STAT 453: Introduction to Deep Learning and Generative Models

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Lecture 03: Stats/Linear algebra review

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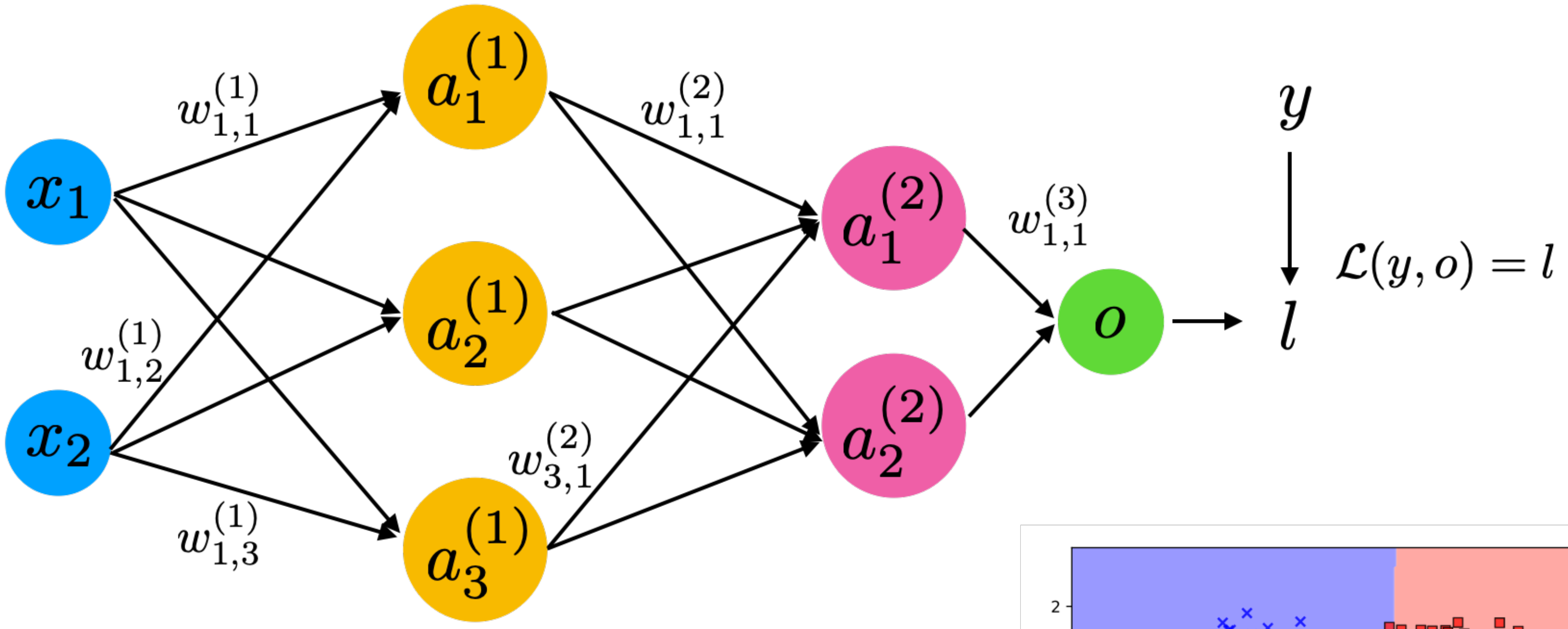
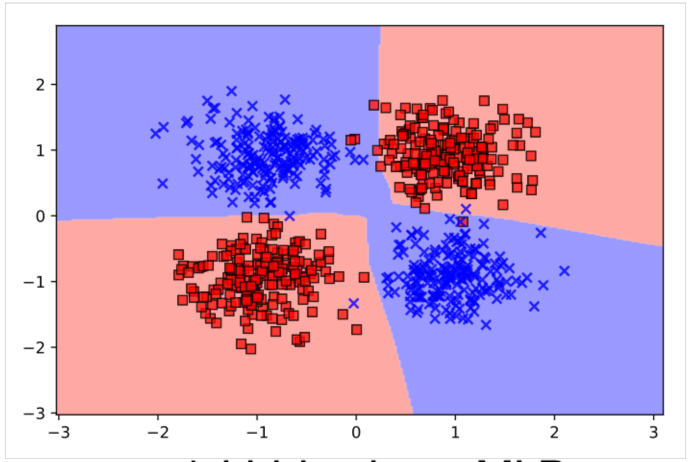
Questions about Course Logistics?

Today: Fundamental Math Skills for DL



So that we can solve the XOR problem, among other things ...



1-hidden layer MLP
with non-linear activation function (ReLU)

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1. **Tensors in Deep Learning**
2. Tensors and PyTorch
3. Vectors, Matrices, and Broadcasting
4. Probability Basics
5. Estimation Methods
6. Linear Regression

Scalars, Vectors, and Matrices

Scalar

(order-0 tensor)

$x \in \mathbb{R}$

e.g.,

$x = 1.23$

Vector

(order-1 tensor)

$\mathbf{x} \in \mathbb{R}^n$

but in this lecture, we will assume

$\mathbf{x} \in \mathbb{R}^{n \times 1}$

e.g.,

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

Matrix

(order-2 tensor)

$\mathbf{X} \in \mathbb{R}^{m \times n}$

e.g.,

$$\mathbf{X} = \begin{bmatrix} x_{1,1} & x_{1,2} & \dots & x_{1,n} \\ x_{2,1} & x_{2,2} & \dots & x_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m,1} & x_{m,2} & \dots & x_{m,n} \end{bmatrix}$$

$$\mathbf{x}^\top = \begin{bmatrix} x_1 & x_2 & \dots & x_n \end{bmatrix}, \text{ where } \mathbf{x}^\top \in \mathbb{R}^{1 \times n}$$

Scalars, Vectors, and Matrices

We will often use $\mathbf{X}$ as a special convention to refer to the "design matrix", “feature matrix”, or “input matrix”. That is, the matrix containing the training examples and features (inputs)

and assume the structure $\mathbf{X} \in \mathbb{R}^{n \times m}$

because *n* is often used to refer to the number of examples in literature across many disciplines.

$$\mathbf{X} = \begin{bmatrix} x_1^{[1]} & x_2^{[1]} & \dots & x_m^{[1]} \\ x_1^{[2]} & x_2^{[2]} & \dots & x_m^{[2]} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{[n]} & x_2^{[n]} & \dots & x_m^{[n]} \end{bmatrix}$$

E.g.,

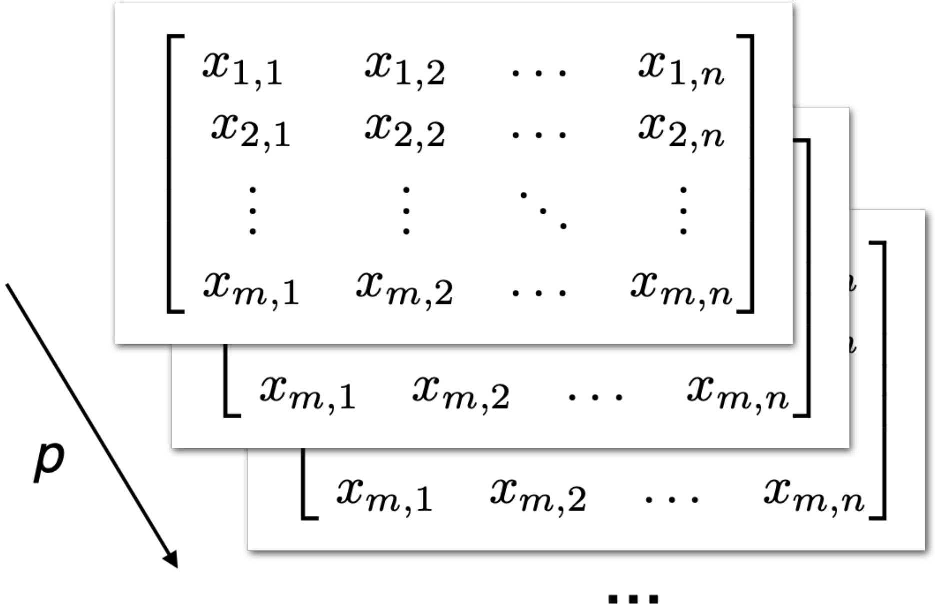
$x_2^{[1]}$ = 2nd feature value of the 1st training example

Tensors

3D Tensor

(order-3 tensor)

$\mathrm{X} \in \mathbb{R}^{m \times n \times p}$ (*n* and *m* are generic indices here)



An Example of a 3D Tensor in DL

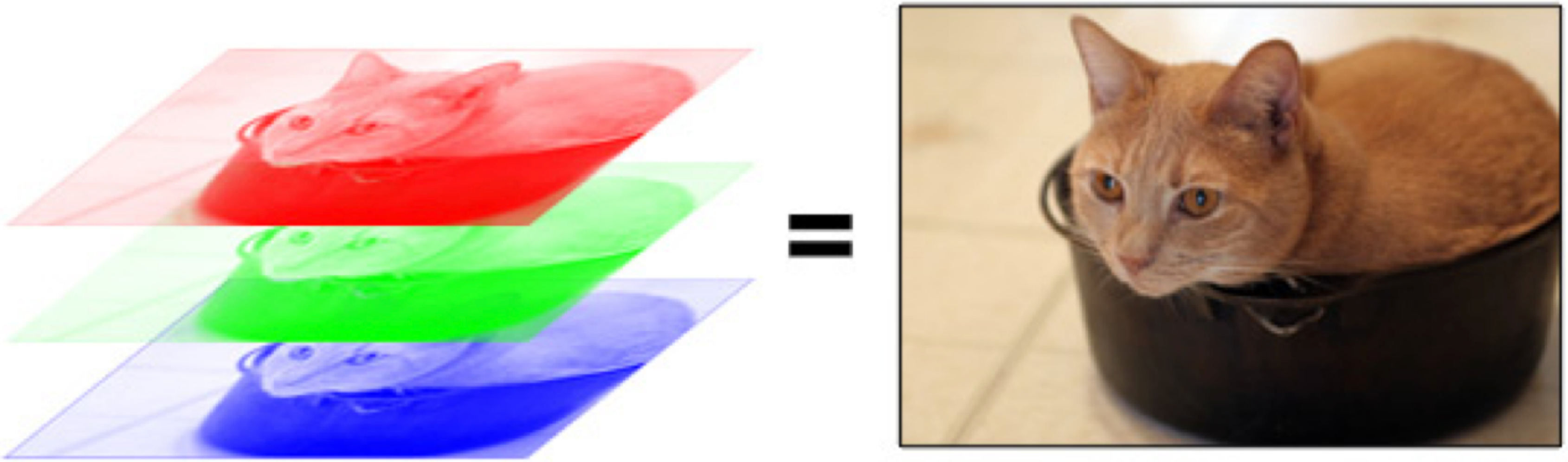
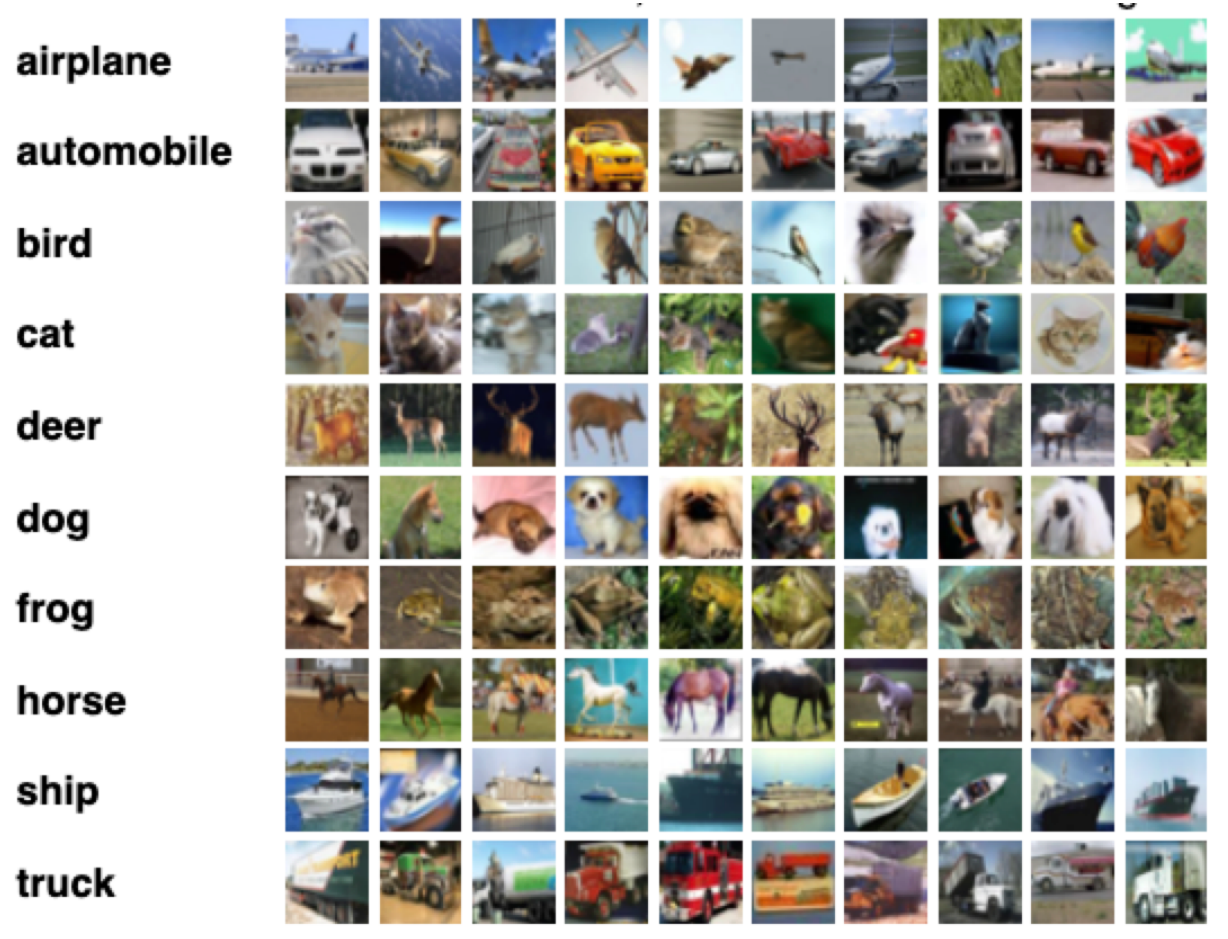


Image Source: https://code.tutsplus.com/tutorials/create-a-retro-crt-distortion-effect-using-rgb-shifting--active-3359

An Example of a 4D Tensor in DL

Batch of images
(as neural network input, more later)



https://www.cs.toronto.edu/~kriz/cifar.html

For our purposes, tensor = multidimensional array

Dimensionality ("order") = # of indices of .shape

```
In [1]: import torch

In [2]: t = torch.tensor([[1, 2, 3], [4, 5, 6]])

In [3]: t
Out[3]:
tensor([[1, 2, 3],
        [4, 5, 6]])

In [4]: t.shape
Out[4]: torch.Size([2, 3])

In [5]: t.ndim
Out[5]: 2

In [6]:
```

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Numpy Arrays → PyTorch Tensors

`numpy.array / numpy.ndarray` = (data structure representation of a tensor)

`pytorch.tensor / pytorch.Tensor` = (data structure representation of a tensor)

Example:

```
In [1]: import numpy as np

In [2]: a = np.array([1., 2., 3.])

In [3]: print(a.dtype)
float64

In [4]: print(a.shape)
(3,)
```

```
In [5]: import torch

In [6]: b = torch.tensor([1., 2., 3.])

In [7]: print(b.dtype)
torch.float32

In [8]: print(b.shape)
torch.Size([3])
```

Numpy and PyTorch Syntax is Similar

Numpy

```
In [9]: a = np.array([1., 2., 3.])

In [10]: print(a.dot(a))
14.0
```

PyTorch

```
In [12]: print(b.matmul(b))
tensor(14.)

In [13]: b
Out[13]: tensor([1., 2., 3.])

In [14]: b.numpy()
Out[14]: array([1., 2., 3.], dtype=float32)
```

PyTorch: `matmul` = `dot` = `@`

```
In [12]: print(b.matmul(b))
tensor(14.)
```

```
In [15]: print(b.dot(b))
tensor(14.)

In [16]: print(b @ b)
tensor(14.)
```

Data types

NumPy data type	Tensor data type	
numpy.uint8	torch.ByteTensor	
numpy.int16	torch.ShortTensor	
numpy.int32	torch.IntTensor	
numpy.int	torch.LongTensor	
numpy.int64	torch.LongTensor	Default int in Numpy & PyTorch
numpy.float16	torch.HalfTensor	
numpy.float32	torch.FloatTensor	Default float in PyTorch
numpy.float	torch.DoubleTensor	
numpy.float64	torch.DoubleTensor	Default float in NumPy

Specify the type with dtype

```
In [21]: c = torch.tensor([1., 2., 3.], dtype=torch.float)

In [22]: c.dtype
Out[22]: torch.float32

In [23]: c = torch.tensor([1., 2., 3.], dtype=torch.double)

In [24]: c.dtype
Out[24]: torch.float64

In [25]: c = torch.tensor([1., 2., 3.], dtype=torch.float64)

In [26]: c.dtype
Out[26]: torch.float64
```

Why not just use NumPy?

- PyTorch is made for DL:
  - GPU support
  - Automatic differentiation
  - DL Convenience functions

Loading Data onto a GPU

```
In [23]: print(torch.cuda.is_available())
True

In [24]: b = b.to(torch.device('cuda:0'))
    ...: print(b)

tensor([1., 2., 3.], device='cuda:0')

In [25]: b = b.to(torch.device('cpu'))
    ...: print(b)
tensor([1., 2., 3.])
```

How to Check Your CUDA Devices

- If you have CUDA installed, you should have access to **`nvidia-smi`**
- However, if you are using a laptop, you probably don't have CUDA compatible graphics cards (my laptops don't)
- We will discuss GPU cloud computing later ...

```
sraschka@gpu03:~$ nvidia-smi
Mon Feb  8 21:05:27 2021
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 455.32.00    Driver Version: 455.32.00    CUDA Version: 11.1     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  GeForce RTX 208...  Off  | 00000000:1A:00.0 Off |                  N/A |
| 24%   37C    P0    71W / 250W |      0MiB / 11019MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+
```

Installing PyTorch

If you want to install PyTorch later (after the lecture) ...

- If you use it on a laptop, you likely don't have a CUDA compatible GPU
- Recommend using CPU version for your laptop (no CUDA)
- Installation on GPU-cloud later ...
- Also, use this selector tool from https://pytorch.org
  (conda is recommended):

PyTorch Build	Stable (1.7.1)	Preview (Nightly)			
Your OS	Linux	Mac	Windows		
Package	Conda	Pip	LibTorch	Source	
Language	Python	C++ / Java			
CUDA	9.2	10.1	10.2	11.0	None
Run this Command:	**NOTE:** Python 3.9 users will need to add '-c=conda-forge' for installation conda install pytorch torchvision torchaudio -c pytorch				

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Vectors

Quiz: How do we call this again in the context of neural nets?

$$\mathbf{w}^\top \mathbf{x} + b = z \quad \text{where} \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{bmatrix}$$

Matrices: Computing Outputs for Multiple Examples

$$\mathbf{X}\mathbf{w} + b = \mathbf{z} \quad \text{where} \quad \mathbf{X} = \begin{bmatrix} x_1^{[1]} & x_2^{[1]} & \dots & x_m^{[1]} \\ x_1^{[2]} & x_2^{[2]} & \dots & x_m^{[2]} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{[n]} & x_2^{[n]} & \dots & x_m^{[n]} \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{bmatrix}$$

What is the Big-O computational cost of matrix multiplication (assume two NxN matrices)?

A common notational convenience

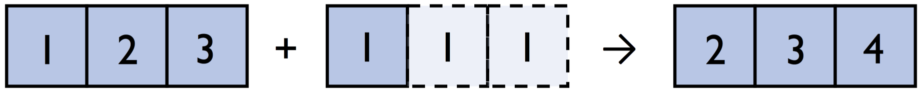
$$\mathbf{X}\mathbf{w} + b = \mathbf{z} \quad \text{where} \quad \mathbf{X} = \begin{bmatrix} x_1^{[1]} & x_2^{[1]} & \dots & x_m^{[1]} \\ x_1^{[2]} & x_2^{[2]} & \dots & x_m^{[2]} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{[n]} & x_2^{[n]} & \dots & x_m^{[n]} \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_m \end{bmatrix}$$

This should really be $\boldsymbol{X}\boldsymbol{w} + \mathbf{1}_{\boldsymbol{n}} b = \boldsymbol{z}$, but in DL notation we drop the $\mathbf{1}_{\boldsymbol{n}}$.

*We assume **broadcasting.***

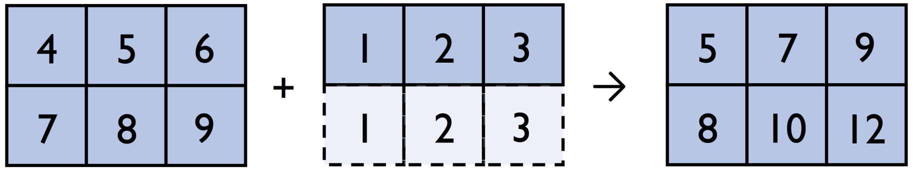
Broadcasting

```
In [4]: torch.tensor([1, 2, 3]) + 1
Out[4]: tensor([2, 3, 4])
```




```
In [5]: t = torch.tensor([[4, 5, 6], [7, 8, 9]])

In [6]: t
Out[6]:
tensor([[4, 5, 6],
        [7, 8, 9]])
```




```
In [7]: t + torch.tensor([1, 2, 3])
Out[7]:
tensor([[ 5,  7,  9],
        [ 8, 10, 12]])
```

Be cautious of this when debugging …

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Probability Basics: Definitions

- Random Variables:
  - Discrete: Values from a countable set (e.g. a coin flip)
  - Continuous: Values from an interval (e.g. a height)
- PMF and PDF:
  - **P**robability **M**ass **F**unction: P(X=x) for discrete X.
  - **P**robability **D**ensity **F**unction: f(x) for continuous X.

Key Distributions

- Bernoulli Distribution:
  - $P(X = x) = \theta^x (1 - \theta)^{1-x}, x \in \{0,1\}$
  - Example: a fair coin flip ($\theta = 0.5$)
- Gaussian Distribution:
  - $f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{(x-\mu)^2}{2\sigma^2}}$
  - **"Normal"** because of Central Limit Theorem
  - "Standard Normal" when $\mu = 0, \sigma = 1$

Central Limit Theorem

- Let $X_1, X_2, \ldots, X_n$ be i.i.d. random variables with mean μ and variance σ^2.
- Define the sample mean:

$$\bar{X}_n = \frac{1}{n}\sum_{i=1}^{n} X_i$$

- Then, as $n \rightarrow \infty$:

$$\frac{\bar{X}_n - \mu}{\frac{\sigma}{\sqrt{n}}} \rightarrow N(0,1)$$

Joint, Marginal, and Conditional Probabilities

- Joint: $P(A, B)$, probability of two events occurring together.
- Marginal: $P(A) = \sum_B P(A, B)$, sum of joint probabilities over one variable.
- Conditional: $P(A|B) = \frac{P(A,B)}{P(B)}$, probability of A given B.

Expectation and Variance

- Expectation:
  - Discrete: $E[X] = \sum_x xP(X = x)$
  - Continuous: $E[X] = \int xf(x)dx$
- Variance: $Var(X) = E[(X - E[X])^2]$
  - Equivalent: $Var(X) = E[X^2] - E[X]^2$

Linearity of Expectation

- Property:
  - $E[aX + b] = aE[X] + b$
- Multiple Variables:
  - $E[X_1 + X_2] = E[X_1] + E[X_2]$

Expectation of Functions

- Formula:
  - $E[g(X)] = \sum_x g(x)P(X = x)$ (discrete)
  - $E[g(X)] = \int_x g(x)f(x)dx$ (continuous)

- Example (Discrete):
  - $X \sim \text{Bernoulli}(\theta), g(X) = X^2$:
  - $E[g(X)] = 1^2\theta + 0^2(1 - \theta) = \theta$
- Example (Continuous):
  - $X \sim \text{Uniform}(0,1), g(X) = X^2$:
  - $E[g(X)] = \int_0^1 x^2 dx = \frac{1}{3}$.

Variance of Functions

- Definition:
  - $Var(g(X)) = E[(g(X) - E[g(X)])^2]$
  - Equivalent: $Var(g(X)) = E[g(X)^2] - (E[g(X)])^2$

Covariance and Correlation

- Covariance:
  - $Cov(X, Y) = E[(X - E[X])(Y - E[Y])]$
- Properties:
  - $Cov(X, X) = Var(X)$
  - If X,Y are independent: $Cov(X, Y) = 0$.
- Correlation:
  - $\rho(X, Y) = \frac{Cov(X,Y)}{\sqrt{Var(X)Var(Y)}}$
  - $\rho = 1$: Perfect positive linear relationship.
  - $\rho = 0$: No linear relationship.
  - $\rho = -1$: Perfect negative linear relationship.

Bayes' Rule

- $P(A|B) = \frac{P(B|A)P(A)}{P(B)}$
- Example: Medical test:
  - $P(disease|positive\ test) = \frac{P(positive\ test\ |disease)\ P(disease)}{P(positive\ test)}$

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Introduction to Estimation

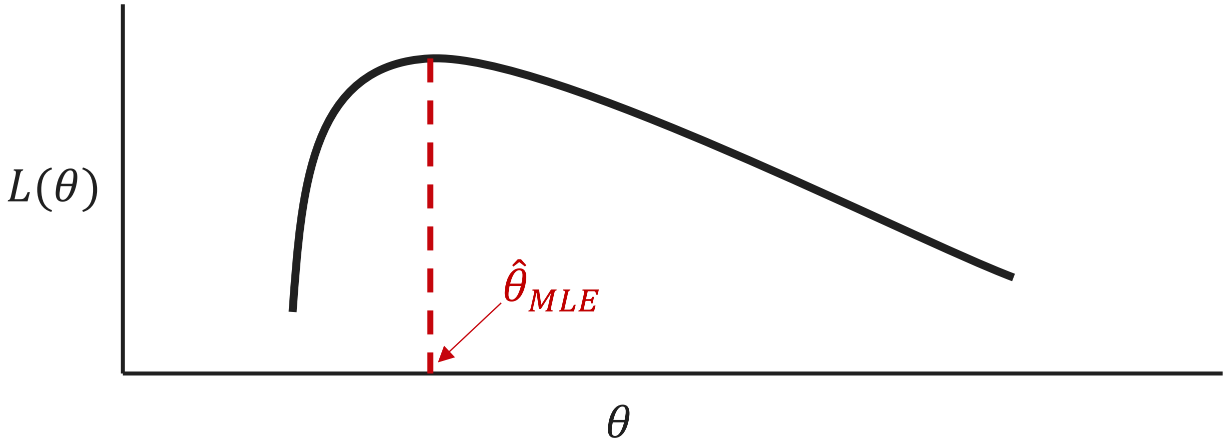
- **Goal of Estimation:**
  - Infer unknown parameters θ from observed data.
- **Types of Estimation:**
  - Point Estimation: Single value (e.g., MLE).
  - Interval Estimation: Range of plausible values (e.g., confidence intervals).
- **Common Methods:**
  - Maximum Likelihood Estimation (MLE)
  - Maximum A Posteriori (MAP)
  - Method of Moments

Maximum Likelihood Estimation (MLE)

- **Definition:**
  - Find $\hat{\boldsymbol{\theta}}$ that maximizes the likelihood of observing the given data.

$$\hat{\boldsymbol{\theta}} = \text{argmax}_\theta L(\theta) \text{ where } L(\theta) = P(\text{data}|\theta).$$

- **Interpretation:**
  - L(θ): Probability of the observed data given θ.
  - MLE chooses the parameter that makes the data most "likely."



Maximum Likelihood Estimation (MLE)

- **Example:**
  - Dataset: X={1,0,1,1,0},
  - Bernoulli distribution with $P(X = 1|\theta) = \theta$:

$$L(\theta) = \prod_i \theta^{x_i} (1-\theta)^{1-x_i}$$

  - Typically solved by maximizing the log-likelihood.

$$\ell(\theta) = \log L(\theta) = \sum_{i=1}^{n} (x_i \log \theta \ + (1-x_i) \log(1-\theta))$$

  - Derivative:

$$\frac{d\ell}{d\theta} = \frac{k}{\theta} - \frac{n-k}{1-\theta}$$

where $k = \sum x_i$

  - Solution:

$$\hat{\boldsymbol{\theta}} = \frac{k}{n}$$

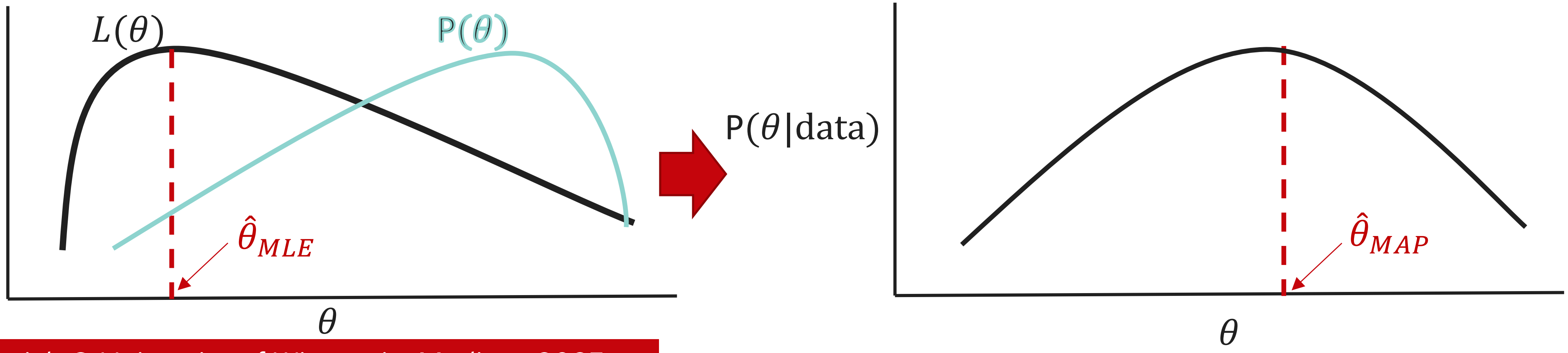
Maximum Likelihood Estimation (MLE)

- The MLE:
  - does not always exist.
  - is not necessarily unique.
  - is not necessarily admissible.

Maximum A Posteriori (MAP) Estimation

- Find
$$\hat{\theta}_{MAP} = argmax_{\theta} P(\theta|\text{data}) \propto argmax_{\theta} P(\text{data}|\theta)P(\theta)$$
- $P(\text{data}|\theta)$: Likelihood
- $P(\theta)$: Prior belief about θ

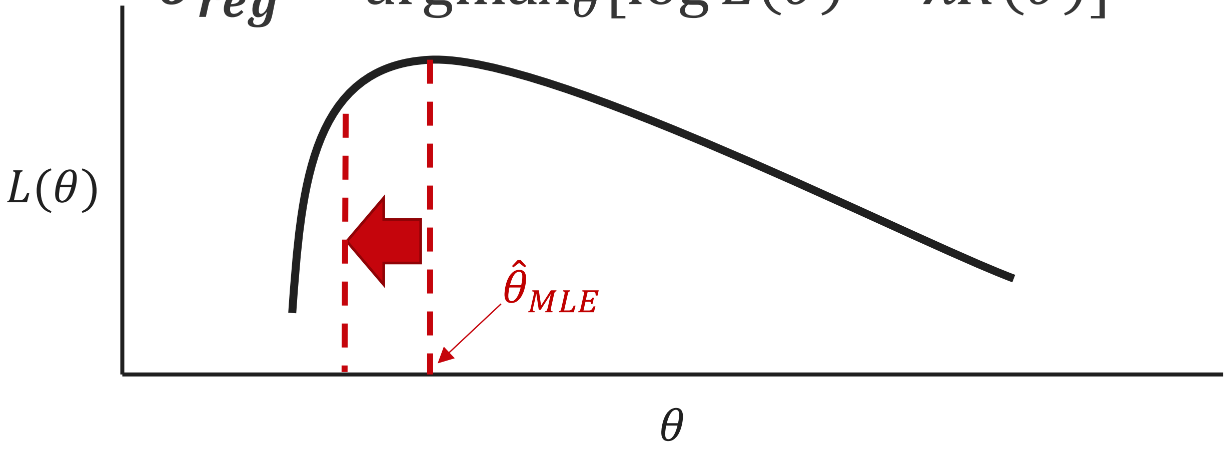
- MLE ignores $P(\theta)$
- MAP incorporates prior information.



Regularization is MAP

- **MLE with Regularization:**
  - Adds a penalty to avoid overfitting

$$\widehat{\boldsymbol{\theta}_{reg}} = \text{argmax}_\theta[\log L(\theta) - \lambda R(\theta)]$$



- **MAP as Penalized MLE:**
  - Let $P(\theta) \propto e^{-\lambda R(\theta)}$. Then

$$\widehat{\boldsymbol{\theta}}_{MAP} = argmax_\theta[\log L(\theta) + \log P(\theta)] = \hat{\theta}_{reg}$$

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Introduction to Linear Regression

- **Model Definition:**
  - $y = X\beta + \epsilon$, where
  - y: Response variable (dependent variable).
  - X: Design matrix (independent variables or features).
  - β: Coefficients (parameters to estimate).
  - ϵ: Error term (often assumed to be $N(0, \sigma^2)$).
- **Goal:**
  - Estimate β.

Linear Regression Evaluation Metrics

- **Coefficient of Determination (R^2):**
  - $R^2 = 1 - \frac{SS_{residual}}{SS_{total}}$
  - Measures the proportion of variance explained by the model.
- **Mean Squared Error (MSE):**
  - $MSE = \frac{1}{n}\sum(y_i - \hat{y}_i)^2$
- **Mean Absolute Error (MAE):**
  - $MSE = \frac{1}{n}\sum\|y_i - \hat{y}_i\|$

Ordinary Least Squares (OLS)

- **Objective:**
  - Minimize the sum of squared residuals:
  - $\hat{\boldsymbol{\beta}}_{OLS} = argmin_{\beta} \|y - X\beta\|^2$
- Residuals:
  - $e_i = y_i - \hat{y}_i$
- **Solution:**
  - $\hat{\boldsymbol{\beta}}_{OLS} = (X^T X)^{-1} X^T Y$

Regularization in Linear Regression (MAP)

- **Ridge Regression (L2 Regularization):**
  - Adds an L2 penalty:
    - $\hat{\boldsymbol{\beta}}_{ridge} = argmin_{\beta}\|y - X\beta\|^2 + \lambda\|\beta\|^2$
  - Equivalent MAP interpretation:
    - Prior on coefficients: $\beta \sim N(0, \frac{\sigma^2}{\lambda})$
    - MAP estimate maximizes: $P(\beta|y) \propto P(y|\beta)P(\beta)$
    - Penalty comes from the Gaussian prior.
- **Lasso Regression (L1 Regularization):**
  - Adds an L1 penalty:
    - $\hat{\boldsymbol{\beta}}_{lasso} = argmin_{\beta}\|y - X\beta\|^2 + \lambda\|\beta\|_1$
  - Equivalent to $\beta \sim \text{Laplace}(0, \frac{\sigma}{\lambda})$

Next Lecture

Single-layer networks

Questions?

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