




MatrixFuns.jl: Matrix functions in Julia

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Summary

The computation of matrix functions (i.e., $f(A)$ for A a $n \times n$ matrix and $f : \mathbb{C} \rightarrow \mathbb{C}$) and their Fréchet derivatives plays a crucial role in many fields of science ([Higham, 2008](#)), and in particular in electronic structure calculations within density functional theory and response calculations. For Hermitian A , computing $f(A)$ can be done efficiently and stably by diagonalization. In the non-normal case, however, diagonalization is unstable and alternative schemes have to be used. Even in the Hermitian case, the evaluation of Fréchet derivatives requires (high-order) divided differences, which by Opitz's formula ([de Boor, 2005](#)) is equivalent to the exact computation of $f(A)$ for non-normal A .

In this work, we develop `MatrixFuns.jl` a Julia package ([Bezanson et al., 2017](#)) to provide the robust computation of matrix functions for arbitrary square matrices and higher-order Fréchet derivatives for Hermitian matrices. This package is tailored towards high accuracy with relatively small matrices and relatively complicated functions f . Our work is based on the Schur-Parlett algorithm ([Davies & Higham, 2003](#); [Higham & Al-Mohy, 2010](#)), with the following modifications:

- It supports functions that are discontinuous, or have sharp variations.
- It does not require the computation of arbitrary-order derivatives of f .
- It exploits existing special-purpose methods for computing matrix functions (e.g., for functions involving exponentials or logarithms) when they exist.

Statement of need

`MatrixFuns.jl` aims to provide high-accuracy computations for general matrix functions and arbitrary-order Fréchet derivatives (including divided differences) in Julia. Julia provides some native matrix functions, but the choice is limited to a few functions for which special-purpose algorithms exist (e.g., exponentials, logarithms, matrix powers). There are no dedicated functions in Julia for computing Fréchet derivatives and divided differences; some Julia packages offer tools for their computation (e.g., `ChainRules.jl` ([White, 2019](#)), `DFTK.jl` ([Herbst et al., 2021](#))), but are typically limited to first order.

Methods

Matrix functions

The basic principle of the Schur-Parlett algorithm is as follows. First, one performs a Schur decomposition to reduce to the case of an upper triangular matrix. Then, one uses the Parlett recursion, which for a block matrix $A = \begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix}$ expresses $B = f(A)$ as $B_{11} = f(A_{11})$, $B_{22} = f(A_{22})$ and B_{12} given by the solution of the Sylvester equation

$A_{11}B_{12} - B_{12}A_{22} = B_{11}A_{12} - A_{12}B_{22}$. In principle, this can be used to compute $f(A)$ by a recursion, but the Sylvester equation becomes ill-conditioned when A_{11} and A_{22} do not have well-separated eigenvalues. In this case, one can use Taylor series, as proposed in Davies & Higham (2003) and Higham & Al-Mohy (2010), but this has the disadvantage of requiring arbitrarily many derivatives of f , which might be impractical in some applications (e.g., when the function is not analytic, or has sharp variations).

Our algorithm attempts to find a partition of the eigenvalues of A (computed using a Schur decomposition) into blocks that are well-separated. The diagonal blocks are then computed using Taylor series, and the Parlett recursion is used to fill out the off-diagonal blocks. The partitioning aims to find small blocks (so that low-order Taylor series can be used) that are well-separated (so that the Parlett recursion is well-conditioned).

To find the partition, we start by partitioning the set of eigenvalues Λ into disjoint clusters Λ_i such that the distance between two such clusters is at least sep , where sep is a user-definable parameter. We then check if the partition is acceptable by estimating the error in all the clusters; if the estimated error is acceptable, we accept the partition; if not, we split the unacceptable clusters further by applying the partitioning algorithm recursively to each unacceptable Λ_i . We estimate the error in a cluster Λ_i of diameter d_i as $\text{err}_i = \left(\frac{d_i}{\text{scale}}\right)^{\text{max_deg}+1}$. We accept a cluster if $\text{err}_i < \varepsilon/\text{sep}$. This choice is made to balance the error originating from the Taylor expansion within a cluster err_i with the error incurred by the use of the Parlett recursion ε/sep .

Therefore, our algorithm has the following parameters:

- `scale`, the characteristic scale of variations of f , set to 1 by default.
- `max_deg`, the order of the Taylor series used, which should be set by the user according to the regularity of the function under consideration and the feasibility of computing high-order derivatives (computed automatically using `TaylorSeries.jl` (Benet & Sanders, 2019) and `Arblib.jl` (Dahne, 2025), where the latter is faster in calculating much larger orders and supports some special functions from `SpecialFunctions.jl` (Johnson, 2025)). By default, set to a large value.
- `sep`, the initial separation distance, set to $0.1 * \text{scale}$ by default following (Davies & Higham, 2003; Higham & Al-Mohy, 2010).
- ε , the target accuracy, set to machine accuracy by default.

In the case where Julia natively supports the computation of $f(A)$ (as determined by trying to compute `f(ones(1,1))` and catching any resulting error), we use them instead of Taylor series to compute diagonal blocks. In the error estimate, we consider `max_deg` = ∞ , and therefore use a partition with maximal diameter `scale`. We partition the eigenvalues rather than simply call the native $f(A)$, because f can still have sharp variations, which would cause inaccuracies in $f(A)$. For example:

```
f(x) = I/(I+exp(50*x));

A = [-0.1 10.0 0.0; 0.0 1 5.0; 0.0 0.0 -0.11];

f(A) # native call
3×3 Matrix{Float64}:
 0.993307 -9.03006 -3.33299e7
 0.0      1.92875e-22 -4.48617
 0.0      0.0      0.99593

mat_fun(f, A; scale=1/50) # Schur-Parlett
3×3 Matrix{Float64}:
 0.993307 -9.03006 -28.8619
 0.0      1.92875e-22 -4.48617
 0.0      0.0      0.99593
```

For discontinuous functions, or functions with sharp variations, our algorithm takes as input a color mapping $\text{color} : \mathbb{C} \rightarrow \mathbb{Z}, \lambda \mapsto a$, and makes sure that all the eigenvalues inside a cluster have the same color. This ensures that Taylor expansions are not used across the discontinuity boundaries.

Fréchet derivatives

For a Hermitian $A \in \mathbb{C}^{n \times n}$, denote the eigenpairs by $\{(\lambda_i, v_i)\}$. The N -th order Fréchet derivative expresses the variation of $f(A)$ with respect to a set of variations H_1, \dots, H_N , and is given by (see the documentation of `MatrixFuns.jl` for details)

$$d^N f(A) H_1 \cdots H_N = \sum_{i_0, \dots, i_N=1}^n v_{i_0} \left(\sum_{p \in \mathcal{P}_N} (H_{p(1)})_{i_0, i_1} \cdots (H_{p(N)})_{i_{N-1}, i_N} \right) f[\lambda_{i_0}, \dots, \lambda_{i_N}] v_{i_N}^*,$$

where $(H_{p(k)})_{i,j} = v_i^* H_{p(k)} v_j$ and $p \in \mathcal{P}_N$ is an arbitrary permutation of $\{1, \dots, N\}$. The higher-order divided differences $f[x_0, \dots, x_N]$ defined recursively by

$$f[x_0, \dots, x_N] = \begin{cases} (f[x_0, \dots, x_{N-1}] - f[x_1, \dots, x_N]) / (x_0 - x_N), & \text{if } x_0 \neq x_N, \\ \frac{\partial}{\partial z} f[z, x_1, \dots, x_{N-1}] \Big|_{z=x_0}, & \text{if } x_0 = x_N. \end{cases}$$

The naive evaluation of this recurrence formula is prone to numerical instabilities. Instead, we compute the divided differences using Opitz's formula

$$f \left(\begin{bmatrix} x_0 & 1 & & \\ & x_1 & \ddots & \\ & & \ddots & 1 \\ & & & x_N \end{bmatrix} \right) = \begin{bmatrix} f[x_0] & f[x_0, x_1] & \cdots & f[x_0, \dots, x_N] \\ & f[x_1] & \ddots & \vdots \\ & & \ddots & f[x_{N-1}, x_N] \\ & & & f[x_N] \end{bmatrix}.$$

Therefore, the key point in evaluating the Fréchet derivative reduces to computing matrix functions for upper triangular matrices.

Examples

We first show how to use `MatrixFuns.jl` to compute the matrix functions, divided differences, and Fréchet derivatives for smooth functions such as `exp`.

using `MatrixFuns`

```
A = [-0.1 1.0 0.0; 0.0 -0.05 1.0; 0.0 0.0 0.01];
```

```
mat_fun(exp, A) # returns exp(A)
```

```
3×3 Matrix{Float64}:
```

```
0.904837  0.92784  0.477323
0.0       0.951229 0.980346
0.0       0.0     1.01005
```

```
div_diff(exp, -0.1, -0.05, 0.01) # returns exp[-0.1,-0.05,0.01]
```

```
0.47732345844677654
```

```
H = 0.5 * (A + A'); # generates a Hermitian matrix
```

```
hs = map(i -> i * H, [1, 2]);
```

```
mat_fun_frechet(exp, H, hs) # returns d^2exp(H)hs[1]hs[2]
```

```
3×3 Matrix{Float64}:
```

```
0.519468 0.347941 0.55445
0.347941 1.10871 0.46992
0.55445 0.46992 0.610653
```

In addition to the usual smooth functions, `MatrixFuns.jl` can also support special functions and discontinuous functions. Here, we use the error function `erf` and the sign function `sign` to show how it can be used to handle functions with different smoothness.

using `MatrixFuns`, `SpecialFunctions`

```
A = [-0.1 1.0 0.0; 0.0 -0.05 1.0; 0.0 0.0 0.01];
```

```
mat_fun(erf, A) # smooth function
```

```
3×3 Matrix{Float64}:
```

```
-0.112463  1.12182  0.0524648
 0.0       -0.056372 1.12759
 0.0        0.0      0.0112834
```

```
mat_fun(x -> erf(500x), A; scale=1/500, color=x->x<0 ? 1 : 2) # singular function
```

```
3×3 Matrix{Float64}:
```

```
-1.0  0.0  303.03
 0.0 -1.0  33.3333
 0.0  0.0   1.0
```

```
mat_fun(sign, A; color=x->Int(sign(x))) # discontinuous function with smooth branches
```

```
3×3 Matrix{Float64}:
```

```
-1.0  0.0  303.03
 0.0 -1.0  33.3333
 0.0  0.0   1.0
```

Reference

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