Multipodal Phases in Dense Networks

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May 8, 2014

Joint work with Rick Kenyon, Kui Ren and Lorenzo Sadun

Abstract. We consider asymptotically large, dense, simple graphs constrained in a set of densities, either edges and triangles or edges and one or more k-stars, and study the associated entropy, the goal being to determine the structure of 'exponentially most' graphs with given variable constraints. We will present evidence - proof for edges/stars, and simulation for edges/triangles - that for all parameter values the optimal graphs have very simple 'multipodal' structure, simple modifications of balanced multipartite graphs.

Consider simple graphs G with vertex set $V(G)$ of (labeled) vertices, with $|V(G)| = n$.

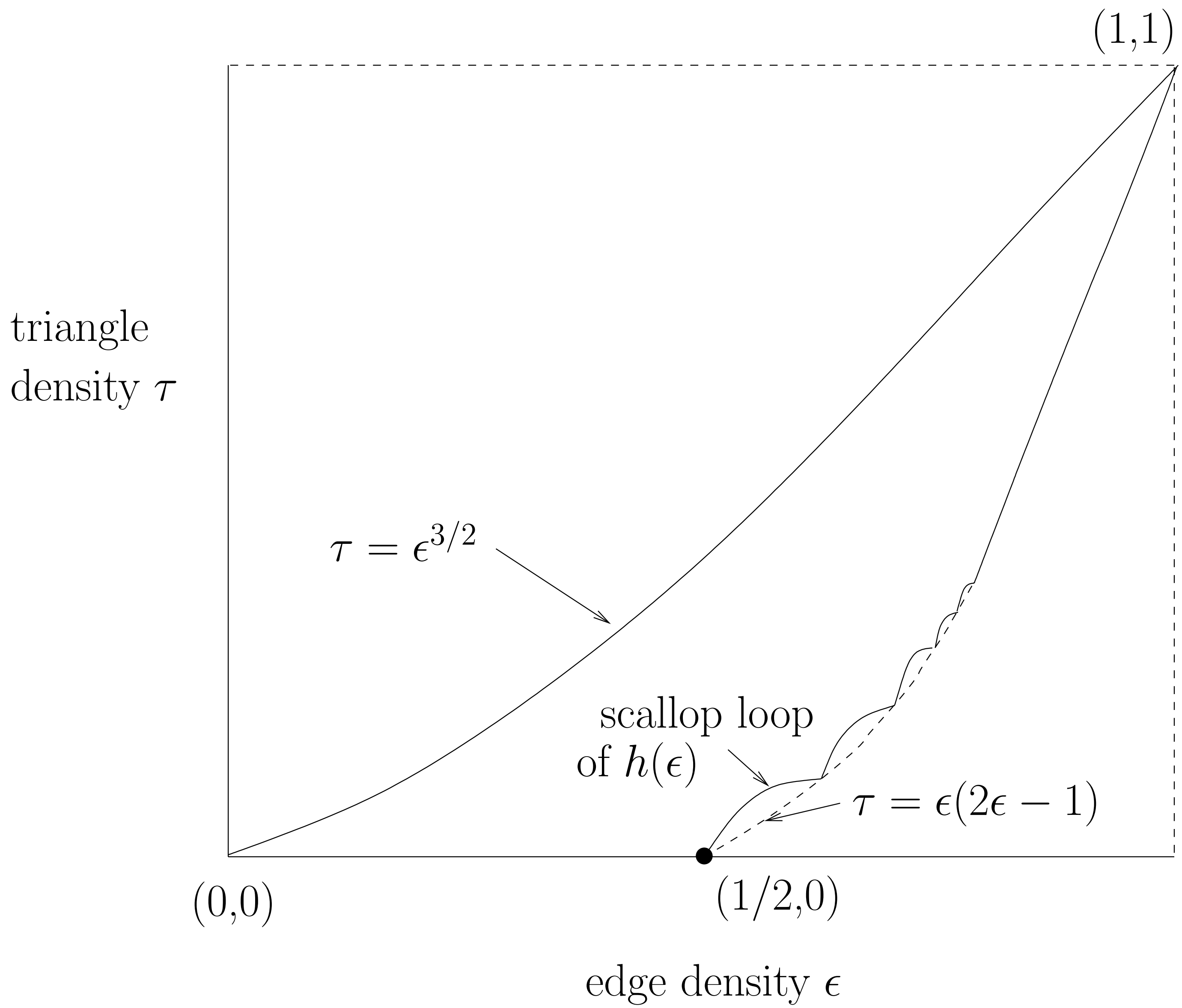
For a simple graph H, its "density" in G is the fraction of all maps, of $V(H)$ into $V(G)$, which preserve edges.

Temporarily specialize constraints to edge density $e(G)$ and triangle densty $t(G)$. Our main tool is $Z^{n,a}_{\epsilon,\tau}$, the number of graphs with densities:

$$e(G) \in (\epsilon - a, \epsilon + a); \quad t(G) \in (\tau - a, \tau + a).$$

By definition $(e(G), t(G)) \in [0, 1]^2$, but in fact the boundary is:

(A. Razborov, Combin. Probab. Comput. 17 (2008) 603-618.)



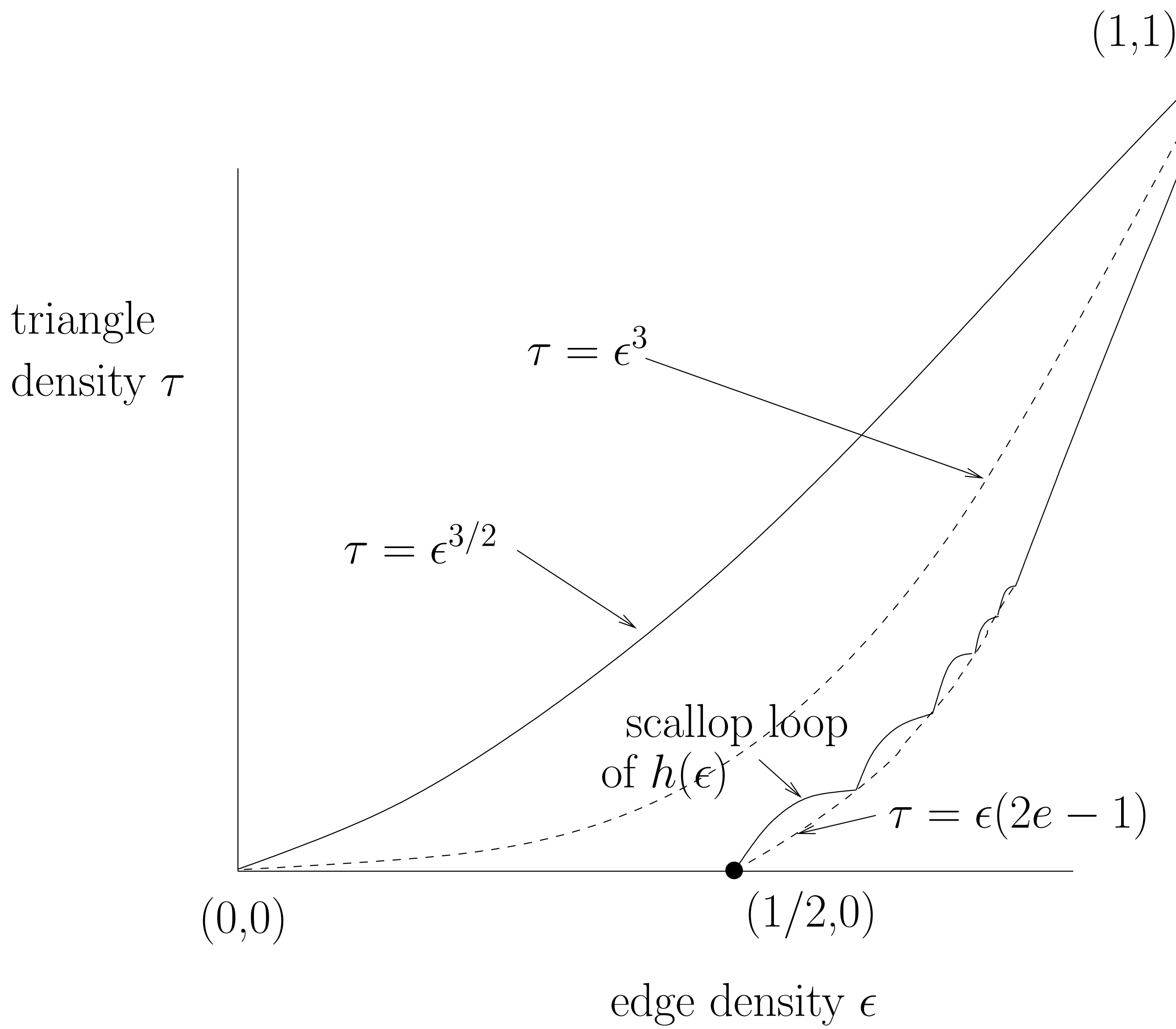
(1,1)
triangle
density τ
$\tau = \epsilon^{3/2}$
scallop loop
of $h(\epsilon)$
$\tau = \epsilon(2\epsilon - 1)$
(0,0)
(1/2,0)
edge density ϵ

Graph for $(\epsilon, \tau) = (0.5, 0)$ is complete, balanced bipartite; it is complete, balanced multipartite for the other vertices, and also known on the rest of the boundary.

This is an example in *extremal graph theory*, the Mantel problem.

We aim to extend to interior, determining 'most' graphs with given constraints.

For instance an optimization principle easily implies that a typical graph with constraints $\tau = \epsilon^3$ has independent edges with probability ϵ.


(1,1)
triangle
density τ
$\tau = \epsilon^3$
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$\tau = \epsilon(2e-1)$
(0,0)
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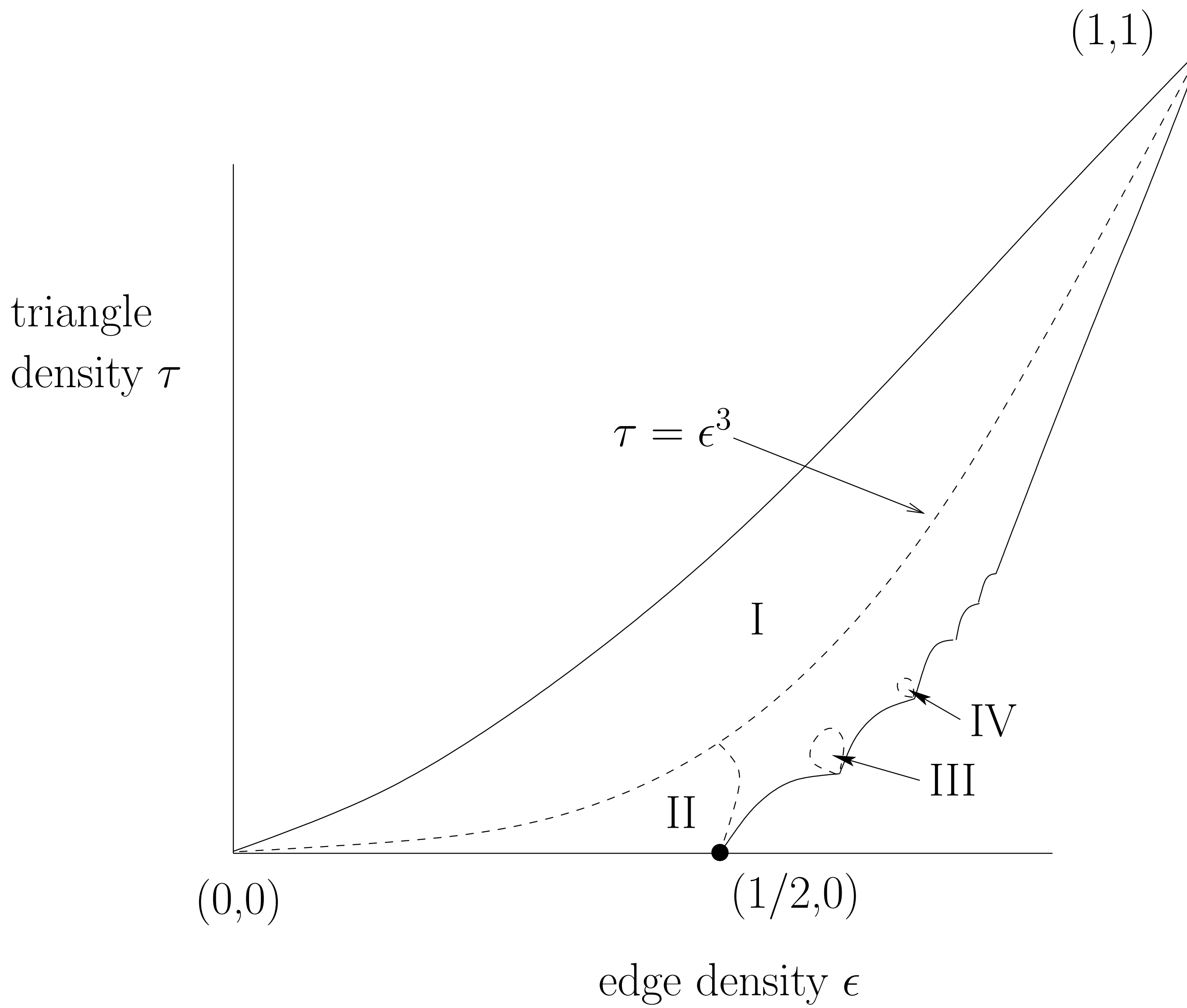
edge density ϵ

Since $Z_{\epsilon,\tau}^{n,a}$ grows like $e^{s(n^2)}$, we normalize as ‘entropy density’:

$$s = s_{\epsilon,\tau}^{n,a} = \frac{\ln(Z_{\epsilon,\tau}^{n,a})}{n^2}, \qquad s(\epsilon,\tau) = \lim_{a\downarrow 0}\lim_{n\to\infty} s_{\epsilon,\tau}^{n,a}.$$

Little is known about $s(\epsilon,\tau)$ beyond existence, but we conjecture it is piecewise smooth in general.

Key definition: A phase is a maximal connected set of parameters where $s(\epsilon,\tau)$ is analytic.


(1,1)
triangle
density τ
$\tau = \epsilon^3$
I
II
III
IV
(0,0)
(1/2,0)
edge density ϵ

Intuitively randomness arises as follows. Start with the assumption that certain kinds of subgraphs $H = (H_1, \ldots, H_m)$ are 'significant' for a large network: edges, triangles, etc. Then determine what most graphs are which have constrained values of the densities $t_H = (t_{H_1}, \ldots, t_{H_m})$ of those type of subgraphs. Large deviations theory gives probabilistic descriptions of such typical graphs through a variational principle for the constrained entropy.

S. Chatterjee, S.R.S. Varadhan, Eur. J. Comb. 32 (2011) 1000-1017

L. Lovász, Large networks and graph limits, AMS, 2012.

Variational Principle (R.-Sadun)

For any (ϵ, τ), $s(\epsilon, \tau) = \max_g[-I(g)]$, where the maximum is over all measurable $g : [0,1]^2 \to [0,1]$, $g(x,y) = g(y,x)$, subject to the constraints

$$e(g) = \int_{[0,1]^2} g(x,y)\,dxdy \ = \ \epsilon$$

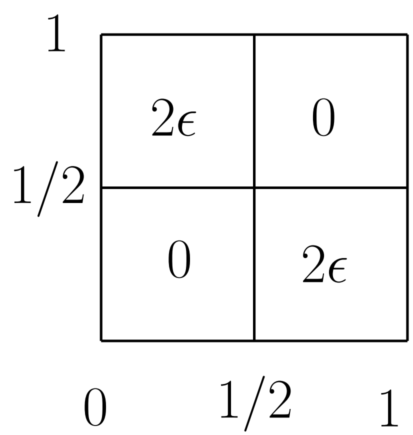
$$t(g) = \int_{[0,1]^3} g(x,y)g(y,z)g(z,x)\,dxdydz \ = \ \tau,$$

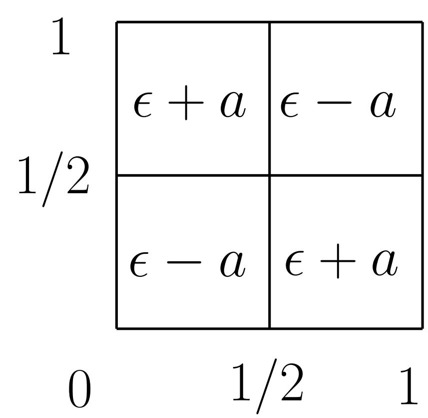
and the 'rate function' $I(g)$ is Shannon entropy:

$$I(g) = \frac{1}{2}\int_{[0,1]^2} g(x,y)\ln[g(x,y)] + [1-g(x,y)]\ln[1-g(x,y)]\,dxdy.$$

Think of points in $[0,1]$ as vertices, and $g(x,y)$ as the probability of an edge between x and y.

Optimizing graphons for phase II (unique up to rearranged vertices):

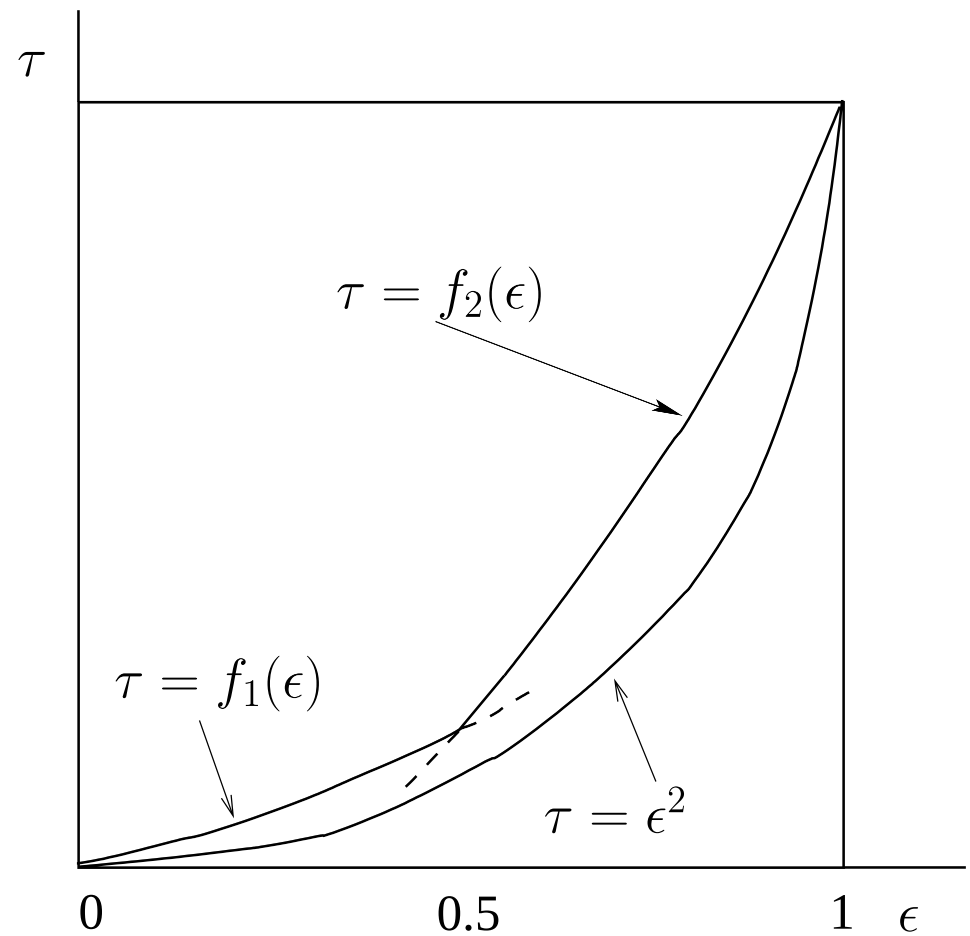




$$a = (\epsilon^3 - \tau)^{1/3}$$

Main result: Simulation suggests for every (ϵ, τ) there is a partition of the vertices into $M < \infty$ subsets $V_1, V_2, \ldots, V_M$, and a set of well-defined probabilities q_{ij} of an edge between any $v_i \in V_i$ and $v_j \in V_j$. We call such states 'multipodal'.

Change constraint from edges/triangles to a finite set of different k-stars, including edges. Phase space for edge/2-star is:



Now the variational principle is to maximize $-I(g)$ subject to

$$t_k(g) = \int_{[0,1]^{k+1}} g(x,y_1)g(x,y_2)\cdots g(x,y_k)\,dxdy_1\cdots dy_k \;=\; \tau_k,$$

for the desired set of $k's$, including $k=1$. (A star model.)

Theorem (Kenyon, R., Ren, Sadun). Every maximizing graphon for a star model is multipodal.

In practice the state is fully described by few variables. We've simulated the edge/triangle model and the 2-star model and so far never seen more than 4 variables, each a function of the constraint values.

Lagrange multipliers; exponential random graphs

Lagrange technique: introduce new variables $\beta = (\beta_1, \cdots, \beta_m)$, one for each constraint, and solve the Euler-Lagrange equations:

$$\delta[-I(g) + \beta \cdot t_H(g)] = 0,$$

together with the constraints $t_H(g) = \tau$, for $s(\epsilon, \tau) = \max_g[-I(g)]$.

Alternate formulation: solve the *unconstrained* problem:

$$\psi(\beta) = \max_g[-I(g) + \beta \cdot t_H(g)],$$

then, if possible, solve for β such that optimizers satisfy constraints.

This optimization problem was first carefully analyzed in:

S. Chatterjee and P. Diaconis, Ann. Statist. 41 (2013) 2428-2461.

However: Any maximizer $\tilde{g}$ of $-I(g) + \beta \cdot t_H(g)$ is automatically a maximizer of $-I(g)$ for some constraints $t_H(g) = \tau'$, namely for $\tau' = t_H(\tilde{g})$. But, as noted by Chatterjee/Diaconis, it is often impossible to find $\beta's$ such that any maximizer of $-I(g)$ with given constraints $t_H(g) = \tau$, will maximize $-I(g) + \beta \cdot t_H(g)$. This is especially true for k-star models; for k-star models all maximizers $\tilde{g}$ of $-I(g) + \beta_1 e(g) + \beta_2 t_k(g)$ satisfy $t_k(\tilde{g}) = e(\tilde{g})^k$, so the two densities cannot be constrained independently.

This phenomenon is known as 'inequivalent ensembles'.