Breaking of ensemble equivalence in networks

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Introduction

It is generally believed that, in the thermodynamic limit, the *microcanonical description* as a function of *energy* coincides with the *canonical description* as a function of *temperature*. However, various examples of systems for which the microcanonical and canonical ensembles are not equivalent have been identified. Here we show that ensemble non-equivalence can manifest itself also in random graphs with topological constraints.

Methods

The difference between the description provided by the microcanonical distribution (heraby indicated with f) and that provided by the canonical distribution (hereby indicated with P) can be compactly expressed via the Kullback-Leibler divergence

$$D_{KL}(f||P)=\sum_{\mathbf{G}\in\mathcal{G}} f(\mathbf{G}^*)\ln\left[\frac{f(\mathbf{G}^*)}{P(\mathbf{G}^*)}\right]$$

that reduces to a difference of entropies (see main box). Upon inspecting its behavior in the thermodynamical limit

$$N\longrightarrow+\infty$$

(i.e. in the limit of infinite networks), we obtain the proper quantification of the ensemble non-equivalence.

Conclusions

While graphs with a given number of links are ensemble-equivalent, graphs with a given degree sequence are not. This result holds irrespective of whether the energy is nonadditive (as in unipartite graphs) or additive (as in bipartite graphs). In contrast with previous expectations, our results show that

- *physically*, nonequivalence can be induced by an extensive number of local constraints, and not necessarily by long-range interactions or nonadditivity;
- *mathematically*, nonquivalence is determined by a different large-deviation behaviour of microcanonical and canonical probabilities for a single microstate and not necessarily for almost all microstates.

The latter criterion, which is entirely local, is not restricted to networks and holds in general.

References

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Ensemble non-equivalence

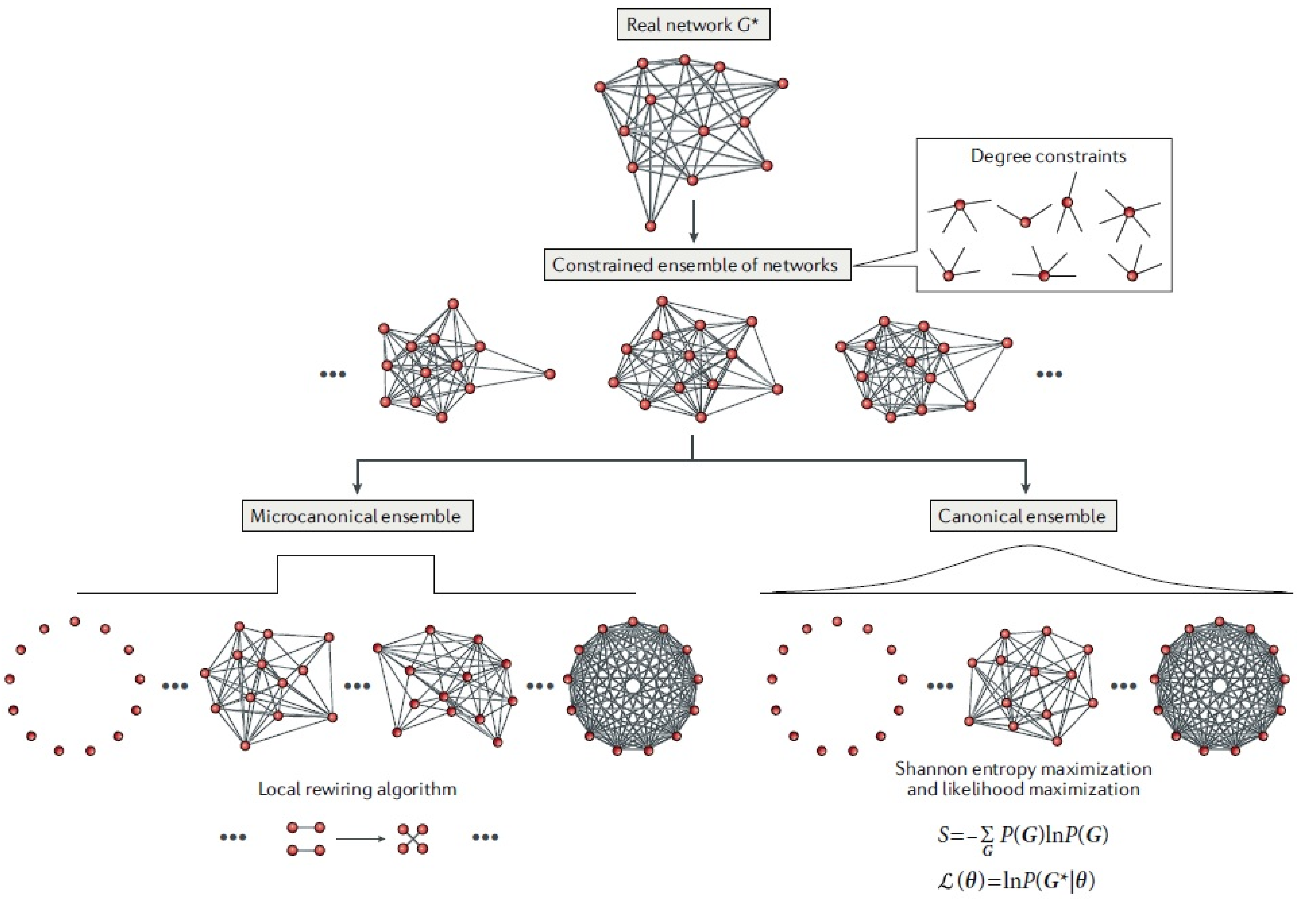

Figure 1: Graphic illustration of the two different network ensembles, i.e. microcanonical and canonical.

The recently-provided definition of *measure equivalence* states that ensembles are (said to be) equivalent when the canonical probability distribution converges to the microcanonical probability distribution in the thermodynamic limit.

The criterion above can be quantified via the Kullback-Leibler (KL) divergence that, in turn, reduces to a difference of entropies. In fact,

$$\begin{aligned}
D_{KL}(f||P) &= \sum_{\mathbf{G}\in\mathcal{G}} f(\mathbf{G}^*)\ln\left[\frac{f(\mathbf{G}^*)}{P(\mathbf{G}^*)}\right]\\
\text{(local criterion)} &= \ln\left[\frac{f(\mathbf{G}^*)}{P(\mathbf{G}^*)}\right]\\
\text{(difference of likelihoods)} &= -\ln P(\mathbf{G}^*)+\ln f(\mathbf{G}^*)=\\
\text{(definition of microcanonical ensemble)} &= -\ln P(\mathbf{G}^*)-\ln\Omega(\mathbf{G}^*)\\
\text{(entropy-likelihood relationship)} &= -\sum_{\mathbf{G}\in\mathcal{G}} P(\mathbf{G}^*)\ln P(\mathbf{G}^*)-\ln\Omega(\mathbf{G}^*)\\
&= S_{can}-S_{mic}\equiv\Delta
\end{aligned}$$

where the property we have employed is indicated in parentheses. Proper ensemble non-equivalence is inspected by calculating the quantity

$$s=\lim_{N\to+\infty}\frac{\Delta}{N}$$

i.e. the KL divergence in the asymptotic limit of infinite networks.

Non-equivalence can be inspected quite easily in the case of the Erdös-Rényi model; in fact, one finds that

$$S_{mic}=\ln\Omega=\ln\binom{\frac{N(N-1)}{2}}{L}\simeq-\binom{N}{2}[(1-p)\ln(1-p)+p\ln p]-\Delta=S_{can}-\Delta$$

where $p=\frac{2L}{N(N-1)}$ and $\Delta=\ln\sqrt{2\pi\sigma^2[L]}$, i.e. it is (proportional to) the logarithm of the standard deviation of the only constraint defining our model, i.e. the total number of links. Since $\sigma[L]\propto N$, one finds that $s\propto\frac{\ln N}{N}\to 0$ in the thermodynamic limit: hence, the microcanonical and the canonical Erdös-Rényi models are equivalent. Generally speaking, however, ensembles are not equivalent: this is the case of the Configuration Model, for which one finds $s>0$ (e.g. for sparse regular networks, it holds that $s=\ln\sqrt{2\pi k}$).

Taken together, the above examples indicate that ensemble equivalence holds when there is a single global constraint, while it is broken when there is an *extensive number* of local constraints. This also indicates that graphs with local constraints are always nonequivalent, irrespectively of the breadth of the degree distribution.