A MATHEMATICAL NOTE

Algorithm for the efficient evaluation of the trace of the inverse of a matrix

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Introductory reminiscence. It was after a physics seminar—therefore on a Wednesday—that Richard Crandall and I, in the company of some colleagues, adjourned to Ye Olde Town Crier for veal birds (Wednesday's special on the invariable menu of that establishment), Kindly Olde Dr. Parkers (to honor the memory of the once-upon-a-time chairman of our department, the inventor of this modified martini and a specialty of the house) and shop talk. Richard, who was working at the time on material subsequently published as "On the quantum zeta function,"[1] was motivated to ask me whether I knew of an efficient way to evaluate the trace of the inverse of a matrix. "I might," said I, "though whether my idea will be of any real use to you I cannot guess." As he was leaving town the next morning, I returned to my office after dinner and wrote out the following material at a single sitting. This I was able to do for a curious reason:

In 1958 I had come by accident (which is to say, while searching for something else) upon Advanced Problem No. 4782 which had been submitted by one V. F. Ivanoff to the American Mathematical Monthly (**65**, 212 (1958)), wherein readers are asked to show that the n^{th} derivative $F^{(n)}(x)$ of a composite function $F(x) = \Phi(f(x))$ can be described

$$\begin{vmatrix} f'D & f''D & f'''D & f''''D & \dots & f^{(n)}D \\ -1 & f'D & 2f''D & 3f'''D & \dots & \binom{n-1}{1}f^{(n-1)}D \\ 0 & -1 & f'D & 3f''D & \dots & \binom{n-1}{2}f^{(n-2)}D \\ 0 & 0 & -1 & f'D & \dots & \binom{n-1}{3}f^{(n-3)}D \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & 0 & \dots & f'D \end{vmatrix} \Phi(f)$$

[1] J. Phys. A: Math. Gen **29** No 21, 7 November 1996, pp. 6795–6816.

where $f^{(k)} \equiv \left(\frac{d}{dx}\right)^k f(x)$ and $D^k\Phi(f) \equiv \left(\frac{d}{df}\right)^k \Phi(f)$. I recognized on the occasion that "Ivanoff's Formula" contained the seed of a solution to the problem that had sent me to the library in the first place, and I discovered subsequently that from it radiates in fact a set of techniques relating usefully to a remarkable variety of topics. Some of that material I pulled together long ago in a seminar "Some applications of an elegant formula due to V. F. Ivanoff" presented on 28 May 1969 to the Applied Math Club at Portland State University (see COLLECTED SEMINARS 1963–1970), and it is from that source that I extracted the germ of the idea developed here.

The computational technique. Let $\mathbb{M}$ be an $N \times N$ matrix. Let its characteristic polynomial be notated

$$p(x) = \det(\mathbb{M} - x\mathbb{I}) = p_0 + p_1 x + p_2 x^2 + \cdots + p_N x^N \tag{1}$$

where clearly

$$\left.\begin{aligned} p_0 &= \det \mathbb{M} \\ &\;\vdots \\ p_{N-1} &= (-)^{N-1}\,\mathrm{tr}\,\mathbb{M} \\ p_N &= (-)^N \end{aligned}\right\} \tag{2}$$

By the Cayley-Hamilton Theorem

$$p_0\mathbb{I} + p_1\mathbb{M} + p_2\mathbb{M}^2 + \cdots + p_N\mathbb{M}^N = \mathbb{O} \tag{3}$$

Therefore

$$\mathbb{M}^{-1} = -\frac{p_1\mathbb{I} + p_2\mathbb{M} + \cdots + p_N\mathbb{M}^{N-1}}{p_0} \tag{4}$$

which would provide an easy way to construct $\mathbb{M}^{-1}$—whence also $\mathrm{tr}\,\mathbb{M}^{-1}$—if there were an easy way to construct the numbers $p_n : n = 1, 2, \ldots, N$. There is. . .

. . . but to describe it I find it convenient to work initially not with $p(x)$ but with the equivalent structure

$$q(y) = \det(\mathbb{I} - y\mathbb{M}) = (-y)^N \cdot p(1/y) \tag{5.1}$$

$$= 1 + q_1 y + q_2 y^2 + \cdots q_N y^N \tag{5.2}$$

The trick now is to notice that

$$q(y) = e^{\mathrm{tr}\log(\mathbb{I} - y\mathbb{M})} \tag{6}$$

and that

$$\log(\mathbb{I} - y\mathbb{M}) = -y\mathbb{M} - \tfrac{1}{2}y^2\mathbb{M}^2 - \tfrac{1}{3}y^3\mathbb{M}^3 - \tfrac{1}{4}y^4\mathbb{M}^4 - \cdots \tag{7}$$

Evidently

$$q(y) = \exp\left\{-T_1 y - \tfrac{1}{2}T_2 y^2 - \tfrac{1}{3}T_3 y^3 - \tfrac{1}{4}T_4 y^4 - \cdots\right\} \tag{8}$$

where

$$T_n = \mathrm{tr}\,\mathbb{M}^n \tag{9}$$

Developing the composite function which appears on the right side of (8), we find

$$\begin{aligned} q(y) = 1 - T_1 y &+ \tfrac{1}{2!}[T_1^2 - T_2]y^2 \\ &- \tfrac{1}{3!}[T_1^3 - 3T_1T_2 + 2T_3]y^3 \\ &+ \tfrac{1}{4!}[T_1^4 - 6T_1^2T_2 + 8T_1T_3 + 3T_2^2 - T_4]y^4 + \cdots \end{aligned} \tag{10}$$

which looks like an infinite series, but actually truncates at the N^{th} term. To get a preliminary sense of how this comes about, consider the case $N = 2$. We have

$$\begin{aligned} p(x) &= p_0 + p_1 x + p_2 x^2 \\ &= \det\mathbb{M} - T_1 x + x^2 \end{aligned}$$

which by (3) entails $\det\mathbb{M}\cdot\mathbb{I} - T_1\cdot\mathbb{M} + \mathbb{M}^2 = \mathbb{O}$, of which we take the trace to obtain

$$2\det\mathbb{M} = T_1^2 - T_2 \tag{11}$$

So we have

$$p(x) = \tfrac{1}{2}[T_1^2 - T_2] - T_1 x + x^2 \tag{12}$$

whence

$$q(y) = y^2 p(1/y) = 1 - T_1 y + \tfrac{1}{2}[T_1^2 - T_2]y^2$$

This is the advertised truncated version of (10), but why does it truncate? Because the Cayley-Hamilton Theorem $p(\mathbb{M}) = \mathbb{O} \implies \mathbb{M}\,p(\mathbb{M}) = \mathbb{O} \implies \mathrm{tr}\{\mathbb{M}\,p(\mathbb{M})\} = 0$, and this, by (11), entails

$$\tfrac{1}{2}[T_1^2 - T_2]T_1 - T_1T_2 + T_3 = \tfrac{1}{2}[T_1^3 - 3T_1T_2 + T_3] = 0$$

which serves to switch off the cubic term in (10). Higher order terms vanish by the same mechanism, but to construct the explicit demonstration one has to dig a bit deeper; the digging will serve also to reduce the phrase "developing the composite function…" to the status of a recursive algorithm. Here I must be content simply to state the results; the arguments are pretty, I think, but of no immediate interest in themselves.

On has $q_n = (-)^n \frac{1}{n!} Q_n$, where

$$Q_n = \begin{vmatrix} T_1 & T_2 & T_3 & T_4 & \dots & T_n \\ 1 & T_1 & T_2 & T_3 & \dots & T_{n-1} \\ 0 & 2 & T_1 & T_2 & \dots & T_{n-2} \\ 0 & 0 & 3 & T_1 & \dots & T_{n-3} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & 0 & \dots & T_1 \end{vmatrix} \tag{13}$$

can be computed recursively from

$$Q_n = \sum_{m=1}^{n} (-)^{m+1} \frac{(n-1)!}{(n-m)!} T_m Q_{n-m} \tag{14}$$

Thus

$$\begin{aligned}
Q_0 &= 1 \\
Q_1 &= T_1 Q_0 \\
Q_2 &= T_1 Q_1 - T_2 Q_0 \\
Q_3 &= T_1 Q_2 - 2T_2 Q_1 + 2T_3 Q_0 \\
Q_4 &= T_1 Q_3 - 3T_2 Q_2 + 6T_3 Q_1 - 6T_4 Q_0 \\
&\ \vdots
\end{aligned} \tag{15}$$

giving

$$\begin{aligned}
Q_0 &= 1 \\
Q_1 &= T_1 \\
Q_2 &= T_1^2 - T_2 \\
Q_3 &= T_1^3 - 3T_1 T_2 + 2T_3 \\
Q_4 &= T_1^4 - 6T_1^2 T_2 + 8T_1 T_3 + 3T_2^2 - 6T_4 \\
&\ \vdots
\end{aligned} \tag{16}$$

One has now enough information to complete the proof (if proof were needed) that

$$\text{Cayley-Hamilton Theorem} \Longrightarrow Q_n = 0 : n > N$$

More interesting, I think, is the universality (i.e., the N-independence) which attaches to (16), and therefore to statements like

$$p(x) = \sum_{n=0}^{N} \tfrac{1}{n!} Q_n (-x)^{N-n} \tag{17}$$

and

$$\det \mathbb{M} = \tfrac{1}{N!} Q_N \quad \text{for any } N \times N \text{ matrix } \mathbb{M} \tag{18}$$

Also interesting are the major simplifications which tend, in my experience, to result when $\mathbb{M}$ is endowed with any kind of specialized structure. For example, if $\mathbb{M}$ is antisymmetric, then so are all of its odd powers, and so also are all its odd traces; in place of (16) one has

$$\begin{aligned}
Q_0 &= 1 \\
Q_1 &= 0 \\
Q_2 &= -T_2 \\
Q_3 &= 0 \\
Q_4 &= 3T_2^2 - 6T_4 \\
&\ \vdots
\end{aligned}$$

Or again, if $\mathbb{M}$ projects ($\mathbb{M}^2 = \mathbb{M}$) onto a d-dimensional domain ($\mathrm{tr}\,\mathbb{M} = d$) then $T_n = d$ (all d) and we have

$$Q_n = \begin{cases} d!/(n-d)! & n = 1, 2, \dots, d \\ 0 & n > d \end{cases}$$

giving $p(x) = (-x)^{N-d}\,(1-x)^d$: the eigenvalues of $\mathbb{M}$ are zero (with multiplicity $N-d$) and unity (with multiplicity d). This is hardly news, but illustrates the elegant swiftness with which strong results can (at least in favorable cases) be obtained by the methods described above. At (7) I made (formal) use of a series which converges conditionally; no lingering condition attaches, however, to our final results. Note also that, according to (18), to compute the determinant of $\mathbb{M}$ we only have to compute $\mathbb{M}^2, \mathbb{M}^3, \dots, \mathbb{M}^N$ (and of the latter we have actually to compute only the diagonal elements); the computational difficulty has been reduced from Laplace's $O(N!)$ to—at worst—$O(N^4)$.

To wrap it up: Compute $\mathbb{M}^0, \mathbb{M}, \mathbb{M}^2, \dots, \mathbb{M}^N$ to get $T_0, T_1, T_2, \dots, T_N$ and use (14) to compute $Q_0, Q_1, Q_2, \dots, Q_N$. Then

$$\mathrm{tr}(\mathbb{M}^{-1}) = -\frac{T_0 p_1 + T_1 p_2 + T_2 p_3 + \cdots + T_{N-1} p_N}{p_0} \tag{19}$$

where

$$\begin{aligned} p_0 &= + \quad \tfrac{1}{N!} Q_N \\ p_1 &= -\tfrac{1}{(N-1)!} Q_{N-1} \\ p_2 &= +\tfrac{1}{(N-2)!} Q_{N-2} \\ &\ \vdots \\ p_N &= (-)^N \end{aligned} \tag{20}$$

Returning with (20) to (4) we obtain an inversion algorithm (i.e., a method for constructing $\mathbb{M}^{-1}$) which is computationally much more efficient than the standard "transpose of the matrix of cofactors" (and from which (19) can be obtained as a corollary), while

$$\det \mathbb{M} = \frac{1}{N} \sum_{m=1}^{N} (-)^{m+1} \frac{1}{(N-m)!} T_m Q_{N-m}$$

provides a description of $\det \mathbb{M}$ which—remarkably—makes no use of the standard "summation over signed permutations" procedure. These expressions are structurally so simple as (in favorable cases) to permit one to contemplate passage to the continuous limit $N \longrightarrow \infty$.