CO 432 Spring 2025:
Lecture Notes

Lecture notes taken, unless otherwise specified, by myself during the Spring 2025 offering of CO 432, taught by Vijay Bhattiprolu.

Lectures

Chapter 1

Introduction

> **Notation.** I will be using my usual LaTeX typesetting conventions:
>
> - $[n]$ means the set $\{1, 2, \dots, n\}$
> - $\{0,1\}^*$ means the set of bitstrings of arbitrary length (i.e., the Kleene star)
> - $\sum_i$ is implicitly $\sum_{i=1}^{n}$
> - $\mathsf{A}, \mathsf{B}, \dots, \mathsf{Z}$ are random variables (in sans-serif)
> - $\mathsf{X} \sim (p_1, p_2, \dots, p_n)$ means X is a discrete random variable with n outcomes such that $\Pr[\mathsf{X} = 1] = p_1$, $\Pr[\mathsf{X} = 2] = p_2$, etc. (abbreviate further as $\mathsf{X} \sim (p_i)$)

1.1 Entropy

—————————————————— ↓ *Lecture 1 adapted from Arthur* ↓ ——————————————————

> **Definition 1.1.1** (entropy)
>
> For a random variable $\mathsf{X} \sim (p_i)$, the <u>entropy</u> $H(\mathsf{X})$ is
>
> $$H(\mathsf{X}) = -\sum_i p_i \log p_i = \sum_i p_i \log \frac{1}{p_i}.$$

> **Convention.** By convention, we usually use $\log_2$. Also, we define entropy such that $\log_2(0) = 0$ so that impossible values do not break the formula.

> **Example 1.1.2.** If X takes on the values a, b, c, d with probabilities 1, 0, 0, 0, respectively, then $H(\mathsf{X}) = 1 \log 1 = 0$.
>
> If X takes on those values instead with probabilities $\frac{1}{2}$, $\frac{1}{4}$, $\frac{1}{8}$, $\frac{1}{8}$, respectively, then $H(\mathsf{X}) = \frac{7}{4}$.

> **Fact 1.1.3.** $H(\mathsf{X}) = 0$ if and only if X is a constant.

Proof. Suppose X is constant. Then, $H(\mathsf{X}) = 1 \log 1 = 0$.

Suppose $H(\mathsf{X}) = 0$. Probabilities are in $[0, 1]$, so $p_i \log \frac{1}{p_i} \geq 0$. Since $H(\mathsf{X}) = \sum_i p_i \log \frac{1}{p_i} = 0$ and each term is non-negative, each term must be zero. Thus, each p_i is either 0 or 1. We cannot have $\sum p_i > 1$, so exactly one $p_i = 1$ and the rest are zero. That is, X is constant. $\qquad\square$

> **Theorem 1.1.4** (Jensen's inequality)
>
> Let $f : \mathbb{R} \to \mathbb{R}$ be concave. That is, for any a and b in the domain of f and $\lambda \in [0, 1)$, $f(\lambda a + (1 - \lambda)b) \geq \lambda f(a) + (1 - \lambda)f(b)$. For any discrete random variable X,
>
> $$\mathbb{E}[f(\mathsf{X})] \leq f(\mathbb{E}[\mathsf{X}])$$

Proof. Consider a random variable X with two values a and b, each with probabilities λ and $1 - \lambda$. Then, notice that

$$\mathbb{E}[f(\mathsf{X})] = \lambda f(a) + (1 - \lambda)f(b) \leq f(\lambda a + (1 - \lambda)b) = f(\mathbb{E}[\mathsf{X}])$$

by convexity of f.

TODO: This can be generalized by induction. $\qquad\square$

> **Fact 1.1.5.** Assume X is supported on $[n]$. Then, $0 \leq H(\mathsf{X}) \leq \log n$.

Proof. Start by claiming without proof that $\log n$ is concave, so we can apply Jensen's inequality. Let $\mathsf{X}' = \frac{1}{p_i}$ with probability p_i. Then,

$$\begin{aligned}
H(\mathsf{X}) &= \sum_i p_i \log \frac{1}{p_i} \\
&= \mathbb{E}\left[\log(\mathsf{X}')\right] \\
&\leq \log(\mathbb{E}[\mathsf{X}']) \\
&= \log\left(\sum p_i \frac{1}{p_i}\right) \\
&= \log n
\end{aligned}$$
$\qquad\square$

It is not a coincidence that $\log_2 n$ is the minimum number of bits to encode $[n]$.

1.2 Entropy as expected surprise

We want $S : [0, 1] \to [0, \infty)$ to capture how "surprised" we are $S(p)$ that an event with probability p happens. We want to show that under some natural assumptions, this is the only function we could have defined as entropy. In particular:

1. $S(1) = 0$, a certainty should not be surprising

2. $S(q) > S(p)$ if $p > q$, less probable should be more surprising

3. $S(p)$ is continuous in p

4. $S(pq) = S(p) + S(q)$, surprise should add for independent events. That is, if I see something twice, I should be twice as surprised.

────────────────── ↑ *Lecture 1 adapted from Arthur* ↑ ──────────────────   *Lecture 2*
May 8

> **Proposition 1.2.1**
>
> If $S(p)$ satisfies these 4 axioms, then $S(p) = c \cdot \log_2(1/p)$ for some $c > 0$.

Proof. Suppose a function $S : [0,1] \to [0,\infty)$ exists satisfying the axioms. Let $c := S(\frac{1}{2}) > 0$.

By axiom 4 (addition), $S(\frac{1}{2^k}) = kS(\frac{1}{2})$. Likewise, $S(\frac{1}{2^{1/k}} \cdots \frac{1}{2^{1/k}}) = S(\frac{1}{2^{1/k}}) + \cdots + S(\frac{1}{2^{1/k}}) = kS(\frac{1}{2^{1/k}})$.

Then, $S(\frac{1}{2^{m/n}}) = \frac{m}{n}S(\frac{1}{2}) = \frac{m}{n} \cdot c$ for any rational m/n.

By axiom 3 (continuity), $S(\frac{1}{2^z}) = c \cdot z$ for all $z \in [0,\infty)$ because the rationals are dense in the reals. In particular, for any $p \in [0,1]$, we can write $p = \frac{1}{2^z}$ for $z = \log_2(1/p)$ and we get

$$S(p) = S\left(\frac{1}{2^z}\right) = c \cdot z = c \cdot \log_2(1/p)$$

as desired. $\square$

We can now view entropy as expected surprise. In particular,

$$\sum_i p_i \log_2 \frac{1}{p_i} = \mathop{\mathbb{E}}_{x \sim \mathsf{X}} [S(p_x)]$$

for a random variable $\mathsf{X} = i$ with probability p_i.

1.3   Entropy as optimal lossless data compression

Suppose we are trying to compress a string consisting of n symbols drawn from some distribution.

> **Problem 1.3.1**
>
> What is the expected number of bits you need to store the results of n independent samples of a random variable X?

We will show this is $nH(\mathsf{X})$.

Notice that we assume that the symbols we are drawn <u>independently</u>, which is violated by almost all data we actually care about.

> **Definition 1.3.2**
>
> Let $C : \Sigma \to (\Sigma')^*$ be a code. We say C is a <u>uniquely decodable</u> code (UDC) if there does not exist a collision $x, y \in \Sigma^*$, with identical encoding $C(x_1)C(x_2)\cdots C(x_k) = C(y_1)C(y_2)\cdots C(y_{k'})$.
>
> Also, C is <u>prefix-free</u> (sometimes called <u>instantaneous</u>) if for any distinct $x, y \in \Sigma$, $C(x)$ is not a prefix of $C(y)$.

> **Proposition 1.3.3**
>
> Prefix-freeness is sufficient for unique decodability.

Example 1.3.4. Let $C : \{A, B, C, D\} \to \{0, 1\}^*$ where $C(A) = 11$, $C(B) = 101$, $C(C) = 100$, and $C(D) = 00$. Then, C is prefix-free and uniquely decodable.

We can easily parse 1011100001100 unambiguously as 101.11.00.00.11.00 ($BADDAD$).

Recall from CS 240 that a prefix-free code is equivalent to a trie, and we can decode it by traversing the trie in linear time.

> **Theorem 1.3.5** (Kraft's inequality)
>
> A prefix-free binary code $C : \{1, \ldots, n\} \to \{0, 1\}^*$ with codeword lengths $\ell_i = |C(i)|$ exists if and only if
> $$\sum_{i=1}^{n} \frac{1}{2^{\ell_i}} \leq 1.$$

Proof. Suppose $C : \{1, \ldots, n\} \to \{0, 1\}^*$ is prefix-free with codeword lengths ℓ_i. Let T be its associated binary tree and let W be a random walk on T where 0 and 1 have equal weight (stopping at either a leaf or undefined branch).

Define E_i as the event where W reaches i and $E_\varnothing$ where W falls off. Then,

$$
\begin{aligned}
1 &= \Pr(E_\varnothing) + \sum_i \Pr(E_i) \\
&= \Pr(E_\varnothing) + \sum_i \frac{1}{2^{\ell_i}} && \text{(by independence)} \\
&\geq \sum_i \frac{1}{2^{\ell_i}} && \text{(probabilities are non-negative)}
\end{aligned}
$$

Conversely, suppose the inequality holds for some ℓ_i. WLOG, suppose $\ell_1 < \ell_2 < \cdots < \ell_n$.

Start with a complete binary tree T of depth ℓ_n. For each $i = 1, \ldots, n$, find any unassigned node in T of depth ℓ_i, delete its children, and assign it a symbol.

Now, it remains to show that this process will not fail. That is, for any loop step i, there is still some unassigned node at depth ℓ_i.

Let $P \leftarrow 2^{\ell_n}$ be the number of leaves of the complete binary tree of depth ℓ_n. After the ith step, we decrease P by $2^{\ell_n - \ell_i}$. That is, after n steps,

$$
\begin{aligned}
P &= 2^{\ell_n} - \sum_{i=1}^{n} \frac{2^{\ell_n}}{2^{\ell_i}} \\
&= 2^{\ell_n} - 2^{\ell_n} \sum_{i=1}^{n} \frac{1}{2^{\ell_i}} \\
&\geq 0
\end{aligned}
$$

by the inequality.   □

Recall the problem we are trying to solve:

> **Problem 1.3.1**
>
> What is the expected number of bits you need to store the results of n independent samples of a random variable X?

Solution (Shannon & Faro). Consider the case where X is symbol i with probability p_i. We want to encode independent samples $x_i \sim \mathsf{X}$ as $C(x_i)$ for some code $C : [n] \to \{0,1\}^*$.

Suppose for simplification that $p_i = \frac{1}{2^{\ell_i}}$ for some integers ℓ_i. Since $\sum p_i = 1$, we must have $\sum \frac{1}{2^{\ell_i}} = 1$. Then, by Kraft's inequality, there exists a prefix-free binary code $C : [n] \to \{0,1\}^*$ with codeword lengths $|C(i)| = \ell_i$. Now,

$$
\mathop{\mathbb{E}}_{x_i \sim \mathsf{X}} \left[\sum_i |C(x_i)| \right] = \sum_i p_i \ell_i = \sum_i p_i \log_2 \frac{1}{p_i} = H(\mathsf{X})
$$

Proceed to the general case. Suppose $\log_2 \frac{1}{p_i}$ are non-integral. Instead, use $\ell_i' = \left\lceil \log_2 \frac{1}{p_i} \right\rceil$. We still satisfy Kraft since $\sum_i \frac{1}{2^{\ell_i'}} \leq \sum_i p_i = 1$. Then,

$$
\mathop{\mathbb{E}}_{x_i \sim \mathsf{X}} \left[\sum_i |C(x_i)| \right] = \sum_i p_i \ell_i' = \sum_i p_i \left\lceil \log_2 \frac{1}{p_i} \right\rceil
$$

which is bounded by

$$
H(\mathsf{X}) = \sum_i p_i \log_2 \frac{1}{p_i} \leq \sum_i p_i \left\lceil \log_2 \frac{1}{p_i} \right\rceil < \sum_i p_i \left(1 + \log_2 \frac{1}{p_i} \right) = H(\mathsf{X}) + 1
$$

We call the code C generated by this process the <u>Shannon–Faro code</u>.   □

We can improve on this bound $[H(\mathsf{X}), H(\mathsf{X}) + 1)$ by amortizing over longer batches of the string.

Solution (batching). For Y defined on $[n]$ equal to i with probability q_i, define the random variable $\mathsf{Y}^{(k)}$ on $[n]^k$ equal to the string $i_1 \cdots i_k$ with probability $q_{i_1} \cdots q_{i_k}$. That is, $\mathsf{Y}^{(k)}$ models k independent samples of Y.

Apply the Shannon–Fano code to $\mathsf{Y}^{(k)}$ to get an encoding of $[n]^k$ as bitstrings of expected length ℓ

satisfying $H(\mathsf{Y}^{(k)}) \le \ell \le H(\mathsf{Y}^{(k)}) + 1$.

$$
\begin{aligned}
H(\mathsf{Y}^{(k)}) &= \mathop{\mathbb{E}}_{i_1 \cdots i_k \sim \mathsf{Y}^{(k)}} \left[\log_2 \frac{1}{q_{i_1} \cdots q_{i_k}} \right] && \text{(by def'n)} \\
&= \mathop{\mathbb{E}}_{i_1 \cdots i_k \sim \mathsf{Y}^{(k)}} \left[\log_2 \frac{1}{q_{i_1}} + \cdots + \log_2 \frac{1}{q_{i_k}} \right] && \text{(log rules)} \\
&= \sum_{j=1}^k \mathop{\mathbb{E}}_{i_1 \cdots i_k \sim \mathsf{Y}^{(k)}} \left[\log_2 \frac{1}{q_{i_j}} \right] && \text{(linearity of expectation)} \\
&= \sum_{j=1}^k \mathop{\mathbb{E}}_{i \sim \mathsf{Y}} \left[\log_2 \frac{1}{q_i} \right] && (q_{i_j} \text{ only depends on one character}) \\
&= kH(\mathsf{Y}) && \text{(by def'n, no } j\text{-dependence in sum)}
\end{aligned}
$$

For every k symbols, we use ℓ bits, i.e., $\frac{\ell}{k}$ bits per symbol. From the Shannon–Faro bound, we have

$$
\frac{H(\mathsf{Y}^{(k)})}{k} \le \frac{\ell}{k} < \frac{H(\mathsf{Y}^{(k)})}{k} + \frac{1}{k}
$$

$$
H(\mathsf{Y}) \le \frac{\ell}{k} < H(\mathsf{Y}) + \frac{1}{k}
$$

Then, we have a code for Y bounded by $[H(\mathsf{Y}), H(\mathsf{Y}) + \frac{1}{k})$.

Taking a limit of some sort, we can say that we need $H(\mathsf{Y}) + o(1)$ bits. $\qquad\square$

> **Definition 1.3.6** (relative entropy)
>
> Given two discrete distributions $p = (p_i)$ and $q = (q_i)$, the relative entropy
>
> $$
> D(p \parallel q) := \sum p_i \log_2 \frac{1}{q_i} - \sum_i p_i \log_2 \frac{1}{p_i} = \sum p_i \log_2 \frac{p_i}{q_i}
> $$
>
> This is also known as the KL divergence.

The KL divergence works vaguely like a "distance" between distributions. (In particular, KL divergence is not a metric since it lacks symmetry and does not follow the triangle inequality, but it can act sorta like a generalized squared distance.)

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May 15

> **Fact 1.3.7.** $D(p \parallel q) \ge 0$ with equality exactly when $p = q$.

Proof. Observe that

$$
-D(p \parallel q) = \sum_i p_i \left(-\log_2 \frac{p_i}{q_i} \right) = \sum_i p_i \log_2 \frac{q_i}{p_i}
$$

and then define $\mathsf{X}' = \frac{q_i}{p_i}$ with probability p_i. By construction, we get

$$
-D(p \parallel q) = \mathbb{E}[\log_2 \mathsf{X}'] \le \log_2(\mathbb{E}[\mathsf{X}'])
$$

by Jensen's inequality (as $f = \log_2$ is concave). Finally,

$$
D(p \parallel q) \ge -\log_2(\mathbb{E}[\mathsf{X}']) = \log_2 \left(\sum_i p_i \frac{q_i}{p_i} \right) = \log_2 1 = 0 \qquad\square
$$

> **Proposition 1.3.8**
>
> Any prefix-free code has an expected length at least $H(\mathsf{X})$.

Proof. Let $\mathsf{X} \sim (p_i)$. Suppose C is a prefix-free code with codeword lengths ℓ_i.

Then, by Kraft's inequality, $\sum_i 2^{-\ell_i} \leq 1$. We want to show that $\sum_i p_i \ell_i \geq H(\mathsf{X})$, and we will prove this by showing that $\sum_i p_i \ell_i - H(\mathsf{X}) = D(p \parallel q)$ for some distribution q (then apply fact 1.3.7).

We will take q to be the random walk distribution corresponding to the binary tree associated to the candidate prefix-free code.

Let T be the binary tree associated to C. Consider the process of randomly going left/right at each node and stopping when either falling off the tree or hitting a leaf.

Let $q_i = 2^{-\ell_i}$ be the probability that this random walk reaches the leaf for the symbol i and let $q_{n+1} = 1 - \sum_i 2^{-\ell_i}$ be the probability that the random walk falls off the tree. Also, to keep ranges identical, let $\tilde{p}_i = p_i$ and $\tilde{p}_{n+1} = 0$. Now,

$$
\begin{aligned}
D(\tilde{p} \parallel q_C) &= \sum_{i=1}^{n+1} \tilde{p}_i \log_2 q_i^{-1} - \sum_{i=1}^{n+1} \tilde{p}_i \log_2 \frac{1}{p_i} \\
&= \sum_{i=1}^{n} p_i \log_2 2^{\ell_i} - \sum_{i=1}^{n} p_i \log_2 \frac{1}{p_i} && (\tilde{p}_{n+1} = 0) \\
&= \sum_{i=1}^{n} p_i \ell_i - H(\mathsf{X})
\end{aligned}
$$

Therefore, by fact 1.3.7, $\sum_i p_i \ell_i \geq H(\mathsf{X})$. $\qquad \square$

This proof technique generalizes. Recall the distinction between UDCs and prefix-free codes:

> **Definition 1.3.2**
>
> Let $C : \Sigma \to (\Sigma')^*$ be a code. We say C is a <u>uniquely decodable</u> code (UDC) if there does not exist a collision $x, y \in \Sigma^*$, with identical encoding $C(x_1)C(x_2)\cdots C(x_k) = C(y_1)C(y_2)\cdots C(y_{k'})$.
>
> Also, C is <u>prefix-free</u> (sometimes called <u>instantaneous</u>) if for any distinct $x, y \in \Sigma$, $C(x)$ is not a prefix of $C(y)$.

> **Example 1.3.9.** The code $C(1, 2, 3, 4) = (10, 00, 11, 110)$ is a uniquely decodable code.
>
> The code $C'(1, 2, 3, 4) = (0, 10, 110, 111)$ is a prefix-free code.

> **Remark 1.3.10.** A natural additional requirement for unique decodability is that for any $k \in \mathbb{N}$, $x \in [n]^k$, $y \in [n]^k$, $C(x) \neq C(y)$.

> **Theorem 1.3.11**
>
> For any uniquely decodable code $C : [n] \to \{0,1\}^*$ of codeword lengths ℓ_i, there is also a prefix-free code $C' : [n] \to \{0,1\}^*$ of lengths ℓ_i.

We will show that for any UDC C, the lengths $\sum_i 2^{-\ell_i} \leq 1$. Then, Kraft's inequality applies and we have a prefix-free code C'.

Partition the code's codomain $C([n]) = C_1 \cup C_2 \cup C_3 \cup \cdots$ by the length of the codeword $C_j \subseteq \{0,1\}^j$. We must instead show $\sum_j \frac{|C_i|}{2^j} \leq 1$.

Consider the easy case $C([n]) = C_2 \cup C_3$. If there are no collisions of length 5, we have

$$2 \cdot |C_2| \cdot |C_3| \leq 2^5$$

because every string in $\{xy : x \in C_2, y \in C_3\} \cup \{yx : x \in C_2, y \in C_3\}$ is unique in $\{0,1\}^5$. That is, $|C_2| \cdot |C_3| \leq 2^4$.

Likewise, if there are no collisions of length $5k$, we get

$$\frac{(2k)!}{k! \cdot k!} \cdot |C_2|^k \cdot |C_3|^k \leq 2^{5k}$$

because the union $\bigcup_{\substack{\alpha \in \{2,3\}^{2k}, \\ \alpha_i = 2 \text{ for} \\ k \text{ choices of } i}} C_{\alpha_i}$ consists of only unique strings.

In the limit, by Sterling's approximation,

$$\frac{2^{2k}}{\sqrt{k}} \cdot |C_2|^k \cdot |C_3|^k \leq 2^{5k}$$

$$|C_2| \cdot |C_3| \leq \frac{2^5}{2^2} (\sqrt{k})^{1/k} \approx 1 + \mathcal{O}(\log k/k)$$

I have no idea where this was going.

Proof. Fix a $k \geq 1$. Let $\ell_{max} = \max \ell_i$. Write $C^{(k)}$ to be the set of encoded k-length strings.

Consider the distribution: sample a length m uniformly from the set $[k \cdot \ell_{max}]$. Also, sample a uniformly random string $s \in \{0,1\}^m$. For each $x \in C^{(k)}$, let E_x be the event where $s = x$.

Now, we can write

$$\sum_{x \in C^{(k)}} \Pr[E_x] \leq 1$$

because the events E_x are mutually exclusive. Then,

$$\sum_{x \in C^{(k)}} \frac{1}{k \cdot \ell_{max}} \cdot \frac{1}{2^{\ell(x)}} \leq 1$$

$$\sum_{x \in C^{(k)}} \frac{1}{2^{\ell(x)}} \leq k \cdot \ell_{max}$$

where $\ell(x)$ is the length of x. Since summing over each codeword $x \in C$ is the same as summing

over each codeword ℓ_i,

$$
\begin{aligned}
\left(\sum_i \frac{1}{2^{\ell_i}}\right)^k &= \left(\sum_{x \in C} \frac{1}{2^{\ell(x)}}\right)^k \\
&= \sum_{x_1, \ldots, x_k \in C} \frac{1}{2^{\ell(x_1)}} \cdot \frac{1}{2^{\ell(x_2)}} \cdots \frac{1}{2^{\ell(x_k)}} \\
&= \sum_{x_1, \ldots, x_k \in C} \frac{1}{2^{\ell(x_1)+\ell(x_2)+\cdots+\ell(x_k)}} \\
&= \sum_{x_1, \ldots, x_k \in C} \frac{1}{2^{\ell(x_1 x_2 \cdots x_k)}} \\
&= \sum_{x \in C^{(k)}} \frac{1}{2^{\ell(x)}}
\end{aligned}
$$

where we can take the last step by uniquely decoding $x_1 x_2 \cdots x_k$ into x. Combining,

$$
\begin{aligned}
\left(\sum_i \frac{1}{2^{\ell_i}}\right)^k &\leq k \cdot \ell_{max} \\
\sum_i \frac{1}{2^{\ell_i}} &\leq (k \cdot \ell_{max})^{\frac{1}{k}} \\
&\leq 1 + \mathcal{O}\left(\frac{\ell_{max} \cdot \log_2 k}{k}\right)
\end{aligned}
$$

which tends to 1 as $k \to \infty$, as desired. $\square$

Chapter 2

Applications of KL divergence

> **Notation.** Write $H(p)$ to denote $H(\mathsf{X})$ for $\mathsf{X} \sim \text{Bernoulli}(p)$.
>
> That is, $H(p) = p \log_2 \frac{1}{p} + (1-p) \log_2 \frac{1}{1-p}$.
>
> Likewise, write $D(q \parallel p)$ to be $D(\mathsf{Y} \parallel \mathsf{X})$ where $\mathsf{Y} \sim \text{Bernoulli}(q)$.

Recall Sterling's approximation (which we have used before):

> **Theorem 2.0.1** (Sterling's approximation)
> $m!$ behaves like $\sqrt{2\pi m} \left(\frac{m}{e}\right)^m \left(1 + \mathcal{O}\left(\frac{1}{m}\right)\right)$

2.1 The boolean k-slice

Consider the boolean k-slice (also known as the Hamming k-slice) of the hypercube $\{0,1\}^n$ defined by

$$B_k := \{x \in \{0,1\}^n : x \text{ has exactly } k \text{ ones}\}$$

> **Remark 2.1.1.**
> $$|B_k| \approx 2^{H\left(\frac{k}{n}\right) \cdot n}$$

Proof. By Sterling's approximation, knowing that $|B_k| = \binom{n}{k}$:

$$|B_k| = \binom{n}{k}$$

$$= \frac{n!}{n!(n-k)!}$$

$$\approx \frac{\sqrt{2\pi n}\left(\frac{n}{e}\right)^n}{\sqrt{2\pi k}\left(\frac{k}{e}\right)^k \sqrt{2\pi(n-k)}\left(\frac{n-k}{e}\right)^{n-k}}$$

$$= \sqrt{\frac{n}{2\pi k(n-k)}} \cdot \frac{n^k \left(\frac{n}{n-k}\right)^{n-k}}{k^k}$$

Now, notice that $\left(\frac{n}{n-k}\right)^{n-k} = \left(1 + \frac{k}{n-k}\right)^{n-k} \approx e^k$ for $k \ll n-k$ because $1 + x \approx e^x$ for small x. Then, $\left(1 + \frac{k}{n-k}\right)^{n-k} \approx \left(e^{k/(n-k)}\right)^{n-k} = e^k$ and

$$|B_k| \approx \left(\frac{ne}{k}\right)^k \tag{2.1}$$

$$= 2^{k \log_2 \frac{ne}{k}}$$

$$= 2^{k \log_2 \frac{n}{k} + k \log_2 e}$$

$$= 2^{\left(\frac{k}{n} \log_2 \frac{n}{k}\right)n + k \log_2 e}$$

$$\approx 2^{\left(\frac{k}{n} \log_2 \frac{n}{k}\right)n}$$

for $1 \ll k \ll n$. Then, given that same assumption,

$$H\left(\frac{k}{n}\right) = \frac{k}{n} \log_2 \frac{n}{k} + \left(1 - \frac{k}{n}\right)\log_2 \frac{1}{1 - \frac{k}{n}} \quad{}^{\nearrow 0}$$

$$\approx \frac{k}{n} \log_2 \frac{n}{k}$$

because if $n \gg k$, $\frac{k}{n} \to 0$ and $1 \log_2 1 = 0$. Combining these approximations yields

$$|B_k| \approx 2^{H\left(\frac{k}{n}\right)n} \qquad\qquad \square$$

Let X be a uniformly chosen point in B_k and $\mathsf{X}_1, \ldots, \mathsf{X}_n \sim \text{Bernoulli}(\frac{k}{n})$.

This means that $H(\mathsf{X}) \approx H((\mathsf{X}_1, \ldots, \mathsf{X}_n))$, which is remarkable because the latter could produce points in B_k or points with n ones or points with no ones.

This seems to imply that the majority of the mass of $(\mathsf{X}_1, \ldots, \mathsf{X}_n)$ lies within the boolean k-slice. Formally, we make the following claim about the <u>concentration of measure</u>:[1]

---

[1] cf. Dvoretzky–Milman theorem

> **Proposition 2.1.2**
>
> Fix any $\varepsilon > 0$. The probability
>
> $$\Pr\left[(\mathsf{X}_1, \dots, \mathsf{X}_n) \notin \bigcup_{\ell=(1-\varepsilon k)}^{(i+\varepsilon)k} B_\ell\right] = \frac{1}{2^{n/\varepsilon^2}}$$
>
> Informally, the probability of the randomly-drawn vector lying outside of the boolean k-slice is exponentially small.

We will prove a stronger claim:

> **Claim 2.1.3.** Fix any $p \in (0, 1)$ and consider any $q > p$. Then,
>
> $$\Pr[w((\mathsf{X}_i)) > q \cdot n] \leq 2^{-D(q\|p)\cdot n}$$
>
> where $w((\mathsf{X}_i))$ is the number of ones. Likewise, consider any $q < p$. Then,
>
> $$\Pr[w((\mathsf{X}_i)) < q \cdot n] \leq 2^{-D(q\|p)\cdot n}$$

Consider a toy example first. Let X be the number of heads after n fair coin tosses. Then, $\mathbb{E}[\mathsf{X}] = \frac{n}{2}$ and

$$\Pr[\mathsf{X} \geq 0.51n] = \frac{1}{2^n} \sum_{k \geq 0.51n}^{n} \binom{n}{k} \approx \frac{1}{2^n} \sum_{k \geq 0.51n}^{n} \left(\frac{ne}{k}\right)^k \to 0 \text{ very quickly}$$

by the same magic that we did in eq. (2.1) and because $\frac{1}{2^n}$ goes to 0 very quickly.

Now we can prove the claim.

Proof. Let $\theta_p(x)$ denote the probability of sampling a vector $x \in \{0, 1\}^n$ where each bit is IID Bernoulli(p). Then,

$$\frac{\theta_p(x)}{\theta_q(x)} = \frac{p^k(1-p)^k}{q^k(1-q)^k}$$

$$= \frac{(1-p)^n}{(1-q)^n}\left(\frac{\frac{p}{1-p}}{\frac{q}{1-q}}\right)^k$$

$$\leq \frac{(1-p)^n}{(1-q)^n}\left(\frac{\frac{p}{1-p}}{\frac{q}{1-q}}\right)^{qn}$$

for any $k \geq qn$ because (1) if $q \geq p$, then $\frac{q}{1-q} \geq \frac{p}{1-p}$ and the ugly fraction is greater than 1 and (2) increasing the exponent increases the quantity if the base is greater than 1.

Let $B_{\geq k} := \bigcup_{\ell \geq k} B_\ell$. Then, for all $x \in B_{\geq qn}$, we must show that

$$\theta_p(x) \leq \frac{(1-p)^n}{(1-q)^n}\left(\frac{\frac{p}{1-p}}{\frac{q}{1-q}}\right)^{qn} \cdot \theta_q(x) = 2^{-nD(q\|p)\cdot\theta_q(x)}$$

Consider the right-hand expression:

$$2^{n \cdot D(q\|p)} = 2^{n \cdot (q \log_2 \frac{1}{p} + (1-q) \log_2 \frac{1}{1-p} - q \log_2 \frac{1}{q} - (1-q) \log_2 \frac{1}{1-q})}$$

$$= \left(\frac{1}{p^q} \cdot \frac{1}{(1-p)^{1-q}} \cdot q^q \cdot (1-q)^{1-q} \right)^n$$

and the left-hand expression:

$$\frac{(1-p)^n}{(1-q)^n} \left(\frac{\frac{p}{1-p}}{\frac{q}{1-q}} \right)^{qn} = \left(\frac{(1-p)^{1-q} p^q}{(1-q)^{1-q} q^q} \right)^n$$

$$= \left(p^q \cdot (1-p)^{1-q} \cdot \frac{1}{q^q} \cdot \frac{1}{(1-q)^{1-q}} \right)^n$$

which is clearly the reciprocal of the right-hand expression.

Now, we know that $\theta_p(x) = 2^{-nD(q\|p)} \theta_q(x)$, so

$$\Pr_{X_1, \ldots, X_n \sim \text{Bernoulli}(p)} [(X_1, \ldots, X_n) \in B_{\geq qn}]$$

$$= \sum_{x \in B_{\geq qn}} \theta_p(x)$$

$$\leq 2^{-nD(q\|p)} \sum_{x \in B_{\geq qn}} \theta_q(x)$$

$$\leq 2^{-nD(q\|p)}$$

since the sum of the probabilities of x being any given entry in $B_{\geq qn}$ must be at most 1. $\square$

2.2 Rejection sampling

The KL divergence can give us a metric of how accurately we can sample one distribution using another distribution.

Example 2.2.1. Suppose $X = \begin{cases} 0 & p = \frac{1}{2} \\ 1 & p = \frac{1}{2} \end{cases}$ and $Y = \begin{cases} 0 & p = \frac{1}{4} \\ 1 & p = \frac{3}{4} \end{cases}$.

How can we sample Y using X?

Solution (naive). Take IID X_1 and X_2. Return 0 if $x_1 = x_2 = 0$ and 1 otherwise. $\square$

Solution (fancy). Take an infinite IID queue $X_1, X_2, \ldots$

Starting at $i = 1$, if $X_i = 0$, then output 0 with probability $\frac{1}{2}$, otherwise increment i until $X_i = 1$. $\square$

———— *↓ Lecture 6 adapted from Arthur ↓* ————

Lecture 6
May 22

Problem 2.2.2 (rejection sampling)

Given access to a distribution $Q = (Q(x))_{x \in \mathcal{X}}$, how efficiently can you simulate $P = (P(x))_{x \in \mathcal{X}}$?

Example 2.2.3. Suppose $Q = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$ and $P = (\frac{1}{2}, \frac{1}{2})$. We want to obtain the P distribution from Q.

Solution. Since Q and P are both uniform, we can just keep sampling from Q until we get something in P. That is, for $i = 1, \dots, \infty$:

1. Sample $\mathsf{X}_i \sim Q$.

2. If $\mathsf{X}_i \in \{1, 2\}$, accept and output $\mathsf{Y} \leftarrow \mathsf{X}_i$.

3. Otherwise, $i \leftarrow i + 1$.

This works because

$$\Pr[\mathsf{Y} = 1] = \Pr[\mathsf{X}_i = 1 \mid \mathsf{X}_i = 1 \vee \mathsf{X}_i = 2] = \frac{1/3}{2/3} = \frac{1}{2}$$

for the final round i, and similarly for $\mathsf{Y} = 2$. $\qquad\square$

Example 2.2.4. Consider a slightly more complex distribution $P = (\frac{1}{3}, \frac{2}{3})$ and $Q = (\frac{1}{2}, \frac{1}{2})$.

Solution. We will create a more complex rejection sampling protocol with some cheating.

Again, iterate and draw independent X_i:

- If $\mathsf{X}_1 = 1$, accept with probability $\frac{2}{3}$. Otherwise, reject and continue to X_2 with probability $\frac{1}{3}$.

- If $\mathsf{X}_1 = 2$, accept.

- For $i \geq 2$, accept if $\mathsf{X}_i = 1$ and reject if $\mathsf{X}_i = 2$.

Then, the probability of accepting $\mathsf{X}_1 = 1$ is $\frac{1}{3}$, $\mathsf{X}_1 = 2$ is $\frac{1}{2}$, and rejecting X_1 is $\frac{1}{6}$.

Since later rounds only output 1, we output 1 with probability $\frac{1}{3} + \frac{1}{6} = \frac{1}{2}$ and 2 with probability $\frac{1}{2}$. $\qquad\square$

Definition 2.2.5 (rejection sampler)

A <u>rejection sampler</u> is a procedure that reads sequentially independent random samples $\mathsf{X}_i \sim Q$ and in each round i either

- accepts the value of X_i and terminates with an index i^*, or
- rejects and continues.

The iteration we terminated on i^* is a random variable since it is a function of other random variables. It satisfies $\mathsf{X}_{i^*} \sim P$, which is weird since for all fixed i, $\mathsf{X}_i \sim Q$.

An interesting application is communication complexity. Suppose Alice has some hidden distribution P. Alice and Bob have access to a shared random IID sequence $\mathsf{X}_i \sim Q$.

Alice can send an encoding of i^* to Bob who outputs $\mathsf{X}_{i^*} \sim P$. This encoding i^* can be encoded using $\log i^*$ bits.

We will show that $\mathbb{E}[\log i^*] \leq D(P \parallel Q) + \mathcal{O}(1)$. You can also show that $D(P \parallel Q) \leq \mathbb{E}[\log i*]$.

For each round i and symbol x, we need to know whether x was sampled before round i, i.e., the probability assigned to x in previous rounds.

For round $i \geq 1$, define:

- $\alpha_i(x)$ to denote the probability that the procedure accepts X_i and that $\mathsf{X}_i = x$
- $p_i(x)$ to denote the probability that the procedure halts at round $i^* \leq i$ and $\mathsf{X}_{i^*} = x$

We want to construct our procedure such that

- for all x, $P(x) = \sum_{i=1}^{n} \alpha_i(x)$
- for all x and i, $p_i(x) = \sum_{k=1}^{i} \alpha_k(x)$
- the probability that we halt on or before round i is $p_i^* := \sum_{x \in \mathcal{X}} p_i(x)$

$$\text{------} \uparrow \textit{Lecture 6 adapted from Arthur} \uparrow \text{------}$$

Algorithm 1 REJECTIONSAMPLING(P, Q)

Require: $\forall x \in \mathcal{X}, Q(x) > 0 \iff D(P \parallel Q) < \infty$
1: **for** $x \in \mathcal{X}$ **do** $p_0(x) \leftarrow 0$
2: $p_0^* \leftarrow 0$
3: **for** $i = 1, \dots, \infty$ **do**
4:     sample $\mathsf{X}_i \sim Q$
5:     **if** $P(\mathsf{X}_i) - P_{i-1}(\mathsf{X}_i) \leq (1 - p_{i-1}^*) \cdot Q(\mathsf{X}_i)$ **then**
6:         **with probability** $\beta_i(\mathsf{X}_i) = \frac{P(\mathsf{X}_i) - p_{i-1}(\mathsf{X}_i)}{(1 - p_{i-1}^*)(Q(\mathsf{X}_i))}$ **do**
7:              $\triangleright$ *so that the net probability of sampling X_i will be $\alpha_i(\mathsf{X}_i) = P(\mathsf{X}_i) - p_{i-1}(\mathsf{X}_i)$* $\triangleleft$
8:             **return** X_i
9:     **else**
10:         **with probability** $\beta_i(\mathsf{X}_i) = 1$ **do**
11:              $\triangleright$ *so that the net probability of sampling X_i is $\alpha_i(1 - p_{i-1}^*) \cdot Q(\mathsf{X}_i)$* $\triangleleft$
12:             **return** X_i

In this case, for all x and for all i:

- the probability of accepting x in round i is $\alpha_i(x) = \min\{P(x) - p_{i-1}(x), (1 - p_{i-1}^*)Q(x)\}$
- the probability of accepting x on or before round i is $p_i(x) = p_{i-1}(x) + \alpha_i(x)$
- the probability of terminating on or before round i is $p_i^* = p_{i-1}^* + \sum_{x \in \mathcal{X}} \alpha_i(x) = \sum_{x \in \mathcal{X}} p_i(x)$

Example 2.2.6. Let $P = (\frac{1}{2}, \frac{3}{8}, \frac{1}{8})$ and $Q = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$. Do the procedure.

Solution. In round 1, sample $\mathsf{X}_1 \sim Q$.

- If $\mathsf{X}_1 = 1$, accept with probability 1.
- If $\mathsf{X}_1 = 2$, accept with probability 1.
- If $\mathsf{X}_1 = 3$, accept with probability $\frac{3}{8}$.

Then, $p_1(1) = \frac{1}{3}$, $p_1(2) = \frac{1}{3}$, $p_1(3) = \frac{1}{8}$, and $p_1^* = \frac{19}{24}$.

In round 2, sample $X_2 \sim Q$.

- If $X_2 = 1$, accept with probability 1. There is a $\frac{5}{72}$ chance of getting here, but deficit probability is $\frac{1}{6}$, so no need to reduce.
- If $X_2 = 2$, accept with probability $\frac{3}{5}$. There is a $\frac{5}{72}$ chance of getting here and deficit probability is $\frac{3}{8} - \frac{1}{3} = \frac{1}{24}$. For equality, use probability $\frac{3}{5} \cdot \frac{5}{72} = \frac{1}{24}$.
- If $X_3 = 3$, accept with probability 0. We already fulfilled $P(3) = p_1(3)$.

Then, $p_2(1) = \frac{29}{72}$, $p_2(2) = \frac{3}{8}$, $p_3(2) = \frac{1}{8}$, and $p_2^* = \frac{19}{24} + \frac{5}{24} \cdot (\frac{1}{3} + \frac{3/5}{5}) = \frac{65}{72}$.

In round 3, sample $X_3 \sim Q$.

- If $X_3 = 1$, accept with probability 1.
- If $X_3 = 2$ or 3, accept with probability 0.

Keep repeating until we accept a 1.   □

Proposition 2.2.7

$(p_i(x))_{x \in \mathcal{X}}$ converges to $P(x)$ as $i \to \infty$. In fact, the residual decays exponentially fast

$$P(x) - p_i(x) \le P(x) \cdot (1 - Q(x))^i.$$

Proof. Begin with the claim that the probability of reaching round i is at least the residual at i for any x:

$$1 - p_{i-1}^* \ge P(x) - p_{i-1}(x) \quad \forall x$$

Intuitively, either you returned prior to round i (i.e., p_{i-1}^*) or you did not (i.e., the residual).

$$
\begin{aligned}
1 - p_{i-1}^* &= \sum_{x \in \mathcal{X}} P(x) - \sum_{x \in \mathcal{X}} p_{i-1}(x) \\
&= \sum_{x \in \mathcal{X}} (P(x) - p_{i-1}(x)) \tag{2.2}
\end{aligned}
$$

Also, claim that

$$\alpha_i \ge (P(x) - p_{i-1}(x)) \cdot Q(x) \tag{2.3}$$

If $\alpha_i = P(x) - p_{i-1}(x)$, then clearly $\alpha_i \ge \alpha_i Q(x)$. Otherwise, if $\alpha_i = (1 - p_{i-1}^*)Q(x)$, then eq. (2.2) applies.

Proceed by induction.

Base case: exercise.

Inductive step: suppose that $P(x) - p_i(x) \le P(x) \cdot (1 - Q(x))^i$. Then,

$$
\begin{aligned}
P(x) - p_{i+1}(x) &= P(x) - p_i(x) - \alpha_{i+1}(x) \\
&\le (P(x) - p_{i-1}(x))(1 - Q(x)) &&\text{(by eq. (2.3))} \\
&\le (P(x) \cdot (1 - Q(x))^i)(1 - Q(x)) &&\text{(by supposition)} \\
&\le P(x) \cdot (1 - Q(x))^{i+1} &&\square
\end{aligned}
$$

Now, we will prove that this is related to relative entropy.

> **Proposition 2.2.8**
>
> Let i^* be the iteration at which the procedure returns. Then, $\mathbb{E}[\log_2 i^*] \leq D(P \parallel Q) + 2\log_2 e$.

Proof. First, claim that for all $x \in \mathcal{X}$ and any $i \geq 2$ such that $\alpha_i(x) > 0$,

$$i \leq \frac{P(x)}{(1 - p^*_{i-1}) \cdot Q(x)} + 1 \tag{2.4}$$

That is, if we reach a particular round i, the probability mass left must be sufficiently large.

We know that $P(x) \geq p_{i-1}(x)$ since we increase to $P(x)$. Then,

$$
\begin{aligned}
P(x) &\geq p_{i-1}(x) \\
&= \alpha_1(x) + \cdots + \alpha_{i-1}(x) \\
&\geq (1 - p^*_1) \cdot Q(x) + \cdots + (1 - p_{i-1}) \cdot Q(x) \\
&\geq (1 - p^*_{i-1}) \cdot Q(x) + \cdots + (1 - p_{i-1}) \cdot Q(x) \\
&= (i - 1)(1 - p^*_{i-1}) \cdot Q(x) \\
i &\leq \frac{P(x)}{(1 - p^*_{i-1}) \cdot Q(x)} + 1
\end{aligned}
$$

as long as $\alpha_{j-1} < \alpha_j$ for all j.

Do a gigantic algebra bash:

$$
\begin{aligned}
\mathbb{E}[\log_2 i^*] &= \sum_{i=1}^{\infty} (p^*_i - p^*_{i-1}) \cdot \log_2 i \\
&= \sum_{i=1}^{\infty} \sum_{x \in \mathcal{X}} \alpha_i(x) \cdot \log_2 i \\
&\leq \sum_{i=1}^{\infty} \sum_{x \in \mathcal{X}} \alpha_i(x) \cdot \log_2 \left[\frac{P(x)}{(1 - p^*_{i-1})Q(x)} + 1 \right] &&\text{(by eq. (2.4))} \\
&\leq \sum_{i=1}^{\infty} \sum_{x \in \mathcal{X}} \alpha_i(x) \cdot \log_2 \left[\frac{1}{(1 - p^*_{i-1})} \left(\frac{P(x)}{Q(x)} + 1 \right) \right] \\
&= \underbrace{\sum_{i=1}^{\infty} \sum_{x \in \mathcal{X}} \alpha_i(x) \log_2 \frac{1}{(1 - p^*_{i-1})}}_{A} + \underbrace{\sum_{i=1}^{\infty} \sum_{x \in \mathcal{X}} \alpha_i(x) \log_2 \left(\frac{P(x)}{Q(x)} + 1 \right)}_{B}
\end{aligned}
$$

Consider the first term A:

$$
\begin{aligned}
A &= \sum_{i=1}^{\infty} \sum_{x \in \mathcal{X}} \alpha_i(x) \log_2 \frac{1}{(1 - p^*_{i-1})} \\
&= \sum_{i=1}^{\infty} (p^*_i - p^*_{i-1}) \log_2 \frac{1}{(1 - p^*_{i-1})}
\end{aligned}
$$

Notice that this is a left-handed Riemann sum of $\log_2 \frac{1}{1-x}$:

$$
\begin{aligned}
A &\leq \int_0^1 \log_2 \frac{1}{1-x} \, dx \\
&= \log_2 e
\end{aligned}
$$

Now, consider the second term B:

$$
\begin{aligned}
B &= \sum_{i=1}^{\infty} \sum_{x \in \mathcal{X}} \alpha_i(x) \log_2 \left(\frac{P(x)}{Q(x)} + 1 \right) \\
&= \sum_{x \in \mathcal{X}} \sum_{i=1}^{\infty} \alpha_i(x) \log_2 \left(\frac{P(x)}{Q(x)} + 1 \right) && \text{(Fubini?)} \\
&= \sum_{x \in \mathcal{X}} P(x) \log_2 \left(\frac{P(x)}{Q(x)} + 1 \right) && \left(P(x) = \textstyle\sum_i \alpha_i(x) \right) \\
&= \sum_{x \in \mathcal{X}} P(x) \log_2 \left(\frac{P(x)}{Q(x)} \cdot \left(1 + \frac{Q(x)}{P(x)} \right) \right) \\
&= \sum_{x \in \mathcal{X}} P(x) \log_2 \left(\frac{P(x)}{Q(x)} \right) + \sum_{x \in \mathcal{X}} P(x) \log_2 \left(1 + \frac{Q(x)}{P(x)} \right) \\
&= D(P \parallel Q) + \sum_{x \in \mathcal{X}} P(x) \log_2 \left(1 + \frac{Q(x)}{P(x)} \right) \\
&\leq D(P \parallel Q) + \sum_{x \in \mathcal{X}} P(x) \log_2 \left(e^{Q(x)/P(x)} \right) && \left(1 + x \leq e^x \text{ for all } x \geq 0 \right) \\
&= D(P \parallel Q) + \sum_{x \in \mathcal{X}} P(x) \frac{Q(x)}{P(x)} \log_2 e \\
&= D(P \parallel Q) + \log_2 e \sum_{x \in \mathcal{X}} Q(x) \\
&= D(P \parallel Q) + \log_2 e
\end{aligned}
$$

Therefore,
$$
\mathbb{E}[\log_2 i^*] \leq A + B \leq D(P \parallel Q) + 2 \log_2 e
$$

completing the proof. $\qquad\square$

Intuition: for any $x \in \mathcal{X}$, if $\alpha_i(x) \leq Q(x) \lll P(x)$, then you need an expected amount of $\frac{P(x)}{Q(x)}$ steps to succeed, because you just won't roll x that often.

Also, if $\alpha_{i+1}(x) > 0$ (any round prior to termination), $(1 - p^*_{i-1}(x))Q(x) \leq \alpha_i(x)$.

> **Proposition 2.2.9**
>
> For any rejection sampler, let i^* be the index where it returns. Then,
> $$
> \mathbb{E}[\ell(i^*)] \geq D(P \parallel Q)
> $$

Proof. For convenience, redefine $\alpha_i(x) := \Pr[i^* = i \wedge \mathsf{X}_i = x]$.

First, observe that for any $x \in \mathcal{X}$, a rejection sampler must have

$$
\alpha_i(x) \leq Q(x)
$$

because we only have a $Q(x)$ chance of rolling x to accept it in round i.

Now, fix $x \in \mathcal{X}$. Consider the random variable $i^*|_{\mathsf{X}_{i^*}=x}$. Then, by Kraft's inequality,

$$
\begin{aligned}
\mathbb{E}[\ell(i^*) \mid \mathsf{X}_{i^*} = x] &\geq H(i^* \mid \mathsf{X}_{i^*} = x) \\
&= \sum_{i=1}^{\infty} \Pr[i^* = i \mid \mathsf{X}_{i^*} = x] \log_2 \frac{1}{\Pr[i^* = i \mid \mathsf{X}_{i^*} = x]} \\
&= \sum_{i=1}^{\infty} \frac{\alpha_i(x)}{P(x)} \log_2 \frac{P(x)}{\alpha_i(x)} \\
&\geq \sum_{i=1}^{\infty} \frac{\alpha_i(x)}{P(x)} \log_2 \frac{P(x)}{Q(x)} \\
&= \log_2 \frac{P(x)}{Q(x)} \cdot \sum_{i=1}^{\infty} \frac{\alpha_i(x)}{P(x)} \\
&= \log_2 \frac{P(x)}{Q(x)}
\end{aligned}
$$

because $\sum_{i=1}^{\infty} \alpha_i(x) = P(x)$. Apply the law of total probability:

$$
\begin{aligned}
\mathbb{E}[\ell(i^*)] &= \sum_{x \in \mathcal{X}} \Pr[\mathsf{X}_{i*} = x] \, \mathbb{E}[\ell(i^*) \mid \mathsf{X}_{i^*} = x] \\
&= \sum_{x \in \mathcal{X}} P(x) \, \mathbb{E}[\ell(i^*) \mid \mathsf{X}_{i^*} = x] \\
&\geq \sum_{x \in \mathcal{X}} P(x) \log_2 \frac{P(x)}{Q(x)} \\
&= D(P \parallel Q)
\end{aligned}
$$

as desired. $\qquad \square$

2.3 Mutual information and communication complexity

> **Notation.** Given two jointly distributed random variables (X, Y) over sample space $\mathcal{X} \times \mathcal{Y}$, write p_{xy} for $\Pr[\mathsf{X} = x, \mathsf{Y} = y]$.

Lecture 9
June 3

> **Definition 2.3.1**
>
> Given two jointly distributed random variables (X, Y) over sample space $\mathcal{X} \times \mathcal{Y}$, define the mutual information $I(\mathsf{X} : \mathsf{Y})$ by
>
> $$
> \begin{aligned}
> I(\mathsf{X} : \mathsf{Y}) &= H(\mathsf{X}) + H(\mathsf{Y}) - H((\mathsf{X}, \mathsf{Y})) \\
> &= H(\mathsf{X}) - H(\mathsf{X} \mid \mathsf{Y}) \\
> &= H(\mathsf{Y}) - H(\mathsf{Y} \mid \mathsf{X})
> \end{aligned}
> $$
>
> where the conditional entropy $H(\mathsf{X} \mid \mathsf{Y})$ is
>
> $$
> \sum_{y \in \mathcal{Y}} p_y \cdot H((\mathsf{X}|_{\mathsf{Y}=y}))
> $$

This is entirely analogous to saying that $|A \cap B| = |A| + |B| - |A \cup B| = |A| - |A \setminus B|$.

Theorem 2.3.2 (chain rule for entropy)

Given two jointly distributed random variables (X, Y) over a discrete sample space $\mathcal{X} \times \mathcal{Y}$,

$$H((\mathsf{X}, \mathsf{Y})) = H(\mathsf{X}) + H(\mathsf{Y} \mid \mathsf{X})$$

Proof. Do a bunch of algebra:

$$
\begin{aligned}
H(\mathsf{X}) + H(\mathsf{Y} \mid \mathsf{X}) &= \sum_{x \in \mathcal{X}} p_x \log \frac{1}{p_x} + \sum_{x \in \mathcal{X}} p_x \sum_{y \in \mathcal{Y}} \Pr[\mathsf{Y} = y \mid \mathsf{X} = x] \log \frac{1}{\Pr[\mathsf{Y} = y \mid \mathsf{X} = x]} \\
&= \sum_{x \in \mathcal{X}} p_x \log \frac{1}{p_x} + \sum_{x \in \mathcal{X}} \cancel{p_x} \sum_{y \in \mathcal{Y}} \frac{p_{xy}}{\cancel{p_x}} \log \frac{p_x}{p_{xy}} \\
&= \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{1}{p_x} + \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{p_x}{p_{xy}} \\
&= \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \left(\log \frac{1}{p_x} + \log \frac{p_x}{p_{xy}} \right) \\
&= \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{1}{p_{xy}} \\
&= H((\mathsf{X}, \mathsf{Y})) \qquad \square
\end{aligned}
$$

Corollary 2.3.3. For two independent variables, since $(\mathsf{Y} \mid \mathsf{X}) = \mathsf{Y}$, we have $H((\mathsf{X}, \mathsf{Y})) = H(\mathsf{X}) + H(\mathsf{Y})$ as expected.

Corollary 2.3.4. $H((\mathsf{X}_1, \mathsf{X}_2, \mathsf{X}_3)) = H(\mathsf{X}_1) + H(\mathsf{X}_2 \mid \mathsf{X}_1) + H(\mathsf{X}_3 \mid (\mathsf{X}_1, \mathsf{X}_2))$

Proof. Consider $(\mathsf{X}_1, \mathsf{X}_2, \mathsf{X}_3) = ((\mathsf{X}_1, \mathsf{X}_2), \mathsf{X}_3)$. Then, by the chain rule for entropy,

$$H(((\mathsf{X}_1, \mathsf{X}_2), \mathsf{X}_3)) = H((\mathsf{X}_1, \mathsf{X}_2)) + H(\mathsf{X}_3 \mid (\mathsf{X}_1, \mathsf{X}_2))$$

and then by another application,

$$H(((\mathsf{X}_1, \mathsf{X}_2), \mathsf{X}_3)) = H(\mathsf{X}_1) + H(\mathsf{X}_2 \mid \mathsf{X}_1) + H(\mathsf{X}_3 \mid (\mathsf{X}_1, \mathsf{X}_2))$$

as desired. $\qquad \square$

Theorem 2.3.5 (general chain rule for entropy)

For k random variables $\mathsf{X}_1, \dots, \mathsf{X}_k$,

$$H((\mathsf{X}_1, \dots, \mathsf{X}_k)) = \sum_{i=1}^{k} H(\mathsf{X}_i \mid (\mathsf{X}_1, \cdots, \mathsf{X}_{i-1}))$$

Proof. By induction on the chain rule for entropy. $\qquad \square$

Notation. Although relative entropy is defined only on *distributions*, write $D(\mathsf{X} \parallel \mathsf{Y})$ to be $D(f_{\mathsf{X}} \parallel f_{\mathsf{Y}})$.

Theorem 2.3.6 (chain rule for relative entropy)

Let $p(x, y)$ and $q(x, y)$ be distributions. Then,

$$D(p(x, y) \parallel q(x, y)) = D(p(x) \parallel q(x)) + D(p(y \mid x) \parallel q(y \mid x))$$

Equivalently, let $(\mathsf{X}_1, \mathsf{Y}_1)$ and $(\mathsf{X}_2, \mathsf{Y}_2)$ be two joint random variables. Then,

$$D((\mathsf{X}_1, \mathsf{Y}_1) \parallel (\mathsf{X}_2, \mathsf{Y}_2)) = D(\mathsf{X}_1 \parallel \mathsf{X}_2) + D(\mathsf{Y}_1|_{(\mathsf{X}_1, \mathsf{X}_2)} \parallel \mathsf{Y}_2|_{(\mathsf{X}_1, \mathsf{X}_2)})$$

Proof (for distributions). Do algebra:

$$
\begin{aligned}
&D(p(x) \parallel q(x)) + D(p(y \mid x) \parallel q(y \mid x)) \\
&= \sum_{x \in \mathcal{X}} p_x \log \frac{p_x}{q_x} + \sum_{x \in \mathcal{X}} p_x \sum_{y \in \mathcal{Y}} p(y \mid x) \log \frac{p(y \mid x)}{q(y \mid x)} \\
&= \sum_{x \in \mathcal{X}} p_x \log \frac{p_x}{q_x} + \sum_{x \in \mathcal{X}} p_x \sum_{y \in \mathcal{Y}} \frac{p_{xy}}{p_x} \log \frac{p_{xy} q_x}{q_{xy} p_x} \\
&= \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{p_x}{q_x} + \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{p_{xy} q_x}{q_{xy} p_x} \\
&= \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \left(\log \frac{p_x}{q_x} + \log \frac{p_{xy} q_x}{q_{xy} p_x} \right) \\
&= \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{p_{xy}}{q_{xy}} \\
&= D(p(x, y) \parallel q(x, y))
\end{aligned}
$$

as in the proof of chain rule for entropy.   □

Fact 2.3.7.
$$I[\mathsf{X} : \mathsf{Y}] = \mathop{\mathbb{E}}_{x \leftarrow \mathsf{X}}[D(\mathsf{Y}|_{\mathsf{X}=x} \parallel \mathsf{Y})] = \sum_{x \in \mathcal{X}} p_x D(\mathsf{Y}|_{\mathsf{X}=x} \parallel \mathsf{Y})$$

Proof. First, claim that
$$I[\mathsf{X} : \mathsf{Y}] = D((\mathsf{X}, \mathsf{Y}) \parallel \tilde{\mathsf{X}} \otimes \tilde{\mathsf{Y}}) \tag{2.5}$$
where $\tilde{\mathsf{X}} \otimes \tilde{\mathsf{Y}}$ denotes a random variable consisting of $\tilde{\mathsf{X}}$ (resp. $\tilde{\mathsf{Y}}$) independently sampled according

to the distribution of X (resp. Y) so that $\Pr\left[\tilde{\mathsf{X}} = x, \tilde{\mathsf{Y}} = y\right] = p_x p_y$. Expand the left-hand side:

$$
\begin{aligned}
I[\mathsf{X} : \mathsf{Y}] &= \sum_{x \in \mathcal{X}} p_x \log \frac{1}{p_x} + \sum_{y \in \mathcal{Y}} p_y \log \frac{1}{p_y} - \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{1}{p_{xy}} \\
&= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p_{xy} \log \frac{1}{p_x} + \sum_y \sum_x p_{xy} \log \frac{1}{p_y} - \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{1}{p_{xy}} \\
&= \sum_{x \in \mathcal{X}} \sum_{y \in \mathcal{Y}} p_{xy} \left(\log \frac{1}{p_x} + \log \frac{1}{p_y} - \log \frac{1}{p_{xy}} \right) \\
&= \sum_{\substack{x \in \mathcal{X} \\ y \in \mathcal{Y}}} p_{xy} \log \frac{p_{xy}}{p_x p_y} \\
&= D((\mathsf{X}, \mathsf{Y}) \parallel \tilde{\mathsf{X}} \otimes \tilde{\mathsf{Y}})
\end{aligned}
$$

Now, apply the chain rule for relative entropy:

$$
\begin{aligned}
D((\mathsf{X}, \mathsf{Y}) \parallel \tilde{\mathsf{X}} \otimes \tilde{\mathsf{Y}}) &= D(\mathsf{X} \parallel \tilde{\mathsf{X}}) + D((\mathsf{X}, \mathsf{Y}) \mid (\mathsf{X}, \tilde{\mathsf{X}}) \parallel (\tilde{\mathsf{X}} \oplus \tilde{\mathsf{Y}}) \mid (\mathsf{X}, \tilde{\mathsf{X}})) \\
&= 0 + \sum_x p_x D(\mathsf{Y}|_{\mathsf{X}=x} \parallel \mathsf{Y}) \\
&= \mathbb{E}_{x \leftarrow \mathsf{X}} D(\mathsf{Y}|_{\mathsf{X}=x} \parallel \mathsf{Y}) \qquad \qquad \square
\end{aligned}
$$

> **Problem 2.3.8**
>
> Suppose there is a joint distribution (X, Y) that Alice and Bob wish to jointly compute. Alice and Bob have access to a shared random string $\mathsf{R} = (\mathsf{R}_i)$. Alice is given $x \in \mathcal{X}$ and wants to send Bob a prefix-free message of minimum length so that Bob can compute a sample from $\mathsf{Y} \mid \mathsf{X} = x$.

> **Definition 2.3.9**
>
> A protocol Π is a pair of functions (M, y) where $M : \mathcal{X} \times \Omega_{\mathsf{R}} \to \{0, 1\}^*$ is the message Alice sends to Bob and $y : \{0, 1\}^* \times \Omega_{\mathsf{R}} \to \mathcal{Y}$ is Bob's output.
>
> The performance of Π is $\mathbb{E}_{\mathsf{X}, \mathsf{R}} |M(\mathsf{X}, \mathsf{R})|$

Suppose X and Y are independent. Then, Bob needs no information so we can use the trivial protocol $M(\mathsf{X}, \mathsf{R}) = \varnothing$ with performance 0.

Otherwise, we can use a strategy of prefix-free encoding x so that $\mathbb{E} |M(\mathsf{X}, \mathsf{R})| \approx H(\mathsf{X})$.

> **Theorem 2.3.10**
>
> There exists a protocol $\Pi = (M, y)$ such that expected message length
>
> $$\mathbb{E}\,|M(\mathsf{X}, \mathsf{R})| \leq I(\mathsf{X} : \mathsf{Y}) + \mathcal{O}(\log I(\mathsf{X} : \mathsf{Y}))$$
>
> For all other protocols $\Pi' = (M', y')$,
>
> $$\mathbb{E}\,|M'(\mathsf{X}, \mathsf{R})| \geq I(\mathsf{X} : \mathsf{Y})$$

Proof. Let X be a random point on the hypercube $\{\pm 1\}^n$. Let Y be a random point on $\{\pm 1\}^n$ that is ε-correlated with X. That is, $\mathsf{Y}_i = \mathsf{X}_i$ with probability ε and is uniformly random otherwise.

Observe that, individually, X and Y have the same distribution. In particular, in the ε case, then $\mathsf{Y}_i = \mathsf{X}_i$ is Uniform$\{\pm 1\}$. In the $1 - \varepsilon$ case, $\mathsf{Y}_i \sim \text{Uniform}\{\pm 1\}$ by definition.

We can calculate $H(\mathsf{X}) = H(\mathsf{Y}) = n$.

Also, $H(\mathsf{Y} \mid \mathsf{X}) = \sum_x p_x H(\mathsf{Y} \mid \mathsf{X} = x) \approx (1 - \varepsilon)n$. One can show that $\mathsf{Y} \mid \mathsf{X} = x$ is approximately uniformly distributed over the vectors of length n that agree on εn coordinates with x. This sample space has size $2^{(1-\varepsilon)n}$.

Therefore, $I(\mathsf{X} : \mathsf{Y}) = H(\mathsf{Y}) - H(\mathsf{Y} \mid \mathsf{X}) \approx \varepsilon n$.

By prop. 2.2.8, there exists a rejection sampler such that $\mathbb{E}[\ell(i^*)] \leq D(P \parallel Q) + \mathcal{O}(\log D(P \parallel Q))$.

Recall from STAT 230 that we can transform R into any distribution with the change of variable bullshit. In particular, transform R_i to IID $\mathsf{Y}_i \sim \mathsf{Y}$ and the biased coins.

Alice will run $\textsc{RejectionSampler}(\mathsf{Y}|_{\mathsf{X}=x}, \mathsf{Y})$ to find a random index i^* such that Y_{i^*} has distribution $\mathsf{Y}|_{\mathsf{X}=x}$.

Alice sends a prefix-free encoding of i^*. Bob outputs Y_{i^*}. The performance is:

$$
\begin{aligned}
\mathbb{E}_{\mathsf{X},\mathsf{R}}|M(\mathsf{X}, \mathsf{R})| &= \sum_{x \in \mathcal{X}} p_x \, \mathbb{E}_{i^*, \mathsf{Y}_1, \mathsf{Y}_2, \dots}[\ell(i^*)] \\
&\leq \sum_{x \in \mathcal{X}} p_x (D(\mathsf{Y}|_{\mathsf{X}=x} \parallel \mathsf{Y}) + \mathcal{O}(\log D(\mathsf{Y}_{\mathsf{X}=x} \parallel \mathsf{Y}))) \\
&= I(\mathsf{X} : \mathsf{Y}) + \sum_{x \in \mathcal{X}} p_x \mathcal{O}(\log D(\mathsf{Y}_{\mathsf{X}=x} \parallel \mathsf{Y})) \\
&\leq I(\mathsf{X} : \mathsf{Y}) + \mathcal{O}(\log I(\mathsf{X} : \mathsf{Y}))
\end{aligned}
$$

where the last step is by Jensen's inequality.

Now, let Π be any protocol. By Kraft's inequality, $\mathbb{E}_{\mathsf{X},\mathsf{R}}|M(\mathsf{X}, \mathsf{R})| \geq H(M(\mathsf{X}, \mathsf{R}))$.

We will also show the data-processing inequality:

$$I(\mathsf{X} : (M(\mathsf{X}, \mathsf{R}), \mathsf{R})) = I(X : M(\mathsf{X}, \mathsf{R})) + \sum_{r \in \Omega} p_r I(\mathsf{X}|_{\mathsf{R}=r} : M(\mathsf{X}, \mathsf{R})|_{\mathsf{R}=r}) \qquad \text{(chain rule)}$$

$$= 0 + \sum_{r \in \Omega} p_r I(\mathsf{X}|_{\mathsf{R}=r} : M(\mathsf{X}, \mathsf{R})|_{\mathsf{R}=r}) \qquad \text{(since } \mathsf{X} \text{ and } \mathsf{R} \text{ are independent)}$$

$$\leq \sum_{r \in \Omega} p_r H(M(\mathsf{X}, \mathsf{R})|_{\mathsf{R}=r}) \qquad \text{(venn diagram logic)}$$

$$= H(M(\mathsf{X}, \mathsf{R}) \mid \mathsf{R})$$

$$\leq H(M(\mathsf{X}, \mathsf{R})) \qquad \text{(conditioning only reduces entropy)}$$

In general,
$$I(\mathsf{A} : f(\mathsf{B})) \leq I(\mathsf{A} : \mathsf{B})$$

and we are doing the case where $\mathsf{A} = \mathsf{X}$, $\mathsf{B} = (M(\mathsf{X}, \mathsf{R}))$, and $f = y$. $\qquad \square$

List of Named Results

Index of Defined Terms