CPE 486/586: Deep Learning for Engineering Applications

04 Training Neural Networks and Computational Thinking

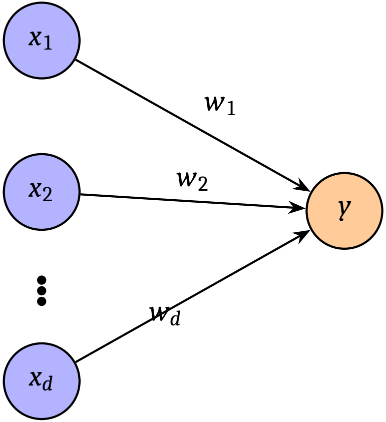
Spring 2026

Rahul Bhadani

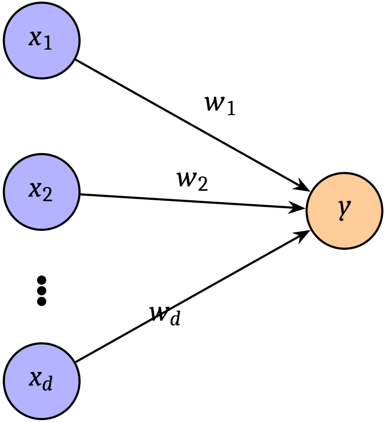
Outline

Recap

Linear Layer

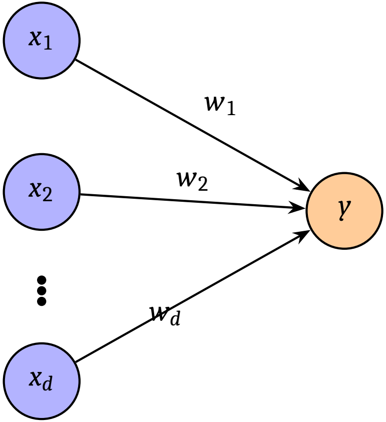


Linear Layer



$$y = \sum_{i=1}^{n} w_i x_i$$

Linear Layer



$$y = \sum_{i=1}^{n} w_i x_i$$

$$\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_d \end{bmatrix} \qquad \mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_d \end{bmatrix}$$

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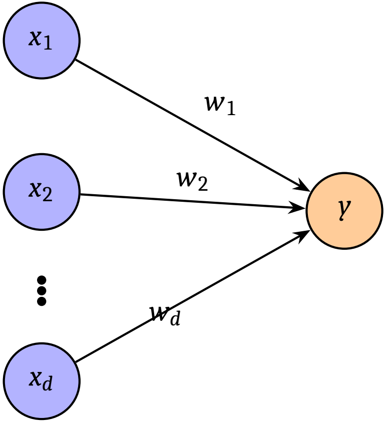

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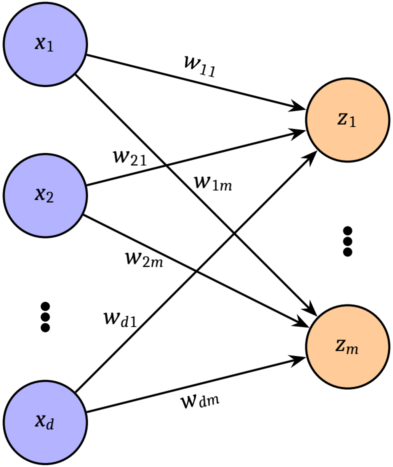
$$\Rightarrow y = \mathbf{x}\mathbf{w}$$

Linear Layer: Case of Hidden Layer



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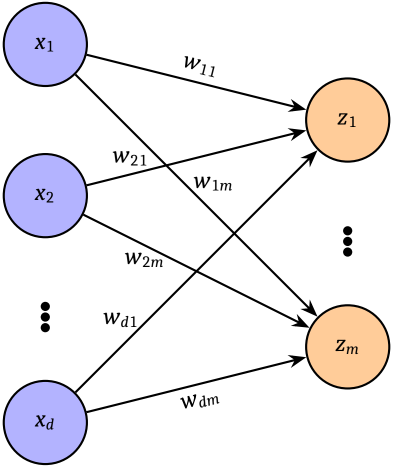

$$z_m = \sum_{i=1}^{n} x_i w_{im}$$

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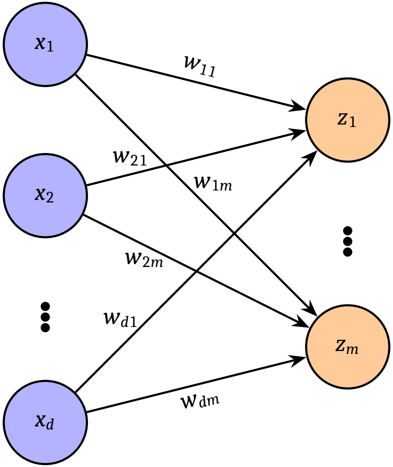

$$z_m = \sum_{i=1}^{n} x_i w_{im}$$

$$\mathbf{z} = \begin{bmatrix} z_1 & z_2 & \vdots & z_m \end{bmatrix}_{1\times m}$$

$$W = \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1m} \\ w_{21} & w_{22} & \cdots & w_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ w_{d1} & w_{m2} & \cdots & w_{dm} \end{bmatrix}_{d\times m} \qquad \mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_d \end{bmatrix}_{1\times d}$$

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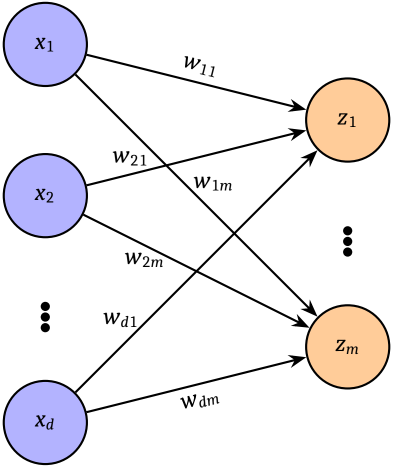

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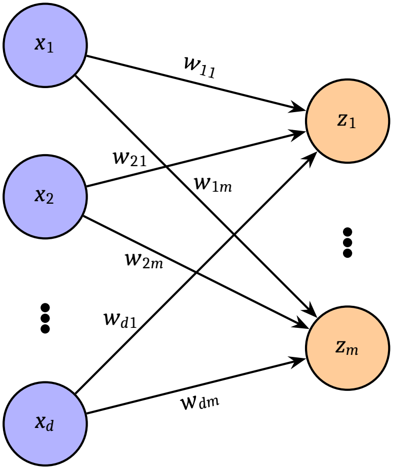
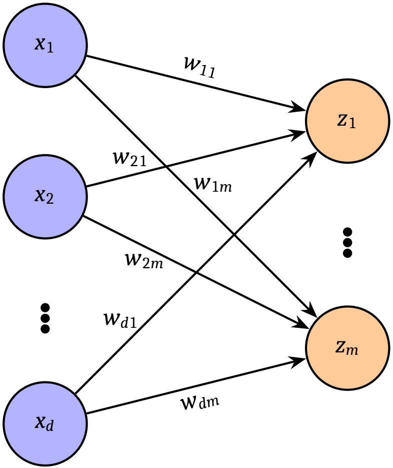
Linear Layer: Case of Hidden Layer



That was the case of one sample, if we consider n sample, then?

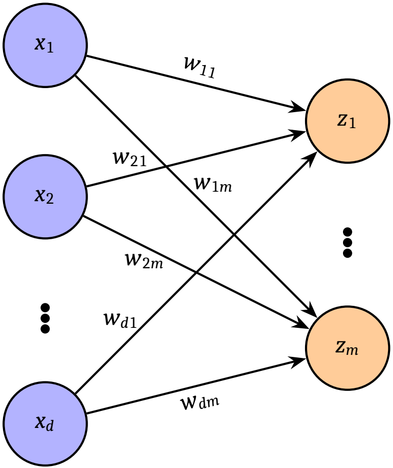
Linear Layer: Case of Hidden Layer



That was the case of one sample, if we consider n sample, then?

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1d} \\ x_{21} & x_{22} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nd} \end{bmatrix}$$

Linear Layer: Case of Hidden Layer



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$$\Rightarrow Z = XW$$

Nonlinear Operation

$$A = \sigma(Z)$$

which will use elementwise operation.

Training a Neural Network

How to Train your Neural Network

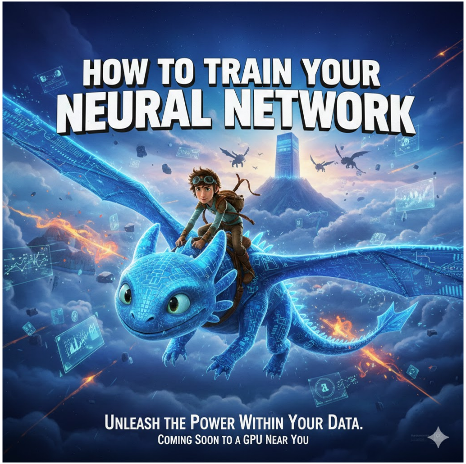

Image generation from Google Gemini.

Training a Neural Network

Some criteria to consider:

1. Data Preprocessing: Normalization/Standardization
2. Batch Size
3. Batch Normalization
4. Dropout
5. Early-Stopping
6. Learning-Rate Scheduling
7. Optimizer Selection
8. Weight Initialization
9. Activation Functions
10. Network Depth & Width
11. Skip/Residual Connections
12. Regularization
13. Loss Functions
14. Gradient Clipping
15. Warm-Up Scheduling

Training a Neural Network

Data Preprocessing

Imputing Missing Values

Definition

The process of filling miss values or correct known errors is called **imputation**.

Feature Index

Sample Index

	x_1	x_2	x_3	x_4	x_5
Sample 0	2.3	4.1	NaN	3.7	1.9
Sample 1	5.2	NaN	2.8	1.5	4.3
Sample 2	1.1	3.4	2.6	NaN	5.1
Sample 3	NaN	2.2	4.0	3.3	2.9
Sample 4	3.5	1.8	2.1	4.5	NaN
Sample 5	2.7	3.9	NULL	1.2	4.6

Legend:
- Feature header
- Valid data
- Missing (NaN)

Figure: Data Table Structure: Features as Columns, Samples as Rows. Red cells indicate missing values (NaN) that require imputation before model training.

Common Types of Missing Values

1. Missing Completely at Random (MCAR), i.e. the probability of being missing is not related to the data and is only dependent on some parameter ϕ.
2. Missing at Random (MAR), i.e., the missingness probability is only related to the observed variables in the data.
3. Missing not at random (MNAR), neither of the above, and the missingness probability is related to missing values of the incomplete variable, which are unknown to us, even after conditioning on observed information

Common Imputation Methods

1. Get rid of those samples where missing # features exceed certain number (or percentage)
2. Get rid of feaures where # missing values exceed certai numbers (or percentage)
3. Sample Mean (only for continuous data)
4. Sample Median (only for continuous data)
5. k-Nearest Neighbors (kNN) imputation
6. Expectation-Maximization (EM) imputation
7. Bayesian Approach

Mean and median approach or anything similar would fail to quantify uncertainty in the estimated missing value.

Bayesian Estimation for Missing Data

1. Model your data first (probabilistic modeling): e.g. normal distribution.
2. Compute prior distribution over uknown parameters.
3. Calculate posterior: update the prior using observed data as (Bayes' Theorem in the play). This gives a posterior distribution over model parameters and missing values.
4. Draw samples using Markov Chain Monte Carlo simulation that will be plausible missing values.

Under a Bayesian framework, missing observations can be thought of as any other parameter in the model whose distribution needs to be determined.

Bayesian Framework

Posterior Distribution

$$p(\boldsymbol{\theta} \mid X) = \frac{p(\mathbf{X} \mid \boldsymbol{\theta})\, p(\boldsymbol{\theta})}{\int_{-\infty}^{\infty} p(\mathbf{X} \mid \boldsymbol{\theta})\, p(\boldsymbol{\theta})\, d\boldsymbol{\theta}} \propto p(\mathbf{X} \mid \boldsymbol{\theta})\, p(\boldsymbol{\theta})$$

$p(\mathbf{X} \mid \boldsymbol{\theta})$ is likelihood, $p(\boldsymbol{\theta})$ is prior.

$$p(\mathbf{X}_{mis} \mid \mathbf{X}_{obs}) = \int p(\mathbf{X}_{mis} \mid \mathbf{X}_{obs}, \boldsymbol{\theta})\, p(\boldsymbol{\theta} \mid \mathbf{X}_{obs})\, d\boldsymbol{\theta}.$$

Calculating posterior is hard, so we use Monte Carlo methods (Markov Chain Monte Carlo (MCMC)).
An example code for MCMC imputation using PyMC is available at
https://www.pymc.io/projects/examples/en/latest/howto/Missing_Data_Imputation.html

Normalization/Standardization

Definition

In simpler terms: adjusting values measured on different scales to a common scale is **Normalization**.

Otherwise, aligning entire probability distribution of adjusted values is **Normalization**.

Standard Normalization

$$\hat{x} = \frac{x - \mu}{\sigma}$$

Minmax Normalization

$$\hat{x} = \frac{x - x_{min}}{x_{max} - x_{min}}$$

Data Preprocessing

0 1 1 1 1 0 1 0 0 0 1 0 1 1 0
0 0 0 0 0 0 1 1 1 0 0 1 0 0 1

Batch Size

References and Additional Reading

1. He, Yulei, Guangyu Zhang, and Chiu-Hsieh Hsu. **Multiple imputation of missing data in practice: basic theory and analysis strategies**. Chapman and Hall/CRC, 2021.
2. Huang, Lei. Normalization Techniques in Deep Learning. Cham: Springer, 2022.