# Pnl Manual

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# 1 Introduction

## 1.1 What is Pnl

Pnl is a scientific library written in C and distributed under the Gnu Lesser General Public Licence (LGPL). This manual is divided into four parts.

• Mathematical functions: complex numbers, special functions, standard financial functions for the Black & Scholes model.

- Linear algebra: vectors, matrices (dense and sparse), hypermatrices, tridiagonal matrices, band matrices and the corresponding routines to manipulate them and solve linear systems.
- Probabilistic functions: random number generators and cumulative distribution functions.
- Deterministic toolbox : FFT, Laplace inversion, numerical integration, zero searching, multivariate polynomial regression, . . .

## 1.2 A few helpful conventions

 All header file names are prefixed by pnl\_ and are surrounded by the preprocessor conditionals

```
#ifndef _PNL_MATRIX_H
#define _PNL_MATRIX_H
...
#endif /* _PNL_MATRIX_H
```

All the header files are protected by an extern "C" declaration for possible use with a C++ compiler. The header files must be include using

```
#include "pnl/pnl_xxx.h"
```

 All function names are prefixed by pnl\_ except those implementing complex number arithmetic which are named following the C99 complex library but using a capitalised first letter C.

For example, the addition of two complex numbers is performed by the function Cadd.

- Function containing \_create in their names always return a pointer to an object created by one or several calls to dynamic allocation. Once these objects are not used, they must be freed by calling the same function but ending in \_free. A function pnl\_foo\_create\_yyy returns a PnlFoo \* object (note the "\*") and a function pnl\_foo\_bar\_create\_yyy returns a PnlFooBar \* object (note the "\*"). These objects must be freed by calling respectively pnl\_foo\_free or pnl\_foo\_bar\_free.
- Functions ending in \_clone take two arguments src and dest and modify dest to make it identical to src, ie. they have the same size and data. Note that no new object is allocated, dest must exist before calling this function.
- Functions ending in \_copy create a new object identical (ie. with the same size and content) as its argument but independent (ie. modifying one of them does not alter the other). Calling A = pnl\_xxx\_copy(B) is equivalent to first calling A = pnl\_xxx\_new() function and then pnl\_xxx\_clone(A, B).

- Every object must implement a pnl\_xxx\_new function which returns a pointer to an empty object with all its elements properly set to 0. This means that the objects returned by the pnl\_xxx\_new functions can be used as output arguments for functions ending in \_inplace for instance. They are suitable for being resized.
- Functions containing \_wrap\_ in their names always return an object, not a pointer to an object, and do not make any use of dynamic allocation. The returned object must not be freed. For instance, a function pnl\_foo\_wrap\_xxx returns an object PnlFoo and a function pnl\_foo\_bar\_wrap\_xxx returns an object PnlFooBar

```
PnlVectComplex *v1;
PnlVectComplex v2;
v1 = pnl_vect_complex_create_from_scalar (5, Complex(0., 1.));
v2 = pnl_vect_complex_wrap_subvect (v1, 1, 2);
...
pnl_vect_complex_free (&v1);
```

The vector v1 is of size 5 and contains the pure imaginary number i. The vector v2 only provides a view to v1(1:1+2), which means that modifying v2 will also modify v1 and vice-versa because v1 shares part of its data with v2. Note that only v1 must be freed and **not** v2.

- Functions ending in \_init do not create any object but only perform some internal initialisation.
- Hypermatrices, matrices and vectors are stored using a flat block of memory obtained by concatenating the matrix rows and C-style pointer-to-pointer arrays. Matrices are stored in row-major order, which means that the column index moves continuously. Note that this convention is not *Blas & Lapack* compliant since Fortran expects 2-dimensional arrays to be stored in a column-major order.
- Type names always begin with Pnl, they do not contain underscores but instead we use capital letters to separate units in type names.

  Examples: PnlMat, PnlMatComplex.
- Object and function names are intimately linked: an object PnlFoo is manipulated by functions starting in pnl\_foo, an object PnlFooBar is manipulated by functions starting in pnl\_foo\_bar. In table 1, we summarise the types and their corresponding prefixes.
- All macro names begin with PNL and are capitalised.
- Differences between **copy** and **clone** methods. The **copy** methods take a single argument and return a pointer to an object of the same type which is an independent copy of its argument. Example:

```
PnlVect *v1, *v2;
```

| Pnl types       | Pnl prefix           |
|-----------------|----------------------|
| PnlVect         | pnl_vect             |
| PnlVectComplex  | $pnl\_vect\_complex$ |
| PnlVectInt      | pnl_vect_int         |
|                 |                      |
| PnlMat          | pnl_mat              |
| PnlMatComplex   | pnl_mat_complex      |
| PnlMatInt       | pnl_mat_int          |
|                 |                      |
| PnlSpMat        | pnl_sp_mat           |
| PnlSpMatComplex | pnl_sp_mat_complex   |
| PnlSpMatInt     | pnl_sp_mat_int       |
|                 |                      |
| PnlHmat         | pnl_hmat             |
| PnlHmatComplex  | pnl_hmat_complex     |
| PnlHmatInt      | pnl_hmat_int         |
|                 |                      |
| PnlTridiagMat   | pnl_tridiag_mat      |
| PnlBandMat      | pnl_band_mat         |
| D. II.          | 1 1                  |
| PnlList         | pnl_list             |
| PnlBasis        |                      |
| r indasis       | pnl_basis            |
| PnlCgSolver     | pnl_cg_solver        |
| PnlBicgSolver   | pnl_bicg_solver      |
| PnlGmresSolver  | pnl_gmres_solver     |
| 1 memressorver  | pm_gmres_sorver      |

Figure 1: Pnl types

```
v1 = pnl_vect_create_from_scalar (5, 2.5);
v2 = pnl_vect_copy (v1);
```

v1 and v2 are two vectors of size 5 with all their elements equal to 2.5. Note that v2 must not have been created by a call to pnl\_vect\_create\_xxx because otherwise it will cause a memory leak. v1 and v2 are independent in the sense that a modification to one of them does not affect the other.

The clone methods take two arguments and fill the first one with the second one. Example:

```
PnlVect *v1, *v2;
v1 = pnl_vect_create_from_scalar (5, 2.5);
v2 = pnl_vect_new ();
pnl_vect_clone (v2, v1);
```

v1 and v2 are two vectors of size 5 with all their elements equal to 2.5. Note that v2 must have been created by a call to pnl\_vect\_new because otherwise the function pnl\_vect\_clone will crash. v1 and v2 are independent in the sense that a modification to one of them does not modify the other.

- All objects are measured using integers int and not size\_t. Hence, iterations over vectors, matrices, ...should use an index of type int.
- In fonctions ending in inplace, the output parameter must be different from any of the input parameters.

## 1.3 Using Pnl

In this section, we assume that the library is installed in the directory \$HOME/pnl-xxx. Once the library has been installed, the libraries can be found in the \$HOME/pnl-xxx/lib directory and the headers in the \$HOME/pnl-xxx/include directory.

## 1.3.1 Compiling and Linking

The header files of the library are installed in a root pnl directory and should always be included with this pnl/ prefix. So, for instance to use random number generators you should include

#include <pnl/pnl\_random.h>

Compiling and linking by hand If gcc is used, you should pass the following options

- -I\$HOME/pnl-xxx/include for compiling
- -L\$HOME/pnl-xxx/lib -lpnl for linking

This does not work straight away on all OS especially if the library is not installed in a standard directory namely /usr/ or /usr/local/ for which you need a privileged writing access. On some systems, you may need to add to the linker flags the dependencies of the library, which can become very tedious. Therefore, we provide a second automatic mechanism which takes care of the dependencies on its own.

Compiling and linking using an automatic Makefile This mechanism only works under Unix (it has been tested under various Linux distributions and Mac OS X).

First, you need to create a new directory wherever you want, put in all your code and create a Makefile as below

To define your target just add the executable name, say my-exec, to the BINS list and create an entry my\_exec\_SRC carrying the list of source files needed to create your executable. Note that if dashes '-' may appear in an executable name, the name of the associated variable holding the list of source files is obtained by replacing dashes with underscores '\_' and adding the SRC suffix.

Assume you want to create two binaries: my-exec based on mixed C and C++ code (file1.c and file2.cpp) and mybinary based on pool.cxx and pool.cxp. You can use the following Makefile.

```
## Flags passed to the linker
I.DFI.AGS=
## Flags passed to the compiler
CFLAGS=
## list of executables to create
BINS=my-exec mybinary
my_exec_SRC=file1.c file2.cpp
# optional flags for compiling and linking
my_exec_CFLAGS=
my_exec_CXXFLAGS=
my_exec_LDFLAGS=
mybinary_SRC=poo1.cxx poo2.cpp
# optional flags for compiling and linking
mybinary_CFLAGS=
mybinary_CXXFLAGS=
mybinary_LDFLAGS=
## This line must be the last one
include full_path_to_pnl_build/CMakeuser.incl
```

Let us comment a little the different variables

- CFLAGS: global flags used for creating objects based on C code
- CXXFLAGS: global flags used for creating objects based on C++ code
- LDFLAGS: gobal linker flags.
- binaryname\_CFLAGS: flags used when creating the objects based on C code and required by binaryname
- binaryname\_CXXFLAGS: flags used when creating the objects based on C++ code and required by binaryname
- binaryname\_LDFLAGS: flags used when linking objects for creating binaryname

An example of such a Makefile can be found in pnl-xxx/perso.

Warning: if a file appears in the source list of several binairies, the flags used to compile this file are determined by the ones of the first binary involving this file. In the following example main.cpp will always be compiled with the flag -03 even for generating bin2

```
BINS=bin1 bin2
```

```
bin1_SRC=main.cpp poo1.c
my_exec_CXXFLAGS=-03
```

```
bin2_SRC=main.cpp poo2.c
mybinary_CXXFLAGS=-g -00

## This line must be the last one
include full_path_to_pnl_build/CMakeuser.incl
```

## 1.3.2 Inline Functions and getters

It it is supported by your compiler, getter and setter functions are declared as inline functions. This is automatically detected when running CMake. By default, setter and getter functions check that the required access is valid, basically it boils down to checking whether the index of the access is within an acceptable range. These extra tests can become very expensive when getter and setter function are intensively called.

Thus, it is possible to alter this default behaviour by defining the macro PNL\_RANGE\_CHECK\_-OFF. This macro is automatically defined when the library is compiled in Release mode, ie. with -DCMAKE\_BUILD\_TYPE=Release passed to CMake.

## 2 Objects

## 2.1 The top-level object

The PnlObject structure is used to simulate some inheritance between the ojbects of Pnl. It must be the first element of all the objects existing in Pnl so that casting any object to a PnlObject is legal

```
typedef unsigned int PnlType;
typedef void (DestroyFunc) (void **);
typedef PnlObject* (CopyFunc) (PnlObject *);
typedef PnlObject* (NewFunc) (PnlObject *);
typedef void (CloneFunc) (PnlObject *dest, const PnlObject *src);
struct _PnlObject
{
  PnlType type; /*!< a unique integer id */
  const char *label; /*!< a string identifier (for the moment not useful) */</pre>
  PnlType parent_type; /*!< the identifier of the parent object is any,
                          otherwise parent_type=id */
  int nref; /*!< number of references on the object */
  DestroyFunc *destroy; /*!< frees an object */
              *constructor; /*! < New function */
  NewFunc
              *copy; /*!< Copy function */
  CopyFunc
              *clone; /*!< Clone function */
  CloneFunc
};
```

Here is the list of all the types actually defined We provide several macros for manipulating PnlObejcts.

| PnlType                        | Description                  |
|--------------------------------|------------------------------|
| PNL_TYPE_VECTOR                | general vectors              |
| PNL_TYPE_VECTOR_DOUBLE         | real vectors                 |
| PNL_TYPE_VECTOR_INT            | integer vectors              |
| PNL_TYPE_VECTOR_COMPLEX        | complex vectors              |
| PNL_TYPE_MATRIX                | general matrices             |
| PNL_TYPE_MATRIX_DOUBLE         | real matrices                |
| PNL_TYPE_MATRIX_INT            | integer matrices             |
| PNL_TYPE_MATRIX_COMPLEX        | complex matrices             |
| PNL_TYPE_TRIDIAG_MATRIX        | general tridiagonal matrices |
| PNL_TYPE_TRIDIAG_MATRIX_DOUBLE | real tridiagonal matrices    |
| PNL_TYPE_BAND_MATRIX           | general band matrices        |
| PNL_TYPE_BAND_MATRIX_DOUBLE    | real band matrices           |
| PNL_TYPE_SP_MATRIX             | sparse general matrices      |
| PNL_TYPE_SP_MATRIX_DOUBLE      | sparse real matrices         |
| PNL_TYPE_SP_MATRIX_INT         | sparse integer matrices      |
| PNL_TYPE_SP_MATRIX_COMPLEX     | sparse complex matrices      |
| PNL_TYPE_HMATRIX               | general hyper matrices       |
| PNL_TYPE_HMATRIX_DOUBLE        | real hyper matrices          |
| PNL_TYPE_HMATRIX_INT           | integer hyper matrices       |
| PNL_TYPE_HMATRIX_COMPLEX       | complex hyper matrices       |
| PNL_TYPE_BASIS                 | bases                        |
| PNL_TYPE_RNG                   | random number generators     |
| PNL_TYPE_LIST                  | doubly linked list           |
| PNL_TYPE_ARRAY                 | array                        |

Table 1: PnlTypes

## • PNL\_OBJECT (o)

Description Cast any object into a PnlObject

## • PNL\_VECT\_OBJECT (o)

Description Cast any object into a PnlVectObject

## • PNL\_MAT\_OBJECT (o)

Description Cast any object into a PnlMatObject

## • PNL\_SP\_MAT\_OBJECT (o)

Description Cast any object into a PnlSpMatObject

## • PNL\_HMAT\_OBJECT (o)

Description Cast any object into a PnlHmatObject

#### • PNL BAND MAT OBJECT (o)

Description Cast any object into a PnlBandMatObject

## • PNL\_TRIDIAGMAT\_OBJECT (o)

Description Cast any object into a PnlTridiagMatObject

#### • PNL\_BASIS\_OBJECT (o)

Description Cast any object into a PnlBasis

## • PNL\_RNG\_OBJECT (o)

Description Cast any object into a PnlRng

## • PNL\_LIST\_OBJECT (o)

Description Cast any object into a PnlList

#### • PNL\_LIST\_ARRAY (o)

Description Cast any object into a PnlArray

#### • PNL GET TYPENAME (o)

Description Return the name of the type of any object inheriting from PnlObject

#### • PNL GET TYPE (o)

Description Return the type of any object inheriting from PnlObject

## • PNL\_GET\_PARENT\_TYPE (o)

Description Return the parent type of any object inheriting from PnlObject

## • PnlObject \* pnl\_object\_create (PnlType t)

Description Create an empty PnlObject of type t which can any of the registered types, see Table 1.

## 2.2 List object

This section describes functions for creating an manipulating lists. Lists are internally stored as doubly linked lists.

The structures and functions related to lists are declared in pnl/pnl\_list.h.

```
typedef struct _PnlCell PnlCell;
struct _PnlCell
{
  struct _PnlCell *prev; /*!< previous cell or 0 */
  struct PnlCell *next; /*!< next cell or 0 */
  PnlObject *self;
                         /*!< stored object */
};
typedef struct _PnlList PnlList;
struct PnlList
{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlList pointer to be cast to a PnlObject
  PnlObject object;
  PnlCell *first; /*!< first element of the list */
  PnlCell *last; /*!< last element of the list */
  PnlCell *curcell; /*!< last accessed element,
                         if never accessed is NULL */
  int icurcell; /*!< index of the last accessed element,
                     if never accessed is NULLINT */
  int len; /*!< length of the list */
};
```

Important note: Lists only store addresses of objects. So when an object is inserted into a list, only its address is stored into the list. This implies that you must not free any objects inserted into a list. The deallocation is automatically handled by the function pnl\_list\_free.

- PnlList \* pnl\_list\_new ()
  Description Create an empty list
- PnlCell \* pnl\_cell\_new ()
  Description Create an cell list
- PnlList \* pnl\_list\_copy (const PnlList \*A)

  Description Create a copy of a PnlList . Each element of the list A is copied by calling the its copy member.
- void pnl\_list\_clone (PnlList \*dest, const PnlList \*src)

  Description Copy the content of src into the already existing list dest. The list dest is automatically resized. This is a hard copy, the contents of both lists are independent after cloning.
- void **pnl\_list\_free** (PnlList \*\*L)

  Description Free a list
- void **pnl\_cell\_free** (PnlCell \*\*c)

  Description Free a list

- PnlObject \* pnl\_list\_get ( PnlList \*L, int i)

  Description This function returns the content of the i-th cell of the list L. This function is optimized for linearly accessing all the elements, so it can be used inside a for loop for instance.
- void pnl\_list\_insert\_first (PnlList \*L, PnlObject \*o)

  Description Insert the object o on top of the list L. Note that o is not copied in L, so do not free o yourself, it will be done automatically when calling pnl\_list\_free
- void pnl\_list\_insert\_last (PnlList \*L, PnlObject \*o)
   Description Insert the object o at the bottom of the list L. Note that o is not copied in L, so do not free o yourself, it will be done automatically when calling pnl\_list\_free
- void pnl\_list\_remove\_last (PnlList \*L)

  Description Remove the last element of the list L and frees it.
- void pnl\_list\_remove\_first (PnlList \*L)

  Description Remove the first element of the list L and frees it.
- void **pnl\_list\_remove\_i** (**PnlList** \*L, int i)

  Description Remove the i-th element of the list L and frees it.
- void pnl\_list\_concat (PnlList \*L1, PnlList \*L2)
   Description Concatenate the two lists L1 and L2. The resulting list is store in L1 on exit.
   Do not free L2 since concatenation does not actually copy objects but only manipulates addresses.
- void pnl\_list\_resize (PnlList \*L, int n)

  Description Change the length of L to become n. If the length of L id increased, the extra elements are set to NULL.
- void **pnl\_list\_print** (const **PnlList** \*L)

  Description Only prints the types of each element. When the **PnlObject** object has a print member, we will use it.

## 2.3 Array object

This section describes functions for creating and manipulating arrays of PnlObjects. The structures and functions related to arrays are declared in pnl/pnl\_array.h.

```
typedef struct _PnlArray PnlArray;
struct _PnlArray
{
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlArray pointer to be cast to a PnlObject
    */
PnlObject object;
int size;
PnlObject **array;
```

```
int mem_size;
};
```

**Important note**: Arrays only store addresses of objects. So when an object is inserted into an array, only its address is stored into the array. This implies that you **must not** free any objects inserted into a array. The deallocation is automatically handled by the function pnl\_array\_free.

- PnlArray \* pnl\_array\_new ()
  Description Create an empty array
- PnlArray \* pnl\_array\_create (int n)
  Description Create an array of length n.
- PnlArray \* pnl\_array\_copy (const PnlArray \*A)

  Description Create a copy of a PnlArray . Each element of the array A is copied by calling the A[i].object.copy.
- void pnl\_array\_clone (PnlArray \*dest, const PnlArray \*src)

  Description Copy the content of src into the already existing array dest. The array dest is automatically resized. This is a hard copy, the contents of both arrays are independent after cloning.
- void **pnl\_array\_free** (**PnlArray** \*\*)

  Description Free an array and all the objects hold by the array.
- int pnl\_array\_resize (PnlArray \*T, int size)

  Description Resize T to be size long. As much as possible of the original data is kept.
- PnlObject \* pnl\_array\_get ( PnlArray \*T, int i)

  Description This function returns the content of the i-th cell of the array T. No copy is made.
- PnlObject \* pnl\_array\_set ( PnlArray \*T, int i, PnlObject \*O)

  Description T[i] = 0. No copy is made, so the object 0 must not be freed manually.
- void pnl\_array\_print (PnlArray \*)

  Description Not yet implemented because it would require that the structure PnlObject has a field copy.

## 3 Mathematical framework

## 3.1 General tools

The macros and functions of this paragraph are defined in pnl/pnl\_mathtools.h.

#### 3.1.1 Constants

A few mathematical constants are provided by the library. Most of them are actually already defined in math.h, values.h or limits.h and a few others have been added.

| meday denned in mach:n;             | varace: if of remittee: if and a  |
|-------------------------------------|---|
| $\mathbf{M}_{\mathbf{L}}\mathbf{E}$ | $e^1$   |
| $M\_LOG2E$                          | $\log_2 e$  |
| $M\_LOG10E$                         | $\log_{10} e$   |
| $M\_LN2$                            | $\log_e 2$  |
| $M_LN10$                            | $\log_e 10$   |
| $M_PI$                              | $\pi$   |
| $M_2PI$                             | $2\pi$  |
| $M_PI_2$                            | $\pi/2$   |
| $M_PI_4$                            | $\pi/4$   |
| $M_1_PI$                            | $1/\pi$   |
| $M_2$ PI                            | $2/\pi$   |
| $M_2_{SQRTPI}$                      | $2/\sqrt{\pi}$  |
| $M_SQRT2PI$                         | $sqrt2\pi$  |
| $M_SQRT2$                           | $\sqrt{2}$  |
| $M\_EULER$                          | $\gamma = \lim_{n \to \infty} \left( \sum_{k=1}^{n} \frac{1}{k} - \ln(n) \right)$ |
| $M_SQRT1_2$                         | $1/\sqrt{2}$  |
| $M_1_SQRT2PI$                       | $1/\sqrt{2\pi}$   |
| $M_SQRT2_PI$                        | $\sqrt{2/\pi}$  |
| INT_MAX                             | 2147483647  |
| MAX_INT                             | INT_MAX   |
| $DBL\_MAX$                          | 1.79769313486231470e + 308  |
| DOUBLE_MAX                          | $DBL\_MAX$  |
| DBL_EPSILON                         | 2.2204460492503131e - 16  |
| PNL_NEGINF                          | $-\infty$   |
| PNL_POSINF                          | $+\infty$   |
| PNL_INF                             | $+\infty$   |
| NAN                                 | Not a Number  |
|                                     |   |

## 3.1.2 A few macros

- PNL\_IS\_ODD (int n)
  Description Return 1 if n is odd and 0 otherwise.
- PNL\_IS\_EVEN (int n)
  Description Return 1 if n is even and 0 otherwise.
- PNL\_ALTERNATE (int n)
  Description Return (-1)<sup>n</sup>.
- MIN (x,y)Description Return the minimum of x and y.
- $\mathbf{MAX}$  (x,y) Description Return the maximum of x and y.

• **ABS** (x)

Description Return the absolute value of x.

• PNL\_SIGN (x)

Description Return the sign of x (-1 if x < 0, 0 otherwise).

• **SQR** (x)

Description Return  $x^2$ .

• **CUB** (x)

Description Return  $x^3$ .

#### 3.1.3 Functions

- double pnl\_nan ()
  Description Return NaN
- double pnl\_posinf()

  Description Return + infinity
- double **pnl\_neginf** ()

  Description Return infinity
- int pnl\_isnan (double x)

  Description Return +1 if x=NaN
- int pnl\_isinf (double x)

  Description Return +1 if x=+Inf, -1 if x=-Inf and 0 otherwise.
- int pnl\_isfinite (double x)

  Description Return 1 if x!=+-Inf
- int pnl\_itrunc (double s)

Description This function is similar to the trunc function (provided by the C library) but the result is typed as an integer instead of a double. Digits may be lost if s exceeds MAX\_INT.

- long int  $\mathbf{pnl\_ltrunc}$  (double s)
  - Description This function is similar to the trunc function (provided by the C library) but the result is typed as a long integer instead of a double.
- double **pnl\_trunc** (double s)

Description Return the nearest integer not greater than the absolute value of s. This function is part of C99 as trunc.

- double pnl\_round (double s)
  - Description Return the integral value nearest to x rounding half-way cases away from zero, regardless of the current rounding direction. This function is part of C99 as round.
- int pnl iround (double s)

Description This function is similar to the round function (provided by the C library) but the result is typed as an integer instead of a double. Digits may be lost if s exceeds MAX\_INT.

- long int **pnl\_lround** (double s)

  Description This function is similar to the **round** function (provided by the C library)
  but the result is typed as a long integer instead of a double.
- double **pnl\_fact** (double x)

  Description See pnl sf fact
- double **pnl\_lgamma** (double x)

  Description See pnl\_sf\_log\_gamma
- double **pnl\_tgamma** (double x) Description See pnl\_sf\_gamma
- double pnl\_acosh (double x)
   Description Compute acosh(x).
- double **pnl\_asinh** (double x)

  Description Compute **asinh**(x).
- double **pnl\_atanh** (double x)

  Description Compute **atanh**(x).
- double pnl\_log1p (double x)
   Description Compute log(1+x) accurately for small values of x
- double pnl\_expm1 (double x)
   Description Compute exp(x)-1 accurately for small values of x
- double pnl\_cosm1 (double x)
   Description Compute cos(x)-1 accurately for small values of x
- double pnl\_pow\_i (double x, int n)
   Description Compute x^n for an integer n.

#### 3.2 Complex numbers

## 3.2.1 Overview

The complex type and related functions are defined in the header pnl/pnl\_complex.h.

The first native implementation of complex numbers in the C language appeared in C99, which is unfortunately not available on all platforms. For this reason, we provide here an implementation of complex numbers.

```
typedef struct {
   double r; /*!< real part */
   double i; /*!< imaginary part */
} dcomplex;</pre>
```

#### 3.2.2 Constants

CZERO 0 as a complex number
CONE 1 as a complex number
CI I the unit complex number

#### 3.2.3 Functions

- double, double CMPLX (dcomplex z)

  Description z.r, z.i
- dcomplex Complex (double x, double y)
   Description x + i y
- dcomplex\_polar (double r, double theta)

  Description r exp(i theta)
- double Creal (dcomplex z) Description R(z)
- double Cimag (dcomplex z) Description Im(z)
- dcomplex Cadd (dcomplex z, dcomplex b)
   Description z+b
- dcomplex CRadd (dcomplex z, double b)
   Description z+b
- dcomplex RCadd (double b, dcomplex z)
   Description b+z
- dcomplex Csub (dcomplex z, dcomplex b)

  Description z-b
- dcomplex **CRsub** (dcomplex z, double b)

  Description z-b
- dcomplex RCsub (double b, dcomplex z)
   Description b-z
- dcomplex Cminus (dcomplex z)
   Description -z
- dcomplex Cmul (dcomplex z, dcomplex b)

  Description z\*b
- dcomplex RCmul (double x, dcomplex z)
   Description x\*z
- dcomplex CRmul (dcomplex z, double x)
   Description z \* x

- dcomplex CRdiv (dcomplex z, double x)
   Description z/x
- dcomplex RCdiv (double x, dcomplex z)
   Description x/z
- dcomplex Conj (dcomplex z) Description  $\overline{z}$
- dcomplex Cinv (dcomplex z)
  Description 1/z
- dcomplex Cdiv (dcomplex z, dcomplex w)

  Description z/w
- double Csqr\_norm (dcomplex z) Description  $Re(z)^2 + im(z)^2$
- double Cabs (dcomplex z)

  Description |z|
- dcomplex Csqrt (dcomplex z)

  Description sqrt(z), square root (with positive real part)
- dcomplex Clog (dcomplex z)

  Description log(z)
- dcomplex Cexp (dcomplex z)

  Description exp(z)
- dcomplex Clexp (double t)

  Description exp( it )
- dcomplex Cpow (dcomplex z, dcomplex w) Description  $z^w$ , power function
- dcomplex Cpow\_real (dcomplex z, double x) Description  $z^x$ , power function
- dcomplex Ccos (dcomplex z)

  Description cos(g)
- dcomplex Csin (dcomplex z)

  Description sin(g)
- dcomplex Ctan (dcomplex z)

  Description tan(z)
- dcomplex Ccotan (dcomplex z)

  Description cotan(z)
- dcomplex Ccosh (dcomplex z)

  Description cosh(g)

- dcomplex Csinh (dcomplex z)
  Description sinh(g)
- dcomplex Ctanh (dcomplex z) Description  $tanh(z) = \frac{1 - e^{-2z}}{1 + e^{-2z}}$
- dcomplex Ccotanh (dcomplex z) Description cotanh(z) =  $\frac{1+e^{-2z}}{1-e^{-2z}}$
- double Carg (dcomplex z)
   Description arg(z)
- dcomplex Ctgamma (dcomplex z)

  Description Gamma(z), the Gamma function
- dcomplex Clgamma (dcomplex z)

  Description log(Gamma (z)), the logarithm of the Gamma function
- void **Cprintf** (dcomplex z)

  Description Print a complex number on the standard output

Most algebraic operations on complex numbers are implemented using the following naming for the functions

- All these function names begin in C\_op\_,
- The small letters a, b denote two complex numbers whereas d is a real number,
- The letter i denotes the multiplication by the pure imagniary number i,
- The letter c indicates that the next coming number is conjugated.
- The letters p, m denote the two standard operations plus and minus respectively.

For example C\_op\_idamcb is  $id(a - \overline{b})$ . So functions are :

- dcomplex C\_op\_apib (dcomplex a, dcomplex b) Description a + ib.
- dcomplex C\_op\_apcb (dcomplex a, dcomplex b) Description  $a + \bar{b}$ .
- dcomplex C\_op\_amcb (dcomplex a, dcomplex b) Description  $a - \overline{b}$ .
- dcomplex C\_op\_amib (dcomplex a, dcomplex b)
   Description a i b
- dcomplex  $C_{op\_dapb}$  (double d, dcomplex a, dcomplex b) Description d(a + b).
- dcomplex C\_op\_damb (double d, dcomplex a, dcomplex b) Description d(a-b).

- dcomplex C\_op\_dapib (double d, dcomplex a, dcomplex b) Description d(a + ib).
- dcomplex C\_op\_damib (double d, dcomplex a, dcomplex b) Description d(a ib).
- dcomplex **C\_op\_dapcb** (double d, dcomplex a, dcomplex b) Description  $d(a + \overline{b})$ .
- dcomplex C\_op\_damcb (double d, dcomplex a, dcomplex b) Description  $d\left(a-\overline{b}\right)$ .
- dcomplex  $C_{op_idapb}$  (double d, dcomplex a, dcomplex b) Description id(a + b).
- dcomplex C\_op\_idamb (double d, dcomplex a, dcomplex b) Description id(a b).
- dcomplex **C\_op\_idapcb** (double d, dcomplex a, dcomplex b) Description  $id(a + \overline{b})$ .
- dcomplex **C\_op\_idamcb** (double d, dcomplex a, dcomplex b) Description  $id(a \overline{b})$ .

# 4 Linear Algebra

#### 4.1 Vectors

#### 4.1.1 Overview

The structures and functions related to vectors are declared in pnl/pnl\_vector.h. Vectors are declared for several basic types: double, int, and dcomplex. In the following declarations, BASE must be replaced by one the previous types and the corresponding vector structures are respectively named PnlVect, PnlVectInt, PnlVectComplex

```
typedef struct _PnlVect {
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlVect pointer to be cast to a PnlObject
    */
PnlObject object;
int size; /*!< size of the vector */
int mem_size; /*!< size of the memory block allocated for array */
double *array; /*!< pointer to store the data */
int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlVect;

typedef struct _PnlVectInt {
    /**</pre>
```

```
* Must be the first element in order for the object mechanism to work
  * properly. This allows any PnlVectInt pointer to be cast to a PnlObject
  */
 PnlObject object;
 int size; /*!< size of the vector */
 int mem_size; /*!< size of the memory block allocated for array */
 int *array; /*!< pointer to store the data */
 int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlVectInt;
typedef struct _PnlVectComplex {
  * Must be the first element in order for the object mechanism to work
  * properly. This allows any PnlVectComplex pointer to be cast
  * to a PnlObject
  */
 PnlObject object;
 int size; /*!< size of the vector */
 int mem_size; /*!< size of the memory block allocated for array */
 dcomplex *array; /*!< pointer to store the data */</pre>
  int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlVectComplex;
```

size is the size of the vector, array is a pointer containing the data and owner is an integer to know if the vector owns its array pointer (owner=1) or shares it with another structure (owner=0). mem\_size is the number of elements the vector can hold at most.

## 4.1.2 Functions

**General functions** These functions exist for all types of vector no matter what the basic type is. The following conventions are used to name functions operating on vectors. Here is the table of prefixes used for the different basic types.

| type     | prefix           | BASE     |
|----------|------------------|----------|
| double   | pnl_vect         | double   |
| int      | pnl_vect_int     | int      |
| dcomplex | pnl_vect_complex | dcomplex |

In this paragraph, we present the functions operating on PnlVect which exist for all types. To deduce the prototypes of these functions for other basic types, one must replace pnl\_vect and double according the above table.

Constructors and destructors There are no special functions to access the size of a vector, instead the field size should be accessed directly.

• PnlVect \* pnl\_vect\_new ()
Description Create a new PnlVect of size 0.

- PnlVect \* pnl\_vect\_create (int size)
  Description Create a new PnlVect pointer.
- PnlVect \* pnl\_vect\_create\_from\_zero (int size)

  Description Create a new PnlVect pointer and sets it to zero.
- PnlVect \* pnl\_vect\_create\_from\_scalar (int size, double x)

  Description Create a new PnlVect pointer and sets all elements t x.
- PnlVect \* pnl\_vect\_create\_from\_ptr (int size, const double \*x)

  Description Create a new PnlVect pointer and copies x to array.
- PnlVect \* pnl\_vect\_create\_from\_mat ( const PnlMat \*M)
   Description Create a new PnlVect pointer of size M->mn and copy the content of M row wise.
- PnlVect \* pnl\_vect\_create\_from\_list (int size, ...)

  Description Create a new PnlVect pointer of length size filled with the extra arguments passed to the function. The number of extra arguments passed must be equal to size and they must be of the type BASE. Example: To create a vector {1., 2.}, you should enter pnl\_vect\_create\_from\_list(2, 1.0, 2.0) and NOT pnl\_vect\_create\_from\_list(2, 1.0, 2) or pnl\_vect\_create\_from\_list(2, 1, 2.0). Be aware that this cannot be checked inside the function.
- PnlVect \* pnl\_vect\_create\_from\_file (const char \*file)

  Description Read a vector from a file and creates the corresponding PnlVect . The data might be stored as a single blank separated line or as a one column file with one element per line.
- PnlVect \* pnl\_vect\_copy (const PnlVect \*v)

  Description This is a copying constructor. It creates a copy of a PnlVect .
- void pnl\_vect\_clone (PnlVect \*clone, const PnlVect \*v)

  Description Clone a PnlVect . clone must be an already existing PnlVect . It is resized to match the size of v and the data are copied. Future modifications to v will not affect clone.
- PnlVect \* pnl\_vect\_create\_subvect\_with\_ind (const PnlVect \*V, const PnlVectInt \*ind)

  Description Create a new vector containing V(ind(:)).
- void pnl\_vect\_extract\_subvect\_with\_ind (PnlVect \*V\_sub, const PnlVect \*V, const PnlVectInt \*ind)
   Description On exit, V\_sub = V(ind(:)).
- PnlVect \* pnl\_vect\_create\_subvect (const PnlVect \*V, int i, int len)

  Description Create a new vector containing V(i:i+len-1). The elements are copied.
- void pnl\_vect\_extract\_subvect (PnlVect \*V\_sub, const PnlVect \*V, int i, int len)

  Description On exit, V\_sub = V(i:i+len-1). The elements are copied.

- void **pnl\_vect\_free** (PnlVect \*\*v)

  Description Free a PnlVect pointer and set the data pointer to NULL
- PnlVect pnl\_vect\_wrap\_array (const double \*x, int size)

  Description Create a PnlVect containing the data x. No copy is made. It is just a container.
- PnlVect pnl\_vect\_wrap\_subvect (const PnlVect \*x, int i, int s)

  Description Create a PnlVect containing x(i:i+s-1). No copy is made. It is just a container. The returned PnlVect has size=s and owner=0.
- PnlVect pnl\_vect\_wrap\_subvect\_with\_last (const PnlVect \*x, int i, int j)

  Description Create a PnlVect containing x(i:j). No copy is made. It is just a container.
- PnlVect pnl\_vect\_wrap\_mat (const PnlMat \*M)

  Description Return a PnlVect (not a pointer) whose array is the row wise array of M.

  The new vector shares its data with the matrix M, which means that any modification to one of them will affect the other.

#### Resizing vectors

- int pnl\_vect\_resize (PnlVect \*v, int size)

  Description Resize a PnlVect . It copies as much of the old data to fit in the resized object.
- int pnl\_vect\_resize\_from\_ptr (PnlVect \*v, int size, double \*t)

  Description Resize a PnlVect and uses t to fill the vector. t must be of size size.

**Accessing elements** If it is supported by the compiler, the following functions are declared inline. To speed up these functions, you can define the macro PNL\_RANGE\_CHECK\_OFF, see Section 1.3.2 for an explanation.

Accessing elements of a vector is faster using the following macros

- **GET** (PnlVect \*v, int i)

  Description Return v[i] for reading, eg. x=GET(v,i)
- GET\_INT (PnlVectInt \*v, int i)

  Description Same as GET but for an integer vector.
- GET\_COMPLEX (PnlVectComplex \*v, int i)

  Description Same as GET but for a complex vector.
- LET (PnlVect \*v, int i)

  Description Return v[i] as a lvalue for writing, eg. LET(v,i)=x
- LET\_INT (PnlVectInt \*v, int i)

  Description Same as LET but for an integer vector.
- LET\_COMPLEX (PnlVectComplex \*v, int i)

  Description Same as LET but for a complex vector.

- void **pnl\_vect\_set** (PnlVect \*v, int i, double x)
  Description Set v[i]=x
- double **pnl\_vect\_get** (const **PnlVect** \*v, int i) Description Return the value of v[i].
- void **pnl\_vect\_lget** (**PnlVect** \*v, int i) Description Return the address of v[i].
- void **pnl\_vect\_set\_all** (**PnlVect** \*v, double x) Description Set all elements to x.
- void pnl\_vect\_set\_zero (PnlVect \*v)

  Description Set all elements to zero.

#### Printing vector

- void **pnl\_vect\_print** (const **PnlVect** \*V)

  Description Print a **PnlVect** as a column vector
- void **pnl\_vect\_fprint** (FILE \*fic, const **PnlVect** \*V)

  Description Print a **PnlVect** in file **fic** as a column vector.
- void pnl\_vect\_print\_asrow (const PnlVect \*V)

  Description Print a PnlVect as a row vector
- void **pnl\_vect\_fprint\_asrow** (FILE \*fic, const **PnlVect** \*V)

  Description Print a **PnlVect** in file fic as a row vector.
- void pnl\_vect\_print\_nsp (const PnlVect \*V)

  Description Print a vector to the standard output in a format compatible with Nsp.
- void **pnl\_vect\_fprint\_nsp** (FILE \*fic, const **PnlVect** \*V)

  Description Print a vector to a file in a format compatible with Nsp.

#### Applying external operation to vectors

- void **pnl\_vect\_minus** (PnlVect \*lhs)

  Description In-place unary minus
- void pnl\_vect\_plus\_scalar (PnlVect \*lhs, double x)
  Description In-place vector scalar addition
- void **pnl\_vect\_minus\_scalar** (PnlVect \*lhs, double x)
  Description In-place vector scalar substraction
- void **pnl\_vect\_mult\_scalar** (**PnlVect** \*lhs, double x)

  Description In-place vector scalar multiplication
- void **pnl\_vect\_div\_scalar** (**PnlVect** \*lhs, double x)

  Description In-place vector scalar division

#### Element wise operations

- void pnl\_vect\_plus\_vect (PnlVect \*lhs, const PnlVect \*rhs)

  Description In-place vector vector addition
- void pnl\_vect\_minus\_vect (PnlVect \*lhs, const PnlVect \*rhs)

  Description In-place vector vector substraction
- void pnl\_vect\_inv\_term (PnlVect \*lhs)

  Description In-place term by term vector inversion
- void pnl\_vect\_div\_vect\_term (PnlVect \*lhs, const PnlVect \*rhs)

  Description In-place term by term vector division
- void pnl\_vect\_mult\_vect\_term (PnlVect \*lhs, const PnlVect \*rhs)

  Description In-place vector vector term by term multiplication
- void pnl\_vect\_map (PnlVect \*lhs, const PnlVect \*rhs, double(\*f)(double))

  Description lhs = f(rhs)
- void pnl\_vect\_map\_inplace (PnlVect \*lhs, double(\*f)(double))

  Description lhs = f(lhs)
- void pnl\_vect\_map\_vect (PnlVect \*lhs, const PnlVect \*rhs1, const PnlVect \*rhs2, double(\*f)(double, double))
   Description 1hs = f(rhs1, rhs2)
- void pnl\_vect\_map\_vect\_inplace (PnlVect \*lhs, PnlVect \*rhs, double(\*f)(double,double))

  Description lhs = f(lhs,rhs)
- void pnl\_vect\_axpby (double a, const PnlVect \*x, double b, PnlVect \*y)
  Description Compute y : = a x + b y. When b==0, the content of y is not used on input and instead y is resized to match x.
- double pnl\_vect\_sum (const PnlVect \*lhs)

  Description Return the sum of all the elements of a vector
- void pnl\_vect\_cumsum (PnlVect \*lhs)

  Description Compute the cumulative sum of all the elements of a vector. The original vector is modified
- double pnl\_vect\_prod (const PnlVect \*V)
   Description Return the product of all the elements of a vector
- void pnl\_vect\_cumprod (PnlVect \*lhs)

  Description Compute the cumulative product of all the elements of a vector. The original vector is modified

#### Scalar products and norms

- double pnl\_vect\_norm\_two (const PnlVect \*V)
   Description Return the two norm of a vector
- double pnl\_vect\_norm\_one (const PnlVect \*V)

  Description Return the one norm of a vector
- double pnl\_vect\_norm\_infty (const PnlVect \*V)

  Description Return the infinity norm of a vector
- double pnl\_vect\_scalar\_prod (const PnlVect \*rhs1, const PnlVect \*rhs2)

  Description Compute the scalar product between 2 vectors
- int pnl\_vect\_cross (PnlVect \*lhs, const PnlVect \*x, const PnlVect \*y)

  Description Compute the cross product of x and y and store the result in lhs. The vectors x and y must be of size 3 and FAIL is returned otherwise.
- double **pnl\_vect\_dist** (const **PnlVect** \*x, const **PnlVect** \*y) Description Compute the distance between x and y, ie  $\sqrt{\sum_i |x_i y_i|^2}$ .

#### Test functions

- int pnl\_vect\_eq (const PnlVect \*V1, const PnlVect \*V2)

  Description Test if two vectors are equal. Returns TRUE or FALSE.
- int pnl\_vect\_eq\_all (const PnlVect \*v, double x)

  Description Test if all the components of v are equal to x. Returns TRUE or FALSE.

**Ordering functions** The following functions are not defined for PnlVectComplex because there is no total ordering on Complex numbers

- double pnl\_vect\_max (const PnlVect \*V)

  Description Return the maximum of a a vector
- double pnl\_vect\_min (const PnlVect \*V)
   Description Return the minimum of a vector
- void **pnl\_vect\_minmax** (double \*m, double \*M, const **PnlVect** \*)

  Description Compute the minimum and maximum of a vector which are returned in m and M respectively.
- void pnl\_vect\_min\_index (double \*m, int \*im, const PnlVect \*)
   Description Compute the minimum of a vector and its index stored in sets m and im respectively.
- void pnl\_vect\_max\_index (double \*M, int \*iM, const PnlVect \*)
   Description Compute the maximum of a vector and its index stored in sets m and im respectively.

• void **pnl\_vect\_minmax\_index** (double \*m, double \*M, int \*im, int \*iM, const **PnlVect** \*)

Description Compute the minimum and maximum of a vector and the corresponding

indices stored respectively in m, M, im and iM.

- void pnl\_vect\_qsort (PnlVect \*, char order)

  Description Sort a vector using a quick sort algorithm according to order ('i' for increasing or 'd' for decreasing).
- void pnl\_vect\_qsort\_index (PnlVect \*, PnlVectInt \*index, char order)

  Description Sort a vector using a quick sort algorithm according to order ('i' for increasing or 'd' for decreasing). On output, index contains the permutation used to sort the vector.
- int pnl\_vect\_find (PnlVectInt \*ind, char \*type, int(\*f)(double \*t), ...)

  Description f is a function taking a C array as argument and returning an integer. type is a string composed by the letters 'r' and 'v' and is used to describe the types of the arguments appearing after f. This function aims at simulating Scilab's find function. Here are a few examples (capital letters are used for vectors and small letters for real values)

```
- ind = find ( a < X )
        int isless ( double *t ) { return t[0] < t[1]; }
        pnl_vect_find ( ind, "rv", isless, a, X );

- ind = find (X <= Y)
        int isless ( double *t ) { return t[0] <= t[1]; }
        pnl_vect_find ( ind, "vv", isless, X, Y );

- ind = find ((a < X) && (X <= Y))
        int cmp ( double *t )
        {
            return (t[0] <= t[1]) && (t[1] <= t[2]);
        }
        pnl_vect_find ( ind, "rvv", cmp, a, X, Y );</pre>
```

ind contains on exit the indices i for which the function f returned 1. This function returns OK or FAIL when something went wrong (size mismatch between matrices, invalid string type).

#### Misc

• void pnl\_vect\_swap\_elements (PnlVect \*v, int i, int j)
Description Exchange v[i] and v[j].

• void pnl\_vect\_reverse (PnlVect \*v)

Description Perform a mirror operation on v. On output v[i] = v[n-1-i] for i=0,...,n-1 where n is the length of the vector.

#### Complex vector functions

- void **pnl\_vect\_complex\_mult\_double** (**PnlVectComplex** \*lhs, double x) Description In-place multiplication by a double.
- PnlVectComplex\* pnl\_vect\_complex\_create\_from\_array (int size, const double \*re, const double \*im)

  Description Create a PnlVectComplex given the arrays of the real parts re and imaginary parts im.
- void pnl\_vect\_complex\_split\_in\_array (const PnlVectComplex \*v, double \*re, double \*im)
   Description Split a complex vector into two C arrays: the real parts of the elements of v are stored into re and the imaginary parts into im.
- void pnl\_vect\_complex\_split\_in\_vect (const PnlVectComplex \*v, PnlVect \*re, PnlVect \*im)

  Description Split a complex vector into two PnlVect 's: the real parts of the elements of v are stored into re and the imaginary parts into im.

There exist functions to directly access the real or imaginary parts of an element of a complex vector. These functions also have inlined versions that are used if the variable HAVE\_INLINE was declared at compilation time.

- double **pnl\_vect\_complex\_get\_real** (const **PnlVectComplex** \*v, int i) Description Return the real part of v[i].
- double pnl\_vect\_complex\_get\_imag (const PnlVectComplex \*v, int i)

  Description Return the imaginary part of v[i].
- double\* pnl\_vect\_complex\_lget\_real (const PnlVectComplex \*v, int i)

  Description Return the real part of v[i] as a lvalue.
- double\* pnl\_vect\_complex\_lget\_imag (const PnlVectComplex \*v, int i)

  Description Return the imaginary part of v[i] as a lvalue.
- void pnl\_vect\_complex\_set\_real (const PnlVectComplex \*v, int i, double re)

  Description Set the real part of v[i] to re.
- void pnl\_vect\_complex\_set\_imag (const PnlVectComplex \*v, int i, double im)

  Description Set the imaginary part of v[i] to im.

Equivalently to these functions, there exist macros. When the compiler is able to handle inline code, there is no gain in using macros instead of inlined functions at least in principle.

• GET\_REAL (v, i)

Description Return the real part of v[i].

- GET\_IMAG (v, i)

  Description Return the imaginary part of v[i].
- LET\_REAL (v, i)

  Description Return the real part of v[i] as a lvalue.
- LET\_IMAG (v, i)

  Description Return the imaginary part of v[i] as a lvalue.

## 4.2 Compact Vectors

#### 4.2.1 Short description

```
typedef struct PnlVectCompact {
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlVectCompact pointer to be cast to a PnlObject
    */
PnlObject object;
int size; /* size of the vector */
double val; /* single value */
double *array; /* Pointer to double values */
char convert; /* 'a', 'd' : array, double */
} PnlVectCompact;
```

#### 4.2.2 Functions

- PnlVectCompact \* pnl\_vect\_compact\_new ()
  Description Create a PnlVectCompact of size 0.
- PnlVectCompact \* pnl\_vect\_compact\_create (int n, double x)
  Description Create a PnlVectCompact filled in with x
- PnlVectCompact \* pnl\_vect\_compact\_create\_from\_ptr (int n, double \*x)

  Description Create a PnlVectCompact filled in with the content of x. Note that x must have at least n elements.
- int pnl\_vect\_compact\_resize (PnlVectCompact \*v, int size, double x) Description Resize a PnlVectCompact .
- PnlVectCompact \* pnl\_vect\_compact\_copy (const PnlVectCompact \*v)
  Description Copy a PnlVectCompact
- void pnl\_vect\_compact\_free (PnlVectCompact \*\*v)
  Description Free a PnlVectCompact
- PnlVect \* pnl\_vect\_compact\_to\_pnl\_vect (const PnlVectCompact \*C)

  Description Convert a PnlVectCompact pointer to a PnlVect pointer.
- double **pnl\_vect\_compact\_get** (const **PnlVectCompact** \*C, int i) Description Access function

- void **pnl\_vect\_compact\_set\_all** (**PnlVectCompact** \*C, double x)

  Description Set all elements of C to x. C is converted to a compact storage.
- void pnl\_vect\_compact\_set\_ptr (PnlVectCompact \*C, double \*ptr)

  Description Copy the array ptr into C. We assume that the sizes match. C is converted to a non compact storage.

#### 4.3 Matrices

#### 4.3.1 Overview

The structures and functions related to matrices are declared in pnl/pnl matrix.h.

```
typedef struct _PnlMat{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlMat pointer to be cast to a PnlObject
  PnlObject object;
  int m; /*! < nb rows */
  int n; /*!< nb columns */
  int mn; /*!< product m*n */</pre>
  int mem size; /*!< size of the memory block allocated for array */
  double *array; /*!< pointer to store the data row-wise */
  int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlMat;
typedef struct _PnlMatInt{
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlMatInt pointer to be cast to a PnlObject
   */
  PnlObject object;
  int m; /*! < nb rows */
  int n; /*!< nb columns */
  int mn; /*!< product m*n */</pre>
  int mem_size; /*!< size of the memory block allocated for array */
  int *array; /*!< pointer to store the data row-wise */
  int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlMatInt;
typedef struct _PnlMatComplex{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlMatComplex pointer to be cast
   * to a PnlObject
   */
  PnlObject object;
```

```
int m; /*!< nb rows */
int n; /*!< nb columns */
int mn; /*!< product m*n */
int mem_size; /*!< size of the memory block allocated for array */
dcomplex *array; /*!< pointer to store the data row-wise */
int owner; /*!< 1 if the object owns its array member, 0 otherwise */
} PnlMatComplex;</pre>
```

m is the number of rows, n is the number of columns. array is a pointer containing the data of the matrix stored line wise, The element (i, j) of the matrix is array[i\*m+j]. owner is an integer to know if the matrix owns its array pointer (owner=1) or shares it with another structure (owner=0). mem\_size is the number of elements the matrix can hold at most.

The following operations are implemented on matrices and vectors. alpha and beta are numbers, A and B are matrices and x and y are vectors.

```
pnl_mat_axpy
                                    B := alpha * A + B
pnl_mat_scalar_prod
                                    x' A y
pnl_mat_dgemm
                                    C := alpha * op (A) * op (B) + beta * C
pnl mat mult vect transpose inplace
                                    y = A' * x
pnl mat mult vect inplace
                                    y = A * x
pnl_mat_lAxpby
                                    y := lambda * A * x + beta * y
pnl_mat_dgemv
                                    y := alpha * op (A) * x + beta * y
pnl mat dger
                                    A := alpha x * y' + A
```

#### 4.3.2 Generic Functions

These functions exist for all types of matrices no matter what the basic type is. The following conventions are used to name functions operating on matrices. Here is the table of prefixes used for the different basic types.

| type     | prefix              | BASE     |
|----------|---------------------|----------|
| double   | pnl_mat             | double   |
| int      | pnl_mat_int         | int      |
| dcomplex | $pnl\_mat\_complex$ | dcomplex |

In this paragraph we present the functions operating on PnlMat which exist for all types. To deduce the prototypes of these functions for other basic types, one must replace pnl\_mat and double according the above table.

Constructors and destructors There are no special functions to access the sizes of a matrix, instead the fields m, n and mn give direct access to the number of rows, columns and the size of the matrix.

```
• PnlMat * pnl_mat_new ()
Description Create a PnlMat of size 0
```

• PnlMat \* pnl\_mat\_create (int m, int n)
Description Create a PnlMat with m rows and n columns.

- PnlMat \* pnl\_mat\_create\_from\_scalar (int m, int n, double x)

  Description Create a PnlMat with m rows and n columns and sets all the elements to x.
- PnlMat \* pnl\_mat\_create\_from\_zero (int m, int n)

  Description Create a PnlMat with m rows and n columns and sets all elements to 0.
- PnlMat \* pnl\_mat\_create\_from\_ptr (int m, int n, const double \*x)

  Description Create a PnlMat with m rows and n columns and copies the array x to the new vector. Be sure that x is long enough to fill all the vector because it cannot be checked inside the function.
- PnlMat \* pnl\_mat\_create\_from\_list (int m, int n, ...)

  Description Create a new PnlMat pointer of size m x n filled with the extra arguments passed to the function. The number of extra arguments passed must be equal to m x n, be aware that this cannot be checked inside the function.
- PnlMat \* pnl\_mat\_copy (const PnlMat \*M)
  Description Create a new PnlMat which is a copy of M.
- PnlMat \* pnl\_mat\_create\_diag\_from\_ptr (const double \*x, int d)

  Description Create a new squared PnlMat by specifying its size and diagonal terms as an array.
- PnlMat \* pnl\_mat\_create\_diag (const PnlVect \*V)

  Description Create a new squared PnlMat by specifying its diagonal terms in a PnlVect
  .
- PnlMat \* pnl\_mat\_create\_from\_file (const char \*file)

  Description Read a matrix from a file and creates the corresponding PnlMat . The following conventions are used for the storage in a file:
  - one row of the matrix corresponds to one line of the file
  - the elements of a row should be separated by blanks (spaces or tabs) and nothing else (no comma or semi-colon separators are detected).
- void pnl\_mat\_free (PnlMat \*\*M)
   Description Free a PnlMat and sets \*M to NULL
- PnlMat pnl\_mat\_wrap\_array (const double \*x, int m, int n)

  Description Create a PnlMat of size m x n which contains x. No copy is made. It is just a container.
- PnlMat pnl\_mat\_wrap\_vect (const PnlVect \*V)

  Description Return a PnlMat (not a pointer) whose array is the array of V. The new matrix shares its data with the vector V, which means that any modification to one of them will affect the other.
- void pnl\_mat\_clone (PnlMat \*clone, const PnlMat \*M)
   Description Clone M into clone. No no new PnlMat is created.
- int pnl\_mat\_resize (PnlMat \*M, int m, int n)

  Description Resize a PnlMat. The new matrix is of size m x n. The old data are lost.

- PnlVect \* pnl\_vect\_create\_submat (const PnlMat \*M, const PnlVectInt \*indi, const PnlVectInt \*indj)

  Description Create a new vector containing the values M(indi(:), indj(:)). indi and indj must be of the same size.
- void pnl\_vect\_extract\_submat (PnlVect \*V\_sub, const PnlMat \*M, const PnlVectInt \*indi, const PnlVectInt \*indj)

  Description On exit, V\_sub = M(indi(:), indj(:)). indi and indj must be of the same size.
- void pnl\_mat\_extract\_subblock (PnlMat \*M\_sub, const PnlMat \*M, int i, int len\_i, int j, int len\_j)

  Description M\_sub = M(i:i+len\_i-1, j:j+len\_j-1). len\_i (resp. len\_j) is the number of rows (resp. columns) to be extracted.
- void pnl\_mat\_set\_subblock (PnlMat \*M, const PnlMat \*block, int i, int j)

  Description If block is a matrix of size m\_block x n\_block, the dimensions of M must satisfy that M->m >= i + m\_block and M->n >= j + n\_block. On output M(i:i+m\_block-1, j:j+n\_block-1) = block.

Accessing elements. If it is supported by the compiler, the following functions are declared inline. To speed up these functions, you can define the macro PNL\_RANGE\_CHECK\_OFF, see Section 1.3.2 for an explanation.

Accessing elements of a matrix is faster using the following macros

- MGET (PnlMat \*M, int i, int j)
  Description Return M[i,j] for reading, eg. x=MGET(M,i,j)
- MGET\_INT (PnlMatInt \*M, int i, int j)
  Description Same as MGET but for an integer matrix.
- MGET\_COMPLEX (PnlMatComplex \*M, int i, int j)
  Description Same as MGET but for a complex matrix.
- MLET (PnlMat \*M, int i, int j)
  Description Return M[i,j] as a lvalue for writing, eg. MLET(M,i,j)=x
- MLET\_INT (PnlMatInt \*M, int i, int j)
  Description Same as MLET but for an integer matrix.
- MLET\_COMPLEX (PnlMatComplex \*M, int i, int j)
  Description Same as MLET but for a complex matrix.
- void **pnl\_mat\_set** (**PnlMat** \*M, int i, int j, double x)
  Description Set the value of M[i, j]=x
- double **pnl\_mat\_get** (const **PnlMat** \*M, int i, int j)

  Description Get the value of M[i, j]
- double \* pnl\_mat\_lget (PnlMat \*M, int i, int j)

  Description Return the address of M[i, j] for use as a lvalue.

- void pnl\_mat\_set\_all (PnlMat \*M, double x)

  Description Set all elements of M to x.
- void **pnl\_mat\_set\_zero** (**PnlMat** \*M)

  Description Set all elements of M to 0.
- void pnl\_mat\_set\_id (PnlMat \*M)

  Description Set the matrix M to the identity matrix. M must be a square matrix.
- void pnl\_mat\_set\_diag (PnlMat \*M, double x, int d)

  Description Set the d<sup>th</sup> diagonal terms of the matrix M to the value x. M must be a square matrix.
- void pnl\_mat\_set\_from\_ptr (PnlMat \*M, const double \*x)

  Description Set M row—wise with the values given by x. The array x must be at least M->mn long.
- void **pnl\_mat\_get\_row** (PnlVect \*V, const PnlMat \*M, int i)

  Description Extract and copies the i-th row of M into V.
- void pnl\_mat\_get\_col (PnlVect \*V, const PnlMat \*M, int j)

  Description Extract and copies the j-th column of M into V.
- PnlVect pnl\_vect\_wrap\_mat\_row (const PnlMat \*M, int i)

  Description Return a PnlVect (not a pointer) whose array is the i-th row of M. The new vector shares its data with the matrix M, which means that any modification to one of them will affect the other.
- PnlMat pnl\_mat\_wrap\_mat\_rows (const PnlMat \*M, int i\_start, int i\_end)

  Description Return a PnlMat (not a pointer) holding rows from i\_start to i\_end (included) of M. The new matrix shares its data with the matrix M, which means that any modification to one of them will affect the other.
- void **pnl\_mat\_swap\_rows** (**PnlMat** \*M, int i, int j) Description Swap two rows of a matrix.
- void **pnl\_mat\_set\_col** (**PnlMat** \*M, const **PnlVect** \*V, int j)

  Description Replace the i-th column of a matrix M by a vector V
- void **pnl\_mat\_set\_row** (**PnlMat** \*M, const **PnlVect** \*V, int i)

  Description Replace the **i**-th row of a matrix M by a vector V
- void pnl\_mat\_add\_row (PnlMat \*M, int i, const PnlVect \*r)
   Description Add a row in matrix M before position i and fill it with the content of r. If r == NULL, row i is left uninitialized. The index i may vary between 0 add a row at the top of the matrix and M->m add a row after all rows.
- void pnl\_mat\_del\_row (PnlMat \*M, int i)
   Description Delete the row with index i (between 0 and M->m-1) of the matrix M.

## **Printing Matrices**

- void pnl\_mat\_print (const PnlMat \*M)
   Description Print a matrix to the standard output.
- void **pnl\_mat\_fprint** (FILE \*fic, const **PnlMat** \*M)

  Description Print a matrix to a file.
- void pnl\_mat\_print\_nsp (const PnlMat \*M)

  Description Print a matrix to the standard output in a format compatible with Nsp.
- void pnl\_mat\_fprint\_nsp (FILE \*fic, const PnlMat \*M)

  Description Print a matrix to a file in a format compatible with Nsp. The saved matrix can be reloaded by the function pnl\_mat\_create\_from\_file.

## Applying external operations

- void **pnl\_mat\_plus\_scalar** (**PnlMat** \*lhs, double x)

  Description In-place matrix scalar addition
- void **pnl\_mat\_minus\_scalar** (**PnlMat** \*lhs, double x)

  Description In-place matrix scalar substraction
- void **pnl\_mat\_mult\_scalar** (**PnlMat** \*lhs, double x)

  Description In-place matrix scalar multiplication
- void **pnl\_mat\_div\_scalar** (**PnlMat** \*lhs, double x)

  Description In-place matrix scalar division

## Element wise operations

- void **pnl\_mat\_mult\_mat\_term** (**PnlMat** \*lhs, const **PnlMat** \*rhs)

  Description In-place matrix matrix term by term product
- void pnl\_mat\_div\_mat\_term (PnlMat \*lhs, const PnlMat \*rhs)

  Description In-place matrix matrix term by term division
- void pnl\_mat\_map\_inplace (PnlMat \*lhs, double(\*f)(double))
  Description lhs = f(lhs).
- void pnl\_mat\_map (PnlMat \*lhs, const PnlMat \*rhs, double(\*f)(double))

  Description lhs = f(rhs).
- void pnl\_mat\_map\_mat\_inplace (PnlMat \*lhs, const PnlMat \*rhs, double(\*f)(double, double))

  Description lhs = f(lhs, rhs).
- void pnl\_mat\_map\_mat (PnlMat \*lhs, const PnlMat \*rhs1, const PnlMat \*rhs2, double(\*f)(double, double))
   Description 1hs = f(rhs1, rhs2).

- double **pnl\_mat\_sum** (const **PnlMat** \*lhs)

  Description Sum matrix component-wise
- void pnl\_mat\_sum\_vect (PnlVect \*y, const PnlMat \*A, char c)

  Description Sum matrix column or row wise. Argument c can be either 'r' (to get a row vector) or 'c' (to get a column vector). When c='r',  $y(j) = \sum_i A_{ij}$  and when c='rc,  $y(i) = \sum_j A_{ij}$ .
- void pnl\_mat\_cumsum (PnlMat \*A, char c)
  Description Cumulative sum over the rows or columns. Argument c can be either 'r' to sum over the rows or 'c' to sum over the columns. When c='r',  $A_{ij}=\sum_{1\leq k\leq i}A_{kj}$  and when c='rc,  $A_{ij}=\sum_{1\leq k\leq j}A_{ik}$ .
- double pnl\_mat\_prod (const PnlMat \*lhs)
   Description Product matrix component-wise
- void pnl\_mat\_prod\_vect (PnlVect \*y, const PnlMat \*A, char c)

  Description Prod matrix column or row wise. Argument c can be either 'r' (to get a row vector) or 'c' (to get a column vector). When c='r',  $y(j) = \prod_i A_{ij}$  and when c='rc,  $y(i) = \prod_j A_{ij}$ .
- void pnl\_mat\_cumprod (PnlMat \*A, char c)

  Description Cumulative prod over the rows or columns. Argument c can be either 'r' to prod over the rows or 'c' to prod over the columns. When c='r',  $A_{ij}=\prod_{1\leq k\leq i}A_{kj}$  and when c='rc,  $A_{ij}=\prod_{1\leq k\leq j}A_{ik}$ .

#### Test functions

- int pnl\_mat\_eq (const PnlMat \*M1, const PnlMat \*M2)

  Description Test if two matrices are equal. Returns TRUE or FALSE.
- int pnl\_mat\_eq\_all (const PnlMat \*M, double x)

  Description Test if all the components of M are equal to x. Returns TRUE or FALSE.

## Ordering operations

- void  $pnl_mat_max$  ( PnlVect \*M, const PnlMat \*A, char d)

  Description On exit,  $M(i) = \max_j(A(i,j))$  when d='c' and  $M(i) = \max_j(A(j,i))$  when d='r' and  $M(0) = \max_{i,j} = A(i,j)$  when d='r'.
- void  $\operatorname{pnl\_mat\_min}$  (  $\operatorname{PnlVect}$  \*m,const  $\operatorname{PnlMat}$  \*A, char d)

  Description On exit,  $\operatorname{m}(i) = \min_{j}(\operatorname{A}(i,j))$  when  $\operatorname{d='c'}$  and  $\operatorname{m}(i) = \min_{j}(\operatorname{A}(j,i))$  when  $\operatorname{d='r'}$  and  $\operatorname{M}(0) = \min_{i,j} = \operatorname{A}(i,j)$  when  $\operatorname{d='*r'}$ .
- void  $\operatorname{pnl\_mat\_minmax}$  (  $\operatorname{PnlVect}$  \*m,  $\operatorname{PnlVect}$  \*M, const  $\operatorname{PnlMat}$  \*A, char d)  $\operatorname{Description}$  On exit,  $\operatorname{m}(i) = \min_j(\operatorname{A}(i,j))$  and  $\operatorname{M}(i) = \max_j(\operatorname{A}(i,j))$  when  $\operatorname{d='c'}$  and  $\operatorname{m}(i) = \min_j(\operatorname{A}(j,i))$  and  $\operatorname{M}(i) = \min_j(\operatorname{A}(j,i))$  when  $\operatorname{d='r'}$  and  $\operatorname{M}(\operatorname{O}) = \max_{i,j} = \operatorname{A}(i,j)$  and  $\operatorname{m}(\operatorname{O}) = \min_{i,j} = \operatorname{A}(i,j)$  when  $\operatorname{d='**}$ .

- void pnl\_mat\_min\_index ( PnlVect \*m, PnlVectInt \*im, const PnlMat \*A, char d) Description Idem as pnl\_mat\_min and index contains the indices of the minima. If index==NULL, the indices are not computed.
- void pnl\_mat\_max\_index ( PnlVect \*M, PnlVectInt \*iM, const PnlMat \*A, char d)
   Description Idem as pnl\_mat\_max and index contains the indices of the maxima. If index==NULL, the indices are not computed.
- void pnl\_mat\_minmax\_index ( PnlVect \*m, PnlVect \*M, PnlVectInt \*im, PnlVectInt \*iM, const PnlMat \*A, char d)

  Description Idem as pnl\_mat\_minmax and im contains the indices of the minima and im contains the indices of the minima. If im==NULL (resp. iM==NULL, the indices of the minima (resp. maxima) are not computed.
- void pnl\_mat\_qsort (PnlMat \*, char dir, char order)

  Description Sort a matrix using a quick sort algorithm according to order ('i' for increasing or 'd' for decreasing). The parameter dir determines whether the matrix is sorted by rows or columns. If dir='c', each row is sorted independently of the others whereas if dir='r', each column is sorted independently of the others.
- void pnl\_mat\_qsort\_index (PnlMat \*, PnlMatInt \*index, char dir, char order)

  Description Sort a matrix using a quick sort algorithm according to order ('i' for increasing or 'd' for decreasing). The parameter dir determines whether the matrix is sorted by rows or columns. If dir='c', each row is sorted independently of the others whereas if dir='r', each column is sorted independently of the others. In addition to the function pnl\_mat\_qsort, the permutation index is computed and stored into index.
- int pnl\_mat\_find (PnlVectInt \*indi, PnlVectInt indj, char \*type, int(\*f)(double \*t), ...)

  Description f is a function taking a C array as argument and returning an integer. type is a string composed by the letters 'r' and 'm' and is used to describe the types of the arguments appearing after f: 'r' for real numbers and 'm' for matrices. This function aims at simulating Scilab's find function. Here are a few examples (capital letters are used for matrices and small letters for real values)

```
- [indi, indj] = find ( a < X )
        int isless ( double *t ) { return t[0] < t[1]; }
        pnl_mat_find ( indi, indj, "rm", isless, a, X );
- ind = find (X <= Y)
        int isless ( double *t ) { return t[0] <= t[1]; }
        pnl_mat_find ( ind, "mm", isless, X, Y );
- [indi, indj] = find ((a < X) && (X <= Y))</pre>
```

```
int cmp ( double *t )
{
  return (t[0] <= t[1]) && (t[1] <= t[2]);
}
pnl_mat_find ( indi, indj, "rmm", cmp, a, X, Y );</pre>
```

(indi, indj) contains on exit the indices (i,j) for which the function f returned 1. Note that if indj == NULL on entry, a linear indexing is used for matrices, which means that matrices are seen as large vectors built up be stacking rows. This function returns OK or FAIL if something went wrong (size mismatch between matrices, invalid string type).

#### Standard matrix operations

- void pnl\_mat\_plus\_mat (PnlMat \*lhs, const PnlMat \*rhs)

  Description In-place matrix matrix addition
- void pnl\_mat\_minus\_mat (PnlMat \*lhs, const PnlMat \*rhs)

  Description In-place matrix matrix substraction
- void pnl\_mat\_sq\_transpose (PnlMat \*M)
  Description On exit, M is transposed
- PnlMat \* pnl\_mat\_transpose (const PnlMat \*M)
  Description Create a new matrix which is the transposition of M
- void pnl\_mat\_tr ( PnlMat \*tM, const PnlMat \*M)
   Description On exit, tM = M'
- double **pnl\_mat\_trace** (const **PnlMat** \*M)

  Description Return the trace of a square matrix.
- void pnl\_mat\_axpy (double alpha, const PnlMat \*A, PnlMat \*B)
   Description Compute B := alpha \* A + B
- void **pnl\_mat\_dger** (double alpha, const **PnlVect** \*x, const **PnlVect** \*y, **PnlMat** \*A)

  Description Compute A := alpha x \* y' + A
- PnlVect \* pnl\_mat\_mult\_vect (const PnlMat \*A, const PnlVect \*x)

  Description Matrix vector multiplication A \* x
- void pnl\_mat\_mult\_vect\_inplace (PnlVect \*y, const PnlMat \*A, const PnlVect \*x)
   Description In place matrix vector multiplication y = A \* x. You cannot use the same vector for x and y.
- PnlVect \* pnl\_mat\_mult\_vect\_transpose (const PnlMat \*A, const PnlVect \*x)

  Description Matrix vector multiplication A' \* x

- void pnl\_mat\_mult\_vect\_transpose\_inplace (PnlVect \*y, const PnlMat \*A, const PnlVect \*x)

  Description In place matrix vector multiplication y = A' \* x. You cannot use the same vector for x and y. The vectors x and y must be different.
- int pnl\_mat\_cross (PnlMat \*lhs, const PnlMat \*A, const PnlMat \*B)

  Description Compute the cross products of the vectors given in matrices A and B which must have either 3 rows or 3 columns. A row wise computation is first tried, then a column wise approach is tested. FAIL is returned in case no dimension equals 3.
- void pnl\_mat\_lAxpby (double lambda, const PnlMat \*A, const PnlVect \*x, double b, PnlVect \*y)
   Description Compute y := lambda A x + b y. When b=0, the content of y is not used on input and instead y is resized to match A\*x. The vectors x and y must be different.
- void pnl\_mat\_dgemv (char trans, double lambda, const PnlMat \*A, const PnlVect \*x, double mu, PnlVect \*b)
  Description Compute b := lambda op(A) x + mu b, where op (X) = X or op (X) = X'. If trans='N' or trans='n', op (A) = A, whereas if trans='T' or trans='t', op (A) = A'.When mu==0, the content of b is not used and instead b is resized to match op(A)\*x. The vectors x and b must be different.
- void pnl\_mat\_dgemm (char transA, char transB, double alpha, const PnlMat \*A, const PnlMat \*B, double beta, PnlMat \*C)

  Description Compute C := alpha \* op(A) \* op (B) + beta \* C. When beta=0, the content of C is unused and instead C is resized to store alpha A \*B. If transA='N' or transA='n', op (A) = A, whereas if transA='T' or transA='t', op (A) = A'. The same holds for transB. The matrix C must be different from A and B.
- PnlMat \* pnl\_mat\_mult\_mat (const PnlMat \*rhs1, const PnlMat \*rhs2)

  Description Matrix multiplication rhs1 \* rhs2
- void pnl\_mat\_mult\_mat\_inplace (PnlMat \*lhs, const PnlMat \*rhs1, const PnlMat \*rhs2)
   Description In-place matrix multiplication lhs = rhs1 \* rhs2. The matrix lhs must be different from rhs1 and rhs2.
- double pnl\_mat\_scalar\_prod (const PnlMat \*A, const PnlVect \*x, const PnlVect \*y)
   Description Compute x' \* A \* y
- void pnl\_mat\_exp (PnlMat \*B, const PnlMat \*A)

  Description Compute the matrix exponential B = exp(A).
- void pnl\_mat\_log (PnlMat \*B, const PnlMat \*A)

  Description Compute the matrix logarithm B = log(A). For the moment, this function only works if A is diagonalizable.
- void **pnl\_mat\_eigen** (PnlVect \*v, PnlMat \*P, const PnlMat \*A, int with\_eigenvector)

Description Compute the eigenvalues (stored in v) and optionally the eigenvectors stored column wise in P when with\_eigenvector==TRUE. If A is symmetric or Hermitian in the complex case, P is orthonormal. When with\_eigenvector=FALSE, P can be NULL.

Linear systems and matrix decompositions The following functions are designed to solve linear system of the from A x = b where A is a matrix and b is a vector except in the functions pnl\_mat\_syslin\_mat, pnl\_mat\_lu\_syslin\_mat and pnl\_mat\_chol\_syslin\_mat which expect the right hand side member to be a matrix too. Whenever the vector b is not needed once the system is solved, you should consider using "inplace" functions. All the functions described in this paragraph return OK if the computations have been carried out successfully and FAIL otherwise.

- int pnl\_mat\_chol (PnlMat \*M)

  Description Compute the Cholesky decomposition of M. M must be symmetric, the positivity is tested in the algorithm. M = L \* L'. On exit, the lower part of M contains the Cholesky decomposition L and the upper part is set to zero.
- int pnl\_mat\_pchol (PnlMat \*M, double tol, int \*rank, PnlVectInt \*p)
   Description Compute the Cholesky decomposition of M with complete pivoting. P' \* A \* P = L \* L'. M must be symmetric positive semi-definite. On exit, the lower part of M contains the Cholesky decomposition L and the upper part is set to zero. The permutation matrix is stored in an integer vector p: the only non zero elements of P are P(p(k),k) = 1
- int pnl\_mat\_lu (PnlMat \*A, PnlPermutation \*p)

  Description Compute a P A = LU factorization. P must be an already allocated PnlPermutation. On exit the decomposition is stored in A, the lower part of A contains L while the upper part (including the diagonal terms) contains U. Remember that the diagonal elements of L are all 1. Row i of A was interchanged with row p(i).
- int pnl\_mat\_upper\_syslin (PnlVect \*x, const PnlMat \*U, const PnlVect \*b)

  Description Solve an upper triangular linear system U x = b
- int pnl\_mat\_lower\_syslin (PnlVect \*x, const PnlMat \*L, const PnlVect \*b)

  Description Solve a lower triangular linear system L x = b
- int pnl\_mat\_chol\_syslin (PnlVect \*x, const PnlMat \*chol, const PnlVect \*b)

  Description Solve a symmetric definite positive linear system A x = b, in which chol is assumed to be the Cholesky decomposition of A computed by pnl\_mat\_chol
- int pnl\_mat\_chol\_syslin\_inplace (const PnlMat \*chol, PnlVect \*b)

  Description Solve a symmetric definite positive linear system A x = b, in which chol is assumed to be the Cholesky decomposition of A computed by pnl\_mat\_chol. The solution of the system is stored in b on exit.
- int pnl\_mat\_lu\_syslin (PnlVect \*x, const PnlMat \*LU, const PnlPermutation \*p, const PnlVect \*b)

  Description Solve a linear system A x = b using a LU decomposition. LU and P are assumed to be the PA = LU decomposition as computed by pnl\_mat\_lu. In particular,

the structure of the matrix LU is the following: the lower part of A contains L while the upper part (including the diagonal terms) contains U. Remember that the diagonal elements of L are all 1.

- int pnl\_mat\_lu\_syslin\_inplace (const PnlMat \*LU, const PnlPermutation \*p, Pn-lVect \*b)
  - Description Solve a linear system A = b using a LU decomposition. LU and P are assumed to be the PA = LU decomposition as computed by pnl\_mat\_lu. In particular, the structure of the matrix LU is the following: the lower part of A contains L while the upper part (including the diagonal terms) contains U. Remember that the diagonal elements of L are all 1. The solution of the system is stored in b on exit.
- int pnl\_mat\_syslin (PnlVect \*x, const PnlMat \*A, const PnlVect \*b)

  Description Solve a linear system A x = b using a LU factorization which is computed inside this function.
- int pnl\_mat\_syslin\_inplace (PnlMat \*A, PnlVect \*b)

  Description Solve a linear system A x = b using a LU factorization which is computed inside this function. The solution of the system is stored in b and A is overwritten by its LU decomposition.
- int pnl\_mat\_syslin\_mat (PnlMat \*A, PnlMat \*B)
   Description Solve a linear system A X = B using a LU factorization which is computed inside this function. A and B are matrices. A must be square. The solution of the system is stored in B on exit. On exit, A contains the LU decomposition of the input matrix which is lost.
- int pnl\_mat\_chol\_syslin\_mat (const PnlMat \*A, PnlMat \*B)
   Description Solve a linear system A X = B using a Cholesky factorization of the symmetric positive definite matrix A. A contains the Cholesky decomposition as computed by pnl\_mat\_chol. B is matrix with the same number of rows as A. The solution of the system is stored in B on exit.
- int pnl\_mat\_lu\_syslin\_mat (const PnlMat \*A, const PnlPermutation \*p, PnlMat \*B)
   Description Solve a linear system A X = B using a P A = L U factorization. A contains the L U factors and p the associated permutation. A and p must have been computed by pnl\_mat\_lu. B is matrix with the same number of rows as A. The solution of the system is stored in B on exit.

The following functions are designed to invert matrices. The authors provide these functions although they cannot find good reasons to use them. Note that to solve a linear system, one must used the syslin functions and not invert the system matrix because it is much longer.

- int pnl\_mat\_upper\_inverse (PnlMat \*A, const PnlMat \*B)

  Description Inversion of an upper triangular matrix
- int pnl\_mat\_lower\_inverse (PnlMat \*A, const PnlMat \*B)

  Description Inversion of a lower triangular matrix

- int pnl\_mat\_inverse (PnlMat \*inverse, const PnlMat \*A)

  Description Compute the inverse of a matrix A and stores the result into inverse. A

  LU factorisation of the matrix A is computed inside this function.
- int pnl\_mat\_inverse\_with\_chol (PnlMat \*inverse, const PnlMat \*A)

  Description Compute the inverse of a symmetric positive definite matrix A and stores the result into inverse. The Cholesky factorisation of the matrix A is computed inside this function.

# 4.3.3 Functions specific to base type double

Linear systems and matrix decompositions The following functions are designed to solve linear system of the from  $A \ x = b$  where A is a matrix and b is a vector except in the functions pnl\_mat\_syslin\_mat, pnl\_mat\_lu\_syslin\_mat and pnl\_mat\_chol\_syslin\_mat which expect the right hand side member to be a matrix too. Whenever the vector b is not needed once the system is solved, you should consider using "inplace" functions. All the functions described in this paragraph return OK if the computations have been carried out successfully and FAIL otherwise.

- int pnl\_mat\_qr (PnlMat \*Q, PnlMat \*R, PnlPermutation \*p, const PnlMat \*A) Description Compute a A P = QR decomposition. If on entry P=NULL, then the decomposition is computed without pivoting, i.e A = QR. When  $P \neq NULL$ , P must be an already allocated PnlPermutation . Q is an orthogonal matrix, i.e Q<sup>-1</sup> = Q<sup>T</sup> and R is an upper triangular matrix. The use of pivoting improves the numerical stability when A is almost rank deficient, i.e when the smallest eigenvalue of A is very close to 0.
- int pnl\_mat\_qr\_syslin (PnlVect \*x, const PnlMat \*Q, const PnlMat \*R, const PnlVectInt \*p, const PnlVect \*b)

  Description Solve a linear system A x = b where A is given by its QR decomposition with column pivoting as computed by the function pnl\_mat\_qr.
- int pnl\_mat\_ls (const PnlMat \*A, PnlVect \*b)

  Description Solve a linear system A x = b in the least square sense, i.e.  $\mathbf{x} = \arg\min_{U} \|A * u b\|^2$ . The solution is stored into b on exit. It internally uses a AP = QR decomposition.
- int pnl\_mat\_ls\_mat (const PnlMat \*A, PnlMat \*B)

  Description Solve a linear system A X = B with A and B two matrices in the least square sense, i.e.  $X = \arg \min_{U} ||A*U B||^2$ . The solution is stored into B on exit. It internally uses a AP = QR decomposition. Same function as pnl mat ls but handles several r.h.s.

## 4.3.4 Functions specific to base type dcomplex

• PnlMatComplex \* pnl\_mat\_complex\_create\_from\_mat (const PnlMat \*R)

Description Create a complex matrix using a real one. The complex parts of the entries of the returned matrix are all set to zero.

#### 4.3.5 Permutations

typedef PnlVectInt PnlPermutation;

The PnlPermutation type is actually nothing else than a vector of integers, i.e. a PnlVectInt. It is used to store the partial pivoting with row interchanges transformation needed in the LU decomposition. We use the Blas convention for storing permutations. Consider a PnlPermutation p generated by a LU decomposition of a matrix A: to compute the decomposition, row i of A was interchanged with row p(i).

- PnlPermutation \* pnl\_permutation\_new ()
  Description Create an empty PnlPermutation .
- PnlPermutation \* pnl\_permutation\_create (int n)
  Description Create a PnlPermutation of size n.
- void **pnl\_permutation\_free** (PnlPermutation \*\*p) Description Free a PnlPermutation .
- void **pnl\_permutation\_inverse** (PnlPermutation \*inv, const PnlPermutation \*p) Description Compute in **inv** the inverse of the permutation **p**.
- void **pnl\_vect\_permute** (PnlVect \*px, const PnlVect \*x, const PnlPermutation \*p) Description Apply a PnlPermutation to a PnlVect .
- void pnl\_vect\_permute\_inplace (PnlVect \*x, const PnlPermutation \*p)

  Description Apply a PnlPermutation to a PnlVect in-place.
- void pnl\_vect\_permute\_inverse (PnlVect \*px, const PnlVect \*x, const PnlPermutation \*p)

  Description Apply the inverse of PnlPermutation to a PnlVect .
- void pnl\_vect\_permute\_inverse\_inplace (PnlVect \*x, const PnlPermutation \*p)

  Description Apply the inverse of a PnlPermutation to a PnlVect in-place.
- void pnl\_mat\_col\_permute (PnlMat \*pX, const PnlMat \*X, const PnlPermutation \*p)
   Description Apply a PnlPermutation to the columns of a matrix. pX contains the result of the permutation applied to X.
- void pnl\_mat\_row\_permute (PnlMat \*pX, const PnlMat \*X, const PnlPermutation \*p)

  Description Apply a PnlPermutation to the rows of a matrix. pX contains the result of the permutation applied to X.
- void **pnl\_permutation\_fprint** (FILE \*fic, const **PnlPermutation** \*p) Description Print a permutation to a file.
- void **pnl\_permutation\_print** (const **PnlPermutation** \*p)

  Description Print a permutation to the standard output.

## 4.4 Tridiagonal Matrices

#### 4.4.1 Overview

The structures and functions related to tridiagonal matrices are declared in pnl/pnl\_tridiag\_matrix.h.

We only store the three main diagonals as three vectors.

```
typedef struct PnlTridiagMat{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlTridiagMat pointer to be cast to a PnlObject
  PnlObject object;
  int size; /*!< number of rows, the matrix must be square */
  double *D; /*!< diagonal elements */</pre>
  double *DU; /*!< upper diagonal elements */</pre>
  double *DL; /*!< lower diagonal elements */</pre>
} PnlTridiagMat;
size is the size of the matrix, D is an array of size size containing the diagonal terms. DU,
DL are two arrays of size size-1 containing respectively the upper diagonal (M_{i,i+1}) and the
lower diagonal (M_{i-1,i}).
typedef struct PnlTridiagMatLU{
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlTridiagMatLU pointer to be cast to a PnlObject
   */
  PnlObject object;
  int size; /*!< number of rows, the matrix must be square */
  double *D; /*!< diagonal elements */
  double *DU; /*!< upper diagonal elements */</pre>
  double *DU2; /*!< second upper diagonal elements */</pre>
  double *DL; /*!< lower diagonal elements */</pre>
  int *ipiv; /*! < Permutation: row i has been interchanged with row ipiv(i) */
```

This type is used to store the LU decomposition of a tridiagonal matrix.

#### 4.4.2 Functions

};

## Constructors and destructors

- PnlTridiagMat \* pnl\_tridiag\_mat\_new ()
  Description Create a PnlTridiagMat with size 0
- PnlTridiagMat \* pnl\_tridiag\_mat\_create (int size)
  Description Create a PnlTridiagMat with size size

- PnlTridiagMat \* pnl\_tridiag\_mat\_create\_from\_scalar (int size, double x)
  Description Create a PnlTridiagMat with the 3 diagonals filled with x
- PnlTridiagMat \* pnl\_tridiag\_mat\_create\_from\_two\_scalar (int size, double x, double y)

  Description Create a PnlTridiagMat with the diagonal filled with x and the upper and lower diagonals filled with y
- PnlTridiagMat \* pnl\_tridiag\_mat\_create\_from\_ptr (int size, const double \*lower\_D, const double \*D, const double \*upper\_D)

  Description Create a PnlTridiagMat
- PnlTridiagMat \* pnl\_tridiag\_mat\_create\_from\_mat (const PnlMat \*mat)

  Description Create a tridiagonal matrix from a full matrix (all the elements but the 3 diagonal ones are ignored).
- PnlMat \* pnl\_tridiag\_mat\_to\_mat (const PnlTridiagMat \*T) Description Create a full matrix from a tridiagonal one.
- PnlTridiagMat \* pnl\_tridiag\_mat\_copy (const PnlTridiagMat \*T)

  Description Copy a tridiagonal matrix.
- void pnl\_tridiag\_mat\_clone (PnlTridiagMat \*clone, const PnlTridiagMat \*T)

  Description Copy the content of T into clone
- void pnl\_tridiag\_mat\_free (PnlTridiagMat \*\*v)
  Description Free a PnlTridiagMat
- int pnl\_tridiag\_mat\_resize (PnlTridiagMat \*v, int size)
  Description Resize a PnlTridiagMat .

Accessing elements. If it is supported by the compiler, the following functions are declared inline. To speed up these functions, you can use the macro constant PNL\_RANGE\_CHECK\_OFF, see Section 1.3.2 for an explanation.

- void pnl\_tridiag\_mat\_set (PnlTridiagMat \*self, int d, int up, double x)

  Description Set self[d, d+up] = x, up can be {-1,0,1}.
- double **pnl\_tridiag\_mat\_get** (const **PnlTridiagMat** \*self, int d, int up) Description Get self[d, d+up], up can be {-1,0,1}.
- double \* pnl\_tridiag\_mat\_lget (PnlTridiagMat \*self, int d, int up)

  Description Return the address self[d, d+up] = x, up can be {-1,0,1}.

#### **Printing Matrix**

- void **pnl\_tridiag\_mat\_fprint** (FILE \*fic, const **PnlTridiagMat** \*M)

  Description Print a tri-diagonal matrix to a file.
- void **pnl\_tridiag\_mat\_print** (const **PnlTridiagMat** \*M)

  Description Print a tridiagonal matrix to the standard output.

# Algebra operations

- void pnl\_tridiag\_mat\_plus\_tridiag\_mat (PnlTridiagMat \*lhs, const PnlTridiag-Mat \*rhs)
  - Description In-place matrix matrix addition
- void pnl\_tridiag\_mat\_minus\_tridiag\_mat (PnlTridiagMat \*lhs, const PnlTridiagMat \*rhs)
  - Description In-place matrix matrix substraction
- void **pnl\_tridiag\_mat\_plus\_scalar** (**PnlTridiagMat** \*lhs, double x) Description In-place matrix scalar addition
- void pnl\_tridiag\_mat\_minus\_scalar (PnlTridiagMat \*lhs, double x)

  Description In-place matrix scalar substraction
- void **pnl\_tridiag\_mat\_mult\_scalar** (**PnlTridiagMat** \*lhs, double x) Description In-place matrix scalar multiplication
- void pnl\_tridiag\_mat\_div\_scalar (PnlTridiagMat \*lhs, double x)

  Description In-place matrix scalar division

#### Element-wise operations

- void pnl\_tridiag\_mat\_mult\_tridiag\_mat\_term (PnlTridiagMat \*lhs, const PnlTridiagMat \*rhs)

  Description In-place matrix matrix term by term product
- void pnl\_tridiag\_mat\_div\_tridiag\_mat\_term (PnlTridiagMat \*lhs, const Pnl-TridiagMat \*rhs)

  Description In-place matrix matrix term by term division
- void pnl\_tridiag\_mat\_map\_inplace (PnlTridiagMat \*lhs, double(\*f)(double))

  Description lhs = f(lhs).
- void pnl\_tridiag\_mat\_map\_tridiag\_mat\_inplace (PnlTridiagMat \*lhs, const PnlTridiagMat \*rhs, double(\*f)(double, double))

  Description lhs = f(lhs, rhs).

## Standard matrix operations & Linear systems

- void pnl\_tridiag\_mat\_mult\_vect\_inplace (PnlVect \*lhs, const PnlTridiagMat \*mat, const PnlVect \*rhs)

  Description In place matrix multiplication. The vector 1hs must be different from rhs.
- PnlVect \* pnl\_tridiag\_mat\_mult\_vect (const PnlTridiagMat \*mat, const PnlVect \*vec)

  Description Matrix multiplication

- void  $pnl\_tridiag\_mat\_lAxpby$  (double lambda, const PnlTridiagMat \*A, const PnlVect \*x, double mu, PnlVect \*b)
  - Description Compute  $b := lambda \ A \ x + mu \ b$ . When mu==0, the content of b is not used on input and instead b is resized to match A\*x. Note that the vectors x and b must be different.
- double pnl\_tridiag\_mat\_scalar\_prod (const PnlVect \*x,const PnlTridiagMat \*A, const PnlVect \*y)
   Description Compute x' \* A \* y
- void pnl\_tridiag\_mat\_syslin\_inplace ( PnlTridiagMat \*M, PnlVect \*b)

  Description Solve the linear system M x = b. The solution is written into b on exit. On exit, M is modified and becomes unusable.
- void  $pnl\_tridiag\_mat\_syslin$  (PnlVect \*x, PnlTridiagMat \*M, const PnlVect \*b) Description Solve the linear system M x = b. On exit, M is modified and becomes unusable.
- PnlTridiagMatLU \* pnl\_tridiag\_mat\_lu\_new ()
  Description Create an empty PnlTridiagMatLU
- PnlTridiagMatLU \* pnl\_tridiag\_mat\_lu\_create (int size)
  Description Create a PnlTridiagMatLU with size size
- PnlTridiagMatLU \* pnl\_tridiag\_mat\_lu\_copy (const PnlTridiagMatLU \*mat)

  Description Create a new PnlTridiagMatLU which is a copy of mat.
- void pnl\_tridiag\_mat\_lu\_clone (PnlTridiagMatLU \*clone, const PnlTridiag-MatLU \*mat)
   Description Clone a PnlTridiagMatLU . clone must already exist, no memory is allocated for the envelope.
- void pnl\_tridiag\_mat\_lu\_free (PnlTridiagMatLU \*\*m)
  Description Free a PnlTridiagMatLU
- int pnl\_tridiag\_mat\_lu\_resize (PnlTridiagMatLU \*v, int size) Description Resize a PnlTridiagMatLU
- int pnl\_tridiag\_mat\_lu\_compute (PnlTridiagMatLU \*LU, const PnlTridiagMat \*A)

  Description Compute the LU factorisation of a tridiagonal matrix A. LU must have already been created using pnl\_tridiag\_mat\_lu\_new. On exit, LU contains the decomposition which is suitable for use in pnl\_tridiag\_mat\_lu\_syslin.
- int pnl\_tridiag\_mat\_lu\_syslin\_inplace (PnlTridiagMatLU \*LU, PnlVect \*b)

  Description Solve a linear system A x = b where the matrix LU is given the LU decomposition of A previously computed by pnl\_tridiag\_mat\_lu\_compute. On exit, b is overwritten by the solution x.
- int  $pnl\_tridiag\_mat\_lu\_syslin$  (PnlVect\*x, PnlTridiagMatLU\*LU, constPnlVect\*b)

Description Solve a linear system A x = b where the matrix LU is given the LU decomposition of A previously computed by pnl\_tridiag\_mat\_lu\_compute.

## 4.5 Band Matrices

#### 4.5.1 Overview

```
typedef struct
{
    /**
    * Must be the first element in order for the object mechanism to work
    * properly. This allows any PnlBandMat pointer to be cast to a PnlObject
    */
PnlObject object;
int m; /*!< nb rows */
int n; /*!< nb columns */
int nu; /*!< nb of upperdiagonals */
int nl; /*!< nb of lowerdiagonals */
int m_band; /*!< nb rows of the band storage */
int n_band; /*!< nb columns of the band storage */
double *array; /*!< a block to store the bands */
} PnlBandMat;</pre>
```

The structures and functions related to band matrices are declared in pnl/pnl\_band\_matrix.h.

## 4.5.2 Functions

# Constructors and destructors

- PnlBandMat \* pnl\_band\_mat\_new ()
  Description Create a band matrix of size 0.
- PnlBandMat \* pnl\_band\_mat\_create (int m, int n, int nl, int nu)

  Description Create a band matrix of size m x n with nl lower diagonals and nu upper diagonals.
- PnlBandMat \* pnl\_band\_mat\_create\_from\_mat (const PnlMat \*BM, int nl, int nu)

  Description Extract a band matrix from a PnlMat .
- void **pnl\_band\_mat\_free** (**PnlBandMat** \*\*) Description Free a band matrix.
- void pnl\_band\_mat\_clone (PnlBandMat \*clone, const PnlBandMat \*M)

  Description Copy the band matrix M into clone. No new PnlBandMat is created.
- PnlBandMat \* pnl\_band\_mat\_copy (PnlBandMat \*BM)

  Description Create a new band matrix which is a copy of BM. Each band matrix owns its data array.

- PnlMat \* pnl\_band\_mat\_to\_mat (PnlBandMat \*BM)
  Description Create a full matrix from a band matrix.
- int pnl\_band\_mat\_resize (PnlBandMat \*BM, int m, int n, int nl, int nu)

  Description Resize BM to store a m x n band matrix with nu upper diagonals and nl lower diagonals.

Accessing elements. If it is supported by the compiler, the following functions are declared inline. To speed up these functions, you can use the macro constant PNL\_RANGE\_CHECK\_OFF, see Section 1.3.2 for an explanation.

- void **pnl\_band\_mat\_set** (PnlBandMat \*M, int i, int j, double x) Description  $M_{i,j} = x$ .
- void  $pnl\_band\_mat\_get$  (PnlBandMat \*M, int i, int j) Description Return  $M_{i,j}$ .
- void pnl\_band\_mat\_lget (PnlBandMat \*M, int i, int j) Description Return the address & $(M_{i,j})$ .
- void pnl\_band\_mat\_set\_all (PnlBandMat \*M, double x)
  Description Set all the elements of M to x.
- void **pnl\_band\_mat\_print\_as\_full** (**PnlBandMat** \*M) Description Print a band matrix in a full format.

# Element wise operations

- void pnl\_band\_mat\_plus\_scalar (PnlBandMat \*lhs, double x)
   Description In-place addition, lhs += x
- void pnl\_band\_mat\_minus\_scalar (PnlBandMat \*lhs, double x)
  Description In-place substraction lhs -= x
- void pnl\_band\_mat\_div\_scalar (PnlBandMat \*lhs, double x)
   Description lhs = lhs ./ x
- void pnl\_band\_mat\_mult\_scalar (PnlBandMat \*lhs, double x)
   Description lhs = lhs \* x
- void pnl\_band\_mat\_plus\_band\_mat (PnlBandMat \*lhs, const PnlBandMat \*rhs)
   Description In-place addition, 1hs += rhs
- void pnl\_band\_mat\_minus\_band\_mat (PnlBandMat \*lhs, const PnlBandMat \*rhs)
   Description In-place substraction 1hs -= rhs
- void pnl\_band\_mat\_inv\_term (PnlBandMat \*lhs)
   Description In-place term by term inversion lhs = 1 ./ rhs

- void pnl\_band\_mat\_div\_band\_mat\_term (PnlBandMat \*lhs, const PnlBand-Mat \*rhs)
  - Description In-place term by term division lhs = lhs ./ rhs
- void pnl\_band\_mat\_mult\_band\_mat\_term (PnlBandMat \*lhs, const PnlBand-Mat \*rhs)
  - Description In-place term by term multiplication lhs = lhs .\* rhs
- void **pnl\_band\_mat\_map** (**PnlBandMat** \*lhs, const **PnlBandMat** \*rhs, double(\*f)(double))
  - Description lhs = f(rhs)
- void pnl\_band\_mat\_map\_inplace (PnlBandMat \*lhs, double(\*f)(double))

  Description lhs = f(lhs)
- void pnl\_band\_mat\_map\_band\_mat\_inplace (PnlBandMat \*lhs, const Pnl-BandMat \*rhs, double(\*f)(double,double))

  Description lhs = f(lhs,rhs)

## Standard matrix operations & Linear system

- void pnl\_band\_mat\_lAxpby (double lambda, const PnlBandMat \*A, const PnlVect \*x, double mu, PnlVect \*b)

  Description Compute b := lambda A x + mu b. When mu==0, the content of b is not used on input and instead b is resized to match the size of A\*x.
- void pnl\_band\_mat\_mult\_vect\_inplace (PnlVect \*y, const PnlBandMat \*BM, const PnlVect \*x)
   Description y = BM \* x
- void pnl\_band\_mat\_syslin\_inplace (PnlBandMat \*M, PnlVect \*b)

  Description Solve the linear system M x = b with M a PnlBandMat . Note that M is modified on output and becomes unusable. On exit, the solution x is stored in b.
- void pnl\_band\_mat\_syslin (PnlVect \*x,PnlBandMat \*M, PnlVect \*b)

  Description Solve the linear system M x = b with M a PnlBandMat . Note that M is modified on output and becomes unusable.
- void pnl\_band\_mat\_lu (PnlBandMat \*BM, PnlVectInt \*p)

  Description Compute the LU decomposition with partial pivoting with row interchanges.

  On exit, BM is enlarged to store the LU decomposition. On exit, p stores the permutation applied to the rows. Note that the Lapack format is used to store p, this format differs from the one used by PnlPermutation .
- void pnl\_band\_mat\_lu\_syslin\_inplace (const PnlBandMat \*M, PnlVectInt \*p, PnlVect \*b)
   Description Solve the band linear system M x = b where M is the LU decomposition computed by pnl\_band\_mat\_lu and p the associated permutation. On exit, the solution x is stored in b.

void pnl\_band\_mat\_lu\_syslin (PnlVect \*x, const PnlBandMat \*M, PnlVectInt \*p, const PnlVect \*b)
 Description Solve the band linear system M x = b where M is the LU decomposition computed by pnl\_band\_mat\_lu and p the associated permutation.

# 4.6 Sparse Matrices

## 4.6.1 Short description

The structures and functions related to matrices are declared in pnl/pnl\_sp\_matrix.h.

```
typedef struct _PnlSpMat
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows a PnlSpMat pointer to be cast to a PnlObject
  PnlObject object;
  int m; /*!< number of rows */
  int n; /*!< number of columns */
  int nz; /*!< number of non-zero elements */</pre>
  int *J; /*!< column indices, vector of size nzmax */</pre>
  int *I; /*!< row offset integer vector,</pre>
            array[I[i]] is the first element of row i.
            Vector of size (m+1) */
  double *array; /*!< pointer to store the data of size nzmax*/
  int nzmax; /*!< size of the memory block allocated for array */
} PnlSpMat;
typedef struct _PnlSpMatInt
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows a PnlSpMat pointer to be cast to a PnlObject
   */
  PnlObject object;
  int m; /*!< number of rows */
  int n; /*!< number of columns */</pre>
  int nz; /*!< number of non-zero elements */
  int *J; /*!< column indices, vector of size nzmax */
  int *I; /*!< row offset integer vector,</pre>
            array[I[i]] is the first element of row i.
            Vector of size (m+1) */
  int *array; /*!< pointer to store the data of size nzmax */
  int nzmax; /*!< size of the memory block allocated for array */
} PnlSpMatInt;
typedef struct _PnlSpMatComplex
```

The non zero elements of row i are stored in array between the indices I[i] and I[i+1]-1. The array J contains the column indices of every element of array.

Sparse matrices are defined using the internal template approach and can be used for integer, float or complex base data according to the following table

| base type | prefix             | type            |
|-----------|--------------------|-----------------|
| double    | pnl_sp_mat         | PnlSpMat        |
| int       | pnl_sp_mat_int     | PnlSpMatInt     |
| dcomplex  | pnl_sp_mat_complex | PnlSpMatComplex |

### 4.6.2 Functions

## Constructors and destructors

- PnlSpMat \* pnl\_sp\_mat\_new ()
  Description Create an empty sparse matrix.
- PnlSpMat \* pnl\_sp\_mat\_create (int m, int n, int nzmax)

  Description Create a sparse matrix with size m x n designed to hold at most nzmax non zero elements.
- void pnl\_sp\_mat\_clone (PnlSpMat \*dest, const PnlSpMat \*src)

  Description Clone src into dest, which is automatically resized. On output, dest and src are equal but independent.
- PnlSpMat \* pnl\_sp\_mat\_copy (PnlSpMat \*src)
  Description Create an independent copy of src.
- void **pnl\_sp\_mat\_free** (PnlSpMat \*\*)
  Description Delete a sparse matrix.

- int pnl\_sp\_mat\_resize (PnlSpMat \*M, int m, int n, int nzmax)

  Description Resize an existing PnlSpMat to become a m x n sparse matrices holding at most nzmax. Note that no old data are kept except if M->m is left unchanged and we only call this function to increase M->nzmax. Return OK or FAIL.
- PnlMat \* pnl\_mat\_create\_from\_sp\_mat (const PnlSpMat \*M)
  Description Create a dense PnlMat from a spare one.
- PnlSpMat \* pnl\_sp\_mat\_create\_from\_mat (const PnlMat \*M)
  Description Create a sparse matrix from a dense one.
- int pnl\_sp\_mat\_eq (const PnlSpMat \*Sp1, const PnlSpMat \*Sp2)

  Description Test if two sparse matrices are equal, ie. if they have the same size (m, n, nz) and hold the same values. Return TRUE or FALSE.

## Accessing elements

- void pnl\_sp\_mat\_set (PnlSpMat \*M, int i, int j, double x)
   Description Set M[i,j] = x. This function increases M->nzmax if necessary.
- double pnl\_sp\_mat\_get (const PnlSpMat \*M, int i, int j)

  Description Return M[i,j]. If M has no entry with such an index, zero is returned.

#### Applying external operations

- void pnl\_sp\_mat\_plus\_scalar (PnlSpMat \*M, double x)

  Description Add x to all non zero entries of M. To apply the operation to all entries including the zero ones, first convert M to a dense matrix and use pnl\_mat\_plus\_scalar.
- void pnl\_sp\_mat\_minus\_scalar (PnlSpMat \*M, double x)

  Description Substract x to all non zero entries of M. To apply the operation to all entries including the zero ones, first convert M to a dense matrix and use pnl\_mat\_minus\_scalar.
- void pnl\_sp\_mat\_mult\_scalar (PnlSpMat \*M, double x) Description In-place matrix scalar multiplication
- void **pnl\_sp\_mat\_div\_scalar** (**PnlSpMat** \*M, double x) Description In-place matrix scalar division

## Standard matrix operations

- void pnl\_sp\_mat\_fprint (FILE \*fic, const PnlSpMat \*M)

  Description Print a sparse matrix to a file descriptor using the format (row, col) -> val.
- void pnl\_sp\_mat\_print (const PnlSpMat \*M)

  Description Same as pnl\_sp\_mat\_fprint but print to standard output.

- void pnl\_sp\_mat\_mult\_vect (()PnlVect \*y, const PnlSpMat \*A, const PnlVect \*x)

  Description y = A x.
- void pnl\_sp\_mat\_lAxpby (double lambda, const PnlSpMat \*A, const PnlVect \*x, double b, PnlVect \*y)

  Description Compute y := lambda A x + b y. When b=0, the content of y is not used on input and instead y is resized to match A\*x. The vectors x and y must be different.

# 4.7 Hyper Matrices

# 4.7.1 Short description

The Hyper matrix types and related functions are defined in the header pnl/pnl\_matrix.h.

```
typedef struct PnlHmat{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlHmat pointer to be cast to a PnlObject
  PnlObject object;
  int ndim; /*!< nb dimensions */
  int *dims; /*!< pointer to store the values of the ndim dimensions */
  int mn; /*!< product dim_1 *...*dim_ndim */</pre>
  int *pdims; /*!< array of size ndim, s.t. pdims[i] = dims[ndim-1] x ... dims[i+1]</pre>
                with pdims[ndim - 1] = 1 */
  double *array; /*!< pointer to store */</pre>
} PnlHmat;
typedef struct PnlHmatInt{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlHmatInt pointer to be cast to a PnlObject
   */
  PnlObject object;
  int ndim; /*!< nb dimensions */
  int *dims; /*!< pointer to store the value of the ndim dimensions */
  int mn; /*!< product dim_1 *...*dim_ndim */</pre>
  int *pdims; /*! < array of size ndim, s.t. pdims[i] = dims[ndim-1] x ... dims[i+1]
                with pdims[ndim - 1] = 1 */
  int *array; /*!< pointer to store */
} PnlHmatInt;
typedef struct PnlHmatComplex{
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlHmatComplex pointer to be cast to a PnlObject
   */
  PnlObject object;
```

ndim is the number of dimensions, dim is an array to store the size of each dimension and nm contains the product of the sizes of each dimension. array is an array of size mn containing the data. The integer array pdims is used to create the one—to—one map between the natural indexing and the linear indexing used in array.

## 4.7.2 Functions

These functions exist for all types of hypermatrices no matter what the basic type is. The following conventions are used to name functions operating on hypermatrices. Here is the table of prefixes used for the different basic types.

| base type | prefix           | $\operatorname{type}$ |  |
|-----------|------------------|-----------------------|--|
| double    | pnl_hmat         | PnlHmat               |  |
| int       | pnl_hmat_int     | PnlHmatInt            |  |
| dcomplex  | pnl hmat complex | PnlHmatComplex        |  |

In this paragraph, we present the functions operating on PnlHmat which exist for all types. To deduce the prototypes of these functions for other basic types, one must replace pnl\_hmat and double according the above table.

# Constructors and destructors

- PnlHmat \* pnl\_hmat\_new ()
  Description Create an empty PnlHmat .
- PnlHmat \* pnl\_hmat\_create (int ndim, const int \*dims)

  Description Create a PnlHmat with ndim dimensions and the size of each dimension is given by the entries of the integer array dims
- PnlHmat \* pnl\_hmat\_create\_from\_scalar (int ndim, const int \*dims, double x) Description Create a PnlHmat with ndim dimensions given by  $\prod_i \text{dims}[i]$  filled with x.
- PnlHmat \* pnl\_hmat\_create\_from\_ptr (int ndim, const int \*dims, const double \*x)
- void **pnl\_hmat\_free** (PnlHmat \*\*H) Description Free a PnlHmat
- PnlHmat \* pnl\_hmat\_copy (const PnlHmat \*H)
  Description Copy a PnlHmat .
- void **pnl\_hmat\_clone** (PnlHmat \*clone, const PnlHmat \*H)

  Description Clone a PnlHmat .

• int pnl\_hmat\_resize (PnlHmat \*H, int ndim, const int \*dims)
Description Resize a PnlHmat .

## Accessing elements

- void **pnl\_hmat\_set** (**PnlHmat** \*self, int \*tab, double x) Description Set the element of index tab to x.
- double pnl\_hmat\_get (const PnlHmat \*self, int \*tab)

  Description Return the value of the element of index tab
- double\* pnl\_hmat\_lget (PnlHmat \*self, int \*tab)

  Description Return the address of self[tab] for use as a lvalue.
- PnlMat pnl\_mat\_wrap\_hmat (PnlHmat \*H, int \*t)
  Description Return a true PnlMat not a pointer holding the data H(t,:,:). Note that t
  must be of size ndim-2 and that it cannot be checked within the function. The returned
  matrix shares its data with H, it is only a view not a true copy.
- PnlVect pnl\_vect\_wrap\_hmat (PnlHmat \*H, int \*t)

  Description Return a true PnlVect not a pointer holding the data H(t,:). Note that t must be of size ndim-1 and that it cannot be checked within the function. The returned vector shares its data with H, it is only a view not a true copy.

## Printing hypermatrices

• void **pnl\_hmat\_print** (const **PnlHmat** \*H) Description Print an hypermatrix.

# Term by term operations

- void pnl\_hmat\_plus\_hmat (PnlHmat \*lhs, const PnlHmat \*rhs)
  Description Compute lhs += rhs.
- void **pnl\_hmat\_mult\_scalar** (**PnlHmat** \*lhs, double x)

  Description Compute **lhs** \*= x where x is a real number.

### 4.8 Iterative Solvers

## 4.8.1 Overview

The structures and functions related to solvers are declared in pnl/pnl\_linalgsolver.h.

```
typedef struct _PnlIterationBase PnlIterationBase;
typedef struct _PnlCgSolver PnlCgSolver;
typedef struct _PnlBicgSolver PnlBicgSolver;
typedef struct _PnlGmresSolver PnlGmresSolver;
struct _PnlIterationBase
{
```

```
/**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlVectXXX pointer to be cast to a PnlObject
  PnlObject object;
  int iteration;
  int max_iter;
  double normb;
  double tol_;
  double resid;
  int error;
  /* char * err_msg; */
};
/* When you repeatedly use iterative solvers, do not malloc each time */
struct _PnlCgSolver
{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlCgSolver pointer to be cast to a PnlObject
   */
  PnlObject object;
  PnlVect * r;
  PnlVect * z;
  PnlVect * p;
  PnlVect * q;
  double rho;
  double oldrho;
  double beta;
  double alpha;
  PnlIterationBase * iter;
} ;
struct _PnlBicgSolver
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlBicgSolver pointer to be cast to a PnlObject
   */
  PnlObject object;
  double rho_1, rho_2, alpha, beta, omega;
  PnlVect * p;
  PnlVect * phat;
  PnlVect * s;
  PnlVect * shat;
  PnlVect * t;
  PnlVect * v;
```

```
PnlVect * r;
  PnlVect * rtilde;
  PnlIterationBase * iter;
} ;
struct _PnlGmresSolver
{
  /**
   * Must be the first element in order for the object mechanism to work
   * properly. This allows any PnlGmresSolver pointer to be cast to a PnlObject
  PnlObject object;
  int restart;
  double beta;
  PnlVect * s;
  PnlVect * cs;
  PnlVect * sn;
  PnlVect * w;
  PnlVect * r;
  PnlMat * H;
  PnlVect * v[MAX_RESTART];
  PnlIterationBase *iter;
  PnlIterationBase *iter_inner;
} ;
```

A Left preconditioner solves the problem :

$$PMx = Pb$$
.

and whereas right preconditioner solves

$$MPy = b, \qquad Py = x.$$

More information is given in Saad, Yousef (2003). Iterative methods for sparse linear systems (2nd ed. ed.). SIAM. ISBN 0898715342. OCLC 51266114. The reader will find in this book some discussion about right or/and left preconditioner and a description of the following algorithms.

These algorithms, we implemented with a left preconditioner. Right preconditioner can be easily computed changing matrix vector multiplication operator from M x to M  $P_R$  x and solving  $P_R y = x$  at the end of algorithm.

#### 4.8.2 Functions

Three methods are implemented: Conjugate Gradient, BICGstab and GMRES with restart. For each of them a structure is created to store temporary vectors used in the algorithm. In some cases, we have to apply iterative methods more than once: for example to solve at each time step a discrete form of an elliptic problem come from parabolic problem. In the cases, do not call the constructor and destructor at each time, but instead use the initialization and solve procedures.

Formally we have,

```
Create iterative method

For each time step
   Initialisation of iterative method
   Solve linear system link to elliptic problem
end for
free iterative method
```

In these functions, we don't use any particular matrix structure. We give the matrix vector multiplication as a parameter of the solver.

Conjugate Gradient method Only available for symmetric and positive matrices.

- PnlCgSolver \* pnl\_cg\_solver\_new ()
  Description Create an empty PnlCgSolver
- PnlCgSolver \* pnl\_cg\_solver\_create (int Size, int max-iter, double tolerance)
  Description Create a new PnlCgSolver pointer.
- void pnl\_cg\_solver\_initialisation (PnlCgSolver \*Solver, const PnlVect \*b) Description Initialisation of the solver at the beginning of iterative method.
- void pnl\_cg\_solver\_free (PnlCgSolver \*\*Solver)
  Description Destructor of iterative solver
- int pnl\_cg\_solver\_solve (void(\*matrix vector-product)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*Matrix-Data, void(\*matrix vector-product-PC)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*PC-Data, PnlVect \*x, const PnlVect \*b, PnlCgSolver \*Solver)

  Description Solve the linear system matrix vector-product is the matrix vector multiplication function matrix vector-product-PC is the preconditionner function Matrix-Data & PC-Data is data to compute matrix vector multiplication.

#### **BICG** stab

- PnlBicgSolver \* pnl\_bicg\_solver\_new ()
  Description Create an empty PnlBicgSolver.
- PnlBicgSolver \* pnl\_bicg\_solver\_create (int Size, int max-iter, double tolerance)
  Description Create a new PnlBicgSolver pointer.
- void pnl\_bicg\_solver\_initialisation (PnlBicgSolver \*Solver, const PnlVect \*b) Description Initialisation of the solver at the beginning of iterative method.
- void pnl\_bicg\_solver\_free (PnlBicgSolver \*\*Solver)

  Description Destructor of iterative solver
- int pnl\_bicg\_solver\_solve (void(\*matrix vector-product)(const void \*, const Pn-lVect \*, const double, const double, PnlVect \*), const void \*Matrix-Data, void(\*matrix vector-product-PC)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*PC-Data, PnlVect \*x, const PnlVect \*b, PnlBicgSolver \*Solver)

Description Solve the linear system matrix vector-product is the matrix vector multiplication function matrix vector-product-PC is the preconditioner function Matrix-Data & PC-Data is data to compute matrix vector multiplication.

**GMRES with restart** See Saad, Yousef (2003) for a discussion about the restart parameter. For GMRES we need to store at the p-th iteration p vectors of the same size of the right and side. It could be very expensive in term of memory allocation. So GMRES with restart algorithm stop if p = restart and restarts the algorithm with the previously computed solution as initial guess.

Note that if restart equals m, we have a classical GMRES algorithm.

- PnlGmresSolver \* pnl\_gmres\_solver\_new ()
  Description Create an empty PnlGmresSolver
- PnlGmresSolver \* pnl\_gmres\_solver\_create (int Size, int max-iter, int restart, double tolerance)

  Description Create a new PnlGmresSolver pointer.
- void pnl\_gmres\_solver\_initialisation (PnlGmresSolver \*Solver, const PnlVect \*b)

  Description Initialisation of the solver at the beginning of iterative method.
- void pnl\_gmres\_solver\_free (PnlGmresSolver \*\*Solver)

  Description Destructor of iterative solver
- int pnl\_gmres\_solver\_solve (void(\*matrix vector-product)(const void \*, const Pn-lVect \*, const double, const double, PnlVect \*), const void \*Matrix-Data, void(\*matrix vector-product-PC)(const void \*, const PnlVect \*, const double, const double, PnlVect \*), const void \*PC-Data, PnlVect \*x, const PnlVect \*b, PnlGmresSolver \*Solver)

  Description Solve the linear system matrix vector-product is the matrix vector multiplication function matrix vector-product-PC is the preconditionner function Matrix-Data & PC-Data is data to compute matrix vector multiplication.

In the next paragraph, we write all the solvers for PnlMat . This will be done as follows: construct an application matrix vector.

In practice, we cannot define all iterative methods for all structures. With this implementation, the user can easily :

- implement right precondioner,
- implement method with sparse matrix and diagonal preconditioner, or special combination of this form ...

## Iterative algorithms for PnlMat

- int pnl\_mat\_cg\_solver\_solve (const PnlMat \*M, const PnlMat \*PC, PnlVect \*x, const PnlVect \*b, PnlCgSolver \*Solver)

  Description Solve the linear system M x = b with preconditionner PC.
- int pnl\_mat\_bicg\_solver\_solve (const PnlMat \*M, const PnlMat \*PC, PnlVect \*x, const PnlVect \*b, PnlBicgSolver \*Solver)

  Description Solve the linear system M x = b with preconditionner PC.
- int pnl\_mat\_gmres\_solver\_solve (const PnlMat \*M, const PnlMat \*PC, PnlVect \*x, PnlVect \*b, PnlGmresSolver \*Solver)

  Description Solve the linear system M x = b with preconditionner PC.

# 5 Cumulative distribution Functions

The functions related to this chapter are declared in pnl/pnl\_cdf.h.

For various distribution functions, we provide functions named pnl\_cdf\_xxx where xxx is the abbreviation of the distribution name. All these functions are based on the same prototype

$$p = 1 - q;$$
  $p = \int_{-\infty}^{\infty} density(u) du$ 

- which If which=1, it computes p and q. If which=2, it computes x. For higher values of which it computes one the parameters characterizing the distribution using all the others, p, q, x.
- p the probability  $\int_{-\infty}^{\infty} density(u) du$
- q = 1 p
- x the upper bound of the integral
- status an integer which indicates on exit the success of the computation. (0) if calculation completed correctly. (-I) if the input parameter number I was out of range. (1) if the answer appears to be lower than the lowest search bound. (2) if the answer appears to be higher than the greatest search bound. (3) if  $p + q \neq 1$ .
- bound is undefined if STATUS is 0. Bound exceeded by parameter number I if STATUS is negative. Lower search bound if STATUS is 1. Upper search bound if STATUS is 2.
- void **pnl\_cdf\_bet** (int \*which, double \*p, double \*q, double \*x, double \*y, double \*a, double \*b, int \*status, double \*bound)

  Description Cumulative Distribution Function BETA distribution.

- void **pnl\_cdf\_bin** (int \*which, double \*p, double \*q, double \*x, double \*xn, double \*pr, double \*ompr, int \*status, double \*bound)

  Description Cumulative Distribution Function BINa distribution.
- void **pnl\_cdf\_chi** (int \*which, double \*p, double \*q, double \*x, double \*df, int \*status, double \*bound)

  Description Cumulative Distribution Function CHI-Square distribution.
- void **pnl\_cdf\_chn** (int \*which, double \*p, double \*q, double \*x, double \*df, double \*pnonc, int \*status, double \*bound)

  Description Cumulative Distribution Function Non-central Chi-Square distribution.
- void **pnl\_cdf\_f** (int \*which, double \*p, double \*q, double \*x, double \*dfn, double \*dfd, int \*status, double \*bound)

  Description Cumulative Distribution Function F distribution.
- void **pnl\_cdf\_fnc** (int \*which, double \*p, double \*q, double \*x, double \*dfn, double \*dfd, double \*pnonc, int \*status, double \*bound)

  Description Cumulative Distribution Function Non-central F distribution.
- void pnl\_cdf\_gam (int \*which, double \*p, double \*q, double \*x, double \*shape, double \*rate, int \*status, double \*bound)

  Description Cumulative Distribution Function GAMma distribution. Note that the parameter rate is 1/scale. The density writes  $f(x) = 1/(s^a\Gamma(a))x^{a-1}e^{-x/s}$  with scale=s and shape=1/rate=a.
- void **pnl\_cdf\_nbn** (int \*which, double \*p, double \*q, double \*x, double \*xn, double \*pr, double \*ompr, int \*status, double \*bound)

  Description Cumulative Distribution Function Negative BiNomial distribution.
- void **pnl\_cdf\_nor** (int \*which, double \*p, double \*q, double \*x, double \*mean, double \*sd, int \*status, double \*bound)

  Description Cumulative Distribution Function NORmal distribution.
- void **pnl\_cdf\_poi** (int \*which, double \*p, double \*q, double \*x, double \*xlam, int \*status, double \*bound)

  Description Cumulative Distribution Function POIsson distribution.
- void **pnl\_cdf\_t** (int \*which, double \*p, double \*q, double \*x, double \*df, int \*status, double \*bound)

  Description Cumulative Distribution Function T distribution.
- double pnl\_cdfchi2n (double x, double df, double ncparam)
   Description Compute the cumulative density function at x of the non central χ² distribution with df degrees of freedom and non centrality parameter ncparam.
- void pnl\_cdfbchi2n (double x, double df, double ncparam, double beta, double \*P)
   Description Store in P the cumulative density function at x of the random variable beta \*X where X is non central χ² random variable with df degrees of freedom and non centrality parameter ncparam.

- double **pnl\_normal\_density** (double x) Description Normal density function.
- double **pnl\_cdfnor** (double x)

  Description Cumulative normal distribution function.
- double **pnl\_cdf2nor** (double a, double b, double r)

  Description Cumulative bivariate normal distribution function, returns  $\frac{1}{2\pi\sqrt{1-r^2}} \int_{-\infty}^{a} \int_{-\infty}^{b} e^{-\frac{x^2-2rxy+y^2}{2(1-r^2)}} dxdy.$
- double pnl\_inv\_cdfnor (double x)
   Description Inverse of the cumulative normal distribution function.

# 6 Random Number Generators

The functionalities described in this chapter are declared in pnl/pnl\_random.h.

Random number generators should be called through the new *rng* interface based on the PnlRng object. This interface uses reentrant functions and is suitable for multi-threaded applications.

The older *rand* interface is kept for compatibility purposes only and should not be used in new code.

| Random generator | index                | Type   | Info                  |
|------------------|----------------------|--------|-----------------------|
| KNUTH            | PNL_RNG_KNUTH        | pseudo |                       |
| MRGK3            | PNL_RNG_MRGK3        | pseudo |                       |
| MRGK5            | PNL_RNG_MRGK5        | pseudo |                       |
| SHUFL            | PNL_RNG_SHUFL        | pseudo |                       |
| L'ECUYER         | PNL_RNG_L_ECUYER     | pseudo |                       |
| TAUSWORTHE       | PNL_RNG_TAUSWORTHE   | pseudo |                       |
| MERSENNE         | PNL_RNG_MERSENNE     | pseudo |                       |
| SQRT             | PNL_RNG_SQRT         | quasi  |                       |
| HALTON           | PNL_RNG_HALTON       | quasi  |                       |
| FAURE            | PNL_RNG_FAURE        | quasi  |                       |
| SOBOL_I4         | PNL_RNG_SOBOL_I4     | quasi  | uses 32 bit intergers |
| SOBOL_I8         | PNL_RNG_SOBOL2_I8    | quasi  | uses 64 bit intergers |
| NIEDERREITER     | PNL_RNG_NIEDERREITER | quasi  |                       |

Table 2: Indices of the random generators

# 6.1 The rng interface

It is possible to create several random number generators each with its own state variable so that they can evolve independently in a shared memory environment. These generators are suitable for use in multi-threaded programs.

```
typedef struct _PnlRng PnlRng;
struct _PnlRng
```

- void pnl\_rng\_free (PnlRng \*\*) Description Free a PnlRng .
- PnlRng \* pnl\_rng\_create (int type)

  Description Create a PnlRng corresponding to type which can be any of the values

  PNL\_RNG\_XXX listed in Table 2 which correspond to pseudo random number generators.

  Once a generator has been created, you must call pnl\_rng\_seed before using it.
- void pnl\_rng\_sseed (PnlRng \*rng, unsigned long int s)

  Description Set the seed of the genrator rng using s. If s=0, then a default seed (depending on the generator) is used.
- int pnl\_rng\_sdim (PnlRng \*rng, int dim)

  Description Set the dimension of the state space for a QMC generator and initializes it accordingly. Returns OK if the generator has been initialized properly and FAIL otherwise.
- PnlRng \* pnl\_rng\_copy (const PnlRng \*rng)
  Description Create a copy of rng.
- void pnl\_rng\_clone (PnlRng \*dest, const PnlRng \*src)

  Description Copy the content of src into the already existing basis dest. On exit, src and dest are identical but independent.
- PnlRng \* pnl\_rng\_dcmt\_create\_id (int id, ulong seed)

  Description Create a generator with type PNL\_RNG\_DCMT and identifier id. Two generators with different ids are independent. Note that the returned generator must be initialized with pnl\_rng\_sseed before usage. The identifier id can for instance correspond to the thread number or the processor rank in parallel computing.
- PnlRng \*\* pnl\_rng\_dcmt\_create\_array\_id (int start\_id, int max\_id, ulong seed, int \*count)

  Description Create an array of generators with types PNL\_RNG\_DCMT and identifiers linearly varying between start\_id and max\_id. The number of generators created is max\_id start\_id + 1. All the generators are independent. Note that each generator of the returned array must be initialized with pnl rng sseed before usage.

• PnlRng \*\* pnl\_rng\_dcmt\_create\_array (int n, ulong seed, int \*count)

Description Create an array of n independent DCMT. seed is the seed used to initialize the Mersenne Twister generator internally used to find new DCMT. On exit, count contains the number of generators actually created. Before using the generators, you must initialize each of them by calling the function pnl\_rng\_sseed count times.

Some auxiliary functions internally used (to be used with caution)

- PnlRng \* pnl\_rng\_new ()
  Description Create an empty PnlRng .
- void pnl\_rng\_init (PnlRng \*rng, int type)

  Description Initialize an empty PnlRng as returned by pnl\_rng\_new to become a generator of type type which can be any of the values PNL\_RNG\_XXX listed in Table 2 which correspond to pseudo random number generators. Calling pnl\_rng\_create is equivalent to calling first pnl\_rng\_new and then pnl\_rng\_init.
- PnlRng \* pnl\_rng\_get\_from\_id (int id)

  Description Return the global generator described by its macro name. The variable id can be any of the values PNL\_RNG\_XXX listed in Table 2.

The following functions return one sample from the specified distribution.

- int pnl\_rng\_bernoulli (double p, PnlRng \*rng)

  Description Generate a sample from the Bernouilli law on {0,1} with parameter p.
- long pnl\_rng\_poisson (double lambda, PnlRng \*rng)
   Description Generate a sample from the Poisson law with parameter lambda.
- double pnl\_rng\_exp (double lambda, PnlRng \*rng)
   Description Generate a sample from the Exponential law with parameter lambda.
- double **pnl\_rng\_dblexp** (double lambda\_p, double lambda\_m, double p, **PnlRng** \*rng)

Description Generate a sample from the asymmetric exponential distribution with density

$$p\lambda_p e^{-\lambda_p y} 1_{\{y>0\}} + (1-p)\lambda_m e^{-\lambda_m |y|} 1_{\{y<0\}}$$

where  $\lambda_p > 0, \lambda_m > 0$  and  $p \in [0, 1]$ .

- double **pnl\_rng\_uni** (**PnlRng** \*rng)

  Description Generate a sample from the Uniform law on [0, 1].
- double  $pnl\_rng\_uni\_ab$  (double a, double b, PnlRng \*rng)

  Description Generate a sample from the Uniform law on [a, b].
- double pnl\_rng\_normal (PnlRng \*rng)
   Description Generate a sample from the standard normal distribution.
- double pnl\_rng\_lognormal (double m, double sigma2, PnlRng \*rng)

  Description Generate a sample from the log-normal distribution. The underlying normal distribution has mean m and variance sigma2.

- double pnl\_rng\_invgauss (double mu, double lambda, PnlRng \*rng)

  Description Generate a sample from the inverse Gaussian distribution with mean mu
  and shape parameter lambda.
- long pnl\_rng\_poisson1 (double lambda, double t,PnlRng \*rng)

  Description Generate a sample from a Poisson process with intensity lambda at time t.
- double pnl\_rng\_gamma (double a, double b, PnlRng \*rng) Description Generate a sample from the  $\Gamma(a,b)$  distribution.
- double pnl\_rng\_chi2 (double df, PnlRng \*rng) Description Generate a sample from the centered  $\chi^2(df)$  distribution.
- double pnl\_rng\_ncchi2 (double df, double xnonc, PnlRng \*rng)

  Description Generate a sample from the non central  $\chi^2$  distribution with df degrees of freedom and non central parameter xnonc.
- double pnl\_rng\_bessel (double v, double a,PnlRng \*rng)
   Description Generate a sample from the Bessel distribution with parameters v > -1 and a > 0.
- double pnl\_rng\_gauss (int d, int create\_or\_retrieve, int index, PnlRng \*rng)
   Description The second argument can be either CREATE (to actually draw the sample)
   or RETRIEVE (to retrieve that element of index index). With CREATE, it draws d random normal variables and stores them for future usage. They can be withdrawn using RETRIEVE with the index of the number to be retrieved.

The following functions take an already existing PnlVect \*as first argument and fill each entry of the vector with a sample from the specified distribution. All the entries are independent. The difference between n-samples from a distribution in dimension 1, and one sample from the same distribution in dimension n only matters when using a **quasi** random number generator.

- void pnl\_vect\_rng\_bernoulli (PnlVect \*V, int samples, double a, double b, double p, PnlRng \*rng)
   Description Simulate an i.i.d. sample from the Bernoulli distribution with values in a,b and parameter p. The result is stored in V.
- void pnl\_vect\_rng\_bernoulli\_d (PnlVect \*V, int dimension, const PnlVect \*a, const PnlVect \*b, const PnlVect \*p, PnlRng \*rng)

  Description Simulate a random vector according to the Bernoulli distribution with values in {a,b} and parameter p. The result is stored in V, ie. V(i) follows a Bernoulli distribution on {a(i), b(i)} with parameter p(i).
- void pnl\_vect\_rng\_poisson (PnlVect \*V, int samples, double lambda, PnlRng \*rng)
   Description Simulate an i.i.d. sample from the Poisson distribution with parameter lambda. The result is stored in V. Note that, we are using double based vectors and not integer based vectors.
- void pnl\_vect\_rng\_poisson\_d (PnlVect \*V, int dimension, const PnlVect \*lambda, PnlRng \*rng)

Description Simulate a random vector according to the Poisson distribution with **vector** parameter lambda. The result is stored in V, ie. V(i) follows a Poisson distribution with parameter lambda(i). Note that, we are using double based vectors and not integer based vectors.

- void **pnl\_vect\_rng\_uni** (PnlVect \*G, int samples, double a, double b, PnlRng \*rng) Description G is a vector of independent and identically distributed samples from the uniform distribution on [a, b].
- void pnl\_vect\_rng\_normal (PnlVect \*G, int samples, PnlRng \*rng)
   Description G is a vector of independent and identically distributed samples from the standard normal distribution.
- void  $pnl\_vect\_rng\_uni\_d$  (PnlVect \*G, int d, double a, double b, PnlRng \*rng) Description G is a sample from the uniform distribution on  $[a, b]^d$ .
- void pnl\_vect\_rng\_normal\_d (PnlVect \*G, int d, PnlRng \*rng)

  Description G is a sample from the d-dimensional standard normal distribution.

The following functions take an already existing PnlMat \*as first argument and fill each entry of the matrix with a sample from the specified distribution. All the entries are independent. On return, the matrix M is of size samples x dimension. The rows of M are independent and identically distributed. Each row is a sample from the given law in dimension dimension.

- void pnl\_mat\_rng\_uni (PnlMat \*M, int samples, int d, const PnlVect \*a, const PnlVect \*b, PnlRng \*rng)

  Description M contains samples samples from the uniform distribution on  $\prod_{i=1}^{d} [a_i, b_i]$ .
- void pnl\_mat\_rng\_uni2 (PnlMat \*M, int samples, int d, double a, double b, PnlRng \*rng)
   Description M contains samples samples from the uniform distribution on [a, b]<sup>d</sup>.
- void pnl\_mat\_rng\_normal (PnlMat \*M, int samples, int d, PnlRng \*rng)
   Description M contains samples samples from the d-dimensional standard normal distribution.
- void pnl\_mat\_rng\_bernoulli (PnlMat \*M, int samples, int dimension, const PnlVect \*a, const PnlVect \*b, const PnlVect \*p, PnlRng \*rng)

  Description Compute a random matrix with independent rows, each of them having a vector Bernoulli distribution, ie. M(i, j) follows a Bernoulli distribution on {a(j), b(j)} with parameter p(j).
- void pnl\_mat\_rng\_poisson (PnlMat \*M, int samples, int dimension, const PnlVect \*lambda, PnlRng \*rng)

  Description Compute a random matrix with independent rows, each of them having a vector Poisson distribution, ie. M(i, j) follows a Poisson distribution with parameter p(j).

Some examples

```
#include <stdlib.h>
#include "pnl/pnl_random.h"
int main ()
  int i, M;
  PnlRng *rng = pnl_rng_create(PNL_RNG_MERSENNE);
  PnlVect *v = pnl_vect_new();
  M = 10000;
  /* rng must be initialized. When sseed=0, a default
     value depending on the generator is used */
     pnl_rng_sseed(rng, 0);
  for (i=0; i<M; i++)
    /* Simulates a normal random vector in R^{10} */
    pnl_vect_rng_normal(v, 10, rng);
    /* Do something with v */
 pnl_vect_free(&v);
  pnl_rng_free(&rng); /* Frees the generator */
  exit(0);
}
#include <stdlib.h>
#include <time.h>
#include "pnl/pnl_random.h"
int main ()
  int i, M;
  double E;
  PnlRng *rng = pnl_rng_create(PNL_RNG_MERSENNE);
  M = 10000;
  /* rng must be initialized. */
  pnl_rng_sseed(rng, time (NULL));
  for (i=0; i<M; i++)
    /* Simulates an exponential random variable */
   E = pnl_rng_exp(1, rng);
    /* Do something with E */
```

```
pnl_rng_free(&rng); /* Frees the generator */
exit(0);
}
```

# 6.2 The rand interface (deprecated)

**Note**: For backward compatibility with older versions of the PNL, we still provide the old rand interface to random number generation although we strongly encourage users to use the new rng interface (see section 6.1).

Every generator is identified by an integer valued macro. One must **NOT** refer to a generator using directly the value of the macro PNL\_RNG\_XXX because there is no warranty that the order used to store the generators will remain the same in future releases. Instead, one should call generators directly using their macro names.

The initial seeds of all the generators are fixed by the function pnl\_rand\_init but you can change it by calling pnl\_rand\_sseed.

Before starting to use random number generators, you must initialize them by calling

- int pnl\_rand\_init (int type\_generator, int simulation\_dim, long samples)

  Description It resets the sample counter to 0 and checks that the generator described by type\_generator can actually generate samples in dimension simulation\_dim and fixes the seed.
- int pnl\_rand\_or\_quasi (int type\_generator)

  Description Return the type the generator of index type\_generator, PNL\_MC or PNL\_QMC
- void pnl\_rand\_sseed ((int type\_generator, unsigned long int seed))

  Description It sets the seed of the generator type generator with seed.
- const char \* pnl\_rand\_name (int type\_generator)

  Description Return the name of the generator of index type\_generator

Once a generator is chosen, there are several functions available in the library to draw samples according to a given law.

The following functions return one sample from a specified law.

- int pnl\_rand\_bernoulli (double p, int type\_generator)

  Description Generate a sample from the Bernoulli law on {0, 1} with parameter p.
- long pnl\_rand\_poisson (double lambda, int type\_generator)

  Description Generate a sample from the Poisson law with parameter lambda.
- double pnl\_rand\_exp (double lambda, int type\_generator)
   Description Generate a sample from the Exponential law with parameter lambda.
- double **pnl\_rand\_uni** (int type\_generator)

  Description Generate a sample from the Uniform law on [0, 1].
- double **pnl\_rand\_uni\_ab** (double a, double b, int type\_generator) Description Generate a sample from the Uniform law on [a, b].

- double **pnl\_rand\_normal** (int type\_generator)

  Description Generate a sample from the standard normal distribution.
- long pnl\_rand\_poisson1 (double lambda, double t, int type\_generator)

  Description Generate a sample from a Poisson process with intensity lambda at time t.
- double **pnl\_rand\_gamma** (double a, double b, int type\_generator) Description Generate a sample from the  $\Gamma(a,b)$  distribution.
- double **pnl\_rand\_chi2** (double n, int type\_generator)

  Description Generate a sample from the centered  $\chi^2(n)$  distribution.
- double pnl\_rand\_bessel (double v, double a, int generator)

  Description Generate a sample from the Bessel distribution with parameters v > -1and a > 0.

The following functions take an already existing PnlVect\* as its first argument and fill each entry of the vector with a sample from the specified law. All the entries are independent. The difference between n-samples from a distribution in dimension 1, and one sample from the same distribution in dimension n only matters when using a **Quasi** random number generator.

- void pnl\_vect\_rand\_uni (PnlVect \*G, int samples, double a, double b, int type\_generator)
   Description G is a vector of independent and identically distributed samples from the uniform distribution on [a, b].
- void pnl\_vect\_rand\_normal (PnlVect \*G, int samples, int generator)
   Description G is a vector of independent and identically distributed samples from the standard normal distribution.
- void **pnl\_vect\_rand\_uni\_d** (**PnlVect** \*G, int d, double a, double b, int type\_generator)

  Description G is a sample from the uniform distribution on  $[a, b]^d$ .
- void pnl\_vect\_rand\_normal\_d (PnlVect \*G, int d, int generator)

  Description G is a sample from the d-dimensional standard normal distribution.

The following functions take an already existing PnlMat \* as first argument and fill each entry of the vector with a sample from the specified law. All the entries are in-dependent. On return, the matrix M is of size samples x dimension. The rows of M are independently and identically distributed. Each row is a sample from the given law in dimension dimension.

- void pnl\_mat\_rand\_uni (PnlMat \*M, int samples, int d, const PnlVect \*a, const PnlVect \*b, int type\_generator)

  Description M contains samples samples from the uniform distribution on  $\prod_{i=1}^{d} [a_i, b_i]$ .
- void **pnl\_mat\_rand\_uni2** (**PnlMat** \*M, int samples, int d, double a, double b, int type\_generator)

  Description M contains samples samples from the uniform distribution on [a, b]<sup>d</sup>.
- void **pnl\_mat\_rand\_normal** (**PnlMat** \*M, int samples, int d, int type\_generator) Description M contains **samples** samples from the **d**-dimensional standard normal distribution.

Because of the use of **Quasi** random number generators, you may need to draw a set of samples at once because they represent one sample from a multi-dimensional distribution. The following function enables to draw one sample from the dimension-dimensional standard normal distribution and store it so that you can access the elements individually afterwards.

• double pnl\_rand\_gauss (int d, int create\_or\_retrieve, int index, int type\_generator)

Description The second argument can be either CREATE (to actually draw the sample)

or RETRIEVE (to retrieve that element of index index). With CREATE, it draws d random normal variables and stores them for future usage. They can be withdrawn using

RETRIEVE with the index of the number to be retrieved.

# 7 Function bases and regression

#### 7.1 Overview

To use these functionalities, you should include pnl/pnl\_basis.h.

```
struct PnlBasis_t {
  PnlObject
                object;
  /** The basis type */
  int
                id;
  /** The string to label the basis */
  const char
               *label;
  /** The number of variates */
  int
                nb_variates;
  /** The total number of elements in the basis */
  int
                nb_func;
  /** The tensor matrix */
  PnlMatInt
               *T;
  /** The sparse Tensor matrix */
  PnlSpMatInt *SpT;
  /** The number of functions in the tensor #T */
                len T;
  /** The i-th element of the one dimensional basis. */
  double
              (*f)(double
                             x, int i);
  /** The first derivative of i-th element of the one dimensional basis */
  double
              (*Df)(double
                             x, int i);
  /** The second derivative of the i-th element of the one dimensional basis */
              (*D2f)(double x, int i);
  /** TRUE if the basis is reduced */
  int
                isreduced;
  /** The center of the domain */
  double
               *center;
  /** The inverse of the scaling factor to map the domain to [-1, 1] nb_variates */
               *scale;
  /** An array of additional functions */
  PnlRnFuncR *func_list;
```

```
/** The number of functions in #func_list */
int len_func_list;
};
```

A PnlBasis is a family of multivariate functions with real values. Tow different kinds of functions can be stored in these families: tensor functions — originally, this was the only possibility, and standard multivariate function typed as PnlRnFuncR.

Tensor functions. Tensors functions are built as a tensor product of one dimensional elements. Hence, we only need a tensor matrix T to describe a multi-dimensional basis in terms of the one dimensional one. These tensors functions can be easily evaluated and differentiated twice, see pnl\_basis\_eval, pnl\_basis\_eval\_vect, pnl\_basis\_eval\_D, pnl\_basis\_eval\_D, pnl\_basis\_eval\_D2\_vect, pnl\_basis\_eval\_derivs, pnl\_basis\_eval\_derivs, pnl\_basis\_eval\_derivs vect.

The two tensors T and SpT do actually store the same information — T(i,j) is the degree w.r.t the j-th variable in the i-th function. Originally, we were only using the dense representation T, which is far more convenient to use when building the basis but it slows down the evaluation of the basis by a great deal. To overcome this lack of efficiency, a sparse storage has been added.

| PNL_BASIS_CANONICAL  | for the Canonical polynomials  |
|----------------------|--------------------------------|
| PNL_BASIS_HERMITE    | for the Hermite polynomials    |
| PNL BASIS TCHEBYCHEV | for the Tchebychev polynomials |

Table 3: Names of the bases. See also function pnl\_basis\_type\_register to register more basis types.

The Hermite polynomials are defined by

$$H_n(x) = (-1)^n e^{\frac{x^2}{2}} \frac{d^n}{dx^n} e^{-\frac{x^2}{2}}.$$

If G is a real valued standard normal random variable,  $\mathbb{E}[H_n(G)H_m(G)] = n!1_{\{n=m\}}$ .

Standard multivariate functions. These functions are supposed to be PnlRnFuncR. To make this toolbox more complete, it is now possible to add some extra functions, which are not tensor product. They are stored using an independent mechanism in func\_list. These additional functions are only taken into account by the methods pnl\_basis\_i, pnl\_basis\_i\_vect, pnl\_basis\_eval and pnl\_basis\_eval\_vect. Note in particular that it is not possible to differentiate these functions. To add an extra function to an existing PnlBasis, call the function pnl\_basis\_add\_function.

#### 7.2 Functions

• int pnl\_basis\_type\_register (const char \*name, double (\*f)(double, int), double (\*Df)(double, int), double (\*Df)(double, int))

Description Register a new basis type and return the index to be passed to pnl\_basis\_create. The variable name is a unique string identifier of the family. The variables f,

Df, D2f are the one dimensional basis functions, its first and second order derivatives. Each of these functions must return a double and take two arguments: the first one is the point at which evaluating the basis functions, the second one is the index of function. Here is a toy example to show how the canonical basis is registered (this family is actually already available with the id PNL\_BASIS\_CANONICAL, so the following example may look a little fake)

```
double f(double x, int n) { return pnl_pow_i(x, n); }
double Df(double x, int n) { return n * pnl_pow_i(x, n-1); }
double f(double x, int n) { return n * (n-1) * pnl_pow_i(x, n-2); }
int id = pnl_basis_register ("Canonic", f, Df, D2f);
/*
   * B is the Canonical basis of polynomials with degree less or equal than 2 in  
   * dimension 5.
   */
PnlBasis *B = pnl_basis_create_from_degree (id, 2, 5);
```

- PnlBasis \* pnl\_basis\_new ()
  Description Create an empty PnlBasis .
- void pnl\_basis\_print (const PnlBasis \*B)

  Description Print the characteristics of a basis.
- PnlBasis \* pnl\_basis\_create (int index, int nb\_func, int nb\_variates)

  Description Create a PnlBasis for the family defined by index (see Table 3 and pnl\_basis\_type\_register) with nb\_variates variates. The basis will contain nb\_func.
- PnlBasis \* pnl\_basis\_create\_from\_degree (int index, int degree, int nb\_variates)
  Description Create a PnlBasis for the family defined by index (see Table 3 and pnl\_basis\_type\_register) with total degree less or equal than degree and nb\_variates variates. The total degree is the sum of the partial degrees.
  For instance, calling pnl\_basis\_create\_from\_degree (index, 2, 4) is equivalent to

calling pnl\_basis\_create\_from\_tensor (index, T) where T is given by

$$\begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

- PnlBasis \* pnl\_basis\_create\_from\_prod\_degree (int index, int degree, int nb\_variates)

  Description Create a PnlBasis for the family defined by index (see Table 3 and pnl\_basis\_type\_register) with total degree less or equal than degree and nb\_variates variates. The total degree is the product of MAX(1, d\_i) where the d\_i are the partial degrees.
- PnlBasis \* pnl\_basis\_create\_from\_tensor (int index, PnlMatInt \*T)

  Description Create a PnlBasis for the polynomial family defined by index (see Table 3) using the basis described by the tensor matrix T. The number of lines of T is the number of functions of the basis whereas the numbers of columns of T is the number of variates of the functions. Note that T is not copied inside this function but only its address is stored, so never free T. It will be freed when calling pnl\_basis\_free on the returned object. i

Here is an example of a tensor matrix. Assume you are working with three variate functions, the basis { 1, x, y, z, x^2, xy, yz, z^3} is decomposed in the one dimensional canonical basis using the following tensor matrix

$$\begin{pmatrix}
0 & 0 & 0 \\
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
2 & 0 & 0 \\
1 & 1 & 0 \\
0 & 1 & 1 \\
0 & 0 & 3
\end{pmatrix}$$

• void pnl\_basis\_add\_function (PnlBasis \*b, PnlRnFuncR \*f)
Description Add the function f to the already existing basis b.

- void pnl\_basis\_clone (PnlBasis \*dest, const PnlBasis \*src)

  Description Clone src into dest. The basis dest must already exist before calling this function. On exit, dest and src are identical and independent.
- PnlBasis \* pnl\_basis\_copy (const PnlBasis \*B)
  Description Create a copy of B.
- void pnl\_basis\_set\_from\_tensor (PnlBasis \*b, int index, const PnlMatInt \*T)

  Description Set an alredy existing basis b to a polynomial family defined by index (see Table 3) using the basis described by the tensor matrix T. The number of lines of T is the number of functions of the basis whereas the numbers of columns of T is the number of variates of the functions.

  Same function as pnl basis create from tensor except that it operates on an already
  - Same function as pnl\_basis\_create\_from\_tensor except that it operates on an already existing basis.
- PnlBasis \* pnl\_basis\_create\_from\_hyperbolic\_degree (int index, double degree, double q, int n)

  Description Create a sparse basis of polynomial with n variates. We give the example of the Canonical basis. A canonical polynomial with n variates writes  $X_1^{\alpha_1}X_2^{\alpha_2}...X_n^{\alpha_n}$ . To be a member of the basis, it must satisfy  $(\sum_{i=1}^n \alpha_i^q)^{1/q} \leq degree$ . This kind of basis based on an hyperbolic set of indices gives priority to polynomials associated to low order interaction.
- void pnl\_basis\_free (PnlBasis \*\*basis)
   Description Free a PnlBasis created by pnl\_basis\_create. Beware that basis is the address of a PnlBasis \*.
- void pnl\_basis\_del\_elt (PnlBasis \*B, const PnlVectInt \*d)

  Description Remove the function defined by the tensor product d from an existing basis

  B
- void pnl\_basis\_del\_elt\_i (PnlBasis \*B, int i)
  Description Remove the i-th element of basis B.
- void pnl\_basis\_add\_elt (PnlBasis \*B, const PnlVectInt \*d)

  Description Add the function defined by the tensor d to the Basis B.

Functional regression based on a least square approach often leads to ill conditioned linear systems. One way of improving the stability of the system is to use centered and renormalised polynomials so that the original domain of interest  $\mathcal{D}$  (a subset of  $\mathbb{R}^d$ ) is mapped to  $[-1,1]^d$ . If the domain  $\mathcal{D}$  is rectangular and writes [a,b] where  $a,b \in \mathbb{R}^d$ , the mapping is done by

$$x \in \mathcal{D} \longmapsto \left(\frac{x_i - (b_i + a_i)/2}{(b_i - a_i)/2}\right)_{i=1,\dots,d}$$
 (1)

• void pnl\_basis\_set\_domain (PnlBasis \*B, const PnlVect \*a, const PnlVect \*b)

Description This function declares B as a centered and normalised basis as defined by

Equation 1. Calling this function is equivalent to calling pnl\_basis\_set\_reduced with

center=(b+a)/2 and scale=(b-a)/2.

• void **pnl\_basis\_set\_reduced** (PnlBasis \*B, const PnlVect \*center, const PnlVect \*scale)

Description This function declares B as a centered and normalised basis using the mapping

$$x \in \mathcal{D} \longmapsto \left( \frac{x_i - \mathtt{center}_i}{\mathtt{scale}_i} \right)_{i=1,\cdots,d}$$

• int pnl\_basis\_fit\_ls (PnlBasis \*P, PnlVect \*coef, PnlMat \*x, PnlVect \*y)

Description Compute the coefficients coef defined by

$$coef = \arg\min_{\alpha} \sum_{i=1}^{n} \left( \sum_{j=0}^{N} \alpha_{j} P_{j}(x_{i}) - y_{i} \right)^{2}$$

where N is the number of functions to regress upon and n is the number of points at which the values of the original function are known.  $P_j$  is the j-th basis function. Each row of the matrix x defines the coordinates of one point  $x_i$ . The function to be approximated is defined by the vector y of the values of the function at the points x.

- double pnl\_basis\_ik\_vect (const PnlBasis \*b, const PnlVect \*x, int i, int k) Description An element of a basis writes  $\prod_{l=0}^{\text{nb}_{variates}} \phi_l(x_l)$  where the  $\phi$ 's are one dimensional polynomials. This functions computes the therm  $\phi_k$  of the i-th basis function at the point x.
- double **pnl\_basis\_i\_vect** (const **PnlBasis** \*b, const **PnlVect** \*x, int i) Description If b is composed of  $f_0, \ldots, f_{nb \text{ func}-1}$ , then this function returns  $f_i(x)$ .
- double **pnl\_basis\_i\_D\_vect** (const **PnlBasis** \*b, const **PnlVect** \*x, int i, int j) Description If b is composed of  $f_0, \ldots, f_{\mathtt{nb\_func}-1}$ , then this function returns  $\partial_{x_i} f_i(x)$ .
- double pnl\_basis\_i\_D2\_vect (const PnlBasis \*b, const PnlVect \*x, int i, int j1, int j2)

  Description If b is composed of  $f_0, \ldots, f_{nb\_func-1}$ , then this function returns  $\partial^2_{x_{j1}, x_{j2}} f_i(x)$ .
- void pnl\_basis\_eval\_derivs\_vect (const PnlBasis \*b, const PnlVect \*coef, const PnlVect \*x, double \*fx, PnlVect \*Dfx, PnlMat \*D2fx)

  Description Compute the function, the gradient and the Hessian matrix of  $\sum_{k=0}^{n} \operatorname{coef}_{k} P_{k}(\cdot)$  at the point x. On output, fx contains the value of the function, Dfx its gradient and D2fx its Hessian matrix. This function is optimized and performs much better than calling pnl\_basis\_eval, pnl\_basis\_eval\_D and pnl\_basis\_eval\_D2 sequentially.
- double pnl\_basis\_eval\_vect (const PnlBasis \*basis, const PnlVect \*coef, const PnlVect \*x)

  Description Compute the linear combination of P\_k(x) defined by coef. Given the coefficients computed by the function pnl\_basis\_fit\_ls, this function returns  $\sum_{k=0}^{n} \operatorname{coef}_{k} P_{k}(\mathbf{x})$ .
- double pnl\_basis\_eval\_D\_vect (const PnlBasis \*basis, const PnlVect \*coef, const PnlVect \*x, int i)

Description Compute the derivative with respect to  $x_i$  of the linear combination of  $P_k(x)$  defined by coef. Given the coefficients computed by the function pnl\_basis\_fit\_ls, this function returns  $\partial_{x_i} \sum_{k=0}^{n} \operatorname{coef}_k P_k(x)$  The index i may vary between 0 and  $P->nb_variates - 1$ .

• double pnl\_basis\_eval\_D2\_vect (const PnlBasis \*basis, const PnlVect \*coef, const PnlVect \*x, int i, int j)

Description Compute the derivative with respect to x\_i of the linear combination of P\_k(x) defined by coef. Given the coefficients computed by the function pnl\_basis\_fit\_ls, this function returns  $\partial_{x_i}\partial_{x_j}\sum_{k=0}^n \operatorname{coef}_k P_k(x)$ . The indices i and j may vary between 0 and P->nb\_variates - 1.

The following functions are provided for compatibility purposes but are marked as deprecated. Use the functions with the \_vect extension.

- double pnl\_basis\_ik (const PnlBasis \*b, const double \*x, int i, int k)

  Description Same as function pnl\_basis\_ik\_vect but takes a C array as the point of evaluation.
- double pnl\_basis\_i (PnlBasis \*b, double \*x, int i)

  Description Same as function pnl\_basis\_i\_vect but takes a C array as the point of evaluation.
- double **pnl\_basis\_i\_D** ( const **PnlBasis** \*b, const double \*x, int i, int j )

  Description Same as function pnl\_basis\_i\_D\_vect but takes a C array as the point of evaluation.
- double **pnl\_basis\_i\_D2** (const **PnlBasis** \*b, const double \*x, int i, int j1, int j2) Description Same as function pnl\_basis\_i\_D2\_vect but takes a C array as the point of evaluation.
- double pnl\_basis\_eval (PnlBasis \*P, PnlVect \*coef, double \*x)

  Description Same as function pnl\_basis\_eval\_vect but takes a C array as the point of evaluation.
- double pnl\_basis\_eval\_D (PnlBasis \*P, PnlVect \*coef, double \*x, int i)
   Description Same as function pnl\_basis\_eval\_D\_vect but takes a C array as the point of evaluation.
- double pnl\_basis\_eval\_D2 (PnlBasis \*P, PnlVect \*coef, double \*x, int i, int j)

  Description Same as function pnl\_basis\_eval\_D2\_vect but takes a C array as the point of evaluation.
- void pnl\_basis\_eval\_derivs (PnlBasis \*P, PnlVect \*coef, double \*x, double \*fx, PnlVect \*Dfx, PnlMat \*D2fx)

  Description Same as function pnl\_basis\_eval\_derivs\_vect but takes a C array as the point of evaluation.

### Numerical integration

#### Overview 8.1

To use these functionalities, you should include pnl/pnl\_integration.h.

Numerical integration methods are designed to numerically evaluate the integral over a finite or non finite interval (resp. over a square) of real valued functions defined on  $\mathbb{R}$  (resp. on  $\mathbb{R}^2$ ).

```
typedef struct {
  double (*function) (double x, void *params);
  void *params;
} PnlFunc;
typedef struct {
  double (*function) (double x, double y, void *params);
  void *params;
} PnlFunc2D;
We provide the following two macros to evaluate a PnlFunc or PnlFunc2D at a given point
#define PNL_EVAL_FUNC(F, x) (*((F)->function))(x, (F)->params)
```

```
#define PNL EVAL_FUNC2D(F, x, y) (*((F)->function))(x, y, (F)->params)
```

#### 8.2 **Functions**

- double **pnl\_integration** (**PnlFunc** \*F, double x0, double x1, int n, char \*meth) Description Evaluate  $\int_{x_0}^{x_1} F$  using n discretization steps. The method used to discretize the integral is defined by meth which can be "rect" (rectangle rule), "trap" (trapezoidal rule), "simpson" (Simpson's rule).
- double pnl\_integration\_2d (PnlFunc2D \*F, double x0, double x1, double y0, double y1, int nx, int ny, char \*meth) Description Evaluate  $\int_{[x_0,x_1]\times[y_0,y_1]} F$  using nx (resp. ny) discretization steps for [x0, x1] (resp. [y0, y1]). The method used to discretize the integral is defined by meth which can be "rect" (rectangle rule), "trap" (trapezoidal rule), "simpson" (Simpson's rule).
- int pnl integration qng (PnlFunc \*F, double x0, double x1, double epsabs, double epsrel, double \*result, double \*abserr, int \*neval) Description Evaluate  $\int_{x_0}^{x_1} F$  with an absolute error less than espabs and a relative error less than esprel. The value of the integral is stored in result, while the variables abserr and neval respectively contain the absolute error and the number of function evaluations. This function returns OK if the required accuracy has been reached and FAIL otherwise. This function uses a non-adaptive Gauss Konrod procedure (qng routine from QuadPack).
- int pnl\_integration\_GK (PnlFunc \*F, double x0, double x1, double epsabs, double epsrel, double \*result, double \*abserr, int \*neval)

Description This function is a synonymous of pnl\_integration\_qng and is only available for backward compatibility. It is deprecated, please use pnl\_integration\_qng instead.

- int pnl\_integration\_qng\_2d (PnlFunc2D \*F, double x0, double x1, double y0, double y1, double epsabs, double epsrel, double \*result, double \*abserr, int \*neval) Description Evaluate  $\int_{[x_0,x_1]\times[y_0,y_1]} F$  with an absolute error less than espabs and a relative error less than esprel. The value of the integral is stored in result, while the variables abserr and neval respectively contain the absolute error and the number of function evaluations. This function returns OK if the required accuracy has been reached and FAIL otherwise.
- int pnl\_integration\_GK2D (PnlFunc \*F, double x0, double x1, double epsabs, double epsrel, double \*result, double \*abserr, int \*neval)

  Description This function is a synonymous of pnl\_integration\_qng\_2d and is only available for backward compatibility. It is deprecated, please use pnl\_integration\_qng\_2d instead.
- int pnl\_integration\_qag (PnlFunc \*F, double x0, double x1, double epsabs, int limit, double epsrel, double \*result, double \*abserr, int \*neval)

  Description Evaluate  $\int_{x_0}^{x_1} F$  with an absolute error less than espabs and a relative error less than esprel. x0 and x1 can be non finite (i.e. PNL\_NEGINF or PNL\_POSINF). The value of the integral is stored in result, while the variables abserr and neval respectively contain the absolute error and the number of iterations. limit is the maximum number of subdivisions of the interval (x0,x1) used during the integration. If on input, limit 0, then 750 subdivisions are used. This function returns 0K if the required accuracy has been reached and FAIL otherwise. This function uses some adaptive procedures (qags and qagi routines from QuadPack). This function is able to handle functions F with integrable singularities on the interval [x0,x1].
- gularities, double epsabs, int limit, double epsrel, double \*result, double \*abserr, int \*neval)

  Description Evaluate  $\int_{x_0}^{x_1} F$  for a function F with known singularities listed in singularities. singularities must be a sorted vector which does not contain x0 nor x1. x0 and x1 must be finite. The value of the integral is stored in result, while the variables abserr and neval respectively contain the absolute error and the number of iterations. limit is the maximum number of subdivisions of the interval (x0,x1) used during the integration. If on input, limit = 0, then 750 subdivisions are used. This

• int pnl integration qapp (PnlFunc \*F, double x0, double x1, const PnlVect \*sin-

function returns OK if the required accuracy has been reached and FAIL otherwise. This

#### 9 Fast Fourier Transform

#### 9.1 Overview

The forward Fourier transform of a vector c is defined by

$$z_j = \sum_{k=1}^{N} c_k e^{-i(j-1)(k-1)2\pi/N}, \quad j = 1, \dots, N$$

The inverse Fourier transform enables to recover c from z and is defined by

$$c_k = \sum_{j=1}^{N} z_j e^{i(j-1)(k-1)2\pi/N}, \quad j = 1, \dots, N$$

The coefficients of the Fourier transform of a real function satisfy the following relation

$$z_k = \overline{z_{N-k}},\tag{2}$$

where N is the number of discretization points.

A few remarks on the FFT of real functions and its inverse transform:

- We only need half of the coefficients.
- When a value is known to be real, its imaginary part is not stored. So the imaginary part of the zero-frequency component is never stored as it is known to be zero.
- For a sequence of even length the imaginary part of the frequency n/2 is not stored either, since the symmetry (2) implies that this is purely real too.

**FFTPack storage** The functions use the fftpack storage convention for half-complex sequences. In this convention, the half-complex transform of a real sequence is stored with frequencies in increasing order, starting from zero, with the real and imaginary parts of each frequency in neighboring locations.

The storage scheme is best shown by some examples. The table below shows the output for an odd-length sequence, n=5. The two columns give the correspondence between the 5 values in the half-complex sequence (stored in a PnlVect V) and the values (PnlVectComplex C) that would be returned if the same real input sequence were passed to pnl\_dft\_complex as a complex sequence (with imaginary parts set to 0),

$$C(0) = V(0) + i0,$$

$$C(1) = V(1) + iV(2),$$

$$C(2) = V(3) + iV(4),$$

$$C(3) = V(3) - iV(4) = \overline{C(2)},$$

$$C(4) = V(1) + iV(2) = \overline{C(1)}$$
(3)

The elements of index greater than N/2 of the complex array, as C(3) C(4), are filled in using the symmetry condition.

The next table shows the output for an even-length sequence, n = 6. In the even case there are two values which are purely real,

$$C(0) = V(0) + i0,$$

$$C(1) = V(1) + iV(2),$$

$$C(2) = V(3) + iV(4),$$

$$C(3) = V(5) - i0 = \overline{C(0)},$$

$$C(4) = V(3) - iV(4) = \overline{C(2)},$$

$$C(5) = V(1) + iV(2) = \overline{C(1)}$$

$$(4)$$

#### 9.2 Functions

To use the following functions, you should include pnl/pnl\_fft.h.

The following functions comes from a C version of the Fortran FFTPack library available on http://www.netlib.org/fftpack.

- int pnl\_fft\_inplace (PnlVectComplex \*data)

  Description Compute the FFT of data in place. The original content of data is lost.
- int pnl\_ifft\_inplace (PnlVectComplex \*data)

  Description Compute the inverse FFT of data in place. The original content of data is lost.
- int pnl\_fft (const PnlVectComplex \*in, PnlVectComplex \*out)

  Description Compute the FFT of in and stores it into out.
- int pnl\_ifft (const PnlVectComplex \*in, PnlVectComplex \*out)

  Description Compute the inverse FFT of in and stores it into out.
- int pnl\_fft2 (double \*re, double \*im, int n)

  Description Compute the FFT of the vector of length n whose real (resp. imaginary)

  parts are given by the arrays re (resp. im). The real and imaginary parts of the FFT are respectively stored in re and im on output.
- int pnl\_ifft2 (double \*re, double \*im, int n)

  Description Compute the inverse FFT of the vector of length n whose real (resp. imaginary) parts are given by the arrays re (resp. im). The real and imaginary parts of the inverse FFT are respectively stored in re and im on output.
- int pnl\_real\_fft (const PnlVect \*in, PnlVectComplex \*out)

  Description Compute the FFT of the real valued sequence in and stores it into out.
- int pnl\_real\_ifft (const PnlVect \*in, PnlVectComplex \*out)

  Description Compute the inverse FFT of in and stores it into out.
- int pnl\_real\_fft\_inplace (double \*data, int n)

  Description Compute the FFT of the real valued vector data of length n. The result is stored in data using the FFTPack storage described above, see 9.1.

- int pnl\_real\_ifft\_inplace (double \*data, int n)

  Description Compute the inverse FFT of the vector data of length n. data is supposed to be the FFT coefficients a real valued sequence stored using the FFTPack storage. On output, data contains the inverse FFT.
- int pnl\_real\_fft2 (double \*re, double \*im, int n)

  Description Compute the FFT of the real vector re of length n. im is only used on output to store the imaginary part the FFT. The real part is stored into re
- int pnl\_real\_ifft2 (double \*re, double \*im, int n)

  Description Compute the inverse FFT of the vector re + i \* im of length n, which is supposed to be the FFT of a real valued sequence. On exit, im is unused.
- int pnl\_fft2d\_inplace (PnlMatComplex \*data)

  Description Compute the 2D FFT of data. This function applies a 1D FFT to each row of the matrix and then a 1D FFT to each column of the modified matrix.
- int pnl\_ifft2d\_inplace (PnlMatComplex \*data)

  Description Compute the inverse 2D FFT of data. This function is the inverse of the function pnl\_fft2d\_inplace.
- int pnl\_fft2d (const PnlMatComplex \*in, PnlMatComplex \*out)

  Description Compute the 2D FFT of in and stores it into out.
- int pnl\_ifft2d (const PnlMatComplex \*in, PnlMatComplex \*out)

  Description Compute the inverse 2D FFT of in and stores it into out.
- int pnl\_real\_fft2d (const PnlMat \*in, PnlMatComplex \*out)

  Description Compute the 2D FFT of the real matrix in and stores it into out.
- int pnl\_real\_ifft2d (const PnlMatComplex \*in, PnlMatComplex \*out)

  Description Compute the inverse 2D FFT of the complex matrix in which is known to be the forward 2D FFT a real matrix. The result id stored it into out. Note that this function modifies the input matrix in.

### 10 Inverse Laplace Transform

For a real valued function f such that  $t \mapsto f(t) e^{-\sigma_c t}$  is integrable over  $\mathbb{R}^+$ , we can define its Laplace transform

$$\hat{f}(\lambda) = \int_0^\infty f(t) e^{-\lambda t} dt$$
 for  $\lambda \in \mathbb{C}$  with  $\operatorname{Re}(\lambda) \ge \sigma_c$ .

To use the following functions, you should include pnl/pnl\_laplace.h.

```
typedef struct
{
  dcomplex (*F) (dcomplex x, void *params);
  void *params;
} PnlCmplxFunc;
```

- double pnl\_ilap\_euler (PnlCmplxFunc \*fhat, double t, int N, int M)

  Description Compute f(t) where f is given by its Laplace transform fhat by numerically inverting the Laplace transform using Euler's summation. The values N = M = 15 usually give a very good accuracy. For more details on the accuracy of the method.
- double pnl\_ilap\_cdf\_euler (PnlCmplxFunc \*fhat, double t, double h, int N, int M)
   Description Compute the cumulative distribution function F(t) where F(x) = \int\_0^x f(t) dt
   and f is a density function with values on the positive real linegiven by its Laplace
   transform fhat. The computation is carried out by numerical inversion of the Laplace
   transform using Euler's summation. The values N = M = 15 usually give a very good
   accuracy. The parameter h is the discretization step, the algorithm is very sensitive to
   the choice of h.
- double  $pnl_ilap_fft$  (PnlVect \*res, PnlCmplxFunc \*fhat, double T, double eps) Description Compute f(t) for  $t \in [h, T]$  on a regular grid and stores the values in res, where h = T/size(res). The function f is defined by its Laplace transform fhat, which is numerically inverted using a Fast Fourier Transform algorithm. The size of res is related to the choice of the relative precision eps required on the value of f(t) for all t < T.
- double pnl\_ilap\_gs (PnlFunc \*fhat, double t, int n)
   Description Compute f(t) where f is given by its Laplace transform fhat by numerically inverting the Laplace transform using a weighted combination of different Gaver Stehfest's algorithms. Note that this function does not need the complex valued Laplace transform but only the real valued one. n is the number of terms used in the weighted combination.
- double pnl\_ilap\_gs\_basic (PnlFunc \*fhat, double t, int n)

  Description Compute f(t) where f is given by its Laplace transform fhat by numerically inverting the Laplace transform using Gaver Stehfest's method. Note that this function does not need the complex valued Laplace transform but only the real valued one. n is the number of iterations of the algorithm. Note: This function is provided for test purposes only. The function pnl\_ilap\_gs gives far more accurate results.

## 11 Ordinary differential equations

#### 11.1 Overview

To use these functionalities, you should include pnl/pnl\_integration.h.

These functions are designed for numerically solving n-dimensional first order ordinary differential equation of the general form

$$\frac{dy_i}{dt}(t) = f_i(t, y_1(t), \cdots, y_n(t))$$

The system of equations is defined by the following structure

```
typedef struct
{
   void (*F) (int neqn, double t, const double *y, double *yp, void *params);
```

```
int neqn;
void *params;
} Pn10DEFunc;
```

- int neqn

  Description Number of equations
- void \* params
   Description An untyped structure used to pass extra arguments to the function f defining the system
- void (\* F) (int neqn, double t, const double \*y, double \*yp, void \*params)
   Description After calling the fuction, yp should be defined as follows yp\_i = f\_i(neqn, t, y, params). y and yp should be both of size neqn

We provide the following macro to evaluate a PnlODEFunc at a given point

```
#define PNL_EVAL_ODEFUNC(Fstruct, t, y, yp) \
    (*((Fstruct)->F))((Fstruct)->neqn, t, y, yp, (Fstruct)->params)
```

#### 11.2 Functions

- int pnl\_ode\_rkf45 (PnlODEFunc \*f, double \*y, double t, double t\_out, double relerr, double abserr, int \*flag)

  Description This function computes the solution of the system defined by the PnlODEFunc f at the point t\_out. On input, (t,y) should be the initial condition, abserr,relerr are the maximum absolute and relative errors for local error tests (at each step, abs(local error) should be less that relerr \* abs(y) + abserr). Note that if abserr = 0 or relerr = 0 on input, an optimal value for these variables is computed inside the function The function returns an error OK or FAIL. In case of an OK code, the y contains the solution computed at t\_out, in case of a FAIL code, flag should be examined to determine the reason of the error. Here are the different possible values for flag
  - flag = 2 : integration reached t\_out, it indicates successful return and is the normal mode for continuing integration.
  - flag = 3: integration was not completed because relative error tolerance was too small. relerr has been increased appropriately for continuing.
  - flag = 4: integration was not completed because more than 3000 derivative evaluations were needed. this is approximately 500 steps.
  - flag = 5 : integration was not completed because solution vanished making a pure relative error test impossible. must use non-zero abserr to continue. using the one-step integration mode for one step is a good way to proceed.
  - flag = 6: integration was not completed because requested accuracy could not be achieved using smallest allowable stepsize. user must increase the error tolerance before continued integration can be attempted.

- flag = 7: it is likely that rkf45 is inefficient for solving this problem. too much output is restricting the natural stepsize choice. use the one-step integrator mode. see pnl\_ode\_rkf45\_step.
- flag = 8: invalid input parameters this indicator occurs if any of the following is satisfied - neqn <= 0, t=tout, relerr or abserr <= 0.</p>
- int pnl\_ode\_rkf45\_step (PnlODEFunc \*f, double \*y, double \*t, double t\_out, double \*relerr, double abserr, double \*work, int \*iwork, int \*flag)

  Description Same as pnl\_ode\_rkf45 but it only computes one step of integration in the direction of t\_out. work and iwork are working arrays of size 3 + 6 \* neqn and 5 respectively and should remain untouched between successive calls to the function. On output t holds the point at which integration stopped and y the value of the solution at that point.

### 12 Optimization

To use the functions described in this section, you should include pnl/pnl\_optim.h.

#### 12.1 Linear constrained optimization (linear programming)

#### 12.1.1 Overview

Consider the minimization problem

$$\min_{x} \quad C^{T} x$$
s.t.  $A_{\text{ineq}} x \leq B_{\text{ineq}}$ 

$$A_{\text{eq}} x = B_{\text{eq}}$$

$$x_{\text{min}} \leq x \leq x_{\text{max}}$$

#### 12.1.2 Functions

To solve such a linear problem, we provide a wrapper to the *LPSolve* library (http://lpsolve.sourceforge.net).

- int pnl\_optim\_linprog (const PnlVect \*C, const PnlMat \*A\_ineq, const PnlVect \*B\_ineq, const PnlMat \*A\_eq, const PnlVect \*B\_eq, const PnlVect \*x\_min, const PnlVect \*x\_max, int debug, PnlVect \*xopt, double \*fobj\_opt)

  Description This function has the following arguments:
  - C The coefficients of the linear objective function.
  - A\_ineq The l.h.s matrix of the inequality constraints. Can be NULL.
  - B\_ineq The r.h.s vector of the inequality constraints. The length of B\_ineq must match the number of rows of A\_ineq.
  - A\_eq The l.h.s matrix of the equality constraints. Can be NULL.
  - B\_eq The r.h.s vector of the equality constraints. The length of B\_eq must match the number of rows of A\_ineq.

- x\_min The lower bound on x. If NULL, it means all the components of x must be non negative.
- x\_max The upper bound on x. If NULL, it means +Infinity for all the components.
- debug TRUE or FALSE. If TRUE some debugging details are printed.
- xopt The argmin of the problem.
- fobj\_opt The value of the obective funtion at the optimum xopt

The function returns OK or FAIL.

- int pnl\_optim\_linprog\_sp (const PnlSpMat \*C, const PnlSpMat \*A\_ineq, const PnlVect \*B\_ineq, const PnlSpMat \*A\_eq, const PnlVect \*B\_eq, const PnlVectInt \*index\_min, const PnlVect \*x\_min, const PnlVect \*x\_max, const PnlVect \*x\_max, int debug, PnlVect \*xopt, double \*fobj\_opt)

  Description This function has the following arguments:
  - C The coefficients of the linear obejctive function, given as a sparse matrix with a single column.
  - A\_ineq The l.h.s matrix of the inequality constraints. Can be NULL.
  - B\_ineq The r.h.s vector of the inequality constraints. The length of B\_ineq must match the number of rows of A\_ineq.
  - A\_eq The l.h.s matrix of the equality constraints. Can be NULL.
  - B\_eq The r.h.s vector of the equality constraints. The length of B\_eq must match the number of rows of A\_ineq.
  - index\_min The indices of the variables with a lower bound constraint. The corresponding lower bound is given in x\_min
  - x\_min The lower bound on x. If NULL, it means all the components of x must be non negative. Can be NULL. For non specified variables, the default lower bound is 0.
  - index\_max The indices of the variables with an upper bound constraint. The corresponding lower bound is given in x\_max. Can be NULL.
  - x\_max The upper bound on x. If NULL, it means +Infinity for all the components.
     For non specified variables, the default upper bound is +Infinity..
  - debug TRUE or FALSE. If TRUE some debugging details are printed.
  - xopt The argmin of the problem.
  - fobj\_opt The value of the obective funtion at the optimum xopt

The function returns OK or FAIL.

#### 12.2 Nonlinear constrained optimization

#### 12.2.1 Overview

A standard Constrained Nonlinear Optimization problem can be written as:

(O) 
$$\begin{cases} \min f(x) \\ c^{I}(x) \ge 0 \\ c^{E}(x) = 0 \end{cases}$$

where the function  $f: \mathbb{R}^n \to \mathbb{R}$  is the objective function,  $c^I: \mathbb{R}^n \to \mathbb{R}^{m_I}$  are the inequality constraints and  $c^E: \mathbb{R}^n \to \mathbb{R}^{m_E}$  are the equality constraints. These functions are supposed to be smooth.

In general, the inequality constraints are of the form  $c^{I}(x) = (g(x), x - l, u - x)$ . The vector l and u are the lower and upper bounds on the variables x and g(x) and the non linear inequality constraints.

Under some conditions, if  $x \in \mathbb{R}^n$  is a solution of problem (O), then there exist a vector  $\lambda = (\lambda^I, \lambda^E) \in \mathbb{R}^{m_I} \times \mathbb{R}^{m_E}$ , such that the well known Karush-Kuhn-Tucker (KKT) optimality conditions are satisfied:

$$(P) \left\{ \begin{array}{l} \nabla \ell(x,\lambda^I,\lambda^E) = \nabla f(x) - \nabla c^I(x)\lambda^I - \nabla c^E(x)\lambda^E = 0 \\ c^E(x) = 0 \\ c^I(x) \geq 0 \\ \lambda^I \geq 0 \\ c^I_i(x)\lambda^I_i = 0, \ i = 1...m_I \end{array} \right.$$

l is known as the Lagrangian of the problem  $(O),\,\lambda^I$  and  $\lambda^E$  as the dual variables while x is the primal variable.

#### 12.2.2 Functions

To solve an inequality constrained optimization problem, ie  $m_E = 0$ , we provide the following function.

• int pnl\_optim\_intpoints\_bfgs\_solve (PnlRnFuncR\*func, PnlRnFuncRm\*grad\_func, PnlRnFuncRm\*nl\_constraints, PnlVect \*lower\_bounds, PnlVect \*upper\_bounds, PnlVect \*x\_input, double tolerance, int iter\_max, int print\_inner\_steps, PnlVect \*output)

Description This function has the following arguments:

- func is the function to minimize f.
- grad is the gradient of f. If this gradient is not available, then enter grad=NULL. In this case, finite difference will be used to estimate the gradient.
- nl\_constraints is the function g(x), ie the non linear inequality constraints.
- lower\_bounds are the lower bounds on x. Can be NULL if there is no lower bound.
- upper\_bounds are the upper bounds on x. Can be NULL if there is no upper bound.
- x\_input is the initial point where the algorithm starts.
- tolerance is the precision required in solving (P).
- iter\_max is the maximum number of iterations in the algorithm.
- print\_algo\_steps is a flag to decide to print information.
- x\_output is the point where the algorithm stops.

The algorithm returns an int, its value depends on the output status of the algorithm. We have 4 cases:

- 0: Failure: Initial point is not strictly feasible.
- 1: Step is too small, we stop the algorithm.
- 2: Maximum number of iterations reached.
- 3: A solution has been found up to the required accuracy.

The last case is equivalent to the two inequalities:

$$||\nabla \ell(x,\lambda^I)||_{\infty} = ||\nabla f(x) - \nabla c^I(x)\lambda^I||_{\infty} < \text{tolerance}$$
 
$$||c^I(x)\lambda^I||_{\infty} < \text{tolerance}$$

where  $c^{I}(x)$  \*  $\lambda^{I}$  where '.\*' denotes the term by term multiplication.

The first inequality is known as the optimality condition, the second one as the complementarity condition.

**Remarks** Our implementation requires the initial point  $x_0$  to be strictly feasible, ie:  $c(x_0) > 0$ . The algorithm tries to find a pair  $(x, \lambda)$  solving the Equations (P), but this does not guarantee that x is a global minimum of f on the set  $\{c(x) \geq 0\}$ .

## 13 Root finding

#### 13.1 Overview

To provide a uniformed framework to root finding functions, we use several structures for storing different kind of functions. The pointer params is used to store the extra parameters. These new types come with dedicated macros starting in PNL\_EVAL to evaluate the function and their Jacobian.

```
/*
 * f: R --> R
 * The function pointer returns f(x)
 *
typedef struct {
  double (*F) (double x, void *params);
  void *params;
} PnlFunc;
#define PNL_EVAL_FUNC(Fstruct, x) (*((Fstruct)->F))(x, (Fstruct)->params)

/*
 * f: R^2 --> R
 * The function pointer returns f(x)
 *
typedef struct {
```

```
double (*F) (double x, double y, void *params);
  void *params;
} PnlFunc2D ;
\#define PNL_EVAL_FUNC2D(Fstruct, x, y) (*((Fstruct)->F))(x, y, (Fstruct)->params)
/*
 * f: R --> R
 * The function pointer computes f(x) and Df(x) and stores them in fx
 * and dfx respectively
typedef struct {
  void (*F) (double x, double *fx, double *dfx, void *params);
  void *params;
} PnlFuncDFunc ;
#define PNL_EVAL_FUNC_FDF(Fstruct, x, fx, dfx) (*((Fstruct)->F))(x, fx, dfx, (Fstruct)->pa
/*
 * f: R^n --> R
 * The function pointer returns f(x)
typedef struct {
  double (*F) (const PnlVect *x, void *params);
  void *params;
} PnlRnFuncR ;
#define PNL_EVAL_RNFUNCR(Fstruct, x) (*((Fstruct)->F))(x, (Fstruct)->params)
/*
 * f: R^n --> R^m
 * The function pointer computes the vector f(x) and stores it in
 * fx (vector of size m)
typedef struct {
  void (*F) (const PnlVect *x, PnlVect *fx, void *params);
  void *params;
} PnlRnFuncRm ;
#define PNL_EVAL_RNFUNCRM(Fstruct, x, fx) (*((Fstruct)->F))(x, fx, (Fstruct)->params)
 * Synonymous of PnlRnFuncRm for f:R^n --> R^n
typedef PnlRnFuncRm PnlRnFuncRn;
#define PNL_EVAL_RNFUNCRN PNL_EVAL_RNFUNCRM
```

```
/*
 * f: R^n --> R^m
* The function pointer computes the vector f(x) and stores it in fx
* (vector of size m)
 * The Dfunction pointer computes the matrix Df(x) and stores it in dfx
  (matrix of size m x n)
typedef struct {
  void (*F) (const PnlVect *x, PnlVect *fx, void *params);
  void (*DF) (const PnlVect *x, PnlMat *dfx, void *params);
  void (*FDF) (const PnlVect *x, PnlVect *fx, PnlMat *dfx, void *params);
  void *params;
} PnlRnFuncRmDFunc ;
#define PNL_EVAL_RNFUNCRM_DF(Fstruct, x, dfx) \
    (*((Fstruct)->Dfunction))(x, dfx, (Fstruct)->params)
#define PNL_EVAL_RNFUNCRM_FDF(Fstruct, x, fx, dfx) \
    (*((Fstruct)->F))(x, fx, dfx, (Fstruct)->params)
#define PNL_EVAL_RNFUNCRM_F_DF(Fstruct, x, fx, dfx)
      if ( (Fstruct)->FDF != NULL )
        {
          PNL_EVAL_RNFUNCRN_FDF (Fstruct, x, fx, dfx);
        }
      else
        {
          PNL_EVAL_RNFUNCRN (Fstruct, x, fx);
          PNL_EVAL_RNFUNCRN_DF (Fstruct, x, dfx);
/*
 * Synonymous of PnlRnFuncRmDFunc for f:R^n --> R^m
typedef PnlRnFuncRmDFunc PnlRnFuncRnDFunc;
#define PNL_EVAL_RNFUNCRN_DF PNL_EVAL_RNFUNCRM_DF
#define PNL_EVAL_RNFUNCRN_FDF PNL_EVAL_RNFUNCRM_FDF
#define PNL_EVAL_RNFUNCRN_F_DF PNL_EVAL_RNFUNCRM_F_DF
```

### 13.2 Functions

To use the following functions, you should include pnl/pnl\_root.h.

#### Real valued functions of a real argument

- double pnl\_root\_brent (PnlFunc \*F, double x1, double x2, double \*tol)

  Description Find the root of F between x1 and x2 with an accuracy of order tol. On exit tol is an upper bound of the error.
- int pnl\_root\_newton\_bisection (PnlFuncDFunc \*Func, double x\_min, double x\_max, double tol, int N\_Max, double \*res)

  Description Find the root of F between x1 and x2 with an accuracy of order tol and

a maximum of N\_max iterations. On exit, the root is stored in res. Note that the function Func must also compute the first derivative of the function. This function relies on combining Newton's approach with a bisection technique.

• int pnl\_root\_newton (PnlFuncDFunc \*Func, double x0, double x\_eps, double fx\_eps, int max\_iter, double \*res)

Description Find the root of f starting from x0 using Newton's method with descent direction given by the inverse of the derivative, ie.  $d_k = f(x_k)/f'(x_k)$ . Armijo's line search is used to make sure |f| decreases along the iterations.  $\alpha_k = \max\{\gamma^j : j \geq 0\}$  such that

$$|f(x_k + \alpha_k d_k)| \le |f(x_k)|(1 - \omega \alpha_k).$$

In this implementation,  $\omega = 10^{-4}$  and  $\gamma = 1/2$ . The algorithm stops when one of the three following conditions is met:

- the maximum number of iterations max\_iter is reached;
- the last improvement over x is smaller that  $x * x_eps$ ;
- at the current position |f(x)| < fx\_eps

On exit, the root is stored in res.

int pnl\_root\_bisection (PnlFunc \*Func, double xmin, double xmax, double epsrel, double espabs, int N\_max, double \*res)
 Description Find the root of F between x1 and x2 with the accuracy |x2 - x1| < epsrel \* x1 + epsabs or with the maximum number of iterations N\_max. On exit, res = (x2 + x1) / 2.</li>

#### Vector valued functions with several arguments

• int pnl\_multiroot\_newton (PnlRnFuncRnDFunc \*func, const PnlVect \*x0, double x\_eps, double fx\_eps, int max\_iter, int verbose, PnlVect \*res)

Description Find the root of func starting from x0 using Newton's method with descent direction given by the inverse of the Jacobian matrix, ie.  $d_k = (\nabla f(x_k))^{-1} f(x_k)$ . Armijo's line search is used to make sure |f| decreases along the iterations.  $\alpha_k = \max\{\gamma^j : j \geq 0\}$  such that

$$|f(x_k + \alpha_k d_k)| \le |f(x_k)|(1 - \omega \alpha_k).$$

In this implementation,  $\omega = 10^{-4}$  and  $\gamma = 1/2$ . The algorithm stops when one of the three following conditions is met:

- the maximum number of iterations max\_iter is reached;
- the norm of the last improvement over x is smaller that  $|x| * x_eps$ ;
- at the current position  $|f(x)| < fx_{eps}$

On exit, the root is stored in res. Note that the function F must also compute the first derivative of the function. When defining Func, you must either define Func->F and Func->DF or Func->FDF.

We provide two wrappers for calling minpack routines.

- int pnl\_root\_fsolve (PnlRnFuncRnDFunc \*f, PnlVect \*x, PnlVect \*fx, double xtol, int maxfev, int \*nfev, PnlVect \*scale, int error\_msg)

  Description Compute the root of a function  $f: \mathbb{R}^n \longmapsto \mathbb{R}^n$ . Note that the number of components of f must be equal to the number of variates of f. This function returns OK or FAIL if something went wrong.
  - f is a pointer to a PnlRnFuncRnDFunc used to store the function whose root is to be found. f can also store the Jacobian of the function, if not it is computed using finite differences (see the file examples/minpack\_test.c for a usage example).
  - x contains on input the starting point of the search and an approximation of the root of f on output,
  - xtol is the precision required on x, if set to 0 a default value is used.

f->FDF can be NULL because it is not used in this function.

- maxfev is the maximum number of evaluations of the function f before the algorithm returns, if set to 0, a coherent number is determined internally.
- nfev contains on output the number of evaluations of f during the algorithm,
- scale is a vector used to rescale x in a way that each coordinate of the solution is approximately of order 1 after rescaling. If on input scale=NULL, a scaling vector is computed internally by the algorithm.
- error\_msg is a boolean (TRUE or FALSE) to specify if an error message should be printed when the algorithm stops before having converged.
- On output, fx contains f(x).
- int pnl\_root\_fsolve\_lsq (PnlRnFuncRmDFunc \*f, PnlVect \*x, int m, PnlVect \*fx, double xtol, double ftol, double gtol, int maxfev, int \*nfev, PnlVect \*scale, int error\_-msg)

Description Compute the root of  $x \in \mathbb{R}^n \longmapsto \sum_{i=1}^m f_i(x)^2$ , note that there is no reason why m should be equal to n.

#### Parameters

**Parameters** 

- f is a pointer to a PnlRnFuncRmDFunc used to store the function whose root is to be found. f can also store the Jacobian of the function, if not it is computed using finite differences (see the file examples/minpack\_test.c for a usage example).
   f->FDF can be NULL because it is not used in this function.
- x contains on input the starting point of the search and an approximation of the root of f on output,
- m is the number of components of f,
- xtol is the precision required on x, if set to 0 a default value is used.
- ftol is the precision required on f, if set to 0 a default value is used.
- gtol is the precision required on the Jacobian of f, if set to 0 a default value is used.

- maxfev is the maximum number of evaluations of the function f before the algorithm returns, if set to 0, a coherent number is determined internally.
- nfev contains on output the number of evaluations of f during the algorithm,
- scale is a vector used to rescale x in a way that each coordinate of the solution is approximately of order 1 after rescaling. If on input scale=NULL, a scaling vector is computed internally by the algorithm.
- error\_msg is a boolean (TRUE or FALSE) to specify if an error message should be printed when the algorithm stops before having converged.
- On output, fx contains f(x).

### 14 Special functions

The special function approximations are defined in the header pnl/pnl\_specfun.h.

Most of these functions rely on the *Cephes* library which uses its own error mechanism which can be activated or deactivated using the two following functions

- void **pnl\_deactivate\_mtherr** ()

  Description Deactivate Cephes error mechanism
- void **pnl\_activate\_mtherr** ()

  Description Activate Cephes error mechanism

### 14.1 Real Bessel functions

- double **pnl\_bessel\_i** (double v, double x)

  Description Modified Bessel function of the first kind of order v.
- double **pnl\_bessel\_i\_scaled** (double v, double x)

  Description Modified Bessel function of the first kind of order v divided by  $e^{|x|}$ .
- double **pnl\_bessel\_rati** (double v, double x)

  Description Ratio of modified Bessel functions of the first kind :  $I_{v+1}(x)/I_v(x)$ .
- double pnl\_bessel\_j (double v, double x)
   Description Bessel function of the first kind of order v.
- double **pnl\_bessel\_j\_scaled** (double v, double x)

  Description Bessel function of the first kind of order v. Same function as pnl\_bessel\_j.
- double pnl\_bessel\_y (double v, double x)
   Description Modified Bessel function of the second kind of order v.
- double pnl\_bessel\_y\_scaled (double v, double x)
   Description Modified Bessel function of the second kind of order v. Same function as pnl\_bessel\_y.
- double pnl\_bessel\_k (double v, double x)
   Description Bessel function of the third kind of order v.

- double  $pnl\_bessel\_k\_scaled$  (double v, double x)

  Description Bessel function of the third kind of order v multiplied by  $e^x$ .
- dcomplex **pnl\_bessel\_h1** (double v, double x)

  Description Hankel function of the first kind of order v.
- dcomplex pnl\_bessel\_h1\_scaled (double v, double x)

  Description Hankel function of the first kind of order v and divided by  $e^{Ix}$ .
- dcomplex **pnl\_bessel\_h2** (double v, double x)

  Description Hankel function of the second kind of order v.
- dcomplex pnl\_bessel\_h2\_scaled (double v, double x)

  Description Hankel function of the second kind of order v and multiplied by  $e^{Ix}$ .

#### 14.2 Complex Bessel functions

- dcomplex pnl\_complex\_bessel\_i (double v, dcomplex z)

  Description Complex Modified Bessel function of the first kind of order v.
- dcomplex pnl\_complex\_bessel\_i\_scaled (double v, dcomplex z) Description Complex Modified Bessel function of the first kind of order v divided by  $e^{|Creal(z)|}$
- dcomplex pnl\_complex\_bessel\_rati (double v, dcomplex x) Description Ratio of complex modified Bessel functions of the first kind :  $I_{v+1}(x)/I_v(x)$ .
- dcomplex **pnl\_complex\_bessel\_j** (double v, dcomplex z)

  Description Complex Bessel function of the first kind of order v.
- dcomplex pnl\_complex\_bessel\_j\_scaled (double v, dcomplex z) Description Complex Bessel function of the first kind of order v divided by  $e^{|Cimag(z)|}$ .
- dcomplex pnl\_complex\_bessel\_y (double v, dcomplex z)

  Description Complex Modified Bessel function of the second kind of order v.
- dcomplex pnl\_complex\_bessel\_y\_scaled (double v, dcomplex z) Description Complex Modified Bessel function of the second kind of order v divided by  $_{\rho}|Cimag(z)|$
- dcomplex pnl\_complex\_bessel\_k (double v, dcomplex z)
   Description Complex Bessel function of the third kind of order v.
- dcomplex pnl\_complex\_bessel\_k\_scaled (double v, dcomplex z)

  Description Complex Bessel function of the third kind of order v multiplied by  $e^z$ .
- dcomplex **pnl\_complex\_bessel\_h1** (double v, dcomplex z)

  Description Complex Hankel function of the first kind of order v.
- dcomplex pnl\_complex\_bessel\_h1\_scaled (double v, dcomplex z)

  Description Complex Hankel function of the first kind of order v and divided by  $e^{Iz}$ .

- dcomplex pnl\_complex\_bessel\_h2 (double v, dcomplex z)

  Description Complex Hankel function of the second kind of order v.
- dcomplex pnl\_complex\_bessel\_h2\_scaled (double v, dcomplex z) Description Complex Hankel function of the second kind of order v and multiplied by  $e^{Iz}$ .

#### 14.3 Error functions

- double pnl\_sf\_erf (double x) Description Compute the error function  $\frac{2}{\pi} \int_0^x e^{-t^2} dt$ .
- dcomplex pnl\_sf\_complex\_erf (dcomplex z)

  Description Same as pnl\_sf\_erf for complex arguments.
- double pnl\_sf\_erfc (double x)
   Description Compute the complementary error function 1. erf(x).
- dcomplex pnl\_sf\_complex\_erfc (dcomplex x)

  Description Same as pnl\_sf\_erfc for complex arguments.
- double  $pnl\_sf\_erfcx$  (double x) Description Compute the scaled complementary error function of x, defined by  $e^{x^2} \operatorname{erfc}(x)$ .
- dcomplex pnl\_sf\_complex\_erfcx (dcomplex z)

  Description Same as pnl\_sf\_erfcx for complex arguments. Note that erfcx(-i x) = w(x).
- dcomplex **pnl\_sf\_w** (dcomplex z) Description Compute  $e^{-z^2}$  erfc(-iz).
- double pnl\_sf\_w\_im (double x) Description Compute 2 Dawson $(x)/\sqrt{\pi}$
- double pnl\_sf\_erfi (double x)

  Description Compute -i erf(i z)
- dcomplex pnl\_sf\_complex\_erfi (dcomplex z)

  Description Same as pnl\_sf\_erfi for complex arguments.
- double **pnl\_sf\_dawson** (double x) Description Compute  $\sqrt{\pi}/2 e^{-x^2}$  erfi(x).
- dcomplex pnl\_sf\_complex\_dawson (dcomplex z)

  Description Same as pnl\_sf\_dawson for complex arguments.
- double **pnl\_sf\_log\_erf** (double x)

  Description Compute log pnl\_sf\_erf(x)
- double pnl\_sf\_log\_erfc (double x)
   Description Compute log pnl\_sf\_erfc(x)

#### 14.4 Gamma functions

For x > 0, the Gamma Function is defined by

$$\Gamma(x) = \int_0^\infty e^{-u} u^{x-1} du.$$

- double  $pnl\_sf\_fact$  (int n) Description Computes factorial of  $n \Gamma(n+1)$ .
- double pnl\_sf\_gamma (double x) Description Computes  $\Gamma(x), x \ge 0$
- double pnl\_sf\_log\_gamma (double x) Description Computes  $\log(\Gamma(x)), x \geq 0$
- int pnl\_sf\_log\_gamma\_sgn (double x, double \*y, int \*sgn)

  Description Computes  $y = \log(|\Gamma(x)|)$  for x > 0 sgn contains the sign of  $\Gamma(x)$  (-1 or +1).
- double **pnl\_sf\_choose** (int n, int k)

  Description Computes the binomial coefficient  $\binom{n}{k} = \frac{n!}{k!(n-k)!}$  for  $0 \le k \le n$  in double precision.

#### 14.5 Digamma function

For x>0, the digamma function  $\psi$  is defined as the logarithmic derivative of the Gamma function  $\Gamma$ 

$$\psi(x) = \frac{d}{dx} \log \Gamma(x) = \frac{\Gamma'(x)}{\Gamma(x)}.$$

The function  $\psi$  admits the following integral representation

$$\psi(x) = \int_0^\infty \left( \frac{e^{-u}}{u} - \frac{e^{-xu}}{1 - e^{-u}} \right).$$

• double  $pnl\_sf\_psi$  (double x) Description Return  $\psi(x)$ .

### 14.6 Incomplete Gamma functions

For  $a \in \mathbb{R}$  and x > 0, the Incomplete Gamma Function is defined by

$$\Gamma(a,x) = \int_{x}^{\infty} e^{-u} u^{a-1} du.$$

A relation similar to the one existing for the standard Gamma function holds

$$\Gamma(a,x) = \frac{-x^a e^{-x} + \Gamma(a+1,x)}{a}.$$

$$\Gamma(a) = \int_0^\infty u^{a-1} e^{-u} du$$

$$P(a,x) = \frac{\Gamma(a) - \Gamma(a,x)}{\Gamma(a)} = \frac{1}{\Gamma(a)} \int_0^x u^{a-1} e^{-u} du$$

$$Q(a,x) = 1 - P(a,x) = \frac{\Gamma(a,x)}{\Gamma(a)} = \frac{1}{\Gamma(a)} \int_x^\infty e^{-u} u^{a-1} du.$$

- double **pnl\_sf\_gamma\_inc** (double a, double x) Description Computes  $\Gamma(a, x)$ ,  $a \in \mathbb{R}, x \geq 0$
- void **pnl\_sf\_gamma\_inc\_P** (double a, double x) Description Computes P(a, x),  $a > 0, x \ge 0$
- void **pnl\_sf\_gamma\_inc\_Q** (double a, double x) Description Computes Q(a, x),  $a > 0, x \ge 0$

### 14.7 Exponential integrals

For x > 0 and  $n \in \mathbb{N}$ , the function  $E_n$  is defined by

$$E_n(x) = \int_1^\infty e^{-xu} u^{-n} du$$

This function is linked to the Incomplete Gamma function by

$$E_n(x) = \int_x^\infty e^{-xu} (xu)^{-n} x^{n-1} d(xu) = x^{n-1} \int_x^\infty e^{-t} t^{-n} dt = x^{n-1} \Gamma(1-n,x),$$

from which we can deduce

$$nE_{n+1}(x) = e^{-x} - xE_n(x).$$

For n > 1, the series expansion is given by

$$E_n(x) = x^{n-1}\Gamma(1-n) + \left[ -\frac{1}{1-n} + \frac{x}{2-n} - \frac{x^2}{2(3-n)} + \frac{x^3}{6(4-n)} - \dots \right].$$

The asymptotic behaviour is given by

$$E_n(x) = \frac{e^{-x}}{x} \left[ 1 - \frac{n}{x} + \frac{n(n+1)}{x^2} + \dots \right].$$

The special case n=1 gives

$$E_1(x) = \int_x^\infty \frac{e^{-u}}{u} du, \quad |\operatorname{Arg}(x)| \ge \pi.$$

For any complex number x with positive real part, this can be written

$$E_1(x) = \int_1^\infty \frac{e^{-ux}}{u} du, \quad \Re(x) \ge 0.$$

By integrating the Taylor expansion of  $e^{-t}/t$ , and extracting the logarithmic singularity, we can derive the following series representation for  $E_1(x)$ ,

$$E_1(x) = -\gamma - \ln x - \sum_{k=1}^{\infty} \frac{(-1)^k x^k}{k \, k!} \qquad |\text{Arg}(x)| < \pi.$$

The function  $E_1$  is linked to the exponential integral  $E_i$ 

$$Ei(x) = \int_{-\infty}^{x} \frac{e^{u}}{u} du = -\int_{-x}^{\infty} \frac{e^{-u}}{u} du \quad \forall x \neq 0.$$

The above definition can be used for positive values of x, but the integral has to be understood in terms of its Cauchy principal value, due to the singularity of the integrand at zero.

$$Ei(-x) = -E_1(x), \quad \Re(x) \ge 0.$$

We deduce,

$$Ei(x) = \gamma + \ln x + \sum_{k=1}^{\infty} \frac{x^k}{k \, k!}, \quad x > 0.$$

For  $x \in \mathbb{R}$ 

$$\Gamma(0,x) = \begin{cases} -Ei(-x) - i\pi & x < 0, \\ -Ei(-x) & x > 0. \end{cases}$$

• double **pnl\_sf\_expint\_En** (int n, double x) Description Computes  $E_n(x)$  for  $n \ge 0, x \ge 0$ , or x > 0 when n = 0 or 1.

#### 14.8 Hypergeometric functions

- double pnl\_sf\_hyperg\_2F1 (double a, double b, double c, double x)
   Description Compute the Gauss hypergeometric function 2F1(a,b,c,x) for |x| < 1 and for x < -1 when b,a,c,(b-a),(c-a),(c-b) are not integers</li>
- double pnl\_sf\_hyperg\_1F1 (double a, double b, double x)

  Description Compute the hypergeometric function 1F1(a,b,x)
- double pnl\_sf\_hyperg\_2F0 (double a, double b, double x)

  Description Compute the hypergeometric function 2F0(a,b,x) for x<0 using the relation  $2F0(a,b,x) = (-x)^{-a}U(a,1+a-b,-\frac{1}{x})$ .
- double pnl\_sf\_hyperg\_0F1 (double c, double x)

  Description Compute the hypergeometric function 0F1(c,x)
- double pnl\_sf\_hyperg\_U (double a, double b, double x)
   Description Compute the confluent hypergeometric function U(a,b,x) with x > 0

### 15 Some bindings

#### 15.1 MPI bindings

#### 15.1.1 Overview

We provide some bindings for the MPI library to natively handle *PnlObjects*. The functionnalities described in this chapter are declared in pnl/pnl\_mpi.h.

#### 15.1.2 Functions

All the following functions return an error code as an integer value. This returned value should be tested against MPI\_SUCCESS to check that no error occurred.

- int pnl\_object\_mpi\_pack\_size (const PnlObject \*Obj, MPI\_Comm comm, int \*size)

  Description Compute in size the amount of space needed to pack Obj.
- int pnl\_object\_mpi\_pack (const PnlObject \*Obj, void \*buf, int bufsize, int \*pos, MPI\_Comm comm)

  Description Pack Obj into buf which must be at least of length size. size must be at least equal to the value returned by pnl\_object\_mpi\_pack\_size.
- int pnl\_object\_mpi\_unpack (PnlObject \*Obj, void \*buf, int bufsize, int \*pos, MPI\_Comm comm)

  Description Unpack the content of buf starting at position pos (unless several objects have been packed contiguously, \*pos should be equal to 0). buf is a contiguous memery area of length bufsize (note that the size is counted in bytes). pos is incremented and is on output the first location in the input buffer after the locations occupied by the message that was unpacked. pos is properly set for a future call to MPI\_Unpack if any.
- int pnl\_object\_mpi\_send (const PnlObject \*Obj, int dest, int tag, MPI\_Comm comm)

  Description Perform a standard-mode blocking send of Obj. The object is sent to the process with rank dest.
- int pnl\_object\_mpi\_ssend (const PnlObject \*Obj, int dest, int tag, MPI\_Comm comm)

  Description Perform a standard-mode synchronous blocking send of Obj. The object is sent to the process with rank dest.
- int pnl\_object\_mpi\_recv (PnlObject \*Obj, int src, int tag, MPI\_Comm comm, MPI\_Status \*status)

  Description Perform a standard-mode blocking receive of Obj. The object is sent to the process with rank dest. Note that Obj should be an already allocated object and that its type should match the true type of the object to be received. src is the rank of the process who sent the object.
- int pnl\_object\_mpi\_bcast (PnlObject \*Obj, int root, MPI\_Comm comm)

  Description Broadcast the object Obj from the process with rank root to all other processes of the group comm.
- int pnl\_object\_mpi\_reduce (PnlObject \*Sendbuf, PnlObject \*Recvbuf, MPI\_Op op, int root, MPI\_Comm comm)

  Description Perform the reduction described by op on the objects Sendbuf and stores the result into Recvbuf. Note that Recvbuf and Sendbuf must be of the same type. The argument root is the index of the root process and comm is a communicator. Not all reductions are implemented for all types. Here is the list of compatible reductions

| MPI_SUM            | PnlVect, PnlVectInt, PnlVectComplex,   |
|--------------------|--|
|                    | PnlMat, PnlMatInt, PnlMatComplex       |
| MPI_PROD, MPI_MAX, | PnlVect, PnlVectInt, PnlMat, PnlMatInt |
| MPI MIN            |  |

For more expect users, we provide the following nonblocking functions.

- int pnl\_object\_mpi\_isend (const PnlObject \*Obj, int dest, int tag, MPI\_Comm comm, MPI\_Request \*request)

  Description Start a standard-mode, nonblocking send of object Obj to the process with rank dest.
- int pnl\_object\_mpi\_irecv (void \*\*buf, int \*size, int src, int tag, MPI\_Comm comm, int \*flag, MPI\_Request \*request)

  Description Start a standard-mode, nonblocking receive of object Obj from the process with rank root. On output flag equals to TRUE if the object can be received and FALSE otherwise (this is the same as for MPI\_Iprobe).

#### 15.2 The save/load interface

The interface is only accessible when the MPI bindings are compiled since it is based on the Packing/Unpacking facilities of MPI.

The functionnalities described in this chapter are declared in pnl/pnl\_mpi.h.

- PnlRng \*\* pnl\_rng\_create\_from\_file (char \*str, int n)

  Description Load n rng from the file of name str and returns an array of n PnlRng.
- int pnl\_rng\_save\_to\_file (PnlRng \*\*rngtab, int n, char \*str)

  Description Save n rng stored in rngtab into the file of name str.
- int pnl\_object\_save (PnlObject \*O, FILE \*stream)

  Description Save the object 0 into the stream stream. stream is typically created by calling fopen with mode="wb". This function can be called several times to save several objects in the same stream.
- PnlObject\* pnl\_object\_load (FILE \*stream)

  Description Load an object from the stream stream. stream is typically created by calling fopen with mode="rb". This function can be called several times to load several objects from the same stream. If stream was empty or it did not contain any PnlObjects, the function returns NULL.
- PnlList\* pnl\_object\_load\_into\_list (FILE \*stream)

  Description Load as many objects as possible from the stream stream and stores them into a PnlList. stream is typically created by calling fopen with mode="rb". If stream was empty or it did not contain any PnlObjects, the function returns NULL.

### 16 Financial functions

The financial functions are defined in the header pnl/pnl\_finance.h.

- int pnl\_cf\_call\_bs (double s, double k, double T, double r, double divid, double sigma, double \*ptprice, double \*ptdelta)
   Description Compute the price and delta of a call option (s k)+ in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid. The parameters ptprice and ptdelta are respectively set to the price and delta on output.
- int pnl\_cf\_put\_bs (double s, double k, double T, double r, double divid, double sigma, double \*ptprice, double \*ptdelta)
   Description Compute the price and delta of a put option (k s)+ in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid. The parameters ptprice and ptdelta are respectively set to the price and delta on output.
- double pnl\_bs\_call (double s, double k, double T, double r, double divid, double sigma)
   Description Compute the price of a call option with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.
- double pnl\_bs\_put (double s, double k, double T, double r, double divid, double sigma)
   Description Compute the price a put option with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.
- double pnl\_bs\_call\_put (int iscall, double s, double k, double T, double r, double divid, double sigma)
   Description Compute the price of a put option if iscall=0 or a call option if iscall=1 with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.
- double pnl\_bs\_vega (double s, double K, double T, double r, double divid, double sigma)
   Description Compute the vega of a put or call option with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.
- double pnl\_bs\_gamma (double s, double k, double T, double r, double divid, double sigma)
   Description Compute the gamma of a put or call option with spot s and strike k in the Black-Scholes model with volatility sigma, instantaneous interest rate r, maturity T and dividend rate divid.

Practitioners do not speak in terms of option prices, but rather compare prices in terms of their implied Black & Scholes volatilities. So this parameter is very useful in practice. Here, we propose two functions to compute  $\sigma_{impl}$ : the first one is for one up-let, maturity, strike, option price. the second function is for a list of strikes and maturities, a matrix of prices (with strikes varying row-wise).

- double pnl\_bs\_implicit\_vol (int is\_call, double Price, double s, double K, double T, double r, double divid, int \*error)

  Description Compute the implied volatility of a put option if iscall=0 or a call option if iscall=1 with spot s and strike K in the Black-Scholes model with instantaneous interest rate r, maturity T and dividend rate divid. On output error is OK if the computation of the implied volatility succeeded or FAIL if it failed.
- int pnl\_bs\_matrix\_implicit\_vol (const PnlMatInt \*iscall, const PnlMat \*Price, double s, double r, double divid, const PnlVect \*K, const PnlVect \*T, PnlMat \*Vol)

  Description Compute the matrix of implied volatilities Vol(i,j) of a put option if iscall(i,j)=0 or a call option if iscall(i,j)=1 with spot s and strike K(j) in the Black-Scholes model with instantaneous interest rate r, maturity T(j) and dividend rate divid. This function returns the number of failures, when everything succeeded it returns 0.

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| PnlRnFuncRn88      |
| PnlRnFuncRnDFunc88 |
| PnlRng63           |
| PnlSpMat51         |
| PnlSpMatComplex51  |
| PnlSpMatInt51      |
| PnlTridiagMat44    |
| PnlTridiagMatLU44  |
| PnlVect            |
| PnlVectCompact     |
| PnlVectComplex20   |
| PnlVectInt         |
|                    |