

**ITERATIVE METHODS FOR FINDING THE
STATIONARY VECTOR FOR MARKOV CHAINS**

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ITERATIVE METHODS FOR FINDING THE STATIONARY VECTOR FOR MARKOV CHAINS

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Abstract. This overview concerns methods for estimating the steady-state vector of an ergodic Markov chain. The problem can be cast as an ordinary eigenvalue problem, but since the eigenvalue is known, it can equally well be studied as a nullspace problem or as a linear system. We discuss iterative methods for each of these three formulations. Many of the applications, such as queuing modeling, have special structure that can be exploited computationally, and we give special emphasis to three ideas for exploiting this structure: decomposability, separability, and multilevel aggregation. Such ideas result in a large number of diverse algorithms, many of which are poorly understood.

Key words. Markov chains, stationary vectors, nullspace, decomposability, separability, multi-level iterations, multigrid, aggregation, small rank corrections, small norm corrections

AMS(MOS) subject classifications.

1. Introduction. This overview concerns the numerical approximation of stationary vectors of discrete Markov chains. The rest of this introductory section contains a sketch of the problem, a classification of the numerical methods, and examples of exploitable structure in Markov chain problems. The three following sections concern methods for the eigenvector formulation, the nullspace formulation, and the linear system formulation. The fifth section focuses on more specialized techniques that can exploit information about nearby problems.

This paper has been structured as an *overview* rather than a *survey*. The goal is to outline major research directions that have proven fruitful, present a sample of successful algorithms and theoretical results, and delineate opportunities for future research. In order to do this within a reasonable amount of space, the completeness of a survey has been sacrificed and many important algorithms, theorems, and references have regrettably been omitted. Related articles in this volume include those of Plemmons and Schweitzer.

1.1. Definitions and Notation. Discrete time Markov chains can be represented by a matrix P , whose (i, j) -element p_{ij} is the probability of a transition from state i to state j . The elements of the rows of P necessarily sum to one; i.e.,

$$(1) \quad Pe = e,$$

where e is the vector with each component equal to 1. If the n states of the Markov chain initially have a probability distribution z^T , where z_i ($i = 1, \dots, n$) is interpreted as the probability that the i th state of the chain is occupied, then at the next time unit the probability distribution is $z^T P$.

Equation (1) implies that 1 is an eigenvalue of P corresponding to the right eigenvector e . If the matrix P is irreducible and acyclic, or, equivalently, if the Markov chain is ergodic (has no transient states and is aperiodic) (see [43] and [18] for definitions), then this eigenvalue is simple and greater in magnitude than the other eigenvalues. Moreover, Perron-Frobenius theory [43, p.30] tells us that, corresponding

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to the eigenvalue 1, P has a positive left eigenvector π^T that is unique under the normalization

$$(2) \quad \pi^T e = 1.$$

The vector π^T is called the *steady state* or *stationary* vector of the chain, since, for almost every vector z of initial probabilities, it is the limit of the transient probabilities of the system:

$$\pi^T = \lim_{k \rightarrow \infty} z^T P^k, \quad z^T \geq 0, \quad z^T e = 1.$$

Iterative methods for estimating π^T are the chief concern of this overview.

The problem can be recast in the form

$$\pi^T Q = 0,$$

where $Q = I - P$. Although this form is a simple algebraic rearrangement of (2), it has important theoretical and computational consequences. In particular, the matrix Q is a *singular M-matrix*; that is, its diagonal elements are positive, its off-diagonal elements are nonpositive, and for any $\epsilon > 0$,

$$(\epsilon I + Q)^{-1} > 0.$$

This means that many of the techniques used for M-matrices can be brought to bear on the solution of Markov chains [43,23].

Two kinds of Markov chain problems have particularly simple solutions. A Markov chain is said to be *completely decomposable* or *uncoupled* if, after a suitable reordering of its states, P is a block diagonal matrix with $k \geq 2$ blocks. A problem in this form can be solved as k independent problems of smaller dimensions.

A Markov chain is *separable* if it can be written in the form

$$P = A \otimes I + I \otimes B,$$

where \otimes denotes the Kronecker tensor product. Many Markov chains arising in queuing networks are separable, or nearly so. Separable chains have a *product form solution* that can be written in closed form (see [19,42] for details and references).

1.2. Classification of Numerical Methods. The computation of the steady state vector of a Markov chain is in principle a remarkably easy eigenvalue problem. The eigenvalue is known to be 1. It is the eigenvalue of largest magnitude, and its multiplicity is 1. We know the right eigenvector, e , and need only find the left eigenvector.

On the other hand, several factors make the problem quite challenging. There may be many other eigenvalues clustered around the value 1, making iterative methods quite slow. Problems arising in many applications (e.g., queuing theory) produce sparse matrices of enormous size, limiting practical methods to a small number of matrix-vector products. Most intriguing of all, many practical problems are *nearly* decomposable or *nearly* separable, and such structure must be exploited in order for algorithms to be practical.

We will discuss the general principle of exploiting information about nearby problems. We consider three meanings of “nearby”:

1. *Nearly decomposable systems.* The matrix P for these problems is equal to a block diagonal matrix plus a correction that is small in norm. Nearly uncoupled Markov chains model systems in which groups of tightly coupled states are loosely coupled to one another. Such chains arise frequently in applications [11].
2. *Nearly separable systems.* The matrix P is equal to a separable matrix plus a small rank correction. Such problems arise in overflow queuing networks [5,6].
3. *Multilevel families of chains.* These models arise from analyzing a system at various levels of granularity. A coarse model may be able to provide approximate information for a more detailed model.

Because we know the eigenvalue, we have three choices for formulating the problem of finding the stationary vector:

1. *an eigenproblem* $\pi^T P = \pi^T$.
2. *a nullspace problem* $Q = I - P$, $\pi^T Q = 0$.
3. *a linear system* $\pi^T Q = 0$ with π_1 fixed to be 1 (or $\pi^T e = 1$, or some other normalization condition).

Various iterations have been proposed for each of these formulations, and we will focus on each in turn. Alternative algorithms that we will not discuss in this overview are direct methods for the second and third formulation (see the paper by G. W. Stewart in this volume) and methods of approximation based on fluid flow approximation and diffusion approximations to queuing networks.

2. Methods for the Eigenproblem Formulation. These methods are based on the fact that $\lim_{k \rightarrow \infty} P^k = e\pi^T$. There are many variants, all having the nice property that they require only the formation of vector-matrix products.

2.1. The Power Method and Subspace Iteration. The method of subspace iteration (also known as simultaneous iteration) extracts approximate solutions from the rows of the matrices $Z^T P^k$. When Z has only one row, the method is called the power method, and the iterates approach the solution by simulating the Markov chain until steady state is reached — often slowly. When Z has more than one row, a nonsymmetric analogue of Rayleigh-Ritz refinement is used to extract an approximation to the steady state vector. The theory and practice of the method are well understood [15,35,36].

Convergence of the power method (or simultaneous iteration) can be accelerated by matrix splitting techniques. A splitting of Q is a decomposition of the form

$$Q = M - N,$$

where M is nonsingular. Since

$$\pi^T M = \pi^T N,$$

a splitting gives rise to an iteration of the form

$$z_{k+1}^T = z_k^T N M^{-1}.$$

Splitting methods include Jacobi's method, successive over-relaxation, and their block variants.

Splittings have been subjected to intense study for solving inhomogeneous systems associated with discretizations of partial differential equations [43,44]. Because Q is

a singular M-matrix, some of the convergence results carry over to the solution of Markov chains (e.g., see [22,23,17,21]). Although splitting methods can be used alone, they are most often used in conjunction with aggregation methods, discussed in §5.

2.2. Krylov Sequence Methods. In many respects these are some of the most promising and least well understood methods. They extract approximate solutions from the Krylov sequence $\{z^T, z^T P, z^T P^2, \dots\}$. The basic algorithm is known as the method of Arnoldi, and some variants have been surveyed by Saad [28]. The nonsymmetric Lanczos method works with Krylov sequences in powers of P and P^T . The symmetric Lanczos method can be applied to PP^T . There are related variants, conjugate gradient methods, for solving linear systems. For brevity we will only discuss the method of Arnoldi here.

Arnoldi's method is based on the observation that if the vectors $\{z^T, z^T P, z^T P^2, \dots\}$ are orthonormalized, say by the Gram-Schmidt algorithm, to produce a sequence $\{v_0^T, v_1^T, \dots\}$, then the matrices $V_k = (v_0, v_1, \dots, v_{k-1})$ satisfy

$$V_{k-1}^T P = H_k^T V_k^T,$$

where H_k is an $(k+1) \times k$ upper Hessenberg matrix. The eigenvalues of \hat{H}_k , the leading $k \times k$ submatrix of H_k , are approximations to eigenvalues of P , and the approximate eigenvectors are V_k times eigenvectors of \hat{H}_k . Under exact arithmetic, the matrix \hat{H}_n^T is similar to P , and the approximate eigenvalues and eigenvectors are exact.

In practice, for the sake of time and storage, the iteration must be terminated long before $k = n$. This leads to the *Arnoldi algorithm with restarts*, in which the iteration is restarted every k steps with a refined z_0 .

Even apart from its use with Markov chains, there are many unanswered questions about convergence properties of this algorithm.

Much study has been devoted to the symmetric version, the Lanczos algorithm [25]. The eigenvalues and eigenvectors of the (now tridiagonal) matrices H_k converge, the convergence being faster for the extreme eigenvalues. Since 1 is an extreme eigenvalue of the positive definite matrix PP^T with eigenvector π , the Lanczos method applied to PP^T is a good candidate for solving large Markov chains. However, some issues are not well resolved — in particular, those relating to restarting the iteration when the reduced system grows too large.

The nonsymmetric iteration has received much less attention. The interlacing properties and monotone convergence are lost. Convergence is no longer assured; the restart strategy must be carefully designed. It is thus necessary to study the local behavior of the iterative Arnoldi algorithm and determine how accurate the initial approximation must be in order to guarantee convergence to the dominant eigenvalue. Other issues such as convergence bounds, computable error bounds, computational variants, the effects of inexact arithmetic, and the need for reorthogonalization of the basis vectors require serious study.

The question arises of how extra information about Markov chain problems might be used to guarantee and accelerate convergence of the Arnoldi algorithm.

One approach is to develop preconditioners appropriate to Markov models:

1. We can use similarity transformations to convert the problem $\pi^T P = \pi^T$ to $\hat{\pi}^T \hat{P} = \hat{\pi}^T$, where $\hat{\pi} = U^{-T} \pi$ and $\hat{P} = U P U^{-1}$ for some matrix U [27]. This does not change the distribution of the eigenvalues but can rotate the solution vector towards a known one.
2. We can choose a polynomial $\mathcal{P}(x)$ such that $\mathcal{P}(1) = 1$ and solve the problem $\pi^T \mathcal{P}(P) = \pi^T$. This changes the distribution of the eigenvalues. [29]

3. Matrix splitting techniques can be used to change the distribution of the eigenvalues. These matrix splittings can be developed from separable queuing models related to the given problem, by multigrid analogues, and by other aggregation ideas as in §5 [26].

Such ideas have been studied in the context of the power method, but their effectiveness in combination with Arnoldi's algorithm or the nonsymmetric Lanczos method is just beginning to be understood.

An alternate approach is to devise an algorithm which forms the Krylov subspace, as in the Arnoldi iteration, but rather than finding eigenvalues of the reduced operator, minimizes a function such as $\|z^T A - z^T\|$ over all vectors z^T of length 1 in the Krylov subspace [26]. Convergence properties and effective preconditioners should be studied.

3. Methods for the Null-Space Formulation. A variety of projection methods have proven effective for solving nonsymmetric systems of linear equations [2], but their behavior for homogeneous systems is less well understood. As an example of this class of methods, we consider the projection method of Kaczmarz [16], which for the solution of $\pi^T Q = 0$ has the following form. Let Q be partitioned by columns:

$$Q = (q_1 \ q_2 \ \dots \ q_n).$$

Let

$$R_i = I - \frac{q_i q_i^T}{q_i^T q_i}$$

be the projection onto the orthogonal complement of the i th column of Q , and let

$$S = R_1 R_2 \dots R_n.$$

Starting with some initial vector z_0 , iterate according to the scheme

$$z_{k+1}^T = z_k^T S.$$

It can be shown that under mild restrictions on z_0^T , the sequence z_k^T converges to a multiple of π^T .

The appealing fact about Kaczmarz' method is its simplicity. It requires only one column of Q at a time, and it requires only one n -vector of storage. For this reason it is well suited to queuing models, where the number of states is very large.

Kaczmarz's method for inhomogeneous systems has been extensively analyzed [14,1,12]. In spite of this, very little is known about the rate of convergence of the method for Markov problems.

Bramley and Sameh [2] have used projection methods as a preconditioner for Krylov subspace methods for nonsymmetric linear systems. A similar idea should be quite effective for Markov chain problems.

4. Methods for the Linear System Formulation. Let P_{n-1} denote a submatrix of P formed by deleting any one column. Then the linear system

$$\pi^T P_{n-1} = 0, \quad \pi^T w = 1,$$

where w is any nonzero vector, is a nonsingular linear system whose solution determines the stationary vector π^T up to a normalization factor. Standard iterative

techniques (Jacobi, successive overrelaxation, Krylov subspace methods) can be applied to this augmented system, and preconditioners can also be used to accelerate convergence.

Although such techniques have been studied, it is perhaps more natural to deal directly with the homogeneous system [17] or with the consistent system of $n + 1$ equations in the n unknowns π . Many of the iterative methods discussed above can be used on this overdetermined system.

5. Exploiting Nearby Problems. Since Markov chain problems tend to be quite enormous in dimension, it is important to minimize the amount of work required to compute the stationary vector. One unifying principle has been used quite successfully: exploit information about nearby, more easily analyzed Markov chains. A prime example of this is the development of successful algorithms for solving nearly decomposable systems. There is potential for progress on other classes of problems as well, in particular, for nearly separable systems and for systems that are naturally part of a multilevel family of problems.

5.1. Nearly Decomposable Systems: Aggregation methods. These methods lump states together and solve the resulting reduced chain. The solution along with auxiliary information is then used to approximate the eigenvector. For nearly uncoupled chains, one step often results in a sufficiently accurate approximation. They can be combined with other iterative methods to yield hybrid methods.

When the Markov chain is nearly uncoupled, the Rayleigh-Ritz refinement is usually called aggregation. For these chains aggregation can be done with the single vector coming from the power method. The resulting algorithm is a method proposed and analyzed by McAllister, Stewart, and Stewart [20]. The surprising fact is that there are theoretical reasons for believing that this method is competitive with simultaneous iteration, though it requires less work.

There are many different aggregation methods, but all are based on a partitioning of π^T into subvectors. The states corresponding to each subvector are then *aggregated* into a single state, and the stationary vector for the aggregate problem is used to improve an approximation to π^T .

When one aggregation step is not enough, aggregation can be coupled with an iterative method (power method, [20], splitting methods [37,4], etc.). Xiaobai Sun [38] has developed a unified theory for these methods.

For general Markov chains, aggregation methods seem to have been first proposed by Takahashi [40,39]. There is an extensive literature on the methods (e.g., [7,8,9,13,31,30]). The performance of aggregation methods in general is spotty; they can be quite slow.

When a chain is nearly uncoupled, one aggregation step often gives a sufficiently accurate approximation. The properties of nearly uncoupled systems were first pointed out by Simon and Ando [32] and have been the subject of many investigations [10,33,34].

5.2. Nearly Separable Systems. Such problems arise in overflow queuing networks, where the matrix P is equal to a separable matrix plus a small rank correction.

Consider a very simple example involving two queues. Suppose that there are $n_k - 1$ spaces and s_k servers in the k th queue ($k = 1, 2$), and that customers arrive at the k th queue at rate λ_k and are served at rate μ_k . If we let state (k, l) correspond to having k customers in queue 1 and l customers in queue 2, then we can define the matrix P for the model.

If there is no interaction between the queues, then the matrix is

$$\hat{P} = P_{n_1}(\lambda_1, \mu_1, s_1) \otimes I + I \otimes P_{n_2}(\lambda_2, \mu_2, s_2),$$

where $P_m(\lambda, \mu, s)$ is the matrix of size m for a single queue with arrival rate λ , s servers, and service rate μ .

If overflow is allowed, e.g., if customers overflow into queue 2 whenever queue 1 is full, then the resulting matrix is

$$P = \hat{P} + E,$$

where E is a matrix with λ_1 in diagonal positions corresponding to queue 1 being full, and $-\lambda_1$ in the off-diagonal position of these rows corresponding to queue 1 being full and queue 2 having one more customer.

The relation between the matrices P and \hat{P} can be exploited. The most obvious way is to use a splitting of P as $M = \hat{P}$ and $N = -E$. This splitting can be used to accelerate the iterative methods discussed above [5,6].

A less expensive way to use the relation between the separable and nonseparable problems is to initialize the iteration for the nonseparable one using the stationary vector for a related separable model. For our example, we model queue 2 as an independent queue with arrival rate $\hat{\lambda}_2 = \lambda_2 + \lambda_1 p_1^{full}$, where p_1^{full} is the probability that queue 1 is full. The resulting matrix is

$$\tilde{P} = P_{n_1}(\lambda_1, \mu_1, s_1) \otimes I + I \otimes P_{n_2}(\hat{\lambda}_2, \mu_2, s_2),$$

The stationary vector for \tilde{P} is the outer product of the stationary vectors for P_{n_1} and P_{n_2} . Since the state of queue 1 is independent of the state of queue 2, the probability that queue 1 is full can be computed directly by finding the stationary vector for $P_{n_1}(\lambda_1, \mu_1, s_1)$, and then we need only find the stationary vector for $P_{n_2}(\lambda_2 + \lambda_1 p_1^{full}, \mu_2, s_2)$.

For more complicated problems, the probabilities that queues are full in the separable model are found by solving a system of nonlinear equations with one equation per queue:

$$p^{full} = f(p^{full}),$$

where f_k is the probability that queue k is full given the probabilities that the other queues are full.

Given an arrival rate for a queue of size m , it is an $O(m)$ process to compute the stationary vector, so the process of solving the nonlinear system of equations costs only a fraction of the time required to compute a single matrix-vector multiplication using the nonseparable model matrix P .

Using the separable problem as an approximation to overflow queuing networks is an old idea, but using it to initialize an iterative algorithm for the overflow network seems to be new.

As a simple example, on a three queue problem with $n = (8, 8, 4)$, $s = (5, 2, 1)$, $\lambda = (.9, .7, .5)$, and $\mu = (.1, .4, .5)$, allowing overflow from queue 1 to queue 2, and from queue 2 to queue 3, the solution to the separable problem is a factor of 4 closer to the stationary vector than is e^T , and the power method converges in 57 iterations to a solution that satisfies $\|\hat{z}^T P - \hat{z}\| \leq 10^{-4}$, a savings of 33 iterations over the iteration started from e^T .

5.3. Multilevel Families of Problems. These models arise from analyzing a system at various levels of granularity. As an example, a coarse model of a queuing system may be able to provide approximate information for a more detailed model.

Much research into such multilevel families has proceeded under the title of *algebraic multigrid methods*. These were an outgrowth of the *geometric* multigrid methods for discretizations of partial differential equations, and correspond to semi-automatic aggregation techniques based on the structure of the matrix rather than the connectivity of the variable dependencies in the underlying model. There is some overlap between these investigations and the aggregation research.

It seems that there is progress to be made in a more geometric approach to Markov chain problems and, in particular, to queuing theory problems. The connectivity of the states imposes a mesh structure on the unknown transition probabilities reminiscent of the mesh structure for discretizations of differential equations. The proportions of the dimensions of the problems are quite different, though. Differential equations typically are solved in 2 or 3 dimensions with a large number of mesh points per dimension. This corresponds to 2 or 3 interacting queues with a large number of waiting spaces in each queue. The Markov problems typically correspond to very high dimensional problems with relatively few mesh points per dimension.

A multigrid approach to a partial differential equation takes advantage of the convergence of discrete approximations as the number of mesh points converges to infinity. This leads to a family of nested grids that can be used in concert to accelerate convergence [3]. For queues, we can build a similar family of nested approximations to states. Chan [5,6] cleverly exploited this relation, and Park [24] made some further progress in understanding the relation between the nested models, but more could be done.

6. Conclusions. In this overview we have considered algorithms for computing the stationary vector of a Markov chain using the eigenproblem formulation, the null-space formulation, and the linear system formulation. Although promising algorithms have been identified for each formulation, we lack data on the comparison of algorithms for different formulations, and much work remains to be done.

Although ideas such as aggregation for nearly decomposable systems have now been rather thoroughly studied, other ideas, such as exploiting the relation to nearby separable problems and to multilevel families, still lack a firm foundation.

These factors, coupled with the importance of Markov models in queuing theory and other applications, ensure that iterative methods for computing the stationary vector of a Markov chain will remain an exciting area for research in the next decade.

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