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KL Divergence Definitions

References

Information Theory

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Entropy, Intuitively

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- Let h(x) be some measure of the "uncertainty" or "surprise" of event x. What are its properties?
- If p(x) = 1, then there's no uncertainty h(x) = 0
- If p(x) < p(y), then h(x) > h(y) if x is rarer than y, then it is more surprising, so it has higher information
- Finally, if x and y are independent, their information should just add h(xy) = h(x) + h(y)
- h(x) looks like log x



Proof of the Form of h(x)

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$$h(xy) = h(x) + h(y) \quad \text{definition}$$

$$yh'(xy) = h'(x) \quad \text{taking } \frac{\partial}{\partial x}$$

$$xyh''(xy) + h'(xy) = 0 \quad \text{taking } \frac{\partial}{\partial y}$$

$$uh''(u) + h'(u) = 0 \quad \text{letting } u = xy$$

$$uf'(u) + f(u) = 0 \quad \text{letting } f(u) = h'(u)$$



Solving the Differential Equation

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$$u\frac{du}{df} + f = 0$$
$$u \, df = -f \, du$$
$$\frac{1}{f} df = -\frac{1}{u} du$$
$$\frac{1}{f} \frac{df}{du} = -\frac{1}{u}$$
$$\int \frac{1}{f} \left(\frac{df}{du}\right) \, du = -\int \frac{1}{u} \, du$$
$$\ln|f| = -\ln|u| + k$$
$$f(u) = k\frac{1}{u}$$

Finishing up h(x)

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$$f(x) = k\frac{1}{x} = h'(x)$$

$$h(x) = k\int \frac{1}{x} dx = k \ln x + 0$$
but we know $h(xy) = h(x) + h(y)$, so
$$C = 0$$
and $x < y$ implies $h(x) > h(y)$ so
$$k < 0$$

$$h(x) = -k \ln x$$



- *k* corresponds to the *base* of the logarithm
- We'll take base e (natural log) for simplicity
- The units are known as "nats", if base 2 is used, "bits"

Expected value of h(x) — Entropy!

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- Suppose *X* is a random variable
- The expected amount of information it takes to encode X will be simply the expected value of h(x):

$$\frac{\mathsf{H}[X] = \mathsf{E}[-\ln(p(X))]}{= -\sum_{x \in X} p(x) \ln(p(x))}$$

H[X] is known as the *entropy* of X. This seems like a natural way to encode the "uncertainty" of a ranvariable, but how precise is this definition?

Heuristical Justification of Entropy



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- The derivation provided earlier seems a bit ... handwavy
- Luckily, we can sometimes ignore how we got to something and simply prove that it makes sense
 - Induction
 - Solving differential and recurrence relations by guessing
 - etc.
- Valid strategy in math when intuition hard to justify a priori

Justification of Expectation

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• Expectation: $E[X] = \sum_{x \in X} x p(x)$

- Frequentist justification: discrete random variable with values *x*₁...*x*_n, probabilities *p*₁...*p*_n.
- **Run** $\lim_{N\to\infty}$ trials, see $p_i N$ of x_i
- Average value $\frac{1}{N} \sum_{i=1}^{n} x_i(p_i N)$

$$\sum_{i=1}^n x_i p_i = \sum_x x p(x)$$

- Doesn't really work with continuous!
- Made rigorous with strong law of large numbers



Strong Justification of Entropy

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- Entropy H[X] lower bound on the (average) number of bits to encode a random variable X [noiseless coding theorem]
- This is quite a strong claim!
- Proved by Shannon, along with many other information-theoretic concepts



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Entropy Coding Example

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- Discrete uniform distribution on 8 states
- $f(x) = \frac{1}{8}$, $H[X] = -8(\frac{1}{8}\log_2\frac{1}{8}) = 3$
- Non-uniform distribution $\left\{ \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64} \right\}$

$$H[X] = -\sum_{i} p(x_i) \log_2 p(x_i)$$

$$= -\left(\frac{1}{2}\log\frac{1}{2} + \frac{1}{4}\log\frac{1}{4} + \frac{1}{8}\log\frac{1}{8} + \frac{1}{16}\log\frac{1}{16} + \frac{1}{64}\log\frac{1}{64} + \frac{1}{64}\log\frac{1}{64} + \frac{1}{64}\log\frac{1}{64} + \frac{1}{64}\log\frac{1}{64}\right)$$
$$= 2$$

= 2

Better than Uniform with Optimal Coding

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KL Divergence Definitions

- $\ \ \, \left\{ \ \ \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \frac{1}{16}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64}, \frac{1}{64} \right\}$
- Use coding with length "proportional" to probability
- 0, 10, 110, 1110, 111100, 111101, 111110, 111111
- Valid code: no code is a prefix of any other (need to be able to uniquely distinguish in a concatenated sequence)
- Length of each code is precisely $\log_2 p(x_i)$
- Expected length also 2 bits!
- In general, *Huffman coding* to generate optimal codes

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Statistical Mechanics Perspective of Entropy

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- N objects placed into bins, the *i*th bin can have n_i objects (∑_i n_i = N). I think physicists call these "microstates".
- The number of ways W to do this is just combinatorial
- Place your objects in a line. Take the first n₁ as bin 1, next n₂ as bin 2, and so on. N! ways to order N objects, but we don't care about order within a bin so divide by each n_i!
- $W = \frac{N!}{\prod_i n_i!}$. I think physicists call this the "macrostate".
- Amount of entropy $H = \frac{1}{N}W$ (normalized uncertainty)
- Take $\lim_{N\to\infty} H$

Statistical Mechanics, Continued



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 $W = \frac{N!}{\prod_{i} n_{i}!}$ definition of W $H = \frac{1}{N} \ln W$ definition of H $= \frac{1}{N} [\ln(N!) - \sum_{i=1}^{N} \ln(n_{i}!)]$ expanding

From Stirling's approximation $n! \sim n \ln n - n$

$$= \frac{1}{N} [N \ln N - N - \sum_{i=1}^{N} (n_i \ln n_i - n_i)]$$

Statistical Mechanics, Continued

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$$H = \frac{1}{N} [N \ln N - N - \sum_{i=1}^{N} (n_i \ln n_i - n_i)]$$

$$= \frac{1}{N} [N \ln N - \sum_{i=1}^{N} (n_i \ln n_i)] \qquad \text{from } \sum_i n_i = N$$

$$= -\sum_{i=1}^{N} \frac{1}{N} (n_i \ln n_i - n_i \ln N) \qquad \text{from } \sum_i n_i = N$$

$$= -\sum_{i=1}^{N} (\frac{n_i}{N}) \ln \left(\frac{n_i}{N}\right)$$

$$= -\sum_{i=1}^{N} p_i \ln p_i$$

Statistical Mechanics, Conclusion

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$$H = -\sum_{i=1}^{N} p_i \ln p_i$$
$$= H[X]$$



Thermodynamic entropy S = k ln W equivalent to information-theoretic entropy!

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Differential Entropy

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KL Divergence Definitions

- Want to generalize entropy to continuous random variable
 Recall: H[X] = E[−ln(p(X))] = −∑_{x∈X} p(X) ln p(X)
- Why not $H[X] = E[-\ln(p(X))] = -\int p(X) \ln p(X)$
- Yes, this quantity is known as differential entropy
- But there is a very important *caveat* we're missing by being cavalier about replacing sums with integrals
- We'll have to actually work through the derivation!



Differential Entropy Derivation



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- Divide X into bins of width Δ
- Need to assign every element that falls into bin i to x_i
- Find x_i such that $p(x_i)$ equals probability of bin i
- Mean value theorem guarantees there exists x_i such that

$$\int_{i\Delta}^{(i+1)\Delta} p(x) \, dx = p(x_i)\Delta$$

- Given these x_i, have discrete distribution with values x_i and corresponding probabilities p(x_i)Δ
- \blacksquare Compute entropy of this discrete distribution as $\lim_{\Delta \to 0}$

Differential Entropy, Continued

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KL Divergence _{Definitions}

 $H_{\Delta} = -\sum_{i} p(x_i) \Delta \ln(p(x_i) \Delta)$ expanding from In, using $\sum_{i} p(x_i) = 1$ $= -\sum p(x_i)\Delta \ln p(x_i) - \ln \Delta$ $\lim_{\Delta \to 0} H_{\Delta} = \lim_{\Delta \to 0} \left| -\sum_{i} p(x_i) \ln p(x_i) \Delta - \ln \Delta \right|$ $= -\int p(x)\ln p(x)\,dx + (-\ln\Delta)$ H_{Δ} infinite bits discretized entropy differential entropy



Differential Entropy, Commentary

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Divergence Definitions

- So, our differential entropy is the entropy of the binned discrete distribution as the discretization gets arbitrarily precise, minus infinite information
- Intuitively, this makes sense, because it takes infinite bits to specify an arbitrary real number
- The fact that we need to subtract infinite bits makes differential entropy less intuitive than its discrete counterpart, for example, it can be negative
- It still has some useful properties though if one quantizes a continuous random variable X to n digits, the cost to encode it will be (approximately) H[X] + n
- It's also useful to define the upcoming KL divergence, which will help quantify the difference between distributions

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Entropy of a Uniform Random Variable

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KL Divergence Definitions

- Now that we've defined both discrete and differential entropy, we can apply them to some simple distributions
- Discrete uniform on 0, 1, ..., *N* − 1 (location doesn't matter, entropy determined by distribution)
- Density $f(x) = \frac{1}{N}$

$$H[X] = -\sum_{i} p(x_{i}) \ln p(x_{i})$$
$$= -N(\frac{1}{N} \ln \frac{1}{N})$$
$$= \ln N$$

 Recall N is the number of states, so this entropy is always positive (N ≥ 1 ⇒ ln N ≥ 0)

Entropy of a Continuous Uniform

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KL Divergence Definitions

Uniform on [0, N], density
$$f(x) = \frac{1}{N}$$

$$H[X] = -\int p(x) \ln p(x) dx$$

$$= -\int_0^N \frac{1}{N} \ln \frac{1}{N} dx$$

$$= \ln N$$

However, a continuous distribution can have N < 1So differential entropy can be negative!

Entropy of a Multivariate Gaussian

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• Recall a multivariate Gaussian $X \sim \mathcal{N}(\mu, \Sigma)$ has density $f(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} e^{-(\mathbf{x}-\mu)^\top \Sigma^{-1}(\mathbf{x}-\mu)}$

$$\begin{split} \mathsf{H}[X] &= -\,\mathsf{E}[\ln\rho(X)] \\ &= -\,\mathsf{E}[\ln\left(\frac{1}{(2\pi)^{\frac{n}{2}}}\frac{1}{|\Sigma|^{\frac{1}{2}}}\right) - \frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\top}\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})] \\ &= \frac{n}{2}\ln(2\pi) + \frac{1}{2}\operatorname{logdet}\Sigma + \frac{1}{2}\,\mathsf{E}[(\mathbf{x}-\boldsymbol{\mu})^{\top}\Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu})] \end{split}$$

Entropy of a Multivariate Gaussian

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Entropy

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KL Divergence Definitions Abusing the fact that the trace of a scalar is a scalar,

$$\mathsf{E}[(\mathbf{x}-\boldsymbol{\mu})^{\top}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})] = \mathsf{E}[\mathsf{trace}\left((\mathbf{x}-\boldsymbol{\mu})^{\top}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)]$$

Using the cyclic property of trace,

$$= \mathsf{E}[\mathsf{trace}\left(\Sigma^{-1}(\pmb{x}-\pmb{\mu})(\pmb{x}-\pmb{\mu})^{\top}\right)]$$

Swapping expectation and trace by linearity of expectation, = trace($E\left[\Sigma^{-1}(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\top}\right]$)

Bringing out Σ^{-1} since it is constant,

$$= \mathsf{trace}(\Sigma^{-1} \,\mathsf{E}\left[(\pmb{x} - \pmb{\mu})(\pmb{x} - \pmb{\mu})^\top\right])$$

Here we recognize the covariance marix of X

$$= { t trace}(\Sigma^{-1}\Sigma) = { t trace}(I_n) = n$$

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$$H[X] = \frac{1}{2}(n \ln(2\pi) + \operatorname{logdet} \Sigma + E[(\mathbf{x} - \boldsymbol{\mu})^{\top} \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu})])$$

= $\frac{1}{2}(n \ln(2\pi) + \operatorname{logdet} \Sigma + n)$
$$H[X] = \frac{n}{2} \ln(2\pi e |\Sigma|^{\frac{1}{n}})$$

For the case of 1D, the entropy reduces to

$$\frac{1}{2}\ln\left(2\pi e\sigma^2\right)$$

 \blacksquare This will again be negative if $\sigma^2 < \frac{1}{2\pi e}$

Perplexity

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The *perplexity* of a random variable is 2^{H[x]}
Entropy is measured in bits (base 2) here

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Cross-Entropy

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KL Divergence Definitions References

- The cross-entropy between distributions p and q is the expected number of bits it takes to specify a sample from p given an (optimal) coding scheme from q
- Coding scheme: a way to encode a sequence as 1's and 0's

KL Divergence

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KL Divergence Definitions

Kullback-Leibler Divergence (KL Divergence)

Conditional Entropy

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