
PSFUN

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MATRIX FUNCTIONS

This library is focused on the computation of matrix-function [1] vector products

$$\mathbf{y} = f(A)\mathbf{x}, A \in \mathbb{R}^{n \times n}, \text{nnz}(A) = O(n), f : \mathbb{R} \rightarrow \mathbb{R}, \quad (1.1)$$

for large and sparse matrices in a distributed setting. Matrix functions are ubiquitous in models for applied sciences. They are involved in the solution of ordinary, partial, and fractional differential equations, systems of coupled differential equations, hybrid differential-algebraic problems, equilibrium problems, measures of complex networks, and many others.

To perform the computation in (1.1), we consider here two main approaches, the first one makes use of a definition based on the *Cauchy integral* for a matrix function: given a closed contour Γ lying in the region of analyticity of the function $f(x)$ and containing the spectrum of A , $f(A)$ can be defined as

$$f(A) = \frac{1}{2\pi i} \int_{\Gamma} f(z)(zI - A)^{-1} dz. \quad (1.2)$$

By applying a quadrature formula on N points to (1.2), with weights $\{c_j\}_{j=1}^N$ and nodes $\{\xi_j\}_{j=1}^N$, it is possible to approximate (1.1) as

$$\mathbf{y} = f(A)\mathbf{x} \approx \sum_{j=1}^N c_j (A + \xi_j I)^{-1} \mathbf{x},$$

that is then computationally equivalent to the solution of N linear systems with the same right-hand side.

The second approach to problem (1.1) resides instead on the use of projection algorithm. Specifically, we suppose having two k -th dimensional subspaces \mathcal{V} and \mathcal{W} spanned by the column of the matrices $V, W \in \mathbb{R}^{n \times k}$. Then, problem (1.1) can be projected and approximated on the two subspaces by doing

$$\mathbf{y} = f(A)\mathbf{x} \approx W f(V^T A W) V^T \mathbf{x},$$

where now $A_k = V^T A W$ is a small matrix of size $k \times k$, to which we can apply many specific algorithms for the particular choice of $f(x)$, [1], or again a quadrature formula.

1.1 The PSFUN Library

The recent developments on softwares for sparse linear algebra have been made essential for a wide variety of scientific applications. Specifically, they have been dedicated to the construction of of massively parallel sparse solvers for a particular matrix function $f(x) = x^{-1}$, i.e., for the solution of large and sparse linear system. A computational framework that lies at the core of pretty much all multi-physics and multi-scale simulations.

With this library, we try to face the analogous challenge of computing matrix-function vector products for more general functions than the inverse.

The library described here is substantially based on the parallel BLAS feature for sparse matrices made available by the [PSBLAS library](#), and is geared towards the possibility of running on machines with thousands of high-performance cores, and is divided in three main modules,

Serial module: this module implements (or interfaces) the computation of $f(A)$, $f(A)\mathbf{x}$ for matrices of small-size that can be handled in a sequential way,

Krylov module: this module implements distributed Krylov based methods for the reduction of problem (1.1) to the solution of problems of small dimensions,

Quadrature module: this module implements the approach in (1.2) by implementing different quadrature formulas.

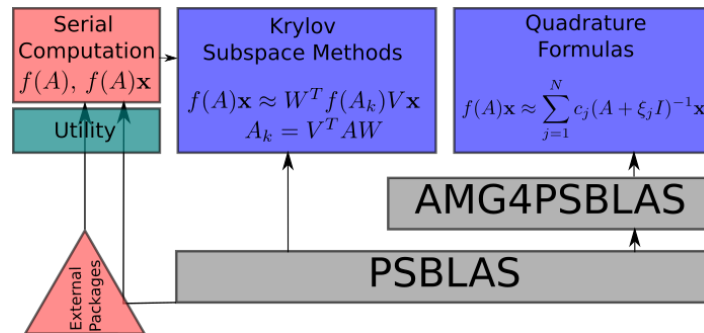


Fig. 1.1: Structure of the PSFUN library.

SERIAL MODULE

This module contains the routines needed for the computation of $f(A)x$ for A a matrix of small size. It interfaces external codes and algorithms that usually work with matrix memorized in dense storage. The intended use of the functions contained here is to use them at the lower level of a Krylov subspace method. The library directly contains the EXPOKIT code [5] for the computation of the matrix exponential, together with the scaling and squaring and Taylor algorithms [3][4] by J. Burkardt. For using the φ -functions, the code from [2] is needed. It can be [downloaded](#), compiled and linked to the main library in the install phase.

All the implemented functions and the keywords needed to load the are given in [Table 2.1](#).

Table 2.1: Implemented Methods

Function	Variant	Matrix	fname	variant	Source
$f(\alpha A)$	Diagonalization	Symmetric	"USERF"	"SYM"	
$\exp(\alpha A)$	Taylor	General	"EXP"	"TAYLOR"	[3][4]
	Scaling and Squaring	General	"EXP"	"SASQ"	[3][4]
	Generalized Padè	General	"EXP"	"GENPADE"	[5]
	Chebyshev	Hessenberg	"EXP"	"CHBHES"	[5]
	Chebyshev	General	"EXP"	"CHBGEN"	[5]
	Chebyshev	Symmetric	"EXP"	"CHBSYM"	[5]
$\varphi_k(\alpha A)$	Scaling and Squaring	Symmetric	"PHI"	"NONE"	[2]

2.1 Module

Description

This module contains the generic interfaces for the computation of the different matrix functions included in the library. The idea is that this modules computes, in a serial way, $y = f(\alpha A)x$.

Quick access

Types *unknown_type*

Routines *psfun_d_serial_apply_array()*, *psfun_d_serial_apply_sparse()*,
psfun_d_setinteger(), *psfun_d_setpointer()*, *psfun_d_setreal()*,
psfun_d_setstring()

Needed modules

- *psb_base_mod*
- *scalesquare*

Types

- **type** *psfun_d_serial_mod/unknown_type*

Type fields

- % **fname** [*character,optional/default='exp'*]
- % **padedegree** [*integer,optional/default=6*]
- % **phiorder** [*integer,optional/default=1*]
- % **scaling** [*real,optional/default=1.0_psb_dpk_*]
- % **variant** [*character,optional/default='expokit'*]

Variables

Subroutines and functions

subroutine *psfun_d_serial_mod/psfun_d_setstring* (*fun, what, val, info*)

Set function for setting options defined by a string

Parameters

- **fun** :: Function object
- **what** [*character,in*] :: String of option to set
- **val** [*character,in*] :: Value of the string
- **info** [*integer,out*] :: Output flag

Use *psb_base_mod*

subroutine *psfun_d_serial_mod/psfun_d_setreal* (*fun, what, val, info*)

Set function for setting options defined by a real

Parameters

- **fun** :: Function object
- **what** [*character,in*] :: String of option to set
- **val** [*real,in*] :: Real Value of the option
- **info** [*integer,out*] :: Output flag

Use `psb_base_mod`

subroutine `psfun_d_serial_mod/psfun_d_setinteger` (*fun, what, val, info*)
Set function for setting options defined by an integer

Parameters

- **fun** :: Function object
- **what** [*character,in*] :: String of option to set
- **val** [*integer,in*] :: Integer Value of the option
- **info** [*integer,out*] :: Output flag

Use `psb_base_mod`

subroutine `psfun_d_serial_mod/psfun_d_setpointer` (*fun, what, val, info*)
To set the function pointer inside the type

Parameters

- **fun** :: Function object
- **what** [*character,in*] :: String of option to set
- **val** :: Function to set
- **info** [*integer,out*] :: Output flag

Use `psb_base_mod`

subroutine `psfun_d_serial_mod/psfun_d_serial_apply_array` (*fun, a, y, x, info*)

This is the core of the function apply on a serial matrix to compute $y = f(\alpha * A)x$. It calls on the specific routines implementing the different functions. It is the function to modify if ones want to interface a new function that was not previously available or a new algorithm (variant) for an already existing function.

Parameters

- **fun** :: Function information
- **a** (*,*) [*real,in*] :: We need to work on a copy of a since the Lapack routine
- **y** (***) [*real,out*] :: Output vector
- **x** (***) [*real,in*] :: Input vector
- **info** [*integer,out*] :: Information on the output

Use `psb_base_mod, scalesquare`

subroutine `psfun_d_serial_mod/psfun_d_serial_apply_sparse` (*fun, a, y, x, info*)

This is the core of the function apply on a serial matrix to compute $y = f(\alpha * A)x$ when A is memorized in a sparse storage. In this case the routine converts it to a dense storage and then calls the array version of itself. That is the one implementing the different functions. It is the function to modify if ones want to interface a new function that was not previously available or a new algorithm (variant) for an already existing function.

Parameters

- **fun** :: Function information
- **a** [*psb_dspmat_type,inout*] :: Matrix
- **y** (***) [*real,out*] :: Output vector
- **x** (***) [*real,in*] :: Input vector
- **info** [*integer,out*] :: Information on the output

Use `psb_base_mod`

KRYLOV MODULE

3.1 Module

Description

The `psfun_d_krylov_mod` contains the generic call to a Krylov subspace method for the computation of $y = f(A)x$, for A large and sparse.

Quick access

Routines `psfun_d_parallel_apply()`

Needed modules

- `psb_base_mod`
- `psfun_d_serial_mod`: This module contains the generic interfaces for the computation of the different matrix functions included in the library. The idea is that this modules computes, in a serial way, $y = f(\alpha A)x \dots$

Types

- **type** `psfun_d_krylov_mod/unknown_type`

Type fields

– % **kname** [*character, optional/default='arnoldi'*]

Variables

Subroutines and functions

subroutine `psfun_d_krylov_mod/psfun_d_setstring` (*meth, what, val, info*)

Set function for setting options defined by a string

Parameters

- **meth**
- **what** [*character, in*]
- **val** [*character, in*]

- **info** [*integer,out*]

Use `psb_base_mod`

subroutine `psfun_d_krylov_mod/psfun_d_parallel_apply` (*meth, fun, a, desc_a, y, x, eps,*
info [, *itmax* [, *itrace* [, *istop* [,
iter [, *err*]]]]])

This is the generic function for applying every implemented Krylov method. The general iteration parameters (like the number of iteration, the stop criterion to be used, and the verbosity of the trace) can be passed directly to this routine. All the constitutive parameters of the actual method, and the information relative to the function are instead contained in the *meth* and *fun* objects. The Descriptor object :p `psb_desc_type desc_a` [*in*]: Descriptor for the sparse matrix

Parameters

- **meth** :: Krylov method object
- **fun** [*psfun_d_serial,inout*] :: Function object
- **a** [*psb_dspmat_type,in*] :: Distribute sparse matrix
- **y** [*psb_d_vect_type,inout*] :: Output vector
- **x** [*psb_d_vect_type,inout*] :: Input vector
- **eps** [*real,in*] :: Requested tolerance
- **info** [*integer,out*] :: Output flag
- **itmax** [*integer,in,*] :: Maximum number of iteration
- **itrace** [*integer,in,*] :: Trace for logoutput
- **istop** [*integer,in,*] :: Stop criterion
- **iter** [*integer,out,*] :: Number of iteration
- **err** [*real,out,*] :: Last estimate error

Use `psb_base_mod, psfun_d_serial_mod`

LIBRARY USAGE EXAMPLES

4.1 Serial examples

program serialtest

Test program for the serial part of the library. This test program loads a matrix from file together with some options to test the serial computation of the matrix functions. Substantially, it test the interfacing with the library doing the serial part.

Use `psb_base_mod, psfun_d_serial_mod, psb_util_mod` (`mm_mat_read()`,
`mm_array_write()`)

4.2 Parallel examples

Polynomial Krylov method examples

program arnolditest

Test for the parallel computation of matrix function by means of the `psfun_d_arnoldi` function. It applies the classical Arnoldi orthogonalization algorithm on a distributed matrix.

Use `psb_base_mod, psfun_d_serial_mod, psfun_d_krylov_mod, psb_util_mod`

- `genindex`

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