NEP-PACK: A Julia package for nonlinear eigenproblems
Release v0.2

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We present NEP-PACK a novel open-source library for the solution of nonlinear eigenvalue problems (NEPs). The package provides a framework to represent NEPs, as well as efficient implementations of many state-of-the-art algorithms. The package makes full use of the efficiency of Julia, yet maintains usability, and integrates well with other software packages. The package is designed to be easy to use for application researchers as well as algorithm developers. Particular attention is paid to algorithm neutrality, in order to make performance comparisons between algorithms easier. This paper describes the main functionality of NEP-PACK, as well as design decisions and theory needed for the design.

1 INTRODUCTION

This package concerns nonlinear eigenvalue problems defined as the problem of determining the singular points of a matrix, i.e., find \((\lambda, v)\) such that

\[
M(\lambda)v = 0
\]

where \(v \neq 0\) and \(M : \mathbb{C} \rightarrow \mathbb{C}^{n \times m}\) is a holomorphic (or meromorphic with only a few poles).

Nonlinear problems which are not the linear or generalized eigenvalue problem, occur in many situations. Some of the most common situations are

- higher order differential equations (references in [71]) leading to matrix polynomials
- systems and control for time-delay systems, leading to exponential nonlinearities [48] [35]
- quantum physics (quantum dots) [5, 6]) leading to rational nonlinear functions
- fluid mechanics (scaling exponent in turbulent flow) [50] leading to exponential nonlinearities
- fluid-solid interations [76, 78] leading to rational terms,
- boundary element method applied to resonance problems [64, 65, 72], see also [19] and the software package [62],
- absorbing boundary conditions (frequency dependent) leading to square root nonlinearities [16, 69, 70] or Bessel functions [2], e.g., in fiber optics design [43],
- chatter in machine tool milling [15, 33, 34, 36, 55],
- periodic structures, e.g., in crystals [20, 23, 24, 57]

In most of these applications there is need for performance, and robustness. Our package is implemented in the Julia programming language [14], in order to obtain efficiency and still have access to high-level functionality. A milestone for computing in the Julia language was carried out within the Celeste project, which qualifies as petascale computation [52].

The numerical treatment of this problem has received attention in a large number of works, see summary papers such as [56], [46] [80] and [28] as well as software packages [8] and [29, 30, 54].

As we shall further describe in Section 3, many applications and algorithms are based on a sum of products representation of the \(M\) matrix. We will provide considerable functionality and efficiency for problems that can be expressed as

\[
M(\lambda) = A_1 f_1(\lambda) + \cdots + A_m f_m(\lambda).
\]
In theory, any NEP can be expressed as (2), if one sets \( m = n^2 \). However, most algorithms based on (2) also assume that \( m \) is not too large, and become less attractive due to an increase in computation time unless \( m \) is relatively small. Our framework is efficient for structures as (2).

Our software is designed to not be based on (2) but rather on certain interface functions, which define a NEP. This allows to represent NEPs, where (2) is not efficient. These framework interfaces are described in Section 3.1.

All of the NEP-algorithms are carefully documented in terms of references, and in order to encourage users to give credit to the original algorithm researchers.

## 2 BASIC USAGE

NEP-PACK is a registered package in the Julia central package repository, which makes it possible to install the package with very little effort

```julia
julia> ]
(0.1.0) pkg> add NonlinearEigenproblems
julia> using NonlinearEigenproblems
```

Nonlinear eigenvalue problems are represented as objects of the type NEP, which can be created in a number of different ways. We have a gallery of problems available, which can be accessed through the `nep_gallery` command (further described in Section 6).

```julia
julia> nep=nep_gallery("neuron0");
```

This creates a NEP object which is used to model a neuron. This gallery problem stems from [60] which is also available as a model problem in DDE-BIFTOOL [21, 22]. The problem describes the stability the delay differential equation

\[
\begin{align*}
\dot{x}_1(t) &= -\kappa x_1(t) + \beta \tanh(x_1(t - \tau_3)) + a_1 \tanh(x_2(t - \tau_2)) \\
\dot{x}_2(t) &= -\kappa x_2(t) + \beta \tanh(x_2(t - \tau_3)) + a_2 \tanh(x_1(t - \tau_1)).
\end{align*}
\]

In particular, the stability of the zero solution is characterized by the eigenvalues with the largest real part of the following NEP

\[
M(\lambda) := -\lambda I + A_0 + A_1 e^{-\gamma_1 \lambda} + A_2 e^{-\gamma_2 \lambda} + A_3 e^{-\gamma_3 \lambda},
\]

which belongs to the class of NEP commonly called a delay eigenvalue problems (DEP), see Section 3.2. The `typeof` command reveals that the problem is represented as a DEP:

```julia
julia> typeof(nep)
DEP{Float64,Array{Complex{Float64},2}}
```

As an illustration we solve this problem with our implementation of the NLEIGS method [27]

```julia
julia> Σ=[-3.0-10im,-3+10im,1+10im,1-10im]; # Region of interest
julia> (λ,V)=nleigs(nep,Σ);
```

The same results are obtained with the infinite Arnoldi method [39]
The result is given in Figure 1.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{neuron_eigenvalues.png}
\caption{The eigenvalues of the neuron example.}
\end{figure}

3 THE NEP REPRESENTATION

3.1 Accessing the data in a NEP

The vast amount of numerical methods and the vast amount of applications that have been developed and formulated in the literature have typically been expressed in the way that is the most natural for that specific method/application. Different methods require data from the NEP in different ways. Different applications are expressed in different ways. Our package is designed for algorithms and problems which can be (efficiently) expressed with the following quantities, which are selected to match the need from as many applications and algorithms as possible.

- **compute_Mder(lambda,k)** computes the kth derivative of $M$ and evaluates it in $\lambda$
  \[ M_k = M^{(k)}(\lambda) \]  

- **compute_Mlincomb(lambda,V)** computes the linear combination
  \[ \sum_{i=1}^{k} M^{(i-1)}(\lambda) v_i \]
  given the evaluation point $\lambda$ and a matrix $V \in \mathbb{C}^{n \times k}$.

- **compute_MM(S,V)** computes the expression
  \[ \mathbb{M}(S,V) = \frac{1}{2\pi i} \int_{\Gamma} M(\xi)V(\xi I - S)^{-1} d\xi \]
  for given matrices $S \in \mathbb{C}^{p \times p}$ and $V \in \mathbb{C}^{n \times p}$, and the contour $\Gamma$ includes the eigenvalues of $S$. The form (7) is more commonly expressed in terms of matrix functions
  \[ \mathbb{M}(S,V) = A_1 V f_1(S) + \cdots + A_m V f_m(S), \]
  if $A_1, \ldots, f_1, \ldots$ are given as in (2).
Note that these compute functions are mathematically equivalent, i.e., there are explicit procedures to compute one quantity from any other quantity. We specify further relations in Section 3.3. Although they are mathematically equivalent, they are computationally very different and the transformations are not necessarily very efficient. For instance, in many applications (particular types of matrix-free situations) the matrix may not be directly available, but only available as a subroutine. In this case the user can specify (6), whereas computing a matrix as in (5) may not be computationally feasible.

Routines for some additional secondary quantities are also available:

- **lin_solve** solves a linear system associated with $M(\lambda)$. Further specifications can be made by inheriting from the type LinSolver.
- **compute_rf** computes the Rayleigh functional for the NEP, i.e., solves the nonlinear (scalar) equation
  \[ y^H M(\lambda) x = 0. \] (8)
- Several algorithms require the solution to a projected problem
  \[ Y^H M(\lambda) X z = 0 \] (9)
  which is again a NEP, see Section 5.3. The fact that projected NEPs are also of the type NEP, allows us to apply any of our methods as an inner solver.
- **errmeasure** is a keyword argument accepted by most functions. The function handle should accept two arguments `errmeasure(lambda, v)` and computes an error estimate based on $\lambda$ and $v$. The `default_errmeasure` computes the relative residual norm
  \[ \frac{\|M(\lambda) v\|}{\|v\|}. \]
  The construction allows the user to specify in which way the error should be measured. Hence other error measurements, such as the backward error presented in [32], can be implemented by the user.

In what follows we describe in what way state-of-the-art algorithms can be implemented with these compute functions.

- A large class of methods can be derived from Newton’s method, e.g., [1, 37, 49, 56, 58, 63, 73]. See also the summary of papers in, e.g., [28, 66–68]. These algorithms have in common that one needs to compute for some vectors $u_1$ and $u_2$
  \[ M(\lambda) u_1 + M'(\lambda) u_2 \]
  where in some settings $u_1$ is zero. This is clearly possible with (6). They also require the solution to one (or many) linear systems, which can be computed with the `lin_solve` functionality.
- The standard application of contour integral methods require the solution to many linear systems (for different evaluation points) and only require a matrix vector product, i.e., (6). Methods in these papers can be classified in this way: [3, 4, 11] and the FEAST software [51], and acceleration techniques [81].
- Jacobi-Davidson methods [10, 18, 61, 79] are projection methods and hence require (9). For the deflation technique presented in [18], the quantity
  \[ U(\mu) = \frac{1}{2\pi} \int_{\Gamma} M(\xi) V(\xi I - S)^{-1}(\xi - \mu)^{-1} d\xi \]
  and its derivatives are required in order for the deflated problem to implement the interfaces desired by the solvers of (9). These derivatives can be computed via the interface (6) and
the observations that \( U^{(k)}(\mu) = (-M^{(k)}(\mu)V + kU^{(k-1)}(\mu))(S - \mu I)^{-1} \), and \( U(\mu) = (M(S, V) - M(\mu I, V))(S - \mu I)^{-1} \). Specifically, due to structure the action of \( M(\mu I, V) \) can be computed using (6), and for an invariant pair \( M(S, V) = 0 \).

• Other projection methods such as the nonlinear Arnoldi method \([77]\) and variation \([42]\) require the projection (9). Also the block preconditioned PCG for NEPs in \([82]\) is a projection method. When solving large-scale problems, the storage of the projection subspace becomes costly as the number of iterations increase. In such cases, we need restarting techniques as discussed in \([7]\), which can be directly implemented with manipulations of the projected NEP.

• Infinite Arnoldi type methods such as \([38, 39, 41]\) and two-sided version \([25]\) require (6). The restarted versions \([40, 47]\) additionally require (7).

• Rayleigh functional methods, e.g., \([49, 58, 59]\) depend on solution methods for the Rayleigh quotient.

• Certain algorithms are based on directly working with the block residual (7), e.g., block Newton \([12, 13, 17, 19, 20, 44]\)

• Methods based on the QR-method, e.g., \([26, 45]\) require (5)

• Rational Krylov methods such as, e.g., \([27, 74, 75]\) requires access to linear solvers. Moreover, for a general NEP either (5) or (6) is used, and in the special case of an SPMF, see Section 3.2, it uses matrix function evaluations \( f_0(S), \ldots, f_m(S) \).

### 3.2 The common types

We provide the user with efficient implementations of the compute functions in the previous section, for many common types:

• **PEP**: \( M(\lambda) = A_1 + \lambda A_2 + \cdots + \lambda^{m-1} A_m \)

• **DEP**: \( M(\lambda) = -\lambda I + A_0 + \sum_{i=1}^{m} e^{-\tau_i \lambda} A_i \)

• **SumNEP**: \( M(\lambda) = A(\lambda) + B(\lambda) \) where \( A \) and \( B \) are also NEPs

• **SPMF\_NEP**: See below.

• **LowRankNEP**: An SPMF where the matrices are represented as low-rank factorizations

The most general of the above is the SPMF\_NEP which represents the sum of products of matrices and functions (2). The functions \( f_i, i = 1, \ldots, m \) have to be defined in scalar sense, as well as in a matrix function sense. The implementation of the SPMF is designed to be efficient when \( m \ll n \).

The example below solves the NEP

\[
M(\lambda) = \lambda A + e^A B + \left(1 + \sqrt{\lambda}\right) C
\]

with the block Newton method \([44]\):

```julia
julia> using LinearAlgebra
julia> A=ones(5,5); B=ones(5,5)+I; C=reverse(B,dims=1)
julia> f1= S-> S;
julia> f2= S-> exp(S)
julia> f3= S-> one(S)+sqrt(S);

julia> nep=SPMF\_NEP([A,B,C],[f1,f2,f3]);

julia> blocknewton(nep,S=[1 0; 0 1 .0 

julia> displaylevel=1)
Iteration 1: Error: 2.112578e+0
Iteration 2: Error: 3.765499e+0
Iteration 3: Error: 2.361554e+0
Iteration 4: Error: 2.955760e+0
Iteration 5: Error: 3.543752e+0
Iteration 6: Error: 4.080188e+0
Iteration 7: Error: 2.885914e+1

(Complex{Float64}
0.557832+0.0im -3.03756e-16+0.0im; -7.18644e-16+0.0im
0.557832+0.0im], Complex{Float64}[-0.617521+0.0im -0.0206428+0.0im;
```
3.3 Equivalence of interfaces
As an example how (6) can be computed from (7): \( M(S, V)e_1 \) is equal to (6) where \( S \in \mathbb{R}^{k \times k} \) is the bidiagonal matrix with \( \lambda \) in the main diagonal, \( S_{i+1,i} = i \) and \( V = [v_1, \ldots, v_k] \). This equivalence follows by expressing \( M(\lambda) \) in SPMF_NEP format (2) in (6) and by using [31, Definition 1.2] with a proper rescaling.

4 PROBLEM TRANSFORMATIONS
The abstraction of the NEPs to be essentially specified by well-defined compute functions (Section 3) leads to the advantage that problems can be transformed leading by defining new compute functions.

We have implemented a number of ways to transform the problem

- One can shift and scale the problem, i.e., define a new NEP
  \[
  \tilde{M}(\lambda) = M(\alpha \lambda + \sigma) \tag{10}
  \]
  This functionality is available in the `shift_and_scale` function.
- One can carry out a Möbius transformation of the problem, i.e., define a new NEP
  \[
  \tilde{M}(\lambda) = M((a \lambda + b)/(c \lambda + d))
  \]
  This functionality is available in the `mobius_transformation` function.
- One can deflate eigenvalue (or invariant pairs) from a NEP as specified, e.g., in [17]. This is provided by the function `effenberger_deflation`

Although the above functions provide convenient features for a user, they may not always lead to extremely efficient algorithms, since a transformed problem may have some computational overhead. Therefore, certain functionality is also provided at an algorithm level, e.g., shifting and scaling is available in the infinite Arnoldi methods.

The deflation can be used to compute one pair at a time and avoid reconvergence, e.g., as follows:

```julia
julia> nep=nep_gallery("dep0");
julia> (s,v)=newton(nep);
julia> n=size(nep,1);
julia> S0=reshape([s],1,1);
julia> V0=reshape(v,n,1);
julia> dnep=effenberger_deflation(nep,S0,V0);
julia> (s2,v2)=augnewton(dnep); # this converges to different eigval
julia> minimum(svdvals(compute_Mder(nep,s2)))
9.323003321058995e-17
```

5 NEP-SOLVER ALGORITHM IMPLEMENTATIONS
We have implemented several algorithms as well as extensions.

5.1 Newton-type methods
Several flavors of Newton’s method are available. Armijo rule steplength combined with deflation increases reliability of these methods considerably.

- `augnewton`: Augmented Newton [73]
- `resinv`: Residual inverse iteration [49]
- `blocknewton`: Block Newton method [44]
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- quasinewton: Quasi-Newton method [37]
- implicitdet: Implicit determinant [63]
- newtonqr: Newton QR approach [45]
- ms1p: Method of successive linear problems [56]
- sgiter: Safe-guarded iteration [77]
- rfi: Rayleigh functional iteration [58]
- broyden: Broyden's method [36]

5.2 Krylov-based methods
- nlArn Nonlinear Arnoldi method [77]
- nleigs NLEIGS [27]
- iar (and variants) infinite Arnoldi method [16, 41]

5.3 Projection methods
- nlArn Nonlinear Arnoldi method [77]
- jd Jacobi-Davidson method [10] and [18]

5.4 Contour integral methods
- beyn_contour [12]

6 BENCHMARK PROBLEMS
We have made a number of benchmark problems available via the nep_gallery command, e.g., a standardized delay eigenvalue problem can be loaded with

```julia
julia> nep=nep_gallery("dep0");
```

Several large-scale problems, such as the model of the waveguide in [16, 53] are available.

The library of Berlin-Manchester benchmark problem in the MATLAB NLEVP package [9], can be accessed in NEP-PACK in two ways. A subset of the problems from that collection have been converted to native NEP-PACK format, e.g., the "gun" problem can be loaded with the commands

```julia
julia> nep=nep_gallery("nlevp_native_gun");
```

Several implementation techniques had to be adapted to Julia in order to become efficient, e.g., the Bessel function nonlinearity in the "fiber" benchmark as described in Section A. The NLEVP problems can also be accessed by using the Julia packages which can communicate with a MATLAB process running in the background. We have provided wrappers such that the problems can be loaded with the command:

```julia
julia> using GalleryNLEVP
julia> nep=nep_gallery(NLEVP_NEP,"fiber")
```

```julia
using newton(nep.x=1e-6)
(7.13949434232901e-7 + 5.12367025712833e-18im, Complex{Float64}[-97388.3
-10508.4im, -2.75452e5-29721.8im, -5.06025e5-54601.1im, -7.79049e5-84060.9im,
-1.0837e6-1.54414e5im, -1.43106e6-1.54414e5im, -1.8322e6-1.54414e5im,
-2.28294e6-2.37702e1im, -2.62842e6-2.37702e1im, -3.07814e6-3.32137e5im,
... -3.67741e7-3.968e6im, -3.6741e7-3.96443e6im, -3.6708e7-3.96087e6im,
-3.675e7-3.95731e6im, -3.66421e7-3.95376e6im, -3.66092e7-3.9582e6im,
-3.65763e7-3.94666e6im, -3.65434e7-3.94311e6im, -3.65106e7-3.93957e6im,
```
Note that the wrapper is completely transparent such that quasinewton makes a call to the NLEVP library (available in a MATLAB process which runs in the background) every time it accesses the NEP. Due to the communication overhead, it is generally preferred to use the native methods for larger problems, due to the overhead generated by the communication between Julia and MATLAB.

7 PERFORMANCE COMPARISON

7.1 NLEIGS Julia implementation

We want to provide empirical support for the performance of our package, and the Julia language. In order to do so, we used the MATLAB NLEIGS implementation\(^1\) described in [27]. For illustration purposes we converted the MATLAB code to Julia and the NEP-PACK procedures to access data, such that it can be considered a good candidate to assess the performance of Julia vs MATLAB.

We used the same two large scale problems as in the above paper and included as benchmarks in the MATLAB implementation; the "gun" problem, and the "particle in a canyon" problem, and we ran the same six experiments. See [27] for full details. The experiments were run on a MacBook Pro, with a 2.9 GHz Intel i7-6920HQ, 2x4 cores, and 16 GB memory. We used MATLAB v8.4.0 (R2014b) and Julia v1.0.2. The results are reported in Table 1. Our Julia reimplementation is faster and consumes less memory. The general explanation is the way Julia handles data structures, which improves the possibility to carry out Just-In-Time compilation. More precisely, we observed that the inner loops (often consisting of orthogonalization) were considerably faster, also handling of sparse matrices differed considerably in performance.

Each MATLAB experiment was carried out 20 times, and the fastest run is reported. For the Julia implementation we used the Benchmark toolbox, with parameter seconds=500. We report the median CPU-time for the NEP-PACK implementation in Table 1. The memory usage is the amount of memory used at the end of the algorithm, including cached LU factors. Note that although the implementations should behave identically, the number of iterations required for convergence may vary a bit due to different start vectors and tiny rounding errors that build up over time.

|                  | MATLAB             | Julia / NEP-PACK |
|------------------|--------------------|------------------|
|                  | Iter | Conv. λ | CPU  | Memory | Iter | Conv. λ | CPU  | Memory |
| Gun P            | 100  | 17      | 6.4 s | 420 MB | 100  | 17      | 3.9 s | 59 MB  |
| Gun R1           | 100  | 21      | 6.9 s | 421 MB | 100  | 21      | 4.0 s | 59 MB  |
| Gun R2           | 95   | 21      | 20.1 s| 413 MB | 95   | 21      | 12.7 s| 51 MB  |
| Gun S            | 70   | 21      | 5.2 s | 408 MB | 71   | 21      | 3.7 s | 46 MB  |
| Particle R2      | 78   | 2       | 16.6 s| 213 MB | 74   | 2       | 7.5 s | 73 MB  |
| Particle S       | 141  | 2       | 13.0 s| 239 MB | 134  | 2       | 5.9 s | 92 MB  |

Table 1. Performance comparison of NLEIGS implementation in NEP-PACK and the original MATLAB implementation

7.2 Computation of many derivatives

In order to show the extendability of our framework, we now show an unusual NEP with 200 terms. It can be created and solved as follows.

\(^1\)NLEIGS version 0.5 available for download at http://twr.cs.kuleuven.be/research/software/nleps/nleigs.html.
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```julia
julia> using Random, BenchmarkTools
julia> Random.seed!(0)

julia> m=200;
julia> fv=Vector{Function}(undef,m);

julia> for i=1:m; fv[i]=(x-> exp(iˆ(1/6)*x)); end;

julia> fv[1]=x->one(x); fv[2]=x->x;

julia> Av=Vector{SparseMatrixCSC}(undef,m);

julia> n=50;

julia> for i=1:m; Av[i]=sprand(n,n,0.01); end;

julia> nep=SPMF_NEP(Av,fv);

julia> v0=ones(n);

julia> @btime iar(nep,maxit=100,v=v0)
7.568 s (13079550 allocations: 3.88 GiB)

Due to the fact that the problem has many exponential terms, the evaluation of the derivatives
required in the infinite Arnoldi method becomes dominant. Precomputation of derivatives are
available through the DerSPMF-type, which essentially precomputes derivatives in a given point,
but otherwise behaves as the parent NEP. The following code shows the improvement.

```julia
julia> dnep=DerSPMF(nep,0.0,100);

julia> @btime iar(dnep,maxit=100,v=v0)
3.365 s (12254494 allocations: 1.07 GiB)
```

Note that DerSPMF is extending the functionality of standard NEPs, by allowing a precomputation
to take place, but maintain all other functionality of the original NEP. The DerSPMF is again a NEP
and precomputation in several points can be achieved by successive application of the DerSPMF.

8 CONCLUSIONS
We have presented and described the current release of the package NEP-PACK. The current state of
the software is ready to be used for many use-cases, e.g., comparison of algorithms and development
of new algorithms, as we have shown in Section 7.1 that it already outperforms other publicly
available implementations of NEP-solvers. Several implementations currently do not have the
full functionality, e.g., some functions do not return eigenvectors but only eigenvalues, although
they are available in theory. Further testing of other NEP-types, applications and algorithms to
obtain improvements of efficiency for large-scale problems. The package has been tested on the
HPC-environment at KTH Royal Institute of Technology, and results will be reported in a later
version. The development of this package is done in a public GIT-HUB repository² and has a public
users manual³, in order to improve possibilities to interact with users and other developers.

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²https://github.com/nep-pack/NonlinearEigenproblems.jl
³https://nep-pack.github.io/NonlinearEigenproblems.jl
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A THE FIBER BENCHMARK

The benchmark problem in [9] called “fiber” contains a term defined as

\[ f(\lambda) = g(\sqrt{\lambda}L) \]
where
\[ g(x) = \frac{L + 0.5}{L^2} x K_1^\prime(x) K_1(x) \]

Bessel matrix functions are not available, so we use an interpolation approach to create a matrix function.
\[ g(x) = \frac{\alpha(x)}{\beta(x)} \]

where
\[
\alpha(x) = \frac{L + 0.5}{L^2} x K_1^\prime(1) K_1(1) \tag{11}
\]
\[
\beta(x) = \frac{1}{K_1(x) K_1(1)} \tag{12}
\]

The functions \(\alpha\) and \(\beta\) are selected such that we can carry out polynomial interpolation. Note that \(K_1(x)\) has a singularity at zero. We create Newton polynomials which interpolate \(\alpha\) and \(\beta\) in certain interpolation points. The interpolation is carried out in \(\text{BigFloat}\), and subsequently rounded to \(\text{Float64}\) in order to lessen the impact of round-off error with many interpolation points.

### B INTERFACE TO IAR CHEBYSHEV VARIANT

The method \(\text{iar\_chebyshev}\) requires, at each iteration, the computation of the vector \(y_0\) defined in \([41, (22)]\). We refer to that paper for all the notation we use. Our interface handles this computation for \(\text{PEP}, \text{DEP}\), with the derivation of \([41]\), and we have further derived the analogous formula for \(\text{SPMF\_NEP}\). More precisely, by using the Taylor series expansion on (2), it holds
\[
y_0 = \sum_{i=0}^{m} A_i X b_i(D_N) \hat{T}_N(0) - Y \hat{T}_N(0)
\]
where \(\hat{T}_N(\theta) := (\hat{T}_0(\theta), \hat{T}_1(\theta), \ldots, \hat{T}_N(\theta))^T\), \(D_N\) is the derivation matrix in Chebyshev basis, defined as
\[
D_N := \begin{pmatrix} 0 \\ I_{N,N+1} L_{N+1}^{-1} \end{pmatrix} \in \mathbb{R}^{(n+1) \times (n+1)}
\]
and derived from \([41, (21)]\) and \(b_i(\lambda) = (f_i(0) - f_i(\lambda))/\lambda = f_i[\lambda, 0]\). With the same technique, this formula can be extended to the computation of \(\hat{y}_0\) for the shifted and scaled problem (10) without explicitly constructing (10) but directly using (2) as follows
\[
\hat{y}_0 = -\alpha \sum_{i=0}^{m} M_i X b_i(\sigma I + \alpha D_N) \hat{T}_N(0) - Y \hat{T}_N(0),
\]
where \(b_i(\sigma + \alpha \lambda) = (f_i(\sigma) - f_i(\sigma + \alpha \lambda))/\lambda = -\alpha f_i[\sigma + \alpha \lambda, \sigma].\) The computation of the divided differences matrices \(b_i(\sigma I + \alpha D_N) = -\alpha f_i[\sigma I + \alpha D_N, \sigma I]\) can be carried out in terms of functions defining the original problem (2) by applying the following result, which is a consequence of the theory for Fréchet derivative in \([31, \text{Section 3.2}].\)

**Lemma B.1.** Given \(S, I \in \mathbb{C}^{n \times n}\) where \(I\) is the identity matrix, \(\sigma, \alpha \in \mathbb{C}\) and \(f\) is a complex analytic function, the following relation is fulfilled
\[
f \begin{pmatrix} \sigma I + \alpha S & I \\ 0 & \sigma I \end{pmatrix} = \begin{pmatrix} f(S) & f[\sigma I + \alpha S, \sigma I] \\ 0 & f(\sigma I) \end{pmatrix}.
\]