Multi-Layer Perceptrons

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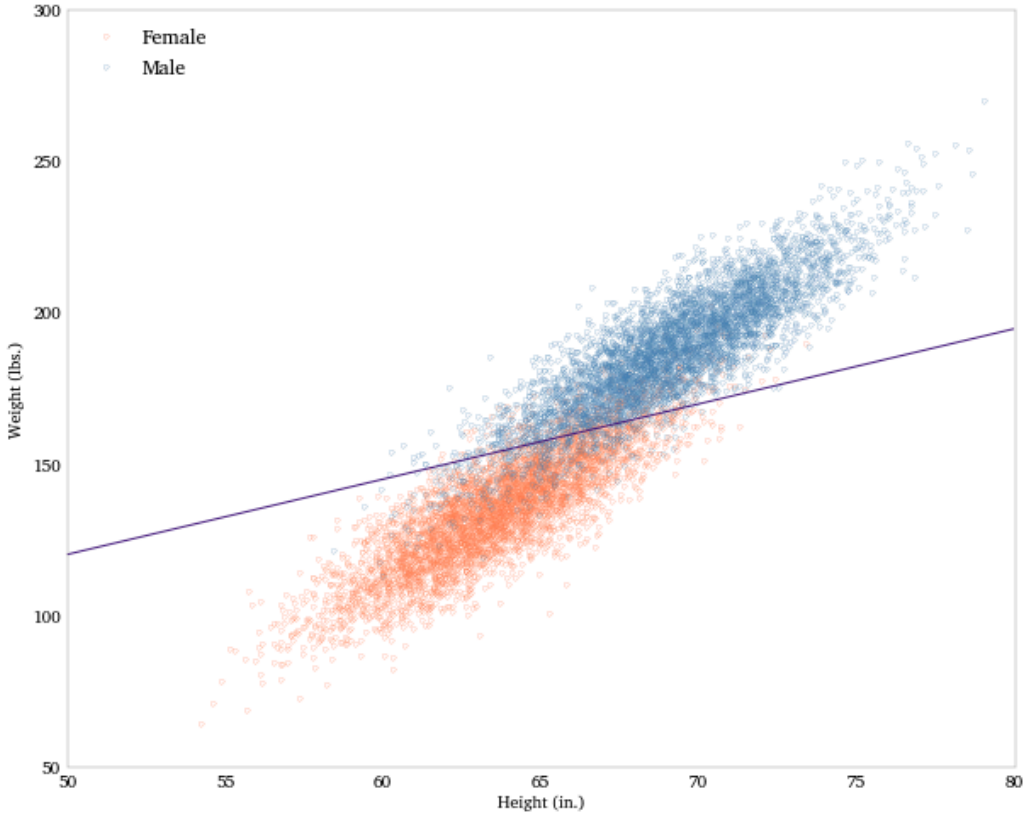
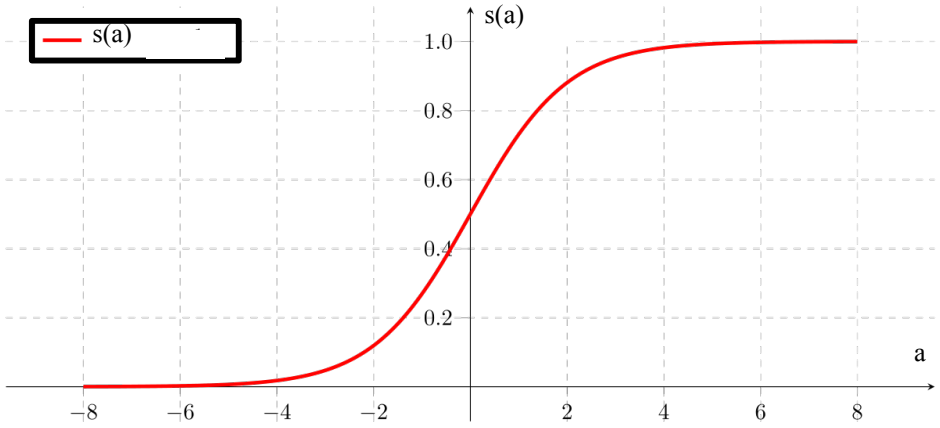
IC-CVLab

Reminder: Logistic Regression



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

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

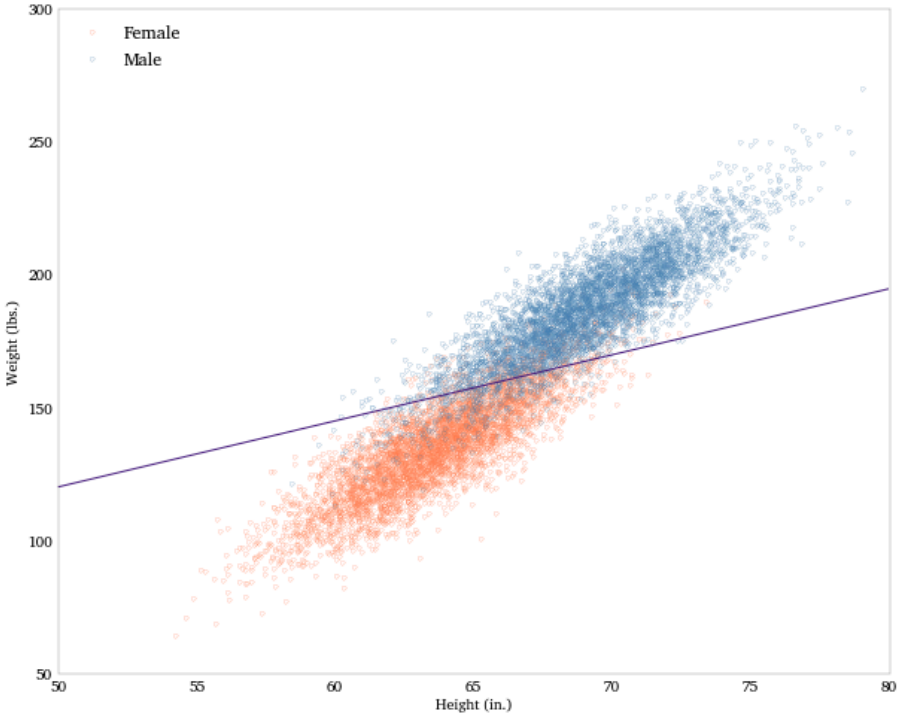


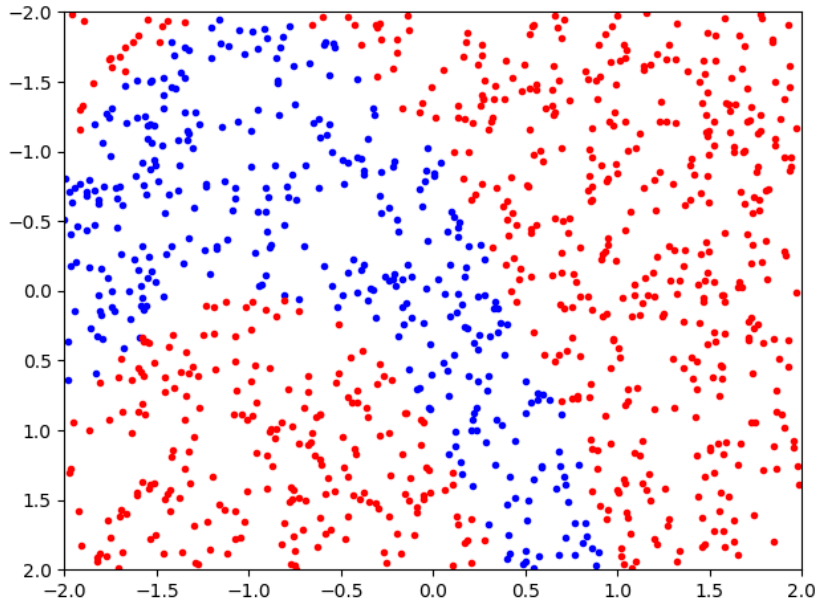
Given a **training** set $\{(\mathbf{x}_n, t_n)_{1 \leq n \leq N}\}$ minimize

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

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

Reminder: Non Separable Distribution



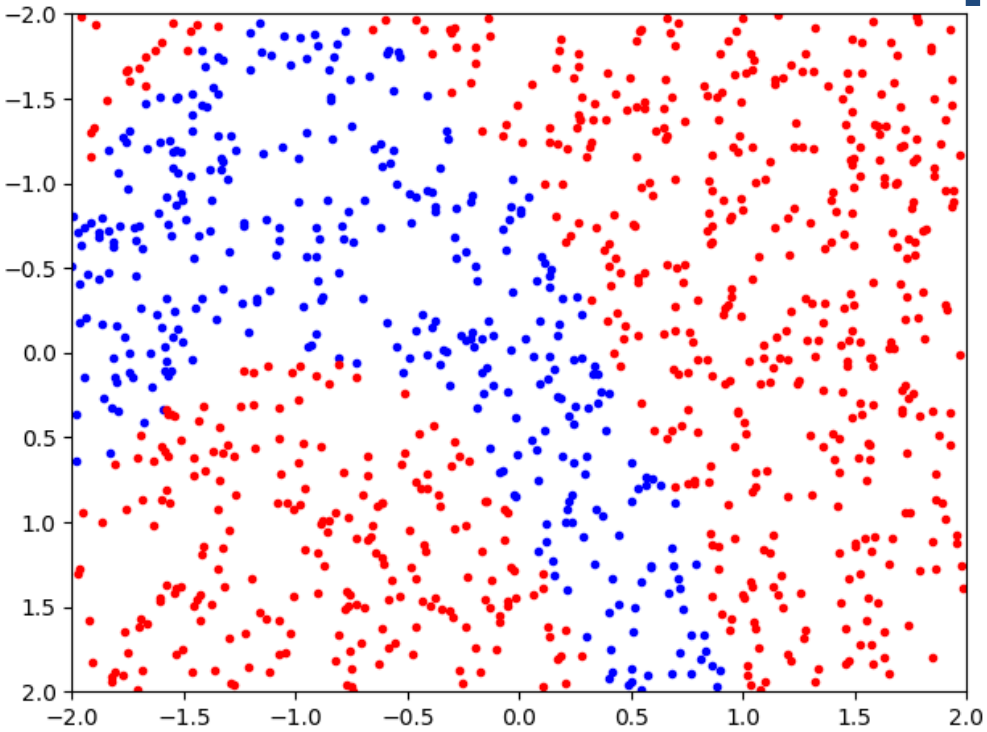


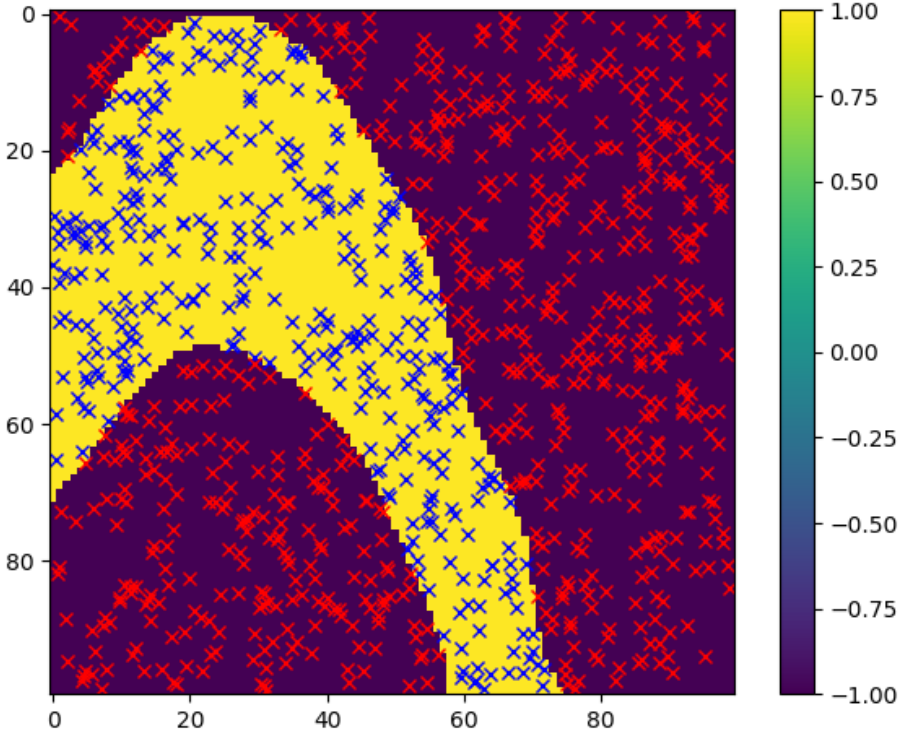
Positive: $100(x_2 - x_1^2)^2 + (1 - x_1)^2 < 0.5$

Negative: Otherwise

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

Reminder: Non Separable Distribution





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

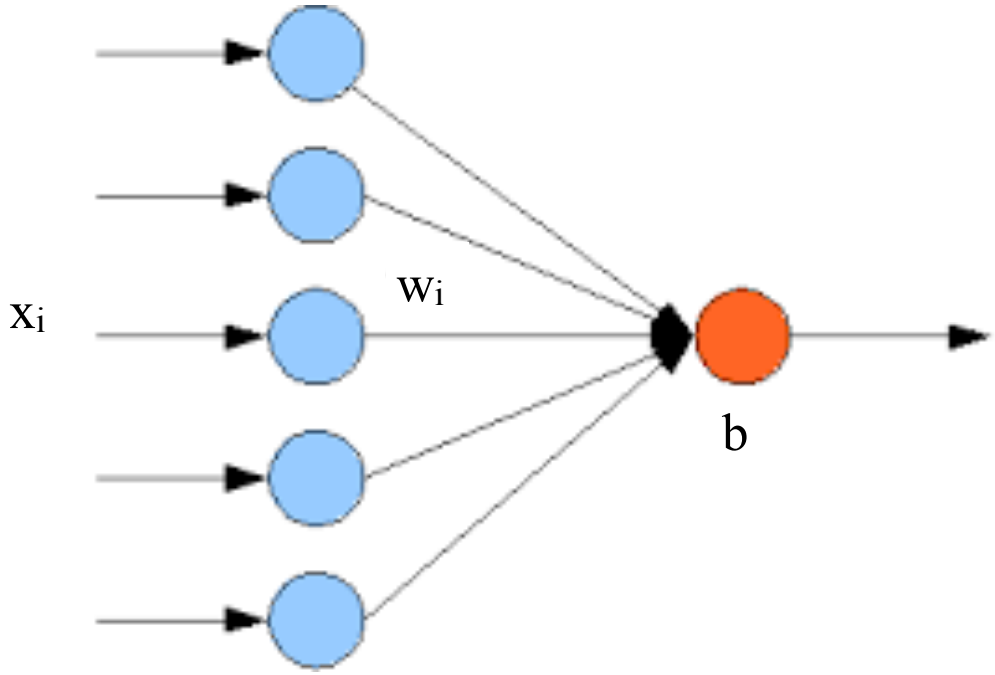
Negative: Otherwise

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

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

Reformulating Logistic Regression

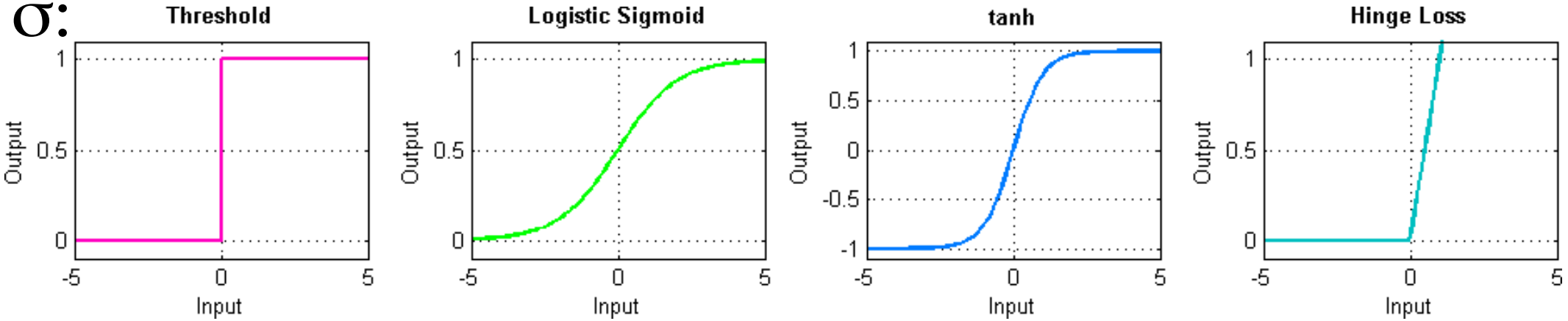


$$y(\mathbf{x}) = \sigma(\mathbf{w} \cdot \mathbf{x} + b)$$

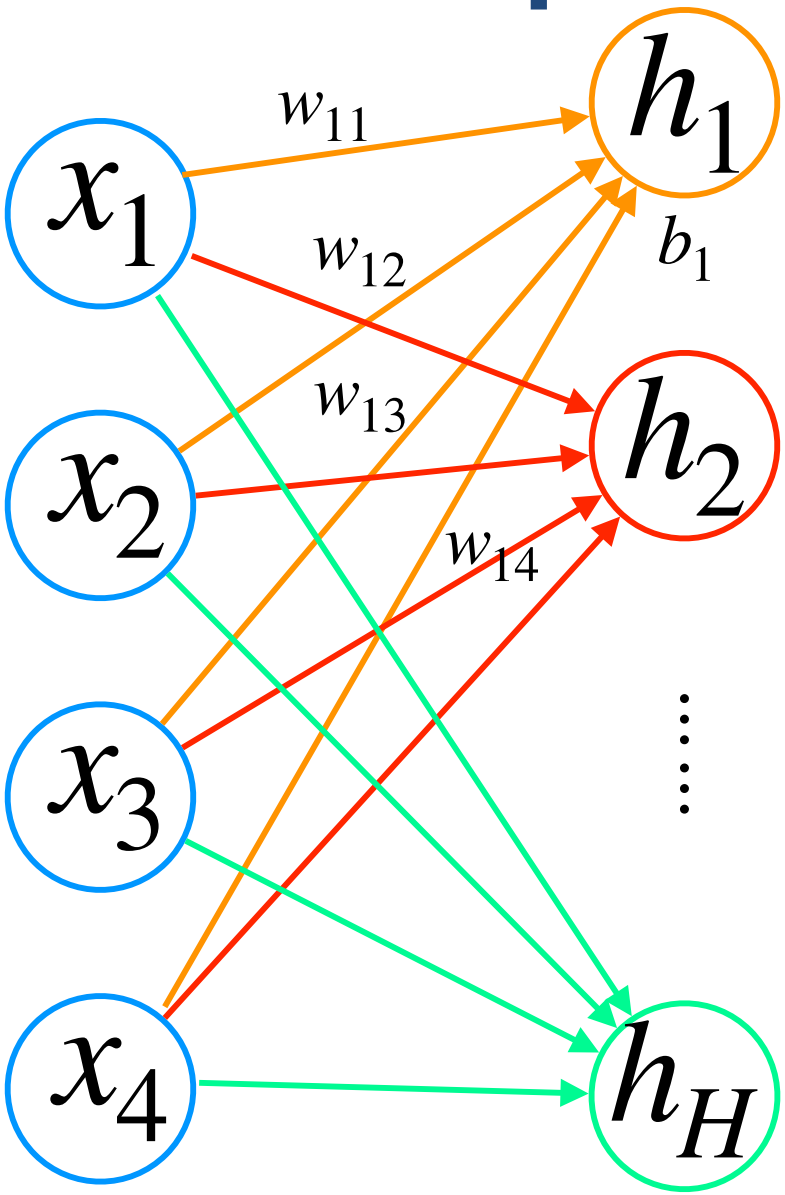
$$\mathbf{x} = \left[x_1, x_2, \ldots, x_n\right]^T$$

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

σ:



Repeating the Process

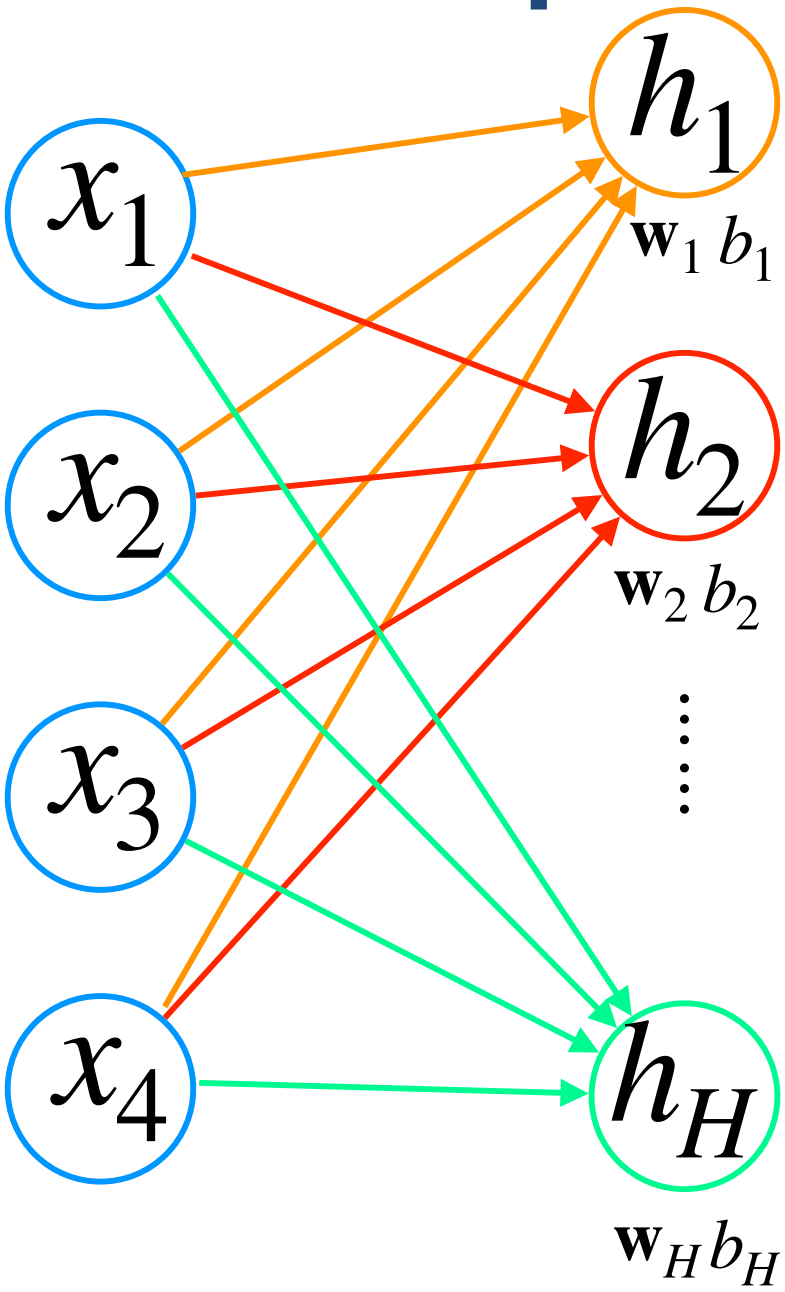


$$h_1 = \sigma(\mathbf{w}_1 \cdot \mathbf{x} + b_1)$$
$$\mathbf{w}_1 = \left[w_{11}, w_{12}, w_{13}, w_{14}\right]^T$$

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

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

Repeating the Process

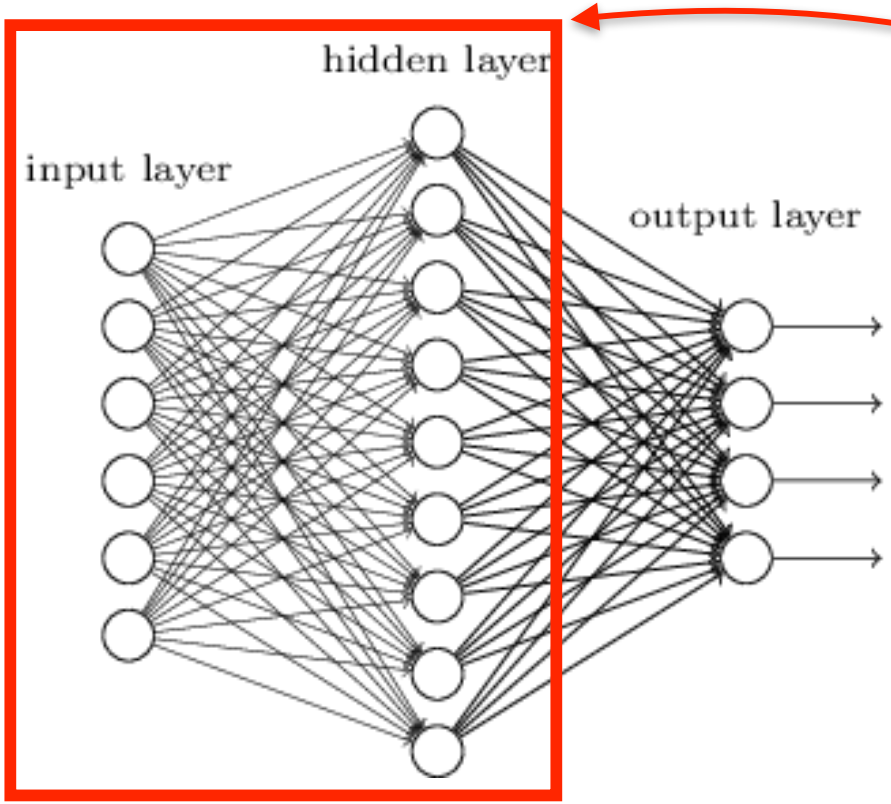


$$\mathbf{h} = \sigma(\mathbf{W}\mathbf{x} + \mathbf{b}) \ ,$$

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

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

Multi-Layer Perceptron (MLP)

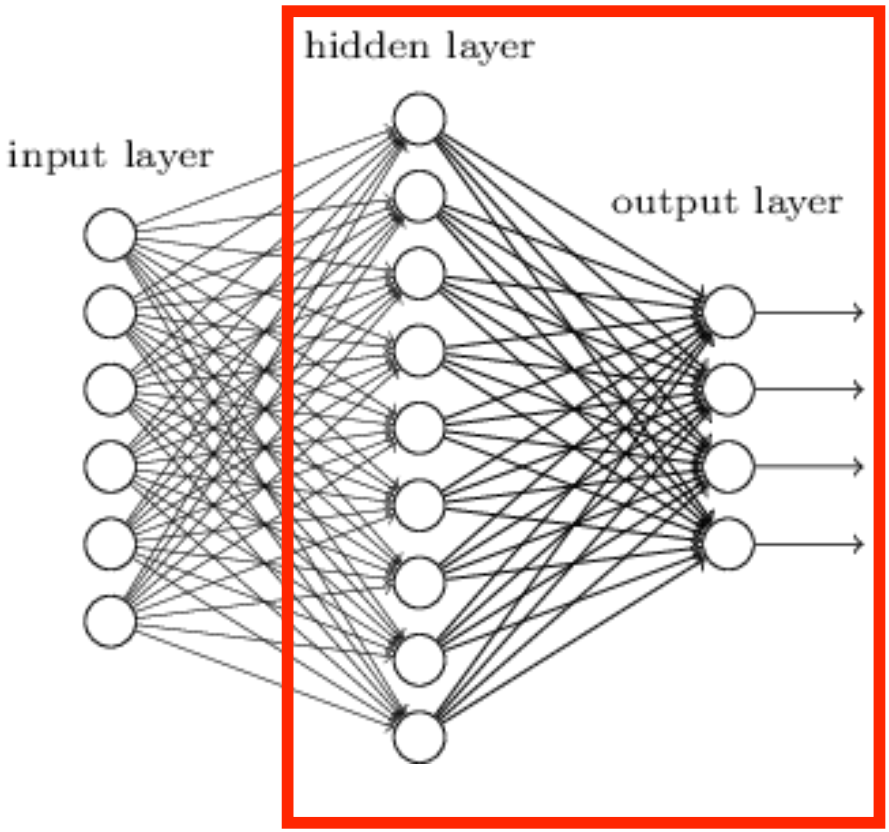


$$\mathbf{h} = \sigma_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$

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

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

Multi-Layer Perceptron (MLP)



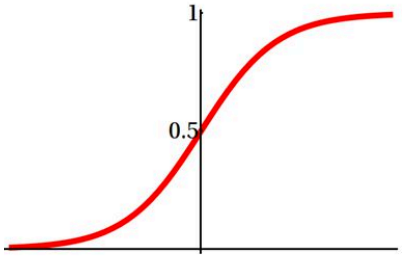
$$\mathbf{h} = \sigma_1(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1)$$

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

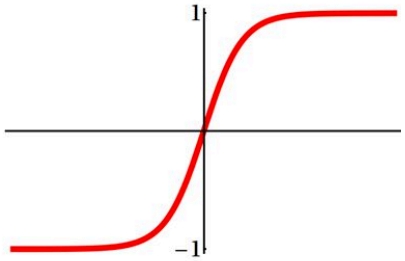
- The process can be repeated several times to create a vector **h**.
- It can then be done again to produce an output **y**.

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

Activation Functions



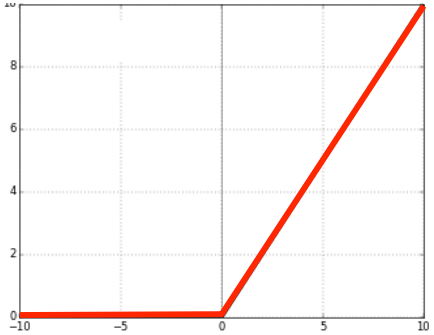
sigm



tanh

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

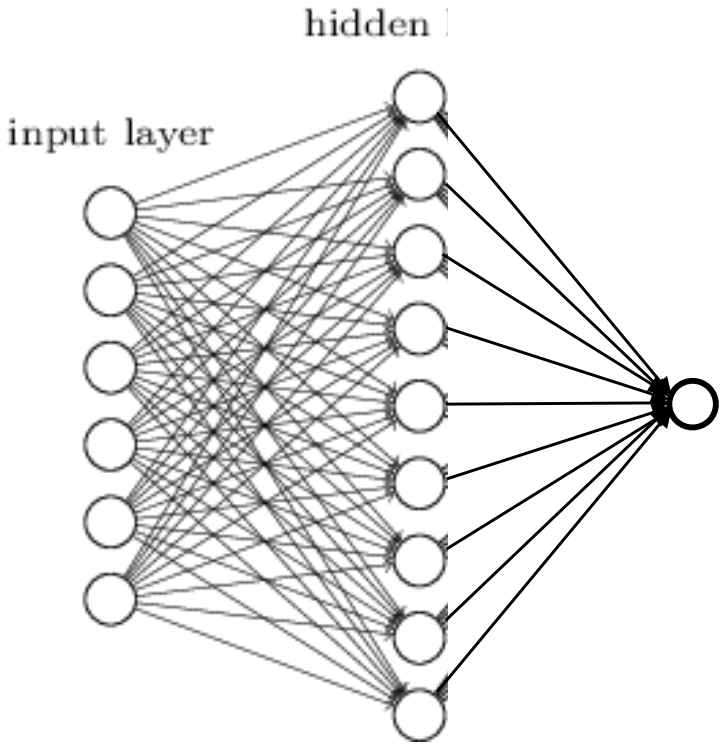
$$\text{tanh:} \quad \sigma(x) = \frac{\exp(x)-\exp(-x)}{\exp(x)+\exp(-x)}$$



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

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

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.

Training

- 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

$$y_n = \sigma_2(\mathbf{w}_2(\sigma_1(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)) + \mathbf{b}_2) \in [0.1]$$

- We want to minimize the binary cross entropy

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

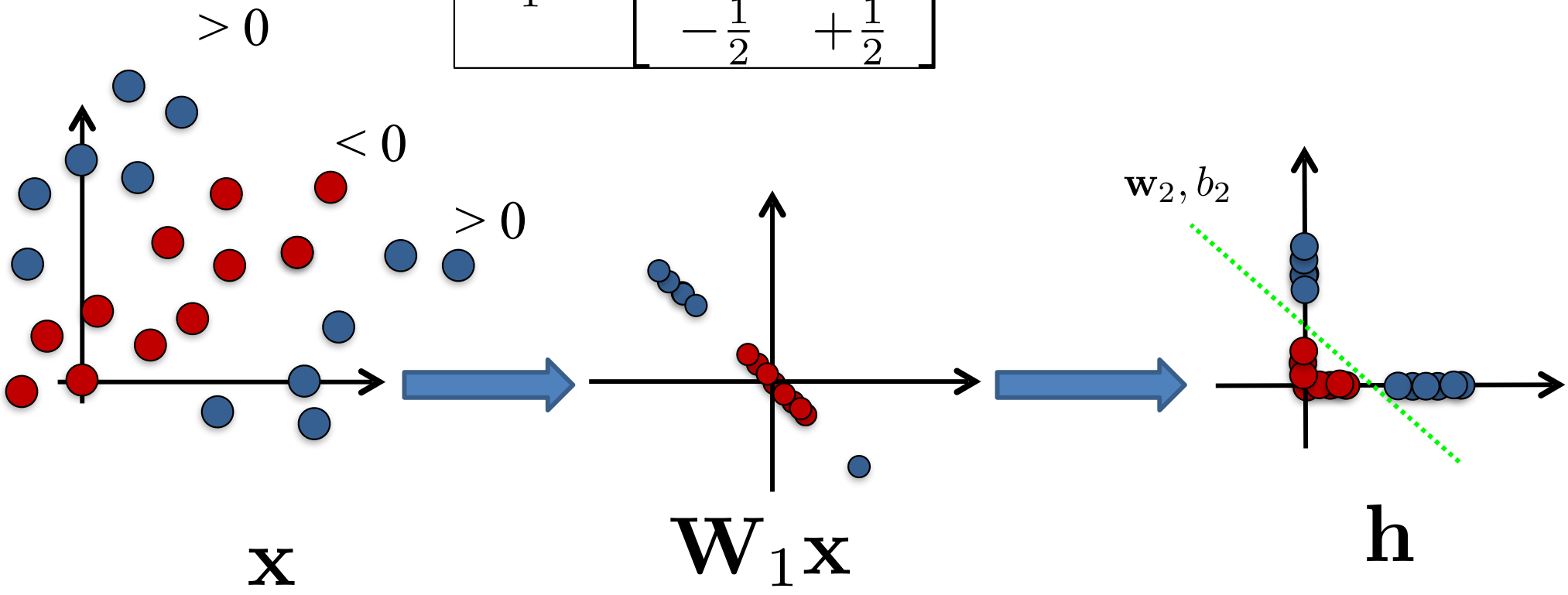
$$E_n(\mathbf{W}_1, \mathbf{w}_2, \mathbf{b}_1, \mathbf{b}_2) = -\left(t_n \ln(y_n) + (1 - t_n)\ln(1 - y_n)\right) \ ,$$

  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.

ReLu Behavior

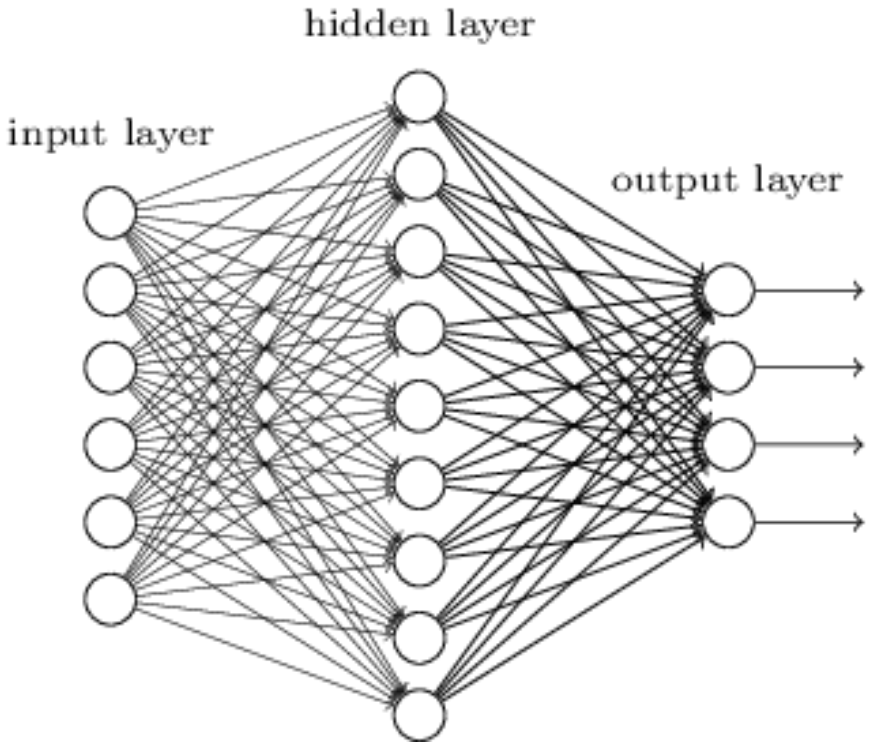
$$\mathbf{W}_1 = \begin{bmatrix} +\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & +\frac{1}{2} \end{bmatrix}$$



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

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

Multi-Class Case



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

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

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

Training

Let the 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

$$\mathbf{y}_n = \mathbf{W}_2(\sigma_1(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)) + \mathbf{b}_2 \in R^K$$

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

- We want to minimize the cross entropy

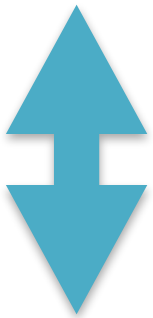
$$E(\mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2) = \frac{1}{N}\sum_{n=1}^{N} E_n(\mathbf{W}_1, \mathbf{W}_2, \mathbf{b}_1, \mathbf{b}_2) \ ,$$

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

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

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.

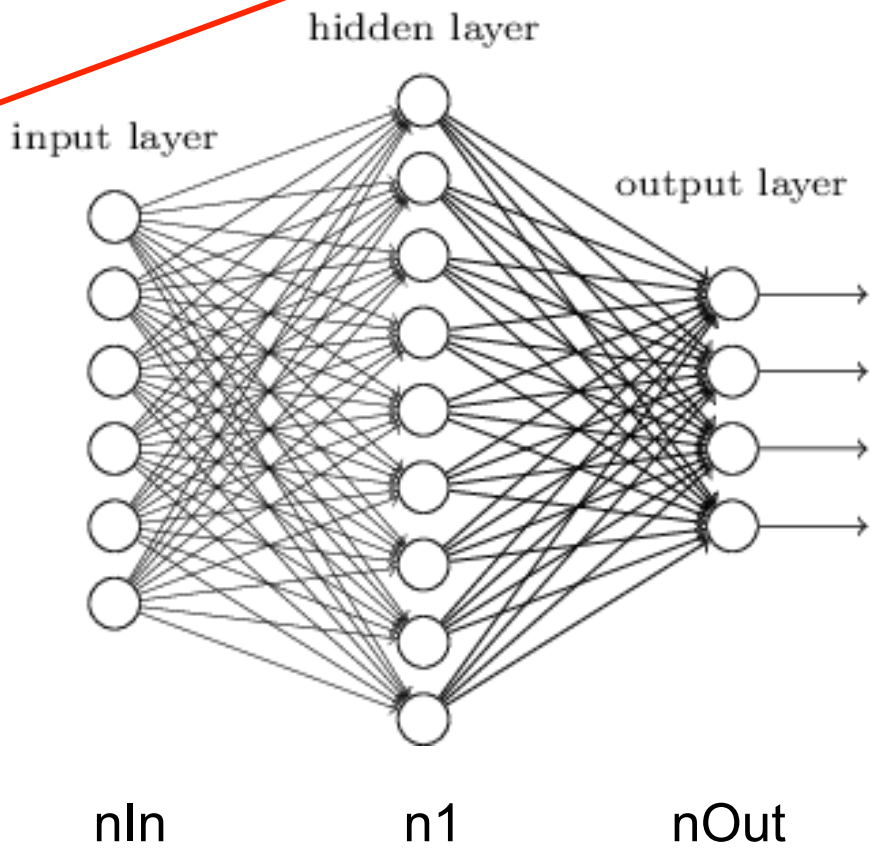
Optional: PyTorch Translation (1)

```
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.

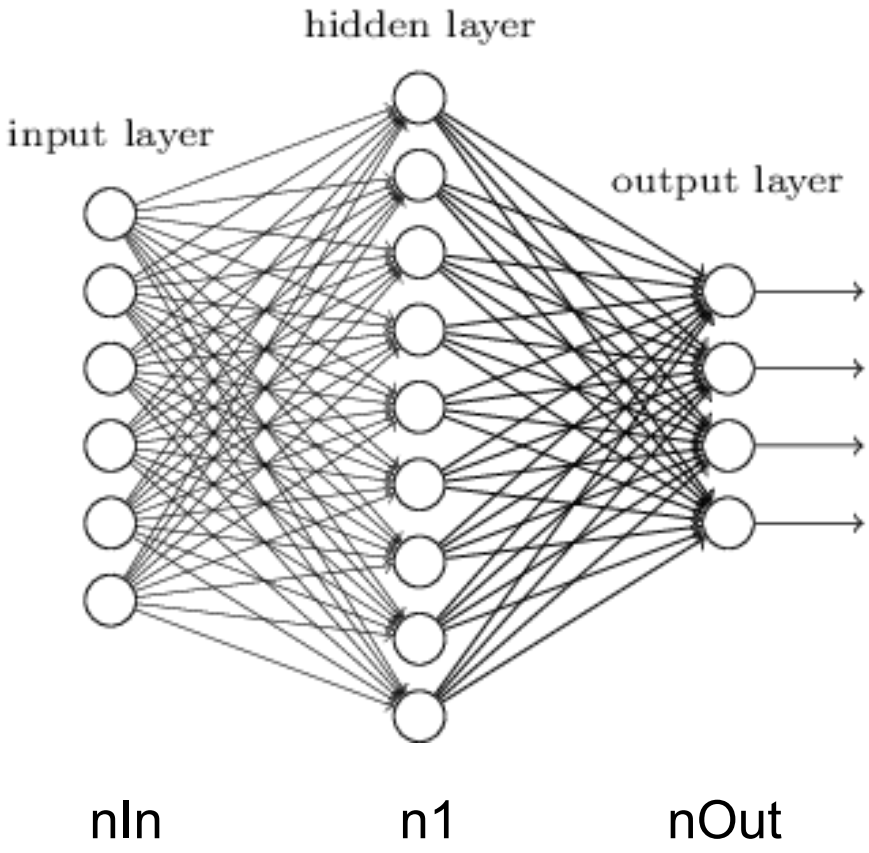
Return $\sigma(\mathbf{W}_2(\sigma(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)) + \mathbf{b}_2)$



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



Multivariate Optimization

- 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:

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

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

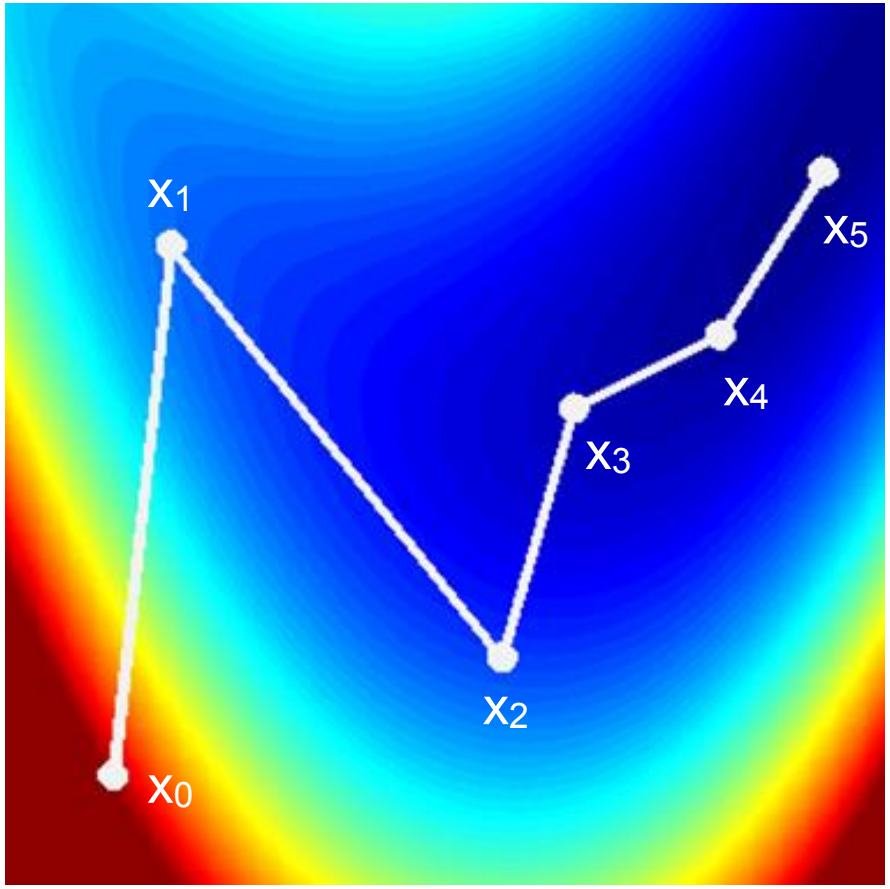
- We want to minimize the cross entropy

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

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

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

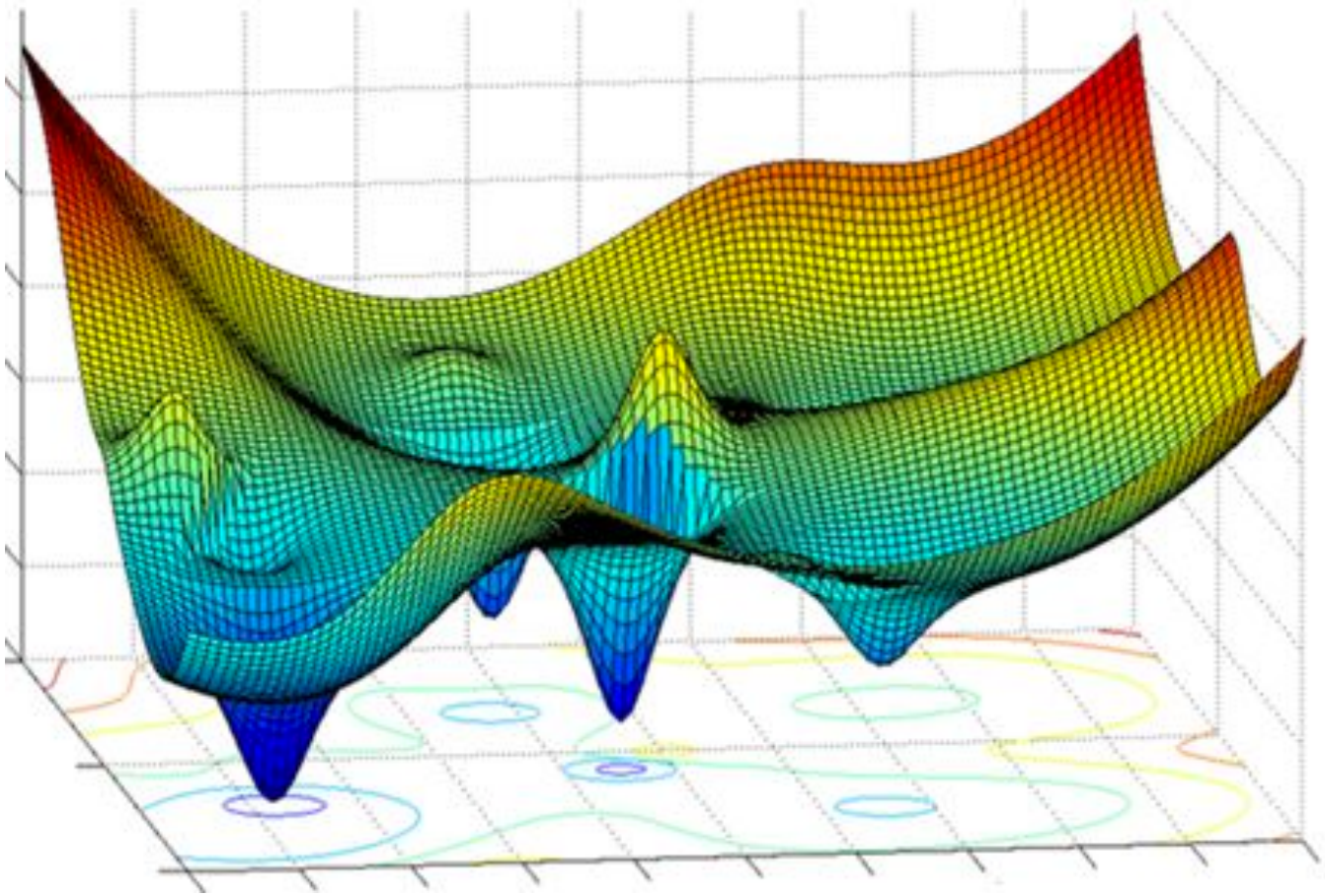
Reminder: Gradient Descent



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

—> η is known as the learning rate and must be carefully chosen.

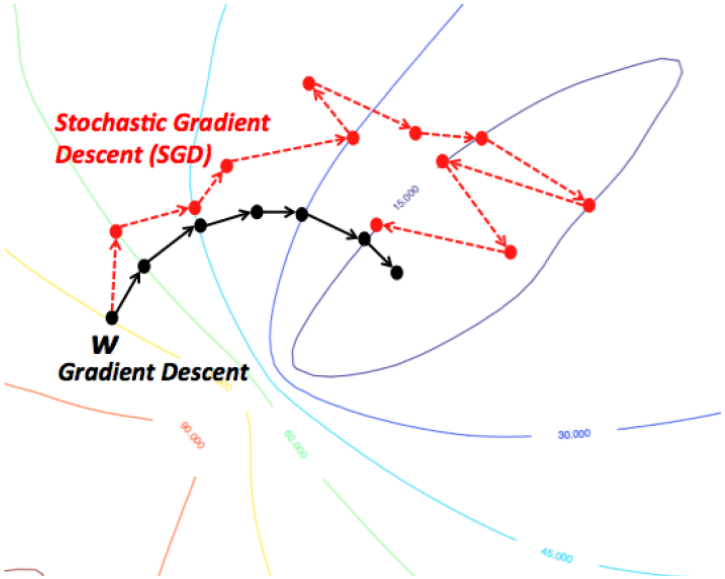
Reminder: Local Minima



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

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



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

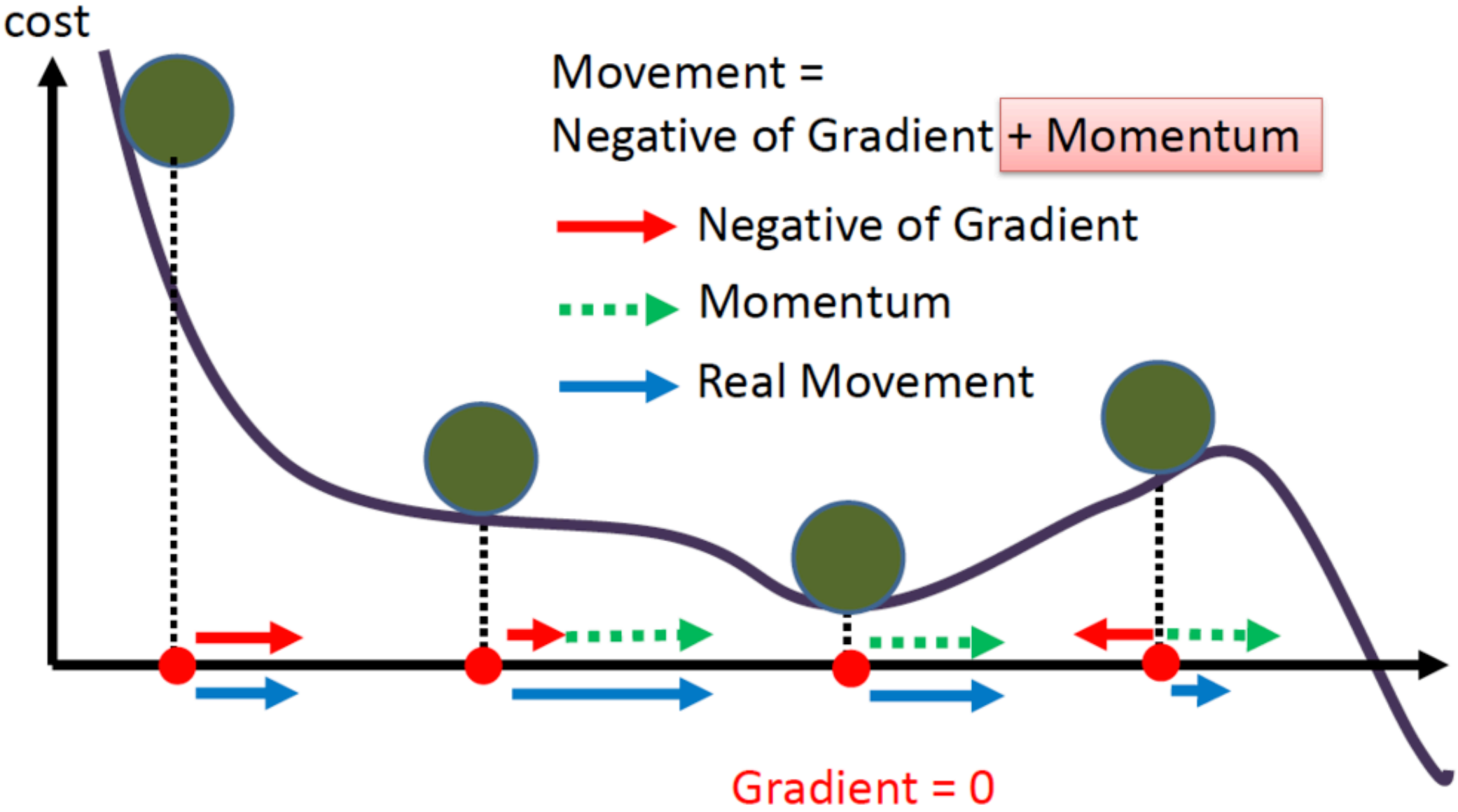
$$\text{Stochastic descent: } \mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \sum_{n \in B^{\tau}} \nabla E_n(\mathbf{w}^{\tau}) \ ,$$

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

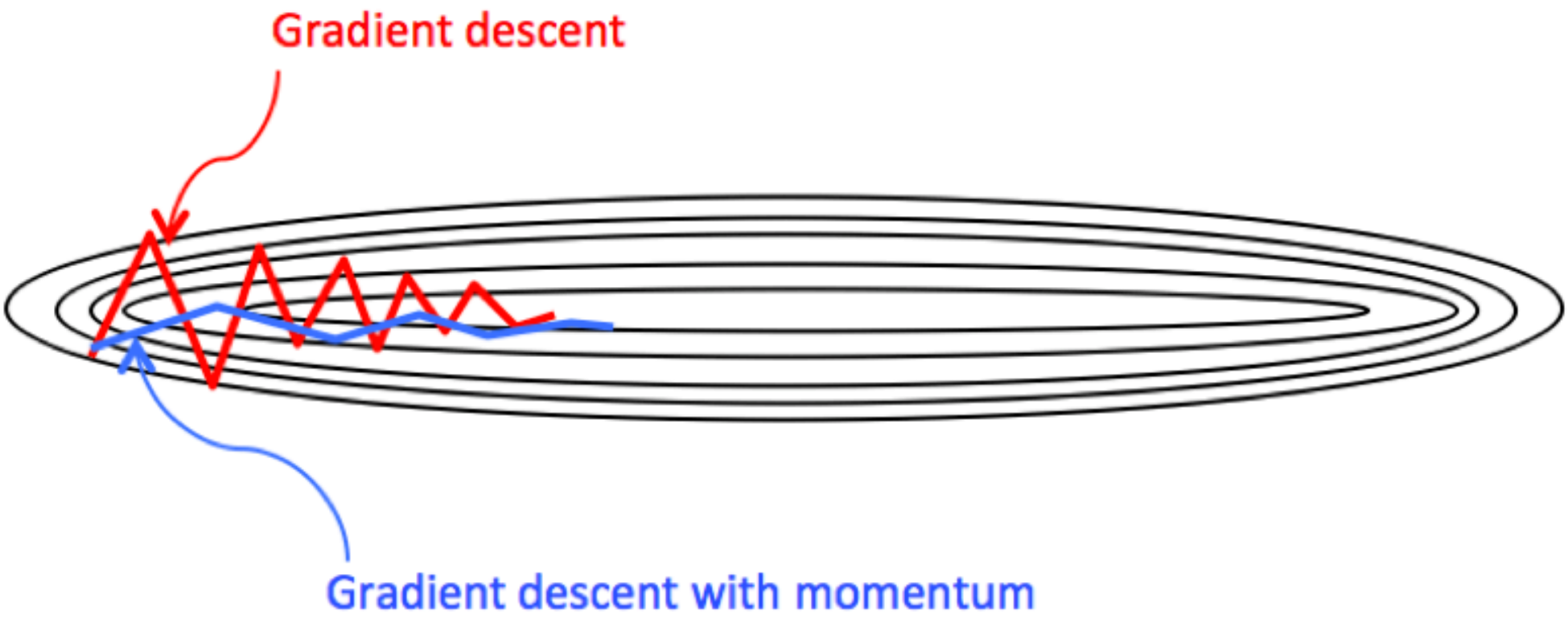
Randomly choosing batches

- 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.

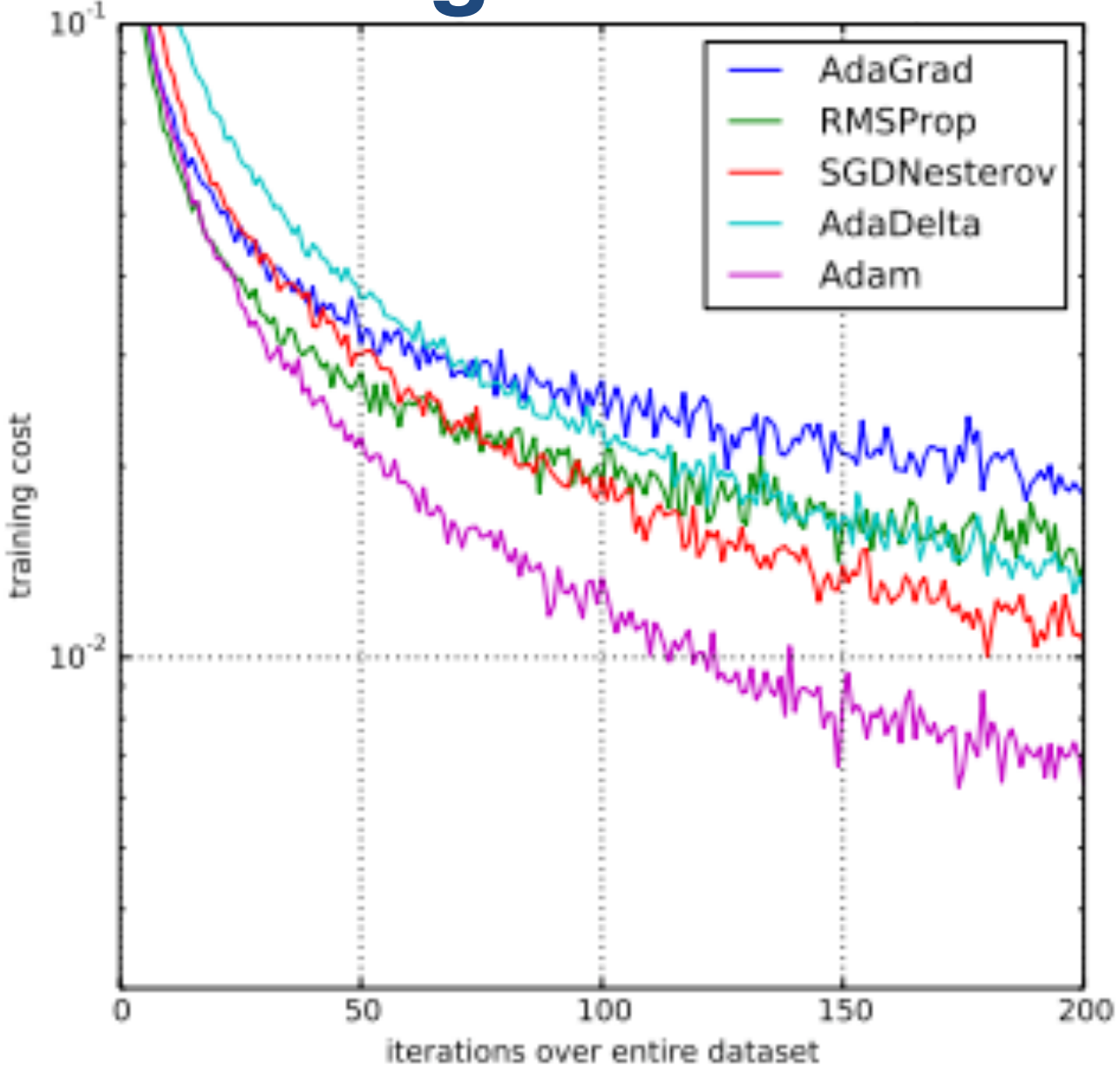
$$\hat{\mathbf{m}}_{\tau+1} = \frac{\mathbf{m}_{\tau+1}}{1-\beta_1^t}$$ Corrective factor.

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

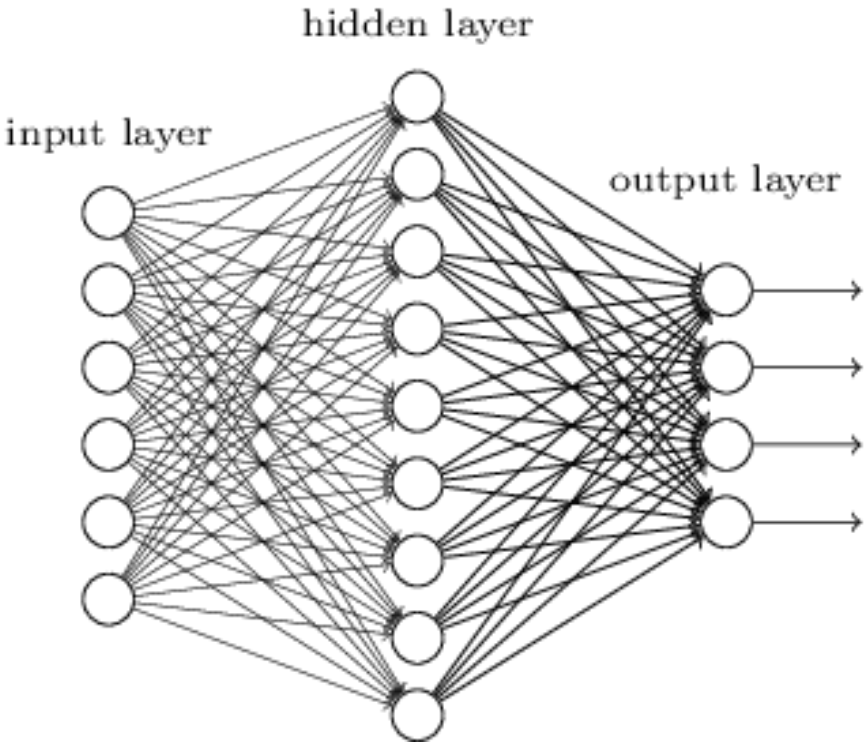
$$\mathbf{m}_0 = \mathbf{v}_0 = 0,$$
$$\beta_1 = 0.9,$$
$$\beta_2 = 0.999,$$
$$\alpha = 0.001,$$
$$\epsilon = 10^{-8}$$

Training the Network



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

Geometric Interpretation

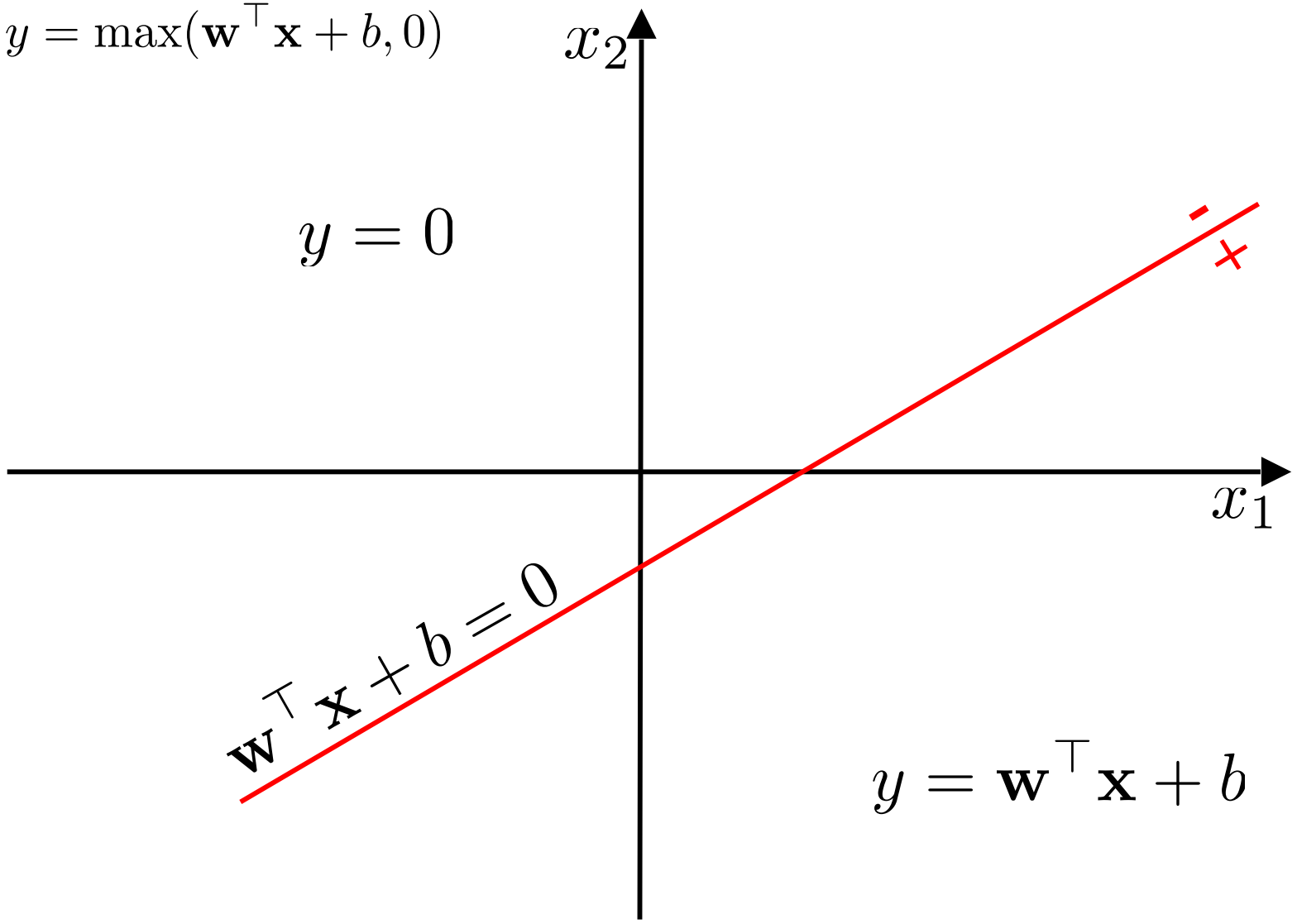


$$\mathbf{h} = \sigma_1(\mathbf{W}_1\mathbf{x}_n + \mathbf{b}_1)$$

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

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

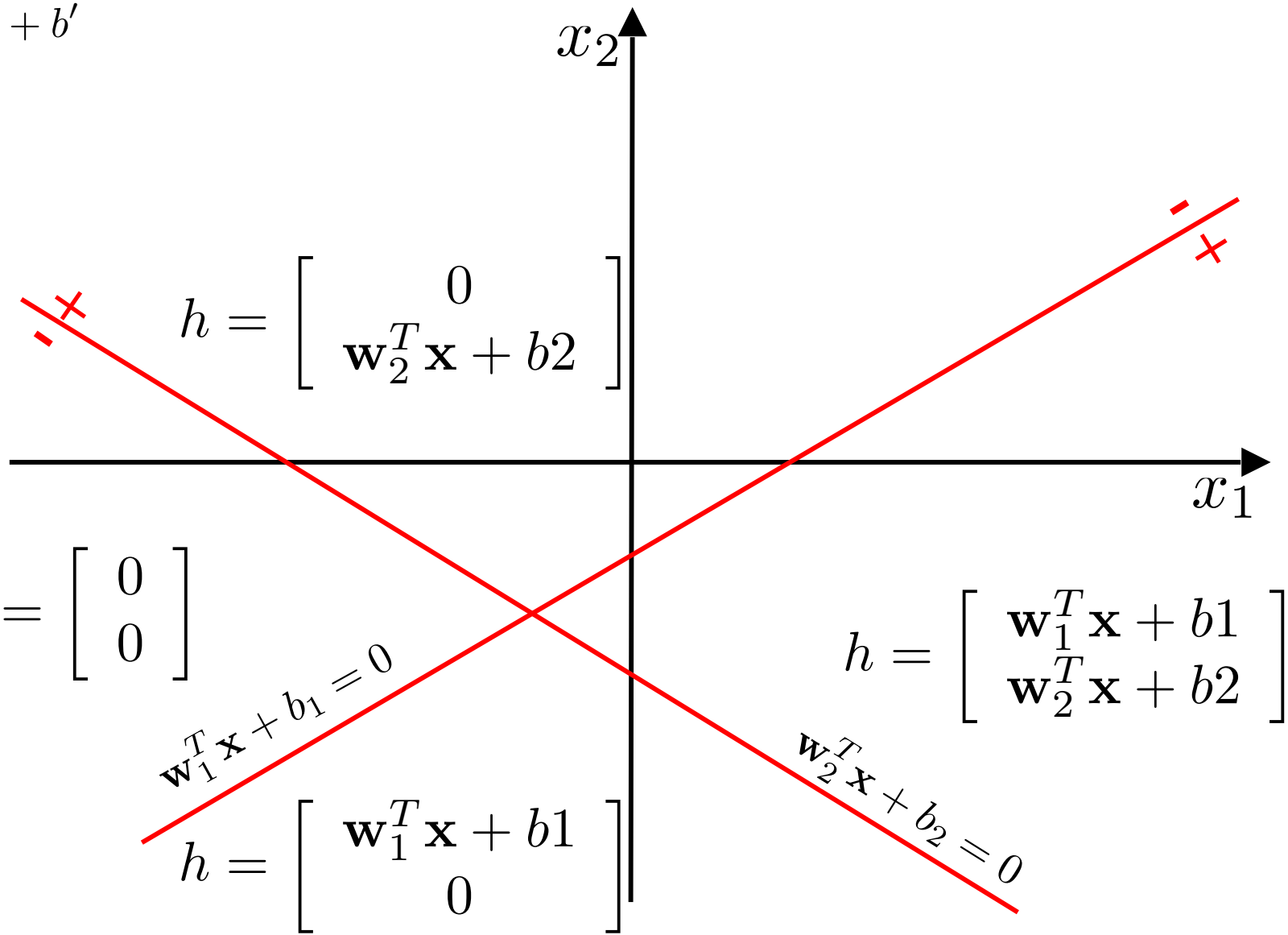
One Single Hyperplane



Two Hyperplanes

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

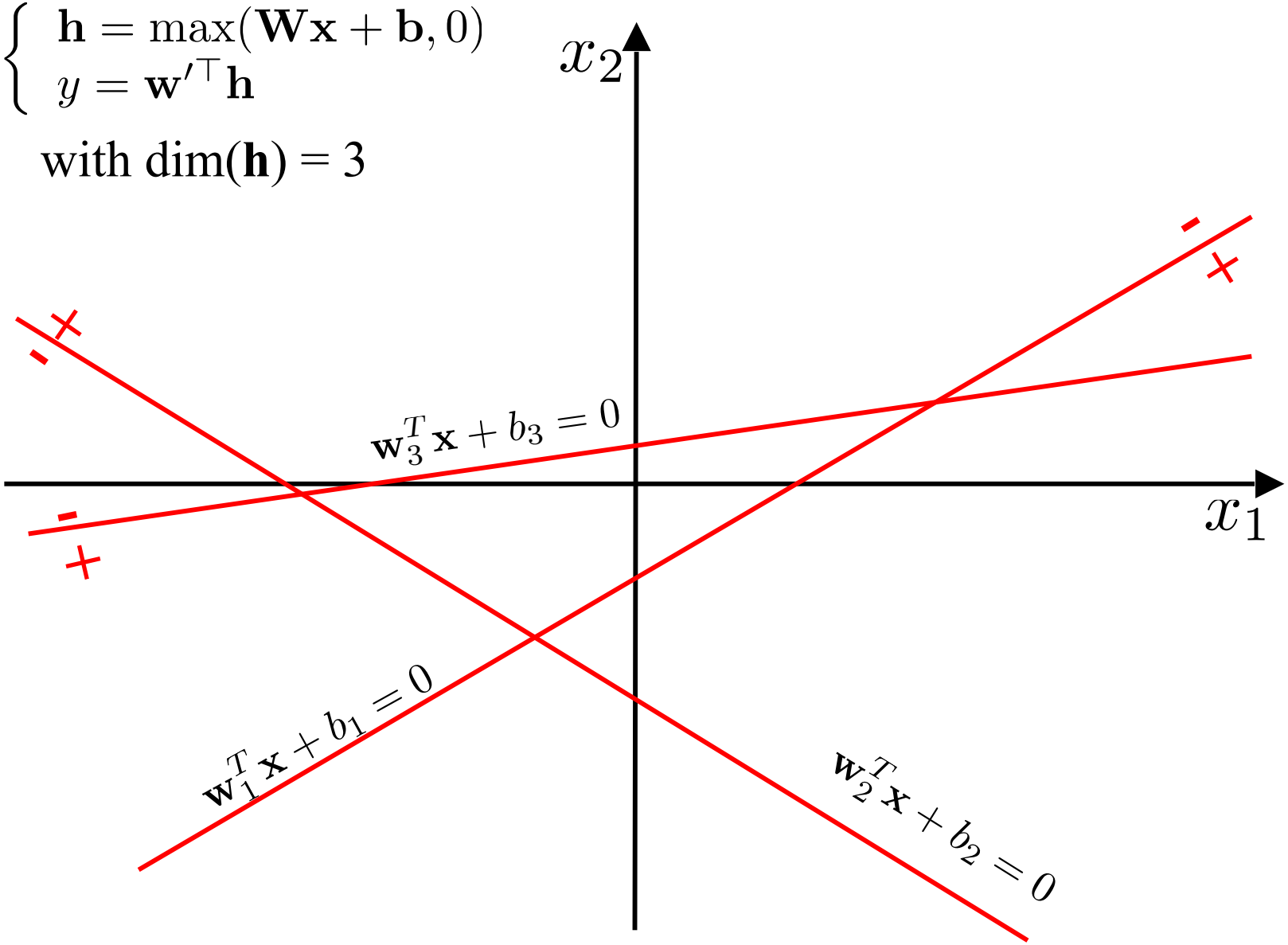
$$y = \mathbf{w}'^T \mathbf{h} + b'$$



Three Hyperplanes

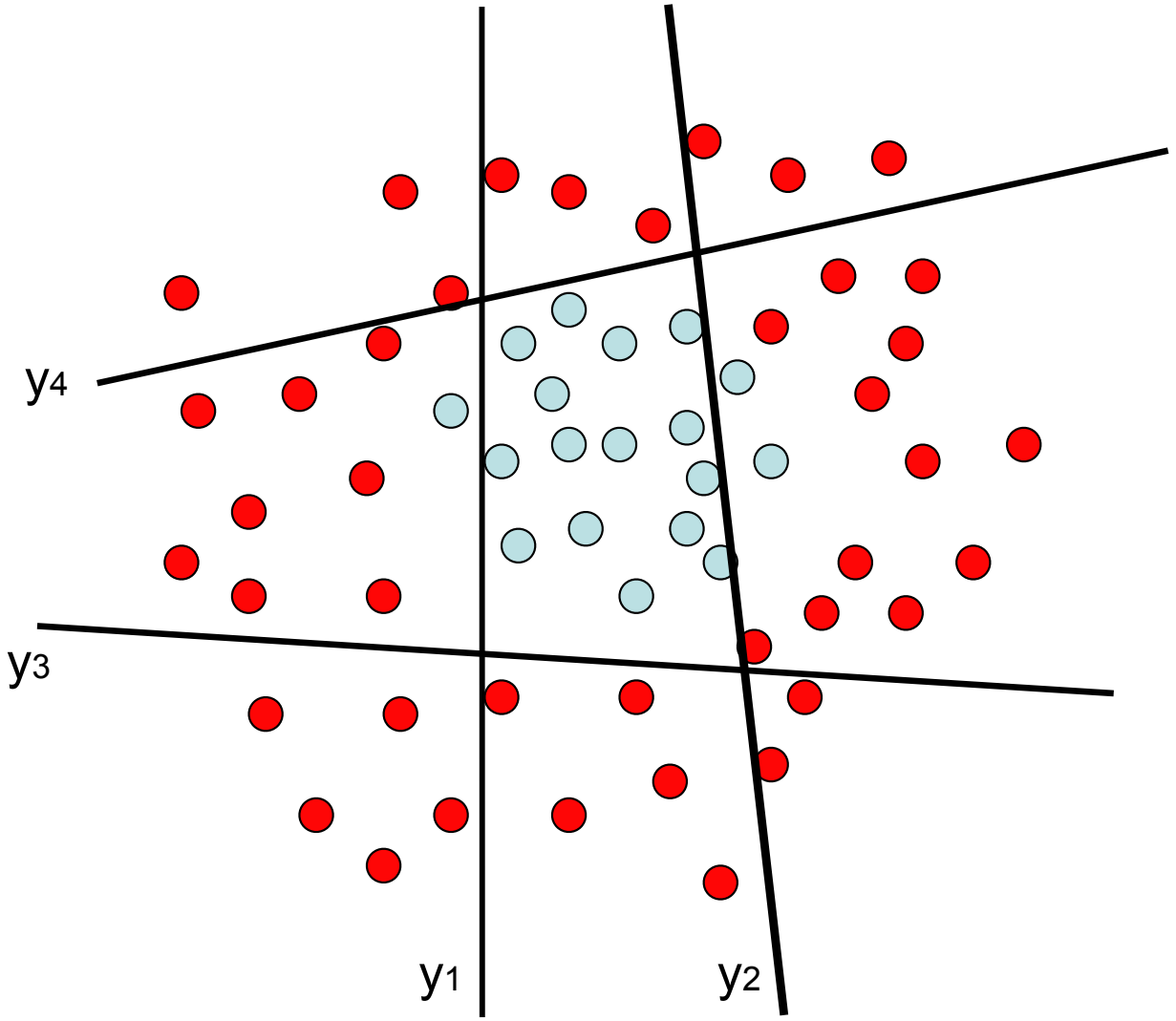
$$\begin{cases} \mathbf{h} = \max(\mathbf{W}\mathbf{x} + \mathbf{b}, 0) \\ y = \mathbf{w}'^{\top}\mathbf{h} \end{cases}$$

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

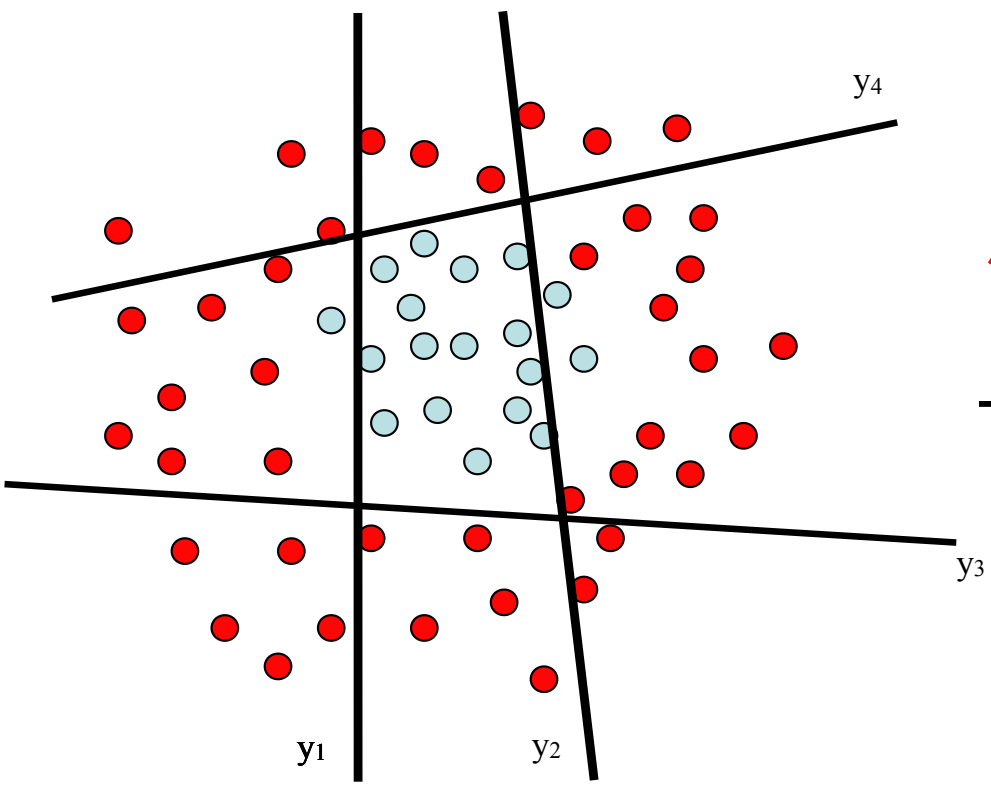


Reminder: AdaBoost

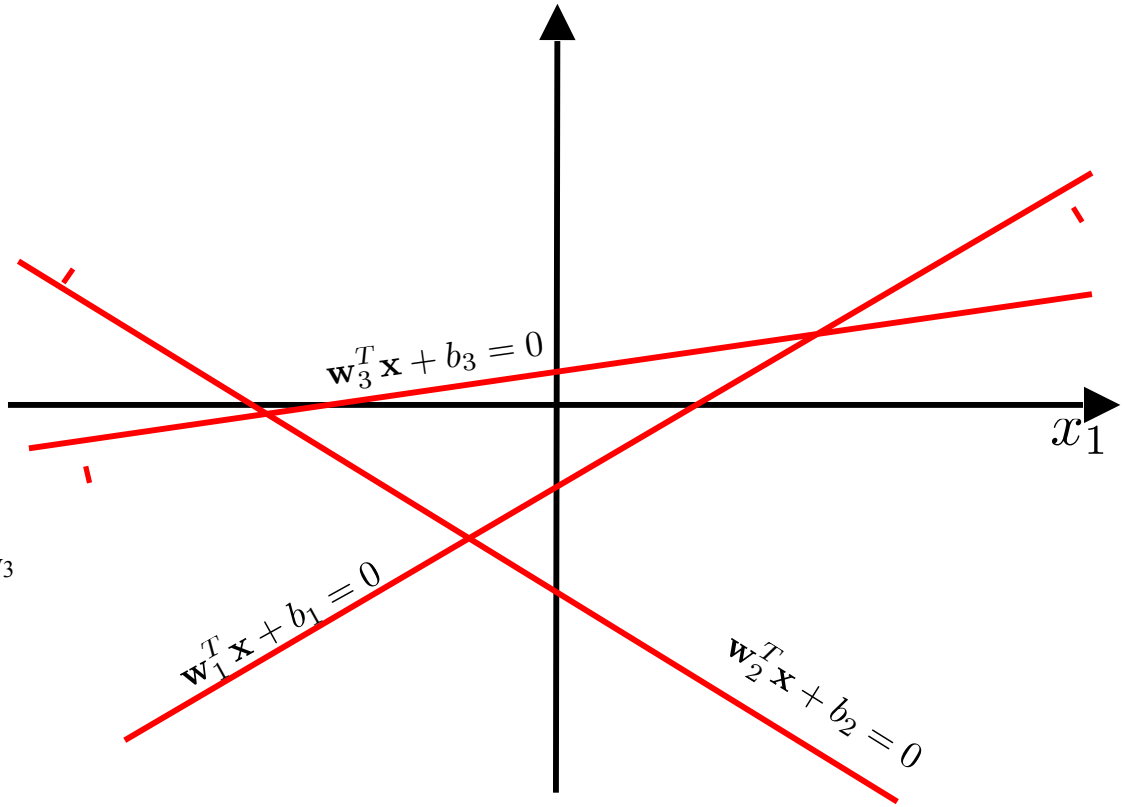
$$y(\mathbf{x}) = \alpha_1 y_1(\mathbf{x}) + \alpha_2 y_2(\mathbf{x}) + \alpha_3 y_3(\mathbf{x}) + \alpha_4 y_4(\mathbf{x})$$



AdaBoost vs MLP



AdaBoost

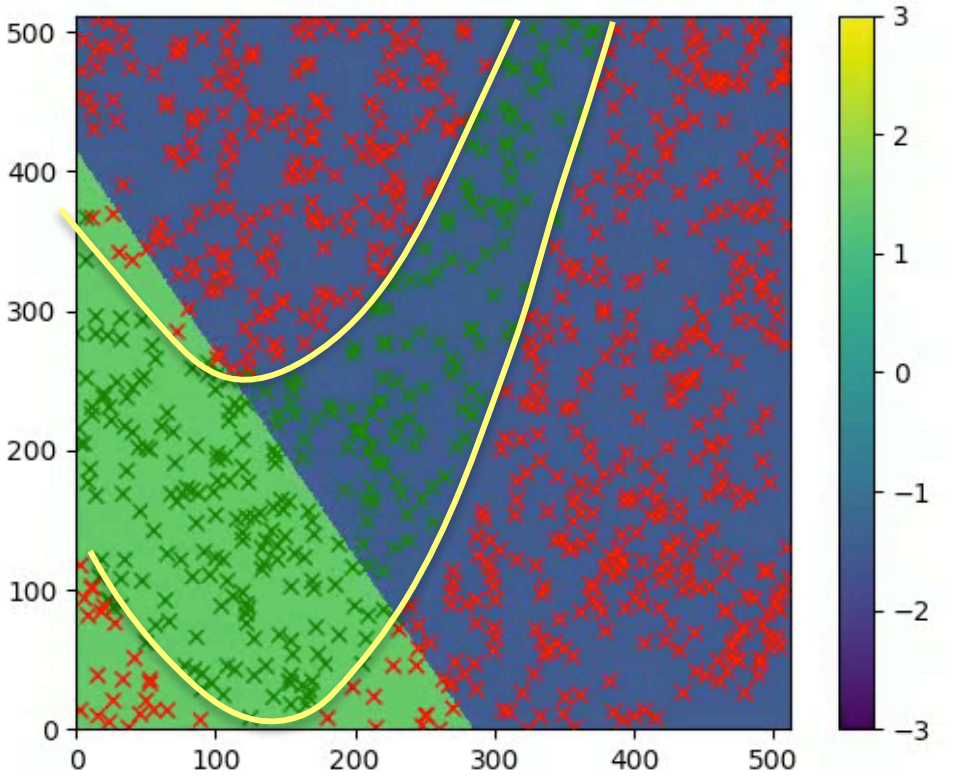


MLP

Both methods find a set of hyperplanes:

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

Rosenbrock using Adaboost



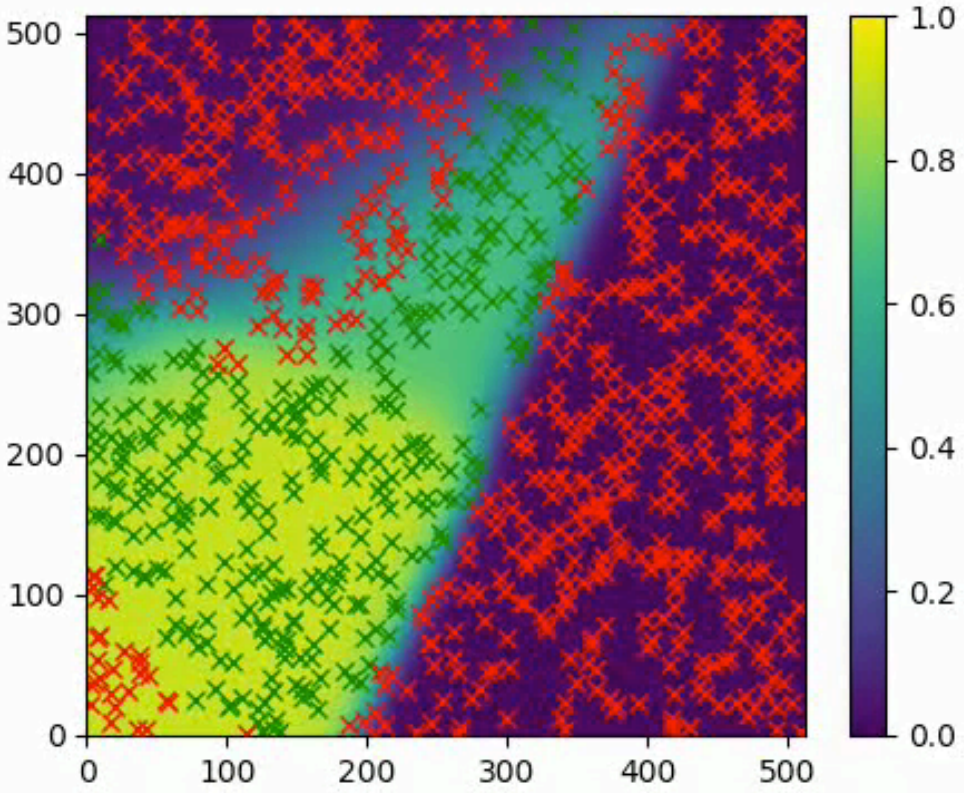
Training (100 iterations)

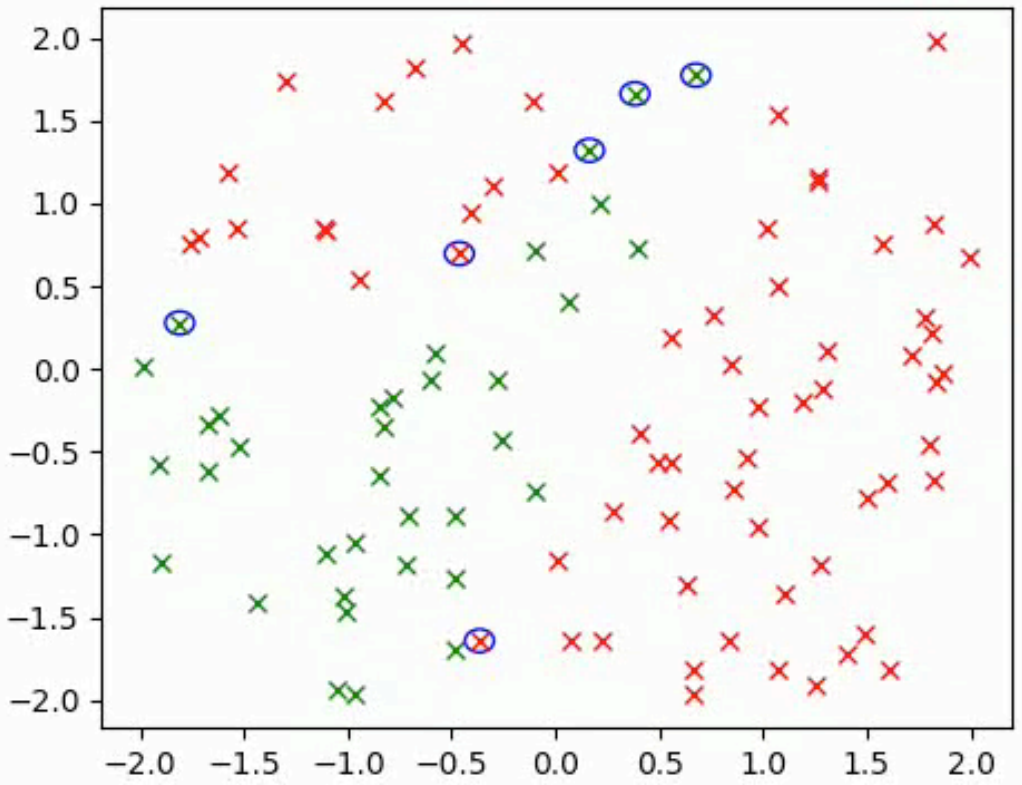
$$r(x,y) = 100 * (y - x^2)^2 + (1 - x)^2$$

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

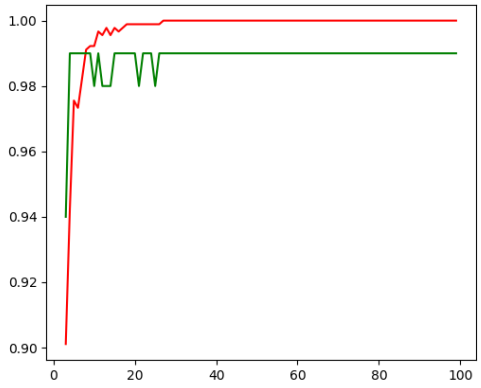
- Adaboost adds one linear classifier at a time.
- MLP works with a fixed number of classifiers and optimizes them all at the same time.

Rosenbrock using a MLP





One hidden layer: 3 < n < 100

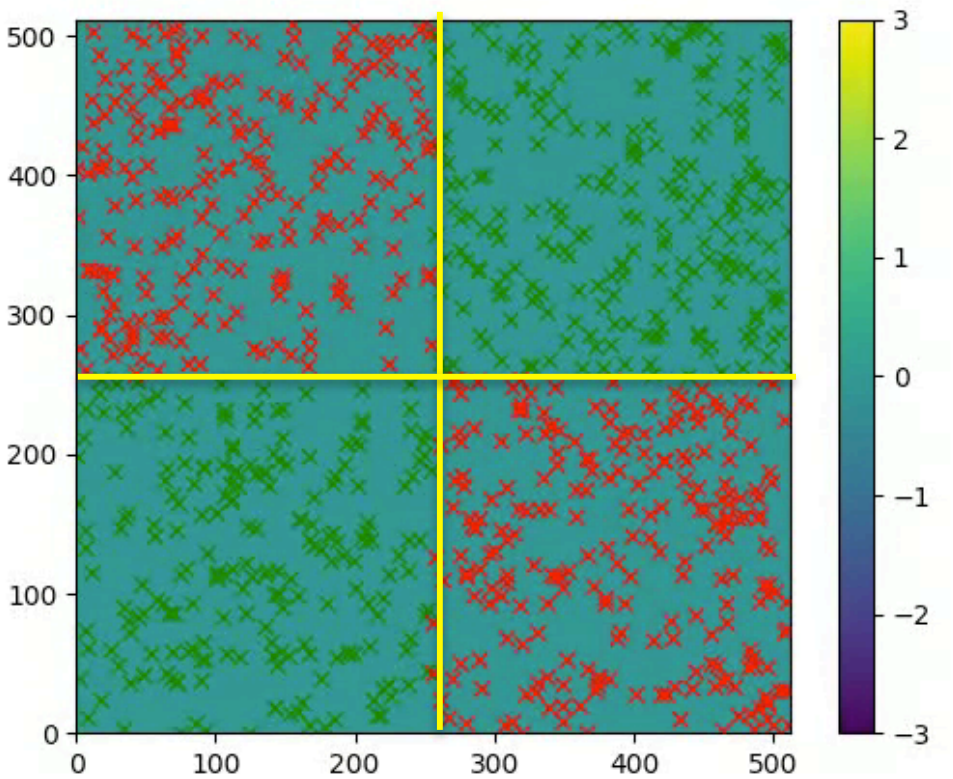


Accuracy as a function of n:

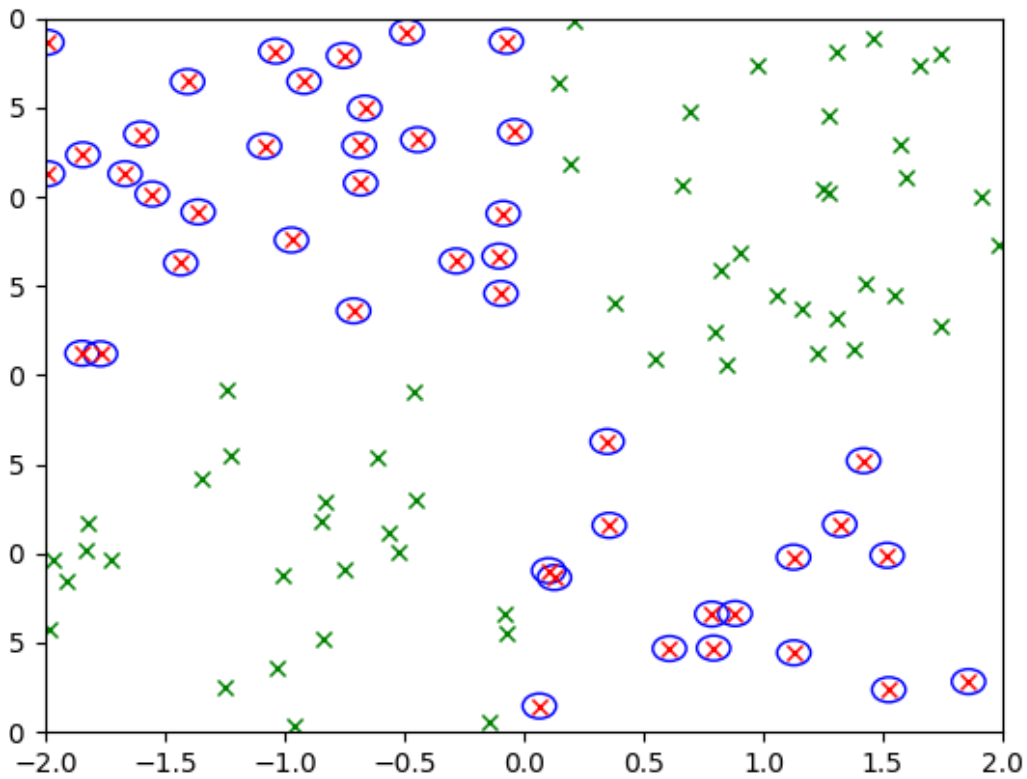
— Adaboost

— MLP

Checker Board using Adaboost



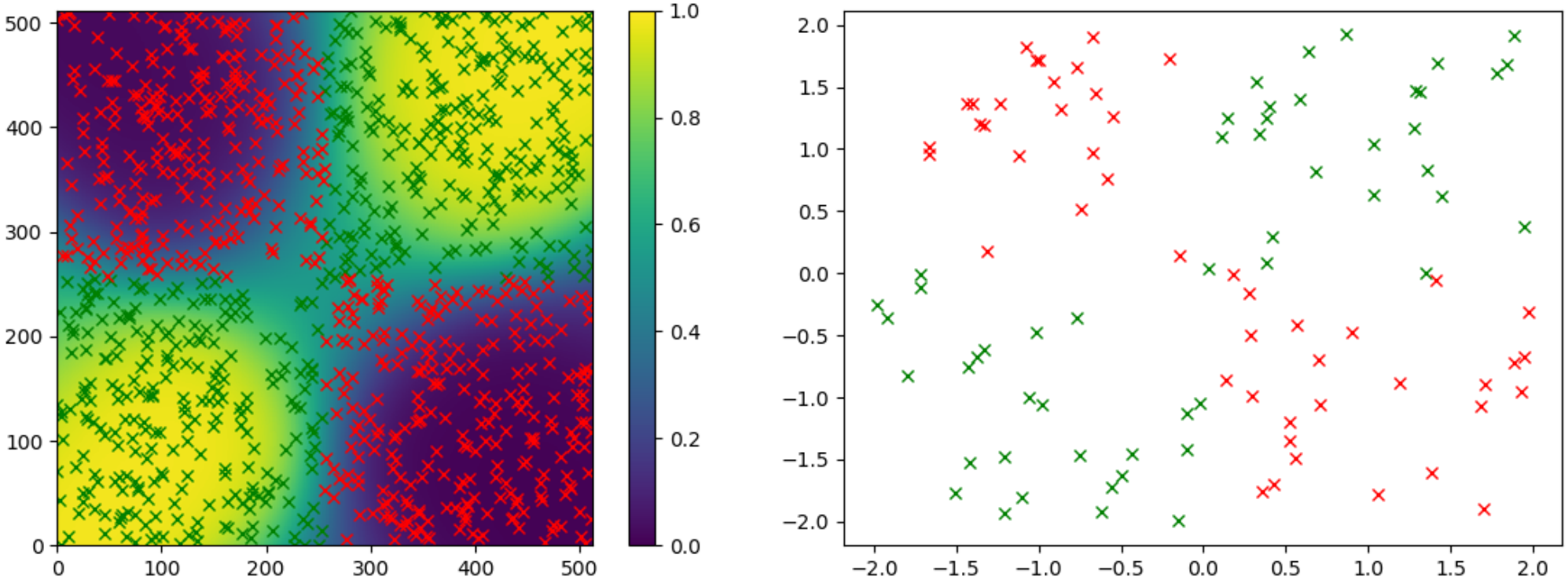
Training (100 iterations)



Validation (56% accuracy)

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

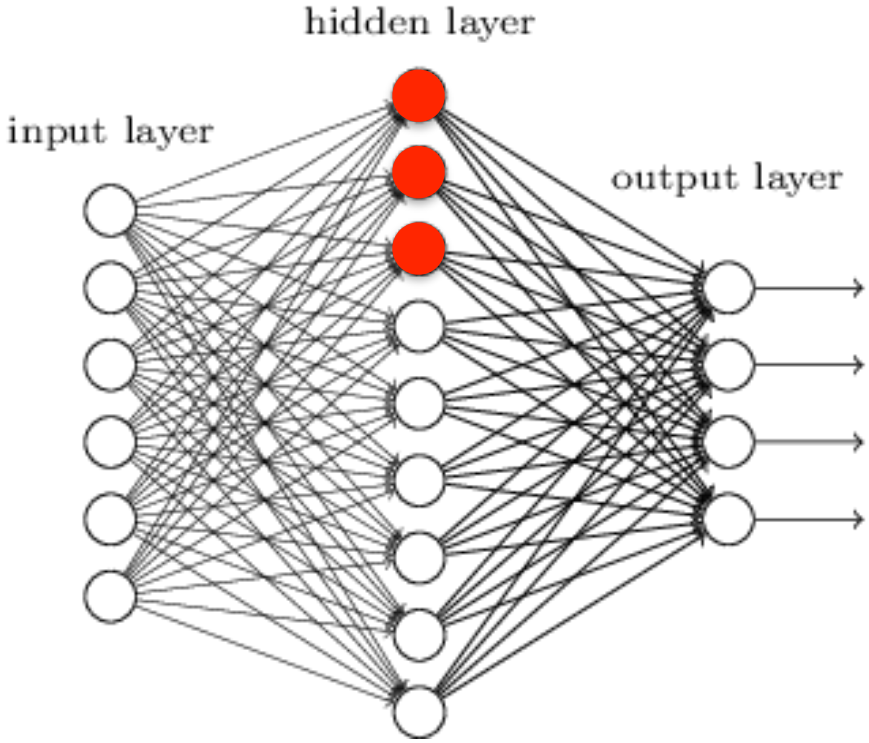
Checkerboard using a MLP

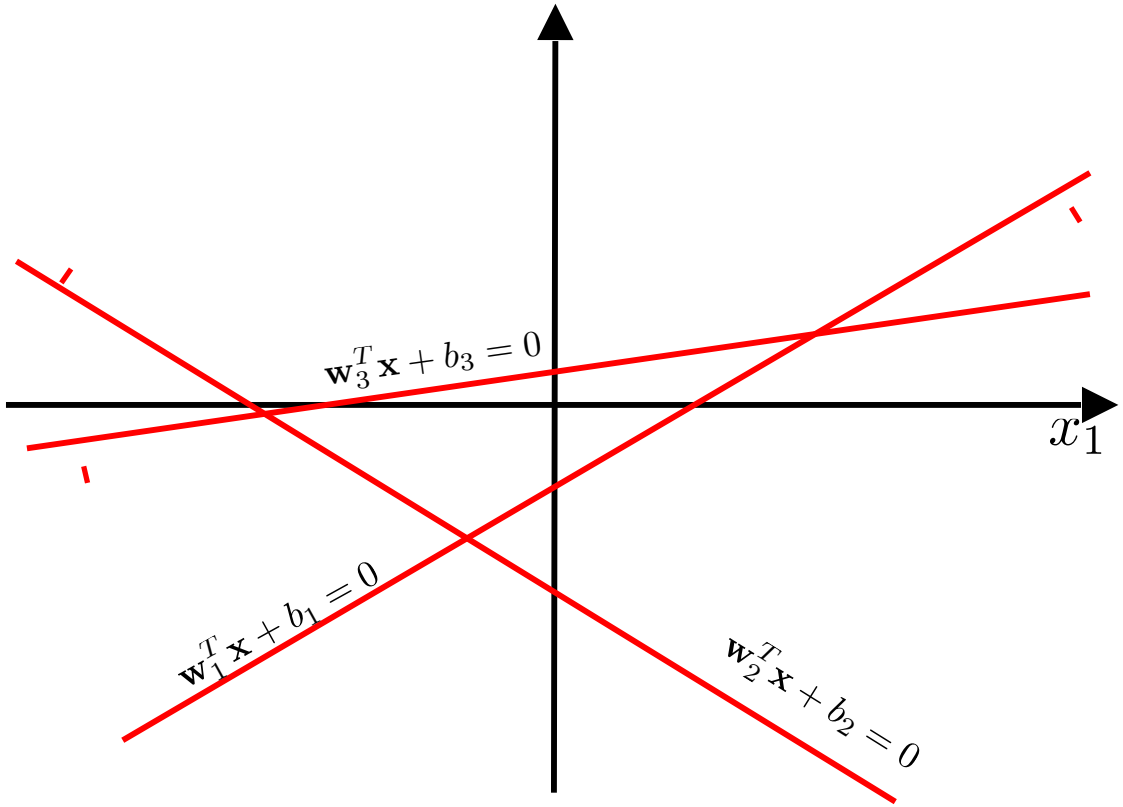


One hidden layer: n=10

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

SVM vs MLP





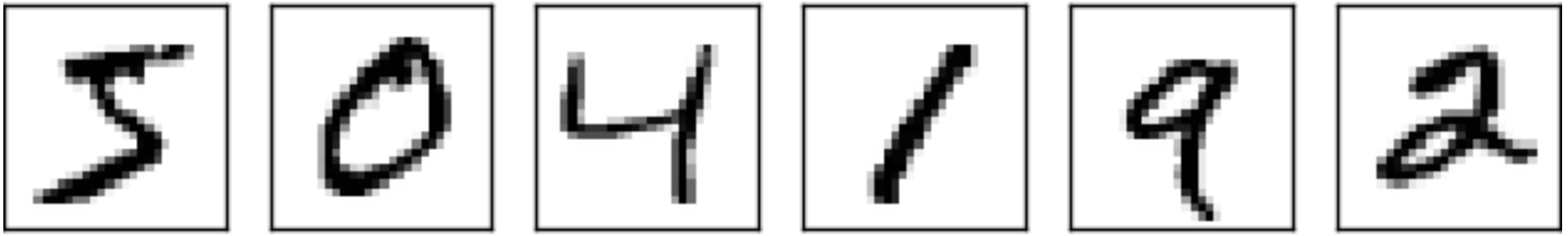
$\mathbf{x}$ $\quad$ $\mathbf{f}(\mathbf{x})$ $\quad$ $\mathbf{W}\mathbf{f}(\mathbf{x})+\mathbf{b}$

Both methods

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

But the form of $\mathbf{f}$ is not defined a priori in a MLP.

Reminder: MNIST



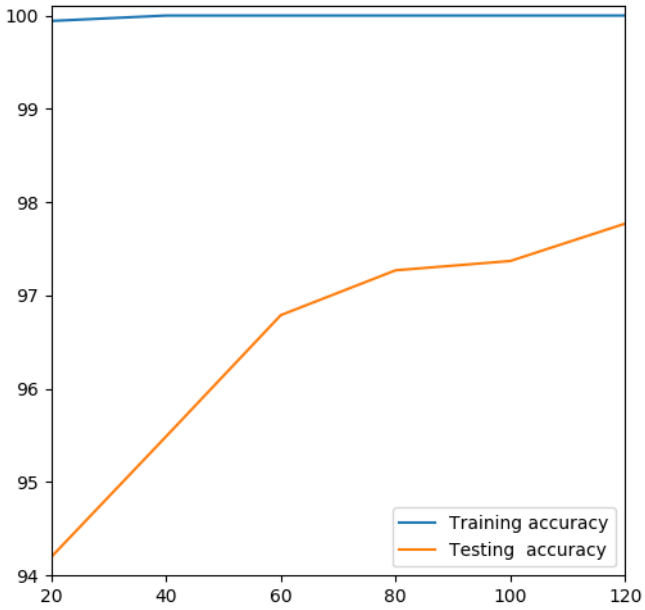
- The network takes as input 28x28 images represented as 784D vectors.
- The output is a 10D vector giving the probability of the image representing any of the 10 digits.
- There are 50'000 training pairs of images and the corresponding label, 10'000 validation pairs, and 5'000 testing pairs.

MNIST Results

nIn =784

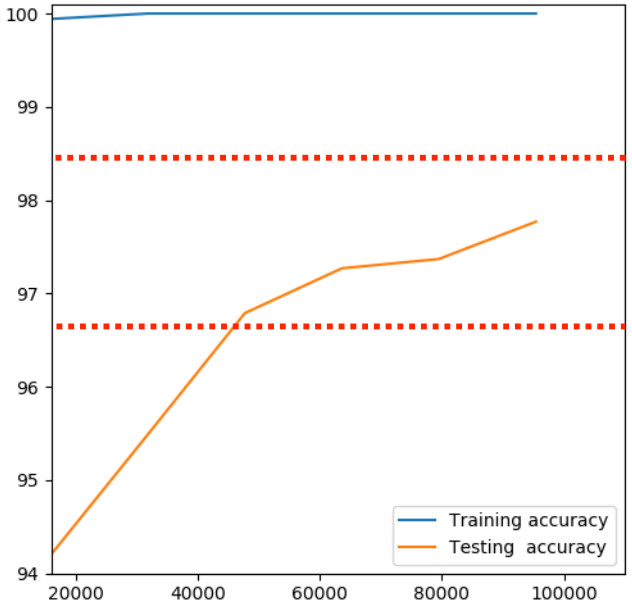
nOut = 10

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 ….

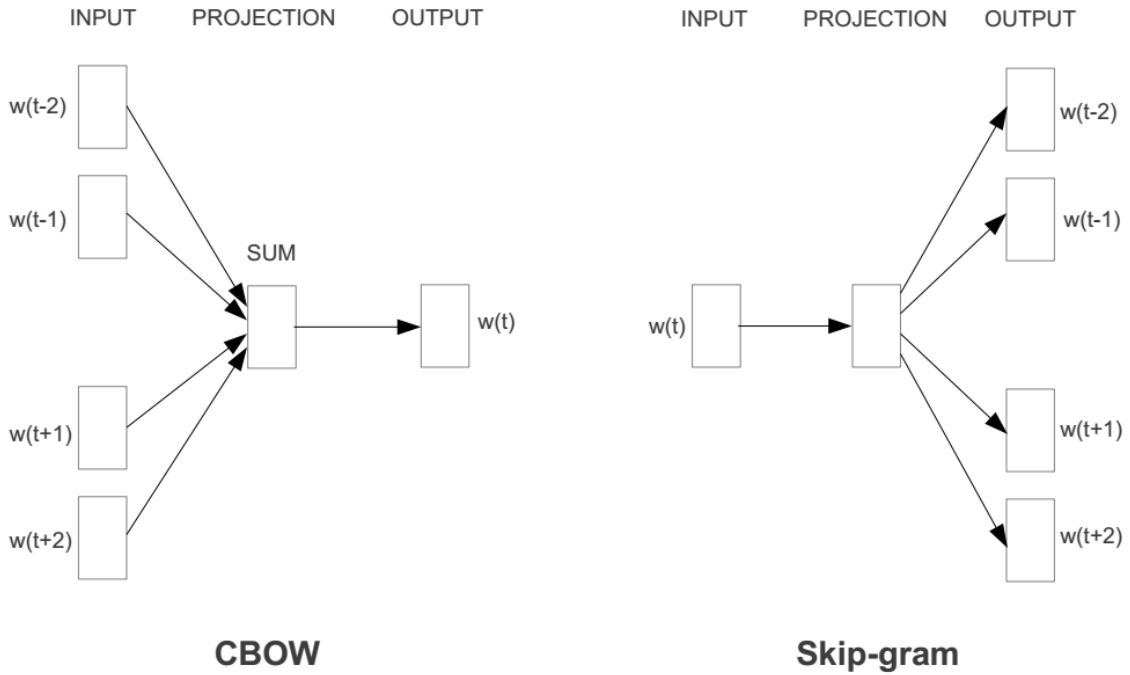
Optional: Converting Words to Vectors

- 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*)

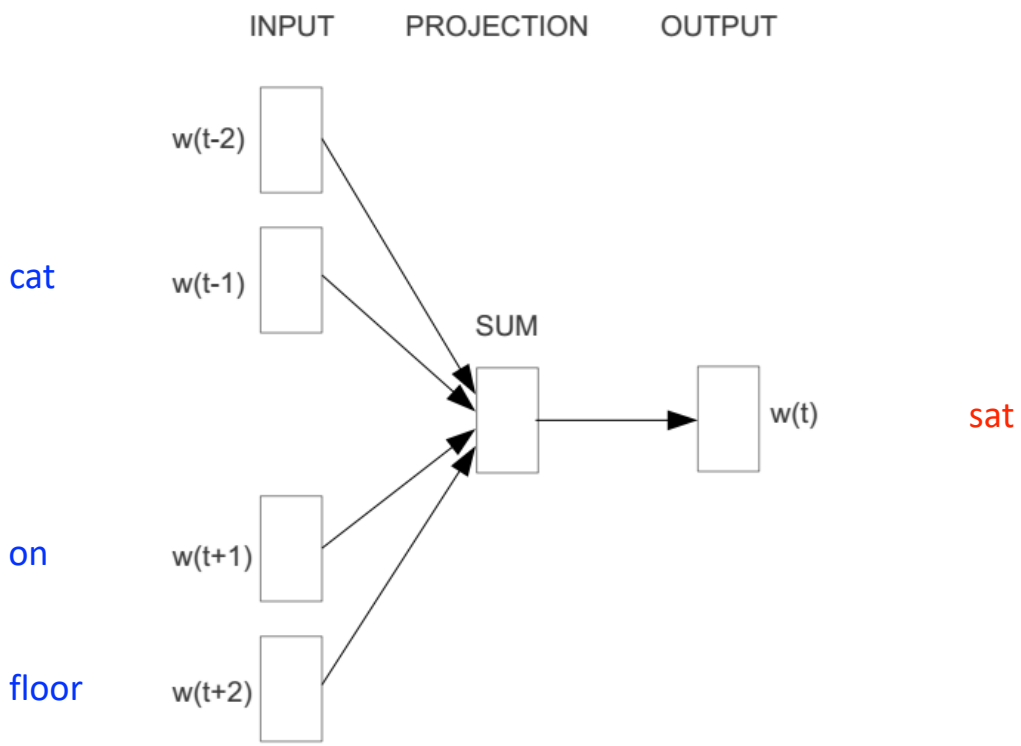


Two basic neural network models:

- 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.

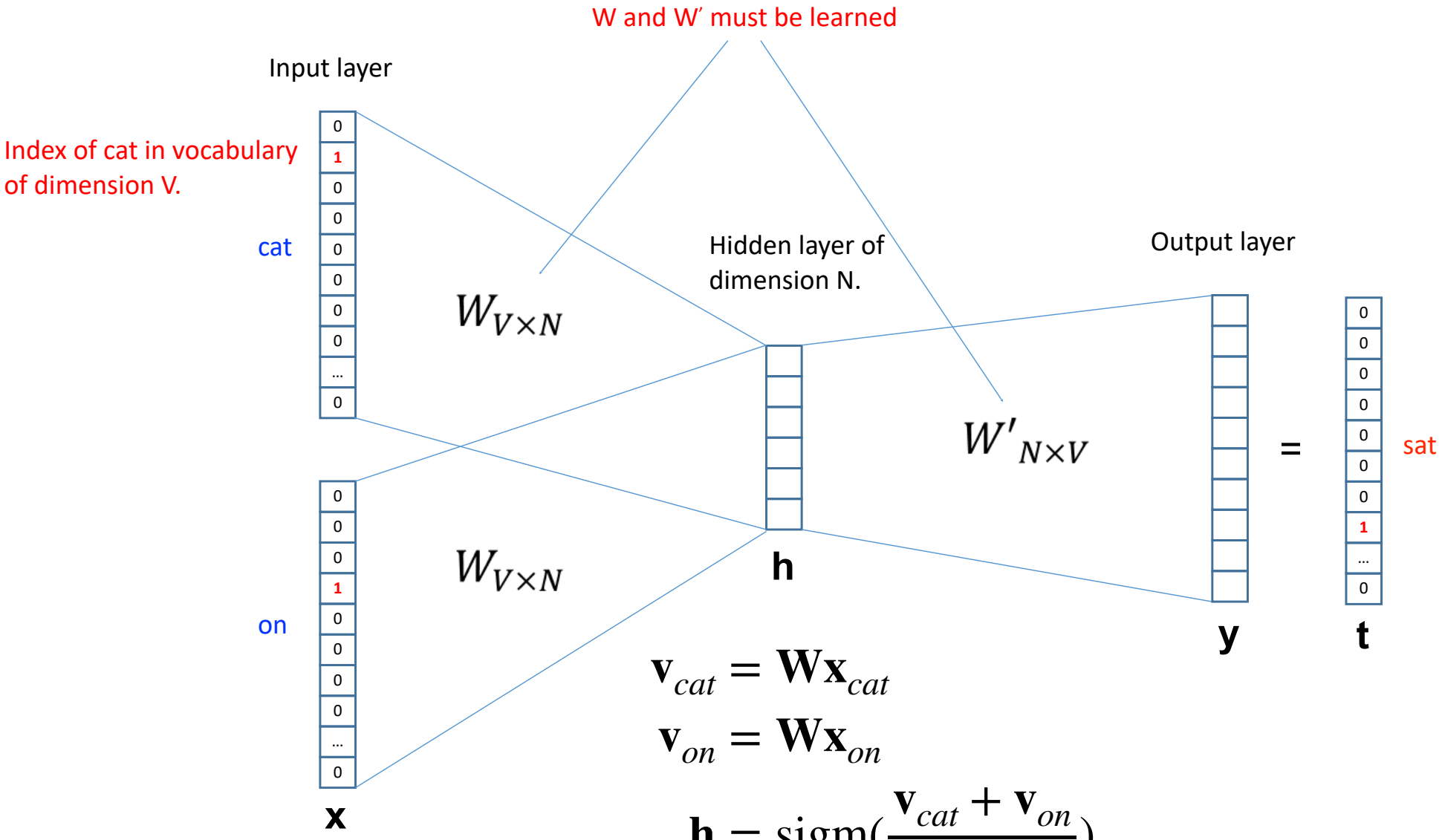
Optional: Continuous Bag of Words

The cat sat on the floor.



sat should be predicted from the words around it.

Optional: Window of Size 3



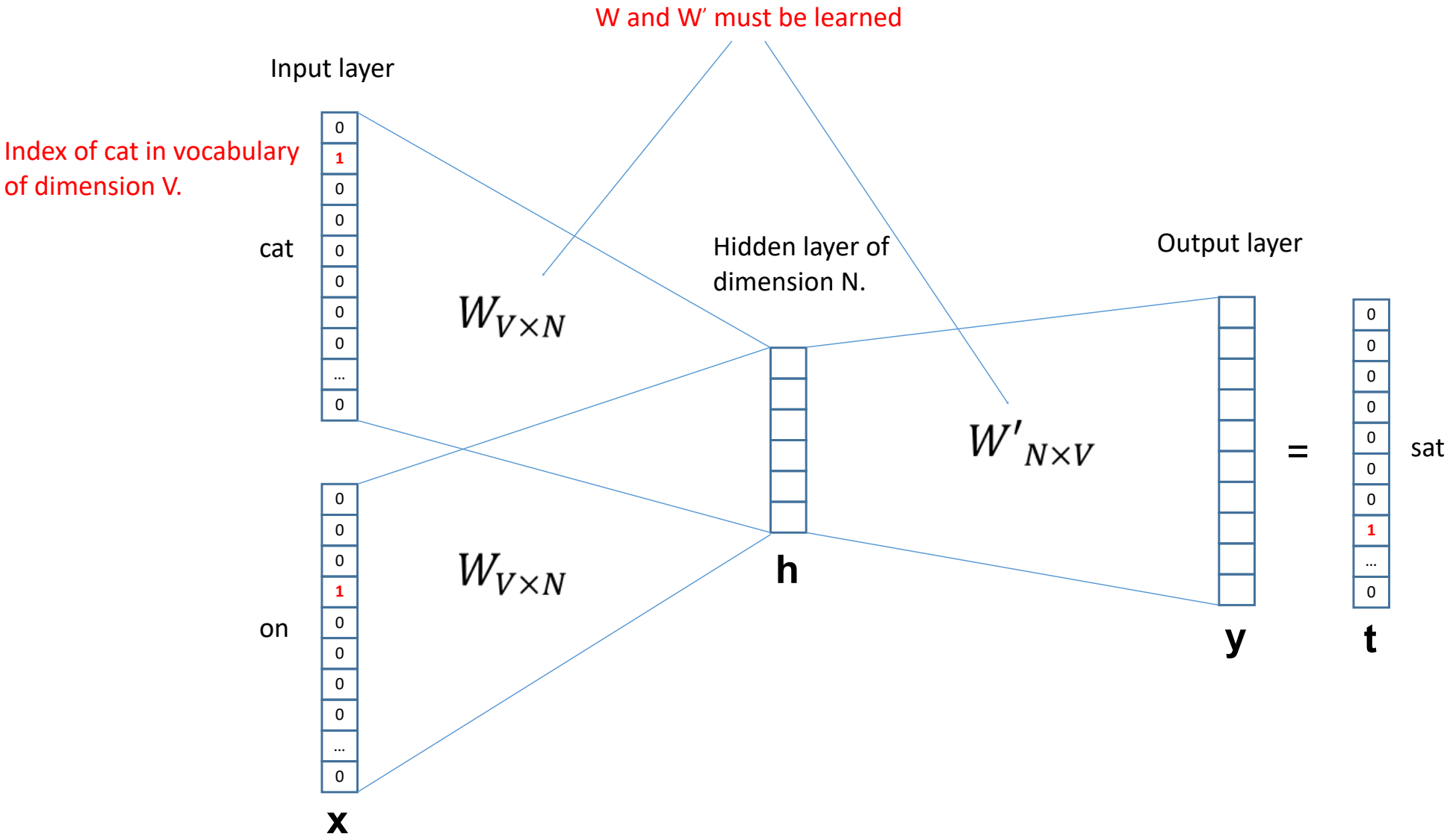
$$\mathbf{v}_{cat} = \mathbf{W}\mathbf{x}_{cat}$$

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

$$\mathbf{h} = \text{sigm}\left(\frac{\mathbf{v}_{cat} + \mathbf{v}_{on}}{2}\right)$$

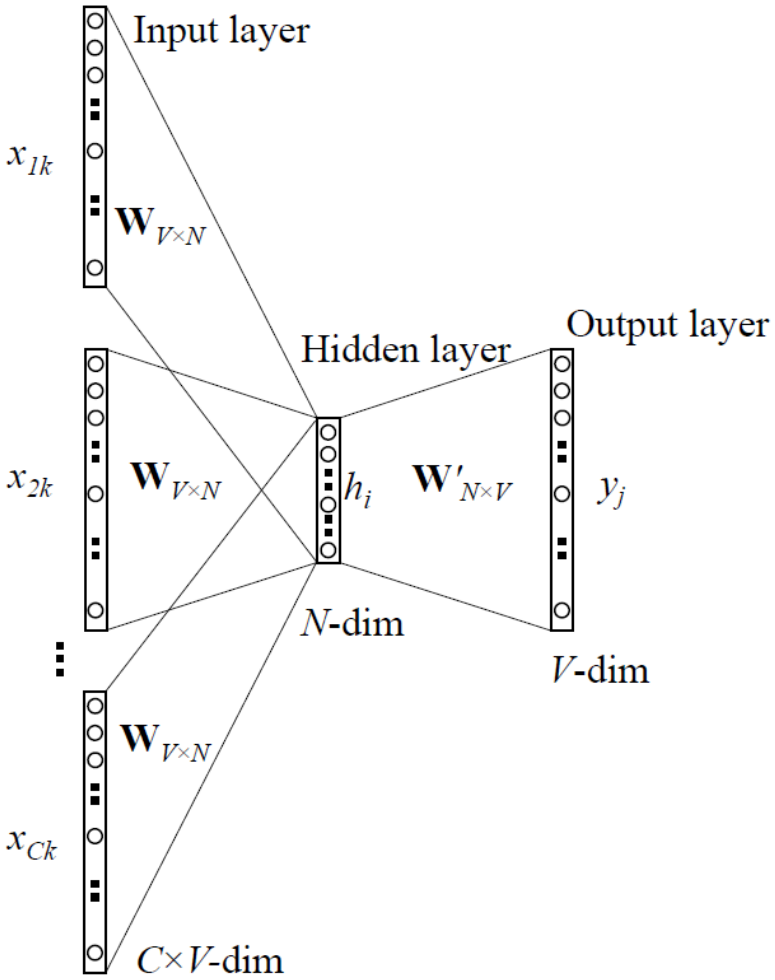
$$\mathbf{y} = \text{softmax}(\mathbf{W}'\mathbf{h})$$

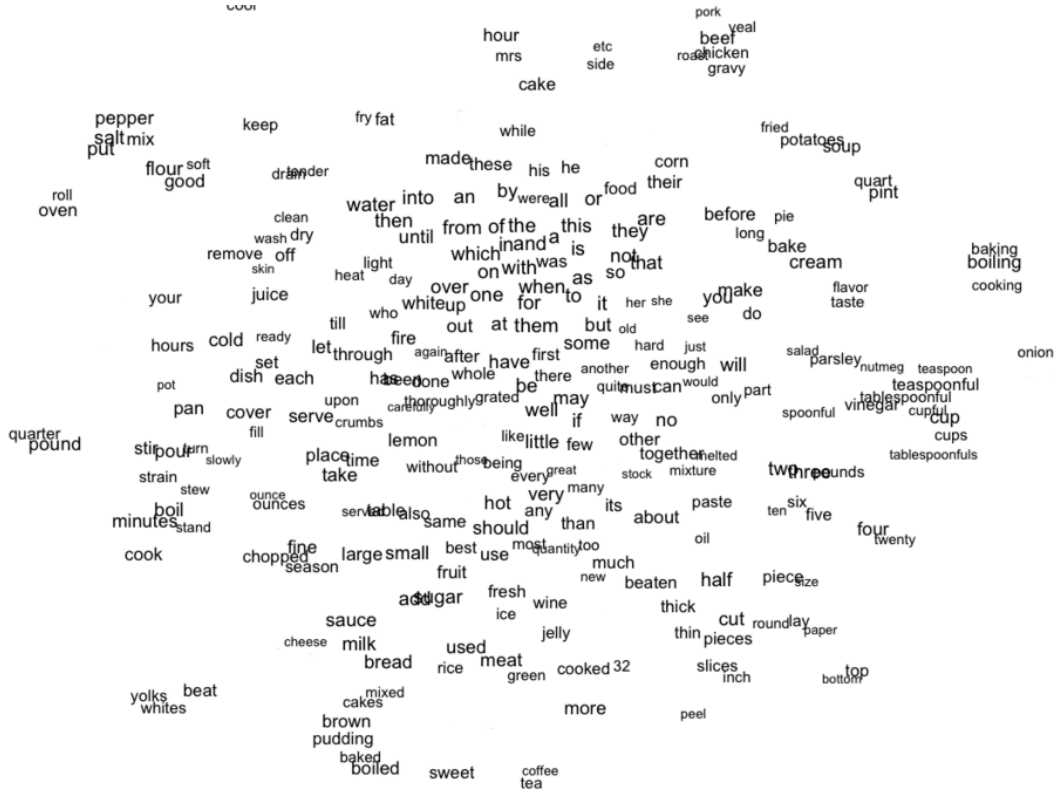
Optional: Window of Size 3



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.

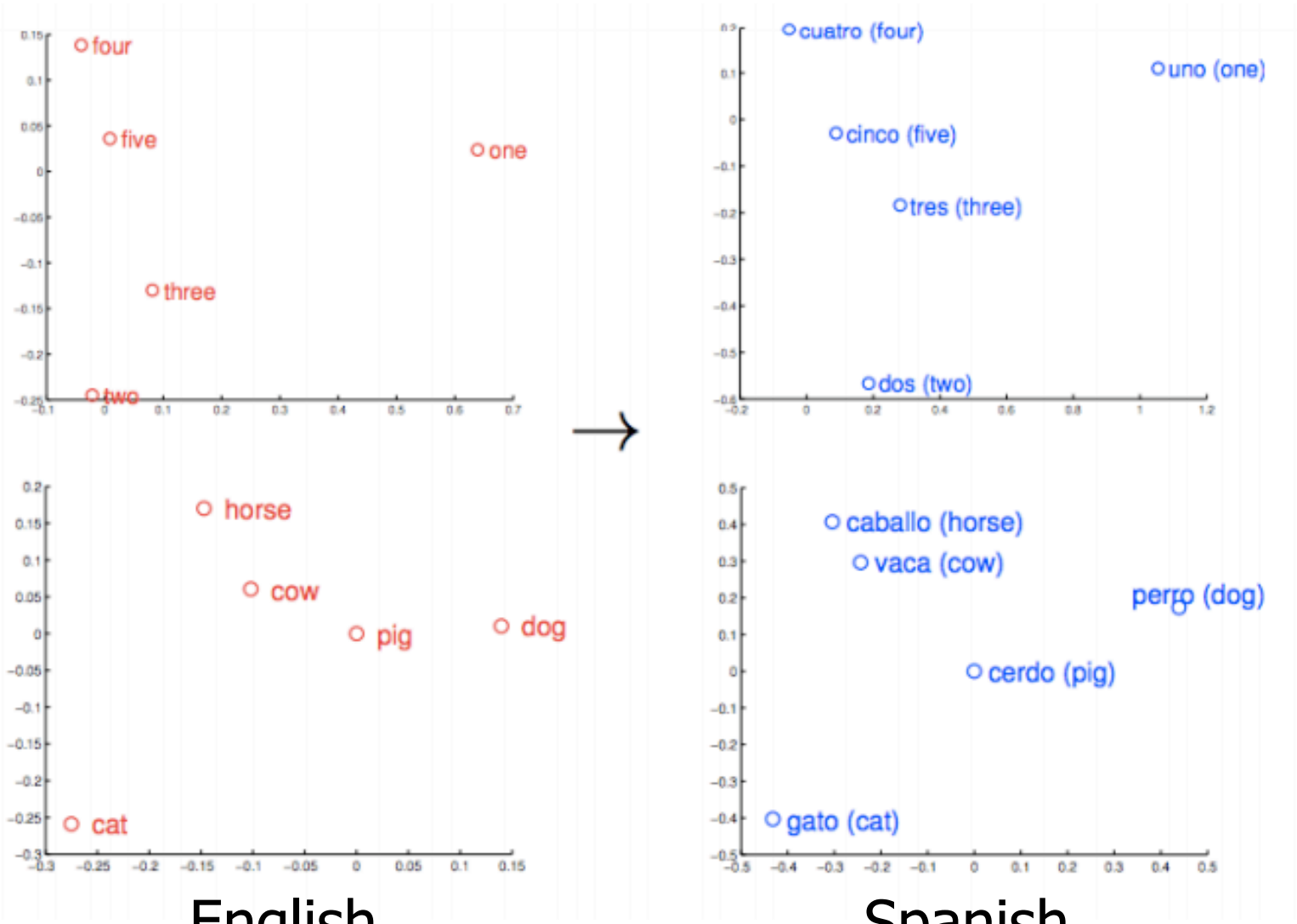
Optional: Code for Windows of Arbitrary Sizes

```
class WordNet(nn.Module):

    def __init__(self,nh,nw):

        super(WordNet, self).__init__()
        self.l1 = nn.Linear(nw,nh,bias=False)
        self.l2 = nn.Linear(nh,nw,bias=False)

    def forward (self,x):

        nb,nc,nw=x.size()

        h = self.l1(x[:,0])
        for i in range(1,nc):
            h = h+self.l1(x[:,i])
        h = sigm(h / nc)
        return self.l2(h)
```

nw: Number of words.
nh: Size of the codes.

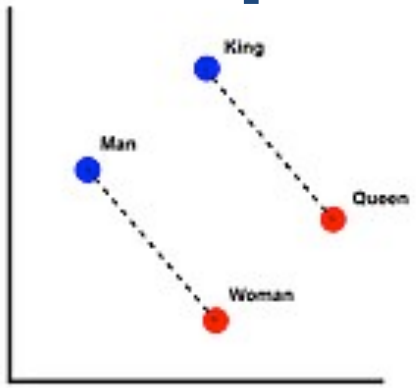
nc: Context size.

Optional: Geometry of Words



English Spanish

Optional: Similarities in Latent Space



Training on Google News Vocab:

- Beijing is to China what Bern is to Switzerland

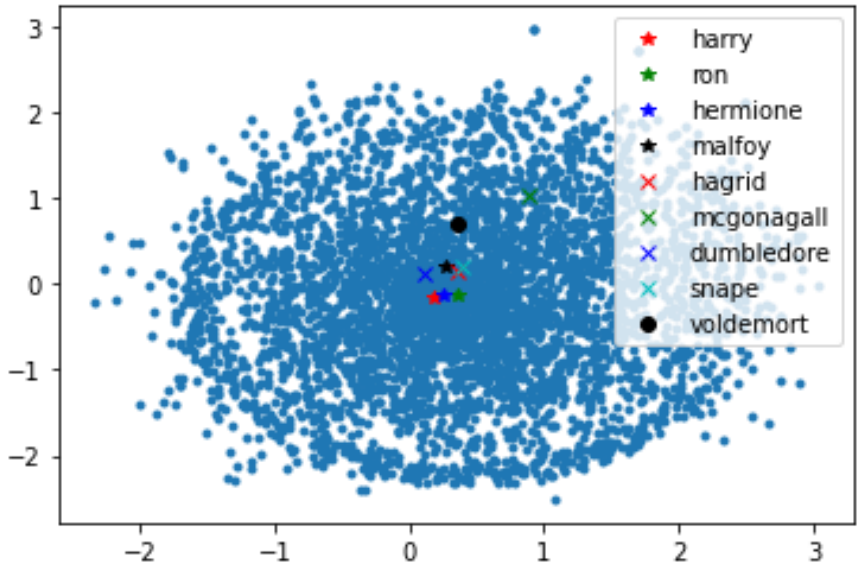
Testing:

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

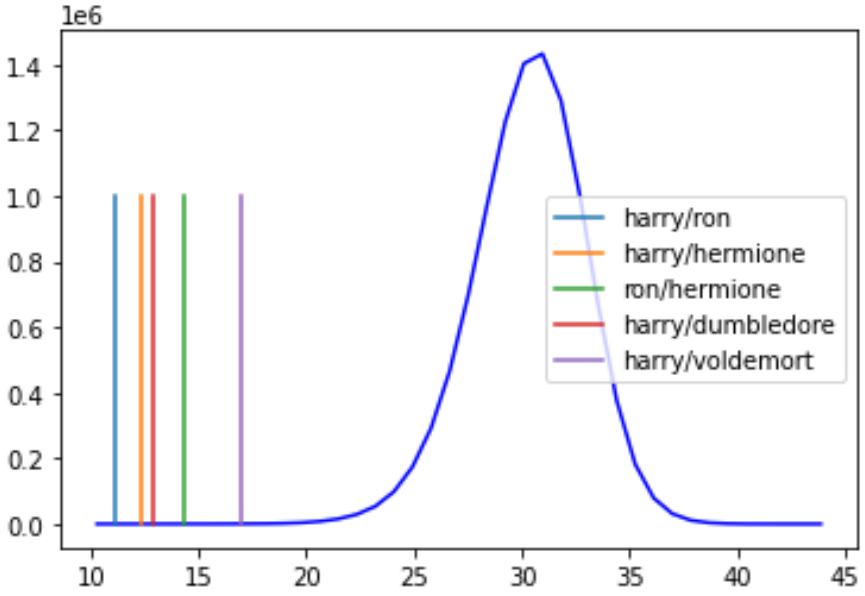
Not bad given that word2vec knows **nothing** about syntax, about the world, or even about logic!!

Optional: It's Magic!

Word2Vec trained on the Harry Potter books:



Tsne Visualization of the embedding

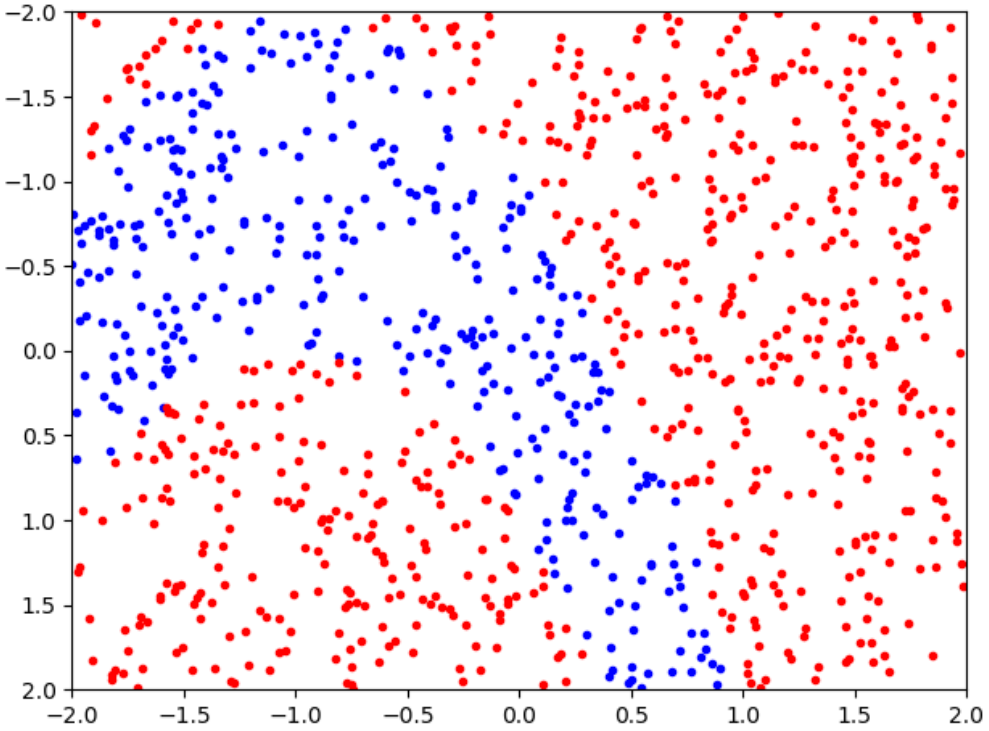


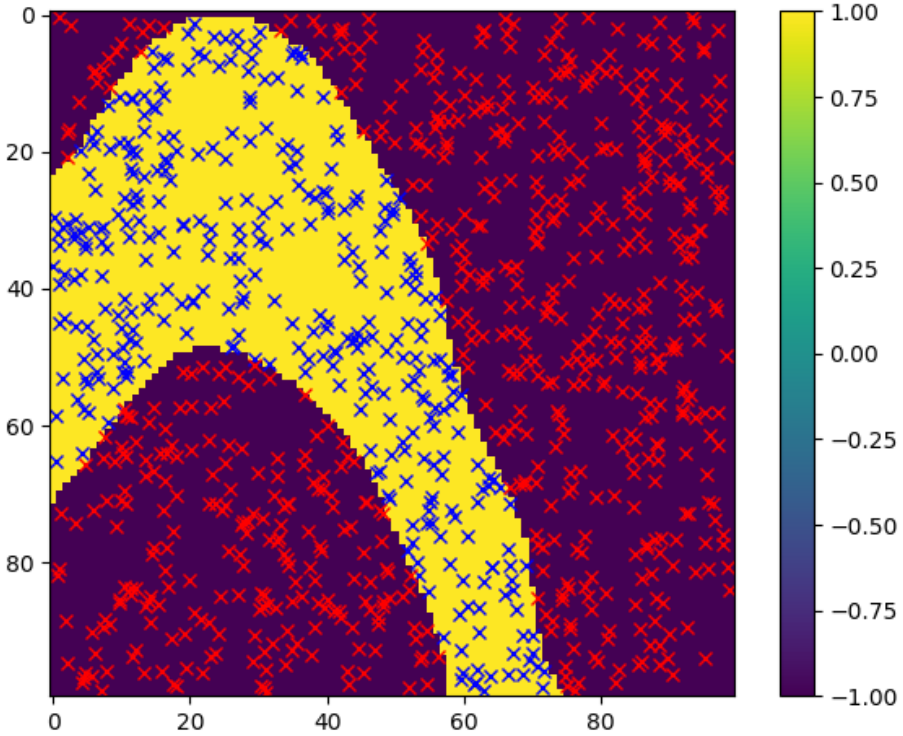
Distances between word pairs

- The reasons for successful word embedding learning in the word2vec framework are poorly understood.
- One potential explanation is that the objective function being minimized results in words occurring in similar contexts to have similar embeddings.

But it works! And the same can be said of more recent techniques.
We'll get back to that when we talk about transformers and LLMs.

From Classification to Regression





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

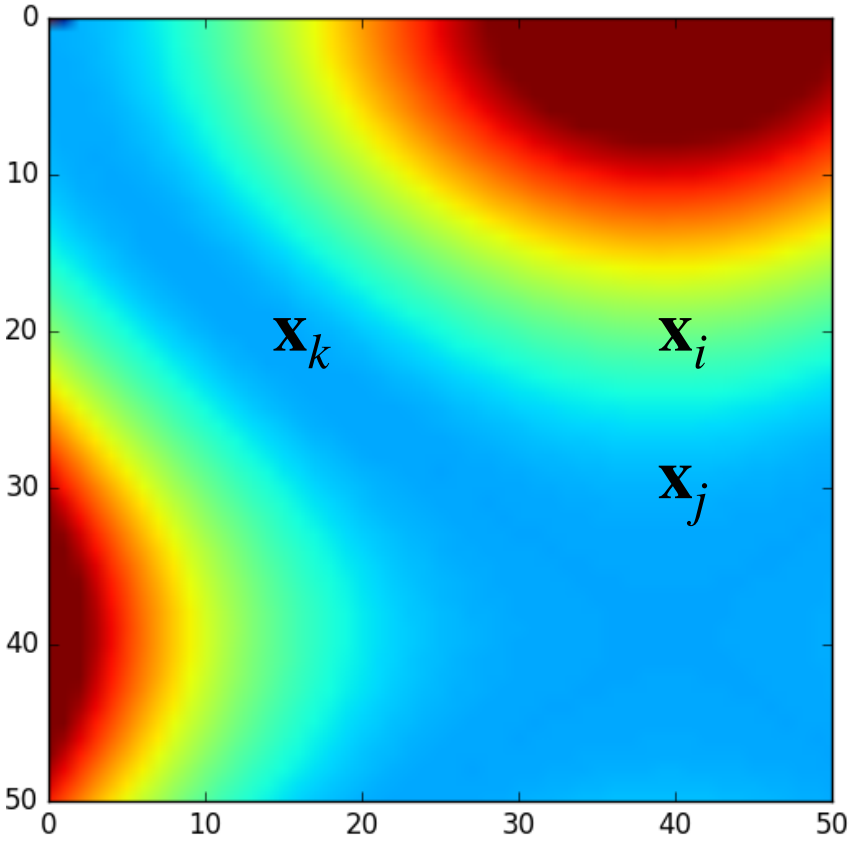
Negative: Otherwise

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

- 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.

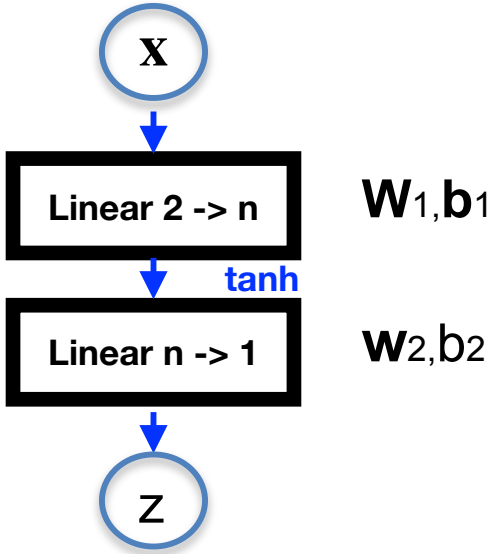
—> This raises a theoretical question: When the probability function is known, how well can a network approximate it?

Approximating the Rosenbrock Function



$$P(\mathbf{x} \text{ in positive class}) = \begin{cases} 1.0 \text{ if } r(\mathbf{x}) < 0.5 \\ 0.0 \text{ otherwise} \end{cases}$$

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



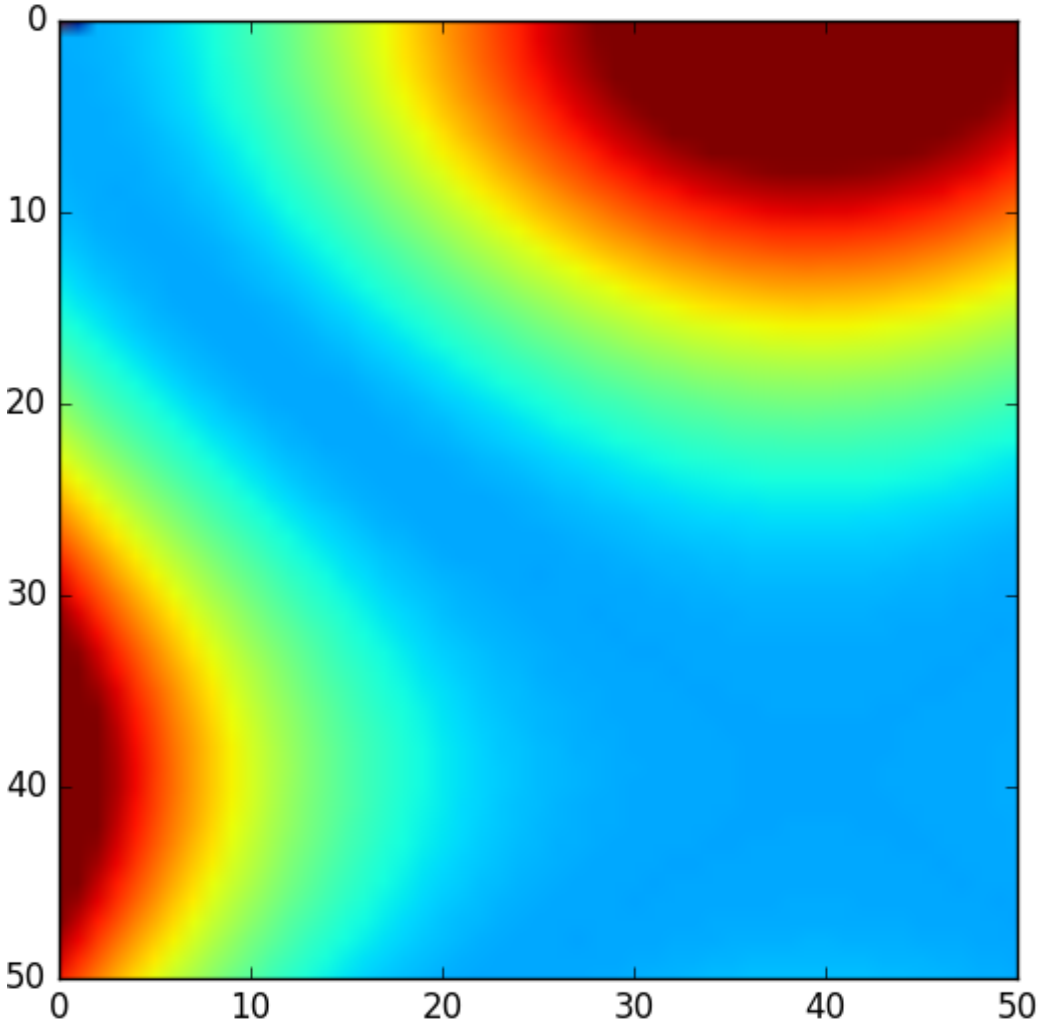
$$y(\mathbf{x}, \tilde{\mathbf{w}}) = \mathbf{w}_2 \tanh(\mathbf{W}_1\mathbf{x} + \mathbf{b}_1) + b_2$$

Problem statement: Given $(\{\mathbf{x}_1, z_1 = r(\mathbf{x_1})\}, \ldots, \{\mathbf{x}_n, z_n = r(\mathbf{x_n})\})$, minimize

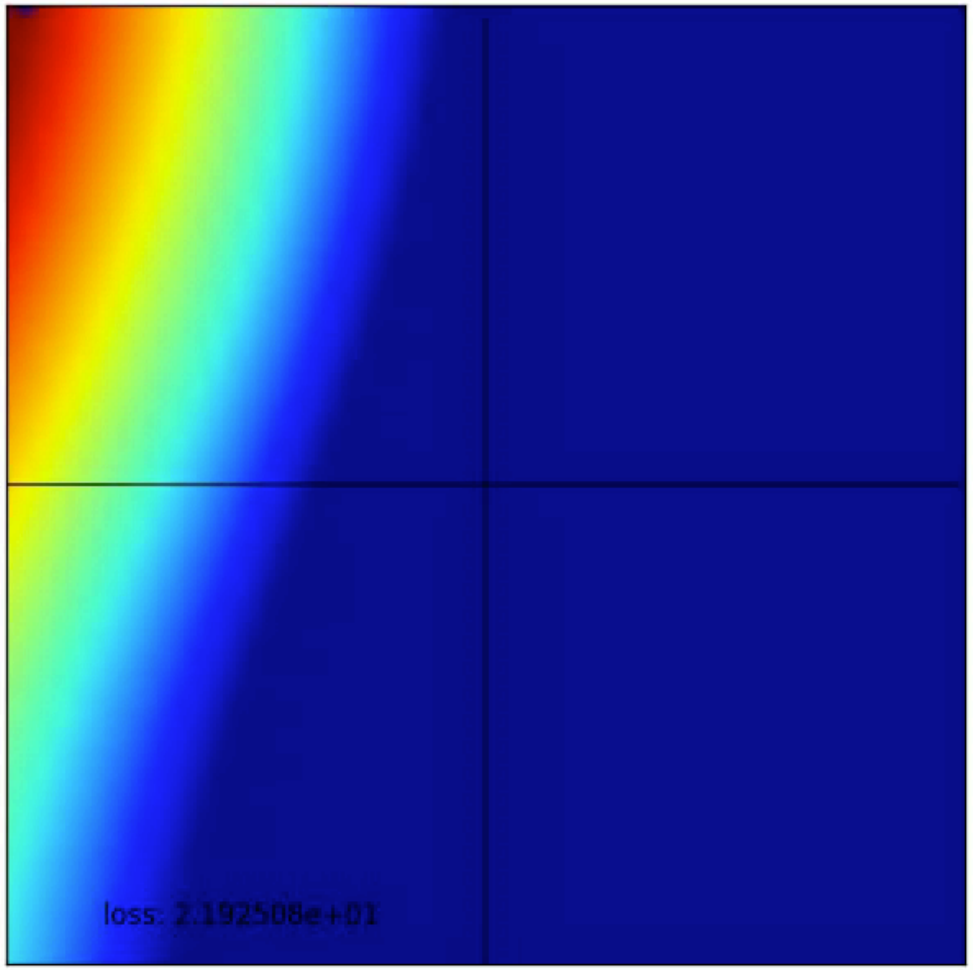
$$\sum_i (z_i - y(\mathbf{x}_i; \tilde{\mathbf{w}}))^2$$

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

Regressing the Rosenbrock Function



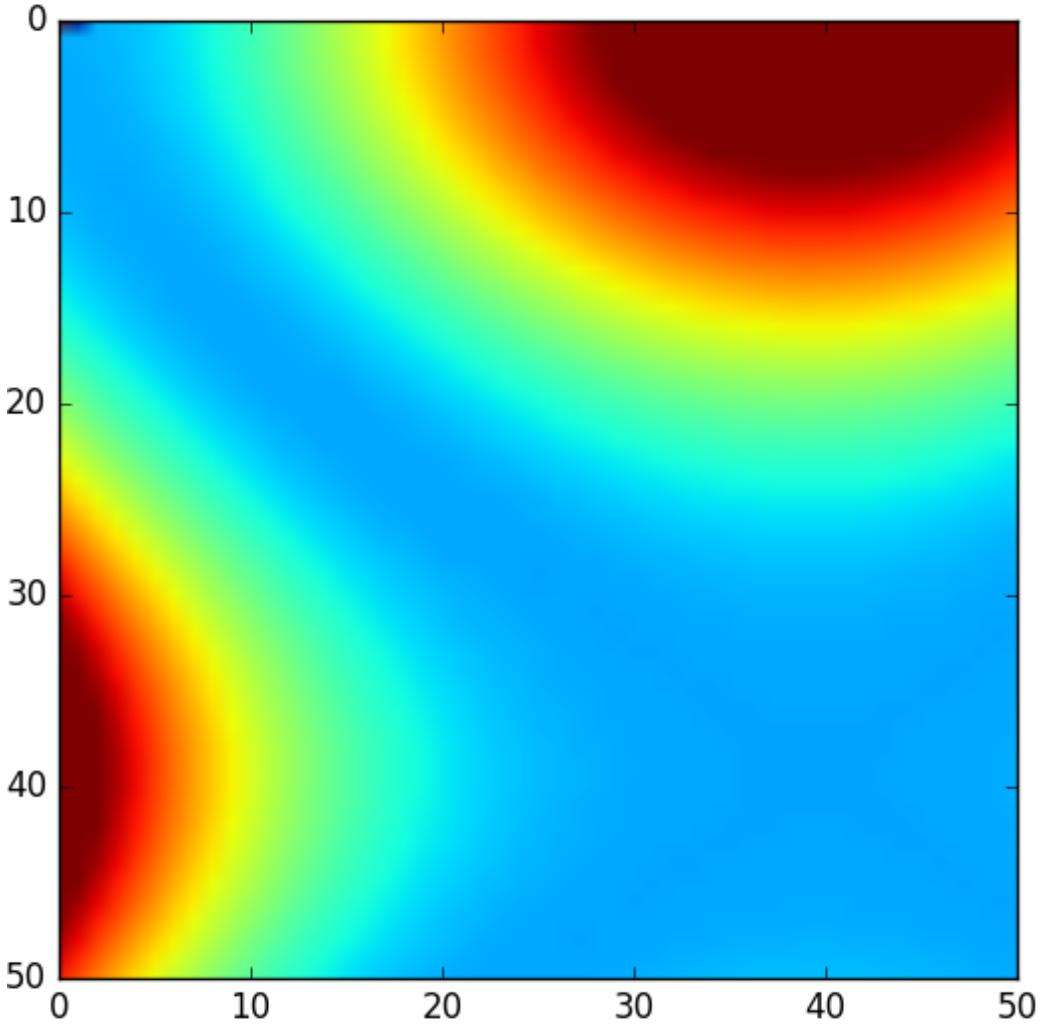
$$z = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



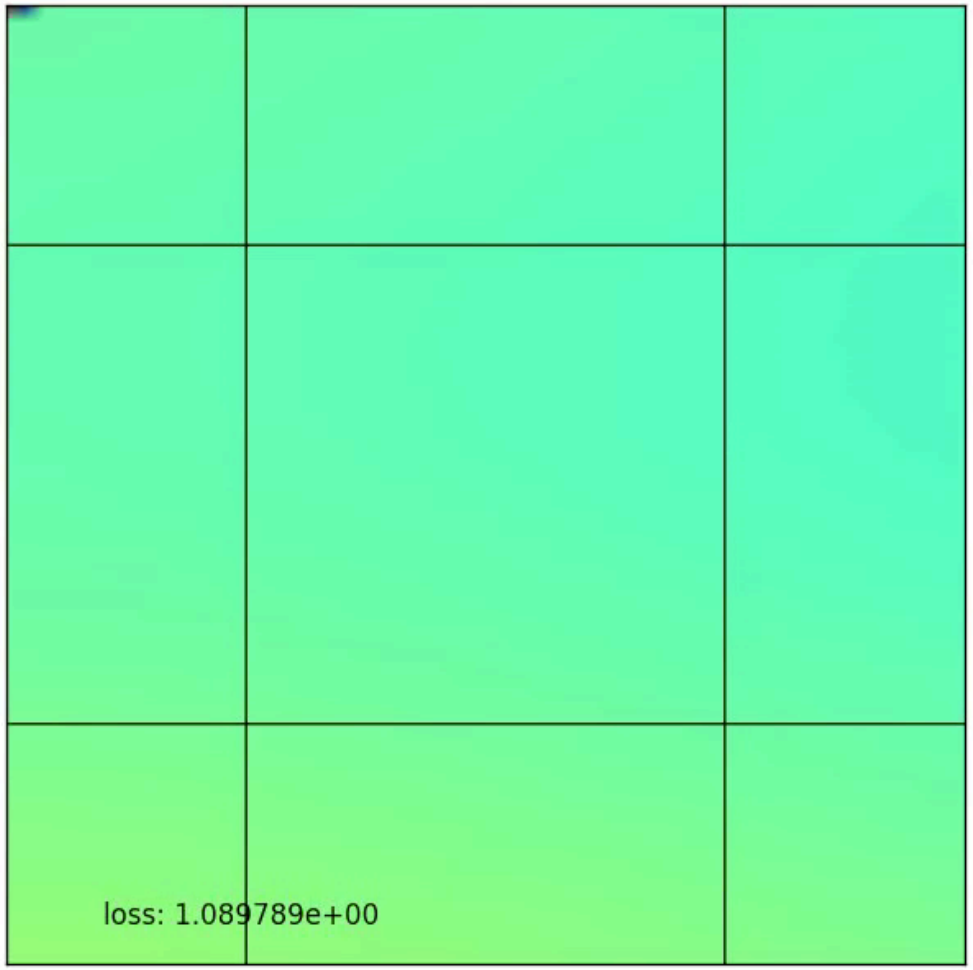
3-node hidden layer

—> 3 nodes is not quite enough.

Regressing the Rosenbrock Function



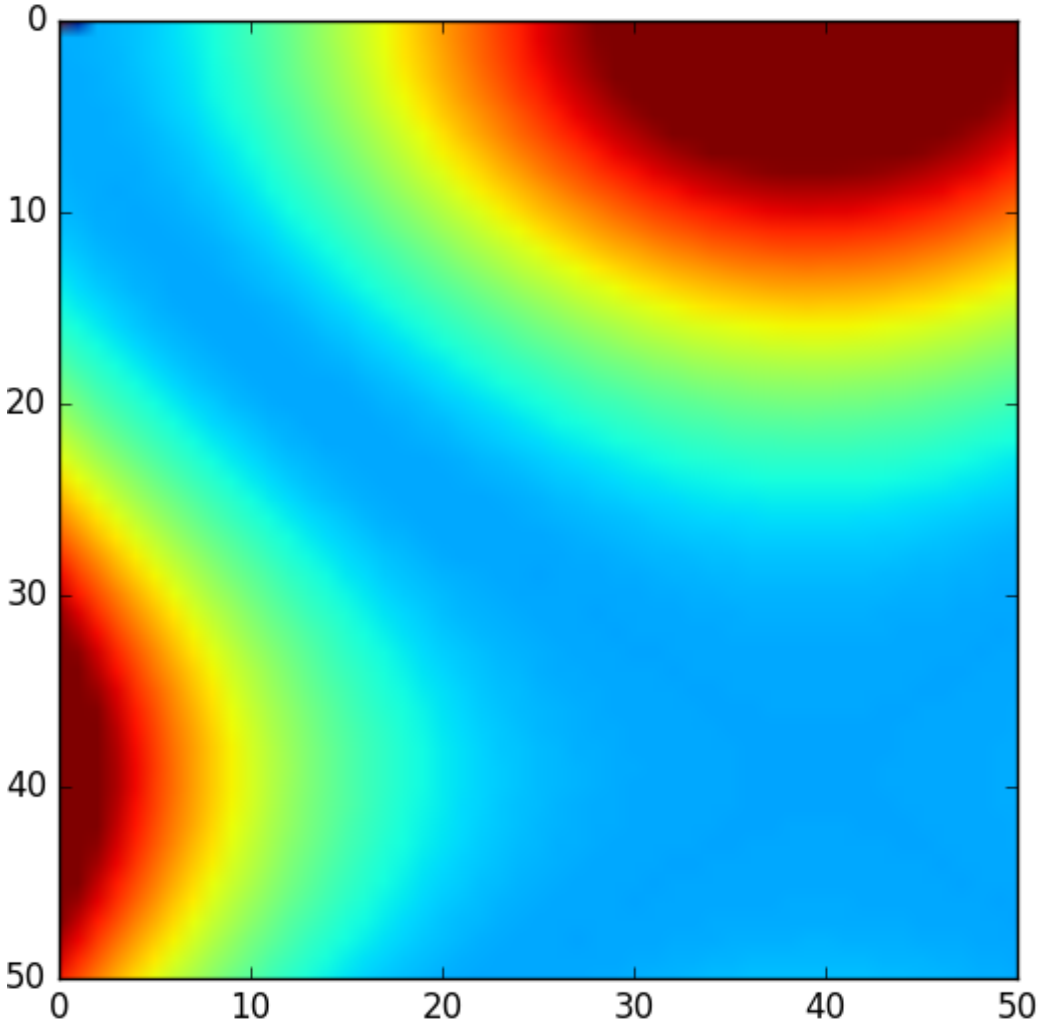
$$z = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



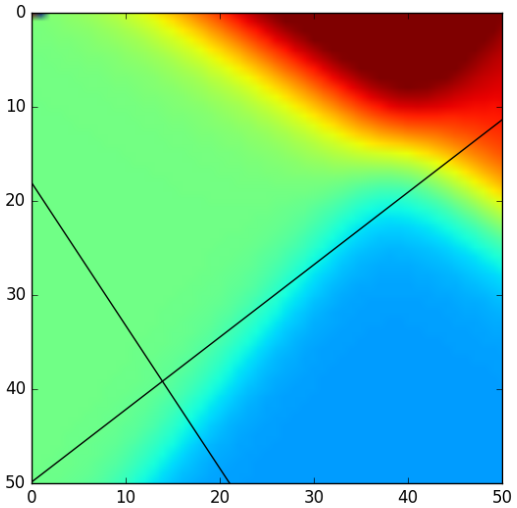
4-node hidden layer

—> 4 nodes is better.

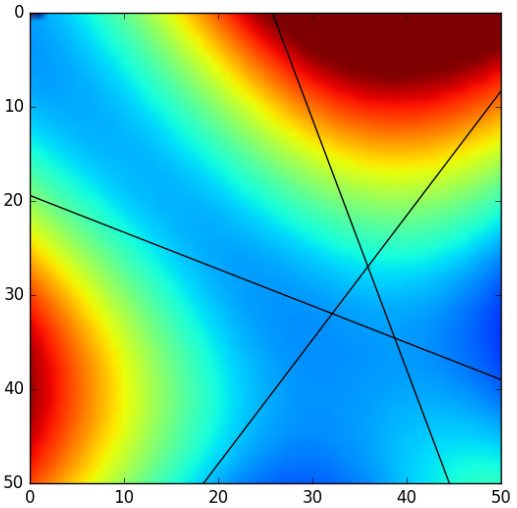
Accuracy as a Function of the Number of Nodes



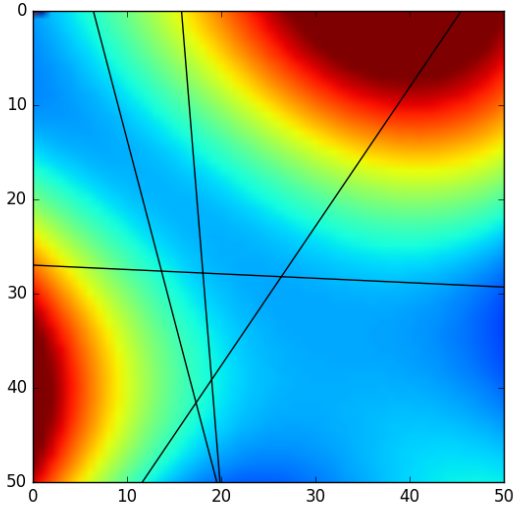
$$z = 100(x_2 - x_1^2)^2 + (1 - x_1)^2$$



2 nodes -> loss 3.02e-01



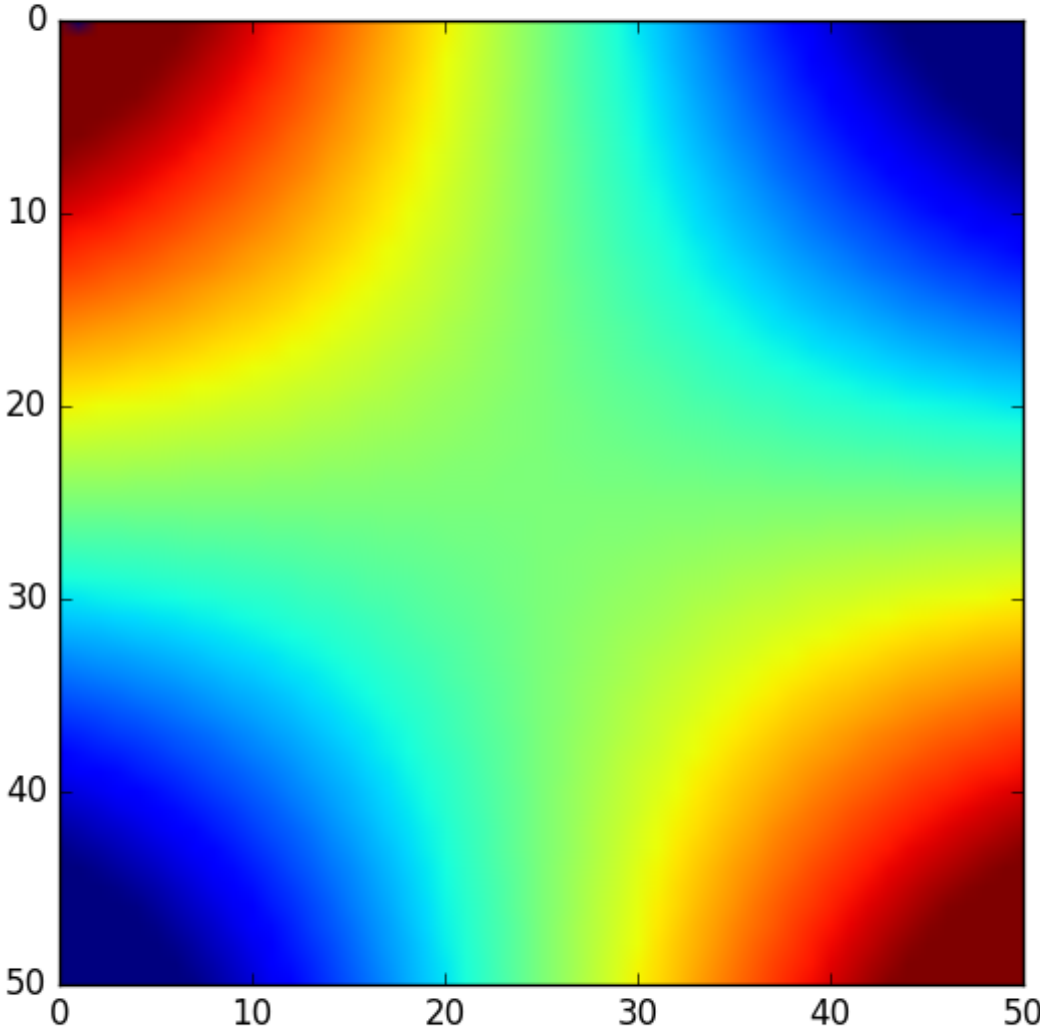
3 nodes -> loss 2.08e-03



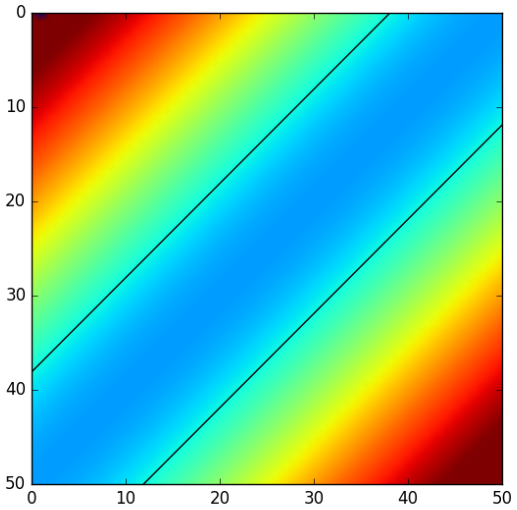
4 nodes -> loss 8.27e-03

—> The more nodes the more accurate the approximation.

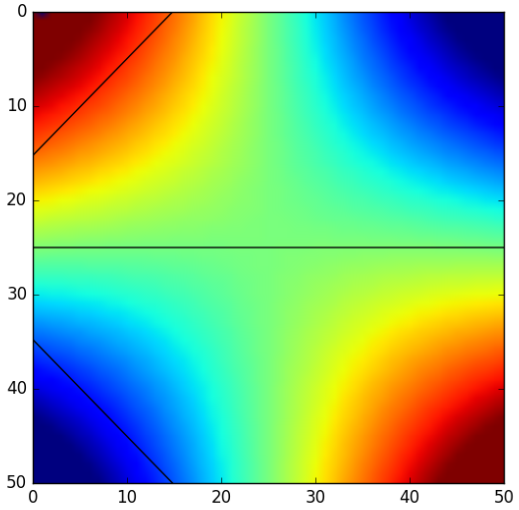
Accuracy as a Function of the Number of Nodes



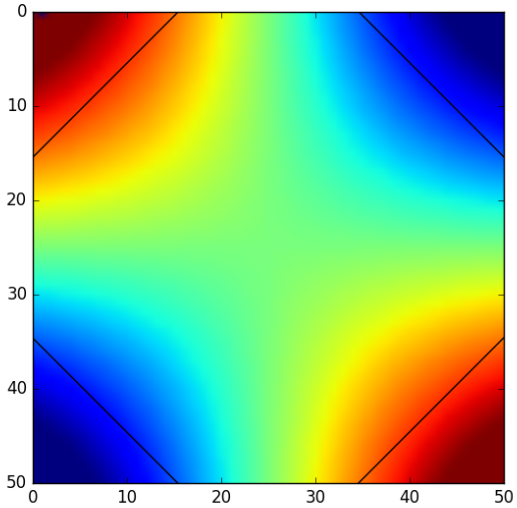
$$z = sin(x)sin(y)$$



2 nodes -> loss 2.61e-01



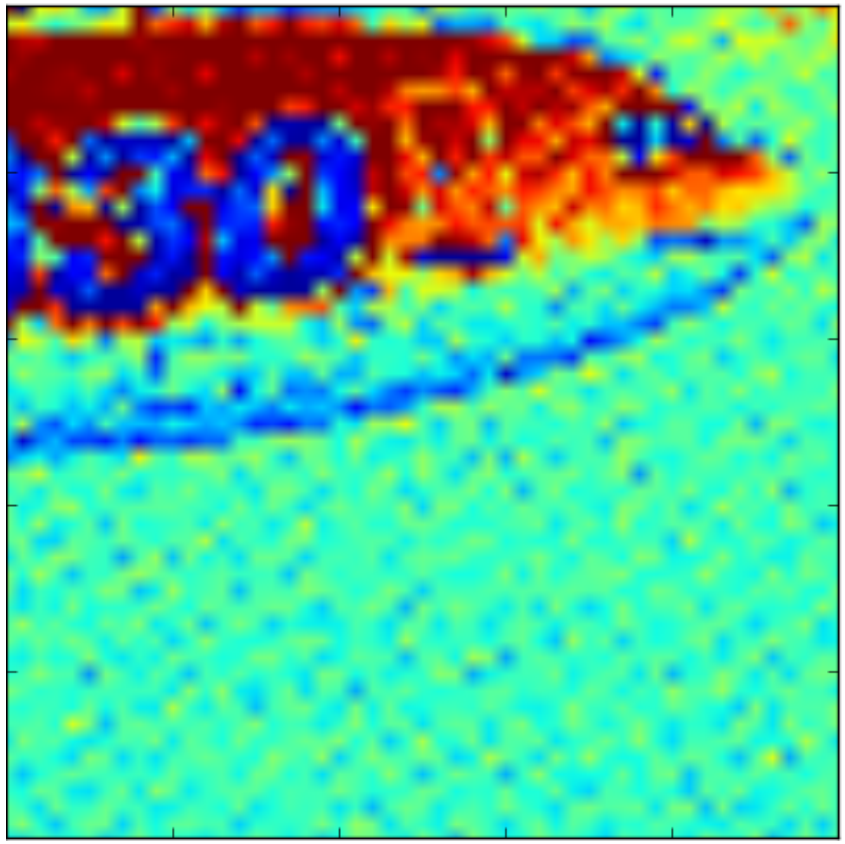
3 nodes -> loss 2.51e-04

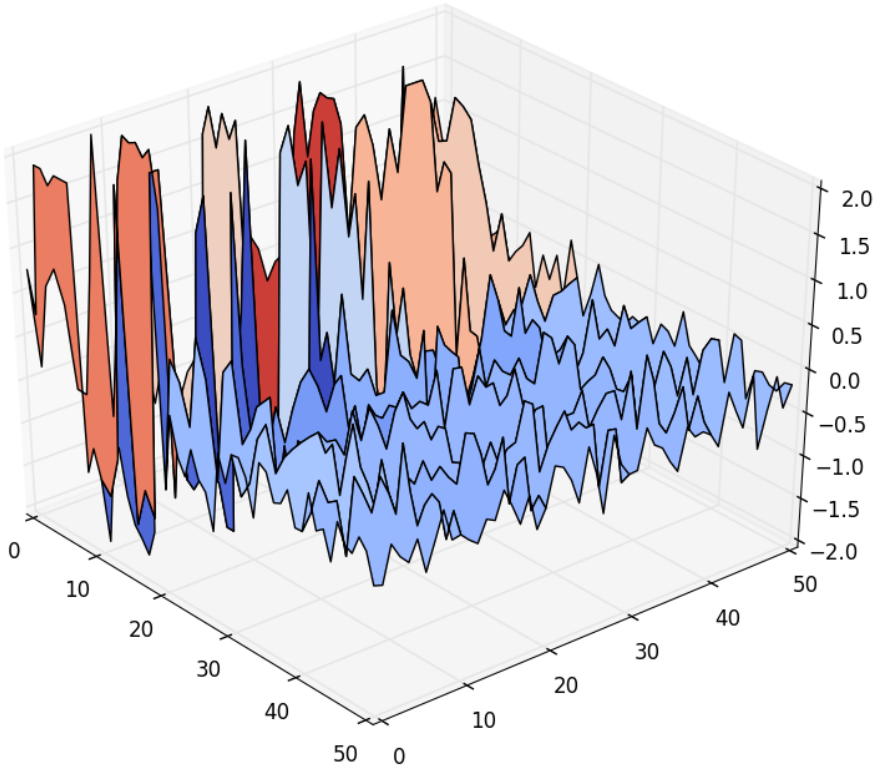


4 nodes -> loss 3.07e-07

—> The more nodes the more accurate the approximation.

Image as a 3D Surface



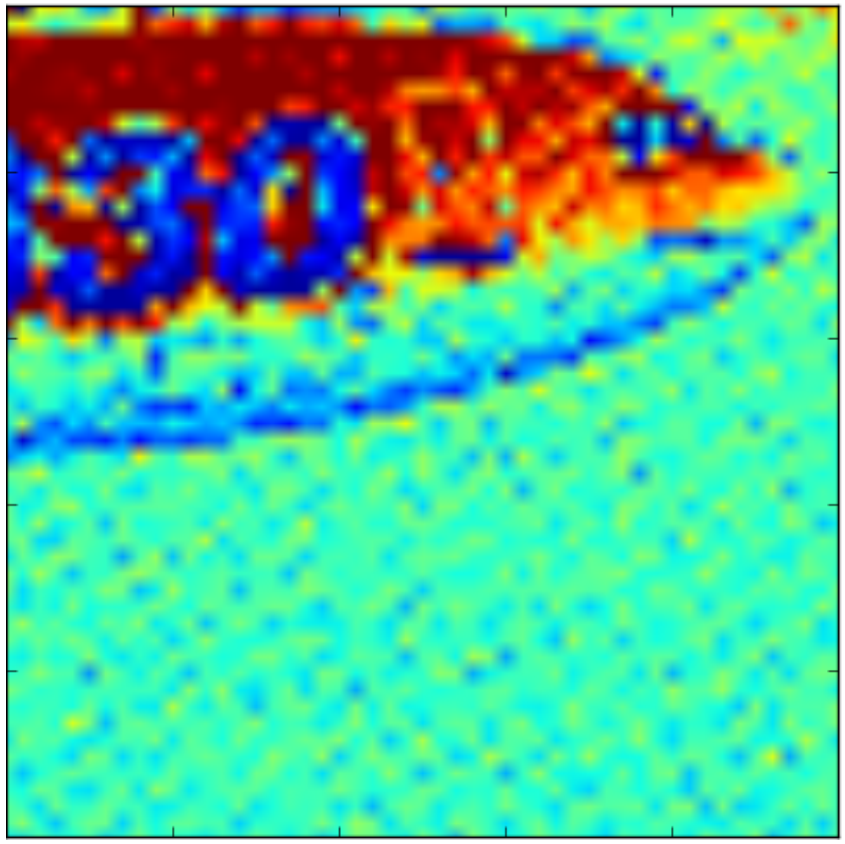


$$I = f(x, y)$$

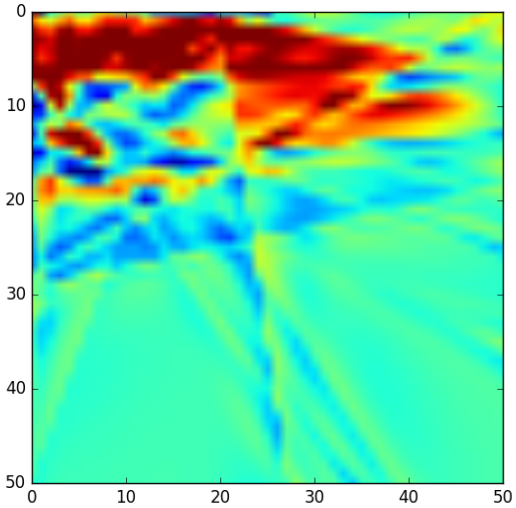
We treat the image as a surface:

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

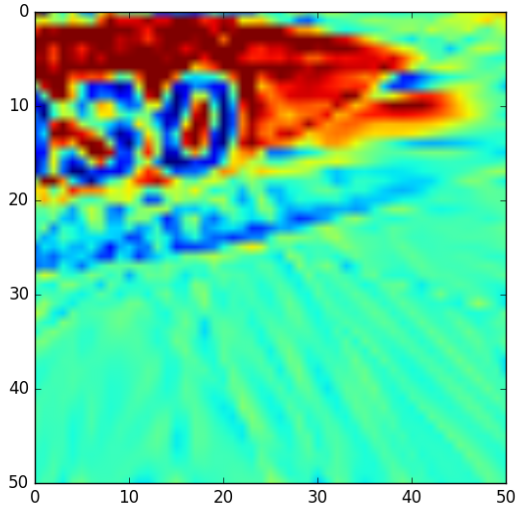
More Complex Surface



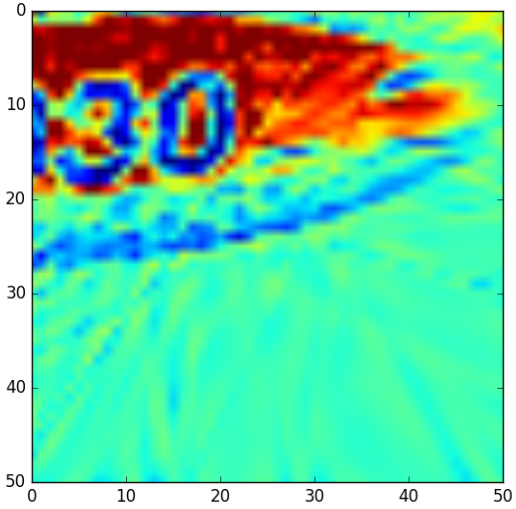
$$I = f(x, y)$$



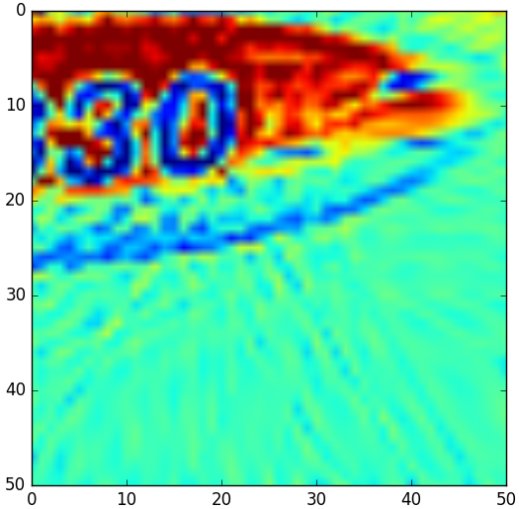
50 nodes -> loss 3.65e-01



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

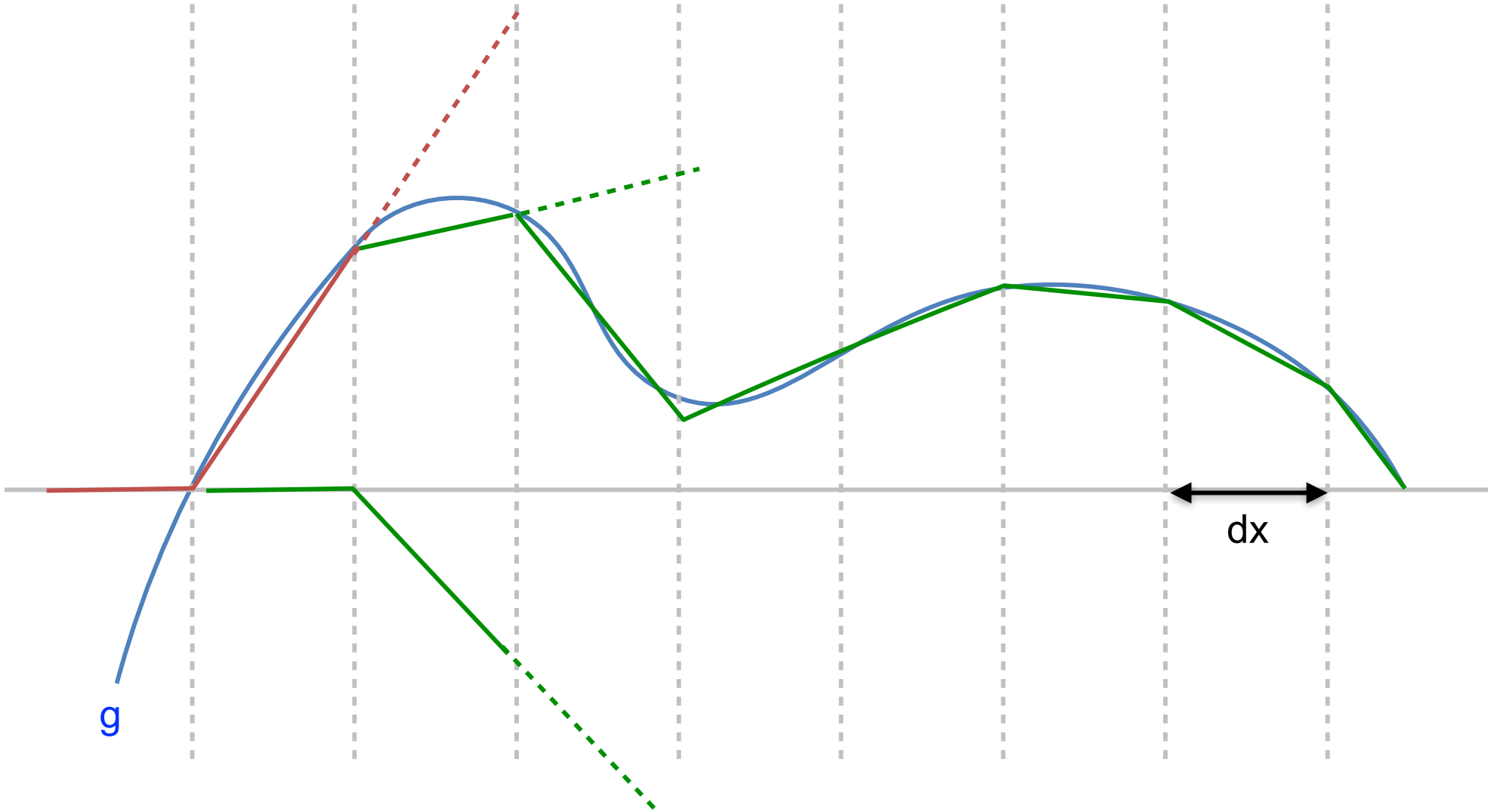
A feedforward network with a linear output layer and at least one hidden layer with any 'squashing' activation function (e.g. logistic sigmoid) can approximate any Borel measurable function (from one finite-dimensional space to another) with any desired nonzero error.

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



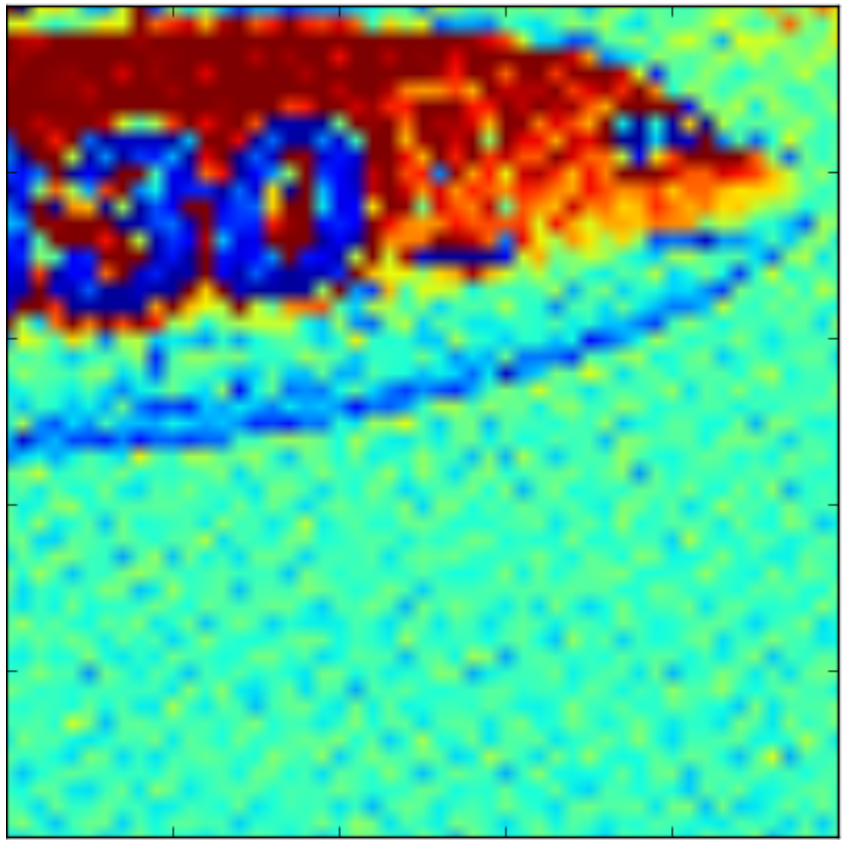
$f(x) = \sigma(w_1 x + b_1) + \sigma(w_2 x + b_2) + \ldots + \sigma(w_n x + b_n)$

When dx —> 0, f —> g.

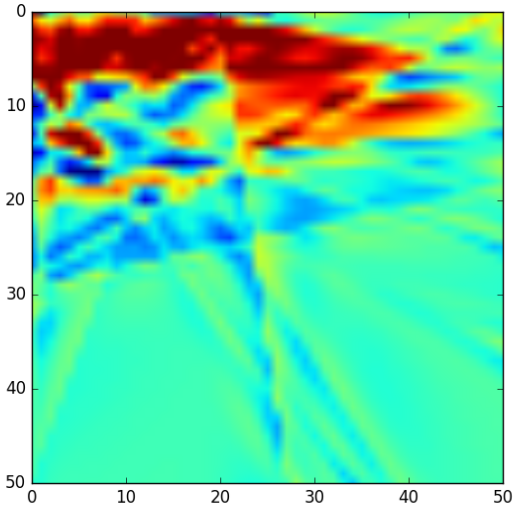
Universal Approximation Theorem in nD

- 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.

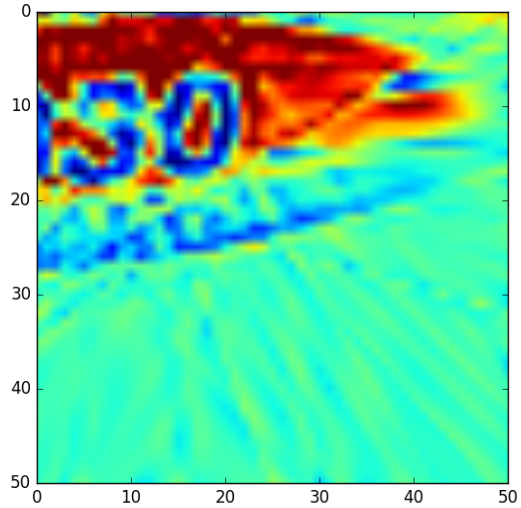
More Complex Surface



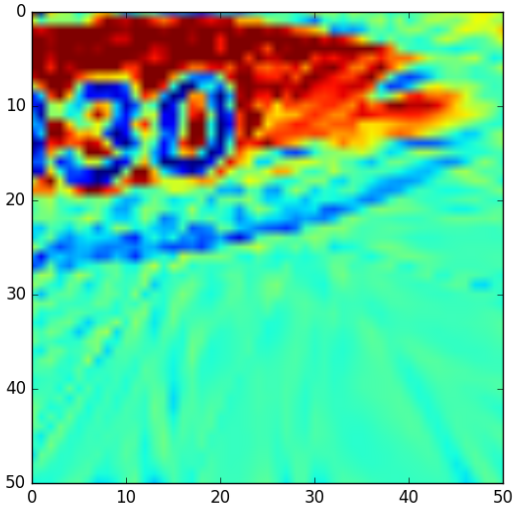
$$I = f(x, y)$$



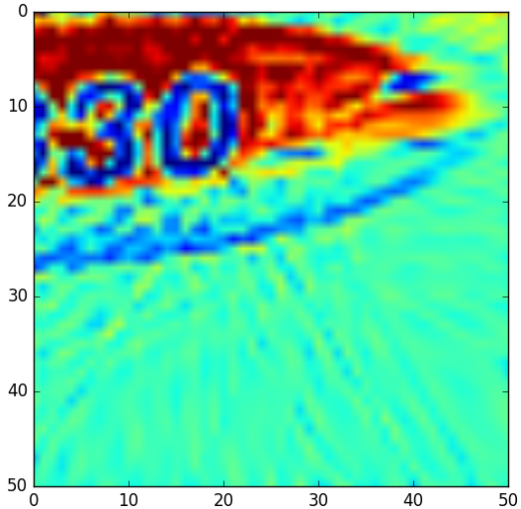
50 nodes -> loss 3.65e-01



100 nodes -> loss 2.50e-01



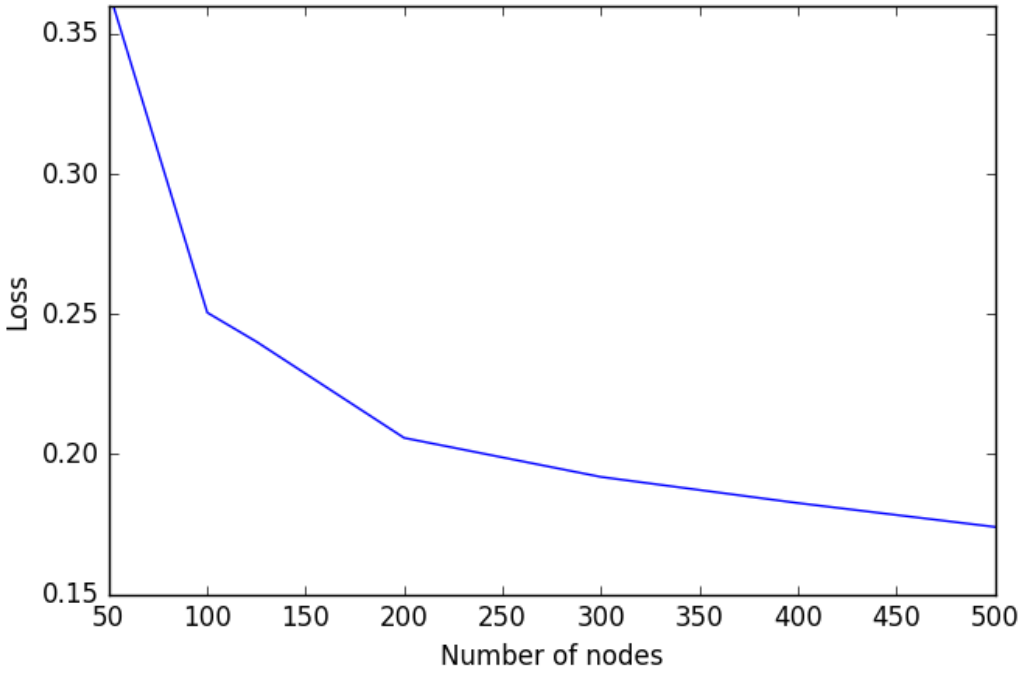
125 nodes -> loss 2.40e-01

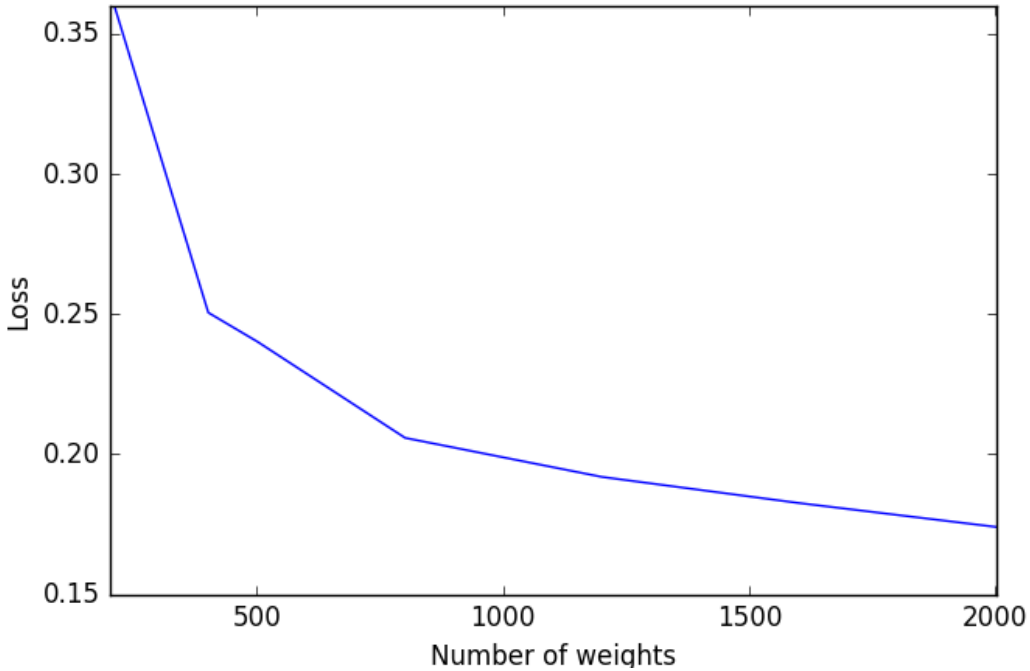


300 nodes -> loss 1.92e-01

—> The more nodes the more accurate the approximation.

In Practice

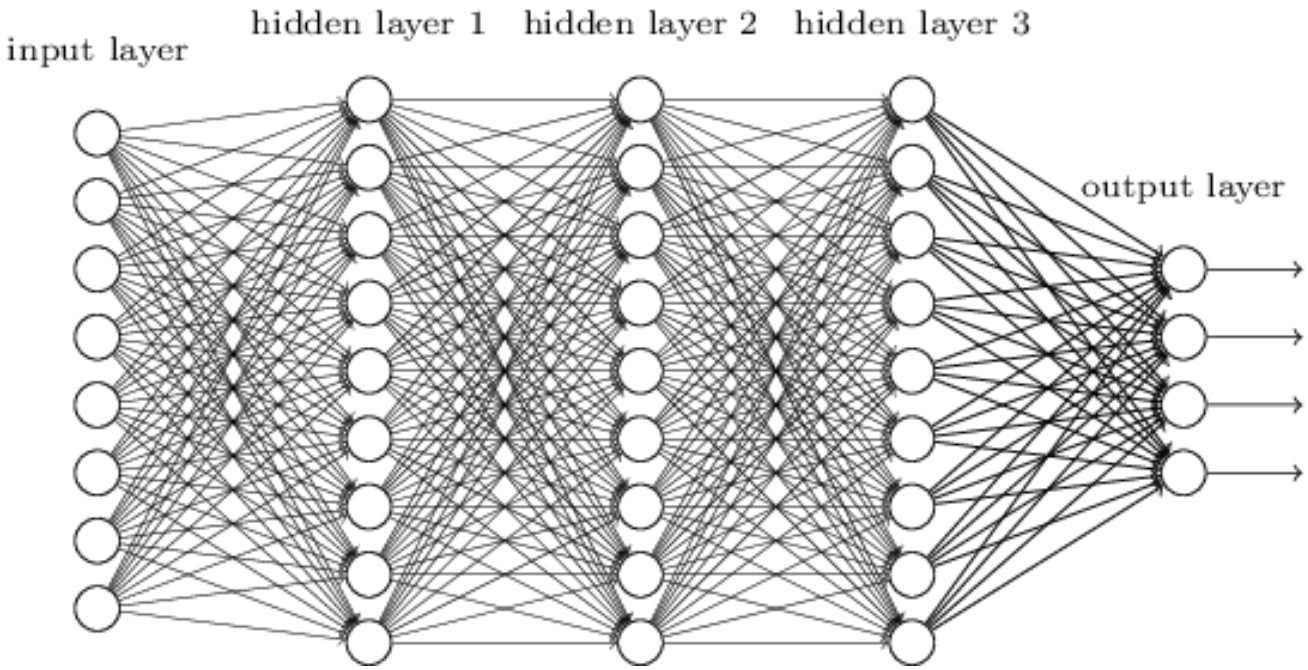




- It may take an exponentially large number of parameters for a good approximation.
- The optimization problem becomes increasingly difficult.

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

From MLP to Deep Learning

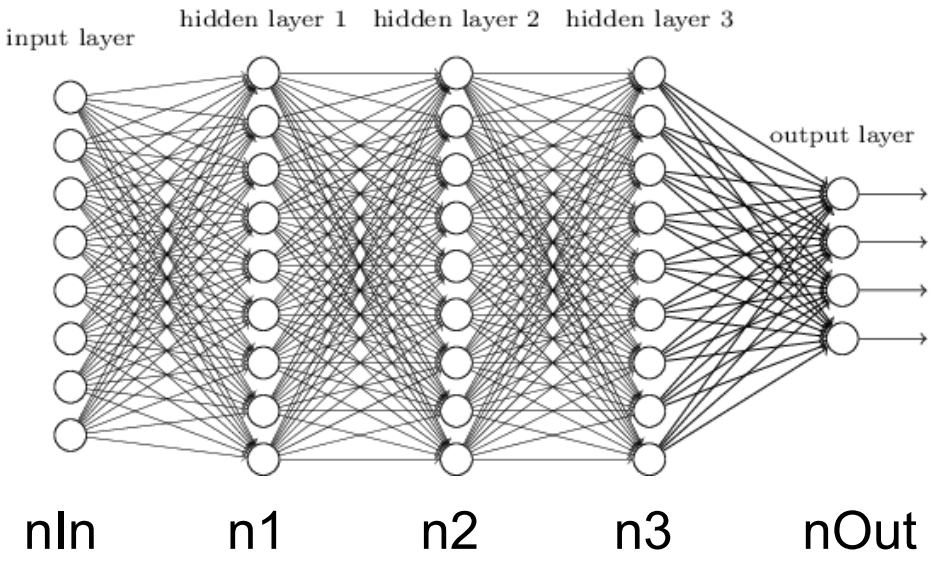


$$
\begin{aligned}
\mathbf{h}_1 &= \sigma_1(\mathbf{W}_1\mathbf{x}_1 + \mathbf{b}_1) \\
\mathbf{h}_2 &= \sigma_2(\mathbf{W}_2\mathbf{h}_1 + \mathbf{b}_2) \\
&\cdots \\
\mathbf{y} &= \sigma_n(\mathbf{W}_n\mathbf{h}_n + \mathbf{b}_n)
\end{aligned}
$$

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

PyTorch Translation

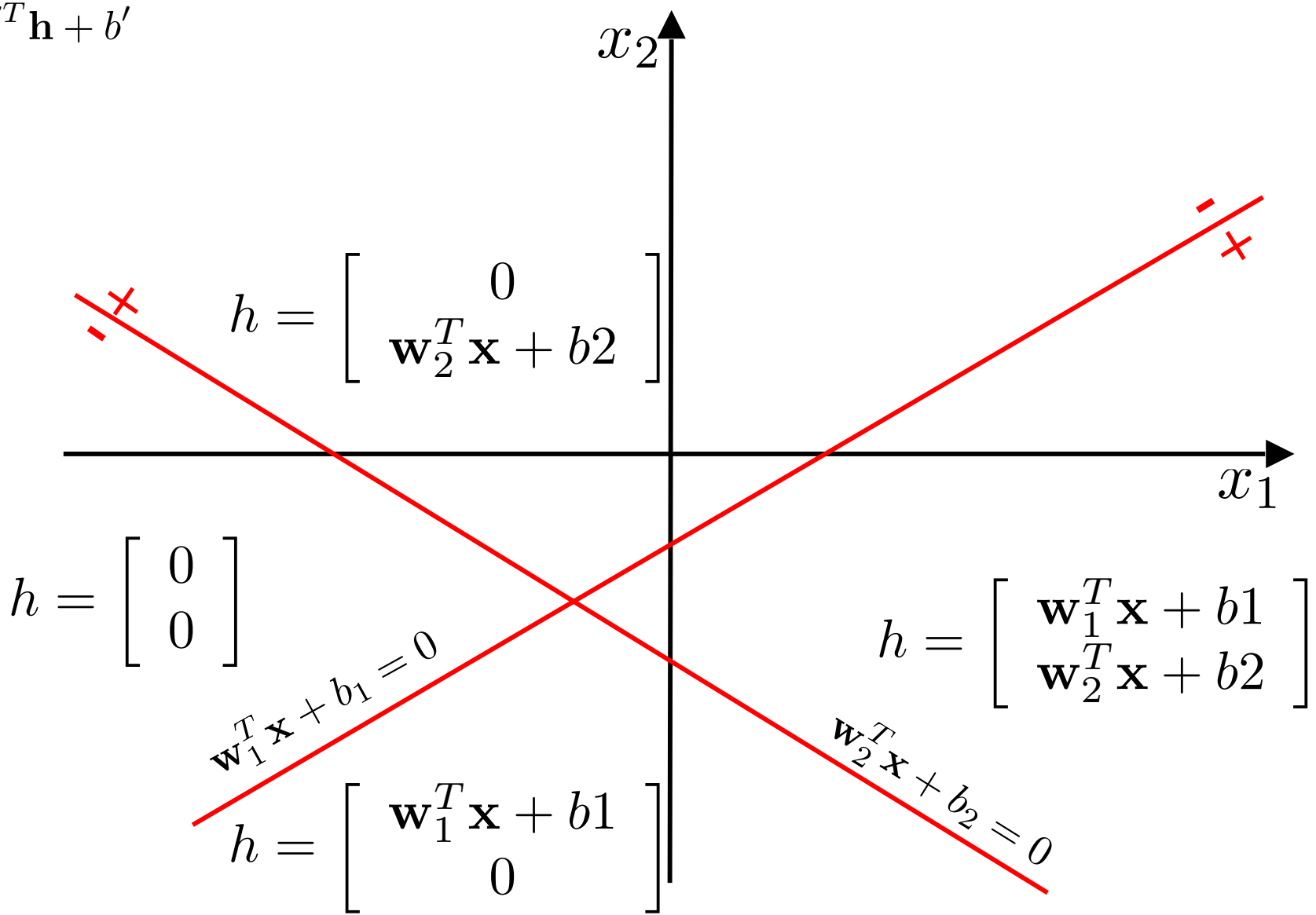
```
class MLP(nn.Module):

    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

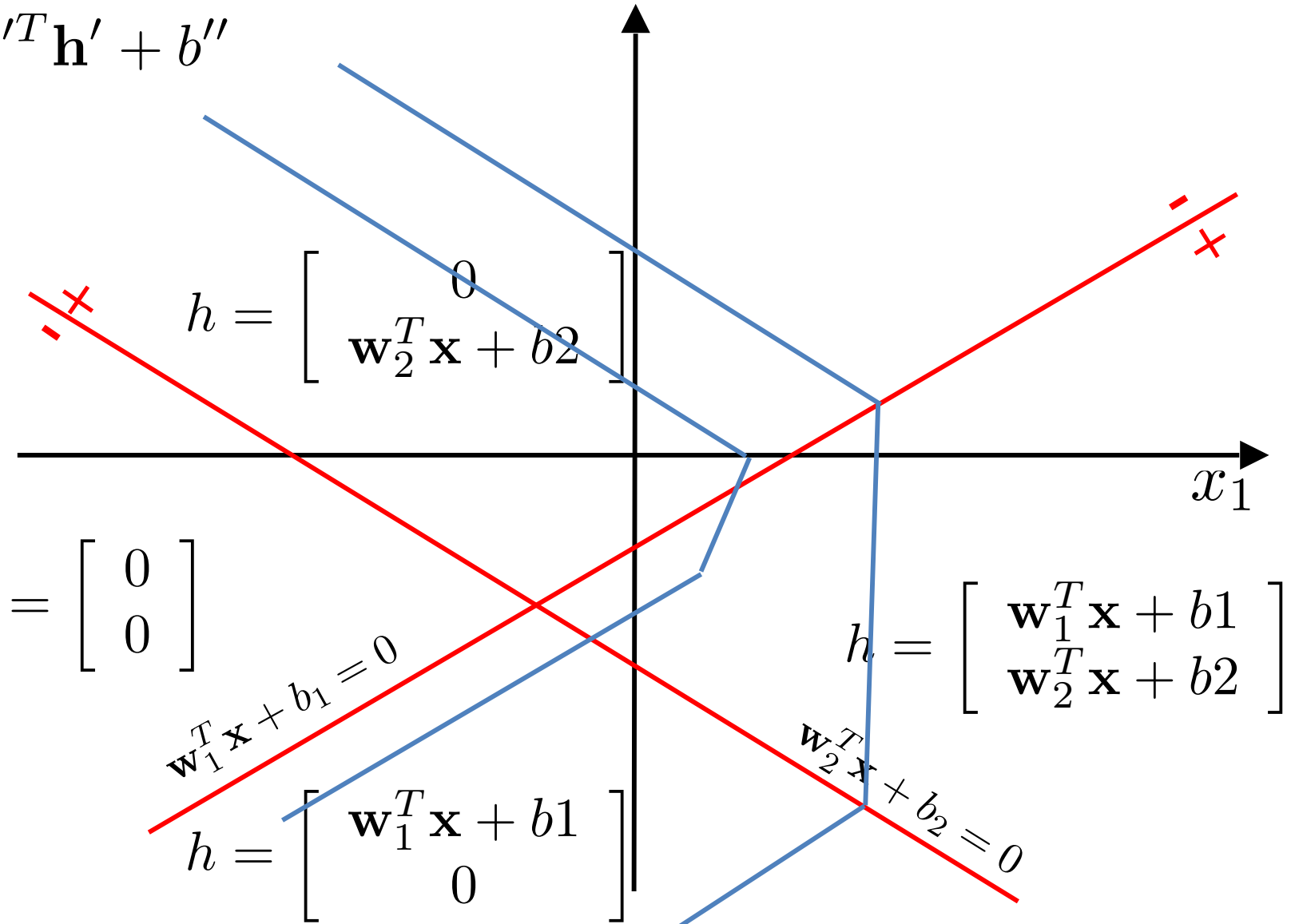
$$\mathbf{h} = \max(\mathbf{W}\mathbf{x} + \mathbf{b}, 0) \text{ with } \mathbf{W} = \begin{bmatrix} \mathbf{w}_1^T \\ \mathbf{w}_2^T \end{bmatrix} \text{ and } \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$$

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



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

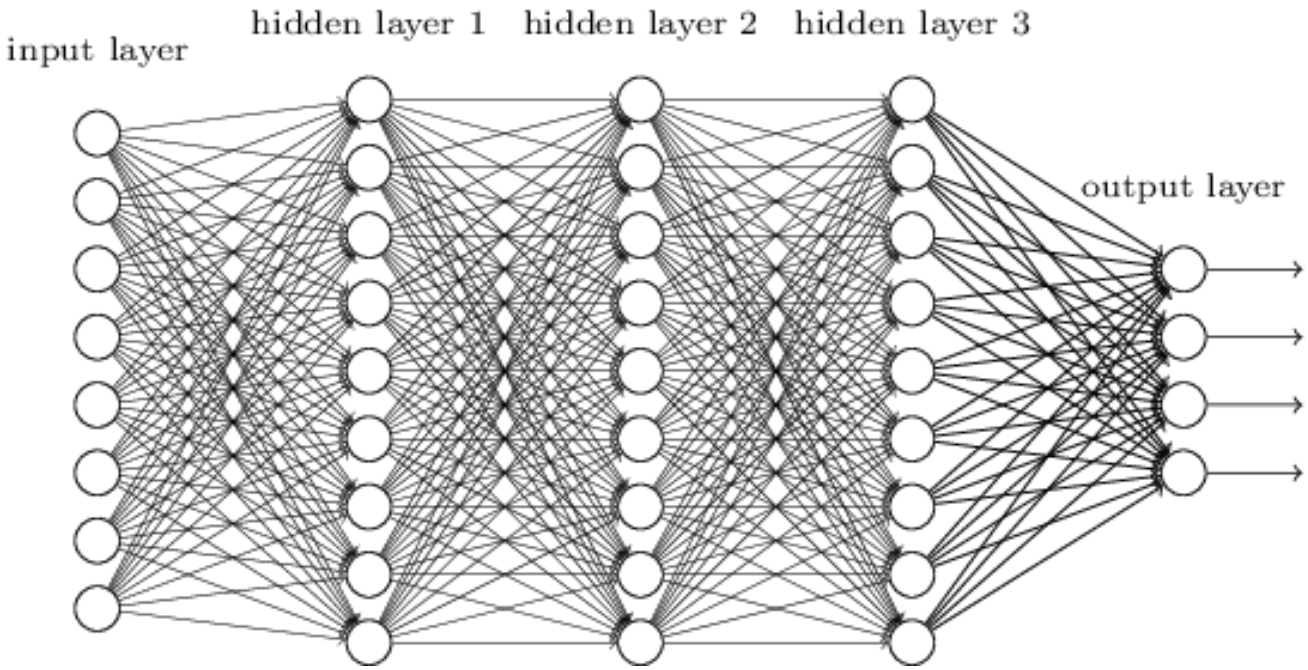
The function learned by a DNN using either ReLU, Sigmoid, or Tanh operators is:

- 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.

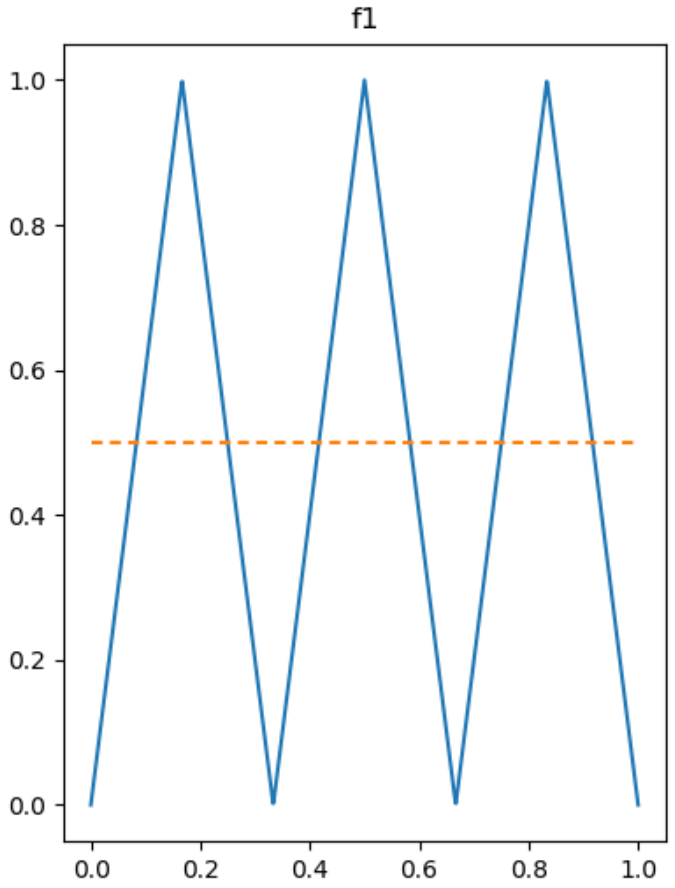
Deep Learning

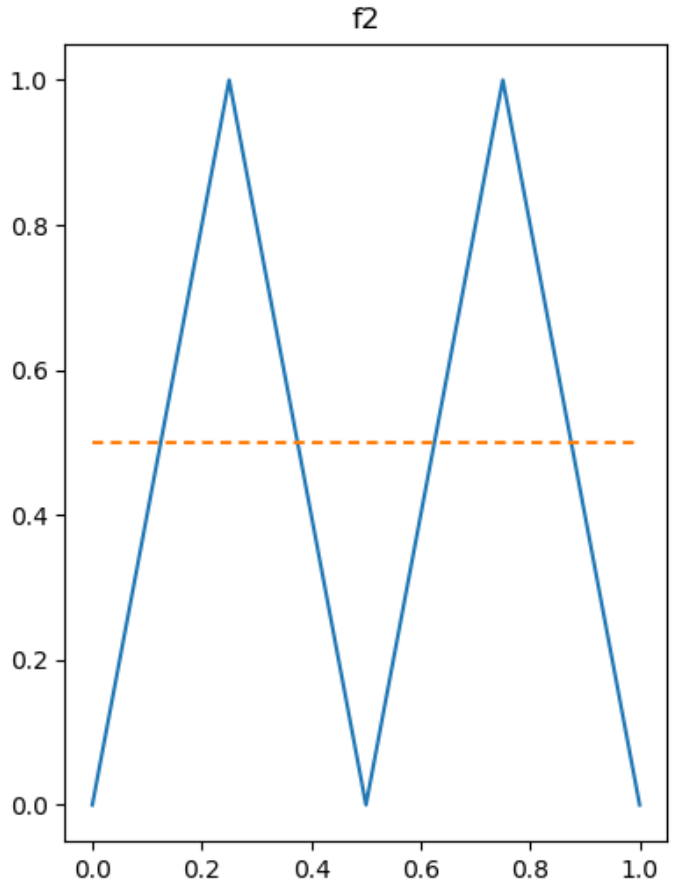


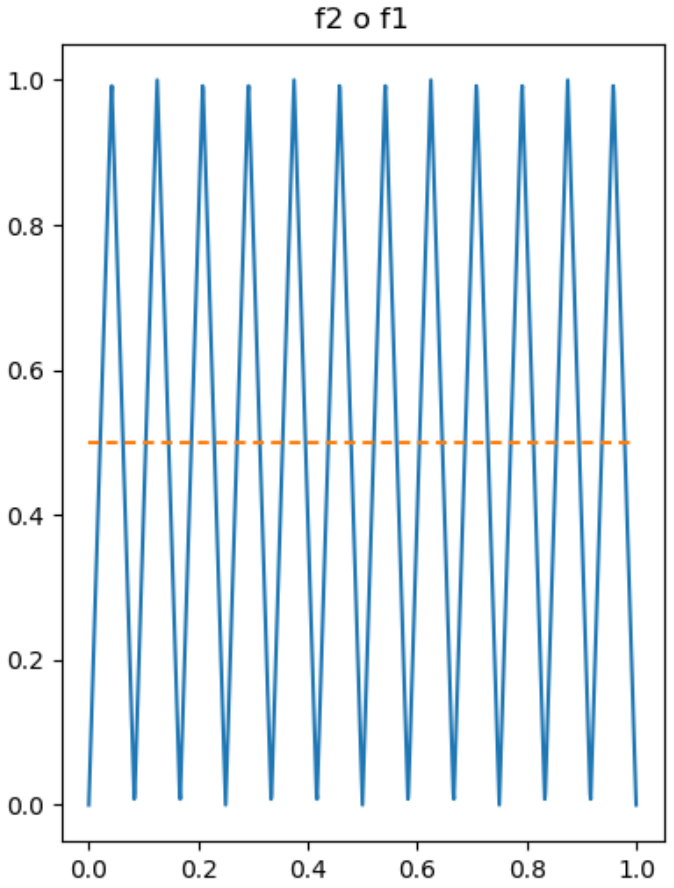
$$\begin{aligned} \mathbf{h}_1 &= \sigma_1(\mathbf{W}_1\mathbf{x}_1 + \mathbf{b}_1) \\ \mathbf{h}_2 &= \sigma_2(\mathbf{W}_2\mathbf{h}_2 + \mathbf{b}_2) \\ &\dots \\ \mathbf{y} &= \sigma_n(\mathbf{W}_n\mathbf{h}_n + \mathbf{b}_n) \end{aligned}$$

- 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

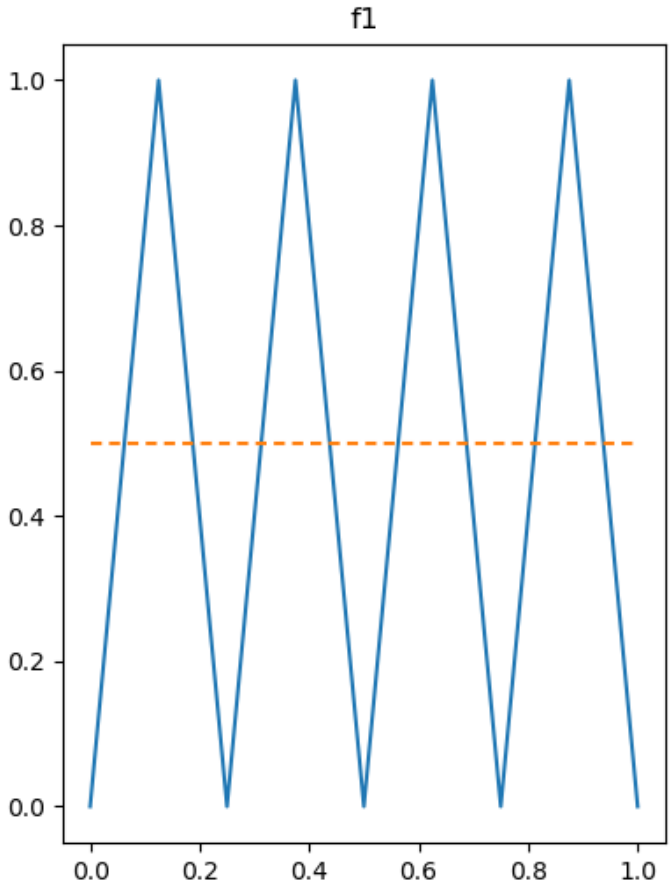


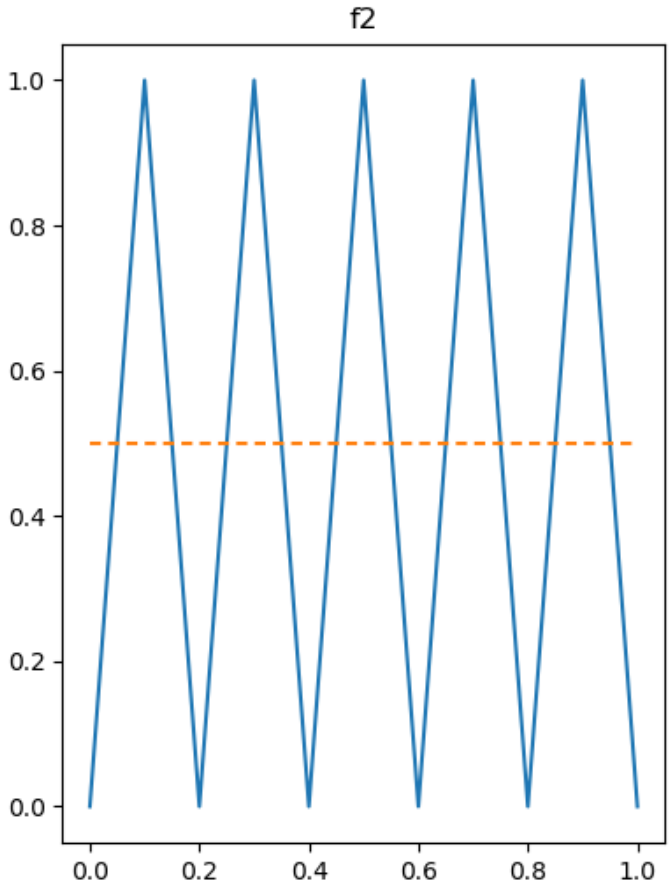


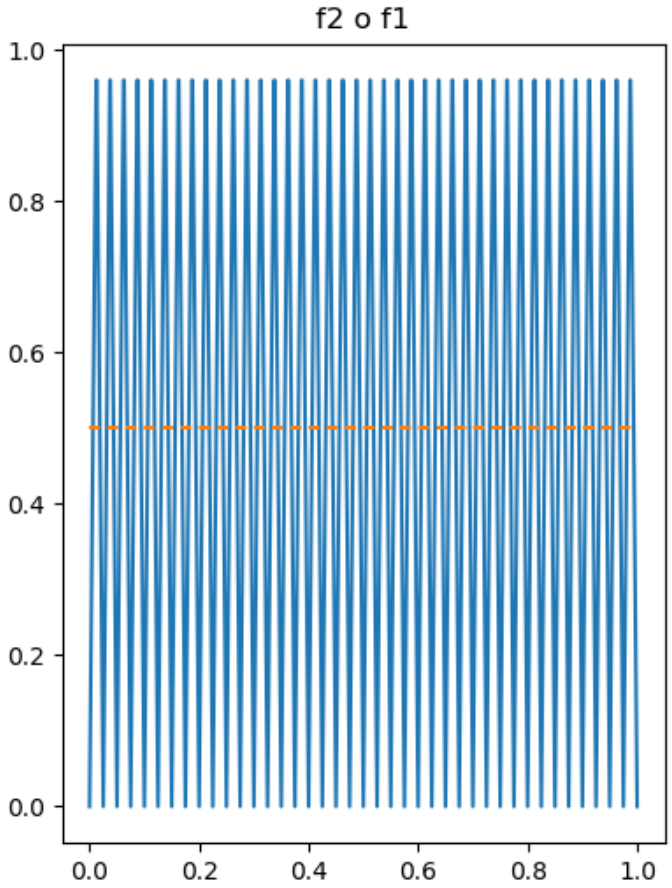


- $f_1(.)$ has $n_1=3$ peaks.
- $f_2(.)$ has $n_2=2$ peaks.
- $f_2(f_1(.))$ has $2n_1n_2=12$ peaks.

The Power of Composition



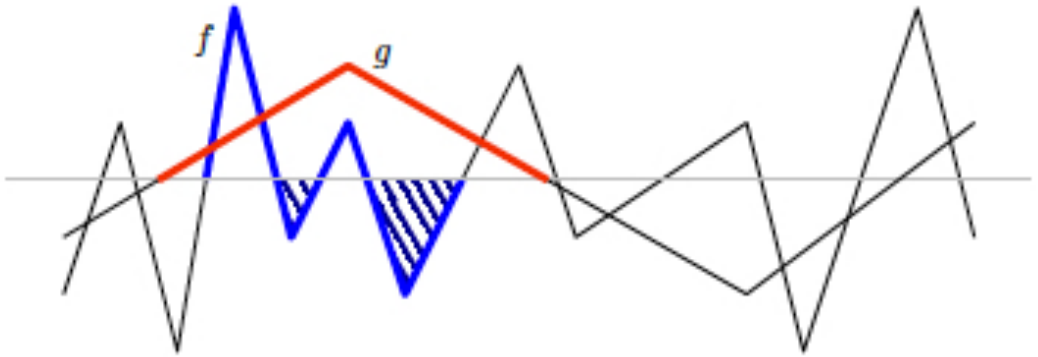




- $f_1(.)$ has $n_1=4$ peaks.
- $f_2(.)$ has $n_2=5$ peaks.
- $f_2(f_1(.))$ has $2n_1n_2=40$ peaks.

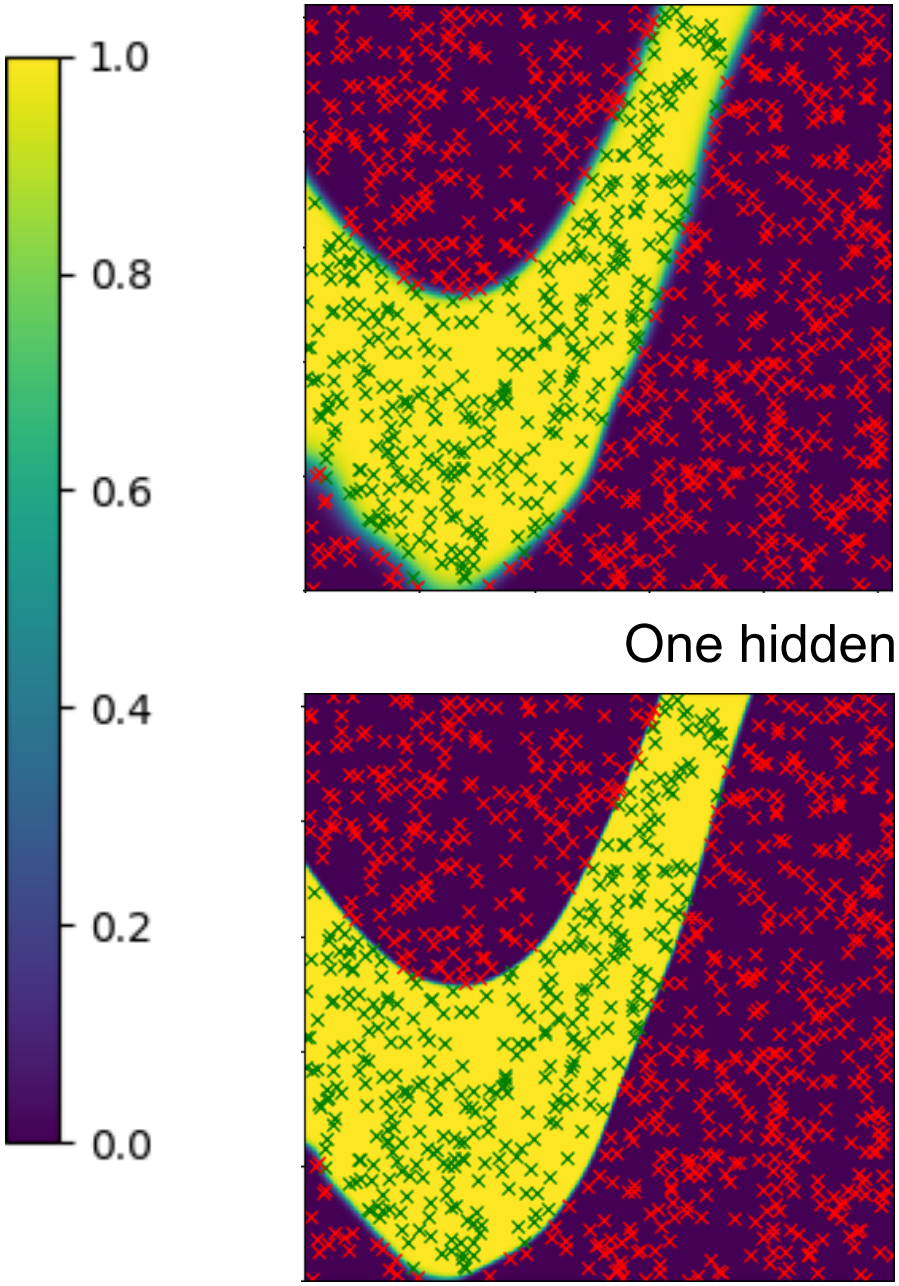
—> Descriptive power is proportional to n_1n_2

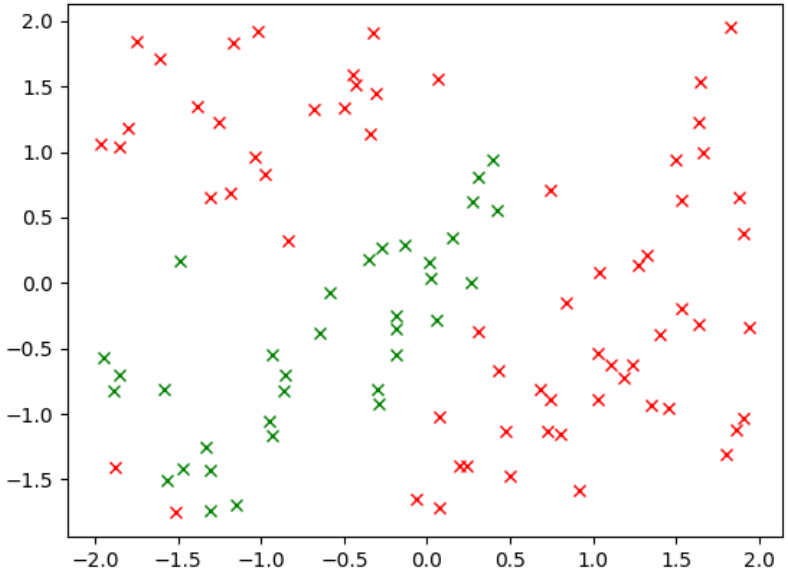
Optional: Proof Sketch



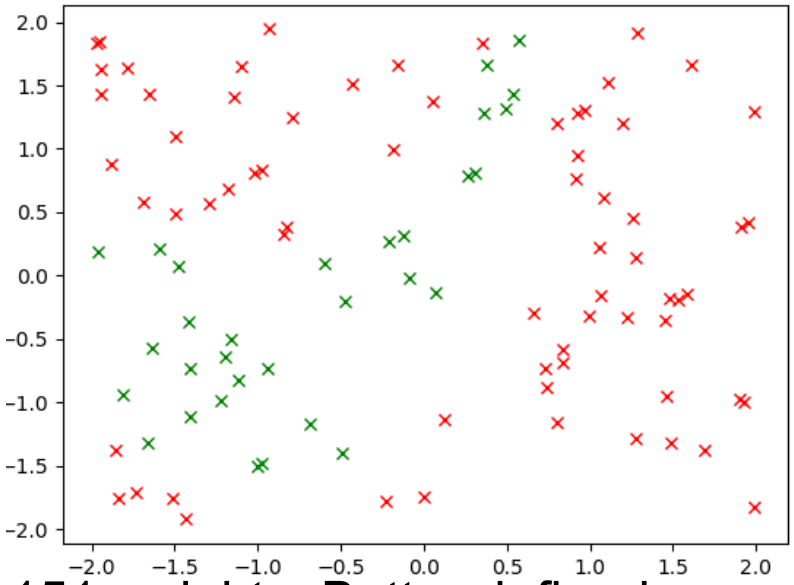
- Functions with few oscillations do not approximate well functions that have many.
- Networks can depict functions that have as many as $\prod_n W_n$ oscillations, where w_n is the width of layer n.
  - Functions computed by networks with few layers have few oscillations.
  - Functions computed by deeper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

Back to Non-Linear Classification



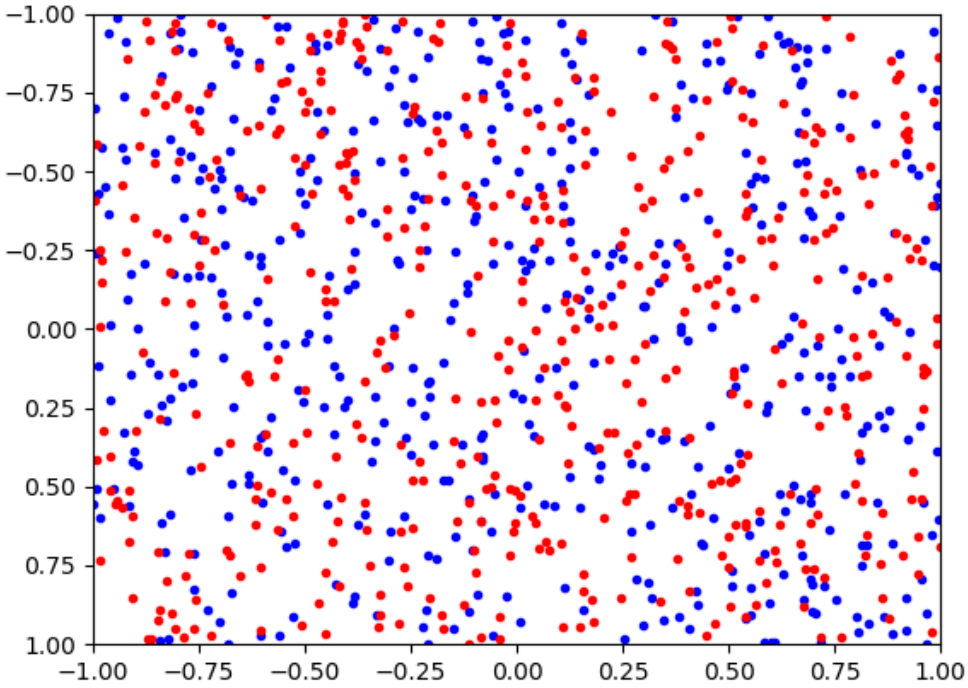


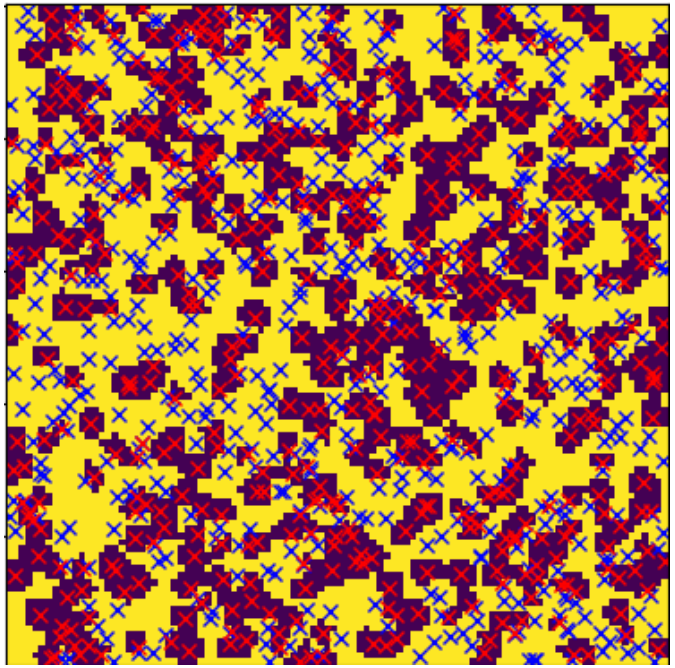
One hidden layer: n=100, 401 weights.



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

Randomly Distributed Points and RBF Kernels



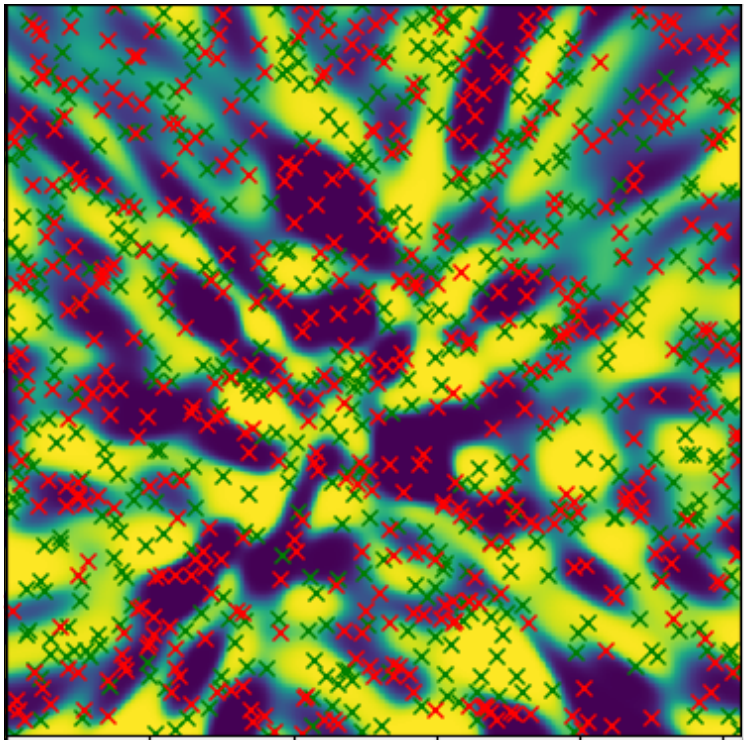


Rbf, $g = 200$

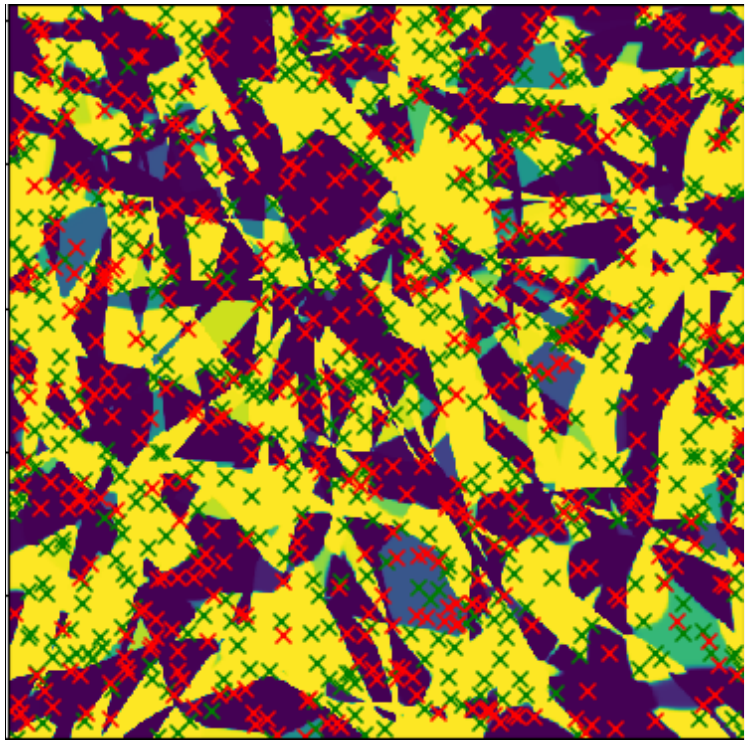
n=100, 72%

n=400, 77%

n=1600,79%



One hidden layer



Two hidden layers

n=10, 70%

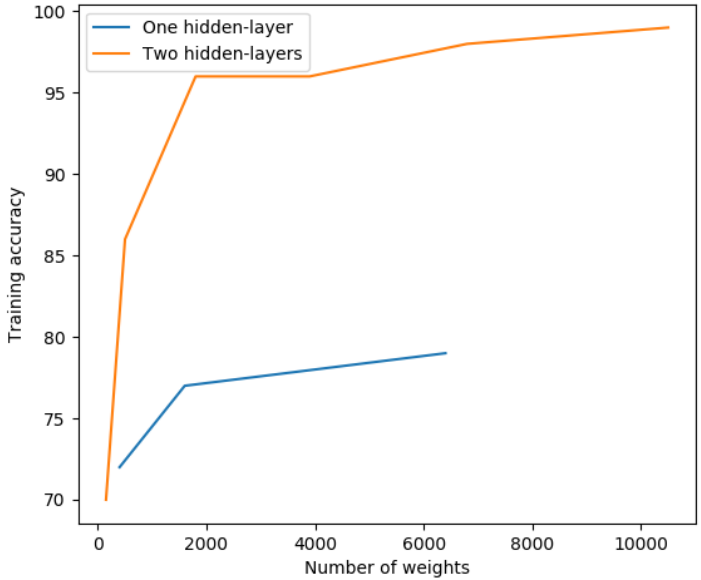
n=20, 86%

n=40, 96%

n=60, 96%

n=80, 98%

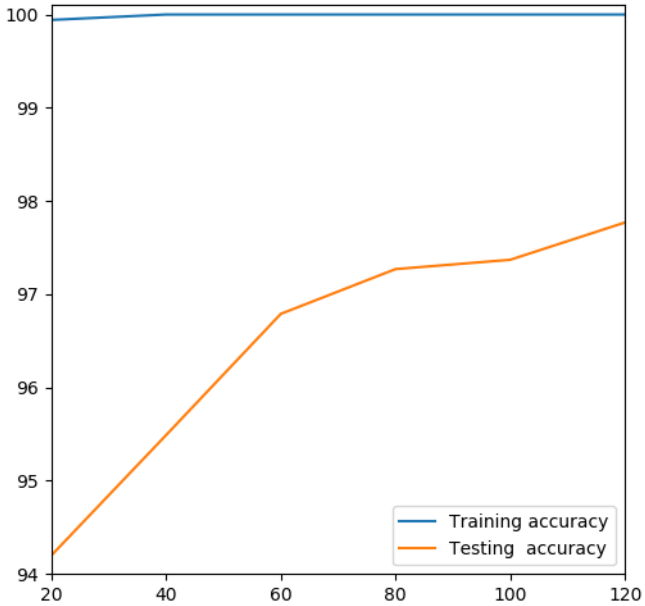
n=100, 99%

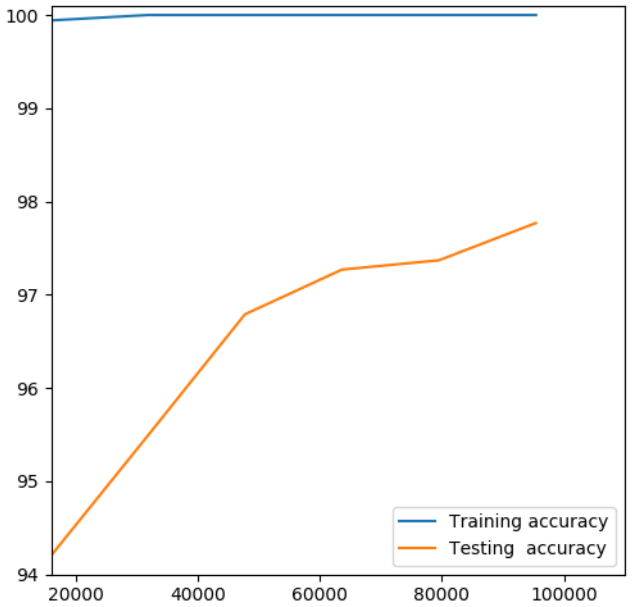


Empirical observation: The two layer networks converge faster and better.

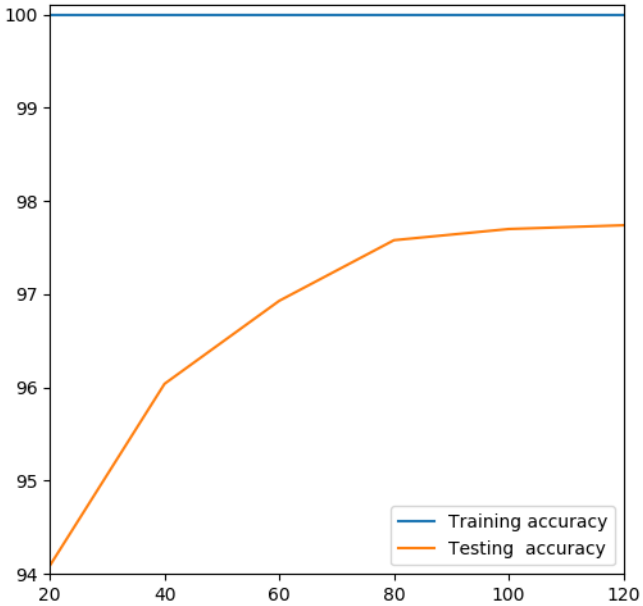
MNIST Results

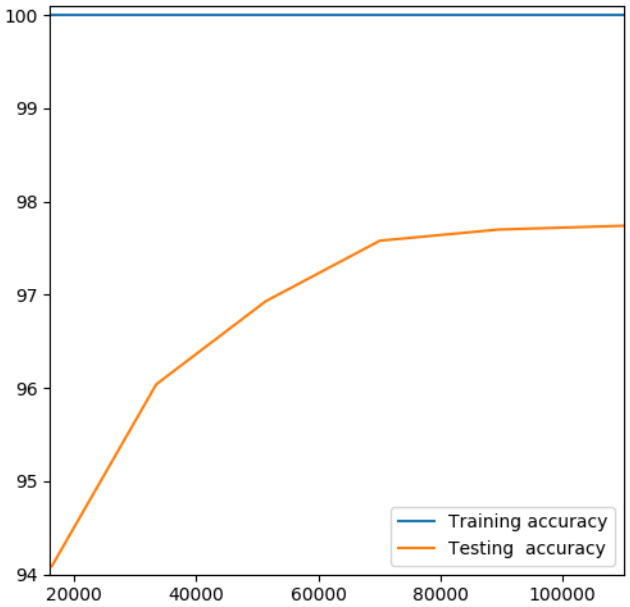
nIn =784
nOut = 10
20 < n1 < 120





One Layer MLP





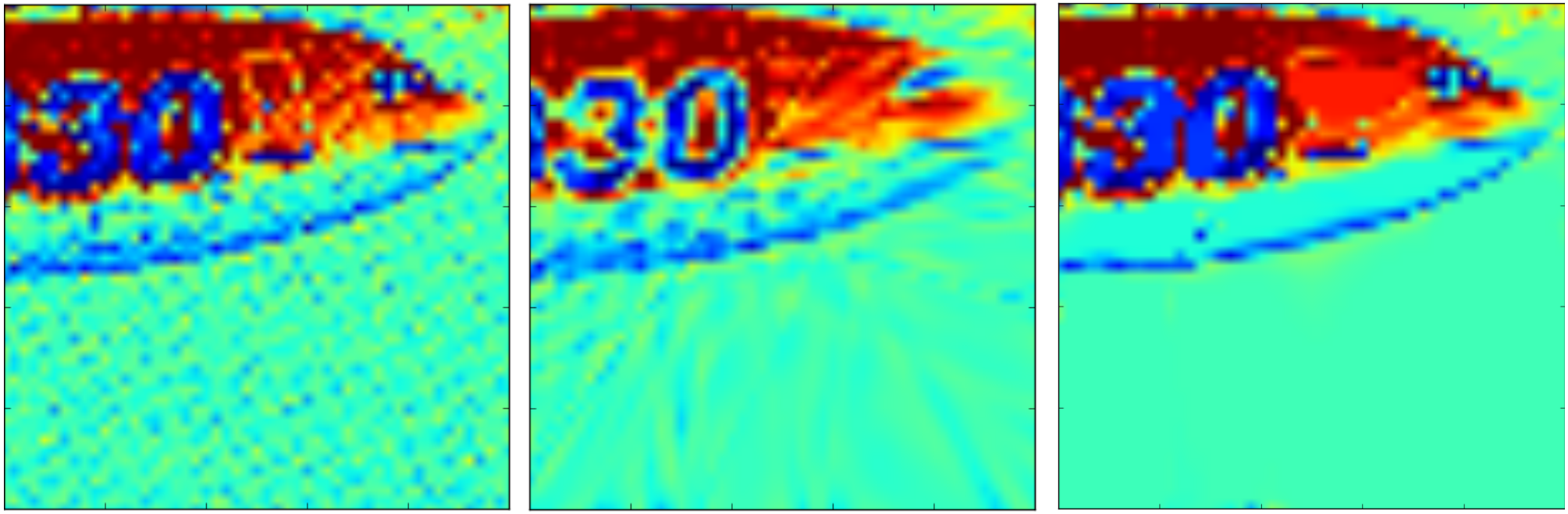
Two-Layer MLP

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 Approximation



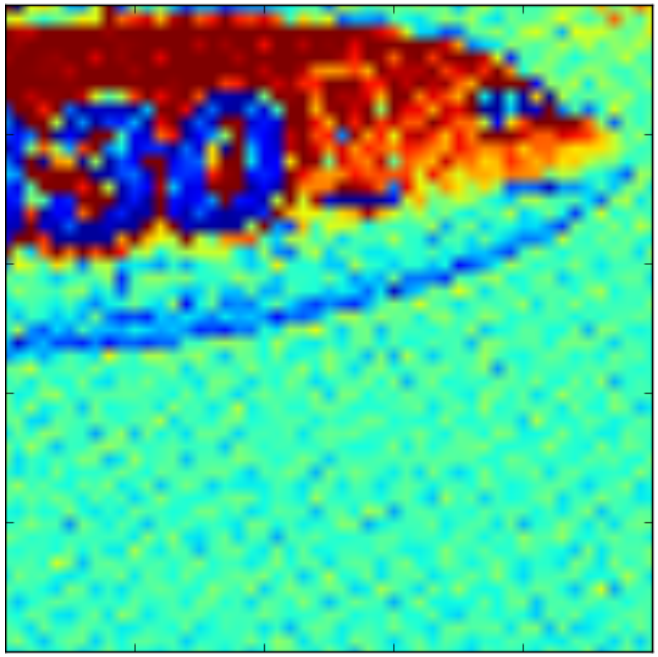
$$I = f(x, y)$$

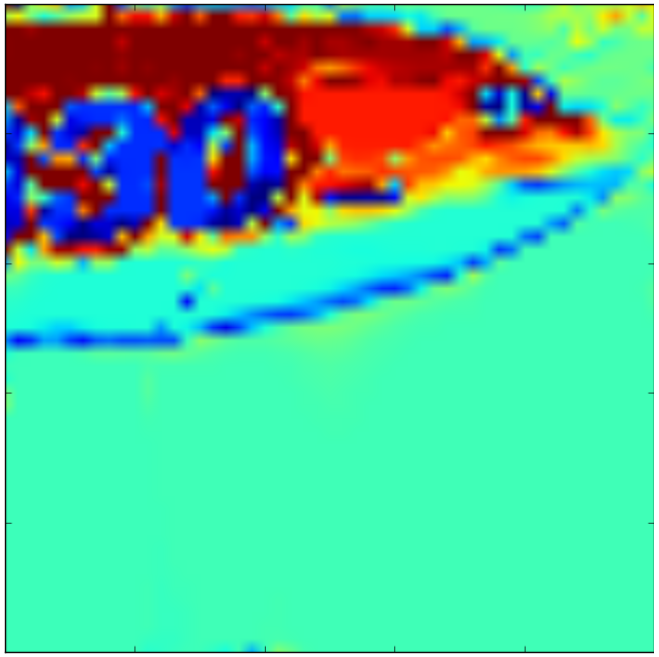
1 Layer: 125 nodes -> loss 2.40e-01 2 Layers: 20 nodes -> loss 8.31e-02

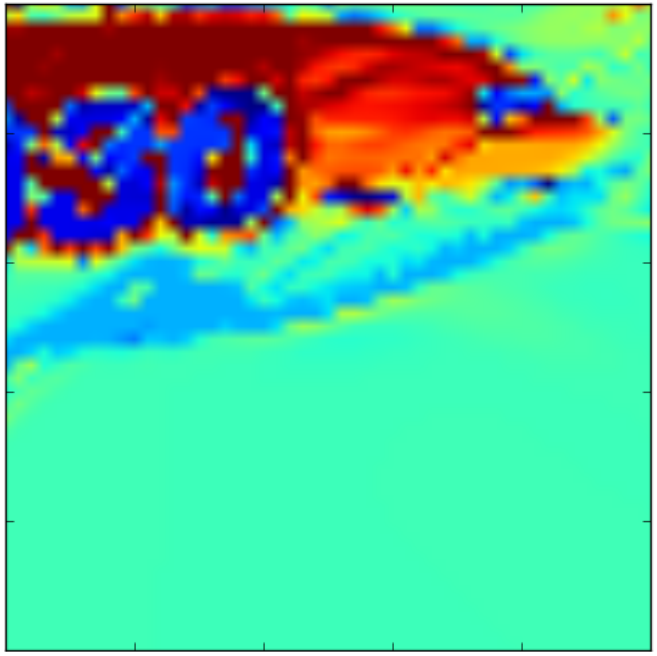
501 weights in both cases

—> 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

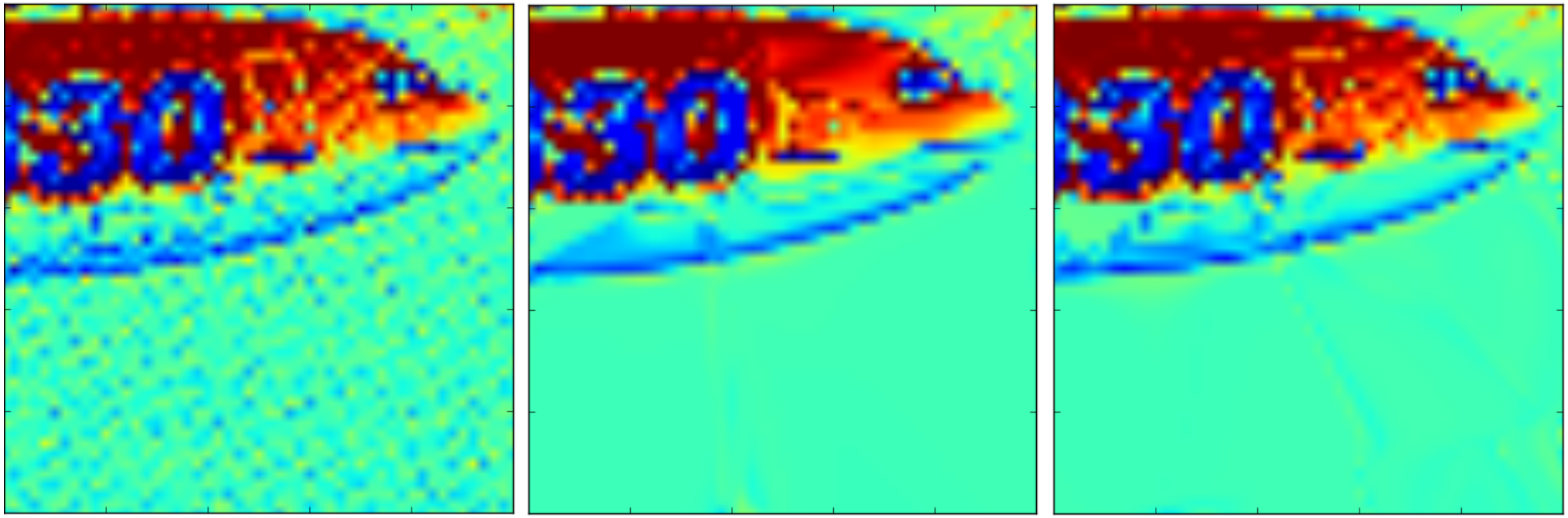
501 weights

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

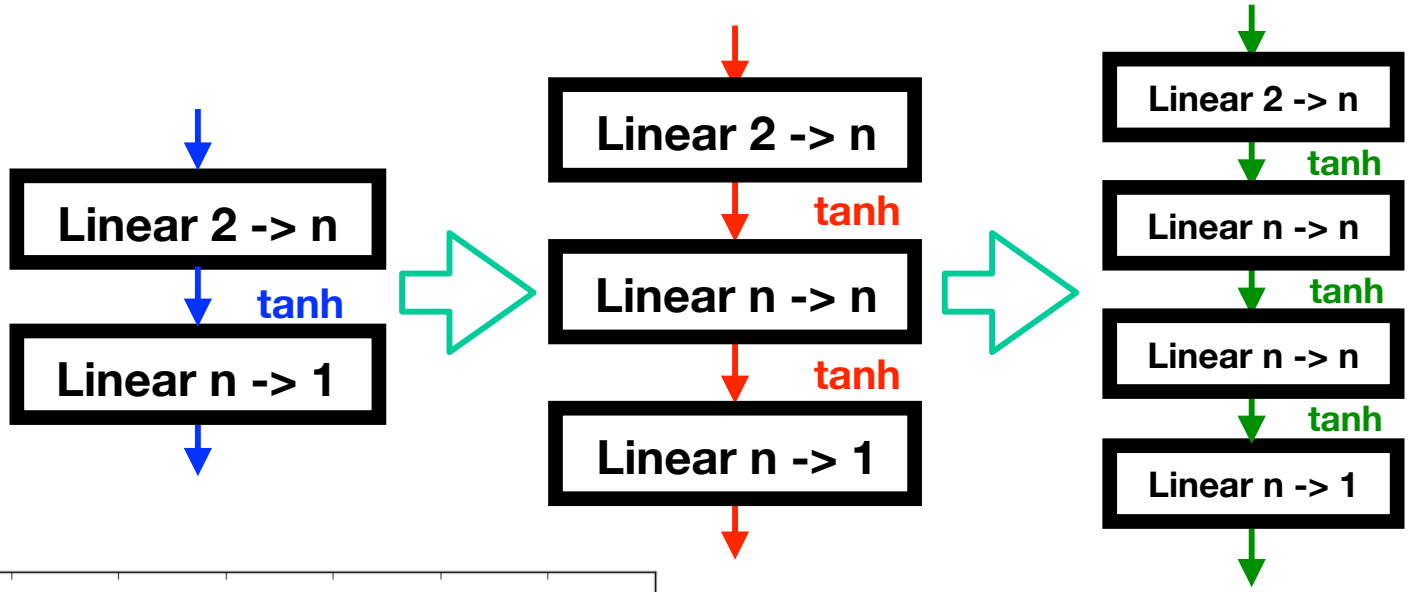
541 weights

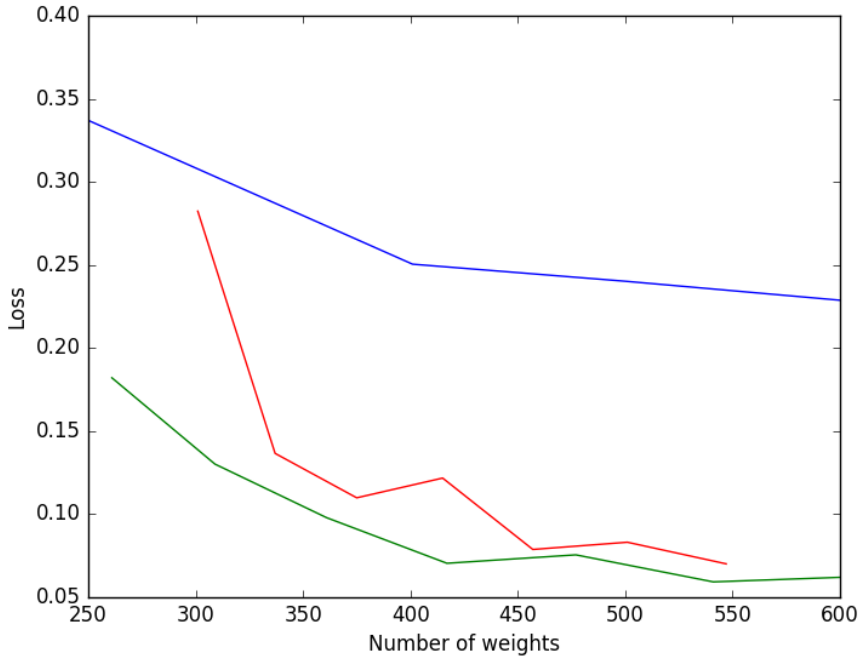
3 Layers: 19 nodes -> loss 4.38e-02

837 weights

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

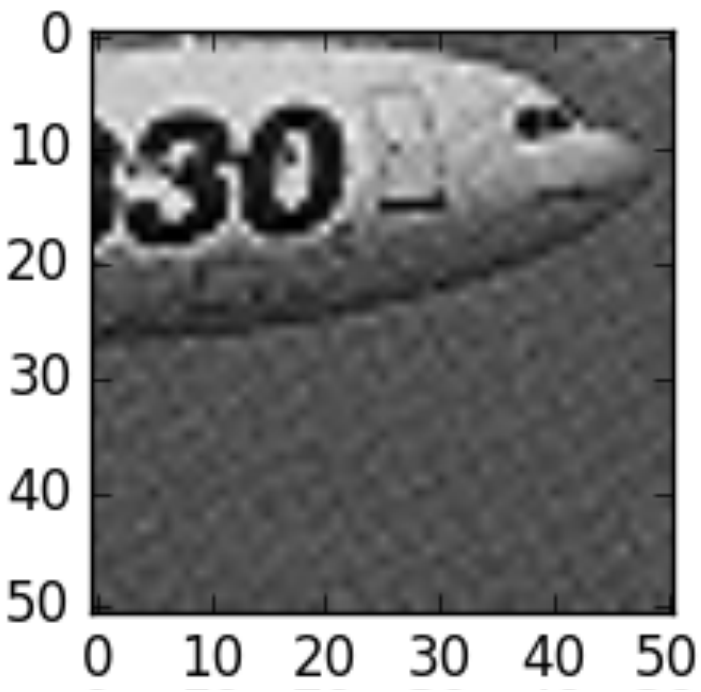
Multi Layer Perceptrons



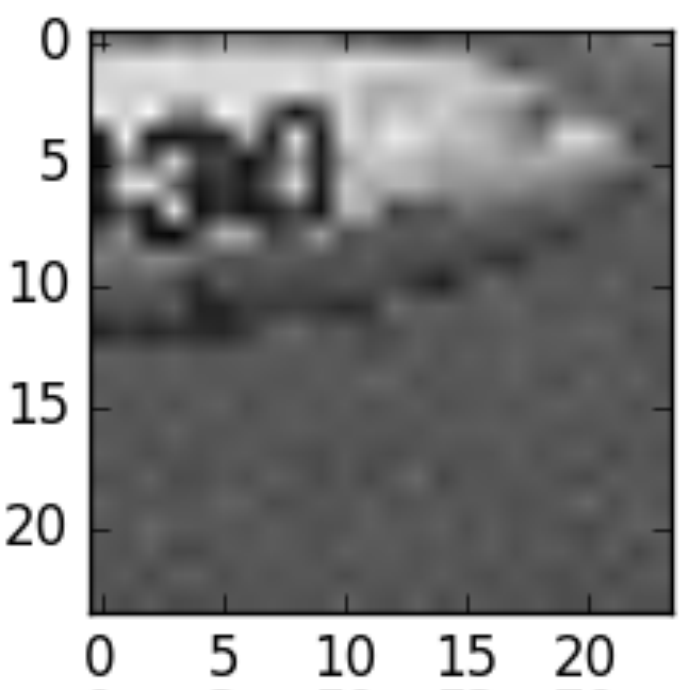


- Adding layers often yields better convergence properties.
- In current practice, deeper is usually better.

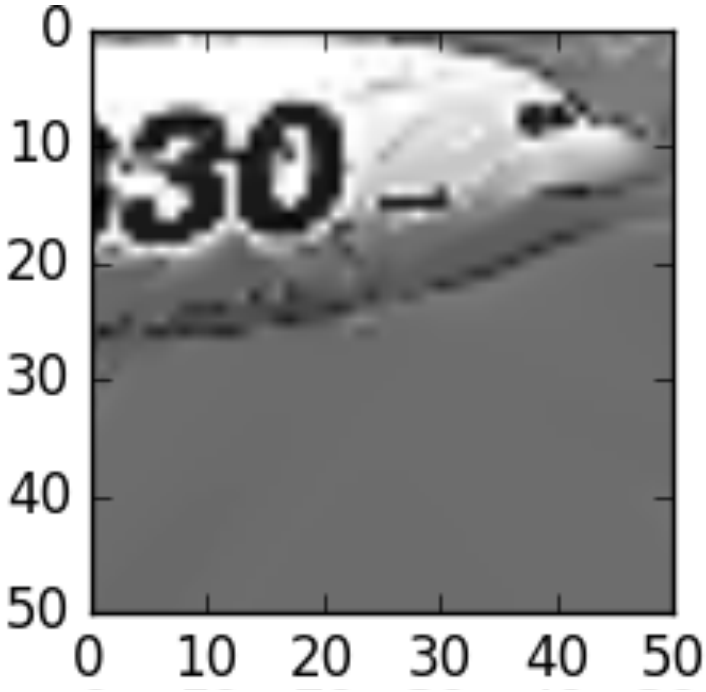
Other Ways to Interpolate



Original 51x51 image:
2601 gray level values.



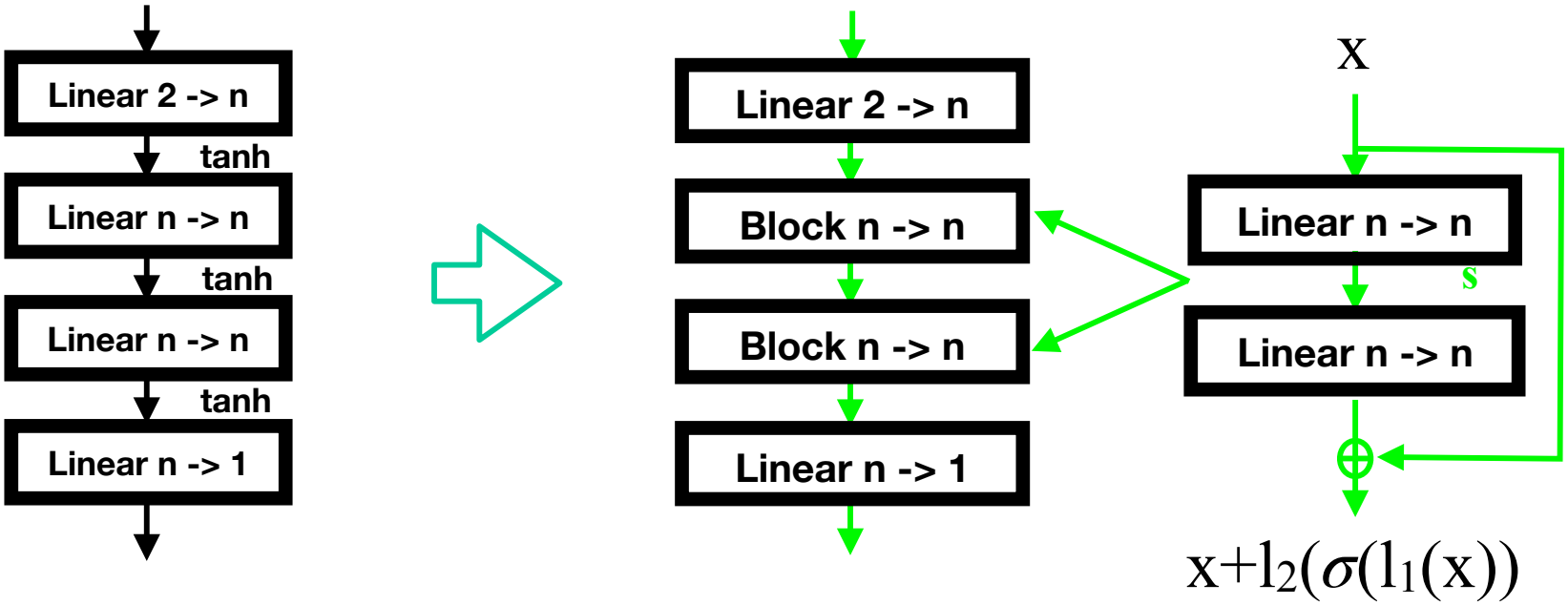
Scaled 24x24 image:
576 gray level values.



MLP 10/20/10 Interpolation:
471 weights.

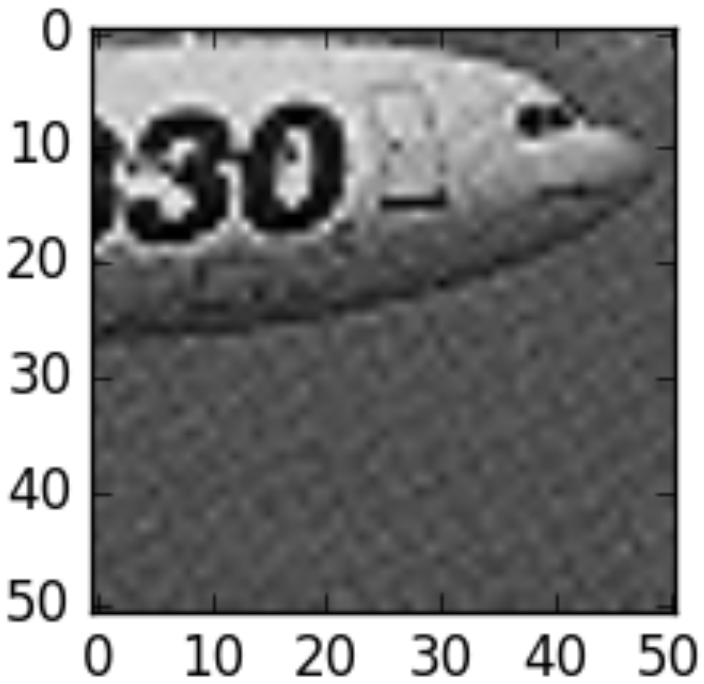
Simpler but not necessarily better!

MLP to ResNet

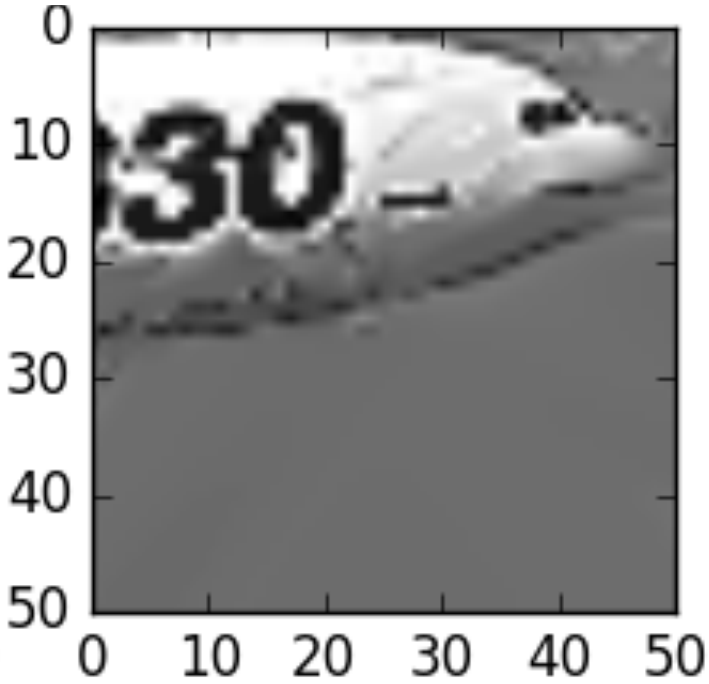


Further improvements in the convergence properties have been obtained by adding a bypass, which allows the final layers to only compute residuals.

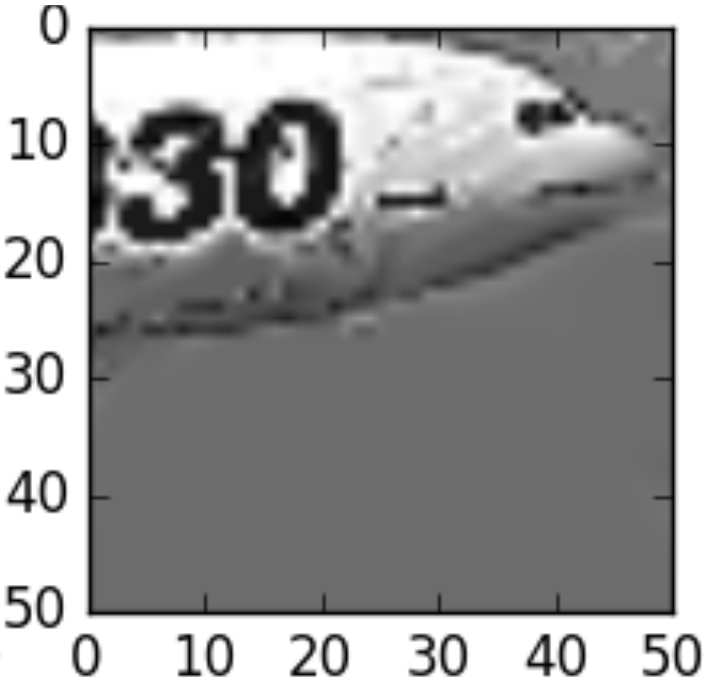
Adding a ResNet Layer



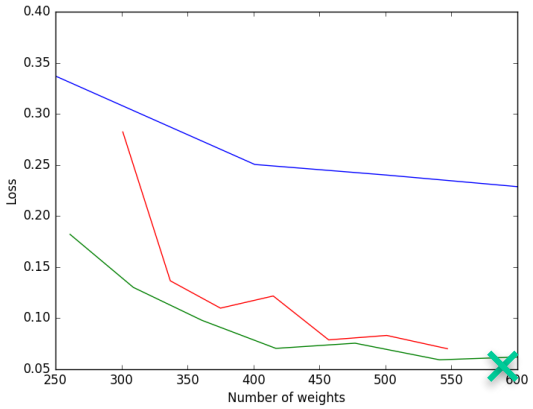
Original 51x51 image:
2601 gray level values.

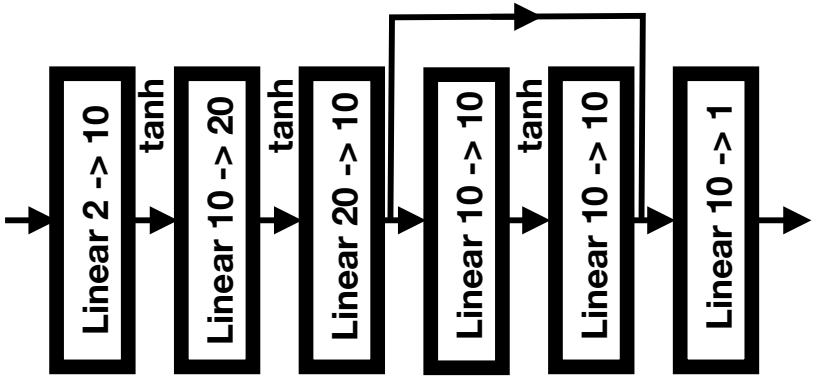


MLP 10/20/10 Interpolation:
471 weights, loss 6.43e-02.



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

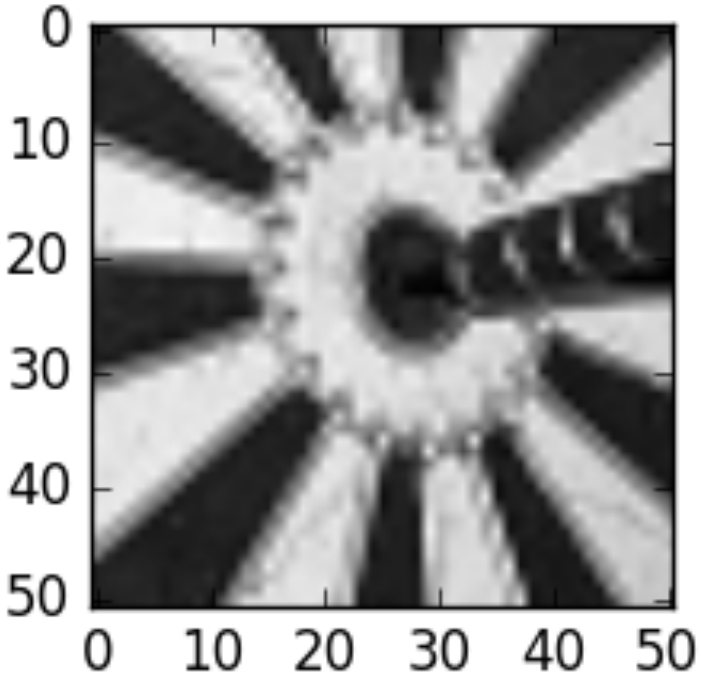




—> Adding a ResNet layer yields a further small improvement.

EPFL

Adding a ResNet Layer



Original 51x51 image:
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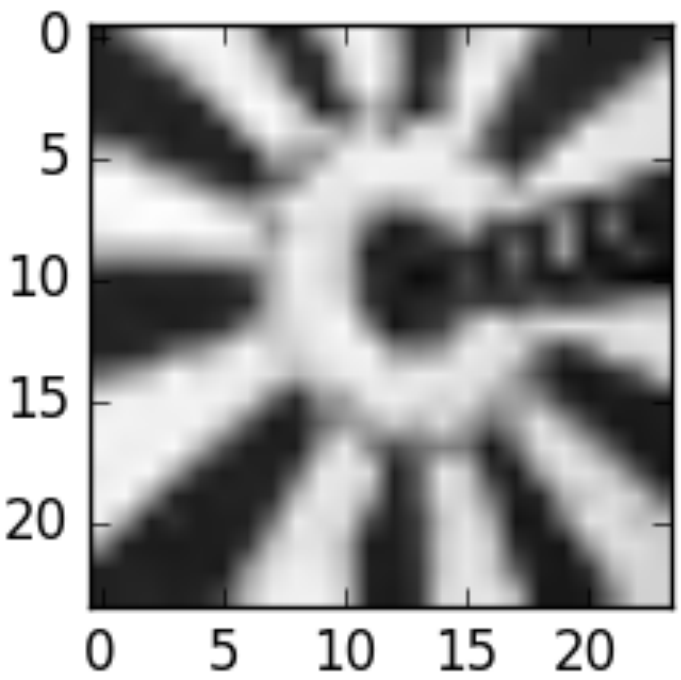
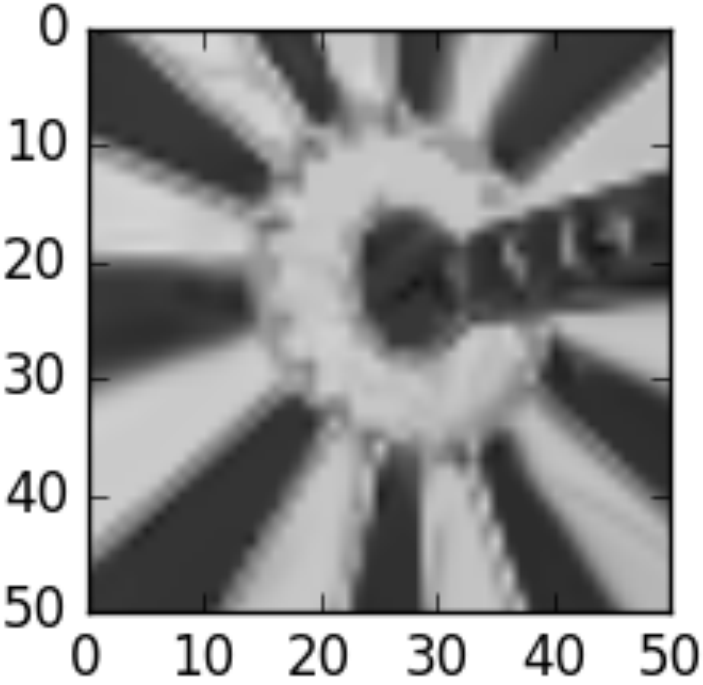


MLP 10/20/10 Interpolation:
471 weights, loss 1.95e-02.

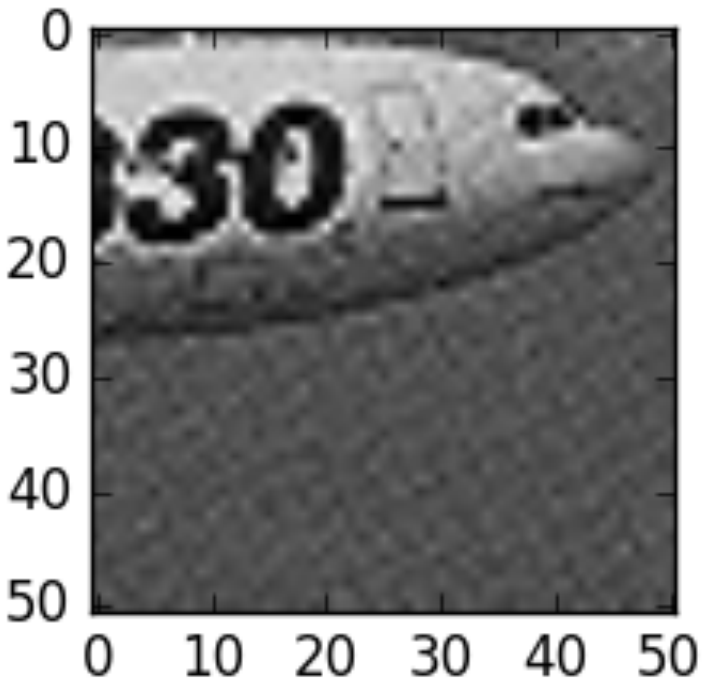


Resnet 10/20/10/10 Interpolation:
581 weights, loss 1.36e-2.

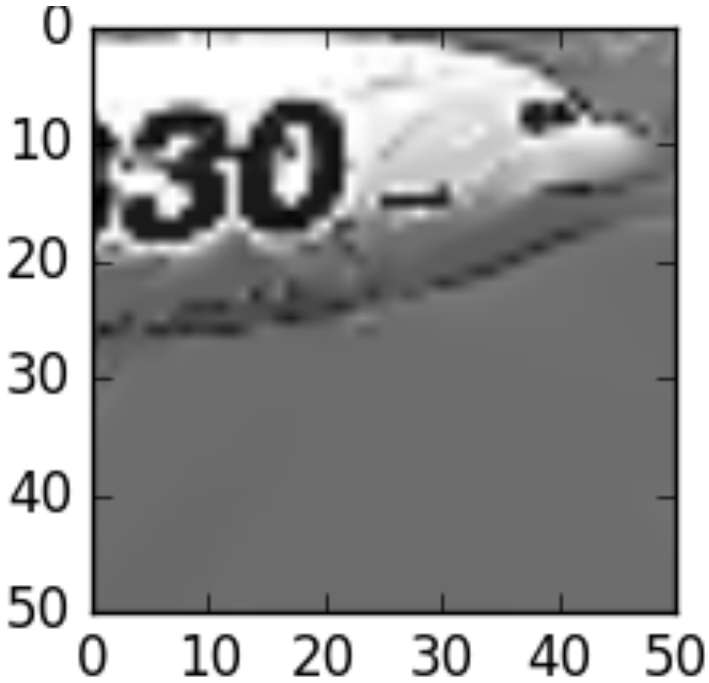
- Relatively small improvement in this case.
- We will see a different behavior for large networks.
- The problem is probably too small.

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

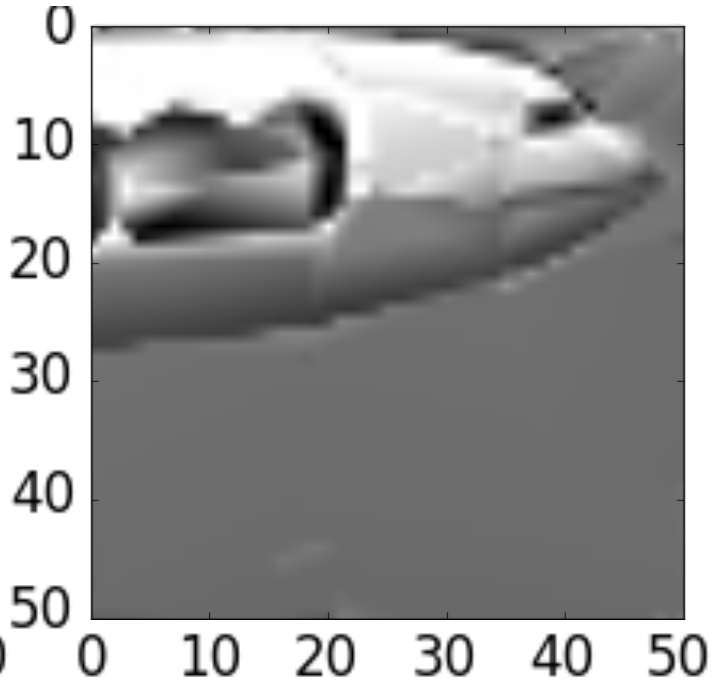
Tanh vs ReLu



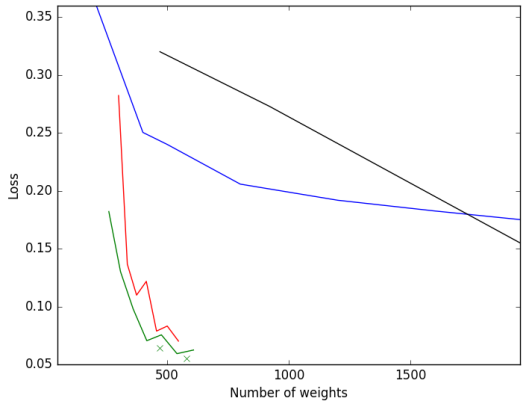
Original 51x51 image:
2601 gray level values.



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



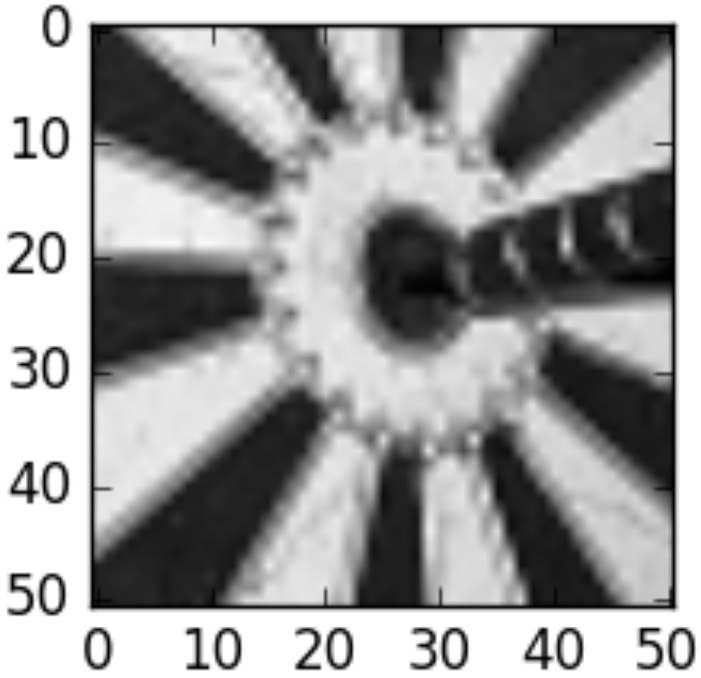
MLP 10/20/10 Interpolation:
ReLU, loss 3.07e-1.



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

—> Tanh works better than ReLU in this case.

Tanh vs ReLu



Original 51x51 image:
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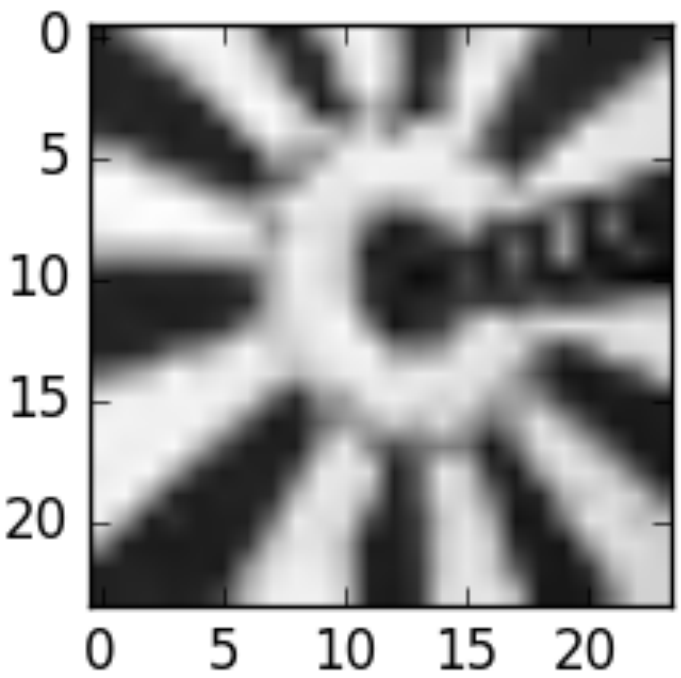
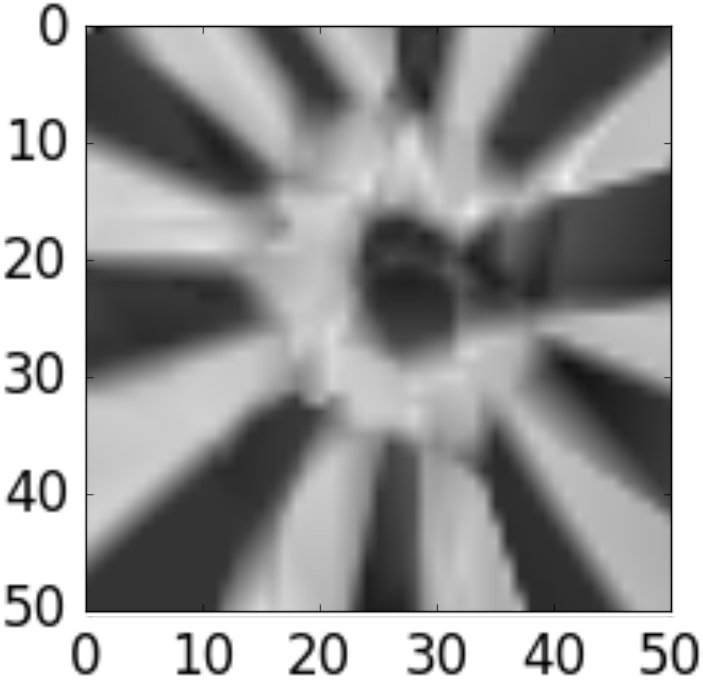


MLP 10/20/10 Interpolation:
tanh, loss 1.95e-02.

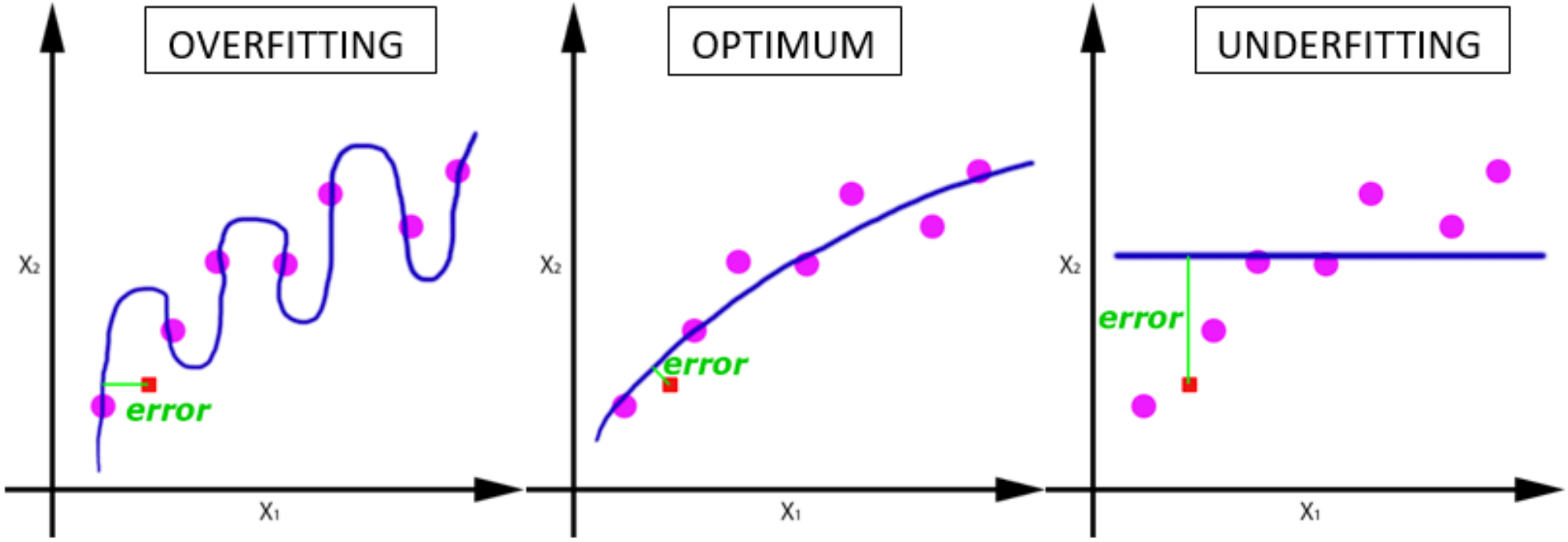


MLP 10/20/10 Interpolation:
relu, loss 7.21e-2.

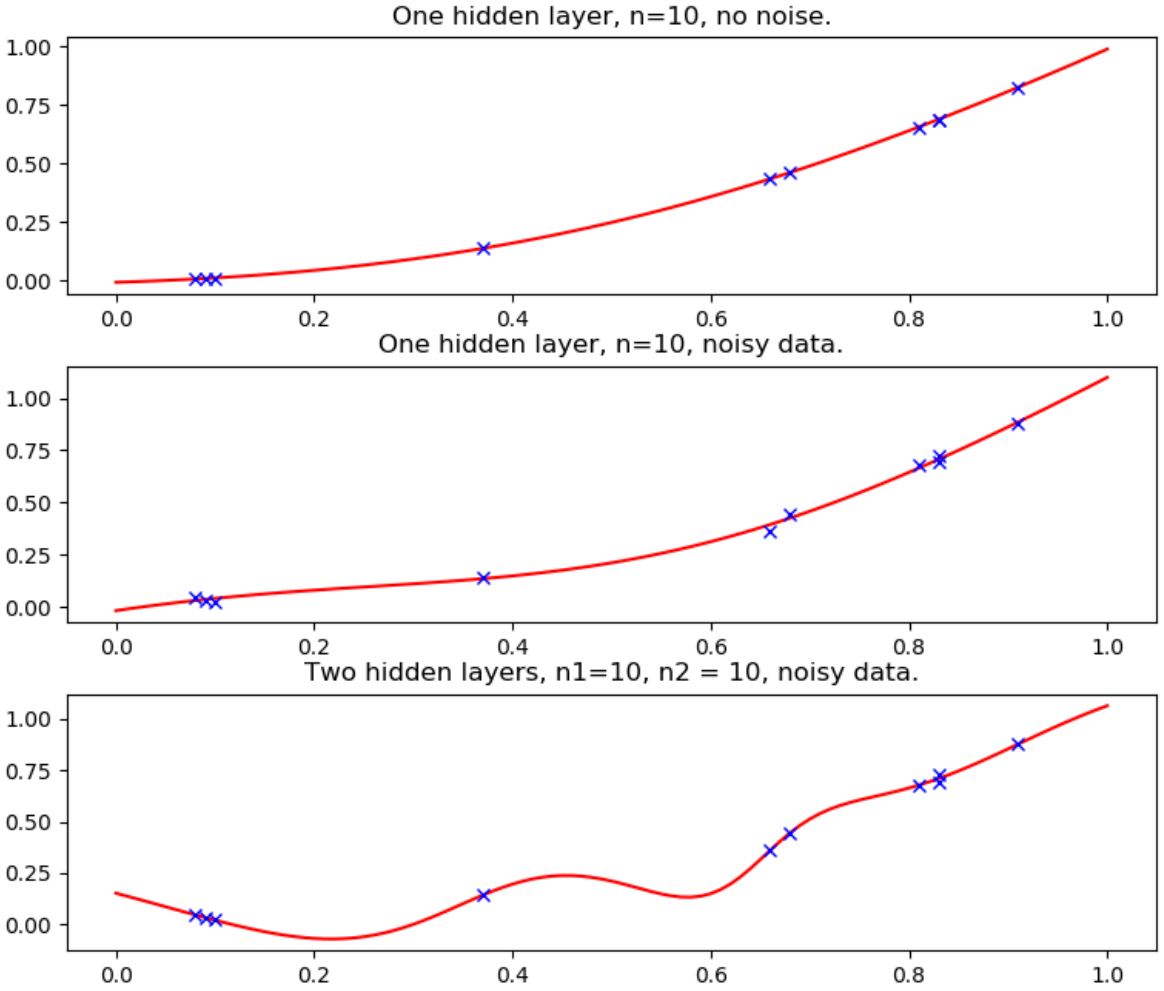
- Tanh works better than ReLU in this case.
- ReLU is widely credited with eliminating the vanishing gradient problem in large networks.

—> There is no substitute for experimentation!

Overfitting vs Underfitting

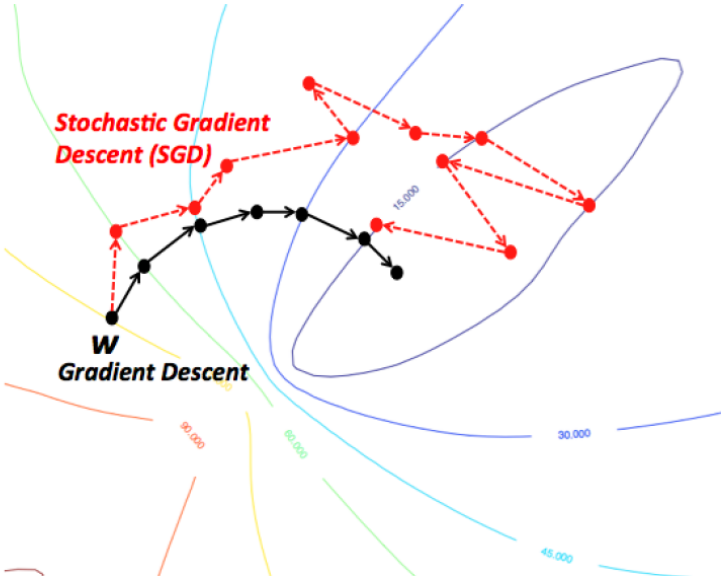


Overfitting



- 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



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

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

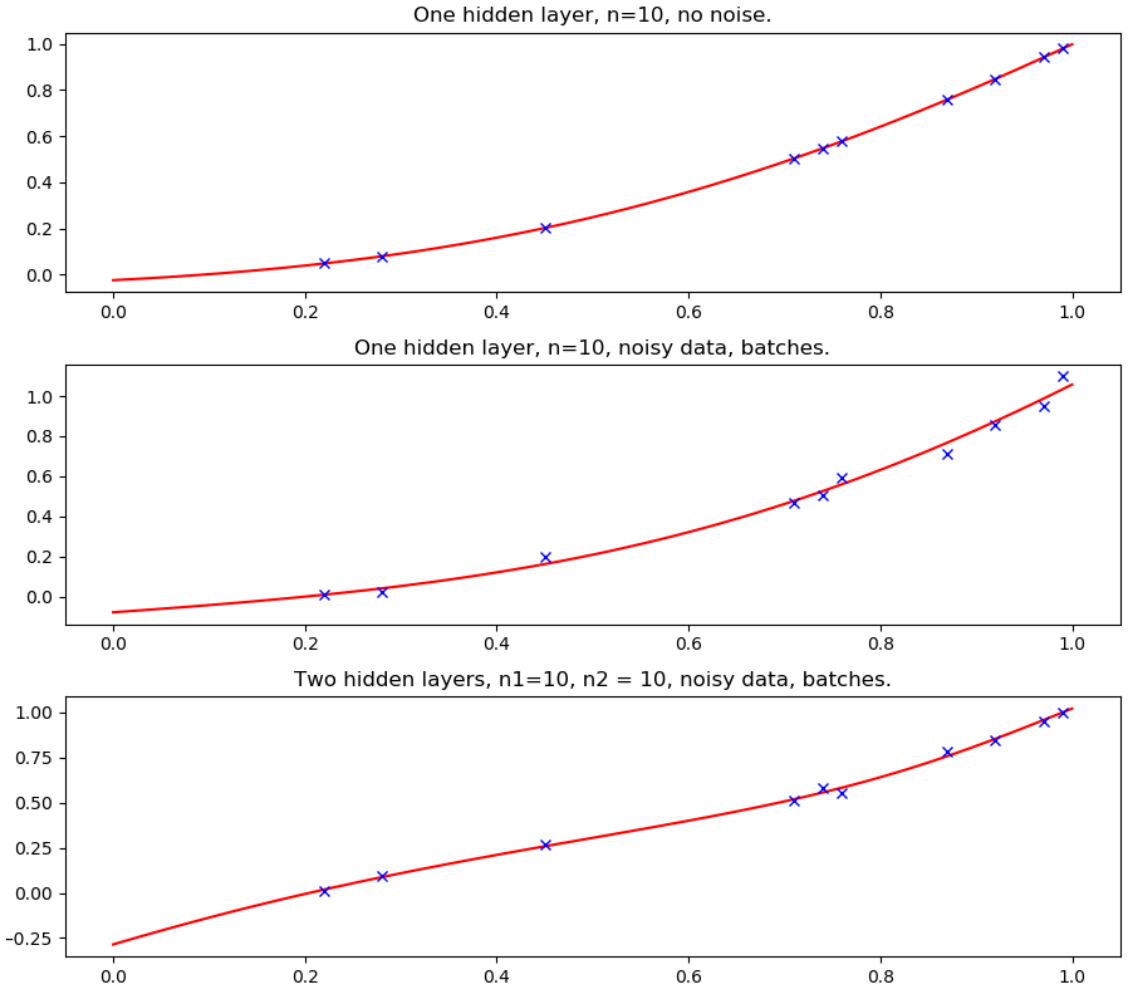
Stochastic descent: $\mathbf{w}^{\tau+1} = \mathbf{w}^{\tau} - \eta \sum_{n \in B^{\tau}} \nabla E_n(\mathbf{w}^{\tau})$,

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

Randomly choosing batches

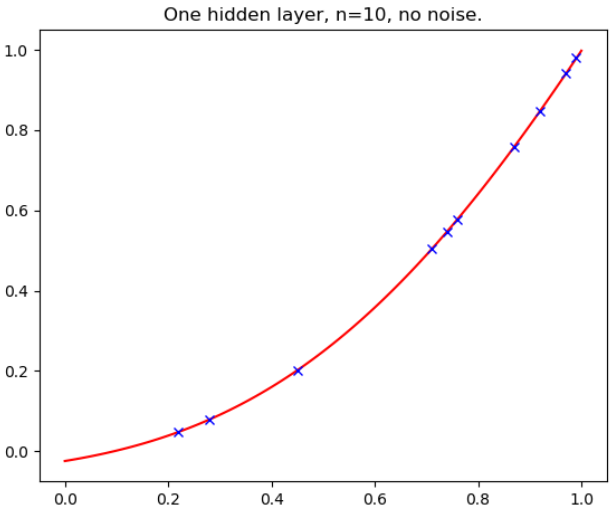
- helps reduce the chances of falling into local minima,
- makes the computation possible on GPUs even when dealing with LARGE databases.

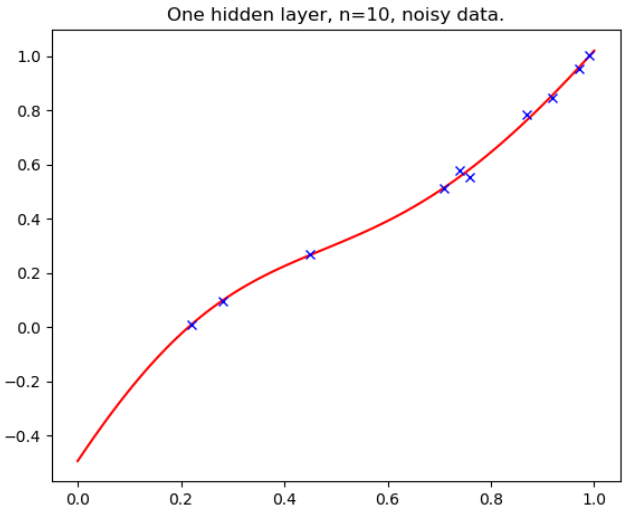
Using Mini-Batches

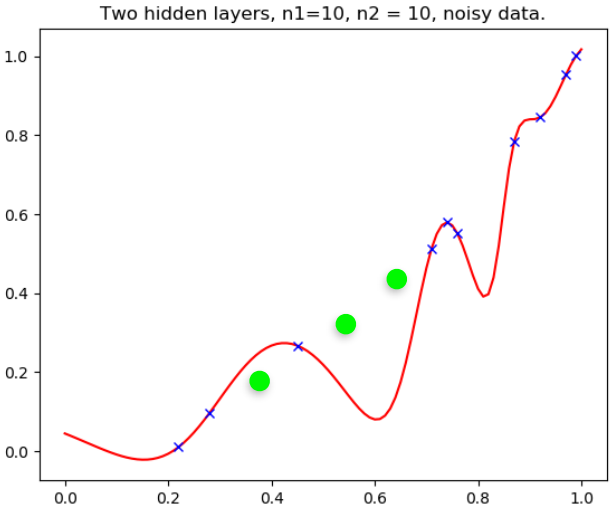


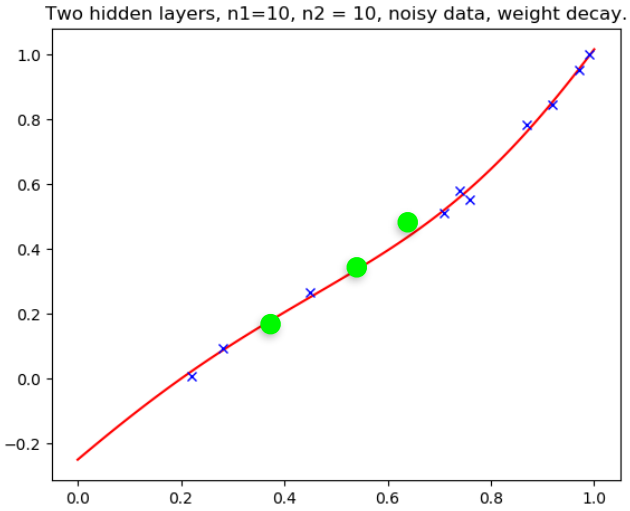
- The element of randomness prevents overfitting.
- No principled way to set the size of the mini-batches to achieve this result.

Weight Decay







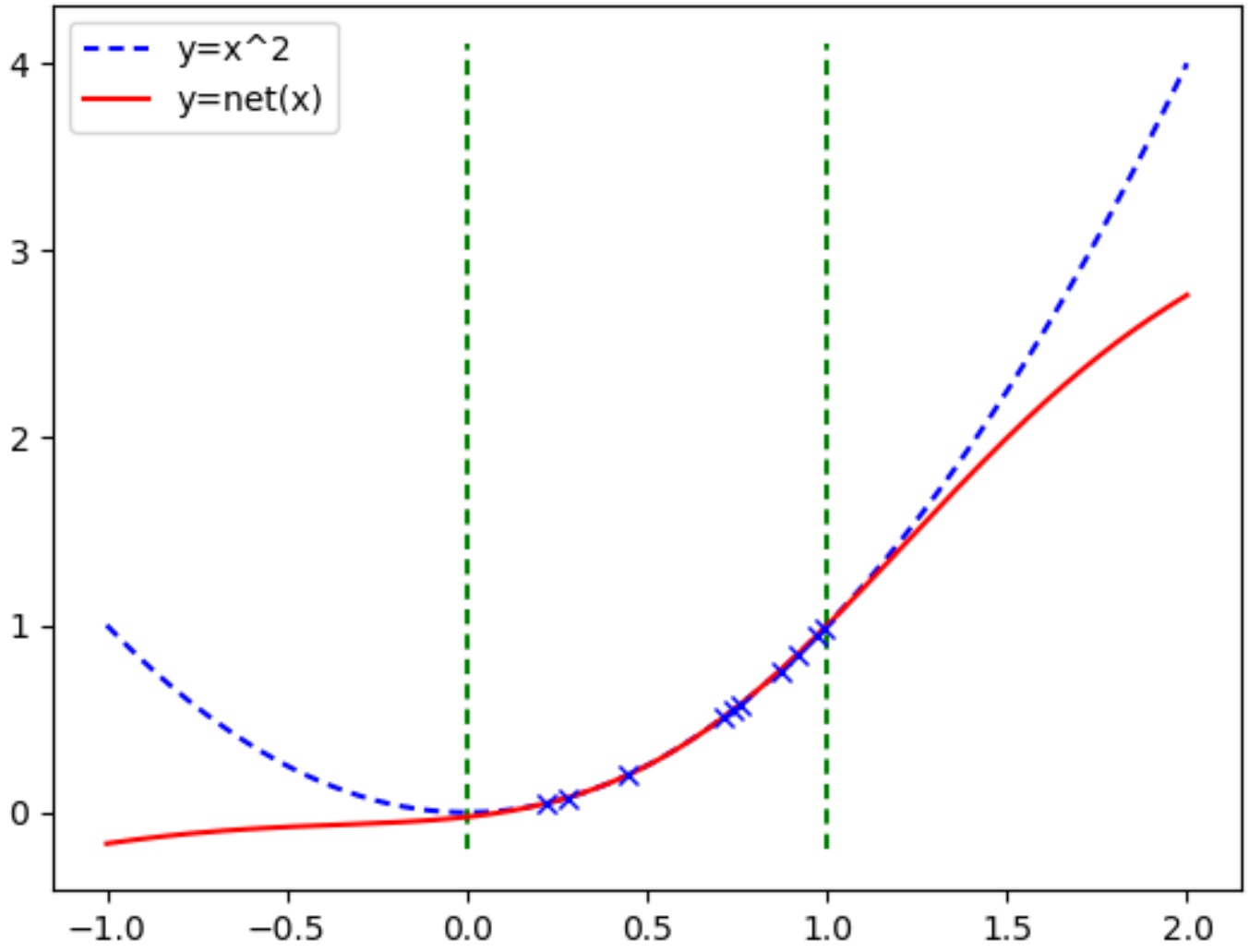


$$E(\mathbf{w}) = \sum_{n=1}^{N} E_n(\mathbf{w}) + \lambda \|\mathbf{w}\|^2$$

How large should λ be?

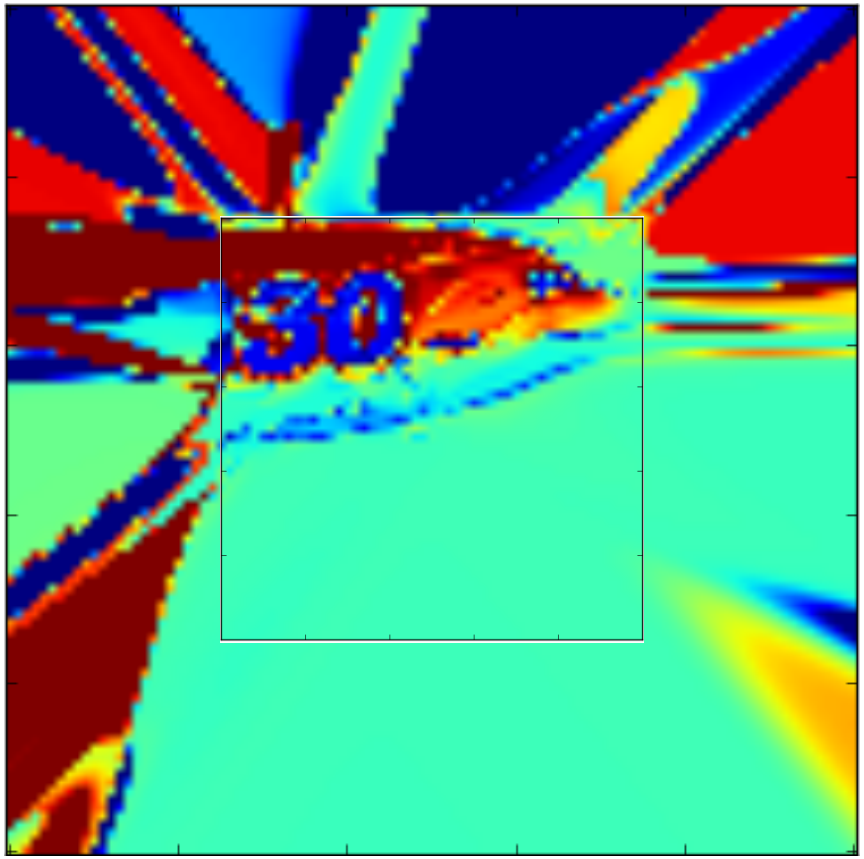
—>Use validation data as usual.

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:

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

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

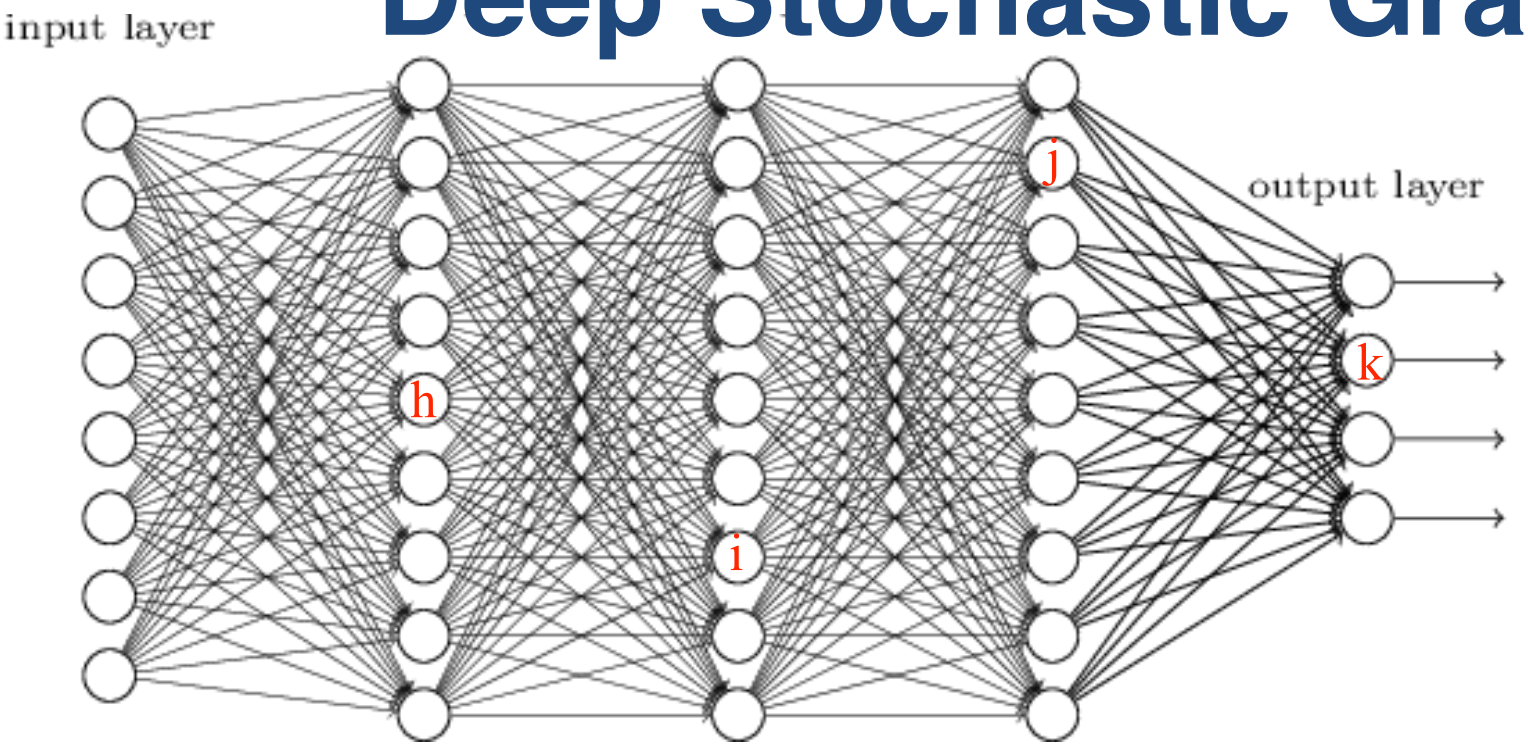
- We want to minimize the cross entropy

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

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

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

Deep Stochastic Gradient



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

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

x_l

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

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

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

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

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

But how do we compute all these derivatives?

Nobel Prize in Physics 2024

© Nobel Prize Outreach. Photo: Nanaka Adachi

John J. Hopfield

Prize share: 1/2

© Nobel Prize Outreach. Photo: Clément Morin

Geoffrey Hinton

Prize share: 1/2

The Nobel Prize in Physics 2024 was awarded jointly to John J. Hopfield and Geoffrey Hinton "for foundational discoveries and inventions that enable machine learning with artificial neural networks"

KUNGL. VETENSKAPS-AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

8 OCTOBER 2024

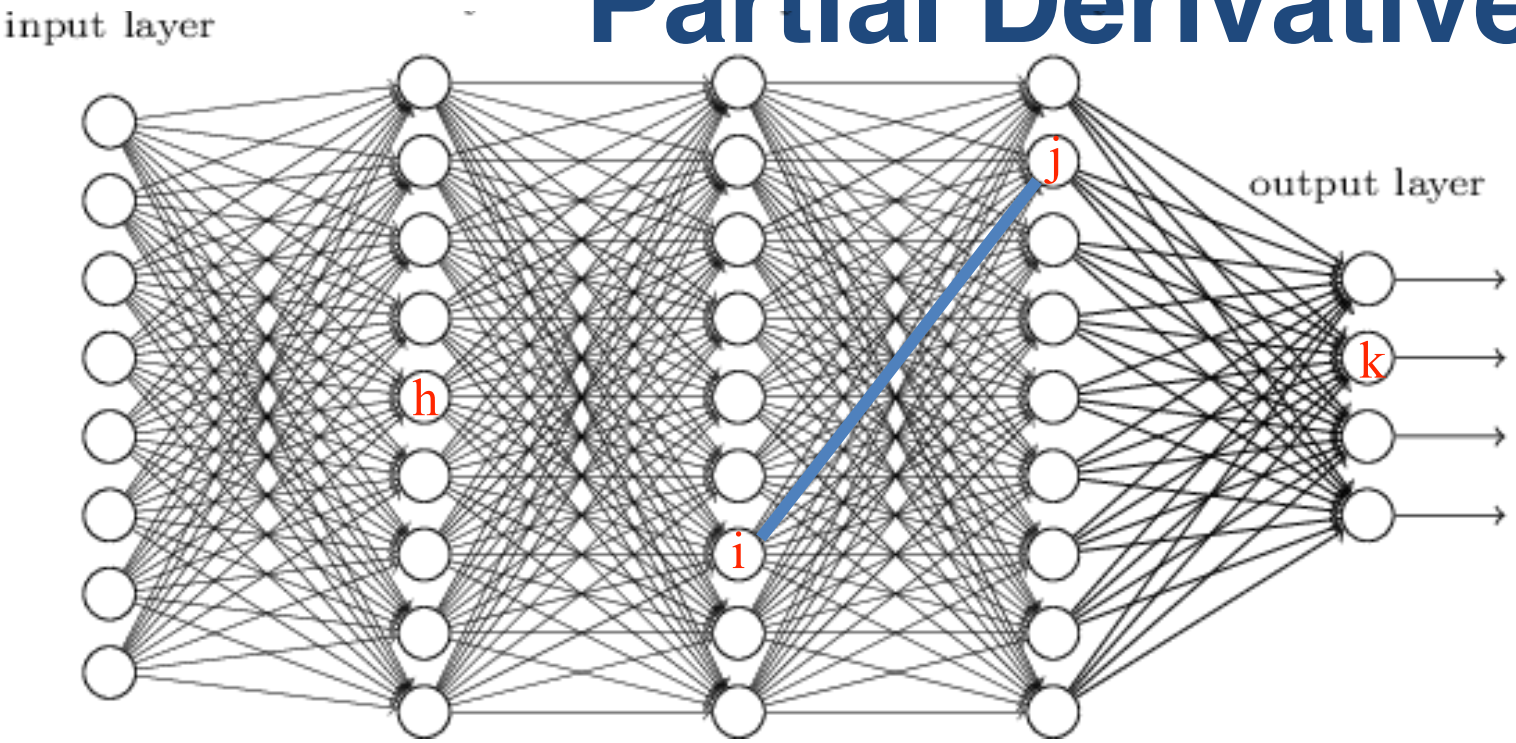
Scientific Background to the Nobel Prize in Physics 2024

"FOR FOUNDATIONAL DISCOVERIES AND INVENTIONS THAT ENABLE MACHINE LEARNING WITH ARTIFICIAL NEURAL NETWORKS"

The Nobel Committee for Physics

… A key advance was the demonstration by David Rumelhart, **Hinton** and Ronald Williams in **1986** of how architectures with one or more hidden layers could be trained for classification using an algorithm known as **backpropagation** …

Partial Derivatives



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

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

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

Hidden vals

Activations

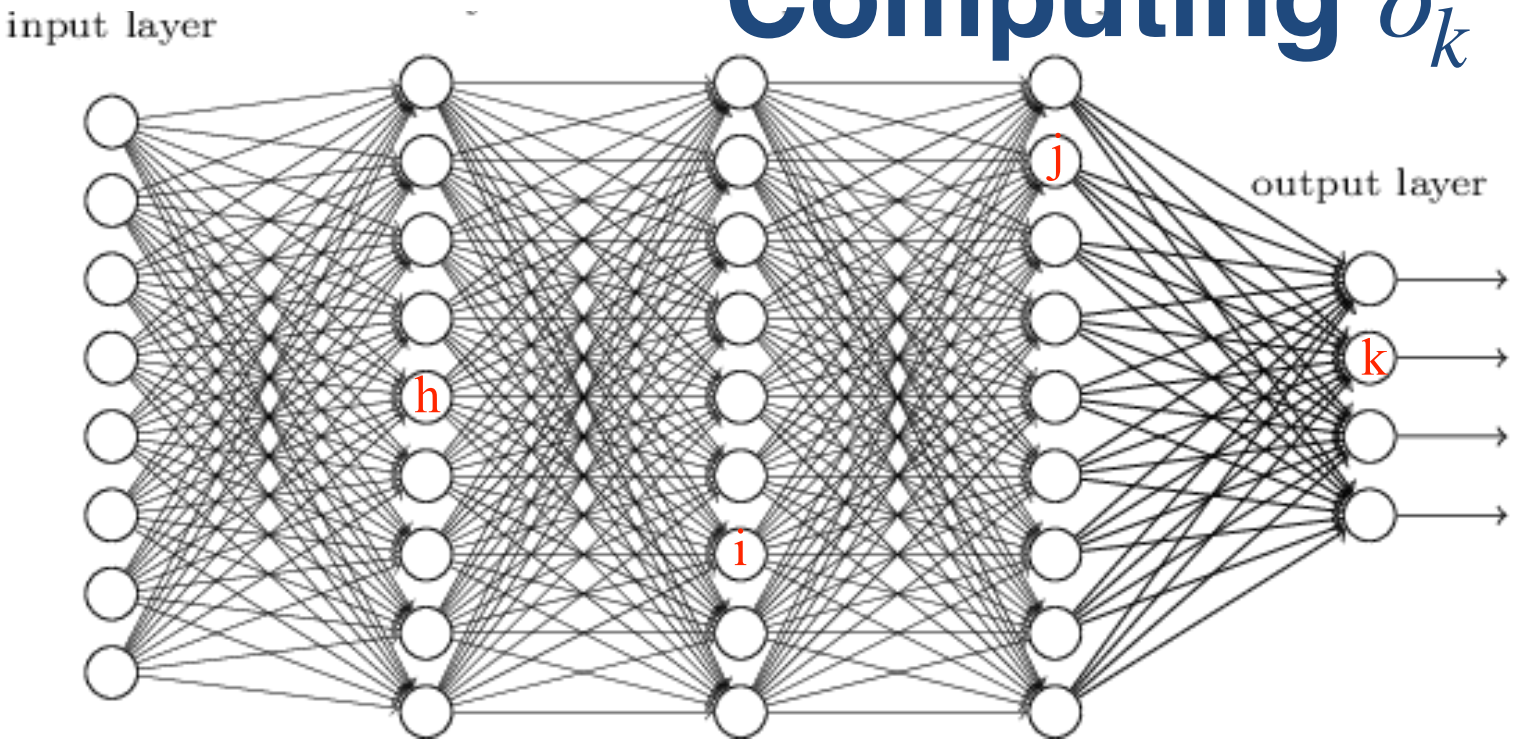
$$\frac{\delta E_n}{\delta w_{ji}} = \frac{\delta E_n}{\delta a_j} \frac{\delta a_j}{\delta w_{ji}}$$

$$= \delta_j z_i$$

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

—> Given the δ_j we can compute all partial derivatives.

Computing δ_k



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

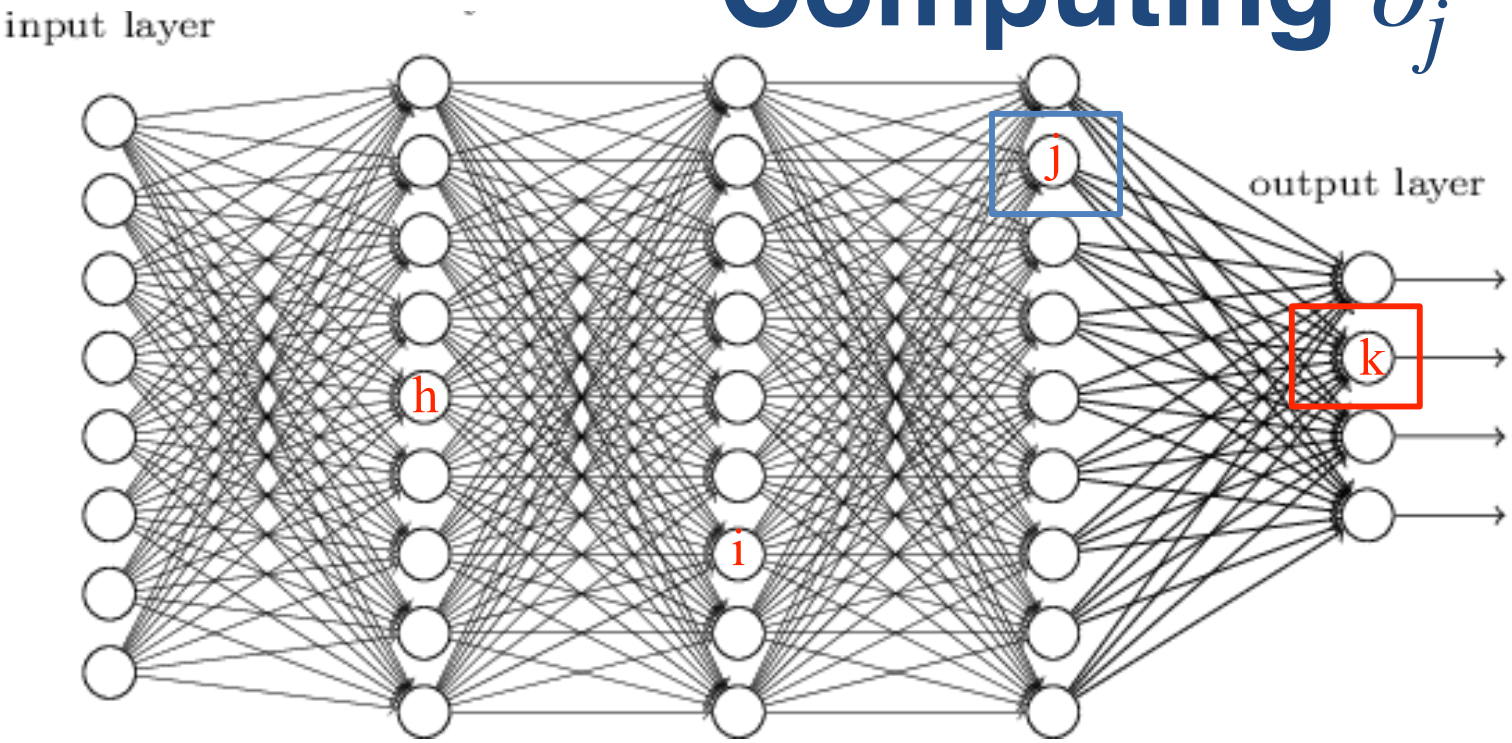
$$z_h = \sigma(a_h) \qquad z_i = \sigma(a_i) \qquad z_j = \sigma(a_j) \qquad y_k = a_k$$

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 δ_j



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

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

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

Other layers:

$$\delta_j = \frac{\delta E_n}{\delta a_j} = \sum_k \frac{\delta E_n}{\delta a_k} \frac{\delta a_k}{\delta a_j}$$

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

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

$$a_k = \sum_j w_{kj} \sigma(a_j)$$

- The δ_j can be computed given the δ_k.
- We can go back and compute all the others.

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:

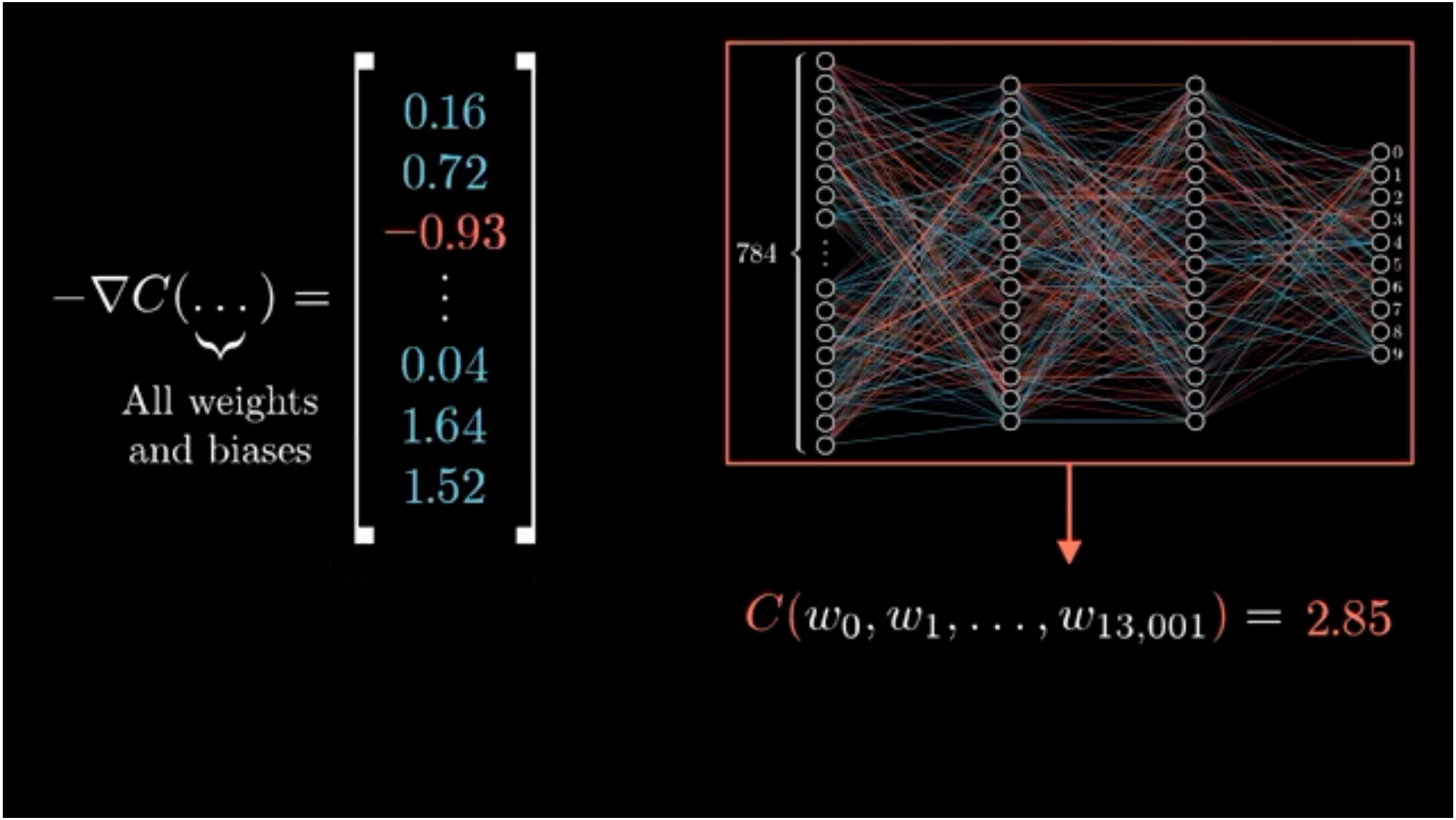
$$\forall k \ , \ \delta_k = \frac{\delta E_n}{\delta a_k}$$

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

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

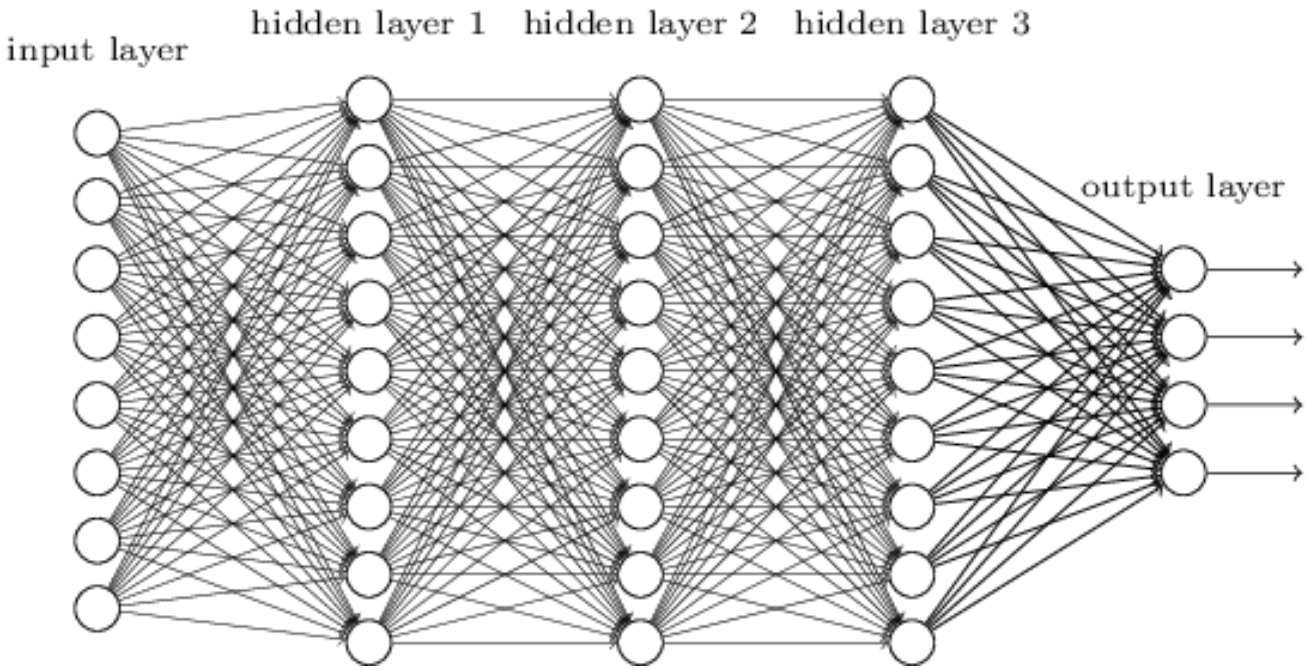
$$\forall h \ , \ \delta_h = \sigma'(a_h) \sum_j w_{ih} \delta_h$$

Back Propagation



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

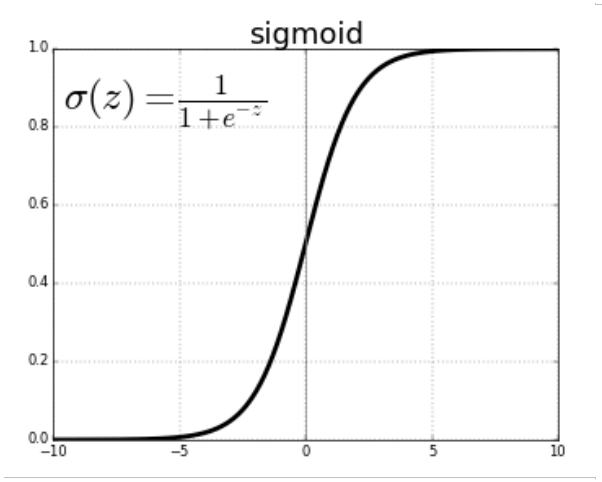
Back Propagation

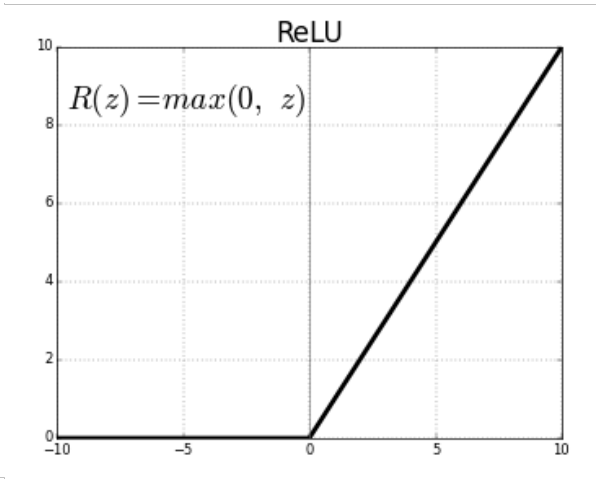


$$
\begin{aligned}
\mathbf{h}_1 &= \sigma_1(\mathbf{W}_1\mathbf{x}_1 + \mathbf{b}_1) \\
\mathbf{h}_2 &= \sigma_2(\mathbf{W}_2\mathbf{h}_2 + \mathbf{b}_2) \\
&\cdots \\
\mathbf{y} &= \sigma_n(\mathbf{W}_n\mathbf{h}_n + \mathbf{b}_n)
\end{aligned}
$$

- 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





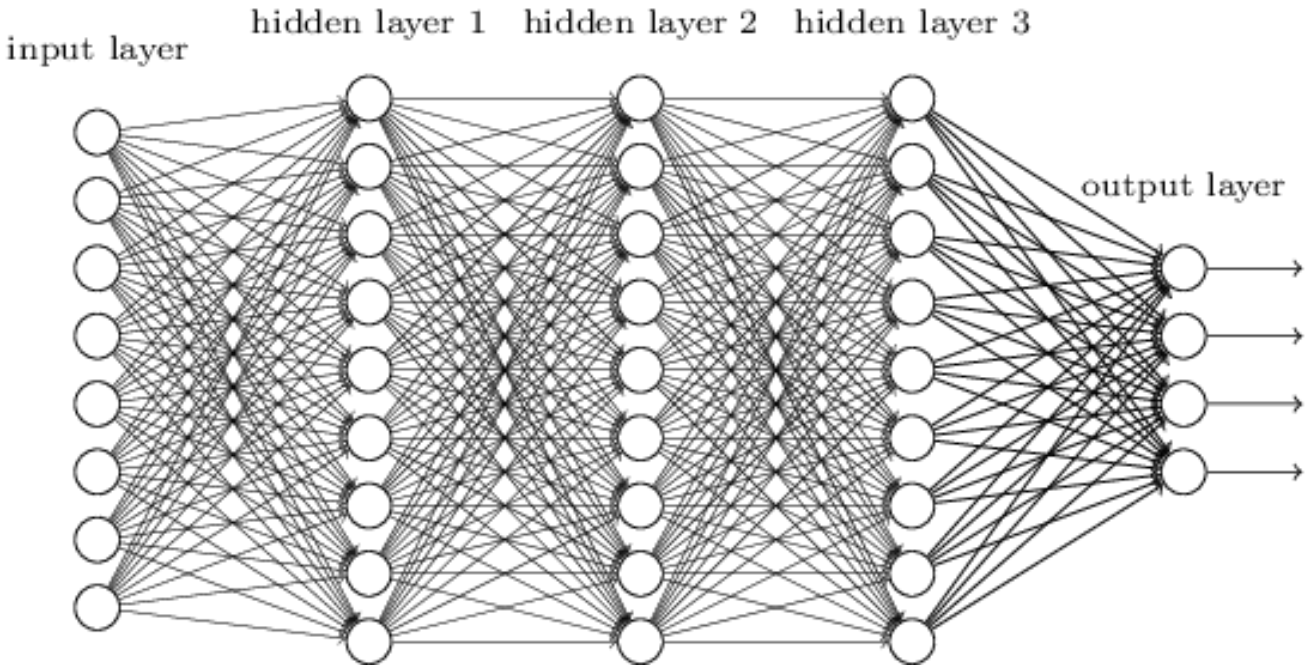
$$\forall i\ ,\ \delta_i = \sigma'(a_i) \sum_j w_{ji}\delta_j$$

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

- As $\sigma(a_i)$ approaches zero, so does δ_i and the gradients in the lower layers are lost. —> Vanishing gradients.
- If the δ_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, …

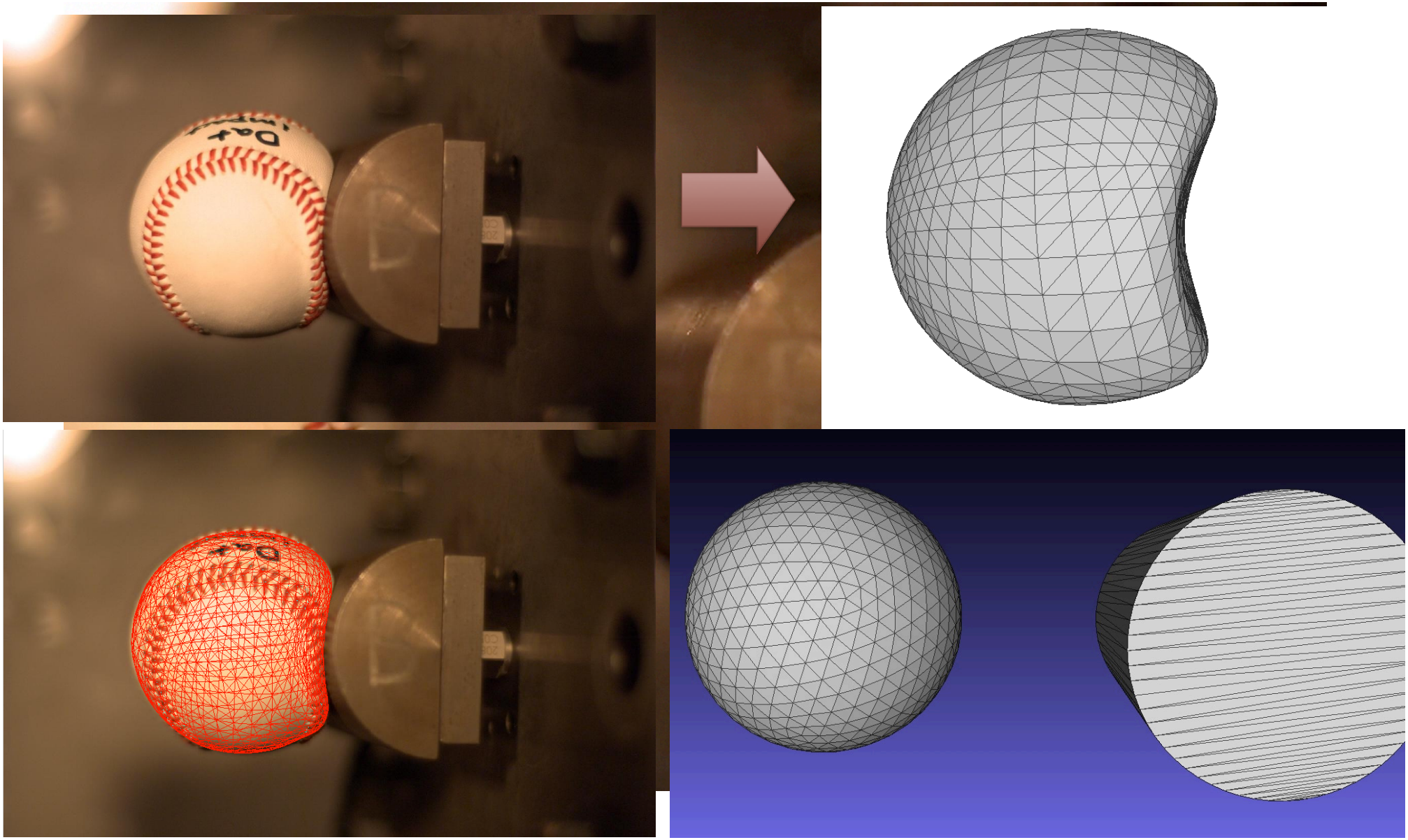
Back Propagation Works!



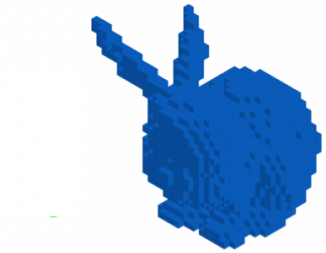
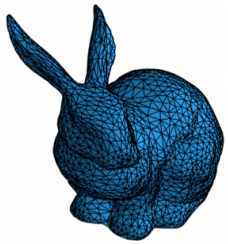
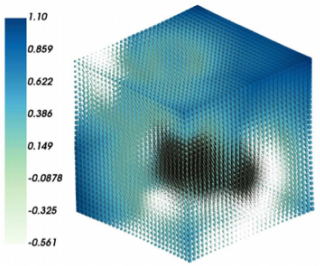
$$
\begin{aligned}
\mathbf{h}_1 &= \sigma_1(\mathbf{W}_1\mathbf{x}_1 + \mathbf{b}_1) \\
\mathbf{h}_2 &= \sigma_2(\mathbf{W}_2\mathbf{h}_2 + \mathbf{b}_2) \\
&\cdots \\
\mathbf{y} &= \sigma_n(\mathbf{W}_n\mathbf{h}_n + \mathbf{b}_n)
\end{aligned}
$$

- 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:

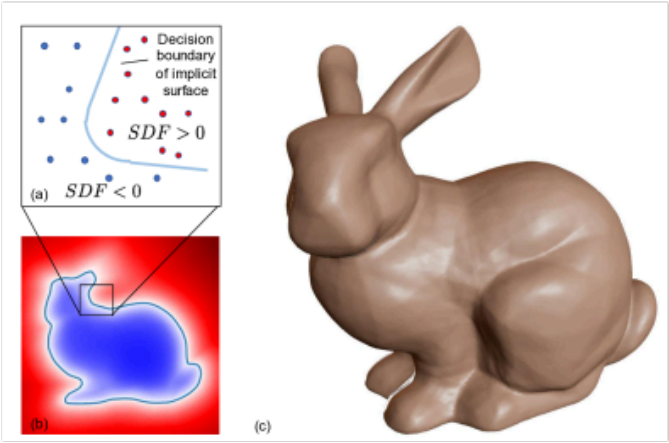
- High-quality rendering in computer graphics.
- Precise modeling of biological structures from biomedical data.
- Computational fluid dynamics in computer assisted design.

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

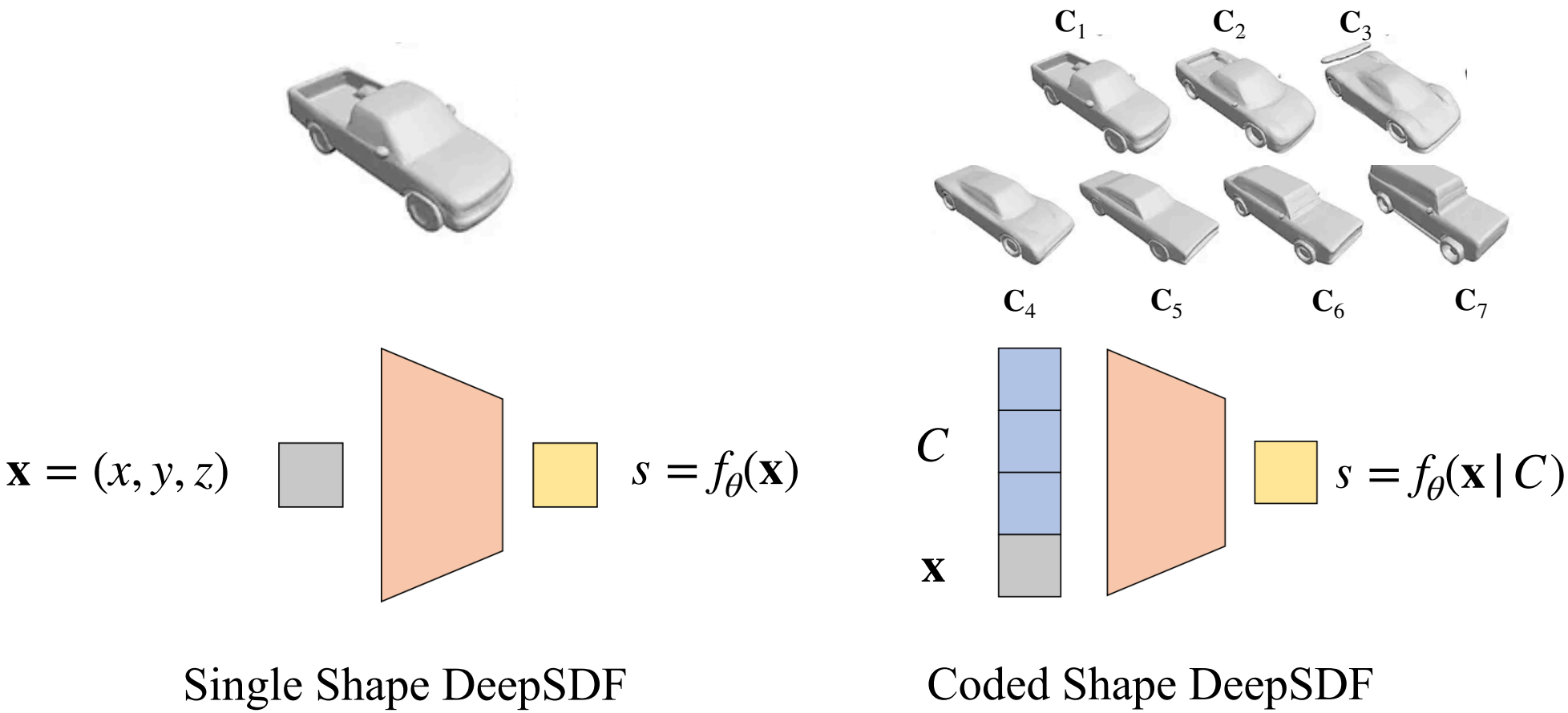
$$f\colon \mathbb{R}^3 \rightarrow \mathbb{R}$$

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

- 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 ….

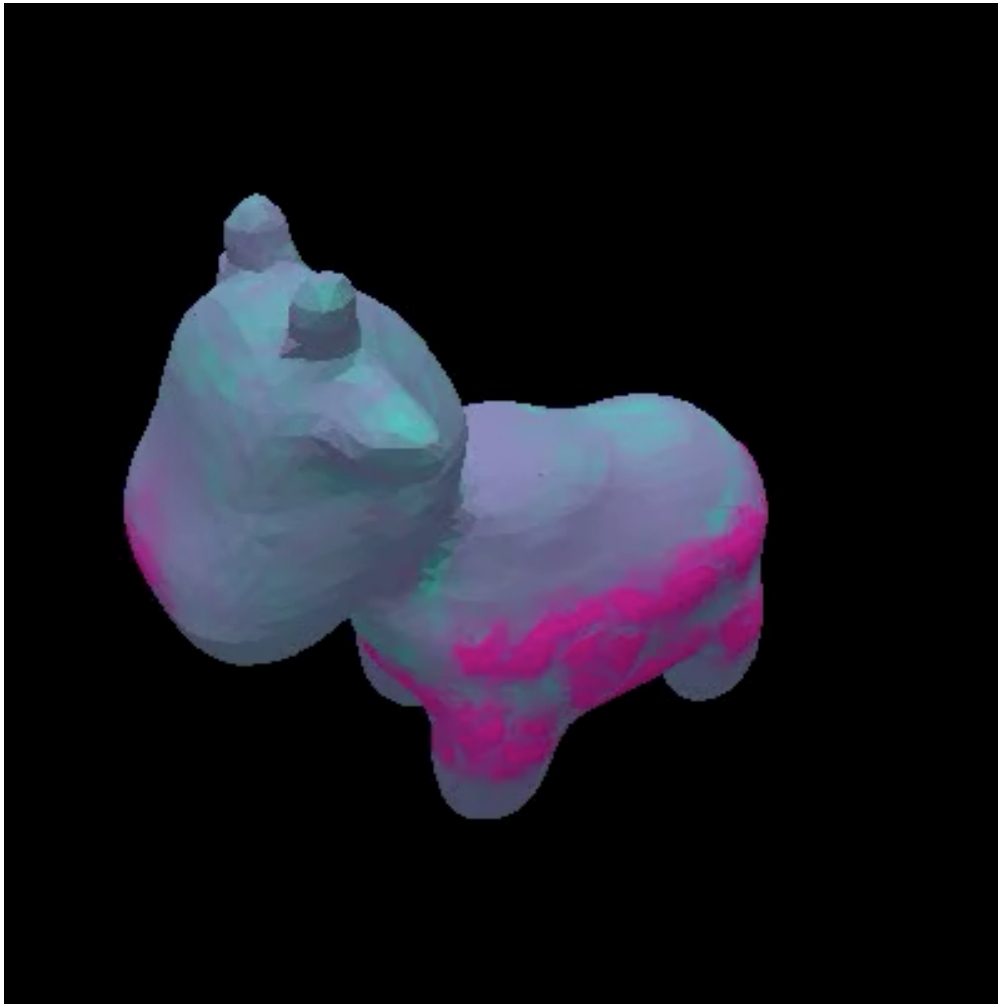
Optional: Deep SDF



C is a latent vector that parameterizes the surface.

[Park et al., CVPR'19]

Optional: From Genus 0 to Genus 1

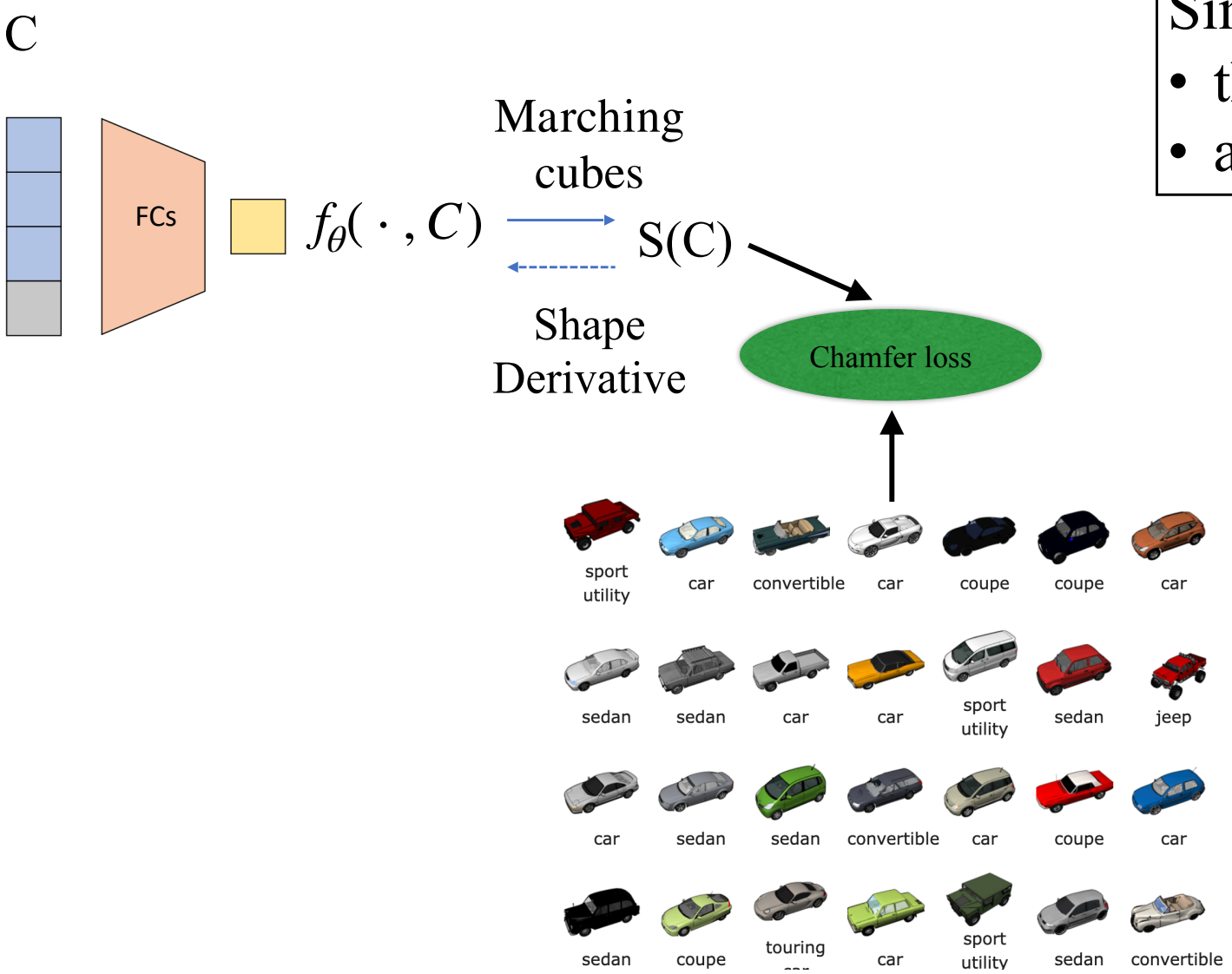


1. Start with a Deep SDF code.
2. Use marching cube to compute vertices and facets.
3. Use them for the forward pass and for backpropagation.
4. Update the SDF code and iterate.

—> We can turn a genus 0 cow into a genus 1 duck by minimizing a differentiable objection function.

[Remelli et al., NeurIPS'20]

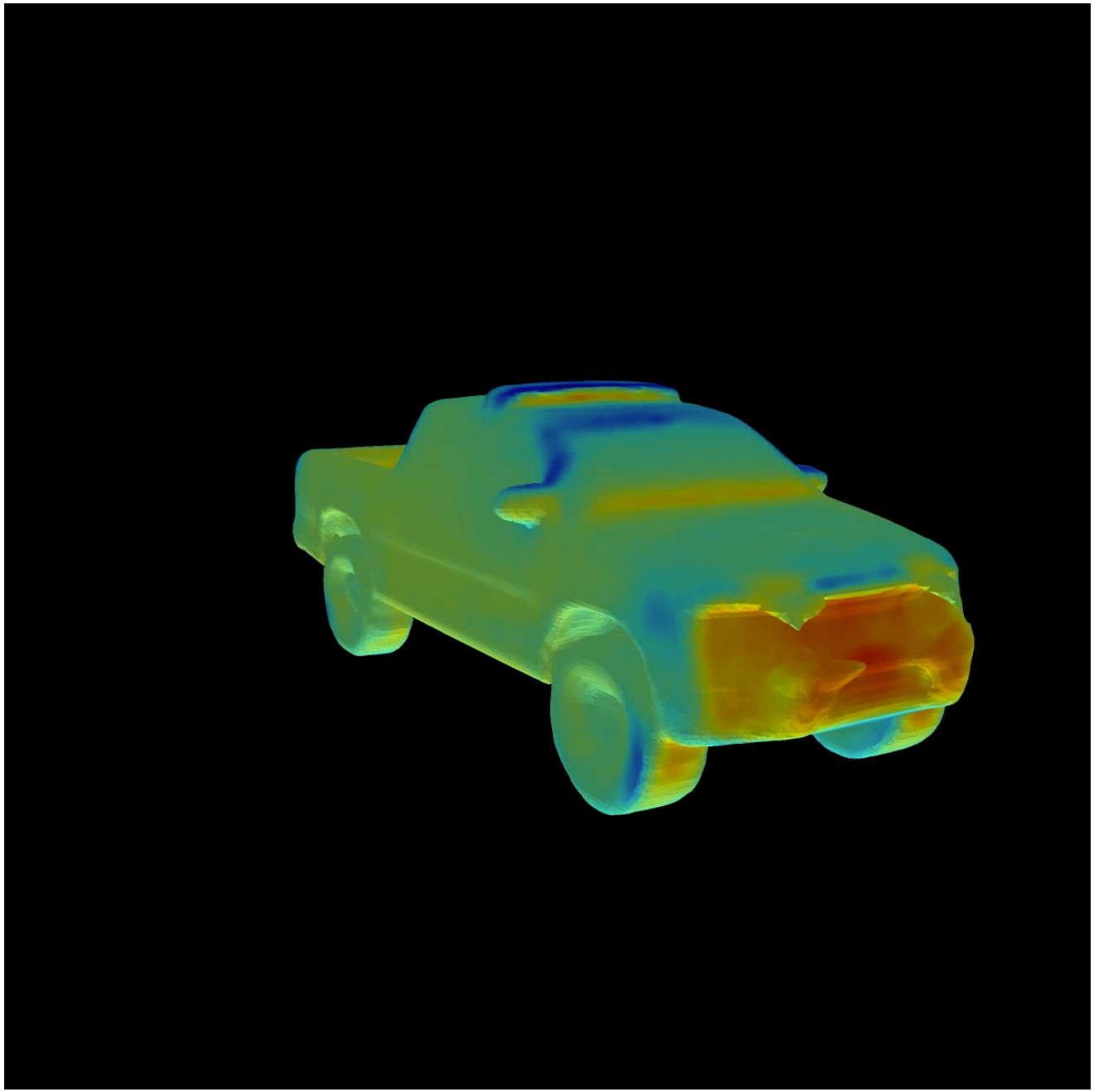
Optional: Introducing Priors



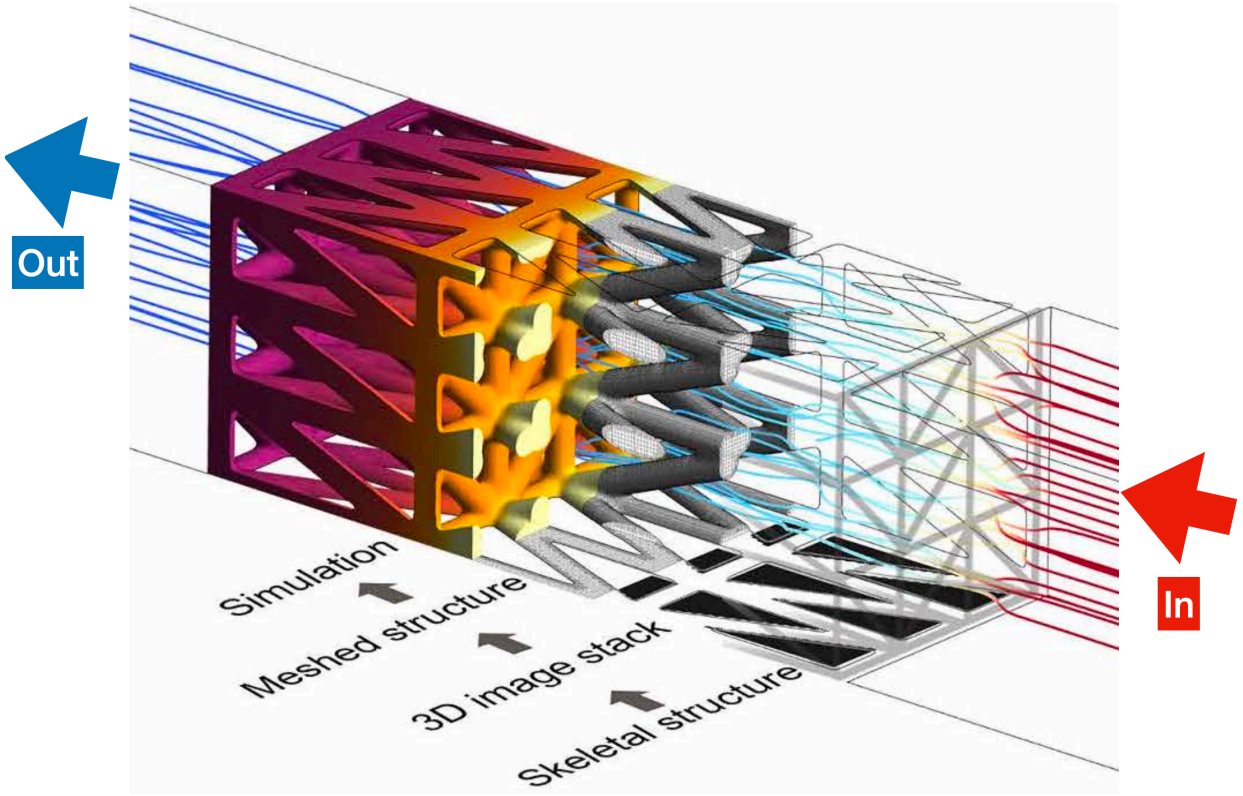
Simultaneously learn
- the network weights θ,
- a code C for each car.

[Guillard et al., PAMI'24]

Optional: From Pickup-Truck to Sports Car



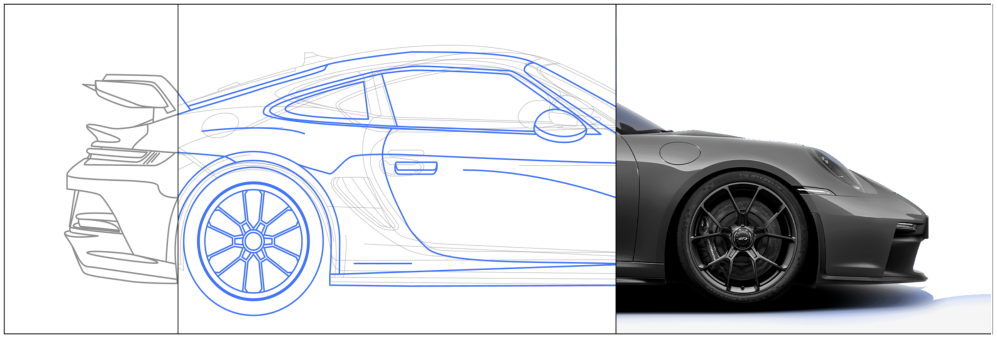
Optional: Heat Exchanger



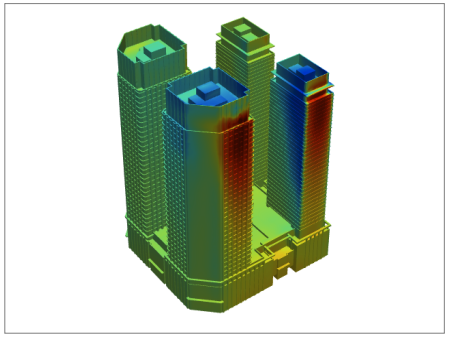
Predict and optimize the heat-exchange performance of 3D monolithic macro-porous structures

Optional: Tech Transfer

Aeronautics

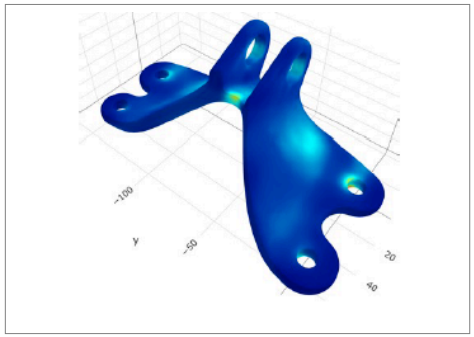


Automotive

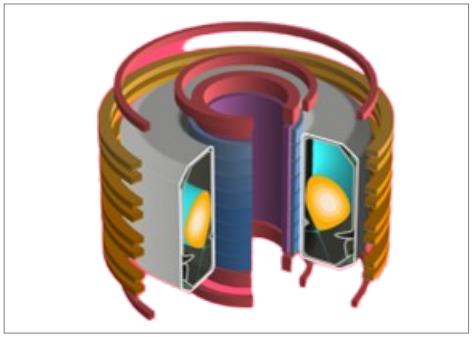


Architecture

Electrification



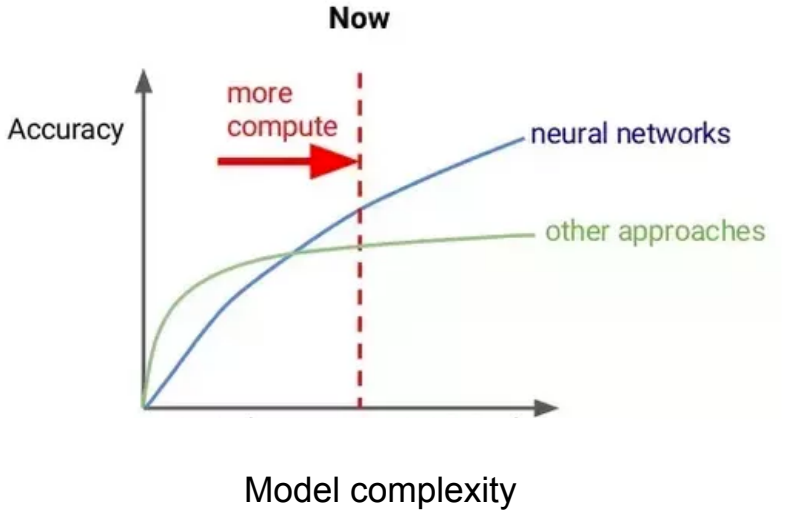
Structural engineering

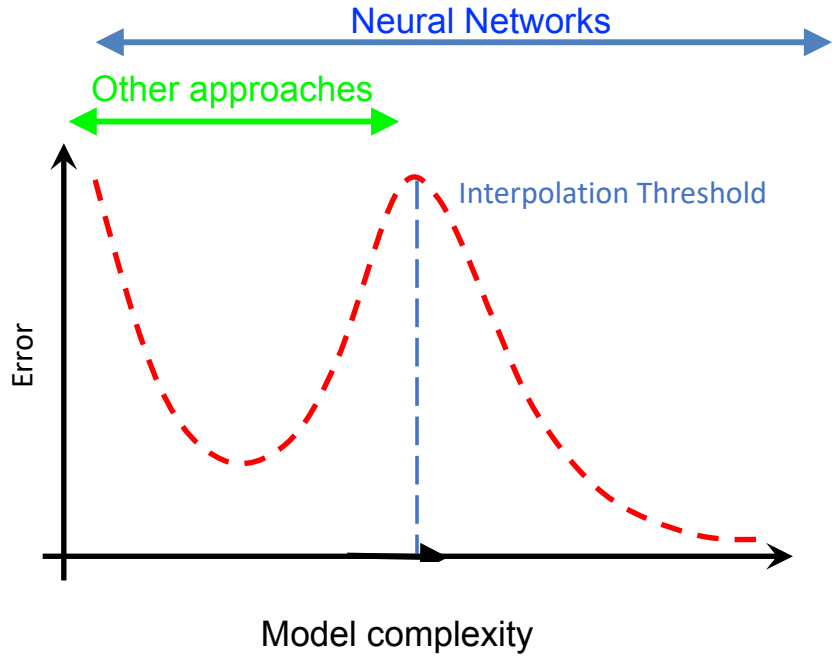


Nuclear fusion

—> A Large Impact in Computer Assisted Engineering

MLPs in Short





- MLPs get their descriptive power from their depth.
- The more training data the better.
- In other ML methods, excessive data complexity yields overfitting.
- No so, in MLPs. Given enough training data, deeper is better.
- MLPs are very good at interpolating.
- Less so at extrapolating.

Much the same thing can be said of other architectures. We'll get back to that.

[Mikhail et al. PNAS'19], [Spigler et al. Journal of Physics'19]