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1. Introduction

It is proved that any 3×3 stochastic matrix P with Det P $\geq \frac{1}{2}$ which is imbeddable in a non-homogeneous Markov chain is the product of 6 Poisson matrices, each of which has at most one positive off-diagonal element.

It follows from this that any imbeddable 3×3 stochastic matrix is the product of a finite number of Poisson matrices.

We consider the imbedding problem for stochastic matrices, see [2] and [3]. The stochastic matrix P is called imbeddable if there exists a bounded measurable intensity matrix valued function Q(t), $0 \leq t \leq 1$, such that the solution P(t), to the backward Kolmogorov equation

$$\frac{d}{dt}P(t,1) = -Q(t)\, P(t,1)$$

with initial condition

$$P(1,1) = I$$

satisfies

$$P(0,1) = P.$$

Here N denotes a null set for Lebesgue measure.

If the initial value is $P(0,1) = P_o$ then we say that P is imbeddable from P_o. Obviously, if P is imbeddable from P_o then there exists an imbeddable matrix P_1, such that $P = P_1 P_o$.

The set of intensity matrices is a convex cone and the extremal elements are characterized by having at most one positive off-diagonal element. If Q is an extremal intensity matrix then exp Q is called a Poisson matrix and is a stochastic matrix with at most one positive off-diagonal element.

It was proved in [2] that finite products of Poisson matrices are dense in the set of imbeddable matrices and in [3] it was proved that any matrix in the interior of the imbeddable matrices had a representation as a finite product of Poisson matrices. For 3×3 matrices we prove that even the boundary matrices have this representation and that in a neighbourhood of I we need only use 6 Poisson matrices. The proof rests on an explicit construction of the set of imbeddable matrices which at least in principle allows one to determine whether a given matrix near I is imbeddable.

The result can be considered a strengthening of the result in [4] (Theorem 3) concerning the configuration of zeroes in an imbeddable stochastic matrix. For 3×3 matrices we prove that the transitive, reflexive relations can be taken as the zero configurations of Poisson matrices.

If Q_{ij} is the extremal intensity matrix with (i,j)'th element 1 then we define the Poisson matrix

$$K_{ij}(u) = e^{tQ_{ij}} = e^{-t}I + (1-e^{-t})(I+Q_{ij}) \qquad (1.1)$$

where

$$u = 1 - e^{-t} \in [0,1].$$

Clearly $K_{ij}(u)$ is imbeddable for $0 \leq u < 1$. For $u = 1$ we get Det $K_{ij}(u) = 0$ and $K_{ij}(1)$ is imbeddable if we use an infinite time interval. It is convenient to call $K_{ij}(u)$ reachable for $u \in [0,1]$.

Let the stochastic matrix P have rows p_1, p_2 and p_3, we write $P = (p_1,p_2,p_3)$, and let $\langle P \rangle$ denote the triangle spanned by p_1, p_2 and p_3. A simple calculation easily yields the following results:

<u>1.1 Lemma</u>. Let $P = (p_1,p_2,p_3)$ then

$$K_{ij}(u)P = (q_1,q_2,q_3)$$

where

$$q_k = \begin{cases} p_k, & k \neq i \\ (1-u)p_i + up_j, & k = i. \end{cases}$$

Thus $\langle K_{ij}(u)P\rangle$ can be reached from $\langle P\rangle$ by moving vertex i towards vertex j a fraction u of the way. If $K_1,\ldots,K_m$ are Poisson matrices we can think of $\langle K_1\cdot\ \ldots\ \cdot K_m\rangle$ as the triangle we get after moving the vertices of $\langle I\rangle$ towards each other, one at a time, a total of m moves, starting with K_m.

Notice that the reachable matrix $K_1\cdot\ \ldots\ \cdot K_m$ is imbeddable if and only if Det $K_1\cdot\ \ldots\ \cdot K_m > 0$.

The following lemma shows how much an imbeddable matrix can move the vertices of a given matrix.

<u>1.2 Lemma</u>. Let P_1 be an imbeddable matrix and let $P = P_1P_o$ where Det $P_o > 0$. Then

$$p_i \in (\mathrm{Det}P_1)p_i^o + (1-\mathrm{Det}P_1)\langle P_o\rangle,\ i = 1,2,3. \qquad (1.2)$$

<u>Proof</u>. If P_1 is a Poisson matrix this follows from Lemma 1.1, and if (1.2) is satisfied for P_1 and P_2 then it is satisfied for P_2P_1, since first of all the product is imbeddable and next if $P = P_2P_1P_o$ then

$$p_i \in (\mathrm{Det}P_2)p_i^{10} + (1-\mathrm{Det}P_2)\langle P_1P_o\rangle$$

and

$$p_i^{10} \in (\mathrm{Det}P_1)p_i^o + (1-\mathrm{Det}P_1)\langle P_o\rangle.$$

If we insert the second relation in the first and use the fact that

$$\langle P_1P_o\rangle \subset \langle P_o\rangle$$

we get that

$$p_i \in (\mathrm{Det}P_2P_1)p_i^o + (1-\mathrm{Det}P_2P_1)\langle P_o\rangle.$$

Thus the set of matrices that satisfy (1.2) is a semigroup that contains the Poisson matrices. Since it is closed it contains the imbeddable matrices.

The idea behind the constructions in the next sections is now to consider the imbedding problem as the control problem of steering the vertices of <I> into the vertices of <P> following the simple rules set out above.

In this way the representation given in Theorem 2.1 and Corollary 2.2 are solutions to the Bang-Bang problem in control theory, i.e. one can reach any imbeddable matrix P by switching between the extremal generators Q a finite number of times.

2. Main Results

We want to prove the following

2.1 Theorem. let P be a 3 × 3 stochastic matrix with Det P $\geqq \frac{1}{2}$. Then P is imbeddable if and only if

$$P = \prod_{i=1}^{6} K_i,$$

where $K_1,\ldots,K_6$ are Poisson matrices.

2.2 Corollary. Let P be a 3 × 3 stochastic matrix, then P is imbeddable if and only if

$$P = \prod_{i=1}^{n} K_i,$$

where $K_1,\ldots,K_n$ are Poisson matrices.

The corollary follows easily since an imbeddable matrix P can be expressed as $P = P_1 \cdot \ldots \cdot P_k$, where $P_1,\ldots,P_k$ are imbeddable stochastic matrices and Det $P_i \geqq \frac{1}{2}$, $i = 1,\ldots,k$. Notice that we can obtain an upper bound on the number of matrices needed in the form

$$n \leq 6\left(1 + \frac{-\ln \mathrm{Det} P}{\ln 2}\right).$$

The proof of the Theorem rests on a rather complicated construction and on Proposition 3.9 which will be given in Section 3.

By means of these results the proof of Theorem 2.1 runs as follows:

What we have to prove is that if P is the product of 7 Poisson matrices and of Det $P \geq \frac{1}{2}$, then P can be expressed as a product of 6 Poisson matrices. An induction proof will then give that any finite product of Poisson matrices with Det $P \geq \frac{1}{2}$ can be expressed as a product of 6. Since the set of matrices, which is a product of 6 Poisson matrices, is closed we get that any limit of a finite product of Poisson matrices and therefore any imbeddable matrix with Det $P \geqq \frac{1}{2}$ is a product of 6 Poisson matrices, see [2].

Let therefore

$$P = K_1 \cdot \ldots \cdot K_7, \text{ Det } P \geqq \frac{1}{2}.$$

We denote by a and b the vertices of $K_2 \cdot \ldots \cdot K_7$ left invariant by K_1 and define c and c' by

$$\langle K_2 \cdot \ldots \cdot K_7 \rangle = \langle a,b,c' \rangle$$

and

$$\langle K_1 \cdot \ldots \cdot K_7 \rangle = \langle a,b,c \rangle.$$

Thus P can be reached in 7 moves. The last move is to take c' towards either a or b into c.

Clearly $\langle a,b,c' \rangle$ is imbeddable in 6 moves and since

$$\text{Det } K_2 \cdot \ldots \cdot K_7 \geq \text{Det } K_1 \cdot \ldots \cdot K_7 \geq \frac{1}{2}$$

it follows from Lemma 3.9 that c' is contained in the set R(I) defined by (3.4). By Proposition 3.10 this set is starshaped around a and b and therefore contains [a,c'] and [b,c'] and hence c. Thus c is contained in R(I) but the construction of R(I) ensures that any $c \in R(I)$ can be reached in 6 moves. Thus (a,b,c) is the product of 6 Poisson matrices, which completes the proof.

Notice that the crucial step in the proof is the construction of R(I). This set is constructed for a fixed a and b as a suitable set of points $c \in \langle I \rangle$ such that $\langle a,b,c \rangle$ is reachable in 6 moves. It is the starshapedness of this set around a and b that allows the induction proof to work.

3. The construction of R(P).

Let $P = \langle A,B,C \rangle$ and let x and y be points in $\langle P \rangle$. We denote by $[x,y]$ the closed interval between x and y and by $M_{x,y}$ the halfline from x through y with the natural order. Let

$$x\dot{y} = \sup\{z \mid z \in M_{x,y} \cap \langle P \rangle\}.$$

Thus xy denotes the projection of x through y onto the boundary of $\langle P \rangle$.

All the proofs in the following will be geometric in nature, using the above projection and it helps the understanding of the constructions to study Fig. 1.

Throughout this section a and b will denote two distinct and fixed points in $\langle I \rangle$. All constructions will be relative to these two points and they will not in general be included in the notation.

Since the set R(I) is defined recursively we can as well define R(P), but this set clearly depends on the relation between the two points a and b and the triangle $\langle P \rangle$.

We shall therefore define 3 sets of matrices as follows: Let $a \in \langle P \rangle$, $b \in \langle P \rangle$ and let $\text{Det } P \geq 0$, we then define

$$P \in P_o \text{ if } ab \in [C,B] \text{ and } ba \in [A,C],$$

$$P \in P_+ \text{ if } ab \in [A,B] \text{ and } ba \in [A,C],$$

$$P \in P_- \text{ if } ab \in [C,B] \text{ and } ba \in [A,B].$$

It is easy to see that $P_o \cup P_+ \cup P_-$ is the set of matrices $P = (A,B,C)$ such that Det $P \geq 0$, $\langle P \rangle$ contains a and b, and Det $(a,b,C) \geq 0$.

One can of course define the similar configurations when Det $(a,b,C) < 0$ but these will not be needed in the constructions.

Notice that the area of $\langle P \rangle$ is proportional to $|\text{Det } P|$ and the orientation of the vertices is determined by the sign of Det P.

<u>3.1 Lemma</u>. If for some c, (a,b,c) is imbeddable from $P(\text{Det } P > 0)$, and if Det $(a,b,c) \geq \frac{1}{2}$ Det P, then

$$P \in P_+ \cup P_o \cup P_-.$$

<u>Proof</u>. If (a,b,c) is imbeddable from $P = (A,B,C)$ then $(a,b,c) = P_1 P$ for some imbeddable P_1, such that Det $P_1 \geq \frac{1}{2}$. It follows from Lemma 1.2 that

$$\begin{aligned} a &\in (\text{Det } P_1)A + (1-\text{Det } P_1)\langle P\rangle \\ &\subset \tfrac{1}{2}A + \tfrac{1}{2}\langle P\rangle \\ &= \text{co}\{A, \tfrac{1}{2}(A+B), \tfrac{1}{2}(A+C)\} \end{aligned}$$

and similarly

$$b \in \text{co}\{B, \tfrac{1}{2}(A+B), \tfrac{1}{2}(B+C)\}.$$

It is easily seen that this implies that Det $(a,b,C) \geq 0$ and hence that

$$P \in P_+ \cup P_o \cup P_-.$$

<u>3.2 Lemma</u>. If $P \in P_o$ and $c \in \langle P \rangle$ then (a,b,c) is reachable in 6 moves from P if and only if Det $(a,b,c) \geq 0$.

Proof. If $P \in P_0$ then Det $P \geq 0$ and anything reachable from P will also have a nonnegative determinant. If Det (a,b,c) $\geq$ 0 then

$$c \in \langle ab, ba, C \rangle$$

and we can reach (a,b,c) as follows: First move A towards C into ba, then B towards C into ab. Then move C into c in two moves and finally take A from ba to a and B from ab to b.

3.3 Corollary. If $I \in P_0$ then any imbeddable matrix (a,b,c) can be reached in 6 moves.

Thus Theorem 1.1 is proved provided a and b have the configuration in relation to I as prescribed by the condition $I \in P_0$.

The difficulties come up if $I \in P_+$ or P_-, where a and b have been tilted such that the line through a and b intersects I in a different way.

Clearly we can treat P_+ and P_- in a similar fashion and we shall therefore concentrate on P_+ in the following.

Let us therefore assume that $P \in P_+$ and let us define the set $S(P) \subset \langle P \rangle$ as the union of co{ab,ba,C,Aa}, co{b,ba,C,Bba} and the smallest region which is starshaped around C and contains the curve ψ defined as follows: Take $B^* \in [ab,B]$ and consider the point

$$c = [B^*, C] \cap [B^*b, B^*ba]. \tag{3.1}$$

As B^* varies from B to ab, c will describe a continuous curve ψ from Bba to ab.

The equation from ψ can be found to be

$$c_3 = \frac{c_2}{a_2} a_3 + \left(1 - \frac{c_2}{a_2}\right) \frac{c_2 b_3}{c_2 - b_2(c_1 + c_2)} \tag{3.2}$$

if we choose P = I and denote the coordinates of a point x by

x_1, x_2, and x_3.

The curve lies inside co$\{ab, ba, C, B\}$ and we shall now describe some properties of ψ and S(P), see Fig. 1.

Notice first that by the geometric construction of S(P) one immidiately gets the following transformation property of S(P):

For any stochastic matrix P we have

$$S_{a,b}(I)\ P = S_{aP,bP}(P), \qquad (3.3)$$

where the points a and b have been introduced as indices.

<u>3.3 Lemma.</u> The curve ψ intersects any line at most twice. If the line separates the end points of ψ, i.e. Bba and ab, then it intersects ψ exactly once.

<u>Proof</u>. This follows easily by observing that the equation for ψ is quadratic in (c_2, c_3).

<u>3.4 Corollary</u>. The set S(P) is starshaped around a,b and C.

<u>Proof</u>. Let c be on the boundary of S(P). We want to prove that $[b,c] \subset S(P)$. If c is on the boundary of co$\{ab, ba, C, Aa\}$ or co$\{b, ba, C, Bba\}$ then this follows by convexity.

The only other possibility is that c is on ψ but outside the two convex sets.

Now take $c' \in [b,c]$. If $Cc' \in [Cb, ab]$ then $c' \in \langle ab, ba, C \rangle \subset S(P)$ and if $Cc' \in [ab, B]$ we consider the point c'' on ψ generated by $B^* = Cc'$, see (3.1).

Clearly the point c'' can not be on the same side of $[b,c]$ as C, since then the curve ψ would intersect $[b,c]$ at least twice which is impossible since the line through b and c separates the end points of ψ. Hence $c' \in [C, c''] \subset S(P)$, which completes the proof that S(P) is starshaped around b.

We also get from this argument that for the point c described above we get $co\{c,b,ba,C\} \subset S(P)$ but this set contains a and c and therefore $[a,c]$. Hence $S(P)$ is also starshaped around a.

<u>3.5 Lemma.</u> Let c be a point on the boundary of $S(P)$ such that $Det(a,b,c) > 0$ or such that $c = ab$ or ba, then (a,b,c) can be reached in 5 moves from P.

<u>Proof</u>. If c is on the curve ψ then c is generated by some $B^* \in [ab,B]$. Now we can reach c as follows: First move B to B^*, then A to B^*b and C to c. Then take B from B^* to b and A from B^*b to a.

If $c \in [Bba,b]$ then we first take A into Bb, then C to Bba and B to b. Then take A to a and C to c.

If $c \in [Aa,ab]$ then we start by taking C into Aa, then B to ab and A into a. Then we take C from Aa to c and finally B to b.

If $c \in [C,Bba] \cup [C,ba]$ we first move A into Bb, then C to c and B to b. Then we have two moves to get A into a.

<u>3.6 Corollary</u>. If $c \in S(P)$ then (a,b,c) can be reached in 6 moves.

<u>Proof</u>. Consider the point:

$$c' = \sup\{z \mid z \in M_{b,c} \cap S(P)\}$$

on the boundary of $S(P)$. Then c' can be reached in 5 moves by Lemma 3.5 and the last move can then take c' into c.

<u>3.7 Lemma.</u> If (a,b,c) can be reached in five moves from P then $c \in S(P)$.

<u>Proof</u>. If $R_i(P)$ denotes the set of points c such that (a,b,c) can be reached from P in i steps, then clearly

$$R_{i+1}(P) = \cup R_i(KP), \quad i = 0,1,\dots ,$$

where the union is taken over all Poisson matrices K.

From the initial value

$$R_o(P) = \{C\} \text{ if, } a = A \text{ and } b = B$$

and $\emptyset$ otherwise we can in principle construct $R_i(P)$ for any value of i.

We have in fact used this relation to construct S(P) as the starshaped (around C) region that contains $R_5(P)$ and [ab,ba].

A complete numeration of all possible cases is rather tedious but we shall give some intermediate results which will allow the reader to get the idea of construction used. The details can then easily be completed.

We find

$$R_3(P) = \begin{cases} \emptyset & \text{if } a \neq ba,\ b \neq ab, \\ \{C, Aa, [C,b] \cap [A,Aa]\}, & \text{if } a \neq ba,\ b = ab, \\ \{C\} & \text{if } a = ba,\ b \neq ab, \\ [C,a] \cap [C,b] & \text{if } a = ba,\ b = ab \end{cases}$$

and

$$R_4(P) = \begin{cases} \{C, Aa, Bba, [Bb,Bba] \cap [C,b], \\ \quad [A,Aa] \cap [C,b],\ [A,Aa] \cap [C,ab]\} & \text{if } a \neq ba,\ b \neq ab \\ [C,ba] \cap [C,a] \cup [C,b] \cup [C,Aa] \cup [Aa,a] \cup [Aa,b] & \text{if } a \neq ba,\ b = ab \\ [C,a] \cup [C,b] \cup [C,ab] & \text{if } a = ba,\ b \neq ab \\ \langle C,a,b \rangle & \text{if } a = ba,\ b = ba. \end{cases}$$

Using these and similar results for other configurations of P in relation to a and b it is easily seen that $R_5(P) \subset S(P)$.

Combining the results in Corollary 3.4, Lemma 3.5, and

Lemma 3.7 we get

<u>3.8 Proposition</u>. The set $S(P)$ is the smallest region containing $R_5(P)$ which is starshaped around a and b.

It was proved in Corollary 3.6 that $S(P)$ is contained in $R_6(P)$. The converse is not in general true, nor is it true that $R_6(P)$ is starshaped in general. We shall now describe a region $R(P)$ which is starshaped and which contains enough points to be of use in the proof of the main theorem.

If $P \in P_o$ we define

$$R(P) = R_6(P) = \langle ab, ba, C \rangle .$$

If $P \in P_+$ we define

$$R(P) = \bigcup R_5(KP) \tag{3.4}$$

where the union is taken over all Poisson matrices K except those that take C into [Ba,ba[. Thus $KP \in P_o \cup P_1$ for all K considered. Only by taking C towards A beyond ba can we change this situation. A similar definition is used for $P \in P_-$.

It is easily seen that $R(P)$ satisfies a relation similar to (3.3), and that every point in $R(P)$ can be reached in 6 moves from P. The following lemma shows to what extend the opposite is true.

<u>3.9 Lemma</u>. Let $(a,b,c) = K_1 \cdot \ldots \cdot K_6 P$, where Det $K_1 \cdot \ldots \cdot K_6 \geqq \frac{1}{2}$ then $c \in R(P)$.

<u>Proof</u>. If $P \in P_o$ then this is obvious since $R(P) = \langle ab, ba, C \rangle$. If $P \in P_+$ we clearly have

$$c \in R_5(K_6 P).$$

It follows from Lemma 1.2 that since

$$\text{Det } K_6 \geq \text{Det } K_1 \cdot \ldots \cdot K_6 \geq \frac{1}{2}$$

then the image of C under K_6 is contained in the triangle

$$\mathrm{co}\{C, \tfrac{1}{2}(A+C), \tfrac{1}{2}(B+C)\}$$

whereas since

$$\mathrm{Det}\ K_1 \cdot \ \ldots \ \cdot K_6 \geq \frac{1}{2}$$

we have

$$ba \in \mathrm{co}\{A,\tfrac{1}{2}(A+C),\tfrac{1}{2}(A+B)\}.$$

Hence K_6 can not move C beyond ba and hence K_6 is one of the Poisson matrices used to define R(P), see (3.4), and hence $c \in R(P)$.

The proof for $P \in P_-$ is similar.

3.10 Proposition. The set R(P) is starshaped around a and b.

Proof. Since the statement is obvious for $P \in P_o$, we shall assume that $P \in P_+$. Let now $K(u) = K_{ij}(u)$ for some fixed i and j, see (1.1). The set $R_5(K(u)P)$, $0 \leq u \leq 1$ is empty for $u > u_o$, where u_o is determined by either a or b being on the boundary of $\langle K(u_o)P\rangle$. Notice also that $K(u)P \in P_+$ except when K(u) takes B into [Cb,ab] in which case $K(u)P \in P_o$ and then

$$R_5(K(u)P) = \langle K(u)P\rangle \cap \langle ab,ba,C\rangle.$$

In all other cases under consideration in the definition of R(P) we get that $R_5(K(u)P)$ has the same shape as $R_5(P)$. In any case let ϕ_u denote the boundary of S(K(u)P), see Proposition 3.8.

Thus ϕ_o is the boundary of S(P) since K(o) = I and ϕ_u, $0 \leq u \leq u_o$ is a continuous family of closed continuous curves each of which determine a region which is starshaped around a and b.

It is easily seen that

$$S(P) \cup \bigcup_{0\leq u\leq u_o} \phi_u = \bigcup_{0\leq u\leq u_o} R_5(K(u)P) \cup S(P) \qquad (3.5)$$

is again starshaped around a and b.

Thus K(u) may squeeze the boundary of S(P) out of S(P), but in a continuous fashion and always in such a way that the inside is starshaped around a and b.

Clearly R(P) is the union of the 6 regions of the form (3.5) which we get for the various choices of i and j. Thus R(P) is itself starshaped around a and b, which completes the proof of Proposition 3.10.

It should be noticed that if $P \in P_+$ and if K takes C beyond ba then we are in an entirely different situation and the corresponding sets need not be starshaped, which is the reason for avoiding them.

Notice also that if K takes C into [C,ba], A into [A,Ca] or moves B then $R_5(KP) \subset S(P)$, but if K takes C towards B or A towards C then points outside S will be in $R_5(KP)$.

One can carry through a more detailed analysis of the set R(P) and obtain an expression for the boundary as an upper envelope of some lines and quadratic curves.

It should finally be pointed out that it is not true that any imbeddable matrix is a product of 6 Poisson matrices. An example of such a matrix can be found if we consider the following situation: Let P = (A,B,C) and assume that ab∈]A,C[, ba ∈]B,C[. Thus a and b are rotated in relation to P and c therefore has to lie in the set co{A,ab,ba,B} in order that (a,b,c) be imbeddable from P. In this case one can again construct $R_5(P)$ by carefully constructing $R_1(P),\dots,R_4(P)$. The boundary can be described as consisting of the lines [Aab,a] and [Bba,b] together with the curves ψ_1 and ψ_2 defined as follows:

Take A^* ∈ [A,Cb] and consider the point

$$c \in [C,A^*] \cap [A^*a, A^*ab].$$

As A^* varies from A to Cb, c describes a continuous curve from Aab to b. The curve ψ_2 is constructed by choosing B^* ∈ [Ca,B] in a similar fashion.

Let us again consider the smallest region containing this boundary which is starshaped around C and intersect with the set co{A,ab,ba,B}. This region S(P) is not starshaped around b or a in general and we let ϕ_o denote its boundary.

Again $R_5(P)$ is constructed by squeezing ϕ_o out of S(P) by first moving one of the vertices A,B, og C by means of K and then find $R_5(KP)$. A careful construction will show that if a and b are sufficiently close then $R_6(P)$ is not starshaped. Thus there exists a $c' \in R_6(P)$ and $c \in [b,c']$ say such that $c \notin R_6(P)$. Hence we can reach (a,b,c') in 6 moves and (a,b,c) in 7 but obviously not in 6.

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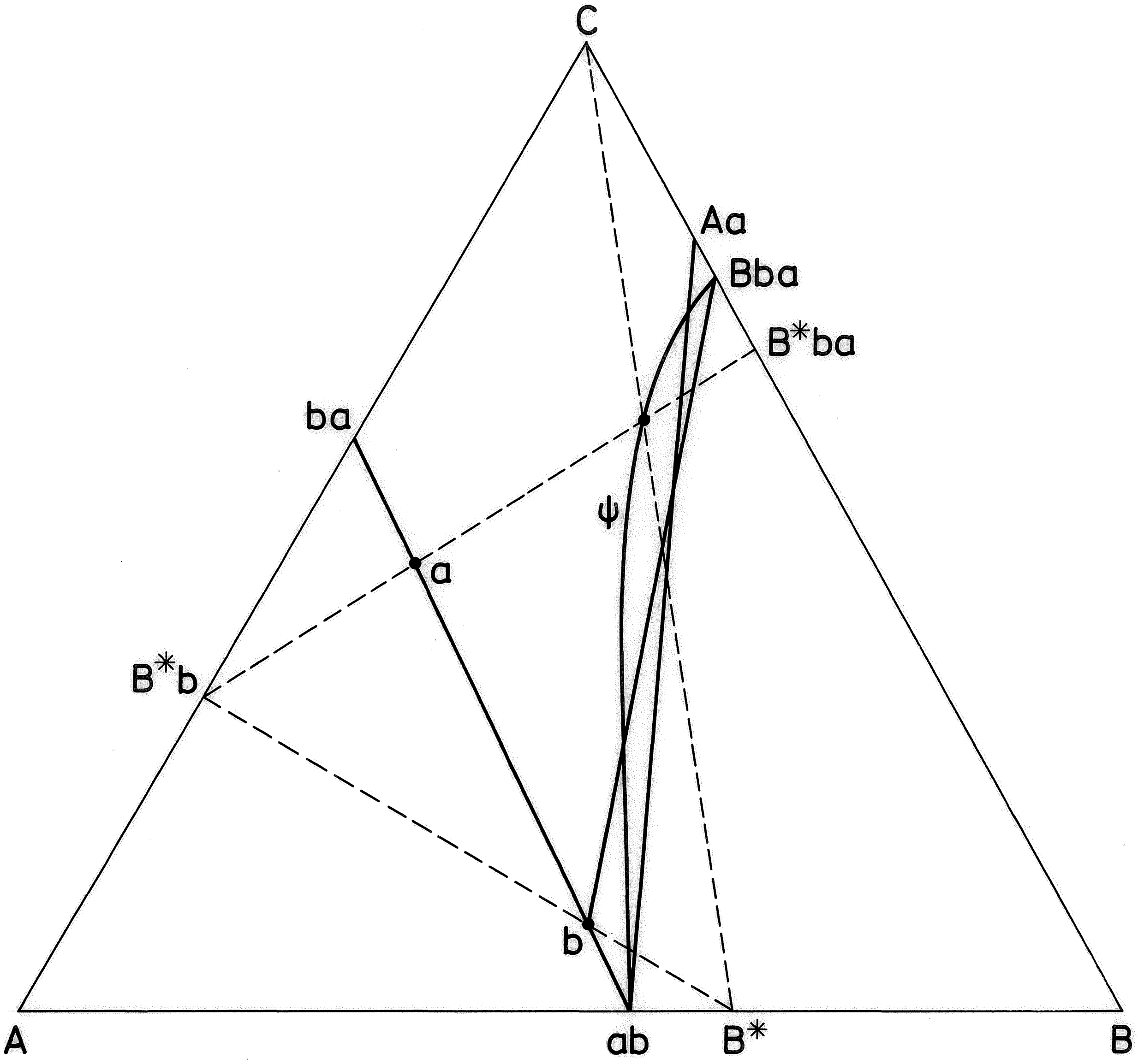

Fig. 1 The construction of ψ and S(P).