# Power-Law and Maximum Entropy Optimization of Large Networks

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Analysis of large networks

The power-law degree sequence

Power-law and maximum entropy

Power-law exponent (inverse temperature)

Free energy and phase transition

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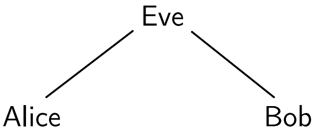
## Definition (Graph)

$G = (V, E)$, where $V = \{v_1, \ldots, v_N\}$ — *vertexes*, $E \subseteq V \times V$ — *edges*.



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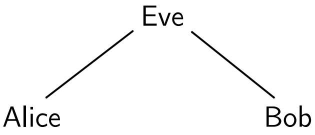


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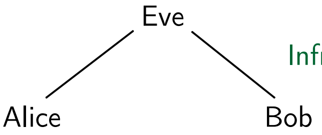


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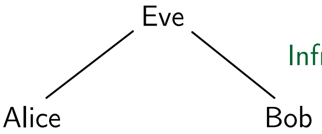


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- Is the graph connected?
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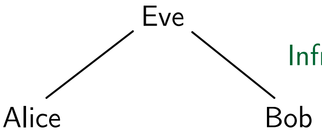


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- Which nodes are the most important (*centrality*)?
- What is the average degree (number of links of a node)?
- What is the average distance between nodes (shortest path length)?

# 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 $(\cdot, v) \in E \subseteq V \times V$):

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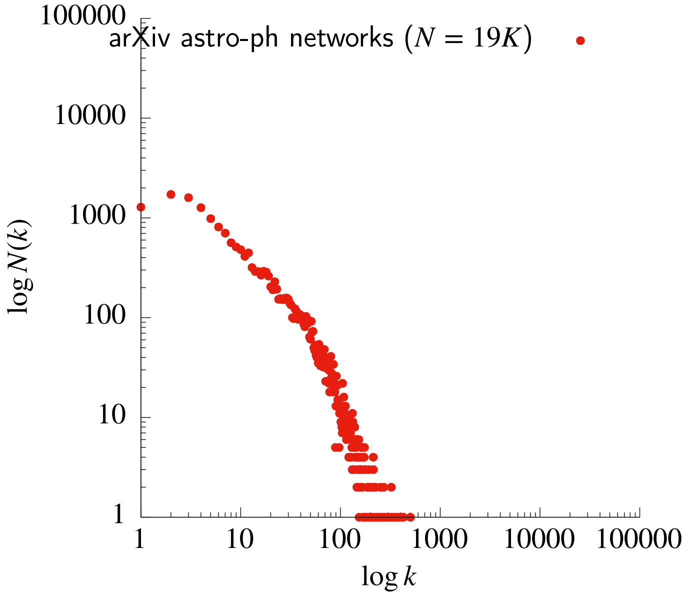
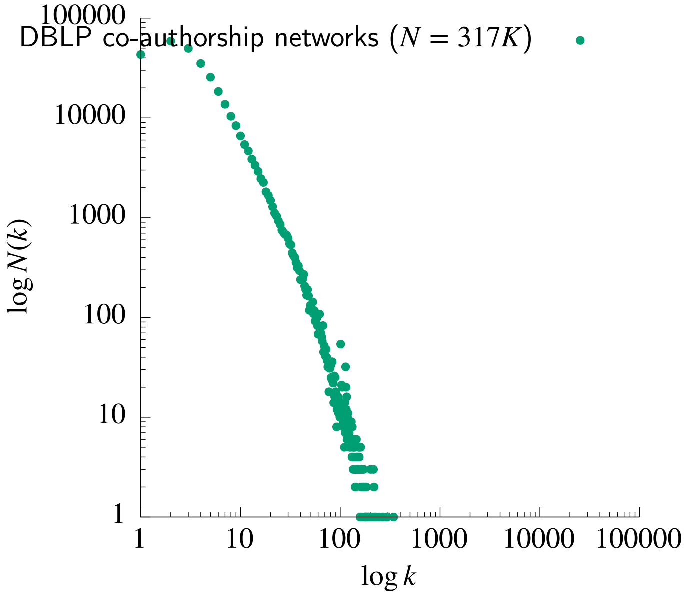
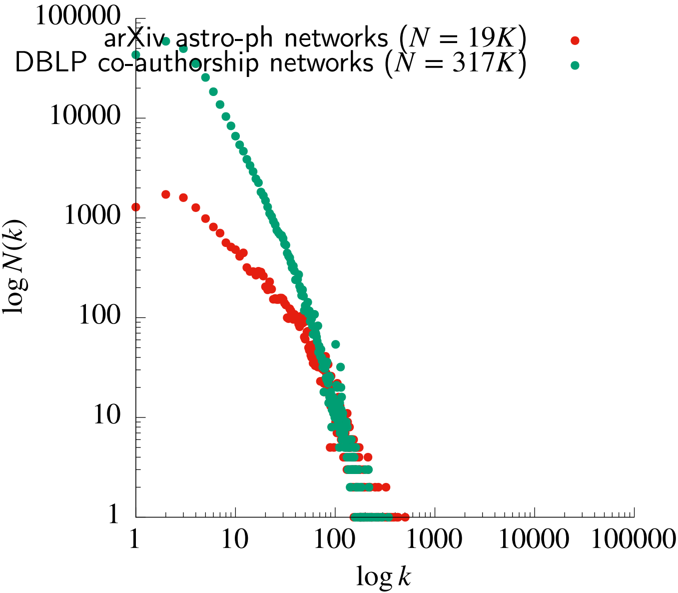
Normalized $N(k)$ is the degree *distribution*

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


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 ($N = 317K$)
$\log N(k)$
$\log k$
100000
10000
1000
100
10
1
1
10
100
1000
10000
100000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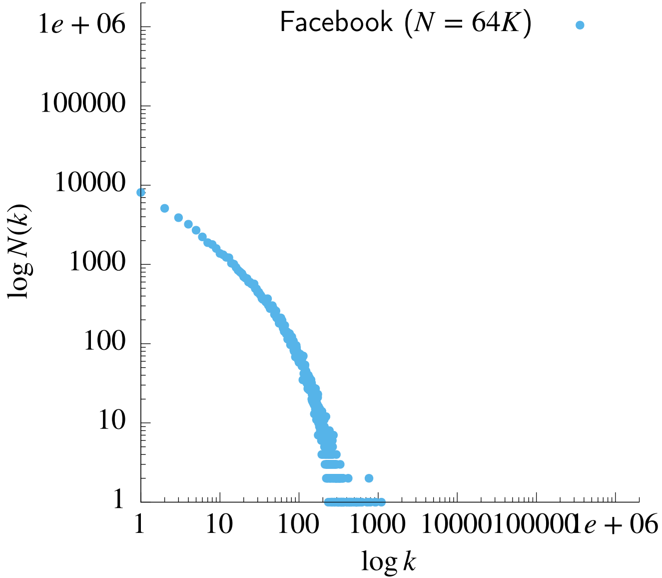
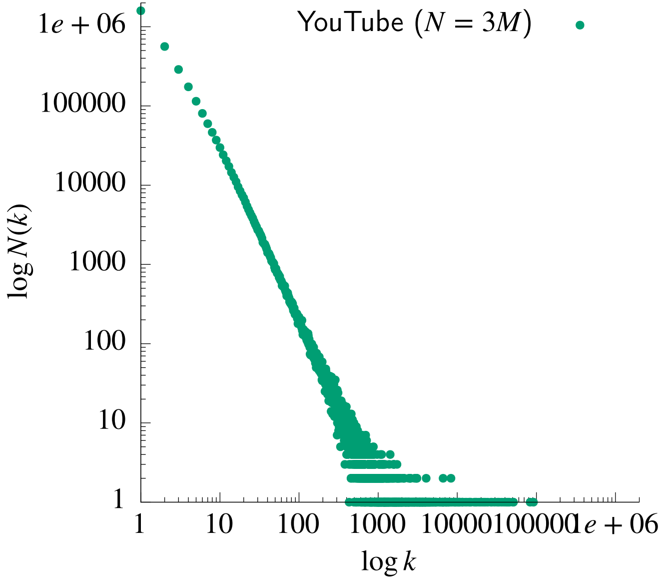
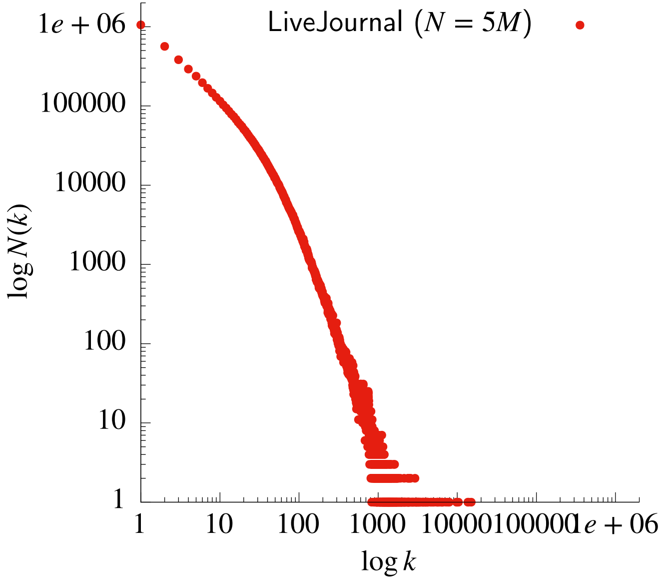
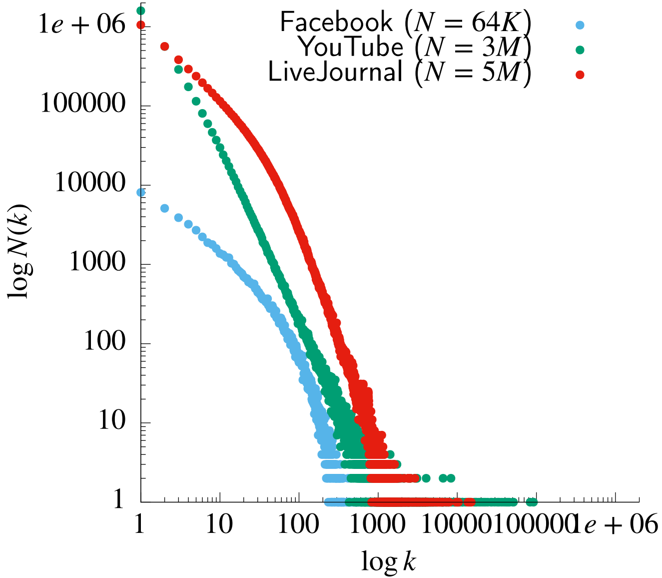

Facebook ($N = 64K$)
1e + 06
100000
10000
1000
100
10
1
log N(k)
1
10
100
1000
10000
100000
1e + 06
log k


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


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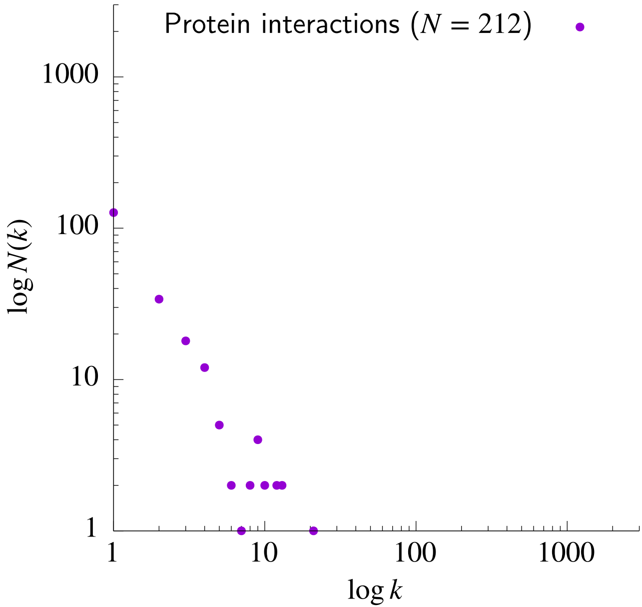
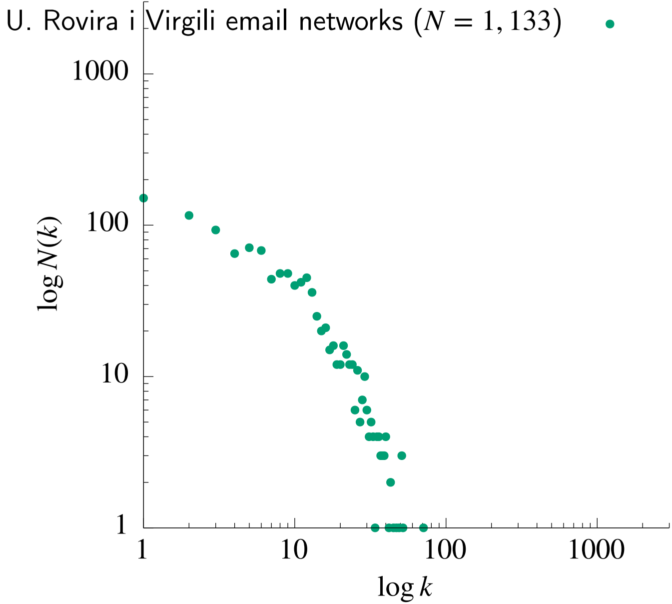
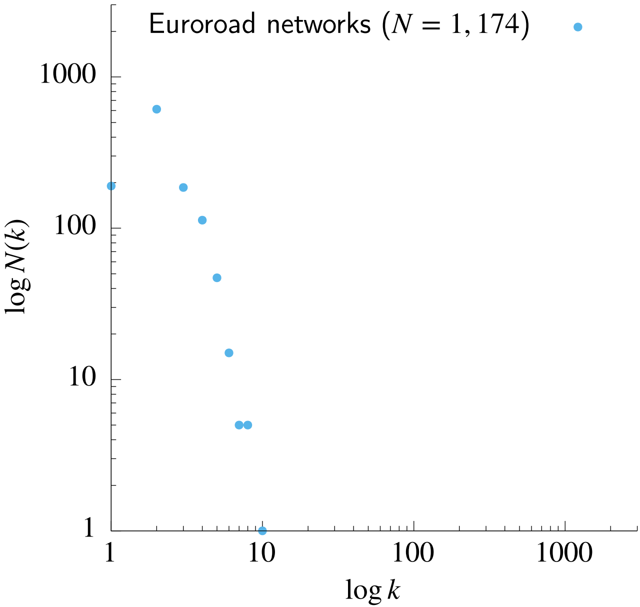
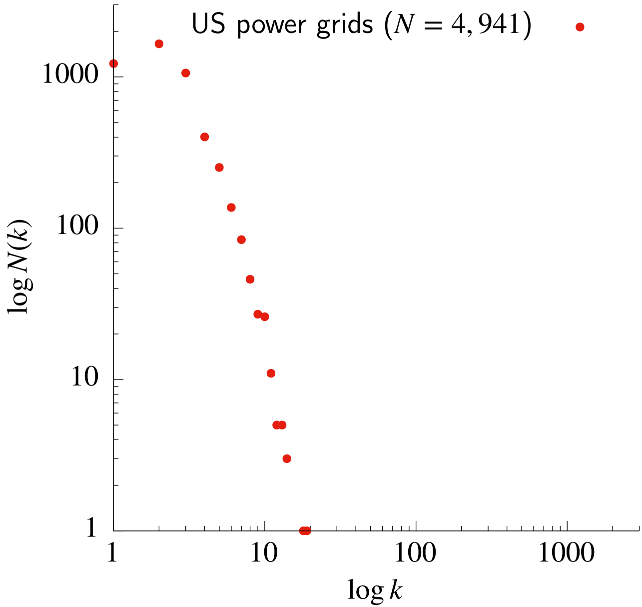
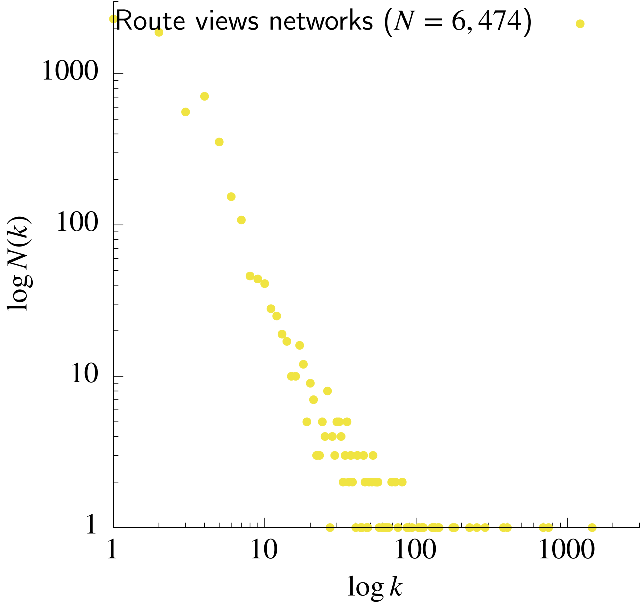

Protein interactions ($N = 212$)
1000
100
10
1
1
10
100
1000
$\log N(k)$
$\log k$


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


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


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
1
10
100
1000
$\log N(k)$
$\log k$

## Power-Law

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

$\alpha$ — intercept

$\beta$ — slope or *exponent*

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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 $\beta_0 \approx 3.47875$ (?, ?, ?).

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

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High robustness : error and attack tolerance (e.g. random edge or node removal).

# Power-Law and maximum entropy

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

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$$\ell(k_i) \sim -\ln k_i$$

# Optimal communication

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

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

- 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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# Duality

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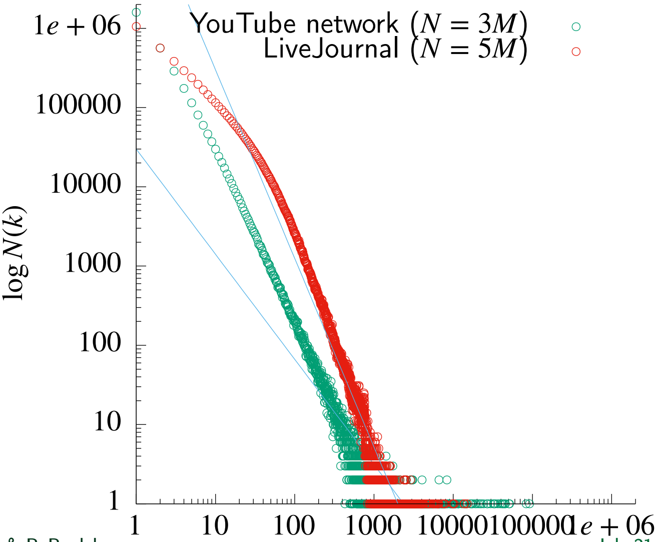
# Exponent as slope



# Maximum likelihood estimation

- Treating $k$ as continuous, the m.l.e is (?, ?)

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

where $k_0$ is the smallest degree corresponding to power-law behaviour (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:

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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

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

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- Compare with our formula

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

Analysis of large networks

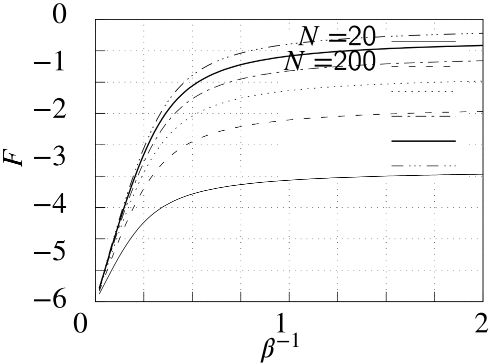
The power-law degree sequence

Power-law and maximum entropy

Power-law exponent (inverse temperature)

Free energy and phase transition

# Free energy




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

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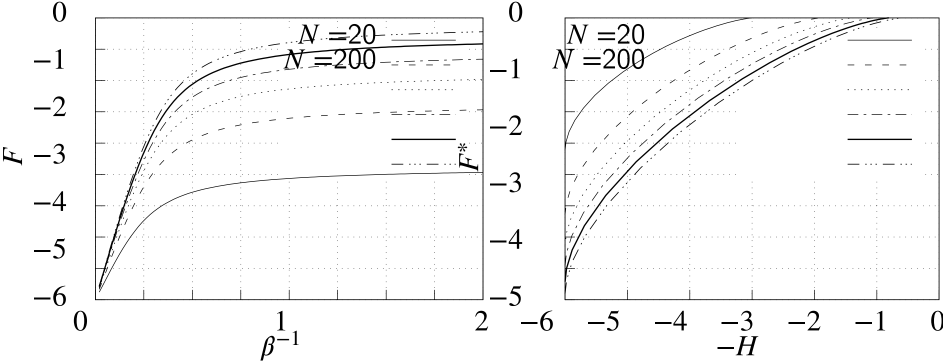


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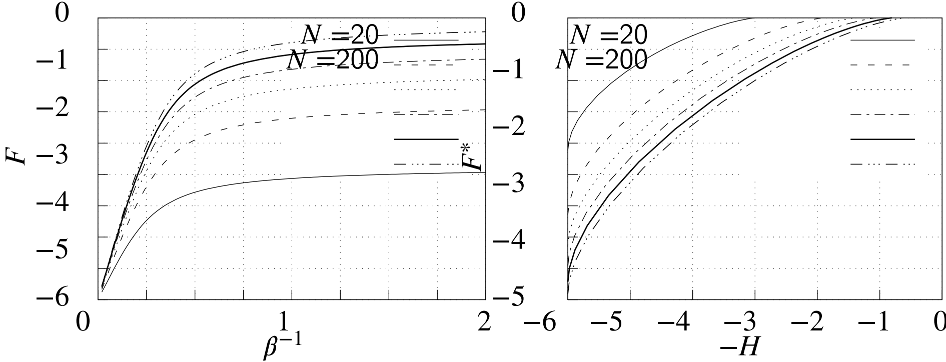


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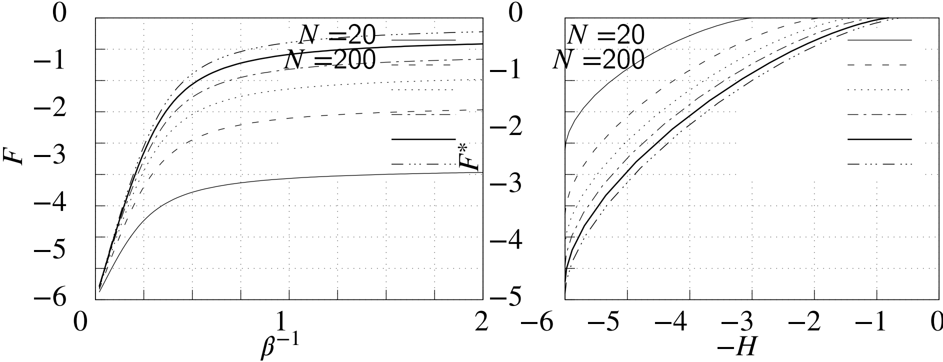


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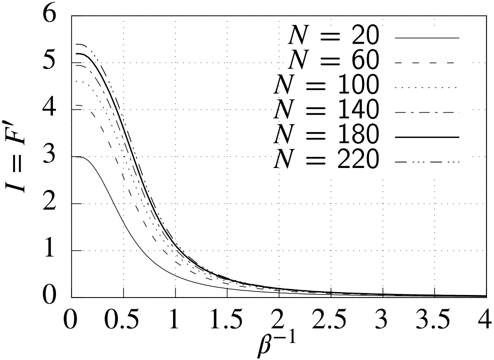
# Information and entropy at $\beta = 1$




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

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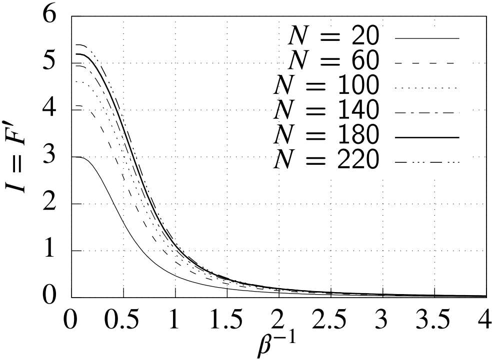


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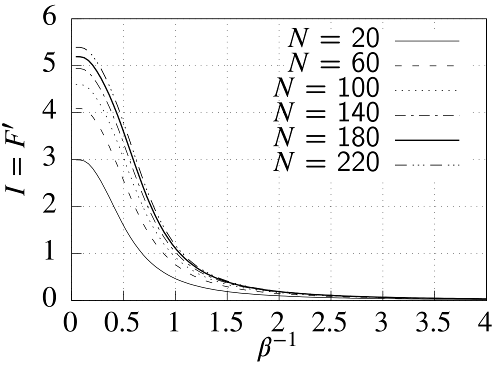


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- *What happens to $F'(\beta^{-1}) = I$ in the limit $N \to \infty$ and $\beta \to 1$?*

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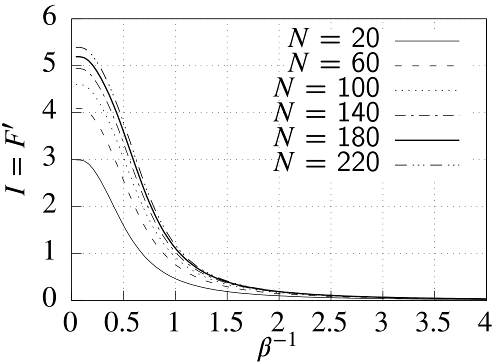


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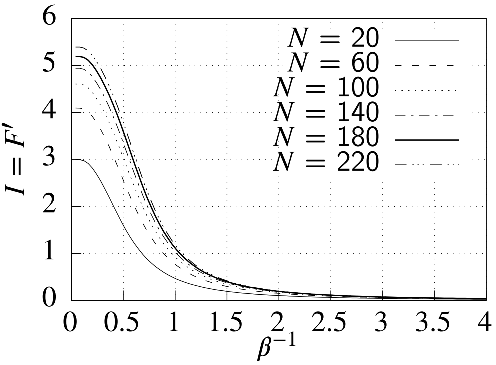


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- $I = \beta\, \Gamma'(\beta) - \Gamma(\beta)$
- $\Gamma'(\beta) = -\mathbb{E}_P\{\ln k\}$, $\Gamma''(\beta) = \sigma^2(\ln k)$.

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

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

$$\begin{aligned}
\Gamma' &= m_1 \\
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\Gamma^{(3)} &= m_3 - 3m_1 m_2 + 2m_1^3 \\
\Gamma^{(4)} &= m_4 - 4m_3 m_1 - 3m_2^2 + 12m_2 m_1^2 - 6m_1^4
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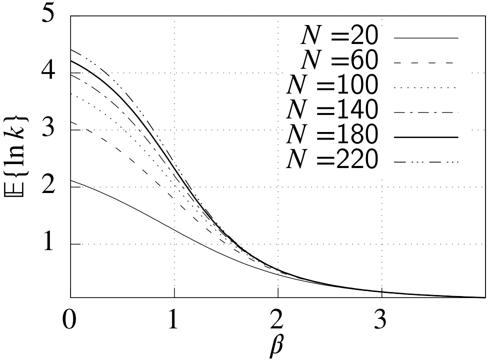
- Using $\int_1^N \frac{dx}{x} = \ln N$:

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

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




$$\mathbb{E}_P\{\ln k\} = -\Gamma'(\beta)$$

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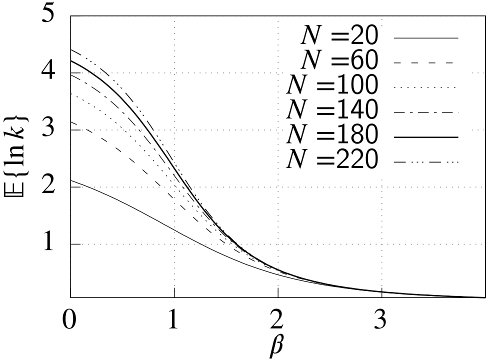


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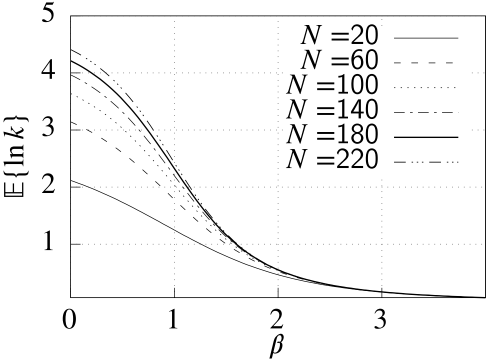


$$
\begin{aligned}
\mathbb{E}_P\{\ln k\} &= -\,\Gamma'(\beta) \\
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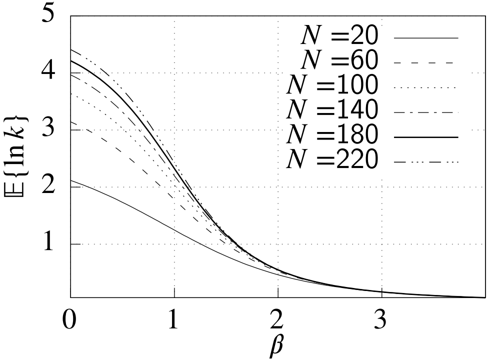
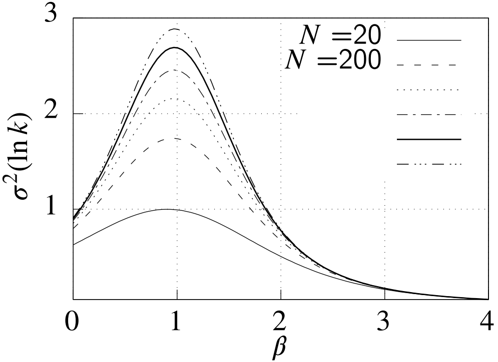



$$\mathbb{E}_P\{\ln k\} = -\Gamma'(\beta) = -\left.\frac{Z'(\beta)}{Z(\beta)}\right|_{\beta=1} \approx \frac{1}{2}\ln N$$

## 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 $\beta = 1$

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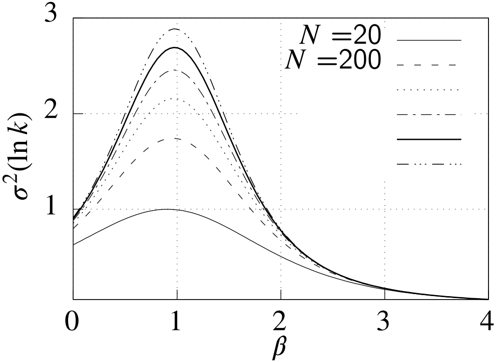


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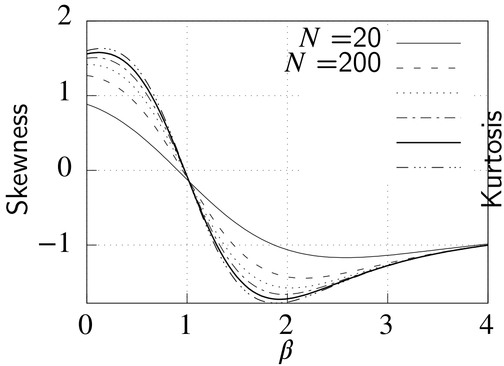
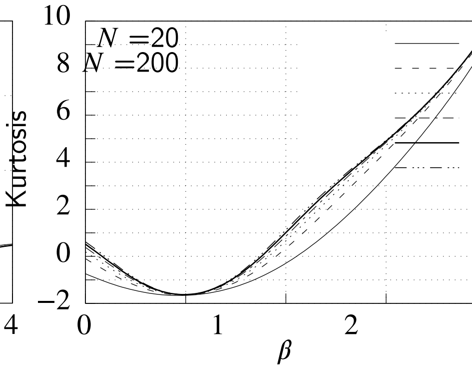
## Remark (Phase transition)

*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 $\beta = 1$




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

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  4. Generate the network using preferential attachment: $P(e \mid k) \propto e^{-\beta f(k)}$.

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  2. Define the cost function $c : V \times V \to \mathbb{R}$ (or utility $u = -c$).
  3. Analyse conditional expected cost $f(k, \dots) = \mathbb{E}\{c \mid k, \dots\}$ as a function of network parameters (e.g. degree $k$).
  4. Generate the network using preferential attachment: $P(e \mid k) \propto e^{-\beta f(k)}$.
  5. Tune parameter $\beta$ (inverse temperature) based on the constraints.

# Conclusions and discussion

- The power-law topology emerges as the solutions to the maximum entropy problem with constraint $\mathbb{E}\{\ln k\} \leq \upsilon$.
- The negative log-degree $-\ln k$ is related to average path length $\ell(k)$.
- The preferential attachment emerges as the solution to the dual problem problem on minimization of the average path length with a constraint on mutual information.
- These principles can be used to optimize various types of networks:
  1. Define the network $G(V, E)$.
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  4. Generate the network using preferential attachment: $P(e \mid k) \propto e^{-\beta f(k)}$.
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- This approach leads to new insights into properties of the power-law graphs (e.g. a phase transition at $\beta = 1$ characterized by maximum variance, zero skewness and minimum kurtosis of $\ln k$).

Analysis of large networks

The power-law degree sequence

Power-law and maximum entropy

Power-law exponent (inverse temperature)

Free energy and phase transition

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