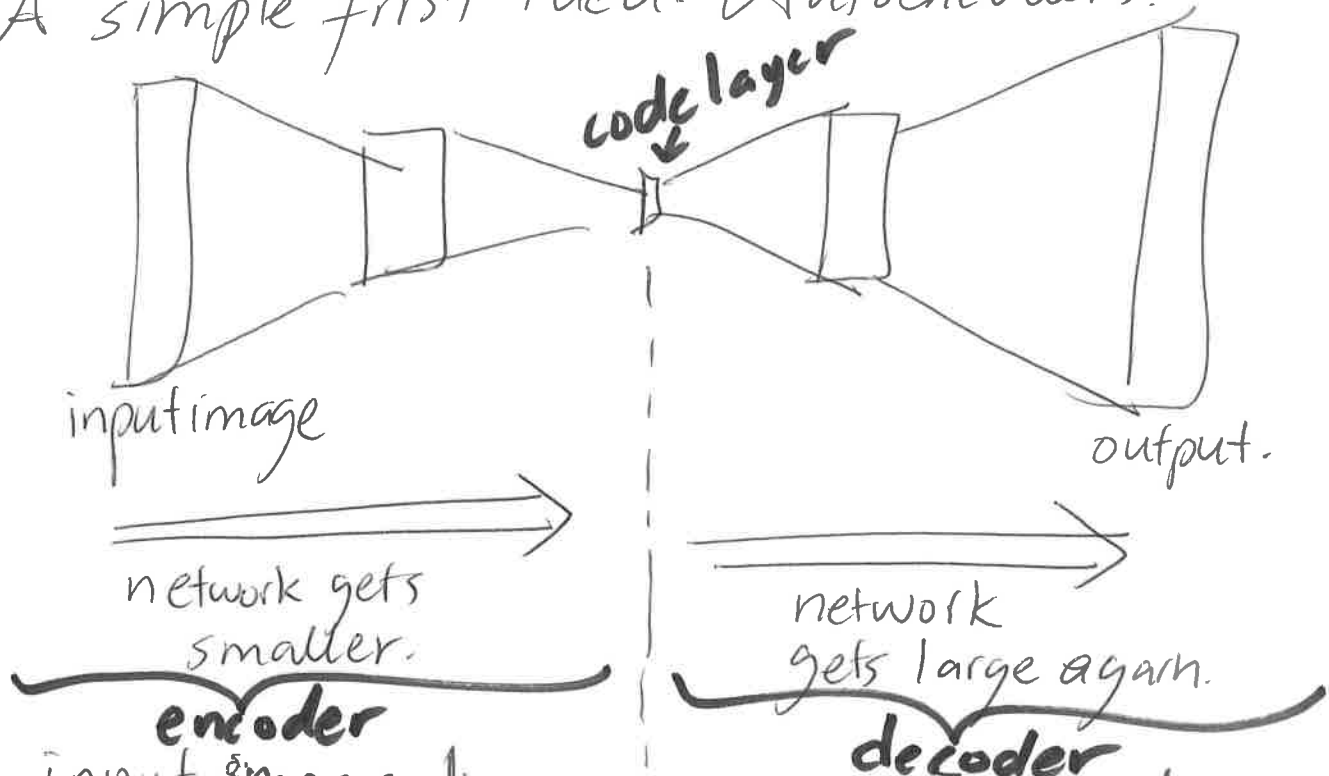
A simple first idea: Autoencoders.



input image dims = output image dims.

IDEA: Desired output for a given input X

=

Input X.

The network learns to compress/encode X to a very-low-dimensional representation (through the encoder layers) and then reconsruct the original X through the decoder layers.

After training, one can use the decoder part of the network as a "generator".

Generative Adversarial Networks. (4)

Introduced by Goodfellow et al 2014.

* **Two main ideas:**

A discriminator network D.

A generator network G.

Ideally $D(x) = \begin{cases} 1, & \text{if } x \text{ is a real image} \\ 0, & \text{if } x \text{ is a fake image provided by e.g. the generator network.} \end{cases}$

In general, D(x) is the likelihood of an image being real.

G takes noise z as an input and generates G(z), a generated image.

* Define the objective

$$\min_G \max_D \mathbb{E}\left[\log D(x) + \log(1 - D(G(z)))\right]$$

* Theorem: The solution satisfies $f_{G(z)}(x) = f_X(x)$.

(f_X: probability density)

Hence, the output of the generator matches the input data distribution.

→ Proof (Sketch): ① For a fixed G, find the optimal discriminator.

② Optimize over G.

How to train GANs?

5.

1. Generate data samples $x_1, \dots, x_m$
2. Generate noise samples $z_1, \dots, z_m$.
3. Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left(\log D(x_i) + \log(1 - D(G(z_i))) \right)$$

θ_d → discriminator parameters.

4. Generate new noise samples $z_1, \dots, z_m$
5. Update the generator by descending its stochastic gradient:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(1 - D(G(z_i))).$$

θ_g → generator parameters

6. Goto (1) until convergence.

At convergence, one arrives at a solution where $p_{G(Z)}(x) = p_X(x)$ and $D(x) = \frac{1}{2}$ $\forall x$. (all images are equally likely to be real or fake as the generator is perfect)

(6) Taken from Goodfellow et al.'s paper.

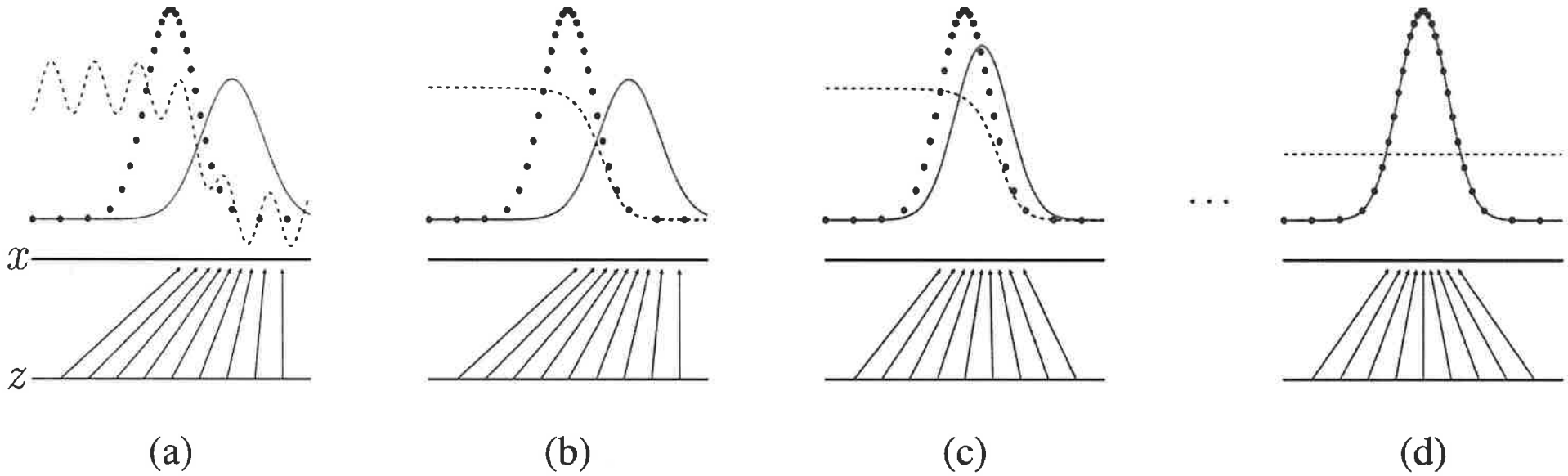


Figure 1: Generative adversarial nets are trained by simultaneously updating the discriminative distribution (D, blue, dashed line) so that it discriminates between samples from the data generating distribution (black, dotted line) $p_{\boldsymbol{x}}$ from those of the generative distribution p_g (G) (green, solid line). The lower horizontal line is the domain from which $\boldsymbol{z}$ is sampled, in this case uniformly. The horizontal line above is part of the domain of $\boldsymbol{x}$. The upward arrows show how the mapping $\boldsymbol{x} = G(\boldsymbol{z})$ imposes the non-uniform distribution p_g on transformed samples. G contracts in regions of high density and expands in regions of low density of p_g. (a) Consider an adversarial pair near convergence: p_g is similar to p_{data} and D is a partially accurate classifier. (b) In the inner loop of the algorithm D is trained to discriminate samples from data, converging to $D^*(\boldsymbol{x}) = \frac{p_{\text{data}}(\boldsymbol{x})}{p_{\text{data}}(\boldsymbol{x}) + p_g(\boldsymbol{x})}$. (c) After an update to G, gradient of D has guided $G(\boldsymbol{z})$ to flow to regions that are more likely to be classified as data. (d) After several steps of training, if G and D have enough capacity, they will reach a point at which both cannot improve because $p_g = p_{\text{data}}$. The discriminator is unable to differentiate between the two distributions, i.e. $D(\boldsymbol{x}) = \frac{1}{2}$.

Conditional GANs.

(7)

GANs cannot natively generate images for a given label. E.g. "Generate an image of a 3". For this purpose, we can use a conditional GAN. All that has to be done is to feed the class label (e.g. as a one-hot-encoded vector) to the generator as well as the discriminator during training (and, of course, during generation). The class label thus becomes an extra input to both D and G.

L17&18

ECE/CS 559 - Neural Networks Lecture Notes: Unsupervised Learning

Erdem Koyuncu

This is also referred to as self-organization. We similarly have a training set. But, for each member of the training set, we do not have a correct output information. The NN is required to organize itself, by possibly detecting the similarities between the patterns (statistical properties) and arranges its outputs accordingly. A typical case is clustering, which may be considered as a form of classification.

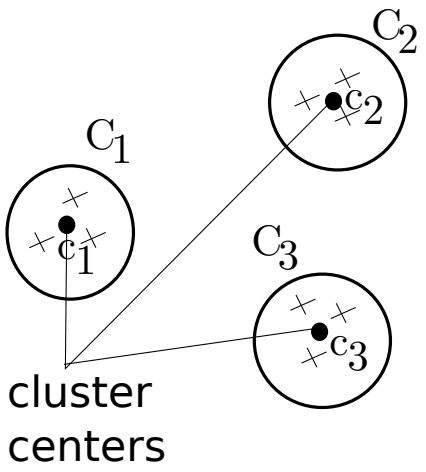


Figure 1: Clustering

- Suppose that the inputs will form clusters $\mathcal{C}_i$ with cluster centers $\mathbf{c}_i$.
- If we know the cluster centers, we can then distinguish the clusters by distance: Given $\mathbf{x} \in \mathcal{S}$, we have $\|\mathbf{x} - \mathbf{c}_i\| < \|\mathbf{x} - \mathbf{c}_j\|, \forall j \neq i \implies \mathbf{x} \in \mathcal{C}_i$.
- Hence one way of looking at unsupervised learning is to find appropriate cluster centers for each clusters, hence detect the clusters in the given training set.
- Here, the cluster centers $\mathbf{c}_i$ are also known as the quantization vectors.
- Unsupervised learning tries to minimize quantization error by finding appropriate cluster centers:
- If we have m clusters, the quantization error given $\mathbf{c}_i$, $i = 1, \ldots, m$ is given by

$$E = \sum_{\mathbf{x} \in \mathcal{S}} \min_i \|\mathbf{x} - \mathbf{c}_i\|^2$$

- The goal is then to minimize E, i.e. finding the appropriate cluster centers (quantization points) $\mathbf{c}_i$ such that E is minimized.

1 k-means algorithm

- In general, the problem of minimizing E can be solved iteratively. Let $\mathcal{V}_i = \{\mathbf{x} : \|\mathbf{x} - \mathbf{c}_i\| \leq \|\mathbf{x} - \mathbf{c}_j\|\}$ denote the Voronoi cell for cluster center i, where ties are broken arbitrarily. Then, we have

$$E = \sum_{i=1}^{m} \sum_{\mathbf{x} \in \mathcal{V}_i} \|\mathbf{x} - \mathbf{c}_i\|^2 \tag{1}$$

  This decomposition suggests the following algorithm:

  1) Initialize cluster centers $\mathbf{c}_1, \ldots, \mathbf{c}_m$ (e.g., arbitrarily).

  2) Until convergence (of the energy E or cluster centers)

  2.1) Calculate Voronoi cells $\mathcal{V}_1, \ldots, \mathcal{V}_m$ given cluster centers $\mathbf{c}_1, \ldots, \mathbf{c}_m$.

  2.2) Set $\mathbf{c}_i \leftarrow \min_{\mathbf{c}} \sum_{\mathbf{x} \in \mathcal{V}_i} \|\mathbf{x} - \mathbf{c}\|^2$, $i = 1, \ldots, m$. In other words, we update each cluster center while considering the corresponding Voronoi cells to be fixed.

  Note that $\arg\min_{\mathbf{c}} \sum_{\mathbf{x} \in \mathcal{V}_i} \|\mathbf{x} - \mathbf{c}\|^2 = \frac{1}{|\mathcal{V}_i|} \sum_{\mathbf{x} \in \mathcal{V}_i} \mathbf{x}$, i.e. the solution of the optimization problem is the geometric centroid of the voronoi region $\mathcal{V}_i$. Thus, instead of 2.2 above, I can equivalently write:

  2.2) Set $\mathbf{c}_i \leftarrow \frac{1}{|\mathcal{V}_i|} \sum_{\mathbf{x} \in \mathcal{V}_i} \mathbf{x}$, $i = 1, \ldots, m$.

  This is known as the k-means algorithm or the Lloyd algorithm. Each step of the algorithm provides a lower energy E, and thus the algorithm is guaranteed to converge in terms of the energy-function sense. The convergence of the cluster centers is another matter that we will not go into, but typically you may assume that you also have the convergence of the cluster centers.

  It is possible to reinterpret the algorithm using neural networks, as we will show soon.

2 Hebbian Learning

Another important case we will look at is Hebbian learning.

- This learning rule was first proposed by D. Webb in 1940's. Hebb's idea was (1949):
- When an axon of a cell A is near enough to excite a cell B and repeatedly or persistently fires it, some growth process or metabolic change takes place in one or both cells such that A's efficiency, as one of the cells firing B, is increased.
- Nodes that tend to be either both positive or both negative at the same time have strong positive weights, while those that tend to be opposite have strong negative weights.
- Mathematically, we have $\mathbf{w}_i(n+1) = \mathbf{w}_i(n) + \eta \mathbf{x} y_i(n)$, where $y_i(n)$ is the output of neuron i for training sample n. This is also called the activity product rule.
- This type of update leads to saturation problems. For example, suppose $y_i(n) = \text{sgn}(\mathbf{x}^T \mathbf{w}_i(n))$, with the initial condition $\mathbf{w}_i(n) = \mathbf{1}$, and consider a fixed input $\mathbf{x} = 1$. We obtain the sequence $\mathbf{1}, \mathbf{2}, \mathbf{4}, \mathbf{8}$, with exponential divergence to infinity.
- So, sometimes, the update $\mathbf{w}_i(n+1) = \alpha \mathbf{w}_i(n) + \eta \mathbf{x} y_i(n)$ is used, where $\alpha < 1$. For the previous example, we obtain $1, 1+\alpha, 1+\alpha(1+\alpha), 1+\alpha(1+\alpha(1+\alpha)), \ldots$. Solution $1 + \alpha x = x$, $x = \frac{1}{1-\alpha}$ (finite).
- Sometimes, this update is also used $\mathbf{w}_i(n+1) = \mathbf{w}_i(n) + \eta(\mathbf{x} - \overline{\mathbf{x}})(y_i(n) - \overline{y_i})$. Here, $\overline{\mathbf{x}}$ and $\overline{y_i}$ are time averages of their respective quantities.
- Example: Suppose $\mathcal{C}_1 = \left\{ \mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \mathbf{x}_2 = \begin{bmatrix} 0.9 \\ 1 \end{bmatrix}, \mathbf{x}_3 = \begin{bmatrix} 1 \\ 1.1 \end{bmatrix} \right\}$, and $\mathcal{C}_2 = \left\{ \mathbf{x}_4 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \mathbf{x}_5 = \begin{bmatrix} 1.1 \\ -1 \end{bmatrix}, \mathbf{x}_6 = \begin{bmatrix} 1 \\ -1.1 \end{bmatrix} \right\}$. The problem is to find a single neuron that can distinguish between the two classes. Although the example introduces the two classes separately, we assume we do not know the desired output for any given pattern. Obviously, if the desired output were given for all patterns, we could have used the perceptron training algorithm to solve the classification task.

- Here, we consider weights without any thresholding. Suppose the initial weights are $\mathbf{w}(1) = \begin{bmatrix}0.1\\0.1\end{bmatrix}$. Note that given input $\mathbf{x}_1$, the output is $\text{sgn}(\mathbf{x}_1^T\mathbf{w}(1)) = 1$. Given input $\mathbf{x}_5$ on the other hand, the output is $\text{sgn}(\mathbf{x}_5^T\mathbf{w}(1)) = 1$. However $\mathbf{x}_1$ and $\mathbf{x}_5$ were supposed to be on different classes. Hence, the initial weights cannot distinguish the two classes.
- Begin Epoch: 1. Suppose $\eta = 1$.
  - Feed $\mathbf{x}_1$, the output is $\text{sgn}(\mathbf{x}_1^T\mathbf{w}(1)) = 1$. Hence, we set $\mathbf{w}(2) = \mathbf{w}(1) + 1 \times 1 \times \mathbf{x}_1 = \begin{bmatrix}1.1\\1.1\end{bmatrix}$.
  - Feed $\mathbf{x}_2$, the output is $\text{sgn}(\mathbf{x}_2^T\mathbf{w}(2)) = 1$. Hence, we set $\mathbf{w}(3) = \mathbf{w}(2) + 1 \times 1 \times \mathbf{x}_2 = \begin{bmatrix}2\\2.1\end{bmatrix}$.
  - Feed $\mathbf{x}_3$, the output is $\text{sgn}(\mathbf{x}_3^T\mathbf{w}(3)) = 1$. Hence, we set $\mathbf{w}(4) = \mathbf{w}(3) + 1 \times 1 \times \mathbf{x}_3 = \begin{bmatrix}3\\3.2\end{bmatrix}$.
  - Feed $\mathbf{x}_4$, the output is $\text{sgn}(\mathbf{x}_4^T\mathbf{w}(4)) = -1$. Hence, we set $\mathbf{w}(5) = \mathbf{w}(4) - 1 \times 1 \times \mathbf{x}_4 = \begin{bmatrix}2\\4.2\end{bmatrix}$.
  - Feed $\mathbf{x}_5$, the output is $\text{sgn}(\mathbf{x}_5^T\mathbf{w}(4)) = -1$. Hence, we set $\mathbf{w}(6) = \mathbf{w}(5) - 1 \times 1 \times \mathbf{x}_5 = \begin{bmatrix}0.9\\5.2\end{bmatrix}$.
  - Feed $\mathbf{x}_6$, the output is $\text{sgn}(\mathbf{x}_6^T\mathbf{w}(4)) = -1$. Hence, we set $\mathbf{w}(7) = \mathbf{w}(6) - 1 \times 1 \times \mathbf{x}_6 = \begin{bmatrix}-0.1\\6.3\end{bmatrix}$.
- We can proceed with more epochs like this, but let us stop at the end of Epoch 1. It can be verified that the final weight vector $\mathbf{w}(7)$ provides an output of 1 for input patterns $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3$, and it provides an output of -1 for input patterns $\mathbf{x}_4, \mathbf{x}_5, \mathbf{x}_6$.

3 Competitive learning

- Also called the winner takes all learning rule.
- Output neurons compete around themselves to be active.
- Consider a one-layer network. Suppose we have m input neurons and n output neurons without any bias, and the activator function is identity. Let $\mathbf{W} \in \mathbb{R}^{n\times m}$ denote the weight matrix with the weight going to output neuron i from neuron j denoted by w_{ij}. Then, given input $\mathbf{x} \in \mathbb{R}^{m\times 1}$, the induced local fields are $\mathbf{v} = \mathbf{W}\mathbf{x} \in \mathbb{R}^{n\times 1}$ and the outputs are $\mathbf{y} = \phi(\mathbf{v}) \in \mathbb{R}^{n\times 1}$. The weights for the ith output neuron is then ith row $\mathbf{w}_i$ of $\mathbf{W}$. We may also use the extended notation.
- After this, we look at the output neuron with the largest output. Due to the monotonicity of the activation function, this neuron is the one with the largest induced local field.
- Suppose that the ith neuron has the largest induced local field, i.e. $v_i = \max_{j\in\{1,\dots,n\}} v_j$ according to some tie-breaking rule. Then, the ith neuron is declared the winning neuron, and its outputs are updated as $\mathbf{w}_i(n+1) = \mathbf{w}_i(n)+\eta(\mathbf{x}-\mathbf{w}_i(n))$. The others remain the same, i.e. $\mathbf{w}_j(n+1) = \mathbf{w}_j(n)$, $j \neq i$. Here, η is the learning constant.
- If $\|\mathbf{w}_i\| = \|\mathbf{w}_j\|$ for every $i \neq j$, then the winning neuron coincides with the neuron whose weight vector is closest to the input $\mathbf{x}$ in terms of the Euclidean distance - prove this. So, roughly speaking: The learning rule has the effect of moving the input $\mathbf{x}$ towards the direction of the winning neuron. The winner is more likely to win next time as well.
- Usually, for the success of the algorithm, most of the time input vectors and weights are normalized.

- Suppose that some input pattern $\mathbf{x}$ is repeatedly applied, and at each time, neuron i wins. We have

$$\begin{aligned}
\mathbf{w}_i(2) &= \mathbf{w}_i(1) + \eta(\mathbf{x} - \mathbf{w}_i(1)) = (1-\eta)\mathbf{w}_i(1) + \eta\mathbf{x} \\
\mathbf{w}_i(3) &= \mathbf{w}_i(2) + \eta(\mathbf{x} - \mathbf{w}_i(2)) = (1-\eta)^2\mathbf{w}_i(1) + \eta(1 + (1-\eta))\mathbf{x} \\
&\vdots \\
\mathbf{w}_i(n+1) &= (1-\eta)^n\mathbf{w}_i(1) + \eta(1 + (1-\eta) + \cdots + (1-\eta)^{n-1})\mathbf{x} \\
&= (1-\eta)^n\mathbf{w}_i(1) + (1 - (1-\eta)^n)\mathbf{x}
\end{aligned}$$

  If $|\eta| < 1$, then we have $\mathbf{w}_i(n+1) \to \mathbf{x}$ as $n \to \infty$. Hence, if we apply patterns from some cluster $\mathcal{C}$, then (eventually) we expect the same neuron to win the competition, and that the weight of the winner neuron converges to the cluster center of $\mathcal{C}$ (Typically, for this to precisely happen, the learning parameter should also go to zero as the number of epochs go to infinity. Otherwise, the winning neuron will oscillate around the cluster center of $\mathcal{C}$).

Example: Say the learning parameter is 0.5 with $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} 0.9 \\ 1 \end{bmatrix}$, $\mathbf{x}_3 = \begin{bmatrix} 1 \\ 1.1 \end{bmatrix}$, $\mathbf{x}_4 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$, $\mathbf{x}_5 = \begin{bmatrix} 1.1 \\ -1 \end{bmatrix}$, $\mathbf{x}_6 = \begin{bmatrix} 1 \\ -1.1 \end{bmatrix}$.

Suppose $\mathbf{w}_1(1) = \begin{bmatrix} 0.8 \\ 0 \end{bmatrix}$, $\mathbf{w}_2(1) = \begin{bmatrix} 0.9 \\ 0.1 \end{bmatrix}$

$[\mathbf{w}_1(1)]^T\mathbf{x}_1 = 0.80$, $[\mathbf{w}_2(1)]^T\mathbf{x}_1 = 1.00 \implies$ 2 wins.
$[\mathbf{w}_1(1)]^T\mathbf{x}_2 = 0.72$, $[\mathbf{w}_2(1)]^T\mathbf{x}_2 = 0.91 \implies$ 2 wins.
$[\mathbf{w}_1(1)]^T\mathbf{x}_3 = 0.80$, $[\mathbf{w}_2(1)]^T\mathbf{x}_3 = 1.01 \implies$ 2 wins.
$[\mathbf{w}_1(1)]^T\mathbf{x}_4 = 0.80$, $[\mathbf{w}_2(1)]^T\mathbf{x}_4 = 0.80 \implies$ Draw.
$[\mathbf{w}_1(1)]^T\mathbf{x}_5 = 0.88$, $[\mathbf{w}_2(1)]^T\mathbf{x}_5 = 0.89 \implies$ 2 wins.
$[\mathbf{w}_1(1)]^T\mathbf{x}_6 = 0.80$, $[\mathbf{w}_2(1)]^T\mathbf{x}_6 = 0.79 \implies$ 1 wins.

Epoch - 1

- $\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$, : $[\mathbf{w}_1(1)]^T\mathbf{x}_1 = 0.80$, $[\mathbf{w}_2(1)]^T\mathbf{x}_1 = 1.00 \implies$ 2 wins. Thus, we update

$$\begin{aligned}
\mathbf{w}_1(2) &= \mathbf{w}_1(1) = \begin{bmatrix} 0.8 \\ 0 \end{bmatrix}, \\
\mathbf{w}_2(2) &= \mathbf{w}_2(1) + \alpha(\mathbf{x}_1 - \mathbf{w}_2(1)) \\
&= \begin{bmatrix} 0.9 \\ 0.1 \end{bmatrix} + 0.5\left(\begin{bmatrix} 1 \\ 1 \end{bmatrix} - \begin{bmatrix} 0.9 \\ 0.1 \end{bmatrix}\right) = \begin{bmatrix} 0.95 \\ 0.55 \end{bmatrix}.
\end{aligned}$$

- $\mathbf{x}_2 = \begin{bmatrix} 0.9 \\ 1 \end{bmatrix}$, : $[\mathbf{w}_1(2)]^T\mathbf{x}_2 = 0.72$, $[\mathbf{w}_2(2)]^T\mathbf{x}_2 = 1.405 \implies$ 2 wins. Thus, we have

$$\begin{aligned}
\mathbf{w}_1(3) &= \begin{bmatrix} 0.8 \\ 0 \end{bmatrix}, \\
\mathbf{w}_2(3) &= \begin{bmatrix} 0.925 \\ 0.775 \end{bmatrix}
\end{aligned}$$

- $\mathbf{x}_3 = \begin{bmatrix} 1 \\ 1.1 \end{bmatrix}$, : $(0.8, 1.7775)$ 2 wins. Thus, we have

$$\begin{aligned}
\mathbf{w}_1(4) &= \begin{bmatrix} 0.8 \\ 0 \end{bmatrix}, \\
\mathbf{w}_2(4) &= \begin{bmatrix} 0.9625 \\ 0.9375 \end{bmatrix}
\end{aligned}$$