INTRODUCTION TO GRAPH ENTROPY

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ABSTRACT. This is an introduction to the notion of (conditional) graph entropy. It is mainly based on [3]. It was created as supplementary material to the website https://www.renyi.hu/~harangi/ge.htm.

1. GRAPH ENTROPY: A VISUAL INTRODUCTION

1.1. A coding problem with indistinguishable letters. Suppose that the discrete random variable X takes values in a finite alphabet \mathcal{X} . If we take a large number of IID copies X_1, \ldots, X_ℓ , then with high probability the outcome will be a so-called *typical sequence*, in which the frequency of each letter $x \in \mathcal{X}$ is close to its probability

$$p_x := \mathbb{P}(X = x).$$

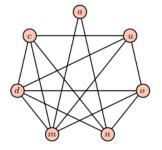
Recall that the Shannon entropy of X is defined as

$$H(X) = \sum_{x} -p_x \log p_x.$$

Loosely speaking, any typical sequence has probability roughly $\exp(-\ell H(X))$, and hence the number of typical sequences is roughly $\exp(\ell H(X))$. This observation essentially proves the following classical result: H(X) gives the minimal *code rate* required to encode the IID sequence (X_i) such that, with high probability, it is uniquely decodable.

Körner introduced [5] a natural variant of this coding problem, where not every pair of letters can be distinguished. Let G be a graph with vertex set $V(G) = \mathcal{X}$ describing which pairs are distinguishable: $x, x' \in \mathcal{X}$ can be distinguished if and only if xx' is an edge of G. Furthermore, we say that the sequences x_1, \ldots, x_ℓ and x'_1, \ldots, x'_ℓ are distinguishable if x_i and x'_i are distinguishable for at least one index *i*. In this variant we wish to encode the IID sequence with high probability in a way that distinguishable sequences are mapped to different codewords. Again, we are interested in the minimal achievable code rate that we call the graph entropy of X w.r.t. G and denote by $H_G(X)$.

For example, consider the alphabet $\mathcal{X} = \{a, c, d, m, n, o, u\}$ with the graph G below:



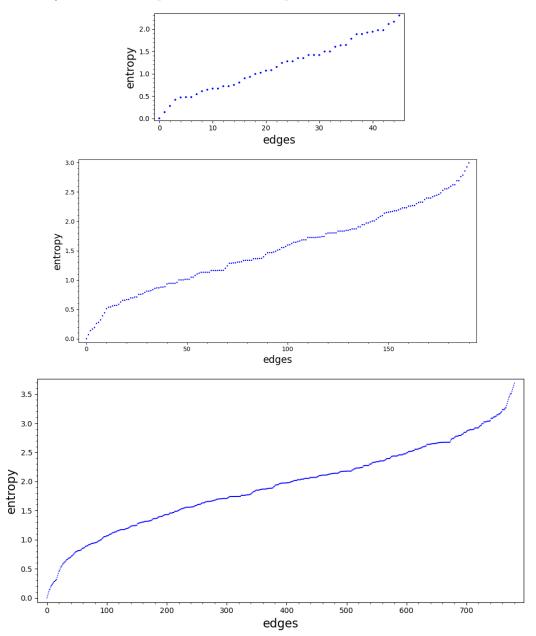
That is, the following pairs of letters are indistinguishable:

Some examples for distinguishable and indistinguishable words (sequences):

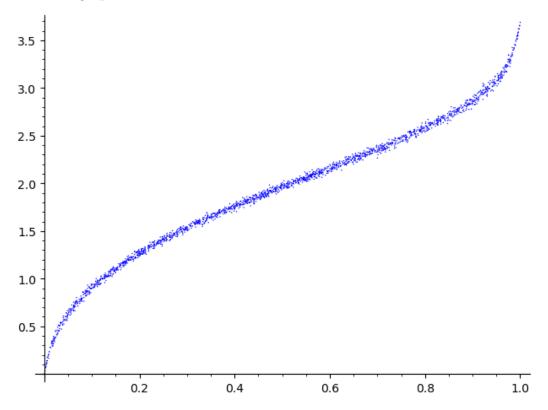
indistinguishable pairs			U I		
moana	uncoad	mad	moan <mark>a</mark>	<u>unco</u> ad	dad
nodua	nuocca	mud	nodun	<u>duon</u> ca	mud

1.2. From empty to complete. For the complete graph G, we get back the original coding problem, so $H_G(X) = H(X)$, while for the empty graph any two sequences are indistinguishable, and hence $H_G(X) = 0$. In general, $0 \le H_G(X) \le H(X)$.

To get an idea how graph entropy typically changes in-between, let us start from the empty graph on N vertices and add edges randomly one by one, computing graph entropy (for uniform X) after each step. The results are plotted below for N = 10, 20, 40.



In a similar experiment, we plotted graph entropy (again for uniform X) and edge density for 2000 random graphs¹ on N = 40 vertices:



1.3. The independent set polytope and a simple formula. In Körner's original paper [5] a fairly simple (non-asymptotic) formula was given for $H_G(X)$. Later, Csiszár, Körner, Lovász, Marton, and Simonyi [1] found an even simpler one, which is based on the following (high-dimensional) polytope.

Definition. Given a simple finite graph G, we say that a subset J of the vertex set V(G) is an *independent set* of G if the induced subgraph G[J] contains no edges. By $\mathcal{J}(G)$ we denote the set of independent sets of G.

The independent set polytope or vertex-packing polytope VP(G) is defined as the convex hull of the characteristic vectors of the independent sets of G:

$$\operatorname{VP}(G) := \operatorname{conv}\left(\{\mathbb{1}_J : J \in \mathcal{J}(G)\}\right) \subseteq [0,1]^{V(G)} \subset \mathbb{R}^{V(G)}.$$

Next we consider the following function:

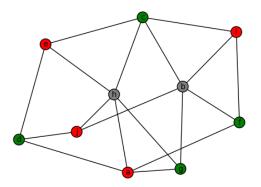
(1)
$$(a_x) \mapsto \sum_{x \in V(G)} -p_x \log(a_x) \quad \text{for } (a_x)_{x \in \mathcal{X}} \in [0, 1]^{\mathcal{X}}.$$

It turns out [1] that graph entropy is the minimum of this function over VP(G):

(2)
$$H_G(X) = \min_{(a_x) \in VP(G)} \sum_{x \in V(G)} -p_x \log(a_x).$$

We explain the details through the following example. Consider the graph below.

¹We considered Erdős–Rényi random graphs G(N, p) for randomly chosen $p \in [0, 1]$.



The vertex set is $V(G) = \{a, b, c, d, e, f, g, h, i, j\}$. Note that the red vertices form an independent set $\{a, e, i, j\}$. For simplicity, we will refer to this set as *aeij*. Similarly, *cdf g* is also an independent set. In fact, this graph has 11 inclusion-maximal² independent sets:

acj, aeij, abe, cfgj, egij, efgj, dgi, dhi, bdh, cdfg, dfh.

The characteristic vector $\mathbb{1}_J$ of an independent set J has ones at the coordinates corresponding to the vertices in J, and has zeros elsewhere. For instance, the vectors corresponding to the sets *aeij*, *cdfg*, *bdh*, *cfgj* are the following:

 $\begin{aligned} &aeij: \begin{pmatrix} a & b & c & d & e & f & g & h & i & j \\ cdfg: & (0,0,1,1,0,1,1,0,0,0) \\ bdh: & (0,1,0,1,0,0,0,1,0,0) \\ cfgj: & (0,0,1,0,0,1,1,0,0,1) \end{aligned}$

The vertex-packing polytope VP(G) consists of points that are convex combinations of such characteristic vectors. For example, if we take the linear combination of the four vectors above with the nonnegative weights 0.4, 0.3, 0.2, 0.1 (note that their sum is 1), then we get the following point:

(3)
$$\left(\begin{array}{c} a \\ 0.4, 0.2, 0.4, 0.5, 0.4, 0.4, 0.4, 0.4, 0.4, 0.2, 0.4, 0.5 \\ 0.4, 0.2, 0.4, 0.5 \\$$

For a uniform random X (i.e., when $p_x = 1/10$ for each x), then the function value (1) at this point is:

$$\frac{1}{10} (6 \log(5/2) + 2 \log(5) + 2 \log(2)) \approx 1.01029.$$

This is, of course, only one possible convex combination. We will later see that there is a simple iterative algorithm for finding the optimal weights. For this particular graph, the optimal weights are $\frac{3}{8}, \frac{1}{4}, \frac{1}{4}, \frac{1}{8}$ (and 0 for the seven remaining maximal independent sets). The corresponding (optimal) point in VP(G) is

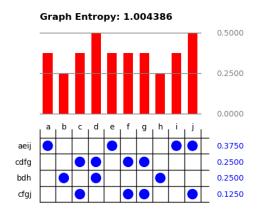
(4)
$$\left(\begin{array}{c} a & b \\ 3/8, 1/4, 3/8, 1/2, 3/8, 3/8, 3/8, 3/8, 1/4, 3/8, 1/2 \\ \end{array} \right) \in \operatorname{VP}(G).$$

The value at this point gives graph entropy:

$$H_G(X) = \frac{1}{10} \left(6\log(8/3) + 2\log(4) + 2\log(2) \right) \approx 1.00438586.$$

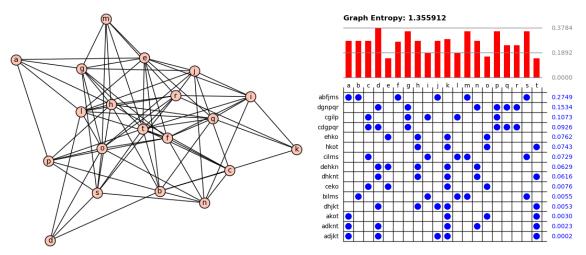
 $^{^{2}}$ When we want to find the optimal convex combination, then it suffices to consider the inclusion-maximal independent sets (not contained by larger independent sets).

This is summarized by the following graphical representation (that our program code generates automatically when graph entropy is computed):



The rows represent independent sets with positive weights, while the columns correspond to the vertices of G (i.e., the letters of our alphabet). The red bar chart shows the corresponding point (a_x) . Given a letter $x \in \mathcal{X} = V(G)$, the height of the bar above x is equal to the coordinate a_x , which is simply the sum of the weights of the sets containing x (that is, the weights at the end of those rows which contain a blue dot • at the column of x).

For a larger example, the graph below has 63 maximal independent sets, out of which 15 are used with positive weights in the optimal convex combination.



1.4. Optimality check and error bound. There is a very simple way to check whether a given point $(a_x) \in VP(G)$ is optimal.

Theorem. Given $(a_x) \in VP(G)$, if

$$\sum_{x \in J} \frac{p_x}{a_x} \le 1 \text{ for all } J \in \mathcal{J}(G),$$

then (a_x) is optimal: $H_G(X) = \sum_{x \in V(G)} -p_x \log(a_x).$

As an illustration, let us confirm that the point given by (4) is indeed optimal: for each independent set J, we need to add up p_x/a_x for $x \in J$, and verify that each sum is at most

one:

$$\begin{array}{ll} acj: & (8/3+8/3+2)/10 = \mathbf{11/15};\\ aeij: & (8/3+8/3+8/3+2)/10 = \mathbf{1};\\ abe: & (8/3+4+8/3)/10 = \mathbf{14/15};\\ cfgj: & (8/3+8/3+8/3+2)/10 = \mathbf{1};\\ egij: & (8/3+8/3+8/3+2)/10 = \mathbf{1};\\ efgj: & (8/3+8/3+8/3+2)/10 = \mathbf{1};\\ dgi: & (2+8/3+8/3)/10 = \mathbf{11/15};\\ dhi: & (2+4+8/3)/10 = \mathbf{13/15};\\ bdh: & (4+2+4)/10 = \mathbf{1};\\ cdfg: & (8/3+2+8/3+8/3)/10 = \mathbf{13/15}.\\ \end{array}$$

In fact, this optimality check is a special case of the following error bound. Given an arbitrary point $(a_x) \in VP(G)$, let us compute the following quantity:

$$\delta := \max_{J \in \mathcal{J}} \left(\sum_{x \in J} \frac{p_x}{a_x} - 1 \right).$$

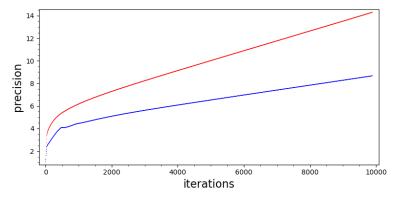
Then the error³ at (a_x) is at most δ :

$$\left(\sum_{x \in V(G)} -p_x \log(a_x)\right) - H_G(X) \in [0, \delta].$$

In particular, δ must always be nonnegative, and if $\delta = 0$, then (a_x) must be optimal (leading to the optimality check described in the theorem above).

As an example, consider the point (a_x) as in (3). It is not optimal because for J = bdh we have (5+2+5)/10 = 1.2, which is greater than 1. In fact, for this point $\delta = 1.2 - 1 = 0.2$, guaranteeing that $H_G(X)$ is at most $\delta = 0.2$ away from the value (1.01029) at (a_x) . The true error for this point is roughly 1.01029 - 1.00439 = 0.0059.

Later we will see that there is a simple iterative algorithm that always converges to graph entropy. However, the rate of convergence may vary. Computing the error bound above, we are guaranteed to be at most δ away from the actual value of $H_G(X)$. The next plot compares the error bound (blue) to the true error (red) through iterations when we run the algorithm for the cycle graph $G = C_{11}$ with some non-uniform X. (Precision means the number of "precise decimal digits", that is, $-\log_{10}$ of the error.)



³By the error at (a_x) we mean the distance of the value at (a_x) from the graph entropy $H_G(X)$.

2. GRAPH ENTROPY: AS AN ALTERNATING OPTIMIZATION PROBLEM

2.1. Körner's original formula. An independent set of G contains no edges, and hence any two letters in the set are indistinguishable. Therefore one possible strategy for encoding a sequence X_1, \ldots, X_ℓ is to replace each X_i with an independent set $J_i \subseteq \mathcal{X}$ containing X_i , and encode the sequence J_1, \ldots, J_ℓ instead. If we do this randomly in a way that (X_i, J_i) are IID samples of some (X, J) where J is a random independent set containing X, then we can encode the J_i sequence with rate H(J). Note that the number of times any given typical X_i sequence is "covered" by typical J_i sequences has exponential rate H(J|X). Based on this, one can design an encoding with rate H(J) - H(J|X) = I(X;J). Then, for a given X, one needs to choose (X, J) in a way that the mutual information I(X; J) is as small as possible. Körner showed [5] that this is the best achievable code rate, and hence we have the following formula for graph entropy:

(5)
$$H_G(X) = \min_{X \in J \text{ ind.set}} I(X; J).$$

2.2. Alternating optimization hidden in the background. We have seen that graph entropy can be obtained as the solution of two different minimization problems; see (2) and (5). In fact, they both stem from the same alternating optimization problem that we introduce next. (This was pointed out in [3] in the more general setting of conditional graph entropy.)

Problem. Suppose that we have probability measures on a given finite set \mathcal{J} :

- a finite family: $\mu_x, x \in \mathcal{X};$
- and a single measure: ν .

For each $x \in \mathcal{X}$ we have the constraint that the support $\sup \mu_x$ must be contained in a given subset \mathcal{J}_x of \mathcal{J} . Find the measures μ_x , ν that minimize the weighted sum of the Kullback–Leibler divergences:

$$\sum_{x} p_x D_{\mathrm{KL}}(\mu_x \parallel \nu) \text{ for some given weights } p_x \ge 0.$$

To summarize, given $\mathcal{J}_x \subseteq \mathcal{J}, x \in \mathcal{X}$ and $p_x \ge 0, x \in \mathcal{X}$, find the minimum of the above sum under the constraint supp $\mu_x \subseteq \mathcal{J}_x$.

In our setting we have a random variable X taking values in the finite set \mathcal{X} , and G is a graph on the vertex set \mathcal{X} . From this point on we will use small j to denote an independent set of G, hence each j is a subset of \mathcal{X} . We choose \mathcal{J} to be the set of all j, while

$$\mathcal{J}_x \coloneqq \{j \, : \, x \in j\}$$

consists of the independent sets containing a fixed x. With this setup and with $p_x := \mathbb{P}(X = x)$, the minimum of the problem above turns out to be precisely $H_G(X)$.

To get concrete formulas, let us represent the distributions μ_x and ν by the following vectors:

$$\boldsymbol{q} = (q_{j|x})_{(j,x)\in\mathcal{J}\times\mathcal{X}} \in \mathbb{R}^{\mathcal{J}\times\mathcal{X}};$$
$$\boldsymbol{r} = (r_j)_{j\in\mathcal{J}}\in\mathbb{R}^{\mathcal{J}},$$

where $q_{j|x}$ and r_j stand for $\mu_x(\{j\})$ and $\nu(\{j\})$, respectively.⁴

⁴We index the coordinates/variables by j|x to emphasize the fact that they express certain conditional probabilities. This notation may also serve as a reminder that $q_{j|x}$ have to sum up to 1 for any fixed x.

Then

$$D_{\mathrm{KL}}(\mu_x \parallel \nu) = \sum_j q_{j|x} \log \frac{q_{j|x}}{r_j}$$

and hence the function to minimize is

$$\varphi(\boldsymbol{q}, \boldsymbol{r}) := \sum_{x,j} p_x q_{j|x} \log \frac{q_{j|x}}{r_j}.$$

The constraints for \boldsymbol{q} and \boldsymbol{r} lead to the following definition. Let $K_{q} \subset \mathbb{R}^{\mathcal{J} \times \mathcal{X}}$ and $K_{r} \subset \mathbb{R}^{\mathcal{J}}$ be the following convex polytopes:

$$K_{q} := \left\{ \boldsymbol{q} = (q_{j|x}) : q_{j|x} \ge 0; \sum_{j \ni x} q_{j|x} = 1 \, (\forall x \in \mathcal{X}); \, q_{j|x} = 0 \text{ if } x \notin j \right\}$$

and

$$K_{\mathbf{r}} := \left\{ \boldsymbol{r} = (r_j) : r_j \ge 0; \sum_j r_j = 1 \right\}.$$

By $int(K_q)$ and $int(K_r)$ we denote the relative interiors of the polytopes (within their affine hull).

With these notation, we need to find $\min_{K_q \times K_r} \varphi(\boldsymbol{q}, \boldsymbol{r})$. This is an alternating minimization problem: the point is that if we fix one of the two variables \boldsymbol{q} and \boldsymbol{r} , then there are explicit formulas for the optimal choice of the other variable.

We define the mappings⁵

$$A: K_{\rm r} \to \mathbb{R}^{\mathcal{X}};$$
$$Q: K_{\rm r} \to K_{\rm q} \subset \mathbb{R}^{\mathcal{J} \times \mathcal{X}};$$
$$R: K_{\rm q} \to K_{\rm r} \subset \mathbb{R}^{\mathcal{J}}$$

by the following coordinate-wise functions $Q_{j|x}$, R_j , A_x :

$$R_{j}(\boldsymbol{q}) := \sum_{x \in j} p_{x} q_{j|x};$$

$$A_{x}(\boldsymbol{r}) := \sum_{j \ni x} r_{j};$$

$$Q_{j|x}(\boldsymbol{r}) := \begin{cases} 0 & \text{if } x \notin j; \\ \frac{r_{j}}{A_{x}(\boldsymbol{r})} & \text{if } x \in j. \end{cases}$$

When minimizing $\varphi(q, r)$, it turns out that r = R(q) is the optimal choice for a fixed q, and similarly q = Q(r) is optimal for a fixed r; that is, for any q and r we have

$$\varphi(\boldsymbol{q},\boldsymbol{r}) \geq \varphi(\boldsymbol{q},R(\boldsymbol{q})) \text{ and } \varphi(\boldsymbol{q},\boldsymbol{r}) \geq \varphi(Q(\boldsymbol{r}),\boldsymbol{r}).$$

So we can explicitly define the following functions:

$$\varphi_{\mathbf{q}}(\boldsymbol{q}) := \min_{\boldsymbol{r}} \varphi(\boldsymbol{q}, \boldsymbol{r}) = \varphi(\boldsymbol{q}, R(\boldsymbol{q})) = \sum_{x} p_{x} \sum_{j \ni x} q_{j|x} \log q_{j|x} - \sum_{j} R_{j}(\boldsymbol{q}) \log R_{j}(\boldsymbol{q});$$
$$\varphi_{\mathbf{r}}(\boldsymbol{r}) := \min_{\boldsymbol{q}} \varphi(\boldsymbol{q}, \boldsymbol{r}) = \varphi(Q(\boldsymbol{r}), \boldsymbol{r}) = -\sum_{x} p_{x} \log A_{x}(\boldsymbol{r}) = -\sum_{x} p_{x} \log \sum_{j \ni x} r_{j}.$$

⁵It is straightforward to check that $Q(\mathbf{r}) \in K_q$ and $R(\mathbf{q}) \in K_r$ always hold. Note that Since the formula for $Q_{j|x}$ involves a division by A_x , it only defines Q over the subset $K_r^* := K_r \setminus \bigcup_x A_x^{-1}(0)$. For $\mathbf{r} \in K_r \setminus K_r^*$

let $Q(\mathbf{r})$ be an arbitrary point in $int(K_q)$.

Then, by definition, $\min_{K_{\mathbf{q}} \times K_{\mathbf{r}}} \varphi = \min_{K_{\mathbf{q}}} \varphi_{\mathbf{q}} = \min_{K_{\mathbf{r}}} \varphi_{\mathbf{r}}$. Note that for

$$\varphi_{\mathbf{a}}(\boldsymbol{a}) := -\sum_{x} p_x \log a_x$$

we clearly have $\varphi_{\mathbf{r}}(\mathbf{r}) = \varphi_{\mathbf{a}}(A(\mathbf{r}))$. It follows that $\min_{K_{\mathbf{r}}} \varphi_{\mathbf{r}} = \min_{K_{\mathbf{a}}} \varphi_{\mathbf{a}}$ if we define $K_{\mathbf{a}}$ as the set of $A(\mathbf{r})$:

$$K_{\mathbf{a}} \coloneqq \{A(\boldsymbol{r}) : \boldsymbol{r} \in K_{\mathbf{r}}\}.$$

Note that $A(\mathbf{r})$ is the convex combination of the characteristic functions of the sets $j \subseteq \mathcal{X}$ (with weights r_j). So if \mathcal{J} consists of the independent sets of a graph G on \mathcal{X} , then $K_a = VP(G)$.

So the q-problem min φ_q is actually equivalent to Körner's original formula (5) while the a-problem (which is just a simple reformulation of the r-problem) gives back (2).

Theorem. We have the following formulas for graph entropy:

$$H_G(X) = \min_{K_q \times K_r} \varphi = \min_{K_q} \varphi_q = \min_{K_r} \varphi_r = \min_{K_a} \varphi_a.$$

2.3. Iterative algorithm. When trying to find the minimum of $\varphi(\boldsymbol{q}, \boldsymbol{r})$, the fact that we can easily optimize in either variable (while the other is fixed) gives rise to the following simple iterative algorithm. Let us start from a point $\boldsymbol{q}^{(0)}$ and apply R and Q alternately:

(6)
$$q^{(0)} \xrightarrow{R} r^{(0)} \xrightarrow{Q} q^{(1)} \xrightarrow{R} r^{(1)} \xrightarrow{Q} q^{(2)} \xrightarrow{R} r^{(2)} \cdots$$

The corresponding φ -value decreases at each step:

$$egin{array}{rll} arphi(m{q}^{(0)},m{r}^{(0)})&=&arphi_{
m q}(m{q}^{(0)})\ &&arphi&arphi\ &&arphi\ &&arph$$

One can also think of this alternating optimization as "jumping" between the q-problem $\min_{K_q} \varphi_q$ and the r-problem $\min_{K_r} \varphi_r$ using the maps $Q: K_r \to K_q$ and $R: K_q \to K_r$. The value to minimize (i.e., the φ_q -value and the φ_r -value, respectively) always decreases, so with each step we get closer to the optimum.

Following the footsteps of the general theory of Csiszár and Tusnády [2], it was shown in [3] that for an arbitrary starting point $q^{(0)}$ in the relative interior $int(K_q)$, the iterative process converges to the minimum.

Theorem ([3]). For an arbitrary starting point $\mathbf{q}^{(0)} \in \text{int}(K_q)$ consider the sequence (6) obtained by alternating optimization. Then $\varphi(\mathbf{q}^{(n)}, \mathbf{r}^{(n)})$ is a decreasing sequence that converges to $\min_{K_q \times K_r} \varphi = H_G(X)$ as $n \to \infty$.

3. Conditional graph entropy

3.1. The generalization of Körner's formula. The analogous problem with side information Y_i at the receiver leads to the notion of *conditional graph entropy* $H_G(X|Y)$. Let (X, Y) be discrete random variables of some given joint distribution and let (X_i, Y_i) be IID samples. We assume that the decoder knows the sequence Y_1, Y_2, \ldots , and, as before, that some of the outcomes of X are indistinguishable, described by a graph G. If we want to use the same approach (i.e., choosing a random independent set J), then J and Y should be independent conditioned on X (because the sender does not know Y_i when choosing J_i). This can be made rigorous, leading to the following formula:

$$H_G(X|Y) = \min_J I(X; J|Y) = \min_J \left(H(J|Y) - \underbrace{H(J|X,Y)}_{H(J|X)} \right),$$

where J is a random independent set of G such that $X \in J$, and J and Y are conditionally independent conditioned on X (which is equivalent to saying that Y - X - J is a Markov chain).

3.2. Compression with side information. Suppose now that the receiver wishes to recover the values $f(X_i, Y_i)$ of some given function $f: \mathcal{X} \times \mathcal{Y} \to \mathcal{Z}$ (with high probability, over long blocks) as depicted in the figure below.

$$X \longrightarrow \boxed{\operatorname{Enc}}^{R = H_G(X|Y)} \xrightarrow{\operatorname{Dec}} f(X,Y)$$

Orlitsky and Roche [6] showed that the minimal rate of information that needs to be transmitted is precisely the conditional graph entropy of the so-called *characteristic graph*, which is defined on the vertex set \mathcal{X} as follows: vertices $x_1, x_2 \in \mathcal{X}$ are connected with an edge if and only if

$$\exists y \in \mathcal{Y} \text{ s.t. } (f(x_1, y) \neq f(x_2, y) \& \mathbb{P}(X = x_1, Y = y) > 0 \& \mathbb{P}(X = x_2, Y = y) > 0).$$

We mention that in the special case f(x, y) = x, which was already studied in Shannon's classical work [7], the optimal rate is given by the conditional entropy H(X|Y) = H(X,Y) - H(Y).

3.3. Generalized formulas. In this conditional setting the alternating optimization problem is as follows.

Problem. Suppose that we have two finite families of probability measures on a given finite set \mathcal{J} : μ_x , $x \in \mathcal{X}$ and ν_y , $y \in \mathcal{Y}$. In the first family for each $x \in \mathcal{X}$ we have a constraint: the support supp μ_x must be contained in a given subset \mathcal{J}_x of \mathcal{J} . Find the measures μ_x , ν_y that minimize the weighted sum of the Kullback–Leibler divergences:

$$\sum_{x,y} p_{x,y} D_{\mathrm{KL}}(\mu_x \parallel \nu_y) \text{ for some given weights } p_{x,y} \ge 0.$$

To summarize, given $\mathcal{J}_x \subseteq \mathcal{J}$, $x \in \mathcal{X}$ and $p_{x,y} \geq 0$, $x \in \mathcal{X}$, $y \in \mathcal{Y}$, find the minimum of the above sum under the constraint supp $\mu_x \subseteq \mathcal{J}_x$.

In our setting we have random variables X and Y taking values in the finite sets \mathcal{X} and \mathcal{Y} , respectively, and G is a graph on the vertex set \mathcal{X} . As before, \mathcal{J} is the set of all independent sets j of G, while

$$\mathcal{J}_x := \{j : x \in j\}$$

consists of the independent sets containing a fixed x. With $p_{x,y} := \mathbb{P}(X = x, Y = y)$, the above minimum is $H_G(X|Y)$.

Let us represent the distributions μ_x and ν_y by the following vectors:

$$\boldsymbol{q} = (q_{j|x})_{(j,x)\in\mathcal{J}\times\mathcal{X}} \in \mathbb{R}^{\mathcal{J}\times\mathcal{X}};$$
$$\boldsymbol{r} = (r_{j|y})_{(j,y)\in\mathcal{J}\times\mathcal{Y}} \in \mathbb{R}^{\mathcal{J}\times\mathcal{Y}},$$

where $q_{j|x}$ and $r_{j|y}$ stand for $\mu_x(\{j\})$ and $\nu_y(\{j\})$, respectively. Then

$$D_{\mathrm{KL}}(\mu_x \parallel \nu_y) = \sum_j q_{j|x} \log \frac{q_{j|x}}{r_{j|y}},$$

so the function to minimize is

$$\varphi(\boldsymbol{q}, \boldsymbol{r}) := \sum_{x,y,j} p_{x,y} q_{j|x} \log rac{q_{j|x}}{r_{j|y}}$$

The constraints for q and r lead to the following definitions:

$$K_{\mathbf{q}} := \left\{ \boldsymbol{q} = \left(q_{j|x}\right) : q_{j|x} \ge 0; \sum_{j \ge x} q_{j|x} = 1 \, (\forall x \in \mathcal{X}); \, q_{j|x} = 0 \text{ if } x \notin j \right\}$$

and

$$K_{\mathbf{r}} := \left\{ \boldsymbol{r} = \left(r_{j|y} \right) : r_{j|y} \ge 0; \sum_{j} r_{j|y} = 1 \, (\forall y \in \mathcal{Y}) \right\}.$$

The general formulas for the mappings $A: K_{\rm r} \to \mathbb{R}^{\mathcal{X}}; Q: K_{\rm r} \to K_{\rm q} \subset \mathbb{R}^{\mathcal{J} \times \mathcal{X}}; R: K_{\rm q} \to K_{\rm r} \subset \mathbb{R}^{\mathcal{J} \times \mathcal{Y}}$ are as follows:

$$R_{j|y}(\boldsymbol{q}) := \sum_{x \in j} p_{x|y} q_{j|x};$$

$$A_x(\boldsymbol{r}) := \sum_{j \ni x} \prod_y (r_{j|y})^{p^{y|x}};$$

$$Q_{j|x}(\boldsymbol{r}) := \begin{cases} 0 & \text{if } x \notin j; \\ \prod_y (r_{j|y})^{p^{y|x}} / A_x(\boldsymbol{r}) & \text{if } x \in j. \end{cases}$$

(Here we define $t^0 = 1$ even for t = 0.)

Remark. Note that R is a linear map and it actually describes how the conditional distributions J | Y = y can be expressed in terms of J | X = x in a Markov chain Y - X - J.

As for φ_{q} and φ_{r} , we have

$$\varphi_{\mathbf{q}}(\boldsymbol{q}) := \varphi(\boldsymbol{q}, R(\boldsymbol{q})) = \sum_{x} p_{x} \sum_{j \ni x} q_{j|x} \log q_{j|x} - \sum_{y} p^{y} \sum_{j} R_{j|y}(\boldsymbol{q}) \log R_{j|y}(\boldsymbol{q})$$

and

$$\varphi_{\mathbf{r}}(\boldsymbol{r}) := \varphi(Q(\boldsymbol{r}), \boldsymbol{r}) = -\sum_{x} p_{x} \log A_{x}(\boldsymbol{r}) = -\sum_{x} p_{x} \log \sum_{j \ni x} \prod_{y} (r_{j|y})^{p^{y|x}}.$$

With these notations, we can express conditional graph entropy in various ways:

$$H_G(X|Y) = \min_{K_q} \varphi_q = \min_{K_r} \varphi_r = \min_{K_r} -\sum_x p_x \log A_x.$$

It can be seen easily that $A_x \colon K_r \to [0,1]$ is a concave function for each x. It means that the set of image points $\boldsymbol{a} = (a_x)_{x \in \mathcal{X}}$ with $a_x = A_x(\boldsymbol{r})$, as \boldsymbol{r} ranges over K_r , (essentially) defines a convex corner⁶ K_a in $\mathbb{R}^{\mathcal{X}}$. Then we have

$$H_G(X|Y) = \min_{K_{\mathbf{a}}} \varphi_{\mathbf{a}}, \text{ where } \varphi_{\mathbf{a}}(\boldsymbol{a}) = -\sum_x p_x \log a_x.$$

A nice feature of this a-problem is that the minimum is attained at a single point $\boldsymbol{a} \in K_{\mathrm{a}}$ because φ_{a} is strictly convex (provided that $p_x = \mathbb{P}(X = x) > 0$ for each x). Also note that φ_{a} depends only on the distribution of X, while the convex corner K_{a} depends only on the graph G and the conditional distributions $Y \mid X = x$ for any given x. Thus, the parameters of the problem are, so to say, split between φ_{a} and K_{a} .

Moreover, in [3] another convex corner, denoted by L, was defined such that

$$H_G(X|Y) = \min_{K_{\mathbf{a}}} \varphi_{\mathbf{a}} = -\min_L \varphi_{\mathbf{a}};$$

a vector $\boldsymbol{a} = (a_x)_{x \in \mathcal{X}} \in K_a$ being optimal (i.e., the minimum point of φ_a) if and only if $\boldsymbol{a}^{-1} := (a_x^{-1})_{x \in \mathcal{X}} \in L$. This provides a fairly simple way to check optimality, and even leading to an error bound for the iterative algorithm, which was shown to converge to $H_G(X|Y)$ in this conditional setting as well.

FURTHER MATERIAL

For a more detailed exposition of the conditional setting, see [3]. Simonyi's excellent survey [8] is a good source for further results on graph entropy. A possible generalization to graphons can be found in [4].

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⁶A convex corner of $\mathbb{R}^{\mathcal{X}}$ is a convex compact set in the positive orthant $[0, \infty)^{\mathcal{X}}$ that is *downward closed*, i.e., if we take any point in the set and decrease some of its coordinates, then the new point still lies in the set.