Entropy Rank and Free Energy: a thermodynamic formalism for Web search

Jean-Charles Delvenne
Imperial College London,
Institute for Mathematical Sciences,
53 Prince’s Gate, South Kensington
London, SW7 2PG
jc.delvenne@imperial.ac.uk

Abstract—We introduce Entropy Rank and Free Energy Rank, two methods to classify pages of the Web according to interest. These variants of PageRank are based on Ruelle’s thermodynamic formalism. They exhibit features from both PageRank and HITS methods.

I. INTRODUCTION

The World Wide Web can be modelled as a graph: pages are vertices, edges are hyperlinks. Google and other Web search engines attribute to each page of the Web a ‘PageRank’ score, which measures how well-connected this page is with respect to other pages [2]. More specifically, a page has a high PageRank if pointed to by pages with a high PageRank. This might be argued as intuitively undesirable, because ‘hubs’ (i.e., they point to good authorities) are not necessarily all equal but can be chosen in order to favor some pages.

Kleinberg [6] has proposed the HITS method, where a page is a good authority if pointed at by good hubs. Other variants have been proposed by several authors, let us mention only Ding et al. [4], who propose a framework generalizing HITS and PageRank and Akian et al. [1], who use thermodynamic concepts in a different way from us.

In this paper we apply methods of dynamical systems theory and statistical physics to the field of large graphs, and in particular we introduce Entropy Rank and Free Energy Rank methods, which rank pages of a Web graph. Their basic idea is to rank paths rather than just vertices, with a probability law given by thermodynamic principles. The last section discusses about the limitations and possible extensions of the Entropy Rank and Free Energy Rank.

In the next two subsections we briefly recall the PageRank method: Entropy Rank and Free Energy Rank methods are outlined. Sections II and III provide formal definitions and results.

A. PageRank: First approach

First, let us normalize every row of the adjacency matrix of the Web graph in such a way that it sums to 1. This is possible if every page contains at least one hyperlink. Then the resulting matrix is row-stochastic and the Web graph is interpreted as a Markov chain. We consider a surfer that moves from page to page following the hyperlinks, choosing randomly with uniform distribution a hyperlink on the current page. The PageRank [2] can be defined as the stationary distribution on the vertices of the graph: a page has a high PageRank if it is visited often by the random surfer. This distribution is computed as the dominant left eigenvector of the row-normalized adjacency matrix.

Some problems arising with this definition are that

• it assumes that all pages contain hyperlinks, which is not true in practice;
• it gives a zero PageRank to pages to which no page points, although these pages might be interesting as ‘hubs’ (i.e., they point to interesting pages);
• the stationary distribution is not unique, e.g., if the graph is not connected.

B. PageRank: Improved approach

To overcome these problems, the possibility is given to the random surfer, with some probability $0 < 1 - \alpha < 1$, to jump to any other page of the web (with uniform distribution). The surfer follows a hyperlink of the current page with probability $\alpha$. Let $\hat{A}$ be the adjacency matrix of the graph, with every non-zero row normalized to 1. Then the stochastic matrix $M$ describing the Markov chain is constructed as follows. Let $e$ be the vector of all ones, normalized in order to sum to one. The $i$th row is equal to $(1 - \alpha) e^T + \alpha \hat{A}_i$ if $\hat{A}_i$ (the $i$th row of $\hat{A}$) is non-zero. If $\hat{A}_i = 0$ then the $i$th row is taken as $e^T$. The left dominant eigenvector of this matrix $M$, normalized in order to sum to one, gives the unique stationary distribution on the vertices. The PageRank is now defined as this stationary distribution. Note that in practice, the entries of $e$ are not necessarily all equal but can be chosen in order to favor some pages.

If $\alpha$ tends toward 1, then we recover the first approach above. If $\alpha$ tends towards 0, then the stationary distribution tends towards the uniform distribution.

However we might argue that this definition still has some questionable aspects. Indeed, take the graph of Figure II Vertices 1, 2, 3 and 4 form a complete directed subgraph, hence they concentrate most of the probability, for values of $\alpha$ close to one, as expected. But they attribute an equal probability to 6 and 8, as we can get easily convinced. This might be argued as intuitively undesirable, because 8 is obviously a better page than 6: it directly points to the most interesting pages.
PageRank

Entropy Rank

C. Introduction to Entropy Rank

We now briefly describe a variant of the PageRank that we call the Entropy Rank method, based on ideas from ergodic theory. We follow the references [3], [7], [8]. Section III explains the algorithm in full depth.

Given the Web graph, we choose probabilities on the edges in such a way that the resulting Markov chain has a maximum entropy rate (defined below). In other words, the behavior of a surfer choosing every edge with these probabilities at every step is maximally unpredictable: even knowing the vertex currently visited, one cannot predict much about the vertex visited next (at least on average). Equivalently, all paths of same (large) length are approximately equiprobable, so one cannot make a good guess about the path that will actually be followed. If we consider an army of random surfers instead of just one, the probabilities are chosen in such a way that the army is maximally dispersing in the graph, exploring every path with an (approximately) equal probability.

More generally, we consider probabilities of transition that depend on the past pages visited by the surfer (loosing the Markov property); however, allowing such a memory of the past is not needed to reach the optimum, for it turns out that there always exists an optimal set of transition probabilities that is Markovian.

We recall the definition of the entropy rate (or Kolmogorov-Sinai entropy): we take the Shannon entropy of all paths of length \( t \), divided by \( t \), taken to the limsup as \( t \to \infty \). The Shannon entropy of a random variable \( X \) taking finitely many values is \(-\sum_x \text{Prob}(X = x) \log \text{Prob}(X = x)\). The logarithm is taken in base \( e \).

The stationary distribution induced by the Markov chain is unique if the graph is strongly connected, and is called the Entropy Rank. It is easily computed from the left and right eigenvectors of the adjacency matrix, as proved by Parry [8] and detailed in Section III.

On the example of Figure I, we observe that the vertex 6 has an Entropy Rank around thirty times lower than the vertex 8, which indicates that the page 8 is more interesting. It illustrates the fact that with the Entropy Rank, a page is good if good pages point to it or it points to good pages.

Also, in the same example, we see that the gap of probabilities between good vertices and poor vertices is higher than given by the PageRank method (at least two orders of magnitude instead of one).

D. Introduction to Free Energy Rank

The Entropy Rank has the same drawbacks than the first approach to the PageRank: it is a meaningful quantity if the graph is strongly connected but otherwise can attribute a probability zero to some vertices, for instance those with zero indegree or zero outdegree. The following modification, which is a particular case of Ruelle’s so-called thermodynamic formalism [9], overcomes this problem in a similar way to the improved version of PageRank.

We allow any transition from any vertex to any vertex, but edges that are not in the graph are pondered with an energy \( U = -\epsilon < 0 \), while the edges of the Web graph have energy \( U = 0 \). We now look for probabilities of transitions such that the resulting Markov chain maximizes the quantity \( S + U \), where \( S \) is the entropy and \( U \) is the expected energy for the stationary distribution of the Markov chain. The maximum value of \( S + U \) is analogous to what is called ‘free energy’ in thermodynamics (with unit temperature and up to the sign). It is also called ‘topological pressure’ in the literature of thermodynamic formalism. Intuitively, the surfer has to find a balance between being as unpredictable as possible and taking the edges with zero energy as often as possible.

The stationary distribution of this Markov chain is always unique and is positive on every vertex. We define the Free Energy Rank to be this distribution. If \( \epsilon \to \infty \) then we find back the Entropy Rank. If \( \epsilon \to 0 \) then the stationary distribution is uniform over the edges.

II. Entropy Rank

We now provide the formal definitions in their full generality. Let \( A \) be the adjacency matrix of a simple directed graph. An infinite path is an infinite sequence of edges such that the terminal vertex of every edge is the initial vertex of the next edge. An infinite path has an initial vertex but no terminal vertex. A finite path is a finite such sequence, and has an initial vertex and a terminal vertex.

Consider a user surfing randomly on the Web, clicking at every step on a hyperlink. Instead of choosing any hyperlink on the page with equal probability (like for the PageRank),
she chooses each hyperlink with a probability that possibly depends on the whole history (list of visited pages up to now). We want these probabilities to be such that the surfing is maximally 'unpredictable'.

Formally, we want a probability distribution over finite paths of length $t$, for any $t > 0$. This is interpreted as the probability that the finite path is actually followed by the random surfer from any given time. We are looking for an invariant, or stationary, distribution which means that the probability for the random surfer to be at time $s$ in a certain vertex and to follow a certain finite path from this vertex, is independent from the time $s$ of observation. Of course this distribution on paths has to satisfy the following constraint: the probability of $e_0 e_1 \ldots e_t$ is the sum over $e_{t+1}$ of all probabilities of paths $e_0 e_1 \ldots e_t e_{t+1}$. We want furthermore the entropy rate of this distribution (defined in Section I-C) to be maximal.

In more concise terms, we are looking for a shift-invariant probability measure on the set of infinite paths with maximal entropy rate. The set of infinite paths is endowed with the Markov property: the random surfer's transition is maximally 'unpredictable'.

Now). We want these probabilities to be such that the surfing right eigenvector for the adjacency matrix $A$ of maximal magnitude, $\lambda$, is replaced by a factor of $\lambda$, $\lambda^{-1}u_i v_i$, which does not depend on the intermediate vertices). We know that the number of paths of length $t$ is in the order of $\lambda^t$ (up to a factor). Hence the probability distribution over paths of fixed length is uniform up to a factor. The Shannon entropy of paths of length $t$ therefore grows as $t \log \lambda$, up to an additive constant. The entropy rate of this distribution is thus $\log \lambda$, which is optimal.

In brief, we have proved the following facts:

- the behavior of a random surfer with maximal entropy rate can be computed from a left and right nonnegative dominant eigenvector, for instance with the power method;
- the resulting distribution on vertices is given by the componentwise product of the two eigenvectors;
- this optimal random surfer need not have a memory of the past (Markov property).

Definition 1: The Entropy Rank of vertex $i$ of an unweighted graph is defined as the probability $u_i v_i$, where $u$ ($v$) is the (right) dominant eigenvector of the adjacency matrix $A$.

If the graph is strongly connected, then $\lambda$, $u$, and $v$ are unique and positive, again by Perron-Frobenius theorem. Then the matrix $\lambda^{-1}A^t$ can be shown to converge to $vu^T$, whose diagonal gives the vertex probability distribution. Actually, as shown in [8], when the graph is strongly connected there is no other probability distribution that maximizes the entropy rate. The Entropy Rank is then uniquely defined and non-zero on every vertex. See an example on Figure [1].

Let us mention some other examples. For the complete graph on $n$ vertices, then $A$ is the matrix of ones (except on the diagonal), and we see that the entropy has the maximal value $\log(n-1)$ for the uniform distribution. If the graph is the union of two complete graphs of different sizes, then the optimal probability distribution is concentrated on the larger component, thus the Entropy Rank of a whole component is zero. If the graph is the union of two copies of the same graph, then the probability distribution can be shared between the two copies in an arbitrary way.

Note also that if we reverse all edges of the graph, then the matrix $A$ is replaced by $A^T$, the vectors $u$ and $v$ switch their roles and the final value for the Entropy Rank is the same. Hence the entropy method takes into account, not only the paths leading to a vertex, but also the paths issued from a vertex.
III. FREE ENERGY RANK

We want a method giving to every graph a unique ranking score, which is non-zero on every vertex. That is why we add the following improvement, which is a particular case of Ruelle’s thermodynamic formalism [9]. On the complete directed graph with self-loops that extends the original graph we attribute an ‘energy’ $U = 0$ to the edges of the original graph and an ‘energy’ $U = -\epsilon < 0$ to the other edges. Now consider the set of all paths in the complete graph. The energy of a path is the energy of its first edge. On this set we want to put an invariant probability measure that maximizes the quantity $S + U$, where $S$ is the entropy rate and $U$ is the expected energy for the probability measure. The maximum of this quantity is analogous to what is called ‘free energy’ in thermodynamics (with unit temperature and up to the sign). It is also called ‘topological pressure’ in the literature of thermodynamic formalism.

This time we consider the matrix $B$ such that $B_{ij} = \exp(U_{ij})$, where $U_{ij}$ is the energy of the edge $ij$. Note that if $\epsilon \to \infty$, then $B$ converges to the adjacency matrix $A$. Note also that the matrix $B$ can be obtained from $A$ by replacing zero entries with $e^{-\epsilon}$.

It is possible to see that the maximizing probability distribution exists and is unique, and we can compute it in the following way. Let $\lambda, u, v$ be such that

- $\lambda$ is the dominant eigenvalue of $B$;
- $u^T B = \lambda u^T$ (left eigenvector);
- $Bv = \lambda v$ (right eigenvector);
- $u > 0$, $\sum_i u_i = 1$;
- $v > 0$, $\sum_i u_i v_i = 1$;

These objects exist and are unique, by Perron-Frobenius theorem. Now, we claim that the maximizing measure gives a probability of $u_i v_j$ to be in vertex $i$. It also gives a probability of $\lambda^{-1} U_{ij} v_j / v_i$ for the transition $i \to j$, of energy $U_{ij}$. And this probability measure is again Markovian. These claims can be derived as corollaries to Ruelle’s more general results [9], but we prefer to give an elementary argument. 

Definition 2: The Free Energy Rank is the probability $u_i v_j$.

Definition 3: For a given $\epsilon > 0$, the Free Energy Rank of vertex $i$ of an unweighted directed graph is defined as the probability $u_i v_j$, where $u_j$ is the left (right) dominant eigenvector of the matrix $B$ obtained from the adjacency matrix by replacing the zero entries with $e^{-\epsilon}$.

The proof of the claim, which we give for the sake of clarity, relies on the following result, well-known in statistical physics; see for instance [9]. Given a finite set endowed with a real-valued energy function, the only distribution that maximizes the free energy (sum of Shannon entropy and expected energy) is the Boltzmann distribution, attributing probability $\exp(U_i) / \sum_i \exp(U_i)$ to element $i$. The free energy is then $\log \sum_i \exp(U_i)$. If a distribution is the Boltzmann distribution up to a factor $\alpha$, meaning that the probability for element $i$ is at most $\alpha \exp(U_i) / \sum_i \exp(U_i)$, then the corresponding free energy is at least $\log \sum_i \exp(U_i) - \log \alpha$. 

The Markov chain described just above gives a probability $\lambda^{-t} \exp(\sum U_{kl}) u_i v_j$ to a path of length $t$ from vertex $i$ to vertex $j$, where $\sum U_{kl}$ is the sum of energies of all edges $(k, l)$ on the path. This has the form of a Boltzmann distribution, up to a factor. Now if we give to a path of length $t$ a ‘path energy’ that is the sum of all energies of its $t$ individual edges, then this probability distribution yields a ‘path free energy’ equal to $\log \sum_{\text{paths of length } t} \exp(\sum U_{kl})$ up to an additive constant (independent of $t$), which is almost maximal. This path free energy, divided by $t$, gives for $t \to \infty$ a maximal $S + U$. Note that the expected energy of a path of length $t$ is exactly $tU$, since the distribution is invariant and the expectation is linear. Note also the maximal free energy is again $\log \lambda$, the logarithm of spectral radius of $B$.

The interpretation of this framework is the following: a random surfer can jump from any page to any page, with an energy cost of $\epsilon$ if no hyperlink is present between the pages. The surfer, whose aim is to optimize the free energy $S + U$, is therefore incited to follow hyperlinks (edges of the graph) in priority. If the energy gap $\epsilon$ is 0, then the optimal probability is uniform. If the energy gap is high, then the surfer is incited to follow hyperlinks most of the time. Such a phenomenon is similar to what is observed when varying the factor $\alpha$ between 0 in 1 in the PageRank method (as detailed in Section I-B). The free energy method also gives a non-zero probability to any vertex of the graph. An example of calculation is shown on Figure 1.

Again, the Free Energy Rank is invariant under reversal of edges.

IV. LIMITATIONS AND EXTENSIONS

There are two ways to get a high Entropy Rank or Free Energy Rank: to be pointed by good pages or to point to good pages. This is reminiscent of HITS method [6], that computes a hub score and authority score for every node from the dominant eigenvectors of $AA^T$ and $A^T A$. The exact relation between HITS and the entropy method remains to be investigated.

Used as a substitute to PageRank to the full web graph, Entropy/Free Energy Rank method can be falsified: to increase the score of a page, it helps to point to many good pages. Used as in HITS method, i.e., on a subgraph of all pages that contain a certain keyword, a page that points to many good pages is a good hub indeed, hence deserves a good score. This indicates however that it might be more indicated to compute the Entropy/Free Energy Rank, not the full web graph but on a subgraph of pages containing a specific keyword or directly linked to such a page, like in the HITS method.

The energies on the edges can be chosen to be unequal, in order to favor some pages, just as for the PageRank (see Section I-B).

Ruelle’s thermodynamic formalism allows to put an energy, not only on the edges, but the paths. In other words, we can define an energy function that depends on a whole path and not only on the first edge. We do not know whether this possibility could find applications in the field of large graphs.

To compute the vectors $u$ and $v$ for the Entropy/Free Energy Rank, one can use the power method, whose rapidity of convergence is determined by the spectral gap of $A$ or $B$.
The spectral gap of a matrix is the ratio of the magnitudes of the first and second eigenvalue. In the PageRank method, the rapidity of convergence is given by the spectral gap of a stochastic matrix $\alpha M + (1 - \alpha) \tilde{A}$.

Instead of maximizing $S$ or $S + \mathcal{U}$, we could also maximize the quantity $(S + \mathcal{U} + \text{spectral gap of the resulting matrix } B)$ over $\epsilon$ and the probability transitions. Indeed, we want to converge as quickly as possible.

The entropy and free energy methods that we propose are not limited to the computation of rankings, but potentially apply any time that we need to transform a graph into a Markov chain. We only mention two examples.

For instance, the following definition of distance between the vertices of an undirected graph has been proposed [5]. We transform the graph into a Markov chain just as in the PageRank method: from every node, choose an outgoing edge with equal probability. Then the distance from vertex $x$ to vertex $y$ is $d_{xy} + d_{yx}$, where $d_{xy}$ is the average first-passage time from $x$ to $y$. Instead of taking this Markov chain, we can choose the Markov chain that maximizes entropy, like in the Entropy Rank method. This would lead to another definition of distance.

Markov chains are also useful in the field of graph clustering: see for instance van Dongen’s Markov clustering algorithm [10]. A variant to van Dongen’s algorithm using the entropy-maximizing Markov chain can be investigated.

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REFERENCES

[1] M. Akian, S. Gaubert, and L. Ninove. The T-PageRank: a model of self-validating effects of web surfing. In Proceedings of the Second Multidisciplinary International Symposium on Positive Systems: Theory and Applications (POSTA06), accepted.

[2] S. Brin and L. Page. The anatomy of a large-scale hypertextual Web search engine. Computer Networks and ISDN Systems, 30(1-7):107–117, 1998.

[3] J. Brown. Ergodic Theory and Topological Dynamics. Academic Press, New York, 1976.

[4] C. Ding, X. He, P. Husbands, H. Zha, and H. Simon. Pagerank, HITS and a unified framework for link analysis. In SIAM International Conference on Data Mining, volume 3, 2003.

[5] F. Fouss, A. Pirotte, J.-M. Renders, and M. Saerens. Random-walk computation of similarities between nodes of a graph, with application to collaborative recommendation. IEEE Transactions on Knowledge and Data Engineering, accepted.

[6] J. Kleinberg. Authoritative sources in a hyperlinked environment. Journal of the ACM, 46(5):604–632, 1999.

[7] P. Kürka. Topological and Symbolic Dynamics, volume 11 of Cours Spécialisés. Société Mathématique de France, 2004.

[8] W. Parry. Intrinsic markov chains. Transactions of the American Mathematical Society, 112:55–66, 1964.

[9] D. Ruelle. Thermodynamic formalism. Addison-Wesley, Reading Mass., 1978.

[10] S. van Dongen. Graph Clustering by Flow Simulation. U. of Utrecht, 2000.