

Patterned Matrices with Explicit Trace Vector and some Consequences

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Most of the results to be presented here have been obtained in collaboration with R. Loewy (Technion, Haifa) and H. Šmigoc (University College Dublin).

Let A be an $n \times n$ complex matrix. Pereira proved that there exists a vector v such that

$$v^* p(A) v = \text{trace}(p(A))/n,$$

for all polynomials $p(x)$.

He calls such a vector v a **trace vector** for A .

Finding a trace vector for general A is difficult. The usual strategy of reducing A to canonical form does not work here, as no such form is available for unitary similarity. However, there are several cases where a trace vector is easy to find and which then yields interesting consequences and we present some of these here.

(1) Suppose that A is diagonal.

Then e/\sqrt{n} , where $e := (1, 1, \dots, 1)^T$, is a trace vector for A .

More generally, if A is a normal matrix, so there exists a unitary matrix U with U^*AU diagonal, then Ue/\sqrt{n} is a trace vector for A .

(2) Suppose that A is in Jordan normal form with consecutive Jordan blocks along the diagonal of sizes k_1, \dots, k_r . Let $e(l, d) := (1, 0, \dots, 0)$ (d components) and let

$$v := (\sqrt{k_1}e(1, k_1), \dots, \sqrt{k_r}e(1, r))^T/\sqrt{n}.$$

Then v is a trace vector for A .

(3) A is a circulant.

Since $p(A)$ is also a circulant, for every polynomial $p(x)$, $p(A)$ has all its diagonal entries equal, so each of the basic unit vectors is a trace vector for A .

A very useful observation of Pereira is that if A is an $n \times n$ matrix with leading principal $(n-1) \times (n-1)$ submatrix A_{11} , then the vector $(0, 0, \dots, 0, 1)^T$ is a trace vector for A if and only if n times the characteristic polynomial of A_{11} equals the derivative of the characteristic polynomial of A . In particular, this holds if A is a circulant.

As an example, let P_n be the permutation matrix corresponding to the n -cycle $(1\ 2\ \dots\ n)$ and $C_n = P_n + P_n^T$. Then C_n is a circulant and thus, for $n > 2$, the characteristic polynomial of the simple $(n-1) \times (n-1)$ path matrix M (so $M = (m_{ij})$ where $m_{ij} = m_{ji} = 1$ when $i - j = \pm 1$ and $m_{ij} = 0$, otherwise) is n times the derivative of $\det(xI_n - C_n)$.

Here $\det(xI_n - M)$ is a Chebyshev polynomial while the eigenvalues of C_n are sums $\omega + \omega^{-1}$, where ω runs through the set of n th roots of unity, so one can deduce identities between roots of unity.

Let $f(x)$ be a monic polynomial of degree n
and C its companion matrix.

Let S_1 be the unipotent lower triangular matrix
with (i,j) entry $\frac{s_{i-1}}{n-j+1}$, for $n \geq i > j \geq 1$, where
 s_k is the k th Newton power sum of f , that is,
 s_k is the sum of the k th powers of the roots of
the equation $f(x) = 0$.

Let $S_2 = CS_1$. So $C = S_2S_1^{-1}$. Let $R = S_1^{-1}S_2$.

For example, if $n = 3$, then

$$S_1 = \begin{pmatrix} 1 & 0 & 0 \\ \frac{s_1}{3} & 1 & 0 \\ \frac{s_2}{3} & \frac{s_1}{2} & 1 \end{pmatrix}, S_2 = \begin{pmatrix} \frac{s_1}{3} & 1 & 0 \\ \frac{s_2}{3} & \frac{s_1}{2} & 1 \\ \frac{s_3}{3} & \frac{s_2}{2} & \frac{s_1}{1} \end{pmatrix}$$

and

$$R = \begin{pmatrix} \frac{s_1}{3} & 1 & 0 \\ \frac{3s_2 - s_1^2}{9} & \frac{s_1}{6} & 1 \\ \frac{s_3}{3} - \frac{5s_1s_2}{18} + \frac{s_1^3}{18} & \frac{2s_2 - s_1^2}{12} & \frac{s_1}{2} \end{pmatrix}.$$

The matrix $R = S_1^{-1}S_2$ was first considered by Reams in his 1994 PhD thesis at University College Dublin and he showed that is useful in the study of the nonnegative inverse eigenvalue problem. If the power sums s_k are nonnegative, then S_1 and S_2 have nonnegative entries and it is possible to write down simple inequalities among the s_k which are sufficient for R to have nonnegative entries.

In seeking examples of matrices with easy-to-describe trace

vectors for this talk, it was discovered that the vector

$$e_1 = (1, 0, \dots, 0)^T$$

is a trace vector for R .

So n times the characteristic polynomial of the trailing $(n - 1) \times (n - 1)$ principal submatrix M of R is the derivative $f'(x)$.

In particular, if R has nonnegative entries, so that the list of roots of the equation $f(x) = 0$ is the spectrum of the nonnegative matrix R , then the list of roots of the polynomial

$$f'(x) = 0$$

is the spectrum of the nonnegative matrix M .

This relates to unsolved questions of Monov (Cybern. Inform. Technol. **2** (2006) 35-11, LAA **429** (2008) 2199-2208) on the spectral properties of the derivatives of the characteristic polynomials of nonnegative matrices. (See also Chapter 4 of the PhD thesis of Anthony Cronin, University College Dublin, 2012).

It also provides a setting for studying the Sendov conjecture on the Hausdorff distance between the spectrum of $g(x)$ and $g'(x)$ for polynomials $g(x)$ with roots inside the unit circle. Pereira has successfully used trace vectors to attack problems of this type, though the Sendov conjecture itself has proved elusive.

We now present another class of examples having trace vector e_n .

Let

$$\tau = (\mu_1, \dots, \mu_n),$$

$$x_k := \mu_1^k + \dots + \mu_n^k, \quad k = 1, 2, 3, \dots$$

$$\begin{aligned} q(x) &:= \prod_{i=1}^n (x - \mu_i) \\ &= x^n + q_1 x^{n-1} + \dots + q_n. \end{aligned}$$

Let $X_n =$

$$\begin{pmatrix} x_1 & 1 & 0 & & . & . & . & & 0 \\ x_2 & x_1 & 2 & 0 & & . & . & . & 0 \\ x_3 & x_2 & x_1 & 3 & 0 & & . & . & 0 \\ . & x_3 & . & . & . & . & & & \\ . & . & & . & . & . & & & \\ . & & & & . & & & & \\ & & & & & . & & & \\ & & & & & & & & \\ x_{n-1} & x_{n-2} & & . & . & . & & x_2 & x_1 & n-1 \\ x_n & x_{n-1} & & & . & . & . & x_3 & x_2 & x_1 \end{pmatrix}$$

The matrix X_n occurs in the context of the Newton identities relating the coefficients of a

polynomial to the power sums of its roots. Let $z = (1, q_1, \dots, q_{n-1})^T, e_n = (0, \dots, 1)^T \in \mathbb{C}^n$. Then the Newton identities can be written as

$$X_n z = -n q_n e_n.$$

If we use Cramer's rule to find the value of the first variable $z_1 = 1$, we obtain the identity

$$\det(X_n) = (-1)^n n! q_n.$$

However, the matrix X_n itself, as distinct from its determinant, does not appear to have been widely investigated.

Laffey (LAA 436(6) (2012)1701-1709) discovered the following universal property of the matrices X_n .

Theorem 1. Let $\sigma = (\lambda_1, \dots, \lambda_m)$ be a list of complex numbers satisfying

- (i) $\lambda_1 > |\lambda_j|$, for $j = 2, 3, \dots, m$ and
- (ii) $s_k := \lambda_1^k + \dots + \lambda_m^k > 0$, for $k = 1, 2, 3, \dots$

Then there exists a positive integer $N = N(\sigma)$ such that, for all integers $n \geq N$, and appropriate nonnegative real numbers x_1, \dots, x_n , the spectrum of the matrix X_n differs from σ only in the number of zeros.

Given σ , one can compute an upper bound on the least such N , and one can then easily compute the required x_i .

In a celebrated paper, using symbolic dynamics, Boyle and Handelman (Annals of Math. (2) 133 (2) (1991) 240-316) found a proof that conditions (i) and (ii) above imply that for sufficiently large n , there exists an $n \times n$ nonnegative matrix with spectrum σ and $n - m$ zeros, but their proof does not lead to a bound on N nor a constructive algorithm.

In their work, condition (ii) is weakened by allowing some of the s_k to be zero under certain circumstances.

It is worth noting that if A is an $m \times m$ square matrix with positive entries, then its spectrum satisfies condition (i) and (ii) above and that, in this case, one can easily modify the matrix X_n to yield a matrix with positive entries having the same spectrum.

Because of this application, Laffey, Loewy and Šmigoc have investigated the properties of the matrices X_n and some of the results obtained are presented next.

It is convenient to regard the entries x_i as commuting indeterminates, but here it is assumed that they are real or complex numbers. Further details are available in the paper "Power series with positive coefficients arising from the characteristic polynomials of positive matrices" currently available on arXiv. 1205.1933v3[math.SP] 17 July 2013.

A key observation in proving Theorem 1 is:

Proposition. The characteristic polynomial of X_n is

$$Q(x) = x^n + nq_1x^{n-1} + n(n-1)q_2x^{n-2} + \dots + n!q_n.$$

Proof.

Let $P =$

$$\begin{pmatrix} 1 & 0 & 0 & & \cdot & \cdot & \cdot & & 0 \\ q_1 & 1 & 0 & 0 & & \cdot & \cdot & \cdot & 0 \\ q_2 & q_1 & \frac{1}{2} & 0 & 0 & & \cdot & \cdot & 0 \\ q_3 & q_2 & \frac{q_1}{2} & \frac{1}{6} & 0 & \cdot & & & \\ \cdot & \cdot & \frac{q_2}{2} & \frac{q_1}{6} & \frac{1}{24} & \cdot & & & \\ \cdot & & & \frac{q_2}{6} & \cdot & \cdot & & & \\ & & & & & \cdot & \cdot & & \\ q_{n-3} & & & & & & \cdot & & \\ q_{n-2} & q_{n-3} & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{1}{(n-2)!} & 0 \\ q_{n-1} & q_{n-2} & \frac{q_{n-3}}{2} & & \cdot & \cdot & \cdot & \cdot & \frac{q_1}{(n-2)!} & \frac{1}{(n-1)!} \end{pmatrix}$$

and let $C =$

$$\begin{pmatrix} 0 & 1 & 0 & & . & . & . & & 0 \\ 0 & 0 & 1 & 0 & & . & . & . & 0 \\ . & . & 0 & 1 & 0 & & . & . & 0 \\ . & & . & . & . & . & & & \\ . & . & & . & . & . & & & \\ . & & & & . & & & & \\ & & & & & . & & & \\ & & & & & & & & \\ 0 & 0 & & . & . & . & & 0 & 0 & 1 \\ -n!q_n & . & & . & . & . & . & . & . & -nq_1 \end{pmatrix}$$

be the companion matrix of

$$Q(x) = x^n + nq_1x^{n-1} + n(n-1)q_2x^{n-2} + \dots + n!q_n$$

Direct multiplication, using the Newton identities, yields $PC = X_n P$.

This proves the proposition.

Let $r(x) = x^{n-1} + q_1x^{n-2} + \dots + q_{n-1}$. Then,

using the Newton identities, x_1, \dots, x_{n-1} are the first $n - 1$ Newton power sums of the polynomial $r(x)$, so, by a similar argument, we have

$$\begin{aligned} F_{n-1}(x) &= \det(xI - X_{n-1}) = x^{n-1} + (n-1)q_1x^{n-2} \\ &\quad + (n-1)(n-2)q_2x^{n-3} + \dots \\ &\quad + (n-1)!q_{n-1}. \end{aligned}$$

Hence the derivative $F'_n(x) = nF_{n-1}(x)$.

So, by Pereira's result, the vector

$$e_n = (0, \dots, 1)^T$$

is a trace vector for X_n .

Let $f_n(t) := t^n X_n(1/t)$ be the reciprocal polynomial of $F_n(x)$.

The equation $F'_n(x) = nF_{n-1}(x)$ transforms to

$$\frac{nf'_n(t)}{f_n(t)} = 1 - \frac{f_{n-1}(t)}{f_n(t)}. \quad (*)$$

Next, expanding $f_n(t) = \det(1 - tX_n)$ yields

$$f_n(t) = (1 - tx_1)f_{n-1}(t) - \sum_{i=2}^n \frac{(n-1)!}{(n-i)!} x_i f_{n-i}(t) t^i.$$

(**)

Suppose now that the numbers x_1, \dots, x_n are real and nonnegative.

Since

$$-\frac{f'_n(t)}{f_n(t)} = T_1(n) + T_2(n)t + T_3(n)t^2 + \dots$$

where $T_j(n) = \text{trace}(X_n^j)$, (*) implies that

$$\frac{f_{n-1}(t)}{f_n(t)} = 1 + \left(\frac{1}{n}\right)(T_1(n)t + T_2(n)t^2 + T_3(n)t^3 + \dots)$$

has all its coefficients nonnegative.

Since e_n is a trace vector for X_n , the (n, n) entry of X_n^j is $\frac{T_j(n)}{n}$,
and thus

$$T_j(n) \geq T_j(n-1) + \frac{T_j(n)}{n}$$

and

$$(n-1)T_j(n) \geq nT_j(n-1).$$

Let $W(t) := f_{n-1}(t)/(f_n(t))^{\frac{n-1}{n}}$, considered as a formal power series in t .

Then the logarithmic derivative

$$\begin{aligned}\frac{W'(t)}{W(t)} &= -\frac{f'_{n-1}(t)}{f_{n-1}(t)} + \frac{(n-1)}{n} \frac{f'_n(t)}{f_n(t)} \\ &= \sum_{j=1}^{\infty} \left[\frac{(n-1)}{n} T_j(n) - T_j(n-1) \right] t^{j-1}\end{aligned}$$

has nonnegative coefficients.

Formally integrating term-by-term and exponentiating, we deduce that $W(t)$ has nonnegative coefficients. Observe that if $0 < c < 1$, the formal expansion of $(1 - h)^c$ in powers of h has all its coefficients negative.

We can write equation (**) in the form

$$\begin{aligned}
 f_n(t)^{\frac{1}{n}} &= ((1 - x_1 t) f_{n-1}(t))^{\frac{1}{n}} \left[1 - \sum_{i=2}^n \frac{(n-1)!}{(n-i)!} \frac{x_i f_{n-i}(t) t^i}{(1 - x_1 t) f_{n-1}(t)} \right]^{\frac{1}{n}} \\
 &= ((1 - x_1 t) f_{n-1}(t))^{\frac{1}{n}} (1 - V_n(t))^{\frac{1}{n}}
 \end{aligned}$$

where

$$V_n(t) = \sum_{i=2}^n \frac{(n-1)!}{(n-i)!} \frac{x_i f_{n-i}(t) t^i}{(1 - tx_1) f_{n-1}(t)}.$$

We now prove by induction that, except for the first term 1, all the coefficients in the formal expansion of $f(t)^{\frac{1}{n}}$ are non-positive.

Note that

$$(f_{n-1}(t))^{\frac{1}{n-1}} = 1 - x_1 t - \sum_{j=2}^{\infty} \gamma_j t^j,$$

with $\gamma_j \geq 0$.

So

$$\begin{aligned}
 ((1 - x_1 t) f_{n-1}(t))^{\frac{1}{n}} &= (1 - x_1 t)^{\frac{1}{n}} (1 - x_1 t - \\
 &\quad \sum_{j=2}^{\infty} \gamma_j t^j)^{\frac{(n-1)}{n}} \\
 &= (1 - x_1 t) (1 - \\
 &\quad \sum_{j=2}^{\infty} \frac{\gamma_j t^j}{1 - x_1 t})^{\frac{(n-1)}{n}} \\
 &= (1 - x_1 t) (1 - \\
 &\quad \sum_{k=1}^{\infty} \beta_k (\sum_{j=2}^{\infty} \frac{\gamma_j t^j}{1 - x_1 t})^k \\
 &= 1 - x_1 t - \\
 &\quad \sum_{k=1}^{\infty} \beta_k \frac{(\sum_{j=2}^{\infty} (\gamma_j t^j))^k}{(1 - x_1 t)^{k-1}},
 \end{aligned}$$

where $(1 - t)^{\frac{n-1}{n}} = 1 - \sum_{k=1}^{\infty} \beta_k t^k$.

Note that $\beta_k > 0$, for $k = 1, 2, 3, \dots$

Note also that the expansion of $(1 - x_1 t)^{-(k-1)}$ has nonnegative coefficients.

Now

$$\begin{aligned}f_n(t)^{\frac{1}{n}} &= ((1 - x_1 t)f_{n-1}(t))^{\frac{1}{n}} (1 - V_n(t))^{\frac{1}{n}} \\&= ((1 - x_1 t)f_{n-1}(t))^{\frac{1}{n}} \left(1 - \sum_{i=1}^{\infty} \alpha_i V_n(t)^i\right) \\&= ((1 - x_1 t)f_{n-1}(t))^{\frac{1}{n}} - \sum_{i=1}^{\infty} \alpha_i ((1 - x_1 t)f_{n-1}(t))^{\frac{1}{n}} V_n(t)^i,\end{aligned}$$

$$\text{where } (1 - t)^{\frac{1}{n}} = 1 - \sum_{i=1}^{\infty} \alpha_i t^i.$$

$$\text{Next}((1 - x_1 t)f_{n-1}(t))^{\frac{1}{n}} V_n(t)$$

$$= \sum_{i=2}^n i \frac{(n-1)!}{(n-i)!} \frac{x_i f_{n-i}(t) t^i}{(1 - tx_1) f_{n-1}(t)}$$

$$\sum_{i=2}^n i \frac{(n-1)!}{(n-i)!} \frac{x_i f_{n-i}(t) t^i}{(1 - tx_1) f_{n-1}(t)} \cdot \frac{x_i f_{n-i}(t)}{f_{n-2}(t)} \cdot$$

$$\frac{f_{n-2}(t)}{(f_{n-1}(t))^{\frac{n-2}{n-1}}}$$

Using (*) and the fact that for a positive integer $k < n - 1$,

$$\frac{f_k(t)}{f_{n-1}(t)} = \frac{f_k(t)}{f_{k+1}(t)} \frac{f_{k+1}(t)}{f_{k+2}(t)} \cdots \frac{f_{n-2}(t)}{f_{n-1}(t)},$$

and the inductive hypothesis that all coefficients except the first term 1 in the expansion of $(f_{n-1}(t))^{\frac{1}{n-1}}$ are non-positive, we deduce that all coefficients in the expansion of $(f_n(t))^{\frac{1}{n}}$, except for the first term 1, are non-positive.

If all the x_j are positive, one can check that "non-positive" can be replaced by "negative".

One has the following consequence:

Theorem 2. Let A be a square matrix with positive entries and let

$f(t) := \det(I - tA)$. Then there exists a positive integer N such

that all coefficients in the formal expansion of $1 - ((f(t))^{\frac{1}{n}})$ are positive, for all $n > N$.

One can write down an upper bound on the least N required in terms of the spectrum of A .

In the special case where

$$A = \text{diag}(a_1, \dots, a_m),$$

where all $a_i > 0$, then $1 - f(t)^{\frac{1}{n}}$ has positive coefficients for all $n \geq m$ and in general this is best possible here (Laffey, Math. Proc.

RIA.112 A (2) (2013) 97-106).

Sign patterns of the coefficients of formal power series also play a role in the study of the spectra of nonnegative integer matrices by Kim, Ormes and Roush (JAMS **13** (2000) 773-806).

Suppose that

$$\sigma = (\lambda_1, \dots, \lambda_n)$$

is a list of complex numbers and

$$\begin{aligned} f(x) &= (x - \lambda_1) \dots (x - \lambda_n) \\ &= x^n + p_1 x^{n-1} + \dots + p_n, \text{ say.} \end{aligned}$$

By comparing power sums of the elements of σ with traces of powers of X_n , for example, one can inductively find unique elements x_1, \dots, x_n , such that the corresponding X_n has characteristic polynomial $f(x)$.

So there is a matrix with entries in the field generated by the coefficients of $f(x)$ which has spectrum σ and trace vector

$$e_n = (0, \dots, 0, 1)^T.$$

If, given σ , we use instead of X_n the matrix Y_n obtained from it by replacing the diagonal $(1, 2, \dots, n-1)$ by $(1, 1, \dots, 1)$ ($n-1$ entries) and then compute the x_j inductively such that the characteristic polynomial of the principal leading $j \times j$ submatrix of Y_n has characteristic polynomial the $(n-j)$ th derivative of $f(x)$, made monic, then the resulting Y_n will also have trace vector e_n .

If the polynomial $f(x)$ has integer coefficients, then the corresponding Y_n will have rational entries, but not necessarily, integer entries. However, if the coefficient p_j is divisible by

$$n(n-1) \dots (n-j+1)$$

for $j=1, \dots, n$, then Y_n will have integer entries.

Finally, we consider a special case of the matrix X_n . Let S_n be the matrix obtained from X_n by putting $x_2 = 1$ and all other $x_j = 0$.

Then S_n has trace vector $(0, \dots, 0, 1)^T$ and characteristic polynomial the (statisticians') Hermite polynomial $He_n(x)$ given by

$$He_n(x) = \exp(x^2/2) D^n(\exp(-x^2/2))$$

where $D = d/dx$.

Let $f_n(t) := \det(I - tS_n)$ be the reciprocal of $\text{He}_n(x)$ and let

$$P(t) := -tf_n'(t)/f_n(t).$$

So

$$P(t) = T_1(n)t + T_2(n)t^2 + \dots$$

where $T_j(n) = \text{trace}(S_n^j)$ is the sum of the j th powers of the roots of $\text{He}_n(x) = 0$.

$P(t)$ satisfies the Riccati equation

$$(1-(2n-1)t^2)P(t)+t^3 P'(t) = t^2 P(t)^2 + n(n-1)t^2.$$

There is a very considerable literature on the roots of $He_n(x)$, especially in the area of combinatorics and theoretical computer science - in studying the average height of plane trees, De Bruijn, Knuth and Rice wrote a famous paper on the subject in 1972 (in which they introduced Mellin transforms into this area) and later, Flajolet, Lagarias, Odlyzko, Zagier and many others, have done so. However, this Riccati equation has no known explicit solution in terms of elementary functions.

The power sum $T_k(n)$ is a polynomial in n of degree $k + 1$ and the coefficient of n^{k+1} is the Catalan number $C_k = \frac{(2k)!}{(k+1)!k!}$.

The Perron root of S_n is close to $\sqrt{2\sqrt{n}}$.

The polynomial $f_n(t)$ is a polynomial in t^2 and, as such, it has positive roots (since, for example, S_n is similar to a real symmetric matrix so the nonzero eigenvalues of S_n^2 are positive) and therefore it follows that the expansion in powers of t of $1 - f_n(t)^{2/n}$ has all its coefficients nonnegative.
