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The power-law degree sequence

Power-law and maximum entropy

Power-law exponent (inverse temperature)

Free energy and phase transition

Graphs

Definition (Graph)

A pair $G = (V, E)$, where $V = \{v_1, \dots, v_N\}$ is a set of *vertexes* (or *nodes*), and $E = \{e_1, \dots, e_M\} \subseteq V \times V$ is a set of *edges* (or *links*, *arrows*).

Example

Social contacts : vertexes represent humans or anumals, edges represent social contacrts (e.g. Zachary karate club, $N = 34$, Zebra network, $N = 27$, Madrid train bombing network, $N = 64$).

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Social networks : edges represent friendships (e.g. subsets of Facebook, $N = 63K$, YouTube, $N = 3M$, LiveJournal, $N = 5M$).

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Degree Sequence

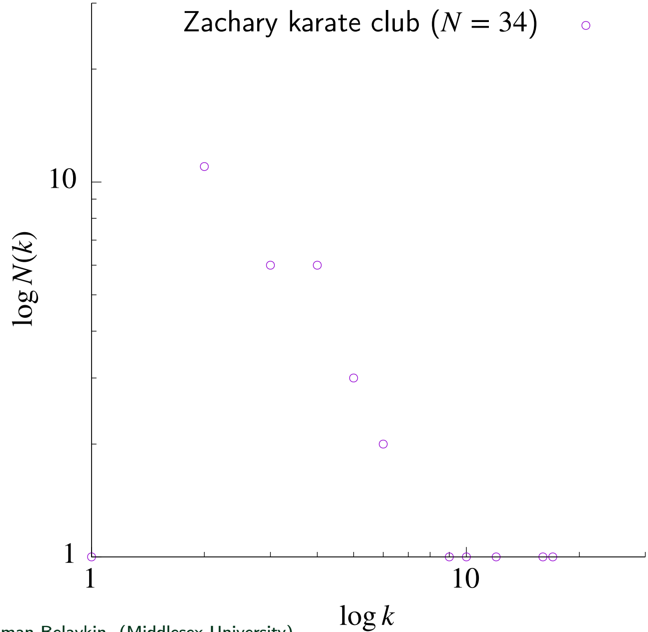
Definition (Degree sequence)

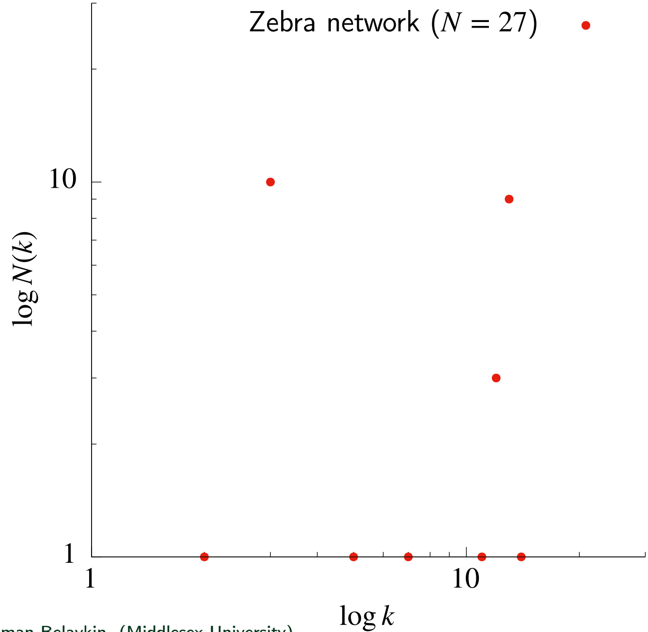
Function $N : \mathbb{N} \to \mathbb{N} \cup \{0\}$ representing the nuber $N(k)$ of vertexes $v \in V$ with degree k (number of edges $(v, \cdot)$ or $(\cdot, v) \in E \subseteq V \times V$):

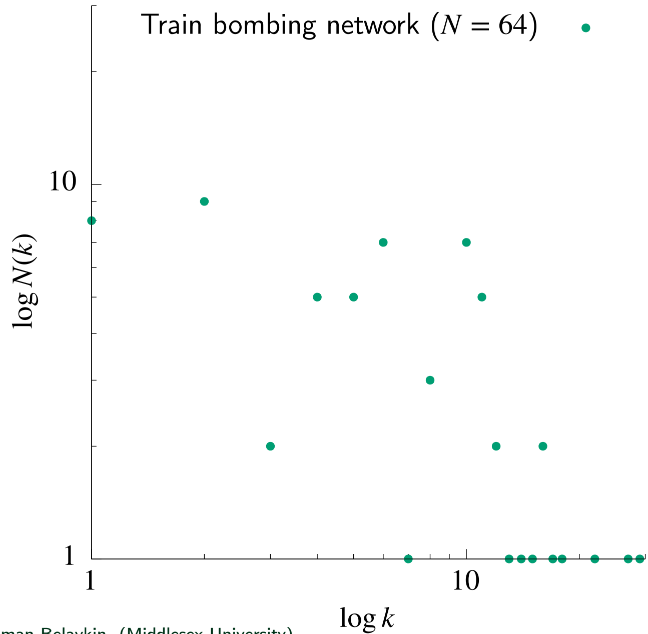
$$N(k) := |\{v \in V : \deg(v) = k\}|$$

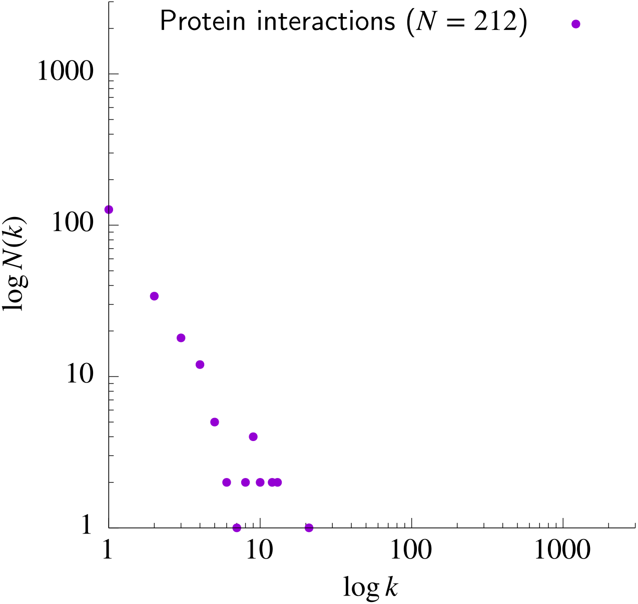
Normalized $N(k)$ is the degree *distribution*

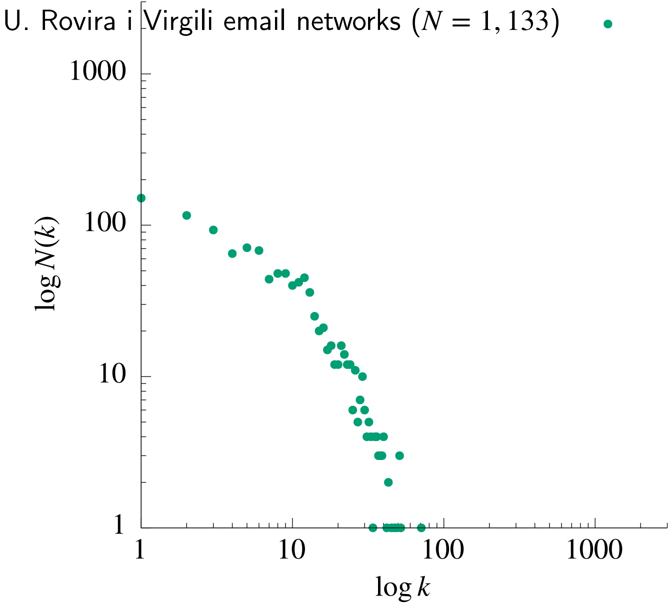
$$P(k) = \frac{N(k)}{N}$$

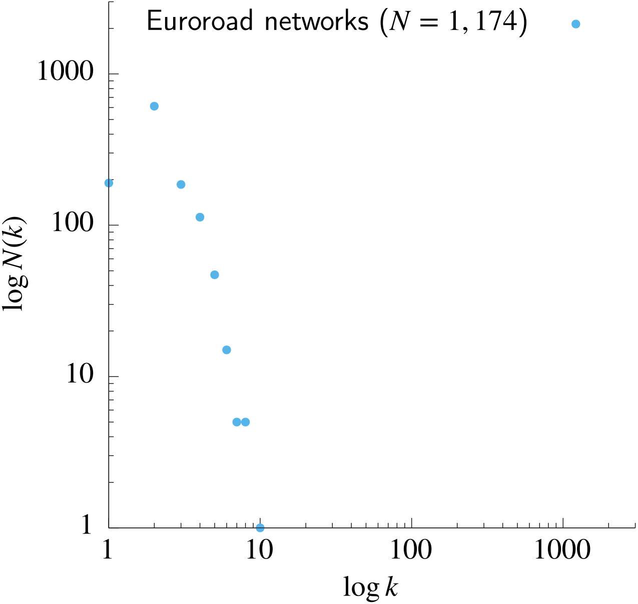

Zachary karate club ($N = 34$)
10
1
$\log N(k)$
1
10
$\log k$

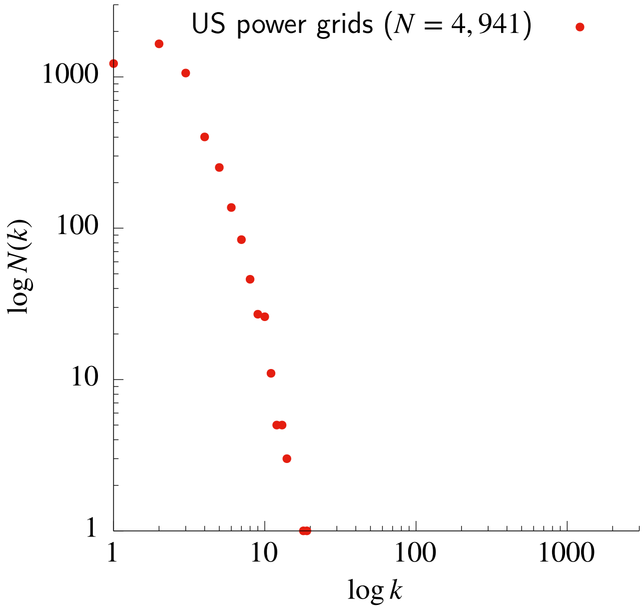

Zebra network ($N = 27$)
10
1
$\log N(k)$
1
10
$\log k$

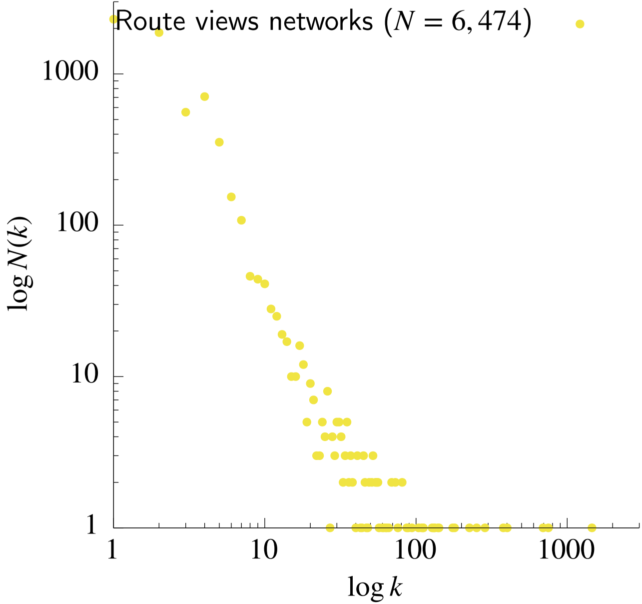

Train bombing network ($N = 64$)
10
1
$\log N(k)$
1
10
$\log k$

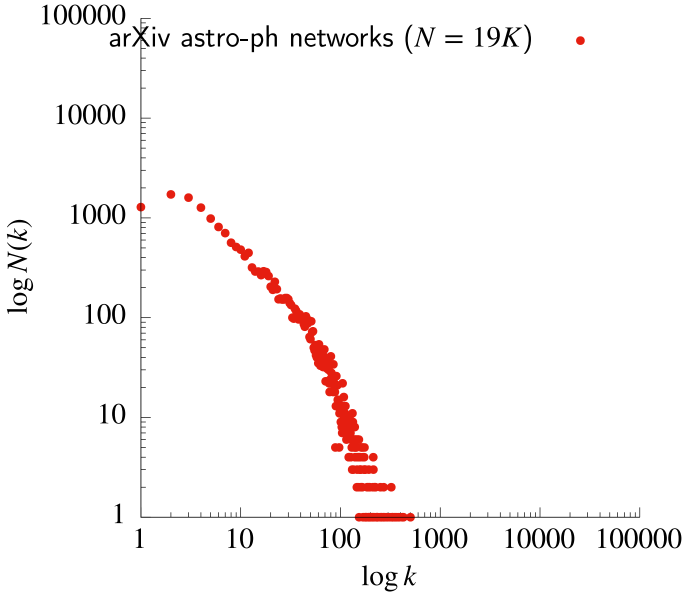

Protein interactions ($N = 212$)
1000
100
10
1
1
10
100
1000
$\log N(k)$
$\log k$

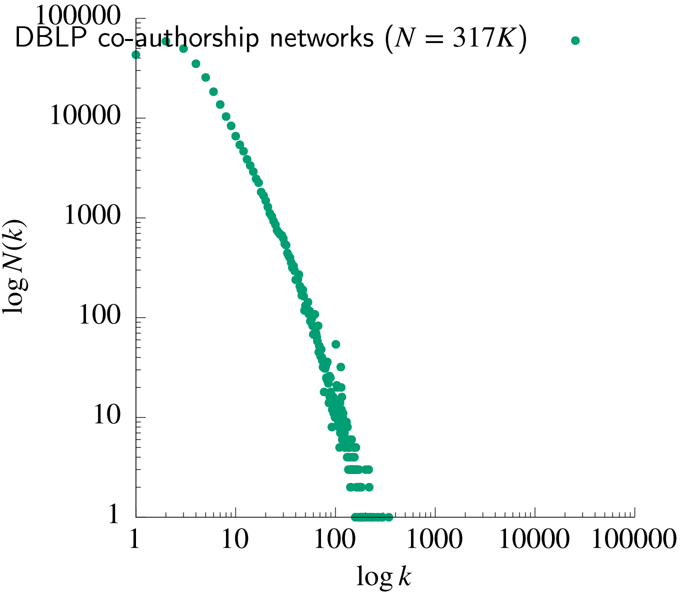

U. Rovira i Virgili email networks ($N = 1,133$)
1000
100
10
1
$\log N(k)$
1
10
100
1000
$\log k$

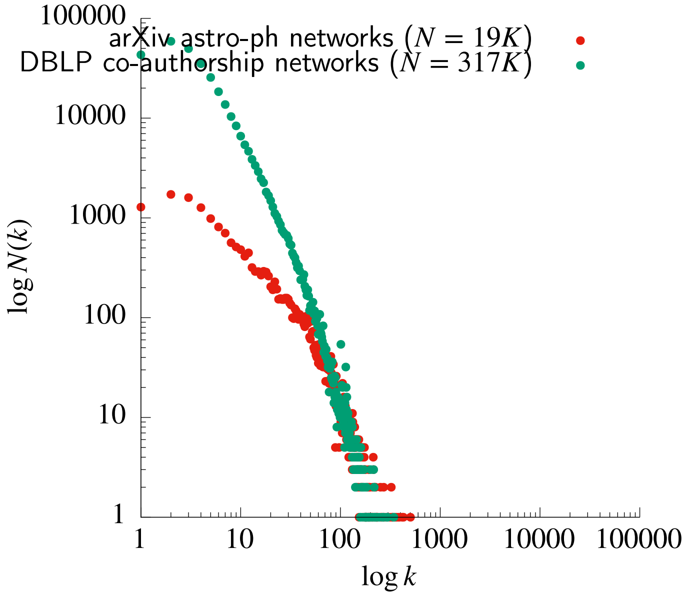

Euroroad networks $(N = 1,174)$
$\log N(k)$
1000
100
10
1
1
10
100
1000
$\log k$


US power grids ($N = 4,941$)
1000
100
10
1
$\log N(k)$
1
10
100
1000
$\log k$


Route views networks ($N = 6,474$)
1000
100
10
1
$\log N(k)$
1
10
100
1000
$\log k$


arXiv astro-ph networks ($N = 19K$)
100000
10000
1000
100
10
1
$\log N(k)$
1
10
100
1000
10000
100000
$\log k$


DBLP co-authorship networks ($N = 317K$)
100000
10000
1000
100
10
1
$\log N(k)$
1
10
100
1000
10000
100000
$\log k$


arXiv astro-ph networks ($N = 19K$)
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100000
10000
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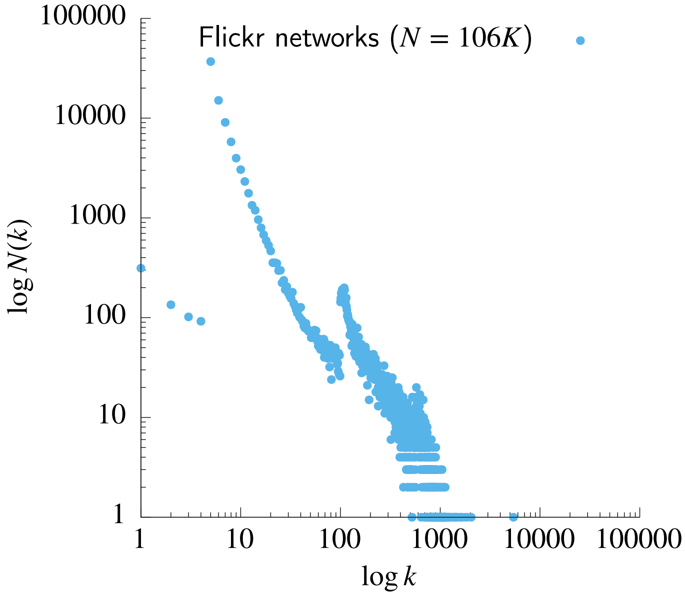
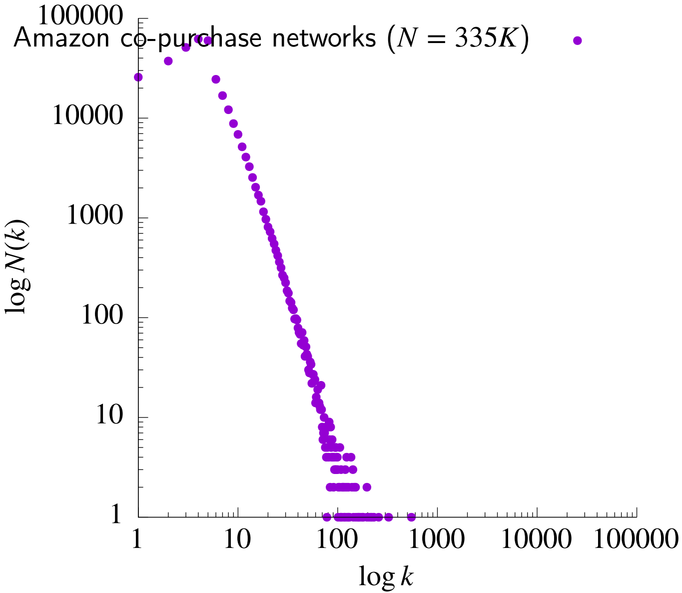
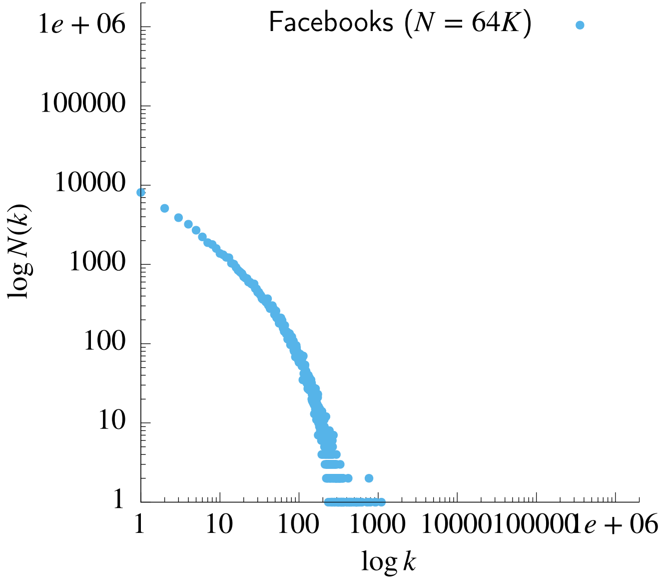
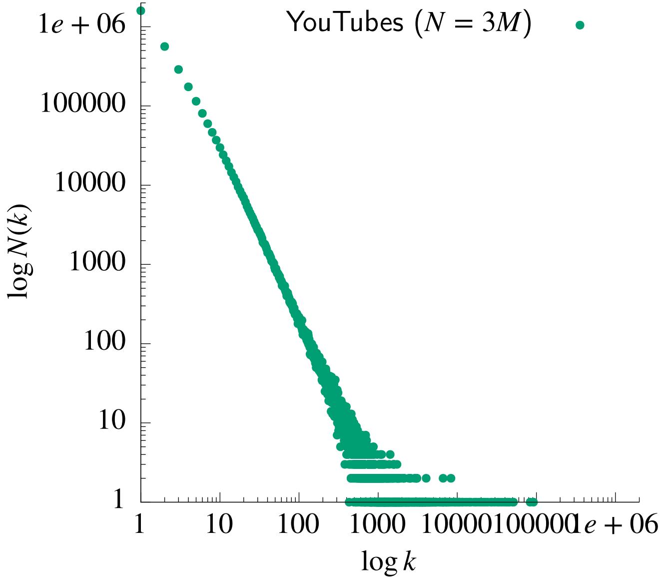
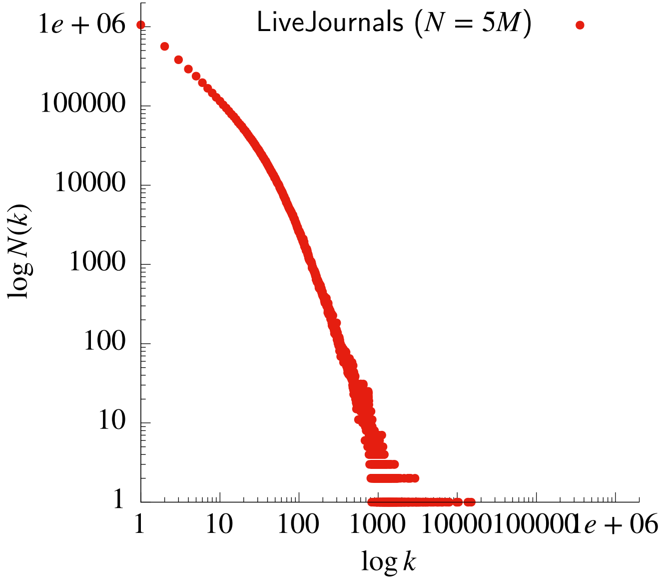
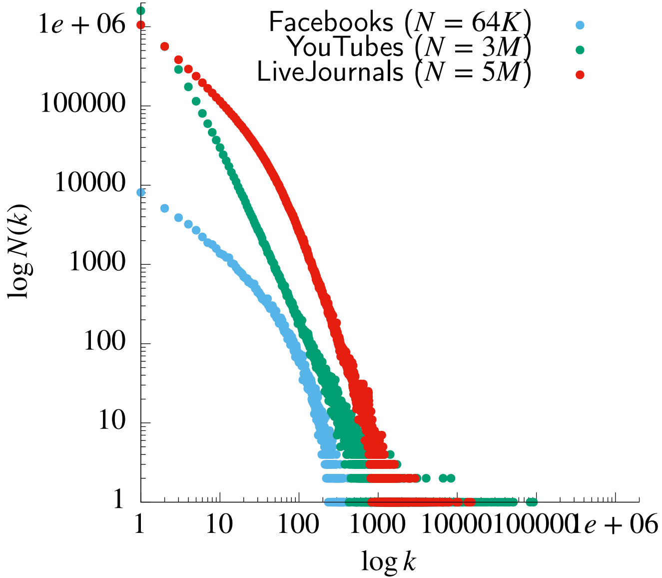

Flickr networks ($N = 106K$)
100000
10000
1000
100
10
1
$\log N(k)$
1
10
100
1000
10000
100000
$\log k$


Amazon co-purchase networks ($N = 335K$)
100000
10000
1000
100
10
1
$\log N(k)$
1
10
100
1000
10000
100000
$\log k$


Facebooks ($N = 64K$)
1e+06
100000
10000
1000
100
10
1
log N(k)
1
10
100
1000
10000
100000
1e+06
log k


YouTubes ($N = 3M$)
1e + 06
100000
10000
1000
100
10
1
log N(k)
1
10
100
1000
10000
100000
1e + 06
log k


LiveJournals ($N = 5M$)
$\log N(k)$
1e + 06
100000
10000
1000
100
10
1
$\log k$
1
10
100
1000
10000
100000
1e + 06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1e+06
100000
10000
1000
100
10
1
1
10
100
1000
10000
100000
1e+06

Power-Law

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$$\ln N(k) = \alpha - \beta \ln k$$

α — intercept

β — slope or *exponent*

$$P(k) = \frac{k^{-\beta}}{\sum_{k=1}^{N} k^{-\beta}}$$

- Almost surely connected for $\beta < 1$, and a.s. disconnected for $\beta > 1$ (Aiello, Chung, & Lu, 2000, 2001).

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- For power-law with $N \to \infty$ ($\sum_{k=1}^{N} k^{-\beta} \to \zeta(\beta)$) this becomes $\zeta(\beta - 2) - 2\zeta(\beta - 1) = 0$, which guves the value $\beta_0 \approx 3.47875$ (Aiello et al., 2000, 2001).

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- Power-law graphs can be generated by preferential attachment:

$$P[(i,j) \in E \mid k_i] = \frac{k_i^{\gamma}}{\sum_{k=1}^{k_{\max}} k_i^{\gamma}}$$

Power-Law as exponential family

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- $\Gamma(\beta) = \ln Z(\beta)$ is the *cumulant generating function*:

$$\Gamma' = m_1 = -\mathbb{E}_P\{\ln k\}$$
$$\Gamma'' = m_2 - m_1^2 = \sigma^2(\ln k)$$

where $m_n = \frac{Z^{(n)}}{Z}$ are nth moments.

Variational problems with entropy

- $P(k) = \exp\{-\beta \ln k - \Gamma(\beta)\}$ is a solution to:

$$\text{maximize} \quad H(P) \quad \text{subject to} \quad \mathbb{E}_P\{\ln k\} \leq \upsilon$$

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- $\ln k$ plays the role of a cost to be minimized.

Solution using Lagrange multipliers

- Lagrange function

$$K(P,\beta,\gamma) = -\sum_{k=1}^{N}[\ln P(k)]\,P(k) + \beta\left[\upsilon - \sum_{k=1}^{N}(\ln k)\,P(k)\right] + \gamma\left[1 - \sum_{k=1}^{N}P(k)\right]$$

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- Necessary and sufficient conditions:

$$\frac{\partial}{\partial P} K(P,\beta,\gamma) = -\ln P(k) - 1 - \beta \ln k + \gamma = 0 \quad \Rightarrow \quad P(k) = e^{-\beta \ln k - \Gamma(\beta)}$$

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$$\frac{\partial}{\partial \gamma}K(P,\beta,\gamma) = 1 - \sum_{k=1}^{N}P(k) = 0 \quad \Rightarrow \quad \Gamma(\beta) = \ln\sum_{k=1}^{N}e^{-\beta\ln k}$$

Optimal communication

- Let $c(x_i, y_j)$ be some cost function for $x_i, y_j \in V$:

$$\text{minimize} \quad \mathbb{E}_P\{c(x_i, y_j)\} \quad \text{subject to} \quad I(x_i, y_j) \le \lambda$$

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- where I is Shannon's mutual information:

$$I(x_i, y_j) := \sum_{(x_i, y_j) \in X \times Y} \left[\ln \frac{P(x_i, y_j)}{P(x_i)P(y_j)} \right] P(x_i, y_j)$$

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- Solution

$$P(x_i, y_i) = e^{-\beta c(x_i, y_j) - \Gamma(\beta, x_i)} P(x_i) P(y_j)$$

Average distance

- Consider $c(x_i, y_j) = d(i,j) - 1$ and denote $\ell := \mathbb{E}_P\{d(i,j)\}$.

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- For $|V| \gg z_1$ and $z_2 \gg z_1$ one can assume

$$|V| = \sum_{m=0}^{\ell} z_m = 1 + \sum_{m=1}^{\ell} \left[\frac{z_2}{z_1}\right]^{m-1} z_1 \approx 1 + \left[\frac{z_2}{z_1}\right]^{\ell-1} z_1$$

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- This leads to

$$\ell = \frac{\ln N - \ln z_1}{\ln(z_2/z_1)} + 1$$

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$$|V| = \sum_{m=0}^{\ell} z_m = 1 + \sum_{m=1}^{\ell} \left[\frac{z_2}{z_1}\right]^{m-1} z_1 \approx 1 + \left[\frac{z_2}{z_1}\right]^{\ell-1} z_1$$

- This leads to

$$\ell = \frac{\ln N - \ln z_1}{\ln(z_2/z_1)} + 1$$

- Relacing $z_1 = \mathbb{E}_P\{k\}$ by the actual degree k_i, we obtain conditional $\ell(k_i) := \mathbb{E}_P\{d(i,j) \mid k_i\}$:

$$\ell(k_i) = \frac{\ln N - \ln k_i}{\ln(z_2/z_1)} + 1$$

Daul problems

- Preferential attachment

$$P[(i,j) \in E \mid k_i)] = e^{-\beta(\ell(k_i)-1)-\Gamma(\beta)} = e^{\gamma \ln k_i - \Gamma(\gamma)} = \frac{k_i^\gamma}{\sum_{k=1}^{k_{\max}} k_i^\gamma}$$

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$$\text{maximize} \quad H(P) \quad \text{subject to} \quad \mathbb{E}_P\{\ln k\} \leq \upsilon$$

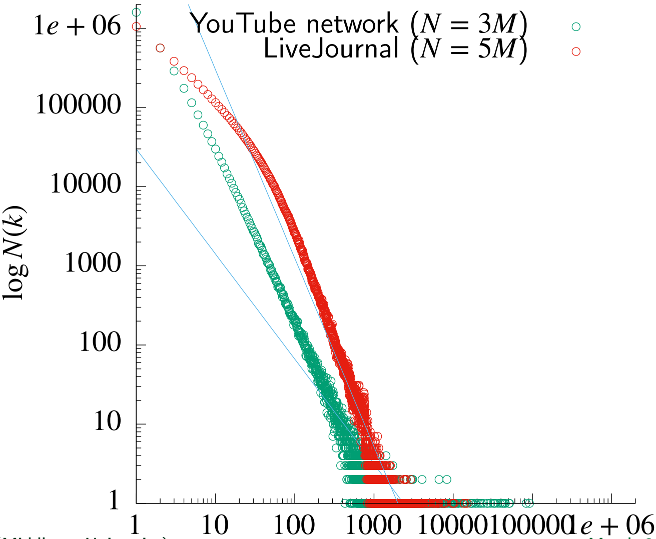
The power-law degree sequence

Power-law and maximum entropy

Power-law exponent (inverse temperature)

Free energy and phase transition

Exponent as slope



Maximum likelihood estimation

- Treating k as continuous, the m.l.e is (Newman, 2005)

$$\beta = 1 + \frac{1}{\mathbb{E}_P\{\ln k\} - \ln k_0}$$

where k_0 is the smallest degree corresponding to power-law behavious (i.e. $P(k_0) = \max P(k)$).

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- Degree k is discrete.
- What about $\beta < 1$ (possible for $N < \infty$)?

Variational approach

- Recall that $P(k) = \exp\{-\beta \ln k - \Gamma(\beta)\}$ is the solution to the maximum entropy problem, where $\beta \geq 0$ is the Lagrange multiplier such that the constraint $\mathbb{E}_P\{\ln k\} \leq \upsilon$ (or $H(P) \geq \ln N - \lambda$) is satisfied with equality:

$$\mathbb{E}_P\{\ln k\} = -\Gamma'(\beta)$$
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- Making the transofrmation $k \mapsto k/k_0$ leads to

$$\beta = \frac{H(P) + \ln P(k_0)}{\mathbb{E}_P\{\ln k\} - \ln k_0}$$

Exponent (inverse temperature)

- Recall the Lagrangian

$$K(P, \beta, \gamma) = H(P) + \beta[\upsilon - \mathbb{E}_P\{\ln k\}] + \gamma\left[1 - \sum P\right]$$

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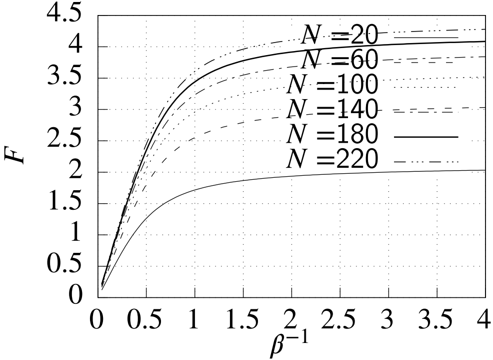
- Compare with our formula

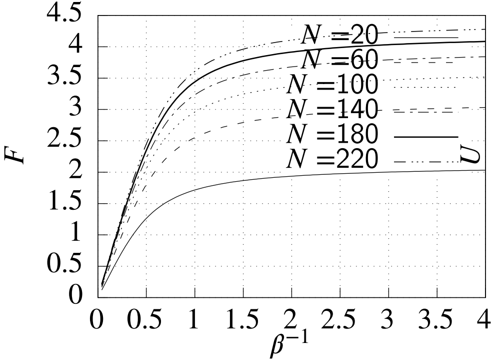
$$\beta = \frac{H(P) - \ln P^{-1}(k_0)}{\mathbb{E}_P\{\ln k\} - \ln k_0} = \frac{\Delta H}{\Delta \upsilon}$$

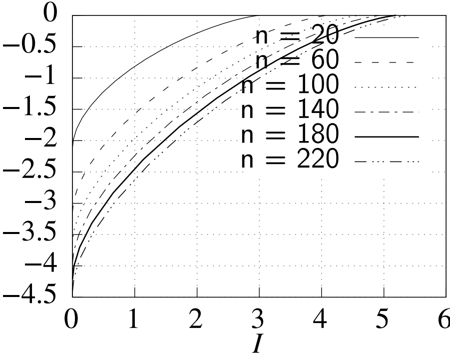
Free energy



$$F(\beta^{-1}) := -\beta^{-1}\Gamma(\beta)$$

Free energy





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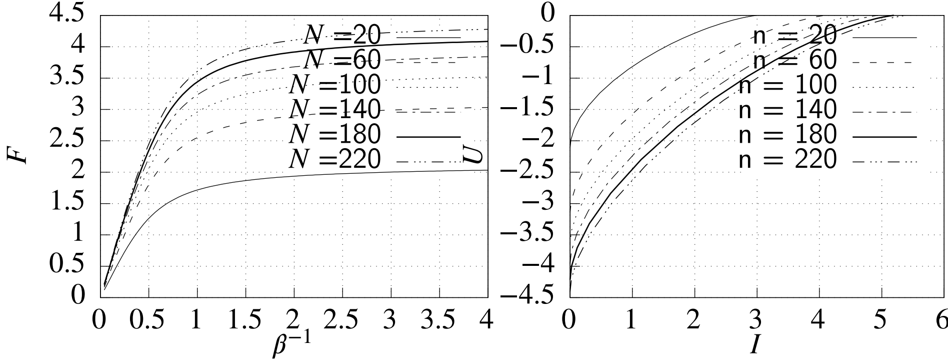

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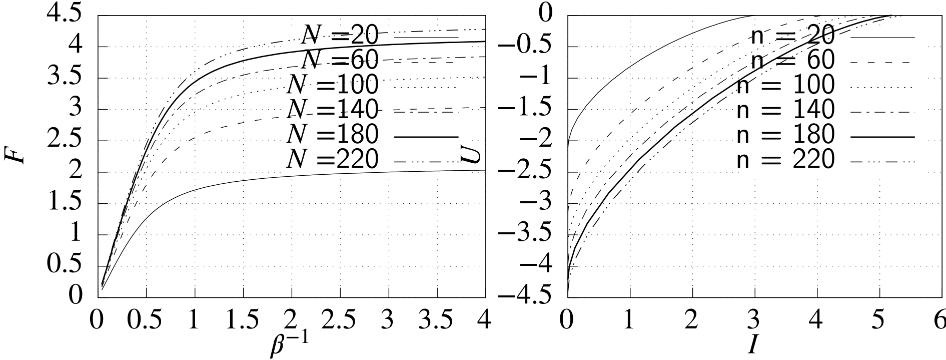

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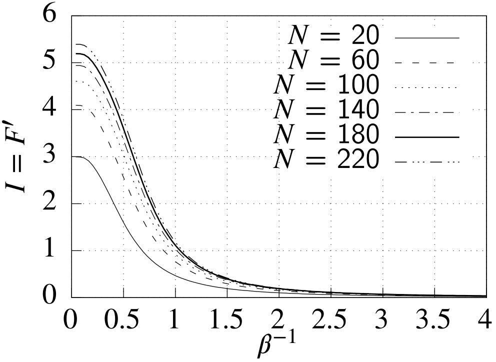
Information and entropy at $\beta = 1$



- $H(\beta) = \ln N - I(\beta)$

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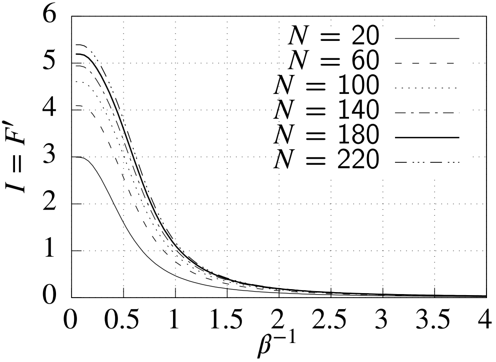

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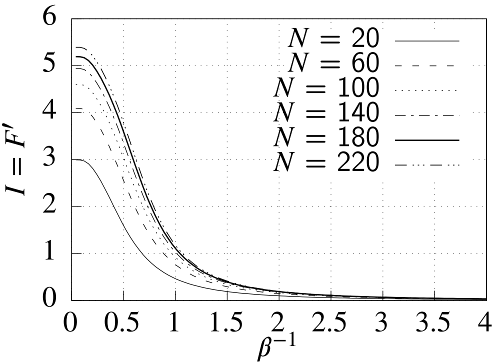

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Question

- *What happens to $F'(\beta^{-1}) = I$ in the limit $N \to \infty$ and $\beta \to 1$?*

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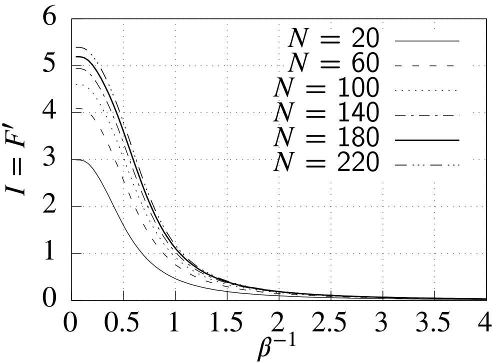

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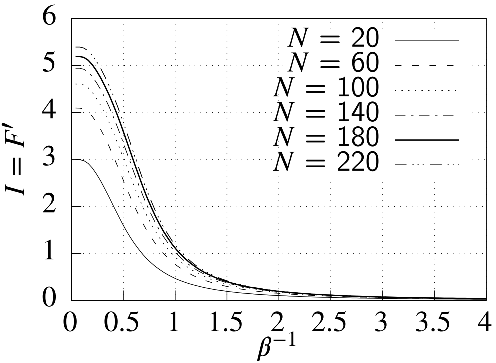

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- $I = \beta\,\Gamma'(\beta) - \Gamma(\beta)$
- $\Gamma'(\beta) = -\mathbb{E}_P\{\ln k\}$, $\Gamma''(\beta) = \sigma^2(\ln k)$.

Approximations at $\beta = 1$ and $N < \infty$

- nth cumulants $\Gamma^{(n)} = (\ln Z)^{(n)}$:

$$\Gamma' = m_1$$
$$\Gamma'' = m_2 - m_1^2$$
$$\Gamma^{(3)} = m_3 - 3m_1 m_2 + 2m_1^3$$
$$\Gamma^{(4)} = m_4 - 4m_3 m_1 - 3m_2^2 + 12 m_2 m_1^2 - 6m_1^4$$

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- where m_n are nth moments of $-\ln k$:

$$m_n(\beta) = \frac{Z^{(n)}(\beta)}{Z(\beta)}, \qquad Z^{(n)}(\beta) = (-1)^n \sum_{k=1}^{N} (\ln k)^n k^{-\beta}$$

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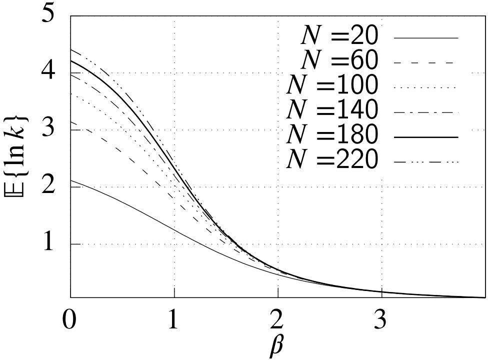
- Using $\int_1^N \frac{dx}{x} = \ln N$:

$$Z(\beta) = \sum_{k=1}^{N} \frac{1}{k^\beta}\bigg|_{\beta=1} \approx \ln N, \quad Z^{(n)}(\beta)\Big|_{\beta=1} \approx \frac{(-1)^n}{n+1} (\ln N)^{n+1}$$

Expectation of $\ln k$ at $\beta = 1$



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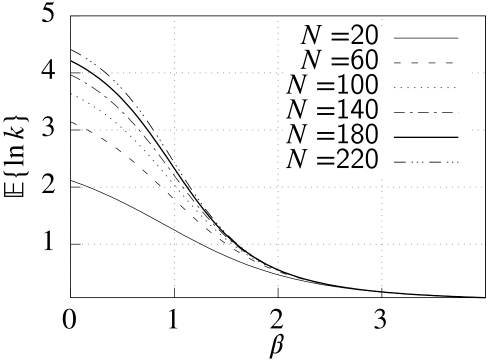

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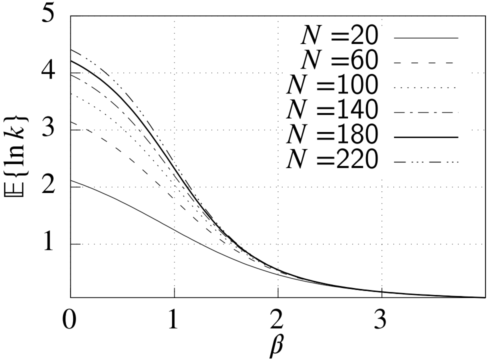

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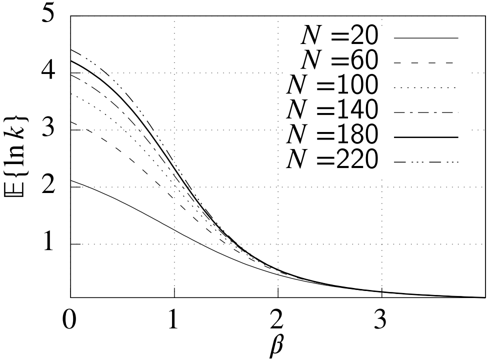

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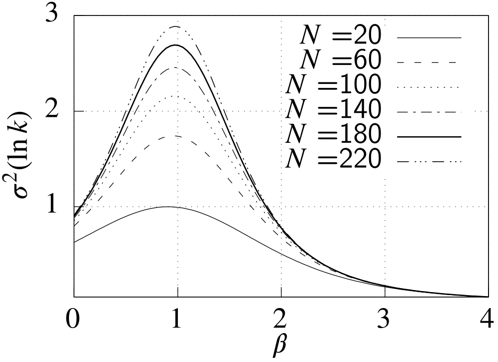
Remark

Using Jenssen's inequality $\ln \mathbb{E}_P\{k\} \geq \mathbb{E}_P\{\ln k\}$ *we also have* $\mathbb{E}_P\{k\} \geq \sqrt{N}$.

Variance of $\ln k$ at $\beta = 1$



$$\sigma^2(\ln k) = \Gamma''(\beta)\big|_{\beta=1} \approx \frac{1}{12}(\ln N)^2$$

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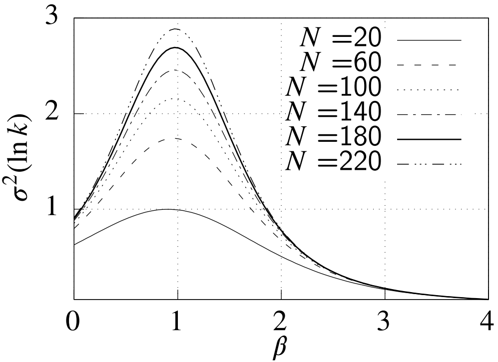

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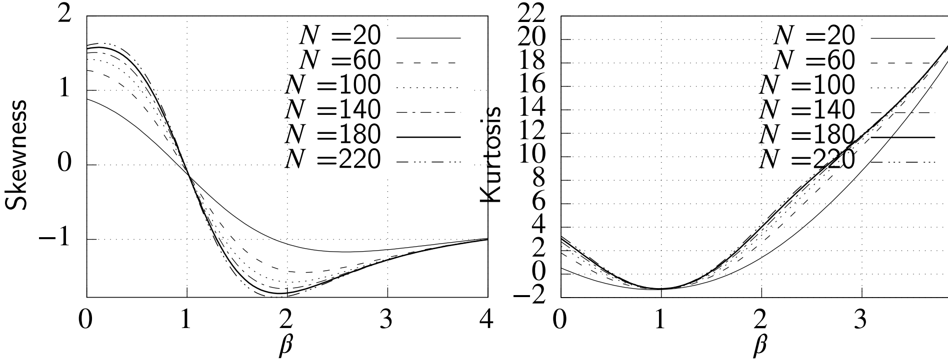
Remark (Phase transition)

The derivative $F'(\beta^{-1}) = I(\beta) = \beta\,\Gamma'(\beta) - \Gamma(\beta)$ *is not differentiable at* $\beta = 1$ *in the limit* $N \to \infty$*, because* $\Gamma''(\beta) \to \infty$*.*

Skewness and kurtosis at $\beta = 1$



$$\frac{\Gamma^{(3)}}{(\Gamma'')^{3/2}} \qquad \frac{\Gamma^{(4)}}{(\Gamma'')^{2}}$$

Giant component

- General condition of existance (Molloy & Reed, 1995; Albert & Barabási, 2002)

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- $k - 1 \geq \ln k$, and $k - 1$ approximates $\ln k$ near $k = 1$.
- $\sigma^2(k) = 1$ gives $\beta_0 \approx 3.466407\ldots$, and $\Gamma'(\beta) = \zeta'(\beta)/\zeta(\beta) = 1$ gives $\beta_0 \approx 1.6042\ldots$.

Network	$\lvert V\rvert$	LCC	$\max k$	$\mathbb{E}\{k\}$	$\mathbb{E}\{\ln k\}$	$\sigma(k)$	H
Zebra	27	23	14	8.2222	1.8819	22.7	49%
Karate club	34	34	17	4.5882	1.2805	14.6	57%
Train bombing	64	64	29	7.5938	1.6586	38.0	64%
Protein	212	161	21	2.3019	0.4918	7.0	26%
Email	1,133	1,133	71	9.6222	1.7822	87.2	45%
Euroroad	1,174	1,039	10	2.4140	0.7753	1.4	20%
US power	4,941	4,941	19	2.6691	0.8021	3.2	58%
Routes	6,474	6,474	1,459	4.2926	0.7948	628.9	22%
arXiv-ph	18,771	17,903	504	21.102	2.2768	934.2	40%
Facebook	63,731	63,392	1,098	25.640	2.3096	1599.4	37%
Flickr	105,938	105,722	5,425	43.742	2.4556	13,359.7	38%
DBLP-authorship	317,080	317,080	343	6.6221	1.3889	100.2	21%
Amazon-purchase	334,863	334,863	549	5.5299	1.4467	33.2	19%
YouTube	3,223,589	3,216,075	91,751	5.8167	0.7474	16,435	17%
LiveJournal	5,204,176	5,189,808	15,016	18.721	1.8562	2557.9	37%

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- The exponent parameter can be estimated as inverse temperature using variational principle.

Conclusions

- We show how the power-law graphs emerge as the solutions to variational problem maximizing entropy with a constraint on $\mathbb{E}\{\ln k\}$.
- The negative log-degree $-\ln k$ is related to average distance $\ell(k)$, and preferential attachment emerges as The dual problem of the solution to variational problem on miniming average distnances with a constraint on mutual information.
- The exponent parameter can be estimated as inverse temperature using variational principle.
- Power-law graphs undergo a phase transition for finite value $\beta \in [1, \beta_0]$:

$$\underbrace{\text{connected}}_{\beta<1}\underbrace{\text{disconnected, giant component}}_{[1,\beta_0]}\underbrace{\text{no giant component}}_{\beta_0<\beta}$$

The power-law degree sequence

Power-law and maximum entropy

Power-law exponent (inverse temperature)

Free energy and phase transition

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