Structural Information

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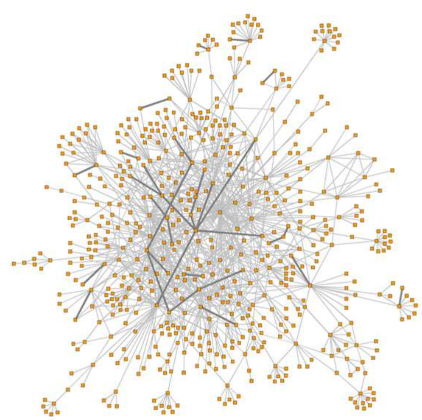
Structural Information

Information Theory of Data Structures: Following Ziv (1997) we propose to explore finite size **information theory** of data structures (i.e., sequences, graphs), that is, to develop information theory of various data structures beyond first-order asymptotics. We focus here on information of graphical structures (unlabeled graphs).

F. Brooks, jr. (JACM, 50, 2003, "Three Great Challenges for . . . CS"):

"We have **no theory** that gives us a metric for the Information embodied in **structure**. This is the most fundamental gap in the theoretical underpinnings of information science and of computer science."

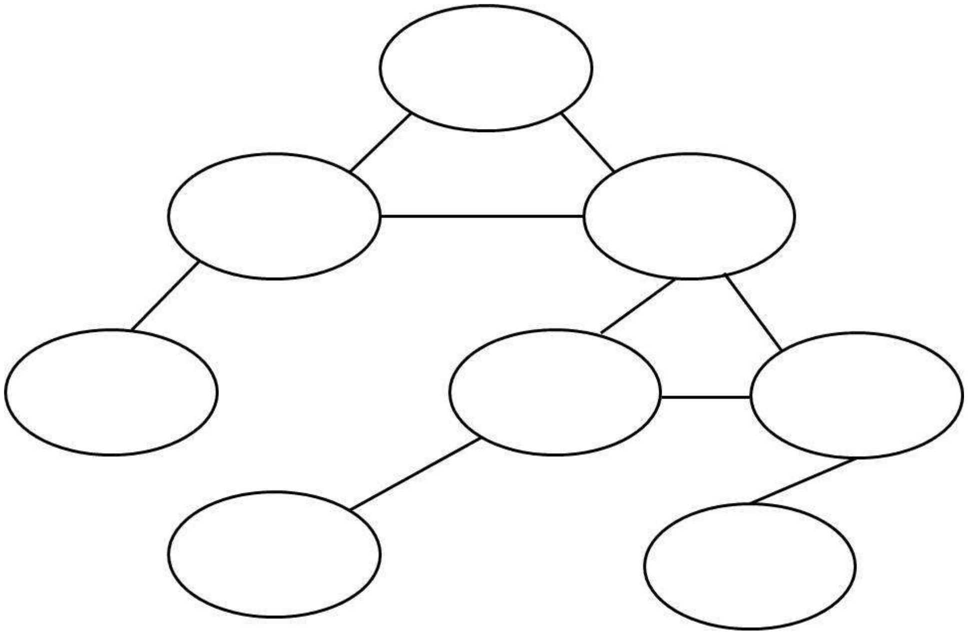
Networks (Internet, protein-protein interactions, and collaboration network) and Matter (chemicals and proteins) have structures.
They can be abstracted by (unlabeled) graphs.

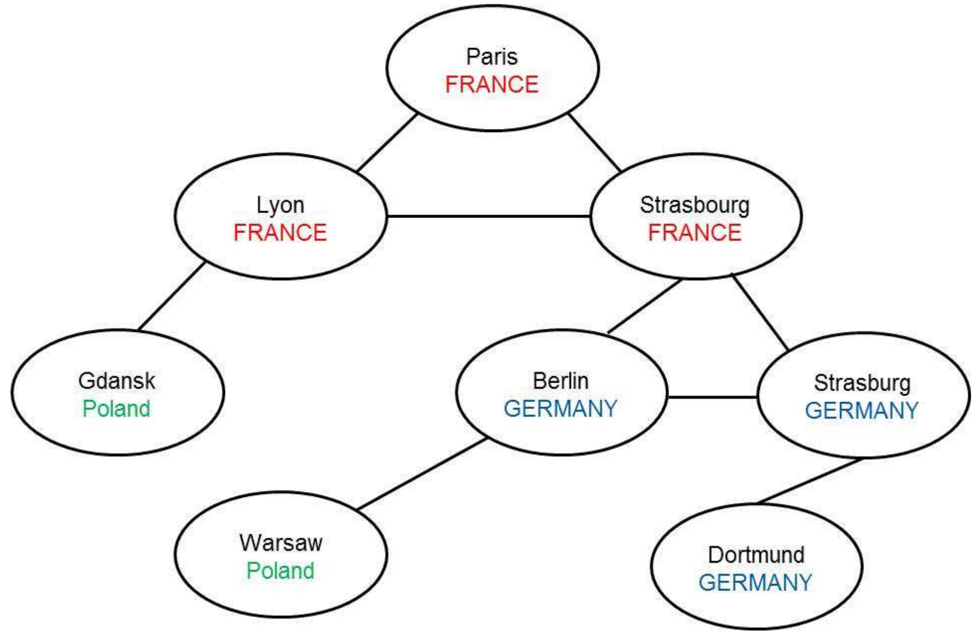


Outline

1. Structural Compression
   - Motivation
   - Unlabeled Graphs
   - SZIP Algorithm and Its Analysis
   - Structural Binary Symmetric Channel
2. Structure of Markov Fields
   - Markov Types
   - One-Dimensional Markov Chains
   - One-Dimensional Universal Types
   - Markov Fields and Tilings
3. Sequence-Structure Protein Folding Channel

Graphs with Locally Correlated Labels





How many bits are required to describe the unlabelled graph on the left, and how many additional bits one needs to represent the correlated labels on the right?

The Real Stuff ...

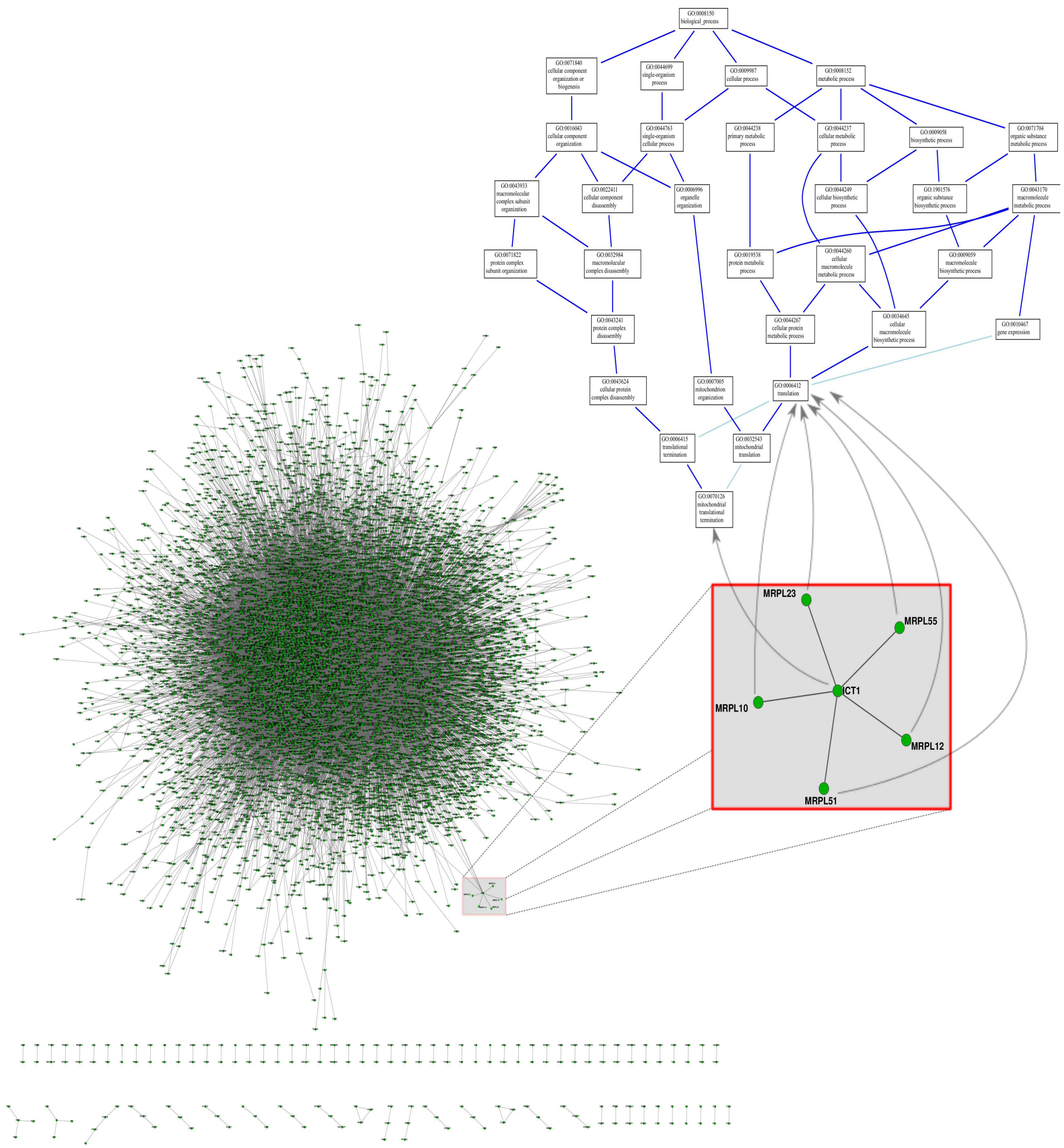


Figure 1: Protein-Protein Interaction Network with BioGRID database

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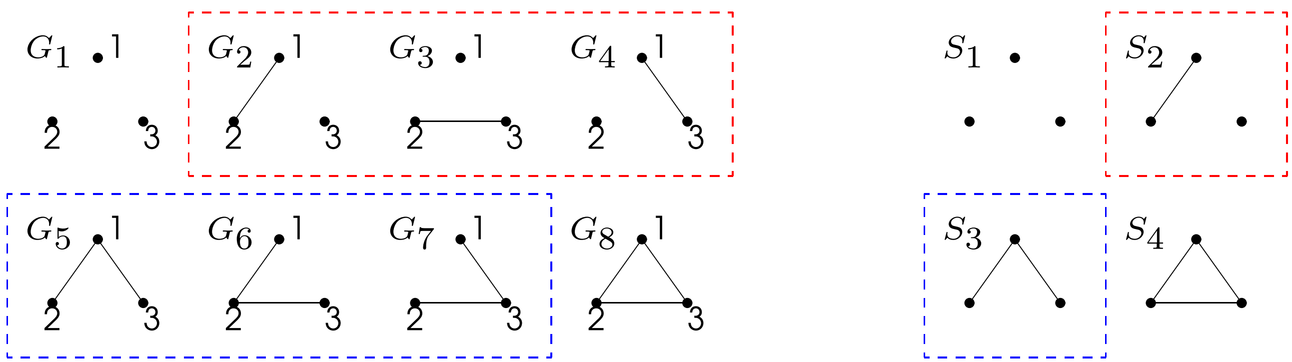
Graph and Structural Entropies

Information Content of Unlabeled Graphs:

A structure model $\mathcal{S}$ of a graph $\mathcal{G}$ is defined for an unlabeled version.
Some labeled graphs have the same structure.



Graph Entropy vs **Structural Entropy**:

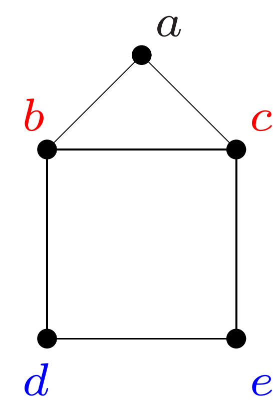
The probability of a structure S is: $P(S) = N(S) \cdot P(G)$
where $N(S)$ is the number of different labeled graphs having the same structure.

$$H_{\mathcal{G}} = \mathbf{E}[-\log P(G)] = -\sum_{G \in \mathcal{G}} P(G) \log P(G), \quad \text{graph entropy}$$

$$H_{\mathcal{S}} = \mathbf{E}[-\log P(S)] = -\sum_{S \in \mathcal{S}} P(S) \log P(S) \quad \text{structural entropy}$$

Relationship between $H_{\mathcal{G}}$ and $H_{\mathcal{S}}$

Two labeled graphs G_1 and G_2 are called *isomorphic* if and only if there is a one-to-one mapping from $V(G_1)$ onto $V(G_2)$ which preserves the adjacency.



Graph Automorphism: For a graph G its automorphism is adjacency preserving permutation of vertices of G.

The collection $\mathrm{Aut}(G)$ of all automorphism of G is called *the automorphism group* of G.

Lemma 1. *If all isomorphic graphs have the same probability, then*

$$H_{\mathcal{S}} = H_{\mathcal{G}} - \log n! + \sum_{S \in \mathcal{S}} P(S) \log |\mathrm{Aut}(S)|,$$

where $\mathrm{Aut}(S)$ is the automorphism group of S.

Proof idea: Using the fact that

$$N(S) = \frac{n!}{|\mathrm{Aut}(S)|}.$$

Erdös-Rényi Graph Model

Our random structure model is the unlabeled version of the binomial random graph model also known as the **Erdös–Rényi** random graph model.

The binomial random graph $\mathcal{G}(n, p)$ generates graphs with n vertices, where edges are chosen independently with probability p.

If a graph G in $\mathcal{G}(n, p)$ has k edges, then (where $q = 1 - p$)

$$P(G) = p^k q^{\binom{n}{2} - k}.$$

Lemma 2 (Kim, Sudakov, and Vu, 2002). *For Erdös-Rényi graphs and all p satisfying*

$$\frac{\ln n}{n} \ll p, \qquad 1 - p \gg \frac{\ln n}{n}$$

a random graph $G \in \mathcal{G}(n, p)$ is symmetric (i.e., $\mathrm{Aut}(G) \approx 1$) with probability $O\left(n^{-w}\right)$ for any positive constant w, that is,

$$P(\mathrm{Aut}(G) = 1) \sim 1 - O(n^{-w}).$$

Symmtery of Power Law Graphs?

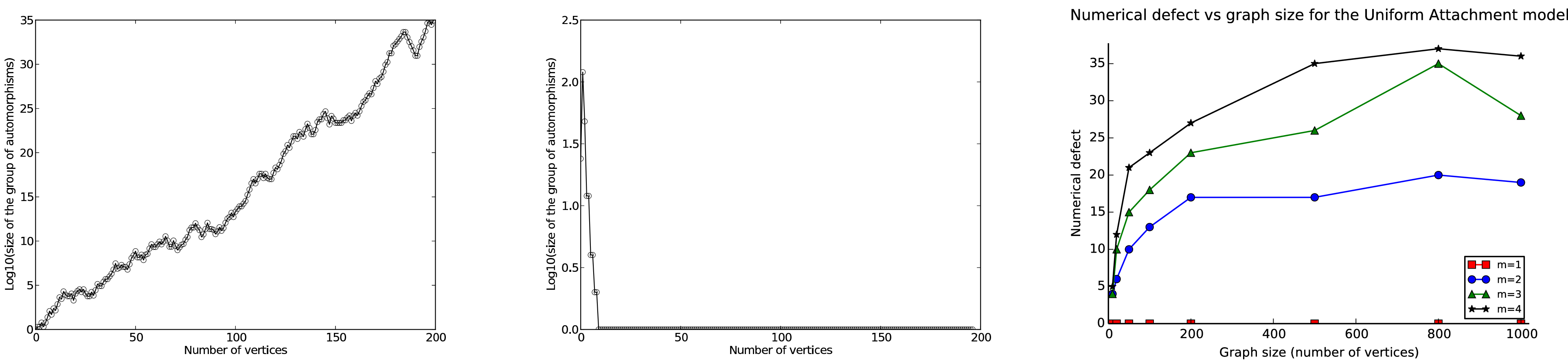


Figure 2: Logarithm of the number of automorphisms versus the number of vertices for $m = 1$ (on the left), $m = 4$ (middle), defect for various m.

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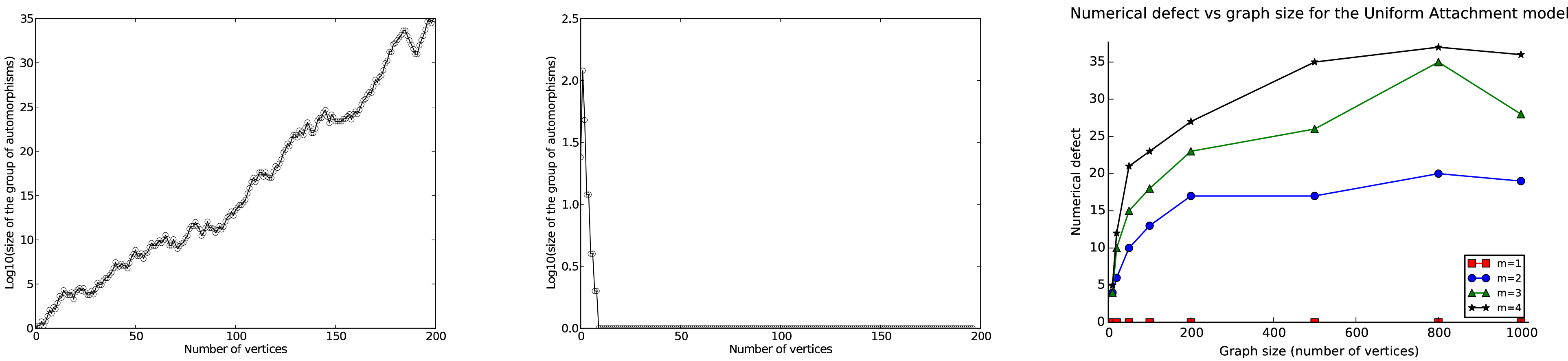

Figure 2: Logarithm of the number of automorphisms versus the number of vertices for $m = 1$ (on the left), $m = 4$ (middle), defect for various m.

Theorem 1 (Symmetry Results for $m = 1, 2$). *Let graph G_n be generated by the preferential model with parameter $m = 1$ or $m = 2$. Then there exists a constant $C > 0$ such that, for n sufficiently large,*

$$\Pr[|\mathrm{Aut}(G_n)| > 1] > C.$$

Conjecture 1. *For $m \geq 3$ a graph G_n generated by the preferential model is asymmetric whp, that is*

$$\Pr[|\mathrm{Aut}(G_n)| > 1] \xrightarrow{n\to\infty} 0.$$

Structural Entropy for Erdös-Rényi Graphs

Theorem 2 (Choi, W.S 2009). *For large n and all p satisfying $\frac{\ln n}{n} \ll p$ and $1-p \gg \frac{\ln n}{n}$ (i.e., the graph is connected w.h.p.),*

$$H_{\mathcal{S}} = \binom{n}{2} h(p) - \log n! + O\left(\frac{\log n}{n^a}\right) = \binom{n}{2} h(p) - n \log n + n \log e + O(\log n), \quad a > 1$$

where $h(p) = -p \log p - (1-p) \log(1-p)$ is the entropy rate.

AEP *for structures:* $\quad 2^{-\binom{n}{2}(h(p)+\varepsilon)+\log n!} \leq P(S) \leq 2^{-\binom{n}{2}(h(p)-\varepsilon)+\log n!}$.

Proof idea:

1. $H_{\mathcal{S}} = H_{\mathcal{G}} - \log n! + \sum_{S \in \mathcal{S}} P(S) \log |\mathrm{Aut}(S)|$.

2. $H_{\mathcal{G}} = \binom{n}{2} h(p)$

3. $\sum_{S \in \mathcal{S}} P(S) \log |\mathrm{Aut}(S)| = o(1)$ by asymmetry of $\mathcal{G}(n,p)$.

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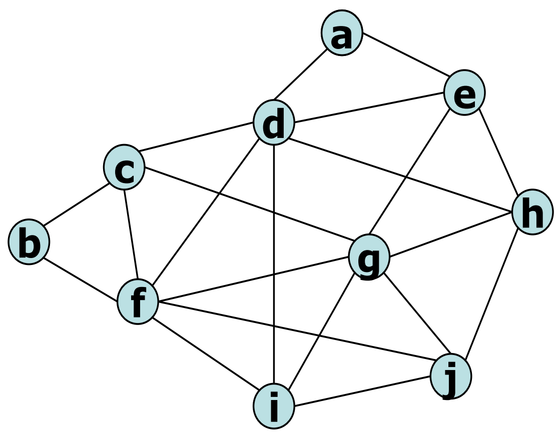
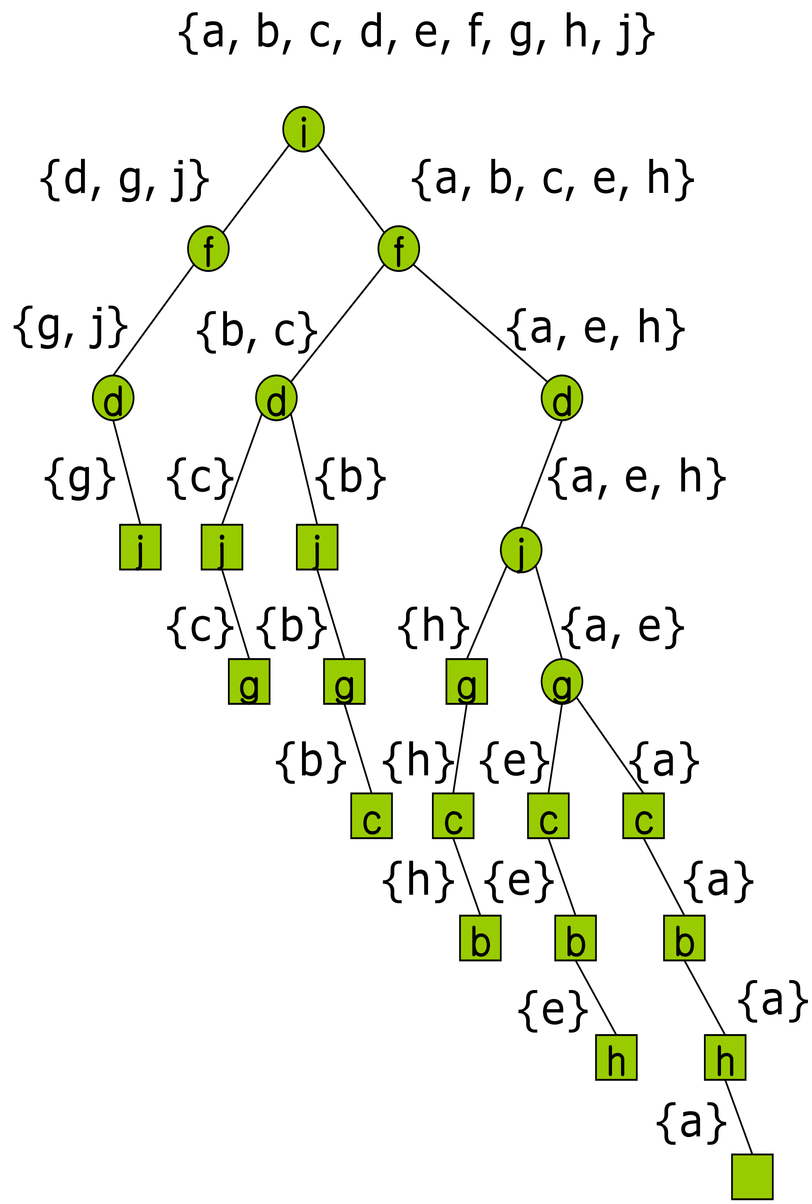
Structural Zip (SZIP) Algorithm

Compression Algorithm called Structural zip, in short SZIP – Demo.





B1 = 010011010000111010 1

B2 = 100101100000010 1

Asymptotic Optimality of SZIP for Erdös-Rényi Graphs

Theorem 3 (Choi, W.S., 2012). *Let $L(S) = |\tilde{B}_1| + |\tilde{B}_2|$ be the code length.*

(i) *For large n,*

$$\mathbf{E}[L(S)] \le \binom{n}{2} h(p) - n \log n + n\,(c + \Phi(\log n)) + o(n),$$

where c is an explicitly computable constant, and $\Phi(x)$ is a fluctuating function with a small amplitude or zero.

(ii) *Furthermore, for any $\varepsilon > 0$,*

$$P\,(L(S) - \mathbf{E}[L(S)] \le \varepsilon n \log n) \ge 1 - o(1).$$

(iii) *The algorithm runs in $O(n+e)$ on average, where e # edges.*

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Table 1: The length of encodings (in bits)

	Networks	# of nodes	# of edges	our algorithm	adjacency matrix	adjacency list	arithmetic coding
Real-world	US Airports	332	2,126	8,118	54,946	38,268	12,991
	Protein interaction (Yeast)	2,361	6,646	46,912	2,785,980	1 59,504	67,488
	Collaboration (Geometry)	6,167	21,535	115,365	19,012, 861	55 9,910	241,811
	Collaboration (Erdös)	6,935	11,857	62,617	24,043,645	308,2 82	147,377
	Genetic interaction (Human)	8,605	26,066	221,199	37,0 18,710	729,848	310,569
	Internet (AS level)	25,881	52,407	301,148	334,900,140	1,572, 210	396,060

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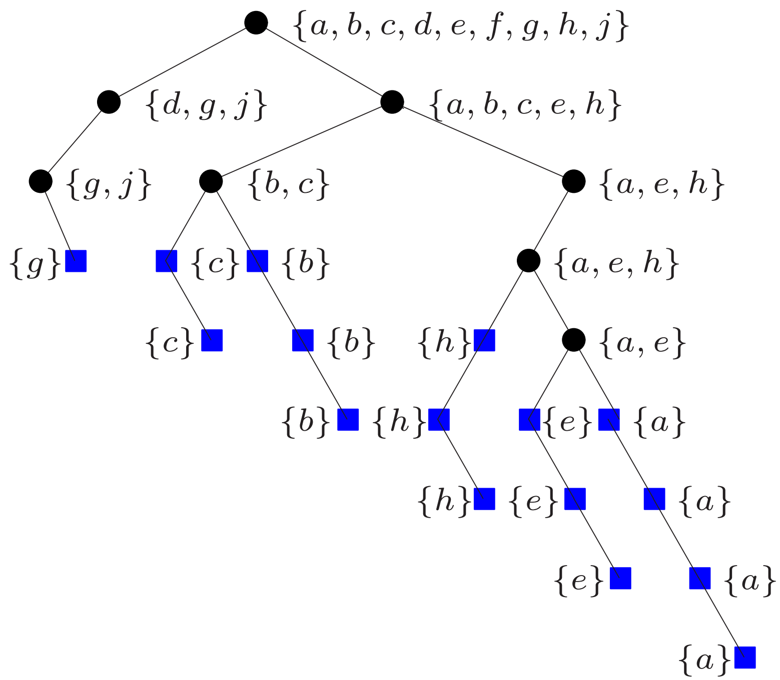
Analysis of Szip: Recurrences for $\mathbf{E}[B_1]$ and $\mathbf{E}[B_2]$

Let N_x be the number of vertices that passed through node x in T_n.

$$|B_1| = \sum_{x \in T_n \text{ and } N_x > 1} \lceil \log(N_x + 1) \rceil$$

$$|B_2| = \sum_{x \in T_n \text{ and } N_x = 1} \lceil \log(N_x + 1) \rceil = \sum_{x \in T_n \text{ and } N_x = 1} 1.$$



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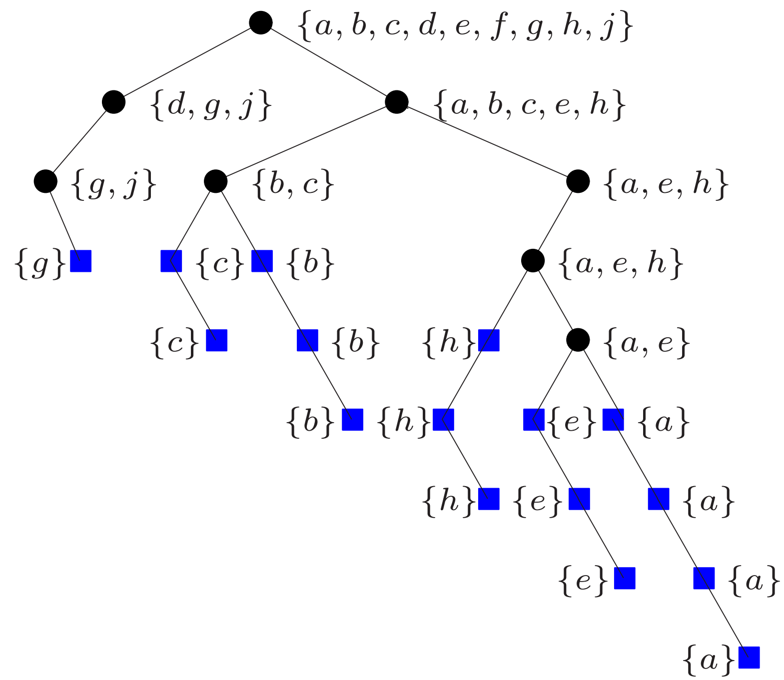
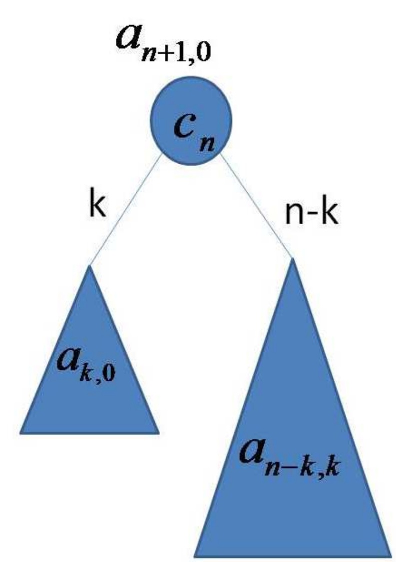


Both $\mathbf{E}[|B_1|]$ and $\mathbf{E}[|B_2|]$ satisfy two-dimensional recurrences for some $d \geq 0$

$$a_{n+1,0} = c_n + \sum_{k=0}^{n} \binom{n}{k} p^k q^{n-k} (a_{k,0} + a_{n-k,k}),$$

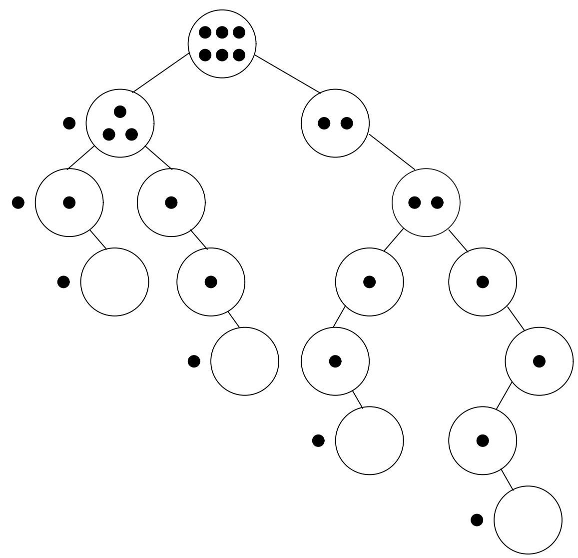
$$a_{n,d} = c_n + \sum_{k=0}^{n} \binom{n}{k} p^k q^{n-k} (a_{k,d-1} + a_{n-k,k+d-1}).$$

for some c_n (e.g., $c_n = \lceil \log(n+1) \rceil$ or $c_n = n$).



Another Look – (n, d)-tries

1. The root of a tree contains n balls.
2. Balls independently move down to the left subtree (with probability p) or the right subtree (with probability $1 - p$).
3. For a non-negative integer d, at level d or greater one ball is removed from the leftmost node.



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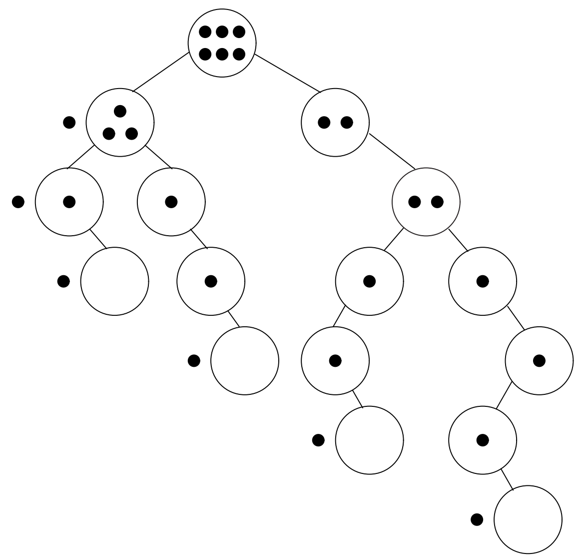

For example for $c_n = n$:

$$a(n,d) = \frac{1}{h} n \log n + \frac{1}{h}\left[\gamma + \frac{h_2}{2h} + \Phi(\log_p n)\right] n + \frac{1}{2h \log p} \log^2 n + \frac{d}{h} \log n + O(1)$$

where $h = -p \log p - q \log q$, $h_2 = p \log^2 p + q \log^2 q$, γ is the Euler constant, and $\Phi(x)$ is the periodic function.

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Structural Binary Symmetric Channel (SBSC)

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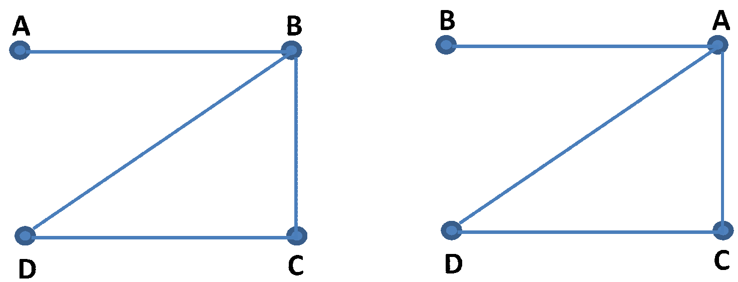
Example: Graph $G_1 = \{A, B, C, D\}$ transmitted with output G_2.



Adjacency matrices are: $G_1 = \begin{vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{vmatrix}$, $G_2 = \begin{vmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{vmatrix}$.

How much structural information can be reliably transmitted over a noisy channel?

Capacity of SBSC

Capacity of SBSC is defined as

$$C = \lim_{n \to \infty} \frac{1}{\binom{n}{2}} \max_{0 \le p \le 1} I(S; S')$$

where $I(S; S')$ is the mutual information between the output structure S' and the input structure S.

Theorem 4. *Capacity of the the structural Binary Symmetric Channel SBSC(ϵ) of Erdös-Rényi graphs is*

$$C = 1 - h(\epsilon)$$

where ε is the error bit rate and

$$h(\varepsilon) = -\varepsilon \log \varepsilon - (1 - \varepsilon) \log(1 - \varepsilon)$$

is the binary entropy.

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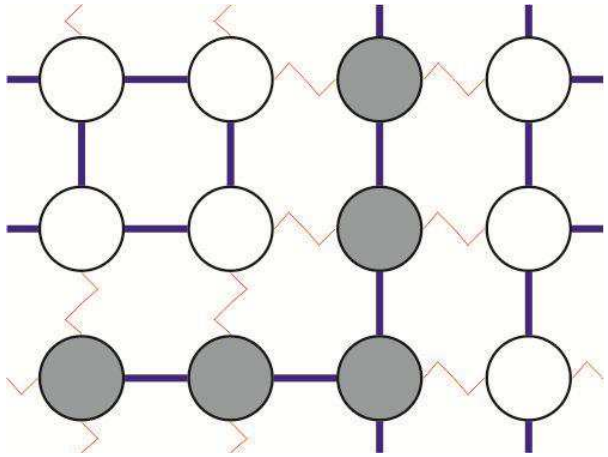
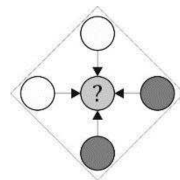
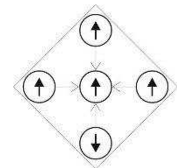
Large Systems with Local Interactions



These local interactions are often represented by shapes and tiles leading to a Markov field.

Markov Field Types:
Two Markov fields have the same type if they have the same empirical distribution.

The method of types is a powerful technique in **information theory**; it reduces calculations of the probability of rare events to combinatorics.

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Let's Begin . . . One-Dimensional Markov Chains

One-Dimensional Markov: Sequences $x^n = x_1 \dots x_n$ over $\mathcal{A} = \{1, 2, \dots, m\}$ alphabet. Define
$\mathcal{T}_n(x^n) = \{y^n : P(x^n) = P(y^n)\}$, and $\mathcal{P}_n := \mathcal{P}_n(m)$ class of distributions.

Consider a **Markov source** with the transition matrix $P = \{p_{ij}\}_{i,j=1}^m$. Then

$$P(x_1^n) = p_{11}^{k_{11}} \cdots p_{mm}^{k_{mm}} = \prod_{i,j \in \mathcal{A}} p_{ij}^{k_{ij}},$$

where k_{ij} is the number of pair symbols (ij) in x_1^n, that is, i followed by j.

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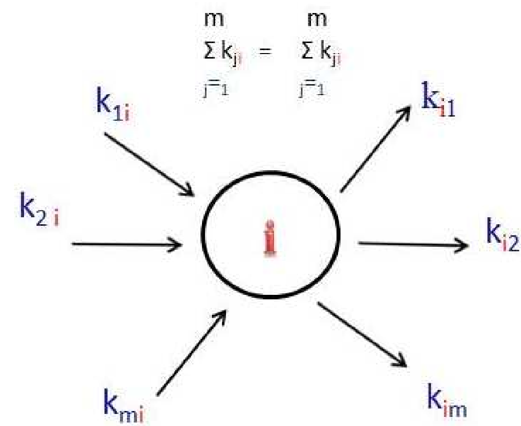
where k_{ij} is the number of pair symbols (ij) in x_1^n, that is, i followed by j.

For circular strings (i.e., after the nth symbol we re-visit the first symbol of x_1^n), the matrix $\mathbf{k} = [k_{ij}]$ satisfies the following constraints denoted as $\boxed{\mathcal{F}_n(m)}$:

$$\sum_{1 \le i,j \le m} k_{ij} = n, \qquad \sum_{j=1}^m k_{ij} = \sum_{j=1}^m k_{ji}$$

For example: m=3

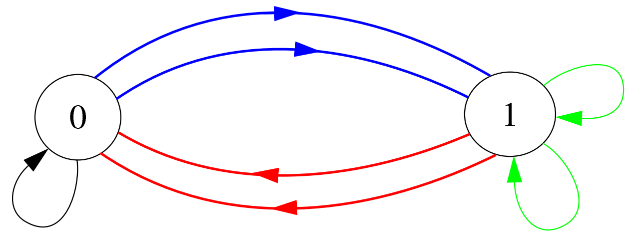
$$k_{11} + k_{12} + k_{13} + k_{21} + k_{22} + k_{23} + k_{31} + k_{32} + k_{33} = n$$
$$k_{12} + k_{13} = k_{21} + k_{31}$$
$$k_{12} + k_{32} = k_{21} + k_{23}$$
$$k_{13} + k_{23} = k_{31} + k_{32}$$



Markov Types and Eulerian Cycles

Example: Let $\mathcal{A} = \{0, 1\}$ and

$$\mathbf{k} = \begin{bmatrix} 1 & 2 \\ 2 & 2 \end{bmatrix}$$



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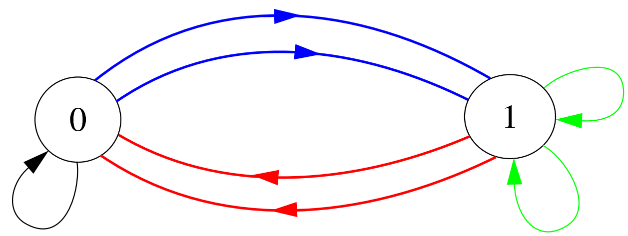
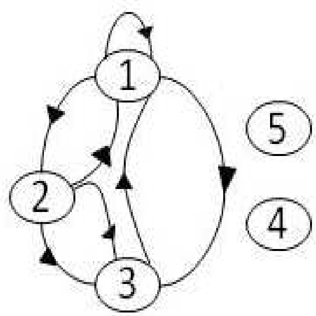
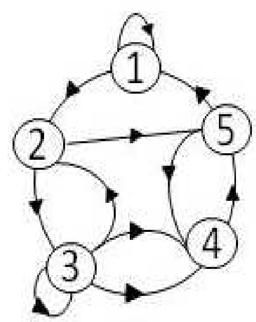


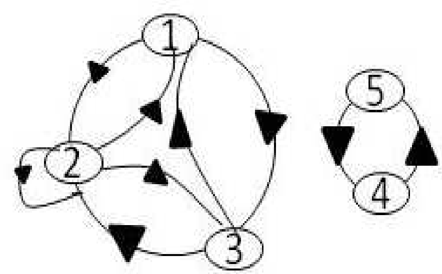
$\mathcal{P}_n(m)$ – Markov types but also ...
a set of all connected Eulerian di-graphs $G = (V(G), E(G))$ such that $V(G) \subseteq \mathcal{A}$ and $|E(G)| = n$.
$\mathcal{E}_n(m)$ – set of connected Eulerian digraphs on $\mathcal{A}$.
$\mathcal{F}_n(m)$ – balanced matrices but also ...
set of (not necessary connected) Eulerian digraphs on $\mathcal{A}$.



$\mathcal{P}_n$



$\mathcal{E}_n$



$\mathcal{F}_n$

Asymptotic equivalence: $|\mathcal{P}_n(m)| = |\mathcal{F}_n(m)| + O(n^{m^2-3m+3}) \sim |\mathcal{E}_n(m)|$.

Main Results for One-Dimensional Markov Chains

Theorem 5. (i) *For fixed m and $n \to \infty$ the number of Markov types is*

$$|\mathcal{P}_n(m)| = d(m)\frac{n^{m^2-m}}{(m^2-m)!} + O(n^{m^2-m-1})$$

where $d(m)$ is a constant that also can be expressed as

$$d(m) = \frac{1}{(2\pi)^{m-1}} \underbrace{\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty}}_{(m-1)-fold} \prod_{j=1}^{m-1} \frac{1}{1+\varphi_j^2} \cdot \prod_{k \neq \ell} \frac{1}{1+(\varphi_k - \varphi_\ell)^2} d\varphi_1 d\varphi_2 \cdots d\varphi_{m-1}.$$

(ii) *When $m \to \infty$ we find that*

$$|\mathcal{P}_n(m)| \sim \frac{\sqrt{2}m^{3m/2}e^{m^2}}{m^{2m^2}2^m\pi^{m/2}} \cdot n^{m^2-m}$$

provided that $m^4 = o(n)$.

Example. The coefficients at n^{m^2-m} are very small.
For $m = 4$ the coefficient is $1.767043356 \; 10^{-11}$.

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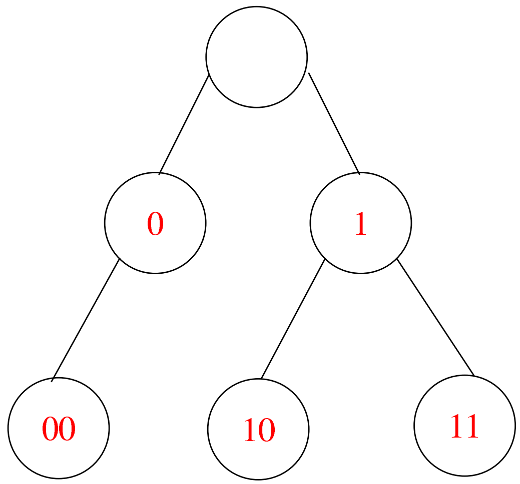
3. Sequence-Structure Protein Folding Channel

Universal Types (Still One-Dimensional)

Seroussi introduced in 2003 **universal types** for stationary ergodic sources:

(0) (1) (00) (10) (11)
(1) (0) (10) (11) (00)



(0) (1) (00) (01) (11)
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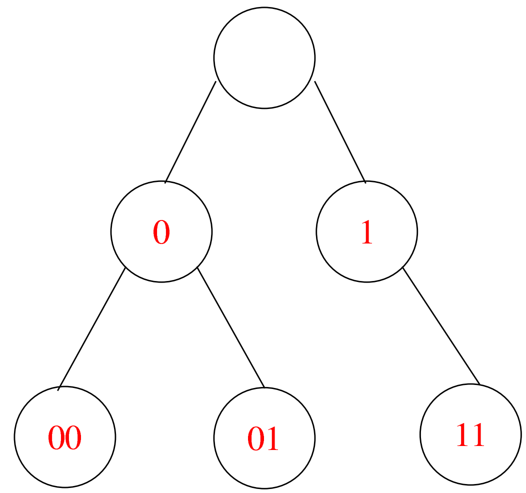


p = path length = 8

Lempel-Ziv'78 parsing scheme of a sequence of length p can be represented by a **binary tree of path length** p.
– $\mathcal{T}_p$ be the set of binary trees with the path length equal to p.

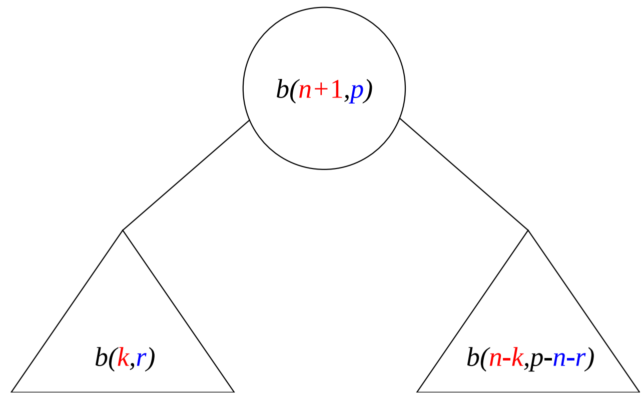
> $\#$ **universal types** over $\mathcal{A}^p$ $\equiv$ $|\mathcal{T}_p|$: $\#$ of trees of a given path p.

How to enumerate binary trees of a given path length p?

Enumeration of Binary Trees: $\mathcal{T}_n$ vs $\mathcal{T}_p$

Let $b(n,p)$ be the number of binary trees with n nodes and path length p. It satisfies:

$$b(n,p) = \sum_{k+\ell=n-1} \sum_{r+s+n-1=p} b(k,r)b(\ell,s)$$



Define $B_n(w) = \sum_{p=0}^{\infty} b(n,p)w^p$, and $B(z,w) = \sum_{n=0}^{\infty} z^n B_n(w)$. Then

$$\boxed{B(z,w) = 1 + zB^2(zw,w)}$$

This **functional equation** is asymmetric with respect to z and w.

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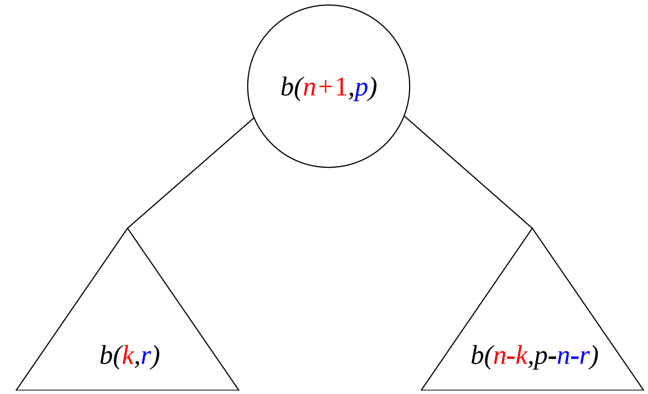

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This **functional equation** is asymmetric with respect to z and w.

We want to study the number of trees in $\mathcal{T}_p$ (of a given path length p). Observe

$$|\mathcal{T}_p| = \sum_{n \geq 0} b(n,p) = [w^p]B(1,w).$$

We set $z = 1$ in the functional equation leading to

$$\boxed{B(1,w) = 1 + B^2(w,w)}$$

which is not algebraically solvable.

Number of Trees with a Given Path Length

These results are obtained using the WKB method of applied mathematics.

Seroussi (2004) and Knessl & W.S (2004) prove that (c_1, c_2 are constants)

$$|\mathcal{T}_p| = \frac{1}{(\log_2 p)\sqrt{\pi p}} 2^{\frac{2p}{\log_2 p}\left(1+c_1 \log^{-2/3} p + c_2 \log^{-1} p + O(\log^{-4/3} p)\right)}.$$

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When randomly selecting a tree from $\mathcal{T}_p$ we may define: N_p, the number of nodes in the $\mathcal{T}_p$-model. Surprisingly, we can prove that N_p is asymptotically normal, that is,

$$\Pr\{N_p = n\} = \frac{b(n,p)}{\sum_{n=0}^{\infty} b(n,p)} \sim \frac{1}{\sqrt{2\pi \mathbf{Var}[N_p]}} \exp\left[-\frac{(n-\mathbf{E}[N_p])^2}{2\mathbf{Var}[N_p]}\right]$$

where

$$\mathbf{E}[N_p] \sim \frac{p}{\log_2 p}, \qquad \mathbf{Var}[N_p] \sim \frac{p}{\log_2 p^{5/3}} \frac{(\log 2) A_0}{6(2^{1/3}}$$

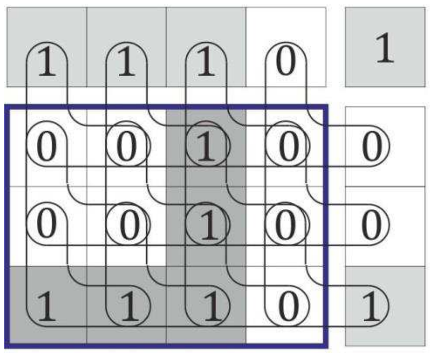
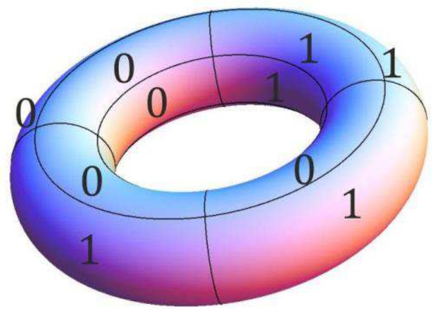
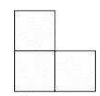
where A_0 is a constant.

Outline Update

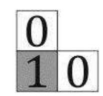
1. Structural Compression
2. Structure of Markov Fields
   - One Dimensional Markov Types
   - Markov Fields and Tilings
3. Sequence-Structure Protein Folding Channel

(Cyclic) Markov Fields and Tilings

d-Dimensional Markov Fields:
Consider a d-dimensional box $(n_1, \ldots, n_d)$ with $N = n_1 \cdots n_d$.
A circular representation of such a box is a **torus** that we denote as $\mathcal{O}_{\mathbf{n}}$.
The shape of interaction is $S \subset \mathbb{Z}^d$.
A tile t is $t : S \to \mathcal{A}$ and $T = \{t : S \to \mathcal{A}\}$.

shape

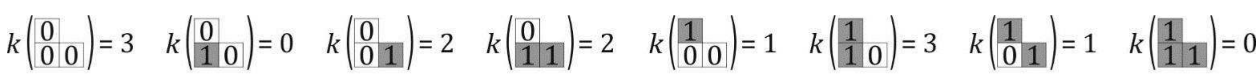


tile

Markov Field Type $\mathcal{X}^{\mathbf{n}} = \{x^{\mathbf{n}} : \mathcal{O}_{\mathbf{n}} \to \mathcal{A}\}$:
Define the frequency vector of dimension $D = |T| = m^{|S|}$:

$$k(t) \equiv k_S(t) = |\{\mathbf{s} \in \mathcal{O}_{\mathbf{n}} \; : \; x|_{S+\mathbf{s}} = t\}| \,, \qquad t \in T.$$

Example:



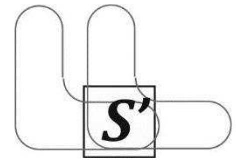
3 + 0 + 2 + 2 + 1 + 3 + 1 + 0 = 12 size of torus

A set of Markov field types or tile types is:

$$\mathcal{P}_{\mathbf{n}}(m, S) = \{\mathbf{k} : \exists_{x \in \mathcal{X}_{\mathbf{n}}} \, x^{\mathbf{n}} \text{is of type } \mathbf{k}\}.$$

Conservation Laws

Conservation Laws:



$$\forall_{\emptyset \neq S' \subset S,\ \mathbf{s} \in \mathbb{Z}^d : (S'+\mathbf{s}) \subset S}\ \forall_{t' : S' \to \mathcal{A}} \quad k_{S'}(t') = k_{S'+\mathbf{s}}(t')$$

with shift $\mathbf{s} \in \mathbb{Z}^d$ subject to $(S' + \mathbf{s}) \subset S$.

Example:

$$k\begin{pmatrix} 0 & \\ 0 & \boxed{0} \end{pmatrix} + k\begin{pmatrix} 0 & \\ 1 & \boxed{0} \end{pmatrix} + k\begin{pmatrix} 1 & \\ 0 & \boxed{0} \end{pmatrix} + k\begin{pmatrix} 1 & \\ 1 & \boxed{0} \end{pmatrix} = \boxed{k\begin{pmatrix} * & \\ * & \boxed{0} \end{pmatrix} = k\begin{pmatrix} * & \\ \boxed{0} & * \end{pmatrix}} = k\begin{pmatrix} 0 & \\ \boxed{0} & 0 \end{pmatrix} + k\begin{pmatrix} 0 & \\ \boxed{0} & 1 \end{pmatrix} + k\begin{pmatrix} 1 & \\ \boxed{0} & 0 \end{pmatrix} + k\begin{pmatrix} 1 & \\ \boxed{0} & 1 \end{pmatrix}$$

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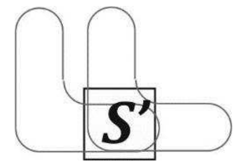

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Example:

$$k\left(\begin{array}{cc} 0 & \\ 0 & 0 \end{array}\right) + k\left(\begin{array}{cc} 0 & \\ 1 & 0 \end{array}\right) + k\left(\begin{array}{cc} 1 & \\ 0 & 0 \end{array}\right) + k\left(\begin{array}{cc} 1 & \\ 1 & 0 \end{array}\right) = \boxed{k\left(\begin{array}{cc} * & \\ * & 0 \end{array}\right) = k\left(\begin{array}{cc} * & \\ 0 & * \end{array}\right)} = k\left(\begin{array}{cc} 0 & \\ 0 & 0 \end{array}\right) + k\left(\begin{array}{cc} 0 & \\ 0 & 1 \end{array}\right) + k\left(\begin{array}{cc} 1 & \\ 0 & 0 \end{array}\right) + k\left(\begin{array}{cc} 1 & \\ 0 & 1 \end{array}\right)$$

The conservation laws can be viewed as *linear equations* with a $1 \times D$ row denoted as $C(\{(S', \mathrm{s}, t')\})$.
The matrix C^* is hugely over determined! Our goal is to find C such that the conservation laws can be written as

$$C\mathbf{k} = \mathbf{0}.$$

Example 1. $d = 1$*-dimensional Markov over* $\mathcal{A} = \{1, 2\}$.
Tiles are $((11), (21), (12), (22))$ and the conservation laws are

$$\begin{aligned} k(11) + k(12) &= k(1*) = k(*1) = k(11) + k(21), \\ k(21) + k(22) &= k(2*) = k(*2) = k(12) + k(22). \end{aligned}$$

leading to **one conservation law** $k(12) - k(21) = 0$ that in the matrix form is

$$(0, -1, 1, 0) \cdot \mathbf{k} = \mathbf{0}.$$

Dimension of the Frequency Vectors

The conservation laws make the vector count $\mathbf{k} \in \mathbb{Z}^D$ to reside in a space of dimensionality

$$\boxed{\mu = D - \mathrm{rk}(C) - 1.}$$

where $\mathrm{rk}(C)$ is the rank of matrix C. I

Theorem 6. *The matrix C has rank*

$$\mathrm{rk}(C) = \sum_{S' \in \mathcal{S}^0} (|\{\mathbf{s} : (S' + \mathbf{s}) \subset S\}| - 1)(m-1)^{|S'|}$$

and consists of a complete set of linearly independent rows.
In particular, for the box shape $S = I_{l_1} \times I_{l_2} \times \ldots \times I_{l_d}$ we find

$$\mu = D - 1 - \mathrm{rk}(C) = \sum_{\mathbf{s} \in \{0,1\}^d} m^{\prod_i (l_i - s_i)} \cdot (-1)^{\sum_i s_i}.$$

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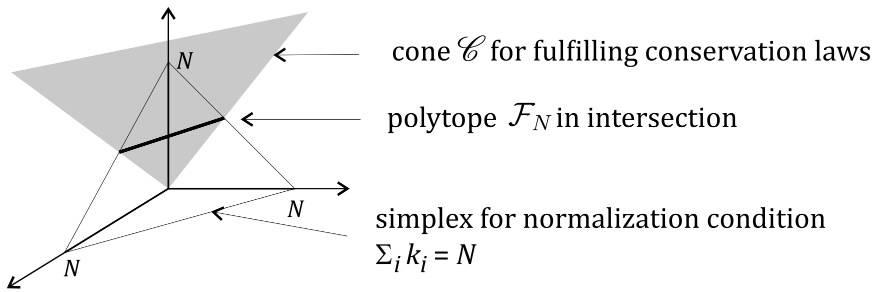
Example: For $d = 2$ and a 2×2 square shape we have $\mu = m^4 - 2m^2 + m$, while for a 3×2 rectangular shape we find $\mu = m^6 - m^4 - m^3 + m^2$.

Geometry

We view the count vector $\mathbf{k} = \{k(t)\}_{t \in T}$ in the $D = m^{|S|}$ space.



$$\mathscr{C} = \{\mathbf{k} \in \mathbb{N}^D \ : \ C_m(S) \cdot \mathbf{k} = \mathbf{0}\}$$
$$\mathcal{F} = \{\mathbf{k} \in \mathscr{C} : \textstyle\sum_i k_i = N\}$$
$$\hat{\mathcal{F}} = \{\hat{\mathbf{k}} \in \{(\mathbb{R}^D_+ \ : \ C \cdot \hat{\mathbf{k}} = \mathbf{0}, \ \textstyle\sum_i \hat{k}_i = 1\}$$
$$\mathcal{F}_N = \{N\hat{\mathbf{k}} : \hat{\mathbf{k}} \in \hat{\mathcal{F}}, \ N\hat{\mathbf{k}} \in \mathbb{Z}^D\}$$

The polytope $\mathcal{F}_N$ is of dimension μ.

Topological Closure of (normalized) $\hat{\mathcal{P}}$ is a convex subset of $\hat{\mathcal{F}}$.

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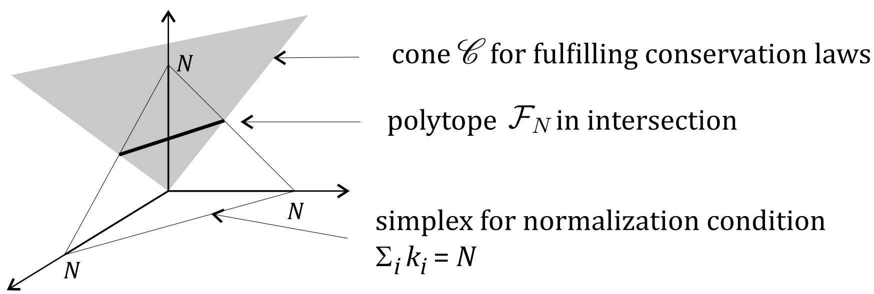

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Topological Closure of (normalized) $\hat{\mathcal{P}}$ is a convex subset of $\hat{\mathcal{F}}$.

The lattice $\mathcal{F}_N$ consists of all integer points inside $\hat{\mathcal{F}}$ scaled by N.
Volume of $\mathcal{F}_N$ is of order N^μ with integer points growing as N^μ.

Theorem 7 (Ehrhart, 1967). *If $\hat{\mathcal{F}}$ is a convex polytope with vertices in $\mathbb{Q}^D$, where $\mathbb{Q}$ is the set of rational numbers, then that $c_{\mu,j} \neq 0$ for some j*

$$|\mathcal{F}_N| = a_{\mu,j} N^\mu + a_{\mu-1,j} N^{\mu-1} + \ldots a_{0,j} \quad N \equiv j \pmod{p}.$$

Main Result for Markov Types

Theorem 8. *Consider the torus* $\mathcal{O}_{\mathbf{n}}$*. There exists* $0 < c^{min} \leq c^{max}$ *such that*

$$c^{min} N^{\mu} \leq |\mathcal{P}_{\mathbf{n}}(m, S)| \leq c^{max} N^{\mu}$$

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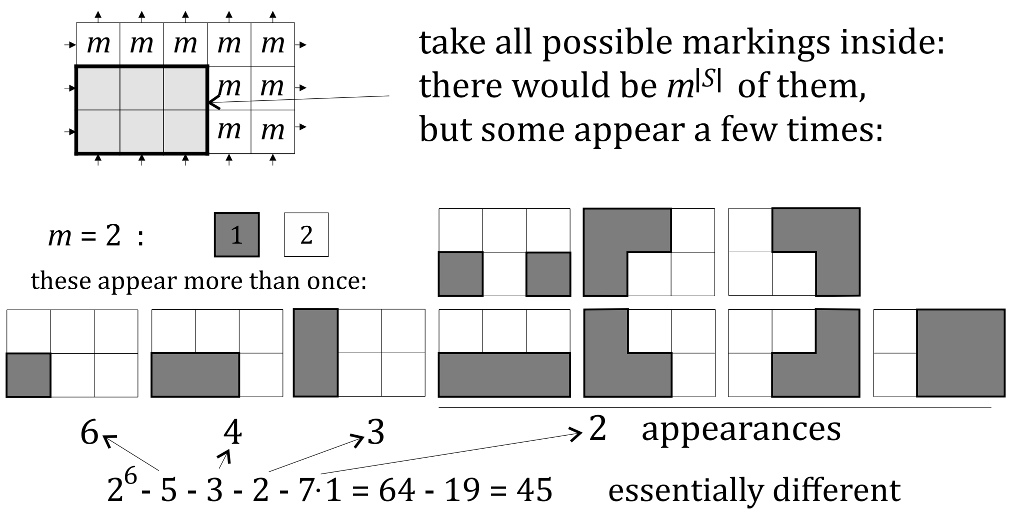
Lemma 3. *There exist* $\mu + 1$ *linearly independent periodic tilings.*



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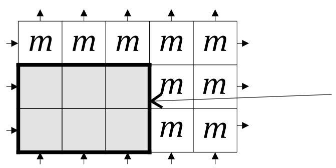
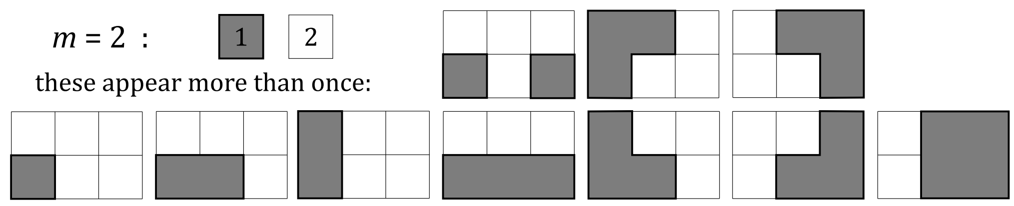


take all possible markings inside:
there would be $m^{|S|}$ of them,
but some appear a few times:

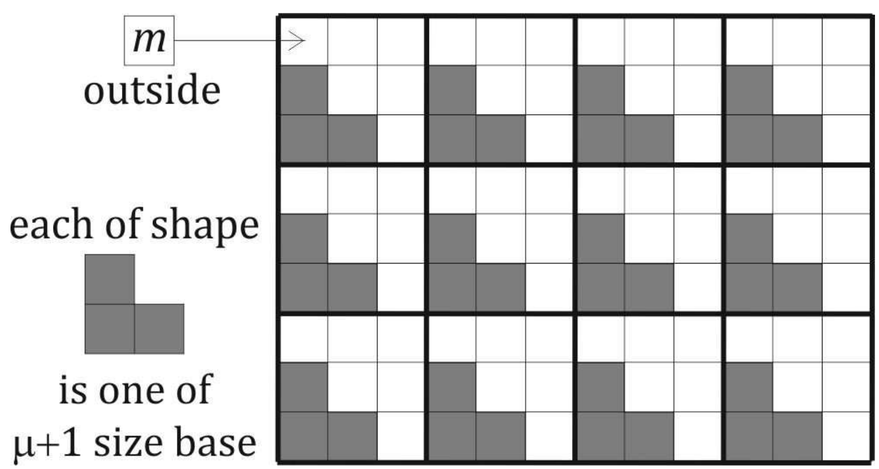
$m = 2$:



these appear more than once:

6 4 3 2 appearances

$2^6 - 5 - 3 - 2 - 7 \cdot 1 = 64 - 19 = 45$ essentially different



$$\frac{a_1 \hat{\mathbf{k}}^1 + .. + a_{\mu+1} \hat{\mathbf{k}}^{\mu+1}}{a_1 + \cdots + a_{\mu+1}} : \forall_i \, a_i \in \mathbb{N}, \; \sum_i a_i = N$$

$$\binom{N+\mu-1}{\mu} = O(N^{\mu})$$

Outline Update

1. Structural Compression
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3. Sequence-Structure Protein Folding Channel

Sequence-Structure Channel

$$p(f|s) := \frac{e^{-\beta\mathcal{E}(s,f)}}{Z(s,\beta)} \qquad Z(s,\beta) := \sum_{f\in\mathcal{F}} e^{-\beta\mathcal{E}(s,f)}$$

Sequence-Structure Channel

$$p(f|s) := \frac{e^{-\beta\mathcal{E}(s,f)}}{Z(s,\beta)} \qquad\qquad Z(s,\beta) := \sum_{f\in\mathcal{F}} e^{-\beta\mathcal{E}(s,f)}$$

Capacity:

$$C = \max_{p(s)} I(S;F) \sim \log|F_N| - \min_{p(s)} H(F|S).$$

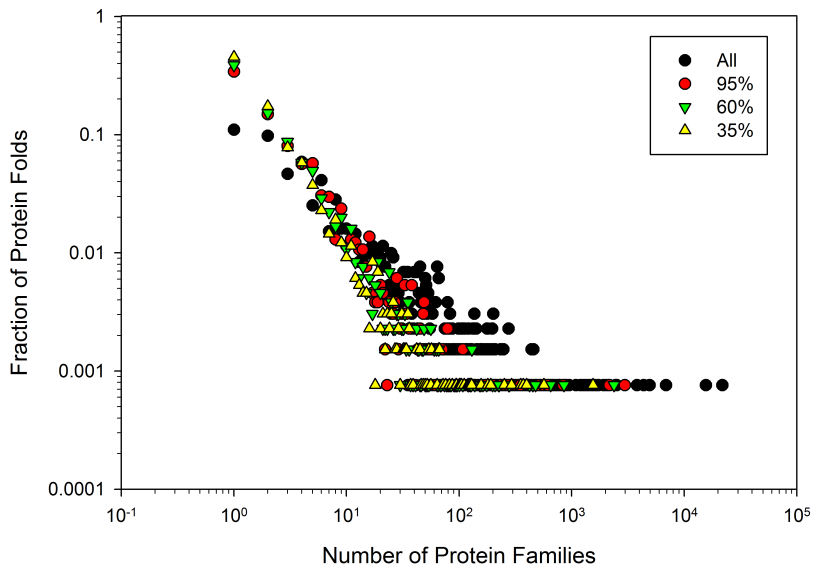
where F_N: set of self-avoiding walks of length N.

Conditional Entropy

$$H(S|F) = \mathbf{E}[\log Z(S,\beta)] + \beta\mathbf{E}[\mathcal{E}(F,S)]$$

where $\mathcal{E}(F,S)$ is energy of a walk F over sequence s.
Clearly, $\mathbf{E}[\mathcal{E}(F,S)] = N\cdot\alpha(S)$ for some $\alpha(S)$.

Motivation & Experimental Results



Protein Folds in Nature

Probability of protein folds vs. sequence rank.

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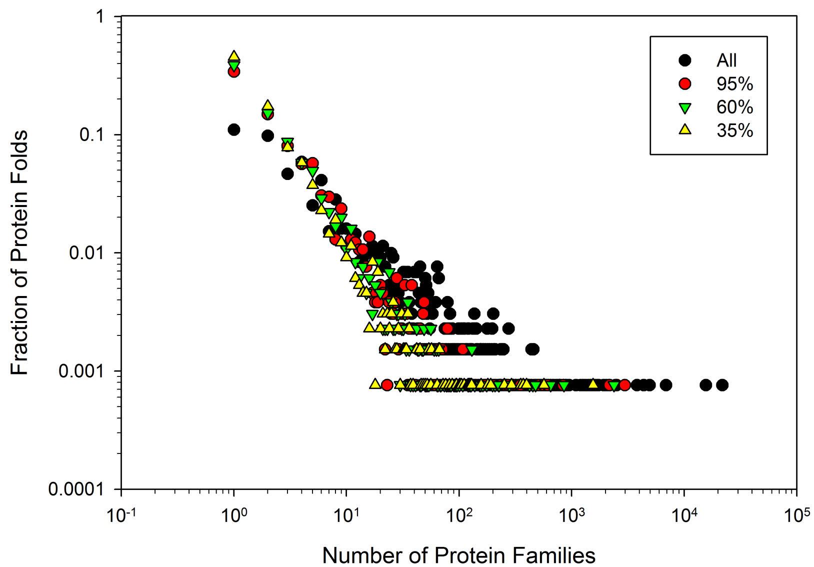
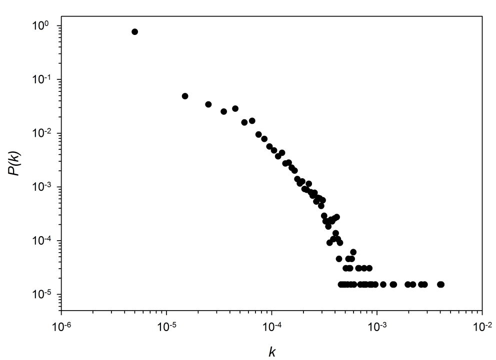
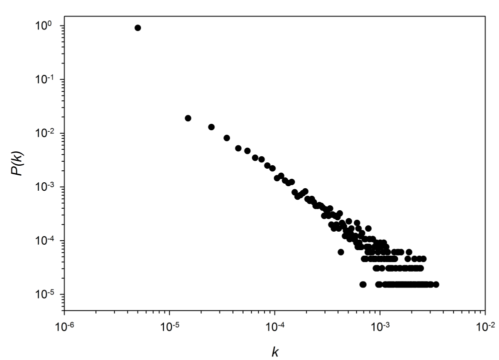


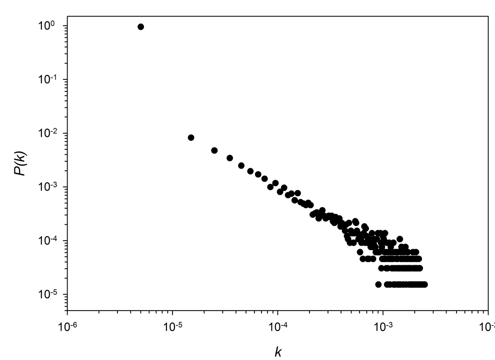
Protein Folds in Nature

Probability of protein folds vs. sequence rank.

Optimal input distribution from **Blahut-Arimoto** algorithm:







Phase Transition

Define free energy $\gamma(\beta, S)$ as

$$\gamma(\beta, S) = \lim_{N \to \infty} \frac{\mathbf{E}[\log Z(S, \beta)]}{\log |\mathcal{F}_N|}.$$

By sub-multiplicative property of F_N we can prove there exists μ such that

$$\frac{\log |F_N|}{N} \xrightarrow{N \to \infty} \log \mu.$$

Then

$$\mathbf{E} \log Z(S, \beta) \sim \log |F_N| \cdot \gamma(\beta, S) \sim N \log \mu \cdot \gamma(\beta, S)$$

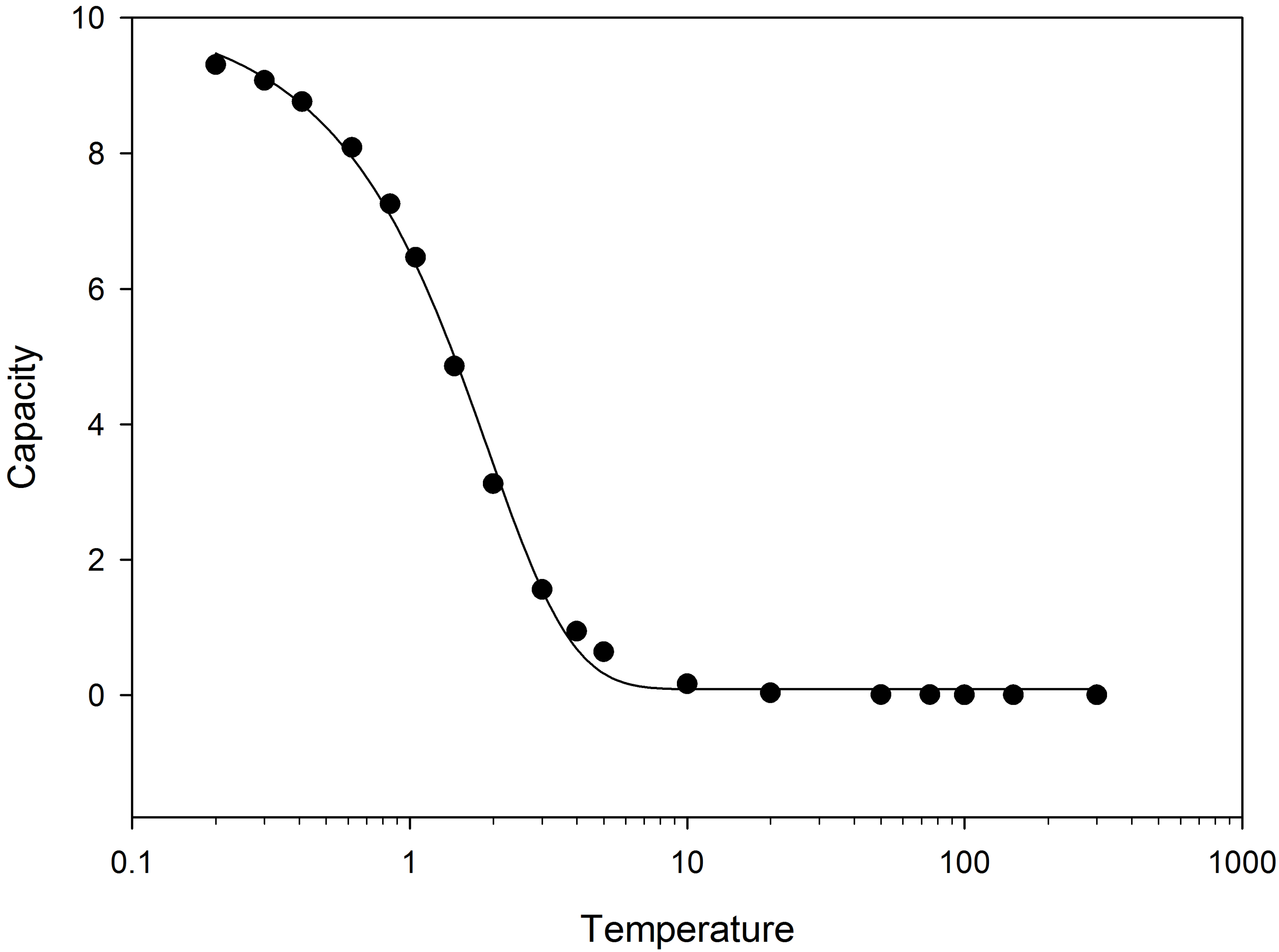
leading to

$$\boxed{H(F|S) \sim N[\gamma(\beta, S) \log \mu + \beta\alpha(S)]}$$

Phase transition of the free energy $\gamma(\beta, S)$ (hence capacity C) leads to

$$\log \mu \cdot \gamma(\beta, S) = \begin{cases} \log \mu - \beta\alpha + \frac{1}{2}\sigma^2\beta^2 & \beta < \frac{\sqrt{2 \log \mu}}{\sigma} \\ \beta\sqrt{2\sigma^2 \log \mu} - \beta\alpha & \beta \geq \frac{\sqrt{2 \log \mu}}{\sigma} \end{cases}$$

Experimental Confirmation of the Phase Transition



That's It

THANK YOU