Numerical Linear Algebra for Computational Science and Information Engineering

Lecture 05
Sparse Data Structures and Basic Linear Algebra Subprograms

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Outline I

Basic linear algebra subprograms (BLAS)

Basic linear algebra subprograms (BLAS)

- What is BLAS?
  - Originated in the 1970s, as a set of **low-level routines** for common **linear algebra operations**, first written in Fortran.
  - Became a **standard** for the specification of linear algebra subroutines.
- Why use BLAS?
  - **Performance**: algorithmic optimizations, multi-threading, vectorization, loop unrolling, cache and register blocking, instruction pipelining, ...
  - **Portability**: Consistent interface across different platforms.
- Over time, **different BLAS libraries** have been developed, in **different languages**, for **different hardware**:
  - Intel oneAPI **MKL**: Proprietary, highly optimized for Intel architectures, GPU support through SYCL, comprehensive.
  - **OpenBLAS**: Open source, multi-architecture support, some GPU support, derived from GotoBLAS, community-driven.
  - **BLIS**: Open source, research-oriented (UT Austin).
  - **ATLAS**: Open source, empirical auto-tuning during build.
  - GPU only: Nvidia **cuBLAS**, AMD **rocBLAS**, ...

Common BLAS subroutines

BLAS routines are **organized into levels**, and follow a **naming convention** for most standard operations.

- **Level 1** (**vector** operations, typically $O(n)$ ops.):
  - Dot product (`DDOT`, `SDOT`, ...): $x^T y$
  - Vector addition (`DAXPY`, `SAXPY`, ...): $y \leftarrow \alpha x + y$
  - Vector norms (`DNRM2`, `SNRM2`, ...): $\|x\|_2$
- **Level 2** (**matrix-vector** operations, typically $O(n^2)$ ops.):
  - Matrix-vector multiply (`DGEMV`, `SGEMV`): $y \leftarrow \alpha A x + \beta y$
  - Rank-1 update (`DGER`, `SGER`): $A \leftarrow \alpha x y^T + A$
  - Triangular solve (`DTRSV`, `STRSV`): $x \leftarrow T^{-1} x$
- **Level 3** (**matrix** operations, typically $O(n^3)$ ops.):
  - Matrix-matrix multiply (`DGEMM`, `SGEMM`, ...): $C \leftarrow \alpha AB + \beta C$
  - Rank-k update (`DSYRK`, `SSYRK`, ...): $C \leftarrow \alpha A A^T + \beta C$

The first letter in the name of a subroutine represents the data type:

`D`: double precision real　　`S`: single precision real

`C`: single precision complex　　`Z`: double precision complex

Common BLAS subroutines, cont'd

Level 1 BLAS

dim scalar vector vector scalars 5-element array		prefixes
`SUBROUTINE xROTG ( A, B, C, S )`	Generate plane rotation	S, D
`SUBROUTINE xROTMG( D1, D2, A, B, PARAM )`	Generate modified plane rotation	S, D
`SUBROUTINE xROT ( N, X, INCX, Y, INCY, C, S )`	Apply plane rotation	S, D
`SUBROUTINE xROTM ( N, X, INCX, Y, INCY, PARAM )`	Apply modified plane rotation	S, D
`SUBROUTINE xSWAP ( N, X, INCX, Y, INCY )`	$x \leftrightarrow y$	S, D, C, Z
`SUBROUTINE xSCAL ( N, ALPHA, X, INCX )`	$x \leftarrow \alpha x$	S, D, C, Z, CS, ZD
`SUBROUTINE xCOPY ( N, X, INCX, Y, INCY )`	$y \leftarrow x$	S, D, C, Z
`SUBROUTINE xAXPY ( N, ALPHA, X, INCX, Y, INCY )`	$y \leftarrow \alpha x + y$	S, D, C, Z
`FUNCTION xDOT ( N, X, INCX, Y, INCY )`	$dot \leftarrow x^T y$	S, D, DS
`FUNCTION xDOTU ( N, X, INCX, Y, INCY )`	$dot \leftarrow x^T y$	C, Z
`FUNCTION xDOTC ( N, X, INCX, Y, INCY )`	$dot \leftarrow x^H y$	C, Z
`FUNCTION xxDOT ( N, X, INCX, Y, INCY )`	$dot \leftarrow \alpha + x^T y$	SDS
`FUNCTION xNRM2 ( N, X, INCX )`	$nrm2 \leftarrow \|\|x\|\|_2$	S, D, SC, DZ
`FUNCTION xASUM ( N, X, INCX )`	$asum \leftarrow \|\|re(x)\|\|_1 + \|\|im(x)\|\|_1$	S, D, SC, DZ
`FUNCTION IxAMAX( N, X, INCX )`	$amax \leftarrow 1^{st} k \ni \|re(x_k)\| + \|im(x_k)\| = max(\|re(x_i)\| + \|im(x_i)\|)$	S, D, C, Z

Level 2 BLAS

options dim b-width scalar matrix vector scalar vector		
`xGEMV ( TRANS, M, N, ALPHA, A, LDA, X, INCX, BETA, Y, INCY )`	$y \leftarrow \alpha Ax + \beta y, y \leftarrow \alpha A^T x + \beta y, y \leftarrow \alpha A^H x + \beta y, A - m \times n$	S, D, C, Z
`xGBMV ( TRANS, M, N, KL, KU, ALPHA, A, LDA, X, INCX, BETA, Y, INCY )`	$y \leftarrow \alpha Ax + \beta y, y \leftarrow \alpha A^T x + \beta y, y \leftarrow \alpha A^H x + \beta y, A - m \times n$	S, D, C, Z
`xHEMV ( UPLO, N, ALPHA, A, LDA, X, INCX, BETA, Y, INCY )`	$y \leftarrow \alpha Ax + \beta y$	C, Z
`xHBMV ( UPLO, N, K, ALPHA, A, LDA, X, INCX, BETA, Y, INCY )`	$y \leftarrow \alpha Ax + \beta y$	C, Z
`xHPMV ( UPLO, N, ALPHA, AP, X, INCX, BETA, Y, INCY )`	$y \leftarrow \alpha Ax + \beta y$	C, Z
`xSYMV ( UPLO, N, ALPHA, A, LDA, X, INCX, BETA, Y, INCY )`	$y \leftarrow \alpha Ax + \beta y$	S, D
`xSBMV ( UPLO, N, K, ALPHA, A, LDA, X, INCX, BETA, Y, INCY )`	$y \leftarrow \alpha Ax + \beta y$	S, D
`xSPMV ( UPLO, N, ALPHA, AP, X, INCX, BETA, Y, INCY )`	$y \leftarrow \alpha Ax + \beta y$	S, D
`xTRMV ( UPLO, TRANS, DIAG, N, A, LDA, X, INCX )`	$x \leftarrow Ax, x \leftarrow A^T x, x \leftarrow A^H x$	S, D, C, Z
`xTBMV ( UPLO, TRANS, DIAG, N, K, A, LDA, X, INCX )`	$x \leftarrow Ax, x \leftarrow A^T x, x \leftarrow A^H x$	S, D, C, Z
`xTPMV ( UPLO, TRANS, DIAG, N, AP, X, INCX )`	$x \leftarrow Ax, x \leftarrow A^T x, x \leftarrow A^H x$	S, D, C, Z
`xTRSV ( UPLO, TRANS, DIAG, N, A, LDA, X, INCX )`	$x \leftarrow A^{-1}x, x \leftarrow A^{-T}x, x \leftarrow A^{-H}x$	S, D, C, Z
`xTBSV ( UPLO, TRANS, DIAG, N, K, A, LDA, X, INCX )`	$x \leftarrow A^{-1}x, x \leftarrow A^{-T}x, x \leftarrow A^{-H}x$	S, D, C, Z
`xTPSV ( UPLO, TRANS, DIAG, N, AP, X, INCX )`	$x \leftarrow A^{-1}x, x \leftarrow A^{-T}x, x \leftarrow A^{-H}x$	S, D, C, Z
options dim scalar vector vector matrix		
`xGER ( M, N, ALPHA, X, INCX, Y, INCY, A, LDA )`	$A \leftarrow \alpha xy^T + A, A - m \times n$	S, D
`xGERU ( M, N, ALPHA, X, INCX, Y, INCY, A, LDA )`	$A \leftarrow \alpha xy^T + A, A - m \times n$	C, Z
`xGERC ( M, N, ALPHA, X, INCX, Y, INCY, A, LDA )`	$A \leftarrow \alpha xy^H + A, A - m \times n$	C, Z
`xHER ( UPLO, N, ALPHA, X, INCX, A, LDA )`	$A \leftarrow \alpha xx^H + A$	C, Z
`xHPR ( UPLO, N, ALPHA, X, INCX, AP )`	$A \leftarrow \alpha xx^H + A$	C, Z
`xHER2 ( UPLO, N, ALPHA, X, INCX, Y, INCY, A, LDA )`	$A \leftarrow \alpha xy^H + y(\alpha x)^H + A$	C, Z
`xHPR2 ( UPLO, N, ALPHA, X, INCX, Y, INCY, AP )`	$A \leftarrow \alpha xy^H + y(\alpha x)^H + A$	C, Z
`xSYR ( UPLO, N, ALPHA, X, INCX, A, LDA )`	$A \leftarrow \alpha xx^T + A$	S, D
`xSPR ( UPLO, N, ALPHA, X, INCX, AP )`	$A \leftarrow \alpha xx^T + A$	S, D
`xSYR2 ( UPLO, N, ALPHA, X, INCX, Y, INCY, A, LDA )`	$A \leftarrow \alpha xy^T + \alpha yx^T + A$	S, D
`xSPR2 ( UPLO, N, ALPHA, X, INCX, Y, INCY, AP )`	$A \leftarrow \alpha xy^T + \alpha yx^T + A$	S, D

Level 3 BLAS

options dim scalar matrix matrix scalar matrix		
`xGEMM ( TRANSA, TRANSB, M, N, K, ALPHA, A, LDA, B, LDB, BETA, C, LDC )`	$C \leftarrow \alpha op(A)op(B) + \beta C, op(X) = X, X^T, X^H, C - m \times n$	S, D, C, Z
`xSYMM ( SIDE, UPLO, M, N, ALPHA, A, LDA, B, LDB, BETA, C, LDC )`	$C \leftarrow \alpha AB + \beta C, C \leftarrow \alpha BA + \beta C, C - m \times n, A = A^T$	S, D, C, Z
`xHEMM ( SIDE, UPLO, M, N, ALPHA, A, LDA, B, LDB, BETA, C, LDC )`	$C \leftarrow \alpha AB + \beta C, C \leftarrow \alpha BA + \beta C, C - m \times n, A = A^H$	C, Z
`xSYRK ( UPLO, TRANS, N, K, ALPHA, A, LDA, BETA, C, LDC )`	$C \leftarrow \alpha AA^T + \beta C, C \leftarrow \alpha A^T A + \beta C, C - n \times n$	S, D, C, Z
`xHERK ( UPLO, TRANS, N, K, ALPHA, A, LDA, BETA, C, LDC )`	$C \leftarrow \alpha AA^H + \beta C, C \leftarrow \alpha A^H A + \beta C, C - n \times n$	C, Z
`xSYR2K( UPLO, TRANS, N, K, ALPHA, A, LDA, B, LDB, BETA, C, LDC )`	$C \leftarrow \alpha AB^T + \bar{\alpha} BA^T + \beta C, C \leftarrow \alpha A^T B + \bar{\alpha} B^T A + \beta C, C - n \times n$	S, D, C, Z
`xHER2K( UPLO, TRANS, N, K, ALPHA, A, LDA, B, LDB, BETA, C, LDC )`	$C \leftarrow \alpha AB^H + \bar{\alpha} BA^H + \beta C, C \leftarrow \alpha A^H B + \bar{\alpha} B^H A + \beta C, C - n \times n$	C, Z
`xTRMM ( SIDE, UPLO, TRANSA, DIAG, M, N, ALPHA, A, LDA, B, LDB )`	$B \leftarrow \alpha op(A)B, B \leftarrow \alpha Bop(A), op(A) = A, A^T, A^H, B - m \times n$	S, D, C, Z
`xTRSM ( SIDE, UPLO, TRANSA, DIAG, M, N, ALPHA, A, LDA, B, LDB )`	$B \leftarrow \alpha op(A^{-1})B, B \leftarrow \alpha Bop(A^{-1}), op(A) = A, A^T, A^H, B - m \times n$	S, D, C, Z

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University of Tennessee, Oak Ridge National Laboratory, Numerical Algorithms Group Ltd. (1997). Basic linear algebra subprograms – A quick reference guide. (`https://www.netlib.org/blas`)

BLAS in practice

- **BLAS interfaces** tend to be **mathematically opaque**.
- Using the **Intel oneAPI MKL C interface**:
  - The Julia code `Ax = A*x; AtAx = A'Ax` becomes:

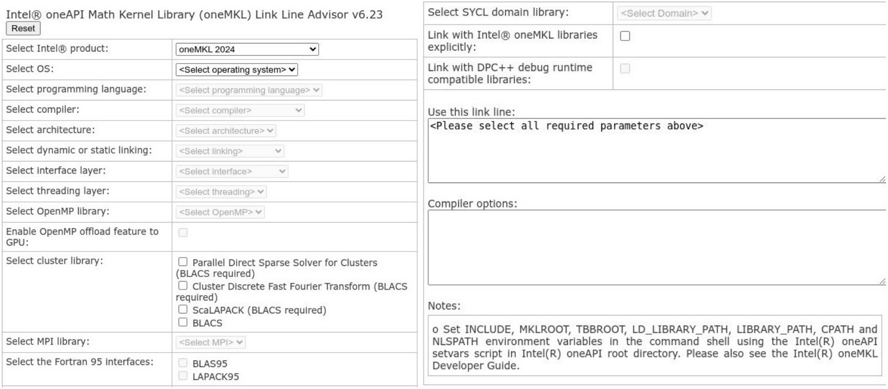
```
double *x = (double*)mkl_malloc(m * sizeof(double), sizeof(double));
double *Ax = (double*)mkl_malloc(n * sizeof(double), sizeof(double));
double *AtAx = (double*)mkl_malloc(m * sizeof(double), sizeof(double));
for (int i=0; i<m; i++)
  x[i] = rand() / (double) RAND_MAX;
for (int i=0; i<maxit; i++) {
  cblas_dgemv(CblasColMajor, CblasNoTrans, n, m, 1., A, n, x, 1, 0., Ax, 1);
  cblas_dgemv(CblasColMajor, CblasTrans, n, m, 1., A, n, Ax, 1, 0., AtAx, 1);
```

  - **Documentation**:

    https://www.intel.com/content/www/us/en/docs/onemkl/developer-reference-dpcpp/2024-2/blas-routines.html
- For interfaces to other implementations, see
  - **OpenBLAS**: https://github.com/OpenMathLib/OpenBLAS
  - **ATLAS**: https://github.com/flame/blis
  - **BLIS**: http://math-atlas.sourceforge.net/

BLAS in practice, cont'd

- The cost of **enhanced portability** often comes in the form of **building challenges**.
  - E.g., MKL and OpenBLAS offer support for various CPU vendors and GPUs.
- For **Intel oneAPI MKL**, there is a dedicated web tool to help with the linking configuration:


Intel® oneAPI Math Kernel Library (oneMKL) Link Line Advisor v6.23

Reset

Select Intel® product:	oneMKL 2024
Select OS:	<Select operating system>
Select programming language:	<Select programming language>
Select compiler:	<Select compiler>
Select architecture:	<Select architecture>
Select dynamic or static linking:	<Select linking>
Select interface layer:	<Select interface>
Select threading layer:	<Select threading>
Select OpenMP library:	<Select OpenMP>
Enable OpenMP offload feature to GPU:	
Select cluster library:	Parallel Direct Sparse Solver for Clusters (BLACS required) Cluster Discrete Fast Fourier Transform (BLACS required) ScaLAPACK (BLACS required) BLACS
Select MPI library:	<Select MPI>
Select the Fortran 95 interfaces:	BLAS95 LAPACK95
Select SYCL domain library:	<Select Domain>
Link with Intel® oneMKL libraries explicitly:	
Link with DPC++ debug runtime compatible libraries:	

Use this link line:

<Please select all required parameters above>

Compiler options:

Notes:

o Set INCLUDE, MKLROOT, TBBROOT, LD_LIBRARY_PATH, LIBRARY_PATH, CPATH and NLSPATH environment variables in the command shell using the Intel(R) oneAPI setvars script in Intel(R) oneAPI root directory. Please also see the Intel(R) oneMKL Developer Guide.

https://www.intel.com/content/www/us/en/developer/tools/oneapi/onemkl-link-line-advisor.html

Linear algebra package (LAPACK)

- What is LAPACK?
  - Set of Fortran 90 routines to solve **linear systems**, **eigenvalue problems**, and **SVDs** with **dense but small to moderately sized** as well as **structured sparse** (banded, tridiagonal, ...) matrices:
  - Successor to LINPACK (1979, for linear systems and least squares pbs.) and EISPACK (1976, for eigenvalue problems).
  - Developed and maintained by an international **team of researchers**.
- Key characteristics:
  - Optimized for **performance**, **portability** and **numerical stability**.
  - **Relies heavily on BLAS**, especially Level 2 and 3.
  - Performance **depends critically** on the **BLAS implementation** used.
  - **Handles higher-level algorithms** and **delegates** operations to **BLAS**.
- Available through various implementations:
  - Reference **LAPACK**: Standard implementation, focus on correctness.
  - Intel **MKL**: Optimized LAPACK routines alongside BLAS.
  - GPU only: Nvidia **cuSOLVER**, AMD **rocSOLVER**.

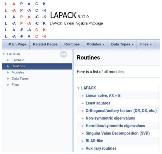
Nomenclature of LAPACK subroutines

LAPACK routines follow a **structured naming convention**: `XYYZZZ`

- **Data types** (`X`):
  - `D`: double precision real
  - `S`: single precision real
  - `C`: single precision complex
  - `Z`: double precision complex
- Common **matrix types** (`YY`):
  - `GE`: general
  - `SY`: symmetric
  - `HG`: upper Hessenberg
  - `PO`: SPD/HPD
  - `TR`: triangular
  - `BD`: bidiagonal
- Common **computational tasks** (`ZZZ`):
  - `SV`: solve linear system
  - `TRF`: triangular factorization
  - `TRS`: solve using factorization
  - `CON`: estimate conditioning
  - `EV`: solve eigenvalue problem
- Examples of (driver) subroutines:
  - `DGESV`: linear solve with real general matrix in double precision.
  - `CPOSV`: linear solve with (complex) HPD matrix in single precision.
  - `ZGEEV`: eigensolve with general complex matrix in double precision.

Structure of LAPACK subroutines

- There are three types of LAPACK routines:
  - **Driver** routines: solves a **complete problem**, e.g.,
    linear systems, eigenvalue problems, least-squares problems, ...
  - **Computational** routines: performs an **intermediate level task**, e.g.,
    LU factorization, tridiagonal reduction, ...
  - **Auxiliary** routines: **unblocked sub-tasks of block algorithms**,
    BLAS-like operations, other low level tasks.
- **Driver** routines listed in the online documentation:



`https://www.netlib.org/lapack/explore-html/modules.html`

- **Computational** routines listed by module:

`https://www.netlib.org/lapack/lug/node37.html`

- **Auxiliary** routines listed by category:

`https://www.netlib.org/lapack/lug/node144.html`

BLAS and LAPACK in Julia

- Default implementation:
  - Ships with **multi-threaded OpenBLAS** and **reference LAPACK**.
  - **Flexible**, i.e., can use other implementations, e.g., **MKL**, **BLIS**, ...
- Three **implementation-independent** levels of **access** (like in Python):
  - **Interface wrappers** via `LinearAlgebra.{BLAS,LAPACK}`:

    `BLAS.gemm!`, `LAPACK.getrf!`, ...

    most control — no extra copies/allocations — math-implicit
  - **Intermediate level functions**:

    `dot(x,y)`, `mul!(C,A,B)`, `lu(A)`, ...

    less control — in-place versions available — good compromise
  - **High-level syntax**:

    `A * x`, `A \ b`, `A / B`, ...

    least control — extra copies/allocations — math-explicit
- Key features:
  - **Matrix type** specified by **data structure**, e.g., `Symmetric`, `Tridiagonal`.
  - **Multiple dispatch**: function behavior depends on types of **all** arguments.
  - Operations **preserve matrix structure** when applicable.

Sparse matrix data structures

Section 9.1 in Darve & Wootters (2021)

Sparse matrices

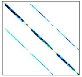
- **Sparse matrices** are **matrices** with relatively **few non-zero components**.
- Natural occurrence in scientific applications:
  - **Discretized differential equations**:
    - ODEs: chemical reactions, multi-body systems with short-range interactions, multi-agent systems with local interactions, ...
    - PDEs: fluid dynamics, solid mechanics, electromagnetics, ...
    - DAEs: circuit simulation, power grid modeling, ...
  - **Networks and graphs**:
    - Adjacency, transition and Laplacian matrices of sparse graphs.
  - **Data science**:
    - Feature matrices in high-dimensional data.
- Important properties:
  - **Inverses** of sparse matrices are generally **dense**, i.e., not sparse.
  - **Factorizations** of sparse matrices **may be reasonably sparse**.
  - **Dense matrices** can be **approximated by sparse matrices**, i.e., using sparse approximate inverses (SPAI).

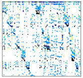
Repository of sparse matrices

- **Researchers** and **developers** often **need** multiple **sparse matrices** with documented characteristics **to benchmark** NLA **algorithms**.
- In particular, the **SuiteSparse Matrix Collection** is widely used for this:

  `https://sparse.tamu.edu/`

  - **Close to 3,000 matrices** available.
  - Matrices **from all sorts of applications**.
  - **Metadata available** include: author, application field, rank, condition number, singular values, definiteness, symmetry and lack thereof, ...
- We can generally distinguish between two types of sparse matrices:
  - **Structured**: typically coming from differential equations discretized on structured grids/meshes.

    E.g., `sherman5` (computational fluid dynamics problem): 
  - **Unstructured**: most other cases.

    E.g., `bp_1000` (optimization problem): 

Sparse matrix data structures

- The use of **proper data structures** is essential **to**

  limit memory requirements and **achieve good performance**

  when deploying basic linear algebra operations and NLA algorithms **with sparse matrices**.
- There is **no unique** sparse matrix **data structure to optimally serve all purposes in all situations**.
- In general, the **choice of** a sparse **data structure** can be **influenced by**
  - **Sparsity pattern** of the matrix.
  - **Hardware architecture**:
    - Memory layout.
    - Sequential vs parallel with shared and/or distributed memory vs GPU.
  - **Algorithm and operations**:
    - Type of access.
    - BLAS level, i.e., 1, 2 or 3.
  - **Implementation requirements**.

Sparse matrix data structures, cont'd$_1$

- There are many sparse matrix data structure formats. In particular:
  - Coordinate (`COO`)

intuitive/explicit	not efficient	large community support
	most convenient/used for construction	

  - Compressed sparse row (`CSR`), compressed sparse column (`CSC`)

lowest memory need	efficient	large community support
	most used	

- Variants of `CSR` and `CSC`:
  - Block sparse row (`BSR`/`BCSR`), block sparse column (`BSC`/`BCSC`)
    good for block matrices **overhead otherwise** **large support**
  - Mapped block row (`MBR`) sparse
    lower memory need **more efficient** **limited community support**
  - Modified sparse row (`MSR`/`MCSR`), modified sparse column (`MSC`/`MCSC`)
    fast diagonal access **square matrices only**
    limited community support

Sparse matrix data structures, cont'd$_2$

- Vector architectures and GPU:
  - Ellpack (`ELL`)
    good for uniform sparsity **community support** **GPU-friendly**
- Banded matrices:
  - Diagonal (`DIA`)
    good for fixed bandwidth **wasteful otherwise**
    moderate support
  - Non-symmetric skyline (`NSK`), symmetric skyline (`SSK`)
    good for variable bandwidth **wasteful for isolated bands**
    moderate support
- Pythonic environment:
  - List of lists (`LIL`)
    used for construction **Python-specific support** **not efficient**
  - Dictionary of keys (`DOK`)
    used for construction **Python-specific support** **not efficient**

Coordinate (`COO`) format

- A COO data structures format is composed of:
  - Array of **non-zero components** (`val`)
  - Array of **row indices of each component** (`row_idx`)
  - Array of **column indices of each components** (`col_idx`)
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix}$$

$$\texttt{val} = [a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{33}, a_{34}, a_{43}]$$

$$\texttt{row\_idx} = [1, 1, 1, 2, 2, 3, 3, 4]$$

$$\texttt{col\_idx} = [1, 2, 3, 1, 2, 3, 4, 3]$$

- Key characteristics:
  - Explicit storage of all indices (higher memory usage)
  - **No particular ordering** required
  - **Duplicates allowed** (values must be summed)
  - **Flexible** for matrix **construction** and **modification**

Compressed sparse row ($\texttt{CSR}$) format

- A CSR data structures format is composed of:
  - Array of **non-zero components** (`val`)
  - Array of **column indices of each component** (`col_idx`)
  - Array of **non-zero value indices where each row starts** (`row_start`)
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix}$$

$$\begin{aligned} \texttt{val} &= [a_{11}, a_{12}, a_{13}, a_{21}, a_{22}, a_{33}, a_{34}, a_{43}] \\ \texttt{col\_idx} &= [1, 2, 3, 1, 2, 3, 4, 3] \\ \texttt{row\_start} &= [1, 4, 6, 8, 9] \end{aligned}$$

- Key characteristics:
  - Compact storage (lower memory than COO)
  - **Fast row access**
  - **Values must be ordered** by row
  - **Difficult to modify** structure dynamically

Compressed sparse column (`CSC`) format

- A CSC data structures format is composed of:
  - Array of **non-zero components** (`val`)
  - Array of **row indices of each component** (`row_idx`)
  - Array of **non-zero indices where each column starts** (`col_start`)
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix}$$

$$\texttt{val} = [a_{11}, a_{21}, a_{12}, a_{22}, a_{13}, a_{33}, a_{43}, a_{34}]$$

$$\texttt{row\_idx} = [1, 2, 1, 2, 1, 3, 4, 3]$$

$$\texttt{col\_start} = [1, 3, 5, 8, 9]$$

- Key characteristics:
  - Compact storage (lower memory than COO)
  - **Fast column access**
  - **Values must be ordered** by column
  - **Difficult to modify** structure dynamically

Block sparse row (BSR) format

- A BSR (or BCSR) data structure format is composed of:
  - **Block dimensions** ($\texttt{r}\times\texttt{c}$)
  - Array (or matrix) of **all components of non-zero blocks** (`val`)
  - Array of **non-zero block column indices** (`col_idx`)
  - Array of **block indices where each block row starts** (`row_start`)
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix}$$

$$\texttt{r} = 2, \texttt{c} = 2$$

$$\texttt{val} = [a_{11}, a_{12}, a_{21}, a_{22}, a_{13}, 0, 0, 0, a_{33}, a_{34}, a_{43}, 0]$$

$$\texttt{col\_idx} = [1, 2, 2]$$

$$\texttt{row\_start} = [1, 3, 4]$$

- Key characteristics:
  - **Zero values within non-zero blocks** are **stored**
  - **Similar to CSR but** operates **on blocks**

Mapped block row (MBR) format

- A MBR data structure format is composed of:
  - **Block dimensions** ($\texttt{r}\times\texttt{c}$)
  - Array of **non-zero components of non-zero blocks** (`val`)
  - Array of **non-zero block column indices** (`col_idx`)
  - Array of **sparsity pattern encoding** (`b_map`)
  - Array of **block indices where each block row starts** (`row_start`)
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix}$$

$$\texttt{r} = 2, \texttt{c} = 2$$

$$\texttt{val} = [a_{11}, a_{12}, a_{21}, a_{22}, a_{13}, a_{33}, a_{34}, a_{43}]$$

$$\texttt{col\_idx} = [1, 2, 2] \quad \texttt{b\_map} = [15, 1, 7] \quad \texttt{row\_start} = [1, 3, 4]$$

- Key characteristic:
  - **Non-zero values within non-zero blocks** are **not stored**

Modified sparse row (MSR) format

- A MSR data structure format is composed of:
  - Array of **diagonal elements first**, then **other non-zeros** (`val`)
  - Composite array $\texttt{idx} := [\texttt{row\_start}, \texttt{col\_idx}]$ where:
    - `row_start` contains the **index of off-diagonal non-zero value where each row starts**.
    - `col_idx` contains **column indices of each off-diagonal non-zero component**.
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix}$$

$$\texttt{val} = [a_{11}, a_{22}, a_{33}, 0, -1, a_{12}, a_{13}, a_{21}, a_{34}, a_{43}]$$

$$\texttt{idx} = [6, 8, 9, 10, 11, 2, 3, 1, 4, 3]$$

- Key characteristics:
  - **Diagonal elements stored first** $\implies$ **Fast diagonal access**
  - Dummy element, here -1, stored in `val` for consistency with `idx` (?).

Ellpack (ELL) format

- An ELL data structure format is composed of:
  - **Maximum number** of **non-zero components on a row** (`row_nnz`)
  - Array of **all components stored in column-major order, from the block of left-aligned non-zero components** (`val`)
  - Array of **column indices of stored components** (`col_idx`)
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix}$$

$$\texttt{row\_nnz} = 3$$

$$\texttt{val} = [a_{11}, a_{21}, a_{33}, a_{43}, a_{12}, a_{22}, a_{34}, 0, a_{13}, 0, 0, 0]$$

$$\texttt{col\_idx} = [1, 1, 3, 3, 2, 2, 4, -1, 3, -1, -1, -1]$$

- Key characteristics:
  - Stores $2\times$`row_nnz` values, including some zeros
  - Wasteful if number of non-zero components varies significantly from one row to another

Diagonal (DIA) format

- A DIA data structure format is composed of:
  - Array of **components on non-zero diagonals** padded to n (`val`)
  - Array of **offset indices** (`ioff`)
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix}$$

$$\texttt{val} = [*, a_{21}, 0, a_{43}, a_{11}, a_{22}, a_{33}, 0, a_{12}, 0, a_{34}, *, a_{13}, 0, *, *]$$

$$\texttt{ioff} = [-1, 0, 1, 2]$$

- Key characteristics:
  - **Fast diagonal access**
  - Wasteful for diagonal with large offset indices (?)

List of list (LIL) format

- A LIL data structure format is composed of:
  - A **list** (`rows`) **of lists**, one per row, **each list storing column indices of non-zero components**.
  - A **list** (`data`) **of lists**, one per row, **each list storing non-zero components, ordered consistently with the indices in** `rows`.
- Example:

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & 0 \\ a_{21} & a_{22} & 0 & 0 \\ 0 & 0 & a_{33} & a_{34} \\ 0 & 0 & a_{43} & 0 \end{bmatrix} \texttt{rows} = \begin{bmatrix} [1, 2, 3] \\ [1, 2] \\ [3, 4] \\ [3] \end{bmatrix} \texttt{data} = \begin{bmatrix} [a_{11}, a_{12}, a_{13}] \\ [a_{21}, a_{22}] \\ [a_{33}, a_{34}] \\ [a_{43}] \end{bmatrix}$$

- Key characteristics:
  - **No particular ordering** required for column indices
  - **Unordered column indices** slows down access
  - Mostly used for matrix **construction**, particularly in **Python**

Sparse matrix data structures in practice

- **Intel oneAPI MKL** supports sparse vectors, and the sparse matrix data structures `CSR`, `CSC`, `COO` and `BSR`.

  For example, using the C interface:

  - A `COO` **matrix** can be **created** as follows:

```
double val[] = {1., 2., 3.};
MKL_INT row_idx[] = {0, 2, 1};
MKL_INT col_idx[] = {0, 1, 2};
sparse_matrix_t A;
mkl_sparse_d_create_coo(&A, SPARSE_INDEX_BASE_ZERO, 3, 3, 3, row_idx, col_idx, val);
```

  - Sparse matrices can be **defined in other formats**, namely `CSR`, `CSC` and `BSR`, **directly from their underlying data structures**.
  - Only two functions to **convert constructed sparse matrices** into

    `CSR` (`mkl_sparse_convert_csr`)

    and `BSR` (`mkl_sparse_convert_bsr`).

    Possible to convert A into `CSC`, by using the `CSR` representation of A^T.
  - **Documentation**:

    https://www.intel.com/content/www/us/en/docs/onemkl/developer-reference-c/2024-2/matrix-manipulation-routines.html

Sparse matrix data structures in practice, cont'd

- **Nvidia cuSPARSE** also supports several vectors, and several sparse matrix data structures:
  - `COO`, `CSR`, `CSC` and `BSR`
  - Sliced Ellpack (`SELL`)
  - Blocked Ellpack (`BLOCKED-ELL`)

  Documentation:

  `https://docs.nvidia.com/cuda/cusparse/#cusparse-storage-formats`

- Other implementations:
  - **AMD ROCsparse**: proprietary, for GPU
  - **SuiteSparse**, **PETSc**,**Trilinos**, **OSKI**, **PSBLAS**, ... : open-source

Sparse matrix data structures in Julia

- Support of basic structured formats through `LinearAlgebra.jl`:

  `Diagonal`, `Bidiagonal`, `Tridiagonal`, `SymTridiagonal`, ...

- Standard library support through `SparseArrays.jl`:
  - **Only** `CSC` (`SparseMatrixCSC`) is **supported by default**:

```
struct SparseMatrixCSC{Tv,Ti<:Integer} <: AbstractSparseMatrixCSC{Tv,Ti}
    m::Int                  # Number of rows
    n::Int                  # Number of columns
    colptr::Vector{Ti}      # Column j is in colptr[j]:(colptr[j+1]-1)
    rowval::Vector{Ti}      # Row indices of stored values
    nzval::Vector{Tv}       # Stored values, typically nonzeros
end
```

  - Construction using `COO`-style input:

```
Is = [1, 3, 2]; Js = [1, 2, 3]; Vs = [1., 2., 3.]
A = sparse(Is, Js, Vs, 3, 3)
```

    with immediate **conversion** to `CSC`.

  - Construction using the `SparseMatrixCSC` struct:

```
A = SparseMatrixCSC(3, 3,
                    [1, 2, 3, 4],
                    [1, 3, 2],
                    [1., 2., 3.])
```

Sparse matrix data structures in Julia, cont'd

- **Random** constructor for **sparse matrix** of density d with iid non-zero elements **distributed uniformly** in $[0, 1)$, `sprand(m,n,d)`.
- **Random** constructor for **sparse matrix** of density d with iid non-zero elements **distributed according to the standard normal distribution**, `sprandn(m,n,d)`.

- More formats supported through other packages:
  - `SparseMatricesCSR.jl`: Julia native implementation of `CSR` formats.
  - `MKLSparse.jl`: Julia wrappers to Intel oneAPI MKL sparse interface.
  - `SuiteSparse.jl`: Julia wrappers to SuiteSparse library.

$\vdots$ $\vdots$

Sparse BLAS

Section 9.1 in Darve & Wootters (2021)

Sparse basic linear algebra subprograms

- **Sparse BLAS** is the extension of BLAS for **sparse matrices and vectors**.
- **Level 1** (**vector** operations):
  Intel oneAPI MKL functions use a compressed sparse vector format:
  https://www.intel.com/content/www/us/en/docs/onemkl/developer-reference-c/2024-2/sparse-blas-level-1-routines.html
  - Sparse $y \leftarrow \alpha x + y$ (`SpAXPY`): `mkl_sparse_x_axpy`
- **Level 2-3** functions have **format-specific implementations**.
  Intel oneAPI MKL offers access through an Inspector-Executor API:
  https://www.intel.com/content/www/us/en/docs/onemkl/developer-reference-c/2024-2/inspector-executor-sparse-blas-execution-routines.html
  - **Level 2** (**matrix-vector** operations):
    - Sparse matrix-vector product (`SpMV`): `mkl_sparse_x_mv`
  - **Level 3** (**matrix-matrix** operations):
    - Sparse matrix-(dense) matrix product (`SpMM`): `mkl_sparse_x_mm`
    - Sparse matrix-(sparse) matrix product (`SpGEMM`): `mkl_sparse_spmm`

Sparse matrices and graphs

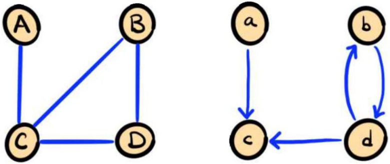
Section 9.2 in Darve & Wootters (2021)

A few definitions

- Basics of graph theory are essential to sparse matrix computation.

Definition (Graph)

- An **undirected graph** is a pair $G = (V, E)$ formed by a non-empty finite set V of **vertices** and a set $E \subseteq V \times V$ of **unordered pairs of vertices** referred to as **edges**.
- A **directed graph** $G = (V, E)$ is formed by a set E of **ordered edges**.



An undirected graph with vertices $V = \{A, B, C, D\}$ and edges $E = \{(A, C), (C, B), (C, D), (B, D)\}$.

A directed graph with vertices $V = \{a, b, c, d\}$ and edges $E = \{(a, c), (d, c), (b, d), (d, b)\}$.

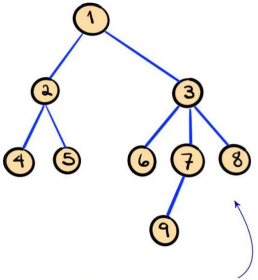
Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

A few definitions, cont'd

- A **path** from a vertex u to another vertex v is a **sequence of edges** $(u_0, u_1), \ldots, (u_{t-1}, u_t)$ such that $u_0 = u$ and $u_t = v$.
- A graph is **connected** if there is a **path from any vertex** u **to any vertex** v.
- A **tree** is a **connected graph without cycles**, i.e., with no path from a vertex to itself.

  A tree has a **root**, i.e., a **designated vertex** represented **at the top** of the tree.
- If a tree has an edge (u, v), and u is **closer to the root** r **than** v **is**, then we say that v is a **parent** and u is a **child**.

  Each vertex in a tree has a unique parent.
- A **leaf** is a **vertex** in a tree **with no children**.
- Family logic applies to define **descendants** and **ancestors**.



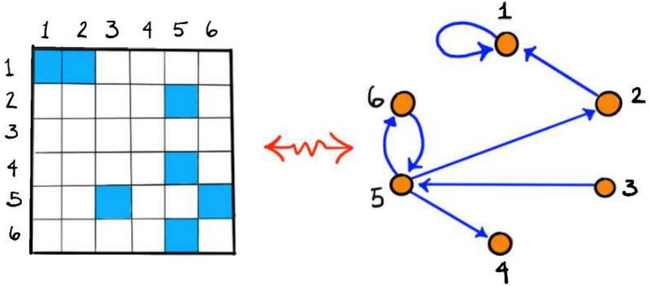
A tree. Vertex 1 is the root, and vertices 4, 5, 6, 9, 8 are leaves. Vertex 8 is 3's child, and 3 is 8's parent. Vertex 9 is 3's descendant, and 3 is 9's ancestor.

Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

Graph representation of sparsity patterns

- The **sparsity pattern** of a square matrix $A \in \mathbb{F}^{n \times n}$ can be represented as a **directed graph** with n **vertices**.
- In Darve and Wooters (2021), the convention is that a **directed edge** (i, j) from vertex j to vertex i exists if and only if $a_{ij} \neq 0$.

  For example:



Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

- The sparsity pattern of **symmetric matrices** can be represented by **undirected graphs**.

Homework problem

Homework problem

Turn in **your own** solution to the following problem:

Pb. 15 Consider the matrices

$$A = \begin{bmatrix} \bullet & \bullet & 0 & \bullet & 0 & 0 \\ 0 & \bullet & 0 & 0 & 0 & \bullet \\ 0 & \bullet & \bullet & 0 & 0 & 0 \\ 0 & \bullet & 0 & 0 & \bullet & 0 \\ 0 & 0 & 0 & 0 & \bullet & 0 \\ 0 & 0 & 0 & 0 & 0 & \bullet \end{bmatrix} \text{ and } B = \begin{bmatrix} \bullet & 0 & 0 & 0 & 0 & 0 \\ \bullet & 0 & \bullet & 0 & \bullet & 0 \\ 0 & \bullet & 0 & 0 & 0 & 0 \\ \bullet & \bullet & 0 & 0 & 0 & 0 \\ 0 & \bullet & 0 & \bullet & \bullet & 0 \\ 0 & 0 & \bullet & 0 & 0 & \bullet \end{bmatrix}$$

where each $\bullet$ denotes a non-zero component.

Show the adjacency graphs of A, B, AB and BA. You may assume that there are no numerical cancellations in computing the products AB and BA.

Problem excerpted from Pb. 4 in Chap. 3 of Saad (2003).

Saad, Y. (2003). Iterative methods for sparse linear systems. Society for Industrial and Applied Mathematics.

Practice session

Practice session

1. Use the `mmread` function from MatrixMarket.jl to read the matrix cage3 from the SuiteSparse website. Investigate the default sparse data structure in which the matrix is stored in Julia.
2. Write a function called `dcscmv` to perform SpMV in CSC format.
3. Write a function called `csc_to_coo` to convert a CSC matrix to COO format. Use the following custom type:

```
mutable struct SparseMatrixCOO
    m::Int # Number of rows
    n::Int # Number of columns
    rowval::Vector{Int} # Starting index for each row
    colval::Vector{Int} # Column indices
    nzval::Vector{Float64} # Matrix entries
end
```

4. Write a function called `dcoomv` to perform SpMV in COO format.
5. Write a function called `coo_to_csr` to convert a COO matrix to CSR format using a custom type `SparseMatrixCSR` with arguments `m::Int`, `n::Int`, `rowptr::Vector{Int}`, `colval::Vector{Int}` and `nzval::Vector{Float64}`.

Practice session, cont'd

6. Write a function called `coo_to_csr2` to convert a COO matrix to CSR format making use of the built-in `sparse` function.
   Hint: Think of the relation between CSC and CSR.
7. Write a function called `dcsrmv` to perform SpMV in CSR format.
8. Write a function called `coo_to_ell` to convert a COO matrix to ELL format using a custom type `SparseMatrixELL` with arguments `m::Int`, `n::Int`, `rownnz::Int`, `colval::Vector{Int}` and `nzval::Vector{Float64}`.
9. Write a function called `dellmv` to perform SpMV in ELL format.