A contour integral approach to the computation of invariant pairs

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Abstract

We study some aspects of the invariant pair problem for matrix polynomials, as introduced by Betcke and Kressner \cite{Betcke:2008} and by Beyn and Thümmler \cite{Beyn:2014}. Invariant pairs extend the notion of eigenvalue-eigenvector pairs, providing a counterpart of invariant subspaces for the nonlinear case. Here, a contour integral formulation is applied to compute condition numbers and backward errors for invariant pairs and solvents. We then adapt the Sakurai-Sugiura moment method \cite{Sakurai:1991} to the computation of invariant pairs, including some classes of problems that have multiple eigenvalues. Numerical refinement via two variants of Newton’s method is also studied. Furthermore, we investigate the relation between the matrix solvent problem and the triangularization of matrix polynomials.

Keywords: matrix polynomials, eigenvalues, invariant pairs, contour integral, moments, solvents, triangularization.

1. Introduction

Invariant pairs, introduced and analyzed in \cite{Betcke:2008, Beyn:2014} and \cite{Segura:2014}, are a generalization of eigenpairs for matrix polynomials. Let \( P(\lambda) = \sum_{j=0}^{n} A_j \lambda^j \) be an \( n \times n \) matrix polynomial, and choose a positive integer \( k \). Then the matrices \( X, S \) of sizes \( n \times k \) and \( k \times k \), respectively, form an invariant pair of size \( k \)
for $P(\lambda)$ if

$$P(X, S) := \sum_{j=0}^{\ell} A_j XS^j = 0.$$  

Invariant pairs offer a unified theoretical perspective on the problem of computing several eigenvalue-eigenvector pairs for a given matrix polynomial. From a numerical point of view, moreover, the computation of an invariant pair tends to be more stable than the computation of single eigenpairs, particularly in the case of multiple or tightly clustered eigenvalues. Observe that the notion of invariant pairs can also be applied to more general nonlinear problems, although here we will limit our presentation to matrix polynomials.

How to compute invariant pairs? Beyn and Thümmler ([6]) adopt a continuation method of predictor-corrector type. Betcke and Kressner ([4]), on the other hand, establish a correspondence between invariant pairs of a given polynomial and of its linearizations. Invariant pairs for $P(\lambda)$ are extracted from invariant pairs of a linearized form and then refined via Newton’s method.

The approach we take in this paper is based on contour integrals, which come into play under two separate forms. First, the definition of invariant pair given above can be rewritten as

$$P(X, S) = \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)X(\lambda I - S)^{-1}d\lambda = 0,$$

where $\Gamma \subseteq \mathbb{C}$ is a smooth closed contour with the spectrum of $S$ in its interior. Being able to specify $\Gamma$ allows us to select invariant pairs that have eigenvalues in a prescribed part of the complex plane. Moreover, this definition is quite convenient for computing a condition number and a backward error.

Contour integrals also play an important role in the definition and computation of moments, which form a Hankel matrix pencil yielding the eigenvalues of the given matrix polynomial that belong to the prescribed contour. The use of Hankel pencils of moment matrices is widespread in several applications such as control theory, signal processing or shape reconstruction, but nonlinear eigenvalue-eigenvector problems can also be tackled through this approach, as suggested for instance in [1] and [5]. E. Polizzi’s FEAST algorithm [32] is also an interesting example of contour-integral based eigensolver applied to large-scale electronic structure computations.

Here we adapt such methods to the computation of invariant pairs. We study in particular the scalar moment method and its relation with the mul-
multiplicity structure of the eigenvalues, but we also explore the behavior of the block version.

The last part of the paper shows an application of our results on invariant pairs to the particular case of matrix solvents, that is, to the matrix equation

\[ P(S) := \sum_{j=0}^{\ell} A_j S^j = 0. \]

The matrix solvent problem has received remarkable attention in the literature, since Sylvester’s work \cite{34} in the 1880s. The relation between the Riccati and the quadratic matrix equation is highlighted in \cite{7}, whereas a study on the existence of solvents can be found in \cite{13}. Several works address the problem of computing a numerical approximation for the solution of the quadratic matrix equation: an approach to compute, when possible, the dominant solvent is proposed in \cite{12}. Newton’s method and some variations are also used to approximate solvents numerically: see for example \cite{11}, \cite{24}, \cite{23}, \cite{29}. The work in \cite{21} uses interval arithmetic to compute an interval matrix containing the exact solution to the quadratic matrix equation. For the case of the general matrix solvent problem, we can also cite \cite{9}, \cite{31} and \cite{25}.

Here we exhibit computable formulations for the condition number and backward error of the general matrix solvent problem, generalizing existing works on the quadratic matrix equation. Moreover, we propose an adaptation of the moment method to the computation of solvents. Finally, we build on existing work on triangularization of matrix polynomials (see \cite{39} and \cite{36}) and explore the relationship between solvents of matrix polynomials in general and in triangularized form.

The paper is organized as follows. Section \ref{sec:prelim} introduces preliminary notions, definitions and notation. The backward error and condition number for the invariant pair problem are computed in Section \ref{sec:condnum}. Section \ref{sec:gamma} addresses some questions on the choice of \( \Gamma \); its content is not new, but it may offer a useful complement to the topics of the paper, particularly regarding the estimation of the number of eigenvalues in a given contour.

Section \ref{sec:algorithm} is devoted to the computation of eigenvalues and invariant pairs through moments and Hankel pencils. Our main results here consist in Remark \ref{rem:main} with the preceding discussion, and Theorem \ref{thm:main}. A comparison of different techniques for numerical refinement of invariant pairs is presented in Section \ref{sec:comparison}.
Finally, Sections 5, 6 and 7 are devoted to the applications to matrix solvents.

The Maple and Matlab implementations of the symbolic and numeric methods presented in the paper are available online at the URL http://www.unilim.fr/pages perso/esteban.segura/software.html

2. Matrix polynomials and invariant pairs

A complex matrix polynomial takes the form:

\[ P(\lambda) = A_0 + A_1 \lambda + A_2 \lambda^2 + \cdots + A_\ell \lambda^\ell \] (1)

where \( \ell \in \mathbb{N} \) is the degree of the matrix polynomial and \( A_0, A_1, \ldots, A_\ell \in \mathbb{C}^{n \times n} \).

A crucial and well-known property of matrix polynomials is the existence of the Smith form (see, e.g., [18]):

**Theorem 1.** Every \( n \times n \) matrix polynomial \( P(\lambda) \) admits the representation

\[ D(\lambda) = E(\lambda)P(\lambda)F(\lambda), \] (2)

where \( D(\lambda) = \text{diag}(d_1(\lambda), \ldots, d_n(\lambda)) \) is a diagonal polynomial matrix with monic scalar polynomials \( d_i(\lambda) \) such that \( d_i(\lambda) \) is divisible by \( d_{i-1}(\lambda) \); \( E(\lambda) \) and \( F(\lambda) \) are matrix polynomials of sizes \( n \times n \) with constant nonzero determinants.

The polynomial eigenvalue problem (PEP) consists in determining right eigenvalue-eigenvector pairs \( (\lambda, x) \in \mathbb{C} \times \mathbb{C}^n \), with \( x \neq 0 \), such that

\[ P(\lambda)x = 0, \]

or left eigenvalue-eigenvector pairs \( (\lambda, y^*) \in \mathbb{C} \times \mathbb{C}^n \), with \( y \neq 0 \), such that

\[ y^*P(\lambda) = 0. \]

A particular case of special interest is the quadratic eigenvalue problem (QEP), where \( \ell = 2 \). Typical applications of the QEP include the vibrational analysis of various physical systems. A considerable amount of work has been done on the theoretical and computational study of the QEP: see for instance [38].

**Invariant pairs**, introduced and analyzed in [4] and [6], are a generalization of the notion of eigenpair for matrix polynomials.
Definition 1. A pair \((X, S) \in \mathbb{C}^{n \times k} \times \mathbb{C}^{k \times k}\) is called an invariant pair if it satisfies the relation:

\[
P(X, S) := A_\ell XS^\ell + \cdots + A_2 XS^2 + A_1 XS + A_0 X = 0,
\]

where we assume \(A_i \in \mathbb{C}^{n \times n}\), \(i = 0, \ldots, \ell\), and \(k\) is an integer between 1 and \(2n\).

The following definitions proposed in [4] and [19] will be helpful for our work, for instance, to allow rank deficiencies in \(X\).

Definition 2. A pair \((X, S) \in \mathbb{C}^{n \times k} \times \mathbb{C}^{k \times k}\) is called minimal if there is \(m \in \mathbb{N}\) such that:

\[
V_m(X, S) := \begin{bmatrix}
XS^m - 1 \\
\vdots \\
XS \\
X
\end{bmatrix}
\]

has full rank. The smallest such \(m\) is called minimality index of \((X, S)\).

Remark 1. We can always construct a minimal pair from a given pair.

Definition 3. An invariant pair \((X, S)\) for a regular matrix polynomial \(P\) of degree \(\ell\) is called simple if \((X, S)\) is minimal and the algebraic multiplicities of the eigenvalues of \(S\) are identical to the algebraic multiplicities of the corresponding eigenvalues of \(P\).

Invariant pairs are closely related to the theory of standard pairs presented in [19], and in particular to Jordan pairs. If \((X, S)\) is a simple invariant pair and \(S\) is in Jordan form, then \((X, S)\) is a Jordan pair.

As an example consider the following quadratic matrix polynomial, discussed in [38]:

\[
p(\lambda) = \lambda^2 \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \lambda \begin{bmatrix} -2 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}
\]

It has eigenvalues \(\lambda_1 = 1\) with algebraic multiplicity 3 and \(\lambda_2 = -1\) with algebraic multiplicity 1. A corresponding Jordan pair \((X, J)\) is given by:

\[
X = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad J = \text{diag} \left( -1, 1, \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \right)
\]
The notion of invariant pairs offers a theoretical perspective and a numerically more stable approach to the task of computing several eigenpairs of a matrix polynomial. Indeed, this problem is typically ill-conditioned in presence of multiple or nearly multiple eigenvalues, whereas the corresponding invariant pair formulation may have better stability properties.

In particular, simple invariant pairs play an important role when using a linearization approach as in [4], and ensure local quadratic convergence of Newton’s method, as shown in [26]; see also [35].

2.1. Formulation of the invariant pair problem using the contour integral

Polynomial eigenpairs and invariant pairs can also be defined in terms of a contour integral. Indeed, an equivalent representation for (3) is the following.

Proposition 1. A pair \((X, S)\) \(\in \mathbb{C}^{n \times k} \times \mathbb{C}^{k \times k}\) is an invariant pair if and only if satisfies the relation:

\[
P(X, S) = \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)X(\lambda I - S)^{-1}d\lambda = 0,
\]

where \(\Gamma \subseteq \mathbb{C}\) is a smooth closed contour with the spectrum of \(S\) in its interior.

This formulation allows us to choose the contour \(\Gamma\) to compute \(S\) with eigenvalues lying in a particular region of the complex plane. We will also use it to compute a condition number and a backward error, which play an important role for a symbolic-numeric approach. See [1], [2], [5], [17] for applications of the contour integral formulation.

2.2. Condition number and backward error of the invariant pair problem

In the following sections, using the contour integral definition, we present formulations of the backward error and condition number for an invariant pair \((X, S)\) of the matrix equation (5). We follow the ideas presented in the articles [37] and [23], which give expressions for backward errors and condition numbers for the polynomial eigenvalue problem and for a solvent of the quadratic matrix equation.
2.2.1. Condition number

Let us compute a condition number for an invariant pair \((X, S)\) of the matrix equation (5).
Consider the perturbed equation:

$$\frac{1}{2\pi i} \oint_{\Gamma} \left[ P(\lambda) + \Delta P(\lambda) \right] (X + \Delta X)(\lambda I - (S + \Delta S))^{-1} d\lambda = 0,$$

where \(\Delta P(\lambda)\) is the perturbation of the matrix polynomial \(P(\lambda)\), defined as:

$$\Delta P(\lambda) = \Delta A_0 + \Delta A_1\lambda + \Delta A_2\lambda^2 + \cdots + \Delta A_\ell\lambda^\ell,$$  \hspace{1cm} (6)

and \(\|\Delta X\| < \Omega, \|\Delta S\| < \Omega\) and \(\|\Delta A_i\| < \Omega\), for \(i = 0, \ldots, \ell\), and \(\Omega\) a first order bound.

Using the formula:

\((A + B)^{-1} = A^{-1} - A^{-1}BA^{-1} + A^{-1}BA^{-1}BA^{-1} - \cdots\)

and expanding we obtain:

$$\frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(X + \Delta X)(\lambda I - S - \Delta S)^{-1} d\lambda = -\frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(X + \Delta X)(\lambda I - S - \Delta S)^{-1} d\lambda.$$

Then we have:

$$\frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)X(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} d\lambda + \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)\Delta X(\lambda I - S)^{-1} d\lambda =$$

$$= -\frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)X(\lambda I - S)^{-1} d\lambda + O(\Omega^2).$$

Now, using the \(\text{vec}\) operator and its property (see \[20\], pp. 28): \(\text{vec}(AXB) = (B^T \otimes A) \text{vec}(X)\),  \hspace{1cm} (7)

and applying it to the last equation, we obtain:

$$\frac{1}{2\pi i} \oint_{\Gamma} \text{vec}(P(\lambda)\Delta X(\lambda I - S)^{-1}) d\lambda + \frac{1}{2\pi i} \oint_{\Gamma} \text{vec}(P(\lambda)X(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1}) d\lambda =$$

$$= -\frac{1}{2\pi i} \oint_{\Gamma} \text{vec}(P(\lambda)X(\lambda I - S)^{-1}) d\lambda + O(\Omega^2)$$

then we have

$$\left[ \frac{1}{2\pi i} \oint_{\Gamma} (\lambda I - S)^{-1} \otimes P(\lambda) d\lambda \right] \text{vec}(\Delta X) + \left[ \frac{1}{2\pi i} \oint_{\Gamma} (\lambda I - S)^{-1} \otimes (P(\lambda)X(\lambda I - S)^{-1}) d\lambda \right] \text{vec}(\Delta S) =$$

$$= -\left[ \frac{1}{2\pi i} \oint_{\Gamma} (X(\lambda I - S)^{-1})^T \otimes I_n d\lambda \right] \text{vec}(\Delta A_0) - \cdots - \left[ \frac{1}{2\pi i} \oint_{\Gamma} (\lambda^\ell X(\lambda I - S)^{-1})^T \otimes I_n d\lambda \right] \text{vec}(\Delta A_\ell) + O(\Omega^2),$$

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where we will measure the relative perturbations normwise by
\[ \epsilon = \| \begin{bmatrix} \alpha_\ell^{-1} \Delta A_\ell & \alpha_{\ell-1}^{-1} \Delta A_{\ell-1} & \ldots & \alpha_1^{-1} \Delta A_1 & \alpha_0^{-1} \Delta A_0 \end{bmatrix} \|_F, \]
with \( \alpha_i \) are nonnegative parameters for \( i = 0, \ldots, \ell \) and \( \| A \|_F = \sqrt{\text{trace}(A^*A)} \) be the Frobenius norm. Now taking:
\[
N = \frac{1}{2\pi i} \oint_{\Gamma} \left( (\lambda I - S)^{-1} \right)^T \otimes P(\lambda) d\lambda, \ N \in \mathbb{C}^{kn \times kn}, \\
M = \frac{1}{2\pi i} \oint_{\Gamma} \left( \left( (\lambda I - S)^{-1} \right)^T \otimes (P(\lambda)X(\lambda I - S)^{-1}) \right) d\lambda, \ M \in \mathbb{C}^{kn \times k^2}, \\
B_j = \frac{1}{2\pi i} \oint_{\Gamma} \left( \lambda^j X(\lambda I - S)^{-1} \right)^T \otimes I_n d\lambda, \ j = 0, \ldots, \ell, \ B_j \in \mathbb{C}^{kn \times n^2}
\]
we have
\[
N \operatorname{vec}(\Delta X) + M \operatorname{vec}(\Delta S) = -B_0 \operatorname{vec}(\Delta A_0) - \cdots - B_\ell \operatorname{vec}(\Delta A_\ell) + O(\epsilon^2) = \\
= - \begin{bmatrix} \alpha_\ell B_\ell & \ldots & \alpha_1 B_1 & \alpha_0 B_0 \end{bmatrix} \begin{bmatrix} \operatorname{vec}(\Delta A_\ell)/\alpha_\ell \\ \vdots \\ \operatorname{vec}(\Delta A_1)/\alpha_1 \\ \operatorname{vec}(\Delta A_0)/\alpha_0 \end{bmatrix} + O(\epsilon^2)
\]
then we obtain
\[
\begin{bmatrix} N & M \end{bmatrix} \begin{bmatrix} \operatorname{vec}(\Delta X) \\ \operatorname{vec}(\Delta S) \end{bmatrix} = - \begin{bmatrix} \alpha_\ell B_\ell & \ldots & \alpha_1 B_1 & \alpha_0 B_0 \end{bmatrix} \begin{bmatrix} \operatorname{vec}(\Delta A_\ell)/\alpha_\ell \\ \vdots \\ \operatorname{vec}(\Delta A_1)/\alpha_1 \\ \operatorname{vec}(\Delta A_0)/\alpha_0 \end{bmatrix} + O(\epsilon^2).
\]
Assuming that the matrix \( \begin{bmatrix} N & M \end{bmatrix} \) has full rank, and multiplying by its pseudo-inverse (that we denote by using the superscript “ + ”), we obtain:
\[
\begin{bmatrix} \operatorname{vec}(\Delta X) \\ \operatorname{vec}(\Delta S) \end{bmatrix} = - \begin{bmatrix} N & M \end{bmatrix}^+ \begin{bmatrix} \alpha_\ell B_\ell & \ldots & \alpha_1 B_1 & \alpha_0 B_0 \end{bmatrix} \begin{bmatrix} \operatorname{vec}(\Delta A_\ell)/\alpha_\ell \\ \vdots \\ \operatorname{vec}(\Delta A_1)/\alpha_1 \\ \operatorname{vec}(\Delta A_0)/\alpha_0 \end{bmatrix} + O(\epsilon^2).
\]
Now, taking 2-norms and using that
\[ \|\text{vec}(X)\|_2 = \|X\|_F, \]
we obtain:
\[
\begin{bmatrix}
\text{vec}(\Delta X) \\
\text{vec}(\Delta S)
\end{bmatrix}
\leq \begin{bmatrix}
N & M^+ & [\alpha_\ell B_\ell & \ldots & \alpha_0 B_0] \\
& & \vdots \\
& & \text{vec}(\Delta A_0)/\alpha_0
\end{bmatrix}
\begin{bmatrix}
\text{vec}(\Delta A_\ell)/\alpha_\ell \\
\vdots \\
\text{vec}(\Delta A_0)/\alpha_0
\end{bmatrix}
+ O(\epsilon^2)
\]
\[
\|\Delta X\|_F^2 + \|\Delta S\|_F^2 \leq \begin{bmatrix}
N & M^+ & [\alpha_\ell B_\ell & \ldots & \alpha_0 B_0] \\
& & \vdots \\
& & \text{vec}(\Delta A_0)/\alpha_0
\end{bmatrix}
\begin{bmatrix}
\text{vec}(\Delta A_\ell)/\alpha_\ell \\
\vdots \\
\text{vec}(\Delta A_0)/\alpha_0
\end{bmatrix}
+ O(\epsilon^2)
\]
\[
\begin{bmatrix}
\|\Delta X\|_F, \|\Delta S\|_F
\end{bmatrix}
\leq \begin{bmatrix}
N & M^+ & [\alpha_\ell B_\ell & \ldots & \alpha_0 B_0] \\
& & \vdots \\
& & \text{vec}(\Delta A_0)/\alpha_0
\end{bmatrix}
\begin{bmatrix}
\text{vec}(\Delta A_\ell)/\alpha_\ell \\
\vdots \\
\text{vec}(\Delta A_0)/\alpha_0
\end{bmatrix}
+ O(\epsilon^2)
\]

Then we have, for first order in \(\epsilon\):
\[
\frac{\|\begin{bmatrix}
\|\Delta X\|_F, \|\Delta S\|_F
\end{bmatrix}
\|_2}{\|\begin{bmatrix}
\|X\|_F, \|S\|_F
\end{bmatrix}
\|_2} \leq \Psi(X,S)\epsilon + O(\epsilon^2)
\]
where
\[
\Psi(X,S) = \frac{\begin{bmatrix}
N & M^+ & [\alpha_\ell B_\ell & \ldots & \alpha_0 B_0]
\end{bmatrix}
}{\|\begin{bmatrix}
\|X\|_F, \|S\|_F
\end{bmatrix}
\|_2}
\]
is the condition number.

2.2.2. Backward error for \(P(X,S)\)

The backward error of an approximate solution \((Y,T)\) to (5) can be defined by:
\[
\eta(Y,T) = \min\{\epsilon : (A_\ell + \Delta A_\ell)YT^\ell + \cdots + (A_0 + \Delta A_0)Y = 0,
\|\begin{bmatrix}
\alpha_\ell^{-1}\Delta A_\ell & \ldots & \alpha_1^{-1}\Delta A_1 & \alpha_0^{-1}\Delta A_0
\end{bmatrix}
\|_F \leq \epsilon\}.
\]
If we define \(R\) as
\[
R = A_\ell YT^\ell + \cdots + A_1 YT + A_0 Y,
\]
then (9) can be written
\[
-R = \Delta A_\ell YT^\ell + \cdots + \Delta A_1 YT + \Delta A_0 Y
\]
We have

$$-R = \begin{bmatrix} \alpha^{-1}_\ell \Delta A_\ell & \ldots & \alpha^{-1}_1 \Delta A_1 & \alpha^{-1}_0 \Delta A_0 \end{bmatrix} \begin{bmatrix} \alpha_\ell Y T^\ell \\ \vdots \\ \alpha_1 Y T \\ \alpha_0 Y \end{bmatrix}$$

If we take the Frobenius norm, we obtain the lower bound for the backward error:

$$\eta(Y, T) \geq \frac{\|R\|_F}{(\alpha^2_\ell\|YT^\ell\|_F^2 + \cdots + \alpha^2_1\|YT\|_F^2 + \alpha^2_0\|Y\|_F^2)^{1/2}}.$$

Now, using (7), we obtain:

$$-\vec(R) = ((YT^\ell)^T \otimes I_n) \vec(\Delta A_\ell) + \cdots + (Y^T \otimes I_n) \vec(\Delta A_0) =$$

$$= \begin{bmatrix} \alpha_\ell (YT^\ell)^T \otimes I_n & \ldots & \alpha_1 (YT)^T \otimes I_n & \alpha_0 Y^T \otimes I_n \end{bmatrix} \begin{bmatrix} \vec(\Delta A_\ell)/\alpha_\ell \\ \vdots \\ \vec(\Delta A_1)/\alpha_1 \\ \vec(\Delta A_0)/\alpha_0 \end{bmatrix},$$

which can be written as:

$$Hz = r, \ H \in \mathbb{C}^{nk \times (\ell+1)n^2}$$

(11)

Here we assume that $H$ is full rank, to guarantee that (11) has a solution (backward error is finite). Then the backward error is the minimum 2-norm solution to:

$$\eta(Y, T) = \|H^+ r\|_2,$$

(12)

where " + " denotes the pseudoinverse.

From (12) we can obtain an upper bound for $\eta(Y, T)$:

$$\eta(Y, T) \leq \|H^+\|_2 \|r\|_2 = \frac{\|r\|_2}{\sigma_{\min}(H)},$$

where $\sigma_{\min}$ denotes the smallest singular value, that by assumption is nonzero. Note that:

$$\sigma_{\min}(H)^2 = \lambda_{\min}(HH^*) = \lambda_{\min}(\alpha^2_\ell(YT^\ell)^T Y T^\ell \otimes I_n + \cdots + \alpha^2_0 Y^T Y \otimes I_n) \geq$$

$$\geq \alpha^2_\ell \sigma_{\min}(YT^\ell)^2 + \cdots + \alpha^2_1 \sigma_{\min}(YT)^2 + \alpha^2_0 \sigma_{\min}(Y)^2.$$

Thus we obtain the upper bound for $\eta(Y, T)$:

$$\eta(Y, T) \leq \frac{\|R\|_F}{(\alpha^2_\ell \sigma_{\min}(YT^\ell)^2 + \cdots + \alpha^2_1 \sigma_{\min}(YT)^2 + \alpha^2_0 \sigma_{\min}(Y)^2)^{1/2}}.$$
2.2.3. Numerical example

Let us consider the power plant problem presented in [3] and in [38]. This is a real symmetric QEP which describes the dynamic behaviour of a nuclear power plant simplified into an eight-degrees-of-freedom system. The problem is ill-conditioned due to the bad scaling of the matrix coefficients. Using the Matlab function \textit{polyeig}, we find that the maximum condition number for the eigenvalues is

$$\Psi = \max_{\lambda \in \Lambda} \\text{condeig}_\lambda = 1.0086e+08.$$ 

But if we choose the contour $\Gamma = \gamma + \rho e^{i\theta}$ ($\gamma = 80 + 10i$, $\rho = 170$), which contains 11 eigenvalues inside (in particular the one with the maximum condition number), and find an invariant pair $(X, S)$ associated with those eigenvalues, we have that

$$\Psi(X, S) = 565.6746$$

and

$$\eta(X, S) = 4.4548e - 017.$$  

Observe that $\Psi(X, S)$ is significantly smaller than the maximum condition number $\Psi = 1.0086e+08$.

3. Choosing the contour

The choice of $\Gamma$ is of course a crucial step when applying the contour integral formulation of the eigenvalue or invariant pair problem. If some information about the localization of the eigenvalues is available, one can choose the contour accordingly. In other cases, $\Gamma$ may be taken as a circle for ease of computation.

A related question is: how many eigenvalues of $P(\lambda)$ live inside a given contour? Even an approximate estimate can be useful to choose $\Gamma$ and $k$ consistently. An answer to this problem is provided in [14] and [15] and it is based on the following result.

**Theorem 2.** Let $F(z)$ be an $n \times n$ regular analytic matrix function and let $\text{tr}(F(z))$ be the matrix trace of $F(z)$. In addition, let $m$ be the number of eigenvalues, counting multiplicity, inside closed curves $\Gamma$ on the complex plane for the nonlinear eigenvalue problem: $F(\lambda)x = 0$. Then we have:

$$m = \oint_{\Gamma} \text{tr} \left( F(z)^{-1} \frac{dF(z)}{dz} \right) dz,$$  \hspace{1cm} (13)
where $\text{det}(F(z)) \neq 0$.

The equation (13) can be approximated by an $N$-point quadrature rule by:

$$m \approx \sum_{j=0}^{N-1} \omega_j \text{tr}(F(z_j)^{-1}F'(z_j)),$$

(14)

where $z_j$ is a quadrature point and $\omega_j$ is a weight.

In the case when we use the trapezoidal rule on a circle with center $C$ and radius $R$, quadrature points and weights are defined by:

$$\omega_j = \frac{R}{N} \exp\left(\frac{2\pi i}{N} \left( j + \frac{1}{2} \right) \right), \quad z_j = C + R \exp\left(\frac{2\pi i}{N} \left( j + \frac{1}{2} \right) \right).$$

To avoid the matrix inversion in (14), an estimate for the trace with an unbiased estimation can be used:

$$\text{tr}(F(z_j)^{-1}F'(z_j)) \approx \frac{1}{L} \sum_{i=1}^{L} (v_i^T F(z_j)^{-1}F'(z_j)v_i),$$

where $v_i$ are the sample vectors, with entries are 1 or -1 with equal probability and $L$ is the number of sample vectors.

The number $m$ of eigenvalues inside the contour can then be estimated as:

$$m \approx \frac{1}{L} \sum_{j=0}^{N-1} \omega_j \sum_{i=1}^{L} (v_i^T F(z_j)^{-1}F'(z_j)v_i).$$

Remark 2. The choice of $\Gamma$ can be combined with shifting techniques for the eigenvalues of $P(\lambda)$: see for instance [30].

4. Computation of invariant pairs

Numerical methods based on contour integrals for the computation of eigenvalues of matrix polynomials and analytic matrix-valued functions have recently met with growing interest. Such techniques are related to the well-known method of moments, where the moments are computed by numerical quadrature.

In this section we explore a similar approach for computing invariant pairs. Our main reference is the Sakurai-Sugiura method (see [1] and [33]), as well as the presentation given in [5].
4.1. The moment method and eigenvalues

Let us begin by briefly recalling a few basic facts about the Sakurai-Sugiura moment method. Here we essentially follow the presentation given in [1].

Let Γ be a smooth closed contour in the complex plane and let \( u \) and \( v \) be arbitrarily given vectors in \( \mathbb{C}^n \). Define the function:

\[
f(\lambda) := u^H P(\lambda)^{-1} v.
\]

The next theorem, which can be found in [1], gives a representation for \( f(\lambda) \) that will prove useful later on.

**Theorem 3.** Let \( D(\lambda) = \text{diag}(d_1(\lambda), \ldots, d_n(\lambda)) \) be the Smith form of \( P(\lambda) \), and let \( E(\lambda) \) and \( F(\lambda) \) be as in (2). Let \( \chi_j(\lambda) = u^H q_j(\lambda) p_j(\lambda)^H v \), \( 1 \leq j \leq n \). Then

\[
f(\lambda) = \sum_{j=1}^{n} \frac{\chi_j(\lambda)}{d_j(\lambda)},
\]

where \( q_j(\lambda) \) and \( p_j(\lambda) \) are the column vectors of \( E(\lambda) \) and \( F(\lambda)^H \), respectively.

**Definition 4.** Let \( k \in \mathbb{N} \). The \( k \)-th moment of \( f(z) \) is:

\[
\mu_k = \frac{1}{2\pi i} \oint_{\Gamma} z^k f(z) dz.
\]

For a positive integer \( m \), define the Hankel matrices \( H_0, H_1 \in \mathbb{C}^{m \times m} \) as follows:

\[
H_0 = \begin{bmatrix}
\mu_0 & \mu_1 & \cdots & \mu_{m-1} \\
\mu_1 & \mu_2 & \cdots & \mu_m \\
\vdots & \vdots & \ddots & \vdots \\
\mu_{m-1} & \mu_m & \cdots & \mu_{2m-2}
\end{bmatrix}, \quad H_1 = \begin{bmatrix}
\mu_1 & \mu_2 & \cdots & \mu_m \\
\mu_2 & \mu_3 & \cdots & \mu_{m+1} \\
\vdots & \vdots & \ddots & \vdots \\
\mu_m & \mu_{m+1} & \cdots & \mu_{2m-1}
\end{bmatrix}
\]

(17)

The eigenvalue algorithm presented in [1] relies on the following result:

**Theorem 4.** Suppose that the polynomial \( P(\lambda) \) has exactly \( m \) eigenvalues \( \lambda_1, \ldots, \lambda_m \) in the interior of \( \Gamma \), and that these eigenvalues are distinct, simple and non degenerated. If \( \chi_n(\lambda_\ell) \neq 0 \) for \( 1 \leq \ell \leq m \), then the eigenvalues of the pencil \( H_1 - \lambda H_0 \) are given by \( \lambda_1, \ldots, \lambda_m \).
So, in order to approximate \( \lambda_1, \ldots, \lambda_m \), it suffices to compute by quadrature the first \( 2m \) moments of \( f(\lambda) \) and then apply an eigensolver, such as the QZ method, to the resulting Hankel pencil. Block versions of this approach have also been proposed; we will say more on this later.

We now wish to investigate the behavior of the above method when the hypothesis that the \( \lambda_i \)'s are distinct is removed. In particular, we aim to generalize the proof of Theorem 4 given in [1], which is based on the Vandermonde factorization of \( H_0 \) and \( H_1 \).

Let \( \lambda_0, \ldots, \lambda_s \) be the eigenvalues of \( P(\lambda) \) that belong to the interior of \( \Gamma \), each with its multiplicity; we can therefore assume w.l.o.g. that \( \lambda_0, \ldots, \lambda_s \) are distinct complex numbers. Suppose that, in the Smith form (2) of \( P(\lambda) \), the matrix \( D(\lambda) \) is in the form

\[
d_n(\lambda) = (\lambda - \lambda_0)^{m_0}(\lambda - \lambda_1)^{m_1} \cdots (\lambda - \lambda_s)^{m_s} \prod_{i=s+1}^r (\lambda - \lambda_i)^{m_i},
\]

and \( \lambda_{s+1}, \ldots, \lambda_r \) are the eigenvalues of \( P(\lambda) \) located outside the contour \( \Gamma \).

Applying Theorem 3, we have:

\[
\mu_k = \frac{1}{2\pi i} \oint_{\Gamma} z^k f(z) dz = \frac{1}{2\pi i} \oint_{\Gamma} \sum_{j=1}^n \frac{\chi_j(z)}{d_j(z)} z^k dz = \frac{1}{2\pi i} \oint_{\Gamma} \varphi(z) z^k dz,
\]

where

\[
\varphi(z) = \sum_{j=1}^n \chi_j(z) h_j(z), \text{ with } h_j(z) = \frac{d_n(z)}{d_j(z)}.
\]

We can introduce partial fraction decompositions and write

\[
\mu_k = \frac{1}{2\pi i} \oint_{\Gamma} \frac{\varphi(z)}{d_n(z)} z^k dz = \frac{1}{2\pi i} \oint_{\Gamma} \left( \sum_{i=1}^{m_0} \frac{c_{0,i} z^k}{(z - \lambda_0)^i} + \cdots + \sum_{i=1}^{m_s} \frac{c_{s,i} z^k}{(z - \lambda_s)^i} \right) dz = \sum_{j=0}^s \sum_{i=1}^{m_j} \frac{1}{2\pi i} \oint_{\Gamma} \frac{c_{j,i} z^k}{(z - \lambda_j)^i} dz,
\]

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where \( c_{j,i} \in \mathbb{C} \), for \( j = 0, \ldots, s \) and \( i = 1, \ldots, m \). Classical results on residues then yield

\[
\begin{align*}
\mu_k &= \sum_{j=0}^{s} \sum_{i=1}^{m_j} c_{j,i} \operatorname{Res} \left( \frac{z^k}{(z - \lambda_j)^i}, \lambda_j \right) = \\
&= \sum_{j=0}^{s} \sum_{i=1}^{m_j} c_{j,i} \frac{1}{(i-1)!} \lim_{z \rightarrow \lambda_j} \frac{d^{i-1}}{dz^{i-1}} \left( \frac{z^k}{(z - \lambda_j)^i} \right) = \\
&= \sum_{j=0}^{s} \sum_{i=1}^{m_j} c_{j,i} \frac{1}{(i-1)!} \lim_{z \rightarrow \lambda_j} \frac{d^{i-1}}{dz^{i-1}} (z^k) = \\
&= \sum_{j=0}^{s} \sum_{i=1}^{m_j} \nu_{j,i} \lambda_j^{k-i+1},
\end{align*}
\]

where

\[
\nu_{j,i} = \begin{cases} 
\frac{c_{j,i}}{(i-1)!} (k - i + 2)(k - i + 3) \cdots k & \text{if } k \geq i - 1, \\
0 & \text{otherwise.}
\end{cases}
\]

Now, consider the pencil \( H_1 - \lambda H_0 \) with \( H_0 \) and \( H_1 \) defined as in (17) of size \( m \times m \), where \( m = m_0 + \cdots + m_s \). We will assume that the coefficients \( \nu_{j,i} \) in (18) are nonzero if \( k \geq i - 1 \). Because of (18), and of the fact that \( \lambda_0, \ldots, \lambda_s \) are roots of \( d_n(\lambda) \), the moments \( \mu_k \) satisfy a linear recurrence equation of the form:

\[
\mu_k = a_{m-1} \mu_{k-1} + a_{m-2} \mu_{k-2} + \cdots + a_0 \mu_{k-r}.
\]

Moreover, \( d_n(\lambda) \) is the polynomial of smallest degree that has roots \( \lambda_0, \ldots, \lambda_s \) with the prescribed multiplicities \( m_0, \ldots, m_s \), so the equation (19) has the shortest possible length. Therefore, the matrices \( H_0 \) and \( H_1 \) have full rank. The same argument shows that \( H_0 \) and \( H_1 \) are rank-deficient if taken of size larger than \( m \times m \).

More on the fascinating relation between the rank of finite or infinite Hankel matrices and linear recurrence equations can be found in [16] (Vol. 2, page 205) and in [8].

As a consequence of the shifted Hankel form of \( H_0 \) and \( H_1 \), we have
$H_0 C = H_1$, where $C$ is a matrix in companion form

$$C = \begin{bmatrix} 0 & 0 & \cdots & 0 & x_0 \\ 1 & 0 & \cdots & 0 & x_1 \\ 0 & 1 & \cdots & 0 & x_2 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & x_{m-1} \end{bmatrix},$$

and its last column is given by the solution of the linear system

$$H_0 \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_{m-1} \end{bmatrix} = \begin{bmatrix} \mu_m \\ \mu_{m+1} \\ \vdots \\ \mu_{2m-1} \end{bmatrix}. \quad (20)$$

The polynomial of degree $m$:

$$p(\lambda) = \lambda^m - x_{m-1}\lambda^{m-1} - \cdots - x_0$$

is a scalar multiple of $d_n(\lambda)$, and its roots are the $\lambda_i$’s generating the entries of the pencil $H_1 - \lambda H_0$. So we also have that the $\mu_i$’s satisfy the recurrence

$$\mu_k = x_{m-1}\mu_{k-1} + x_{m-2}\mu_{k-2} + \cdots + x_0\mu_{k-m},$$

where $k = m, m + 1, \ldots, 2m$.

Consider now the Jordan matrix

$$J = \begin{bmatrix} J_1 \\ \vdots \\ J_s \end{bmatrix},$$

where each block $J_i$ is a square matrix of the form

$$J_i = \begin{bmatrix} \lambda_i & 1 \\ \lambda_i & \ddots \\ \vdots & \ddots & \ddots \\ \lambda_i & \cdots & 1 \end{bmatrix},$$

and define the confluent Vandermonde matrix

$$V = (v \ J^T v \ \cdots \ (J^T)^{r-1}v),$$
where $\mathbf{v}^T = \left(e_1^{[m_1]T} \ldots e_1^{[m_s]T}\right)$ is a partitioned conformally with $J$ and $e_1^{[m_\ell]T} = (1 \ 0 \ldots 0)^T$ is the $m_\ell$ dimensional unit coordinate vector. Then we have

$$VC = (\mathbf{v} \ J^T \mathbf{v} \ldots (J^T)^{r-1} \mathbf{v}) C$$

$$= (J^T \mathbf{v} \ldots (J^T)^{r-1} \mathbf{v} -(x_0 I + x_1 J + \cdots + x_{m-1} J^{r-1})^T \mathbf{v})$$

$$= (J^T \mathbf{v} \ldots (J^T)^{r-1} \mathbf{v} (J^T)^r \mathbf{v})$$

$$= J^T V,$$

where we have used the property $p(J) = 0$, that is, the Cayley-Hamilton theorem.

We can now introduce the Vandermonde decomposition of our Hankel matrices $H_0$ and $H_1$. By applying the results presented in [8], we deduce that there exist block matrices $B_0 = \text{diag}(D_1^{(0)},\ldots,D_s^{(0)})$ and $B_1 = \text{diag}(D_1^{(1)},\ldots,D_s^{(1)})$, partitioned conformally with $J$, satisfying the conditions $B_0 J^T = J B_0$ and $B_1 J^T = J B_1$, so that

$$H_i = V^T B_i V, \quad \text{for } i = 0, 1.$$

Moreover, we can prove that $J B_0 = B_1$:

$$H_0 C = H_1 \iff (V^T B_0 V) C = V^T B_1 V \iff V^T B_0 J^T V = V^T B_1 V$$

$$\iff V^T J B_0 V = V^T B_1 V \iff J B_0 = B_1,$$

where we used the properties $V C = J^T V$ and $B_i J^T = J B_i$.

Therefore, we have:

$$H_1 - \lambda H_0 = V^T B_1 V - \lambda V^T B_0 V = V^T J B_0 V - \lambda V^T B_0 V$$

$$= V^T (J - \lambda I) B_0 V.$$

So the eigenvalues of $H_1 - \lambda H_0$ are $\lambda_0,\ldots,\lambda_s$ with respective multiplicities $m_0,\ldots,m_s$.

**Remark 3.** We conclude that the scalar moment method can be used to compute the (possibly multiple) eigenvalues of $P(\lambda)$ that belong to the interior of $\Gamma$ and that are roots of the polynomial $d_m(\lambda)$. The method misses the additional multiplicities associated with the polynomials $d_1(\lambda),\ldots,d_{n-1}(\lambda)$. 
The above remark is consistent with the fact that the Jordan form of a companion matrix only contains one Jordan block for each eigenvalue: it is not possible to capture multiple eigenvalues associated with several Jordan blocks.

In order to “see” the additional eigenvalues that are roots of $d_1(\lambda), \ldots, d_{n-1}(\lambda)$, one needs to apply the block version of the moment method.

4.2. Example

Consider the matrix polynomial:

$$P(\lambda) = \lambda^2 I + \lambda \begin{bmatrix} -2 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -6 & 0 \\ 0 & 0 & 0 & -5 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & \frac{1}{4} & 0 & 0 \\ 0 & 0 & 9 & 0 \\ 0 & 0 & 0 & 6 \end{bmatrix}.$$  

$P(\lambda)$ has eigenvalues: $\lambda_1 = \frac{1}{2}, \lambda_2 = 1, \lambda_3 = 2, \lambda_4 = 3$ with algebraic multiplicities: $m_1 = 2, m_2 = 2, m_3 = 1, m_4 = 3$. The associated Smith form is:

$$D(\lambda) = \text{diag} \left( 1, 1, 1, (\lambda - \frac{1}{2})^2 (\lambda - 1)^2 (\lambda - 2)(\lambda - 3)^3 \right).$$

Choosing vectors $u = [2 \ -2 \ 1 \ -1]^T$ and $v = [0 \ 1 \ 0 \ 2]^T$, we find that:

$$H_0 = \begin{bmatrix} -3 & -7 & -9 & -\frac{21}{2} \\ -7 & -9 & -\frac{21}{2} & -12 \\ -9 & -\frac{21}{2} & -12 & -\frac{109}{8} \\ -\frac{21}{2} & -12 & -\frac{109}{8} & -\frac{651}{32} \end{bmatrix}, \quad H_1 = \begin{bmatrix} -7 & -9 & -\frac{21}{2} & -12 \\ -9 & -\frac{21}{2} & -12 & -\frac{109}{8} \\ -\frac{21}{2} & -12 & -\frac{109}{8} & -\frac{651}{32} \\ -\frac{21}{2} & -12 & -\frac{109}{8} & -\frac{651}{32} \end{bmatrix}.$$  

Then, we have:

$$C = H_0^{-1} H_1 = \begin{bmatrix} 0 & 0 & 0 & -\frac{1}{3} \\ 1 & 0 & 0 & \frac{1}{2} \\ 0 & 1 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & 3 \end{bmatrix}.$$  

The companion matrix $C$ is associated with the monic polynomial:

$$p(\lambda) = \lambda^4 - 3\lambda^3 + \frac{13}{4} \lambda^2 - \frac{3}{2} \lambda + \frac{1}{4},$$

whose roots (that is, the eigenvalues of $H_1 - \lambda H_0$) are indeed $\frac{1}{2}, \frac{1}{2}, 1, 1$.  

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In fact, the Vandermonde factorization for $H_0$ and $H_1$ is $H_i = V^T B_i V$, $i = 0, 1$, where

$$V = \begin{bmatrix}
1 & \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\
0 & 1 & 1 & \frac{3}{4} \\
1 & 1 & 1 & 1 \\
0 & 1 & 2 & 3
\end{bmatrix}, \quad B_0 = \begin{bmatrix}
0 & -2 & 0 & 0 \\
-2 & 0 & 0 & 0 \\
0 & 0 & -3 & -2 \\
0 & 0 & -2 & 0
\end{bmatrix}, \quad B_1 = \begin{bmatrix}
-2 & -1 & 0 & 0 \\
-1 & 0 & 0 & 0 \\
0 & 0 & -5 & -2 \\
0 & 0 & -2 & 0
\end{bmatrix},$$

and $J B_0 = B_1$, with

$$J = \begin{bmatrix}
\frac{1}{2} & 1 & 0 & 0 \\
0 & \frac{1}{2} & 0 & 0 \\
0 & 0 & 1 & 1 \\
0 & 0 & 0 & 1
\end{bmatrix}.$$

### 4.3. Computing invariant pairs via moment pencils

As above, let $\Gamma$ be a smooth closed contour, $\lambda_1, \ldots, \lambda_m$ eigenvalues of $P(\lambda)$ in the interior of $\Gamma$ and the matrices $H_0$ and $H_1$ defined as in (17). For $k = 0, 1, \ldots, m - 1$ and a nonzero vector $v \in \mathbb{C}^n$, consider the vectors:

$$s_k = \frac{1}{2\pi i} \oint_{\Gamma} z^k P(z)^{-1} v dz,$$  \hspace{1cm} (21)

The method proposed in [1] for the computation of the eigenvectors of $P(\lambda)$ is based on the following result:

**Theorem 5.** Let $(\lambda_i, w_i), \; i = 1, \ldots, m$ be eigenpairs for the matrix pencil $H_1 - \lambda H_0$, where the simple, distinct, nondegenerate eigenvalues $\lambda_i$ belong to the interior of a given smooth closed contour $\Gamma$. Let $S = [s_0, \ldots, s_{m-1}]$. Then, for $i = 1, \ldots, m$, the vector $y_i = S w_i$ is an eigenvector of $P(\lambda)$ corresponding to the eigenvalue $\lambda_i$.

Theorem 5 is readily applied to invariant pairs: $(Y, \Lambda)$, where $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_m)$ and $Y = [y_1, \ldots, y_m]$, is clearly an invariant pair for $P(\lambda)$, that is,

$$P(Y, \Lambda) = \sum_{j=0}^{\ell} A_j Y \Lambda^j = 0.$$

Moreover, we know that $C = H_0^{-1} H_1 = V^{-1} \Lambda V$, where $V$ is the classical Vandermonde matrix associated with $\lambda_1, \ldots, \lambda_m$, and that the columns of
are eigenvectors of $H_1 - \lambda H_0$. So we have

$$0 = \sum_{j=0}^{\ell} A_j Y \Lambda^j = \sum_{j=0}^{\ell} A_j Y^j V =$$

$$= \sum_{j=0}^{\ell} A_j Y V V^{-1} \Lambda^j V = \sum_{j=0}^{\ell} A_j S C^j = P(S, C),$$

that is, $(S, C)$ is also an invariant pair of $P(\lambda)$.

What can we say about more general cases, where some of the hypotheses of Theorem 5 are removed? Because of Remark 3, we will only look for simple invariant pairs and we will assume that the polynomials $d_1, \ldots, d_{n-1}$ have no roots inside the given contour $\Gamma$. As in the previous section, we take $d_n(\lambda) = \prod_{j=0}^{s}(\lambda - \lambda_j)^{m_j}$. We will call $q_1(\lambda), \ldots, q_n(\lambda)$ the columns of the matrix $F(\lambda)$ in the Smith form of $P(\lambda)$.

Consider the definition of $s_k$ given in (21). A similar computation to (18) shows that

$$S = [s_0, \ldots, s_{m-1}] = QV,$$

where

$$Q = [Q_0, \ldots, Q_s],$$

$$Q_j = [\gamma_{0,j} q_n(\lambda_j), \gamma_{1,j} q_n'(\lambda_j), \ldots, \gamma_{m_j-1,j} q^{(m_j-1)}(\lambda_j)]$$

for $j = 0, \ldots, s$,

the $\gamma_{i,j}$'s are complex coefficients and $V$ is the confluent Vandermonde matrix defined above.

It is shown in [1] (Lemma 2.4) that, if a complex number $\zeta$ is a root of $d_j(\lambda)$ for some index $1 \leq j \leq n$, then $P(\zeta)q_j(\zeta) = 0$. In our case, this implies that the vector $q_n(\lambda)$ is a root polynomial of $P(\lambda)$ corresponding to the eigenvalue $\lambda_j$, for each $j = 0, \ldots, s$; see [18], section 1.5, for the definition and properties of root polynomials. It follows that $[q_n(\lambda_j), q_n'(\lambda_j), \ldots, q^{(m_j-1)}(\lambda_j)]$ forms a Jordan chain for the eigenvalue $\lambda_j$. So we have that $(Q, J)$ is an invariant pair for $P(\lambda)$. Moreover, if $C = H_0^{-1} H_1$ as usual, we have

$$0 = \sum_{j=0}^{\ell} A_j Q J^j = \sum_{j=0}^{\ell} A_j Q J^j V =$$

$$= \sum_{j=0}^{\ell} A_j Q V V^{-1} J^j V = \sum_{j=0}^{\ell} A_j S C^j = P(S, C).$$

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So we have proved:

**Theorem 6.** With the hypotheses above, let $S = [s_0, s_1, \ldots, s_{m-1}]$ and $C = H_0^{-1}H_1$. Then the pair $(S, C)$ satisfies $P(S, C) = 0$, i.e., $(S, C)$ is a simple invariant pair for $P(\lambda)$.

Note that this property still holds when the size of the invariant pair is larger than the coefficients of $P(\lambda)$, as illustrated in the following example.

4.3.1. Example

Consider the matrix polynomial:

$$P(\lambda) = \lambda^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \lambda \begin{bmatrix} -2 & 0 \\ 2 & -1 \end{bmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix},$$

which has eigenvalues $\lambda_1 = 0$ with algebraic multiplicity 1 and $\lambda_2 = 1$ with algebraic multiplicity 3.

Suppose we are interested in the eigenvalues $\lambda_2$. Then we can choose a contour $\Gamma(t) = z_0 + Re^{it}$, $t \in [0, 2\pi]$, where $z_0 = 1$ and $R = \frac{1}{2}$.

Choosing the vectors $u = \begin{bmatrix} 1 & -1 \end{bmatrix}^T$ and $v = \begin{bmatrix} -1 & 1 \end{bmatrix}^T$, we find that:

$$H_0 = \begin{bmatrix} -1 & -2 & -5 \\ -2 & -5 & -10 \\ -5 & -10 & -17 \end{bmatrix}, \quad H_1 = \begin{bmatrix} -2 & -5 & -10 \\ -5 & -10 & -17 \\ -10 & -17 & -26 \end{bmatrix}$$

Then, we have that the pair $(S, C)$ given by Theorem 6

$$S = H_0^{-1}H_1 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & -3 \\ 0 & 1 & 3 \end{bmatrix} \quad \text{and} \quad C = \begin{bmatrix} 0 & -1 & -2 \\ 1 & 1 & 3 \end{bmatrix}$$

is an invariant pair, i.e., it satisfies $P(S, C) = 0$.

Note that the companion matrix $C$ is associated with the monic polynomial:

$$p(\lambda) = \lambda^3 - 3\lambda^2 + 3\lambda - 1,$$

which has as roots: 1,1,1.
4.4. The block moment method

Instead of the scalar version of the moment method, we can consider a Hankel pencil constructed by block moments $M_k \in \mathbb{C}^{L \times L}$.

**Definition 5.** Let $k$ be a positive integer. For $k = 0, 1, \ldots$, define the block moment $M_k$ as:

$$
M_k = \frac{1}{2\pi i} \oint_{\Gamma} z^k U^H P(z)^{-1} V dz,
$$

where $U, V \in \mathbb{C}^{n \times L}$ are nonzero matrices with linearly independent columns.

Then the block Hankel matrices $H_{L0}, H_{L1} \in \mathbb{C}^{\tilde{m}L \times \tilde{m}L}$ are defined as:

$$
H_{L0} = \begin{bmatrix}
M_0 & M_1 & \cdots & M_{\tilde{m}-1} \\
M_1 & M_2 & \cdots & M_{\tilde{m}} \\
\vdots & \vdots & \ddots & \vdots \\
M_{\tilde{m}-1} & M_{\tilde{m}} & \cdots & M_{2\tilde{m}-2}
\end{bmatrix},
H_{L1} = \begin{bmatrix}
M_1 & M_2 & \cdots & M_{\tilde{m}} \\
M_2 & M_3 & \cdots & M_{\tilde{m}+1} \\
\vdots & \vdots & \ddots & \vdots \\
M_{\tilde{m}} & M_{\tilde{m}+1} & \cdots & M_{2\tilde{m}-1}
\end{bmatrix}
$$

Polynomial eigenvalue computation via the eigenvalues of the pencil $H_{L1} - \lambda H_{L0}$ is discussed in [1] and [5]. See also [28] for an application to acoustic nonlinear eigenvalue problems.

Invariant pairs can be computed from block moments by applying an approach that is similar to the one described in the previous section for the scalar version. An invariant pair $(Y, T)$ can be obtained as $T = H_{L1}^{-1} H_{L0}$ and $Y = [S_0, \ldots, S_{\tilde{m}-1}]$, where

$$
S_k = \frac{1}{2\pi i} \oint_{\Gamma} z^k P(z)^{-1} V dz.
$$

Recall that

$$
T = H_{L0}^{-1} H_{L1} = \begin{bmatrix}
0 & 0 & \cdots & 0 & -X_0 \\
1 & 0 & \cdots & 0 & -X_1 \\
0 & 1 & \cdots & 0 & -X_2 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & -X_{\tilde{m}-1}
\end{bmatrix},
$$

where

$$
\begin{bmatrix}
-X_0 \\
-X_1 \\
\vdots \\
-X_{\tilde{m}-1}
\end{bmatrix} = H_{L0}^{-1} \begin{bmatrix}
M_m \\
M_{m+1} \\
\vdots \\
M_{2\tilde{m}-1}
\end{bmatrix},
$$

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Remark 4. Since $T$ has a block companion form, the problem of finding the eigenvalues $\lambda_1, \ldots, \lambda_m$ of $T$ is equivalent to the problem of finding the eigenvalues of the matrix polynomial:

$$L(\lambda) := \lambda^\ell + X_{\ell-1}\lambda^{\ell-1} + \cdots + X_1\lambda + X_0 = 0.$$  

In principle, the block method allows us to better “capture” the multiplicity structure of eigenvalues, when there are several Jordan blocks per eigenvalue. From a numerical point of view, it often appears to be more stable. Further investigation of this approach will be the topic of future work.

4.4.1. Example

Consider the matrix polynomial:

$$P(\lambda) = \lambda^4I + \lambda^3 \begin{bmatrix} -12 & 0 & 0 \\ 0 & -12 & 0 \\ 0 & 0 & -12 \end{bmatrix} + \lambda^2 \begin{bmatrix} 41 & 0 & 0 \\ 0 & 41 & 0 \\ 0 & 0 & 41 \end{bmatrix} + \lambda \begin{bmatrix} -30 & 0 & 0 \\ 0 & -30 & 0 \\ 0 & 0 & -30 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

which has eigenvalues: 0, 0, 0, 1, 1, 5, 5, 6, 6, 6.

Suppose that in this example we only wish to compute the eigenvalues 0 and 1. We choose a contour $\Gamma$ enclosing just those eigenvalues; for example we can take the circle $\Gamma(t) = z_0 + Re^{it}$, where $z_0 = \frac{1}{2}$, $R = 1$. For $L = 3$, we find

$$T = H_{L0}^{-1}H_{L1} = \begin{bmatrix} 0 & 0 & 0 & \frac{1}{30} & \frac{1}{30} & \frac{1}{30} \\ 0 & 0 & 0 & -\frac{1}{30} & -\frac{1}{30} & -\frac{1}{30} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & \frac{61}{60} & \frac{1}{60} & \frac{1}{60} \\ 0 & 1 & 0 & -\frac{59}{60} & \frac{1}{60} & \frac{1}{60} \\ 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix}.$$  

The companion matrix $T$ is associated with the monic quadratic matrix polynomial:

$$H(\lambda) = \lambda^2I + \lambda X_1 + X_0,$$

where

$$X_0 = -\begin{bmatrix} \frac{1}{30} & \frac{1}{30} & \frac{1}{30} \\ -\frac{1}{30} & -\frac{1}{30} & -\frac{1}{30} \\ 0 & 0 & 0 \end{bmatrix}, \quad X_1 = -\begin{bmatrix} \frac{61}{60} & \frac{1}{60} & \frac{1}{60} \\ -\frac{59}{60} & \frac{1}{60} & \frac{1}{60} \\ 0 & 0 & 1 \end{bmatrix},$$

which has as eigenvalues: 0,0,0,1,1,1 as sought.
4.5. Numerical refinement of invariant pairs

Once an invariant pair has been numerically computed or approximated, it can be refined using an iterative method such as Newton: this is, for instance, the strategy proposed in [4]. Here we experiment with some modifications to the classical Newton’s method applied to the equation $P(X, S) = 0$.

4.5.1. Incorporating line search into Newton’s method

Newton’s method defines $(\Delta X, \Delta S)$ by

$$P(X, S) + \mathbb{D}P_{(X,S)}(\Delta X, \Delta S) = 0 \quad (22)$$

In this section we show how to incorporate exact line searches into Newton’s method for solving the invariant pair problem $P(X, S)$. Line searches are relatively inexpensive and improve the global convergence properties of Newton’s method.

A line search algorithm generally relies on iteration of the form $x_{k+1} = x_k + t_k d_k$, where $d_k$ is a search direction and $t_k$ is the step length.

In our specific problem (5), we must study the minimization problem:

$$p(t) = \| P(X + t\Delta X, S + t\Delta S) \|^2_F.$$

Using the formula for the total derivative of $P$ at $(X, S)$ in direction $(\Delta X, \Delta S)$:

$$\mathbb{D}P_{(X,S)}(\Delta X, \Delta S) = \frac{1}{2\pi i} \int_{\Gamma} P(\lambda) (\Delta X + X(\lambda I - S)^{-1}\Delta S) (\lambda I - S)^{-1} d\lambda,$$

we have, at second order in $\|\Delta X\|$ and $\|\Delta S\|$:

$$P(X + t\Delta X, S + t\Delta S) = \frac{1}{2\pi i} \int_{\Gamma} P(\lambda)(X + t\Delta X)(\lambda I - S)^{-1}d\lambda \approx$$

$$= \frac{1}{2\pi i} \int_{\Gamma} P(\lambda)(X + t\Delta X) \left( (\lambda I - S)^{-1} + (\lambda I - S)^{-1}t\Delta S(\lambda I - S)^{-1} + (\lambda I - S)^{-1}t\Delta S(\lambda I - S)^{-1} \cdots \right) d\lambda \approx$$

$$\approx \frac{1}{2\pi i} \int_{\Gamma} P(\lambda)(X + t\Delta X) \left( (\lambda I - S)^{-1} + t(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} + t^2(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} \Delta S(\lambda I - S)^{-1} \right) d\lambda =$$

$$= \frac{1}{2\pi i} \int_{\Gamma} P(\lambda)(\lambda I - S)^{-1}d\lambda + \int_{\Gamma} P(\lambda) \left[ X + X(\lambda I - S)^{-1}\Delta S \right] (\lambda I - S)^{-1} d\lambda +$$

$$+ t\left[ \frac{1}{2\pi i} \int_{\Gamma} P(\lambda) \left[ X + X(\lambda I - S)^{-1}\Delta S \right] (\lambda I - S)^{-1} d\lambda \right] +$$

$$+ t^2 \left[ \frac{1}{2\pi i} \int_{\Gamma} P(\lambda) (\lambda I - S)^{-1}d\lambda \right] =$$

$$= P(X, S) + \mathbb{D}P_{(X,S)}(\Delta X, \Delta S) + t^2 \left[ \frac{1}{2\pi i} \int_{\Gamma} P(\lambda) \left[ X + X(\lambda I - S)^{-1}\Delta S \right] (\lambda I - S)^{-1} d\lambda \right] +$$

$$+ t^3 \left[ \frac{1}{2\pi i} \int_{\Gamma} P(\lambda) (\lambda I - S)^{-1}d\lambda \right]$$

Recalling that Newton’s method defines $(\Delta X, \Delta S)$ by (22), we have:

$$P(X + t\Delta X, S + t\Delta S) = (1 - t)P(X, S) +$$

$$+ t^2 \left[ \frac{1}{2\pi i} \int_{\Gamma} P(\lambda) \left[ X + X(\lambda I - S)^{-1}\Delta S \right] (\lambda I - S)^{-1} d\lambda \right] +$$

$$+ t^3 \left[ \frac{1}{2\pi i} \int_{\Gamma} P(\lambda) (\lambda I - S)^{-1}d\lambda \right].$$
Thus
\[ p(t) = (1 - t)^2 \| P(X_S) \|^2_F + t^4 \| A \|^2_F + t^6 \| B \|^2_F + \\
+ t^2 (1 - t) \text{trace}(P(X_S)\*A + A\*P(X_S)) + \\
+ t^5 (1 - t) \text{trace}(P(X_S)\*B + B\*P(X_S)) + \\
+ t^6 \text{trace}(A\*B + B\*A) \\
\equiv (1 - t)^2 \alpha + t^4 \theta + t^6 \phi + t^5 (1 - t) \gamma + t^5 \eta \\
= t^6 \varphi + t^5 \eta + t^4 (\theta - \gamma) + t^3 (\gamma - \beta) + t^2 (\alpha + \beta) - 2at + \alpha \] (23)

where:
\[ A = \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda) [\Delta X + X(\lambda I - S)^{-1}\Delta S] (\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} d\lambda, \]
\[ B = \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda) \Delta X (\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} d\lambda, \]
\[ \alpha = \| P(X_S) \|^2_F, \quad \theta = \| A \|^2_F, \quad \varphi = \| B \|^2_F, \quad \eta = \text{trace}(A\*B + B\*A), \]
\[ \beta = \text{trace}(P(X_S)\*A + A\*P(X_S)), \quad \gamma = \text{trace}(P(X_S)\*B + B\*P(X_S)). \]

4.5.2. Šamanskii’s technique

Another variation on Newton’s method is Šamanskii’s technique, which accelerates the quadratic convergence to cubic. Therefore, we must ensure we have quadratic convergence in order to use this technique (see [40]).

4.5.3. Algorithm

Given an initial approximation \((X_0, S_0)\) to the solution of (5), tolerances \(\epsilon\) and \(\epsilon_0\) and a contour \(\Gamma \in \mathbb{C}\) (with the spectrum of \(S_p\) in its interior), we have:

**Algorithm 1. (Newton’s Method with Line Search and Šamanskii Technique)**

**STEP 1:** Set \(k = 0\)

**STEP 2:** If \(\text{error}_k \leq \epsilon\): **STOP**

**STEP 3:** Solve for \((\Delta X_k, \Delta S_k)\) the equation:
\[ \mathbb{D}P_{(X_S)}(\Delta X_k, \Delta S_k) = -(P(X_k, S_k), 0) \]

**STEP 4:** If \(\text{error}_k < \epsilon_0\): go to **STEP 7**.

**STEP 5:** Find by exact line searches a \(t\) that minimizes the function:
\[ \min_{t \in [0,2]} \| P(X + t\Delta X, S + t\Delta S) \|^2_F. \]

**STEP 6:** Update
• \( X_{k+1} = X_k + t\Delta X_k \), \( S_{k+1} = S_k + t\Delta S_k \).

• \( k = k + 1 \) and go to STEP 2.

**STEP 7:** Update \( X_{k,1} = X_k + \Delta X_k \) and \( S_{k,1} = S_k + \Delta S_k \).

**STEP 8:** Solve for \((\Delta X_{k,1}, \Delta S_{k,1})\) the equation:

\[
\mathbb{D}P(X,S)(\Delta X_{k,1}, \Delta S_{k,1}) = -(P(X_{k,1}, S_{k,1}), 0)
\]

**STEP 9:** Update

• \( X_{k+1} = X_{k,1} + \Delta X_{k,1} \), \( S_{k+1} = S_{k,1} + \Delta S_{k,1} \).

• \( k = k + 1 \) and go to STEP 2.

### 4.6. More numerical results

We have implemented Newton’s method with the above variants in Mat- lab and applied it to several problems taken from the NLEVP collection (see [3]). The results are shown in Table 1. For each problem, an invariant pair has first been computed following the classical Sakurai-Sugiura method with 20 integration nodes, and then refined using different variants of Newton’s method. We observe that line search and Šamanskii’s technique are generally effective in reducing the number of iterations and the overall computation time.

| Problem       | Deg P | Size X | Ite | Time   | Ite | Time   | Ite | Time   |
|---------------|-------|--------|-----|--------|-----|--------|-----|--------|
| N.M.          |       |        |     |        |     |        |     |        |
| N.M.L.S.      |       |        |     |        |     |        |     |        |
| N.M.L.S.S.    |       |        |     |        |     |        |     |        |
| bicycle       | 2     | 2 × 2  | 23  | 0.082  | 16  | 0.112  | 12  | 0.05   |
| butterfly     | 4     | 64 × 5 | 67  | 3.174  | 22  | 1.567  | 19  | 1.37   |
| cd_player     | 2     | 60 × 6 | 500 | N.C.   | 19  | 1.021  | 19  | 1.15   |
| closed_loop   | 2     | 2 × 2  | 8   | 0.016  | 7   | 0.02   | 6   | 0.02   |
| damped_beam   | 2     | 200 × 5| 28  | 6.109  | 4   | 0.664  | 3   | 0.80   |
| dirac         | 2     | 80 × 5 | 500 | N.C.   | 27  | 1.394  | 27  | 2.23   |
| hospital      | 2     | 24 × 24| 53  | 5.65   | 51  | 6.21   | 48  | 6.29   |
| metal_strip   | 2     | 9 × 9  | 500 | N.C.   | 28  | 0.589  | 23  | 0.48   |
| mobile_manipulator | 2 | 5 × 2  | 8   | 0.014  | 7   | 0.030  | 6   | 0.03   |
| pdde_stability| 2     | 225 × 6| 29  | 9.644  | 16  | 5.622  | 17  | 8.17   |
| planar_waveguide | 4  | 129 × 5| 72  | 11.148 | 19  | 3.682  | 17  | 5.34   |
| plasma_drift  | 3     | 128 × 6| 69  | 13.059 | 26  | 5.596  | 23  | 6.33   |
| power_plant   | 2     | 8 × 8  | 15  | 0.34   | 13  | 0.39   | 11  | 0.50   |
| railtrack     | 2     | 1005 × 3| 32  | 199.365| 28  | 209.471| 25  | 216.53 |

Table 1: Comparison of results for classical Newton, Newton with line search and Newton with line search and Šamanskii’s technique.
5. Matrix solvents

In this section we study the matrix solvent problem as a particular case of the invariant pair problem, and we apply to solvents some results we have obtained for invariant pairs.

**Definition 6.** A matrix $S \in \mathbb{C}^{n \times n}$ is called a solvent for $P(S)$ if satisfies the relation:

$$P(S) := A_\ell S^\ell + \cdots + A_2 S^2 + A_1 S + A_0 = 0.$$  \hfill (24)

A special case is, for $\ell = 2$, the quadratic matrix equation $A_2 S^2 + A_1 S + A_0 = 0$, which has received considerable attention in the literature. For instance, in [22] and [23] the authors find formulations for the condition number and the backward error. They also propose functional iteration approaches based on Bernoulli’s method and Newton’s method with line search to compute the solution numerically.

The relation between eigenvalues of $P(\lambda)$ and solvents is highlighted in [27]: a corollary of the generalized Bézout theorem states that if $S$ is a solvent of $P(S)$ then:

$$P(\lambda) = L(\lambda)(\lambda I - S),$$

where $L(\lambda)$ is a matrix polynomial of degree $\ell - 1$. Then any eigenpair of the solvent $S$ is an eigenpair of $P(\lambda)$.

5.1. Matrix solvents via contour integral

An equivalent representation for [24] the uses the contour integral is:

**Proposition 2.** $S \in \mathbb{C}^{n \times n}$ is a solvent if and only if

$$P(S) = \frac{1}{2\pi i} \oint_\Gamma P(\lambda)(\lambda I - S)^{-1} d\lambda = 0,$$  \hfill (25)

for any smooth closed contour $\Gamma \subseteq \mathbb{C}$ with the spectrum of $S$ in its interior.

As for invariant pairs, this formulation allows us to choose the contour $\Gamma$ to compute $S$ with specific eigenvalues lying in a particular region of the complex plane and we can use it to compute a condition number of $P(S)$. 

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5.2. **Condition number and backward error**

An analysis and a computable formulation for the condition number and backward error of a solvent can be found in [22] and [23]. These results are given using definition (24) and for the case of the quadratic solvent problem, using definition (24).

This section presents computable expressions for the condition number and backward error for the general matrix solvent problem, using the contour integral formulation (25). We follow the ideas presented in [22], [23] and [37].

### 5.2.1. **Condition number of \( P(S) \)**

We perform here a similar analysis as we did in Section 2.2.1.

Consider the perturbed equation:

\[
\frac{1}{2\pi i} \oint_{\Gamma} \left[ P(\lambda) + \Delta P(\lambda) \right] (\lambda I - S - \Delta S)^{-1} d\lambda = 0,
\]

where \( \Delta P(\lambda) \) is defined in (6).

Measuring the relative perturbations normwise by:

\[
\epsilon = \left\| \begin{bmatrix} \alpha_\ell^{-1} \Delta A_\ell & \ldots & \alpha_1^{-1} \Delta A_1 & \alpha_0^{-1} \Delta A_0 \end{bmatrix} \right\|_F
\]

where the \( \alpha_i \)'s are nonnegative parameters for \( i = 0, \ldots, \ell \). For first order in \( \epsilon \), computations yield to:

\[
\frac{\| \Delta S \|_F}{\| S \|_F} \leq \Psi(S) \epsilon + O(\epsilon^2)
\]

where

\[
\Psi(S) = \frac{\left\| M^{-1} \begin{bmatrix} \alpha_\ell B_\ell & \ldots & \alpha_1 B_1 & \alpha_0 B_0 \end{bmatrix} \right\|_2}{\| S \|_F}
\]

is the condition number and

\[
M = \frac{1}{2\pi i} \oint_{\Gamma} \left( (\lambda I - S)^{-1} \right)^T \otimes (P(\lambda)(\lambda I - S)^{-1}) d\lambda, \quad M \in \mathbb{C}^{n^2 \times n^2}
\]

\[
B_j = \frac{1}{2\pi i} \oint_{\Gamma} \left( \lambda^j (\lambda I - S)^{-1} \right)^T \otimes I_n d\lambda, \quad j = 0, \ldots, \ell, \quad B_j \in \mathbb{C}^{n^2 \times n^2}.
\]
5.2.2. Backward error of $P(S)$

The backward error of an approximate solution $T$ to (24) can be defined by:

$$
\eta(T) = \min\{ \epsilon : (A_\ell + \Delta A_\ell)T^\ell + \cdots + (A_0 + \Delta A_0) = 0, \\
\| [\alpha_\ell^{-1} \Delta A_\ell \cdots \alpha_1^{-1} \Delta A_1 \alpha_0^{-1} \Delta A_0] \|_F \leq \epsilon \} \quad (26)
$$

We proceed as in Section 2.2.2 and we obtain bounds for the backward error of $P(S)$:

$$
\eta(T) \geq \frac{\|P(T)\|_F}{(\alpha_\ell^2\|T^\ell\|_F^2 + \cdots + \alpha_1^2\|T\|_F^2 + \alpha_0^2)^{1/2}}, \\
\eta(T) \leq \frac{\|P(T)\|_F}{(\alpha_\ell^2\sigma_{\min}(T^\ell)^2 + \cdots + \alpha_1^2\sigma_{\min}(T)^2 + \alpha_0^2)^{1/2}},
$$

where the $\alpha_i$'s are nonnegative parameters and $\sigma_{\min}$ denotes the smallest singular value, that by assumption is nonzero.

6. Computation of solvents

The question of designing symbolic algorithms for computing solvents remains relatively unexplored. Attempts have been made to formulate the problem as a system of polynomial equations which can be solved via standard methods. However, this approach becomes cumbersome for problems of large size (see [22]).

Motivated by applications to differential equations [10], we study an approach to the symbolic or symbolic-numeric computation of solvents based on the moment method, by specializing the results presented in Section 4.

Let us recall some results that will be needed later. The next result is a generalization of a theorem presented in [23] which gives information about the number of solvents of $P(S)$.

**Theorem 7.** Suppose $P(\lambda)$ has $p$ distinct eigenvalues $\{\lambda_i\}_{i=1}^p$, with $n \leq p \leq \ell n$, and that the corresponding set of $p$ eigenvectors $\{v_i\}_{i=1}^p$ satisfies the Haar condition (every subset of $n$ of them is linearly independent). Then there are at least $\left(\begin{array}{c} p \\ n \end{array}\right)$ different solvents of $P(\lambda)$, and exactly this many if $p = \ell n$, which are given by

$$
S = W\text{diag}(\mu_i)W^{-1}, \quad W = \begin{bmatrix} w_1 & \cdots & w_n \end{bmatrix},
$$

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where the eigenpairs \((\mu_i, w_i)_{i=1}^n\) are chosen from among the eigenpairs \((\lambda_i, v_i)_{i=1}^p\) of \(P\).

Note that if we have that \(p = n\) in Theorem 7, the distinctness of the eigenvalues is not needed, and then we have a sufficient condition for the existence of a solvent.

**Corollary 1.** If \(P(\lambda)\) has \(n\) linearly independent eigenvectors \(v_1, v_2, \ldots, v_n\) then \(P(S)\) has a solvent.

An example which illustrates this last result is the following. Consider the quadratic matrix solvent problem (see [13], [23])

\[
Q(S) = S^2 + \begin{bmatrix} -1 & -6 \\ 2 & -9 \end{bmatrix} S + \begin{bmatrix} 0 & 12 \\ -2 & 14 \end{bmatrix}
\]

\(Q(\lambda)\) has eigenpairs: \((1, \begin{bmatrix} 1 \\ 0 \end{bmatrix})\), \((2, \begin{bmatrix} 0 \\ 1 \end{bmatrix})\), \((3, \begin{bmatrix} 1 \\ 1 \end{bmatrix})\) and \((4, \begin{bmatrix} 1 \\ 1 \end{bmatrix})\). For this example, the complete set of solvents is:

\[
\begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}, \begin{bmatrix} 1 & 2 \\ 0 & 3 \end{bmatrix}, \begin{bmatrix} 3 & 0 \\ 1 & 2 \end{bmatrix}, \begin{bmatrix} 1 & 3 \\ 0 & 4 \end{bmatrix} \text{ and } \begin{bmatrix} 4 & 0 \\ 2 & 2 \end{bmatrix}.
\]

Note that we cannot construct a solvent whose eigenvalues are 3 and 4 because the associated eigenvectors are linearly dependent.

Our approach is based on the relation between the matrix solvent problem (24) and the invariant pair problem (3), in the special case when in the invariant pair \((Y, T)\), the matrix \(Y\) has size \(n \times n\) and is invertible. Note that taking \(S = YTY^{-1}\) then \(S\) will satisfy (24):

\[
A_\ell Y T^{\ell} + \cdots + A_2 Y T^2 + A_1 Y T + A_0 Y = 0 \iff
A_\ell Y T^{\ell} Y^{-1} + \cdots + A_2 Y T^2 Y^{-1} + A_1 Y T Y^{-1} + A_0 Y = 0 \iff
A_\ell S^\ell + \cdots + A_2 S^2 + A_1 S + A_0 = 0.
\]

So, one can first compute invariant pairs \((Y, T)\) \(\in \mathbb{C}^{n \times n} \times \mathbb{C}^{n \times n}\) with the condition that \(Y\) is invertible, and then determine the associated solvents.

### 6.1. Numerical refinement of solvents

As pointed out before, the use of Newton’s method incorporating line searches to find solvents is not new. For instance, in [23], [29] this approach
is used to approximate solvents for the quadratic matrix equation. Here we apply this method to approximate solvents for the general matrix solvent problem $P(S) = 0$. For that, we use the contour integral formulation \(^{(25)}\).

For the general problem we have the minimization problem:

$$p(t) = \| P(S + t\Delta S) \|^2_F,$$

Using the formula for the derivative of the matrix inverse:

$$\frac{dA^{-1}}{dt} = -A^{-1}\frac{dA}{dt}A^{-1},$$

we write the formula for the total derivative of $P$ at $S$ in direction $\Delta S$ as follows:

$$\mathbb{D}P_S(\Delta S) = \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1}d\lambda. \quad (27)$$

Then we have:

$$P(S + t\Delta S) = \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(\lambda I - S - t\Delta S)^{-1}d\lambda =$$

$$= \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda) \left[(\lambda I - S)^{-1} + (\lambda I - S)^{-1}t\Delta S(\lambda I - S)^{-1} + (\lambda I - S)^{-1}t^2\Delta S(\lambda I - S)^{-1} + \cdots \right] d\lambda$$

$$\approx \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda) \left[(\lambda I - S)^{-1} + t(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} + t^2(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} \right] d\lambda =$$

$$= \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(\lambda I - S)^{-1}d\lambda + t \left[ \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} d\lambda \right] +$$

$$+ t^2 \left[ \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} d\lambda \right] =$$

$$= P(S) + \mathbb{D}P_S(\Delta S) + t \left[ \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} d\lambda \right]$$

Recalling that Newton’s method defines $\Delta S$ by

$$P(S) + \mathbb{D}P_S(\Delta S) = 0$$

then we have:

$$P(S + t\Delta S) = (1 - t)P(S) +$$

$$+ t^2 \left[ \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1} d\lambda \right]$$

Thus

$$p(t) = (1 - t)^2\| P(S) \|^2_F + t^4\| A \|^2_F + t^2(1 - t)\text{trace}(P(S)^*A + A^*P(S))$$

$$\equiv (1 - t)^2\alpha + t^4\theta + t^2(1 - t)\beta =$$

$$= t^4\theta - t^3\beta + t^2(\alpha + \beta) - 2at + \alpha$$

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where:

\[ A = \frac{1}{2\pi i} \oint_{\Gamma} P(\lambda)(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1}\Delta S(\lambda I - S)^{-1}d\lambda, \]
\[ \alpha = \|P(S)\|_F^2, \quad \theta = \|A\|_F^2, \quad \beta = \text{trace}(P(S)^*A + A^*P(S)). \]

7. Solvents and triangularized matrix polynomials

Motivated by the results in [36] and [39], where the authors analyze a method for triangularizing the matrix polynomial \( P(\lambda) \), we aim here to study the relation between solvents of general and triangularized matrix polynomials.

7.1. Triangularizing matrix polynomials

For any algebraically closed field \( \mathbb{F} \), any matrix polynomial \( P(\lambda) \in \mathbb{F}[\lambda]^{n \times m} \), with \( n \leq m \), can be reduced to triangular form via unimodular transformations, preserving the degree and the finite and infinite elementary divisors [36], [39].

**Theorem 8.** [36] For an algebraically closed field \( \mathbb{F} \), any \( P(\lambda) \in \mathbb{F}[\lambda]^{n \times m} \) with \( n \leq m \) is triangularizable.

What can we say about solvents for a given matrix polynomial \( P(\lambda) \) and for the associated triangularized polynomial? A partial answer will be given in Theorem 10.

**Theorem 9.** For any \( \ell n \times \ell n \) monic linearization \( \lambda I - A \) of \( P(\lambda) \in \mathbb{C}[\lambda]^{n \times n} \) with nonsingular leading coefficient, there exists \( U \in \mathbb{C}^{n \times \ell n} \) with orthogonal columns such that \( M = [U; \ UA; \ldots; \ UA^{\ell-1}] \) is nonsingular and \( \lambda I - MAM^{-1} \) is a linearization for the polynomial \( T(\lambda) = \lambda^\ell I + \lambda^{\ell-1}T_{\ell-1} + \cdots + \lambda^2 T_2 + \lambda T_1 + T_0 \), which is upper triangular and equivalent to \( P(\lambda) \).

Theorem 9 is a straightforward generalization of a result found in [39]. Note that, for the time being, we assume that the leading coefficient \( A_\ell \) is nonsingular. Block matrices are written according to Matlab notation.

**Theorem 10.** Let \( M \) be as in Theorem 9 and let \( Y_1 \) be the first \( n \times n \) block of the matrix \( M^{-1} [I_n; \ S_\ell; \ \cdots; \ S_{\ell-1}^\ell] \). If \( Y_1 \) is nonsingular and \( S_\ell \) is a solvent for the triangularized problem, i.e., \( T(S_\ell) = 0 \), then \( S = Y_1 S_\ell Y_1^{-1} \) is a solvent for \( P(S) \).

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Here we use the linearization:

\[
A = \begin{bmatrix}
0 & I_n & 0 & \cdots & 0 \\
0 & 0 & I_n & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & I_n \\
-A_0 & -A_1 & -A_2 & \cdots & -A_{\ell-1}
\end{bmatrix}.
\]

**Proof.** Note that:

\[
\begin{bmatrix}
0 \\
0 \\
\vdots \\
0
\end{bmatrix} = \begin{bmatrix}
S_t - S_t \\
S_t^2 - S_t^2 \\
\vdots \\
-T_0 - T_1 S_t - S_t^2 - \cdots - S_t^\ell
\end{bmatrix} = 
\begin{bmatrix}
0 & I_n & 0 & \cdots & 0 \\
0 & 0 & I_n & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & I_n \\
-T_0 & -T_1 & -T_2 & \cdots & -T_{\ell-1}
\end{bmatrix} \begin{bmatrix}
I_n \\
S_t \\
\vdots \\
S_{t-1}^\ell
\end{bmatrix} - \begin{bmatrix}
I_n \\
S_t \\
\vdots \\
S_{t-1}^\ell
\end{bmatrix} = 
\begin{bmatrix}
0 & I_n & 0 & \cdots & 0 \\
0 & 0 & I_n & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & I_n \\
-A_0 & -A_1 & -A_2 & \cdots & -A_{\ell-1}
\end{bmatrix} \begin{bmatrix}
I_n \\
S_t \\
\vdots \\
S_{t-1}^\ell
\end{bmatrix} - \begin{bmatrix}
I_n \\
S_t \\
\vdots \\
S_{t-1}^\ell
\end{bmatrix} S_t^{(iii)} = 
\begin{bmatrix}
0 & I_n & 0 & \cdots & 0 \\
0 & 0 & I_n & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & I_n \\
-A_0 & -A_1 & -A_2 & \cdots & -A_{\ell-1}
\end{bmatrix} \begin{bmatrix}
I_n \\
S_t \\
\vdots \\
S_{t-1}^\ell
\end{bmatrix} - \begin{bmatrix}
I_n \\
S_t \\
\vdots \\
S_{t-1}^\ell
\end{bmatrix} S_t.
\]

Since \( M^{-1} \) has size \( \ell n \times n \), let us partition it as

\[
\begin{bmatrix}
I_n \\
S_t \\
\vdots \\
S_{t-1}^\ell
\end{bmatrix}, \text{ where}
\begin{bmatrix}
Y_1 \\
Y_2 \\
\vdots \\
Y_\ell
\end{bmatrix}
\]
$Y_i \in \mathbb{C}^{n \times n}$ for $i = 1, \ldots, \ell$. Then:

$$
\begin{bmatrix}
0 & I_n & 0 & \cdots & 0 \\
0 & 0 & I_n & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \cdots & I_n \\
-A_0 & -A_1 & -A_2 & \cdots & -A_{\ell-1}
\end{bmatrix}
\begin{bmatrix}
Y_1 \\
Y_2 \\
\vdots \\
Y_\ell
\end{bmatrix}
- 
\begin{bmatrix}
Y_1 \\
Y_2 \\
\vdots \\
Y_\ell
\end{bmatrix}
S_i = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.
$$

Then we have:

$$
Y_i = Y_1 S_i^{i-1}, \text{ for } i = 2, \ldots, \ell; 
- A_0 Y_1 - A_1 Y_2 - \cdots - A_{\ell-1} Y_\ell - Y_\ell S_i = 0.
$$

Substituting equations (28) in (29) we obtain:

$$
0 = Y_1 S_1^\ell + A_{\ell-1} Y_1 S_1^{\ell-1} + \cdots + A_1 Y_1 S_1 + A_0 Y_1.
$$

If $Y_1$ is invertible we have:

$$
0 = Y_1 S_1^\ell Y_1^{-1} + A_{\ell-1} Y_1 S_1^{\ell-1} Y_1^{-1} + \cdots + A_1 Y_1 S_1 Y_1^{-1} + A_0.
$$

Taking $S = Y_1 S_1 Y_1^{-1}$ we have:

$$
0 = S^\ell + A_{\ell-1} S^{\ell-1} + \cdots + A_2 S^2 + A_1 S + A_0 := P(S).
$$

Then $S = Y_1 S_1 Y_1^{-1}$ is a solvent for $P(S)$.

### 7.2. A problem with an infinite number of solvents

What happens to the ideas outlined above when working on problems with an infinite number of solvents? Here is an example taken from [31].

Consider the matrix polynomial:

$$
P(\lambda) = \lambda^2 I + \lambda \begin{bmatrix}
-7 & -2 \\
\frac{3}{31} & \frac{-203}{31} & \frac{3}{31} \\
\frac{31}{3} & \frac{31}{3} & \frac{31}{3}
\end{bmatrix}
+ \begin{bmatrix}
13 & 9 & 7 \\
\frac{-21}{31} & \frac{294}{31} & \frac{-36}{31} \\
\frac{31}{31} & \frac{31}{31} & \frac{31}{31}
\end{bmatrix}
$$

Triangularizing $T(\lambda)$ we find:

$$
T(\lambda) = \begin{bmatrix}
(\lambda - 3)(\lambda - 4) & (\lambda - 3) & 0 \\
0 & (\lambda - 3)^2 & 1 \\
0 & 0 & (\lambda - 4)^2
\end{bmatrix}
= \lambda^2 I_2 + \lambda T_1 + T_0 =
$$

$$
= \lambda^2 I + \lambda \begin{bmatrix}
-7 & 1 & 0 \\
0 & -6 & 0 \\
0 & 0 & -8
\end{bmatrix}
+ \begin{bmatrix}
12 & -3 & 0 \\
0 & 9 & 1 \\
0 & 0 & 16
\end{bmatrix}.
$$
Now, suppose that the solvent $S_t \in \mathbb{C}^{3\times3}$ of the triangularized problem is in upper triangular form, i.e.:

$$S_t = \begin{bmatrix} x_{11} & x_{12} & x_{13} \\ 0 & x_{22} & x_{23} \\ 0 & 0 & x_{33} \end{bmatrix},$$

then we have:

$$T(S_t) = S_t^2 + T_1 S_t + T_0 = \begin{bmatrix} (x_{11} - 3)(x_{11} - 4) & x_{22} - 7x_{11} + x_{11}x_{12} + x_{12}x_{22} - 3 & x_{23} - 7x_{13} + x_{11}x_{13} + x_{12}x_{23} + x_{13}x_{33} \\ x_{22} - 3 & 0 & 0 \\ 0 & 0 & (x_{33} - 4)^2 \end{bmatrix}.$$ 

In the task of solving the problem $T(S_t) = 0$, we see that: $x_{11} = 3$ or $x_{11} = 4$, $x_{22} = 3$ and $x_{33} = 4$. Then we have two cases:

I. If $x_{11} = 3$, $x_{22} = 3$ and $x_{33} = 4$:
Then we find that $x_{23} = -1$, $x_{12} = 0$ and $x_{12} = -1$, which is a contradiction. In this case there is no solution and then we can’t construct a solvent.

II. If $x_{11} = 4$, $x_{22} = 3$ and $x_{33} = 4$:
Then we find that $x_{23} = -1$ and $x_{13} = x_{12} + 1$. In this case the solvent $S_t$ has the form:

$$S_t = \begin{bmatrix} 4 & x_{12} & x_{12} + 1 \\ 0 & 3 & -1 \\ 0 & 0 & 4 \end{bmatrix} = \begin{bmatrix} 4 & 0 & 1 \\ 0 & 3 & -1 \\ 0 & 0 & 4 \end{bmatrix} + x_{12} \begin{bmatrix} 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

for $x_{12} \in \mathbb{C}$.

Thus $T(\lambda)$ has an infinite number of solvents and the same holds for $P(\lambda)$.

8. Conclusion

In this paper we have explored several questions related to invariant pairs and solvents of matrix polynomials. In particular, preliminary results on the use of scalar or block moment Hankel pencils to compute invariant pairs and solvents suggest that this approach may present several points of interest. A more detailed analysis, along with the design and development of effective symbolic-numeric algorithms and extensive numerical tests, will be the topic of future work.
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