# Exponential random graphs

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## Shi Zhou and Raúl Mondragón

- *Accurately modeling the internet topology* Phys. Rev. E **70** 066108 (2004)
- Network parameters:
  - *number of nodes, number of links, average degree, exponent of power law, rich-club connectivity, maximum degree, degree distribution, characteristic path length, average triangle coefficient, maximum triangle coefficient, average quadrangle coefficient, maximum quadrangle coefficient, average $k_{mn}$, average betweenness, maximum betweenness. . .*
  - *girth, spectrum, . . .*



## Motivation

- we use many random graph models in network applications. . .
- but rarely specify the statistical ensemble precisely
- so even the averages we compute are suspect
- and even the famous Barabási-Albert scale-free model has known problems

we need a unified, rigorous framework

- related ideas in earlier literature:
  - *Markov random fields*
  - *$p^*$ models of social networks*
  - *Ising-type models in physics*
  - *agricultural field trials*
  - *image processing*
  - *. . .*



## Dependency graphs (Frank, Strauss, Besag, . . . )

- consider a random vector $X=(X_1,X_2,\dots,X_m)$
- $P(x)=\exp(Q(x))/\sum\exp Q(x) \Leftrightarrow Q(x)=\log P(x)+$const
  - *only restriction $P(x)>0 \quad \forall x$*
- let $D$ be the *dependency graph* of $X$; i.e. $i\sim j \Leftrightarrow x_i$ not independent of $x_j$
  - *e.g. all $x_i$ independent: empty graph*
  - *e.g. Markov chain: line graph*
  - *e.g. multivariate Gaussian: complete graph (generically)*
- inclusion-exclusion principle $Q(x)=\sum_{s\subseteq\{1,2,\dots,m\}}\lambda_s(x_s)$
  - *$x_s\equiv$ components of $x$ corresponding to elements of $s$*
  - *Pr $[\cap_i A_i]=\sum_i$ Pr $[A_i]-\sum_{i<j}$ Pr $[A_i\cup A_j]+\dots$*
- Hammersley-Clifford theorem: $\lambda_s\equiv 0$ unless $s$ is a clique of $D$
  - *a clique is a complete subgraph*

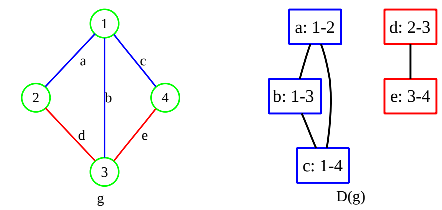


## Markov graphs

- to apply to a graph $g$ with edge dependencies, let $X$ be the edge indicator functions
- this defines the dependency graph $D(g)$ of $g$: $D(g)$ contains and edge $(i,j)$ if $X_i$ and $X_j$ $(i\neq j)$ are dependent
- definition: $g$ is *Markov* if $D(g)$ contains no edge between edges which are disjoint in $E(g)$
- in other words, edges can only 'interact' if they share a common end-point



## Markov graph example $(n=4,m=5)$




- cliques: $\{\{a\},\{b\},\{c\},\{d\},\{e\},\{a,b\},\{b,c\},\{a,c\},\{d,e\},\{a,b,c\}\}$
- thus

$$\begin{aligned}Q(x) &= \lambda_a(x_a)+\lambda_b(x_b)+\lambda_c(x_c)+\lambda_d(x_d)+\lambda_e(x_e)\\ &+ \lambda_{ab}(x_a,x_b)+\lambda_{bc}(x_b,x_c)+\lambda_{ac}(x_a,x_c)+\lambda_{de}(x_d,x_e)\\ &+ \lambda_{abc}(x_a,x_b,x_c)\end{aligned}$$



## Homogeneous Markov graphs 1

- if we require all isomorphic graphs to have the same probability, then a further simplification results:
- let $t(g)$ be the number of triangles in $g$
- let $s_k(g)$ be the number of $k$-stars in $g$
- then $P(g)$ can *only* depend on $t(g)$ and $s_k(g)$, in the form

$$P_\beta(g)=\frac{1}{Z(\beta)}\exp\left[\beta_0 t(g)+\sum_{k=1}^{n-1}\beta_k\, s_k(g)\right]$$

where $\beta_i$ are fixed parameters

- here $Z(\beta)=\sum_g \exp\left[\beta_0 t(g)+\sum_{k=1}^{n-1}\beta_k\, s_k(g)\right]$



## Homogeneous Markov graphs 2

- alternatively, we may use $d_j$, the number of nodes of degree $j$ $(s_k(g)\equiv\sum_{j\geqslant k}\binom{j}{k}d_j(g))$
- and let $\theta_k(g)\equiv\sum_{k\leqslant j}\binom{j}{k}\beta_k$; then

$$P_\theta(g)=\frac{1}{Z(\theta)}\exp\left[\theta_0 t(g)+\sum_{j=1}^{n-1}\theta_j\, d_j(g)\right]$$

- in other words, the Hamiltonian *can only be* a linear function of the number of triangles and $k$-stars
- note: if $A$ if the adjacency matrix of $g$, then $m(g)=d_1(g)=\operatorname{tr}\left(A^2\right)/2$ is the number of edges and $t(g)=\operatorname{tr}\left(A^3\right)/6$



## Exponential random graphs

- fix a number of nodes $n$
- consider the set $G(n)$ of all graphs on $n$ nodes
- we will assign to each $g\in G(n)$ a probability $P(g)$
- let $x=\{x_1,x_2,\dots\}$ be a set of functions on $G(n)$ representing properties we are interested in, for example
  - *$x_1(g)$=number of edges*
  - *$x_2(g)$=number of nodes of degree 3*
  - *$x_3(g)$=number of triangles*
- we then assign the probabilities $P$ by

$$P_\theta(g)=\frac{1}{Z(\theta)}\exp\left(\theta_1 x_1+\theta_2 x_2+\dots\right)$$

where $Z(\theta)=\sum_{g\in G(n)}\exp\left(\theta_1 x_1+\theta_2 x_2+\dots\right)$

## Statistical mechanics

- Hamiltonian: $H(\theta, g) = \sum_i \theta_i x_i(g)$
- probability of $g$: $P_\theta(g) = \exp(H(\theta, g))/Z(\theta)$
- partition function: $Z(\theta) = \sum_g \exp(H(\theta, g))$
- entropy $S(\theta) = -\sum_g P_\theta(g) \log(P_\theta(g))$
- $S$ is maximized by our choice of $P$
- free energy: $F(\theta) = \log(Z(\theta))$
- $\mathsf{E}[x_i] = \frac{\mathsf{d}F(\theta)}{\mathsf{d}\theta_i}$



## Exactly soluble example - Bernoulli model $G\{n,p\}$

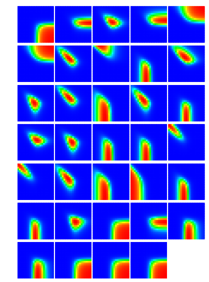
- $g \in G\{n,p\}$ has $n$ nodes and each possible edge appears independently with fixed probability $p$
- let $x(g) =$ number of edges in graph $g$
- $H(\theta, g) = \theta\, m(g)$
- $Z(\theta) = (1+\exp(-\theta))^{\binom{n}{2}}$
- $p = 1/(1+\exp(\theta))$
- $F(\theta) = \binom{n}{2} \log(1+\exp(-\theta))$
- which gives $P_p(g) = \binom{n}{m(g)} p^{m(g)} (1-p)^{\binom{n}{2}-m(g)}$ as expected
- $\mathsf{E}[x] = m = \binom{n}{2} p$



## Example - exact likelihood for all 5-node graphs

Likelihood of parameters, given a graph: $L(\theta|g) \propto P_\theta(g)$. (Loglikelihood: $l(\theta|g) \equiv \log P_\theta(g) + \text{const.}$)

Each figure shows the likelihood for one of the 34 graphs, the parameters corresponding to the number of nodes of degrees one and two. i.e. $H_\theta(g) = \theta_1 d_1(g) + \theta_2 d_2(g)$





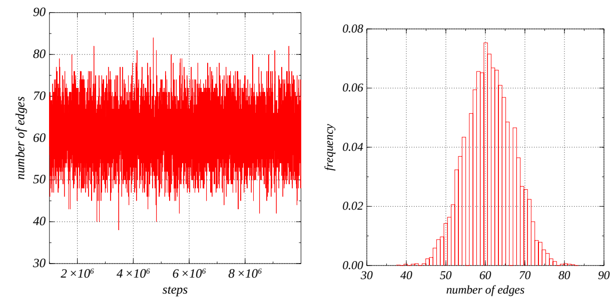
## Metropolis simulation

- works by defining a random walk in $G$ which has equilibrium distribution equal to our desired $P$
- typically we choose a pair of nodes, and then flip its state depending on whether the flip is energetically favourable
  - *(1) choose a proposal dyad $i, j \in N(g)$ uniformly at random*
  - *(2) compute the energy change $\delta H$ that would occur if the dyad $(i, j)$ were flipped*
  - *(3) if $\delta H$ or $u < \exp(\delta H)$, $u \sim U(0,1)$, then accept the proposal; i.e. flip the edge*
  - *(4) go to (1)*
- estimate loglikelihood by (where $x$ is the vector of graph statistics, $\theta_{\text{ref}}$ a reference value of graph parameters (hopefully close to the true ones) and $x_{\text{data}}$ the statistics from the data):

$$l(\theta) - l(\theta_{\text{ref}}) \approx -\log \langle \exp[(l(\theta) - l(\theta_{\text{ref}})) \cdot (x(t) - x_{\text{data}})] \rangle$$



## Metropolis simulation example

- 18 nodes; graph shows fluctuations in $m(g)$
- 




## Metropolised independence sampling (MIS) 1

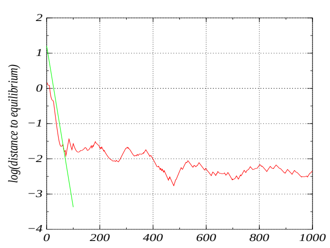
- consider the target distribution $\pi_\theta(j) = \exp(j \log\theta)/Z(\theta)$, $Z(\theta) \equiv (1-\theta^n)/(1-\theta)$ on the set $\{0, 1, 2, \ldots, n-1\}$
- an MIS scheme is
  - *(0) start at $x = n-1$*
  - *(1) choose a proposal $y \in X$ uniformly at random*
  - *(2) if $y < x$ or $u < \theta^{y-x}$, $u \sim U(0,1)$, then accept the proposal; i.e. set $x = y$*
  - *(3) go to (1)*
- note that this scheme ignores the current position $x$ and assumes no knowledge of $\pi$. In general, we can do better



## Metropolised independence sampling 2

- for this example, it can be proven [Diaconis & Saloff-Coste 1998] that

$$4\,||M^k - \pi|| \leqslant \frac{1}{(1-\theta)(\theta^{n-1})} \left(1 - \frac{1}{n}\right)^{2k}$$






## What next?

- directed graphs
- perturbation theory (around Bernoulli model?)
- more rapidly converging sampling schemes
- parameter estimation for real examples by maximum likelihood (e.g. internet AS graph)
- . . . ?



## Some references (amongst many)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