A GEOMETRIC INTERPRETATION OF 2×2 MARKOV TRANSITION MATRICES

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Abstract. By creating a geometric interpretation for 2×2 Markov chain transition matrices, we obtain a simple graphical method for finding the limiting probability vector. As a bonus, the interpretation gives a geometric method for finding powers and roots of transition matrices.

1. Introduction. How would you find a "square root" of the matrix

$$P = \begin{bmatrix} .8 & .2 \\ .3 & .7 \end{bmatrix}$$

if you were not allowed to use eigenvalues and eigenvectors? If you wanted to construct two (different) matrices that commute, how would you do so, if diagonal matrices were not allowed? If you wanted to find a 2×2 matrix A, not equal to I, such that $A^2 = A$, how would you proceed? These questions have easy answers. We will answer them using a geometric interpretation of 2×2 Markov chain transition matrices.

The study of Markov chains is often included in an applications section of a linear algebra text. For example, see Nicholson [3] and Norman [4]. Markov chains have many uses. For example, two state Markov chains are useful in systems with only ON/OFF states. Also, 2×2 Markov transition matrices can be helpful for understanding results involving $n \times n$ Markov transition matrices.

Let $P = [p_{ij}]$ be an $n \times n$ transition matrix where p_{ij} represents the probability of moving to state j on the next step given that the system is currently in state i. In what follows, we will talk about irreducible aperiodic Markov chains. Markov chains having transition matrices with all nonzero entries form a subset of those chains, so anyone unfamiliar with such terminology can focus on matrices with all nonzero entries.

For irreducible aperiodic Markov chains, it is well-known that the limiting probability of being in state i on the nth step, denoted by $v_i = \lim_{n \to \infty} p_i^{(n)}$, exists and does not depend on the initial state probabilities. Let $\underline{v}$ be the limiting probability (row) vector. For such Markov chains, with a finite number of states, $\underline{v}$ can be found by solving

$$\underline{v} = \underline{v}P \text{ subject to } \sum_i v_i = 1, \quad 0 \le v_i \le 1. \tag{1}$$

It can also be found as any row $\underline{v}$ of

$$\lim_{n\to\infty} P^n \tag{2}$$

where P^n is the nth power of P.

One of the most frequently asked questions for Markov chains is, "Given a transition matrix, what is the limiting probability vector?" Algebraic solutions are given by solving (1) in the previous paragraph. An important but less frequently asked question is, "Given a limiting probability vector, what is the corresponding set of transition matrices?" In this paper, both questions will be answered for 2×2 matrices, via a novel geometric interpretation.

2. Transition Matrices and Limiting Vectors. Because transition matrix entries are probabilities and the rows must sum to 1, any 2×2 transition matrix

$$P = \begin{bmatrix} x & 1-x \\ y & 1-y \end{bmatrix}$$

can be represented by the point $[x, y]$ in the unit square bounded by $[0, 0]$, $[1, 0]$, $[1, 1]$, and $[0, 1]$. Square parentheses $[*, *]$ will be used to represent such a matrix, and round parentheses $(*, *)$ will be reserved for limiting probability vectors of the Markov chain. It is very fortunate that four dimensional 2×2 matrices can be reduced to a two dimensional vector by adding the constraint on the row sums of the matrix.

The matrices represented on the sides of the unit square $[x, 0]$, $[1, y]$, $[x, 1]$, $[0, y]$ include transition matrices for Markov chains which are periodic or have absorbing states, or are not irreducible. These are special cases. All points $[x, y]$ strictly within the unit square represent transition matrices of irreducible aperiodic Markov chains. Unless otherwise stated, only irreducible aperiodic Markov chains are being considered.

We first solve the problem of finding all transition matrices with a given limiting vector.

Property. Let $\underline{v} = (a, 1-a)$ be a known probability vector, with $0 < a < 1$. For $0 < x < 1$, $0 < y < 1$, let the transition matrix

$$P = \begin{bmatrix} x & 1-x \\ y & 1-y \end{bmatrix}$$

be represented by $[x, y]$. Then the set of 2×2 transition matrices P having $\underline{v}$ as the limiting vector, when represented in $\mathbb{R}^2$, form a straight line through the points $[1, 0]$, $[a, a]$, and $[0, a/(1-a)]$.

Proof. From (1), solving $\underline{v} = \underline{v}P$ yields

$$\begin{aligned} a &= ax + (1-a)y \\ 1-a &= a(1-x) + (1-a)(1-y). \end{aligned} \tag{3}$$

The second equation is redundant. The first equation represents a straight line, containing the points $[1, 0]$, $[a, a]$, and $[0, a/(1-a)]$.

Each value of a corresponds to a line through the points $[1, 0]$ and $[a, a]$ representing matrices with limiting vector $(a, 1-a)$. In Diagram 1, (3) is plotted in $\mathbb{R}^2$

for $a = 1/3, 1/2, 2/3$.

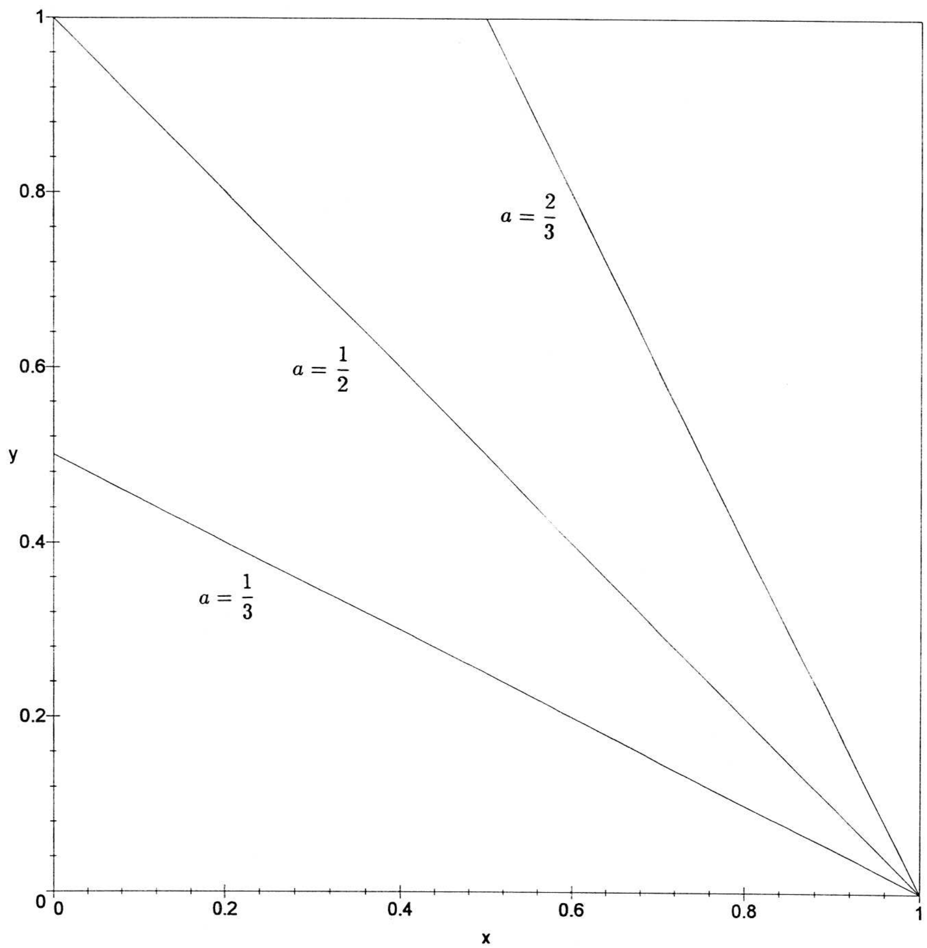

Diagram 1

Now, instead of finding the collection of matrices with a given limiting vector, we reverse the procedure to find geometrically the limiting vector for a given matrix.

Finding the Limiting Vector. For $0 < x < 1$, $0 < y < 1$, let

$$P = \begin{bmatrix} x & 1-x \\ y & 1-y \end{bmatrix}$$

be represented by $[x, y]$. Let the limiting vector be $\underline{v} = (a, 1-a)$ for some a. By (2), the limiting matrix must be $[a, a]$. Since the limiting matrix $[a, a]$ is on the line $y = x$, it can be found from the intersection of $y = x$ with the line passing through the points $[1, 0]$ and $[x, y]$.

Diagram 2 illustrates the technique for

$$P = \begin{bmatrix} .8 & .2 \\ .3 & .7 \end{bmatrix},$$

represented by the point $[.8, .3]$. The intersection point is $[.6, .6]$, which represents the limiting matrix

$$\begin{bmatrix} .6 & .4 \\ .6 & .4 \end{bmatrix}$$

so the limiting vector is $\underline{v} = (.6, .4)$.

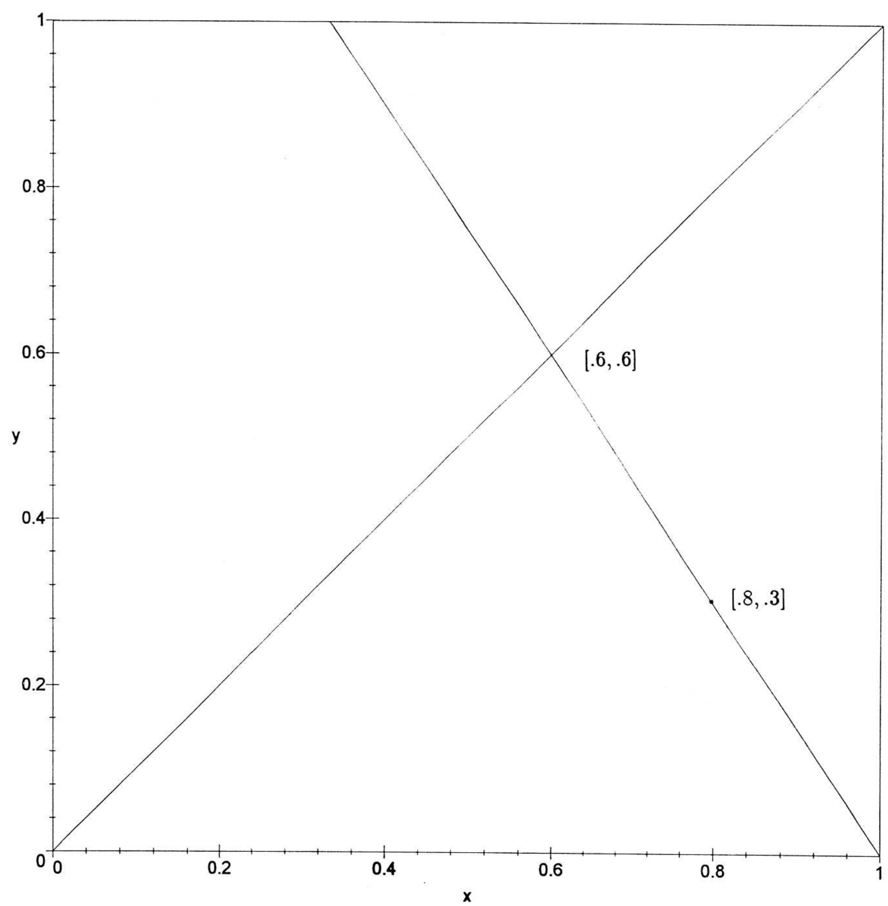

Diagram 2

3. Convergence. An interesting geometric picture can be obtained of convergence for transition matrices of two state Markov chains.

Let P, represented by $[x, y]$, be a Markov transition matrix for a two state irreducible aperiodic Markov chain. Then all positive integer powers of P are on the straight line through $[1, 0]$ and $[x, y]$ and inside the unit square. To see this, let $\underline{v} = (a, 1-a)$ be the limiting vector. Then $\underline{v} = \underline{v}P$. For $n > 1$, $\underline{v}P^n = \underline{v}P(P^{n-1}) =$

$\underline{v}P^{n-1} = \cdots = \underline{v}$. So all positive integer powers of P have the same limiting vector and must lie on the same straight line.

If the position of the point representing P^n, denoted by $[x_n, y_n]$, is needed, it is sufficient to determine x_n, because the second coordinate can be determined by knowing the point is on the straight line through $[1,0]$ and $[x,y]$. Equivalently only the $(1,1)$ coefficient of the 2×2 matrix P^n is needed. Denote x_n by $f_n(x)$ to emphasize that x_n is some function of x.

Let the limiting vector for P be $(a, 1-a)$. It is easy to show that the $(1,1)$ entry of P^n is

$$f_n(x) = (x-a)^n(1-a)^{1-n} + a, \tag{4}$$

which passes through the points $[1,1]$ and $[a,a]$. This expression for $f_n(x)$ can be used to find the position of P^n in the unit square for any positive integer n.

Diagram 3 illustrates using the function $f_2(x)$. Here

$$P = \begin{bmatrix} .8 & .2 \\ .1 & .9 \end{bmatrix},$$

which is represented by the point $[x,y] = [.8, .1]$. Thus,

$$P^2 = \begin{bmatrix} .66 & .34 \\ .17 & .83 \end{bmatrix},$$

which is represented by the point $[x_2, y_2] = [.66, .17]$. The Y coordinate of the quadratic $f_2(x)$ (at P) is equal to the X coordinate of P^2. Continuing in this manner,

$$P^4 = \begin{bmatrix} .4934 & .5066 \\ .2533 & .7467 \end{bmatrix}.$$

These matrices are labeled in Diagram 3. Note that if a matrix P is selected, then the powers of P along a straight line will give an idea of how fast or slow

$\{P^n\}$ converges to its limit. Careful initial choices of P can result in fast or slow convergence.

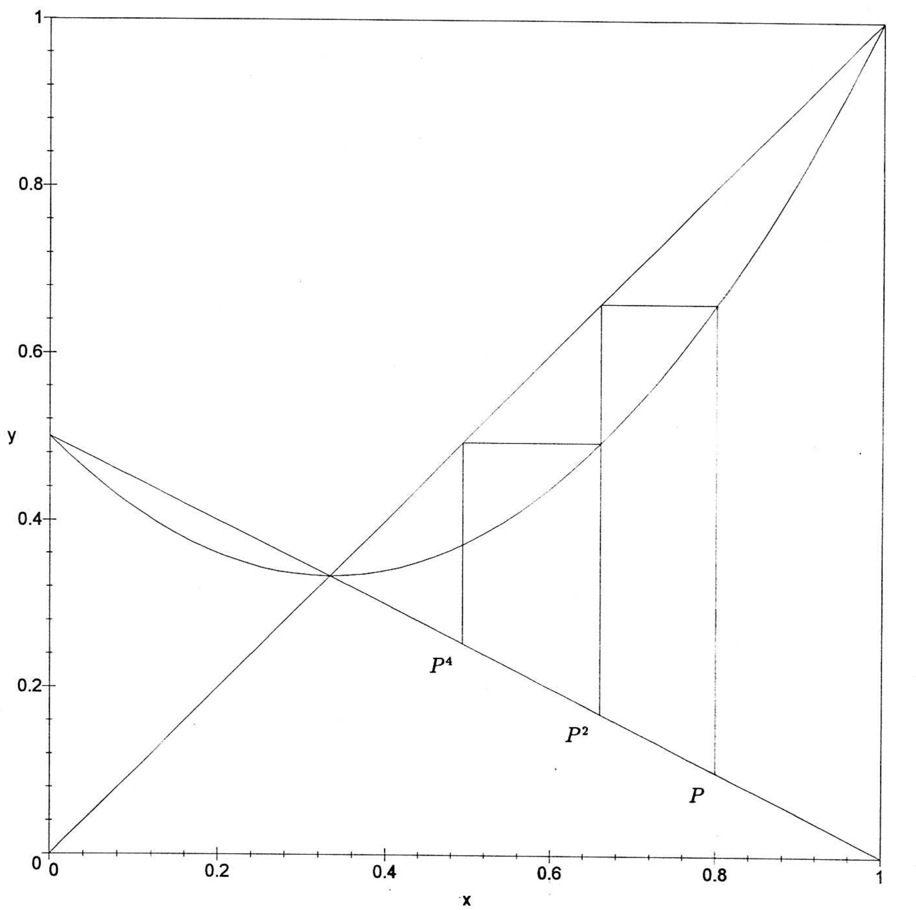

Diagram 3

In Diagram 4, both $f_2(x)$ and $f_3(x)$ are plotted, and the position of P^2 and P^3 are indicated.

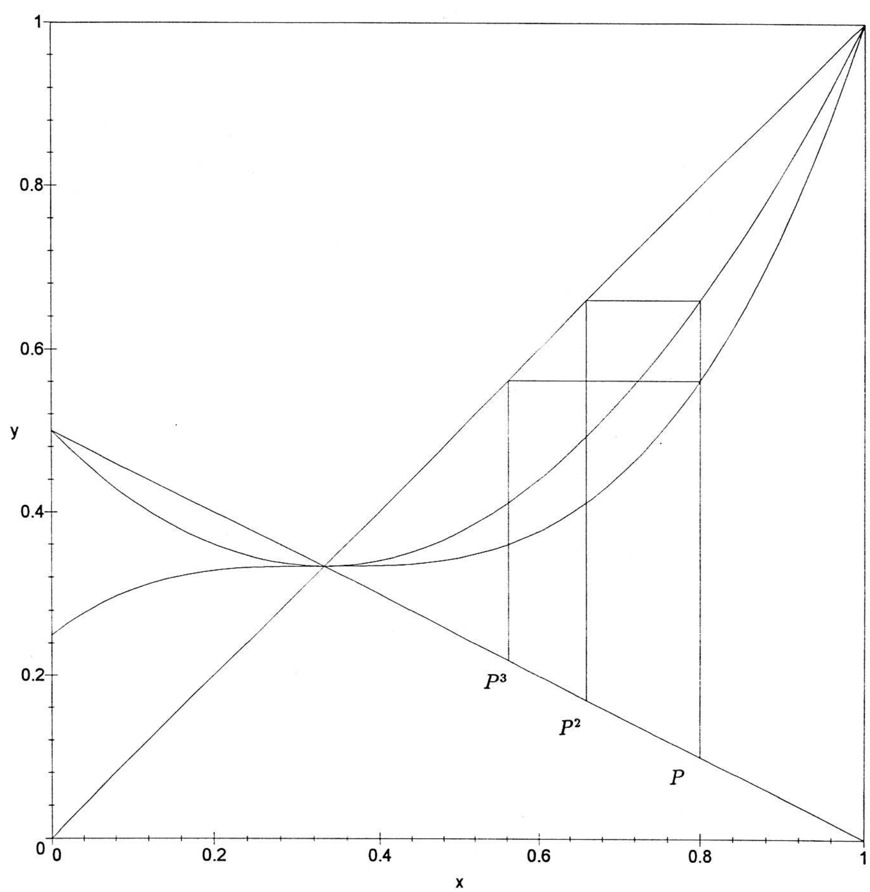

Diagram 4

In the appendix, a geometric method of multiplying any 2×2 transition matrices with the same limiting probabilites, is given. This would give another method of computing P^2 geometrically.

Consider again the quadratic $f_2(x)$. It is interesting to note that by moving backwards $P^{1/2}$ can be found using this geometric method (see Diagram 5).

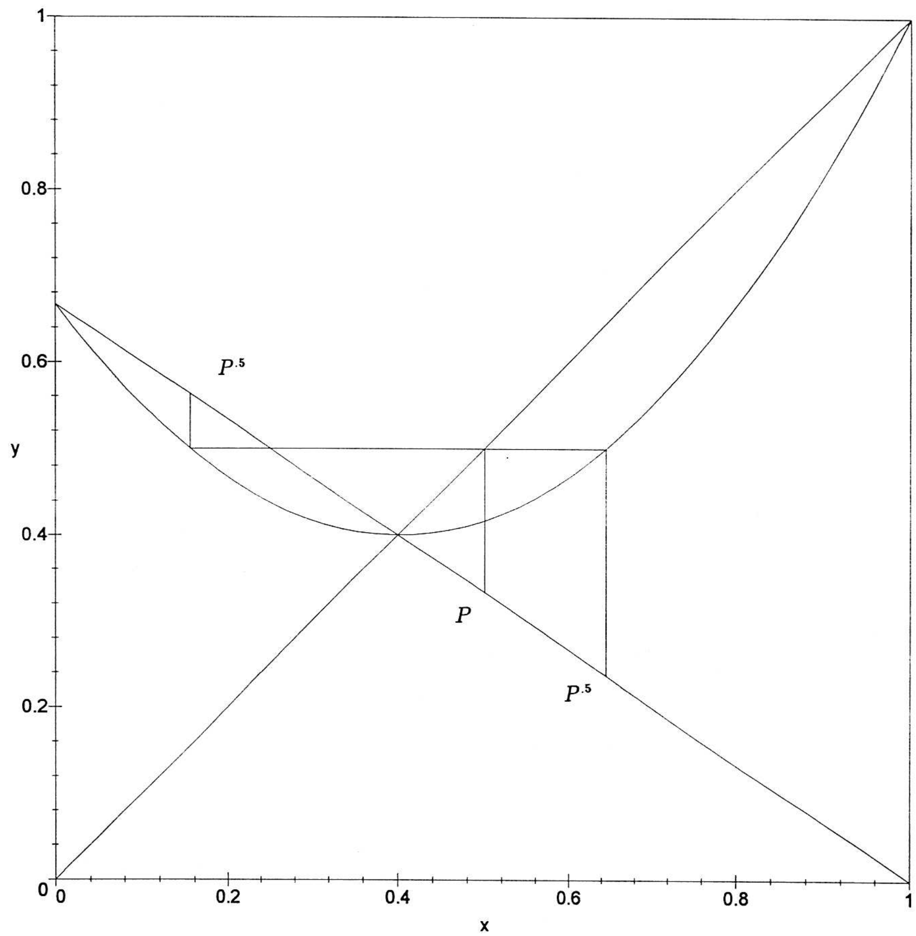

Diagram 5

Two square roots are obtained – one to the left of the point (a, a) and one to the right. Sometimes the point representing the square root matrix on the left is not in the unit square. In Diagram 5, take

$$P = \begin{bmatrix} 1/2 & 1/2 \\ 1/3 & 2/3 \end{bmatrix},$$

which is represented by the point $[1/2, 1/3]$. The two points representing square roots of P are shown in the diagram. Label both of these as $P^{.5}$. These square root matrices represent transition matrices for Markov chains which have two step transition probabilities which are the same as the one step transition probabilities of the original Markov chain with transition matrix P!

Next, some additional properties are stated about the transition matrices represented by the straight line through $[1, 0]$ and $[a, a]$. These are all easy to prove, especially from the probabilistic viewpoint, and may be useful if one wishes to construct matrices with certain given properties. These properties will answer some of the questions posed in the first paragraph of the introduction.

1. The product of two matrices on the line will again be on that line.
2. Matrix multiplication of any two matrices on the line is commutative.
3. The inverse of a matrix which is on the line and strictly within the unit square, is again on the line, but outside the unit square. Note that the inverse always exists except for the matrices represented by $[a, a]$. The inverse must lie outside the unit square since it is not a transition matrix. In Diagram 6, this is illustrated with

$$P = \begin{bmatrix} .1 & .9 \\ .6 & .4 \end{bmatrix}, \quad P^{-1} = \begin{bmatrix} -.8 & 1.8 \\ 1.2 & -.2 \end{bmatrix}, \quad \text{and } P^2 = \begin{bmatrix} .55 & .45 \\ .30 & .70 \end{bmatrix}.$$

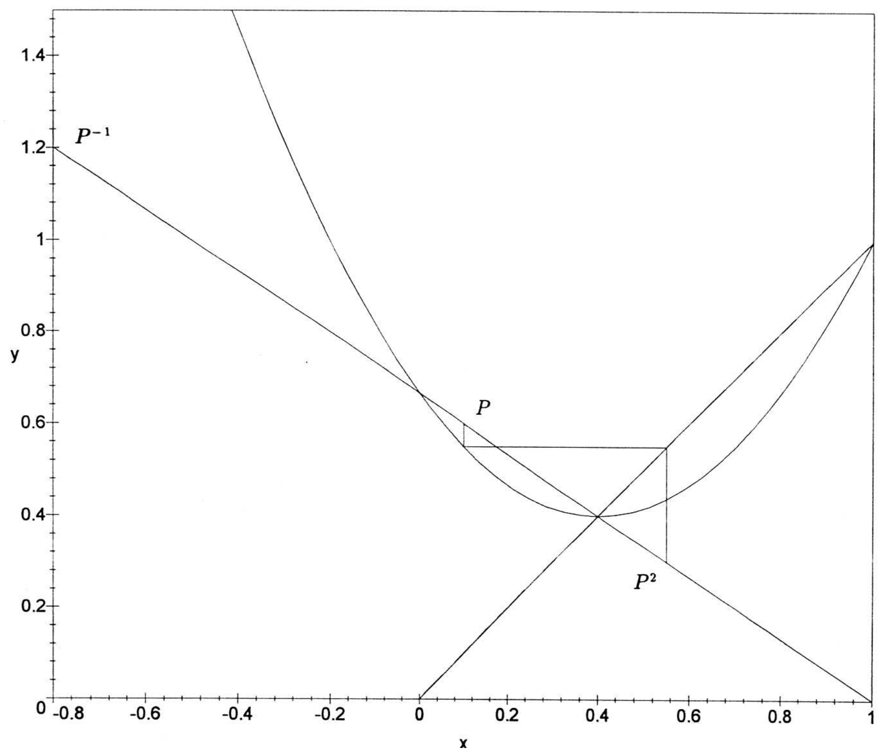

Diagram 6

4. Multiplying any matrix on the line by the matrix represented by $[a, a]$ gives the result $[a, a]$.
5. Matrices of type $[a, a]$ are idempotent (i.e. $P^2 = P$), and no other 2×2 transition matrices (with all nonzero entries) are idempotent.
6. The limiting vector is $(.5, .5)$ if and only if P is a symmetric matrix.

One advantage of the geometric approach is that some properties of transition matrices become immediately recognizable. It is easy to see that very different transition matrices may have the same limit. An example, apparent in the geometric approach, would be the matrices

$$P_1 = \begin{bmatrix} .9 & .1 \\ .05 & .95 \end{bmatrix} \text{ and } P_2 = \begin{bmatrix} .1 & .9 \\ .45 & .55 \end{bmatrix},$$

which both have limiting vector $(1/3, 2/3)$. It is also possible to find matrices which appear to be very close to each other but which have very different limiting vectors. An example would be

$$P_1 = \begin{bmatrix} .990 & .010 \\ .005 & .995 \end{bmatrix},$$

which has limiting vector $(1/3, 2/3)$, and

$$P_2 = \begin{bmatrix} .995 & .005 \\ .010 & .990 \end{bmatrix},$$

which has limiting vector $(2/3, 1/3)$.

4. Conclusion. This paper has demonstrated how 2×2 Markov transition matrices can be interpreted in a geometric manner, which provides insights and aids in understanding Markov chains. In particular, the convergence of powers of the transition matrix become simple motions in $\mathbb{R}^2$. As a bonus, we have found a method of obtaining square roots of transition matrices, identified a class of idempotent matrices, and found some matrices which commute with each other.

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References

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Appendix. A geometric method of computing P_1P_2 when P_1 and P_2 have the same limiting vector.

Description. Assume that P_1 and P_2 have the same limiting vector. Then their "point" representations $[a, b]$ and $[c, d]$ lie on the same line L passing through $[1, 0]$.

The product is

$$P_1P_2 = \begin{bmatrix} ac + (1-a)d & * \\ * & * \end{bmatrix}.$$

Note that $ac + (1-a)d$ is a convex combination of c and d. A construction to locate $ac + (1-a)d$ on the X axis is given. Then the point is projected vertically to the line L. The result will be the point representation of P_1P_2. The construction to find $ac + (1-a)d$ on the X axis is as follows.

1. Project $[c, d]$ vertically to the X axis to obtain $[c, 0]$.
2. Project $[c, d]$ horizontally to $[0, d]$ followed by a $45°$ motion to obtain the point $[d, 0]$.
3. Draw the two lines from $[0, 1]$ to $[d, 0]$ and from $[1, 1]$ to $[c, 0]$ and find their intersection point.

4. Draw the line connecting the intersection point from step 3 to the point $[a, 1]$. This line will intersect the X axis at the point $[ac+(1-a)d, 0]$, as desired. See Diagram 7.

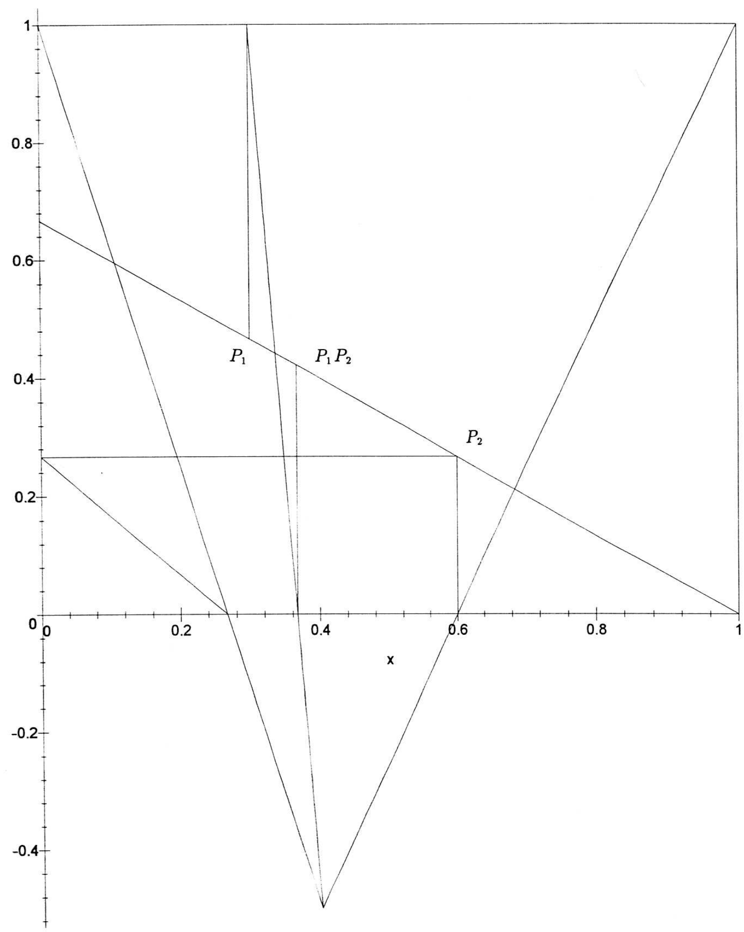

Diagram 7

Note that this method of multiplying any two matrices with the same limiting vector gives a second method of computing P^2. In addition, it gives a way of finding any positive integral multiple of P without requiring the function $f_n(x)$ in (4).

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