On Equilibrium Metropolis Simulations on Self-Organized Urban Street Networks

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Abstract. The complexity of urban street networks is well recognised to reside in their information networks. An information network maps roads to nodes and maps junctions to edges. Information networks of self-organized cities typically have a scale-free degree distribution. A recent fluctuating mesoscopic model links their scale-freeness to the preservation of their average amount of surprisal. Here the surprisal measures the astonishment and indecision of city-dwellers. The Metropolis algorithm may in theory allow to generate fluctuating information networks, with the scaling exponent acting as inverse temperature, in thermal-like equilibria. In this paper, we show how the Metropolis algorithm can apply to urban street networks along a case study. Our case study, Old Ahmedabad, sustains Metropolis equilibria and offers promising thermodynamic-like results. Our work opens doors to a statistical physics framework for understanding how self-organized urban street networks develop.

Keywords: urban street network · spatial network · self-organization · scale-freeness · Metropolis algorithm · MaxEnt · complex system · statistical physics

1 Introduction

The information network that maps roads to nodes and junctions to edges is well acknowledged to capture the complexity of urban street networks [1–5]. Actual information networks of self-organized urban street networks typically undergo a scale-free coherence [2–5]. We recently explained this puzzling pattern within the framework of statistical physics in terms of fluctuating Boltzmann-mesoscopic systems [4, 5]. Scale-free Boltzmann-mesoscopic systems appears indeed to evolve by maintaining their amount of surprisal — an information measure which quantifies our “surprise” of seeing an outcome — constant on average [4, 5]. This undergoing conservation (along its derivation) carries a striking similarity between the scaling exponent \( \lambda \) (along average amounts of surprisal \( \langle S \rangle \)) and the inverse temperature \( \beta = (kT)^{-1} \) (along average amounts of energy \( \langle E \rangle \)). This similarity \( (\lambda, S) \leftrightarrow (\beta, E) \) with fluctuating systems that preserve their amount of energy on average offers new perspectives.

The single-spin-flip Metropolis algorithm used to generate equilibrium states of Ising-like models embodies well the idea of fluctuating systems [6]. If adaptable to information networks, the single-spin-flip Metropolis algorithm will definitely provide
an expressive and intuitive perspective. To achieve this, the model has to fulfil two condi-
tions [6]. First, the model must rely on a Markov process to generate new information
networks from old ones. That is, the transition probability to a new information net-
work from an old one must both be invariant over time and depend only on the old
and new information networks. Second, the condition of ergodicity must assure that the
Markov process can reach any information network from any other one. As the proba-
bility of a scale-free information network depends only on its actual configuration, the
Markov process conditions are both readily satisfied. On the other hand, the condition
of ergodicity relies on how nodes are actually constructed.

Here nodes are roads, basically an exclusive sequence of successive street-segments
joined according to some paradigms [3]. Exclusive means that a street-segment can only
belong to a single road. An immediate paradigm is the “named street” paradigm which
simply reproduces cadasters. Since for some cities a cadaster may not exist, or sim-
ply reflect local habits and customs, generic substitutes are generally employed instead.
The choice of the paradigm may ponder social and geographical criteria. However,
the deflection angle between two adjacent street-segments has appeared to be a rele-
vant parameter [3, 7]. If beyond some threshold angle any joining has to be excluded,
many possibilities remain open. A multi-random-walk-like process based on deflection
angles, meant to mimic behavioural principles, has been used with good success [3].
The self-fit joint principle, as it was coined, readily inspires a single-junction-swap er-
godic iteration. Similarly to the single-spin-flip (ergodic) iteration that flips spins at
Ising sites [6], the single-junction-swap (ergodic) iteration swaps direction at junctions.
Thusly, the condition of ergodicity can be fulfilled.

Our Metropolis generation series simulated for Old Ahmedabad (India) are very
promising and confirm the potential of the Boltzmann-mesoscopic approach. We were
able to simulate Metropolis equilibria for a large range of effective scaling exponents.
The plots of the total and average amounts of surprisal as a function of the scaling
exponent are monotonically smooth, so that we can possibly infer quantitative data as
specific-heat-like capacities. This definitely places us to the frontier of a thermodynamic-
like framework.

The rest of the paper is organized as follows. Section 2 discusses background con-
cepts and presents the adopted Metropolis algorithm. In Section 3, along some plots of
typical Metropolis generation series against self-fit join principle outputs, we present
the total and average amounts of surprisal versus scaling exponent plots. Finally, in
Section 4, we discuss and offer perspectives.

2 Background

2.1 Behavioural based join principles

The aforementioned self-fit joint principle belongs to a family of join paradigms iden-
tified as behavioural based join principles [3]. They are governed by the deflection an-
gles. One can find three main principles. The every-best-fit join principle acts at every
junction by joining its street-segment pairs in increasing order of their deflection angles
— until the threshold angle is reached. The self-best-fit and self-random-fit join prin-
ciples act sequentially on growing roads, until applicable, by randomly seeding them
with a not-yet-selected street-segment before recursively appending, until applicable, one of the not-yet-appended street-segments — whose deflection angle against the end-street-segment is smaller than the threshold angle. The self join principles differ only in the choice of the not-yet-selected street-segment to append. The self-best-fit join principle selects the not-yet-appended street-segments forming the smallest deflection angle. By contrast, the self[-random]-fit join principle selects at random.

By construction, the fit joint principles categorise themselves in two main groups. The every-best-fit join principle is local and almost deterministic. It is almost deterministic in the sense that it resolves at random the very rare occurrences of equality between deflection angles. The two self join principles are global and random to a certain degree. Both inherits randomness from the underlying spatial network, the random seeding, and their respective walk. By spatial network we denote the network whose nodes are junctions and edges are street-segments. For the self-best-fit principle, in the same sense as above, the walk is almost deterministic; for the self[-random]-fit principle, the walk is random. Along this line, as suggested in Introduction, the self-fit join principle can be looked at as a saturated set of nonoverlapping random walks occurring on urban street networks.

In practice, the self join principles have appeared more realistic than the every-best-fit join principle against well-founded cadasters and transportation traffic in terms of correlation [3]. The random variant generally gives the best “fit” [3]. Here the goodness-of-fit (or p-value) quantifies for an information-network-output the plausibility for the valence distribution to follow a power law. Its estimation is done according to the state-of-the-art statistical method for power law distributions which is based on Maximum Likelihood Estimations (MLE) [8]. Notice however that since only one of the random information-network-outputs appears to be considered, this estimation method is in fact applied ad hoc.

This behavioural model along its validation scheme is not entirely satisfactory for at least two reasons. First, from a mathematical viewpoint, any proper validating data analysis must take explicitly into account the random nature of the information-network-outputs. Second, from a physics viewpoint, the nature of the possible behavioural choices at junctions is extreme. It is either absolutely rational (self-best-fit) or absolutely irrational (self[-random]-fit). Namely the city-dwellers are implicitly assumed without comprehension (or perception) of their own city. These two questions can be bypassed at once by embracing the idea that information networks are Boltzmann-mesoscopic systems preserving their average amount of surprisal as follows.

### 2.2 Single-direction-swap Metropolis algorithm

To describe a Boltzmann-mesoscopic system conserving its amount of surprisal on average, let us first denote by \( \Pr(\Omega_o) \) the distribution of the numbers of configurations \( \Omega_o \) of its mesoscopic objects \( o \). The average amount of surprisal \( \langle S \rangle \) expresses then as \( \langle S \rangle = \sum_{\Omega_o} \Pr(\Omega_o) \ln \Omega_o \). The distribution \( \Pr(\Omega_o) \) most plausibly follows, by Jaynes’s Maximum Entropy principle [5,9–11], a scale-free distribution \( \Pr(\Omega_o) \propto \Omega_o^{-\lambda} \) [4,5,12]. That is, the system is scale-free with \( \lambda \) as characterizing scaling exponent. If we assume that an information network is such a system, then the probability \( p_{\mu} \) of its state (or con-
configuration) \( \mu \) readily yields

\[
p_\mu \propto \prod_{\alpha \mu \in \{r_\mu, j_\mu \}} \Omega_{\alpha \mu}^{-\lambda} = e^{-\lambda S_\mu}
\]

with

\[
S_\mu = \sum_{\alpha \mu \in \{r_\mu, j_\mu \}} \ln \Omega_{\alpha \mu}
\]

the total amount of surprisal in state \( \mu \); the product (the sum) is over the roads \( r_\mu \) and junctions \( j_\mu \) of state \( \mu \). Surprisal measures astonishment and indecision when facing arbitrary event [13]. Along this line, the total amount of surprisal \( S_\mu \) quantifies the comprehension of the city-dwellers for state \( \mu \) [4, 5]. The comprehension of the city-dwellers is thusly reflected in information network probability distribution (1). Probability distribution (1) also reveals that the scaling exponent \( \lambda \) acts towards their comprehension as a regulator. That is, the scaling exponent \( \lambda \) may lead or not, by favouring certain states over others, our fluctuating system to equilibria.

Fluctuating systems are generally treated by performing Monte Carlo simulations [6]. The Monte Carlo method of first choice remains the historical method introduced by Nicolas Metropolis [6, 14]. Its simplest application to the Ising model serves as a classic in statistical physics known as the single-spin-flip Metropolis algorithm. Before seeking to adapt the single-spin-flip variant to our system, we must verify two conditions. First, our system must be able to undergo Markov iterations [6], that is, time invariant transitions whose probabilities depend only on their initial and final states. This condition is satisfied given that the probability \( p_\mu \) of any state \( \mu \) depends only on its actual configuration. Second, our system must be able to undergo ergodicity [6], namely Markov iterations that reach any state of our system from any other state after enough iterations. This requirement is met by elaborating an iteration that mimics the random flip of a spin at Ising sites. Our elaboration goes as follows.

The ergodicity condition is related to how information networks can be, in one combined step, unknitted and reknitted. Knitting operations occur concretely at junctions. This is implicit for the above behavioural based joint principles. Their appending subparadigms, which select the street-segment to join, look immediately like reknittings. The reverse of these reknittings, which select the street-segment to detach, look consequently like unknittings. Here, however, both unknittings and reknittings must be imposed, in order to satisfy the ergodicity condition, to detach and join, respectively, at random. These observations leads to the following single-direction-swap ergodic iteration: pick at random a street-segment, then move at random to one of its two end-junctions, then choose at random a new street-segment nominee, then detach the old nominee and attach the new one, finally recombine at random the remaining detached street-segments until applicable. To summarize, the single-direction-swap iteration acts the random swap of a road at junctions. This operation might be named in the above behavioural nomenclature single-[random]-refit. The hyphenated compound single-direction-swap expresses however better both what the iteration actually does and the similarity with the single-spin-flip iteration.

Featuring any single-direction-swap at junctions as a single-spin-flip at sites of an Ising model allows a literal application of the single-spin-flip Metropolis algorithm [6].
Metropolis algorithms hold their specificity among Monte Carlo algorithms in the implementation details of the condition of detailed balance [6]. The condition of detailed balance assures both that each Markov chain (or sequence) reaches an equilibrium and that the equilibrium states follow a desired probability distribution. The condition applies, technically, to the probability \( P(\mu \rightarrow \nu) \) of generating a state \( \nu \) from a given state \( \mu \), which is called the transition probability. The transition probability can be split into two parts as \( P(\mu \rightarrow \nu) = g(\mu \rightarrow \nu) A(\mu \rightarrow \nu) \). The selection probability \( g(\mu \rightarrow \nu) \) is the probability for our algorithm to generate a new state \( \nu \) given a state \( \mu \), while the acceptance ratio \( A(\mu \rightarrow \nu) \) gives the odds of accepting or rejecting the move to state \( \nu \) from state \( \mu \). In Metropolis algorithms, the selection probability \( g(\mu \rightarrow \nu) \) is uniform and the acceptance ratio \( A(\mu \rightarrow \nu) \) is adjusted to minimize the number of rejections. For the derivation, we refer to the literature [6]. For our model, the emblematic Metropolis acceptance ratio \( A(\mu \rightarrow \nu) \) to accept a new state \( \nu \) from state \( \mu \) becomes

\[
A(\mu \rightarrow \nu) = \begin{cases} 
e^{-\tilde{\lambda}(S_\nu - S_\mu)} & \text{if } S_\nu - S_\mu > 0 \\ 1 & \text{otherwise}. \end{cases}
\] (3)

For early investigations, we have made two suppositions. First, we have assumed that information networks reduce to their roads. This means that the Galois lattice underlying each information network is approximated by a network [4, 5]. Second, we have described the mesoscopic roads as asymptotic agent systems driven by social interactions [4,5,12]. Accordingly, the number of configurations \( \Omega_{r_\mu} \) of road \( r_\mu \) becomes proportional to a power of its number of junctions \( n_{r_\mu} \) [4, 5]; we have

\[
\Omega_{r_\mu} \propto n_{r_\mu}^{2\upsilon}
\] (4)

with \( \upsilon \) the number of vital connections for roads. Therefore the total amount of surprisal \( S_\mu \) (2) in state \( \mu \) computes then as

\[
S_\mu = 2\upsilon \sum_{r_\mu} \ln n_{r_\mu}
\] (5)

up to an irrelevant constant; the sum is over the roads \( r_\mu \) of state \( \mu \). Thusly our working assumptions bring out an effective scaling exponent \( \tilde{\lambda} \) along an effective total amount of surprisal \( \tilde{S}_\mu \); we read

\[
\tilde{\lambda} = 2\lambda \upsilon \quad \text{along} \quad \tilde{S}_\mu = \sum_{r_\mu} \ln n_{r_\mu}. \] (6)

The corresponding effective acceptance ratio is literally the tilde version of formula (3).

3 Simulations

This paper selects the walled urban street network of Old Ahmedabad (India), which is a classical example of self-organized urban street network [15], as case study.
3.1 Behavioural based join outputs

Figure 1 shows typical sequences of self-best-fit and self-fit outputs. They are shown, for the sake of comparison with real Metropolis-Markov chains, as if they were generated as Markov chains [6, 16]. The difference is marked in the time-axis legend by using ‘output’ instead of the expected ‘generation’. The two family of output sequences look actually very similar. Nevertheless, the self-fit outputs have in average a slightly smaller effective total amount of surprisal $\tilde{S}_\mu$, while their standard-deviation is slightly larger. However, given that self-fit outputs have been considered to give the best “fits”, sequences of self-fit outputs will serve in the remaining as in-background references.

![Fig. 1. Typical behavioural-based-join output series for Old Ahmedabad (India): the foreground purple output series plot a typical sequence of self-best-fit outputs in (a) and a typical sequence of self-fit outputs in (b); the background light-grey output series plot typical sequences of self-fit outputs. The self-fit principle is used as reference, here and in Figure 2, because it generally offers the best “fit” [3]. The plots adopt, as in Figure 2, the modus operandi customarily used for Metropolis generation series [6, 16].](image)

3.2 Equilibrium Metropolis simulations

Old Ahmedabad offers, as shown in Figure 2, single-direction-swap Metropolis generation series that reach equilibria. The equilibria were attained from self-fit outputs through a basic algebraic annealing schedule [6, 16, 17]. To paraphrase: increase (resp. decrease) the control effective-scaling-exponent $\tilde{\lambda}_c$ to $\tilde{\lambda}_c(1 + \epsilon)$ (resp. $\tilde{\lambda}_c/(1 + \epsilon)$) after every $m$ accepted/rejected single-direction-swap moves up (resp. down) to the desired equilibrium effective-scaling-exponent $\tilde{\lambda}$; the initial control effective-scaling-exponent $\tilde{\lambda}_0$ and the parameters $\epsilon$ and $m$ are determined by experiment. This annealing schedule allows to reach equilibria for a range of effective-scaling-exponent $\tilde{\lambda}$ values long enough to capture noteworthy behaviours.

The behaviours of the effective total and average amounts of surprisal, $\tilde{S}_\mu$ and $\langle \tilde{S}_\mu \rangle$ respectively, as the effective scaling exponent $\tilde{\lambda}$ varies exhibit in Figure 3 at least two promising properties. First, their means and their standard-deviations are functions of
Fig. 2. Typical single-direction-swap Metropolis generation series for Old Ahmedabad (India): the foreground purple generation series plot, for different effective scaling exponents $\tilde{\lambda} = 2\lambda \nu$, typical simulations starting from a self-fit output; the background light-grey generation series plot, according to the same modus operandi, typical sequences of self-fit outputs. The following annealing parameters were used to algebraically cool down to the desired $\tilde{\lambda}$: $\tilde{\lambda}_0 = \frac{6}{5} \gamma = 10^{-3}$ and $m = 500$. (The starting cooling value $\tilde{\lambda}_0 = \frac{6}{5}$ was chosen as rational interpolation for which the Metropolis equilibrium approaches in average self-fit outputs — as illustrated in (c); the special case $\tilde{\lambda} = \infty$ in (h) corresponds to a full 'simulated annealing' process [16, 17].)
Fig. 3. Effective total and average amounts of surprisal versus effective scaling exponent for Old Ahmedabad (India); green solid lines plot the mean (top) and standard-deviation (bottom) of the effective average amount of surprisal $\langle \tilde{S}_\mu \rangle$; purple dashed lines plot the mean (top) and standard-deviation (bottom) of the effective total amount of surprisal $\tilde{S}_\mu$; the main plots exhibit their behaviours around the point of inflection $\tilde{\lambda} \approx 3.5$; the insets show their asymptotic behaviours. Around the point of inflection, the standard-deviation rates vary essentially linearly; the value of the rates at the point of inflection may characterize the urban street network of Old Ahmedabad among others. The annealing parameters are the same as in Figure 2, the mean and standard-deviation values were computed over 250000 in-equilibrium generations and averaged over 10 simulations. The equilibria were assumed reached after the $5000^{th}$ generation — see Figure 2. (We attribute the noise that waves the asymptotic branches to the poor quality of our map data in their small streets.)
the effective scaling exponent $\hat{\lambda}$ which vary very smoothly and asymptotically to a constant for large values. This means that they can certainly be interpolated as rational fractions. Such interpolations will allow to compute quantitative data as specific-heat-like capacities. Second, their standard-deviations have around $\hat{\lambda} = 3.5$ a point of inflection. Around the same value, the mean of the average amount of surprisal $\langle \tilde{S}_\mu \rangle$ experiences a significant change of rate; the mean of the total amount of surprisal $\tilde{S}_\mu$ appears to experience there a noticeable change of rate as well. This point of inflection is certainly for our system a quantitative characteristic. These two properties are simply reminiscence of thermodynamic properties that must be investigated in an appropriate thermodynamic-like framework.

4 Discussion and Perspectives

Information networks of self-organized urban street networks undergo a scale-free coherence that we have recently interpreted in terms of a fluctuating system which preserves its amount of surprisal on average [4, 5]. The similitude with fluctuating systems that preserve their amount of energy on average is immediate. It needs to be reinforced. This paper sketches how the Metropolis algorithm, which embodies well the idea of fluctuating systems [6], can apply to information networks once our interpretation is embraced. Our preliminary simulations on a recognized self-organized urban street network, Old Ahmedabad, sustain Metropolis equilibria for a large range of effective scaling exponents (see Figures 2 and 3). The range runs from vanishing values to values ten times the state-of-art estimation $\hat{\lambda}^* = 2.66 (18)$ [4, 5] — beyond this range, simulations show asymptotic behaviours (see insets in Figure 3). Mean and standard-deviation plots of the effective total and average amounts of surprisal along this range (Figure 3) are smooth enough to possibly interpolate quantitative data as specific-heat-like capacities [6]. Meanwhile, we can observe more than slightly beyond the state-of-art estimation $\hat{\lambda}^* = 2.66 (18)$ [4, 5] a point of inflection around $\hat{\lambda} = 3.5$. This point of inflection certainly characterizes our system both qualitatively and quantitatively. This quick analysis of our system plots is a promising prelude to a thermodynamic-like framework for urban street networks. The resulting specific-heat-like capacities may permit to compare quantitatively urban street networks along time and with each others.

The fluctuating nature of our system along the existence of equilibria is not compatible with current approaches, since they assume nonfluctuating systems, for determining the effective scaling exponent of an urban street network. This is issue may have to be resolved in a thermodynamic-like framework. Meanwhile, let us notice that the effective scaling exponent breaks into two coefficients of different nature: a scaling exponent that reflects the structuration of the urban street network and a number of vital connections that reflect social interactions between city-dwellers. Here the urban street network is essentially fixed, so that only the number of vital connections can vary. As different number of vital connections may corresponds to different city-dweller flows, the determination of the effective scaling exponent may take into account the actual fluctuation in city-dweller flows. Along this line, a thermodynamic-like framework may provide new ways to act on the behaviour of city-dweller flows by altering specific-heat-like capacities, namely the structuration of the urban street network.
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