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Abstract. Using parallels with the quantum scattering theory, developed for processes in nuclear and mesoscopic physics and quantum chaos, we construct a reduced Google matrix G_R which describes the properties and interactions of a certain subset of selected nodes belonging to a much larger directed network. The matrix G_R takes into account effective interactions between subset nodes by all their indirect links via the whole network. We argue that this approach gives new possibilities to analyze effective interactions in a group of nodes embedded in a large directed networks. Possible efficient numerical methods for the practical computation of G_R are also described.

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1. Introduction

At present the concept of Markov chains finds impressive applications in descriptions of directed networks including the World Wide Web (WWW) [1, 2], citation networks [3], Perron-Frobenius operators of dynamical systems [4], software architecture [5], Ulam networks of chaotic maps, world trade flows, network of Wikipedia articles and many other networks [6]. Such directed networks are well described by the Google matrix usually presented in the form

$$G_{ij} = \alpha S_{ij} + (1 - \alpha)/N , \qquad (1)$$

where S_{ij} describes Markov transitions on the network typically given by the inverse number of outgoing links from the node j in presence of a link $j \to i$ or 0 in absence of such a link. In case of total absence of outgoing links from the node j one replaces $S_{ij} = 1/N$ for all values of i, i. e. for the full column j [1, 2]. A random surfer follows with probability α , called damping factor, the dynamics fixed by the Markov transitions S_{ij} and with the complementary probability $(1-\alpha)$ he jumps with uniform probability to any node of the N nodes of the network. The elements of G are nonnegative and the sum of elements in each column is equal to unity corresponding to probability conservation. As a result the product of two different Google matrices is also a Google matrix, respecting these two properties.

The eigenvalues λ_i and right eigenvectors $\psi_i(j)$ of G are defined by

$$\sum_{j'} G_{jj'} \psi_i(j') = \lambda_i \psi_i(j) .$$
⁽²⁾

The eigenvector at maximal $\lambda = 1$ is called the PageRank vector. It has only nonnegative elements and, after normalizing its sum to unity, P(j) has the meaning of the probability to find a random surfer on a given node j in the stationary long time limit of the Markov process. Left eigenvectors are biorthogonal to right eigenvectors of different eigenvalues. The left eigenvector for $\lambda = 1$ has identical (unit) entries due to the column sum normalization of G. One can show that the damping factor, when replacing S by G according to (1), only affects the PageRank vector (or other eigenvectors for $\lambda = 1$ of S in case of a degeneracy) while other eigenvectors are independent of α due to their orthogonality to the left unit eigenvector for $\lambda = 1$ [2] but their (complex) eigenvalues are reduced by a factor α when replacing S by G. In the following we use the notations ψ_L^T and ψ_R for left and right eigenvectors respectively (here T means vector transposition).

In many real networks the number of nonzero elements in a column of S is significantly smaller then the whole matrix size N that allows to find efficiently the PageRank vector by the PageRank algorithm of power iterations. Also a certain number of largest eigenvalues (in modulus) and related eigenvectors can be efficiently computed by the Arnoldi algorithm (see e.g. [7, 8, 9]).

At present directed networks of real systems can be very large (e.g. 4.5 millions for the English Wikipedia edition in 2013 [6] or 3.5 billion web pages for a publicly accessible web crawl that was gathered by the Common Crawl Foundation in 2012 [10]). In certain cases one may be interested in the particular interactions among a small reduced subset of N_r nodes with $N_r \ll N$ instead of the interactions of the entire network. However, the interactions between these N_r nodes should be correctly determined taking into account that there are many indirect links between the N_r nodes via all other $N_s = N - N_r$ nodes of the network. This leads to the problem of

the reduced Google matrix G_R with N_r nodes which describes the interactions of a subset of N_r nodes.

In a certain sense we can trace parallels with the problem of quantum scattering appearing in nuclear and mesoscopic physics (see e.g. [11, 12, 13, 14, 15]) and quantum chaotic scattering (see e.g. [16]). Indeed, in the scattering problem there are effective interactions between open channels to localized basis states in a well confined scattering domain where a particle can spend a certain time before its escape to open channels. Having this analogy in mind we construct the reduced Google matrix G_R which describes interactions between selected N_r nodes and satisfies the standard requirements of the Google matrix. This construction is described in the next Section 2 and the discussion of the results is given in Section 3.

2. Determination of reduced Google matrix

Let G be a typical Google matrix of Perron-Frobenius type for a network with N nodes such that $G_{ij} \geq 0$ and the column sum normalization $\sum_{i=1}^{N} G_{ij} = 1$ are verified. We consider a sub-network with $N_r < N$ nodes, called "reduced network". In this case we can write G in a block form :

$$G = \begin{pmatrix} G_{rr} & G_{rs} \\ G_{sr} & G_{ss} \end{pmatrix}$$
(3)

where the index "r" refers to the nodes of the reduced network and "s" to the other $N_s = N - N_r$ nodes which form a complementary network which we will call "scattering network".

Let us introduce the PageRank vector of the full network

$$P = \left(\begin{array}{c} P_r \\ P_s \end{array}\right) \tag{4}$$

which satisfies the equation GP = P or in other words P is the right eigenvector of G for the unit eigenvalue. This eigenvalue equation reads in block notations:

$$(1 - G_{rr}) P_r - G_{rs} P_s = 0, (5)$$

$$-G_{sr} P_r + (\mathbf{1} - G_{ss}) P_s = 0.$$
(6)

Here **1** is a unit diagonal matrix of corresponding size N_r or N_s . Assuming that the matrix $\mathbf{1} - G_{ss}$ is not singular, i.e. all eigenvalues G_{ss} are strictly smaller than unity (in modulus), we obtain from (6) that $P_s = (\mathbf{1} - G_{ss})^{-1}G_{sr}P_r$ which gives together with (5):

$$G_{\rm R}P_r = P_r$$
 , $G_{\rm R} = G_{rr} + G_{rs}(\mathbf{1} - G_{ss})^{-1}G_{sr}$ (7)

where the matrix $G_{\rm R}$ of size $N_r \times N_r$, defined for the reduced network, can be viewed as an effective reduced Google matrix. In this expression the contribution of G_{rr} accounts for direct links in the reduced network and the second term with the matrix inverse corresponds to all contributions of indirect links of arbitrary order. We note that in mesocopic scattering problems one typically uses an expression of the scattering matrix which has a similar structure where the scattering channels correspond to the reduced network and the states inside the scattering domain to the scattering network [13].

The matrix elements of G_R are non-negative since the matrix inverse in (7) can be expanded as:

$$(\mathbf{1} - G_{ss})^{-1} = \sum_{l=0}^{\infty} G_{ss}^{l} \quad .$$
(8)

In (8) the integer l represents the order of indirect links, i. e. the number of indirect links which are used to connect indirectly two nodes of the reduced network. The matrix inverse corresponds to an exact resummation of all orders of indirect links. According to (8) the matrix $(\mathbf{1} - G_{ss})^{-1}$ and therefore also $G_{\mathbf{R}}$ have non-negative matrix elements. It remains to show that $G_{\mathbf{R}}$ also fulfills the condition of column sum normalization being unity. For this let us denote by $E^T = (1, \ldots, 1)$ the line vector of size N with unit entries and by E_r^T (or E_s^T) the corresponding vectors for the reduced (or scattering) network with N_r (or N_s) unit entries such that $E^T = (E_r^T, E_s^T)$. The column sum normalization for the full Google matrix G implies that $E^T G = E^T$, i. e. E^T is the left eigenvector of G with eigenvalue 1. This equation becomes in block notation:

$$E_r^T (\mathbf{1} - G_{rr}) - E_s^T G_{sr} = 0, (9)$$

$$-E_r^T G_{rs} + E_s^T (1 - G_{ss}) = 0. (10)$$

From (10) we find that $E_s^T = E_r^T G_{rs} (\mathbf{1} - G_{ss})^{-1}$ which implies together with (9) that $E_r^T G_R = E_r^T$ using G_R as in (7). This shows that the column sum normalization condition is indeed verified for G_R justifying that this matrix is indeed an effective Google matrix for the reduced network.

The question arises how to evaluate practically the expression (7) of $G_{\rm R}$ for a particular sparse and quite large network with a typical situation when $N_r \sim 10^2 \cdot 10^3$ is small compared to N and $N_s \approx N \gg N_r$. If N_s is too large (e. g. $N_s \sim 10^5$) a direct naive evaluation of the matrix inverse $(\mathbf{1} - G_{ss})^{-1}$ in (7) by Gauss algorithm is not possible. In this case we can try the expansion (8) provided it converges sufficiently fast with a modest number of terms. However, this is most likely not the case for typical applications.

Let us consider the situation where the full Google matrix has a well defined gap between the leading unit eigenvalue and the second largest eigenvalue (in modulus). For example if G is defined using a damping factor α in the standard way, as in (1), the gap is at least $1 - \alpha$ which is 0.15 for the standard choice $\alpha = 0.85$ [2]. For such a situation we expect that the matrix G_{ss} has a leading real eigenvalue close to unity (but still different from unity so that $1 - G_{ss}$ is not singular) while the other eigenvalues are clearly below this leading eigenvalue with a gap comparable to the gap of the full Google matrix G. In order to evaluate the expansion (8) efficiently, we need to take out analytically the contribution of the leading eigenvalue close to unity which is responsible for the slow convergence.

In the following, we denote by λ_c this leading eigenvalue and by ψ_R (ψ_L^T) the corresponding right (left) eigenvector such that $G_{ss}\psi_R = \lambda_c\psi_R$ (or $\psi_L^TG_{ss} = \lambda_c\psi_L^T$). Both left and right eigenvectors as well as λ_c can be efficiently computed by the power iteration method in a similar way as the standard PageRank method. We note that one can easily show that λ_c must be real and that both left/right eigenvectors can be chosen with positive elements. Concerning the normalization for ψ_R we choose $E_s^T\psi_R = 1$ and for ψ_L we choose $\psi_L^T\psi_R = 1$. It is well known (and easy to show) that ψ_L^T is orthogonal to all other right eigenvectors (and ψ_R is orthogonal to all other left eigenvectors) of G_{ss} with eigenvalues different from λ_c . We introduce the operator $\mathcal{P}_c = \psi_R \psi_L^T$ which is the projector onto the eigenspace of λ_c and we denote by $\mathcal{Q}_c = \mathbf{1} - \mathcal{P}_c$ the complementary projector. One verifies directly that both projectors commute with the matrix G_{ss} and in particular $\mathcal{P}_c G_{ss} = G_{ss} \mathcal{P}_c = \lambda_c \mathcal{P}_c$. Therefore we can write:

$$(\mathbf{1} - G_{ss})^{-1} = (\mathcal{P}_c + \mathcal{Q}_c)(\mathbf{1} - G_{ss})^{-1}(\mathcal{P}_c + \mathcal{Q}_c)$$
(11)

$$= \mathcal{P}_c \frac{1}{1 - \lambda_c} + \mathcal{Q}_c (1 - G_{ss})^{-1} \mathcal{Q}_c$$
(12)

$$= \mathcal{P}_c \frac{1}{1 - \lambda_c} + (1 - \bar{G}_{ss})^{-1} \mathcal{Q}_c \tag{13}$$

$$= \mathcal{P}_c \frac{1}{1 - \lambda_c} + \mathcal{Q}_c \sum_{l=0}^{\infty} \bar{G}_{ss}^l$$
(14)

with $\bar{G}_{ss} = \mathcal{Q}_c G_{ss} \mathcal{Q}_c$ and using the standard identity $\mathcal{P}_c \mathcal{Q}_c = 0$ for complementary projectors. The expansion in (14) has the advantage that it converges rapidly since $\bar{G}_{ss}^l \sim |\lambda_{c,2}|^l$ with $\lambda_{c,2}$ being the second largest eigenvalue which is significantly lower than unity (e. g. $|\lambda_{c,2}| \approx \alpha = 0.85$ for the case with a damping factor). The first contribution due to the leading eigenvalue λ_c close to unity is taken out analytically once the left and right eigenvectors, and therefore also the projector \mathcal{P}_c , are known. The combination of (7) and (14) provides an explicit algorithm feasible for a numerical implementation for the case of modest values of N_r , large values of N_s and of course for sparse matrices G, G_{ss} etc.

The method can also be modified to take out analytically the contributions of several leading eigenvalues close to unity if the latter are sufficiently well separated (non-degenerate) such that these eigenvalues and left/right eigenvectors can be determined by the Arnoldi method (applied to G_{ss}). Then Eq. (14) is modified as:

$$(\mathbf{1} - G_{ss})^{-1} = \sum_{j} \mathcal{P}_{c}^{(j)} \frac{1}{1 - \lambda_{c,j}} + \mathcal{Q}_{c} \sum_{l=0}^{\infty} \bar{G}_{ss}^{l}$$
(15)

with $\mathcal{P}_{c}^{(j)} = \psi_{R}^{(j)}(\psi_{L}^{(j)})^{T}$ being the projector on the eigenspace of the eigenvalue $\lambda_{c,j}$ with right (left) eigenvector $\psi_{R}^{(j)}$ [or $(\psi_{L}^{(j)})^{T}$] obeying, after proper normalization, the bi-orthogonality identity $(\psi_{L}^{(j)})^{T}\psi_{R}^{(k)} = \delta_{jk}$ and with $\mathcal{Q}_{c} = \mathbf{1} - \sum_{j} \mathcal{P}_{c}^{(j)}$ being the total complementary projector. The expression (15) is in principle also suitable for a numerical evaluation provided that the number of leading eigenvalues $\lambda_{c,j}$ is modest.

We note that the numerical methods described in [17] allow to determine the eigenvalues λ_c (and corresponding eigenvectors) which are exponentially close to unity (e.g. $1 - \lambda_c \sim 10^{-16}$) so that the expression (15) can be efficiently computed numerically.

In the case when N < 20000 an exact diagonalization of G_{ss} can be done numerically and then the presentation $G_{ss} = QD_{\lambda}Q^{-1}$ allows to obtain the simple expression $(\mathbf{1} - G_{ss})^{-1} = Q[\mathbf{1}/(\mathbf{1} - D_{\lambda})]Q^{-1}$. Here Q is the regular matrix formed by eigenvectors of G_{ss} (in its columns) and D_{λ} is the diagonal matrix of corresponding (complex) eigenvalues λ .

There is also an additional possibility to avoid the problem of slow convergence in $G_{\rm R}$ by a slight modification of the initial Google matrix to the form

$$G_{\rm mod} = \begin{pmatrix} \mathbf{1} & (1-\eta)U_{rs} \\ 0 & \eta \mathbf{1} \end{pmatrix} \times \begin{pmatrix} G_{rr} & G_{rs} \\ G_{sr} & G_{ss} \end{pmatrix} .$$
(16)

Here $0.5 \leq \eta < 1$ is an additional damping factor, U_{rs} is a rectangular $N_r \times N_s$ matrix with non-negative elements and whose columns are sum normalized. A possible choice is $U_{rs} = (1/N_r)E_rE_s^T$ with E_r or E_s as defined in the paragraph preceeding Eq. (9) or more generally $U_{rs} = v_p E_s^T$ where v_p is a sum normalized vector with N_r non-negative entries and representing somehow a kind of preferential vector on the reduced network.

Therefore the first matrix in the product of (16) belongs to the Google matrix class (sum of non-negative elements in each column is equal to unity). Thus, the product of both matrices also belongs to the class of Google matrices and hence G_{mod} is also a matrix of Google type. Then for G_{mod} , in analogy with (7), we obtained the modified reduced Google matrix

$$G_{\text{Rmod}} = G_{rr} + (1 - \eta)U_{rs}G_{sr} + \eta[G_{rs} + (1 - \eta)U_{rs}G_{ss}](1 - \eta G_{ss})^{-1}G_{sr} .$$
(17)

If η is sufficiently smaller than unity, e. g. $1 - \eta \approx 0.1$ -0.2, then the geometric series expansion analogous to (8) converges rapidly allowing for an efficient numerical computation even if G_{ss} has a maximal eigenvalue close to unity. We note that a similar expansion has been used for the ImpactRank in [18] where the rapid numerical convergence allowed for an efficient computation.

Finally we note that in a similar way it is possible to construct the reduced matrix for the network of same N nodes with the inverted direction of links. This gives the Google matrix G^* with the CheiRank eigenvector P^* of G^* at $\lambda = 1$ [5, 6]. Then from G^* using (7) we obtain the reduced matrix G_R^* .

3. Discussion

The obtained expression (7) for the reduced Google matrix G_R allows to analyze effective interactions between a selected subset of nodes of a given large network. We expect that this will allow to understand in a better way hidden indirect dependencies existing between specific nodes in small subsets of large networks. The geometric series expansion of the propagator $(1 - G_{ss})^{-1}$ in (8) is similar to the propagators appearing in the theory of quantum scattering [12, 13, 16] corresponding to summation over all periods of particle motion inside the confined scattering domain. In our case N_s nodes correspond to localized basis states in the scattering domain while the subset of N_r nodes in the reduced network describes interactions (scattering) between open channels. We think that such an analogy will find further useful applications. The reduced Google matrix should allow to study effective interactions between a small group of friends. For a group of three, four friends it would be interesting to compare results from real networks with the known results for the ensemble of random orthostochastic matrices [19]. It would be also interesting to analyze the properties of G_R for a class of random RPFM matrices considered in [18] (see Fig.16 there).

Thus we expect that the description of specific subsets of directed networks with the help of the reduced Google matrix will find many interesting applications.

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