CS 480/680
Introduction to Machine Learning

Lecture 3
Maximum Likelihood Estimation and Entropy

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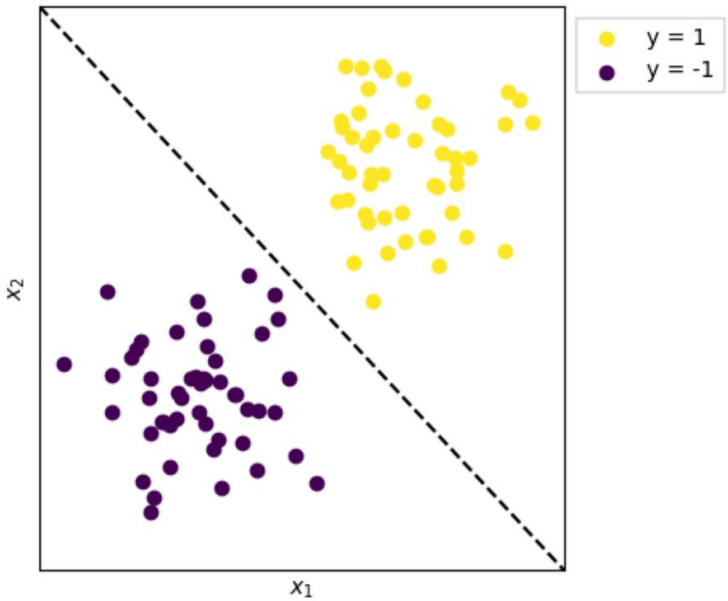
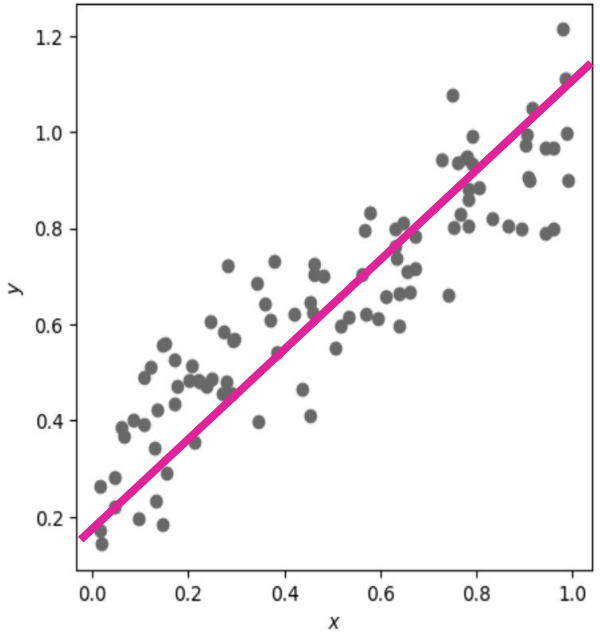
17 September 2024

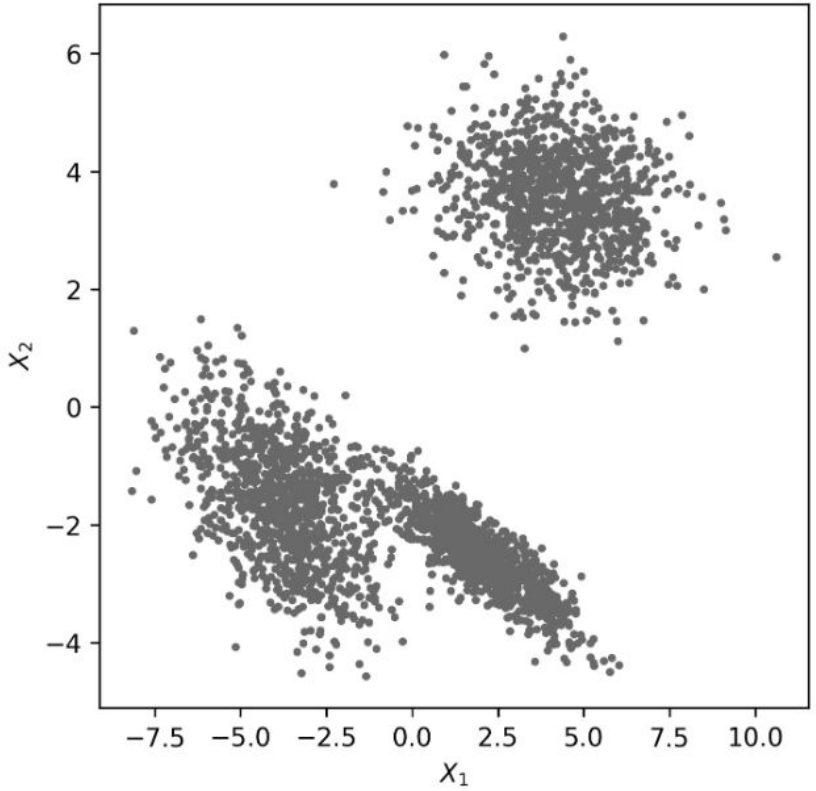
UNIVERSITY OF WATERLOO | FACULTY OF MATHEMATICS

Classification and regression are supervised learning tasks





Unsupervised learning concerns pattern identification



Lecture	Date	Topics
0	05/09/2024	Introduction + Administrative Remarks
1	10/09/2024	Halfspaces the Perceptron Algorithm
2	12/09/2024	Linear Regression and Convexity
3	17/09/2024	Maximum Likelihood Estimation
4	19/09/2024	k-means Clustering
5	24/09/2024	k-NN Classification and Logistic Regression
6	26/09/2024	Hard-margin SVM
7	01/10/2024	Soft-margin SVM
8	03/10/2024	Kernel methods
9	08/10/2024	Decision Trees
10	10/10/2024	Bagging and Boosting
	15/10/2024	NO LECTURE - MIDTERM BREAK
	17/10/2024	NO LECTURE- MIDTERM BREAK
11	22/10/2024	Expectation Maximization Algorithm
12	24/10/2024	MLPs and Fully-Connected NNs
	29/10/2024	NO LECTURE - MIDTERM EXAM
13	31/10/2024	Convolutional Neural Networks
14	05/11/2024	Recurrent Neural Networks
15	07/11/2024	Attention and Transformers
16	12/11/2024	Graph Neural Networks (Time permitting)
17	14/11/2024	VAEs and GANs
18	19/11/2024	Flows
19	21/11/2024	Contrastive Learning (Time permitting)
20	26/11/2024	Robustness
21	28/11/2024	Privacy (Saber Malekmohammadi)
22	03/12/2024	Fairness

Key Questions

I. How can we represent and sample from a distribution?

II. How do you estimate the parameters and evaluate the model?

III. Could this also apply to supervised learning?

IV. Summary + Housekeeping

Lecture Objectives

At the end of the lecture, we should be able to:

- ★ Identify the probability density function and parameterization of widely used distributions and relate it to their use in constructing likelihood functions.
- ★ Construct the likelihood function for a dataset and maximize it to find the maximum likelihood estimates (MLE) of the parameters.
- ★ Define and apply information theoretic measures such as entropy and KL divergence to characterize and compare distributions.
- ★ Reformulate the linear regression objective using likelihood principles, and demonstrate that it can be viewed as a special case of MLE.

Key Questions

I. **How can we represent and sample from a distribution?**

II. How do you estimate the parameters and evaluate the model?

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The PDF of a univariate Gaussian (normal) distribution

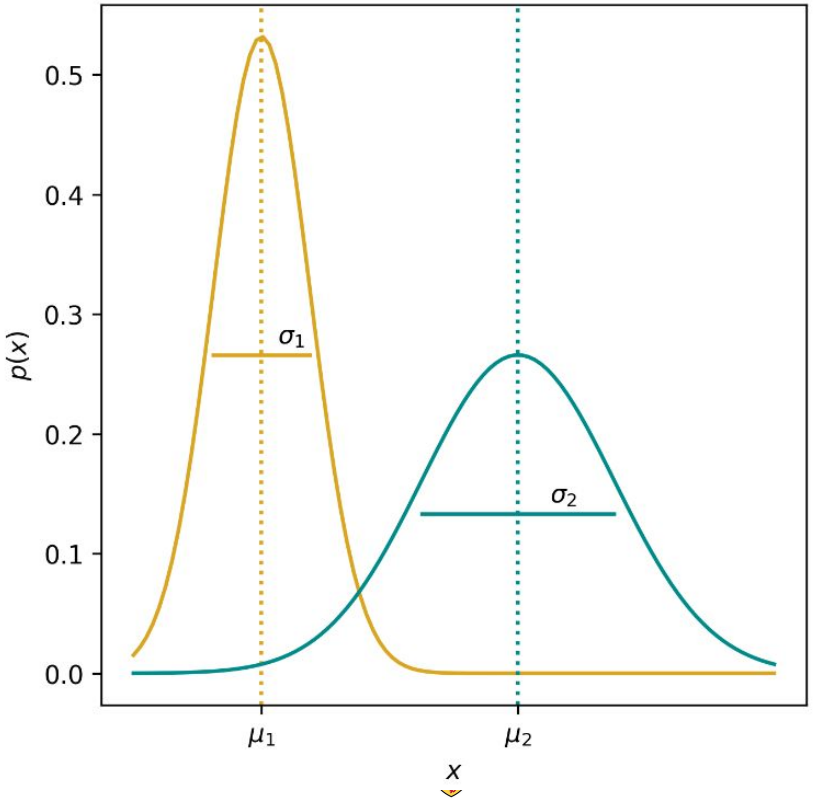
The probability density at a point x under a Gaussian distribution is given by:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x-\mu)^2}$$

Where μ and σ^2 parameters referring to the mean (or center) and variance, respectively.

Probability density functions must satisfy

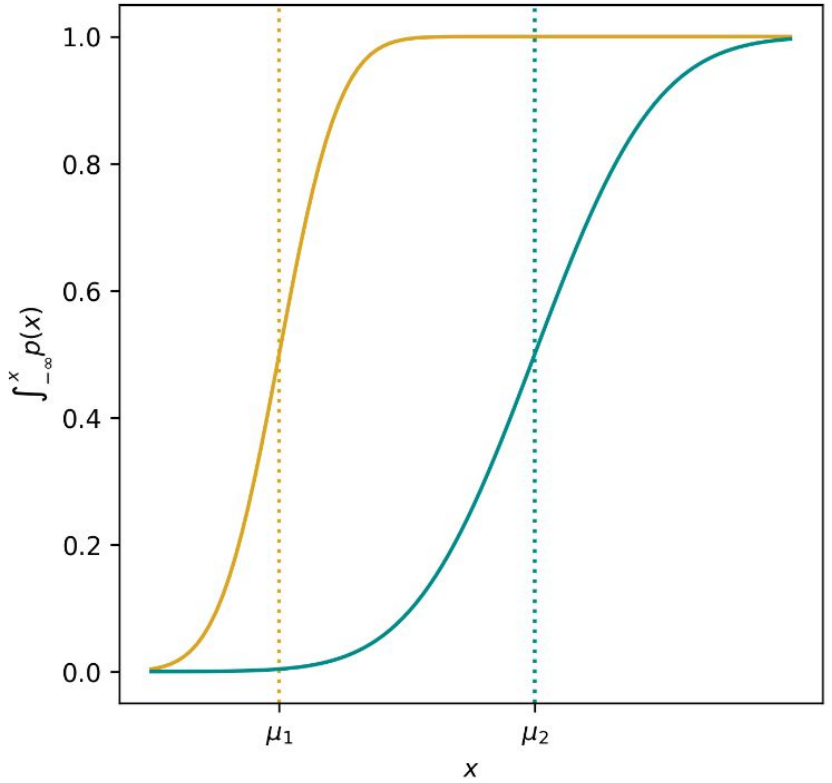
$$\int_{-\infty}^{\infty} p(x) = 1$$



The CDF of a univariate Gaussian (normal) distribution

Cumulative distribution function (CDF):

$$\Pr[X \leq x] = \int_{-\infty}^{x} p(x)$$



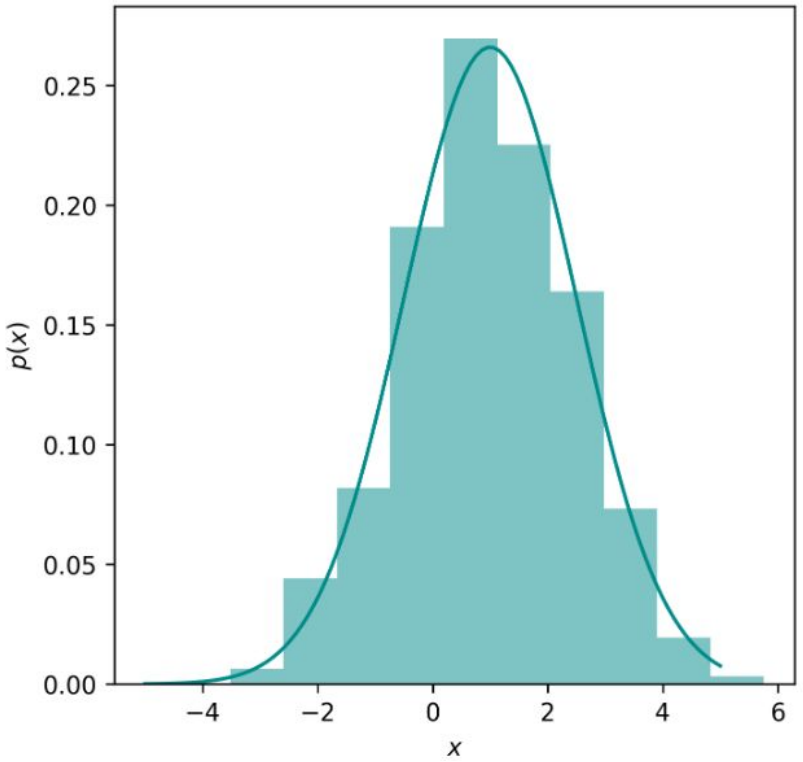
Expectation and the first moment

We denote a continuous random variable X that follows a normal distribution with mean μ and variance σ^2 as

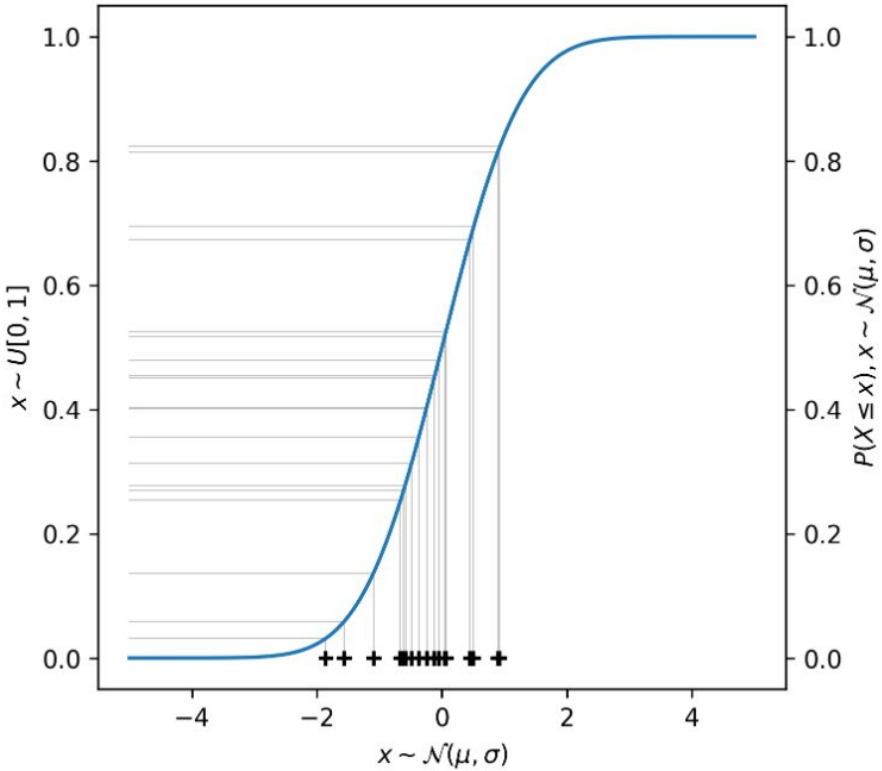
$$X \sim \mathcal{N}(\mu, \sigma^2).$$

The expectation of X is given by:

$$E[X] = \int xp(x)dx = \mu$$
$$\approx \frac{1}{n}\sum_{i=1}^{n} X_i$$



Inverse transform sampling from a parameterized distribution

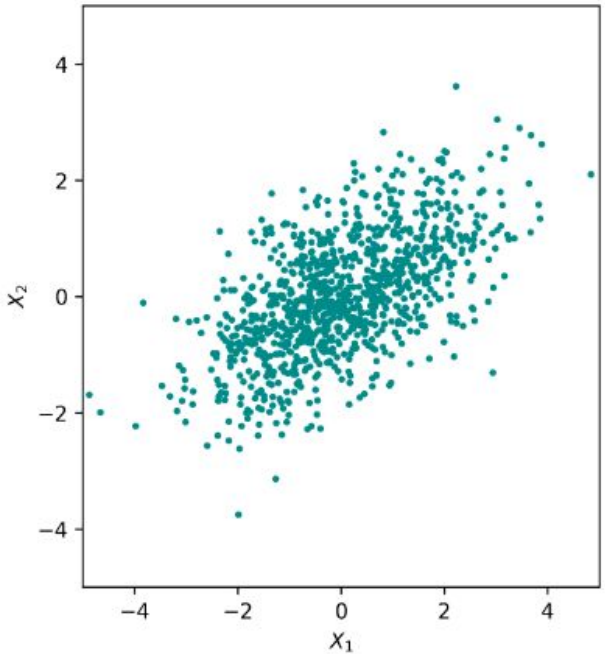


Covariance: generalization for multidimensional data

A random vector $\boldsymbol{X}, \boldsymbol{X} \in \mathbb{R}^d$ has covariance matrix

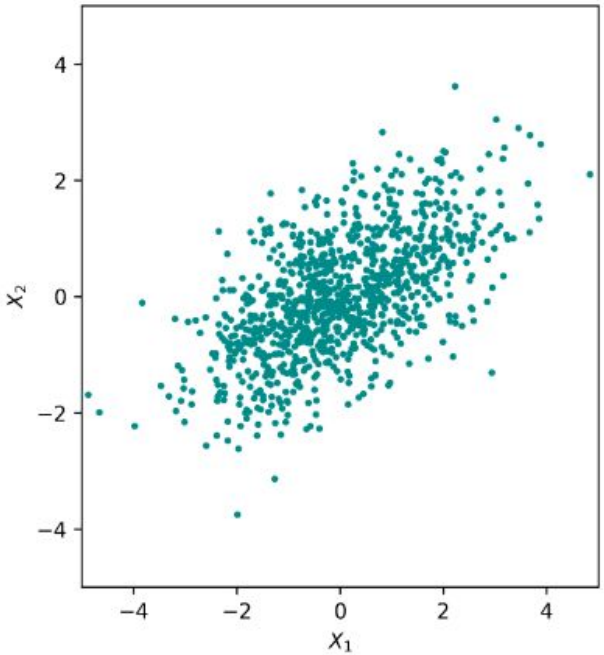
$$
\begin{aligned}
\boldsymbol{\Sigma} &= \mathrm{Cov}(\boldsymbol{X}) \\
&= E[(\boldsymbol{X} - E[\boldsymbol{X}])^T (\boldsymbol{X} - E[\boldsymbol{X}])] \\
&= \begin{bmatrix}
\mathrm{Var}(X_1) & \mathrm{Cov}(X_1, X_2) & \dots & \mathrm{Cov}(X_1, X_d) \\
\mathrm{Cov}(X_2, X_1) & \mathrm{Var}(X_2) & \dots & \mathrm{Cov}(X_2, X_d) \\
\vdots & \vdots & \ddots & \vdots \\
\mathrm{Cov}(X_d, X_1) & \mathrm{Cov}(X_d, X_2) & \dots & \mathrm{Var}(X_d)
\end{bmatrix},
\end{aligned}
$$

which is symmetric and positive semidefinite.

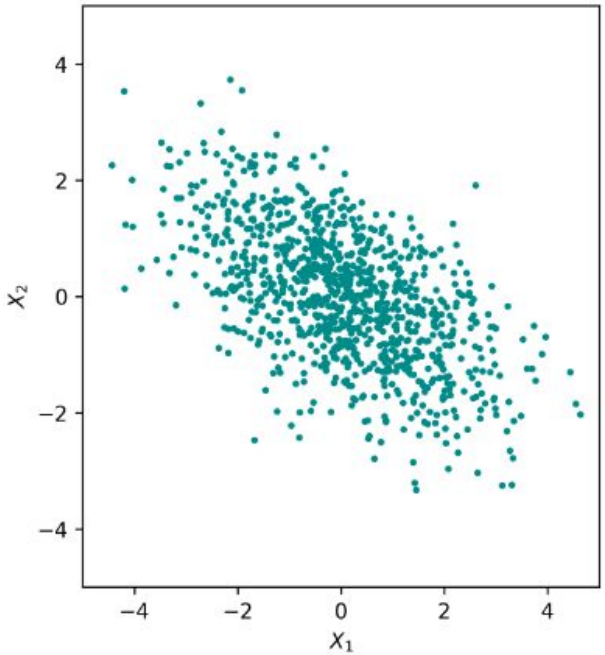


$$
\begin{aligned}
\boldsymbol{X} &\sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \\
&\sim \frac{1}{\sqrt{2\pi^d \det(\boldsymbol{\Sigma})}} e^{-\frac{1}{2}(\boldsymbol{X}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{X}-\boldsymbol{\mu})}
\end{aligned}
$$

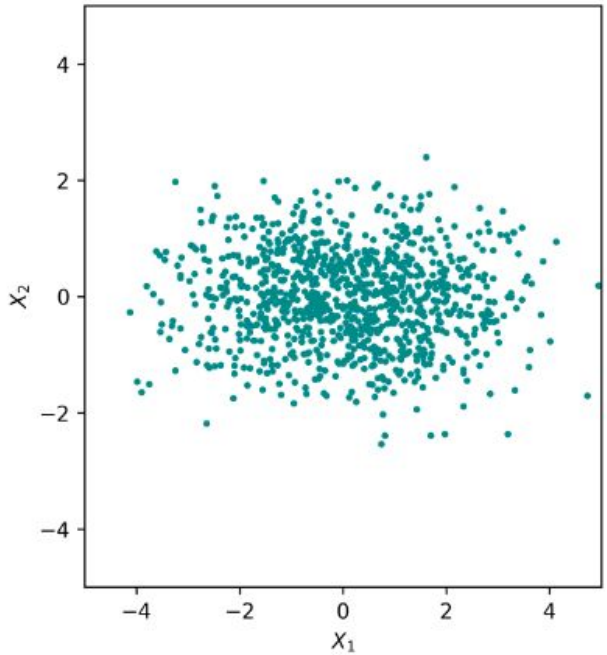
Covariance matrix examples




```
[[2.05764803 0.86381417]
 [0.86381417 1.04250702]]
```




```
[[ 2.23043927 -0.85443664]
 [-0.85443664  1.15488608]]
```




```
[[ 2.66695315 -0.05916988]
 [-0.05916988  0.65315518]]
```

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The joint distribution describes behavior of combined densities

Suppose we have two independent univariate random variables, X_1 and X_2. Their joint probability distribution,

$$p(X_1, X_2) = p(X_2 \mid X_1)p(X_1),$$

describes the probability of the variables occurring together. If variables X_1 and X_2 are *independent*, this simplifies to:

$$p(X_1, X_2) = p(X_2)p(X_1).$$

Pr[A = H]

Pr[A = T]

Pr[B = H|A = H]Pr[A = H]
= Pr[B=H]Pr[A=H]
= (0.5)(0.5) = 0.25

Pr[B=T]Pr[A=H]

Pr[B=H]Pr[A=T]

Pr[B=T]Pr[A=T]

Example: estimating the parameters of a distribution

Suppose we have a set of n observations $\{x_1, x_2, \ldots, x_n\}$, $x_i \in \mathbb{R}$, and we assume that they are realizations of a univariate Gaussian (normal) distribution with some mean μ and variance σ^2:

$$x_i \sim \mathcal{N}(\mu, \sigma^2)$$

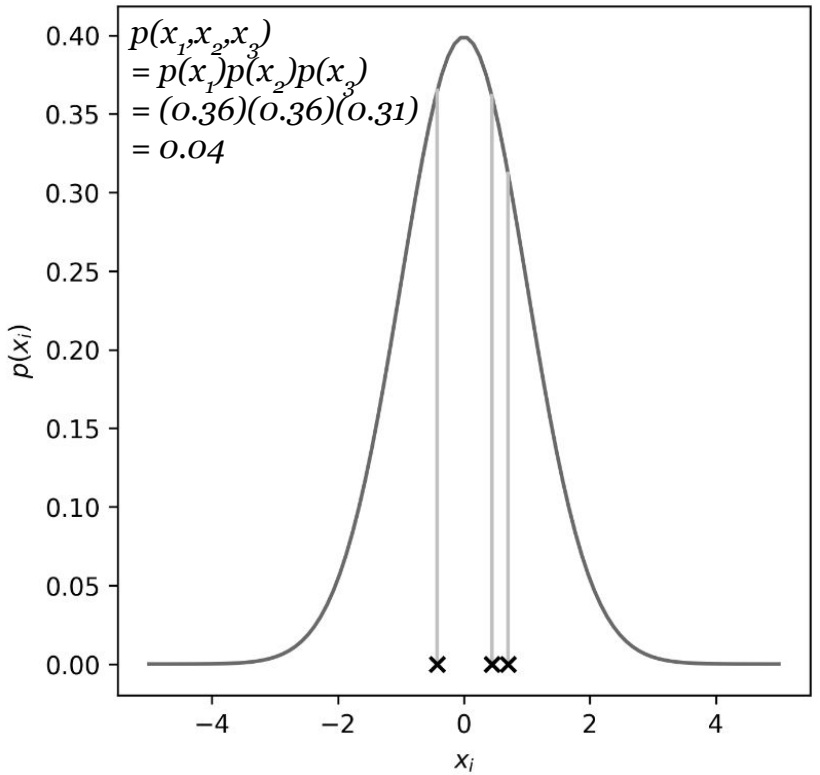
The probability density for each observation x_i is

$$p(x_i \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x_i - \mu)^2},$$

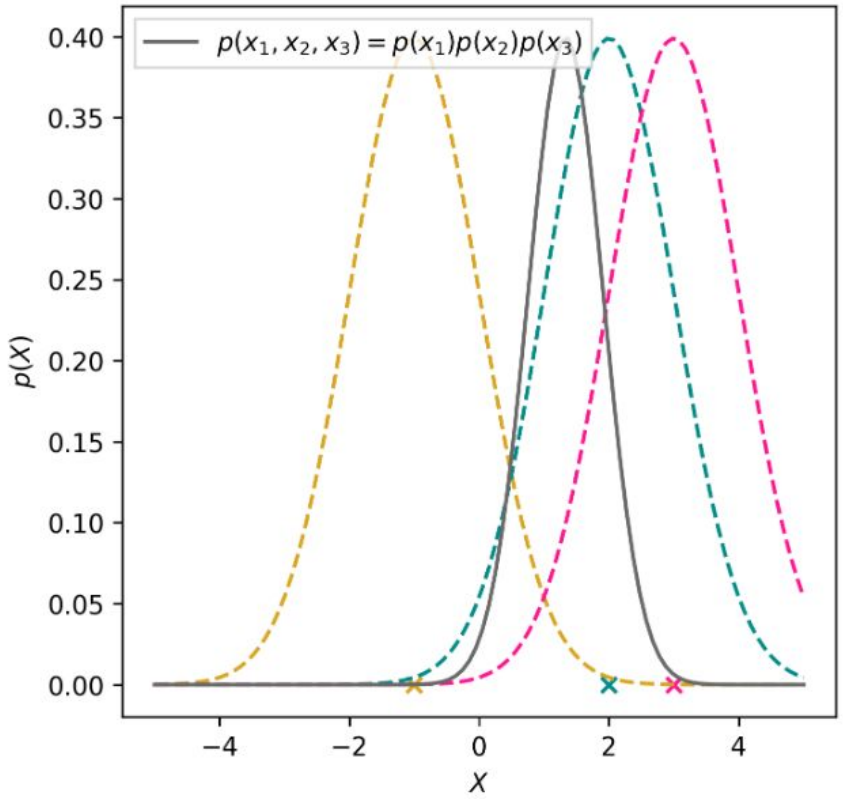
with joint density

$$p(\boldsymbol{x} \mid \mu, \sigma^2) = \prod_{i=1}^{n} p(x_i \mid \mu, \sigma^2)$$

$$= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} se^{-\frac{1}{2\sigma^2}(x_i - \mu)^2}$$



Visual interpretation of joint probability distribution



Likelihood considers the probability of parameters, given data

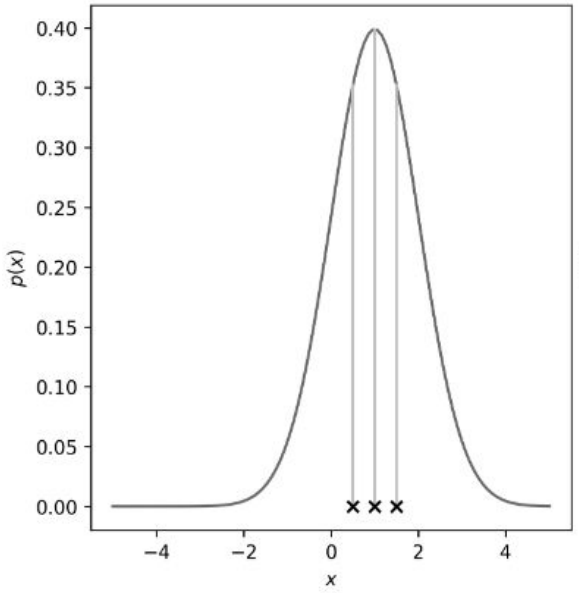
Joint density:

$$p(\boldsymbol{x} \mid \mu, \sigma^2) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x_i-\mu)^2}$$

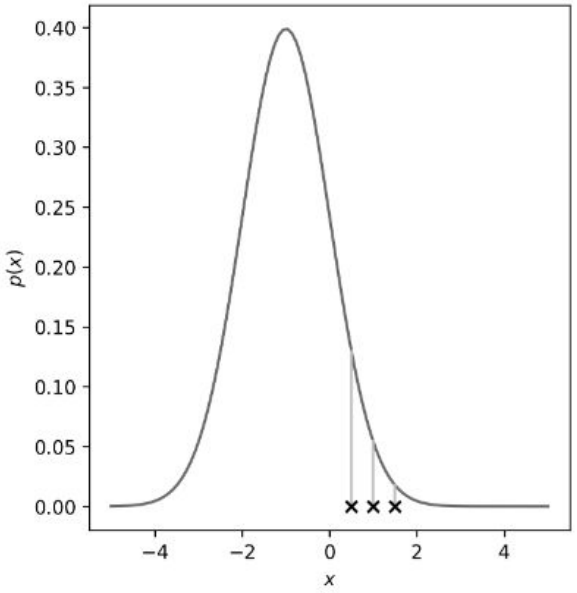
Likelihood:

$$\mathcal{L}(\mu, \sigma^2 \mid \boldsymbol{x}) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(x_i-\mu)^2}$$

$\mu = 1, \sigma = 1$



$\mu = -1, \sigma = 1$



Finding the Maximum Likelihood Estimate (MLE)

$$\mathcal{L}(\mu, \sigma^2 \mid \boldsymbol{x}) = \prod_{i=1}^{n} \frac{1}{\sigma^2} e^{-\frac{1}{2\sigma^2}(x_i - \mu)^2}$$

Finding the Maximum Likelihood Estimate (MLE)

$$\mathcal{L}(\mu, \sigma^2 \mid \boldsymbol{x}) = \prod_{i=1}^{n} \frac{1}{\sigma^2} e^{-\frac{1}{2\sigma^2}(x_i-\mu)^2}$$

$$\log\mathcal{L}(\mu, \sigma^2) = -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2$$

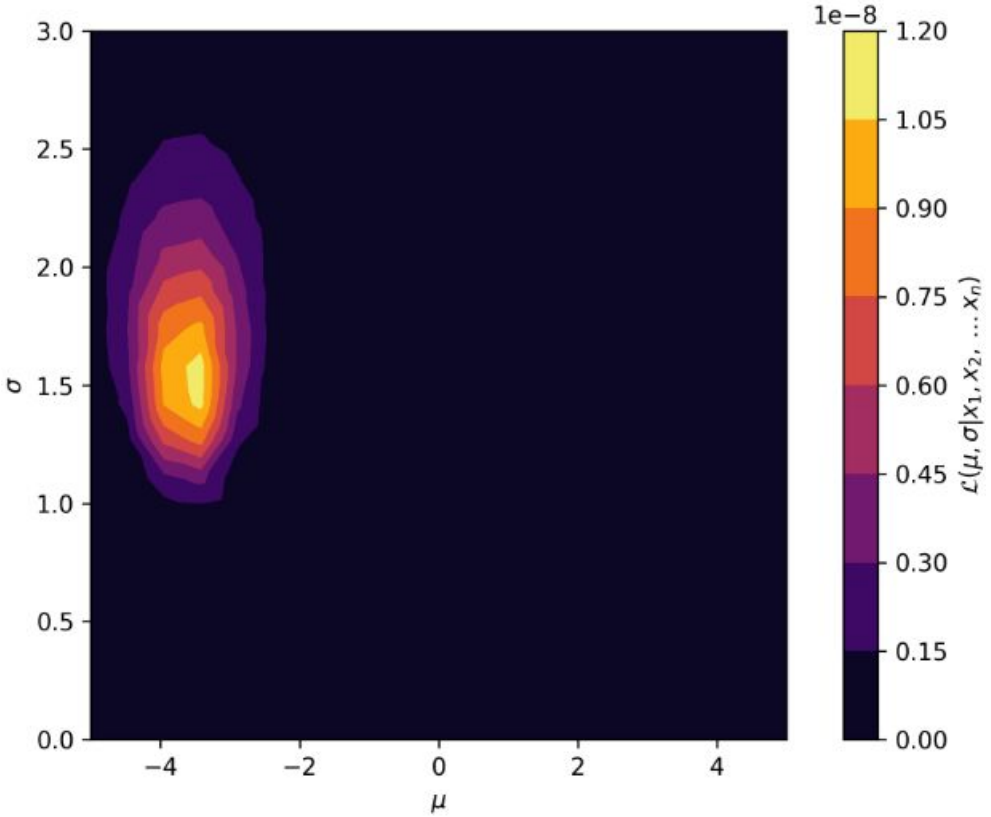
With partial derivatives:

$$\frac{\partial \log\mathcal{L}}{\partial \mu} = -\frac{1}{\sigma^2}\sum_{i=1}^{n}(x_i-\mu)$$

$$\frac{\partial \log\mathcal{L}}{\partial \sigma^2} = \frac{1}{2\sigma^2}\left[\frac{1}{\sigma^2}\sum_{i=1}^{n}(x_i-\mu)^2 - n\right]$$

$$\frac{\partial \log\mathcal{L}}{\partial \mu} = 0 \implies \hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

$$\frac{\partial \log\mathcal{L}}{\partial \sigma^2} = 0 \implies \hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu)^2$$

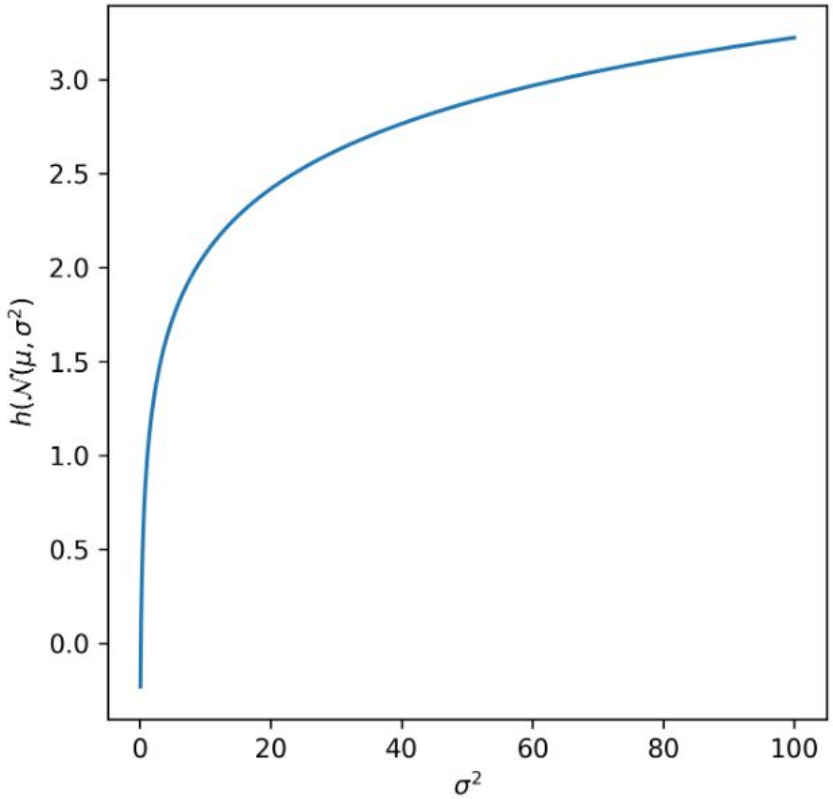


Entropy characterizes the uncertainty in a distribution

$$
\begin{aligned}
h(X) &= E[-\log p(X)] \\
&= -\sum_{i=1}^{n} \Pr[x_i] \log \Pr[x_i] \text{ (Discrete Random Variable)} \\
&= -\int_{\mathcal{X}} p(x) \log p(x) dx \text{ (Continuous Random Variable)}
\end{aligned}
$$

Example: Entropy of a Gaussian (normal) distribution

$$h(X) = E[-\log p(X)]$$
$$= -\int_{\mathcal{X}} p(x)\log p(x)dx$$
$$h(X \sim \mathcal{N}(\mu, \sigma^2)) = \frac{1}{2}\log[2\pi e\sigma^2]$$



Example: Entropy of a Bernoulli random variable

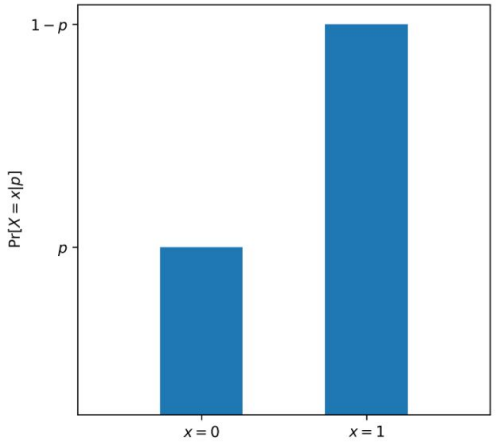
Bernoulli random variable:

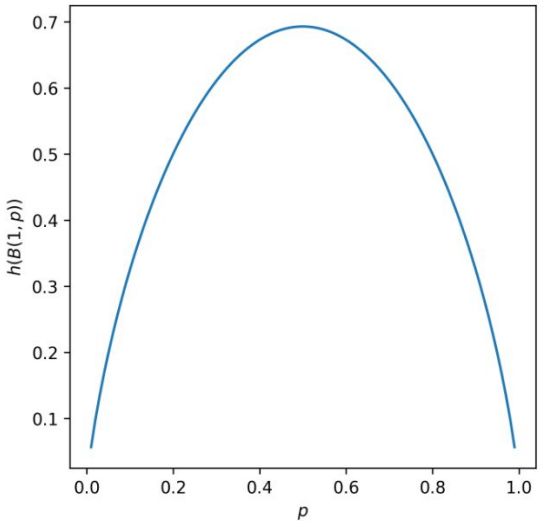
$$\Pr[X = x] = \begin{cases} p & \text{if } x = 1, \\ 1 - p & \text{if } x = 0, \end{cases}$$

where $0 \leq p \leq 1$.

Entropy:

$$\begin{aligned} H(X) &= -\sum_{i=1}^{n} \Pr[x_i] \log \Pr[x_i] \\ &= -\left[P(X = 1) \log P(X = 1) + P(X = 0) \log P(X = 0)\right] \\ &= -\left[p \log p + (1 - p) \log (1 - p)\right] \end{aligned}$$

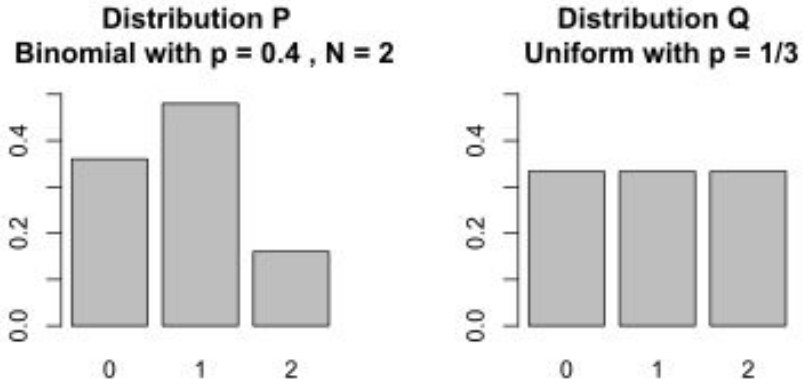




Kullback-Leibler divergence measures dissimilarity between a reference and model distribution (aka relative entropy)

$$D_{\mathrm{KL}}(P \,||\, Q) = \sum_{x \in \mathcal{X}} P(x) \log \frac{P(x)}{Q(x)} \text{ (Discrete Random Variable)}$$

$$D_{\mathrm{KL}}(P \,||\, Q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx \text{ (Continuous Random Variable)}$$



	P	Q	Plog(P/Q)
X = 0	0.36	≅ 0.33	≅ 1.08
X = 1	0.48	≅ 0.33	≅ 1.44
X = 2	0.16	≅ 0.33	≅ -0.11
			D_{KL} ≅ 0.085

Source: Wikipedia

Key Questions

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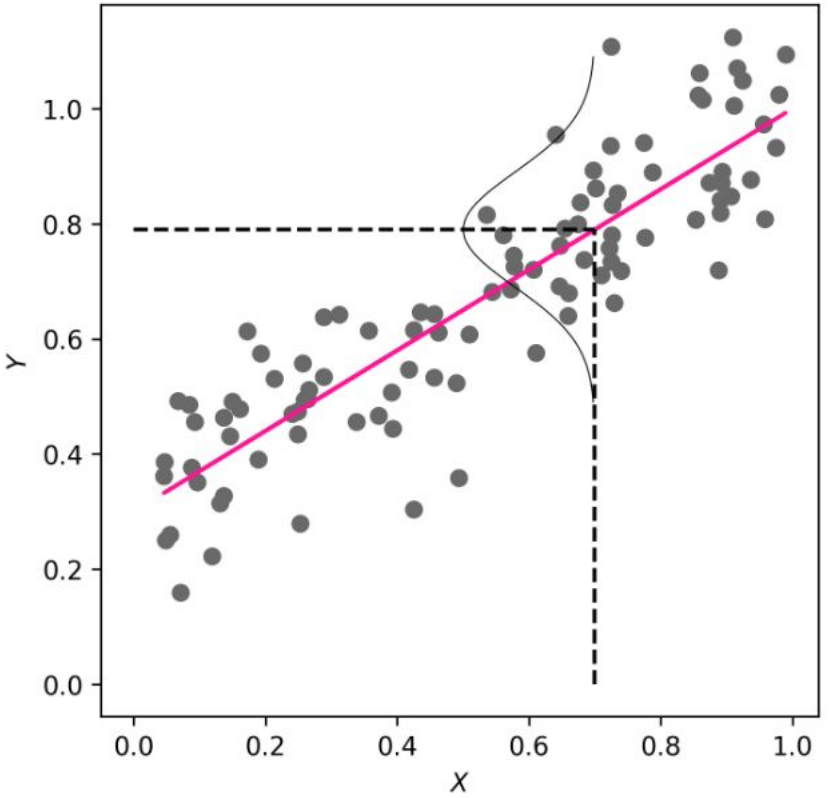
Interpreting the linear regression problem with MLE

Consider a random variable Y that follows a normal distribution with mean $\mu = w^T X$, where X is another random variable, and variance σ^2:

$$Y \sim \mathcal{N}(w^T X, \sigma^2)$$
$$y_i = w^T x_i + \mathcal{N}(0, \sigma^2)$$
$$\text{c.f. } X \sim \mathcal{N}(\mu, \sigma^2)$$

$$\mathcal{L}(\boldsymbol{y} \mid \boldsymbol{x}, w, \sigma^2) = \prod_{i=1}^{n} p(y_i \mid x_i, w, \sigma^2)$$

$$\mathcal{L}(z \mid A, w, \sigma^2) = \prod_{i=1}^{n} p(z_i \mid a_i, w, \sigma^2)$$



Maximizing the likelihood with respect to the parameters $\boldsymbol{w}$

$$\mathcal{L}(z \mid A, w, \sigma^2) = \prod_{i=1}^{n} p(z_i \mid a_i, w, \sigma^2)$$

$$= \prod_{i=1}^{n} \frac{1}{2\pi\sigma^2} e^{-\frac{1}{2\sigma^2}(z_i - w^T a_i)^2}$$

expected / mean

expected / mean

$$\log\mathcal{L}(z \mid A, w, \sigma^2) = -\frac{n}{2}\log(2\pi\sigma^2) - \frac{1}{2\sigma^2}(\boldsymbol{z} - Aw)^T(\boldsymbol{z} - Aw)$$

$$\text{argmax}_w \log\,\mathcal{L} = \text{argmin}_w - \log\,\mathcal{L}$$

$$-\log\,\mathcal{L} = \frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}(\boldsymbol{z} - Aw)^T(\boldsymbol{z} - Aw)$$

$$\frac{\partial - \log\,\mathcal{L}}{\partial w} = \frac{1}{2\sigma^2}(\boldsymbol{z} - Aw)^T(\boldsymbol{z} - Aw)$$

$$= \frac{1}{2\sigma^2}\left(w^T A^T A w - 2A^T w^T \boldsymbol{z} + \boldsymbol{z}^T \boldsymbol{z}\right)$$

$$\frac{\partial - \log\,\mathcal{L}}{\partial w} = 0$$

$$\implies w = (A^T A)^{-1} A^T z$$

What about the variance?

$$\frac{\partial - \log \mathcal{L}}{\partial \sigma} = \frac{\partial}{\partial \sigma}\left[\frac{n}{2}\log(2\pi\sigma^2) + \frac{1}{2\sigma^2}(\boldsymbol{z} - Aw)^T(\boldsymbol{z} - Aw)\right]$$

$$= -\frac{n}{\sigma} + \frac{1}{\sigma^3}(\boldsymbol{z} - Aw)^T(\boldsymbol{z} - Aw)$$

$$\frac{\partial - \log \mathcal{L}}{\partial \sigma} = 0$$

$$\implies \frac{n}{\sigma} = \frac{1}{\sigma^3}(\boldsymbol{z} - Aw)^T(\boldsymbol{z} - Aw)$$

$$\implies \sigma^2 = \frac{1}{n}(\boldsymbol{z} - Aw)^T(\boldsymbol{z} - Aw)$$

$$= \frac{1}{n}\sum_{i=1}^{n}(a_i w - z_i)^2$$

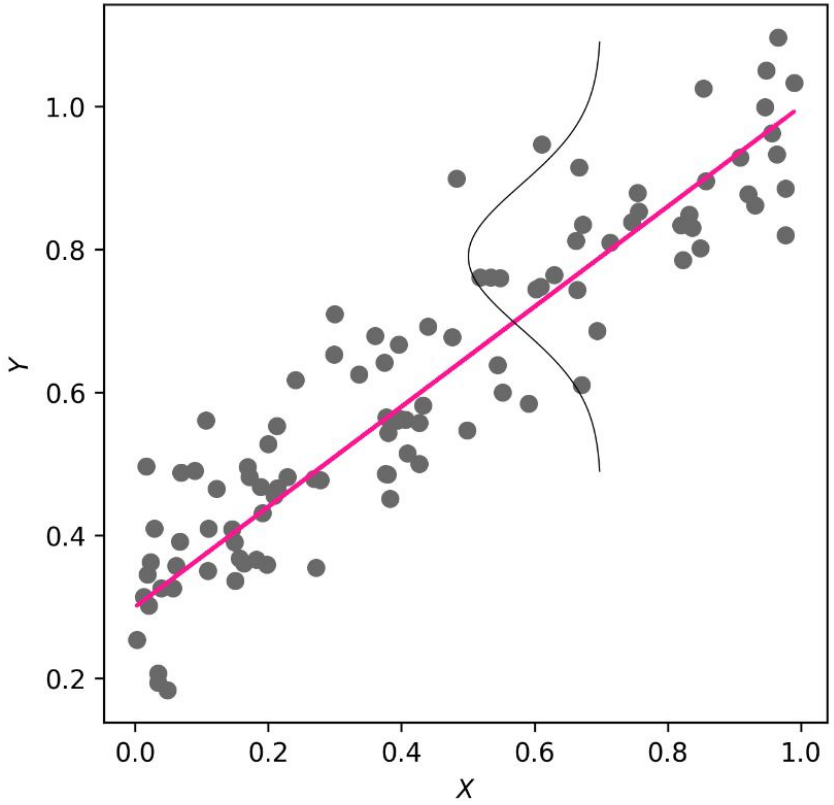
If $y = \log[f(x)]$, then

$$\frac{dy}{dx} = \frac{1}{f(x)}f'(x)$$

$$\implies \frac{d}{d\sigma}\left(-\frac{n}{2}\log(2\pi\sigma^2)\right) = -\frac{n}{2}\frac{1}{2\pi\sigma^2}4\pi\sigma$$

$$= -\frac{n}{\sigma}$$

Under assumption of normally distributed errors, least-squares regression can be viewed as maximizing likelihood



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- ★ Reformulate the linear regression objective using likelihood principles, and demonstrate that it can be viewed as a special case of MLE.

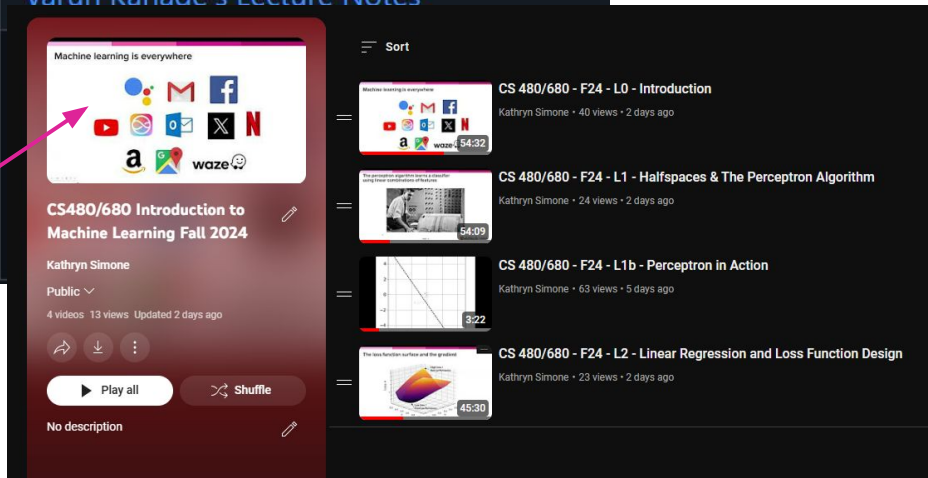
Last lecture's slides have been updated

Errata

- On the slide titled, "Equivalent notation of loss to leverage the gradient" a reference was made to constructing a loss *matrix*. This has been corrected to "We can write the total loss, L as ...".
- A previous version of the slide deck had a slide titled "If a function is convex, its second derivative is positive." This statement was incorrect because a convex function requires the second derivative to be non-negative (≥ 0, not strictly positive, > 0). Additionally, a function may be convex but not necessarily everywhere twice differentiable. The corrected statement reads: "A twice-differentiable function of more than one variable is convex *if and only if* its Hessian is everywhere positive semidefinite," emphasizing that this condition must hold for all points in the function's domain. This clarification highlights that having a positive semidefinite Hessian matrix everywhere in the domain is a sufficient and necessary condition for convexity in the context of twice-differentiable functions. However, convexity as a broader property does not inherently require the function to be twice differentiable or the Hessian to be defined everywhere.

Lecture videos linked from course homepage, playlist also on YouTube

LECTURE	TITLE	MATERIALS	SUPPLEMENTARY READINGS
0	Logistics & Introduction	Slides Video Lecture	N/A
1	Halfspaces & The Perceptron Algorithm	Slides Video Lecture Perceptron Video	UML Section 9.1 ESL Section 4.5 Yaoliang Yu's Lecture Notes Varun Kanade's Lecture Notes
2	Linear Regression & Loss Function Design	Slides Video Lecture	



Lecture	Date	Topics
0	05/09/2024	Introduction + Administrative Remarks
1	10/09/2024	Halfspaces the Perceptron Algorithm
2	12/09/2024	Linear Regression and Convexity
3	17/09/2024	Maximum Likelihood Estimation
4	19/09/2024	k-means Clustering
5	24/09/2024	k-NN Classification and Logistic Regression
6	26/09/2024	Hard-margin SVM
7	01/10/2024	Soft-margin SVM
8	03/10/2024	Kernel methods
9	08/10/2024	Decision Trees
10	10/10/2024	Bagging and Boosting
	15/10/2024	NO LECTURE - MIDTERM BREAK
	17/10/2024	NO LECTURE- MIDTERM BREAK
11	22/10/2024	Expectation Maximization Algorithm
12	24/10/2024	MLPs and Fully-Connected NNs
	29/10/2024	NO LECTURE - MIDTERM EXAM
13	31/10/2024	Convolutional Neural Networks
14	05/11/2024	Recurrent Neural Networks
15	07/11/2024	Attention and Transformers
16	12/11/2024	Graph Neural Networks (Time permitting)
17	14/11/2024	VAEs and GANs
18	19/11/2024	Flows
19	21/11/2024	Contrastive Learning (Time permitting)
20	26/11/2024	Robustness
21	28/11/2024	Privacy (Saeed Mahloujifar Malekmohammadi)
22	03/12/2024	Fairness

Non-parametric methods:

- Kernel Density Est.
- K-means Clustering
- K-NN Classification

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21	28/11/2024	Privacy (Saber Malekmohammadi)
22	03/12/2024	Fairness

On the horizon

Questions? Ask Saber! :) →

Table 2: Grading Scheme

Assessment	Assessment Date	Weighting (CS480)	Weighting (CS680)
Assignment 1	September 27	7.5%	7.5%
Assignment 2	October 14	7.5%	7.5%
Assignment 3	November 8	7.5%	7.5%
Assignment 4	November 22	7.5%	7.5%
Exams			
Midterm	October 29	30%	15%
Final	TBD	40%	30%
Project (CS 680 only)			
Pitch	September 19	N/A	2%
Proposal	October 8	N/A	8%
Report	December 3	N/A	15%
Total		100%	100%

Thursday! →

Errata and Changes

- On slides 17-8, the square root in the denominator of the formulae provided for the probability density function of a Gaussian distribution. This has been fixed (03/12/2024).