GSLSP

Extensions to the GNU Scientific Library

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1 Introduction

These routines provide support for constructing and manipulating sparse matrices in GSL, using an API similar to the `gsl_matrix` machinery. The basic structure is called `gsl_spmatrix`. There are two supported storage formats for sparse matrices: the triplet and compressed column storage (CCS) formats. The triplet format stores triplets (i, j, x) for each non-zero element of the matrix. This notation means that the (i, j) element of the matrix A is $A_{ij} = x$. Compressed column storage stores each column of non-zero values in the sparse matrix in a continuous memory block, keeping pointers to the beginning of each column in that memory block, and storing the row indices of each non-zero element. The triplet format is ideal for adding elements to the sparse matrix structure while it is being constructed, while the compressed column storage is better suited for matrix-matrix multiplication or linear solvers.

GSL does not provide a linear sparse matrix solver for $Ax = b$, since this is a highly complex problem and many advanced software packages already exist to efficiently solve it. The routines in this section provide a simple interface to construct a sparse matrix and convert it to a compressed format, where it can easily be passed to external linear sparse matrix solvers.

The `gsl_spmatrix` structure is defined as

```
typedef struct
{
  size_t size1;
  size_t size2;
  size_t *i;
  double *data;
  size_t *p;
  size_t nzmax;
  size_t nz;
  size_t *work;
  size_t flags;
} gsl_spmatrix;
```

This defines a *size1*-by-*size2* sparse matrix. The number of non-zero elements currently in the matrix is given by *nz*. For the triplet representation, *i*, *p*, and *data* are arrays of size *nz* which contain the row indices, column indices, and element value, respectively. So if $data[k] = x$, then $x = A(i[k], p[k])$. For compressed column storage, *i* and *data* are arrays of size *nz* containing the row indices and element values, similar to the triplet case. *p* is an array of size $size2 + 1$ where $p[j]$ points to the index in *data* of the start of column *j*. Thus, if $data[k] = A(i, j)$, then $i = i[k]$ and $p[j] <= k < p[j + 1]$.

work is additional workspace needed for various operations like converting from triplet to compressed column storage. *flags* indicates the type of storage format being used (triplet or compressed column).

The routines in this extension are defined in the header file '`gsl_spmatrix.h`'.

2 Sparse matrix allocation

The functions for allocating memory for a sparse matrix follow the style of `malloc` and `free`. They also perform their own error checking. If there is insufficient memory available to allocate a matrix then the functions call the GSL error handler with an error code of `GSL_ENOMEM` in addition to returning a null pointer.

`gsl_spmatrix * gsl_spmatrix_alloc` (*const size_t* `n1`, *const size_t* `n2`) [Function]

This function allocates a sparse matrix of size *n1*-by-*n2* and initializes it to all zeros. If the size of the matrix is not known at allocation time, both *n1* and *n2* may be set to 1, and they will automatically grow as elements are added to the matrix. This function sets the matrix to the triplet representation, which is the easiest for adding and accessing matrix elements. This function tries to make a reasonable guess for the number of non-zero elements (*nzmax*) which will be added to the matrix by assuming a sparse density of 10%. The function `gsl_spmatrix_alloc_nzmax` can be used if this number is known more accurately. The workspace is of size $O(nzmax)$.

`gsl_spmatrix * gsl_spmatrix_alloc_nzmax` (*const size_t* `n1`, *const size_t* `n2`, *const size_t* `nzmax`, *const size_t* `flags`) [Function]

This function allocates a sparse matrix of size *n1*-by-*n2* and initializes it to all zeros. If the size of the matrix is not known at allocation time, both *n1* and *n2* may be set to 1, and they will automatically grow as elements are added to the matrix. The parameter *nzmax* specifies the maximum number of non-zero elements which will be added to the matrix. It does not need to be precisely known in advance, since storage space will automatically grow using `gsl_spmatrix_realloc` if *nzmax* is not large enough. Accurate knowledge of this parameter reduces the number of reallocation calls required. The parameter *flags* specifies the storage format of the sparse matrix. Possible values are

`GSL_SPMATRIX_TRIPLET`
: This flag specifies triplet storage.

`GSL_SPMATRIX_COMPCOL`
: This flag specifies compressed column storage.

The allocated `gsl_spmatrix` structure is of size $O(nzmax)$.

`int gsl_spmatrix_realloc` (*const size_t* `nzmax`, *gsl_spmatrix ** `m`) [Function]

This function reallocates the storage space for *m* to accomodate *nzmax* non-zero elements. It is typically called internally by `gsl_spmatrix_set` if the user wants to add more elements to the sparse matrix than the previously specified *nzmax*.

`void gsl_spmatrix_free` (*gsl_spmatrix ** `m`) [Function]

This function frees the memory associated with the sparse matrix *m*.

3 Accessing sparse matrix elements

`double gsl_spmatrix_get` (*const gsl_spmatrix * `m`, const size_t `i`, const size_t `j`*) [Function]

This function returns element (*i*,*j*) of the matrix *m*. The matrix may be in triplet or compressed format.

`int gsl_spmatrix_set` (*gsl_spmatrix * `m`, const size_t `i`, const size_t `j`, const double `x`*) [Function]

This function sets element (*i*,*j*) of the matrix *m* to the value *x*. The matrix must be in triplet representation.

4 Initializing sparse matrix elements

Since the sparse matrix format only stores the non-zero elements, it is automatically initialized to zero upon allocation. The function `gsl_spmatrix_set_zero` may be used to re-initialize a matrix to zero after elements have been added to it.

`int gsl_spmatrix_set_zero` (*gsl_spmatrix * m*) [Function]

This function sets (or resets) all the elements of the matrix *m* to zero.

5 Copying sparse matrices

`gsl_spmatrix * gsl_spmatrix_memcpy` (*const gsl_spmatrix * `src`*) [Function]

This function makes a copy of the sparse matrix *src* and returns a pointer to a newly allocated copy, which must be freed by the caller when no longer needed. The matrix *src* may be in either triplet or compressed format.

`gsl_spmatrix * gsl_spmatrix_transpose_memcpy` (*const gsl_spmatrix * `src`*) [Function]

This function computes the transpose of *src* and stores it in a newly allocated matrix which is returned by the function. This matrix should be freed by the caller using `gsl_spmatrix_free` when no longer needed. The matrix *src* may be in either triplet or compressed format.

6 Sparse matrix operations

`gsl_spmatrix * gsl_spmatrix_add` (*const gsl_spmatrix* * `a`, *const gsl_spmatrix* * `b`) [Function]

This function adds the two matrices $a + b$ and stores the result in a newly allocated matrix which is returned. The result should be freed with `gsl_spmatrix_free` when no longer needed. The two matrices must have the same dimensions.

`int gsl_spmatrix_scale` (*gsl_spmatrix* * `m`, *const double* `x`) [Function]

This function scales all elements of the matrix m by the constant factor x. The result $m(i, j) \leftarrow xm(i, j)$ is stored in m.

7 Sparse matrix properties

`size_t gsl_spmatrix_nnz` (*const gsl_spmatrix * `m`*) [Function]

This function returns the number of non-zero elements in *m*.

`int gsl_spmatrix_equal` (*const gsl_spmatrix * `a`, const gsl_spmatrix * `b`*) [Function]

This function returns 1 if the matrices *a* and *b* are equal (by comparison of element values) and 0 otherwise. The matrices *a* and *b* must be either both triplet format or both compressed format for comparison.

8 Finding maximum and minimum elements of sparse matrices

int gsl_spmatrix_minmax (*const gsl_spmatrix* * m, *double* * min_out, *double* * max_out) [Function]

This function returns the minimum and maximum elements of the matrix *m*, storing them in *min_out* and *max_out*.

9 Sparse matrix compressed format

GSL supports the compressed column format, in which the non-zero elements in each column are stored contiguously in memory.

`gsl_spmatrix * gsl_spmatrix_compress` (*const gsl_spmatrix * T*) [Function]

This function creates a sparse matrix in compressed column format from the input sparse matrix T which must be in triplet format. A pointer to a newly allocated matrix is returned. The calling function should free the newly allocated matrix when it is no longer needed.

10 Conversion between sparse and dense matrices

The `gsl_spmatrix` structure can be converted into the dense `gsl_matrix` format and vice versa with the following routines.

`int gsl_spmatrix_d2sp` (*gsl_spmatrix * S*, *const gsl_matrix * A*) [Function]

This function converts the dense matrix A into sparse triplet format and stores the result in S.

`int gsl_spmatrix_sp2d` (*gsl_matrix * A*, *const gsl_spmatrix * S*) [Function]

This function converts the sparse matrix S into a dense matrix and stores the result in A. S must be in triplet format.

11 Sparse BLAS operations

GSL supports a limited number of BLAS operations for sparse matrices.

`int gsl_spblas_dgemv` (*const double* `alpha`, *const gsl_spmatrix ** `A`, *const gsl_vector ** `x`, *const double* `beta`, *gsl_vector ** `y`) [Function]

This function computes the matrix-vector product and sum $y \leftarrow \alpha A x + \beta y$, where A is sparse and the vectors x and y are dense. The matrix A may be in triplet or compressed format.

`gsl_spmatrix * gsl_spblas_dgemm` (*const double* `alpha`, *const gsl_spmatrix ** `A`, *const gsl_spmatrix ** `B`) [Function]

This function computes the sparse matrix-matrix product $C = \alpha AB$. A pointer to the newly allocated matrix C is returned and should be freed using `gsl_spmatrix_free` when no longer needed. The matrices A and B must be in compressed format.

12 Examples

This example program demonstrates the sparse matrix routines on the solution of a simple 1D Laplace equation on $[0, 1]$:

$$\frac{d^2u(x)}{dx^2} = f(x) = -\pi^2 \sin(\pi x)$$

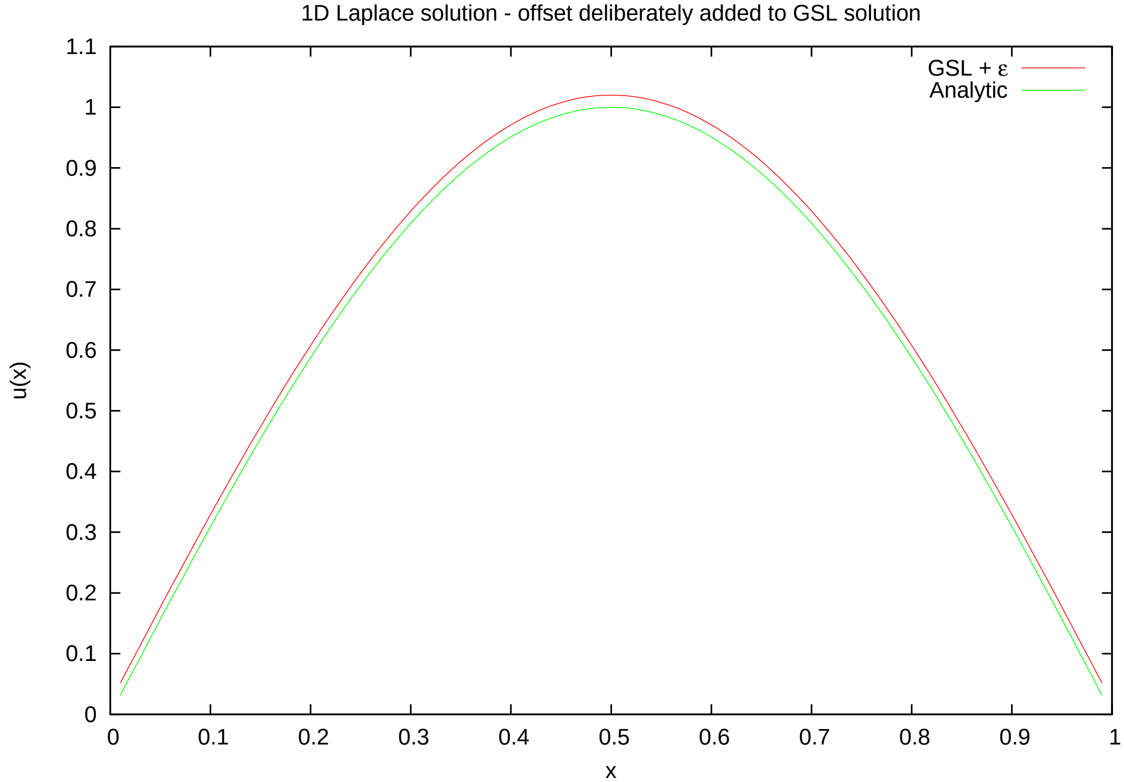
with boundary conditions $u(0) = u(1) = 0$. The analytic solution of this simple problem is $u(x) = \sin \pi x$. We will solve this problem by finite differencing the left hand side to give

$$\frac{1}{h^2}(u_{i+1} - 2u_i + u_{i-1}) = f_i$$

Defining a grid of N points, $h = 1/(N-1)$. In the finite difference equation above, $u_0 = u_{N-1} = 0$ are known from the boundary conditions, so we will only put the equations for $i = 1...N-2$ into the matrix system. The resulting matrix equation is

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 & \dots \\ 1 & -2 & 1 & 0 & 0 & \dots \\ 0 & 1 & -2 & 1 & 0 & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots & \dots \\ 0 & \dots & \dots & 1 & -2 & 1 \\ 0 & \dots & \dots & \dots & 1 & -2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-3} \\ u_{N-2} \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{N-3} \\ f_{N-2} \end{pmatrix}$$

An example program which constructs this system using the `gsl_spmatrix` framework is given below. The system is solved using the dense GSL LU solver. The program output is shown in the following plot.




```
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

#include <gsl/gsl_math.h>
#include <gsl/gsl_vector.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_linalg.h>

#include <gslsp/gsl_spmatrix.h>

/* exact solution */
double u_exact(const double x) { return sin(M_PI * x); }

int
main()
{
  const size_t N = 100;                        /* number of grid points */
  const size_t n = N - 2;                      /* subtract 2 to exclude boundaries */
  const double h = 1.0 / (N - 1.0);            /* grid spacing */
  gsl_spmatrix *T = gsl_spmatrix_alloc(n ,n); /* triplet format */
  gsl_spmatrix *C;                             /* compressed format */
  gsl_vector *f = gsl_vector_alloc(n);         /* right hand side vector */
  gsl_vector *u = gsl_vector_alloc(n);         /* solution vector */
  size_t i;
```

```
  /* construct the sparse matrix for the finite difference equation */

  /* loop over interior grid points */
  for (i = 0; i < n; ++i)
    {
      /* u_{i+1} term, ignore at the boundary */
      if (i + 1 < n)
        gsl_spmatrix_set(T, i, i + 1, 1.0);

      gsl_spmatrix_set(T, i, i, -2.0);

      /* u_{i-1} term, ignore at the boundary */
      if (i > 0)
        gsl_spmatrix_set(T, i, i - 1, 1.0);
    }

  /* scale by h^2 */
  gsl_spmatrix_scale(T, 1.0 / (h * h));

  /* construct right hand side vector */
  for (i = 0; i < n; ++i)
    {
      double xi = (i + 1) * h;
      double fi = -M_PI * M_PI * sin(M_PI * xi);
      gsl_vector_set(f, i, fi);
    }

  /* convert to compressed column format */
  C = gsl_spmatrix_compress(T);

  /*
   * At this point, C->i, C->p, C->data contain the
   * row indices, column pointers, and matrix elements
   * of the compressed column storage format. These 3
   * arrays can be passed to external linear solvers.
   *
   * For illustration purposes, we will convert the
   * sparse matrix to a dense gsl_matrix and complete
   * the solution using a dense LU solver.
   */

  {
    gsl_matrix *A = gsl_matrix_alloc(n, n);
    gsl_permutation *p = gsl_permutation_alloc(n);
    int s;
```

```
      /* convert sparse to dense */
      gsl_spmatrix_sp2d(A, T);

      /* solve linear system A u = f */
      gsl_linalg_LU_decomp(A, p, &s);
      gsl_linalg_LU_solve(A, p, f, u);

      /* output solution */
      for (i = 0; i < n; ++i)
        {
          double xi = (i + 1) * h;
          double u_analytic = u_exact(xi);
          double u_gsl = gsl_vector_get(u, i);

          printf("%f %.12e %.12e\n", xi, u_gsl, u_analytic);
        }

      gsl_matrix_free(A);
      gsl_permutation_free(p);
    }

  gsl_spmatrix_free(T);
  gsl_spmatrix_free(C);
  gsl_vector_free(f);
  gsl_vector_free(u);

  return 0;
} /* main() */
```

13 References and Further Reading

The algorithms used by these functions are described in the following sources:

T. A. Davis, Direct Methods for Sparse Linear Systems, SIAM, 2006.

CSparse software library, https://www.cise.ufl.edu/research/sparse/CSparse/

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