THERMODYNAMIC & ALGORITHMIC EFFICIENCY IN HETEROGENEOUS NETWORKS

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ABSTRACT

Why complex structures emerge in a real world environment is a fascinating question which has not found any fully satisfactory answer at the point of today. At the border between statistical physics, machine learning and network theory, we provide some computational empirical evidence indicating that the emergence of complex structures in a real world environment is the macroscopic thermodynamic result of the optimal trade-off between the ability to encode information about the environment in the very features of the network and the ability to transmit information across it. While the former is quantified by the von Neumann network entropy and the latter by the Helmholtz free energy, the two are gathered into a single quantity tantamount to the thermodynamic efficiency. We take as a case study an algorithm originally proposed for creating and searching trees of patterns under the assumption that, akin to living system, the algorithm seeks the best internal representation of the outer world, namely a real world dataset of patterns. Remarkably, optimal thermodynamic efficiency overlaps with the optimal algorithmic efficiency, defined in terms of accuracy and computational cost, whether the former is measured at the resolution scale in where the network transits from exhibiting a specific heat with a single peak to a scale-invariant region. Moreover the critical hypothesis is investigated and empirical evidence suggests that the system benefits from the critical-state when it confronts with higher-complexity environments, while it does not when the environment is simpler.

Keywords von Neumann entropy · Specific heat · Thermodynamics · Statistical physics · Machine Learning

1 Introduction

Why complex structures emerge in a real world environment is a fascinating question which has not found any fully satisfactory answer at the point of today. We aim at some computational empirical evidence suggesting that the emergence of complex structures is the macroscopic thermodynamic result of optimal ability to store the information about the environment and the ability to transmit information across the structure \cite{1,2}. The latter is defined in terms of microscopic quantities thanks to the fairly newly developments in statistical physics of fields in network theory \cite{2,3,4,5}. In living systems, natural selection is the way the information about the environment flows into the system’s genome which will than encode such information in the structural traits of the organisms which in turn reflect the functional capability of the system. Thus the structural traits of a system could themselves enclose the complexity of the environmental conditions the system needs to adapt to, or in other words, to represent into its very own structure \cite{6}. How these traits are optimized to maximize the fitness to the environment is an open question. The hypothesis of optimal functioning at the border of order and disorder suggests the critical point as the potential candidate to obtain functional advantages \cite{7,8,9,10} and maximize the fitness to the outer world, or to obtain a better performance in a
statistical generalization problem in the context of learning machines. Here we challenge this hypothesis. In our work a system seeks the best-fitness configuration given some external constraints $r$ and the dataset $D$.

We take as case study the algorithm introduced by Portegys [11] for nearest-neighbour (1-NN) pattern recognition tasks and subsequently extended to k-NN [12]. The algorithm employs a tree formation protocol where raw data are reorganized into tree structures using a recursive tree-formation method in which samples are randomly selected and inserted into the growing tree structure. At each step the new pattern is linked to either the currently parent pattern or to one of the k-NN children of the parent pattern. The choice is based on the relative distance between the parent and the new pattern and the one evaluated between the child pattern and the new pattern. The parameter $r$ modulates the relative importance of these two distances creating a larger or smaller region of influence of the parent in the sample space. Figure 1 shows the three structure prototypes produced depending on the value of the control parameter $r$. For $r \sim 0$, every node is linked to the root node (see the central node, which is the first node selected in the process) and a star-graph turns out. For some intermediate value of $r$ a ragged tree structure is produced, while for $r \rightarrow 2$ a 1d-lattice is created. Remarkably, the algorithm produces exclusively trees, i.e. number of spanning trees is always 1, which are sparse $|E| = N - 1$ where $|E|$ and $N$ are the number of links and nodes respectively. Using the metaphor introduced by Jacob for natural selection [13], the algorithm does act as a tinkerer that creates a structure using what is available at the time, collocating one node after the other across the tree formation process according to a distance based rule.

Depending on the structural traits of the networks, an optimal trade-off between fast search of the best-matching pattern and accuracy in terms of node-class labels can be defined.

The Portegys algorithm has the desirable properties of being simple, explainable and subject to a single control parameter $r$. Thanks to these features, we can work on the bridge between three disciplines: statistical physics, machine learning and network science, and we can show that information-theoretical tools as the von Neumann entropy and its derivative reflect the functional capabilities of the network. Most notably thermodynamic efficiency and algorithmic efficiency demonstrate noticeable overlap.

Figure 1: **The three prototypical structures generated by the Portegys algorithm.** The algorithm creates star-like networks up to 1d lattice when $r \rightarrow 2$. For intermediate values of $r$, networks resembling an arborescent tree are produced. The process is reminiscent of the transition vapor/liquid $\rightarrow$ amorphous solid $\rightarrow$ 1d lattice. Depicted networks are generated from a subset of 50 samples randomly extracted from the MNIST dataset with $r = 0.05, 0.95, 1.50$ respectively. Classes are indicated by the 10 different colors in the color-bar.

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"Natural selection does not work as an engineer works. It works like a tinkerer - who does not know exactly what he is going to produce but uses whatever he finds around him whether it be pieces of string, fragments of wood, or old cardboards; in short works like a tinkerer who uses everything at his disposal to produce some kind of workable object."
2 Theoretical framework

2.1 Statistical physics of networks

Information spreading over networked structures is governed by the Laplacian matrix \[ \mathbf{L} \] and its spectrum of eigenvalues encodes many relevant topological properties of the graph \[ \mathbf{G} \] \cite{14}. Let us consider an undirected and unweighted network \( \mathbf{G}(V, E) \) of order \( |V| = N \) with number of links equal to \( |E| = m \). The network Laplacian is defined as \( \mathbf{L} = \mathbf{D} - \mathbf{A} \), where \( \mathbf{D} \) and \( \mathbf{A} \) are the diagonal matrix of the node degrees and the adjacency matrix respectively. The Laplacian operator can be used to define a density operator \[ \mathbf{\rho} \], where the Laplacian takes the role of the Hamiltonian of statistical physics \cite{17} as in equation (1).

\[
\mathbf{\rho}_\tau = e^{-\tau \mathbf{L}}
\]

The elements \( \rho_{ij} \) represent the normalized amount of information transferred in a diffusion process between nodes \( i \) and \( j \) at time \( \tau \). Remarkably, \( \rho_{ij} \) takes into account all possible topological pathways between the two nodes and assigns smaller weights to longer ones tantamount to path-integrals \cite{18,20}. The partition function \( Z = \text{Tr}[\mathbf{\rho}] = \sum_{i=1}^{N} e^{-\tau \lambda_i (\mathbf{L})} \) is a function of the eigenvalues, \( \lambda_i \), of the Laplacian and is proportional to the average return probability of a edge-centric random walker to be back in its initial location at time \( \tau \) \cite{4}. Note that the object \( \mathbf{\rho} \) is a positive semi-definite and Hermitian matrix whose trace sums to unity which has allowed its eigenvalues to be interpreted as probabilities.

Finally, the network von Neumann entropy can be introduced \[ \mathbf{5} \] as a multi-scale descriptor of the network structure:

\[
S(\mathbf{\rho}(\tau)) = - \sum_{i=1}^{N} \mu_i(\tau) \log \mu_i(\tau)
\]

where \( \{\mu_i(\tau)\}_{i=1}^{N} \) is the set of \( \mathbf{\rho}(\tau) \) eigenvalues that are related to the set of Laplacian eigenvalues through \( \mu_i(\tau) = e^{-\tau \lambda_i}/Z \). The entropy \( S(\mathbf{\rho}(\tau)) \) is a function of the normalized time \( \tau \) and is bounded between \( \log C_{\text{conn}}, \log N \) where \( C_{\text{conn}} \) is the number of connected components and \( N \) is the number of nodes. Thus the von Neumann entropy \( S \) as a function of \( \tau \) reflects the entropic phase transition of information propagation (or loss) over the network \cite{20} as illustrated in figure 2. Specifically for a connected network, at \( \tau \to 0 \), \( S(\tau) = \log N \) reflects the segregated heterogeneous phase where information diffuses from the single nodes to the very local neighborhood; at \( \tau \to \infty \), \( S(\tau) = 0 \) the diffusion is governed by the smallest non-zero eigenvalue of the Laplacian, associated with the so-called Fiedler eigenvector, reflecting the homogeneous phase where the information has propagated all over the network.

The network entropy thus counts the (logarithmic) number of informationally connected component on the heterogeneous network and by the inspection of the entropy \( S \) and its generalized susceptibility (or specific heat) \( C = -dS/\log \tau \) it is possible to identify the characteristic resolution scales of the network \cite{20,3}. For instance, a constant specific heat reflects the scale-invariance of the network where information is lost at a constant rate. Such a situation is typical of d-dimensional lattices and scale invariant networks with power law distributed spectrum. On the contrary, a single large peak of the specific heat \( C \) identifies a single scale where there is a fast and unique information diffusion (or information lost) across the network. The latter is the typical situation of a star-graph, depicted in figure 1 or an Erdős-Rényi network, see purple curve in figure 1. Before the peak the informationally connected components are the single nodes and after the peak the informationally connected components is the full-network reviling a single trivial-scale.

From this considerations, a Laplacian-Renormalization group theory has been recently developed allowing for a coarse-graining of the network structures into super-nodes unraveling the mesoscale structures \[ \text{3,20} \]. In this context, the peaks of the specific heat, \( C \), or a marked change in its slope, identify the most convenient resolution scales where to perform the coarse-graining over the informationally connected nodes, as it allows the iteration of the procedure without an excessive network reduction.
To conclude, we can intuitively use the diffusion parameter $\tau$ to resolve the network topological structures at different resolution scales. Thus, the necessity of analyzing complex networked systems at all levels is solved by resorting to the conjugate Fourier space, the $k$-space, defined by the Laplacian spectrum and the "wavelengths" of its modes.

**Figure 2:** Von Neumann entropy as a function of the diffusion time. Panel (a) depicts diffusion over two exemplary networks with analogous topological features to those depicted in panel (b): in blue a stochastic block model network exhibiting tripartite modular structure, and in purple a Erdős-Rényi random network with the same number of nodes of the blue one. For small $\tau \sim 0$, both networks exhibit the maximum spectral entropy value $\log N$, where $N$ is the number of nodes, reflecting the segregated phase. For $\tau \to \infty$, the spectral entropy converges to $\log C$, where $C$ is the number of connected components, thus reflecting the integrated phase. For intermediate values of $\tau$, the Erdős-Rényi network shows a single critical scale at which the network transitions from the segregated to the integrated phase. The position on the horizontal axis of the critical scale is related to the edge density of the network as well as the heterogeneity in the degree distribution. On the contrary, the blue network exhibits two critical resolution scales in the entropic transition. At smaller $\tau$, information initially diffuses within the modules ending into a plateau. A later slower diffusion process between the three modules completes the transition to the integrated phase. The insets show the density matrix $\hat{\rho}(\tau)$ across the entropic transition on the blue curve. The tripartite modular structure of the network is shown by the emergence of the three blocks in the density matrix. Graphs depicted in (b) have only illustration purpose. Illustration from [21].

### 2.2 Thermodynamics of networks

The beauty of the statistical physics theory for networks introduced above is that it naturally allows to view network phenomena from a new perspective and to bridge the gap to network macroscopic observables. To this regard network thermodynamic quantities as work, $W$, and heat, $Q$, can be defined in (at least mathematical) analogy to their thermodynamic counterparts [2]. Since a network of isolated nodes is the only network with maximum entropy $S_{iso} = \log N$ for $\tau > 0$, progressively adding edges results in diminishing the entropy of the network. In turns, lower entropy reflects the diminished ability of the network to express diversity to a stochastic perturbation, or in other terms, the loss in the internal representation capabilities encoded in the network topological traits. The entropic cost is given by:

$$Q = \frac{-dS}{\tau} = - \frac{\log N - S}{\tau} \leq 0$$

which resembles the heat dissipation in a thermodynamic process.

On the other hand, it is obvious that adding edges increases the information flow quantified by the (Helmholtz) free energy $F = -\log Z/\tau$ [2,3]. Less obvious is how, for fixed number of edges, the degree distribution influences the flow of information. As the Laplacian governs the continuous-time edge-centric random walk, the presence of large hubs implies an enhancement of the process with faster propagation of the diffusing quantity [14,22]. As the free energy is inversely related to the partition function, $Z = \sum_{i=1}^{N} e^{-\tau \lambda_i}$, the bounds of the former are given by the bounds of the latter. From $1 \leq Z \leq \log N$, where the lower bound is given for the connected network at large $\tau \gg 1$, while
the upper bound is given by a network of isolated nodes \( \forall \tau \), or for a connected one at small scales \( \tau = 0 \). Thus, the \(- \log N/\tau \leq F \leq 0\) and the gain in information flow is reflected by the variation of the free energy from the case of isolated nodes:

\[
W = dF = F - F_{iso} = F + \frac{\log N}{\tau} \geq 0
\]

which is tantamount to the work in the canonical ensemble. Moreover, \(U = W + Q \geq 0\) which implies \(W \geq |Q|\). A formation process can be depicted as the trade-off between this two necessities of a networked complex systems: the maximization of information flow, while at the same time maintaining an amount of entropy such that the network can encode and express sufficient amount of diversity through its traits.

Thus, to complete the analogy to thermodynamics, the trade-off between diversity of information and information flow is captured by the efficiency \(2\):

\[
\eta = \frac{W + Q}{W} = 1 - \frac{|Q|}{W} = \frac{U}{W}
\]

where \(0 \leq \eta \leq 1\) and \(U = -\partial_r \log Z \equiv \text{Tr}[\hat{L}\hat{\rho}]\). The variational principle here exposed has been devised to macroscopically explain the sparsity and its empirical scaling law, as well as the emergence of topological features such as modularity, small-worldness and heterogeneity \(2\). In our work we make use of this variational principle to explain the structural properties of a network that is required to encode the diversity expressed in the environment, where the environment is defined by a real-world dataset of patterns. We also make use of the specific heat to identify which is the resolution scale at which such variational principle is effective for heterogeneous networks constrained to a sparsity regime.

3 Results

Our results are evaluated over subsets of three different datasets: the NIST \(23\), the MNIST \(24\) and the FashionMNIST \(25\) datasets. These data sets contain randomly collected instances of image samples out of 10 classes. It should be noted that in this type of data, a pattern class can generally not be represented by a single centroid vector, but will contain multiple densities (‘sub-style patterns’) such that the sample point cloud can be ordered naturally in a network structure. The MNIST database contains 24 \(\times\) 24 grey-scale images of handwritten digits [0-9] commonly used to benchmark machine- and deep- learning algorithms. The NIST dataset is the ancestor of the MNIST, it contains 16 \(\times\) 16 black-and white images of the handwritten digits [0-9]. The FashionMNIST is a large dataset of 28 \(\times\) 28 grey-scale images of fashion products from 10 categories. In all our experiments a subset of 2000 samples is extracted from the train-set and the test-set independently. In the Suppplementary we show also the same results for larger networks generated from 4000 samples from the MNIST and FashionMNIST. The 10 classes are equally represented both in the test and in training set. We limit to \(r \leq 0.85\) as the accuracy, and hence the algoritmic efficiency quickly drops for larger \(r\), moreover the algorithm shows instability as it doesn’t necessarily converge for \(r \geq 0.9\).

3.1 Algorithmic efficiency

After the tree formation described in section\(1\) the Portegys algorithm enters the search phase, where the best match to a test pattern is given using a first-best approach. The original goal of this algorithm was to restructure a list of examples in a tree-based way, such that the performance would not be much worse than nearest-neighbor matching on a full list, while providing a considerable speed up due to the tree-based structure. The search process is an iterative process which begins with the computation of the distance between the test pattern and the root-node pattern scaled by \(r\). The distance is then compared to the distance between the test pattern and all of the root node’s children. The first node with a pattern that has a smaller distance is than selected as the new root node, and the process starts over with the newly selected node as root. The search phase terminates when no node whose pattern has smaller distance to the test pattern than the current one can be found.

It is natural to define an algorithmic efficiency, \(\theta\), in terms of class match accuracy, \(A\), and the number of distances computed, \(N_{\text{dist}}\):

\[
\theta = \frac{A}{\log N_{\text{dist}}}
\]

the logarithm is taken as the range of \(N_{\text{dist}}\) can virtually span the interval \(N_{\text{dist}} \in (0,N]\) where \(N\) is the number of nodes. For the case of a star-graph, \(r \to 0\), the number of computed distances is maximum \(N_{\text{dist}} = N\), for lower values of \(r\) the number of computed distances decreases as does the accuracy but at a different pace, thus, it is possible to identify an optimal trade-off between the gain in computational burden and the loss in performance, as depicted in panel (c) of figure\(3\).
Figure 3: **Algorithmic efficiency**, (c), is defined as the trade-off between the classification accuracy, (a), and the logarithm of the number of distances computed to find the best-match, (b). The dashed-red vertical line indicates the optimal $r$ value in terms of efficiency. The shaded grey area designates the standard deviation. The purple shaded area in panel (c) indicates the intersection between the blue curve and the standard deviation at the optimal point whose y-axis projection is indicated by yellow shaded area. Curves are computed over 50 independent simulations with a subset of 2000 samples extracted from the NIST dataset. The 10 digit-classes are equally represented both in the train- and test-set.

### 3.2 Thermodynamic and algorithmic efficiency at the emergence of new C-peaks

In figures [4 to 6] methodology and results showing the coherence between algorithmic and thermodynamic efficiency are replicated for the three investigated datasets. For each dataset, panel (a) depicts the $\tau$-resolution scales identified by the first peak (blue curve), $\tau_{\text{peak}}^{(1)}$, and last peak (green curve), $\tau_{\text{peak}}^{(2)}$, of the specific heat, $C$, as a function over the control parameter $r$. See figure S5 in the Supplementary for more von Neumann entropy and specific heat curves as a function of $r$.

Similar to what would be the transition from vapor/liquid to an amorphous solid, at a critical value of $r$ topological complexity increases from the trivial traits of a star-graph. Thus, structure emerges reflected by the rise of a second peak in $C$ and a roughly $C = c_0 > 0$ plateau in between the first and the last peak. Such transition can be identified by the bifurcation of the blue and green curves for $\tau_{\text{peak}}^{(1)}$ and for $\tau_{\text{peak}}^{(2)}$ respectively.

Before the bifurcation the two curves overlap, and the single peak in the specific heat identifies a single resolution scale below which the informationally connected components are the single nodes, and after which the informationally connected component is the full graph. The emergence of a plateau $C = c_0 > 0$ for $r \rightarrow 2$ reflects the emergence of a progressively larger scale invariant structure. For $r \rightarrow 2$ we expect the plateau height to converge to the theoretical value $C \rightarrow c_0 = 1/2$ of the 1d-lattice [3]. The observation is cross-validated by the color code in panel (d) showing the specific heat as a function of both parameters $r$ and $\tau$. The two curves $\tau_{\text{peak}}^{(1)}$ and $\tau_{\text{peak}}^{(2)}$ are projected onto the specific heat surface in panel (d).

In panels (b), (c) the overlap between the thermodynamic efficiency, $\eta$, and the algorithmic efficiency, $\theta$, is illustrated. The dashed lines indicate where best trade-off is obtained, while the shaded purple region indicate a tolerance region for $\theta$ defined by the intersection between the points on the efficiency curve and the standard deviation computed at the best trade-off. Striking overlap between the two efficiency is observed for the NIST and the FashionMNIST dataset, suggesting that, whether thermodynamic or algorithmic, the two objects are the same thing just viewed from different angles. Remarkably, the efficiency $\eta$ is computed at the $\tau$-resolution scales in the proximity of the transition depicted in panels (a), namely at the $\tau$ values where the bifurcation between $\tau_{\text{peak}}^{(1)}$ and $\tau_{\text{peak}}^{(2)}$ appears in panel (a).

In the seminal work [2], it was indicated to compute the thermodynamics efficiency, $\eta$, using as a reference the $\tau$-scale equal to the inverse of the smallest non-zero Laplacian eigenvalue $\lambda_2 = 1/\tau_{\text{diff}}$, as this might give the time-scale where the diffusion process has reached equilibrium and then logarithmically divide $\tau_{\text{diff}}$ to progressively define the large propagation scales, the middle scales and the small scales. Nevertheless, $\tau_{\text{diff}}$ only approximates the end of the diffusion process which is better reflected by $\tau_{\text{peak}}^{(2)}$. Panels (a) for all three figures 4 to 6 show the numerical average $< \tau_{\text{peak}}^{(2)} >$ in red next to the $\tau_{\text{peak}}^{(1)}$ curves discussed above. While the mentioned strategy is effective in the case of a transition from sparse to connected networks [2], it is less so in a transition that exclusively involves the heterogeneity of the degree distribution. We remind that the Portegy’s algorithm allows us to stay in the regime of sparsity, symbolically $\delta((N-1)/|E| - 1)$.

Thus, it is crucial to identify which is the $\tau$-scale involved in the phase transition from a single trivial scale, i.e. the star-graph, to more complex topological traits. Such resolution scale is the relevant scale for the computation of the
Thermodynamic & algorithmic efficiency in heterogeneous networks

efficiency $\eta$ and defines an "ultra-violet" cut-off in the characteristic frequency of the network across the transformation, similarly to what was discussed in the context of the Laplacian-Renormalization group $^3$. In section S3 of the Supplementary the efficiency, $\eta$, is computed in the range interval indicated by $< \tau_{\text{diff}} >$, i.e. the red curves depicted in panels (a). Whether computed at those scales, $\eta$ shows a change in concavity and no consistent relation with the algorithmic accuracy.

![Figure 4: Thermodynamic & algorithmic efficiency - NIST.](image)

In (a) the bifurcation of $\tau_{\text{peak}}^{(2)}$ and $\tau_{\text{peak}}^{(2)}$ curves identify the $\tau$-scale relevant for the transition from the single-peak to $C = c_0 > 0$ plateau reflecting the emergence of a roughly scale-invariant structure. The numerical average of the diffusion time $\tau_{\text{diff}} = \langle 1/\lambda^2 \rangle$ is plotted in red for reference, see the main text for discussion. In (d) the specific heat, $C$, surface is illustrated and the $\tau_{\text{peak}}^{(1,2)}$ are projected on it. In (b)-(c) the thermodynamic efficiency, $\eta$, and the algorithmic efficiency, $\theta$, are functions of $r$. Vertical dashed-lines indicate the global maxima of the efficiencies. Remarkably, the thermodynamic efficiency is computed in the $\tau$-range of one order of magnitude from the bifurcation between $\tau_{\text{peak}}^{(1)}$ and $\tau_{\text{peak}}^{(2)}$ in (a). Note that both maxima in the efficiencies are located where a discontinuity in $\tau_{\text{peak}}^{(2)}$ is observed at $r = 0.7$, far away from the transition. This is in line with the argument that indicates the NIST as a fairly simple dataset that does not benefit from the critical point. Curves are averaged over 50 independent simulations.

3.3 Criticality or not to criticality

We now focus the discussion of the results obtained for the NIST and MNIST datasets. As it is shown in both panels (a) and (b) of figures 4 and 6, the "plateau" region of the specific heat has a contraction and an expansion for $r = 0.7$ for the NIST and $r = 0.6$ for the MNIST. For the latter the contraction is such that the two $\tau_{\text{peak}}^{(1,2)}$ curves overlap. We mention that this effect is mitigated for larger datasets, i.e. larger networks, as we show in section S2 of the Supplementary. Moreover, for the MNIST case, the contraction of the plateau region is sufficiently strong to reflect on a local maximum in the efficiency, $\eta$, but not registered by the algorithmic efficiency $\theta$.

Note that the mentioned values of $r$ where the (largest) jump in the $\tau_{\text{peak}}^{(2)}$ is observed correspond to the $r$ values where both the best algorithmic efficiencies, $\eta$ and $\theta$, are found, as indicated by the red dashed lines in panels (c) and the multi-colored dashed lines in panels (b) (valid also for the MNIST if we include points in the one standard deviation illustrated by the shaded-purple). Nevertheless, we stress that we did not compute the efficiency at the corresponding $\tau$ scale where such discontinuity appears.

In fact, the $\tau$-scale at which the bifurcation in panels (a) shows up indicates the scale interested in the phase transition and it is the resolution scale where the thermodynamic efficiency overlaps with algorithmic efficiency as a function of $r$. 

7
Figure 5: **Thermodynamic & algorithmic efficiency - FashionMNIST.** As for the case of the NIST, in (a) the bifurcation of $\tau_{\text{peak}}^{(2)}$ and $\tau_{\text{peak}}^{(2)}$ curves identify the $\tau$-scale relevant for the topological transition. In red the numerical average of the diffusion time $< \lambda_2 = 1/\tau_{\text{diff}} >$ is plotted for reference, see the main text for discussion. In (d) the specific heat, $C$, surface is illustrated. In (b)-(c) the efficiencies $\eta$ and $\theta$ are plotted as a function of $r$ with the dashed-lines indicating the global maxima. The $\eta$ is computed in the $\tau$-range of one order of magnitude from the $\tau$-scale indicated by the bifurcation of $\tau_{\text{peak}}^{(1,2)}$ in (a). Note that the maxima of the efficiencies is posited at the edge of the critical value of $r \sim 0.35$ indicating the FashionMNIST as a dataset more complex than the other two investigated, that does benefit from the critical region. Curves are averaged over 50 independent simulations.

Nevertheless, the critical value of $r$ where such transition appears is not necessarily the value where the efficiencies have the global maximum. To explain this we turn to the argument, already present in the literature [26, 10], that indicates the necessity of tuning a system, or of a system to self-tune, at border of a phase transition only weather the task shows a high level of complexity. While for the FashionMNIST, a notoriously more complex dataset when compared to both the MNIST and NIST, the optimal value for the efficiency is posited in the proximity of the critical value of $r \sim 0.35$, the optimal values of $r$ for the NIST and MNIST datasets are evidently far away from their respective transition values. The MNIST in figure 6, which is the intermediate case in terms of complexity, is an interesting case as it shows two maxima. While the global maximum is far away from the critical value of $r$ in panel (a), the local maxima is at $r \sim 0.35$ which corresponds to the critical value of $r$ indicated by the bifurcation in panel (a). This observation is in line with the hypothesis that the system takes advantage from the critical behaviour only when a fairly complex task is presented to it and in line with other observations discussed in the literature [26,10]. Thus, it stresses the importance of dataset under analyses.

Moreover, while the value of $r$ where a structural transition appears is dependent on the dataset, the $\tau \sim 10^3$ scale identified is the same for all the three datasets. Interestingly that $\tau$-scale is also unaffected by the number of nodes in the network (see Supplementary S3). We speculate about the possibility that this is due to the constraint on sparsity.

## 4 Discussion

The ability of a system to survive is the capability of concentrating a flow of order from the environment - “drinking order from the environment” [27]. In other words, systems, whether living systems or machine(-learning) systems, need to learn an efficient internal representation of the complex world - or the dataset- they are posed in contact with. Such internal representation can be encoded in terms of abstract probability distributions [9,10] or in the very network-features of the system, as it happens in genetic regulatory networks playing a central role in morphogenesis [28], or in a mixed-way as in artificial neural networks where the engineer designs a complicated distribution through the definition
Figure 6: **Thermodynamic & algorithmic efficiency - MNIST.** See the main text and the caption of figure 4 for a detailed explanation. The MNIST does not fully benefit from the transition point $r = 0.3$, nevertheless we still observe a local maxima in the efficiency. The contraction of the $\tau_{\text{peak}}^{(2)}$ is reflected in the local maxima of $\eta$ in (b), but not in the efficiency (c). Overlap between the two efficiencies is less striking when compared to figures 4 and 5 but still valid if we include points in one standard deviation, see shaded purple area in (c), from the maximum of $\theta$. Note that the shaded area in (c) extends and includes local to global maxima in (c). Curves are averaged over 50 independent simulations.

of an architecture and the training phase fills in the parameters in order to obtain the desired function-approximation machine to achieve statistical generalization [29].

When confronted to real world environment, in order to survive, living systems not only need the capability of interpreting the environment, but they also need the capability to quickly react with a coherent response to stimuli possibly drawn from the same distribution they adapted to [30]. Moreover the same system needs to cope with cost of sending information across its structure which can cause an enhanced exploitation of resources. In the context of machine-learning, cost can be quantified by the number of computations to be done before the satisfying answer to a task can be reported, e.g. class-matching. By using the recently developed theoretical tools of statistical physics for networks [5, 4, 31, 20, 3, 2], we have quantified diversity in the traits of the network with the von Neumann entropy and transmission flow of information as the Helmholtz free energy. As fastness of information flow and sufficiently rich representation of the outer world are two competing capabilities [2], the formation process of a networked structure is depicted as the trade-off between the two, and a variational principle in terms of thermodynamic efficiency can be devised to explain why a certain structure emerge in place of an other. We have shown that such a thermodynamic efficiency strictly overlaps with the algorithmic efficiency defined in terms of accuracy and computational costs, suggesting that the two can be regarded as the same thing but viewed from different angles.

Notably, we have shown that the thermodynamic efficiency needs to be computed at a specific resolution scale $\tau$. We have used the specific heat $C = -dS/d\log \tau$ to identify the $\tau$-resolution involved in the transition from the trivial-structure with a single specific heat peak to emergence of more complex structures, where the specific heat shows some plateau reflecting the growth of a scale-invariant region where information is integrated at a constant rate. Such $\tau$-resolution scale is akin to an “ultra-violet” cut-off delimiting the frequency of the network structure across the heterogeneity-transition from star-graph to 1d-lattice. While the transition point reflects the network resolution scale where the efficiency needs to be measured, the corresponding transition value of the control parameter $r$ does not coincide with the global maximum in efficiency. We explain this with the statement that a system benefits from the critical point only when it confronts with environments of higher complexity, while it does not benefit from it when the environmental complexity is lower. This is elucidated by the use of three different datasets of increasing complexity and supported by other works in the literature [26, 10].
Conflict of Interest Statement

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Author Contributions

DC: Theoretical framework, Conceptualization, Methodology, Simulations, Data curation, Software, Writing – original draft, Writing – review & editing. LS: Writing – review & editing, Conceptualization, Supervision, Funding acquisition.

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We are thankful to Jos van Goor for providing some of the scripts that enabled efficient grid-search across parameters and to Federico Balducci for the useful discussions.

Supplemental Data

Supplementary Material include figures that are mentioned in the main text but are omitted from it to the purpose of clarity.

Data Availability Statement

The original contributions presented in the study are included in the article/supplementary material, further inquiries can be directed to the corresponding author/s. Datasets and scripts can be found at https://github.com/CipolliniDavide/LaplacianTrees.

References

Thermodynamic & algorithmic efficiency in heterogeneous networks


Supplementary Information: Thermodynamic & Algorithmic Efficiency in Heterogeneous Networks

A Preprint

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S1 Laplacian spectrum

Figure S1: **Laplacian spectrum** for multiple values of $r$. The red-dashed line indicates the limit of 1-d dimensional lattice converging towards a power law with exponent $\gamma = 2$, corresponding to the plateau height of the specific heat $c_0 = 1/\gamma$ in the limit of continuous spectrum. The greater is the degeneracy in the eigenvalue spectrum larger is the peak in the specific heat (see figure S5). For the case of the star graph $r = 0.05$ the maximum eigenvalue is equal to the maximum number of nodes $\lambda_{\text{max}} = 2000$. Points are averaged over 50 independent network generations from the subset of 2000 MNIST samples.
S2   Larger networks: N=4000

Figure S2: MNIST - N=4000. Same tables reported in the main text (refer to those captions for detailed discussion). For larger networks N=4000 optimal $r$ remains unchanged as it is a property mostly dependent on the dataset complexity. Shaded area in (c) spans over the two local maxima in panel (b). In (d) contraction of the specific heat is less pronounced compared to networks of 2000 nodes.
Figure S3: **FashionMNIST - N=4000.** No changes are observed for larger networks in the case of the FashionMNIST. See main text and caption of figure 5 for detailed discussion.

S3  Thermodynamic efficiency change in concavity
Figure S4: Thermodynamic efficiency change concavity across the transition from single peak of the specific heat to the emergence of a scale-invariant region. Remarkably, the coherence between thermodynamic and algorithmic efficiency for resolution $\tau$-scales above and below the order of magnitude where the transition appears. Panels (a) through (c) show the transition for trees of order $N = 2000$, hence 2000 samples from the datasets NIST, FashionMNIST and MNIST. Curves are averaged over 50 iterations.
S4  Von Neumann entropy and specific heat

Figure S5: Von Neumann and specific heat - FashionMNIST. The table shows the von Neumann entropy (blue) and the specific heat (red) for $r = 0.10, 0.85$ for the case of 2000 samples from the FashionMNIST database. Vertical dashed lines indicate the peaks corresponding to $\tau_{\text{peak}}^{(2)}$ in the main text. Shaded areas represent the standard deviation. Curves are averaged over 50 simulations.
Author Contributions

DC: Theoretical framework, Conceptualization, Methodology, Simulations, Data curation, Software, Writing – original draft, Writing – review & editing. LS: Writing – review & editing, Conceptualization, Supervision, Funding acquisition.

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