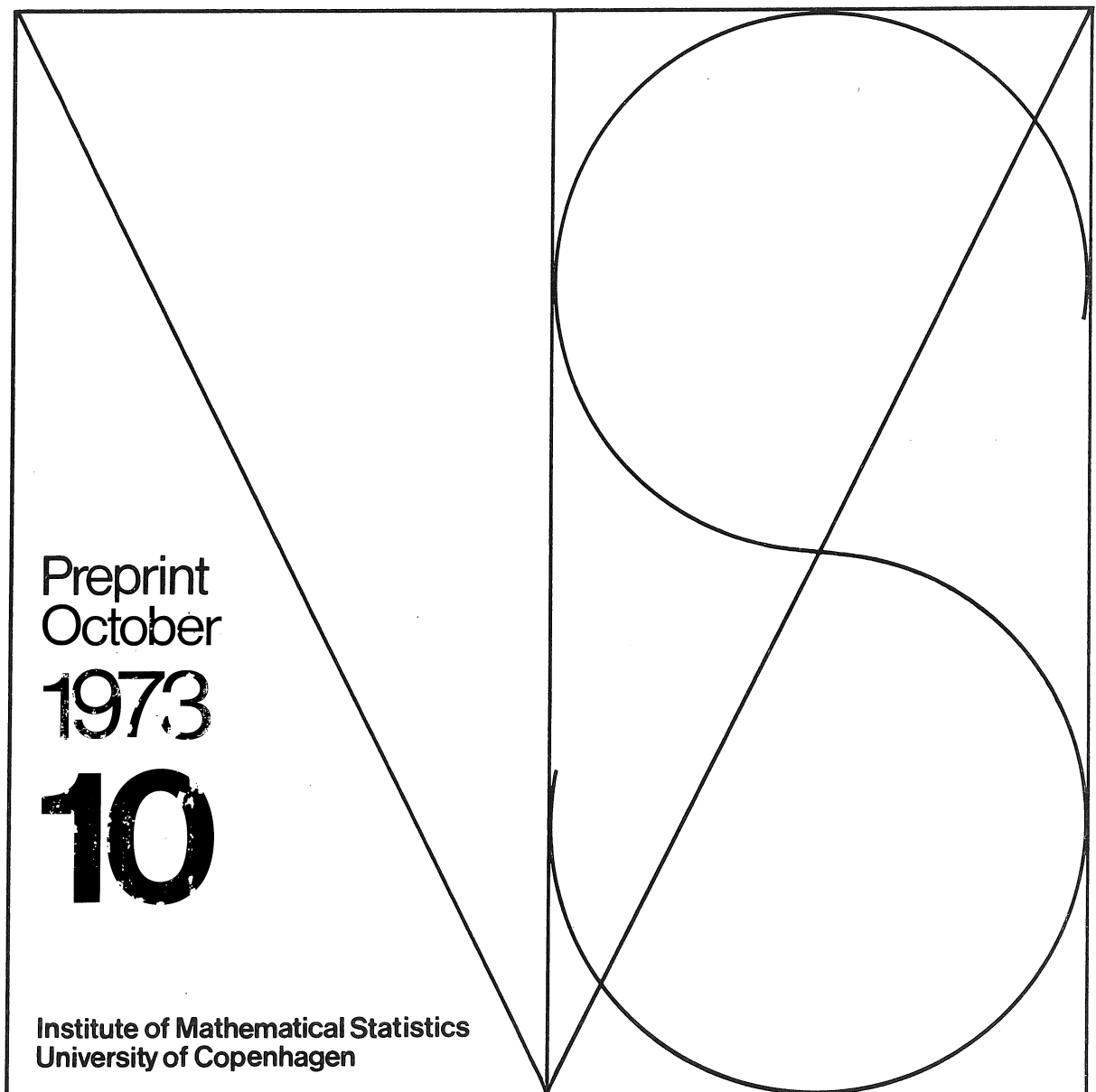


Søren Johansen

The Imbedding Problem
for Markov Chains



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Preface

The work summarized in this report has mainly been carried out in the period from 1970 to 1973 and was initiated by Professor Gerald S. Goodman, who presented his results on the change of time scale for Markov chains and its implications to the imbedding problem in a lecture at the Institute of Mathematical Statistics in Copenhagen.

Since then I have been collaborating closely with Gerald Goodman and most of the results have grown out of discussions with him and I wish to thank him sincerely for his continuing interest in my work and for insisting that the imbedding problem was important.

In 1972/1973 Professor F.L. Ramsey visited the Institute and I want to thank him for discussions which eventually led to one of the few explicit results in the theory.

I also want to thank Professor D.R. Cox for allowing me to spend a fruitful year at Imperial College in 1971/72 and to Professor G.E.H. Reuter for many valuable comments.

Finally I wish to thank my colleagues at the Institute of Mathematical Statistics for patiently listening to a long series of seminars all having to do with the imbedding problem and all having the same title as the present report.

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Søren Johansen.

1. Introduction

The problem of characterizing the stochastic matrices which can occur in a continuous time Markov chain was first formulated by Elfving in 1937, see [7] and [8]. This problem was mentioned by Chung in 1960, [1] p. 203, and in the last 10 years a number of papers have appeared.

In this note we shall present a brief outline of the methods and results in the papers [13] - [20] and relate them to the other work in the area.

We first introduce the basic notation and definitions for finite state chains. Let P denote an $n \times n$ stochastic matrix with elements p_{ij} , i.e.

$$p_{ij} \geq 0, \sum_j p_{ij} = 1.$$

An intensity matrix Q is a matrix with elements q_{ij} , such that

$$q_{ij} \geq 0, i \neq j, \sum_j q_{ij} = 0.$$

A Markov chain is a continuous family

$$\{P(s,t), 0 \leq s \leq t < t_0\} \quad (1.1)$$

of stochastic matrices satisfying the Chapman-Kolmogorov equations:

$$P(s,t) = P(s,u)P(u,t), 0 \leq s \leq u \leq t < t_0, \quad (1.2)$$

and

$$P(s,s) = I, 0 \leq s < t_0. \quad (1.3)$$

The stochastic matrix P is called imbeddable if there exists a Markov chain such that

$$P(0,1) = P. \quad (1.4)$$

We say that P is imbeddable in a homogeneous chain if

the family (1.1) depends only on $t-s$.

An important idea in the discussion of the equations (1.2) is the following: The equations are clearly invariant under a homeomorphic change of time scale and it was observed by Goodman [10] that if one chooses

$$\varphi(t) = - \ln \text{Det } P(0,t) \quad (1.5)$$

as the new time scale, then the functions $P(.,t)$ and $P(s,.)$ become absolutely continuous and can be characterized as the unique solution to the Kolmogorov differential equations:

$$\partial_t P(s,t) = P(s,t)Q(t), \quad t \in N, \quad (1.6)$$

$$\partial_s P(s,t) = - Q(s)P(s,t), \quad s \in N, \quad (1.7)$$

$$P(s,s) = I, \quad (1.8)$$

where N is a null set for Lebesgue measure, and $Q(.)$ is a bounded measurable function with values in the set of intensity matrices.

The solution to these equations can be constructed as a product integral

$$P(s,t) = \prod_s^t (I + Q(u)du), \quad (1.9)$$

see Schlesinger [38] and Dobrušin [6].

In view of these results the imbedding problem can be formulated by means of the theory of differential equations. More specifically, consider the controlsystem (1.6) for $s = 0$ and $P(t) = P(0,t)$:

$$DP(t) = P(t)Q(t), \quad t \in N, \quad (1.9)$$

where the controller $Q(.)$ is chosen in the convex cone of intensity matrices. In this language a matrix P can be imbedded if it can be reached using a bounded measurable controller in a finite time, and the imbedding problem is that of charac-

terizing the reachable set.

In this formulation one naturally asks for a Bang-Bang representation of an imbeddable matrix, i.e. a representation of P as a finite product of matrices generated by the extremal intensity matrices since this corresponds to reaching P by switching the controller a finite number of times between the extremal controllers. This problem has been treated in [16] and [19].

For countable state chains the definitions are similar to (1.1), (1.2), (1.3) and (1.4) but one will have to specify in each case which concept of continuity is required.

Clearly the determinant need not exist and one will have to choose another time scale. In [14] it is shown that under the assumption of continuity of $p_{ij}(s,t)$ uniformly in (i,j) one can use the expected number of jumps and in [20] it is shown that for a class of Markov branching processes one can choose the expected size of the population provided it is assumed to be finite and continuous in (s,t) .

One can think of the above as a semigroup approach, since clearly the set of stochastic matrices as well as the set of imbeddable matrices form a semigroup.

It is, however, also possible to apply a convex analysis to the set of stochastic matrices, which clearly form a convex compact set. The extreme points are easily identified with the matrices with entries 0 and 1 and they form a semigroup under multiplication. A stochastic matrix can then be represented as a convex combination of the extreme points or as a probability measure on a semigroup. Conversely given a probability measure on a semigroup one can construct the corresponding random walk which is a Markov chain with discrete time.

It is easily seen that convolution of the probability measures corresponds to multiplication of the stochastic matrices, see [15],[20] and also Maksimov [29].

Thus the stochastic matrices can be thought of as a representation of the measures on semigroups, and there is a close connection between stochastic processes with independent increments and imbeddable stochastic matrices. This relation is used in [17] and [20] to suggest the definitions and results for Markov chains as well as a central limit theorem for random variables on finite semigroups and the definition of infinite factorizability.

There is also a relation between the Lévy-Khinchin representation of infinitely divisible distributions see [13] and the Bang-Bang representation as presented in [16] and [19] in that they both clarify the rôle of the extreme intensities as generating the "building blocks" of the semigroup.

The basic structure of the stochastic matrices that is used is that they form a convex semigroup. The set has many other properties, like the extreme points form a semigroup, the multiplication is bilinear and for finite state space there exists a homomorphism onto $[0,1]$ with multiplication, namely the determinant.

There are many other examples of convex semigroups, the most obvious is that the set of probability measures on a semigroup is itself a semigroup under convolution. The set of doubly stochastic matrices with multiplication, the set of characteristic functions of probability measures on \mathbb{R} again with multiplication, but also the set of generating functions of probability measures on the positive integers with composition as the semigroup operation form convex semigroups see [20].

Many of the results derived here for finite stochastic matrices can be proved for convex semigroups with some extra structure as indicated above, but we shall only be concerned here with results that have a direct interpretation in terms of Markov chains.

2. Non-homogeneous finite state Markov chains.

In this section we shall give some of the results obtained on the imbedding problem for finite state non-homogeneous Markov chains and in particular for processes with independent increments and values in a finite semigroup.

2.1. Definition. A stochastic matrix P is called infinitely factorizable if for all $\epsilon > 0$ there exist P_1, \dots, P_n such that

$$P = P_1 \cdot \dots \cdot P_n \quad (2.1)$$

$$\|I - P_i\| \leq \epsilon, \quad i = 1, \dots, n, \quad (2.2)$$

where

$$\|I - P\| = \sup_i \sum_j |\delta_{ij} - p_{ij}| = 2 \sup_i (1 - p_{ii}).$$

This concept was first used by Loewner [28] who studied the semigroup of schlicht mappings of the unit disc into itself but has also been used by Maksimov [31] and [32] in the discussion of probability measures on groups.

2.2. Definition. A triangular array is a family $\{P_{m,k}, k = 1, \dots, m, m = 1, 2, \dots\}$ of stochastic matrices. The marginal products are

$$P_m = \prod_{k=1}^m P_{m,k}$$

and the limit is $\lim_m P_m$. The array is a null array if

$$\lim_m \sup_k \|I - P_{m,k}\| = 0.$$

The concept of a triangular array is well known in probability, see Grenander [11], Kendall [23], Davidson [5] and Gnedenko and Kolmogorov [9].

The relation between probability measures on semigroups and stochastic matrices suggests the following results, which

has been proved in [17]:

2.3. Theorem. Let P be a non-singular stochastic matrix, then the following statements are equivalent:

P is imbeddable. (2.3)

P is infinitely factorizable (2.4)

P is the limit of a triangular null array (2.5)

The basic idea of the proof is to find the proper notion of a companion array as in the classical theory of infinitely divisible distributions.

If we consider the problem as a control problem we have to discuss the extremal controllers. The intensity matrices form a convex cone and an extremal element has at most one positive off-diagonal element. The stochastic matrix generated by an extremal intensity is called a Poisson matrix and is characterized by having at most one positive off-diagonal element.

By means of this we prove in [17] the following theorem:

2.4. Theorem. Let P be a non-singular stochastic matrix, then P is imbeddable if and only if P can be approximated by a finite product of Poisson matrices.

Using this result and the techniques from control theory see Lee and Markus [26] we get the following Bang-Bang representation [16]:

2.5. Theorem. Let P be in the interior of the imbeddable matrices, then P has a representation as a finite product of Poisson matrices.

Finally one would like to extend this result to hold for all imbeddable matrices.

This has been proved in [19] for 3×3 matrices, and in fact if $\text{Det } P \geq \frac{1}{2}$ we need only use 6 Poisson matrices to re-

présent P.

Kingman and Williams [25] have studied the zero configuration of the imbeddable matrices and shown that it can be represented as a finite product of zero configurations which are reflexive and transitive.

The set of imbeddable matrices is not convex, but in [16] it is proved that it is starshaped around the stochastic matrix with equal entries, and it is quite easily seen that the convex hull is the set of all stochastic matrices.

In [18] another semigroup is considered namely the set of matrices that can be imbedded using symmetric intensity matrices. This problem continues an investigation by Loewner [27] who considered the control problem

$$DX(t) = - Q(t)X(t), X(t) \in R^n$$

where $Q(t)$ is a symmetric intensity matrix.

It can easily be seen that the symmetric stochastic matrices with two off-diagonal elements equal to $\frac{1}{2}$ and the rest equal to 0 are on the boundary of the imbeddable set. There are $\frac{1}{2}n(n-1)$ such matrices, and one can prove that the convex hull of the set we get by taking products of not more than $\frac{1}{2}n(n-1)$ of these equals the closed convex hull of the imbeddable matrices. Thus we have found the smallest convex semigroup containing the matrices imbeddable by symmetric intensities. The result is proved for $n = 3$ in [18], where also the supporting hyperplanes of the set are found. This gives thus a lot of necessary conditions for imbeddability.

The semigroup of probability measures on a finite semigroup is studied to give results about the special type of Markov chains formed by processes with independent increments.

The semigroup has all the properties of the set of stochastic matrices, in particular we have a homomorphism defined by

$$h(\nu) = |\text{Det } P(\nu)|$$

where $P(\nu)$ denote the transition probability matrix for the random walk determined by the probability measure ν .

Martin-Löf [33] used results about Markov chains to derive results about random walks and infinitely divisible distributions. In [17] we prove a central limit theorem and characterize the marginal distributions in processes with independent increments in a manner analogous to Theorem 2.3. This generalizes some results by Maksimov [30] and [31].

Finally we can turn these results around and obtain a criterion for imbeddability:

2.6. Theorem. A stochastic matrix is imbeddable if and only if it can be represented by a non-singular infinitely factorizable probability measure on the extreme stochastic matrices.

3. Homogeneous finite state Markov chains

For homogeneous chains the imbedding problem is that of finding a continuous one parameter semigroup of stochastic matrices that contains P . Since any continuous one parameter semigroup is of the form $\{P(t) = \exp tQ, 0 \leq t < \infty\}$ for some intensity matrix Q , this problem is closely related to finding the logarithm of P . In fact Elfving [7] assumed that P had distinct eigenvalues, which then have to be positive or come in complex conjugate pairs, and then determined the various logarithms by diagonalizing the matrix.

He proved that only finitely many logarithms were admissible and the solution to the imbedding problem is then to search among these logarithms for an intensity matrix.

Cuthbert [3] and [4] discusses the logarithm function by means of the Jordan form and finds criteria for a unique imbedding. He also gives a criterion for imbeddability in terms

of a series expansion for the logarithm. Speakman [39] gave an example of a stochastic matrix which could be imbedded in two different ways.

Elfving [7] obtained some simple inequalities for the eigenvalues of an imbeddable matrix and Runneburg [36] described the region of the complex plane where the eigenvalues can be found, using results of Karpelewitch [22].

In [15] a criterion for imbeddability is given in terms of a power series expression for the logarithm. For $n = 3$ this gives manageable conditions for imbeddability in terms of P, P^2 and the eigenvalues of P .

Conditions of a different kind can be found using infinite divisibility.

3.1. Definition. The stochastic matrix P is called infinitely divisible if for all n there exists P_n such that $P = (P_n)^n$.

The basic result is due to Kingman [24] who proved that a non-singular P is imbeddable in a homogeneous chain if and only if P is infinitely divisible. It was this result that revived the interest in the imbedding problem and it has inspired almost all the subsequent work in this area.

Ott [35] extended this result to singular P and Vere-Jones proved the result for the semigroup of stochastic matrices that reduce to diagonal form by a fixed non-singular transformation.

In [17] we also prove Kingman's result and characterize the non-singular imbeddable P as limits of triangular null arrays with commuting elements in each row.

We also obtain results for processes with independent increments similar to the results in the non-homogeneous case and then apply them to the imbedding problem as follows:

3.2. Theorem. A stochastic matrix P can be imbedded in a homogeneous Markov chain if and only if it can be represented by an infinitely divisible probability measure on the extreme stochastic matrices.

This result is proved in [15]. It should be emphasized that the notions of infinite factorizability and infinite divisibility coincide if the semigroup is commutative.

Finally Cohen [2] has defined a class of semigroups obtained from a given semigroup and a kernel. He then applies this result to characterize a subclass of infinitely divisible matrices by means of a positive definiteness condition.

4. Countable state Markov chains.

No results are known for the general imbedding problem for countable state Markov chains. For certain classes of Markov chains, however, the problem has been studied.

The first example is the set of random walks on the integers which are Markov chains. The multiplication of the matrices corresponds to convolution of the measures underlying the random walks.

Since this convolution is commutative there is no distinction between the homogeneous and the non-homogeneous imbedding and the imbeddable matrices just correspond to the classical infinitely divisible distributions, see Gnedenko and Kolmogorov [9] or [13].

Another example is the Markov branching processes. The stochastic matrices considered here have the property that the s 'th row is the s -fold convolution of the first row. These matrices form a semigroup and one can prove the analogue of Theorems 2.3, and 2.4 for this semigroup with an appropriate definition of infinite factorizability and the continuity of the imbedding family, see [20].

The homogeneous imbedding problem has been considered by Karlin and Mc Gregor [21] who gave many necessary conditions for imbeddability thereby proving that many of the wellknown distributions on the integers can not occur as distributions in continuous time Markov branching processes, see also Wang [41].

5. Dansk resume

Indlejningsproblemet for Markov processer blev formuleret af Elfving i 1937 se [7] og [8]. I 1962 beviste Kingman, at en regulær stokastisk matrix kan indlejres i en tidshomogen Markovkæde, hvis og kun hvis den er uendelig delbar, og i 1970 viste Goodman [10] at indlejningsproblemet kunne formuleres som et kontrolproblem for en bilinear differential-ligning og knyttede forbindelsen til Loewners arbejde [28].

Disse arbejder sammen med den simple observation, at en stokastiskmatrix kan skrives som en konveks kombination af de ekstreme stokastiske matrixer danner grundlaget for den teori jeg har arbejdet med i artiklerne [13] til [20].

Vi definerer en Markovkæde som en familie (1.1), der opfylder betingelserne (1.2) og (1.3), og vi siger, at P kan indlejres hvis der findes en Markovkæde således, at (1.4) er opfyldt. Hvis denne familie alene afhænger af $(t-s)$ siger vi, at P kan indlejres i en homogen kæde.

Betragter vi mængden af regulære $n \times n$ stokastiske matrixer, som en semigruppe, vil de matrixer, der kan indlejres udgøre en undersemigruppe.

I [17] karakteriseres denne undersemigruppe som de elementer, der er uendelig faktoriserbare, se definition 2.1, eller som de elementer, der er grænseværdi af trekantsskemaer, se definition 2.2.

Ved at udnytte Goodman's ide om at formulere indlejnings-

problemet som et kontrolproblem for Kolmogorov' differential ligninger (1.6), (1.7) og (1.8) er der i [16] bevist, at enhver matrix idet indre af de indlejrlige matricer kan repræsenteres som et endeligt produkt af stokastiske matricer med præcis eet positivt led uden for diagonalen og i [19] har jeg sammen med Fred Ramsey vist, at for 3×3 matricer kan alle matricer, der kan indlejres repræsenteres på denne måde. Denne repræsentation kaldes i kontrolteorien en Bang-Bang repræsentation, idet den svarer til, at man har styret processen ved at skifte et endelig antal gange mellem de ekstremale kontroller.

Ved at repræsentere en stokastisk matrix, som en konveks kombination af de ekstreme stokastiske matricer, der udgør en semigruppe, kan man knytte en forbindelse mellem foldning af mål på endelige semigrupper og multiplikation af de tilsvarende stokastiske matricer.

Ved at udnytte disse ideer er der i [17] bevist en central grænseværdisætning for stokastiske variable med værdier i endelige semigrupper, og vi kan derfor karakterisere de indlejrlige matricer som de, der kan repræsenteres ved et uendeligt faktoriserbart sandsynlighedsmål.

I [18] er der undersøgt en anden semigruppe bestående af de stokastiske matricer, der kan frembringes af symmetriske intensiteter. Jeg finder her det konvekse hylster af de indlejrlige matricer, og kan derfor finde en række nødvendige betingelser for at en matrix kan indlejres.

For det homogene indlejningsproblem har jeg i [15] angivet et kriterium for at en $n \times n$ stokastisk matrix P med forskellige egenverdier kan indlejres. For 3×3 matricer reducerer dette til en relativt simpel betingelse udtrykt ved P, P^2 og egenverdierne.

For processer med numerabelt tilstandsrum er resultaterne sparsomme. Problemet omkring tidsskift er behandlet sammen med Goodman [14] for processer med ligelig kontinuerte over-

gangssandsynligheder og for forgreningsprocesser i [20]. I [20] har jeg vist, at de forskellige karakteriseringer af de indlejrlige matricer, der gælder for endeligt tilstandsrum, også kan gennemføres for forgreningsprocesser på de hele positive tal. I [13] har jeg vist Lévy-Khinchin formlen ved hjælp af ekstremalpunkts metode, hvilket kan fortolkes som en repræsentation af de indlejrlige random walks på \mathbb{R} .

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