Maximum Entropy Analysis of Flow and Reaction Networks

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Abstract. We present a generalised MaxEnt method to infer the stationary state of a flow network, subject to "observable" constraints on expectations of various parameters, as well as "physical" constraints arising from frictional properties (resistance functions) and conservation laws (Kirchhoff laws). The method invokes an entropy defined over all uncertainties in the system, in this case the internal and external flow rates and potential differences. The proposed MaxEnt framework is readily extendable to the analysis of networks with uncertainty in the network structure itself.

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1. INTRODUCTION

The concept of a "flow network" – a set of nodes connected by flow paths – unites many different disciplines, including electrical, communications, pipe flow, fluid flow, transportation, chemical reaction, ecological and human systems. Historically, the state of a flow network has been analysed by conservation (Kirchhoff's) laws and to some extent by network mappings (e.g. Tellegen's theorem), and more recently by numerous dynamical simulation and optimisation methods. A less well explored approach, however, is the use of Jaynes' maximum entropy (MaxEnt) method [1, 2], in which an entropy – defined over the total uncertainty in the network – is maximised subject to constraints, to give the stationary state of the network. Several workers have applied MaxEnt methods to the analysis of transportation [3] and hydraulic networks [4], but not always correctly, e.g. in many cases without considering the frictional properties. MaxEnt methods have also been applied directly to network structures (graph ensembles) subject to various configurational constraints (e.g. expected degree of each node, k-core structure, etc) [5, 6], but without consideration of flows and potentials on the network.

This study examines the application of MaxEnt to the prediction of flows and potential differences on a flow network. It builds upon previous MaxEnt analyses of the steady state of flow and dissipative systems [7, 8, 9] and flow networks [10, 11].

2. THEORY

2.1. Network Specifications

We consider a generalised undirected graph network, with the following properties:

(1) N nodes;

(2) M edges each defined by an adjacency parameter $A_{ij} \in \{\mathbb{N} \cup 0\}$, equal to the number of connections from node i to node j, giving give the adjacency tensor $\boldsymbol{\mathcal{A}} \in \mathbb{R}^{N \times N}$. We here consider only simple graphs without self-loops or multiple connections, whence $A_{ii} = 0, \forall i$, and $A_{ij} \in \{0, 1\}$.

(3) A set of M internal flow rates $Q_{ij} \in \mathbb{R}$ for each edge $i, j \in \{1, ..., N\}$ of some extensive quantity B along the ijth edge, measured in units of B s^{-1}. These give the internal flow rate tensor $\boldsymbol{\mathcal{Q}} \in \mathbb{R}^{N \times N}$.

(4) A set of K external flow rates $\Theta_i \in \mathbb{R}$ for each node $i \in \{1, ..., N\}$ of B to each node i, defined positive for an inwards flow. In this study, we amalgamate all multiple external flows to node i into the single flow rate Θ_i, hence $0 \leq K \leq N$. These give the external flow rate vector $\boldsymbol{\Theta} = [\Theta_1, ..., \Theta_N]^\top \in \mathbb{R}^N$.

(5) A set of N potentials $E_i \in \mathbb{R}$ at each node $i \in \{1, ...N\}$, measured in units of the intensive variable conjugate to B, in this case B^{-1} s. These lead to a set of M potential differences $\Delta\!\!\!^{*} E_{ij} = -\Delta E_{ij} = E_i - E_j$ for $i, j \in \{1, ..., N\}$. These give the potential vector $\boldsymbol{E} \in \mathbb{R}^N$ and potential difference tensor $\Delta\!\!\!^{*}\boldsymbol{\mathcal{E}} \in \mathbb{R}^{N \times N}$.

(6) A set of M resistance functions $R_{ij} : \mathbb{R} \to \mathbb{R}$, for each edge $i, j \in \{1, ..., N\}$. In their simplest formulation, these convert each flow rate into an *equivalent potential difference*, using a local functional form:

$$\widetilde{\Delta\!\!\!^{*} E}_{ij} = R_{ij}(Q_{ij}) \tag{1}$$

For example, in electrical circuits or pipe flow networks, the resistance functions may consist of linear or power law relations $\widetilde{\Delta\!\!\!^{*} E}_{ij} = R_{ij} Q_{ij} |Q_{ij}|^{a-1}$, where R_{ij} is the resistance of the ijth edge and a is a coefficient (e.g. Ohm's law with $a = 1$; Blasius' law with $1 \leq a \leq 2$). For road and air traffic networks, the resistance functions obey an asymptotic rule such that $\widetilde{\Delta\!\!\!^{*} E}_{ij} \to \infty$ as Q_{ij} approaches a carrying capacity Q_{ij}^{max}. The resistance functions are assembled into the tensor operator $\boldsymbol{\mathcal{R}} \in (\mathbb{R} \to \mathbb{R})^{N \times N}$, here assumed known, such that

$$\widetilde{\Delta\!\!\!^{*}\boldsymbol{\mathcal{E}}} = \boldsymbol{\mathcal{R}}(\boldsymbol{\mathcal{Q}}) \tag{2}$$

In the above vectors and tensors, any non-existent internal or external flow rate can simply be assigned to zero, while the potential differences and resistance functions for non-existent edges are left undefined.

The above variables are not independent. Firstly, for an undirected graph $Q_{ij} = -Q_{ji}$ and $\Delta\!\!\!^{*} E_{ij} = -\Delta\!\!\!^{*} E_{ji}$, hence the flow rate and potential difference tensors must be diagonally antisymmetric. For graphs without self-loops, the diagonal terms (and trace) of $\boldsymbol{\mathcal{Q}}$, $\Delta\!\!\!^{*}\boldsymbol{\mathcal{E}}$ and $\boldsymbol{\mathcal{R}}$ must also be zero. Secondly – as will be examined – the resistance

functions create a dependence between the flow rates and potential differences. Thirdly, the potential differences and potentials are connected by the relation:

$$\overset{\Delta}{\boldsymbol{\mathcal{E}}} = \boldsymbol{E}\,\mathbf{1}^\top - \mathbf{1}\,\boldsymbol{E}^\top \tag{3}$$

where $\mathbf{1}$ is an $N \times 1$ column vector of 1's, and $\boldsymbol{a}\,\boldsymbol{b}^\top = [a_i b_j]$ is a vector product. For the purpose of flow calculations, only the differences in potentials – not their absolute values – are important, hence the information contained in $\overset{\Delta}{\boldsymbol{\mathcal{E}}}$ is fully conveyed by $\boldsymbol{E} - \boldsymbol{E}_0$, where $\boldsymbol{E}_0$ is an N-dimensional vector of a reference potential E_0.

2.2. Probability Space and Entropy

We consider a flow network in which the graph structure based on M, N and $\boldsymbol{\mathcal{A}}$ is specified, but there is uncertainty in some (or all) of the flow rates $\boldsymbol{\mathcal{Q}}$ and $\boldsymbol{\Theta}$ and the potential differences $\overset{\Delta}{\boldsymbol{\mathcal{E}}}$. We therefore consider the joint probability over these unknowns, subject to what is known, given by:

$$p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \overset{\Delta}{\boldsymbol{\mathcal{E}}} | M, N, \boldsymbol{\mathcal{A}}, I) d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\overset{\Delta}{\boldsymbol{\mathcal{E}}}$$
$$= \text{Prob}\left(\begin{array}{ccccc} \boldsymbol{\mathcal{Q}} & \leq & \boldsymbol{\Upsilon}_{\boldsymbol{\mathcal{Q}}} & \leq & \boldsymbol{\mathcal{Q}} + d\boldsymbol{\mathcal{Q}} \\ \boldsymbol{\Theta} & \leq & \boldsymbol{\Upsilon}_{\boldsymbol{\Theta}} & \leq & \boldsymbol{\Theta} + d\boldsymbol{\Theta} \\ \overset{\Delta}{\boldsymbol{\mathcal{E}}} & \leq & \boldsymbol{\Upsilon}_{\overset{\Delta}{\boldsymbol{\mathcal{E}}}} & \leq & \overset{\Delta}{\boldsymbol{\mathcal{E}}} + d\overset{\Delta}{\boldsymbol{\mathcal{E}}} \end{array} \middle| M, N, \boldsymbol{\mathcal{A}}, I \right) \tag{4}$$

where $p(...)$ is a probability density function (pdf), $\boldsymbol{\Upsilon}_{\boldsymbol{\mathcal{X}}}$ is the random variable for the vector or tensor $\boldsymbol{\mathcal{X}}$, $d\boldsymbol{\mathcal{X}} = \prod_i dX_i$ based on each element $X_i \in \boldsymbol{\mathcal{X}}$, and I contains the background knowledge to the problem. This leads naturally to the relative entropy function, which expresses the spread of uncertainties:

$$\mathfrak{H} = -\int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\overset{\Delta}{\boldsymbol{\mathcal{E}}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \overset{\Delta}{\boldsymbol{\mathcal{E}}} | M, N, \boldsymbol{\mathcal{A}}, I) \ln \frac{p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \overset{\Delta}{\boldsymbol{\mathcal{E}}} | M, N, \boldsymbol{\mathcal{A}}, I)}{q(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \overset{\Delta}{\boldsymbol{\mathcal{E}}} | M, N, \boldsymbol{\mathcal{A}}, I)} \tag{5}$$

where $q(...)$ is the joint prior pdf and $\boldsymbol{\Omega}$ is the entire domain of all parameters.

2.3. The constraints

Firstly, $p(...)$ is subject to the normalisation constraint:

$$1 = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\overset{\Delta}{\boldsymbol{\mathcal{E}}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \overset{\Delta}{\boldsymbol{\mathcal{E}}} | M, N, \boldsymbol{\mathcal{A}}, I) \tag{6}$$

Secondly, the network may be constrained by global mean values of some of the internal flow rate(s), external flow rate(s) and/or potential difference(s), respectively:

$$\langle Q_{ij} \rangle^{spec} = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\overset{\Delta}{\boldsymbol{\mathcal{E}}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \overset{\Delta}{\boldsymbol{\mathcal{E}}} | M, N, \boldsymbol{\mathcal{A}}, I)\, Q_{ij} \tag{7}$$

$$\langle \Theta_i \rangle^{spec} = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I)\, \Theta_i \tag{8}$$

$$\langle \dot{\Delta} E_{ij} \rangle^{spec} = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I)\, \dot{\Delta} E_{ij} \tag{9}$$

The above sets can be assembled into the tensor or vector forms:

$$\langle \boldsymbol{\mathcal{Q}} \rangle^{spec} = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I)\, \boldsymbol{\mathcal{Q}} \tag{10}$$

$$\langle \boldsymbol{\Theta} \rangle^{spec} = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I)\, \boldsymbol{\Theta} \tag{11}$$

$$\langle \dot{\Delta}\boldsymbol{\mathcal{E}} \rangle^{spec} = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I)\, \dot{\Delta}\boldsymbol{\mathcal{E}} \tag{12}$$

in which those values which are not constrained can be left unspecified. Furthermore, it is important that the constrained flow rates selected from $\langle \boldsymbol{\mathcal{Q}} \rangle$ and $\langle \boldsymbol{\Theta} \rangle$ not be in contradiction, and also that any constrained potential differences $\langle \dot{\Delta}\boldsymbol{\mathcal{E}} \rangle$ be compatible with the flow rates $\langle \boldsymbol{\mathcal{Q}} \rangle$ and $\langle \boldsymbol{\Theta} \rangle$.

Thirdly, the network is constrained by the resistance functions, which are applied in the mean:

$$\langle \dot{\Delta} E_{ij} \rangle = \langle \widetilde{\dot{\Delta} E_{ij}} \rangle = R_{ij}(\langle Q_{ij} \rangle) \tag{13}$$

using the moment shorthand

$$\langle r \rangle = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I)\, r \tag{14}$$

This gives the integral tensor form:

$$\int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I)\, \dot{\Delta}\boldsymbol{\mathcal{E}} = \boldsymbol{\mathcal{R}}(\langle \boldsymbol{\mathcal{Q}} \rangle) \tag{15}$$

Note (13) and (15) are based on functional operation on mean flow rates, a more general formulation [10].

Fourthly, the network is constrained by conservation – in the mean – of quantity B at each node (Kirchhoff's first law). For each node i on an undirected graph, this gives:

$$0 = \langle \Theta_i \rangle - \sum_{j=1}^{N} \langle Q_{ij} \rangle, \quad \forall i \in \{1, ..., N\} \tag{16}$$

In vector-tensor form this gives:

$$\mathbf{0} = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I) \left(\boldsymbol{\Theta} - \sum_{j=1}^{N} \boldsymbol{\mathcal{Q}}_{\cdot j} \right), \tag{17}$$

where $\boldsymbol{Q}_{\cdot j}$ is the jth column vector of $\boldsymbol{\mathcal{Q}}$.

Finally, the network will be constrained by a mean formulation of conservation of energy (Kirchhoff's second law), for which the mean potential difference around any flow loop must vanish. For each loop ℓ on an undirected graph with single connections between nodes, this gives:

$$0 = \sum_{ij \in \ell} \langle \dot{\Delta} E_{ij} \rangle, \quad \forall \ell \in \{1, ..., \mathcal{L}\} \tag{18}$$

where $\mathcal{L}$ is the total number of independent loops. A number of search algorithms are available to identify a linearly independent set of loops, expressed by the loop adjacency tensors $\boldsymbol{\mathcal{M}}^{(\ell)}, l \in \{1, ..., \mathfrak{L}\}$ with elements $M_{ij}^{(\ell)} \in \{0, 1\}$ for each loop ℓ, indicating a specified orientation. Eq. (18) can then be rewritten with ij indices:

$$\mathbf{0} = \sum_{i=1}^{N} \sum_{j=1}^{N} \mathcal{M}_{ij}^{(\ell)} \langle \dot{\Delta} E_{ij} \rangle = \boldsymbol{\mathcal{M}}^{(\ell)} : \langle \dot{\Delta} \boldsymbol{\mathcal{E}} \rangle, \quad \forall \ell \in \{1, ..., \mathcal{L}\} \tag{19}$$

where $\boldsymbol{\mathcal{V}} : \boldsymbol{\mathcal{W}} = \text{trace}\,(\boldsymbol{\mathcal{V}}^\top \boldsymbol{\mathcal{W}}) = \sum_{i=1}^{N} \sum_{j=1}^{N} V_{ij} W_{ij}$ is the tensor scalar product [12]. This gives the integral form:

$$\mathbf{0} = \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta} \boldsymbol{\mathcal{E}}\, p(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta} \boldsymbol{\mathcal{E}} | M, N, \boldsymbol{\mathcal{A}}, I)\, \boldsymbol{\mathcal{M}}^{(\ell)} : \dot{\Delta} \boldsymbol{\mathcal{E}}, \qquad \forall \ell \in \{1, ..., \mathcal{L}\} \tag{20}$$

2.4. MaxEnt Analysis

In the MaxEnt method, we extremise the entropy, subject to the constraints on the system, to determine its most probable or least informative state (here denoted $*$). Using the moment shorthand (14) and dropping the functional dependencies of p and q, the entropy (5) subject to the constraints (6), (10)-(12), (15), (17) and (20) gives the Lagrangian:

$$\begin{aligned} L = &- \left\langle \ln \frac{p}{q} \right\rangle - \kappa \big(\langle 1 \rangle - 1 \big) - \boldsymbol{\lambda} : \big(\langle \boldsymbol{\mathcal{Q}} \rangle - \langle \boldsymbol{\mathcal{Q}} \rangle^{spec} \big) - \boldsymbol{\mu} \cdot \big(\langle \boldsymbol{\Theta} \rangle - \langle \boldsymbol{\Theta} \rangle^{spec} \big) \\ &- \boldsymbol{\nu} : \big(\langle \dot{\Delta} \boldsymbol{\mathcal{E}} \rangle - \langle \dot{\Delta} \boldsymbol{\mathcal{E}} \rangle^{spec} \big) - \boldsymbol{\rho} : \big(\langle \dot{\Delta} \boldsymbol{\mathcal{E}} \rangle - \boldsymbol{\mathcal{R}}(\langle \boldsymbol{\mathcal{Q}} \rangle) \big) - \boldsymbol{\alpha} \cdot \left\langle \boldsymbol{\Theta} - \sum_{j=1}^{N} \boldsymbol{Q}_{\cdot j} \right\rangle \\ &- \sum_{\ell=1}^{\mathcal{L}} \beta_\ell \left\langle \boldsymbol{\mathcal{M}}^{(\ell)} : \dot{\Delta} \boldsymbol{\mathcal{E}} \right\rangle \end{aligned} \tag{21}$$

where $\boldsymbol{a} \cdot \boldsymbol{b} = \boldsymbol{a}^\top \boldsymbol{b} = \sum_{i=1}^{N} a_i b_i$ is the vector scalar product, $\top$ is the transpose, and we use the following Lagrangian multipliers: κ for normalisation, $\boldsymbol{\lambda}$ (tensor) for internal flow rates, $\boldsymbol{\mu}$ (vector) for external flow rates, $\boldsymbol{\nu}$ (tensor) for potential differences, $\boldsymbol{\rho}$ (tensor) for the resistance function relations, $\boldsymbol{\alpha}$ (vector) for Kirchhoff node constraints and β_ℓ

(scalar) for each Kirchhoff loop constraint. If any constraint within $\langle \boldsymbol{\mathcal{Q}} \rangle$, $\langle \boldsymbol{\Theta} \rangle$, $\langle \dot{\Delta} \boldsymbol{\mathcal{E}} \rangle$ or within the resistance relation (2) is unspecified, the corresponding multiplier λ_{ij}, μ_i, ν_{ij} or ρ_{ij} can be fixed to zero. In contrast, all Kirchhoff constraints will be present. Combining integrals and simplification gives:

$$\begin{aligned} L = \Bigg\langle & -\ln\frac{p}{q} - \kappa - \boldsymbol{\lambda} : \boldsymbol{\mathcal{Q}} - \boldsymbol{\mu} \cdot \boldsymbol{\Theta} - \boldsymbol{\nu} : \dot{\Delta}\boldsymbol{\mathcal{E}} - \boldsymbol{\rho} : \dot{\Delta}\boldsymbol{\mathcal{E}} - \boldsymbol{\alpha} \cdot \boldsymbol{\Theta} + \boldsymbol{\alpha}\mathbf{1}^\top : \boldsymbol{\mathcal{Q}} \\ & - \sum_{\ell=1}^{\mathcal{L}} \beta_\ell \boldsymbol{\mathcal{M}}^{(\ell)} : \dot{\Delta}\boldsymbol{\mathcal{E}} \Bigg\rangle + \boldsymbol{\rho} : \boldsymbol{\mathcal{R}}(\langle \boldsymbol{\mathcal{Q}} \rangle) + \kappa + \boldsymbol{\lambda} : \langle \boldsymbol{\mathcal{Q}} \rangle^{spec} + \boldsymbol{\mu} \cdot \langle \boldsymbol{\Theta} \rangle^{spec} + \boldsymbol{\nu} : \langle \dot{\Delta}\boldsymbol{\mathcal{E}} \rangle^{spec} \end{aligned} \tag{22}$$

which uses the identity:

$$\boldsymbol{\alpha} \cdot \sum_{j=1}^{N} \boldsymbol{Q}_{\cdot j} = \sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i Q_{ij} = \boldsymbol{\alpha} \cdot \boldsymbol{\mathcal{Q}}\mathbf{1} = \boldsymbol{\alpha}\mathbf{1}^\top : \boldsymbol{\mathcal{Q}} \tag{23}$$

The total variation of the Lagrangian is:

$$\delta L = 0 = \frac{\partial L}{\partial p}\delta p \tag{24}$$

from which $\partial L/\partial p = 0$ for all p. Within this, by the chain rule

$$\frac{\partial \boldsymbol{\mathcal{R}}\langle \boldsymbol{\mathcal{Q}} \rangle}{\partial p} = \frac{\partial \boldsymbol{\mathcal{R}}\langle \boldsymbol{\mathcal{Q}} \rangle}{\partial \langle \boldsymbol{\mathcal{Q}} \rangle} \odot \frac{\partial \langle \boldsymbol{\mathcal{Q}} \rangle}{\partial p} = \boldsymbol{\mathcal{R}}'(\langle \boldsymbol{\mathcal{Q}} \rangle) \odot \frac{\partial \langle \boldsymbol{\mathcal{Q}} \rangle}{\partial p} \tag{25}$$

where $\boldsymbol{\mathcal{V}} \odot \boldsymbol{\mathcal{W}}$ is the element-wise tensor (Hadamard) product, in which $(\boldsymbol{\mathcal{V}} \odot \boldsymbol{\mathcal{W}})_{ij} = V_{ij}W_{ij}$ [12]. The extremum is therefore:

$$\begin{aligned} 0 = & -\ln\frac{p}{q} - 1 - \kappa - \boldsymbol{\lambda} : \boldsymbol{\mathcal{Q}} - \boldsymbol{\mu} \cdot \boldsymbol{\Theta} - \boldsymbol{\nu} : \dot{\Delta}\boldsymbol{\mathcal{E}} - \boldsymbol{\rho} : \dot{\Delta}\boldsymbol{\mathcal{E}} - \boldsymbol{\alpha} \cdot \boldsymbol{\Theta} + \boldsymbol{\alpha}\mathbf{1}^\top : \boldsymbol{\mathcal{Q}} \\ & - \sum_{\ell=1}^{\mathcal{L}} \beta_\ell \boldsymbol{\mathcal{M}}^{(\ell)} : \dot{\Delta}\boldsymbol{\mathcal{E}} + \boldsymbol{\rho} : \boldsymbol{\mathcal{R}}'(\langle \boldsymbol{\mathcal{Q}} \rangle) \odot \boldsymbol{\mathcal{Q}} \end{aligned} \tag{26}$$

Defining the partition function $Z = e^{1+\kappa}$, this gives the Boltzmann equation:

$$\begin{aligned} p^* = \frac{q}{Z}\exp\Bigg[& -\big(\boldsymbol{\lambda} - \boldsymbol{\alpha}\mathbf{1}^\top\big) : \boldsymbol{\mathcal{Q}} - \big(\boldsymbol{\mu} + \boldsymbol{\alpha}\big) \cdot \boldsymbol{\Theta} - \Big(\boldsymbol{\nu} + \boldsymbol{\rho} + \sum_{\ell=1}^{\mathcal{L}} \beta_\ell \boldsymbol{\mathcal{M}}^{(\ell)}\Big) : \dot{\Delta}\boldsymbol{\mathcal{E}} \\ & + \boldsymbol{\rho} : \boldsymbol{\mathcal{R}}'(\langle \boldsymbol{\mathcal{Q}} \rangle) \odot \boldsymbol{\mathcal{Q}} \Bigg] \end{aligned} \tag{27}$$

This can be inserted into the seven sets of constraints (6), (10)-(12), (15), (17) and (20) to calculate the partition function Z and multipliers $\boldsymbol{\lambda}$, $\boldsymbol{\mu}$, $\boldsymbol{\nu}$, $\boldsymbol{\rho}$, $\boldsymbol{\alpha}$ and β_ℓ. Any other moment, for example of the quantity $F(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \dot{\Delta}\boldsymbol{\mathcal{E}})$, can then be calculated over p^*:

$$\langle F \rangle = \frac{1}{Z} \int_{\boldsymbol{\Omega}} \cdots \int d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\dot{\Delta}\boldsymbol{\mathcal{E}}\, p^*\, F \tag{28}$$

2.5. Prior Probabilities

In the MaxEnt formulation, the joint prior probability $q(\boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \Delta\!\!\!^{\backprime}\boldsymbol{\mathcal{E}}|M, N, \boldsymbol{\mathcal{A}}, I)$ expresses the expected joint distribution of the uncertain parameters in the absence of any physical constraints. Commonly, the prior encodes information extracted from the symmetry or geometry of the problem, which can be expected to restrict the solution domain and hence will alter the solution inferred by MaxEnt.

In analyses of simple undirected flow networks, it is necessary to allow the internal flow rates to vary over the entire real domain $\mathbb{R}$, which gives rise to the possibility of flow reversal in any edge as a function of the constraints. From the resistance constraints (15), the potential differences must also be real-valued, and so may also undergo sign reversal. It is also convenient to allow the external flow rates to extend over the real domain, to encompass inflows and outflows. However, for a physically realizable network, it is important to ensure that the flow rates and potential differences each be centred somewhere within the "middle" of the real domain, with vanishing probability of approaching $\pm\infty$. While many functions satisfy this choice, we have found it useful to adopt Gaussian priors for each variable, since these will – to a fair degree – express the information inherent in the problem specification, while remaining analytically tractable. The prior can then be written as a separable product of individual priors:

$$q = \frac{\prod\limits_{ij\in\boldsymbol{\mathcal{A}}} \frac{1}{\sigma_{Q_{ij}}} e^{-\frac{(Q_{ij}-m_{Q_{ij}})^2}{2\sigma_{Q_{ij}}^2}} \prod\limits_{i=1}^{N} \frac{1}{\sigma_{\Theta_i}} e^{-\frac{(\Theta_i-m_{\Theta_i})^2}{2\sigma_{\Theta_i}^2}} \prod\limits_{ij\in\boldsymbol{\mathcal{A}}} \frac{1}{\sigma_{\Delta\!\!\!^{\backprime}E_{ij}}} e^{-\frac{(\Delta\!\!\!^{\backprime}E_{ij}-m_{\Delta\!\!\!^{\backprime}E_{ij}})^2}{2\sigma_{\Delta\!\!\!^{\backprime}E_{ij}}^2}}}{(2\pi)^{(2M+N)/2}} \tag{29}$$

where m_X is the mean and σ_X is the standard deviation of parameter X. If the mean is specified by a constraint $\langle X\rangle^{spec}$ in (10)-(12), this can be used in the prior; otherwise we have found zero mean priors to be a good choice. Similarly, if a standard deviation is known from constraints $\langle X^2\rangle^{spec}$ and $\langle X\rangle^{spec}$, this can be used in the prior; otherwise a broad standard deviation is useful for numerical solution purposes.

3. GENERAL FORMULATION

As a final comment, we may consider a network in which there is uncertainty in both the network formulation itself, as expressed by M, N and $\boldsymbol{\mathcal{A}}$, as well as the flow rates and potential differences. This gives the joint pdf $p(M, N, \boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \Delta\!\!\!^{\backprime}\boldsymbol{\mathcal{E}}|I)$, leading to the relative entropy:

$$\mathfrak{H}_{gen} = -\int\limits_{\boldsymbol{\Omega}_{gen}}\!\!\cdots\!\!\int d\boldsymbol{\mathcal{A}} d\boldsymbol{\mathcal{Q}} d\boldsymbol{\Theta} d\Delta\!\!\!^{\backprime}\boldsymbol{\mathcal{E}}\, p(M, N, \boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \Delta\!\!\!^{\backprime}\boldsymbol{\mathcal{E}}|I) \ln \frac{p(M, N, \boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \Delta\!\!\!^{\backprime}\boldsymbol{\mathcal{E}}|I)}{q(M, N, \boldsymbol{\mathcal{A}}, \boldsymbol{\mathcal{Q}}, \boldsymbol{\Theta}, \Delta\!\!\!^{\backprime}\boldsymbol{\mathcal{E}}|I)} \tag{30}$$

where $\boldsymbol{\Omega}_{gen}$ is the more general domain. This will also be subject to constraints on the network structure itself, in addition to the above flow constraints (6), (10)-(12), (15),

(17) and (20). The MaxEnt formulation readily lends itself to the analysis of both the inferred structure and flow properties of such a network.

4. CONCLUSIONS

We present a generalised MaxEnt method to infer the stationary state of a flow network. The method invokes a relative entropy over all uncertainties within the system, in this case the internal flow rates, external flow rates and potential differences, which is constrained by "observable" constraints on expectations of various parameters, as well as "physical" constraints arising from frictional properties and network conservation laws (Kirchhoff laws). The resulting Boltzmann equation can contain non-linearities, depending on the form of the resistance equations. The MaxEnt framework is readily extendable to the analysis of networks in which there is uncertainty in the network structure itself.

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