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Recursive Evaluation of Padé Approximants for Matrix Sequences

Abstract: An algorithm is described for calculating the existing Padé approximants to any sequence $A_0, A_1, \cdots$ of $s \times t$-matrices. As an application the algorithm gives a new way for finding the minimal polynomial of any square matrix A and the inverse of the characteristic matrix $xI - A$.

Introduction

The classical Padé approximation problem [1] is to find two polynomials of prescribed degree, $P(x) = \sum_{i=0}^{m} p_i x^i$ and $Q(x) = \sum_{i=0}^{n} q_i x^i$, with $q_0 = 1$, such that for a given function $f(x) = \sum_{i=0}^{\infty} a_i x^i$,

$$f(x)Q(x) - P(x) = Ax^{m+n+1} + Bx^{m+n+2} + \cdots. \qquad (1)$$

The rational form $P(x)/Q(x)$ is called the $[n, m]$ *Padé approximant* to $f(x)$.

Recently studies have been made to generate the Padé approximants recursively; several algorithms are described in [2] and an improved recursion scheme is given in [3]. In both of these studies it is assumed that the function $f(x)$ is such that all the Padé approximants not only exist but also are in their reduced form; i.e., there are no common factors in $P(x)$ and $Q(x)$. This assumption seems to be a severe restriction because it is not easy to tell when a function has that property, and moreover, the algorithms fail if just one of the intermediately calculated approximants either is not in its reduced form or, worse yet, does not exist.

In [4] the Padé problem was generalized for the case where the coefficients of the power series expansion of $f(x)$ are $s \times t$-matrices. An approximant was then taken of the form $P(x)Q^{-1}(x)$, where $P(x)$ is an $s \times t$ and $Q(x)$ a $t \times t$ matrix polynomial. In addition, recurrence equations for evaluating the approximants were derived for certain special cases.

We shall study another generalization of the Padé problem that differs from the preceding one in that $Q(x)$ is taken to be a scalar polynomial. We also relax the requirement that all the approximants exist.

Our version of the problem, although no less general than the previous one, has its most natural applications in certain special cases. One such is the problem of finding the inverse of the characteristic matrix $xI - A$ in the form $P(x)/q(x)$, where $q(x)$ is the minimal polynomial of A. Other applications appear in the area of systems identification, where the so-called transfer function of the system has precisely the form $P(x)/q(x)$. In this context a criterion for the existence of the approximants was given in [5]. Our algorithm is an outgrowth of one studied in [6].

Generalized Padé approximants

Let $P(x) = \sum_{i=0}^{m} P_i x^i$ and $Q(x) = \sum_{i=0}^{n} Q_i x^i$ be $s \times t$- and $s \times s$-matrix polynomials, respectively, where the matrices P_i and Q_i have real-valued elements. If the determinant $q(x) = |Q(x)|$ does not vanish for all values of x, the rational form

$$C(x) = Q^{-1}(x)P(x) = T(x)/q(x) = \sum_{i=0}^{\infty} C_i x^i \qquad (2)$$

may be defined. Here, $T(x)$ is a matrix polynomial determined by $P(x)$ and $Q(x)$.

We define the Padé-approximants in the following way:

If a subset $A_0, A_1, \cdots, A_N$ of an infinite set of $s \times t$-matrices $A_0, A_1, \cdots$ determines two polynomials

$P_{n,m}(x) = \sum_{i=0}^{m} P_i(n,m)x^i$ and $q_{n,m}(x) = \sum_{i=0}^{n} q_i(n,m) x^i$, $q_0(n,m) = 1$, of prescribed degree m and n, respectively; i.e., $P_m(n,m) \neq 0$ and $q_n(n,m) \neq 0$, such that in the expansion of the rational form,

$$P_{n,m}(x)/q_{n,m}(x) = \sum_{i=0}^{\infty} C_i x^i,$$

1) $C_i = A_i$ for $i = 0, 1, \cdots, N$ and (3a)
2) there is no common factor other than ± 1 in $q_{n,m}(x)$ and all the elements of $P_{n,m}(x)$, (3b)

then the pair $(P_{n,m}(x), q_{n,m}(x))$, also denoted $[n,m]$, is said to be a *Padé approximant to the series* A_0, $A_1, \cdots$.

Requirement (3b) implies that $[n,m]$ is unique. Further, the approximants do not depend on N; hence N need not appear in the polynomials nor in the approximant $[n,m]$.

The present definition extends those in [1 to 3] in that all the approximants need not exist. Moreover, if one exists it is unique; in other words, the rational form in question is in its reduced form.

Conditions for approximants

Consider the equation

$$\left(\sum_{i=0}^{N} A_i x^i\right)\left(\sum_{i=0}^{n} q_i x^i\right) - \sum_{i=0}^{m} P_i x^i = B_1 x^{N+1} + \cdots + B_n x^{N+n}, \tag{4}$$

where $N \geq \max(n,m)$, $q_0 = 1$, and

$$B_1 = q_1 A_N + q_2 A_{N-1} + \cdots + q_n A_{N-n+1}$$

$$B_2 = q_2 A_N + \cdots + q_n A_{N-n+2}$$

$$\vdots$$

$$B_n = q_n A_N.$$

Define $P_i = 0$ for $i > m$, $q_i = 0$ for $i > n$, and $A_i = 0$ for $i < 0$. Then the coefficients of x^r in (4) yield

$$\sum_{i=0}^{r} q_i A_{r-i} - P_r = 0 \qquad \text{for } r = 0, 1, \cdots, N. \tag{5}$$

Equations (5) are equivalent to the pair of systems

$$\sum_{i=0}^{m} q_i A_{r-i} = P_r \qquad \text{for } r = 0, 1, \cdots, m \tag{6}$$

and

$$\sum_{i=0}^{n} q_i A_{r-i} = 0 \qquad \text{for } r = m+1, \cdots, N. \tag{7}$$

Since any solution $(q_0, \cdots, q_n)$ of (7) defines through (6) a solution $(q_0, \cdots, q_n, P_0, \cdots, P_m)$ of (5), the existence of a unique solution for (7) is equivalent to the existence of a unique solution for (5).

For each i, $i \leq N$, write $A_i = [a_{jk}(i)]$, $1 \leq j \leq s$, $1 \leq k \leq t$, as the $1 \times st$ vector,

$$a_i = [a_{11}(i), \cdots, a_{1t}(i), \cdots, a_{s1}(i), \cdots, a_{st}(i)]. \tag{8}$$

Further, define the $1 \times (N-m)st$ vector

$$h_j = (a_{m-n+j+1}, a_{m-n+j+2}, \cdots, a_{N-n+j}) \qquad \text{for } j = 0, \cdots, n. \tag{9}$$

Finally, for $k = n - m$ define $H(k,n,N)$ as the $(n+1) \times (N-m)st$ matrix whose jth row for $j = 0, 1, \cdots, n$ is given by h_j.

Then the system (7) can be written as

$$(q_n, q_{n-1}, \cdots, q_0)H(k,n,N) = 0. \tag{10}$$

For this equation a unique solution with $q_0 = 1$ exists if and only if the rows $h_0, \cdots, h_{n-1}$ are linearly independent and h_n is linearly dependent on them.

Suppose that (10) has a unique solution and suppose further that P_m with $m = n - k$ from (6) and q_n turn out to be nonzero. Then $P(x) = \sum_{i=0}^{m} P_i x^i$ and $q(x) = \sum_{i=0}^{n} q_i x^i$ define the approximant $[n,m]$ for the sequence $A_0, A_1, \cdots$. Conversely, suppose there is an approximant $[n,m] = [P_{n,m}(x), q_{n,m}(x)]$ for the same sequence. Then by (3a), Eqs. (6)-(7) with $q_i(n,m) = q_i$ and $P_i(n,m) = P_i$ hold. Also, both P_m and q_n are nonzero. The existence of $[n,m]$ implies that h_n is linearly dependent on $h_0, \cdots, h_{n-1}$, and the requirement (3b) further implies that $h_0, \cdots, h_{n-1}$ forms a linearly independent set.

It is clear by (3b) that the existence of an approximant $[n, n-k]$ satisfying (3a) for some N implies that no approximant of the type $[n', n'-k]$ for $n' < n$ and satisfying (3a) for the same N can exist. Another line of reasoning leads to the same result: each of the first $n'+1$ rows of $H(k,n,N)$ appears as a subrow in the corresponding row of $H(k,n',N)$. Since this makes all the rows of $H(k,n',N)$ linearly independent, the result follows.

In general cases where the matrices A_i have no special properties it is necessary for an approximant to exist so that $n = (N-m)st$. This means that the degree of $q(x)$ grows rapidly when s and t are large, which makes these kinds of approximants less attractive than those of the type $P(x)Q^{-1}(x)$. In special cases, however, such as those studied in the last section and in systems identification problems, where $q(x)$ has a special meaning, our types of approximants are the only ones of interest.

A factoring problem

Suppose k, n, and N are such that the first n rows of $H(k,n,N)$ are linearly independent. Consider the following factorization of $H(k,n,N)$ (and although we illustrate the case $k > 0$, the given rules apply to the case $k \leq 0$ as well):

$$
\underbrace{\begin{bmatrix} 0 & \cdots & 0 & a_0 & a_1 & \cdots & a_{N-n} \\ \vdots & \cdot^{\cdot^{\cdot}} & a_0 & a_1 & & \cdots & a_{N-n+1} \\ 0 & \cdot^{\cdot^{\cdot}} & & & & & \\ a_0 & & & & & & \vdots \\ \vdots & & & & & & \\ a_{m+1} & \cdots & & & & & a_N \end{bmatrix}}_{H(k,n,N)}
$$

$$
= \underbrace{\begin{bmatrix} 1 & & & & \\ r_{10} & 1 & & & \\ r_{20} & r_{21} & 1 & & \\ \vdots & \vdots & & \ddots & \\ r_{n,0} & r_{n,1} & \cdots & r_{n,n-1} & 1 \end{bmatrix}}_{R(n)} \underbrace{\begin{bmatrix} q_{00} & \cdots & q_{0,(N-m)st-1} \\ & & \\ \vdots & & \vdots \\ & & \\ q_{n,0} & \cdots & q_{n,(N-m)st-1} \end{bmatrix}}_{Q(k,n,N)} . \tag{11}
$$

The elements of $R(n)$ and $Q(k,n,N)$ are uniquely determined by the following rules, which allow their calculation recursively one-by-one. At the same time we also calculate the inverse $D(n) = R(n)^{-1}$ which is lower-triangular. Observe, that for each pair n' and n such that $n' \le n$, $D(n')$ is a submatrix of $D(n)$.

Step 1. Set the first row of $Q(k,n,N)$ equal to the first row of $H(k,n,N)$. Set $R(0) = D(0) = (1)$.

Step 2. Proceeding recursively we shall have determined at the ith row all the r_{hj}'s and q_{hj}'s for $h = 0, 1, \cdots, i$ as well as $R(i)$ and $D(i)$. Let $s(i)$ be the least integer such that $q_{i,s(i)} \ne 0$. For $i < n+1$, $s(i)$ exists. Set $q_{h,s(i)} = 0$ for all $h > i$. Equation (11) leads to a set of $i+1$ equations, one for each column $s(j)$, $j = 0, \cdots, i$. From these equations the unknowns $r_{i+1,0}, \cdots, r_{i+1,i}$ can be found recursively one-by-one, which gives $R(i+1)$ and $D(i+1)$. The latter further determines the $q_{i+1,j}$'s, which terminates the cycle.

If now, in addition, the last row of $H(k,n,N)$ is linearly dependent on the first n, the last row of $Q(k,n\,N)$ is zero and is the only such row. But then the last row of $D(n)$, namely $(d_{n,0}, d_{n,1}, \cdots, d_{n,n-1}, 1)$, spans the space of solutions to the equation

$$
x'H(k,n,N) = 0. \tag{12}
$$

In that case we define

$$
q_{n,m}(x) = \sum_{i=0}^{n} q_i(n,m)x^i
$$

$$
P_{n,m}(x) = \sum_{i=0}^{m} P_i(n,m)x^i, \tag{13}
$$

where $q_i(n,m) = d_{n,n-i}$ and the $P_i(n,m)$'s are determined by (6) with $q_i = q_i(n,m)$.

We conclude that the approximant $[n,m] = [P_{n,m}(x), q_{n,m}(x)]$ obtained from (13) exists if and only if $q_n(n,m)$ and $P_m(n,m)$ both turn out to be nonzero.

The preceeding factoring algorithm is clearly related to a Gauss-elimination scheme with a particular choice of the pivoting elements [7]. This choice is so made that the following is true: For any n' and N', $n' \le n$ and $N' \le N$, the last row of the corresponding submatrix $H(k,n',N')$ of $H(k,n,N)$ is in the linear span of the other rows if and only if the last row of $Q(k,n',N')$ is a row of zeros. Then as above the last row of $D(n')$ satisfies the equation $x'H(k,n',N') = 0$. This means that the one and the same factorization will also give us the approximant $[n', n'-k]$ if it exists. Hence, we can continue the factorization indefinitely and obtain all the existing approximants with $n - m = k$ as fixed just by picking out certain rows of $D(n)$. The details of the resulting algorithm are described in the next section.

Observe that we need not—and to get recursion we must not—perform any apriori reshuffling of rows and columns of $H(k,n,N)$ in order to guarantee that the principal minors be nonzero, as must be done by applying the other versions of the Gauss-elimination scheme. Then, naturally, we cannot get $Q(k,n,N)$ as upper-triangular in general, but that is no disadvantage whatsoever. However, our fixed rules may cause difficulties due to round-off errors in inverting $R(n)$ if $H(k,n,N)$ is ill-conditioned. As a safeguard to this, one should check that any picked last row of $D(n)$ indeed produces a zero-row in $Q(k,n,N)$. If that does not happen, one may recalculate that particular row by refactoring $H(k,n,N)$ by a different choice of the pivotal points. For instance, change the rules above by letting $s(i)$ be the integer for which $|q_{i,s(i)}|$ is maximum. After the correct row of $D(n)$ is found, the original factorization routine will be continued. It is possible to devise other variations of the rules to preserve recursion while handling various types of numerical difficulties. See, e.g., the analysis in the last section.

Algorithm

In order for the desired conditions to be maintained, the main algorithm need only take care of how $H(k,n,N)$ is to be grown. We illustrate the algorithm described by the flow chart in Fig. 1 by calculating the approximants of several sequences, where the input in each example is a given sequence $A_0, A_1, \cdots, A_{N_0}$ and k.

- *Example 1*

We calculate the first three approximants with $k = 0$ for the sequence $1, 1, \frac{1}{2}, \frac{1}{6}, \frac{1}{24}$ which constitutes the first five coefficients in the series expansion of e^x. The first approximant is $[0,0]=(1,1)$. We obtain after $H(0,1,2)$ the second approximant, $[1,1]=[(1+\frac{1}{2}x),\ (1-\frac{1}{2}x)]$. Continuing, the factorization of $H(0,2,4)$ becomes

$$\begin{bmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{6} \\ \frac{1}{6} & \frac{1}{24} \end{bmatrix} = \begin{bmatrix} 1 & & \\ \frac{1}{2} & 1 & \\ \frac{1}{6} & \frac{1}{2} & 1 \end{bmatrix} \begin{bmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{12} \\ 0 & 0 \end{bmatrix}.$$

This gives

$$D(2) = \begin{bmatrix} 1 & & \\ -\frac{1}{2} & 1 & \\ \frac{1}{12} & -\frac{1}{2} & 1 \end{bmatrix}$$

and the third approximant, $[2,2]=[(1+\frac{1}{2}x+\frac{1}{12}x^2),\ (1-\frac{1}{2}x+\frac{1}{12}x^2)]$.

- *Example 2*

For the sequence $0,0,1,1,1,2$ and $k=1$ we calculate all the approximants. We have in Fig. 1 $M=2$ which gives the initial matrix $H(1,3,5)$. Hence there is no approximant for $N \leq 4$. The factorization of $H(1,3,5)$ becomes

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ 1 & 1 & 1 & \\ 2 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

and we get $[3,2]=[(x^2,\ (1-x-x^3)]$. This time $Q(1,3,5)$ cannot be made upper-triangular, and this example is not calculable by the methods in [2] or [3].

- *Example 3*

Let $s=t=2$ and consider the sequence

$$\begin{bmatrix} 1 & 3 \\ 1 & 2 \end{bmatrix}, \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \begin{bmatrix} 4 & 3 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 10 & 10 \\ 3 & 3 \end{bmatrix}.$$

We wish to calculate the first Padé-approximant for $k=1$. Proceeding analogously to the scalar-valued case we have after a few steps the factorization of $H(1,3,3)$:

$$\begin{bmatrix} 1 & 3 & 1 & 2 \\ 1 & 1 & 0 & 1 \\ 4 & 3 & 1 & 0 \\ 10 & 10 & 3 & 3 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ 4 & \frac{9}{2} & 1 & \\ 10 & 10 & 2 & 1 \end{bmatrix} \begin{bmatrix} 1 & 3 & 1 & 2 \\ 0 & -2 & -1 & -1 \\ 0 & 0 & \frac{3}{2} & -\frac{7}{2} \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

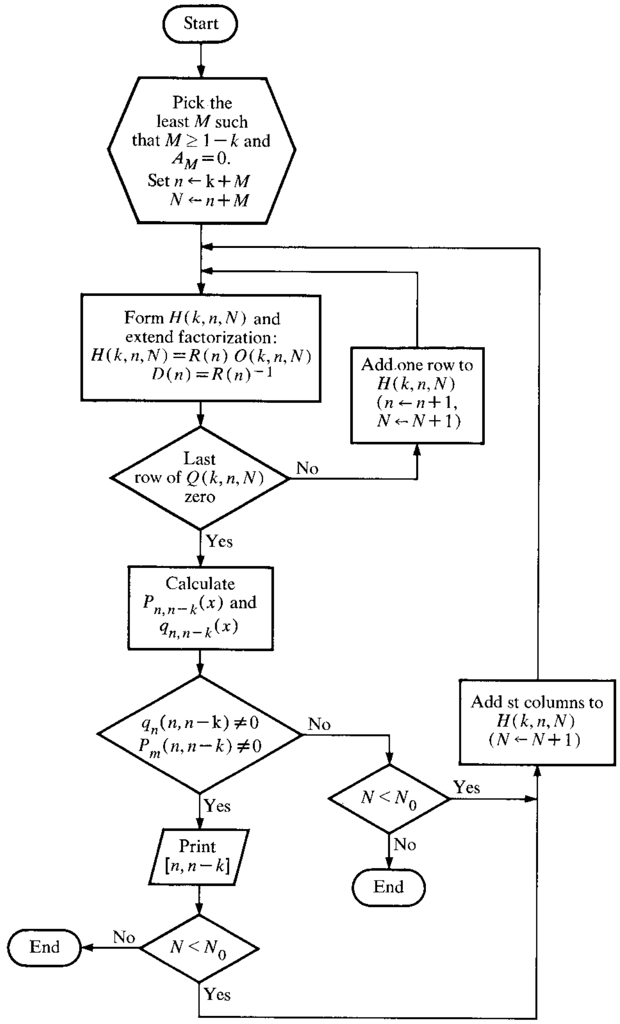

Figure 1 Main algorithm for the Padé approximants.

We then obtain

$$[3,2] = \frac{\begin{bmatrix} 1 & 3 \\ 1 & 2 \end{bmatrix} - \begin{bmatrix} 1 & 5 \\ 2 & 3 \end{bmatrix} x + \begin{bmatrix} 1 & -2 \\ 0 & -4 \end{bmatrix} x^2}{1-2x-x^2-x^3}.$$

To compare the efficiency of our algorithm to those in [3] we assume that $s=t=1$. The number of arithmetic operations required to calculate $[n+1,\ m+1]$ from $[n,m]$ is about n^2+m^2; to obtain $[n,m]$ it takes n^3+m^2 operations. The algorithm in [3], taking advantage of the special Hankel-structure of the matrix $H(k,n,N)$ and the assumption that all the principal minors of this matrix are nonzero, only requires about n^2+m^2 operations to get $[n,m]$. However, as that algorithm works through the Padé-table along the upper right row-lower left diagonal it still takes $(n+1)^2+(m+1)^2$ operations to pass from $[n,m]$ to $[n+1,m+1]$; i.e., the given recursion is useless for the diagonal direction, which is the direction of most interest.

Finally, we mention that by setting $k = 1$ and relaxing the requirement that $P_m \neq 0$, see Fig. 1, we can determine all the partial transfer function realizations for a linear system defined by its impulse response series A_0, $A_1, \cdots$.

Inverse of $xI - A$

An immediate application of our solution to the matrix-valued Padé problem is to calculate the inverse of the characteristic matrix $xI - A$ for any $t \times t$ matrix A as well as the minimal polynomial of A. Our solution turns out to be somewhat simpler than the formulas due to Faddeev. See Ref. 7.

We begin by considering the formula

$$(xI - A)^{-1} = \bar{A}(x)/\Delta(x) , \tag{14}$$

where $\Delta(x) = \det (xI - A)$, and the matrix polynomial $\bar{A}(x)$, the adjoint of A, has degree one less than the degree t of $\Delta(x)$. This means that if the coefficients of the expansion in the parentheses in Eq. (15)

$$(xI - A)^{-1} = x^{-1}(I + x^{-1}A + x^{-2}A^2 + \cdots) , \tag{15}$$

are fed into our algorithm with $k = 1$, the algorithm will produce as a last printout the approximant $[n, n-1] = P'(x^{-1})/q'(x^{-1})$ for some n no greater than t. We then have the formulas

$$(xI - A)^{-1} = x^{-1}\frac{P'(x^{-1})}{q'(x^{-1})} = \frac{P(x)}{q(x)}, \; q_n = q'_0 = 1 , \tag{16}$$

where $q(x)$, rather than $q'(x^{-1})$, is the minimal polynomial of A. But since $q(x)$ is the lowest degree polynomial for which $q(A) = 0$, the approximant $[n, n-1]$ is at the same time the first and only printout of the algorithm!

Because of the importance of this application we give an analysis of the behavior of the algorithm using $P(x)$ and $q(x)$ rather than $P'(x^{-1})$ and $q'(x^{-1})$. With $A_i = A^i$, $i = 0, 1, \cdots$, and a_i as defined in (8) the algorithm will find the least integer n such that a_{n+1} is a linear combination of the a_i's for $i = 0, \cdots, n$, and will determine that linear combination. This is done by factoring the downwards-growing matrix

$$\begin{matrix} a_0 \\ a_1 \\ \vdots \\ a_n \\ \vdots \end{matrix}$$

as in (11) until a zero-row appears in the second factor. Inverting the triangular first factor gives the minimal polynomial of A as the last row of the inverse: If that last row is $(d_{n,0}, d_{n,1}, \cdots, d_{n,n-1}, 1)$ then $q_i = d_{n,i}$, $q_n = 1$, and $q(x) = \sum_{i=0}^{n} q_i x^i$. The coefficients of $P(x)$ are then given by

$$\begin{aligned} P_{n-1} &= I \\ P_{n-2} &= q_{n-1}I + A \\ &\vdots \\ P_1 &= q_2 I + q_3 A + \cdots + q_{n-1}A^{n-3} + A^{n-2} \\ P_0 &= q_1 I + q_2 A + \cdots + q_{n-1}A^{n-2} + A^{n-1} . \end{aligned} \tag{17}$$

This algorithm requires of the order of $t^3 n$ operations for finding the inverse and the minimal polynomial of a $t \times t$ matrix, where n is the degree of the minimal polynomial. This compares well with the Faddeev-formulas, which require of the order of t^4 operations. Our method also gives the minimal polynomial directly without a need to find the common factors in the elements of $\bar{A}(x)$ and $\Delta(x)$ in (14).

As an example take

$$A = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

A factorization of the matrix defined by a_0, a_1, and a_2 results in:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & & \\ -1 & 1 & \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and we get

$$(xI - A)^{-1} = xI + A/x^2 - 1 .$$

Finally, for better numerical performance in this application we should replace the rule for choosing the pivotal point in the algorithm of the factoring problem section by the following: Let $s(i)$ be the least integer such that $q_{i,s(i)} \neq 0$ and that $|q_{i,s(i)}|$ is maximum.

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