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*
  - . . .

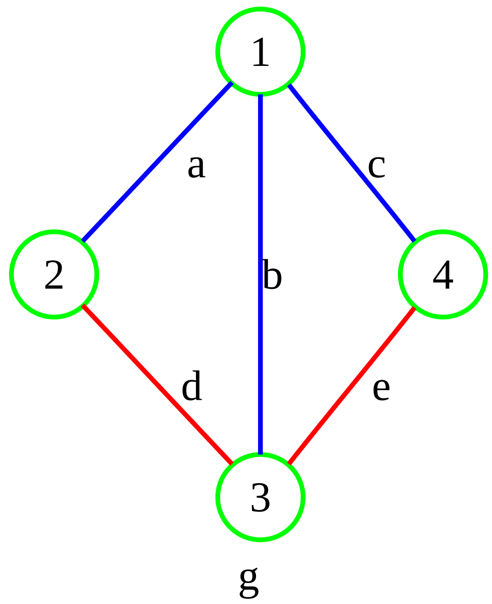
Dependency graphs (Frank, Strauss, Besag, . . .)

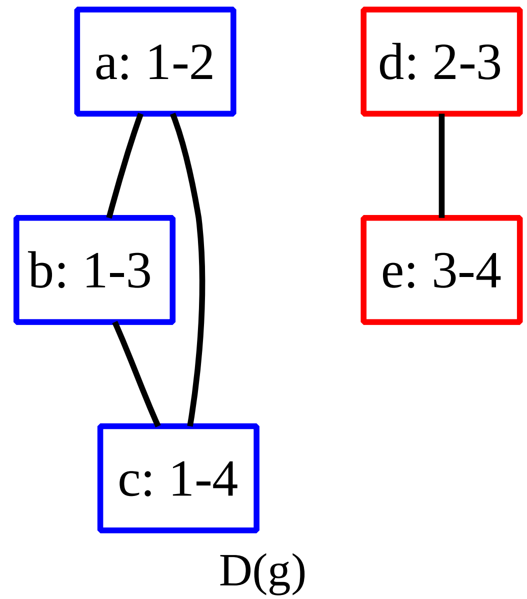
- ★ consider a random vector $X = (X_1, X_2, \ldots, X_m)$
- ★ $P(x) = \exp(Q(x))/\sum \exp Q(x) \Leftrightarrow Q(x) = \log P(x) +$ const
  - ▷ *only restriction* $P(x) > 0 \quad \forall x$
- ★ let D be the *dependency graph* of X; i.e. $i \sim j \Leftrightarrow x_i$ not independent of x_j
  - ▷ *e.g. all* x_i *independent: empty graph*
  - ▷ *e.g. Markov chain: line graph*
  - ▷ *e.g. multivariate Gaussian: complete graph (generically)*
- ★ inclusion-exclusion principle $Q(x) = \sum_{s \subseteq \{1,2,\ldots,m\}} \lambda_s(x_s)$
  - ▷ $x_s \equiv$ *components of* x *corresponding to elements of* s
  - ▷ *Pr* $[\cap_i A_i] = \sum_i$ *Pr* $[A_i] - \sum_{i<j}$ *Pr* $[A_i \cup A_j] + \ldots$
- ★ 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 β_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 $m(g) = d_1(g) = \text{tr}\left(A^2\right)/2$ is the number of edges and $t(g) = \text{tr}\left(A^3\right)/6$

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

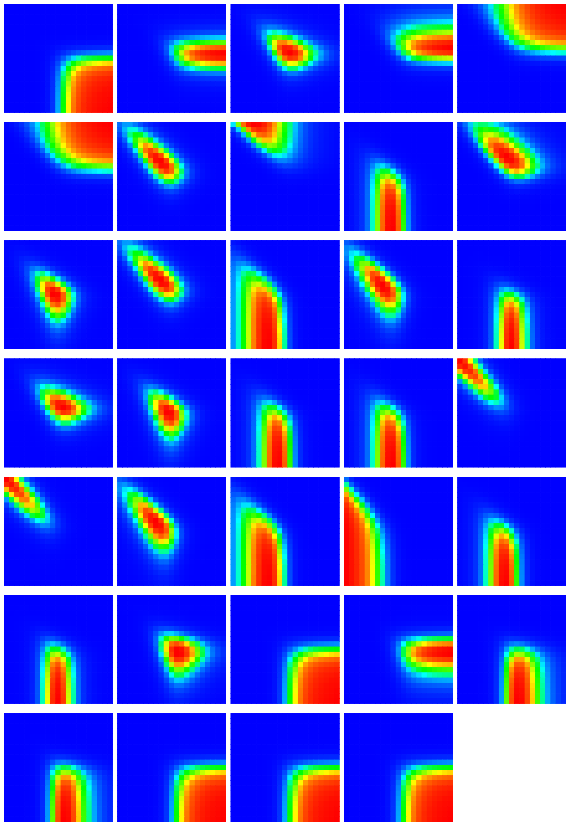
Exactly soluble example - Bernoulli model $G\{n,p\}$

- $g \in G\{n,p\}$ 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: $l(\theta|g) \equiv \log P_\theta(g)+$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. $H_\theta(g) = \theta_1 d_1(g) + \theta_2 d_2(g)$



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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 δH that would occur if the dyad (i, j) were flipped

  (3) if δH or $u < \exp(\delta H)$, $u \sim U(0, 1)$, then accept the proposal; i.e. flip the edge

  (4) go to (1)

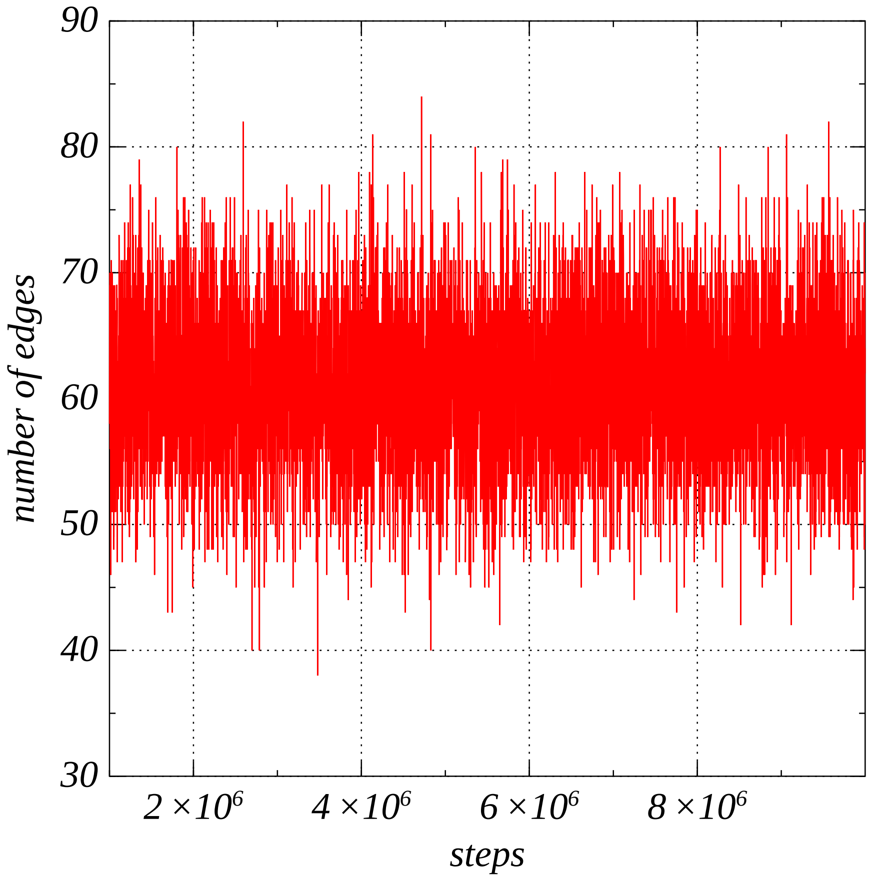
- estimate loglikelihood by (where x is the vector of graph statistics, θ_{ref} a reference value of graph parameters (hopefully close to the true ones) and x_{data} the statistics from the data):

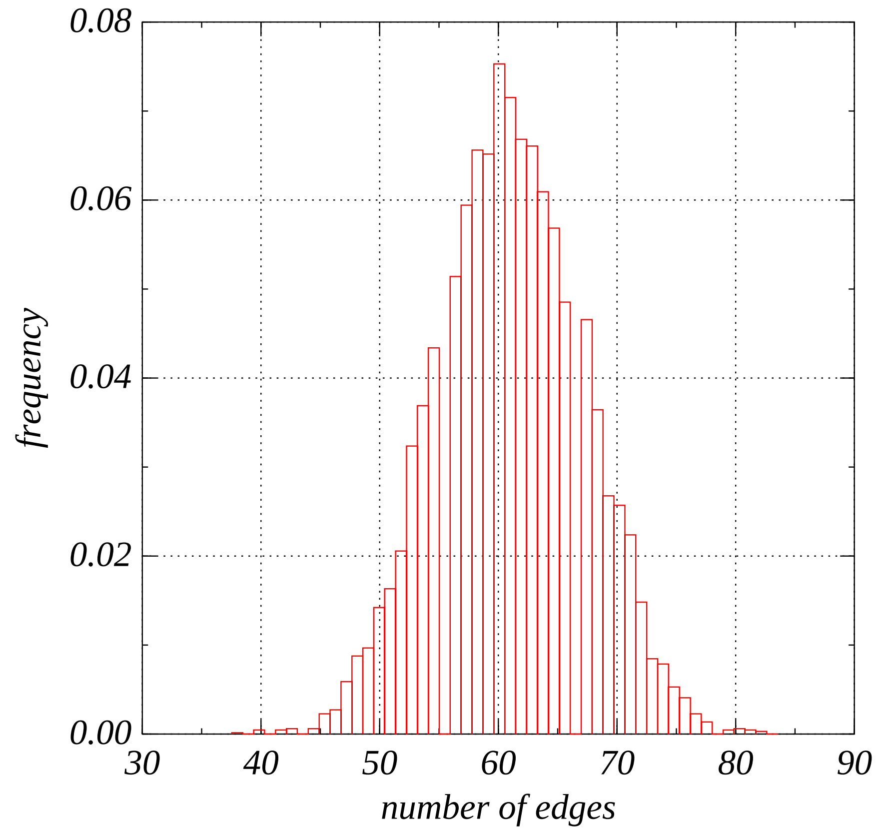
$$l(\theta) - l(\theta_{\text{ref}}) \approx -\log \langle \exp[(l(\theta) - l(\theta_{\text{ref}})) \cdot (x(t) - x_{\text{data}})] \rangle$$

Metropolis simulation example

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

★





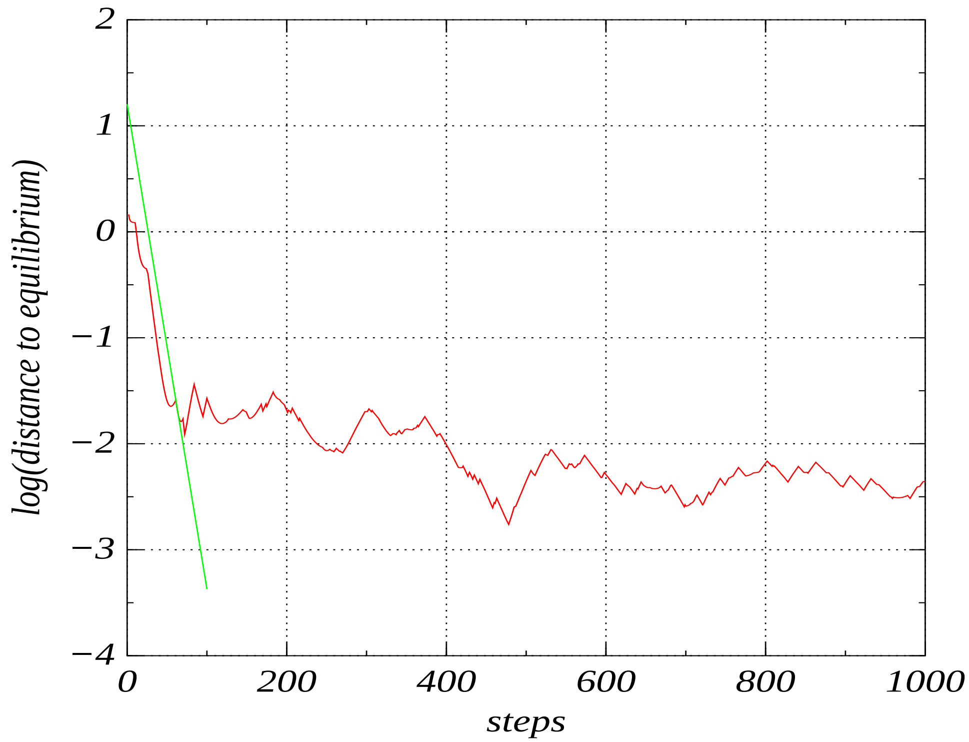
Metropolised independence sampling (MIS) 1

- 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 π. 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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O Frank & D Strauss *Markov graphs* J Am Stat Ass **81**, 832-842 (1986)

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J Berg & M Lässig *Correlated random networks* `http://xxx.soton.ac.uk/abs/cond-mat/0205589`

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K M Briggs *graphlib-1.0* `http://keithbriggs.info/graphlib.html`