

A Markov chain representation of the normalized Perron–Frobenius eigenvector

Raphaël Cerf* Joseba Dalmau†

Abstract

We consider the problem of finding the Perron–Frobenius eigenvector of a primitive matrix. Dividing each of the rows of the matrix by the sum of the elements in the row, the resulting new matrix is stochastic. We give a formula for the normalized Perron–Frobenius eigenvector of the original matrix, in terms of a realization of the Markov chain defined by the associated stochastic matrix. This formula is a generalization of the classical formula for the invariant probability measure of a Markov chain.

Keywords: Perron Frobenius; eigenvector; Markov chain.

AMS MSC 2010: 15A18; 60J10.

Submitted to ECP on February 23, 2017, final version accepted on July 20, 2017.

Let A be a primitive matrix of size N , i.e., a non–negative matrix whose m –th power is positive for some natural number m . The Perron–Frobenius theorem (Theorem 1.1 in [7]) states that there exist a positive real number λ and a vector u on the unit simplex $\{x \in \mathbb{R}_+^N : x_1 + \dots + x_N = 1\}$ such that $u^T A = \lambda u^T$. Moreover, the eigenvalue λ is simple, is larger in absolute value than any other eigenvalue of A , and any non–negative eigenvector of A is a multiple of u . The eigenvalue λ is the Perron–Frobenius eigenvalue of A and u is a Perron–Frobenius eigenvector of A . The purpose of this note is to give a Markov chain representation of the normalized Perron–Frobenius eigenvector $u/|u|_1$.

The matrix A can be decomposed as $A(i, j) = f(i)M(i, j)$ with $f(i)$ being the sum of the elements in the i –th row of A and $M(i, j) = A(i, j)/f(i)$. The matrix M is now primitive and stochastic, so that it naturally defines an ergodic Markov chain. Let $(X_n)_{n \in \mathbb{N}}$ be a Markov chain with state space $\{1, \dots, N\}$ and transition matrix M , denote by E_k the expectation of the Markov chain issued from k and τ_k the time of the first return of the chain to k . We have the following result.

Theorem. *Let $1 \leq k \leq N$. The normalized Perron–Frobenius eigenvector u of A is given by the formula*

$$\forall i \in \{1, \dots, N\} \quad u_i = \frac{E_k \left(\sum_{n=0}^{\tau_k-1} \left(1_{\{X_n=i\}} \lambda^{-n} \prod_{t=0}^{n-1} f(X_t) \right) \right)}{E_k \left(\sum_{n=0}^{\tau_k-1} \left(\lambda^{-n} \prod_{t=0}^{n-1} f(X_t) \right) \right)}.$$

*Département de mathématiques et applications, École normale supérieure, CNRS, PSL Research University, 75005 Paris, France. E-mail: Raphaël.Cerf@gmail.com

†Département de mathématiques et applications, École normale supérieure, CNRS, PSL Research University, 75005 Paris, France. E-mail: joseba.dalmau@polytechnique.edu

Representation of the Perron–Frobenius eigenvector

By taking $i = k$ in the above formula we obtain the following corollary.

Corollary. *The normalized Perron–Frobenius eigenvector u of A is given by the formula*

$$\forall k \in \{1, \dots, N\} \quad u_k = \frac{1}{E_k \left(\sum_{n=0}^{\tau_k-1} \left(\lambda^{-n} \prod_{t=0}^{n-1} f(X_t) \right) \right)}.$$

This formula is a generalization of the classical formula for the invariant probability measure of a Markov chain. Indeed, in the particular case where A is stochastic, f is constant equal to 1, λ is also equal to 1, and u corresponds to the invariant probability measure of the Markov chain. Thus, the formula of the corollary becomes the well-known formula

$$\forall k \in \{1, \dots, N\} \quad u_k = \frac{1}{E_k(\tau_k)}.$$

Before proving the theorem, we state a preparatory lemma.

Lemma. *Let A be a non-negative primitive matrix of size N . Its Perron–Frobenius eigenvalue λ satisfies the following identity: for any $k \in \{1, \dots, N\}$,*

$$\begin{aligned} 1 &= \frac{1}{\lambda} A(k, k) + \frac{1}{\lambda^2} \sum_{i_1 \neq k} A(k, i_1) A(i_1, k) + \dots \\ &\quad + \frac{1}{\lambda^n} \sum_{i_1, \dots, i_{n-1} \neq k} A(k, i_1) A(i_1, i_2) \cdots A(i_{n-1}, k) + \dots \end{aligned}$$

Proof. Let $(x_i)_{1 \leq i \leq N}$ be a non-negative eigenvector associated to the Perron–Frobenius eigenvalue λ of A :

$$\forall j \in \{1, \dots, N\} \quad \sum_{i=1}^N x_i A(i, j) = \lambda x_j.$$

Since A is primitive, all the components of x are positive. Let $k \in \{1, \dots, N\}$ be fixed. We have thus

$$1 = \frac{1}{\lambda x_k} \sum_{i=1}^N x_i A(i, k) = \frac{1}{\lambda} A(k, k) + \sum_{i \neq k} \frac{x_i}{\lambda x_k} A(i, k).$$

We replace x_i in the last sum and we get

$$\begin{aligned} 1 &= \frac{1}{\lambda} A(k, k) + \sum_{i \neq k} \sum_{i'=1}^N \frac{x_{i'}}{\lambda^2 x_k} A(i', i) A(i, k) \\ &= \frac{1}{\lambda} A(k, k) + \sum_{i \neq k} \frac{1}{\lambda^2} A(k, i) A(i, k) + \sum_{i, i' \neq k} \frac{x_{i'}}{\lambda^2 x_k} A(i', i) A(i, k). \end{aligned}$$

Iterating this procedure, we obtain, for $n \geq 1$,

$$\begin{aligned} 1 &= \sum_{t=0}^{n-1} \frac{1}{\lambda^{t+1}} \sum_{i_1, \dots, i_t \neq k} A(k, i_1) A(i_1, i_2) \cdots A(i_t, k) + \\ &\quad \frac{1}{\lambda^n} \sum_{i_1, \dots, i_{n-1} \neq k} \frac{x_{i_1}}{x_k} A(i_1, i_2) \cdots A(i_{n-1}, k). \end{aligned}$$

Let B be the matrix obtained from A by filling with zeroes the line and the column associated to k . The last term of the previous identity can be rewritten as

$$\frac{1}{\lambda^n} \sum_{i, j \neq k} \frac{x_i}{x_k} B(i, j)^{n-2} A(j, k).$$

Representation of the Perron–Frobenius eigenvector

Yet it follows from part (e) of Theorem 1.1 of [7] that the spectral radius of B is strictly less than λ , whence

$$\forall i, j \in \{1, \dots, N\} \quad \lim_{n \rightarrow \infty} \frac{1}{\lambda^n} B(i, j)^{n-2} = 0.$$

Thus the previous sum vanishes as n goes to ∞ . Passing to the limit, we obtain the desired identity. \square

We now proceed to the proof of the theorem.

Proof. Let us note E_k and τ_k simply by E and τ . We set, for $1 \leq i \leq N$,

$$y_i = E \left(\sum_{n=0}^{\tau-1} \left(1_{\{X_n=i\}} \lambda^{-n} \prod_{t=0}^{n-1} f(X_t) \right) \right).$$

Obviously, the vector $(y_i)_{1 \leq i \leq N}$ is non-null (notice that $y_k = 1$) and its components are non-negative. Let us compute

$$\begin{aligned} \sum_{i=1}^N y_i f(i) M(i, j) &= \\ &= \sum_{i=1}^N \sum_{n \geq 0} E \left(1_{\{\tau > n\}} \lambda^{-n} \left(\prod_{t=0}^{n-1} f(X_t) \right) 1_{\{X_n=i\}} f(i) M(i, j) \right) \\ &= \sum_{i=1}^N \sum_{n \geq 0} E \left(1_{\{\tau > n\}} \lambda^{-n} \left(\prod_{t=0}^n f(X_t) \right) 1_{\{X_n=i\}} 1_{\{X_{n+1}=j\}} \right) \\ &= E \left(\sum_{n=0}^{\tau-1} 1_{\{X_{n+1}=j\}} \lambda^{-n} \left(\prod_{t=0}^n f(X_t) \right) \right) \\ &= \lambda E \left(\sum_{n=1}^{\tau} 1_{\{X_n=j\}} \lambda^{-n} \left(\prod_{t=0}^{n-1} f(X_t) \right) \right). \end{aligned}$$

Suppose that $j \neq k$. Then the term in the last sum vanishes for $n = 0$ or $n = \tau$, and we recover the identity

$$\sum_{i=1}^N y_i f(i) M(i, j) = \lambda y_j.$$

For $j = k$, we obtain

$$\sum_{i=1}^N y_i f(i) M(i, j) = \lambda E \left(\lambda^{-\tau} \prod_{t=0}^{\tau-1} f(X_t) \right).$$

The last expectation can be rewritten as

$$\begin{aligned} E \left(\lambda^{-\tau} \prod_{t=0}^{\tau-1} f(X_t) \right) &= \sum_{n \geq 1} E \left(1_{\{\tau=n\}} \lambda^{-n} \prod_{t=0}^{n-1} f(X_t) \right) \\ &= \sum_{n \geq 1} \sum_{i_1, \dots, i_{n-1} \neq k} \lambda^{-n} f(k) f(i_1) \cdots f(i_{n-1}) \\ &\quad \times P(X_1 = i_1, \dots, X_{n-1} = i_{n-1}, X_n = k) \\ &= \sum_{n \geq 1} \sum_{i_1, \dots, i_{n-1} \neq k} \lambda^{-n} f(k) M(k, i_1) \cdots f(i_{n-1}) M(i_{n-1}, k). \end{aligned}$$

This last sum is equal to 1 by Lemma. Noticing that $y_k = 1$, we conclude that

$$\sum_{i=1}^N y_i f(i) M(i, k) = \lambda y_k.$$

Therefore the vector $(y_i)_{1 \leq i \leq k}$ is an eigenvector of A associated to λ . We normalize it so that it belongs to the unit simplex and we obtain the formula stated in the theorem. \square

Examples

The decomposition of the matrix A in terms of f and M might seem artificial. However, it arises naturally in several situations. We illustrate this fact in the following two examples, which also provided us with the motivation to construct the probabilistic representation of the normalized Perron–Frobenius eigenvector given in the above results.

Mutation–selection equilibrium. Consider a mutation–selection model in which individuals have an associated type, the possible types being numbered from 1 to m . Individuals reproduce and mutate, and mutations, which only happen during the reproduction events, change the type of the offspring. We fix a function $f : \{1, \dots, m\} \rightarrow]0, +\infty[$ and a primitive stochastic matrix $(M(i, j))_{1 \leq i, j \leq m}$. An individual of type i reproduces at rate $f(i)$, and the offspring mutates to type j with probability $M(i, j)$. Let the vector $(N_k(t))_{1 \leq k \leq m}$ represent the numbers of the different types at time t in an evolving population. We assume that the evolution is driven by the following linear system of differential equations,

$$N'_k(t) = \sum_{i=1}^m N_i(t) f(i) M(i, k), \quad 1 \leq k \leq m.$$

Let us consider the vector $(x_k(t))_{1 \leq k \leq m}$ of the proportions associated to the linear system, i.e.,

$$x_k(t) = \frac{N_k(t)}{N_1(t) + \dots + N_m(t)}, \quad 1 \leq k \leq m.$$

A simple computation shows that the vector of proportions follows the following system of differential equations:

$$x'_k(t) = \sum_{i=1}^m x_i(t) f(i) M(i, k) - x_k(t) \sum_{i=1}^m x_i(t) f(i), \quad 1 \leq k \leq m. \quad (\mathcal{E})$$

We look now for the equilibrium solutions of this system of differential equations, and we obtain the mutation–selection equilibrium equation

$$\forall k \in \{1, \dots, N\} \quad x_k \sum_{i=1}^N x_i f(i) = \sum_{i=1}^N x_i f(i) M(i, k). \quad (\mathcal{S})$$

This equilibrium equation is of high interest and it arises in a wide variety of models, for instance in Eigen’s quasispecies model [1, 2], which is just the system of differential equations (\mathcal{E}) for $(x_k(t))_{1 \leq k \leq m}$, or in the evolutionary dynamics of grammar learning [5], for a more detailed account of its wide applicability, see [6]. The main question is whether a solution of (\mathcal{S}) exists in the $N - 1$ dimensional unit simplex, and whether the solution, if it exists, is unique or not. In view of the Perron–Frobenius Theorem [8, 4], the unique solution of (\mathcal{S}) in the unit simplex is given by the normalized Perron–Frobenius eigenvector u of the matrix $A = (f(i)M(i, j))_{1 \leq i, j \leq m}$. The Perron–Frobenius eigenvalue

λ corresponds to the mean fitness at equilibrium $\lambda = \sum_{1 \leq i \leq m} x_i f(i)$. In this particular setting, the Markov chain $(X_n)_{n \geq 0}$ can be naturally interpreted as the random walk of a mutant in a neutrally evolving population, that is, if f is constant equal to 1.

Multitype Galton–Watson process. We describe next a probabilistic counterpart of the mutation–selection equilibrium above. Consider a multitype Galton–Watson process in which individuals of type i produce offspring according to a Poisson law with mean $f(i)$, and the offspring of a type i individual becomes of type j with probability $M(i, j)$. The multitype Galton–Watson process is a Markov chain

$$Z_n = (Z_n(1), \dots, Z_n(m)), \quad n \geq 0.$$

The number $Z_n(i)$ represents the number of individuals having type i in generation n . In order to build generation $n + 1$ from generation n , each individual of type i present in generation n produces a random number of offspring, distributed according to a Poisson random variable with mean $f(i)$, and each of the offspring then mutates according to the matrix M . All these events happen independently of each other, as well as of the past of the process. The ensemble of all the offspring forms the generation $n + 1$. The null vector is an absorbing state. For each $i \in \{1, \dots, m\}$, we denote by P_i and E_i the probabilities and expectations for the process started from a population consisting of a single individual of type i . The mean matrix of the process $(Z_n)_{n \geq 0}$ is defined by

$$\forall i, j \in \{1, \dots, m\} \quad A(i, j) = E_i(Z_1(j)).$$

The matrix A is nothing but the matrix $(f(i)M(i, j))_{1 \leq i, j \leq m}$. Indeed, for $i, j \in \{1, \dots, m\}$, conditioning on the number of children of the individual in the initial population, we obtain

$$\begin{aligned} E_i(Z_1(j)) &= \sum_{k=1}^{\infty} E_i(Z_1(j) \mid |Z_1|_1 = k) P_i(|Z_1|_1 = k) \\ &= \sum_{k=1}^{\infty} k M(i, j) e^{-f(i)} \frac{f(i)^k}{k!} = f(i) M(i, j). \end{aligned}$$

It is well-known (Chapter 2 of [3]) that if the Perron–Frobenius eigenvalue λ of A is strictly larger than one, then the multitype Galton–Watson process has a positive probability of survival. Conditionally on the survival event, the vector of proportions of the different types converges to u when time goes to ∞ , u being the normalized Perron–Frobenius eigenvector of A , i.e., conditionally on the survival event

$$\forall k \in \{1, \dots, m\} \quad \lim_{n \rightarrow \infty} \frac{Z_n(k)}{Z_n(1) + \dots + Z_n(m)} = u_k.$$

References

- [1] Manfred Eigen, *Self-organization of matter and the evolution of biological macromolecules*, *Naturwissenschaften* **58** (1971), no. 10, 465–523.
- [2] Manfred Eigen, John McCaskill, and Peter Schuster, *The molecular quasi-species.*, *Advances in Chemical Physics* **75** (1989), 149–263.
- [3] Theodore E. Harris, *The theory of branching processes*, Springer-Verlag, Berlin; Prentice-Hall, Inc., Englewood Cliffs, N.J., 1963. MR-0163361
- [4] B. L. Jones, R. H. Enns, and S. S. Rangnekar, *On the theory of selection of coupled macromolecular systems*, *Bulletin of Mathematical Biology* **38** (1976), no. 1, 15–28.
- [5] Martin A. Nowak, Natalia L. Komarova, and Partha Niyogi, *Evolution of universal grammar*, *Science* **291** (2001), no. 5501, 114–118.

Representation of the Perron–Frobenius eigenvector

- [6] Karen M. Page and Martin A. Nowak, *Unifying evolutionary dynamics*, Journal of Theoretical Biology **219** (2002), no. 1, 93–98.
- [7] E. Seneta, *Nonnegative matrices and Markov chains*, second ed., Springer Series in Statistics, Springer-Verlag, New York, 1981. MR-719544
- [8] Colin J. Thompson and John L. McBride, *On eigen's theory of the self-organization of matter and the evolution of biological macromolecules*, Mathematical Biosciences **21** (1974), no. 1, 127–142.