SyLVER Documentation

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Florent Lopez

CONTENTS:

		luction				
	1.1	Purpose	3			
	1.2	Usage overview	3			
2	Basic	c Subroutines	5			
		SpLDLT				
	2.2	SpLU	5			
3	Deriv	ved types	7			
4	Indic	ces and tables	11			
In	dex		13			

SyLVER

CONTENTS: 1

2 CONTENTS:

CHAPTER

ONE

INTRODUCTION

1.1 Purpose

SyLVER is a sparse direct solver for computing the solution of **large sparse symmetrically-structured linear systems** of equations. This includes both positive-definite and indefinite sparse symmetric systems as well as unsymmetric system whose sparsity pattern is symmetric.

The solution of the system of equations:

$$AX = B$$

is achived by computing a factorization of the input matrix. the following cases are covered:

1. A is symmetric positive-definite, we compute the sparse Cholesky factorization:

$$PAP^T = LL^T$$

where the factor L is a lower triangular matrix and the matrix P is a permutation matrix used to reduce the fill-in generated during the factorization. Following the matrix factorization the solution can be retrieved by successively solving the system LY = PB (forward substitution) and $L^T PX = Y$ (backward substitutions).

2. A is symmetric indefinite, then we compute the sparse LDL^T decomposition:

$$A = PLD(PL)^T$$

where P is a permutation matrix, L is unit lower triangular, and D is block diagonal with blocks of size 1×1 and 2×2 .

3. A is **unsymmetric**, then we compute the sparse :math LU decomposition:

$$P_s A P_s^T = P_n L U Q_n$$

where P_s is a permutation matrix corresponding to the fill-reducing permutation whereas P_n and Q_n are meant to improve the numerical property of the factorization algorithm. L is lower triangular, and U is unit upper triangular.

The code optionally supports hybrid computation using one or more NVIDIA GPUs.

1.2 Usage overview

Solving AX = B using SyLVER is a four stage process.

- If *A* is *symmetric*:
 - 1. Call <code>spldlt_analyse()</code> to perform a symbolic factorization, stored in <code>spldlt_akeep</code>.

- 2. Call <code>spldlt_factor()</code> to perform a numeric factorization, stored in <code>spldlt_fkeep</code>. More than one numeric factorization can refer to the same <code>spldlt_akeep</code>.
- 3. Call <code>spldlt_solve()</code> to perform a solve with the factors. More than one solve can be performed with the same <code>spldlt_fkeep</code>.
- 4. Once all desired solutions have been performed, free memory with spldlt_free().

• If A is unsymmetric:

- 1. Call <code>splu_analyse()</code> to perform a symbolic factorization, stored in <code>splu_akeep</code>.
- 2. Call splu_factor() to perform a numeric factorization, stored in *splu_fkeep*. More than one numeric factorization can refer to the same *splu_akeep*.
- 3. Call splu_solve() to perform a solve with the factors. More than one solve can be performed with the same *splu_fkeep*.
- 4. Once all desired solutions have been performed, free memory with splu_free().

BASIC SUBROUTINES

In the below, all reals are double precision unless otherwise indicated.

2.1 SpLDLT

subroutine spldlt_analyse (akeep, n, ptr, row, options, inform, ncpu[, order, val])

Perform the analyse (symbolic) phase of the factorization for a matrix supplied in Compressed Sparse Column (CSC) format. The resulting symbolic factors stored in *spldlt_akeep* should be passed unaltered in the subsequent calls to ssids_factor().

Parameters

- **akeep** [spldlt_akeep,out] :: returns symbolic factorization, to be passed unchanged to subsequent routines.
- **n** [integer,in] :: number of columns in A.
- **integer** (long) ptr(n+1) [in] :: column pointers for A (see CSC format).
- \mathbf{row} (ptr(n+1)-1) [integer,in] :: row indices for A (see CSC format).
- **options** [sylver_options,in] :: specifies algorithm options to be used (see sylver_options).
- **inform** [sylver_inform, out] :: returns information about the execution of the routine (see sylver_inform).
- **ncpu** [integer,in] :: Number of CPU available for the execution.

Options

- **order** (n) [integer,inout] :: on entry a user-supplied ordering (options%ordering=0). On return, the actual ordering used (if present).
- val (ptr(n+1)-1) [real,in] :: non-zero values for A (see CSC format). Only used if a matching-based ordering is requested.

subroutine spldlt_factor(akeep, fkeep, posdef, val, options, inform[, scale, ptr, row])

2.2 SpLU

subroutine splu_analyse (*akeep*, *n*, *ptr*, *row*, *options*, *inform*, *ncpu*[, *order*, *val*])

Perform the analyse (symbolic) phase of the factorization for a matrix supplied in Compressed Sparse Column

(CSC) format. The resulting symbolic factors stored in *splu_akeep* should be passed unaltered in the subsequent calls to ssids_factor().

Parameters

- **akeep** [splu_akeep,out] :: returns symbolic factorization, to be passed unchanged to subsequent routines.
- \mathbf{n} [integer,in] :: number of columns in A.
- **integer** (long) ptr(n+1) [in] :: column pointers for A (see CSC format).
- row (ptr(n+1)-1) [integer,in] :: row indices for A (see CSC format).
- **options** [sylver_options, in] :: specifies algorithm options to be used (see sylver_options).
- **inform** [sylver_inform,out] :: returns information about the execution of the routine (see sylver_inform).
- **ncpu** [integer,in] :: Number of CPU available for the execution.

Options

- **order** (n) [integer,inout] :: on entry a user-supplied ordering (options%ordering=0). On return, the actual ordering used (if present).
- val (ptr(n+1)-1) [real,in] :: non-zero values for A (see CSC format). Only used if a matching-based ordering is requested.

DERIVED TYPES

type sylver_options

The derived data type sylver_options is used to specify the options used within SyLVER. The components, that are automatically given default values in the definition of the type, are:

Type fields

• % **print_level** [integer,default=0] :: the level of printing. The different levels are:

< 0	No printing.
= 0	Error and warning messages only.
= 1	As 0, plus basic diagnostic printing.
> 1	As 1, plus some additional diagnostic printing.

- % unit_diagnostics [integer,default=6] :: Fortran unit number for diagnostics printing. Printing is suppressed if <0.
- % unit_error [integer, default=6] :: Fortran unit number for printing of error messages. Printing is suppressed if <0.
- % unit_warning [integer,default=6] :: Fortran unit number for printing of warning messages. Printing is suppressed if <0.
- % **ordering** [integer,default=1] :: Ordering method to use in analyse phase:

0	User-supplied ordering is used (order argument to spldlt_analyse() or
	splu_analyse()).
1	METIS ordering with default settings.
(de-	
fault)	
2	Matching-based elimination ordering is computed (the Hungarian algorithm is
	used to identify large off-diagonal entries. A restricted METIS ordering is then
	used that forces these on to the subdiagonal).
	Note: This option should only be chosen for indefinite systems. A scaling is also
	<pre>computed that may be used in spldlt_factor() or splu_factor() (see</pre>
	%scaling below).

- % **nemin** [integer,default=32]:: supernode amalgamation threshold. Two neighbours in the elimination tree are merged if they both involve fewer than nemin eliminations. The default is used if nemin<1.
- % use_gpu [logical,default=true] :: Use an NVIDIA GPU if present.

• % scaling [integer, default=0] :: scaling algorithm to use:

<=0	No scaling (if scale(:) is not present on call to <code>spldlt_factor()</code> or
(de-	<pre>splu_factor(), or user-supplied scaling (if scale(:) is present).</pre>
fault)	
=1	Compute using weighted bipartite matching via the Hungarian Algorithm (MC64
	algorithm).
=2	Compute using a weighted bipartite matching via the Auction Algorithm (may
	be lower quality than that computed using the Hungarian Algorithm, but can be
	considerably faster).
=3	Use matching-based ordering generated during the analyse phase using op-
	tions%ordering=2. The scaling will be the same as that generated with op-
	tions%scaling= 1 if the matrix values have not changed. This option will generate
	an error if a matching-based ordering was not used during analysis.
>=4	Compute using the norm-equilibration algorithm of Ruiz.

- % **nb** [integer,default=256]:: Block size to use for parallelization of large nodes on CPU resources.
- % pivot_method [integer, default=1] :: Pivot method to be used on CPU, one of:

0	Aggressive a posteori pivoting. Cholesky-like communication pattern is used, but
	a single failed pivot requires restart of node factorization and potential recalcula-
	tion of all uneliminated entries.
1	Block a posteori pivoting. A failed pivot only requires recalculation of entries
(de-	within its own block column.
fault)	
2	Threshold partial pivoting. Not parallel.

- % small [real,default=1d-20]:: threshold below which an entry is treated as equivalent to 0.0.
- % u [real,default=0.01]:: relative pivot threshold used in symmetric indefinite case. Values outside of the range [0, 0.5] are treated as the closest value in that range.

type sylver_inform

Used to return information about the progress and needs of the algorithm.

Type fields

- % cpu_flops [integer] :: number of flops performed on CPU
- % cublas_error [integer] :: CUBLAS error code in the event of a CUBLAS error (0 otherwise).
- % cuda_error [integer] :: CUDA error code in the event of a CUDA error (0 otherwise). Note that due to asynchronous execution, CUDA errors may not be reported by the call that caused them.
- % flag [integer] :: exit status of the algorithm (see table below).
- % integer (long) :: number of flops performed on GPU
- % matrix_dup [integer] :: number of duplicate entries encountered (if ssids_analyse() called with check=true, or any call to ssids_analyse_coord()).

- % matrix_missing_diag [integer] :: number of diagonal entries without an explicit value (if ssids_analyse() called with check=true, or any call to ssids_analyse_coord()).
- % matrix_outrange [integer] :: number of out-of-range entries encountered (if ssids_analyse() called with check=true, or any call to ssids_analyse_coord()).
- % matrix_rank [integer] :: (estimated) rank (structural after analyse phase, numerical after factorize phase).
- % maxdepth [integer] :: maximum depth of the assembly tree.
- % maxfront [integer] :: maximum front size (without pivoting after analyse phase, with pivoting after factorize phase).
- % num_delay [integer] :: number of delayed pivots. That is, the total number of fully-summed variables that were passed to the father node because of stability considerations. If a variable is passed further up the tree, it will be counted again.
- % integer :: number of entries in L (without pivoting after analyse phase, with pivoting after factorize phase).
- % **integer**:: number of floating-point operations for Cholesky factorization (indefinte needs slightly more). Without pivoting after analyse phase, with pivoting after factorize phase.
- % num_neg [integer] :: number of negative eigenvalues of the matrix D after factorize phase.
- % num_sup [integer] :: number of supernodes in assembly tree.
- % num_two [integer] :: number of 2×2 pivots used by the factorization (i.e. in the matrix D).
- % **stat** [integer] :: Fortran allocation status parameter in event of allocation error (0 otherwise).

in-	Return status
form%flag	
0	Success.
-1	Error in sequence of calls (may be caused by failure of a preceding call).
-2	n<0 or ne<1.
-3	Error in ptr(:).
-4	CSC format: All variable indices in one or more columns are out-of-range.
	Coordinate format: All entries are out-of-range.
-5	Matrix is singular and options%action=.false.
-6	Matrix found not to be positive definite but posdef=true.
-7	ptr(:) and/or row(:) not present, but required as ssids_analyse() was called with
	check=.false,.
-8	options%ordering out of range, or options%ordering=0 and order parameter not provided or not
	a valid permutation.
-9	options%ordering=-2 but val(:) was not supplied.
-10	ldx <n nrhs<1.<="" or="" td=""></n>
-11	job is out-of-range.
-13	Called ssids_enquire_posdef() on indefinite factorization.
-14	Called ssids_enquire_indef() on positive-definite factorization.
-15	options%scaling=3 but a matching-based ordering was not performed during analyse phase.
-50	Allocation error. If available, the stat parameter is returned in inform%stat.
-51	CUDA error. The CUDA error return value is returned in inform%cuda_error.
-52	CUBLAS error. The CUBLAS error return value is returned in inform%cublas_error.
+1	Out-of-range variable indices found and ignored in input data. inform%matrix_outrange is set
	to the number of such entries.
+2	Duplicate entries found and summed in input data. inform%matrix_dup is set to the number of
	such entries.
+3	Combination of +1 and +2.
+4	One or more diagonal entries of A are missing.
+5	Combination of +4 and +1 or +2.
+6	Matrix is found be (structurally) singular during analyse phase. This will overwrite any of the
	above warning flags.
+7	Matrix is found to be singular during factorize phase.
+8	Matching-based scaling found as side-effect of matching-based ordering ignored (consider set-
	ting options%scaling=3).

CHAPTER

FOUR

INDICES AND TABLES

- genindex
- modindex
- search

INDEX

S

```
spldlt_analyse() (fortran subroutine), 5
spldlt_factor() (fortran subroutine), 5
splu_analyse() (fortran subroutine), 5
sylver_inform (fortran type), 8
sylver_options (fortran type), 7
```