Universal emergence of PageRank

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Universal emergence of PageRank

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Abstract

The PageRank algorithm enables us to rank the nodes of a network through
a specific eigenvector of the Google matrix, using a damping parameter
$\alpha \in ]0, 1[$. Using extensive numerical simulations of large web networks, with
a special accent on British University networks, we determine numerically and
analytically the universal features of the PageRank vector at its emergence
when $\alpha \to 1$. The whole network can be divided into a core part and a group of
invariant subspaces. For $\alpha \to 1$, PageRank converges to a universal power-law
distribution on the invariant subspaces whose size distribution also follows a
universal power law. The convergence of PageRank at $\alpha \to 1$ is controlled by
eigenvalues of the core part of the Google matrix, which are extremely close to
unity, leading to large relaxation times as, for example, in spin glasses.

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(Some figures may appear in colour only in the online journal)

1. Introduction

The PageRank algorithm (PRA) [1] is a cornerstone element of the Google search engine,
which allows us to perform an efficient information retrieval from the World Wide Web
(WWW) and other enormous directed networks created by modern society over the last two
decades [2]. The ranking based on the PRA finds applications in such diverse fields as the
Physical Review citation network [3, 4], scientific journals rating [5], ranking of tennis players
[6] and many others [7]. The PRA allows us to efficiently find the PageRank vector of the
Google matrix of the network, whose values enable us to rank the nodes. For a given network
with $N$ nodes, the Google matrix is defined as

$$
\mathbf{G} = \alpha \mathbf{S} + (1 - \alpha) \mathbf{e} \mathbf{e}^T / N,
$$

where the matrix $\mathbf{S}$ is obtained from an adjacency matrix $\mathbf{A}$ by normalizing all nonzero columns
to 1 ($\sum_j S_{ij} = 1$) and replacing columns with only zero elements by $1/N$ (dangling nodes). For
the WWW, an element $A_{ij}$ of the adjacency matrix is equal to unity if a node $j$ points to node $i$.
and zero otherwise. Here $e = (1, \ldots, 1)^T$ is the unit column vector and $e^T$ is its transposition. The damping parameter $\alpha$ in the WWW context describes the probability $(1 - \alpha)$ to jump to any node for a random surfer. For the WWW, the Google search uses $\alpha \approx 0.85$ [2].

The matrix $G$ belongs to the class of Perron–Frobenius operators naturally appearing for Markov chains and dynamical systems [2, 8]. For $0 < \alpha < 1$, there is only one maximal eigenvalue $\lambda = 1$ of $G$. The corresponding eigenvector is the PageRank vector which has non-negative components $P(i)$ with $\sum_i P(i) = 1$, which can be ranked in decreasing order to give the PageRank index $K(i)$. For the WWW, it is known that the probability distribution $w(P)$ of $P(i)$ values is described by a power law $w(P) \propto 1/P^\mu$ with $\mu \approx 2.1$ [9], corresponding to the related cumulative dependence $P(i) \propto 1/K^{\beta}$, where $\beta = 1/(\mu - 1) \approx 0.9$ at $\alpha \sim 0.85$.

PageRank performs ranking, which on average is proportional to the number of ingoing links [2, 10], putting at the top the best known and popular nodes. However, in certain networks outgoing links also play an important role. Recently, in examples of the procedure call for the network of Linux Kernel software [11] and the Wikipedia article network [12], it was shown that a relevant additional ranking is obtained by considering the network with inverse link directions in the adjacency matrix corresponding to $A_{ij} \rightarrow A^T_{ij} = A_{ji}$ and constructing from it a reverse Google matrix $G^*$ according to relation (1) at the same $\alpha$. The eigenvector of $G^*$ with eigenvalue $\lambda = 1$ gives then a new PageRank $P^*(i)$ with the ranking index $K^*(i)$, which was named CheiRank [12]. This rates nodes on average in proportion to the number of outgoing links highlighting their communicative properties [11, 12]. For the WWW, one finds $\mu \approx 2.7$ [9] so that the decay of CheiRank $P^* \propto 1/K^{\star \beta}$ is characterized by a slower decay exponent $\beta \approx 0.6$ compared to PageRank. In figure 1, we show PageRank and CheiRank distributions for the WWW networks of the Universities of Cambridge and Oxford (2006), obtained from the database [13].

Due to the importance of PageRank for information retrieval and ranking of various directed networks [7] it is important to understand how it is affected by variation of the damping parameter $\alpha$. In the limit $\alpha \rightarrow 1$, PageRank is determined by the eigenvectors of the highly degenerate eigenvalue $1$ [14]. These eigenvectors correspond by definition to invariant subspaces through the matrix $S$. It is known [15] that in general these subspaces correspond to sets of nodes with ingoing links from the rest of the network but no outgoing link to it. These parts of the network have been given different names in the literature (rank sink, out component, bucket, and so on). In this paper, we show that for large matrices (of size up to
several millions) the structure of these invariant subspaces is universal and we study in detail the universal behavior of PageRank at $\alpha \to 1$ related to the spectrum of $G$, using an optimized Arnoldi algorithm.

We note that this behavior is linked to the internal structure of the network. Indeed, it is possible to randomize real networks by randomly exchanging the links while keeping exactly the same number of ingoing and outgoing links. It was shown in [16] that this process generally destroys the structure of the network and creates a huge gap between the first unit eigenvalue and the second eigenvalue (with modulus below 0.5). In this case, PageRank simply goes for $\alpha \to 1$ to the unique eigenvector of the matrix $S$ associated with the unit eigenvalue.

The paper is organized as follows: in section 2 we discuss the spectrum and subspace structure of the Google matrix, in section 3 we present the construction of invariant subspaces, the numerical method of PageRank computation at small damping factors is given in section 4, the projected power method is described in section 5, universal properties of PageRank are analyzed in section 6 and a discussion of the results is given in section 7.

2. Spectrum and subspaces of the Google matrix

In order to obtain the invariant subspaces, for each node we determine iteratively the set of nodes that can be reached by a chain of non-zero matrix elements. If this set contains all nodes of the network, we say that the initial node belongs to the core space $V_c$. Otherwise, the limit set defines a subspace which is invariant with respect to the applications of the matrix $S$. In a second step, we merge all subspaces with common members, and obtain a sequence of disjoint subspaces $V_j$ of dimension $d_j$ invariant by applications of $S$. This scheme, which can be efficiently implemented using a computer program, provides a subdivision of network nodes in $N_c$ core space nodes (typically 70–80% of $N$) and $N_s$ subspace nodes belonging to at least one of the invariant subspaces $V_j$ inducing the block triangular structure,

$$S = \begin{pmatrix} S_{ss} & S_{sc} \\ 0 & S_{cc} \end{pmatrix}$$

where the subspace–subspace block $S_{ss}$ is actually composed of many diagonal blocks for each of the invariant subspaces. Each of these blocks corresponds to a column sum normalized matrix of the same type as $G$ and has therefore at least one unit eigenvalue, thus explaining the high degeneracy. Its eigenvalues and eigenvectors are easily accessible by numerical diagonalization (for full matrices) thus allowing us to count the number of unit eigenvalues, e.g., 1832 (2360) for the WWW networks of Cambridge 2006 (Oxford 2006) and also to verify that all eigenvectors of the unit eigenvalue are in one of the subspaces. The remaining eigenvalues of $S$ can be obtained from the projected core block $S_{cc}$ which is not column sum normalized (due to non-zero matrix elements in the block $S_{sc}$) and therefore has eigenvalues strictly inside the unit circle $|\lambda_j^{(\text{core})}| < 1$. We have applied the Arnoldi method (AM) [17–19] with Arnoldi dimension $n_A = 20,000$ to determine the largest eigenvalues of $S_{cc}$. For both example networks, this provides at least about 4000 numerical accurate eigenvalues in the range $|\lambda| \geq 0.7$. For the two networks the largest core space eigenvalues are given by $\lambda_1^{(\text{core})} = 0.999 874 353 718$ (0.999 982 435 081) with a quite clear gap $1 - \lambda_1^{(\text{core})} \sim 10^{-4}$ ($\sim 10^{-5}$). We also mention that the largest subspace eigenvalues with modulus below 1 also have a comparable gap $\sim 10^{-5}$. In order to obtain this accuracy it is highly important to apply the AM to $S_{cc}$ and not to the full matrix $S$ (see more details below). In the latter case the AM fails to determine the degeneracy of the unit eigenvalue, and for the same value of $n_A$ it produces less accurate results.
In figure 2, we present the spectra of subspace and core space eigenvalues in the complex plane $\lambda$ as well as the fraction of eigenvalues with modulus larger than $|\lambda|$, showing that subspace eigenvalues are spread around the unit circle being closer to $|\lambda| = 1$ than core eigenvalues. The fraction of states with $|\lambda| > |\lambda_j|$ has a sharp jump at $\lambda = 1$, corresponding to the contribution of $N_s$, followed by an approximate linear growth.

We now turn to the implications of this structure to the PageRank vector $P$; it can be formally expressed as

$$ P = (1 - \alpha) (1 - \alpha S)^{-1} e/N. $$

(3)
Let us first assume that \( S \) is diagonalizable (with no non-trivial Jordan blocks). We denote by \( \psi_j \) its (right) eigenvectors and expand the vector \( N^{-1}e = \sum_j c_j \psi_j \) in this eigenvector basis with coefficients \( c_j \). Inserting this expansion in equation (3), we obtain

\[
P = \sum_{j_{\neq 1}} c_j \psi_j + \sum_{\lambda_k \neq 1} \frac{1 - \alpha}{(1 - \alpha) + \alpha(1 - \lambda_j)} c_j \psi_j.
\]

In the case of non-trivial Jordan blocks, we may have in the second sum contributions \( \sim (1 - \alpha) / (1 - \alpha \lambda_j)^q \) with some integer \( q \) smaller or equal to the size of the Jordan block [14]. Suppose we have, for example, a Jordan block of dimension 2 with a principal vector \( \tilde{\psi}_j \) such that \( S \tilde{\psi}_j = \lambda_j \tilde{\psi}_j + \psi_j \), with \( \psi_j \) being the corresponding eigenvector. From this we obtain, for an arbitrary integer \( n \), the following condition on the 1-norm of these vectors: \( \| \tilde{\psi}_j \|_1 \geq \| \lambda_j \tilde{\psi}_j + \psi_j \|_1 \geq \| \lambda_j^n \tilde{\psi}_j \|_1 - n | \lambda_j |^{n-1} \| \psi_j \|_1 \) showing that one should have \( \psi_j = 0 \) if \( | \lambda_j | = 1 \). Even if \( | \lambda_j | < 1 \), this condition is hard to fulfil for all \( n \) if \( | \lambda_j | \) is close to 1. In general, the largest eigenvalues with modulus below 1 are not likely to belong to a non-trivial Jordan block; this is indeed well verified for our university networks since the largest core space eigenvalues are not degenerate.

Here equation (4) indicates that in the limit \( \alpha \to 1 \) PageRank converges to a particular linear combination of the eigenvectors with \( \lambda = 1 \), which are all localized in one of the subspaces. For a finite value of \( 1 - \alpha \) the scale of this convergence is set by the condition \( 1 - \alpha \ll 1 - \lambda^{(\text{core})} \sim 10^{-4} (10^{-5}) \) and the corrections for the contributions of the core space nodes are \( \sim (1 - \alpha) / (1 - \lambda^{(\text{core})}) \). In order to test this behavior we have numerically computed the PageRank vector for values \( 10^{-8} \leq 1 - \alpha \leq 0.15 \). For \( 1 - \alpha \approx 10^{-8} \), the usual power method (iterating the matrix \( G \) on an initial vector) is very slow and in many cases fails to converge with a reasonable precision. In order to get the PageRank vector in this regime, we use a combination of power and AMs that allows us to reach the precision \( \| P - G(\alpha) P \|_1 < 10^{-13} \); after each \( n_1 \) iteration with the power method, we use the resulting vector as an initial vector for an Arnoldi diagonalization, choosing an Arnoldi matrix size \( n_2 \); the resulting eigenvector for the largest eigenvalue is used as a new vector to which we apply the power method and so on until convergence by the condition \( \| P - G(\alpha) P \|_1 < 10^{-13} \) is reached. For the university network data of [13] in most cases the values \( n_1 = 10^4 \) and \( n_2 = 100 \) (\( n_3 = 500 \) for Cambridge 2006) provide convergence with \( \sim 10 \) iterations of the process (for \( 1 - \alpha = 10^{-8} \)). Additional details are given below.

3. Construction of invariant subspaces

In order to construct the invariant subspaces we use the following scheme which we implemented using an efficient computer program.

For each node \( j = 1, \ldots, N \) we determine iteratively a sequence of sets \( E_n \), with \( E_0 = \{ j \} \) and \( E_{n+1} \) containing the nodes \( k \) which can be reached by a non-zero matrix element \( \delta_{ik} \) from one of the nodes \( l \in E_n \). Depending on the initial node \( j \) there are two possibilities: (a) \( E_n \) increases with the iterations until it contains all nodes of the network, especially if one set \( E_n \) contains a dangling node connected (by construction of \( S \)) to all other nodes, or (b) \( E_n \) saturates at a limit set \( E_\infty \) of small or modest size \( d_j < N \). In the first case, we say that the node \( j \) belongs to the core space \( V_c \). In the second, the limit set defines a subspace \( V_j \) of dimension \( d_j \), which is invariant with respect to the applications of the matrix \( S \). We call the initial node \( j \) the root node of this subspace; subsequently, the members of \( E_\infty \) do not need to be tested themselves as initial nodes since they are already identified as subspace nodes. If during the iterations a former root node appears as a member in a new subspace one can absorb its subspace in the new one and this node loses its status as a root node. Furthermore, the
scheme is greatly simplified if during the iterations a dangling node or another node already identified as a core space node is reached. In this case one can immediately attribute the initial node \( j \) to the core space as well.

For practical reasons it may be useful to stop the iteration if the set \( E_n \) contains a macroscopic number of nodes larger than \( B N \), where \( B \) is some constant of order 1, and in this case to attribute the node \( j \) to the core space. This does not change the results provided that \( B N \) is above the maximal subspace dimensions. For the university networks we studied, the choice \( B \geq 0.1 \) turned out to be sufficient since there is always a considerable number of dangling nodes.

In this way, we obtain a subdivision of the nodes of the network in \( N_c \) core space nodes (typically 70–80\% of \( N \)) and \( N_s \) subspace nodes belonging to at least one of the invariant subspaces \( V_j \). However, at this point it is still possible, even likely, that two subspaces have common members. Therefore, in a second step we merge all subspace with common members and choose arbitrarily one of the root nodes as the ‘root node’ of the new bigger subspace, which is of course also invariant with respect to \( S \).

We can also mention that most of the subspaces contain one or more ‘zero nodes’ (of first order) with outgoing links to the subspace but no incoming links from the same or other subspaces (but they may have incoming links from core space nodes as every subspace node). These nodes correspond to complete zero lines in the corresponding diagonal block for this subspace in the matrix \( S \) and therefore they produce a trivial eigenvalue zero. Furthermore, there are also zero nodes of higher order \( j (\geq 2) \) which have incoming subspace links only from other zero nodes of order \( j - 1 \) resulting in a non-trivial Jordan block structure with eigenvalue zero. In other words, when one applies the matrix \( S \) to a vector with non-zero elements on all nodes of one subspace, one eliminates successively the zero nodes of orders 1, 2, 3, . . . and finally the resulting vector will have non-zero values only for the other ‘non-zero nodes’. Due to this any subspace eigenvector of \( S \) with an eigenvalue different from zero (and in particular the PageRank vector) cannot have any contribution from a zero node.

In a third step of our scheme we therefore determined the zero nodes (of all orders) and the reduced subspaces without these zero nodes. The results of the distribution of subspace dimensions are discussed in section 6 (see the left panel of figure 7). The distribution is essentially unchanged if we use the reduced subspaces since the number of zero nodes is below 10\% of \( N_s \) for most of the universities. Only for the matrix \( S^* \) of Wikipedia, we have about 45\% of zero nodes, that reduces the value of \( N_s \) from 21 198 to 11 625.

Once the invariant subspaces of \( S \) are known it is quite easy to obtain numerically the exact eigenvalues of the subspaces, including the exact degeneracies. Thus, using the AM we determine the largest remaining eigenvalues of the core-projected block \( S_{cc} \). In figure 2, the complex spectra of subspace and core space eigenvalues of \( S \) and \( S^* \) are shown for the two networks of Cambridge 2006 and Oxford 2006 as well as the fraction of eigenvalues with modulus larger than \( |\lambda| \), indicating a macroscopic fraction of about 2\% of eigenvalues with \( |\lambda| = 1 \).

In table 1, we summarize the main quantities of the networks studied: network size \( N \), number of network links \( L \), number of subspace nodes \( N_s \) and average subspace dimension \( \langle d \rangle \) for the university networks considered in figure 4 and the matrix \( S^* \) of Wikipedia.

4. Numerical method of PageRank computation

Let us now discuss the numerical techniques that we developed in order to compute PageRank. The standard method to determine PageRank is the power method [1, 2]. However, this method fails to converge at a sufficient rate in the limit \( \alpha \to 1 \) and therefore we need a more refined
method. First, we briefly discuss how the power method works and then how it can be modified to improve the convergence.

Let \( P_0 \) be an initial vector which is more or less a good approximation of PageRank. Typically, one may choose \( P_0 = e/N \), where \( e = (1, \ldots, 1)^T \). For simplicity, let us also suppose that the matrix \( G(\alpha) \) can be diagonalized. The eventual existence of principal vectors and non-trivial Jordan blocks does not change the essential argument and creates only minor technical complications. The initial vector can be developed in the eigenvector basis of \( G(\alpha) \) as

\[
P_0 = P + \sum_{j \geq 2} C_j \phi_j,
\]

where \( P = \phi_1 \) is the exact PageRank, which is for \( \alpha < 1 \) the only (right) eigenvector of \( G(\alpha) \) with eigenvalue 1. Here, \( \phi_j \) denote for \( j \geq 2 \) other (right) eigenvectors with eigenvalues \( \lambda_j \) such that \( |\lambda_j| < \alpha \) and \( C_j \) are the expansion coefficients. We note that \( e^T \phi_j = 0 \) for \( j \geq 2 \), since \( e \) is the first left eigenvector bi-orthogonal to other right eigenvectors, and for sufficiently small \( C_j \) the expansion coefficient of \( P \) in \( P_0 \) is exactly 1, if \( P_0 \) and \( P \) are both normalized by the 1-norm. Iterating the initial vector by \( G(\alpha) \) one obtains after \( i \) iterations:

\[
P_i = G(\alpha) P_0 = P + \sum_{j \geq 2} C_j \lambda_j^i \phi_j.
\]

Therefore, the convergence of the power method goes with \( \sim \lambda_2^i \), where \( \lambda_2 \) is the second largest eigenvalue. In the case of realistic networks, \( \lambda_2 \) is typically highly degenerate and equal to \( \alpha \). Typically, there are also complex eigenvalues with non-trivial phases where only the modulus is equal to \( \alpha \) and whose contributions imply the same speed of convergence. In the limit \( \alpha \to 1 \), the power method becomes highly ineffective due to these eigenvalues. For example, to verify the condition \( \alpha^i < \epsilon \) one needs \( i > 3 \times 10^6 \) iterations for \( 1 - \alpha = 10^{-8} \) and \( \epsilon = 10^{-13} \).

In order to obtain a faster convergence we propose a different method based on the AM [17–19]. The idea of the AM is to diagonalize the matrix representation of \( G(\alpha) \) on the Krylov space generated by \( P_0, P_1, \ldots, P_{n_A-1} \), where \( n_A \) is the Arnoldi dimension. For reasons of

### Table 1. Network parameters.

<table>
<thead>
<tr>
<th></th>
<th>( N )</th>
<th>( L )</th>
<th>( N_s )</th>
<th>( \langle d \rangle )</th>
</tr>
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<tr>
<td>Cambridge 2002</td>
<td>140,256</td>
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</tr>
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</tr>
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<td>Oxford 2005</td>
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<td>135,193</td>
<td>36,014</td>
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</tr>
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<td>Wikipedia (S^*)</td>
<td>3282,257</td>
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<td>21,198</td>
<td>3.96</td>
</tr>
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</table>
Figure 3. Convergence of the combined power–AM to calculate the PageRank for $1 - \alpha = 10^{-8}$. Shown is the quantity $\|P_i - G(\alpha)P_i\|_1$ to characterize the quality of the approximate PageRank $P_i$ versus the number of iterations $i$ made by the power method. The green line at $10^{-13}$ shows the line below which convergence is reached. The upper-left panel shows the data for Oxford 2006 with $n_A = 100$ and $n_i = 10000$. The upper-right panel corresponds to Cambridge 2006 with $n_A = 500$ and $n_i = 50000$ (red dots) or $n_i = 10000$ (blue crosses). The lower-left panel shows the case of Cambridge 2003 with $n_A = 500$ and $n_i = 50000$, for which it is particularly hard to obtain convergence. The lower-right panel compares for the case of Cambridge 2002 the choice $n_A = 500$ and $n_i = 50000$ (red dots) with $n_A = 500$ and $n_i$ determined by the criterion that the relative change of $\|P_i - G(\alpha)P_i\|_1$ between $i$ and $i + 100$ is less than $10^{-4}$.

For numerical stability, one constructs by Gram–Schmidt orthogonalization an orthogonal basis of the Krylov space, which also provides the matrix elements of the matrix representation of $G(\alpha)$ in this basis. In the particular case, where the number of non-vanishing coefficients $C_j$ in equation (5) is not too large, the AM should even provide the exact PageRank, obtained as the eigenvector of the largest eigenvalue on the Krylov space, and exactly suppress the other eigenvector contributions provided that the dimension $n_A$ of the Krylov space is sufficiently large to contain all other eigenvectors contributing in equation (5). Of course, in reality the number of non-vanishing coefficients $C_j$ is not small, but one can use a strategy which consists first of applying the power method with $n_i$ iterations to reduce the contributions of the large majority of eigenvectors whose eigenvalues have a reasonable gap from the unit circle, and in a second step the AM to eliminate the remaining ‘hard’ eigenvectors whose eigenvalues are too close to the unit circle for the power method. Even though this strategy does not provide the numerical ‘exact’ PageRank, it considerably improves the quality of the initial vector as an approximation of the PageRank, and repeating this scheme with the new approximation as an initial vector (with suitable values for $n_i$ and $n_A$) one obtains an algorithm which efficiently computes the PageRank to a high precision as can be seen in figure 3. To measure the quality of the PageRank vector we compute the quantity $\|P_i - G(\alpha)P_i\|_1$ and iterate our algorithm.
until this is below $10^{-13}$. Using this convergence criterion for most university networks from the database [13], the choice of $n_l = 10000$ and $n_A = 100$ provides convergence typically with about ten steps of this procedure.

In figure 3, we show the convergence of this method for several university network cases with the initial vector $P_0 = e/N$ and $1 - \alpha = 10^{-8}$. The typical situation is shown in the upper-left panel for Oxford 2006. During the first power method cycle there is nearly no improvement in the quality of PageRank. This is completely normal in view of the small value of $1 - \alpha$. However, the first Arnoldi step improves the quality by four orders of magnitude. The subsequent power method iterations of the second cycle continue to improve the convergence quality but their effect saturates after a certain number of iterations. The second Arnoldi step seems at first to reduce the PageRank quality, but after a few power method iterations (in the third cycle) this loss is compensated for and its quality improves until the next saturation and the next Arnoldi step. In total, this provides a nice exponential convergence and after seven Arnoldi steps and 75 000 power method iterations the convergence is reached with very high accuracy. Apparently, the AM is efficient at reducing the coefficients $C_j$ associated with the eigenvectors with eigenvalues close to the circle of radius $\alpha$, but the approximation due to the truncation of the Arnoldi matrix to the Krylov space at $n_A$ creates some artificial contributions from other eigenvectors whose eigenvalues have a quite big gap from 1 and whose contributions may be eliminated by a relatively modest number of power method iterations.

The number $n_A = 100$ appears very modest if compared to the degeneracy of the second eigenvalue $\lambda_2 = \alpha$, which may easily be about 1000–2000. Fortunately, the exact degeneracy of the eigenvalues close to or on the circle of radius $\alpha$ does not really count, since for each degenerate eigenspace only one particular eigenvector appears in the expansions (5) and (6), which can be relatively easily ‘eliminated’ by an Arnoldi step with the modest value of $n_A$. However, the total number of different eigenvalues (with different phases) on the circle of radius $\alpha$ is important and if this number is too big the convergence of the method is more difficult. This is actually the case for the university networks of Cambridge as can be seen in the upper-left panel of figure 2, where the subspace eigenvalues of $S$ for Cambridge 2006 nearly fill out the unit circle and indeed for these cases we have to increase the Arnoldi dimension to $n_A = 500$ in order to achieve a reasonable convergence. In the upper-right panel of figure 3, we show the PageRank convergence for Cambridge 2006 with $n_A = 500$ and two choices of $n_l = 10000$ and $n_l = 50000$. For this particular example, the first choice is more efficient, but this is not systematic and is different for other cases. We also see that by increasing the value of $n_l$ the convergence is not immediately improved (the PageRank error does not really decrease during the power method cycle), but the positive effect of the next Arnoldi step will be much better, because the bigger number of power method iterations allows us to reduce the effect of more eigenvectors in the eigenvector expansion of $P_i$. In the lower-left panel of figure 3, we show the case of Cambridge 2003 which is particularly hard to converge and requires 28 Arnoldi steps with $n_l = 50000$ and $n_A = 500$. Actually, the choice $n_l = 10000$ (not shown in the figure) is less efficient with nearly doubled power method iterations and about 235 Arnoldi steps. In the lower-right panel, we consider the case of Cambridge 2002 where we need three Arnoldi steps for the parameters $n_A = 500$ and $n_l = 50000$. For this case, we also tried a different strategy which consists of using a variable value of $n_l$ determined by the criterion that when the relative change of $\|P_i - G(\alpha)P_i\|_1$ from $i$ to $i + 100$ is below $10^{-4}$ we perform one Arnoldi step but at the latest after 50 000 power method iterations for each cycle. For this example, this strategy does not really pay off since the overall number of power method iterations is even slightly increased and additionally we have 11 instead of 3 quite expensive Arnoldi steps. However, this approach has the advantage that one does not need to search in advance for which $n_l$ parameters work best. In practical calculations when calculating the
PageRank for a continuous set of values of $\alpha$ one may also improve convergence simply by using PageRank at a certain value of $\alpha$ as the initial vector for the next value $\alpha + \Delta \alpha$. However, in figure 3, we simply used the same initial vector $P_0 = e/N$ for all cases in order to study the effectiveness of the method.

The computational costs of the method are increased quite strongly with $n_A$, since the Arnoldi steps correspond to $n_A^2 N + n_A L$ elementary operations (with $L$ being the number of links in the network) due to the Gram–Schmidt orthogonalization scheme and $n_A$ applications of $G(\alpha)$ on a vector, while one step with the power method costs $L$ operations. Therefore, one Arnoldi step corresponds to $\sim (n_A^2 (N/L) + n_A)$ steps of the power method, which is $\sim 1000$ ($\sim 25000$) for $n_A = 100$ ($n_A = 500$) and $L/N \sim 10$ (typical value for most university networks of [13]).

We mention that the method does not converge if we use only Arnoldi steps without intermediate power method iterations (i.e. $n_i = 0$). Golub et al [18] have suggested a different variant of the AM, where they determine the improved vector not as the eigenvector of the largest eigenvalue of the truncated squared Arnoldi matrix but as the vector corresponding to the smallest singular value of a matrix obtained from the full non-truncated rectangular Arnoldi matrix. We have also implemented this variant and confirmed for some examples that convergence by simply repeating these ‘refined’ Arnoldi steps is possible, but in general the computational time for convergence is much longer if compared to our method. We have also tested the combination of power method and refined Arnoldi steps and find that this approach is in general comparable to our first method, with a slight advantage for one or the other method depending on the network that is studied.

5. Projected power method for the case of a small core space eigenvalue gap

The behavior of PageRank in the limit $\alpha \to 1$ is determined by the core space eigenvalue gap $1 - \lambda_1^{(\text{core})}$, where $\lambda_1^{(\text{core})} < 1$ is the maximal eigenvalue of the core space projected matrix $S_{cc}$ (see equation (2)). This eigenvalue and its eigenvector $\psi_1^{(\text{core})}$ can in principle be determined by the AM applied to $S_{cc}$. However, for certain university networks of [13], Cambridge 2002, 2003, 2005 and Leeds 2006, we find that $\lambda_1^{(\text{core})}$ is extremely close to 1. Since the results of the AM are obtained by standard double precision arithmetic operations, it gives a largest core space eigenvalue which is numerically equal to 1 for these cases (up to an error of order $\sim 10^{-14}$). This is not sufficient to provide an accurate value for the gap $1 - \lambda_1^{(\text{core})}$ apart from the information that this gap is below $10^{-14}$.

To overcome this computational problem we note that $\lambda_1^{(\text{core})}$ and $\psi_1^{(\text{core})}$ can also be numerically determined by a different algorithm. The main idea is to apply the power method, eventually with intermediate Arnoldi steps to accelerate convergence, as described in the previous section, to the matrix $S_{cc}$ which first provides the eigenvector $\psi_1^{(\text{core})}$ and once the eigenvector is known, its eigenvalue is simply obtained as $\lambda_1^{(\text{core})} = \|S_{cc} \psi_1^{(\text{core})}\|_1$ if the normalization is given by $\|\psi_1^{(\text{core})}\|_1 = 1$. In this section, it is understood that $S_{cc}$ is the matrix $S$ multiplied left and right by the projection operator on the core space (and similarly for $S_{sc}$ and $S_{ss}$). We have implemented this method and verified for some examples that it indeed provides the same results as the AM. Actually, it may even be more efficient than the direct AM which may require a quite large Arnoldi dimension for a reliable first eigenvector. However, at this stage this approach also suffers from the same problem concerning the numerical inaccuracy for the cases of a very small core space gap.

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Fortunately, the approach can be modified to be more accurate. To see this, we use equation (2) and the fact that the columns of $S$ are sum normalized which implies \[ \| S_{\text{sc}} \psi_1^{(\text{core})} \|_1 + \| S_{\text{core}} \psi_1^{(\text{core})} \|_1 = 1 \] and therefore
\[
1 - \lambda_1^{(\text{core})} = \| S_{\text{sc}} \psi_1^{(\text{core})} \|_1 = \sum_{j \in V_{\text{SP}}} \sum_{l \in V_{\text{core}}} S_{jl} \psi_1^{(\text{core})}(l),
\]
where $V_{\text{SP}}$ denotes the set of subspace nodes and $V_{\text{core}}$ is the set of core space nodes (note that $\psi_1^{(\text{core})}(l) \geq 0$). This expression, which relates the core space gap to the sum of all transitions from a core space node to a subspace node (the ‘escape probability’ from the core space), is the key to determining the gap accurately.

First, we note that a numerically small core space gap (below $10^{-14}$) implies that the eigenvector components $\psi_1^{(\text{core})}(l)$ are also numerically small for the core space nodes $l$ which are directly connected to a subspace node $j$ by a non-vanishing matrix element $S_{jl} > 0$. To be more precise, it turns out that for this situation the eigenvector $\psi_1^{(\text{core})}$ is strongly localized on a modest number of about 100 nodes out of $10^5$ nodes in total and numerically small on the other nodes. Obviously, the nodes inside the small localization domain are not directly connected to a subspace node (by the matrix $S$). The important point is that we can also determine the eigenvector accurately for the very small tails (below $10^{-15}$) by the pure power method (without intermediate Arnoldi steps) if we choose as an initial vector a vector localized at the maximum node. The reason is that the non-vanishing matrix elements $S_{jl}$ connect only sites for which the eigenvector components are comparable to the order of magnitude. Therefore, numerical round-off errors are minimized despite the fact that the resulting vector will contain components with a size ratio significantly above $10^{15}$ between maximal and minimal components. This is similar to certain localization problems in disordered quantum systems where it is in certain cases possible to numerically determine exponentially small tails of localized eigenvectors even if these tails are far below $10^{-15}$.

Therefore, in practice, we implement the following projected power method.

(i) Determine the first approximation of $\psi_1^{(\text{core})}$ by the direct AM, which is accurate inside the localization domain but numerically incorrect for the very small tails on the nodes outside the localization domain. From these data we determine the node $l_{\text{max}}$ at which $\psi_1^{(\text{core})}(l_{\text{max}})$ is maximal.

(ii) Choose as an initial vector (on the full space including core space and subspace nodes) the vector localized on the node $l_{\text{max}}$, i.e. $\psi(l) = \delta_{l,l_{\text{max}}}$.

(iii) Make a copy of the vector: $\psi_{\text{old}} = \psi$.

(iv) Apply the matrix $S$ to the actual vector: $\psi = S \psi$, which produces artificially non-zero values $\psi(j)$ on certain subspace nodes $j$.

(v) According to equation (7) compute the quantity $\sum_{j \in V_{\text{SP}}} \psi(j)$ as an approximation of the gap $1 - \lambda_1^{(\text{core})}$.

(vi) Project the vector on the core space: $\psi(j) = 0$ for all subspace nodes $j \in V_{\text{SP}}$.

(vii) Normalize the vector by the 1-norm: $\psi = \psi / \| \psi \|_1$.

(viii) Stop the iteration if \[ \| \psi - \psi_{\text{old}} \|_1 < \varepsilon_1 \] and \[ \max_{j \in V_{\text{core}}} | \psi(l) - \psi_{\text{old}}(l) | / | \psi(l) | < \varepsilon_2. \] Otherwise go back to step (iii).

This algorithm produces an accurate vector very rapidly on the localization domain (less than 100 iterations), but in order to obtain an accurate value of the gap by equation (7) the eigenvector needs to be accurate with a small relative error also in the very small tails and therefore the convergence criterion has to take into account the relative error for each component. We have chosen $\varepsilon_1 = 10^{-13}$ and $\varepsilon_2 = 10^{-6}$ which provides convergence with $10^6$ iterations for the cases of Cambridge 2002, 2003 and 2005. In the case of Leeds 2006, we
even obtain convergence with $\varepsilon_1 = \varepsilon_2 = 10^{-15}$ after $2 \times 10^5$ iterations. For the particular case of Cambridge 2004 (where the gap $\sim 10^{-9}$ is still ‘accessible’ by the AM) the convergence is more difficult and we have stopped the iteration at $\varepsilon_1 = 10^{-12}$ and $\varepsilon_2 = 3.2 \times 10^{-6}$.

The choice of the initial vector localized at the maximum node is very important for the speed of the convergence. If we choose the delocalized vector $e/N$ as the initial vector, it is virtually impossible to obtain convergence in the tails which stay at ‘large’ values $\sim 10^{-8}$, unless we use intermediate Arnoldi steps, but this destroys the fine structure of the tails below $10^{-15}$ which is crucial to determine the very small gap.

Using the above algorithm we obtain the gap values given in table 2. In figure 4 we compare these gap values to the other university networks, which we found by the AM larger gaps $1 - \lambda_1^{(\text{core})} > 10^{-7}$.

In figure 5, we show the eigenvectors $\psi_i^{(\text{core})}$ obtained by the projected power method versus their rank index $K^{(\text{core})}$ defined by the ordering of the components of these vectors. We can clearly identify the exponential localization on 40 nodes for Leeds 2006 or 110 nodes for Cambridge 2002, 2003 and 2005, with values below $10^{-14}$ (Leeds 2006) or $10^{-18}$ (Cambridge 2002, 2003 and 2005). The case of Cambridge 2004 with a quite large gap $\sim 10^{-9}$ provides at first the same exponential localization as the other three cases of Cambridge but after 50 nodes goes over to a tail in the range of $10^{-8}$ to $10^{-10}$. In all cases the range of values of the small tail is in qualitative agreement with the gap values in the table 2 and expression (7).
When the iteration with the matrix $S$ starts at the maximal node, the vector diffuses first quite slowly inside the localization domain for a considerable number of iterations (46 for Leeds 2006 and 35 for Cambridge 2002, 2003 and 2005) until it reaches a dangling node, at which point the diffusion immediately extends to the full network since the dangling node is artificially connected to all nodes. However, at this point the probability of the amplitude is already extremely small. Therefore, the initial node belongs technically to the core space (since it is ‘connected’ to all other nodes), but practically it defines a quasi-subspace (since the probability of leaving the localization domain is very small $\sim 10^{-19}$ or $\sim 10^{-17}$). At $1 - \alpha = 10^{-8}$, which is much larger than the gap, this quasi-subspace also contributes to the PageRank in the same way as the exact invariant subspaces. This provides somehow a slight increase in the effective value of $N_s$, but it does not change the overall picture as described in section 2.

Figure 5 also shows that apparently the particular network structure responsible for this quasi-subspace behavior is identical for the three cases: Cambridge 2002, 2003 and 2005. For Cambridge 2004, this structure also exists but there is one additional dangling node which is reached at an earlier point of the initial slow diffusion providing delocalization on a scale $\sim 10^{-10}$–$10^{-8}$. For the case of Cambridge 2006 with a ‘large’ gap $\sim 10^{-4}$ this structure seems to be completely destroyed but this may be due to one single modified matrix element $S_{ji}$ if compared to the networks of previous years.

6. Universal properties of PageRank and subspace distribution

Using the powerful numerical methods described above, we turn to the analysis of universal properties of PageRank. Figure 6 clearly confirms the theoretical picture given in section 2 of the limit behavior for PageRank at $\alpha \to 1$. In particular, one can clearly identify the limit where it is localized in the invariant subspaces\(^{1}\) with only small corrections $\sim (1 - \alpha)$ at the core space nodes. We also determine the eigenvector of the largest core space eigenvalue $\lambda_1^{(\text{core})}$ of the projected matrix $S_{ct}$. In the lower panels of figure 6, we compare PageRank at $1 - \alpha = 10^{-8}$ with this vector (normalized by the 1-norm) multiplied by $(1 - \alpha)/(1 - \lambda_1^{(\text{core})})$.

\(^{1}\) In certain invariant subspaces, there are nodes with no ingoing links from the same subspace, which do not contribute to PageRank for $\alpha \to 1$. Except for Wikipedia (CheiRank), they are very few in our data and their effect is not visible in the figures.
Figure 6. Left panels (right panels) correspond to Cambridge 2006 (Oxford 2006). Top row: PageRank $P(K)$ for $1 - \alpha = 0.1$, $10^{-3}$, $10^{-5}$, $10^{-7}$. Numerical precision is such that $\|P - G(\alpha)P\|_1 < 10^{-13}$. Bottom row: $P(K)$ at $1 - \alpha = 10^{-8}$. Blue crosses correspond to the eigenvector of the largest core space eigenvalue $\lambda_1^{(\text{core})} = 0.999 \, 874 \, 353 \, 718$ (0.999 \, 982 \, 435 \, 081) multiplied by $(1 - \alpha)/(1 - \lambda_1^{(\text{core})})$. The arrow indicates the first position where a site of the core space $V_c$ contributes to the rank index; all sites at its left are in an invariant subspace. The Inset shows the residual weight $w(\alpha)$ with $w(\alpha) = \sum_{j \in V_c} P^\alpha(j)$ of the core space $V_c$ in PageRank and the difference $f(\alpha) - f(1)$ versus $1 - \alpha$, where $f(\alpha)$ is the PageRank fidelity with respect to $\alpha = 0.85$, i.e., $f(\alpha) = \langle P(\alpha) \rangle_{\text{PageRank}} \approx f(\alpha) = \langle P(\alpha) \Vert_{1.0} \Vert_{2}$. Note that $\|P^\alpha\|_2 \neq 1$ since the PageRank is normalized through the 1-norm: $\|P^\alpha\|_1 = 1$. The limiting value $f(1) = 0.188 \, 400 \, 463 \, 202$ (0.984 \, 882 \, 016) is obtained from linear extrapolation from the data with smallest values of $1 - \alpha$ which we verified to be exact up to machine precision.

We observe that except for a very small number of particular nodes, this vector approximates quite well the core space correction of PageRank even though the corrections due to the second term in (4) are more complicated with contributions from many eigenvectors. In the insets, we also show the fidelity of PageRank, which decays from 1 at $1 - \alpha = 0.1$ to about 0.188 (0.097) at $1 - \alpha = 10^{-8}$, and the residual weight $w(\alpha) = \sum_{j \in V_c} P^\alpha(j)$ of the core space $V_c$ in PageRank, which behaves as $w(\alpha) \approx 221.12 \, (1 - \alpha) \approx 607.12 \, (1 - \alpha)$ for $1 - \alpha < 10^{-5}$.

As mentioned in the previous section, we also determine the subspace structure and the PageRank at $1 - \alpha = 10^{-8}$ for other university networks available in [13] and for the matrix $S^*$ of Wikipedia [12] with $N = 3282 \, 257$ and $N_c = 21 \, 198$ (it turns out that the matrix $S$ for Wikipedia provides only very few small size subspaces with no reliable statistics). A striking feature is that the distribution of subpace dimensions $d_j$ is universal for all networks considered (figure 7 left panel). The fraction of subspaces with dimensions larger than $d$ is well described by the power law $F(x) = (1 + x/(b - 1))^{-b}$ with the dimensionless variable $x = d/\langle d \rangle$, where $\langle d \rangle$ is the average subspace dimension. The fit of all cases gives $b = 1.608 \pm 0.009 \approx 1.5$. 
It is interesting to note that the value of $b$ is close to the exponent of Poincaré recurrences in dynamical systems [19]. Possible links with the percolation on directed networks (see e.g. [20]) are still to be elucidated. The rescaled PageRank $P_{\text{N}}$ (or CheiRank $P^*_{\text{N}}$ for the case of Wikipedia) takes a universal form with a power law $P \sim K^{-c}$ for $K < N$ with an exponent $c = 0.698 \pm 0.005 \approx 1/b = 2/3$ and $P \sim (1 - \alpha)$ close to zero for $K > N$ (see the right panel of figure 7). For certain university networks, Cambridge 2002, 2003 and 2005 and Leeds 2006, there is a specific complication. Indeed, the AM (with $n_A = 10,000$) provides a maximal core space eigenvalue $\lambda_1(\text{core})$ numerically equal to 1, which should not be possible. A more careful evaluation by a different algorithm, based on the power method (iterating $S$ with a subsequent core space projection) and measuring the loss of probability at each iteration, shows that this eigenvalue is indeed very close but still smaller than 1. For the three cases of Cambridge, we find $1 - \lambda_1(\text{core}) \approx 4.0 \times 10^{-17}$ and for Leeds 2006: $1 - \lambda_1(\text{core}) \approx 3.1 \times 10^{-20}$ (see details in section 5). The corresponding eigenvectors are exponentially localized on a small number of nodes (about 110 nodes for Cambridge and 40 nodes for Leeds 2006) being very small ($<10^{-14}$ for Cambridge and $<10^{-18}$ for Leeds 2006) on other nodes. These quasi-subspaces with a small number of nodes belong technically to the core space, since they are eventually linked to a dangling node, but when starting from the maximal node of these eigenvectors, it takes a considerable number of iterations with a strong reduction of probability to reach the dangling node. Since their eigenvalue is very close to 1, these quasi-subspaces also contribute to PageRank at $1 - \alpha = 10^{-8}$ in the same way as the exact invariant subspaces. However, since the size of these quasi-subspaces is small they do not change the overall picture and we can still identify a region of large PageRank with $N_{\text{subspace}}$ or quasi-subspace nodes and vanishing PageRank for the other core space nodes. For most of the other universities and also the matrix $S^*$ of Wikipedia, we have $1 - \lambda_1(\text{core}) \gg 10^{-6}$ (and $1 - \lambda_1(\text{core}) \sim 10^{-9}$ for Cambridge 2004).
7. Discussion

Our results show that for $\alpha \rightarrow 1$, the PageRank vector converges to a universal distribution $P \sim 1/K^c$ determined by the invariant subspaces (with $c \approx 2/3$). The fraction of nodes which belong to these subspaces varies greatly depending on the network, but the distribution of the subspace sizes is described by a universal function $F(x) = 1/(1 + 2x)^{3/2}$ that reminds the properties of critical percolation clusters. When $\alpha$ decreases from 1, PageRank undergoes a transition which allows us to properly rank all nodes. This process is controlled by the largest eigenvalues of the core matrix $S_{cc}$, which are strictly below 1 but can be extremely close to it. Their distance from 1 sets the scale of the transition, and the associated eigenvectors of $S_{cc}$ control the new ranking of nodes. Although at $\alpha = 1$ the eigenspace for eigenvalue 1 can be very large, for $\alpha$ sufficiently larger in norm than the eigenvalues of $S_{cc}$, PageRank remains fixed when $\alpha \rightarrow 1$, in a way reminiscent of degenerate perturbation theory in quantum mechanics. Our highly accurate numerical method based on alternations of Arnoldi iterations and direct iterations of the G matrix enables us to determine the correct PageRank even where the scale of this transition is extremely small ($1 - \lambda_{\text{core}}^1 \approx 10^{-20}$) and the matrix size is very large (up to several millions). The very slow convergence of the power method in this regime is reminiscent of very long equilibration times in certain physical systems (e.g. spin glasses), and thus Arnoldi iterations can be viewed as a certain kind of a simulated annealing process which enables us to select the correct eigenvector among many others with very close eigenvalues. PageRank in this regime of $\alpha \rightarrow 1$ shows universal properties different from the usual PageRank at $\alpha \approx 0.85$, with a different statistical distribution. This can be used to refine search and ranking in complex networks and hidden communities extraction.

Finally, we note that usually in quantum physics one deals with unitary matrices with a real spectrum. In the case of directed Markov chains, we naturally obtain a complex spectrum. In physical quantum systems a complex spectrum appears in positive quantum maps [21], problems of decoherence and quantum measurements [22] and random matrix theory of quantum chaotic scattering [23]. Thus we hope that a cross-fertilization between complex matrices and directed network will highlight in a new way the properties of complex networks.

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References