

Universal Emergence of PageRank

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The PageRank algorithm enables 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, we determine numerically and analytically the universal features of PageRank vector at its emergence when $\alpha \rightarrow 1$. The whole network can be divided into a core part and a group of invariant subspaces. For $\alpha \rightarrow 1$ the 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 $\alpha \rightarrow 1$ is controlled by eigenvalues of the core part of the Google matrix which are exponentially close to unity leading to large relaxation times as for example in spin glasses.

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

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

where the matrix \mathbf{S} is obtained by normalizing to unity all columns of an adjacency matrix \mathbf{A} , 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 $\mathbf{e} = (1, \dots, 1)^T$ is the unit column vector and \mathbf{e}^T is its transposition. The damping parameter α in the WWW context describes the probability $(1 - \alpha)$ to jump to any node for a random surfer. For WWW the Google search uses $\alpha \approx 0.85$ [2].

The matrix \mathbf{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 \mathbf{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 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 $P(i) \propto 1/K^\beta(i)$ with $\beta = 1/(\mu - 1) \approx 0.9$ at $\alpha \sim 0.85$. The PageRank performs ranking which in average is proportional to the number of ingoing links [2, 10], putting at the top the most known and popular nodes. However, in

certain networks outgoing links also play an important role. Recently, on the examples of the procedure call network of Linux Kernel software [11] and the Wikipedia articles 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 $(A_{ij}) \rightarrow \mathbf{A}^T = (A_{ji})$ and constructing from it a reverse Google matrix \mathbf{G}^* according to relation (1) at the same α . The eigenvector of \mathbf{G}^* with eigenvalue $\lambda = 1$ gives then a new PageRank $P^*(i)$ with ranking index $K^*(i)$, which was named CheiRank [12]. It rates nodes in average proportionally to the number of outgoing links highlighting their communicative properties [11, 12]. For WWW one finds $\mu \approx 2.7$ [9] so that the decay of CheiRank $P^* \propto 1/K^{*\beta}$ is characterized by a slower decay exponent $\beta \approx 0.6$ compared to PageRank. In Fig. 1, we show PageRank and CheiRank distributions for the WWW networks of the Universities of Cambridge and Oxford (2006), obtained from the database [13].

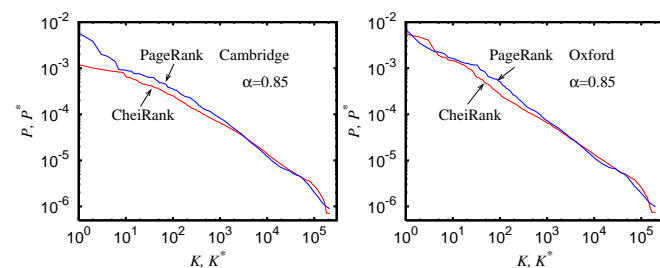


FIG. 1: (Color online) PageRank P and CheiRank P^* versus the corresponding rank indexes K and K^* for the WWW networks of Cambridge 2006 (left panel) and Oxford 2006 (right panel); here $N = 212710$ (200823) and the number of links is $L = 2015265$ (1831542) for Cambridge (Oxford).

Due to importance of PageRank for information retrieval and ranking of various directed networks [7] it is important to understand how it is affected by the variation of the damping parameter α . In the limit $\alpha \rightarrow 1$ the PageRank is determined by the eigenvectors of the highly degenerate eigenvalue 1 [14]. These eigenvectors

correspond by definition to invariant subspaces through the matrix \mathbf{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 study in detail the universal behavior of the PageRank at $\alpha \rightarrow 1$ related to the spectrum of \mathbf{G} , using an optimized Arnoldi algorithm.

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 applications of the matrix \mathbf{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 \mathbf{S} . This scheme, which can be efficiently implemented in 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,

$$\mathbf{S} = \begin{pmatrix} \mathbf{S}_{ss} & \mathbf{S}_{sc} \\ 0 & \mathbf{S}_{cc} \end{pmatrix} \quad (2)$$

where the subspace-subspace block \mathbf{S}_{ss} is actually composed of many diagonal blocks for each of the invariant subspaces. Each of these blocks correspond to a column sum normalized matrix of the same type as \mathbf{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 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 \mathbf{S} can be obtained from the projected core block \mathbf{S}_{cc} which is not column sum normalized (due to non-zero matrix elements in the block \mathbf{S}_{sc}) and has therefore eigenvalues strictly inside the unit circle $|\lambda_j^{(\text{core})}| < 1$. We have applied the Arnoldi method (AM) [16–18] with Arnoldi dimension $n_A = 20000$ to determine the largest eigenvalues of \mathbf{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 $\lambda_1^{(\text{core})} = 0.999874353718$ (0.999982435081) 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 \mathbf{S}_{cc} and not to the full matrix \mathbf{S} (see more detail in Appendix). 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.

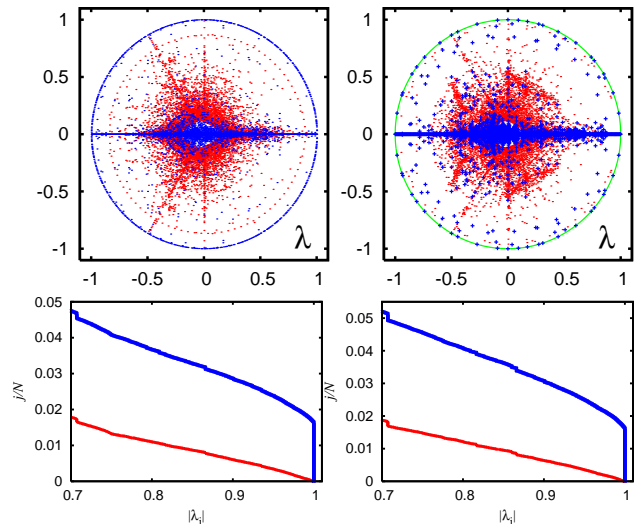


FIG. 2: (Color online) Left panels (right panels) correspond to Cambridge 2006 (Oxford 2006). *Top row*: Subspace eigenvalues of the matrix \mathbf{S} (blue dots or crosses) and core space eigenvalues (red dots) in λ -plane (green curve shows unit circle). Here $N_s = 48239$ (30579), more details are given in Appendix. There are 1543 (1889) invariant subspaces, with maximal dimension 4656 (1545) and the sum of all subspace dimensions is $N_s = 48239$ (30579). The core space eigenvalues are obtained from the Arnoldi method applied to the block S_{cc} with Arnoldi dimension 20000 and are numerically accurate for $|\lambda| \geq 0.7$. *Bottom row*: Fraction j/N of eigenvalues with $|\lambda| > |\lambda_j|$ for the core space eigenvalues (red bottom curve) and all eigenvalues (blue top curve) from top row data. The number of eigenvalues with $|\lambda_j| = 1$ is 3508 (3275) of which 1832 (2360) are at $\lambda_j = 1$; it larger than the number of invariant subspaces which have each at least one unit eigenvalue.

In Fig. 2 we present the spectra of subspace and core space eigenvalues in the complex plane λ 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

$$P = (1 - \alpha) (\mathbf{1} - \alpha \mathbf{S})^{-1} \mathbf{e}/N. \quad (3)$$

Let us first assume that \mathbf{S} is diagonalizable (with no non-trivial Jordan blocks). We denote by ψ_j its (right) eigenvectors and expand the vector $N^{-1} \mathbf{e} = \sum_j c_j \psi_j$ in this

eigenvector basis with coefficients c_j . Inserting this expansion in Eq. (3), we obtain

$$P = \sum_{\lambda_j=1} c_j \psi_j + \sum_{\lambda_j \neq 1} \frac{1-\alpha}{(1-\alpha) + \alpha(1-\lambda_j)} c_j \psi_j. \quad (4)$$

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 $\mathbf{S}\tilde{\psi}_j = \lambda_j\tilde{\psi}_j + \psi_j$ with ψ_j the corresponding eigenvector. From this we obtain for arbitrary integer n the following condition on the 1-norm of these vectors: $\|\tilde{\psi}_j\|_1 \geq \|\mathbf{S}^n\tilde{\psi}_j\|_1 = \|\lambda_j^n\tilde{\psi}_j + n\lambda_j^{n-1}\psi_j\|_1 \geq \left| |\lambda_j|^n\|\tilde{\psi}_j\|_1 - n|\lambda_j|^{n-1}\|\psi_j\|_1 \right|$ showing that one should have $\psi_j = 0$ if $|\lambda_j| = 1$. Even if $|\lambda_j| < 1$ this condition is hard to fulfill 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.

Eq. (4) indicates that in the limit $\alpha \rightarrow 1$ the 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 $1-\alpha \ll 1-\lambda_1^{(\text{core})} \sim 10^{-4}$ (10^{-5}) and the corrections for the contributions of the core space nodes are $\sim (1-\alpha)/(1-\lambda_1^{(\text{core})})$. 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 \mathbf{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 Arnoldi methods that allowed us to reach the precision $\|P - \mathbf{G}(\alpha)P\|_1 < 10^{-13}$: after each n_i iterations with the power method we use the resulting vector as initial vector for an Arnoldi diagonalization choosing an Arnoldi matrix size n_A ; 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 $\|P - \mathbf{G}(\alpha)P\|_1 < 10^{-13}$ is reached. For the university network data of [13] in most cases the values $n_i = 10^4$ and $n_A = 100$ ($n_A = 500$ for Cambridge 2006) provide convergence with about ~ 10 iterations of the process (for $1-\alpha = 10^{-8}$). Additional details are given in Appendix.

Fig. 3 clearly confirms the existence of limit behavior for the PageRank at $\alpha \rightarrow 1$. In particular one can clearly identify the limit where it is localized in the invariant subspaces [19] 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 \mathbf{S}_{cc} . In the lower panels of Fig. 3, we compare the

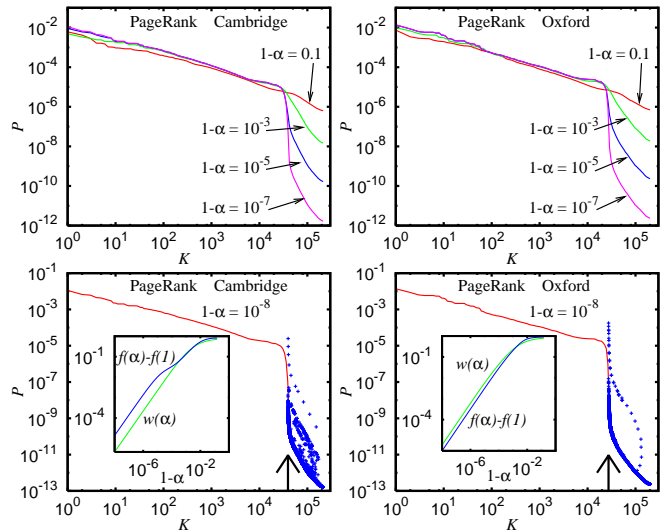


FIG. 3: (Color online) Left panels (right panels) correspond to Cambridge 2006 (Oxford 2006). *Top row*: PageRank $P(K)$ for $1-\alpha = 0.1, 10^{-3}, 10^{-5}, 10^{-7}$. Numerical precision is such that $\|P - \mathbf{G}(\alpha)P\|_1 < 10^{-13}$. *Bottom row*: $P(K)$ at $1-\alpha = 10^{-8}$. Blue crosses correspond to the eigenvector of the largest core space eigenvalue $\lambda_1^{(\text{core})} = 0.999874353718$ (0.999982435081) 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. Insert shows the residual weight $w(\alpha)$ with $w(\alpha) = \sum_{j \in V_c} P_j(\alpha)$ of the core space V_c in the 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. $f(\alpha) = \langle P(\alpha) | P(0.85) \rangle / (\|P(\alpha)\|_2 \|P(0.85)\|_2)$. Note that $\|P(\alpha)\|_2 \neq 1$ since the PageRank is normalized through the 1-norm: $\|P(\alpha)\|_1 = 1$. The value $f(1) = 0.188400463202$ (0.097481331613) is obtained from linear extrapolation from the data with smallest values of $1-\alpha$.

PageRank at $1-\alpha = 10^{-8}$ with this vector (normalized by the 1-norm) multiplied by $(1-\alpha)/(1-\lambda_1^{(\text{core})})$. We observe that except for a very small number of particular nodes this vector approximates quite well the core space correction of the PageRank even though the corrections due to the second term in (4) are more complicated with contributions from many eigenvectors. In the inserts, we also show the fidelity of the PageRank, which decays from 1 at $1-\alpha = 0.15$ to about 0.188 (0.097) at $1-\alpha = 10^{-8}$, and the residual weight $w(\alpha) = \sum_{j \in V_c} P_j(\alpha)$ of the core space V_c in the PageRank which behaves as $w(\alpha) \approx 221.12(1-\alpha) [\approx 607.12(1-\alpha)]$ for $1-\alpha < 10^{-5}$.

We also determine the subspace structure and the PageRank at $1-\alpha = 10^{-8}$ for other university networks available at [13] and for the matrix \mathbf{S}^* of Wikipedia [12] with $N = 3282257$ and $N_s = 21198$ (it turns out that the matrix \mathbf{S} for Wikipedia provides only very few small size subspaces with no reliable statistics). A striking feature is that the distribution of subspace dimensions d_j is uni-

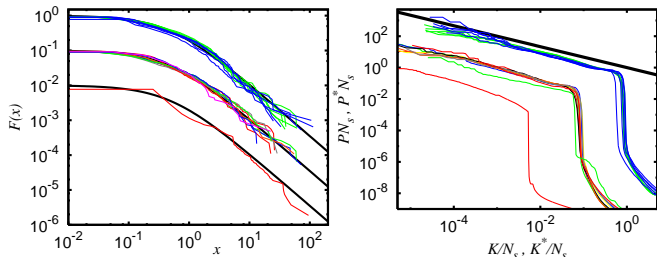


FIG. 4: (Color online) *Left panel:* Fraction of invariant subspaces F with dimensions larger than d as a function of the rescaled variable $x = d/\langle d \rangle$. Upper curves correspond to Cambridge (green) and Oxford (blue) for years 2002 to 2006 and middle curves (shifted down by a factor of 10) to the university networks of Glasgow, Cambridge, Oxford, Edinburgh, UCL, Manchester, Leeds, Bristol and Birkbeck for year 2006 with $\langle d \rangle$ between 14 and 31. Lower curve (shifted down by a factor of 100) corresponds to the matrix \mathbf{S}^* of Wikipedia with $\langle d \rangle = 4$. The thick black line is $F(x) = (1 + 2x)^{-1.5}$. *Right panel:* Rescaled PageRank PN_s versus rescaled rank index K/N_s for $1 - \alpha = 10^{-8}$ and $3974 \leq N_s \leq 48239$ for the same university networks as in the left panel (upper and middle curves, the latter shifted down and left by a factor of 10). The lower curve (shifted down and left by a factor of 100) shows the rescaled CheiRank of Wikipedia P^*N_s versus K^*/N_s with $N_s = 21198$. The thick black line corresponds to a power law with exponent $-2/3$.

versal for all networks considered (Fig. 4 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 [18]. Possible links with the percolation on directed networks (see e.g. [20]) are still to be elucidated. The rescaled Pagerank PN_s (or CheiRank P^*N_s for the case of Wikipedia) takes a universal form with a power law $P \sim K^{-c}$ for $K < N_s$ with an exponent $c = 0.698 \pm 0.005 \approx 1/b = 2/3$ and $P \sim (1 - \alpha)$ close to zero for $K > N_s$.

For certain university networks, Cambridge 2002, 2003 and 2005 and Leeds 2006, there is a specific complication. Indeed, the AM (with $n_A = 10000$) 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 \mathbf{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 $1 - \lambda_1^{(\text{core})} \approx 4.0 \cdot 10^{-17}$ and for Leeds 2006: $1 - \lambda_1^{(\text{core})} \approx 3.1 \cdot 10^{-20}$ (see details in Appendix). 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 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 the 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_s subspace or quasi-subspace nodes and vanishing PageRank for the other core space nodes. For most of the other universities and also the matrix \mathbf{S}^* of Wikipedia we have $1 - \lambda_1^{(\text{core})} \geq 10^{-6}$ (and $1 - \lambda_1^{(\text{core})} \sim 10^{-9}$ for Cambridge 2004).

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 α decreases from 1, the PageRank undergoes a transition which allows to properly rank all nodes. This process is controlled by the largest eigenvalues of the core matrix \mathbf{S}_{cc} , which are strictly below 1 but can be exponentially close to it. Their distance from 1 sets the scale of the transition, and the associated eigenvectors of \mathbf{S}_{cc} control the new ranking of nodes. Although at $\alpha = 1$ the eigenspace for eigenvalue 1 can be very large, for α sufficiently larger in norm than the eigenvalues of \mathbf{S}_{cc} , the 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 \mathbf{G} matrix enables to determine the correct PageRank even where the scale of this transition is extremely small ($1 - \lambda_1^{(\text{core})} \approx 10^{-20}$) 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 simulated annealing process which enables to select the correct eigenvector among many others with very close eigenvalues. The PageRank in this regime of $\alpha \rightarrow 1$ shows universal properties being 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.

We thank CalMiP for supercomputer access and A.D.Chepelianskii for help in data collection from [13].

APPENDIX

A1. Construction of invariant subspaces

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

For each node $j = 1, \dots, N$ 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 S_{kl} 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 \mathbf{S}) to all other nodes, or b) E_n saturates at a limit set E_∞ 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 case the limit set defines a subspace V_j of dimension d_j which is invariant with respect to applications of the matrix \mathbf{S} . We call the initial node j the *root node* of this subspace; the members of E_∞ do not need to be tested themselves as initial nodes subsequently 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 root node. Furthermore, the scheme is greatly simplified if during the iterations a dangling node or another node already being identified as 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 BN where B is some constant of order one and to attribute in this case the node j to the core space. This does not change the results provided that BN 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. However, for networks without dangling nodes or for a strongly localized personalization vector v , with a small number of non-zero elements placed in the column corresponding to the dangling node (instead of the generic choice $v = N^{-1}(1, \dots, 1)^T$), the situation changes and one may have very large invariant subspaces so that an exact choice of B becomes more important.

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 \mathbf{S} .

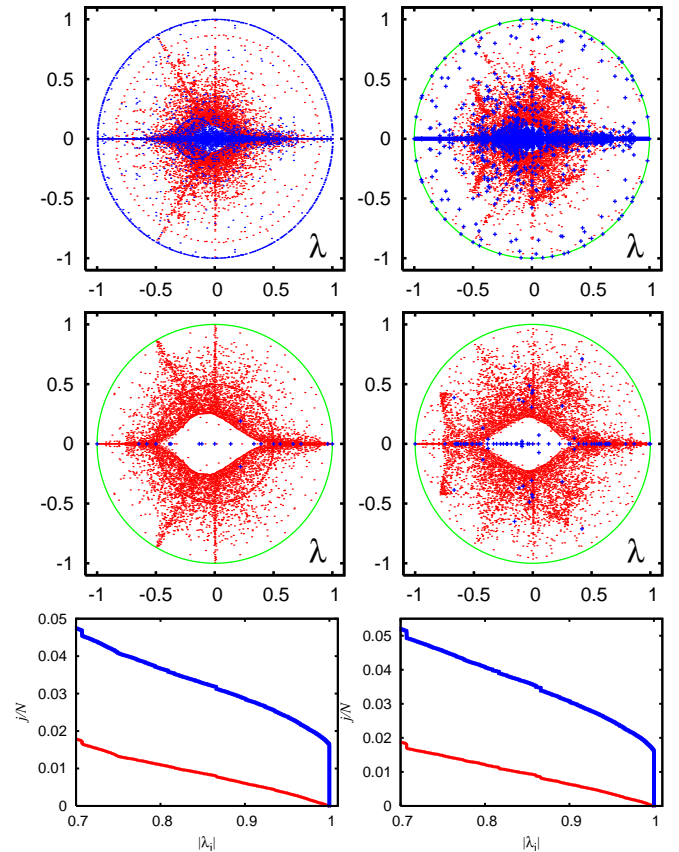


FIG. 5: *Top and bottom rows:* same as top and bottom rows of Fig. 2. *Middle row:* Eigenvalue spectrum for the matrix \mathbf{S}^* , corresponding to the CheiRank, for Cambridge 2006 (left panel) and Oxford 2006 (right panel) with red dots for core space eigenvalues (obtained by the Arnoldi method applied to \mathbf{S}_{cc}^* with $n_A = 15000$), blue crosses for subspace eigenvalues and the green curve showing the unit circle.

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 \mathbf{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 \mathbf{S} to a vector with non-zero elements on all nodes of one subspace one eliminates successively the zero nodes of order 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 \mathbf{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 for the distribution of subspace dimensions and the function $F(x)$ shown in the left panel of Fig. 4 are essentially unchanged if we use the reduced subspaces since the number of zero nodes is below 10% of N_s for most of universities. Only for the matrix \mathbf{S}^* of Wikipedia we have about 45% of zero nodes that reduces the value of N_s from 21198 to 11625.

Once the invariant subspaces of \mathbf{S} are known it is quite obvious to obtain numerically the exact eigenvalues of the subspaces, including the exact degeneracies. Thus, using the Arnoldi method we determine the largest remaining eigenvalues of the core projected block \mathbf{S}_{cc} . In Fig. 5 the complex spectra of subspace and core space eigenvalues of \mathbf{S} and \mathbf{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 $|\lambda_j| = 1$.

In the following table, we summarize the main quantities of 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 Fig. 4 and the matrix \mathbf{S}^* of Wikipedia.

	N	L	N_s	$\langle d \rangle$
Cambridge 2002	140256	752459	23903	20.36
Cambridge 2003	201250	1182527	45495	24.97
Cambridge 2004	206998	1475945	44181	26.14
Cambridge 2005	204760	1505621	44978	29.30
Cambridge 2006	212710	2015265	48239	31.26
Oxford 2002	127450	789090	14820	14.01
Oxford 2003	144783	883672	19972	19.85
Oxford 2004	162394	1158829	29729	19.18
Oxford 2005	169561	1351932	36014	23.34
Oxford 2006	200823	1831542	30579	16.19
Glasgow 2006	90218	544774	20690	28.54
Edinburgh 2006	142707	1165331	24276	26.24
UCL 2006	128450	1397261	25634	28.64
Manchester 2006	99930	1254939	23648	26.07
Leeds 2006	94027	862109	12605	31.20
Bristol 2006	92262	1004175	9143	19.49
Birkbeck 2006	54938	1186854	3974	19.11
Wikipedia (\mathbf{S}^*)	3282257	71012307	21198	3.96

A2. Numerical method of PageRank computation

The standard method to determine the PageRank is the power method [1, 2]. However, this method fails to

converge at a sufficient rate in the limit $\alpha \rightarrow 1$ 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 the PageRank. Typically one may choose $P_0 = \mathbf{e}/N$ where $\mathbf{e} = (1, \dots, 1)^T$. For simplicity let us also suppose that the matrix $\mathbf{G}(\alpha)$ 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 $\mathbf{G}(\alpha)$ as:

$$P_0 = P + \sum_{j \geq 2} C_j \varphi_j \quad (5)$$

where $P = \varphi_1$ is the exact PageRank, which is for $\alpha < 1$ the only (right) eigenvector of $\mathbf{G}(\alpha)$ with eigenvalue 1. Here φ_j denote for $j \geq 2$ other (right) eigenvectors with eigenvalues λ_j such that $|\lambda_j| \leq \alpha$ and C_j are the expansion coefficients. We note that $\mathbf{e}^T \varphi_j = 0$ for $j \geq 2$ since \mathbf{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 $\mathbf{G}(\alpha)$ one obtains after i iterations :

$$P_i = \mathbf{G}^i(\alpha) P_0 = P + \sum_{j \geq 2} C_j \lambda_j^i \varphi_j . \quad (6)$$

Therefore the convergence of the power method goes with $\sim \lambda_2^i$ where λ_2 is the second largest eigenvalue. In the case of realistic networks λ_2 is typically highly degenerate and equal to α . Typically there are also complex eigenvalues with non-trivial phases where only the modulus is equal to α and whose contributions imply the same speed of convergence. In the limit $\alpha \rightarrow 1$ the power method becomes highly ineffective due to these eigenvalues. For example to verify the condition $\alpha^i < \varepsilon$ one needs $i > 3 \cdot 10^9$ iterations for $1 - \alpha = 10^{-8}$ and $\varepsilon = 10^{-13}$.

In order to obtain a faster convergence we propose a different method based on the Arnoldi method [16–18]. The idea of the Arnold method is to diagonalize the matrix representation of $\mathbf{G}(\alpha)$ on the Krylov space generated by $P_0, P_1, \dots, P_{n_A-1}$ where we call n_A the Arnoldi dimension. For reasons of 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 $\mathbf{G}(\alpha)$ in this basis. In the particular case where the number of non-vanishing coefficients C_j in Eq. (5) is not too large the Arnoldi method 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 Eq. (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 to apply the power method with n_i iterations to reduce the contributions of the big majority of eigenvectors whose eigenvalues have a reasonable gap from the unit circle and in a second step the Arnoldi method 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 approximation of the PageRank and repeating this scheme on the new approximation as initial vector (with suitable values for n_i and n_A) one obtains an algorithm which efficiently computes the PageRank up to a high precision as can be seen in Fig. 6. To measure the quality of the PageRank vector we compute the quantity $\|P_i - \mathbf{G}(\alpha)P_i\|_1$ and iterate our algorithm until this quantity is below 10^{-13} . Using this convergence criterion for most university networks from the database [13] the choice of $n_i = 10000$ and $n_A = 100$ provides convergence with typically about 10 steps of this procedure.

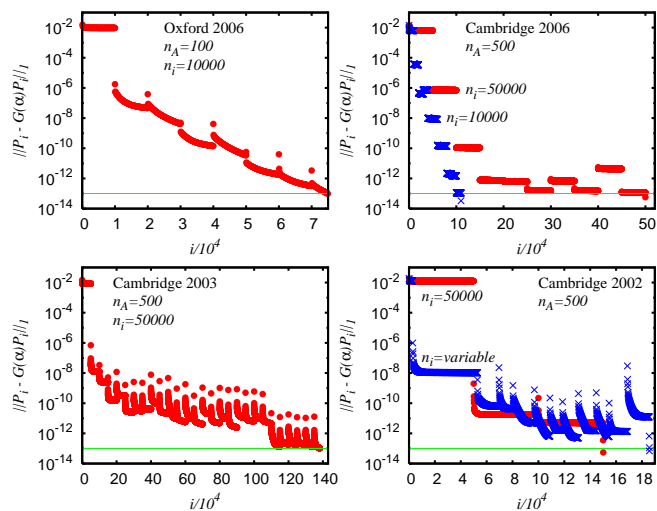


FIG. 6: Convergence of the combined power-Arnoldi method to calculate the PageRank for $1 - \alpha = 10^{-8}$. Shown is the quantity $\|P_i - \mathbf{G}(\alpha)P_i\|_1$ to characterize the quality of the approximate PageRank P_i versus the number of iterations i done by the power method. The green line 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 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 Cambridge 2002 the choice $n_A = 500$ and $n_i = 50000$ (red dots) with $n_A = 500$ and $n_i = \text{variable}$ (blue crosses) with n_i determined by the criterion that the relative change of $\|P_i - \mathbf{G}(\alpha)P_i\|_1$ between i and $i + 100$ is less than 10^{-4} .

In Fig. 6 we show the convergence of this method for

several university network cases with the initial vector $P_0 = \mathbf{e}/N$ 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 of the quality of the PageRank. This is completely normal in view of the small value of $1 - \alpha$. However, the first Arnoldi step improves the quality by 4 orders of magnitude. Then 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 number of power method iterations (in the third cycle) this loss is compensated and its quality improves until the next saturation and the next Arnoldi step. In total this provides a nice exponential convergence and after 7 Arnoldi steps and 75000 power method iterations in total the convergence is reached with very high accuracy. Apparently the Arnoldi method is rather efficient to reduce the coefficients C_j associated to the eigenvectors with eigenvalues close to the circle of radius α but the approximation due to 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 α does not really count, since for each degenerate eigenspace only *one* particular eigenvector appears in the expansions (5), (6) which can be relatively easily “eliminated” by an Arnoldi step with modest value of n_A . However, the total number of *different* eigenvalues (with different phases) on the circle of radius α 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 Fig. 2 where the subspace eigenvalues of \mathbf{S} for Cambridge 2006 nearly fill out the unit circle and indeed we have to increase for these cases the Arnoldi dimension to $n_A = 500$ in order to achieve a reasonable convergence. In the upper right panel of Fig. 6 we show the PageRank convergence for Cambridge 2006 with $n_A = 500$ and two choices of $n_i = 10000$ and $n_i = 50000$. 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 increasing the value of n_i 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, apparently because the bigger number of power method iterations allows to reduce the effect of more eigenvectors in the eigenvector expansion of P_i . In the lower

left panel of Fig. 6 we show the case of Cambridge 2003 which is particularly hard for the convergence and requires 28 Arnoldi steps with $n_i = 50000$ and $n_A = 500$. Actually here the choice $n_i = 10000$ (not shown in the figure) is less efficient with nearly the doubled number of power method iterations and about 235 Arnoldi steps. In the lower right panel we consider the case of Cambridge 2002 where we need 3 Arnoldi steps for the parameters $n_A = 500$ and $n_i = 50000$. For this case, we also tried a different strategy which consists of using a variable value of n_i determined by the criterion that when the relative change of $\|P_i - \mathbf{G}(\alpha)P_i\|_1$ from i to $i + 100$ is below 10^{-4} we perform one Arnoldi step but at latest after 50000 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 which exact choice of n_i parameters works best. In practical calculations when calculating the PageRank for a continuous set of values of α one may also improve convergence simply by using the PageRank at a certain value of α as initial vector for the next value $\alpha + \Delta\alpha$. However, in Fig. 6, we simply used the same initial vector $P_0 = \mathbf{e}/N$ for all cases in order to study the effectiveness of the method as such.

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 $\mathbf{G}(\alpha)$ 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 ~ 1000 (~ 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.* [17] has suggested a different variant of the Arnoldi method 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 we have 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 we 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.

A3. Projected power method for the case of small core space eigenvalue gap

The behavior of the PageRank in the limit $\alpha \rightarrow 1$ 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 \mathbf{S}_{cc} [see Eq. (2)]. This eigenvalue and its eigenvector $\psi_1^{(\text{core})}$ can in principle be determined by the Arnoldi method applied to \mathbf{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 Arnoldi method 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 Appendix section, to the matrix \mathbf{S}_{cc} which first provides the eigenvector $\psi_1^{(\text{core})}$ and once the eigenvector is known its eigenvalue is simply obtained as $\lambda_1^{(\text{core})} = \|\mathbf{S}_{\text{cc}} \psi_1^{(\text{core})}\|_1$ if the normalization is given by $\|\psi_1^{(\text{core})}\|_1 = 1$. We have implemented this method and verified for some examples that it indeed provides the same results as the Arnoldi method. Actually it may even be more efficient than the direct Arnoldi method 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.

Fortunately the approach can be modified to be more accurate. To see this we use Eq. (2) and the fact that the columns of \mathbf{S} are sum normalized which implies $\|\mathbf{S}_{\text{sc}} \psi_1^{(\text{core})}\|_1 + \|\mathbf{S}_{\text{cc}} \psi_1^{(\text{core})}\|_1 = 1$ and therefore

$$1 - \lambda_1^{(\text{core})} = \|\mathbf{S}_{\text{sc}} \psi_1^{(\text{core})}\|_1 = \sum_{j \in V_{\text{SP}}} \sum_{l \in V_c} S_{jl} \psi_{1,l}^{(\text{core})} \quad (7)$$

where V_{SP} denotes the set of subspace nodes and V_c is the set of core space nodes (note that $\psi_{1,l}^{(\text{core})} \geq 0$). 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 determine the gap accurately.

First, we note that an exponentially small core space gap implies that the eigenvectors components $\psi_{1,l}^{(\text{core})}$ are also exponentially 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

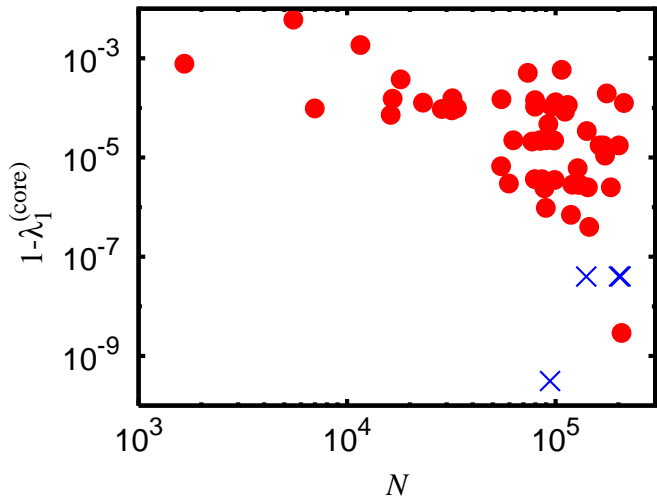


FIG. 7: Core space eigenvalue gap $1 - \lambda_1^{(\text{core})}$ versus network size N for the universities Glasgow, Cambridge, Oxford, Edinburgh, UCL, Manchester, Leeds, Bristol and Birkbeck (years 2002 to 2006) and Bath, Hull, Keele, Kent, Nottingham, Aberdeen, Sussex, Birmingham, East Anglia, Cardiff, York (year 2006). Red dots correspond to data with $1 - \lambda_1^{(\text{core})} > 10^{-9}$ and blue crosses (shifted up by a factor of 10^9) to the cases Cambridge 2002, 2003 and 2005 and Leeds 2006 with $1 - \lambda_1^{(\text{core})} < 10^{-16}$ where the maximal core space eigenvalue is determined by the projected power method. The data point at $1 - \lambda_1^{(\text{core})} = 2.91 \cdot 10^{-9}$ is for Cambridge 2004.

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 exponentially small on the other nodes. Obviously, the nodes inside the small localization domain are not directly connected to a subspace node (by the matrix \mathbf{S}). The important point is that we can determine the eigenvector accurately also for the exponentially small tails (below 10^{-15}) by the *pure* power method (without intermediate Arnoldi steps) if we choose as 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 in 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 determine numerically 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:

1. Determine a first approximation of $\psi_1^{(\text{core})}$ by the direct Arnoldi method which is accurate inside the localization domain but numerically incorrect for

the exponentially small tails on the nodes outside the localization domain. From these data we determine the node l_{max} at which $\psi_{1,l_{\text{max}}}^{(\text{core})}$ is maximal.

2. Choose as initial vector (on the full space including core space *and* subspace nodes) the vector localized on the node l_{max} , i.e. $\psi_l = \delta_{l,l_{\text{max}}}$.
3. Make a copy of the vector: $\psi_{\text{old}} = \psi$.
4. Apply the matrix \mathbf{S} to the actual vector: $\psi = \mathbf{S}\psi$ which produces artificially non-zero values ψ_j on certain subspace nodes j .
5. According to Eq. (7) compute the quantity $\sum_{j \in V_{\text{SP}}} \psi_j$ as approximation of the gap $1 - \lambda_1^{(\text{core})}$.
6. Project the vector on the core space: $\psi_j = 0$ for all subspace nodes $j \in V_{\text{SP}}$.
7. Normalize the vector by the 1-norm: $\psi = \psi / \|\psi\|_1$.
8. Stop the iteration if $\|\psi - \psi_{\text{old}}\|_1 < \varepsilon_1$ and $\max_{l \in V_c} |\psi_l - \psi_{\text{old},l}| / |\psi_l| < \varepsilon_2$. Otherwise go back to step 3.

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 Eq. (7) the eigenvector needs to be accurate with a small relative error also in the exponentially 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 $2 \cdot 10^5$ iterations. For the particular case of Cambridge 2004 (where the gap $\sim 10^{-9}$ is still “accessible” by the Arnoldi method) the convergence is more difficult and we have stopped the iteration at $\varepsilon_1 = 10^{-12}$ and $\varepsilon_2 = 3.2 \cdot 10^{-6}$.

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 \mathbf{e}/N as 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 following gap values:

	$1 - \lambda_1^{(\text{core})}$
Cambridge 2002	$3.996 \cdot 10^{-17}$
Cambridge 2003	$4.01 \cdot 10^{-17}$
Cambridge 2004	$2.91 \cdot 10^{-9}$
Cambridge 2005	$4.01 \cdot 10^{-17}$
Leeds 2006	$3.126 \cdot 10^{-19}$

In Fig. 7 we compare these gap values to the other university networks for which we found by the Arnoldi method larger gaps $1 - \lambda_1^{(\text{core})} > 10^{-7}$.

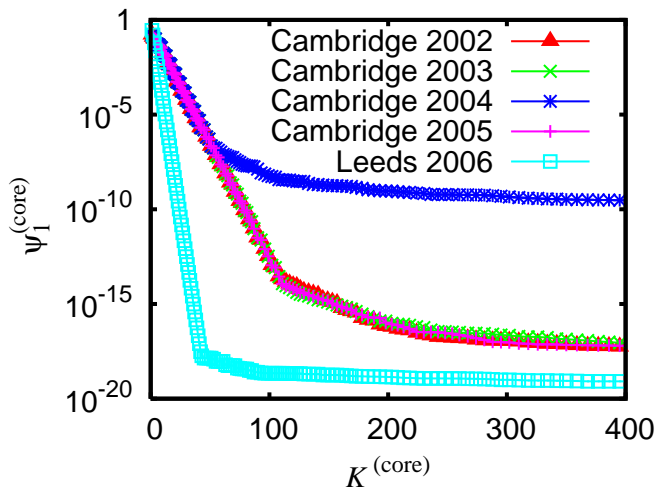


FIG. 8: First core space eigenvector $\psi_1^{(\text{core})}$ versus its rank index $K^{(\text{core})}$ for the university networks with a small core space gap $1 - \lambda_1^{(\text{core})} < 10^{-8}$.

In Fig. 8 we show the eigenvectors $\psi_1^{(\text{core})}$ 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^{-18} (Leeds 2006) or 10^{-14} (Cambridge 2002, 2003 and 2005). The case Cambridge 2004 with a quite larger gap $\sim 10^{-9}$ provides at first the same exponential localization as the other three cases of Cambridge but after 50 nodes it goes over to a tail in the range 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 above table and the expression (7).

When the iteration with the matrix \mathbf{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 exponentially 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 to leave 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 of the effective value of N_s but

it does not change the overall picture.

Fig. 8 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 here 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_{jl} if compared to the networks of the previous years.

The numerical methods described above give powerful tools for detailed analysis of eigenvalue spectrum and eigenstates of Google matrices of complex directed networks of large scale.

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