Maximum Entropy Analysis of Flow Networks with Structural Uncertainty (Graph Ensembles)

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Abstract This study examines MaxEnt methods for probabilistic inference of the state of flow networks, including pipe flow, electrical and transport networks, subject to physical laws and observed moments. While these typically assume networks of invariant graph structure, we here consider higher-level MaxEnt schemes, in which the network structure constitutes part of the uncertainty in the problem specification. In physics, most studies on the statistical mechanics of graphs invoke the Shannon entropy $H_G^{Sh} = -\sum_{\Omega_G} P(G) \ln P(G)$, where G is the graph and Ω_G is the graph ensemble. We argue that these should adopt the relative entropy $H_G = -\sum_{\Omega_G} P(G) \ln P(G)/Q(G)$, where $Q(G)$ is the graph prior associated with the graph macrostate G. By this method, the user is able to employ a simplified accounting over graph macrostates rather than need to count individual graphs. Using

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combinatorial methods, we here derive a variety of graph priors for different graph ensembles, using different macrostate partitioning schemes based on the node or edge counts. A variety of such priors are listed herein, for ensembles of undirected or directed graphs.

Keywords Maximum entropy · Graphs · Networks · Graph priors · Graph ensemble

1 Introduction

Over the past few years, we have developed a MaxEnt framework to infer the state of flow on all types of flow networks, for example, pipe flow, electrical, communications and transport networks [1–4]. In this approach, the user adopts the relative entropy:

$$H_{\mathbf{X}} = -\int_{\Omega_{\mathbf{X}}} P(\mathbf{X}) \ln \frac{P(\mathbf{X})}{Q(\mathbf{X})} d\mathbf{X} \tag{1}$$

in which $\mathbf{X}$ are the unknown network parameters (such as flow rates and potentials), $P(\mathbf{X})$ is a joint probability density function (pdf) over $\mathbf{X}$, $Q(\mathbf{X})$ is the prior pdf, and $\Omega_{\mathbf{X}}$ is the domain of $\mathbf{X}$. The entropy (1) is maximized, subject to the constraints on the network, to infer the state of the network. The constraints necessarily include all relevant physical laws (such as Kirchhoff's node and loop laws), as well as any physical observations measured at particular nodes, edges or over components of the network. The resulting inference is expressed in terms of the pdf $P(\mathbf{X})$, which can either be used directly, or from which the moments or other statistical features of the flow (e.g., mean, mode, variances) can be extracted. The MaxEnt method, therefore, provides one approach to extend previous deterministic methods for flow network analysis, applicable only to fully determined networks, to a probabilistic framework which can handle incomplete information.

In the past decade, there has been a tremendous surge of interest in the structural properties of networks in statistical physics (and other fields), especially the emergent scaling features of the Internet and human social networks [5–8]. Such studies generally consider the probability $P(G)$ of a graph G within a graph ensemble Ω_G, almost always inferred by maximizing the Shannon entropy [9]:

$$H_G^{Sh} = -\sum_{G \in \Omega_G} P(G) \ln P(G) \tag{2}$$

While correct, this formulation does not exploit the fundamental advantage of statistical mechanics, based on the separate counting of observable macrostates and their underlying microstates. Instead of (2), network analysts and graph theorists would be better advised to adopt the discrete relative entropy (negative Kullback–Leibler) function [10]

$$H_G = -\sum_{G \in \Omega_G} P(G) \ln \frac{P(G)}{Q(G)} \tag{3}$$

now based on the graph macrostates G, defined as equivalence classes (sets) of graphs which partition the ensemble Ω_G. $P(G)$ and $Q(G)$ now represent the posterior and prior probabilities of the macrostate G within the graph ensemble Ω_G. Eq. (3) ensures that maximizing (3), subject only to normalization, gives the inferred state $P^*(G) = Q(G)$ [11]. Further constraints will then restrict the ensemble, either by removing (microcanonical ensemble) or weighting (canonical ensemble) its constituent graphs, causing $P^*(G)$ to deviate from $Q(G)$ consistent with these constraints. In contrast, the Shannon form (2) requires the counting of each individual graph in an ensemble, which may be quite onerous for large ensembles, and does not provide the user with any insights from the network structure.

We can indeed unite the above fields, to present a MaxEnt framework for probabilistic inference of flows on a network, subject to uncertainty in the flow parameters and *in the network structure itself*. This entails use of the relative entropy function:

$$H_{G,\mathbf{X}(G)} = -\sum\nolimits_{\Omega_G} \int_{\Omega_{\mathbf{X}(G)}} P(\mathbf{X}(G), G) \ln \frac{P(\mathbf{X}(G), G)}{Q(\mathbf{X}(G), G)} d\mathbf{X} \tag{4}$$

where $P(\mathbf{X}(G), G)$ and $Q(\mathbf{X}(G), G)$ are the joint posterior and prior pdfs, defined over parameters $\mathbf{X}$ and graph macrostates G. As a first step, analyzes using (4) will generally invoke the Bayesian separation:

$$Q(\mathbf{X}(G), G) = Q(G)Q(\mathbf{X}(G)|G) \tag{5}$$

based on the distinct graphical and flow priors $Q(G)$ and $Q(\mathbf{X}(G)|G)$. For some flow networks, complete separability $Q(\mathbf{X}(G), G) = Q(G)Q(\mathbf{X})$ may be possible.

The aim of this study is to formally derive the priors $Q(G)$ for graph macrostates in a variety of graph ensembles, as a prelude to later studies on the joint graph and flow parameter priors $Q(\mathbf{X}(G), G)$. We here note that graph priors will not only depend on the graph ensemble selected, but also on the rule (equivalence relation) used to partition the ensemble into graph macrostates. Different partitioning rules will obviously give rise to different priors —there are many ways to count cats in a collection of user-selected baskets of cats. The choice of ensemble and partitioning scheme must, therefore, be made by the user, and so will depend on his/her purpose, although some approaches will be more mathematically tractable or fruitful.

2 Derivation of Graph Priors

In statistical physics, the *degeneracy* $g(G)$ of a discrete macrostate G can be defined as its statistical weight or number of occurrences in the ensemble [12], counting each component graph (or microstate) once each. If the entire ensemble Ω_G is also countable and finite, then the prior can be calculated by

$$Q(G) = \frac{g(G)}{|\Omega_G|} \tag{6}$$

where $|\Omega_G|$ is the cardinal number of Ω_G. If the macrostate and ensemble are both countably infinite or uncountable, it may be possible to define the prior by a limiting process applied to (6), although many such priors will be found to vanish asymptotically.

We here calculate priors for various graph macrostates G in a range of graph ensembles Ω_G, using partitioning rules based on the numbers of nodes and/or edges. These include both undirected and directed graph ensembles, each discussed in turn. The complete sets of results are summarized, respectively, in Tables 1 and 2. In the following, all nodes and edges are considered distinguishable (are labeled), and so are counted according to their multiplicities in each macrostate and the ensemble. Where present, self-edges are each counted only once.

2.1 Undirected Graph Priors

In turn, we discuss various partitioning schemes for undirected graph ensembles, which are appropriate for the analysis of potential-driven flows, such as electricity, pipe flow and chemical networks. All results are tabulated in Table 1.

(1) We first consider an ensemble of simple graphs with N nodes, which can be partitioned into macrostates based on the number of edges M. We disallow self-loops. By a little consideration, it will be seen that the degeneracy of each such macrostate can be derived by the allocation of M indistinguishable digits (such as 1s) to the upper triangle of elements A_{ij} of the adjacency matrix $\mathcal{A}$, with all occupancies restricted to $\{0, 1\}$. This gives degeneracy $g = \binom{T_{N-1}}{M}$, based on the $(N-1)$th triangle number $T_{N-1} = \frac{1}{2}N(N-1)$ of independent matrix elements. By summation or direct allocation, the ensemble itself can be shown to have cardinal number $2^{T_{N-1}}$, hence, the prior is obtained as $Q(G) = \binom{T_{N-1}}{M}/2^{T_{N-1}}$.

(2) We then embed the above 'microcanonical' ensemble into a 'canonical' ensemble of all simple undirected graphs with $n \leq N$ nodes, for fixed N. We consider three different partitioning schemes:

(a) A partitioning scheme based on the macrostates with n nodes and M edges. By construction from (1), we directly obtain the degeneracy $g = \binom{T_{n-1}}{M}$ and ensemble dimension $\sum_{n=1}^{N} 2^{T_{n-1}}$, hence giving the corresponding prior.
(b) A partitioning scheme based on the macrostates with M edges, regardless of the number of nodes. From (a), the degeneracy is then $g = \sum_{n=1}^{N} \binom{T_{n-1}}{M}$, while the ensemble dimension is unchanged, giving the corresponding prior.
(c) A partitioning scheme based on the macrostates with n nodes, regardless of the number of edges. The degeneracy is then given by the subset ensemble with n nodes, of dimension $2^{T_{n-1}}$; using the known ensemble dimension then gives the prior.

(3) We now consider the ensemble of single-edge undirected graphs with N nodes, now allowing for self-loops. We consider two partitioning schemes:

(a) In the first scheme, we partition the ensemble into macrostates of graphs with N nodes, L self-edges and m non-self-edges. The number of graphs in each such macrostate is given by the number of ways to allocate m elements in the upper triangle of the adjacency matrix, without self-loops $\binom{T_{N-1}}{m}$, multiplied by the number of ways to allocate L self-loops amongst the N diagonal elements $\binom{N}{L}$. The ensemble now has dimension 2^{T_N}, based on the Nth triangle number $T_N = \frac{1}{2}(N+1)N$, since it includes the diagonal adjacency elements A_{ii}. The prior is thus $Q(G) = \binom{T_{N-1}}{m}\binom{N}{L}/2^{T_N}$.
(b) In the second scheme, we form graph macrostates with N nodes and M edges, regardless of the number of self-loops. We now use a simpler allocation scheme of elements to the upper triangle of the adjacency matrix, including diagonal elements, giving the degeneracy $\binom{T_N}{M}$, and corresponding prior. For $m = M - L$, it can be verified that $\sum_{L=0}^{N} \binom{T_{N-1}}{m}\binom{N}{L} = \binom{T_N}{M}$, so the two partitions give the same results (although the first requires more information).

(4) We again embed the above 'microcanonical' ensembles into a 'canonical' ensemble of all undirected graphs with $n \leq N$ nodes, allowing self-loops. We again consider several partitioning schemes:

(a) Graphs with n nodes, m non-self-edges and L self-edges;
(b) Graphs with any nodes, m non-self-edges and L self-edges;
(c) Graphs with any nodes, M total edges including self-edges;
(d) Graphs with n nodes and any edges including self-edges.

The resulting degeneracies, ensemble dimension, and priors follow by construction from those in (3), and are set out in Table 1.

(5) We now consider the ensemble of undirected multigraphs — i.e., with the possibility of parallel edges including self-loops —and with N nodes. To keep the ensemble finite, we restrict the total number of edges to C. We wish to examine graph macrostates with N nodes and $M \leq C$ edges. Following the previous logic, we must now consider the allocation of M edges to T_N adjacency matrix

elements, without restriction on occupancy, giving the degeneracy $g = \binom{T_N+M-1}{M}$ (n.b., similar to the allocation scheme for Bose–Einstein statistics [12–14]). By summation of this result over $M = 0...C$, it can be shown the ensemble has dimension $\binom{T_N+C}{C}$, leading to the corresponding prior.

(6) We can further embed the above ensemble (5) in a larger 'canonical ensemble' of undirected multigraphs with $n \leq N$ nodes, again with the restriction of maximum C edges. We again consider several partitions:

  (a) Graphs with n nodes, M total edges;
  (b) Graphs with any nodes, M total edges
  (c) Graphs with n nodes and any total edges.

  The degeneracies, ensemble dimension, and priors follow by construction from (5), and are set out in Table 1.

2.2 Directed Graph Priors

We now replicate the above ensembles and partitioning schemes, but this time for directed graph structures, generally required for the analysis of transportation networks. These results are set out in the same pattern in Table 2 as for the undirected graph ensembles, and mostly exhibit the same features, but with the following distinctions:

(i) The macrostates of simple or single-edge digraphs, based on the allocation of edges to the $N \times N$ adjacency matrix, now must account for $2T_{N-1}$ independent elements if there are no self-loops, or N^2 elements with self-loops.

(ii) The macrostates of multidigraphs are now based on the allocation of M edges to N^2 elements, without restriction on occupancies, giving the degeneracy $g = \binom{N^2+M-1}{M}$ and a corresponding ensemble dimension of $\binom{N^2+C}{C}$.

2.3 Asymptotic Limits

From Tables 1 and 2, most of the calculated priors for the canonical ensembles (those with $n \leq N$) vanish in the asymptotic limit $N \to \infty$. Interestingly, some do not appear to do so. One such prior is that for multigraph macrostates identified by $U_N^{\text{multi},M}$ in the undirected multigraph ensemble (Table 1). While, we do not have a mathematical proof, numerical analyses suggest the following limits:

Table 1 Dimensions, degeneracies and prior probabilities for various partitions of undirected graph ensembles

Ensemble			Macrostate				
Symbol Ω_G	Description	Dimension $\lvert\Omega_G\rvert$	Symbol G	Description	Degeneracy $g(G)$	Prior Prob. $Q(G)$	Label
Ω_{U_N}	All simple undirected graphs with N nodes	$2^{T_{N-1}}$	U_N^M	Graphs with N nodes, M edges	$\binom{T_{N-1}}{M}$	$\dfrac{\binom{T_{N-1}}{M}}{2^{T_{N-1}}}$	(U1)
$\Omega_{U_{n \le N}}$	All simple undirected graphs with $n \le N$ nodes	$\sum\limits_{n=1}^{N} 2^{T_{n-1}}$	U_n^M	Graphs with n nodes, M edges	$\binom{T_{n-1}}{M}$	$\dfrac{\binom{T_{n-1}}{M}}{\sum\limits_{n=1}^{N} 2^{T_{n-1}}}$	(U2)
			U^M	Graphs with any nodes, M edges	$\sum\limits_{n=1}^{N} \binom{T_{n-1}}{M}$	$\dfrac{\sum\limits_{n=1}^{N} \binom{T_{n-1}}{M}}{\sum\limits_{n=1}^{N} 2^{T_{n-1}}}$	(U3)
			U_n	Graphs with n nodes, any edges	$2^{T_{n-1}}$	$\dfrac{2^{T_{n-1}}}{\sum\limits_{n=1}^{N} 2^{T_{n-1}}}$	(U4)

(continued)

Table 1 (continued)

Ensemble			Macrostate				
Symbol Ω_G	Description	Dimension $\|\Omega_G\|$	Symbol G	Description	Degeneracy $g(G)$	Prior Prob. $Q(G)$	Label
$\Omega_{U_N^{\circlearrowleft}}$	All single-edge undirected graphs with N nodes, incl. self-edges	2^{T_N}	$U_N^{L\circlearrowleft,m}$	Graphs with N nodes, m non-self-edges, L self-edges	$\binom{T_{N-1}}{m}\binom{N}{L}$	$\frac{\binom{T_{N-1}}{m}\binom{N}{L}}{2^{T_N}}$	(U5)
			$U_N^{\circlearrowleft,M}$	Graphs with N nodes, M total edges incl. self-edges	$\binom{T_N}{M}$	$\frac{\binom{T_N}{M}}{2^{T_N}}$	(U6)
$\Omega_{U_{n\le N}^{\circlearrowleft}}$	All single-edge undirected graphs with $n \le N$ nodes, incl. self-edges	$\sum\limits_{n=1}^{N} 2^{T_n}$	$U_n^{L\circlearrowleft,m}$	Graphs with n nodes, m non-self-edges, L self-edges	$\binom{T_{n-1}}{m}\binom{n}{L}$	$\frac{\binom{T_{n-1}}{m}\binom{n}{L}}{\sum\limits_{n=1}^{N} 2^{T_n}}$	(U7)
			$U^{L\circlearrowleft,m}$	Graphs with any nodes, m non-self-edges, L self-edges	$\sum\limits_{n=1}^{N}\binom{T_{n-1}}{m}\binom{n}{L}$	$\frac{\sum\limits_{n=1}^{N}\binom{T_{n-1}}{m}\binom{n}{L}}{\sum\limits_{n=1}^{N} 2^{T_n}}$	(U8)
			$U^{\circlearrowleft,M}$	Graphs with any nodes, M total edges incl. self-edges	$\sum\limits_{n=1}^{N}\binom{T_n}{M}$	$\frac{\sum\limits_{n=1}^{N}\binom{T_n}{M}}{\sum\limits_{n=1}^{N} 2^{T_n}}$	(U9)

(continued)

Table 1 (continued)

Ensemble			Macrostate				
Symbol Ω_G	Description	Dimension $\|\Omega_G\|$	Symbol G	Description	Degeneracy $g(G)$	Prior Prob. $Q(G)$	Label
			$U_n^{\circlearrowleft}$	Graphs with n nodes, any edges incl. self-edges	2^{T_n}	$\dfrac{2^{T_n}}{\sum\limits_{n=1}^{N} 2^{T_n}}$	(U10)
$\Omega_{U_N^{\text{multi},M\le C}}$	All undirected multigraphs with N nodes, up to C edges incl. self-edges	$\binom{T_N+C}{C}$	$U_N^{\text{multi},M}$	Multigraphs with N nodes, M total edges	$\binom{T_N+M-1}{M}$	$\dfrac{\binom{T_N+M-1}{M}}{\binom{T_N+C}{C}}$	(U11)
$\Omega_{U_{n\le N}^{\text{multi},M\le C}}$	All undirected multigraphs with $n \le N$ nodes, up to C edges incl. self-edges	$\sum\limits_{n=1}^{N}\binom{T_n+C}{C}$	$U_n^{\text{multi},M}$	Multigraphs with n nodes, M total edges	$\binom{T_n+M-1}{M}$	$\dfrac{\binom{T_n+M-1}{M}}{\sum\limits_{n=1}^{N}\binom{T_n+C}{C}}$	(U12)
			$U^{\text{multi},M}$	Multigraphs with any nodes, M total edges	$\sum\limits_{n=1}^{N}\binom{T_n+M-1}{M}$	$\dfrac{\sum\limits_{n=1}^{N}\binom{T_n+M-1}{M}}{\sum\limits_{n=1}^{N}\binom{T_n+C}{C}}$	(U13)
			U_n^{multi}	Multigraphs with n nodes, any total edges	$\binom{T_n+C}{C}$	$\dfrac{\binom{T_n+C}{C}}{\sum\limits_{n=1}^{N}\binom{T_n+C}{C}}$	(U14)

Table 2 Dimensions, degeneracies and prior probabilities for various partitions of directed graph ensembles

Ensemble			Macrostate				
Symbol Ω_G	Description	Dimension $\lvert\Omega_G\rvert$	Symbol G	Description	Degeneracy $g(G)$	Prior Prob. $Q(G)$	Label
Ω_{D_N}	All simple digraphs with N nodes	$4^{T_{N-1}}$	D_N^M	Digraphs with N nodes, M edges	$\binom{2T_{N-1}}{M}$	$\dfrac{\binom{2T_{N-1}}{M}}{4^{T_{N-1}}}$	(D1)
$\Omega_{D_{n \le N}}$	All simple digraphs with $n \le N$ nodes	$\sum\limits_{n=1}^{N} 4^{T_{n-1}}$	D_n^M	Digraphs with n nodes, M edges	$\binom{2T_{n-1}}{M}$	$\dfrac{\binom{2T_{n-1}}{M}}{\sum\limits_{n=1}^{N} 4^{T_{n-1}}}$	(D2)
			D^M	Digraphs with any nodes, M edges	$\sum\limits_{n=1}^{N} \binom{2T_{n-1}}{M}$	$\dfrac{\sum\limits_{n=1}^{N} \binom{2T_{n-1}}{M}}{\sum\limits_{n=1}^{N} 4^{T_{n-1}}}$	(D3)
			D_n	Digraphs with n nodes, any edges	$4^{T_{n-1}}$	$\dfrac{4^{T_{n-1}}}{\sum\limits_{n=1}^{N} 4^{T_{n-1}}}$	(D4)

(continued)

Table 2 (continued)

Ensemble			Macrostate				
Symbol Ω_G	Description	Dimension $\lvert\Omega_G\rvert$	Symbol G	Description	Degeneracy $g(G)$	Prior Prob. $Q(G)$	Label
$\Omega_{D_N^{\circlearrowleft}}$	All non-multiedge digraphs with N nodes, incl. self-edges	2^{N^2}	$D_N^{L\circlearrowleft,m}$	Digraphs with N nodes, m non-self-edges, L self-edges	$\binom{2T_{N-1}}{m}\binom{N}{L}$	$\dfrac{\binom{2T_{N-1}}{m}\binom{N}{L}}{2^{N^2}}$	(D5)
			$D_N^{\circlearrowleft,M}$	Digraphs with N nodes, M total edges incl. self-edges	$\binom{N^2}{M}$	$\dfrac{\binom{N^2}{M}}{2^{N^2}}$	(D6)
$\Omega_{D_{n\le N}^{\circlearrowleft}}$	All non-multiedge digraphs with $n \le N$ nodes, incl. self-edges	$\sum\limits_{n=1}^{N} 2^{n^2}$	$D_n^{L\circlearrowleft,m}$	Digraphs with n nodes, m non-self-edges, L self-edges	$\binom{2T_{n-1}}{m}\binom{n}{L}$	$\dfrac{\binom{2T_{n-1}}{m}\binom{n}{L}}{\sum\limits_{n=1}^{N} 2^{n^2}}$	(D7)
			$D^{L\circlearrowleft,m}$	Digraphs with any nodes, m non-self-edges, L self-edges	$\sum\limits_{n=1}^{N} \binom{2T_{n-1}}{m}\binom{n}{L}$	$\dfrac{\sum\limits_{n=1}^{N} \binom{2T_{n-1}}{m}\binom{n}{L}}{\sum\limits_{n=1}^{N} 2^{n^2}}$	(D8)
			$D^{\circlearrowleft,M}$	Digraphs with any nodes, M total edges incl. self-edges	$\sum\limits_{n=1}^{N} \binom{n^2}{M}$	$\dfrac{\sum\limits_{n=1}^{N} \binom{n^2}{M}}{\sum\limits_{n=1}^{N} 2^{n^2}}$	(D9)

(continued)

Table 2 (continued)

Ensemble			Macrostate				
Symbol Ω_G	Description	Dimension $\|\Omega_G\|$	Symbol G	Description	Degeneracy $g(G)$	Prior Prob. $Q(G)$	Label
			$D_n^{\circlearrowleft}$	Digraphs with n nodes, any edges incl. self-edges	2^{n^2}	$\frac{2^{n^2}}{\sum_{n=1}^{N} 2^{n^2}}$	(D10)
$\Omega_{D_N^{\text{multi},M \le C}}$	All multidigraphs with N nodes, up to C edges	$\binom{N^2+C}{C}$	$D_N^{\text{multi},M}$	Multidigraphs with N nodes, M total edges	$\binom{N^2+M-1}{M}$	$\frac{\binom{N^2+M-1}{M}}{\binom{N^2+C}{C}}$	(D11)
$\Omega_{D_{n \le N}^{\text{multi},M \le C}}$	All multidigraphs with $n \le N$ nodes, up to C edges	$\sum_{n=1}^{N} \binom{n^2+C}{C}$	$D_n^{\text{multi},M}$	Multidigraphs with n nodes, M total edges	$\binom{n^2+M-1}{M}$	$\frac{\binom{n^2+M-1}{M}}{\sum_{n=1}^{N} \binom{n^2+C}{C}}$	(D12)
			$D^{\text{multi},M}$	Multidigraphs with any nodes, M total edges	$\sum_{n=1}^{N} \binom{n^2+M-1}{M}$	$\frac{\sum_{n=1}^{N} \binom{n^2+M-1}{M}}{\sum_{n=1}^{N} \binom{n^2+C}{C}}$	(D13)
			D_n^{multi}	Multidigraphs with n nodes, any total edges	$\binom{n^2+C}{C}$	$\frac{\binom{n^2+C}{C}}{\sum_{n=1}^{N} \binom{n^2+C}{C}}$	(D14)

$$Q(U_N^{\text{multi},M}) = \frac{\binom{T_N+M-1}{M}}{\binom{T_N+C}{C}} \xrightarrow{N\to\infty} \begin{cases} 0 & \text{if } M < C \\ & \text{or } M = C > O(N^2) \\ \frac{1}{2\alpha-1} & \text{if } M = C = O(\alpha N^2) \\ 1 & \text{if } M = C < O(N^2) \end{cases} \tag{7}$$

For the analogous multidigraph macrostate identified by $D_N^{\text{multi},M}$ in the multidigraph ensemble (Table 2), the above limits appear to be repeated, but with limit $\frac{1}{\alpha-1}$ for $M = C = \alpha N^2$. In both cases, the prior appears to vanish asymptotically for $C \to \infty$.

If these asymptotic limits (and others) can be established more rigorously, they provide the means to derive graph priors for macrostates in countably infinite graph ensembles, for which it is not possible to conduct statistical mechanics based on the counting of individual graphs.

3 Conclusions

We consider graph priors for various ensembles of undirected and directed graphs, to simplify the analysis of flow networks with uncertainty in the network structure. By combinatorial reasoning, we formally derive a collection of graph priors for various choices of graph macrostates in graph ensembles, partitioned according to the numbers of nodes and/or edges of graphs in the macrostate. The results are discussed and listed in tabular form. For simple graphs (no self-edges), single-edge graphs (allowing self-edges) or multigraphs, the 'microcanonical ensemble' constructed with a fixed number of nodes N can be embedded in a higher order 'canonical ensemble' with up to N nodes, allowing construction of more and more complicated ensembles. While most calculated priors appear to vanish asymptotically for countably infinite ensembles, some asymptotic limits have been identified numerically, for multigraphs and multidigraphs macrostates in certain ensembles. Such asymptotic results suggest a method to derive graph priors for macrostates in countably infinite graph ensembles, which cannot be handled by the counting of individual graphs.

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