Numerical Linear Algebra for Computational Science and Information Engineering

Sparse Data Structures and Basic Linear Algebra Subroutines

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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)	$nrm2 \leftarrow \lVert x \rVert_2$	S, D, SC, DZ
FUNCTION xASUM (N, X, INCX)	$asum \leftarrow \lVert re(x) \rVert_1 + \lVert im(x) \rVert_1$	S, D, SC, DZ
FUNCTION IxAMAX(N, X, INCX)	$amax \leftarrow 1^{st} k \ni \lvert re(x_k)\rvert + \lvert im(x_k)\rvert = max(\lvert re(x_i)\rvert + \lvert im(x_i)\rvert)$	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:

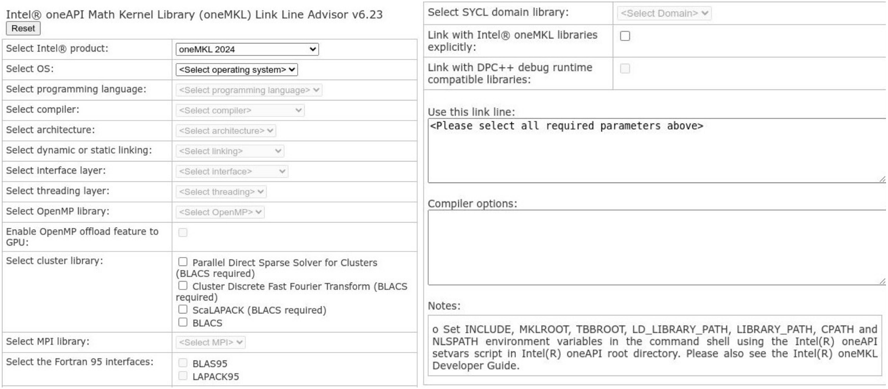
```
double *x = (double*)mkl_malloc(m * sizeof(double), sizeof(double));
double *Ax = (double*)mkl_malloc(n * sizeof(double), sizeof(double));
double *AtAx = (double*)mkl_malloc(m * sizeof(double), sizeof(double));
for (int i=0; i<m; i++)
  x[i] = rand() / (double) RAND_MAX;
for (int i=0; i<maxit; i++) {
  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:



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**.

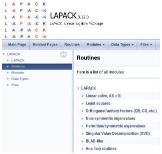
Nomenclature of LAPACK subroutines

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

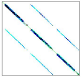
- **Sparse matrices** are **matrices** with relatively **few non-zero components**.
- Natural occurrence in scientific applications:
  - **Discretized differential equations**:
    - ODEs: chemical reactions, multi-body systems with short-range interactions, multi-agent systems with local interactions, ...
    - 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

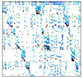
- **Researchers** and **developers** often **need** multiple **sparse matrices** with documented characteristics **to benchmark** NLA **algorithms**.
- In particular, the **SuiteSparse Matrix Collection** is widely used for this:

  `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 (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:

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

$$\begin{aligned} \texttt{r} &= 2, \texttt{c} = 2 \\ \texttt{val} &= [a_{11}, a_{12}, a_{21}, a_{22}, a_{13}, 0, 0, 0, a_{33}, a_{34}, a_{43}, 0] \\ \texttt{col\_idx} &= [1, 2, 2] \\ \texttt{row\_start} &= [1, 3, 4] \end{aligned}$$

- 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** ($\mathtt{r}\times\mathtt{c}$)
  - 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:

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

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

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

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

- 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 `idx` $:= [$`row_start`$,$ `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:

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

- 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

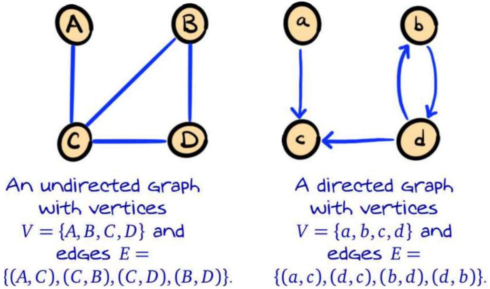
Section 9.2 in Darve & Wootters (2021)

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**.



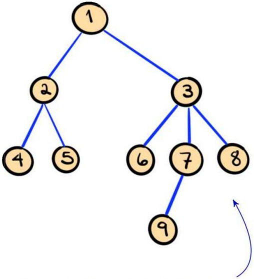
Darve, E., & Wootters, M. (2021). Numerical linear algebra with Julia. Society for Industrial and Applied Mathematics.

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**.



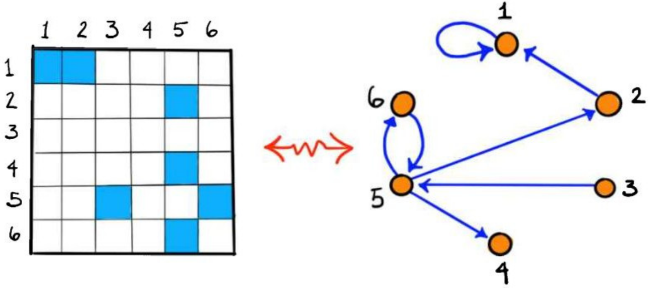
A tree. Vertex 1 is the root, and vertices 4, 5, 6, 9, 8 are leaves. Vertex 8 is 3's child, and 3 is 8's parent. Vertex 9 is 3's descendant, and 3 is 9's ancestor.

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**.