Machine Learning CS 4641-B Summer 2020



Lecture 03. Information theory

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These slides are based on slides from Mahdi Roozbahani

Outline

- Logistics -
- Motivation
- Entropy
- Conditional Entropy and Mutual Information
- Cross-Entropy and KL-Divergence

Logistics

- Create your team as soon as possible.
- Textbook and reading materials
- Homework 1 will come out by the end of this week.
- Attendance sheet will be posted.
- We start our office hour this week.

Recap

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Uncertainty and Information

Information is processed data whereas **knowledge** is **information** that is modeled to be useful.

You need **information** to be able to get **knowledge**

information ≠ knowledge
 Concerned with abstract possibilities, not their meaning

Uncertainty and Information



Which day is more uncertain?

How do we quantify uncertainty?

High entropy correlates to high information or the more uncertain 7

Physics and chemistry





How to explain these behaviors?







Design English Dictionary

- Each word is used in people's lives with various frequencies
 - ► Frequent: a, an, the
 - Infrequent: adomania, opia
- The question is how to encode these words.
- The goal is to minimize the size of the information.
 - Intuitively, you don't want to say a long sentence for: "how are you?", "this is an apple."

An example with Probability



Assume that the particles are can move to anywhere in the container.

An example with Probability



An example with Probability



Q1: What is the relationships among these states?

Q2: Can we have a single term to represent the information as knowledge?

- Suppose we observe a sequence of events:
 - Coin tosses
 - Words in a language
 - notes in a song
 - ► etc.
- We want to record the sequence of events in the smallest possible space.
- In other words we want the shortest representation which preserves all information.
- Another way to think about this: How much information does the sequence of events actually contain?

To be concrete, consider the problem of recording coin tosses in unary.

T, T, T, T, H

Approach 1:

Η	Т		
0	00		

00, 00, 00, 00, 0

We used 9 characters

To be concrete, consider the problem of recording coin tosses in unary.

T, T, T, T, H

Approach 2:

0, 0, 0, 0, 00

We used 6 characters

- Frequently occuring events should have short encodings
- We see this in english with words such as "a", "the", "and", etc.
- ► We want to maximise the information-per-character
- seeing common events provides little information
- seeing uncommon events provides a lot of information

Application examples



Entropy is a direct measure of disorder.

Information Theory

- Information theory is a mathematical framework which addresses questions like:
 - How much information does a random variable carry about?
 - How efficient is a hypothetical code, given the statistics of the random variable?
 - How much better or worse would another code do?
 - Is the information carried by different random variables complementary or redundant?



Claude Shannon

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Entropy

• Entropy H(Y) of a random variable Y

$$H(Y) = -\sum_{k=1}^{K} P(y=k) \log_2 P(y=k)$$

- H(Y) is the expected number of bits needed to encode a randomly drawn value of Y (under most efficient code)
- Information theory:

Most efficient code assigns $-\log_2 P(Y = k)$ bits to encode the message Y = k, So, expected number of bits to code one random Y is:

$$\sum_{k=1}^{K} P(y=k) \log_2 \overline{P(y=k)}$$



- S is a sample of coin flips
- p_+ is the proportion of heads in S
- p_{-} is the proportion of tails in S
- Entropy measure the uncertainty of S

$$H(S) \equiv -p_{+} \log_2 p_{+} - p_{-} \log_2 p_{-}$$

Entropy Computation: An Example



head	1
tail	5

P(h) = 1/6	P(t) = 5/6	
Entropy = -	(1/6) log ₂ (1/6)-	- (5/6) log ₂ (1/6) = 0.65

head	2		
tail	4		

P(h) = $\frac{2}{6}$ P(t) = $\frac{4}{6}$ Entropy = - (2/6) $\log_2(2/6)$ - (4/6) $\log_2(4/6)$ = 0.92

Information

Let X be a random variable with distribution p(x)

$$I(X) = \log(\frac{1}{p(x)})$$

Have you heard a picture is worth 1000 words?

Information obtained by random word from a 100,000 word vocabulary:

$$I(word) = \log\left(\frac{1}{p(x)}\right) = \log\left(\frac{1}{1/100000}\right) = 16.61 \ bits$$

A 1000 word document from same source:

$$I(document) = 1000 \times I(word) = 16610$$

A 640*480 pixel, 16-greyscale video picture (each pixel has 16 bits information):

$$I(Picture) = \log\left(\frac{1}{1/16^{640*480}}\right) = 1228800$$

A picture is worth (a lot more than) 1000 words!

Understand entropy with the example



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Understand entropy with the example



The Probability Example



Physics and chemistry



Entropy(solid water) < Entropy (liquid water)</pre>



Entropy(compressed air) < Entropy (air outside)</pre>



Understand entropy with the example

Entropy is a direct measurement of disorder.



Entropy is an average number of bits needed encodes an variable.

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More disordered means needing more bits for the encoding Less disordered means needing less bits for the encoding

How to explain?







Water in solid Low entropy



Water in liquid Medium entropy Water in vapor High entropy





Properties of Entropy

$$H(P) = \sum_{i} p_{i} \cdot \log \frac{1}{p_{i}}$$

- 1. Non-negative: $H(P) \ge 0$
- 2. Invariant wrt permutation of its inputs: $H(p_1, p_2, \dots, p_k) = H(p_{\tau(1)}, p_{\tau(2)}, \dots, p_{\tau(k)})$
- 3. For any *other* probability distribution $\{q_1, q_2, \ldots, q_k\}$:

$$H(P) = \sum_{i} \underline{p_i} \cdot \log \frac{1}{p_i} < \sum_{i} \underline{p_i} \cdot \log \frac{1}{q_i}$$

4. $H(P) \leq \log k$, with equality iff $p_i = 1/k \ \forall i$

5. The further P is from uniform, the lower the entropy.

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Joint Entropy

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			Tem	perati	ıre	۲	
			cold	mild	hot		
	1 16 • 1 • .	low	0.1	0.4	0.1	<u>0.</u> 6	FV.
J	hu <u>Midi</u> ty	high	0.2	0.1	0.1	0.4	
			0.3	0.5	0.2	1.0	

- H(T) = H(0.3, 0.5, 0.2) = 1.48548
- H(M) = H(0.6, 0.4) = 0.970951
- H(T) + H(M) = 2.456431
- Joint Entropy: consider the space of (t, m) events $H(T, M) = \sum_{t,m} P(T = t, M = m) \cdot \log \frac{1}{P(T = t, M = m)}$ H(0.1, 0.4, 0.1, 0.2, 0.1, 0.1) = 2.32193

Notice that H(T, M) < H(T) + H(M) !!!

Conditional Entropy

$$P(T=t|M=m)$$

 $P(\chi, y)$

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[aald	in a il d	bot]
	cold	mila	not	
low	1/6	4/6	1/6	1.0
high	2/4	1/4	1/4	1.0

Conditional Entropy:

- H(T|M = low) = H(1/6, 4/6, 1/6) = 1.25163
- H(T|M = high) = H(2/4, 1/4, 1/4) = 1.5
- Average Conditional Entropy (aka equivocation): $H(T/M) = \sum_m P(M = m) \cdot H(T|M = m) =$ $0.6 \cdot H(T|M = low) + 0.4 \cdot H(T|M = high) = 1.350978$

Conditional Entropy

$$P(M=m|T=t)$$

	cold	mild	hot
low	1/3	4/5	1/2
high	2/3	1/5	1/2
	1.0	1.0	1.0

Conditional Entropy:

- H(M|T = cold) = H(1/3, 2/3) = 0.918296
- H(M|T = mild) = H(4/5, 1/5) = 0.721928
- H(M|T = hot) = H(1/2, 1/2) = 1.0
- Average Conditional Entropy (aka Equivocation): $\frac{H(M/T)}{H(M/T)} = \sum_{t} P(T = t) \cdot H(M|T = t) = 0.3 \cdot H(M|T = cold) + 0.5 \cdot H(M|T = mild) + 0.2 \cdot H(M|T = hot) = 0.8364528$

Conditional Entropy

• Conditional entropy H(Y|X) of a random variable Y given X_i

Discrete random variables:

$$H(Y|X_i) = \sum_{x \in X} p(x_i) H(Y|X = x_i) = \sum_{x \in X, y \in Y} p(x_i, y_i) \log \frac{p(x_i)}{p(x_i, y_i)}$$
Continuous: $H(Y|X_i) = -\int \left(\sum_{k=1}^{K} P(y = k|x_i) \log_2 P(y = k)\right) p(x_i) dx_i$

- Quantify the uncerntainty in Y after seeing feature X_i
- H(Y) is the expected number of bits needed to encode a randomly drawn value of Y
 - given X_i , and
 - average over the likelihood of seeing particular value of x_i

Mutual Information

 Mutual information: quantify the reduction in uncerntainty in Y after seeing feature X_i

$$I(X_i, Y) = \underline{H(Y)} - \underline{H(Y|X_i)}$$

- The more the reduction in entropy, the more informative a feature.
- Mutual information is symmetric
 - $I(X_i, Y) = I(Y, X_i) = H(X_i) H(X_i|Y)$

•
$$I(Y, X_i) = \int \sum_{k}^{K} p(x_i, y = k) \log_2 \frac{p(x_i, y = k)}{p(x_i)p(y = k)} dx_i$$

• =
$$\int \sum_{k}^{K} p(x_i | y = k) p(y = k) \log_2 \frac{p(x_i | y = k)}{p(x_i)} dx_i$$

Properties of Mutual Information

$$I(X;Y) = H(X) - H(X/Y)$$

= $\sum_{x} P(x) \cdot \log \frac{1}{P(x)} - \sum_{x,y} P(x,y) \cdot \log \frac{1}{P(x|y)}$
= $\sum_{x,y} P(x,y) \cdot \log \frac{P(x|y)}{P(x)}$
= $\sum_{x,y} P(x,y) \cdot \log \frac{P(x,y)}{P(x)P(y)}$

Properties of Average Mutual Information:

- Symmetric (but $H(X) \neq H(Y)$ and $H(X/Y) \neq H(Y/X)$)
- Non-negative (but H(X) H(X/y) may be negative!)
- Zero iff X, Y independent

CE and MI: Visual Illustration

H(X,Y)				
H(X)		H(Y X)		
H(X Y)	H((Y)		



Image Credit: Christopher Olah.

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An example that motivates Cross



Cross Entropy

Cross Entropy: The expected number of bits when a wrong distribution Q is assumed while the data actually follows a distribution P

$$H(p,q) = -\sum_{x \in \mathcal{X}} p(x) \log q(x)$$

This is because:

$$egin{aligned} H(p,q) &= \mathrm{E}_p[l_i] = \mathrm{E}_p\left[\lograc{1}{q(x_i)}
ight] \ H(p,q) &= \sum_{x_i} p(x_i)\,\lograc{1}{q(x_i)} \ H(p,q) &= -\sum_x p(x)\,\log q(x). \end{aligned}$$

Kullback-Leibler Divergence

Another useful information theoretic quantity measures the difference between two distributions.

$$\begin{aligned} \mathsf{KL}[P(S) \| Q(S)] &= \sum_{s} P(s) \log \frac{P(s)}{Q(s)} \\ &= \sum_{s} P(s) \log \frac{1}{Q(s)} - \mathsf{H}[P] \\ &\text{cross entropy} \end{aligned}$$

$$\begin{aligned} \mathsf{KL} \text{ Divergence} &= \sum_{s} P(s) \log \frac{1}{Q(s)} - \mathsf{H}[P] \\ &\text{cross entropy} \end{aligned}$$

$$\begin{aligned} \mathsf{KL} \text{ Divergence} &= \sup_{s} P(s) \log \frac{1}{Q(s)} - \mathsf{H}[P] \\ &\text{cross entropy} \end{aligned}$$

$$-\mathbf{KL}[P||Q] = \sum_{s} P(s) \log \frac{Q(s)}{P(s)}$$
$$\sum_{s} P(s) \log \frac{Q(s)}{P(s)} \le \log \sum_{s} P(s) \frac{Q(s)}{P(s)} \qquad \text{by Jensen}$$
$$= \log \sum_{s} Q(s) = \log 1 = 0$$

So $\mathbf{KL}[P \| Q] \ge 0$. Equality iff P = Q

When P = Q, KL[P||Q] = 0

Entropy and KL Divergence in Machine learning

- Construct a model with high entropy or low entropy?
- How a modle is related to cross entropy and **KL Divergence?**

Take-Home Messages

- Entropy
 - A measure for disorder
 - Why it is defined in this way (optimal coding)
 - ► Its properties
- Joint Entropy, Conditional Entropy, Mutual Information
 - The physical intuitions behind their definitions
 - The relationships between them
- Cross Entropy, KL Divergence
 - The physical intuitions behind them
 - The relationships between entropy, cross-entropy, and KL divergence

Lagrange Multipliers

- Min/Max a function f(x, y, z), where x, y, z are subject to the constraint g(x, y, z)=c
- Lagrange Multipliers
 - •Define $F(x, y, z, \lambda) = f(x, y, z) + \lambda g(x, y, z)$
 - Take partial derivative with regarding to each parameter
 - Solve all the associated equations as the potential min/max value.
- Example
 - ►Max $f(x, y) = x^2 y$, s.t. $x^2 + y^2 = 1$ ►Max f(x, y, z) = 8xyz, s.t. $\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1$