Overview of UMass Research

W. Gong, D. Towsley

Networks with MVHT distributions

- MVHT distributions ubiquitous in networks
  - in-degree, out-degree, reciprocated degree, labels, aggregate weights, …

Q: How to model, generate, estimate, classify, learn network structures?

How do networks evolve?

Outline

- outline (D. Towsley)
- modeling, generating, estimating networks (Towsley)
- classifying networks, distributions (Gong)
- competition in growing networks (Jiang)
- learning networks from data (Atwood)

Kaprivsky model [Krapivsky et al 2001]

- with prob. p
  - new node attaches to existing node v, with prob. proportional to $d_v^{\mathrm{in}} + \lambda$
- with prob. q = 1 - p
  - new edge $u \to v$ connects existing nodes, with prob. proportional to $(d_v^{\mathrm{in}} + \lambda)(d_u^{\mathrm{out}} + \mu)$
- joint distribution
  - when $v_{in} = v_{out}$

$$\mathbb{P}(d_{in} = i, d_{out} = j) \sim C \frac{i^{\lambda-1} j^{\mu}}{(i+j)^{2\lambda+1}}$$

Kaprivsky model

- efficient network generation algorithm – Atwood (UMass)
  - $O(n \ \log n)$
  - generates 10^6 node networks in seconds
  - node fitness, edge weights, other variants
- analysis – Gena
- parameter estimation – Jiang (UMass), Davis

Kaprivsky model: limitations

- cannot control in/out degree correlation
- cannot directly account for reciprocity
- network datasets exhibit significant variations in both

More useful models?

A versatile network model (UMass, UMN)

- generate undirected CA network
  - attach to i in proportion to $\deg(i) + \lambda, \quad \lambda > -1$
- assign directions randomly
  - undirected, prob. p
  - directed, prob. 1 - p, each direction prob. (1 - p)/2
- marginal unreciprocated in-, out-, reciprocated degree distr.

$$P(d_k = i) \propto i^{-3-\lambda}, \qquad k = in, out, re$$

- asymptotic joint distribution

$$P(d_{in} = i, d_{out} = j, d_{re} = j) \sim \frac{C}{(i+j+k)^{3+\lambda}} \binom{i+j+k}{i \;\; j \;\; k} p^k \left(\frac{1-p}{2}\right)^{i+j}$$

Ongoing work (UMass, UMN)

- explore other network models
  - model clustering (HT cluster sizes)

- place joint distributions in MRV framework
  - leverage Gena's recent work

Complex Graph Similarity Testing and Multivariate Distribution Comparison Using Random Walks

Shan Lu, Jieqi Kang, Weibo Gong, Don Towsley

UMASS Amherst

Outline of the approach

- Need for fast similarity testing among large data group/complex networks
- Existing algorithms are combinatorial in nature
- Small-time asymptotic results for diffusion on manifold motivated our approach
- Analogues on graphs/large data groups
- 1d experiments to seek understanding
- Analyzing graphs with 2d distributions
- Collaborations (Zhi-Li, Gena)
- Future work

Consider diffusion on Riemannian manifold M:

$$\Delta_M u = \frac{\partial u}{\partial t}, \quad t > 0,$$

with initial condition $u(x,0) = 1$

and boundary conditions $u(x,t) = 0, \quad x \in \partial M, t > 0$

Using the Δ_M spectral resolution $\{\lambda_k, \phi_k, \}$, $\lambda_1 < \lambda_2 < \cdots < \lambda_k < \cdots$

The Dirichlet heat kernel for M is $p(x,y,t) = \sum_{k=1}^{\infty} e^{-\lambda_k t} \phi_k(x) \phi_k(y)$

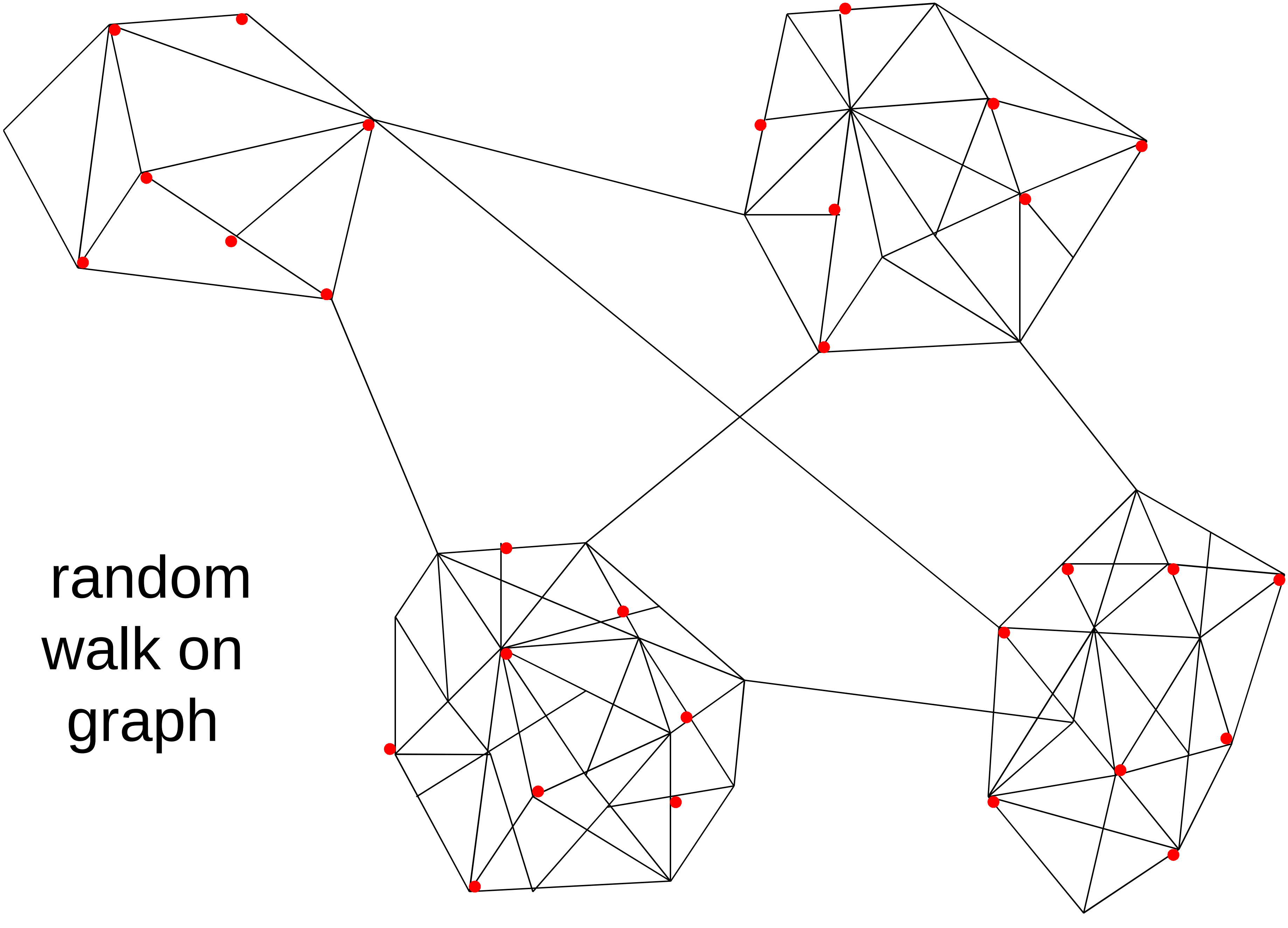
and the heat content

$$h(t) = \int_M u(x,t)dx = \int_M \int_M p(x,y,t)dydx = \sum_{k=1}^{\infty} e^{-t\lambda_k} \left(\int_M \phi_k(x)dx \right)^2$$

Note $\int_M \phi_k(x)dx = \int_M \phi_k(x)u(x,0)dx$ is the Fourier coefficient of the

initial condition in the eigen space spanned by $\{\phi_1, \phi_2, \cdots, \}$!

random walk on graph



Notations

Laplacian matrix: $L = D - A$

Normalized Laplacian: $\mathcal{L} = D^{-1/2} L D^{-1/2}$

Random walk Laplacian: $L_r = D^{-1} L$

Let $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$ be the eigenvalues of $\mathcal{L}$ and $\phi_i, i = 1, \ldots, N$ the corresponding eigenvectors. With $\Lambda = diag[\lambda_i]$ and $\Phi = [\phi_1, \ldots, \phi_N]$,

$$\mathcal{L} = \Phi \Lambda \Phi^{-1} \qquad L_r = (D^{-1/2}\Phi)\Lambda(\Phi^{-1}D^{1/2})$$

where $\Phi^{-1} = [\pi_1; \ldots; \pi_N]$.

Notations

Partition vertex set V *into two subsets, the set of all interior nodes* iD *and the set of all boundary nodes* ∂D*.*
Label the interior vertices $1, \cdots, m$ *and the boundary vertices* $m+1, \cdots, n$*. The normalized* $\mathcal{L}$ *can be partitioned into:*

$$\mathcal{L} = \begin{bmatrix} \mathcal{L}_{iD,iD} & \mathcal{L}_{\partial D,iD} \\ \mathcal{L}_{iD,\partial D} & \mathcal{L}_{\partial D,\partial D} \end{bmatrix}$$

Let the boundary vertices be absorbing in the heat equation in next page. Use $\mathcal{L}$ *for* $\mathcal{L}_{iD,iD}$ *for convenience henceforth.*

Heat Equation and Heat Content

Heat Equation is associated with the normalized graph Laplacian

$$\frac{\partial h_t}{\partial t} = -\mathcal{L} h_t \quad \Rightarrow \quad h_t = e^{-\mathcal{L}t}$$

with a given initial condition.

Heat Content:

$$Q(t) = \sum_{u \in iD} \sum_{v \in iD} h_t(u,v) = \sum_{u \in iD} \sum_{v \in iD} \sum_{i=1}^{m} e^{-\lambda_i t} \phi_i(u) \pi_i(v)$$

$$\alpha_i = \sum_{u \in iD} \sum_{v \in iD} \phi_i(u) \pi_i(v)$$

$$\boxed{Q(t) = \sum_{i=1}^{m} \alpha_i e^{-\lambda_i t}}$$

Heat Equation and Heat Content

- Time derivatives of the heat content:

$$\dot{Q}(t) = -\sum_{i=1}^{m} \alpha_i \lambda_i e^{-\lambda_i t}$$

$$\ddot{Q}(t) = \sum_{i=1}^{m} \alpha_i \lambda_i^2 e^{-\lambda_i t}$$

- When $t \to 0$,

$$Q(t)|_{t\to 0} = \sum_i \alpha_i = 1 \qquad \dot{Q}(t)|_{t\to 0} = -\sum_i \alpha_i \lambda_i \qquad \ddot{Q}(t)|_{t\to 0} = \sum_i \alpha_i \lambda_i^2$$

Lazy Random Walk Approximation

1. *Transition matrix* $M = D^{-1}A$.

2. *Lazy random walk* $M_L = (1-\delta)I + \delta M$.

3. For any given time $t = k\delta$, take the limit with $k \to \infty$ ($\delta \to 0$),

$$P_t = M_L^k P_0 = [I - \frac{t}{k} L_r]^k P_0 \to e^{-L_r t} P_0$$

$$M_L^k(u,v) \to \sum_{i=1}^{m} e^{-\lambda_i t} \phi_i(u) \pi_i(v) (\frac{d_v}{d_u})^{1/2}$$

$$\hat{Q}(t) = \sum_{u \in iD} \sum_{v \in iD} M_L^k(u,v) (\frac{d_u}{d_v})^{1/2} \to Q(t)$$

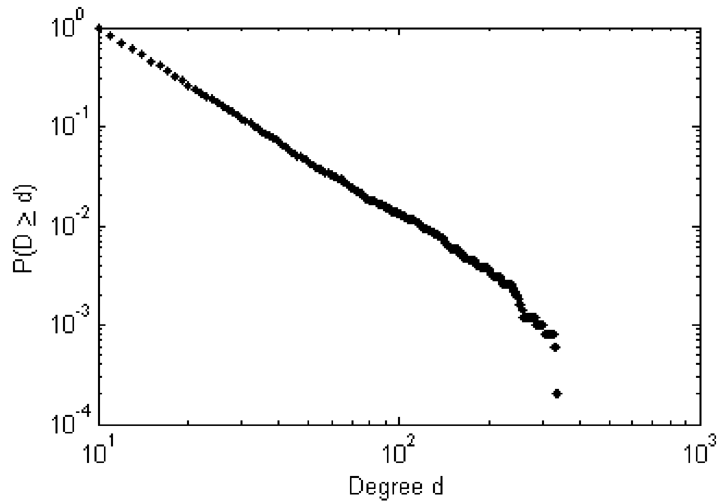
Graph Similarity Testing

- Undirected Graphs
  - Barabási–Albert model vs. Erdős–Rényi model

- Directed Graphs
  - Krapivsky's model (2001)
  - Multivariate power law degree distribution
  - Krapivsky's model vs. Erdős–Rényi model

Barabási–Albert vs. Erdős–Rényi Model

Barabási–Albert model**:** starts with s_0 nodes; each new node is connected to s existing nodes with a probability proportional to the degree of the existing nodes.
Degree distribution follows $P(D = d) \sim d^{-3}$.

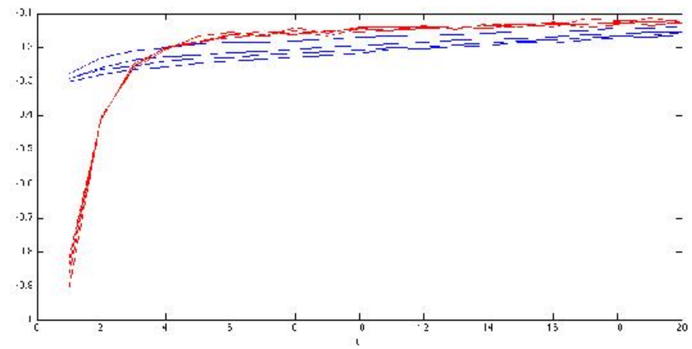


Erdős–Rényi model : $G(n, p)$, each edge is included in the graph with probability p independent from other edges.

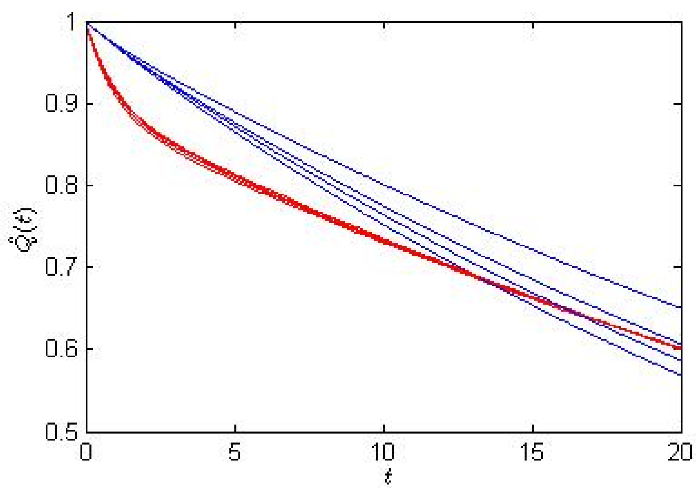
Barabási–Albert vs. Erdős–Rényi Model

Two groups of graphs: power law graphs generated by B-A model and random graphs generated by E-R model. Average degree varies from 20 to 50. Heat content in each group are plotted in the same color.

Boundary selection: nodes with the smallest degrees.

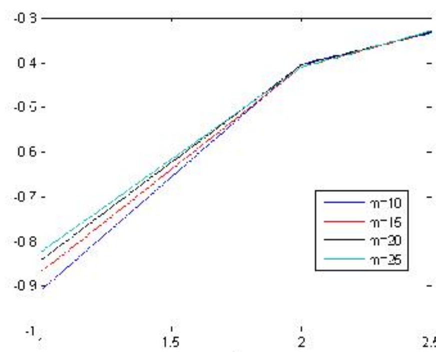


The time derivatives of the heat contents for the two groups of graphs



Power Law graphs generated by B-A model

Random graphs generated by E-R model

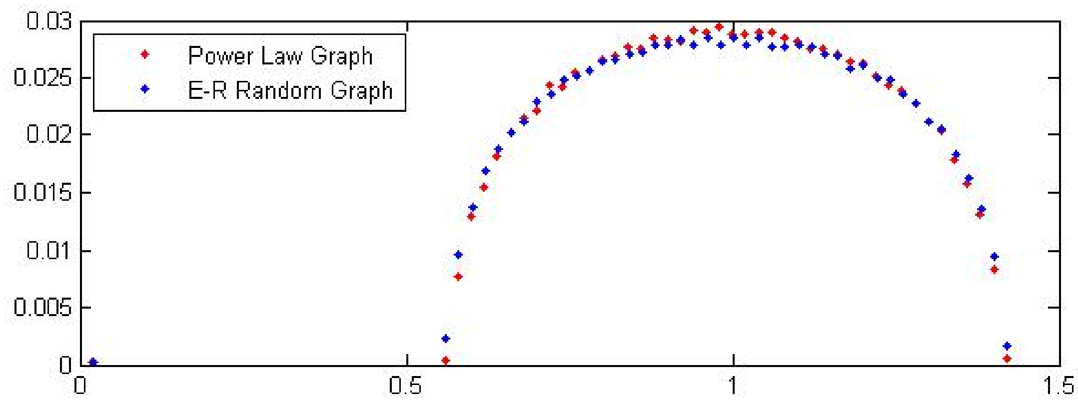


The initial time derivative of the heat contents for power law graphs with different mean degrees

Barabási–Albert vs. Erdős–Rényi Model

Laplacian Spectrum of two graphs with mean degree 20

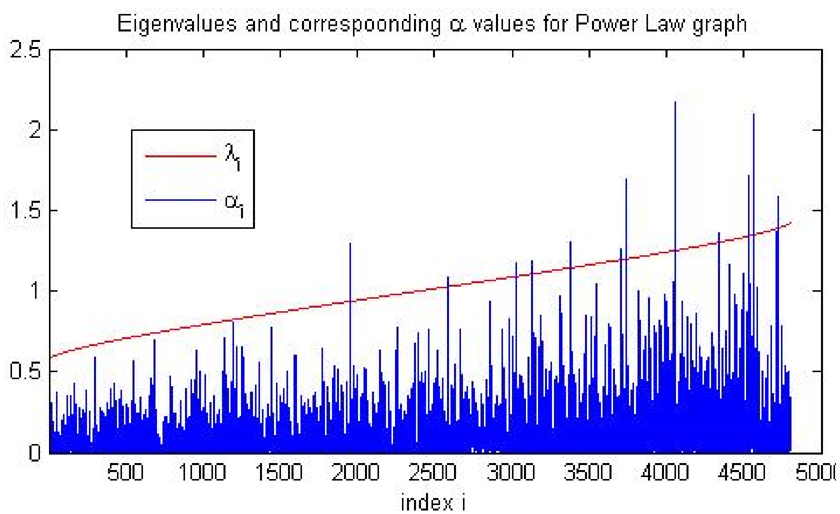
- The eigenvalues of the normalized Laplacian satisfy the semicircle law under the condition that the minimum expected degree is relatively large. (*Chung et. al. 2003*)



Laplacian eigenvalues

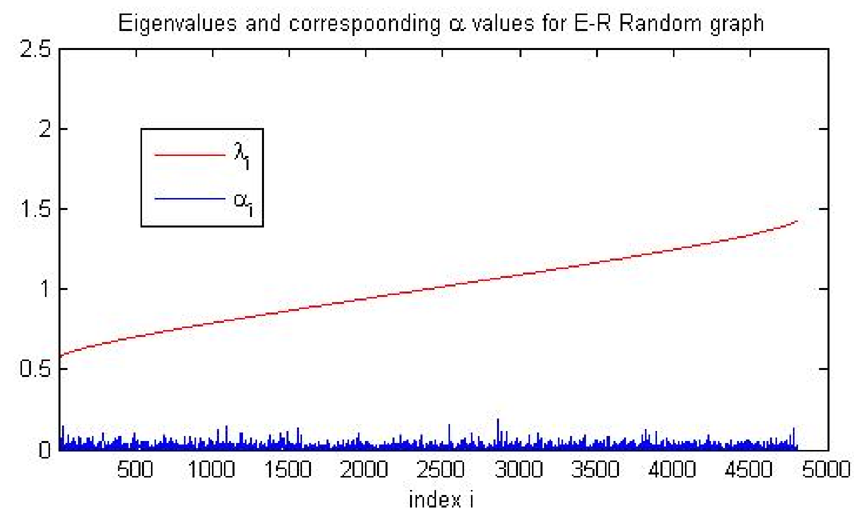
Barabási–Albert vs. Erdős–Rényi Model

$$\boxed{Q(t) = \sum_{i=1}^{m} \alpha_i e^{-\lambda_i t}}$$



$$\lambda_1 = 0.0195 \quad \alpha_1 = 4260.2$$

Power Law graph generated by B-A model



$$\lambda_1 = 0.0210 \quad \alpha_1 = 4745.6$$

Random graph generated by E-R model

Krapivsky vs. Erdős–Rényi Model

- Krapivsky's Model (*'Degree distributions of growing networks'* , 2001)
  - ➢ With probability p , a new node is introduced and attached to a target node u *with probability proportional to* $d_u^{\text{in}} + \lambda_{\text{in}}$ *.*
  - ➢ With probability $q = 1 - p$, a new link from node v to node u is created with probability proportional to $(d_u^{\text{in}} + \lambda_{\text{in}})(d_v^{\text{out}} + \lambda_{\text{out}})$.
- Degree distribution

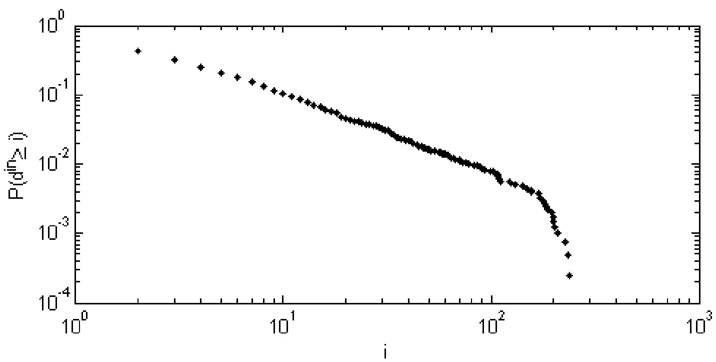
$$P(d^{\text{in}} = i) \sim i^{-v_{\text{in}}} \qquad P(d^{\text{out}} = j) \sim j^{-v_{\text{out}}}$$

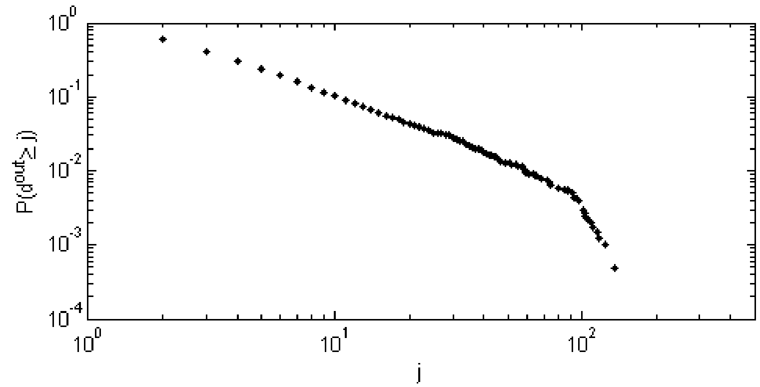
$$v_{\text{in}} = 2 + p\lambda_{\text{in}} \qquad v_{\text{out}} = 1 + q^{-1} + p\lambda_{\text{out}}/q$$

- Average in-degree and out-degree: $1/p$

Krapivsky vs. Erdős–Rényi Model

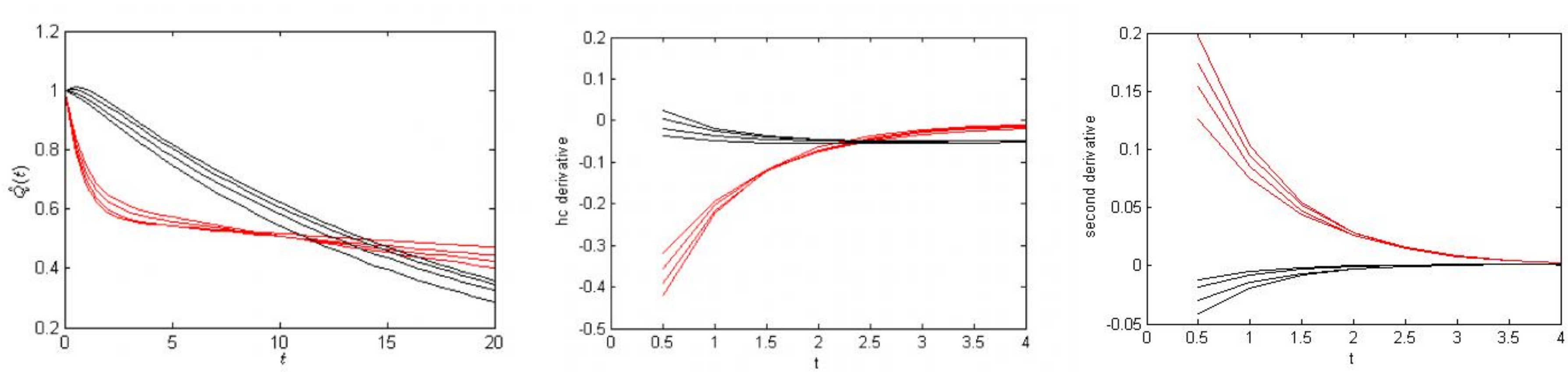
Generated a 2000 nodes' directed graph using Krapivsky's model with $p = 0.2,\ \lambda_{\rm in} = 2$ *and* $\lambda_{out} = 1$ *. CCDF of the in-degrees and out-degrees of the generated graph:*





Krapivsky vs. Erdős–Rényi Model

Generated four 2000 nodes' directed graphs using Krapivsky's model with p=0.1 , 0.15, 0.2 and 0.25 , respectively. Also generated four directed graphs using E-R model with the same average degrees. Heat contents in each group are plotted in the same color.

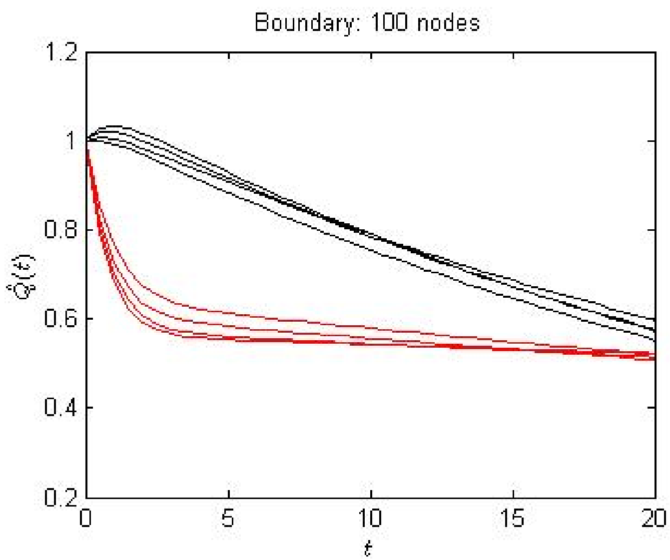


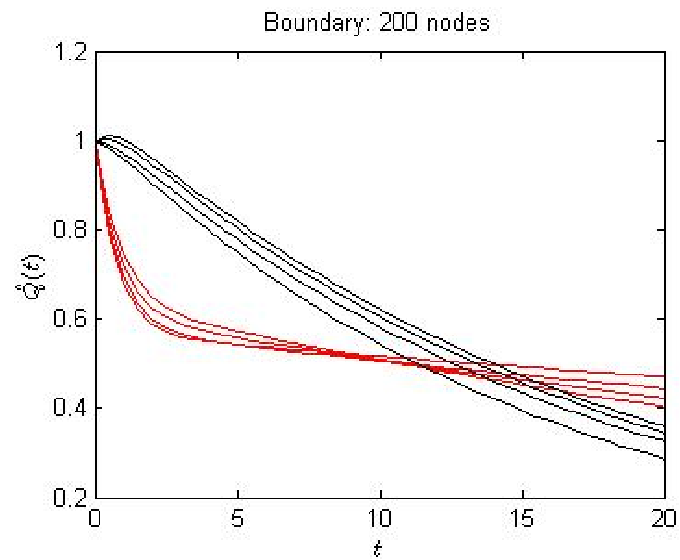
Directed graphs with bivariate power Law degree distributions

Directed E-R random graphs

Krapivsky vs. Erdős–Rényi Model

Boundary selection : nodes with smallest values of $d^{\text{in}} \times d^{\text{out}}$





The number of boundary vertices impacts the heat contents of directed E-R random graphs more.

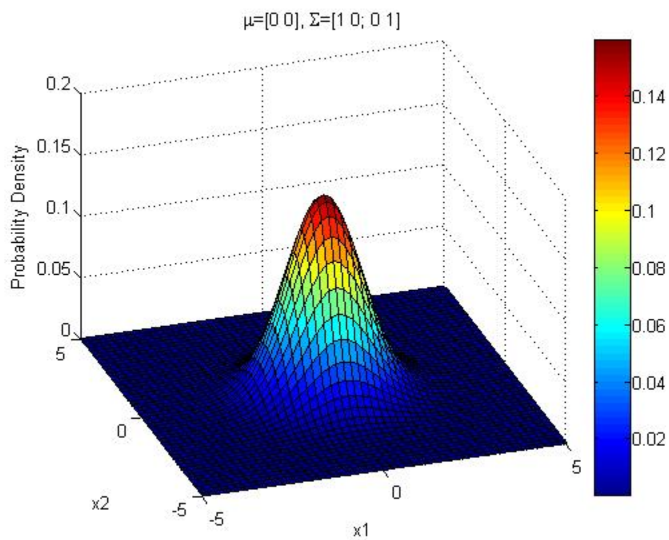
Multivariate Distribution Comparison

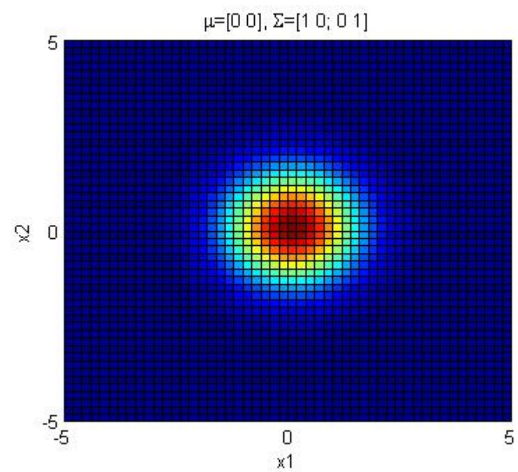
- Multivariate Normal Distributions
  - Compare bivariate normal distributions with different covariance matrices
- Multivariate Power Law Distributions
  - Krapivsky's model, 2002
  - Correlated bivariate power law degree distributions
  - Correlated distributions vs. independent distributions

Multivariate Normal Distribution

- Probability density function of the 2-dimensional bivariate normal distribution

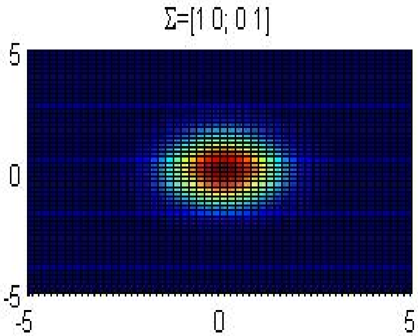
$$y = f(x, \mu, \Sigma) = \frac{1}{\sqrt{|\Sigma|(2\pi)^2}} e^{-\frac{1}{2}(x-\mu)\Sigma^{-1}(x-\mu)'}$$

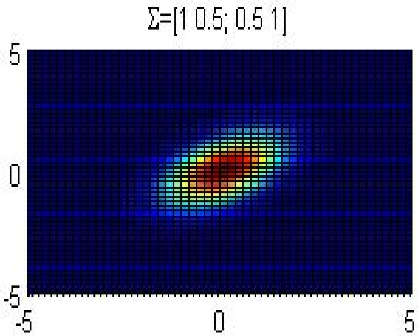


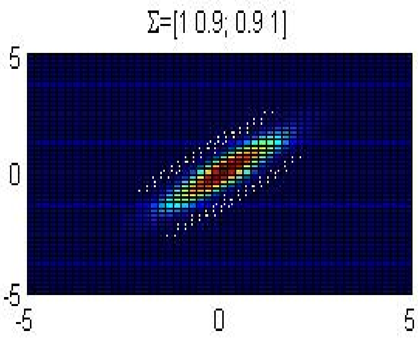


$$W(p_1, p_2) = \frac{|f(p_1, \mu, \Sigma) - f(p_2, \mu, \Sigma)|}{\|p_1 - p_2\|^2}$$

Multivariate Normal Distribution





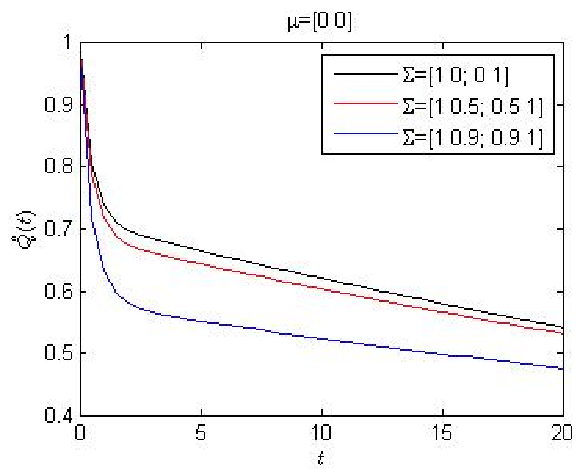


The Kullback–Leibler divergence from $\mathcal{N}_0(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ to $\mathcal{N}_1(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1)$, for non-singular matrices Σ_0 and Σ_1, is:

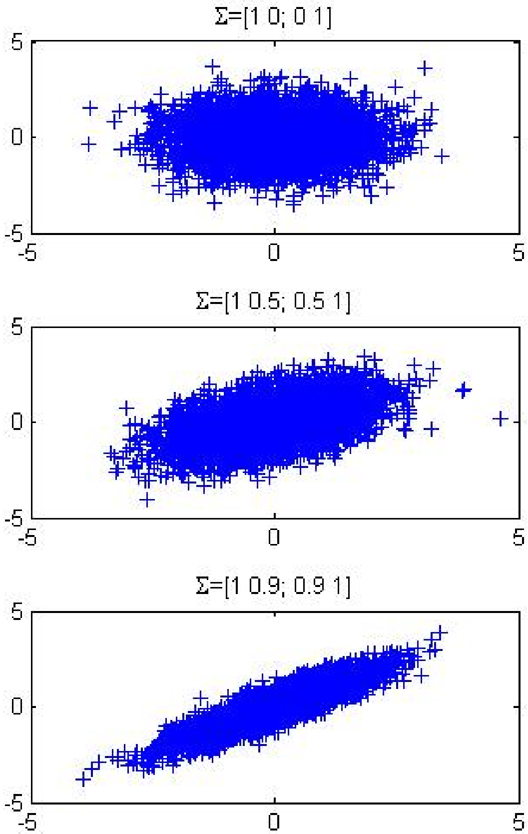
$$D_{\mathrm{KL}}(\mathcal{N}_0 \| \mathcal{N}_1) = \frac{1}{2}\left\{ \mathrm{tr}\left(\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_0\right) + \left(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0\right)^{\mathrm{T}} \boldsymbol{\Sigma}_1^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_0) - K - \ln \frac{|\boldsymbol{\Sigma}_0|}{|\boldsymbol{\Sigma}_1|} \right\},$$

where K is the dimension of the vector space.

$\mathcal{N}_0(\mu, \Sigma_0)$ vs. $\mathcal{N}_1(\mu, \Sigma_1)$ ($\mu = [0\ 0]$)	$D_{KL}(\mathcal{N}_1 \| \mathcal{N}_0)$	$D_{KL}(\mathcal{N}_0 \| \mathcal{N}_1)$	Symmetrised divergence
$\Sigma_0 = [1, 0; 0, 1]$ vs. $\Sigma_1 = [1, 0.5; 0.5, 1]$	0.1438	0.1895	0.3333
$\Sigma_0 = [1, 0.5; 0.5, 1]$ vs. $\Sigma_1 = [1, 0.9; 0.9, 1]$	0.4199	1.2082	1.6281
$\Sigma_0 = [1, 0; 0, 1]$ vs. $\Sigma_1 = [1, 0.9; 0.9, 1]$	0.8304	3.4328	4.2632



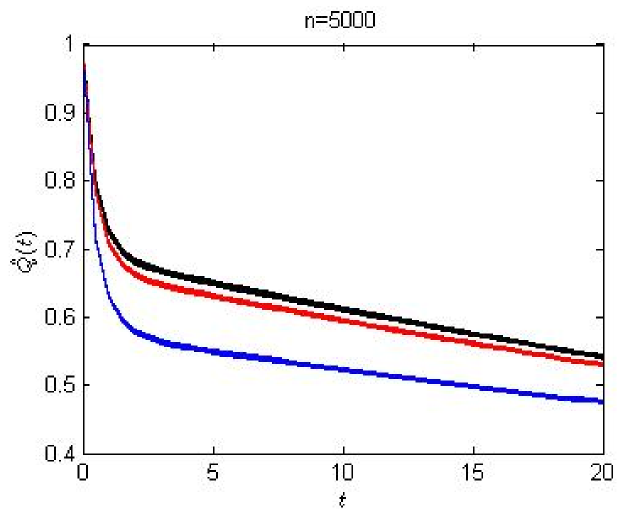
Multivariate Normal Distribution



20 samples for each distribution with 5000 random numbers in each sample.

Histogram is used for density estimation.

Heat contents for samples of the same distribution are plotted in the same color.



Multivariate distribution with power law marginal

- Krapivsky's Model (*'A statistical physics perspective on web growth'*, 2002) :
  - Some new node is introduced as isolated for webnet reality.
- Degree distribution
  - *Marginal distribution* $P(d^{\text{in}} = i) \sim i^{-v_{\text{in}}}$ $P(d^{\text{out}} = j) \sim j^{-v_{\text{out}}}$

    $v_{\text{in}} = 2 + p\lambda_{\text{in}}/q$ $v_{\text{out}} = 2 + p\lambda_{\text{out}}/q$

  - *Joint Distribution* (*when* $\lambda_{\text{in}} = \lambda_{\text{out}} \equiv \lambda$)

$$P(d^{\text{in}} = i, d^{\text{out}} = j) \sim C \frac{(ij)^{\lambda-1}}{(i+j)^{1+\lambda+\lambda/q}}$$

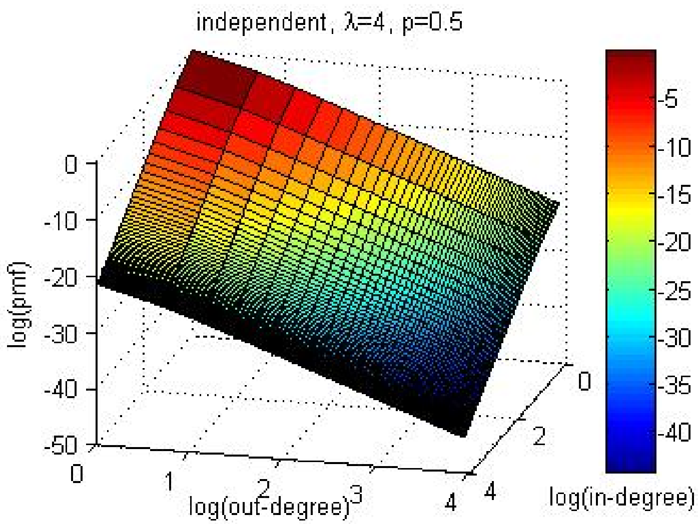
In-degree and out-degree of a node are correlated

$$P(d^{\text{in}} = i, d^{\text{out}} = j) \neq P(d^{\text{in}} = i)P(d^{\text{out}} = j)$$

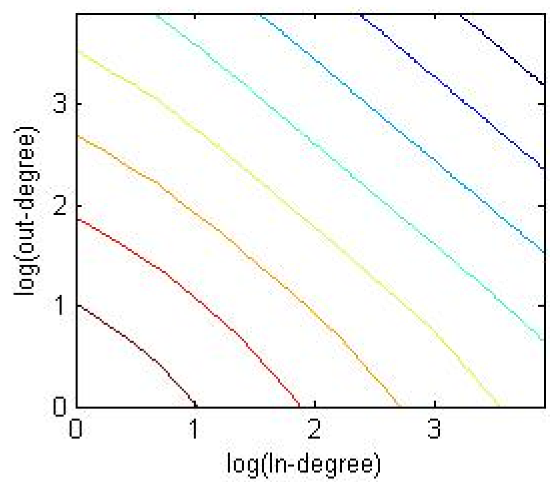
Multivariate distribution with power law marginal

Independent bivariate power law distribution with the same marginal distributions as in Krapivsky's model
($\lambda_{in} = \lambda_{out} = 4, \; p = 0.5$ in the figures below)

$$P(d^{\text{in}} = i, d^{\text{out}} = j) = P(d^{\text{in}} = i)P(d^{\text{out}} = j)$$

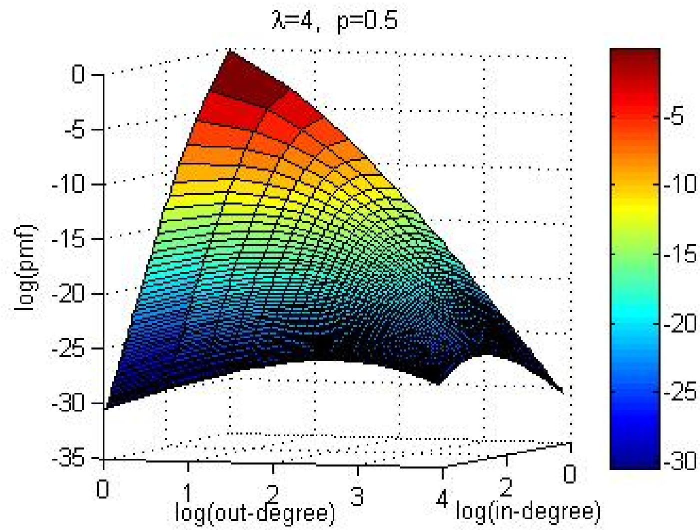


level curves

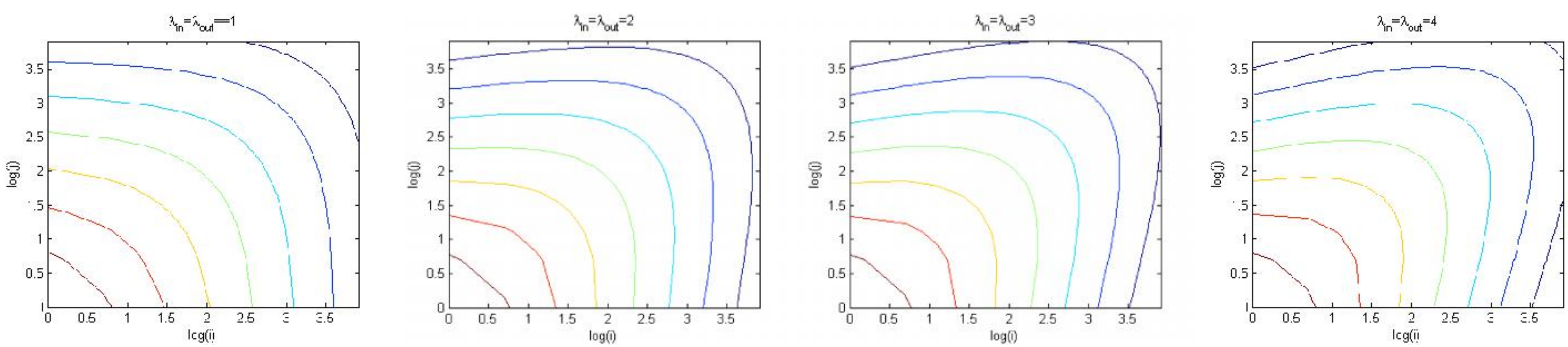


Multivariate distribution with power law marginal

The joint degree distribution generated by Krapivsky's model
($\lambda_{in} = \lambda_{out} = 4,\ p = 0.5$ in the figure on right)

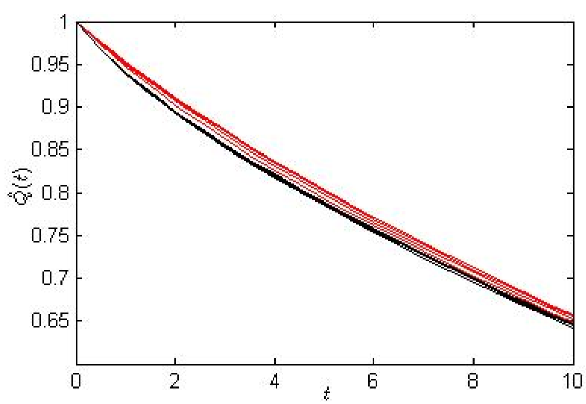


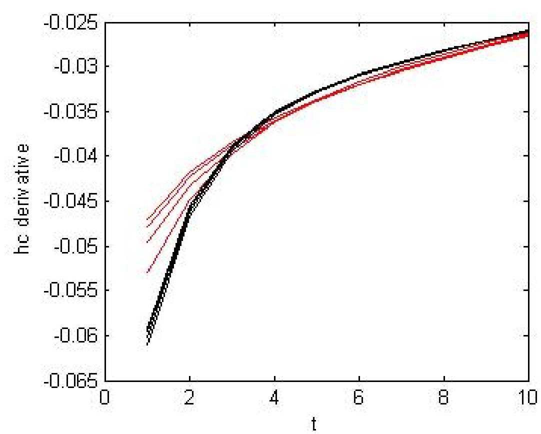
The level curves for Krapivsky's distribution with different λ *values*

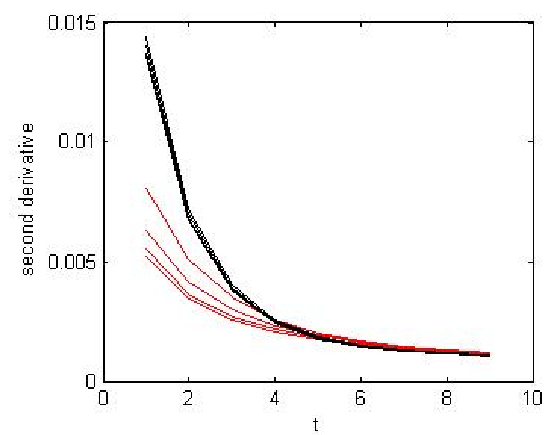


Multivariate distribution with power law marginal

Heat contents and time derivatives of the two groups of distributions: distributions generated by Krapivsky's model with different λ values and the corresponding independent ones.





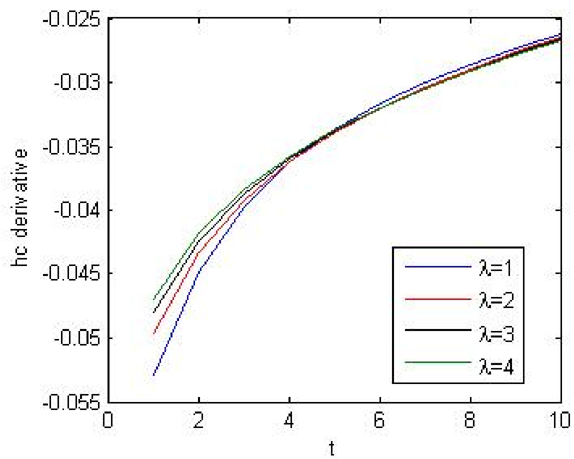


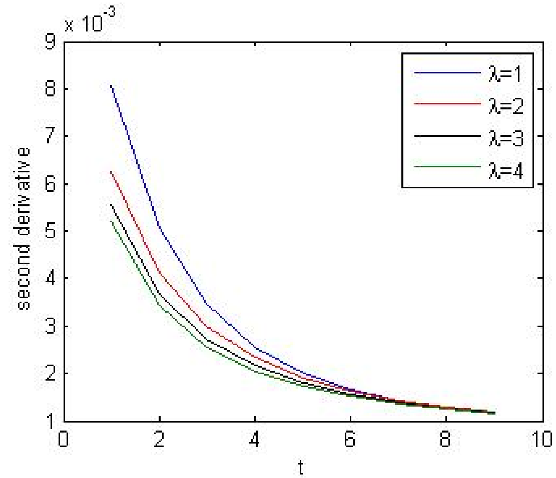
Distributions generated by Krapivsky's model

Independent bivariate power law distributions

Multivariate distribution with power law marginal

Heat content derivatives of the distributions generated by Krapivsky's model with different λ *values.*





Ongoing Work

- Mathematical definition and properties
  - L2 difference does not account for decreasing importance in time
- Graph Similarity Testing
  - *Consider other graph generative models*
  - *Consider real world network datasets*
- Multivariate Distribution Comparison
  - *Real data; higher dimension;*
  - *Theoretical understanding of correlation impact*
- Collaborations
  - UMASS-Cornell
  - UMASS-UMN