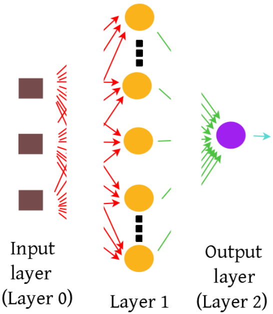
Deep Learning - Theory and Practice

IE 643
Lectures 11 & 12

September 9 & 13, 2022.

1. Popular examples of MLP
   - MLP with Single Hidden Layer
   - Encoder-Decoder Architecture

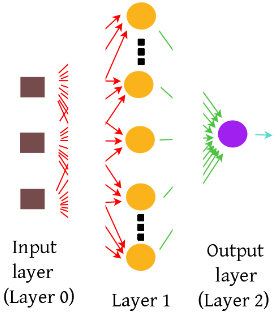
MLP with Single Hidden Layer: Approximation Properties



In the MLP with single hidden layer, consider:

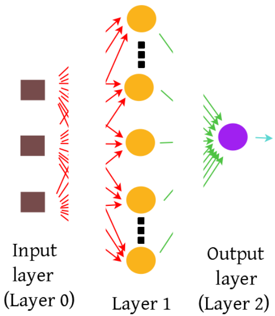
- d neurons in input layer accepting inputs from $[0, 1]^d$.
- N neurons in hidden layer.
- Single neuron in the output layer.

MLP with Single Hidden Layer: Approximation Properties



- All hidden layer neurons have sigmoidal activations.

MLP with Single Hidden Layer: Approximation Properties



- All hidden layer neurons have sigmoidal activations.
  - **Recall:** A sigmoidal activation $\sigma : \mathbb{R} \to (0, 1)$ is a montonically increasing continuous function with the property $\sigma(z) \to 0$ as $z \to -\infty$ and $\sigma(z) \to 1$ as $z \to +\infty$.

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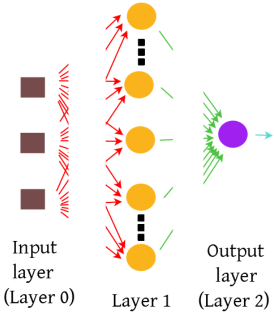

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- The output layer neuron has linear activation function.

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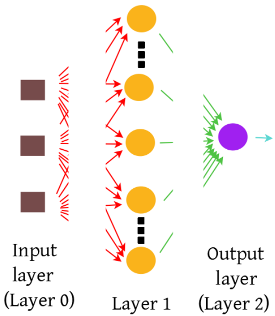

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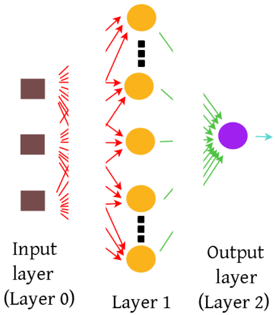
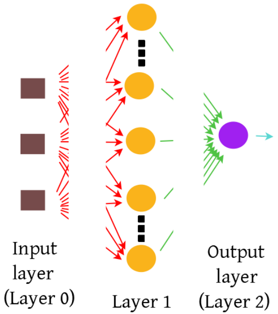
- The output layer neuron has linear activation function.
  - **Recall:** A linear activation function $\phi : \mathbb{R} \to \mathbb{R}$ is given by $\phi(z) = z$.

MLP with Single Hidden Layer: Approximation Properties



- Weights connecting the input layer neurons to the j-th neuron in the hidden layer are collected into the vector w_j and the associated bias be b_j.
- Weight connecting the j-th neuron in hidden layer to the output layer neuron is denoted by α_j.

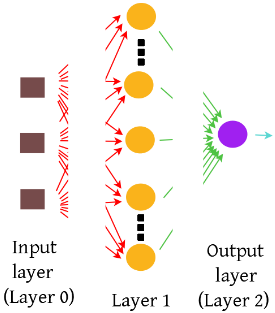
MLP with Single Hidden Layer: Approximation Properties



- Then for an input $x \in [0,1]^d$ the prediction or last layer output can be represented as:

$$\hat{y} = G(x) = \sum_{j=1}^{N} \alpha_j \sigma(w_j^\top x + b_j).$$

MLP with Single Hidden Layer: Approximation Properties

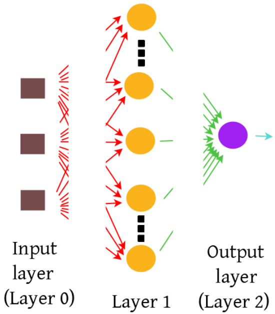


From a famous result of Cybenko (1989)† we have:

Let $\mathcal{C}([0,1]^d)$ denote the set of continuous functions over $[0,1]^d$ and let $\epsilon > 0$. Then for any $f \in \mathcal{C}([0,1]^d)$, there is a sum of the form $G(x) = \sum_{j=1}^{N} \alpha_j \sigma(w_j^\top x + b_j)$ such that $|G(x) - f(x)| < \epsilon, \ \forall x \in [0,1]^d$.

† G. Cybenko, Approximations by Superpositions of a Sigmoidal Function, Math. Control Signals Systems, 1989.

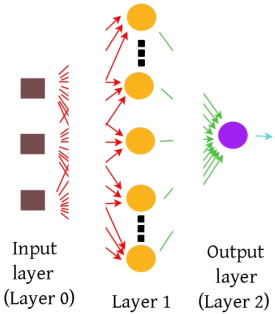
MLP with Single Hidden Layer: Approximation Properties



The result of Cybenko (1989) implies:

- Single hidden layer networks where hidden layer neurons have sigmoidal activation functions and an output neuron with linear activation can approximate any continuous function over $[0, 1]^d$ to any arbitrarily precision $\epsilon > 0$.

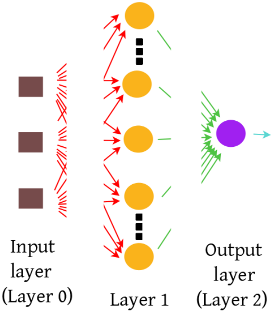
MLP with Single Hidden Layer: Approximation Properties



The result of Cybenko (1989) implies:

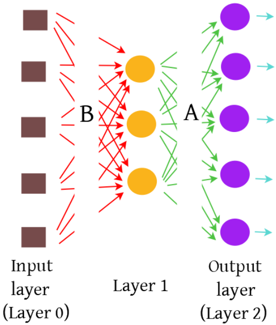
- Single hidden layer networks with hidden layer neurons with sigmoidal activation functions and an output neuron with linear activation can approximate any continuous function over $[0, 1]^d$ to any arbitrarily precision $\epsilon > 0$.
- This result is about the **approximation capability** of single hidden layer networks.

MLP with Single Hidden Layer: Approximation Properties



- Caveat: How many neurons N do we require in the hidden layer to achieve the approximation?

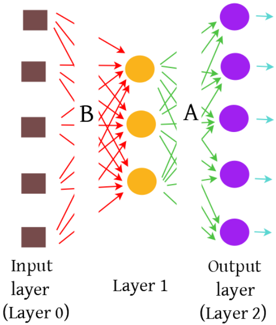
Multi Layer Perceptron: Encoder-Decoder Architecture



We consider a simple MLP architecture with:

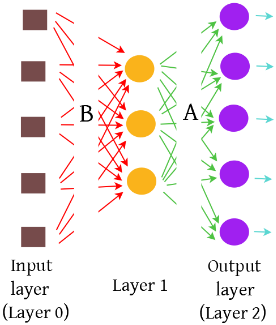
- An input layer with n neurons
- A hidden layer with p neurons, where $p \leq n$
- An output layer with n neurons
- All neurons in hidden and output layers have linear activations.

Multi Layer Perceptron: Encoder-Decoder Architecture



This architecture is popularly called **Encoder-Decoder Architecture**.

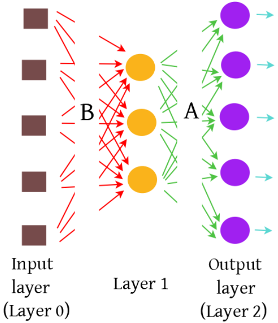
Multi Layer Perceptron: Encoder-Decoder Architecture



Let B denote the $p \times n$ matrix connecting input layer and hidden layer.

Let A denote the $n \times p$ matrix connecting hidden layer and output layer.

Multi Layer Perceptron: Encoder-Decoder Architecture



- **Input:** Training Data $D = \{(x^i, y^i)\}_{i=1}^{S}$, $x^i \in \mathbb{R}^n$, $y^i \in \mathbb{R}^n$, $\forall i \in \{1, \ldots, S\}$.
- **MLP Parameters:** Weight matrices B and A.

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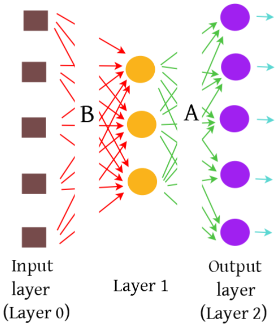

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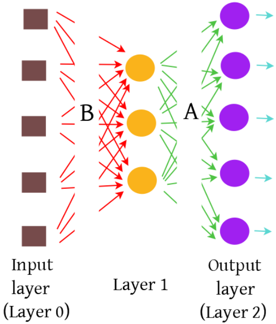
Error: $E(B, A) = \sum_{i=1}^{S} \|ABx^i - y^i\|_2^2$.

Multi Layer Perceptron: Encoder-Decoder Architecture



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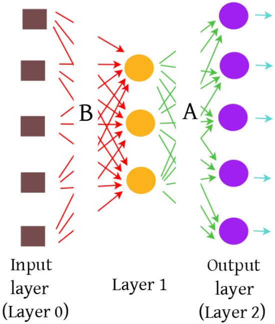
Special case: When $y^i = x^i$, $\forall i$, the architecture is called **Autoencoder**.

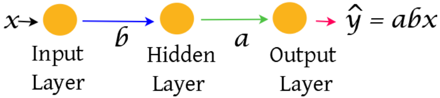
Multi Layer Perceptron: Encoder-Decoder Architecture



- **Input:** Training Data $D = \{(x^i, y^i)\}_{i=1}^{S}$, $x^i \in \mathbb{R}^n$, $y^i \in \mathbb{R}^n$, $\forall i \in \{1, \ldots, S\}$.
- **MLP Parameters:** Weight matrices B and A.

Error for autoencoder: $E(B, A) = \sum_{i=1}^{S} \|ABx^i - x^i\|_2^2$.

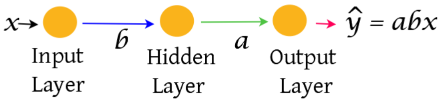
Multi Layer Perceptron: Encoder-Decoder Architecture



Example: Consider the case: $n = p = 1$.

Error: $E(b, a) = \sum_{i=1}^{S}(abx^i - y^i)^2$.

Multi Layer Perceptron: Encoder-Decoder Architecture

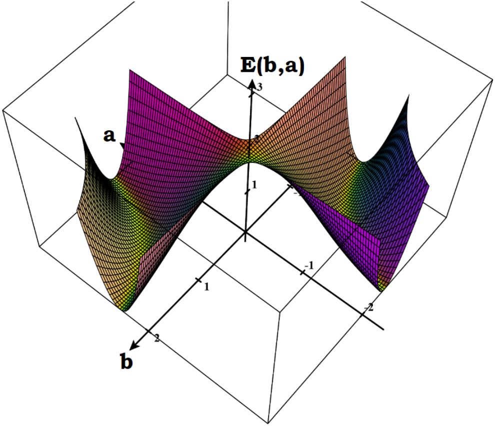


Sample Training Data:

x^i	y^i
.708333	.708333
.583333	.583333
.166667	.166667
.458333	.458333
.875	.875

Multi Layer Perceptron: Encoder-Decoder Architecture

Loss surface for the sample training data:



Multi Layer Perceptron: Encoder-Decoder Architecture

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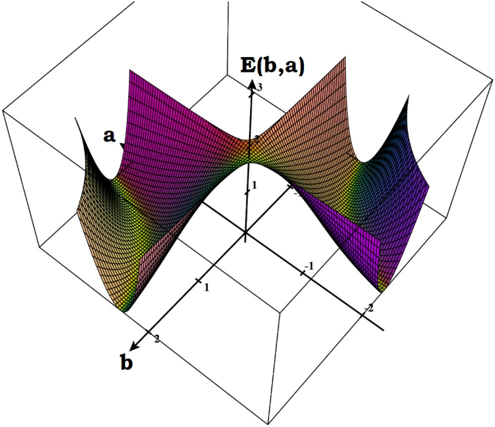
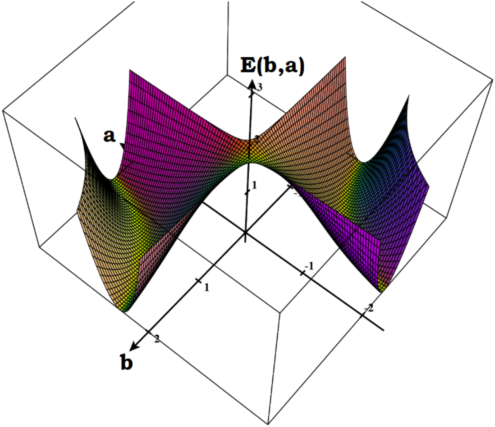


Observation: Though there are two valleys in the loss surface, they look symmetric.

Multi Layer Perceptron: Encoder-Decoder Architecture

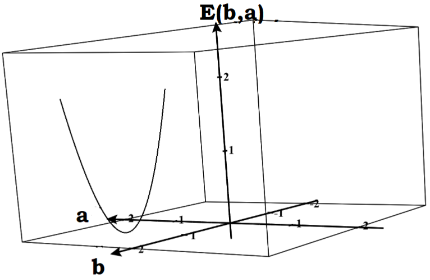
Loss surface for the sample training data:



Question: Does this extend to cases where $y^i \neq x^i$ and for $n \geq 2,\ n \geq p$?

Multi Layer Perceptron: Encoder-Decoder Architecture

However, when we fix *a*, we have:



Multi Layer Perceptron: Encoder-Decoder Architecture

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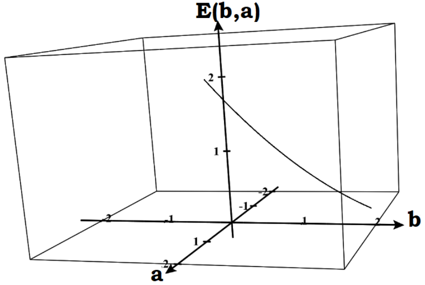

Multi Layer Perceptron: Encoder-Decoder Architecture

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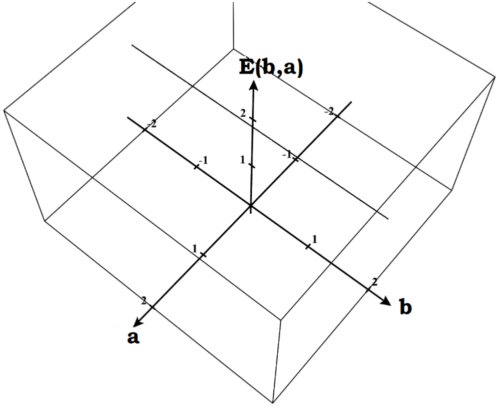
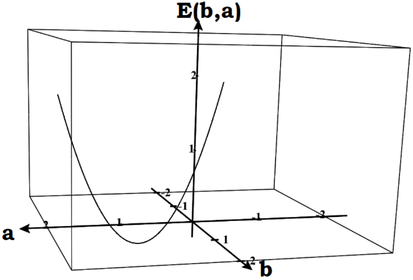


Multi Layer Perceptron: Encoder-Decoder Architecture

Similarly, when we fix b, we have:



Multi Layer Perceptron: Encoder-Decoder Architecture

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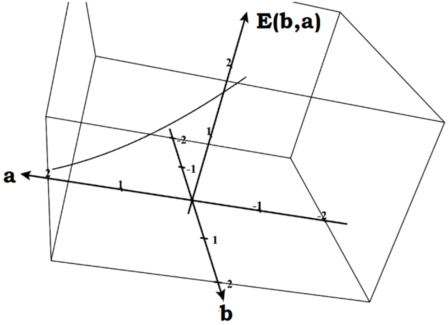

Multi Layer Perceptron: Encoder-Decoder Architecture

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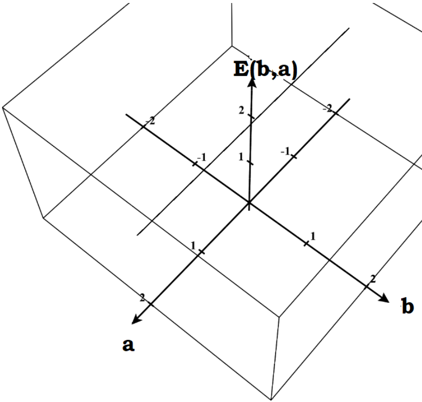
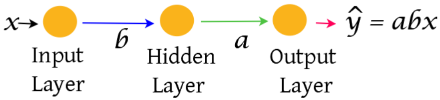


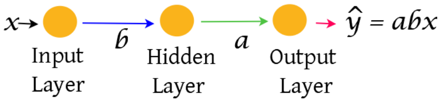
Multi Layer Perceptron: Encoder-Decoder Architecture



Error: $E(b, a) = \sum_{i=1}^{S}(abx^i - y^i)^2$.

When we fix a or when we fix b, we observe that the graph does not contain multiple valleys.

Multi Layer Perceptron: Encoder-Decoder Architecture



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Thus when we fix a or when we fix b, we observe that the graph looks as if every local optimum is a global optimum.

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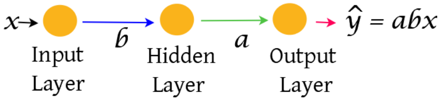

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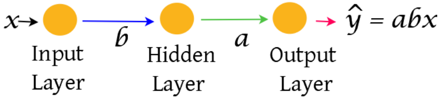
Question: Does this behavior extend to higher dimensions?

Multi Layer Perceptron: Encoder-Decoder Architecture



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Question: Does this behavior extend to higher dimensions?

We shall investigate this in higher dimensions !

Multi Layer Perceptron: Encoder-Decoder Architecture

Some notations:

Let $X = \begin{bmatrix} \uparrow & \uparrow & \dots & \uparrow \\ x^1 & x^2 & \dots & x^S \\ \downarrow & \downarrow & \dots & \downarrow \end{bmatrix}$, $Y = \begin{bmatrix} \uparrow & \uparrow & \dots & \uparrow \\ y^1 & y^2 & \dots & y^S \\ \downarrow & \downarrow & \dots & \downarrow \end{bmatrix}$.

Note: X and Y are $n \times S$ matrices.

Multi Layer Perceptron: Encoder-Decoder Architecture

Some notations:

For a $n \times q$ matrix $H = \begin{bmatrix} h_{11} & h_{12} & \dots & h_{1q} \\ \vdots & \vdots & \dots & \vdots \\ h_{n1} & h_{n2} & \dots & h_{nq} \end{bmatrix}$,

let $\text{vec}(H) = \begin{bmatrix} h_{11} & \dots & h_{n1} & h_{12} & \dots & h_{n2} & \dots & h_{1q} & \dots & h_{nq} \end{bmatrix}^\top$

denote a $nq \times 1$ vector.

Note: $vec(H)$ contains the columns of matrix H stacked upon one another.

Multi Layer Perceptron: Encoder-Decoder Architecture

Recall:

- **Input:** Training Data $D = \{(x^i, y^i)\}_{i=1}^S$, $x^i \in \mathbb{R}^n$, $y^i \in \mathbb{R}^n$, $\forall i \in \{1, \dots, S\}$.
- **MLP Parameters:** Weight matrices B and A.

Error: $E = \sum_{i=1}^S \|ABx^i - y^i\|_2^2$. (We have used E since the context is clear!)

Multi Layer Perceptron: Encoder-Decoder Architecture

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- Using the new notations, we write: $E = \|\text{vec}(ABX - Y)\|_2^2$. (Homework!)

Note: The norm is a simple vector norm.

Multi Layer Perceptron: Encoder-Decoder Architecture

We have: $E = \|\text{vec}(ABX - Y)\|_2^2$.

Now note: $\text{vec}(ABX - Y) = \text{vec}(ABX) - \text{vec}(Y)$. (Homework: Verify this claim!)

Multi Layer Perceptron: Encoder-Decoder Architecture

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Now note: $\text{vec}(ABX - Y) = \text{vec}(ABX) - \text{vec}(Y)$. (Homework: Verify this claim!)

Thus we have: $E = \|\text{vec}(ABX) - \text{vec}(Y)\|_2^2$.

Multi Layer Perceptron: Encoder-Decoder Architecture

Some more new notations:

For a $m \times n$ matrix $G = \begin{bmatrix} g_{11} & \cdots & g_{1n} \\ \vdots & \ldots & \vdots \\ g_{m1} & \cdots & g_{mn} \end{bmatrix}$

and a $p \times q$ matrix $H = \begin{bmatrix} h_{11} & \ldots & h_{1q} \\ \vdots & \ldots & \vdots \\ h_{p1} & \ldots & h_{pq} \end{bmatrix}$,

define: $G \otimes H = \begin{bmatrix} g_{11}H & \ldots & g_{1n}H \\ \vdots & \ldots & \vdots \\ g_{m1}H & \ldots & g_{mn}H \end{bmatrix}$ as Kronecker product of G and H.

Note: $G \otimes H$ is of size $mp \times nq$.

Multi Layer Perceptron: Encoder-Decoder Architecture

Claim:

$$\mathrm{vec}(ABX) = (X^\top \otimes A)\mathrm{vec}(B).$$

Proof idea:

Multi Layer Perceptron: Encoder-Decoder Architecture

Using:

$$\mathrm{vec}(ABX) = (X^\top \otimes A)\mathrm{vec}(B).$$

we can write:

$$\begin{aligned} E &= \|\mathrm{vec}(ABX - Y)\|_2^2 = \|\mathrm{vec}(ABX) - \mathrm{vec}(Y)\|_2^2 \\ &= \|(X^\top \otimes A)\mathrm{vec}(B) - \mathrm{vec}(Y)\|_2^2. \end{aligned}$$

Multi Layer Perceptron: Encoder-Decoder Architecture

Using:

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This is of the form: $F(z) = \|Mz - c\|_2^2$, where $M = (X^\top \otimes A)$, $z = \text{vec}(B)$ and $c = \text{vec}(Y)$.

Multi Layer Perceptron: Encoder-Decoder Architecture

Using:

$$\text{vec}(ABX) = (X^\top \otimes A)\text{vec}(B).$$

we can write:

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This is of the form: $F(z) = \|Mz - c\|_2^2$, where $M = (X^\top \otimes A)$, $z = \text{vec}(B)$ and $c = \text{vec}(Y)$.

Observe: M is of size $nS \times np$, z is a $np \times 1$ vector and c is a $nS \times 1$ vector.

Multi Layer Perceptron: Encoder-Decoder Architecture

Consider the function $F(z) = \|Mz - c\|_2^2$. We have the following result:

Convexity of function F

The function $F(z)$ is convex.

Multi Layer Perceptron: Encoder-Decoder Architecture

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The function $F(z)$ is convex.

Question: What is a convex function?

Multi Layer Perceptron: Encoder-Decoder Architecture

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The function $F(z)$ is convex.

Question: What is a convex function?

We discuss convex sets and convex functions in Part 2 of this lecture !

Multi Layer Perceptron: Encoder-Decoder Architecture

Consider the function $F(z) = \|Mz - c\|_2^2$. We have the following result:

Convexity of function F

The function $F(z)$ is convex.

Hence $\min_z F(z)$ is a **convex optimization problem**.

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Hence $\min_z F(z)$ is a **convex optimization problem**.

Note:

$$\underset{z}{\operatorname{argmin}}\, F(z) = \underset{z}{\operatorname{argmin}}\, \|Mz - c\|_2^2$$

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The function $F(z)$ is convex.

Hence $\min_z F(z)$ is a **convex optimization problem**.

Note:

$$\operatorname*{argmin}_z F(z) = \operatorname*{argmin}_z \|Mz - c\|_2^2 = \operatorname*{argmin}_z (Mz - c)^\top (Mz - c)$$

Multi Layer Perceptron: Encoder-Decoder Architecture

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Convexity of function F

The function $F(z)$ is convex.

Hence $\min_z F(z)$ is a **convex optimization problem**.

Note:

$$\begin{aligned}\underset{z}{\operatorname{argmin}}\, F(z) &= \underset{z}{\operatorname{argmin}}\, \|Mz - c\|_2^2 = \underset{z}{\operatorname{argmin}} (Mz - c)^\top (Mz - c) \\ &= \underset{z}{\operatorname{argmin}}\, z^\top M^\top Mz - 2z^\top M^\top c + c^\top c\end{aligned}$$

Multi Layer Perceptron: Encoder-Decoder Architecture

Consider the function $F(z) = \|Mz - c\|_2^2$. We have the following result:

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Multi Layer Perceptron: Encoder-Decoder Architecture

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Multi Layer Perceptron: Encoder-Decoder Architecture

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Multi Layer Perceptron: Encoder-Decoder Architecture

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Multi Layer Perceptron: Encoder-Decoder Architecture

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- $\implies 2M^\top Mz^* - 2M^\top c = 0$.
- $\implies M^\top Mz^* = M^\top c$.

Further if $M^\top M$ is positive definite, z^* is the unique optimal solution and is given by $z^* = (M^\top M)^{-1} M^\top c$.

Multi Layer Perceptron: Encoder-Decoder Architecture

Recall:

$$\min_{z} F(z) = \|Mz - c\|_2^2 \text{ is same as } \min_{\text{vec}(B)} \|(X^\top \otimes A)\text{vec}(B) - \text{vec}(Y)\|_2^2.$$

Hence from $M^\top M z^* = M^\top c$, we have:

$$(X^\top \otimes A)^\top (X^\top \otimes A) z^* = (X^\top \otimes A)^\top c.$$

Multi Layer Perceptron: Encoder-Decoder Architecture

Some properties of Kronecker Product:

(P1) $\mathrm{vec}(ABC) = (C^\top \otimes A)\mathrm{vec}(B)$.

(P2) $(G \otimes H)^\top = (G^\top \otimes H^\top)$.

(P3) $(G \otimes H)^{-1} = (G^{-1} \otimes H^{-1})$.

(P4) $(G \otimes H)(U \otimes V) = (GU \otimes HV)$

(P5) If G and H are symmetric and positive (semi-)definite, then $(G \otimes H)$ is also symmetric and positive (semi-)definite.

Multi Layer Perceptron: Encoder-Decoder Architecture

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$$\begin{aligned} (X^\top \otimes A)^\top (X^\top \otimes A) z^* &= (X^\top \otimes A)^\top c \\ \implies (X \otimes A^\top)(X^\top \otimes A) z^* &= (X \otimes A^\top) c \text{ (from (P2))} \\ \implies (XX^\top \otimes A^\top A) z^* &= (X \otimes A^\top) c \text{ (from (P4))} \end{aligned}$$

Multi Layer Perceptron: Encoder-Decoder Architecture

Recall: $X = \begin{bmatrix} \uparrow & \uparrow & \dots & \uparrow \\ x^1 & x^2 & \dots & x^S \\ \downarrow & \downarrow & \dots & \downarrow \end{bmatrix}$, $Y = \begin{bmatrix} \uparrow & \uparrow & \dots & \uparrow \\ y^1 & y^2 & \dots & y^S \\ \downarrow & \downarrow & \dots & \downarrow \end{bmatrix}$.

Also note:

$$XX^\top = \sum_{i=1}^{S} x^i (x^i)^\top,$$

$$YY^\top = \sum_{i=1}^{S} y^i (y^i)^\top,$$

$$XY^\top = \sum_{i=1}^{S} x^i (y^i)^\top$$

$$\text{and } YX^\top = \sum_{i=1}^{S} y^i (x^i)^\top.$$

(Homework: try to see if these equalities are true!)

Denote $XX^\top$ by Σ_{XX}, $YY^\top$ by Σ_{YY}, $XY^\top$ by Σ_{XY} and $YX^\top$ by Σ_{YX}.

Multi Layer Perceptron: Encoder-Decoder Architecture

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Denote $XX^\top$ by Σ_{XX}, $YY^\top$ by Σ_{YY}, $XY^\top$ by Σ_{XY} and $YX^\top$ by Σ_{YX}.

Also note Σ_{XX}, Σ_{YY} are symmetric and $(\Sigma_{XY})^\top = (XY^\top)^\top = YX^\top = \Sigma_{YX}$.

Multi Layer Perceptron: Encoder-Decoder Architecture

Recall:

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Multi Layer Perceptron: Encoder-Decoder Architecture

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\implies (\Sigma_{XX} \otimes A^\top A)(\text{vec}(B^*)) &= (X \otimes A^\top)(\text{vec}(Y))
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Multi Layer Perceptron: Encoder-Decoder Architecture

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\implies A^\top A B^* \Sigma_{XX} &= A^\top Y X^\top \text{ (from (P1))}
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\implies A^\top A B^* \Sigma_{XX} &= A^\top \Sigma_{YX}
\end{aligned}$$

Multi Layer Perceptron: Encoder-Decoder Architecture

We have the following result:

The minimizer z^* of $\min_z \|(X^\top \otimes A)z - \text{vec}(Y)\|_2^2$ satisfies

$$A^\top A B^* \Sigma_{XX} = A^\top \Sigma_{YX}$$

where $\text{vec}(B^*) = z^*$.

Multi Layer Perceptron: Encoder-Decoder Architecture

Assume:

- Σ_{XX} is invertible.

Multi Layer Perceptron: Encoder-Decoder Architecture

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Multi Layer Perceptron: Encoder-Decoder Architecture

Assume:

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  - Recall: $\Sigma_{XX} = XX^\top = \sum_{j=1}^{S} x^i (x^i)^\top$.
  - Hence Σ_{XX} is symmetric and positive semi-definite.

Multi Layer Perceptron: Encoder-Decoder Architecture

Assume:

- Σ_{XX} is invertible.
  - Recall: $\Sigma_{XX} = XX^\top = \sum_{j=1}^{S} x^i (x^i)^\top$.
  - Hence Σ_{XX} is symmetric and positive semi-definite.
  - Now invertibility of Σ_{XX} implies that Σ_{XX} is symmetric and positive definite.

Multi Layer Perceptron: Encoder-Decoder Architecture

Assume:

- Σ_{XX} is invertible.
- A is full rank.

Multi Layer Perceptron: Encoder-Decoder Architecture

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Multi Layer Perceptron: Encoder-Decoder Architecture

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  - Also recall: A is of size $n \times p$ and $p \leq n$.

Multi Layer Perceptron: Encoder-Decoder Architecture

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Multi Layer Perceptron: Encoder-Decoder Architecture

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  - A is full rank $\implies \text{rank}(A) = \min\{n, p\} = p$.

The full rank assumption on $A \implies A^\top A$ is symmetric and positive definite and hence invertible.

Multi Layer Perceptron: Encoder-Decoder Architecture

Recall:

$$\min_{z} F(z) = \|Mz - c\|_2^2 \text{ is same as } \min_{\text{vec}(B)} \|(X^\top \otimes A)\text{vec}(B) - \text{vec}(Y)\|_2^2.$$

Hence from $M^\top M z^* = M^\top c$, we have:

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\implies (\Sigma_{XX} \otimes A^\top A) z^* &= (X \otimes A^\top) c
\end{aligned}$$

If the assumptions that Σ_{XX} is invertible and A is full rank hold, then we have Σ_{XX} and $A^\top A$ are symmetric and positive definite, hence

$$M^\top M = (\Sigma_{XX} \otimes A^\top A) \text{ is also symmetric and positive definite(by (P5)).}$$

Multi Layer Perceptron: Encoder-Decoder Architecture

Recall:

$$\min_z F(z) = \|Mz - c\|_2^2 \text{ is same as } \min_{\text{vec}(B)} \|(X^\top \otimes A)\text{vec}(B) - \text{vec}(Y)\|_2^2.$$

Since $M^\top M$ is positive definite, the function $\|Mz - c\|_2^2$ is strictly convex and admits a unique minimizer.

Multi Layer Perceptron: Encoder-Decoder Architecture

Consider the result:

For a fixed A, the minimizer z^* of $\min_z \|(X^\top \otimes A)z - \text{vec}(Y)\|_2^2$ satisfies

$$A^\top AB^*\Sigma_{XX} = A^\top \Sigma_{YX}$$

where $\text{vec}(B^*) = z^*$.

If the assumptions that Σ_{XX} is invertible and A is full rank hold, then we have

$$B^* = (A^\top A)^{-1} A^\top \Sigma_{YX} {\Sigma_{XX}}^{-1}$$

as the unique minimizer.

Multi Layer Perceptron: Encoder-Decoder Architecture

Recall: $E = \|\text{vec}(ABX) - \text{vec}(Y)\|_2^2$.

Homework: **Fix B and vary weights of A matrix and check for convexity of the loss function and solution characteristics of the associated minimization problem.**

Multi Layer Perceptron: Encoder-Decoder Architecture

We have the corresponding result:

For a fixed B, the loss function is convex with respect to $\text{vec}(A)$ and the minimizer A satisfies the following relation:

$$AB\Sigma_{XX}B^\top = \Sigma_{YX}B^\top$$

If the assumptions that Σ_{XX} is invertible and B is full rank hold, then we have

$$A^* = \Sigma_{YX}B^\top(B\Sigma_{XX}B^\top)^{-1}$$

as the unique minimizer.

Multi Layer Perceptron: Encoder-Decoder Architecture

Further, we have the corresponding result:

Assume Σ_{XX} is invertible and A is of full rank. Then A and B denote the critical points of the loss (or error) function E, that is,
$\frac{\partial E}{\partial A_{ij}} = 0, \ \forall i \in \{1, \ldots, n\}, j \in \{1, \ldots, p\}$ and
$\frac{\partial E}{\partial B_{ij}} = 0, \ \forall i \in \{1, \ldots, p\}, j \in \{1, \ldots, n\}$, if and only if A satisfies:

$$P_A \Sigma = \Sigma P_A = P_A \Sigma P_A, \text{ where } P_A = A(A^\top A)^{-1} A^\top, \Sigma = \Sigma_{YX} \Sigma_{XX}^{-1} \Sigma_{XY}.$$

and $W = AB$ is of the form:

$$W = P_A \Sigma_{YX} \Sigma_{XX}^{-1}.$$