CS 446/ECE 449: Machine Learning

Lecture 19: Information Theory 101

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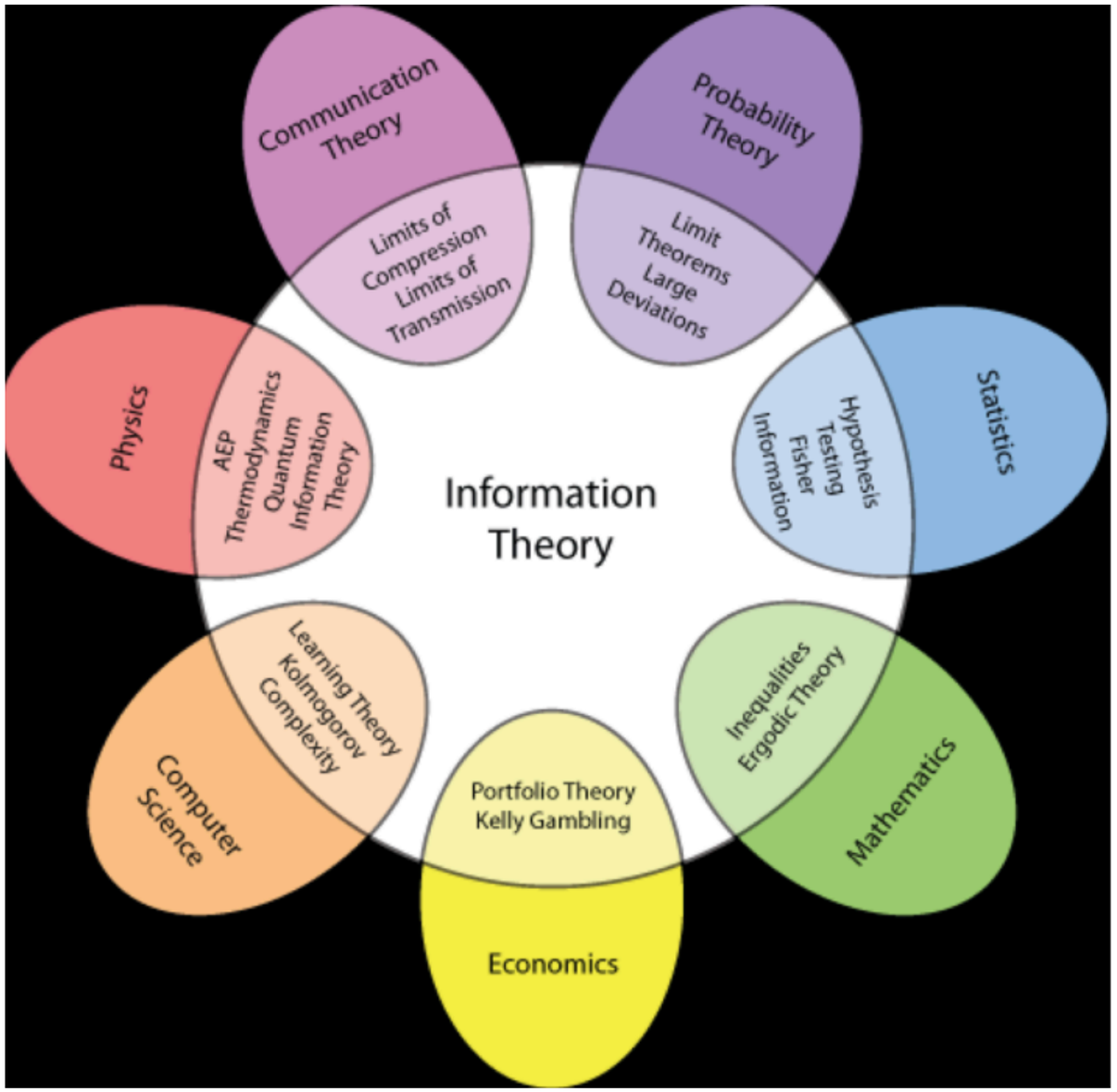
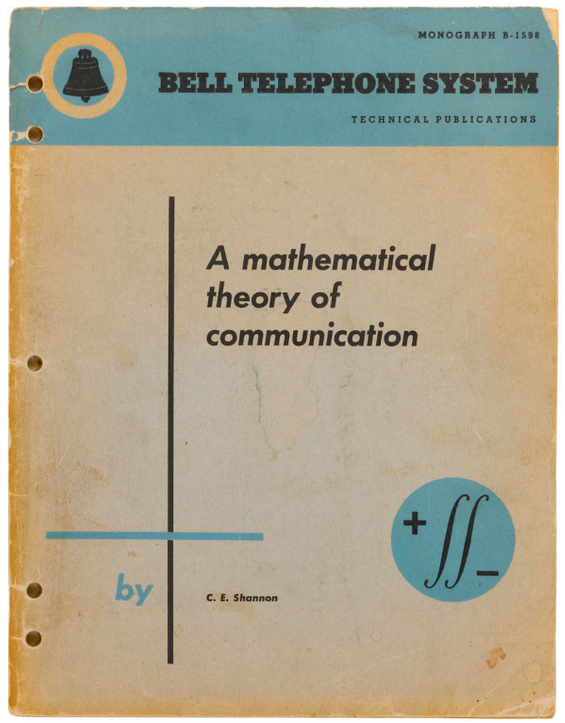
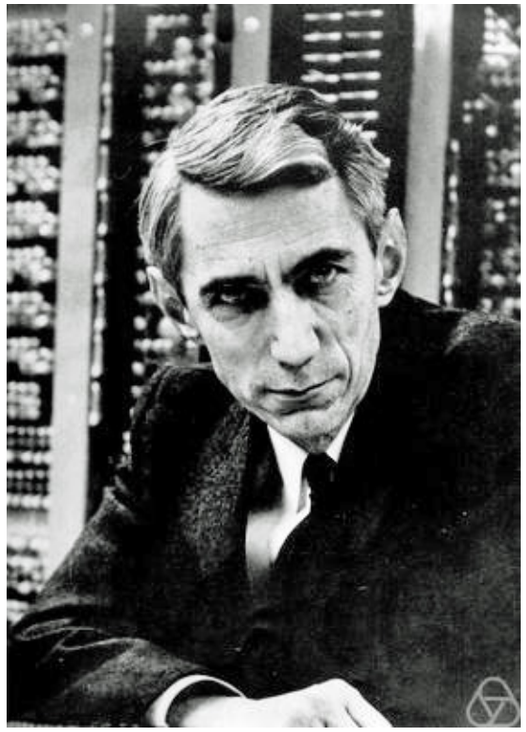
Today

- Entropy, KL-divergence, Mutual Information
- Total Variation distance & the distinguishing game
- Data-processing Inequality

Information Theory 101







Claude E. Shannon, 1948

Information theory is the scientific study of the quantification, storage and communication of digital information

—Wikipedia

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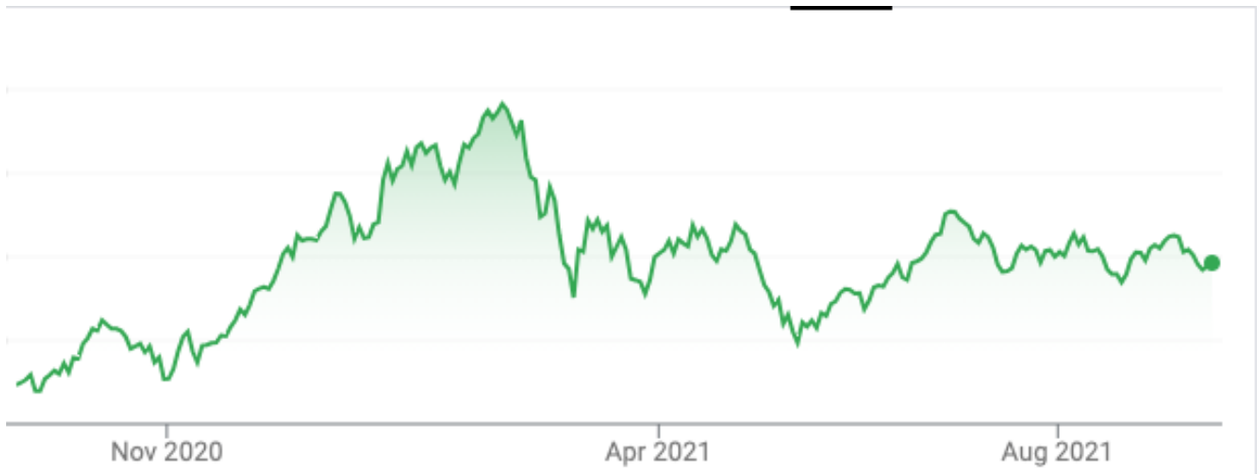
How to quantify information: information content of a random outcome

The sun always rises everyday, no uncertainty here



The price of a stock fluctuates, full of uncertainty

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How to quantify information:

Let X be a discrete random variable taking n different values:

- Example of X: English letter in a document
- Example of X: last digit of S&P 500 index
- Example of X: result of a coin tossing
- ……

X takes n values with probability:

$$p_1, \ldots, p_n, \sum_{i=1}^{n} p_i = 1, p_i \geq 0$$

What's the uncertainty associated with X ?

Information Theory 101

X takes n values with probability:

$$p_1, \ldots, p_n, \sum_{i=1}^{n} p_i = 1, p_i \geq 0$$

What's the uncertainty associated with X ?

Intuitively:

- It should only depend on $p = (p_1, \ldots, p_n)$, independent of the alphabet
- Let's use $H(X) := H(p_1, \ldots, p_n)$ to denote this measure of uncertainty

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Monotonicity:

Let $f(n) := H(1/n, \ldots, 1/n)$. If $n \leq m$, then $f(n) \leq f(m)$.

Grouping rule:

Let $p = (p_1, \ldots, p_m)$ be a probability distribution on m elements. Define a new distribution q on $m-1$ elements as $q_i = p_i, \forall i < m-1$ and $q_{m-1} = p_{m-1} + p_m$. We ask that the following equality holds:

$$H(p) = H(q) + (p_{m-1} + p_m) \cdot H\left(\frac{p_{m-1}}{p_{m-1} + p_m}, \frac{p_m}{p_{m-1} + p_m}\right)$$

Continuity

$H(p_1, \ldots, p_n)$ is continuous in $p = (p_1, \ldots, p_n)$.

Theorem (informal, Shannon 1948):

Under the three axioms above, (up to multiplicative constant $c > 0$), the Shannon entropy admits the following unique form:

$$H(p) = -\sum_{i=1}^{n} p_i \log p_i$$

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X takes n values with probability: an axiomatic approach

$$p_1, \ldots, p_n, \sum_{i=1}^{n} p_i = 1, p_i \geq 0$$

What's the uncertainty associated with X ?

Theorem (informal, Shannon 1948):

Under the three axioms above, (up to multiplicative constant $c > 0$), the Shannon entropy admits the following unique form:

$$H(p) = -\sum_{i=1}^{n} p_i \log p_i$$

Note: 0 log(0) = 0

$$H(X) = \mathbb{E}[\log(1/p(X))]$$

Alternative perspective: the optimal average coding length

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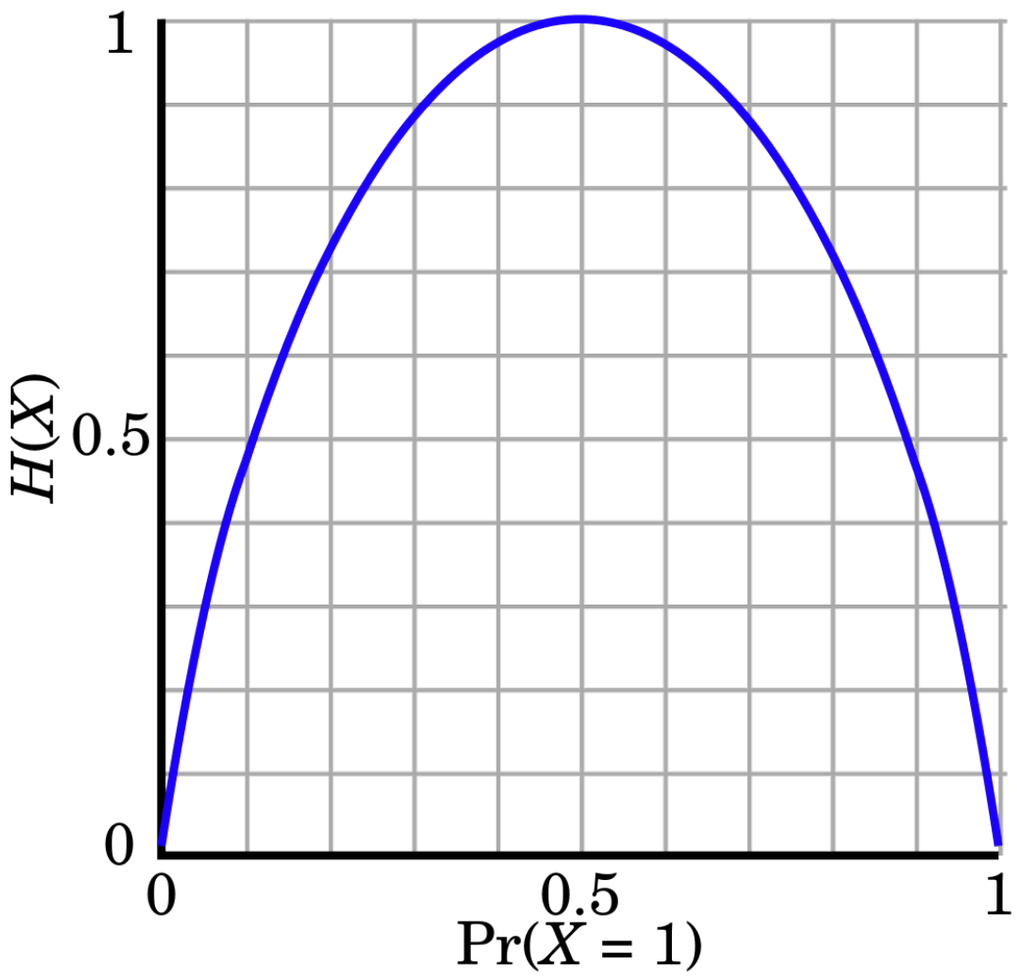
Some properties of entropy:

- For discrete RV, always nonnegative
- Concave in p
- Maximum entropy achieved with uniform distribution



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Other related notions:

- For a pair of RV (X, Y) with joint probability $p(X, Y)$, the joint entropy is

$$H(X, Y) = -\mathbb{E}[\log p(X, Y)]$$

- Conditional entropy: the uncertainty of one variable given the knowledge of another

$$\begin{aligned} H(Y \mid X) &= \mathbb{E}[H(Y \mid X = x)] \\ &= \sum_x p(x) H(Y \mid X = x) \\ &= -\sum_x p(x) \sum_y p(y \mid x) \log p(y \mid x) \end{aligned}$$

- Chain rule:

$$H(X, Y) = H(X) + H(Y \mid X)$$

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How to measure the discrepancy between two distributions, P, Q?

Kullback-Leibler divergence (KL-div, aka relative entropy):

Discrete: $$D_{\mathrm{KL}}(P \parallel Q) := \sum_{x \in \mathcal{X}} P(x) \log \left(\frac{P(x)}{Q(x)} \right)$$

Continuous: $$D_{\mathrm{KL}}(P \parallel Q) := \int_{-\infty}^{\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx$$

Notes:

- Always non-negative
- Not symmetric, hence not a distance
- No upper bound in general (think about one example)

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Kullback-Leibler divergence (KL-div, aka relative entropy):

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$$D_{\mathrm{KL}}(P \parallel Q) := \sum_{x \in \mathcal{X}} P(x) \log \left(\frac{P(x)}{Q(x)} \right)$$

Continuous:
$$D_{\mathrm{KL}}(P \parallel Q) := \int_{-\infty}^{\infty} p(x) \log \left(\frac{p(x)}{q(x)} \right) dx$$

Notes:

- Additive for independent distributions, i.e., if

$$P(x, y) = P_1(x) P_2(y), \; Q(x, y) = Q_1(x) Q_2(y)$$

then,

$$D_{\mathrm{KL}}(P \parallel Q) = D_{\mathrm{KL}}(P_1 \parallel Q_1) + D_{\mathrm{KL}}(P_2 \parallel Q_2)$$

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Kullback-Leibler divergence (KL-div, aka relative entropy):

Discrete:
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Continuous:
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Examples:

- For two Bernoulli distributions $\mathrm{Bern}(p)$ and $\mathrm{Bern}(q)$,
$$D_{\mathrm{KL}}(p_1 \parallel p_2) = p \log \frac{p}{q} + (1-p) \log \frac{1-p}{1-q}$$

- For two Gaussian distributions $\mathcal{N}(\mu_0, \Sigma), \mathcal{N}(\mu_1, \Sigma)$,
$$D_{\mathrm{KL}}(\mathcal{N}_0 \parallel \mathcal{N}_1) = \frac{1}{2}(\mu_1 - \mu_0)^T \Sigma^{-1} (\mu_1 - \mu_0)$$
$$= \frac{1}{2} \|\mu_0 - \mu_1\|_{\Sigma}^2$$ Mahalanobis distance

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Mutual Information: the reduction of uncertainty of one RV given the knowledge of another

$$\begin{aligned} I(X;Y) &= H(X) - H(X \mid Y) \\ &= H(Y) - H(Y \mid X) \end{aligned}$$

Equivalently,

$$\begin{aligned} I(X;Y) &= \sum_x \sum_y p(x,y) \log \frac{p(x,y)}{p(x)p(y)} \\ &= D_{\mathrm{KL}}(p(X,Y) \parallel p(X) \otimes p(Y)) \end{aligned}$$

Some identities:

$$I(X;X) = H(X)$$

$$H(X,Y) = H(X) + H(Y) - I(X;Y)$$

$I(X;Y) = 0$ iff X, Y independent with each other.

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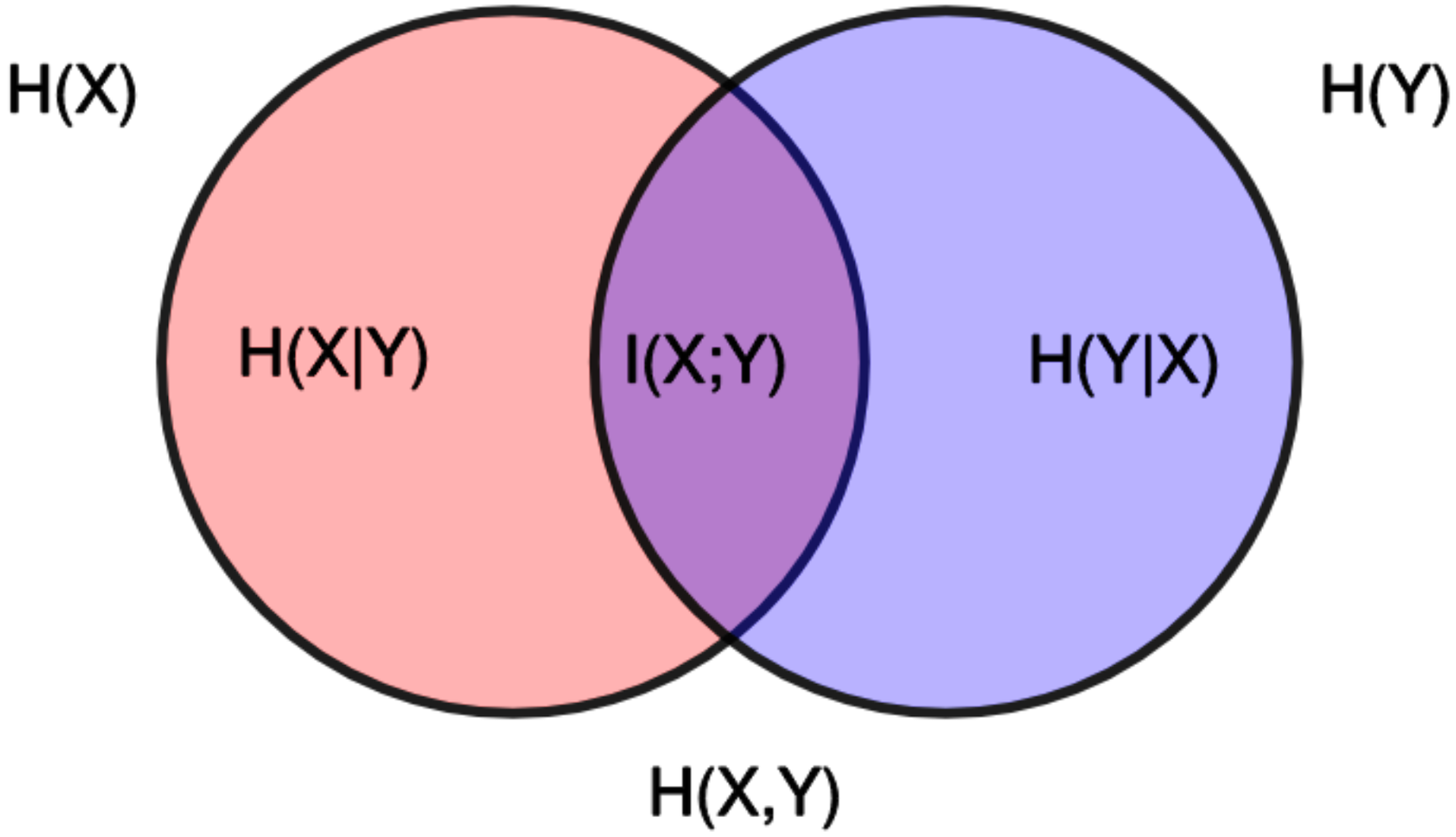
Venn diagram between entropy, conditional entropy, joint entropy and mutual information



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Total variation (TV) distance:

$$d_{\mathrm{TV}}(P, Q) := \sup_{A \subseteq \mathbb{R}^d} |P(A) - Q(A)|$$

Examples:

- TV-distance between two Bernoulli distributions $\mathrm{Bern}(p_0)$ and $\mathrm{Bern}(p_1)$: $|p_0 - p_1|$

Notes:

- Always non-negative, symmetric and bounded between [0, 1]
- TV-distance does not use the underlying geometry of $\mathbb{R}^d$
- TV-distance is a strong one, e.g., if μ is continuous, then

$$d_{\mathrm{TV}}(\hat{\mu}_n, \mu) = 1, \ \forall n$$

Information Theory 101

Total variation (TV) distance:

$$d_{\mathrm{TV}}(P,Q) := \sup_{A \subseteq \mathbb{R}^d} |P(A) - Q(A)|$$

Proposition:

Let P, Q be two probability distributions over the same space, then

$$d_{\mathrm{TV}}(P,Q) = \frac{1}{2}\sum_{x \in \mathcal{X}} |P(x) - Q(x)| =: \frac{1}{2}\|P - Q\|_1$$

Proof:

Let A^* be the event such that $d_{\mathrm{TV}}(P,Q) = P(A^*) - Q(A^*)$. Then

$$\forall x \in \mathcal{X} \backslash A^*,\ P(x) < Q(x)$$

Hence,

$$\begin{aligned}
\|P - Q\|_1 &= \sum_{x \in \mathcal{X}} |P(x) - Q(x)| \\
&= \sum_{x \in A^*} (P(x) - Q(x)) + \sum_{x \in \mathcal{X} \backslash A^*} (Q(x) - P(x)) \\
&= (P(A^*) - Q(A*)) + (1 - Q(A^*) - (1 - P(A^*))) \\
&= 2\,(P(A^*) - Q(A*)) = 2 d_{\mathrm{TV}}(P,Q)
\end{aligned}$$

Information Theory 101

Total variation (TV) distance:

$$d_{\mathrm{TV}}(P, Q) := \sup_{A \subseteq \mathbb{R}^d} |P(A) - Q(A)|$$

Interpretation of the TV-distance as a binary classification problem:

- Let P, Q be two known distributions
- An adversary chooses a distribution D as follows:

$$D = \begin{cases} P & w.p.\ 0.5 \\ Q & w.p.\ 0.5 \end{cases}$$

- You get to see a sample from D, and then make a (possibly randomized) guess about whether D is P or Q?
- Given knowledge about P, Q, upon receiving the sample x, what's your best strategy?

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Interpretation of the TV-distance as a binary classification problem:

$$\eta(x) := \Pr(\text{my guess is } P \mid x)$$

Then, the error probability of using strategy $\eta(\cdot)$ when seeing x is:

$$\begin{aligned}\Pr(\text{error}, x) &= \Pr(\text{guess } P, x \sim Q) + \Pr(\text{guess } Q, x \sim P) \\ &= \frac{1}{2}Q(x)\eta(x) + \frac{1}{2}P(x)(1-\eta(x))\end{aligned}$$

Hence, the overall error probability is given by:

$$\begin{aligned}\Pr(\text{ error }) &= \sum_{x\in\mathcal{X}} \Pr(\text{ error }, x) \\ &= \sum_{x\in\mathcal{X}} \frac{1}{2}Q(x)\eta(x) + \frac{1}{2}P(x)(1-\eta(x)) \\ &= \frac{1}{2} + \frac{1}{2}\sum_{x\in\mathcal{X}} \eta(x)(Q(x)-P(x))\end{aligned}$$

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Interpretation of the TV-distance as a binary classification problem:

$$\eta(x) := \Pr(\text{my guess is } P \mid x)$$

Hence, the overall error probability is given by:

$$\Pr(\text{error}) = \frac{1}{2} + \frac{1}{2} \sum_{x \in \mathcal{X}} \eta(x) \left(Q(x) - P(x)\right)$$

So, clearly, to minimize the overall guessing error, the best strategy is given by:

$$\eta(x) = \begin{cases} 1 & P(x) \geq Q(x) \\ 0 & P(x) < Q(x) \end{cases}$$

Under this optimal strategy, the optimal distinguishing error is:

$$\begin{aligned} \Pr(\text{error}) &= \frac{1}{2} + \frac{1}{2} \sum_{x : P(x) \geq Q(x)} Q(x) - P(x) \\ &= \frac{1}{2} - \frac{1}{2} d_{\mathrm{TV}}(P, Q) \end{aligned}$$

Consider some extremal cases of this distinguishing game

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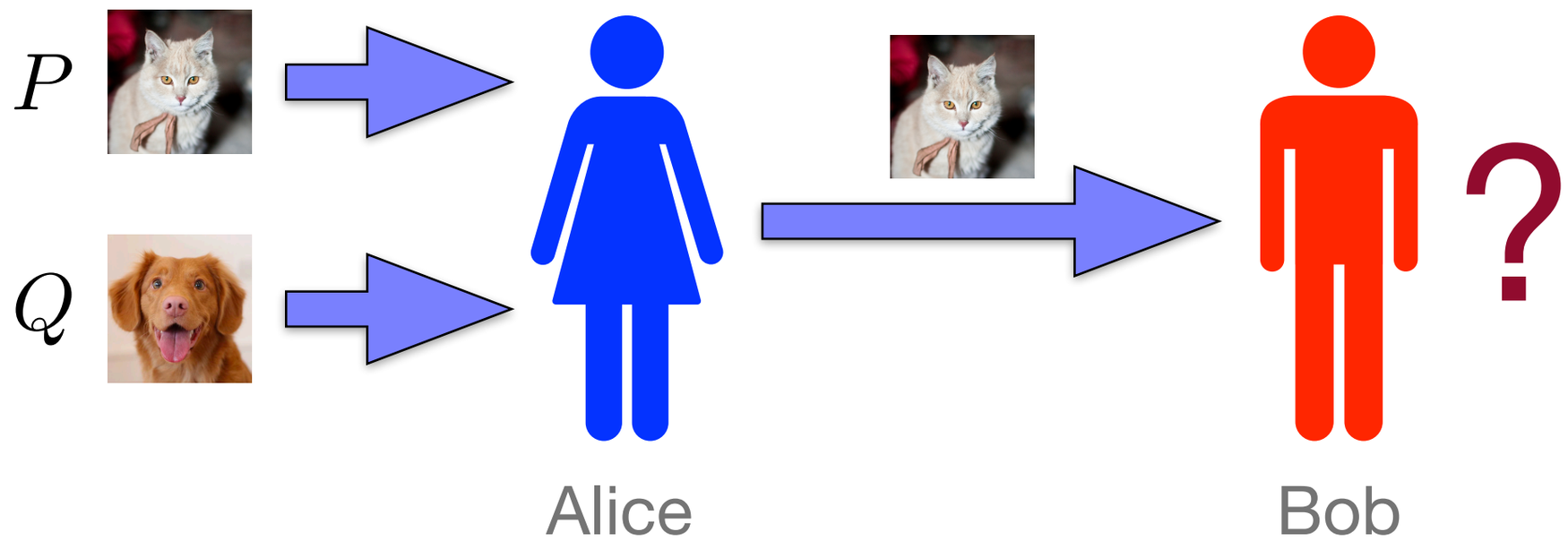
Total Variation (TV) distance & the distinguishing game

TV distance: $d_{\mathrm{TV}}(P, Q) := \sup_{A \subseteq \mathbb{R}^d} |P(A) - Q(A)|$



Bob's optimal error: $\Pr(\text{error}) = \frac{1}{2} + \frac{1}{2} \sum_{x : P(x) \geq Q(x)} Q(x) - P(x)$

$$= \frac{1}{2} - \frac{1}{2} d_{\mathrm{TV}}(P, Q)$$

Information Theory 101

Relationship between the two divergence measures we discussed so far:

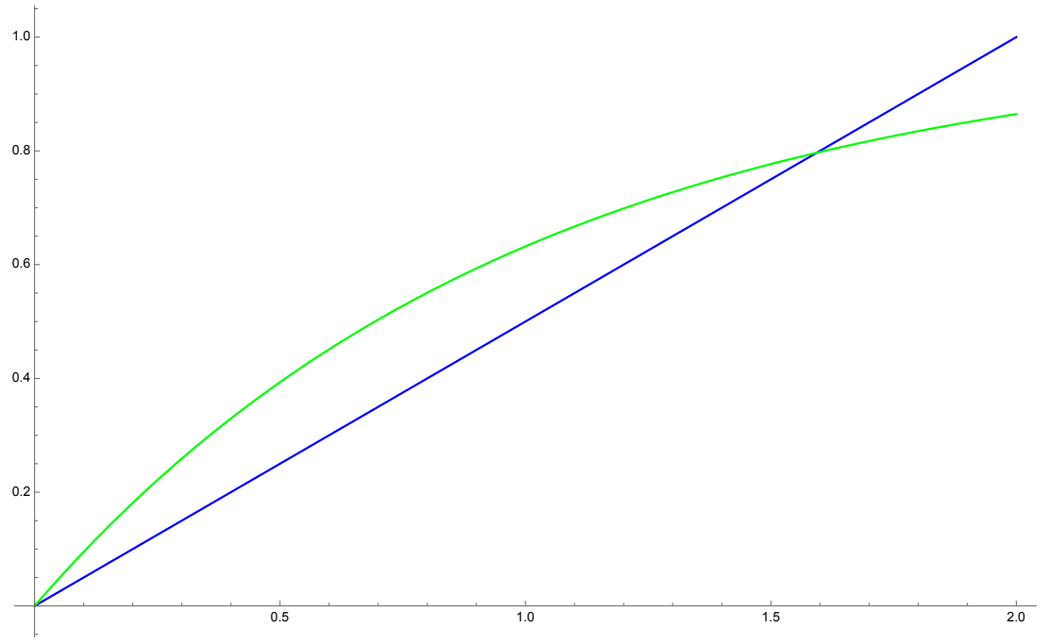
Pinsker's inequality

$$d_{\mathrm{TV}}(\cdot,\cdot) \leq \sqrt{\frac{1}{2} D_{\mathrm{KL}}(\cdot\|\cdot)}$$

Additionally, for TV and KL, we have:

$$d_{\mathrm{TV}}(\cdot,\cdot) \leq \sqrt{1-\exp(-D_{\mathrm{KL}}(\cdot \parallel \cdot))}$$

The second one is better when KL is large:



Information Theory 101

Data processing pipeline:

Nature Camera CD

Information Theory 101

Markov chain: we say that X, Y, Z forms a Markov chain in this order, denoted as $X \to Y \to Z$, if

$$p(x, y, z) = p(x)p(y \mid x)p(z \mid y)$$

Intuitively, given the knowledge of Y, X, Z are conditionally independent from each other.

- Example (coin tossing): probability of getting a head is p. Generate a sequence of independent tosses $X_1, \ldots, X_n$, then

$$p \to \{X_1, \ldots, X_n\} \to \bar{X}_n$$

- Example (multilayer perceptron): X the input image. $Z_i = f_i(Z_{i-1})$ the i-th layer representation with $Z_0 = X$, then

$$X \to Z_1 \to Z_2 \to \cdots \to Z_L$$

Information Theory 101

Data Processing Inequality: If $X \to Y \to Z$, then

$$I(X;Y) \geq I(X;Z), \quad I(Y;Z) \geq I(X;Z)$$

Intuitively:

- Further processing of data cannot increase mutual information

Proof:

$$\begin{aligned} I(X;Y,Z) &= I(X;Z) + I(X;Y \mid Z) \\ &= I(X;Y) + I(X;Z \mid Y) \end{aligned}$$

But

$$I(X;Z \mid Y) = 0$$

So,

$$I(X;Y) \geq I(X;Z)$$

The other one follows since Z, Y, X also forms a Markov chain