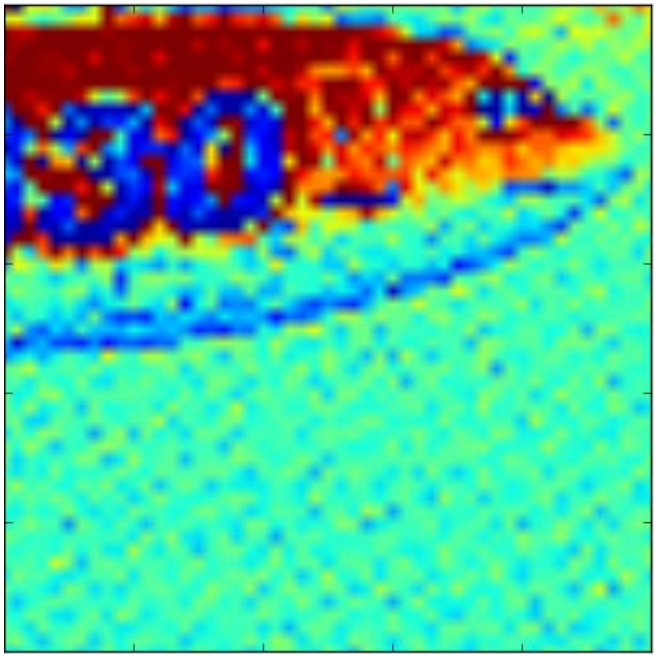
501 weights

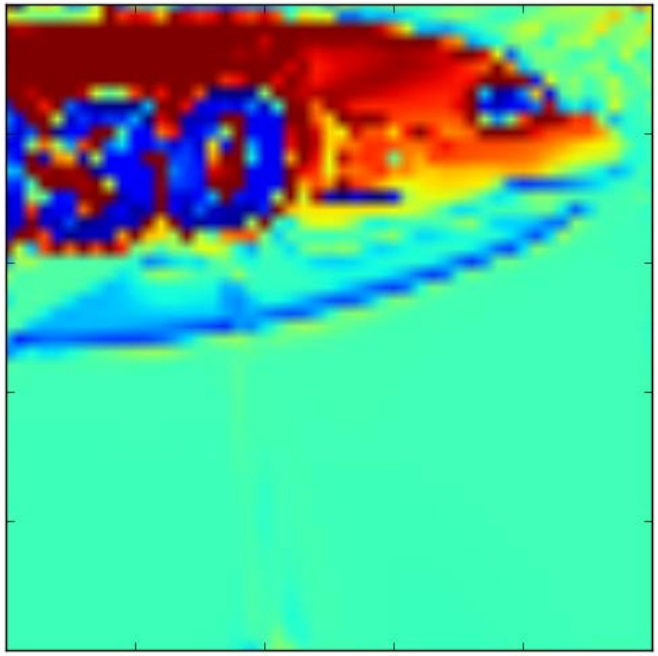
3 Layers: 14 nodes -> loss 7.55e-02

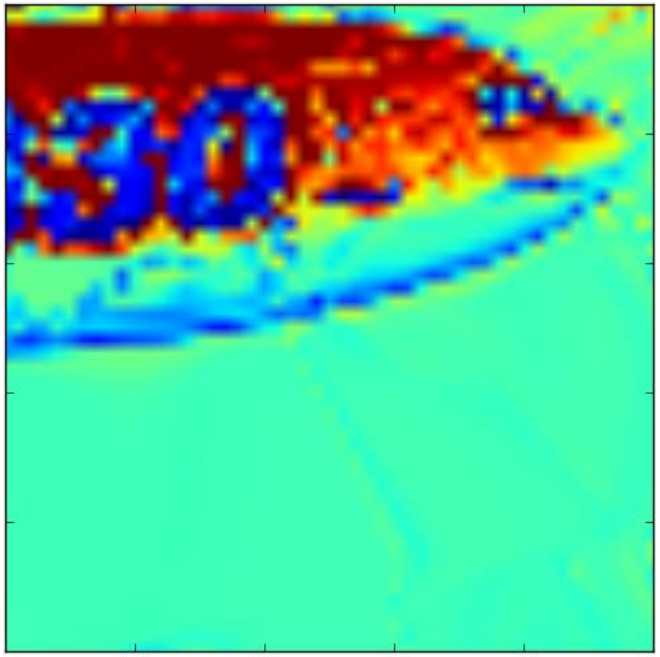
477 weights

—> The three-layer MLP does even better but the difference is less striking. Diminishing returns?

# Adding a Third Layer







$$I = f(x, y)$$

3 Layers: 15 nodes -> loss 5.93e-02

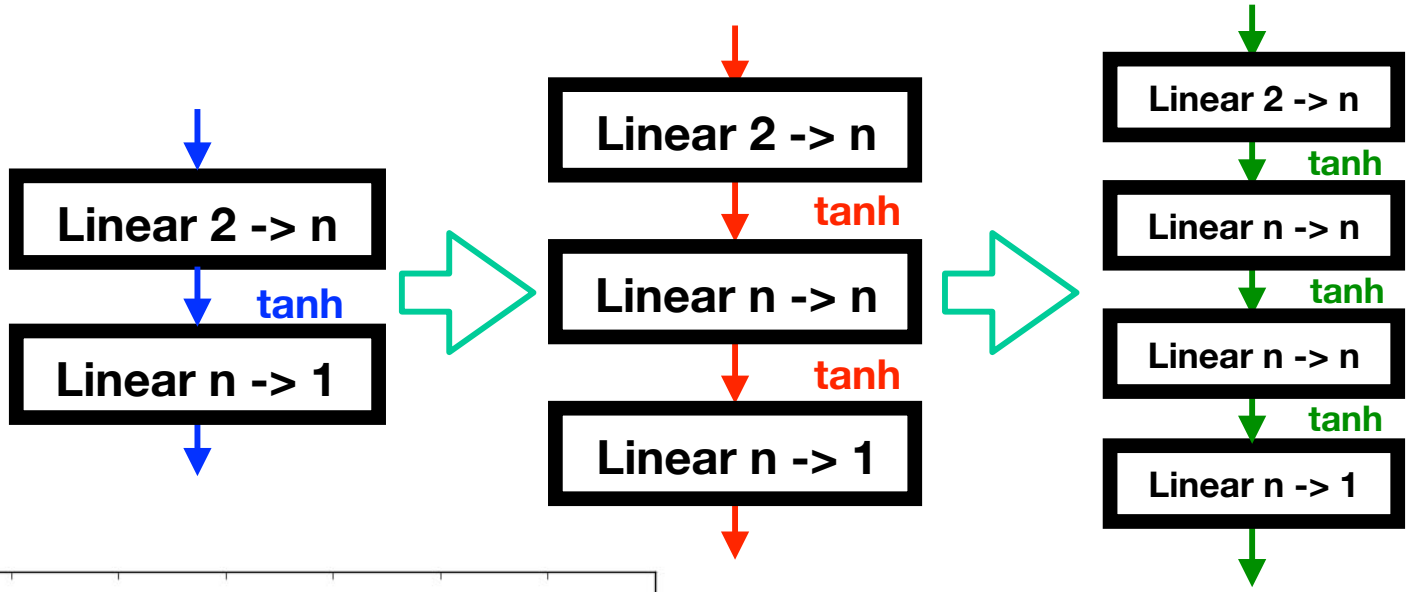
541 weights

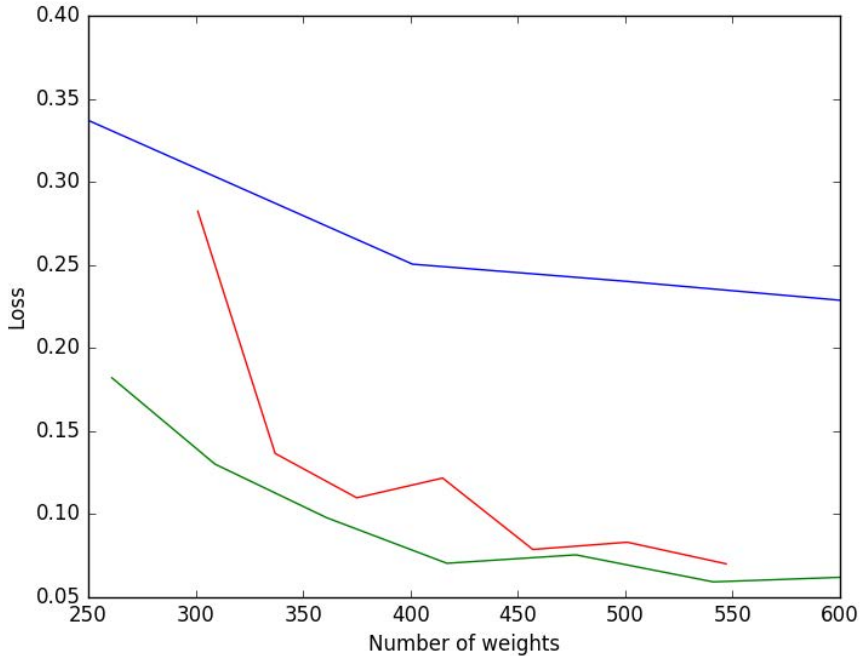
3 Layers: 19 nodes -> loss 4.38e-02

837 weights

—> The three-layer MLP does even better but the difference is less striking. Diminishing returns?

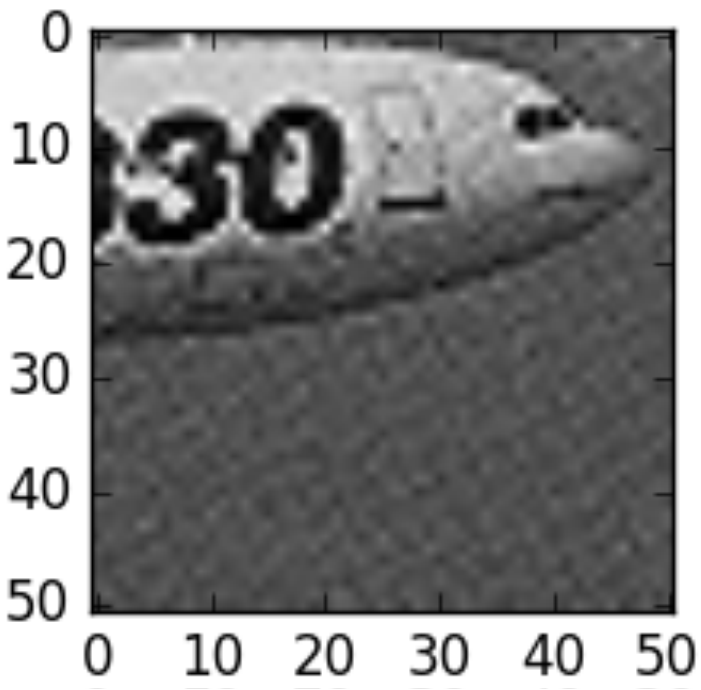
# Multi Layer Perceptrons



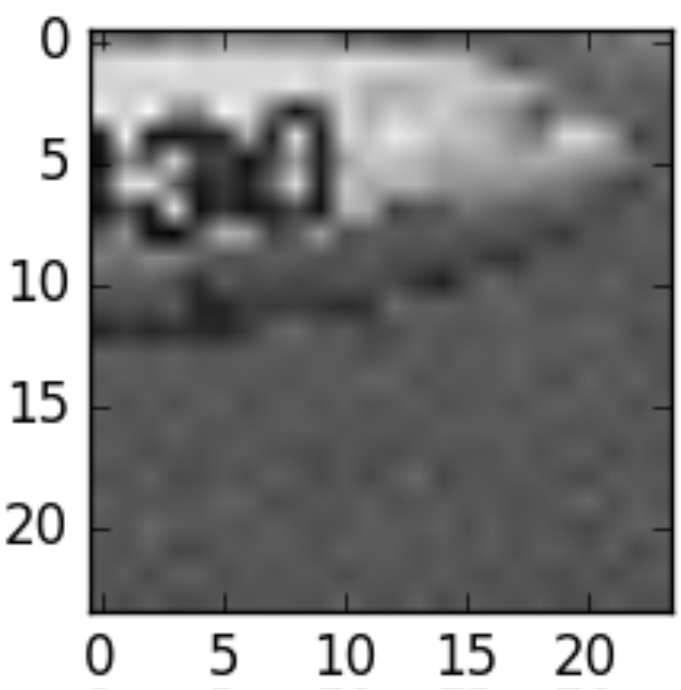




- Adding layers often yields better convergence properties.
- In current practice, deeper is usually better.

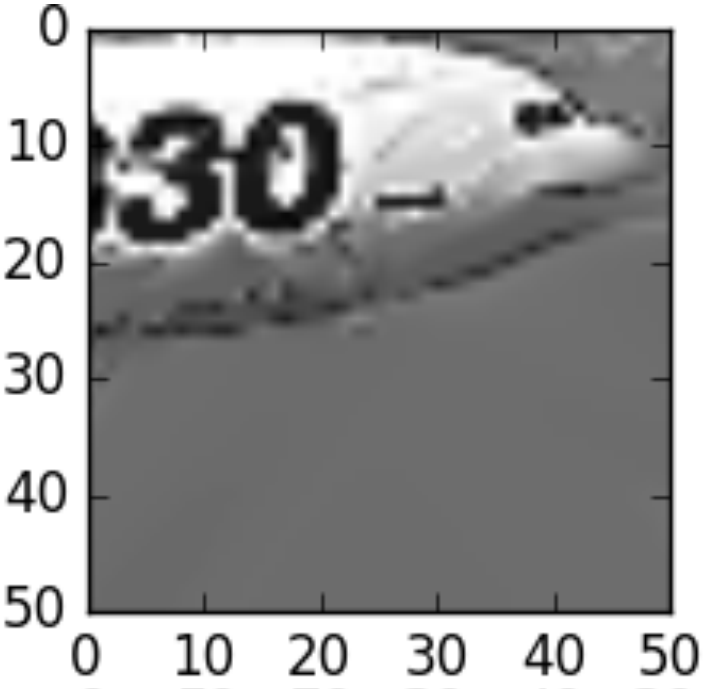
# Other Ways to Interpolate




Original 51x51 image:
2601 gray level values.



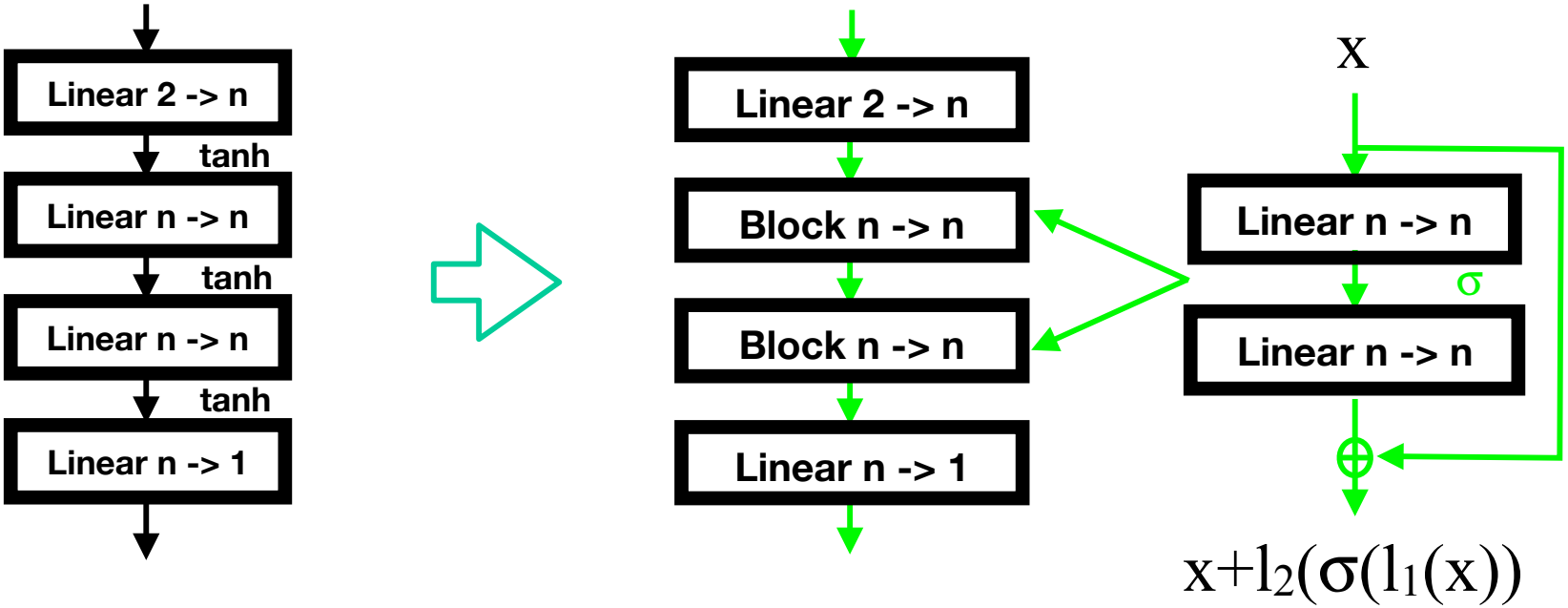

Scaled 24x24 image:
576 gray level values.




MLP 10/20/10 Interpolation:
471 weights.

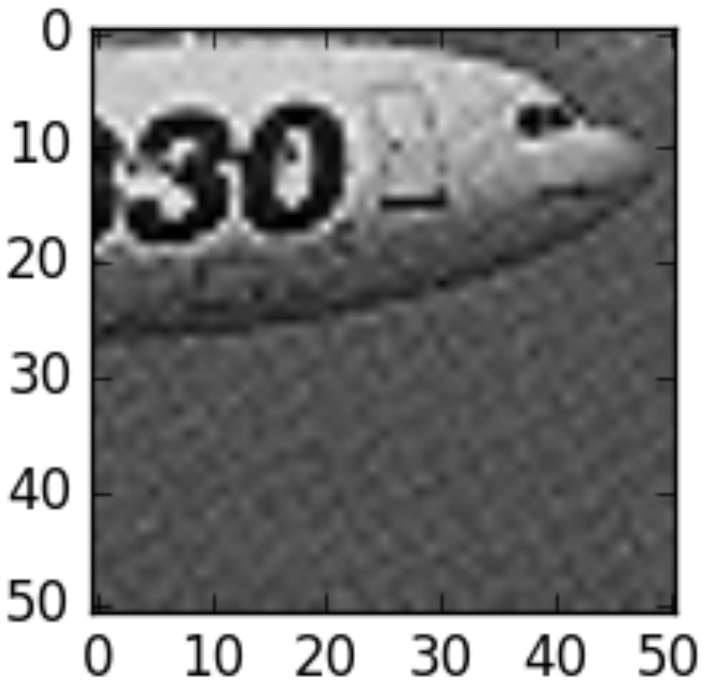
Simpler but not necessarily better!

# MLP to ResNet

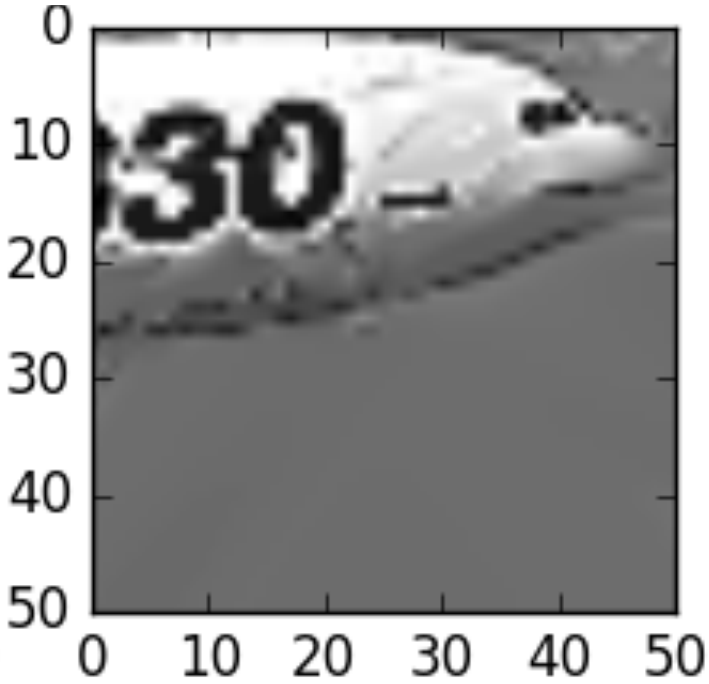



Further improvements in the convergence properties have been obtained by adding a bypass, which allows the final layers to only compute residuals.

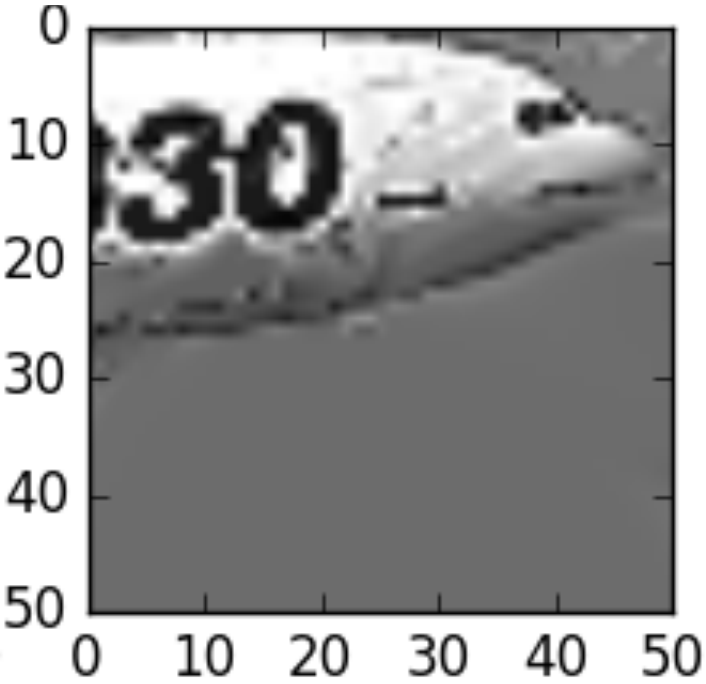
# Adding a ResNet Layer



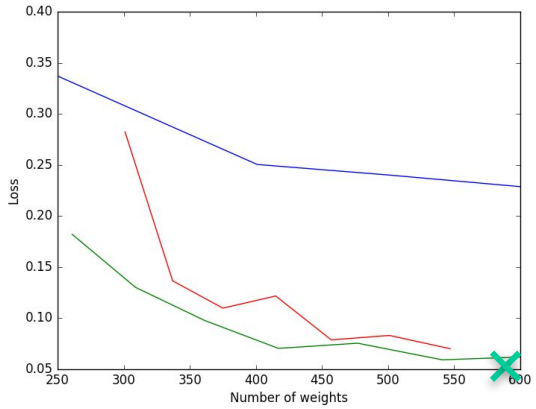

Original 51x51 image:
2601 gray level values.

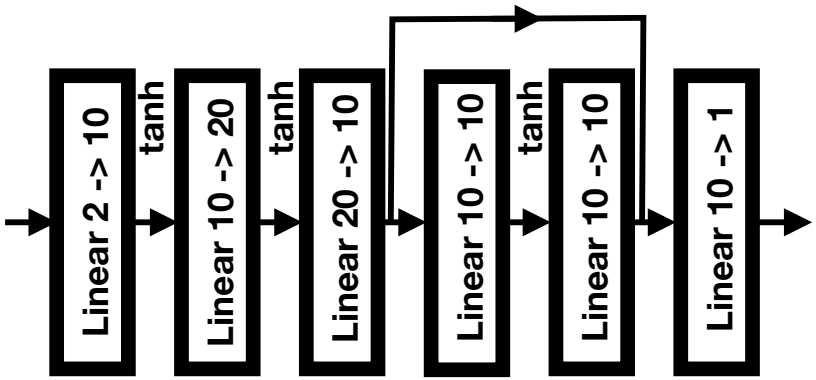



MLP 10/20/10 Interpolation:
471 weights, loss 6.43e-02.



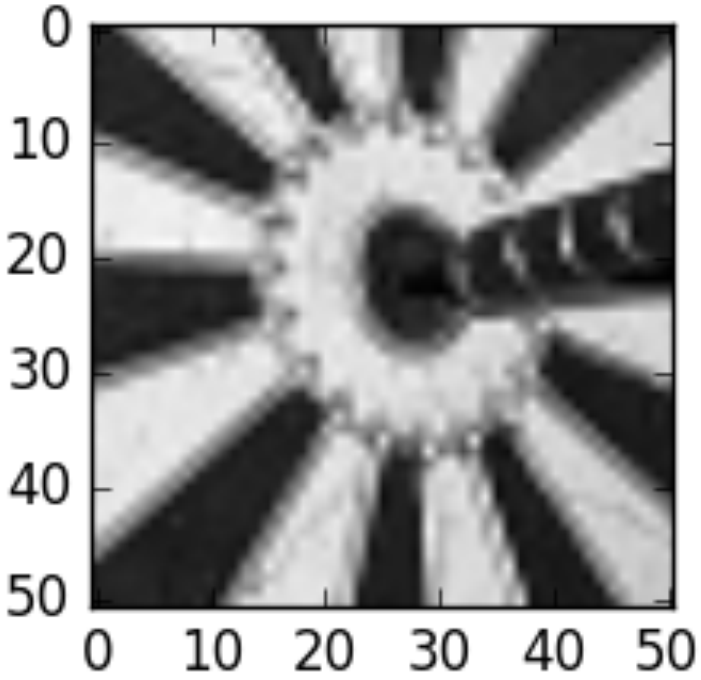

Resnet 10/20/10/10 Interpolation:
581 weights, loss 5.30e-2.



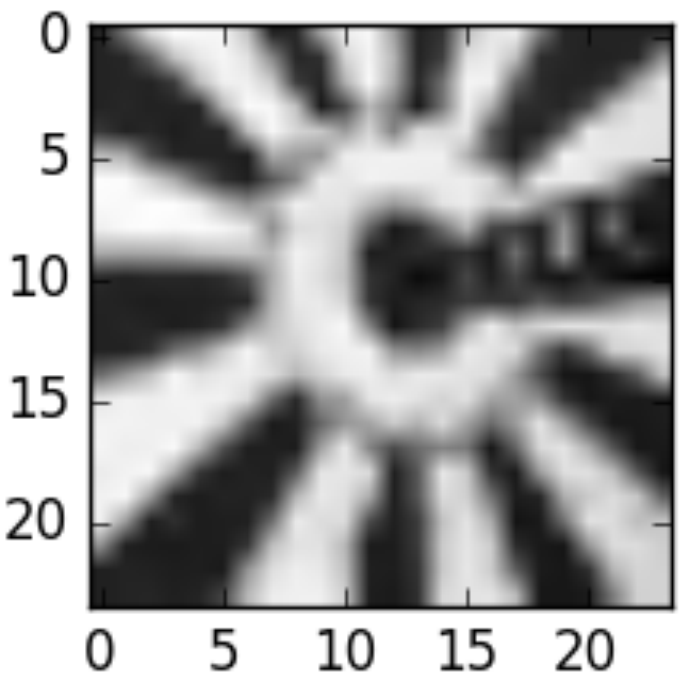




—> Adding a ResNet layer yields a further small improvement.

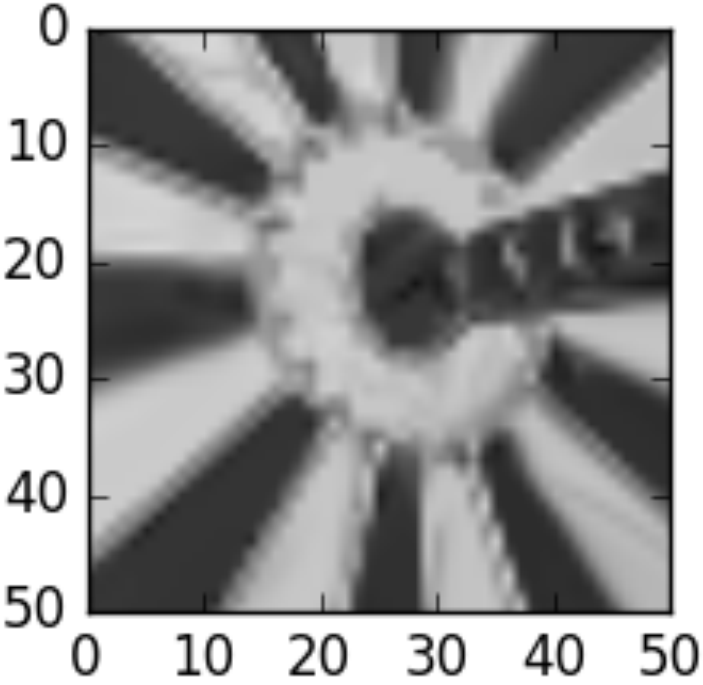
# Adding a ResNet Layer




Original 51x51 image:
2601 gray level values.




MLP 10/20/10 Interpolation:
471 weights, loss 1.95e-02.

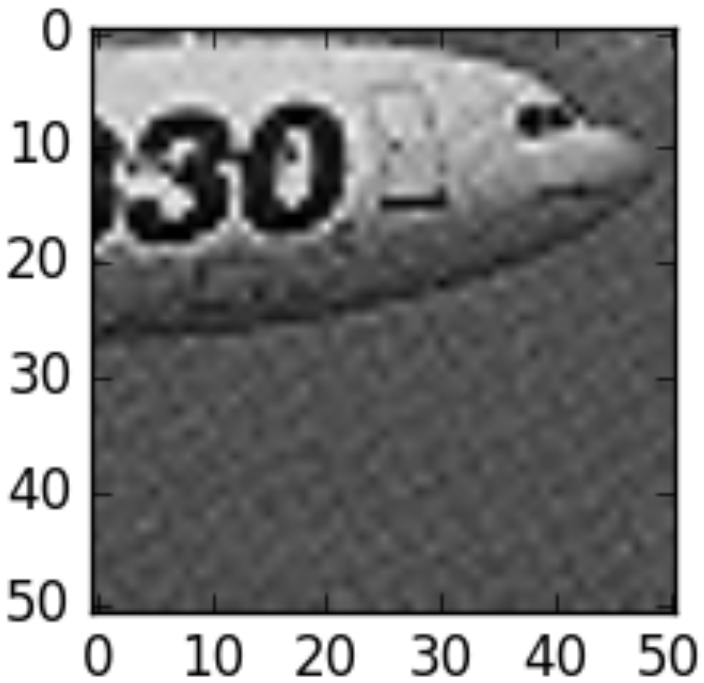



Resnet 10/20/10/10 Interpolation:
581 weights, loss 1.36e-2.

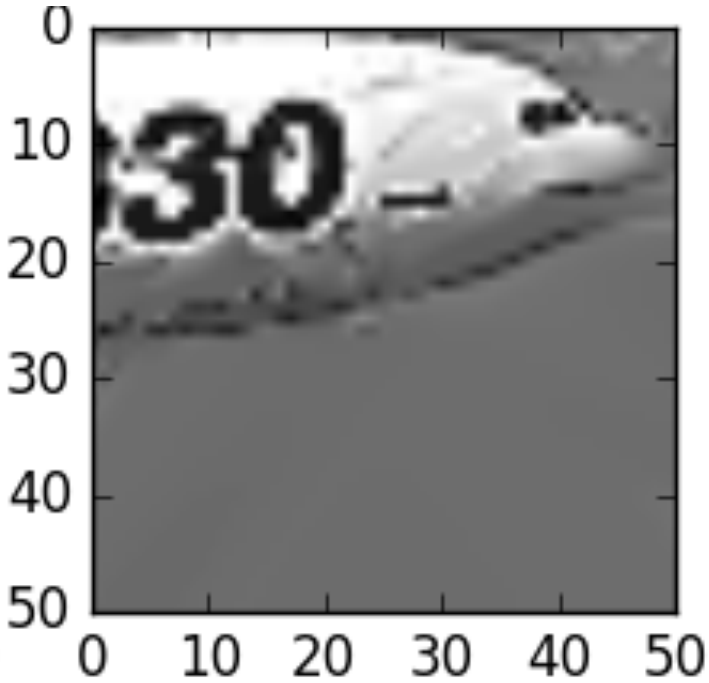
- Relatively small improvement in this case.
- We will see a different behavior for large networks.
- The problem is probably too small.

—> Networks can behave very differently for small and large problems!

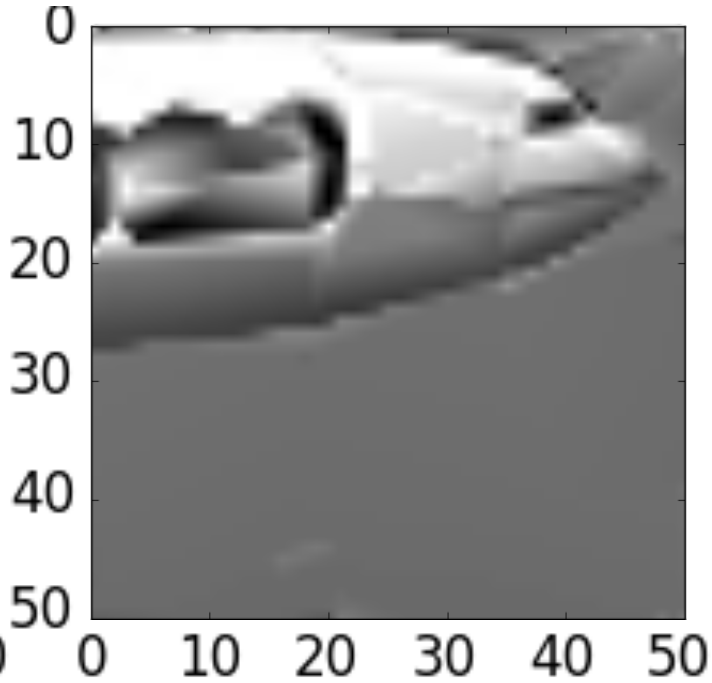
# Tanh vs ReLu



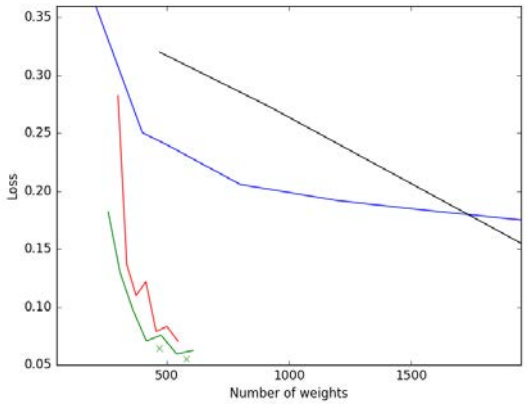
Original 51x51 image:
2601 gray level values.



MLP 10/20/10 Interpolation:
Tanh, loss 6.43e-02.



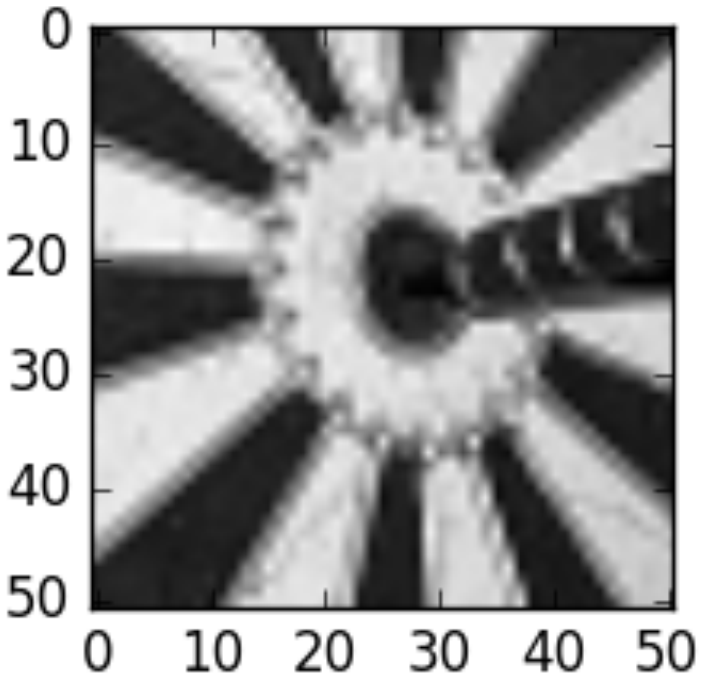
MLP 10/20/10 Interpolation:
ReLU, loss 3.07e-1.



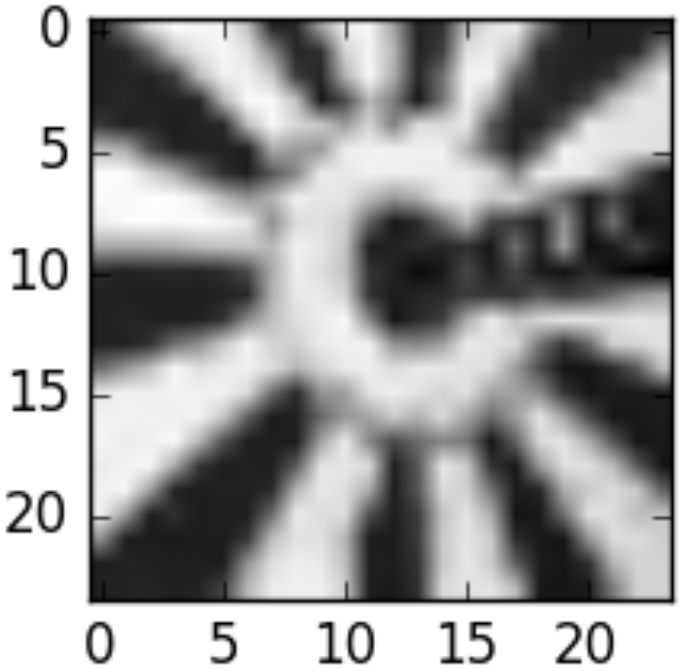

Tanh, 1 layers
Tanh, 2 layers
Tanh, 3 layers
ReLU, 3 layers
Tanh, 4 layers

—> Tanh works better than ReLU in this case.

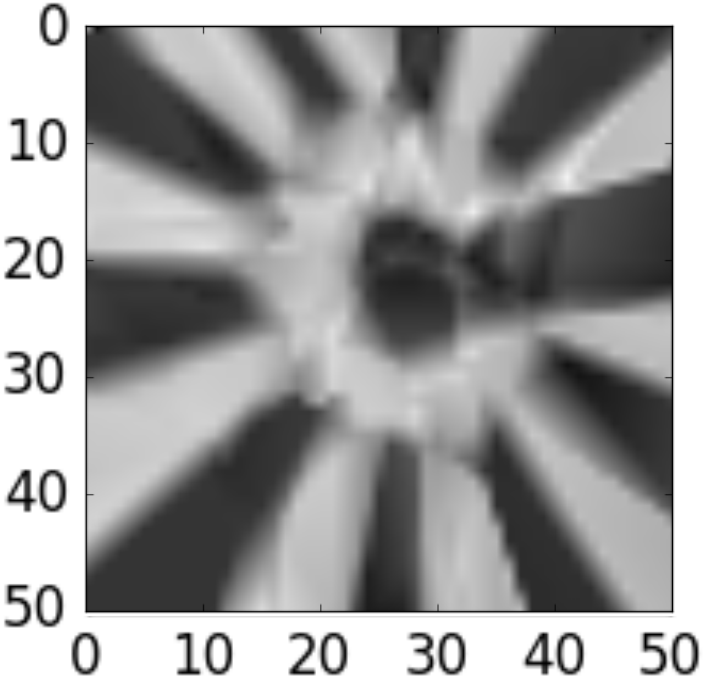
# Tanh vs ReLu




Original 51x51 image:
2601 gray level values.




MLP 10/20/10 Interpolation:
tanh, loss 1.95e-02.

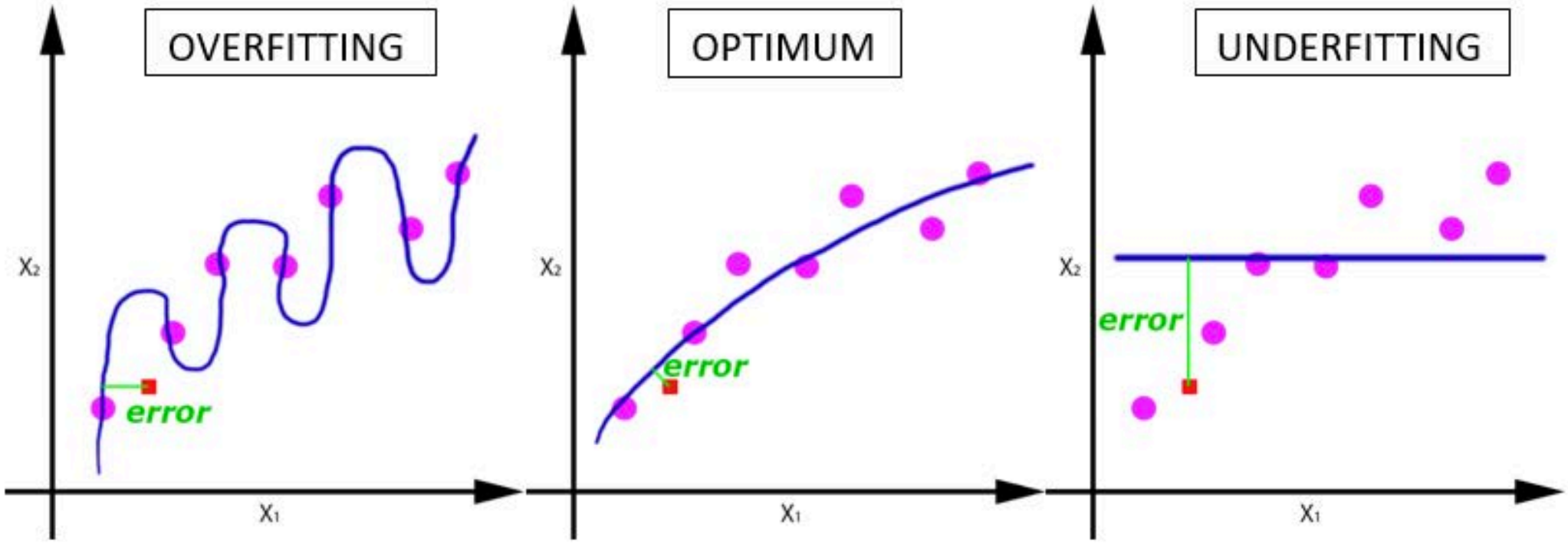



MLP 10/20/10 Interpolation:
relu, loss 7.21e-2.

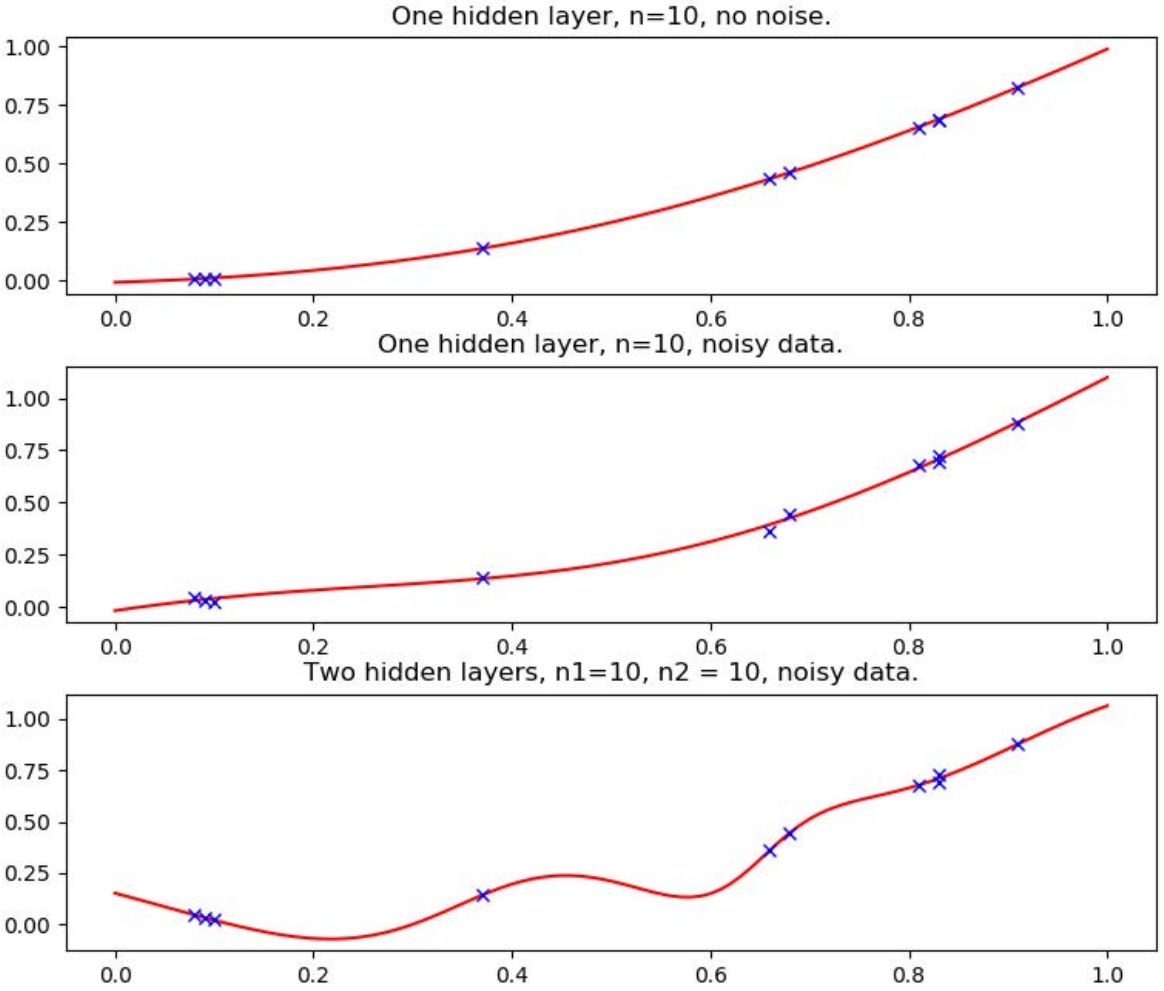
- Tanh works better than ReLU in this case.
- ReLU is widely credited with eliminating the vanishing gradient problem in large networks.

—> There is no substitute for experimentation!

# Overfitting vs Underfitting

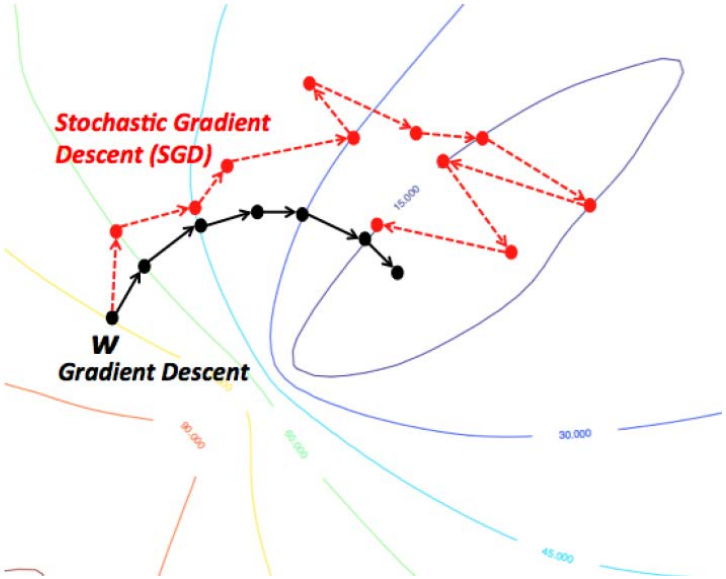


# Overfitting




- Multi-layer perceptrons have great descriptive power and can approximate almost any reasonable function.
- But they can also overfit.
- There is no truly automated way to set the number and width of the layers.

# Reminder: Stochastic Gradient Descent




$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

$$\text{Gradient descent: } \mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \sum_{n=1}^{N} \nabla E_n(\mathbf{w}^{\tau}) \ .$$

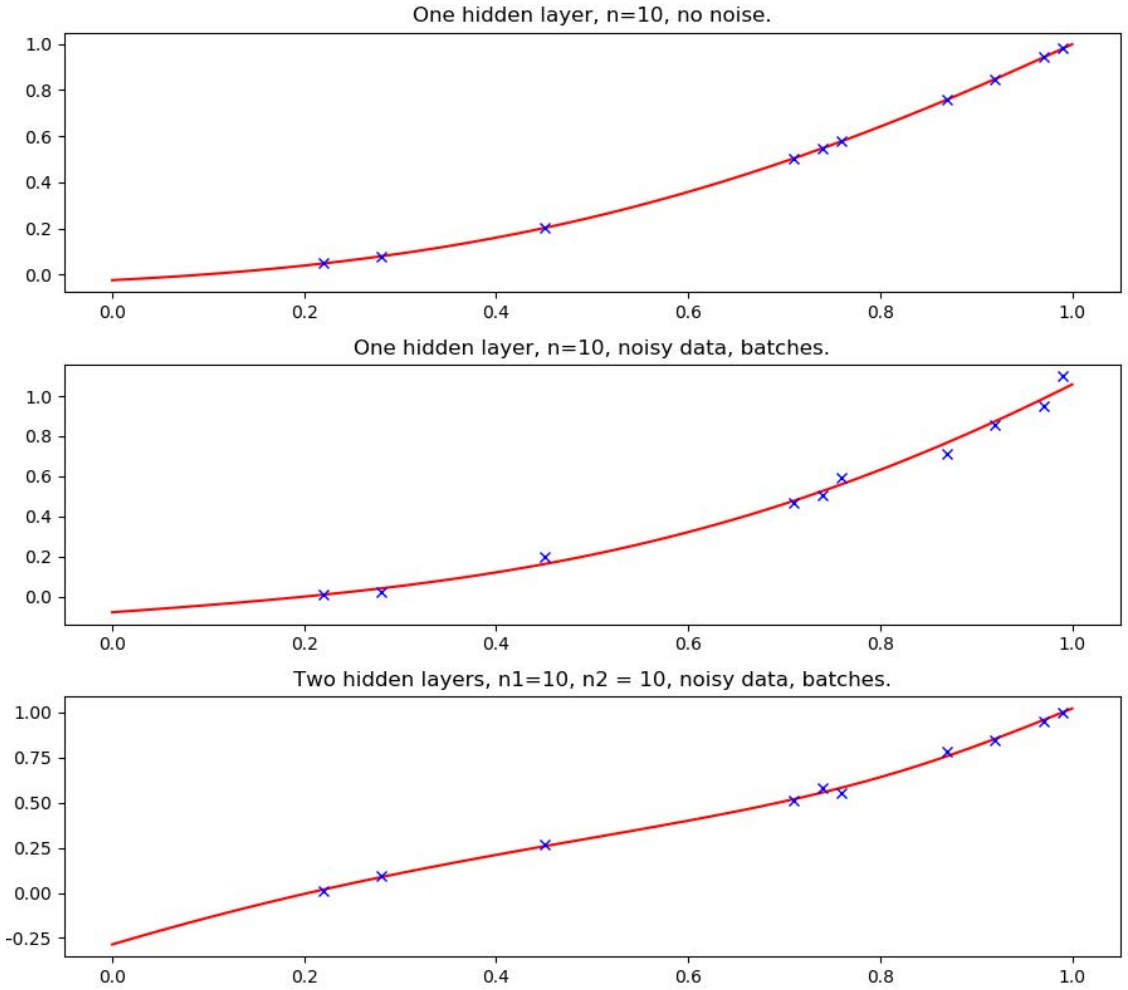
$$\text{Stochastic descent: } \mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \sum_{n \in B^{\tau}} \nabla E_n(\mathbf{w}^{\tau}) \ ,$$

where $B^{\tau}$ represents a different randomly chosen set of indices at each iteration, also known as a mini-batch.

Randomly choosing batches

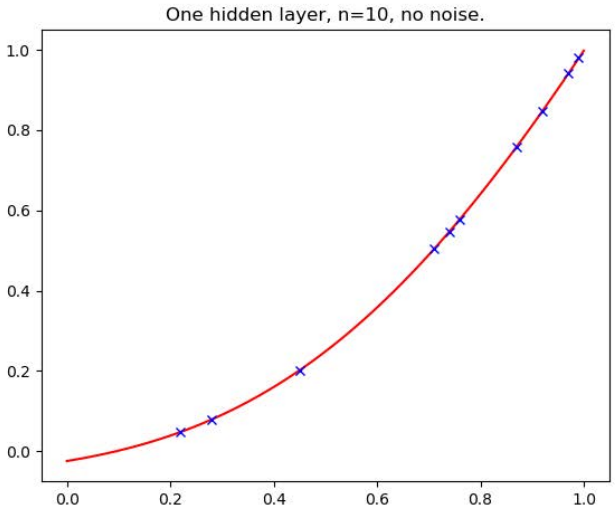
- helps reduce the chances of falling into local minima,
- makes the computation possible on GPUs even when dealing with LARGE databases.

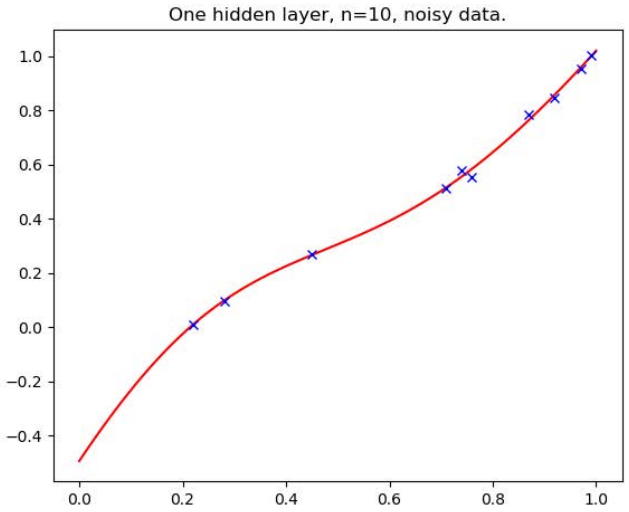
# Using Mini-Batches

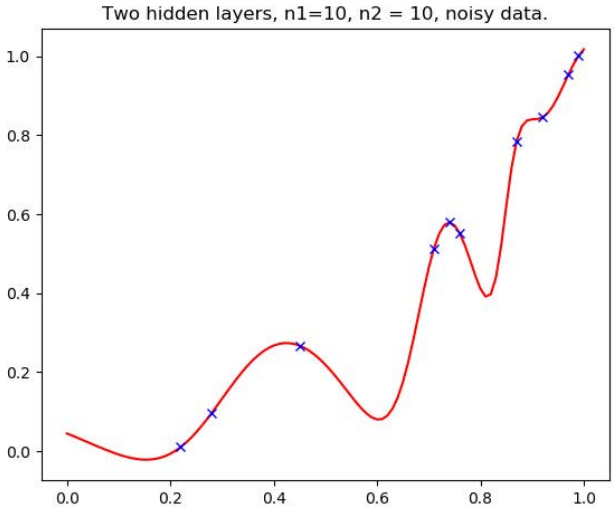


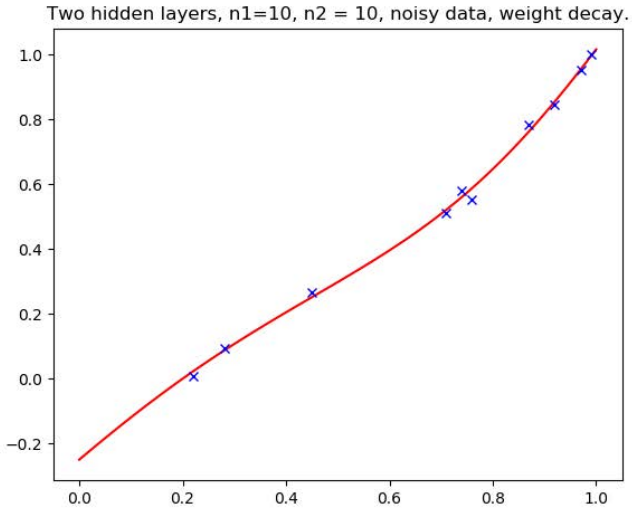

- The element of randomness prevents overfitting.
- No principled way to set the size of the mini-batches to achieve this result.

# Weight Decay



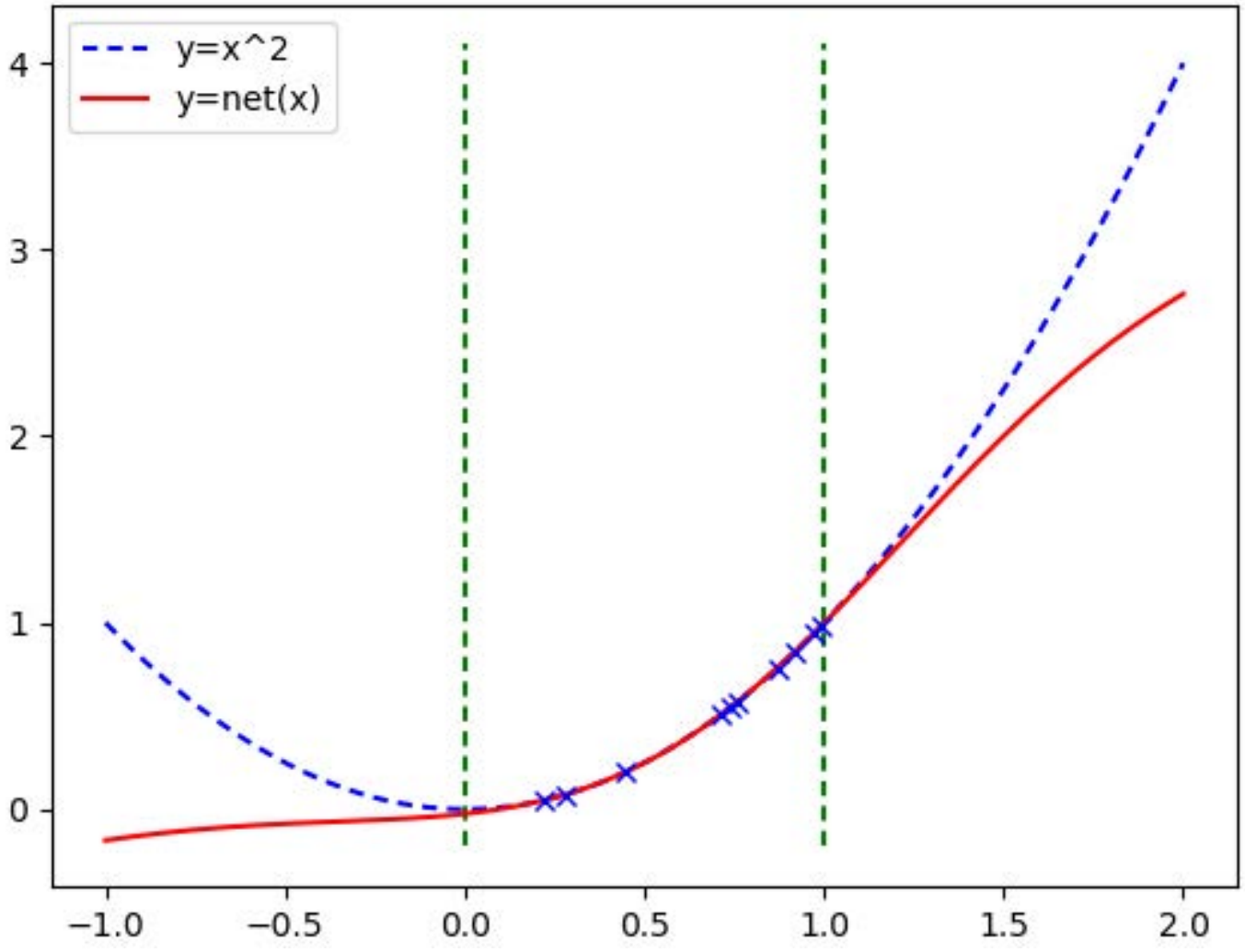




$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w}) + \lambda \|\mathbf{w}\|^2$$

How large should λ be?

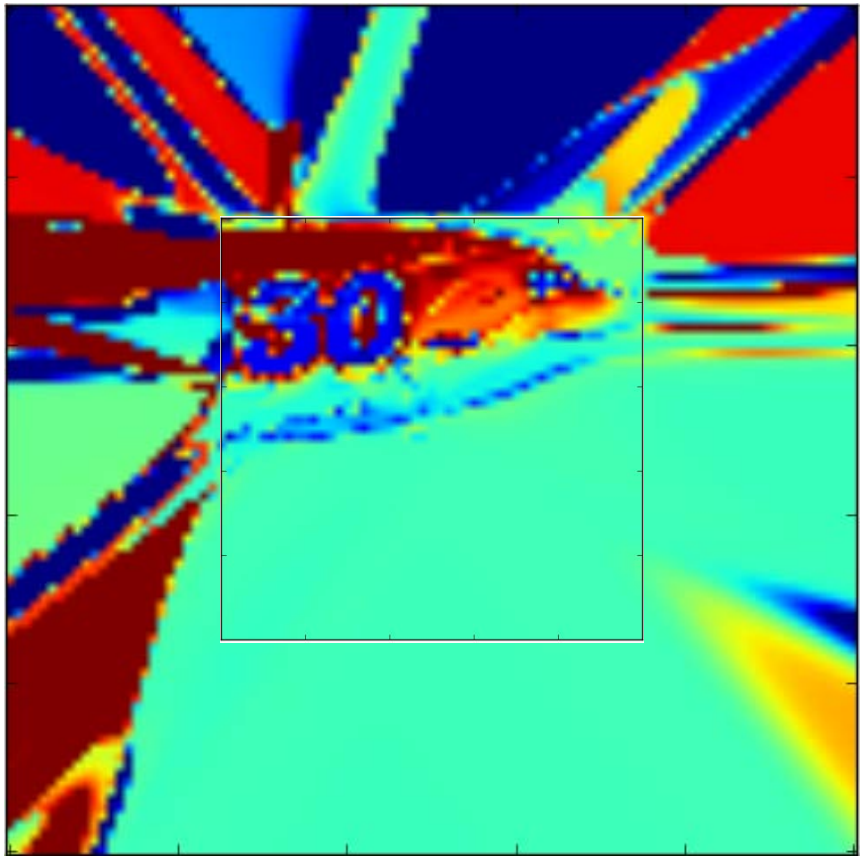
—>Use validation data as usual.

# Interpolation vs Extrapolation




—> Perceptrons do **not** extrapolate well

# Interpolation vs Extrapolation



—> Perceptrons do **not** extrapolate well

# Reminder: Learning the Weights

- Given a training set be $\{(\mathbf{x}_n, [t_n^1, \ldots, t_n^K])_{1 \leq n \leq N}\}$ where $t_n^k \in \{0,1\}$ is the probability that sample $\mathbf{x}_n$ belongs to class k, we write:

$$\mathbf{y}_n = f_{\mathbf{w}}(\mathbf{x}_n) \in R^K$$

$$p_n^k = \frac{\exp(\mathbf{y}_n[k])}{\sum_j \exp(\mathbf{y}_n[j])}$$

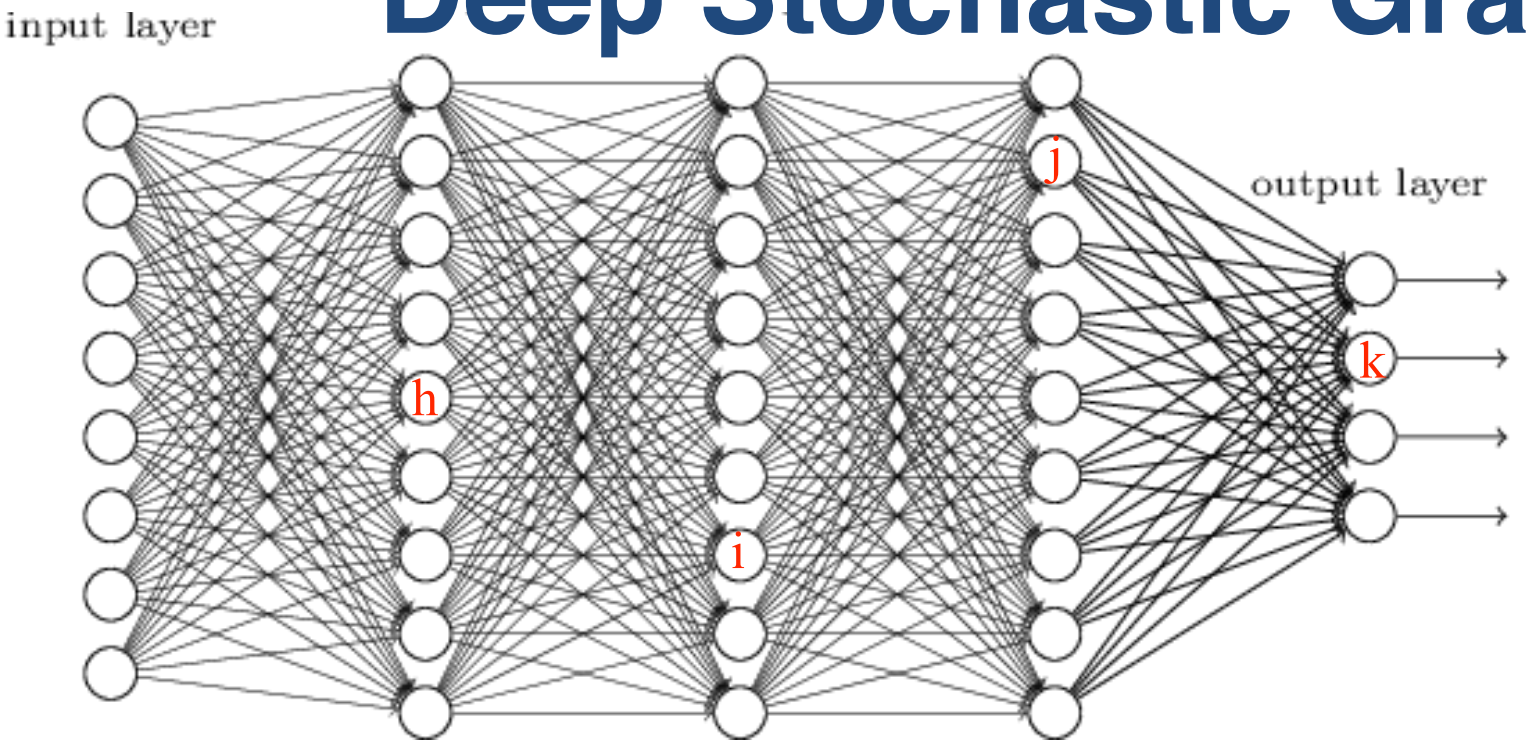
- We want to minimize the cross entropy

$$E(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} E_n(\mathbf{w}) \ ,$$

$$E_n(\mathbf{w}) = - \sum t_n^k \ln(p_n^k) \ ,$$

with respect to the coefficients of $\mathbf{w}$.

# Deep Stochastic Gradient




$$E_n(\mathbf{w}) = -\sum_{k=1}^{K} t_n^k \ln(p_n^k) \,,$$
$$= L_n(y_1, \ldots y_K)$$
$$= L_n(a_1, \ldots a_K)$$

$x_l$

$$z_h = \sigma(a_h) \qquad z_i = \sigma(a_i) \qquad z_j = \sigma(a_j) \qquad y_k = a_k$$
$$a_h = \sum_l w_{hl} x_l \qquad a_i = \sum_h w_{ih} z_h \qquad a_j = \sum_i w_{ji} z_i \qquad a_k = \sum_j w_{kj} z_j$$

$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w})$$

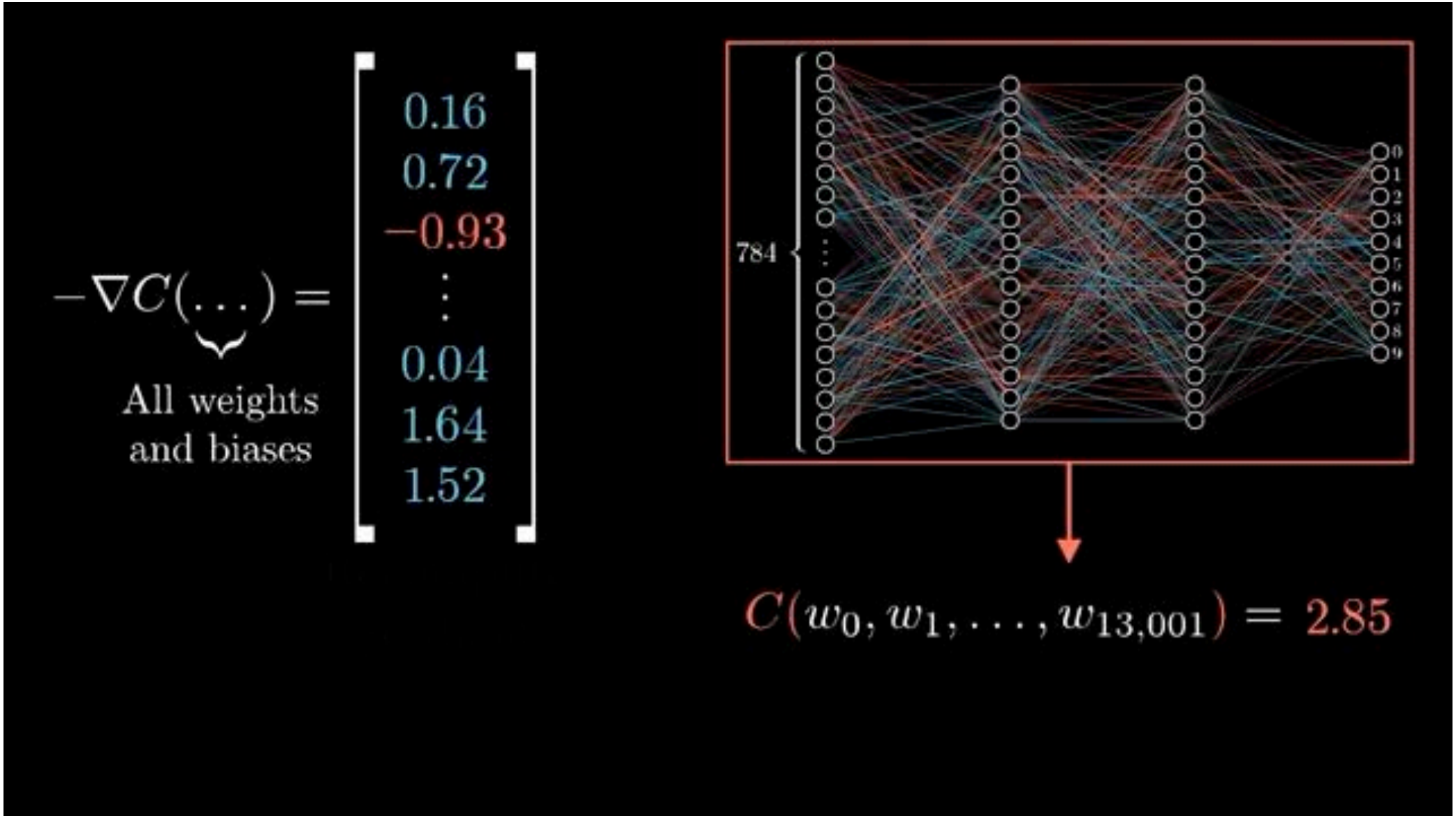
$$\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \sum_{n \in B^{\tau}} \nabla E_n(\mathbf{w}^{\tau})$$

$$\mathbf{w} = [w_{ji}]$$

$$\nabla E_n = \left[ \frac{\delta E_n}{\delta w_{ji}} \right]$$

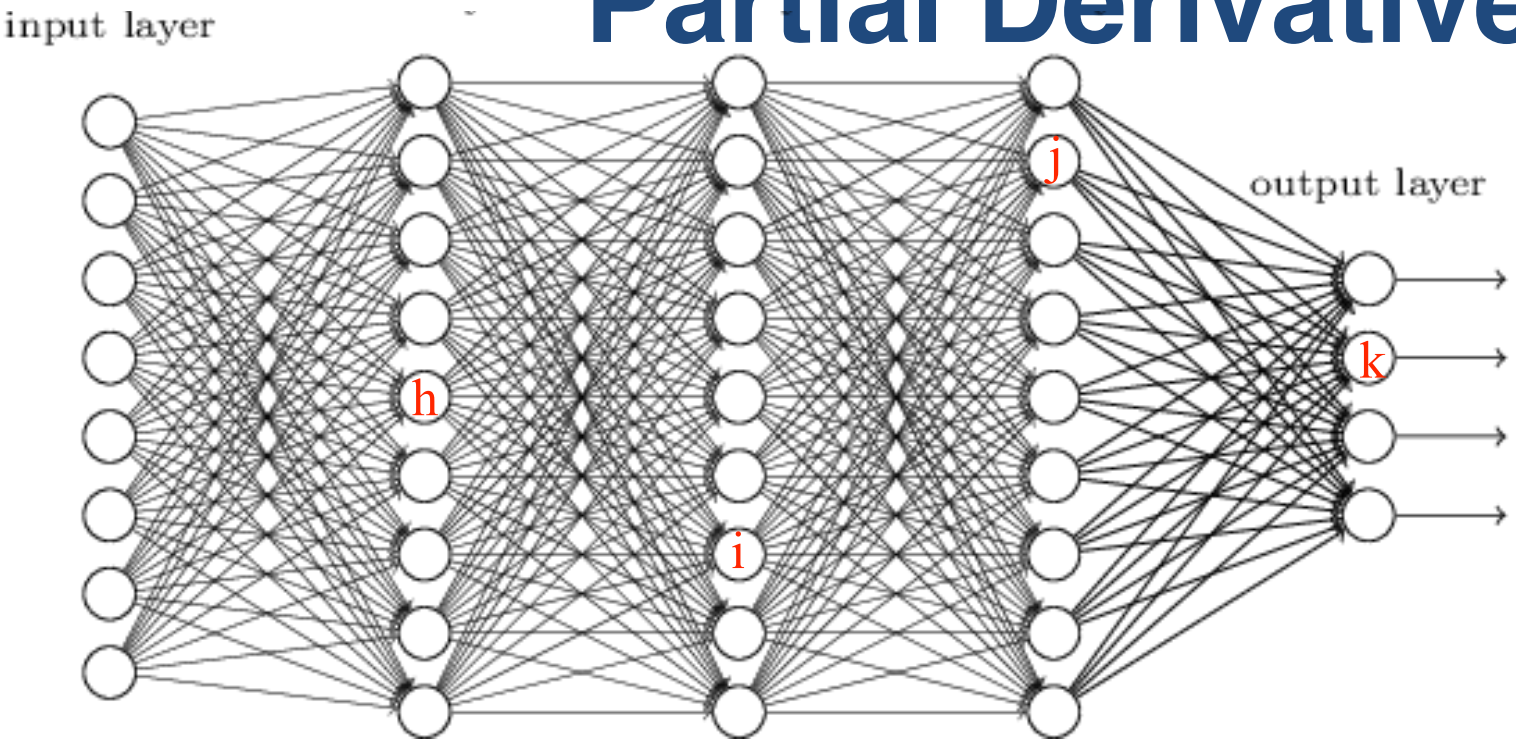
But how do we compute all these derivatives?

# Back Propagation




3Blue1Brown: https://www.youtube.com/watch?v=Ilg3gGewQ5U

# Partial Derivatives




$$E_n = L_n(a_1, \ldots, a_K)$$

$$z_h = \sigma(a_h) \qquad z_i = \sigma(a_i) \qquad z_j = \sigma(a_j) \qquad y_k = a_k$$

$x_l$

$$a_h = \sum_l w_{hl} x_l \qquad a_i = \sum_h w_{ih} z_h \qquad a_j = \sum_i w_{ji} z_i \qquad a_k = \sum_j w_{kj} z_j$$

Hidden vals

Activations

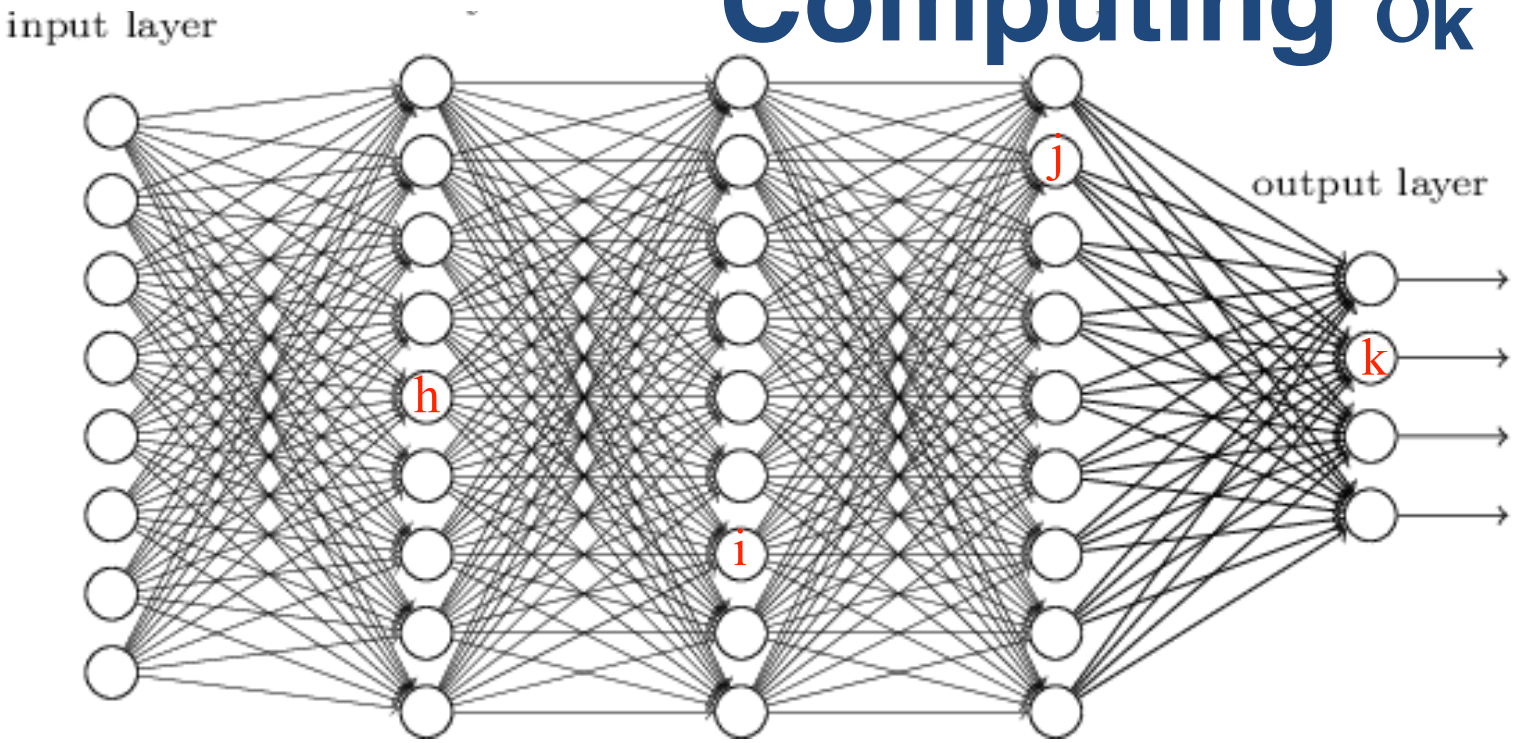
$$\frac{\delta E_n}{\delta w_{ji}} = \frac{\delta E_n}{\delta a_j} \frac{\delta a_j}{\delta w_{ji}}$$

$$= \delta_j z_i$$

$$\text{with } \delta_j \equiv \frac{\delta E_n}{\delta a_j}$$

—> Given the $\delta_j$ we can compute all partial derivatives.

# Computing $\delta_k$




$$E_n = L_n(a_1, \ldots, a_K)$$

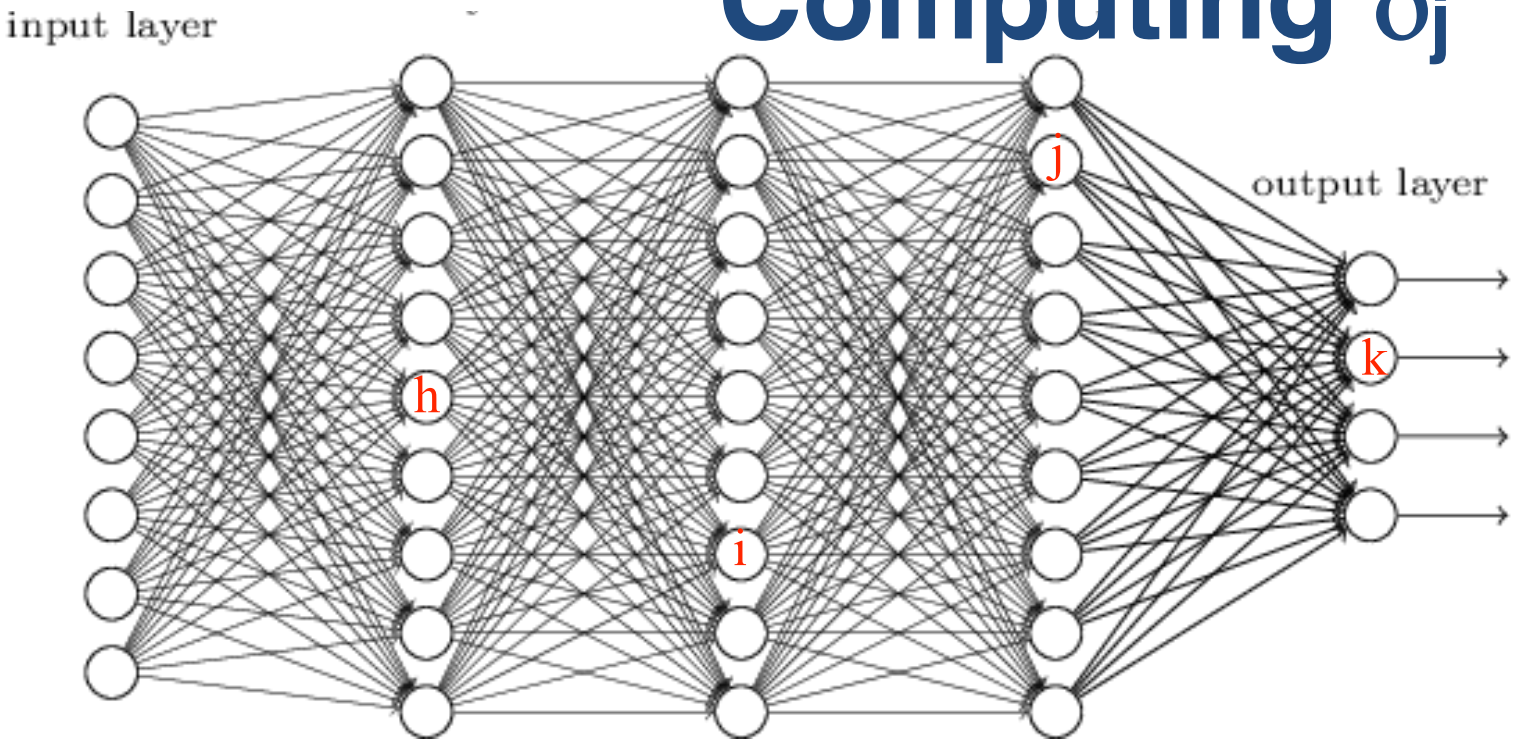
$$z_h = \sigma(a_h) \qquad z_i = \sigma(a_i) \qquad z_j = \sigma(a_j) \qquad y_k = a_k$$

$x_l$

$$a_h = \sum_l w_{hl} x_l \qquad a_i = \sum_h w_{ih} z_h \qquad a_j = \sum_i w_{ji} z_i \qquad a_k = \sum_j w_{kj} z_j$$

Output layer: $\delta_k = \dfrac{\delta E_n}{\delta a_k}$ No $w_{ij}$ here.

# Computing $\delta_j$




$$E_n = L_n(a_1, \ldots, a_K)$$

$$z_h = \sigma(a_h) \qquad z_i = \sigma(a_i) \qquad z_j = \sigma(a_j)$$

$x_l$

$$a_h = \sum_l w_{hl} x_l \qquad a_i = \sum_h w_{ih} z_h \qquad a_j = \sum_i w_{ji} z_i \qquad y_k = \sum_j w_{kj} z_j$$

Other layers: $\delta_j = \dfrac{\delta E_n}{\delta a_j} = \sum_k \dfrac{\delta E_n}{\delta a_k} \dfrac{\delta a_k}{\delta a_j}$ $\qquad a_k = \sum_j w_{kj} \sigma(a_j)$

$$= \sigma'(a_j) \sum_k w_{kj} \delta_k$$

# Back Propagation

Forward pass:

$$\forall h \ , \ a_h = \sum_l w_{hl} x_l \ , \ z_h = \sigma(a_h)$$

$$\forall i \ , \ a_i = \sum_h w_{ih} z_h \ , \ z_i = \sigma(a_i)$$

$$\forall j \ , \ a_j = \sum_i w_{ji} z_i \ , \ z_j = \sigma(a_j)$$

$$\forall k \ , \ a_k = \sum_j w_{kj} z_j$$

Backward pass:

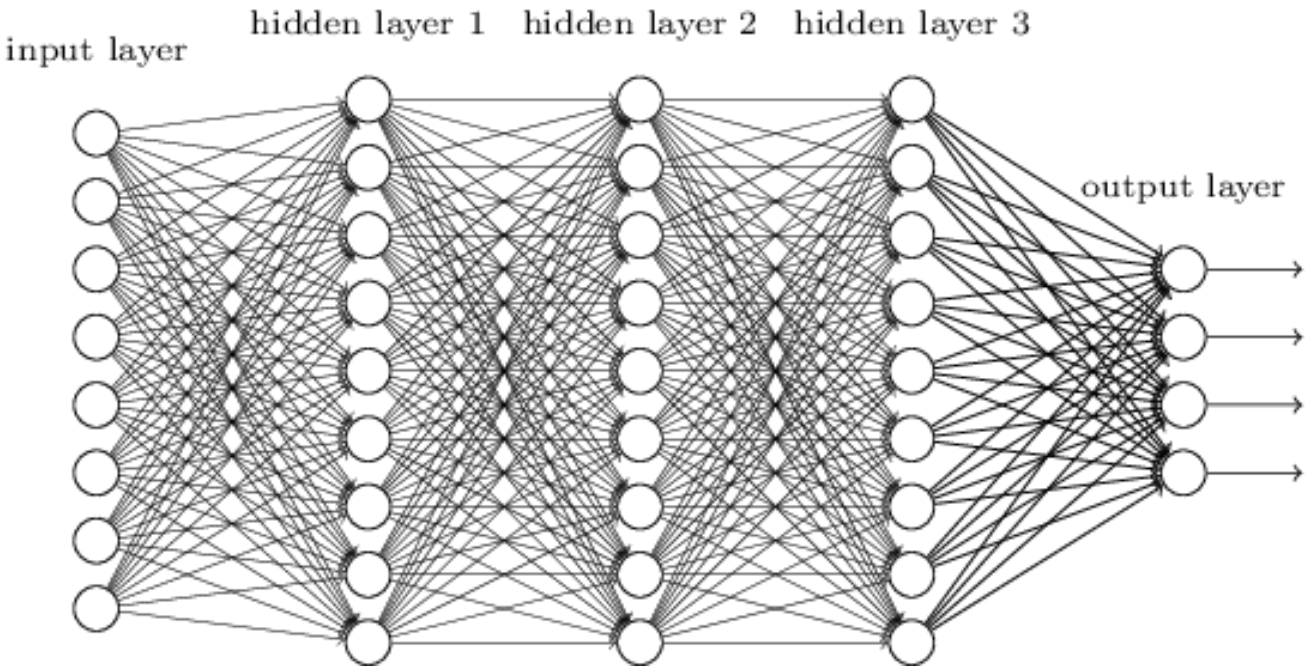
$$\forall k \ , \ \delta_k = \frac{\delta E_n}{\delta a_k}$$

$$\forall j \ , \ \delta_j = \sigma'(a_j) \sum_k w_{kj} \delta_k$$

$$\forall i \ , \ \delta_i = \sigma'(a_i) \sum_j w_{ji} \delta_j$$

$$\forall h \ , \ \delta_h = \sigma'(a_h) \sum_j w_{ih} \delta_h$$

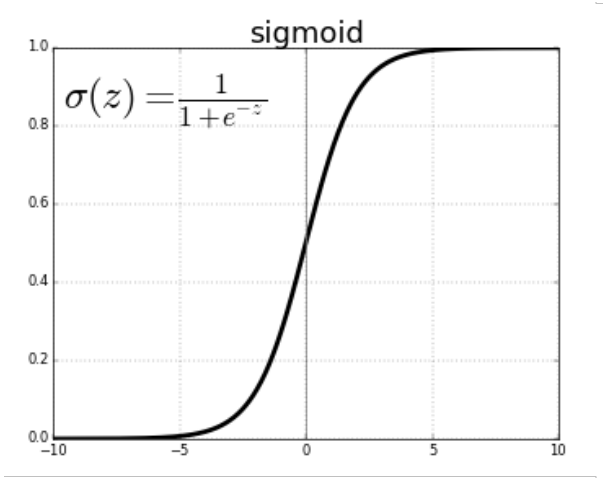
# Back Propagation

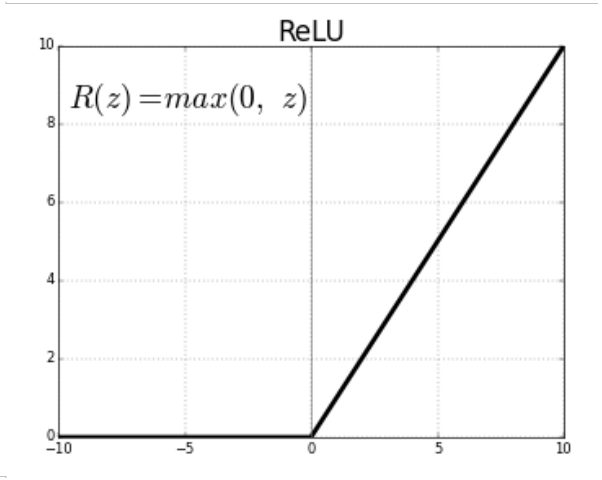



$$\begin{aligned} \mathbf{h}_1 &= \sigma_1(\mathbf{W}_1\mathbf{x}_1 + \mathbf{b}_1) \\ \mathbf{h}_2 &= \sigma_2(\mathbf{W}_2\mathbf{h}_2 + \mathbf{b}_2) \\ &\cdots \\ \mathbf{y} &= \sigma_n(\mathbf{W}_n\mathbf{h}_n + \mathbf{b}_n) \end{aligned}$$

- Both the loss and its derivatives can be computed using simple and regular operations.
- Can be implemented on GPUs and runs much faster than on CPUs.

# Vanishing and Exploding Gradients



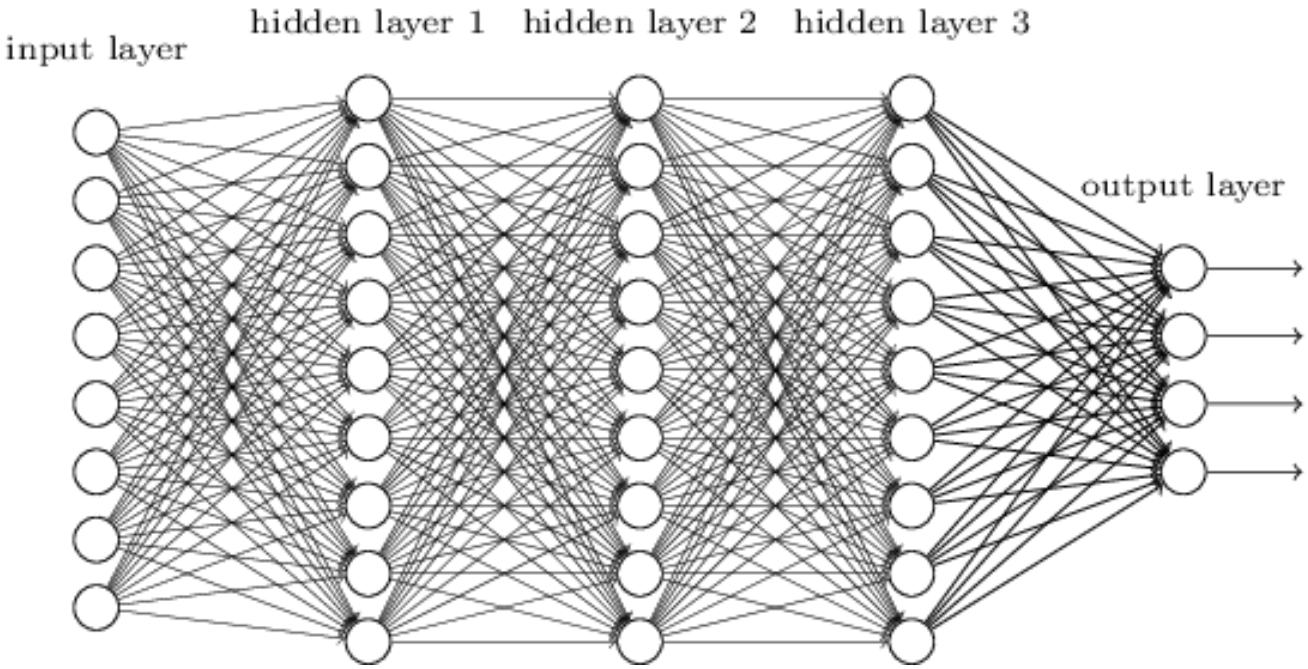

$$\forall i\ ,\ \delta_i = \sigma'(a_i) \sum_j w_{ji}\delta_j$$

In a very deep network, the derivatives at all levels are multiplied by each other:

- As $\sigma(a_i)$ approaches zero, so does $\delta_i$ and the gradients in the lower layers are lost. —> Vanishing gradients.
- If the $\delta_i$ become large in several consecutive layers, their product can become exponentially large —> Exploding gradients.

The problem can be mitigated by using ReLU, clipping the gradients, relying on gated or resnet-type architectures, …

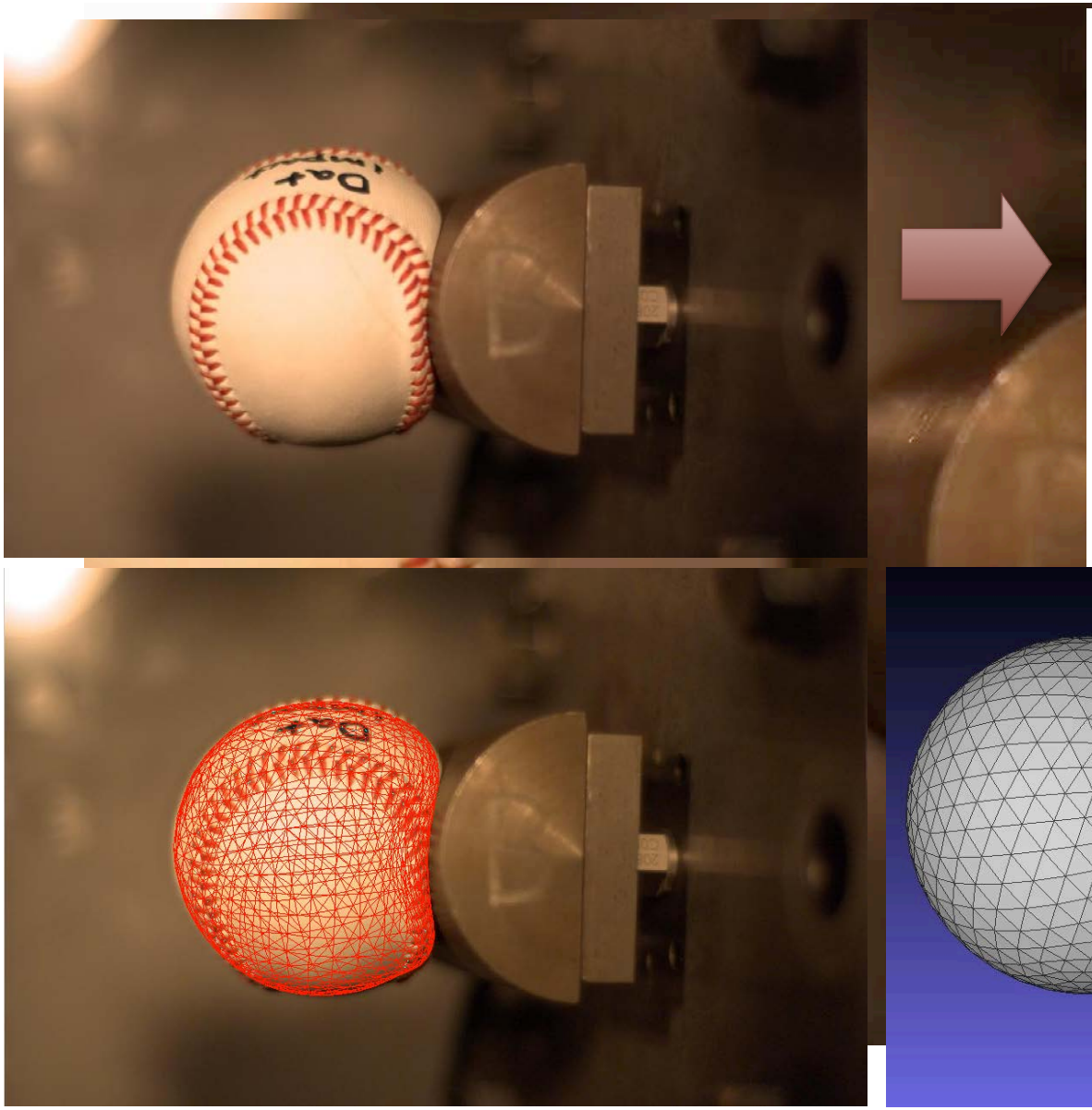
# Back Propagation Works!



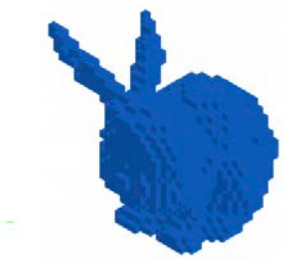
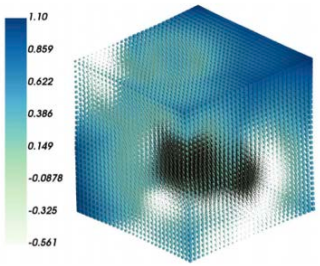

$$
\begin{aligned}
\mathbf{h}_1 &= \sigma_1(\mathbf{W}_1\mathbf{x}_1 + \mathbf{b}_1) \\
\mathbf{h}_2 &= \sigma_2(\mathbf{W}_2\mathbf{h}_2 + \mathbf{b}_2) \\
&\cdots \\
\mathbf{y} &= \sigma_n(\mathbf{W}_n\mathbf{h}_n + \mathbf{b}_n)
\end{aligned}
$$

- Both the loss and its derivatives can be computed using simple and regular operations.
- Can be implemented on GPUs and runs much faster than on CPUs.
- Vanishing and exploding gradients can be handled through a number of methods, the simplest of which is to use reLU to introduce the non-linearities.

# Optional: Deforming 3D Surfaces



# Optional: 3D Surface Representations

| | Voxels | Explicit surface mesh | Point sets | Continuous implicit fields |
|---|---|---|---|---|
| |  |  |  |   |
| High frequency details? | -- | ++ | + | ++ |
| Arbitrary topology? | + | - | + | ++ |
| Regularity? | + | + | - | ++ |

There are many applications at which explicit representations excel:

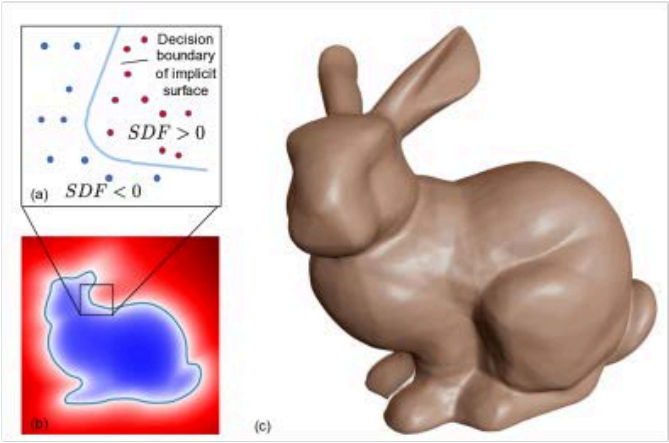
- High-quality rendering in computer graphics.
- Precise modeling of biological structures from biomedical data.
- Computational fluid dynamics in computer assisted design.

But:

- Their topology is fixed.
- They are not particularly deep learning friendly.

—> Implicit Surface Representations

# Optional: Signed Distance Fields (SDF)




- Represent a 3D surface S by the zero crossings of a signed distance function

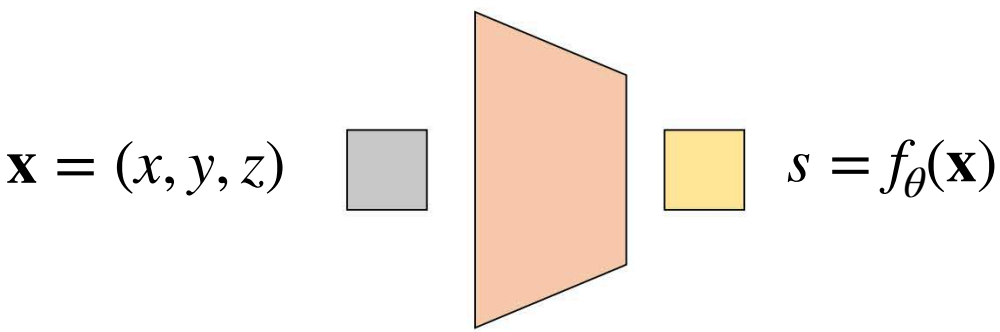
$$f\colon \mathbb{R}^3 \rightarrow \mathbb{R}$$

$$\forall \mathbf{x} \in \mathbb{R}^3,\ f(\mathbf{x}) \text{ is the signed distance to the surface.}$$

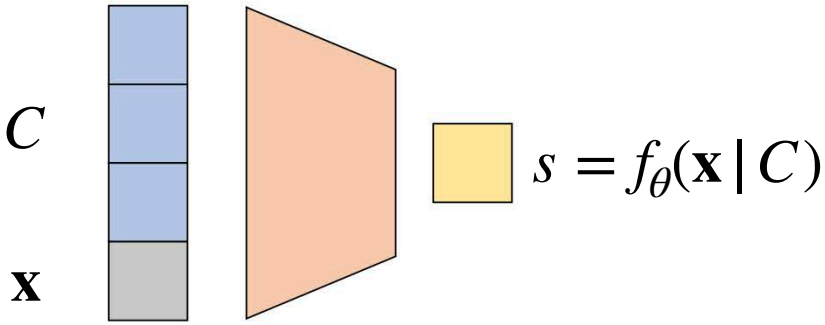
- Such surfaces can easily change topology, which is harder to do with explicit surface representations.

- SDFs have long been appealing in theory but hard to use in practice because it it was necessary to store the 3D values of $f$ in a cube like structure until ….

# Optional: Deep SDF




Single Shape DeepSDF




Coded Shape DeepSDF

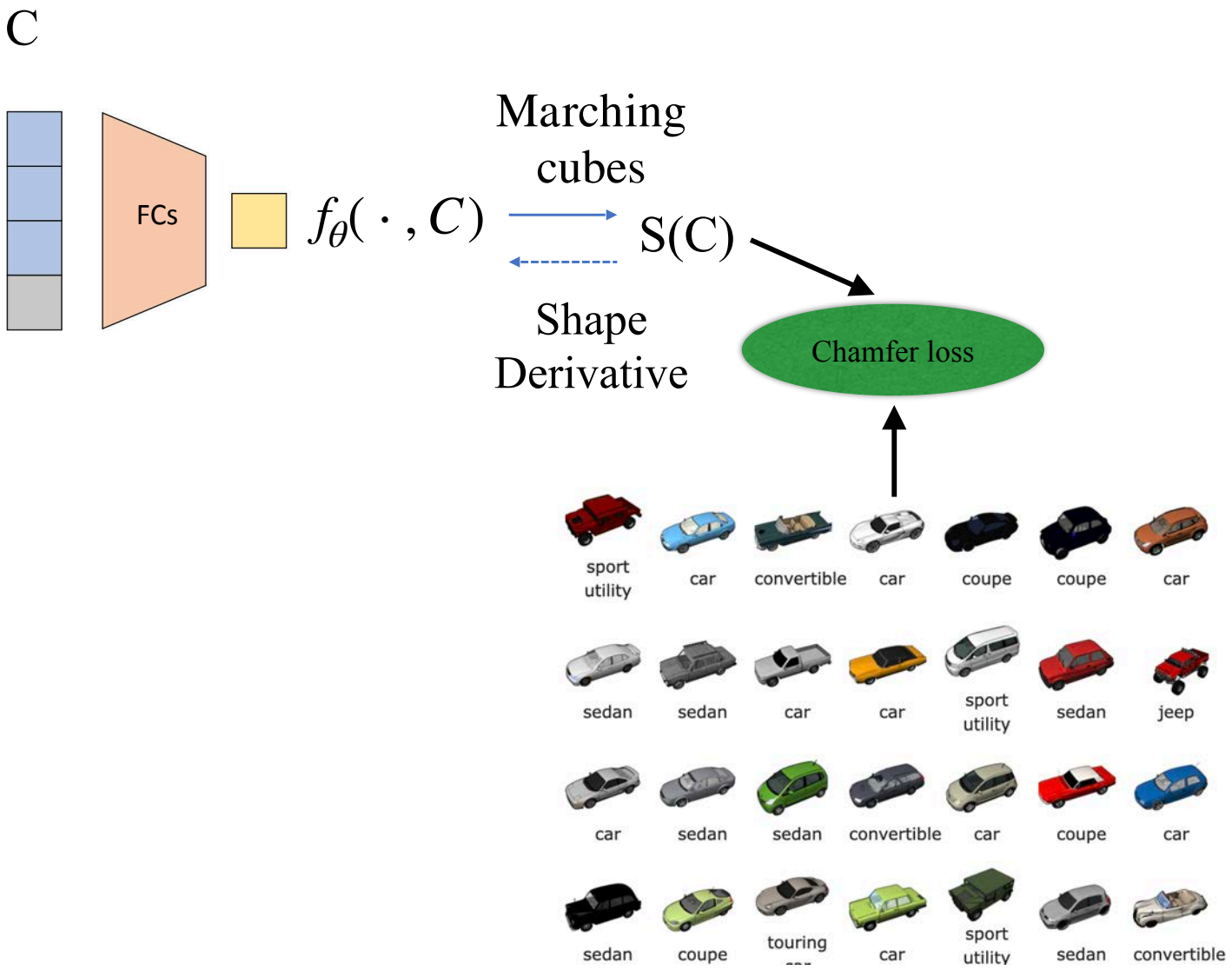
[Park et al., CVPR'19]

C is a latent vector that parameterizes the surface.

# Optional: From Genus 0 to Genus 1

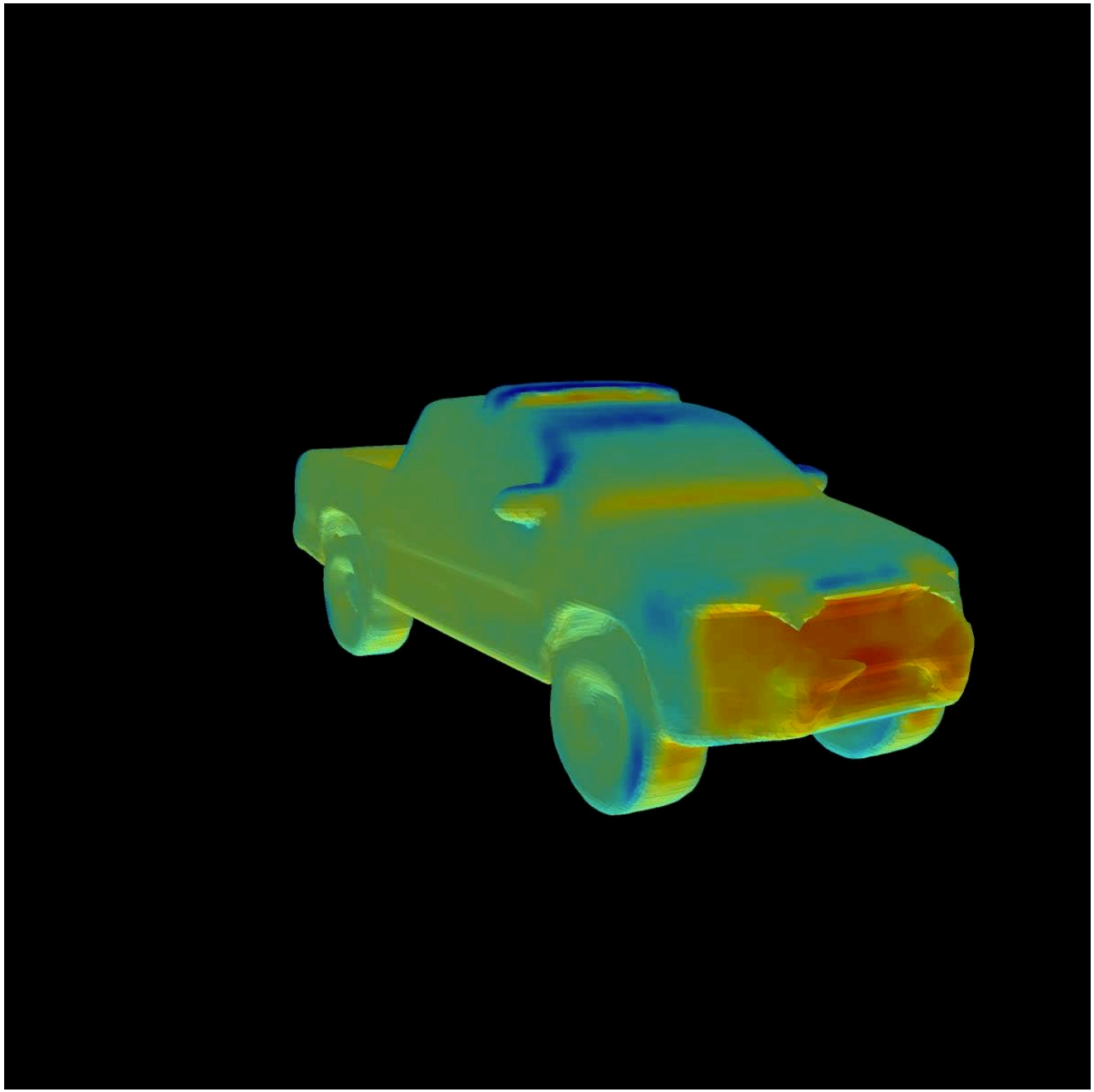
[Remelli et al., NeurIPS'20]

# Optional: Introducing Priors

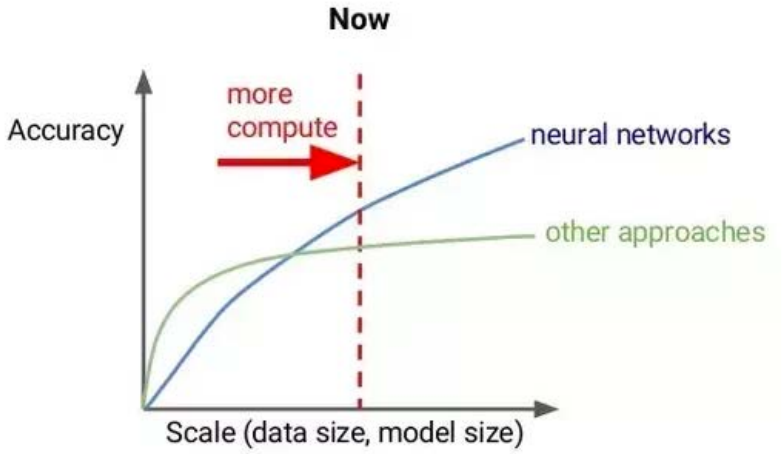



Train an auto-decoder using ShapeNet cars.

# Optional: From Pickup-Truck to Sports Car



# MLPs in Short




- Deep Neural Networks can handle huge training databases.
- When the objective function can be minimized, the results are outstanding.
- There are failure cases and performance is hard to predict.

—> Many questions are still open and there is much theoretical work left to do.