2 Numerical solution of equilibrium equations: iterative methods

In this chapter we treat several iterative methods to solve the equilibrium equations

$$p = pP, \qquad pe = 1, \tag{1}$$

where p denotes the row vector of equilibrium probabilities, P the transition probability matrix of an irreducible Markov chain and e the column vector with ones. To analyze their convergence properties, we first need some general properties of nonnegative matrices (see, e.g., [1, 4]).

2.1 Nonnegative matrices

Let Q be a nonnegative, irreducible and aperiodic $N \times N$ matrix. The spectral radius $\rho(Q)$ of Q is defined by

$$\rho(Q) = \max\{|\lambda|; \lambda \text{ is an eigenvalue of } Q\}.$$

From the assumptions on Q it follows that there is a unique and simple eigenvalue $\lambda_1(Q)$ with $|\lambda_1(Q)| = \rho(Q)$, even $\lambda_1(Q) = \rho(Q)$. The corresponding right-eigenvector, called the *Perron-Frobenius or spectral eigenvector*, will be denoted by y^*. This eigenvector satisfies $y_i^* > 0$ for all i. Further let $\rho_2(Q)$ denote the *subradius of* Q, defined by

$$\rho_2(Q) = \max\{|\lambda|; \lambda \text{ is an eigenvalue of } Q \text{ with } |\lambda| < \rho(Q)\}.$$

Now the following proposition holds.

Proposition 2.1 *Let u be an N-column vector with $u \geq 0$ and $u \neq 0$. Then there exist a constant $a > 0$ and an integer k, with $0 \leq k < N$, such that*

$$Q^n u = a\rho^n(Q)y^* + O(n^k \rho_2^n(Q)), \qquad (n \to \infty).$$

Remark 2.2 The constant k will be unequal to zero only if there are generalized eigenvectors corresponding to the subdominant eigenvalue(s), see e.g. [3].

Remark 2.3 The same proposition is of course valid for vQ^n where v is an N-row vector with $v \geq 0$ and $v \neq 0$.

2.2 Matrix powers

A simple method which provides bounds on the equilibrium distribution p is to calculate the matrix powers $P, P^2, P^4, P^8, \ldots$ until P^{2^n} is nearly a constant matrix. If P is aperiodic, then $(P^{2^n})_{ij}$ converges to p_j and the bounds are $\max_i(P^{2^n})_{ij} \downarrow p_j$ and $\min_i(P^{2^n})_{ij} \uparrow p_j$ (see p. 173 in [2]). Note that we can always achieve that P is aperiodic by the transformation $\widetilde{P} = \alpha I + (1-\alpha)P$, where $0 < \alpha < 1$ and I denotes the identity matrix. This transformation leaves the equilibrium distribution intact (cf. [5]).

This method is impractical if N is large, since P^{2^n} becomes a dense matrix, so each iteration will require $O(N^3)$ operations.

2.3 Power method

The most popular iterative method, which exploits the sparsity of P, is the *power method* (see, e.g., [7]). This method is described in Figure 1.

POWER METHOD

Choose an initial vector $p^{(0)} \geq 0$, $p^{(0)} \neq 0$, and compute for $n = 0, 1, \ldots$

$$p^{(n+1)} = p^{(n)} P, \tag{2}$$

until $p^{(n+1)} - p^{(n)}$ is sufficiently small.

Figure 1: Power method

The stopping criterion is based on the difference between $p^{(n+1)}$ and $p^{(n)}$. For example, the stopping criterion can be taken to be

$$\sum_{i=0}^{N} |p_i^{(n+1)} - p_i^{(n)}| \leq \epsilon \sum_{i=0}^{N} |p_i^{(n)}|,$$

where ϵ is some small positive number. When the method has converged, an approximation of p is obtained by normalization of the final $p^{(n)}$. Note that, if $p^{(0)}$ is a probability distribution, then $p^{(n)}$ is the probability distribution of the Markov chain P after n transitions (given that the initial distribution is $p^{(0)}$).

If P is *aperiodic* (which can always be achieved, see Exercise 2), then this method converges geometrically. From Proposition 2.1 it follows that for some constant $a > 0$ and nonnegative integer $k < N$,

$$p^{(n)} = p^{(0)} P^n = ap + O(n^k \rho_2^n(P)), \qquad (n \to \infty).$$

Hence the rate of convergence is determined by the subradius of P.

Example 2.4
Consider the periodic Markov chain with transition probability matrix

$$P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

When we start with $p^{(0)} = (0, 1)$, then we obtain the alternating sequence

$$p^{(1)} = (1, 0), \quad p^{(2)} = (0, 1), \quad p^{(3)} = (1, 0), \ldots$$

So there is no convergence. But for the transformed matrix

$$\widetilde{P} = \frac{1}{2} I + \frac{1}{2} P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix},$$

we have convergence after one iteration.

Example 2.5
Consider the Markov chain with transition probability matrix

$$P = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{4} & \frac{3}{4} \end{pmatrix}.$$

The eigenvalues of P are given by $\sigma_1 = 1$ and $\sigma_2 = 1/4$, with corresponding row eigenvectors $x_1 = (1, 2)$ and $x_2 = (1, -1)$. When we start with the initial distribution

$$p^{(0)} = (0, 1) = \frac{1}{3}\, x_1 - \frac{1}{3}\, x_2,$$

then for $n = 0, 1, \ldots$

$$p^{(n)} = \frac{1}{3}\, \sigma_1^n x_1 - \frac{1}{3}\, \sigma_2^n x_2 = \frac{1}{3}\, (1, 2) - \frac{1}{3} \left(\frac{1}{4}\right)^n (1, -1).$$

Hence $p^{(n)}$ converges geometrically fast to the equilibrium distribution $p = (1/3, 2/3)$.

2.4 Gauss-Seidel variant of the Power method

The power method recursively computes the components of $p^{(n+1)}$ from

$$p_i^{(n+1)} = \sum_{j=0}^{N} p_j^{(n)} p_{ji}, \qquad i = 0, 1, \ldots, N.$$

The Gauss-Seidel approach uses for the computation of $p_i^{(n+1)}$ the new estimates $p_j^{(n+1)}$ for $j \leq i$. Then the recursive scheme becomes

$$p_i^{(n+1)} = \sum_{j=0}^{i} p_j^{(n+1)} p_{ji} + \sum_{j=i+1}^{N} p_j^{(n)} p_{ji}, \qquad i = 0, 1, \ldots, N.$$

In vector-matrix notation this reads

$$p^{(n+1)} = p^{(n+1)} P_U + p^{(n)} P_L,$$

with P_U the upper triangular matrix with the diagonal of P, and P_L the lower diagonal matrix without the diagonal of P. This can be rewritten as

$$p^{(n+1)} = p^{(n)} P_{gs}, \tag{3}$$

with

$$P_{gs} = P_L (I - P_U)^{-1}. \tag{4}$$

Note that the inverse of $I - P_U$ exists, since P_U is a transient Markov chain. Since P_{gs} is a non-negative matrix with spectral radius 1 (see Exercise 4), the convergence properties

of scheme (3) can be analyzed along the same lines as scheme (2). The structure of P_{gs}, however, may differ from the structure of P. Clearly, P_{gs} is never irreducible (the first row has only zeros), and it may be periodic even if P is not.

In practice the convergence of the Gauss-Seidel scheme is usually much faster than the Power method.

Example 2.6
Consider the Markov chain in Example 2.5 again. The Gauss-Seidel scheme becomes

$$\begin{aligned} p_0^{(n+1)} &= p_0^{(n+1)}\frac{1}{2} + p_1^{(n)}\frac{1}{4}, \\ p_1^{(n+1)} &= p_0^{(n+1)}\frac{1}{2} + p_1^{(n+1)}\frac{3}{4}, \end{aligned}$$

which can be rewritten as

$$\begin{aligned} p_0^{(n+1)} &= p_1^{(n)}\frac{1}{2}, \\ p_1^{(n+1)} &= p_1^{(n)}. \end{aligned}$$

Hence

$$P_{gs} = \begin{pmatrix} 0 & 0 \\ \frac{1}{2} & 1 \end{pmatrix}.$$

Note that P_{gs} is not stochastic. Its eigenvalues are given by $\sigma_1 = 1$ and $\sigma_2 = 0$. When we start with the initial distribution $p^{(0)} = (0, 1)$, then $p^{(1)} = (1/2, 1)$, $p^{(2)} = (1/2, 1), \ldots$. So convergence is reached after one iteration.

Remark 2.7 Another variant of the Power method is the method of successive overrelaxation, see e.g. [6]. Here the components $p_i^{(n+1)}$ are recursively computed from

$$p_i^{(n+1)} = (1-\omega)p_i^{(n)} + \omega\left(\sum_{j=0}^{i-1} a_{ij}p_j^{(n+1)} + \sum_{j=i+1}^{N} a_{ij}p_j^{(n)}\right), \qquad i = 0, 1, \ldots, N,$$

where

$$a_{ij} = \frac{p_{ji}}{1-p_{ii}}, \qquad i, j = 0, 1, \ldots, N, \quad j \neq i,$$

and ω is the relaxation factor. Usually $1 \leq \omega \leq 2$. The iteration method with $\omega = 1$ is the Gauss-Seidel method.

2.5 Iterative bounds

In this section we provide another iteration scheme which also produces bounds on the equilibrium distribution. This scheme is obtained by reformulating (1) as a *contraction scheme* (see [8]).

Define

$$v_i = \frac{p_i}{p_0}, \qquad i = 0, 1, \ldots, N.$$

Then $v_0 = 1$ and (1) becomes

$$v_i = p_{0i} + \sum_{j=1}^{N} v_j p_{ji}, \qquad i = 1, \ldots, N. \tag{5}$$

Note that v_i is the expected number of visits to state i between two successive visits to state 0. Writing $r_i = p_{0i}$ and $q_{ij} = p_{ji}$, equation (5) turns into

$$v_i = r_i + \sum_{j=1}^{N} q_{ij} v_j, \qquad i = 1, \ldots, N. \tag{6}$$

This set of equations is contractive (cf. Exercise 3). To see this, note that since P is irreducible, the system ultimately leaves the set of states $\{1, 2, \ldots, N\}$, whence $Q^n \to 0$ and thus $\rho(Q) < 1$. Therefore the solution v can be approximated recursively by

$$v^{(n+1)} = r + Q v^{(n)}, \tag{7}$$

where $v^{(n)}$ and r are the N-column vectors with elements $v_i^{(n)}$ and r_i, $i = 1, \ldots, N$. Once v is known, p can be recovered via

$$p_i = \frac{v_i}{\sum_{j=0}^{N} v_j} \qquad i = 0, 1, \ldots, N,$$

and from lower and upper bounds on v,

$$\underline{v}_i \le v_i \le \overline{v}_i, \qquad i = 0, 1, \ldots, N,$$

bounds on p are determined via

$$\frac{\underline{v}_i}{\sum_{j=0}^{N} \overline{v}_j} \le p_i \le \frac{\overline{v}_i}{\sum_{j=0}^{N} \underline{v}_j}, \qquad i = 0, 1, \ldots, N.$$

In the remainder of this section we will derive the bounds on v. It will be assumed that Q is irreducible and aperiodic. The following two examples show that this is not an immediate consequence of the assumption that P is irreducible and aperiodic.

Example 2.8
The matrix P defined by

$$P = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{4} & 0 & \frac{3}{4} \end{pmatrix}$$

is irreducible, but the corresponding Q,

$$Q = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{3}{4} \end{pmatrix}$$

is not irreducible.

Example 2.9
The matrix P defined by

$$P = \begin{pmatrix} 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & 0 & \frac{1}{2} \\ \frac{1}{4} & \frac{3}{4} & 0 \end{pmatrix}$$

is aperiodic, but the corresponding Q,

$$Q = \begin{pmatrix} 0 & \frac{3}{4} \\ \frac{1}{2} & 0 \end{pmatrix}$$

is periodic.

For the difference between $v^{(n+1)}$ and $v^{(n)}$ it follows that

$$v^{(n+1)} - v^{(n)} = r + Qv^{(n)} - r - Qv^{(n-1)} = Q(v^{(n)} - v^{(n-1)}) = \cdots = Q^n(v^{(1)} - v^{(0)}).$$

Hence, when we take as initial vector $v^{(0)} = 0$, then $v^{(1)} - v^{(0)} = r \geq 0$, $r \neq 0$, and thus $v^{(n+1)} - v^{(n)} \geq 0$ for all n. Further, by Proposition (2.1),

$$v^{(n+1)} - v^{(n)} = a\rho^n(Q)y^* + O(n^k\rho_2^n(Q)), \qquad (n \to \infty), \tag{8}$$

where a is some positive constant and y^* is the positive right-eigenvector corresponding to the largest eigenvalue $\rho(Q)$ of Q. So $v^{(n+1)} - v^{(n)} > 0$ for n sufficiently large (and of course, once the difference is positive, it remains positive in all subsequent iterations).

Now define α_n and β_n by (if $v^{(n)} - v^{(n-1)} > 0$)

$$\alpha_n = \min_i \frac{v_i^{(n+1)} - v_i^{(n)}}{v_i^{(n)} - v_i^{(n-1)}}, \qquad \beta_n = \max_i \frac{v_i^{(n+1)} - v_i^{(n)}}{v_i^{(n)} - v_i^{(n-1)}}.$$

The numbers α_n and β_n are monotonically converging lower- and upperbounds on $\rho(Q)$,

$$\alpha_n \uparrow \rho(Q), \qquad \beta_n \downarrow \rho(Q), \qquad (n \to \infty).$$

The monotonicity $\alpha_{n+1} \geq \alpha_n$ follows from

$$v^{(n+2)} - v^{(n+1)} = Q(v^{(n+1)} - v^{(n)}) \geq Q\alpha_n(v^{(n)} - v^{(n-1)}) = \alpha_n(v^{(n+1)} - v^{(n)}).$$

Similarly $\beta_{n+1} \leq \beta_n$ and obviously $\alpha_n \leq \beta_n$. Further, relation (8) implies that

$$\frac{v_i^{(n+2)} - v_i^{(n+1)}}{v_i^{(n+1)} - v_i^{(n)}} = \rho(Q) + O\left(n^k \left(\frac{\rho_2(Q)}{\rho(Q)}\right)^n\right), \qquad (n \to \infty), \tag{9}$$

from which we can conclude that α_n and β_n converge to $\rho(Q)$.

So for n sufficiently large $\beta_n < 1$. In this case we can derive the following upperbound for v. Clearly

$$\begin{aligned} v &= v^{(n+1)} + (v^{(n+2)} - v^{(n+1)}) + (v^{(n+3)} - v^{(n+2)}) + \cdots \\ &= v^{(n+1)} + \sum_{k=1}^{\infty} (v^{(n+k+1)} - v^{(n+k)}). \end{aligned}$$

For $k \geq 1$ we have, by using that $\beta_{n+1} \leq \beta_n$,

$$\begin{aligned} v^{(n+k+1)} - v^{(n+k)} &\leq \beta_{n+k}(v^{(n+k)} - v^{(n+k-1)}) \\ &\leq \beta_n(v^{(n+k)} - v^{(n+k-1)}) \\ &\vdots \\ &\leq \beta_n^k(v^{(n+1)} - v^{(n)}). \end{aligned}$$

Hence,

$$v \leq v^{(n+1)} + \sum_{k=1}^{\infty} \beta_n^k (v^{(n+1)} - v^{(n)}) = v^{(n+1)} + \frac{\beta_n}{1-\beta_n}(v^{(n+1)} - v^{(n)}).$$

Similarly we can derive the following lowerbound,

$$v \geq v^{(n+1)} + \frac{\alpha_n}{1-\alpha_n}(v^{(n+1)} - v^{(n)}).$$

These bounds are easy to implement: while executing scheme (7), α_n and β_n can be computed and the bounds become better if α_n and β_n get closer to $\rho(Q)$. From the relation $v - v^{(n+1)} = Q(v - v^{(n)})$ we immediately see that $v^{(n)}$ converges to v with rate $\rho(Q)$. But the power of scheme (7) is not determined by the rate of convergence of $v^{(n)}$, but by *the rate of convergence of the bounds*. From (9) it is readily verified that the difference between the upper- and lowerbound converges to 0 with rate $\rho_2(Q)$. The contraction scheme with bounds is summarized in Figure 2. The bounds used in this scheme can be computed as soon as $v^{(n)} - v^{(n-1)}$ is strictly positive and β_n drops below 1.

Remark 2.10
The method (i.e., the number of iterations required) is sensitive to the choice of state 0. Choosing state 0 as a *likely* state is strongly recommended.

Remark 2.11
Let P denote the transition probability matrix of a Markov chain, and let r be the reward vector and β the discount factor. Then the total discounted reward vector v_β can be determined by successive iterations,

$$v^{(n+1)} = r + \beta P v^{(n)}, \qquad n = 0, 1, 2, \ldots,$$

and in each iteration,

$$v^{(n+1)} + \frac{\beta}{1-\beta} \min_i (v_i^{(n+1)} - v_i^{(n)}) e \leq v \leq v^{(n+1)} + \frac{\beta}{1-\beta} \max_i (v_i^{(n+1)} - v_i^{(n)}) e,$$

where e is the all one vector. The derivation of these bounds for v_β is very similar to the one for v (Verify!).

ITERATIVE BOUNDS

Set $v^{(0)} = 0$ and compute for $n = 0, 1, \ldots$

$$v^{(n+1)} = r + Qv^{(n)},$$

until $\overline{v}^{(n+1)} - \underline{v}^{(n+1)}$ is sufficiently small, where

$$\begin{aligned} \overline{v}^{(n+1)} &= v^{(n+1)} + \frac{\beta_n}{1-\beta_n}\,(v^{(n+1)} - v^{(n)}) \\ \underline{v}^{(n+1)} &= v^{(n+1)} + \frac{\alpha_n}{1-\alpha_n}\,(v^{(n+1)} - v^{(n)}). \end{aligned}$$

Then lower- and upperbounds for the equilibrium distribution p are obtained from the last $\underline{v}^{(n)}$ and $\overline{v}^{(n)}$ via

$$\frac{\underline{v}_i^{(n)}}{\sum_{j=0}^{N} \overline{v}_j^{(n)}} \le p_i \le \frac{\overline{v}_i^{(n)}}{\sum_{j=0}^{N} \underline{v}_j^{(n)}}\,, \qquad i = 0, 1, \ldots, N,$$

where by convention $\overline{v}_0^{(n)} = \underline{v}_0^{(n)} = 1$.

Figure 2: Iterative bounds

2.6 Gauss-Seidel variant of the iterative bounds

The set of equations (6) can of course also be solved by Gauss-Seidel iteration. Then the recursive scheme becomes

$$v_i^{(n+1)} = r_i + \sum_{j=1}^{i} q_{ij} v_j^{(n+1)} + \sum_{j=i+1}^{N} q_{ij} v_j^{(n)}, \qquad i = 1, \ldots, N.$$

In vector-matrix notation this reads as

$$v^{(n+1)} = r + Q_L v^{(n+1)} + Q_U v^{(n)},$$

where Q_L is the lower triangular matrix with the diagonal, and Q_U the upper triangular matrix without the diagonal of Q. This can be rewritten as

$$v^{(n+1)} = r_{gs} + Q_{gs} v^{(n)}, \tag{10}$$

with $r_{gs} = (I - Q_L)^{-1} r$ and $Q_{gs} = (I - Q_L)^{-1} Q_U$. From (10) we see that the Gauss-Seidel variant can be analyzed along the same lines as scheme (6). Thus we may conclude that the convergence behavior of Gauss-Seidel iteration is determined by the spectral radius and even more by the subradius of Q_{gs}. For the spectral radius we know that, if $\rho(Q) < 1$, then

$\rho(Q_{gs}) \leq \rho(Q)$ (see, e.g., p. 70 in [7]). For the subradius the situation is more complicated: the subradius of Q_{gs} may be less, but also greater than the subradius of Q. In practice, however, usually $\rho_2(Q_{gs}) < \rho_2(Q)$.

2.7 Exercises

Exercise 1.
Consider a Markov chain with transition probability matrix P. Define

$$m_j^n = \min_i (P^n)_{ij}, \qquad M_j^n = \max_i (P^n)_{ij}.$$

Prove that for all n,

$$m_j^n \leq m_j^{n+1} \leq M_j^{n+1} \leq M_j^n.$$

Exercise 2.
Consider an irreducible Markov chain with transition probability matrix P. Define

$$\widetilde{P} = \alpha I + (1-\alpha)P,$$

where $0 < \alpha < 1$ and I denotes the identity matrix.

(i) Show that $\widetilde{P}$ is aperiodic.

(ii) Show that P and $\widetilde{P}$ have the same equilibrium distribution.

Exercise 3.
Let Q be an irreducible aperiodic non-negative matrix and let y^* denote the positive right-eigenvector corresponding to the maximal eigenvalue of Q (see Proposition 2.1). Define the following norm,

$$\|x\|_{y^*} = \max_i \frac{|x_i|}{y_i^*}.$$

(i) Show that for all x we have $|x_i| \leq y_i^* \|x\|_{y^*}$ for each i.

(ii) Prove that $\|Qx\|_{y^*} \leq \rho(Q)\|x\|_{y^*}$ for all vectors x.

Hence, if $\rho(Q) < 1$, then Q is a *contraction*.

Exercise 4.
Let p be the equilibrium distribution of an irreducible Markov chain with transition probability matrix P.

(i) Show that p is a positive (left) eigenvector of P_{gs} as defined by (4).

(ii) Prove that $\|xP_{gs}\|_p \leq \|x\|_p$ for all vectors x, where the norm $\|\cdot\|_p$ is defined in Exercise 3.

(iii) Prove that $\rho(P_{gs}) \leq 1$.

References

[1] A. Berman, R.J. Plemmons, *Nonnegative matrices in the mathematical sciences*, Academic Press, New York, 1979.

[2] J.L. Doob, *Stochastic processes*, Wiley, New York, 1953.

[3] M.C. Pease, *Methods of matrix algebra*, Academic Press, New York, 1965.

[4] E. Seneta, *Nonnegative matrices and Markov chains*, 2nd edition, Springer-Verlag, Berlin, 1980.

[5] P.J. Schweitzer, *Iterative solution of the functional equations of undiscounted Markov renewal programming*, J. Math. Anal. Appl., 34 (1971), pp. 495–501.

[6] H.C. Tijms, *Stochastic modelling and analysis: a computational approach*, John Wiley & Sons, Chichester, 1990.

[7] R. Varga, *Matrix iterative analysis*, Prentice Hall, Englewood Cliffs, 1962.

[8] J. van der Wal, P.J. Schweitzer, *Iterative bounds on the equilibrium distribution of a finite Markov chain*, Prob. Eng. Inf. Sci., 1 (1987), pp. 117–131.