Linear Algebra Libraries

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How to deal with linear algebra in code

As much as possible, rely on existing, mature software libraries to perform linear algebra computations.

By doing so you...

- Focus on your code details.
- Reduce the amount of code to write and debug
- Libraries are tuned and optimized, i.e., your code will run faster
- More options to switch methods if necessary.

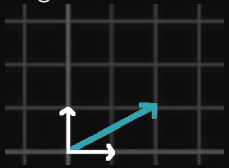
BLAS

Basic Linear Algebra Subroutines

- A well-defined standard interface for linear algebra routines.
- Many highly-tuned implementations exist for various platforms.
  (MKL, BLIS, Atlas, OpenBLAS, PLASMA, cuBLAS, ...)
- Interface vs. Implementation!
  Trick is designing a sufficiently general interface.
- Higher-order operations (e.g. factorizations, solving) defined in LAPACK, on top of BLAS.

Linear algebra recap: vectors

- Basic building block is the **vector**.

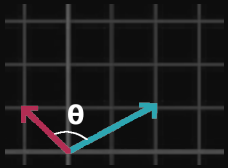


N numbers for a N-dimensional vector. Each number says how far along each axes $\hat{e}_i$.

- Magnitude of a vector by the square root of the sum of the squares of the components:

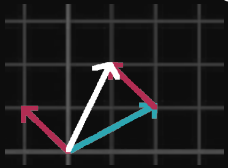
$$\|\vec{a}\| = \sqrt{\sum_i a_i^2}$$

- Inner product of two vectors:



$$\vec{a} \cdot \vec{b} = \sum_i a_i b_i = \|a\| \, \|b\| \, \cos\theta$$
$$a_i = \hat{e}_i \cdot \vec{a}$$

- Vectors addition means adding components.



- Scaling vectors means one scalar multiplying all components: $(\lambda\vec{a})_i = \lambda a_i$

Linear algebra recap: matrices

- We can look at the vector space in different coordinates.
- Individual new components of a vector in new coodinates can be found by inner product with unit vectors corresponding to the new axes:

$$(\vec{a}')_i = \hat{e}'_i \cdot \vec{a}$$

$$a'_i = \hat{e}'_i \cdot \vec{a}$$

$$a'_i = \hat{e}'_i \cdot \sum_j a_j \hat{e}_j$$

$$a'_i = \sum_j (\hat{e}'_i \cdot \hat{e}_j) a_j$$

- So the transformation from one to the other is given by an N x N matrix.

$$Q_{ij} = \hat{e}'_i \cdot \hat{e}_j$$

- And we need matrix vector multiplication to apply this matrix:

$$a'_i = \sum_j Q_{ij} a_j \quad \textit{i.e.} \quad \vec{a}' = \mathbf{Q} \cdot \vec{a}$$

- This is a special matrix called an orthogonal matrix, which preserves angles and sizes.
- General matrices can also scale and skew.

Finally, applying several matrices results in applying a matrix product:

$$(\mathbf{A} \cdot \mathbf{B})_{ij} = \sum_k A_{ik} B_{kj}$$

Typical BLAS routines

- Level 1: vector operations
  - `sdot` (dot product, single)
  - `zaxpy` ($ax + y$, dbl complex)
- Level 2: matrix-vector operations
  - `dgemv` (dbl matrix*vec)
  - `dsymv` (dbl symmetric matrix*vec)
- Level 3: matrix-matrix operations
  - `sgemm` (general matrix-matrix)
  - `ctrmm` (triangular matrix-matrix)

Somewhat cryptic names, interfaces.

Prefixes

S: Single
D: Double
C: Complex
Z: Double Complex Matrix

Types

GE: General
HY: Hermetian
SY: Symmetric
TR: Triangular
GB: General Banded
HB: Hermetian Banded
SB: Symmetric Banded
TB: Triangular Banded
TP: Triangular Packed

Why using Linear Algebra Packages?

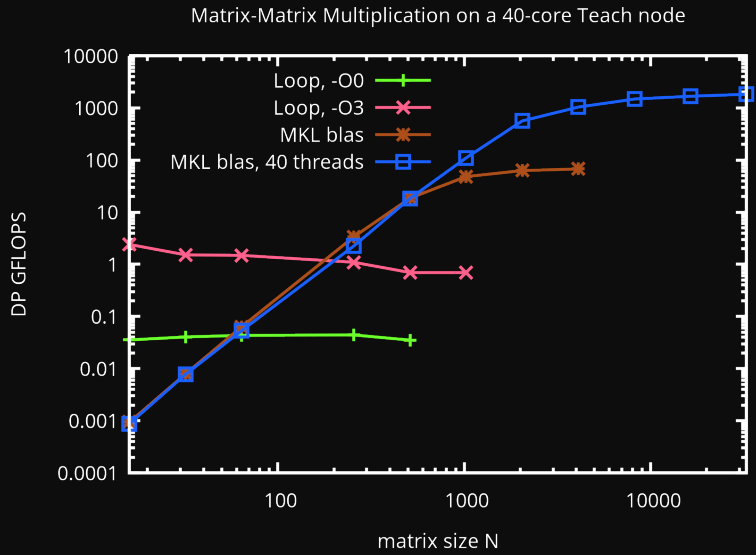
- Why bother?
- Finding, downloading, installing the library
- Figuring out how to link
- C/Fortran issues
- Why not just write it?
  (It's not rocket science)

$$\mathbf{C} = \mathbf{A} \cdot \mathbf{B}$$

$$C_{ij} = \sum_k A_{ik} B_{kj}$$

```
for (i=0; i<N; i++) {
    for (j=0; j<N; j++) {
        c[i,j] = 0.0;
        for (k=0; k<N; k++) {
            c[i,j] += a[i,k]*b[k,j];
        }
    }
}
```

Never, ever, write your own...



Using BLAS


SciNet
ADVANCED RESEARCH COMPUTING at the UNIVERSITY OF TORONTO

Using BLAS

- Netlib provides *reference* implementation
- Most vendors provide optimized versions
- Vendor-specific: Intel (MKL), AMD (AMD-BLIS), IBM (ESSL)
- Open Source: ATLAS, BLIS, OpenBLAS
- Fortran functions
- C interface using CBLAS and LAPACKE

Install OpenBLAS

```
$ module load gcc/14.3
$ git clone https://github.com/xianyi/OpenBLAS.git openblasbuild
$ cd openblasbuild
$ git checkout v0.3.31
$ make USE_LOCKING=1 USE_OPENMP=0 USE_THREAD=1 CC=gcc
$ make PREFIX=~/myopenblas install
```

Create a script to set variables:

```
echo 'LD_LIBRARY_PATH=$LD_LIBRARY_PATH:~/myopenblas/lib' >> ~/myopenblas/setup
echo 'LIBRARY_PATH=$LIBRARY_PATH:~/myopenblas/lib'       >> ~/myopenblas/setup
echo 'CPATH=$CPATH:~/myopenblas/lib'                     >> ~/myopenblas/setup
echo 'MANPATH=$MANPATH:~/myopenblas/man'                 >> ~/myopenblas/setup
```

Before using OpenBLAS, you must do

```
source ~/myopenblas/setup
```

Install manpages (optional, but useful)

```
$ wget http://www.netlib.org/lapack/lapack-3.1.1.tgz
$ tar -C ~/myopenblas --strip-components=3 -xaf lapack-3.1.1.tgz lapack-3.1.1/manpages/blas/man/manl
$ tar -C ~/myopenblas --strip-components=2 -xaf lapack-3.1.1.tgz lapack-3.1.1/manpages/man/manl
```

BLAS Examples

BLAS Example: DSCAL (x $\leftarrow \alpha$ x)

```cpp
// dscalex.cpp
#include <print>
#include <rarray>
#include <cblas.h>

int main() {
  rvector x = make_rarray({ 1.0, 2.0, 3.0 });

  cblas_dscal(x.size(), 4.323, &x[0], 1);

  std::println("{} ",x);
}
```

```
$ module load gcc/14.3 rarray/2.8.2
$ source ~/myopenblas/setup
$ g++ -c -std=c++23 dscalex.cpp -o dscalex.o
$ g++ dscalex.o -o dscalex -lopenblas
$./dscalex
{4.323,8.646,12.969}
```

BLAS Example: DSCAL (x $\leftarrow \alpha$ x)

Documentation

- https://www.netlib.org/blas/blast-forum
- `man dscal`

```
NAME
       DSCAL - a vector by a constant

SYNOPSIS
       SUBROUTINE DSCAL(N,DA,DX,INCX)

           DOUBLE PRECISION          DA
           INTEGER                   INCX,N
           DOUBLE PRECISION          DX(*)

PURPOSE
         scales a vector by a constant.
         uses unrolled loops for increment equal to one.
```

Function name + order and names of arguments

Says that DA is a double precision scalar

Says that INCX and N are integers.

Says that DX is a double precision array

Yep, that's the Fortran version, but the C/C++ versions are (nearly) the same.

BLAS Example: DSCAL (x $\leftarrow \alpha$ x)

```cpp
#include <print>
#include <rarray>
#include <cblas.h>

int main() {
  rvector x = make_rarray({ 1.0, 2.0, 3.0 });

  // DSCAL(N,DA,DX,INCX):

  // number of elements (x.extent(0) works too)
  int N = x.size();
  // scalar to multiply with
  double DA = 4.323;
  // point to first element (x.data() works too)
  double* DX = &x[0];
  // all elements are contiguous
  int    INCX = 1;
  cblas_dscal(N, DA, DX, INCX);

  std::println("{} ",x);
}
```

```
$ module load gcc/14.3 rarray/2.8.2
$ source ~/myopenblas/setup
$ g++ -c -std=c++23 dscalex2.cpp -o dscalex2.o
$ g++ dscalex2.o -o dscalex2 -lopenblas
$./dscalex2
{4.323,8.646,12.969}
```

Let's try something a bit more involved...

Matrix Multiply Documentation

- man dgemm

```
NAME
       DGEMM - performs one of the matrix-matrix operations   C := alpha*op( A )*op( B ) + beta*C,
SYNOPSIS
       SUBROUTINE DGEMM(TRANSA,TRANSB,M,N,K,ALPHA,A,LDA,B,LDB,BETA,C,LDC)

           DOUBLE PRECISION     ALPHA,BETA
           INTEGER              K,LDA,LDB,LDC,M,N
           CHARACTER            TRANSA,TRANSB
           DOUBLE PRECISION     A(LDA,*),B(LDB,*),C(LDC,*)

PURPOSE
       DGEMM  performs one of the matrix-matrix operations

       where  op( X ) is one of
          op( X ) = X   or   op( X ) = X',

       alpha and beta are scalars, and A, B and C are matrices, with op( A ) an m by k matrix,
       op( B ) a  k by n matrix and C an m by n matrix.
```

LDA? Leading Dimension?

Miscellaneous Details

- CBLAS calls involving matrices have an additional first argument `CblasRowMajor`, `CblasColMajor`
- LDA - *Leading dimension of* `A` used to access subblocks of the matrix.
- The *leading dimension* is the number of elements to skip to get to the next row (when row major) or column (when column major).
- For full matrices, this is the number of columns (for row major)
  or the number of rows (for column major).
- This allows you to use submatrices without making a copy.

BLAS Example: DGEMM (C $\leftarrow \alpha$ A · B + β C)

```
$ g++ -std=c++23 dgemmex.cpp -o dgemmex -lopenblas
```

```
#include <cblas.h>
#include <print>
#include <rarray>
void printmatrix(const rmatrix<double>& a) {
   std::println("{} by {}\n{}", a.extent(0), a.extent(1), a);
}
int main() {
   int m = 3, k = 5, n =4;
   double alpha = 1.0, beta = 0.0;
   rmatrix<double> A(m,k), B(k,n);
   rmatrix<double> C(m,n);
   for (int i=0; double& a: A) a = ++i;
   for (int i=0; double& b: B) b = --i;
   C.fill(0.0);
   cblas_dgemm(CblasRowMajor, CblasNoTrans, CblasNoTrans,
               m, n, k, alpha, &A[0][0], k, &B[0][0], n,
               beta, &C[0][0], n);
   std::print("A:"); printmatrix(A);
   std::print("B:"); printmatrix(B);
   std::print("C:"); printmatrix(C);
}
```

```
$ ./dgemmex
```

```
A:3 by 5
{
{1,2,3,4,5},
{6,7,8,9,10},
{11,12,13,14,15}
}
B:5 by 4
{
{-1,-2,-3,-4},
{-5,-6,-7,-8},
{-9,-10,-11,-12},
{-13,-14,-15,-16},
{-17,-18,-19,-20}
}
C:3 by 4
{
{-175,-190,-205,-220},
{-400,-440,-480,-520},
{-625,-690,-755,-820}
}
```

LAPACK

Linear Algebra PACKage (LAPACK)

LAPACK contains a variety of subroutines for solving linear systems, matrix decompositions, and factorizations.

- Internally uses BLAS calls
- Supports the same data types (single/double precision, real/complex and matrix structure types (symmetric, banded, etc.) as BLAS
- Three categories: auxiliary routines, computational routines, and driver routines
- C interface with prefix `LAPACKE_`
  https://www.netlib.org/lapack/lapacke.html

Linear Algebra PACKage (LAPACK)

Computational routines are designed to perform single, specific computational tasks:

- factorizations:
  - LU , LL^T /LL^H, LDL^T /LDL^H ,
  - QR, LQ, QRZ generalized QR and RQ
- symmetric/Hermitian and nonsymmetric eigenvalue decompositions
- singular value decompositions
- generalized eigenvalue and singular value decompositions

LAPACK Example: DGESV (Solve A x = b)

```
NAME
       DGESV - computes the solution to a real system of linear equations  A * X = B,

SYNOPSIS
       SUBROUTINE DGESV( N, NRHS, A, LDA, IPIV, B, LDB, INFO )

           INTEGER          INFO, LDA, LDB, N, NRHS
           INTEGER          IPIV( * )
           DOUBLE PRECISION A( LDA, * ), B( LDB, * )
PURPOSE
       DGESV computes the solution to a real system of linear equations
          A  *  X = B, where A is an N-by-N matrix and X and B are N-by-NRHS matrices.
       The LU decomposition with partial pivoting and row interchanges is used to factor A as
          A = P * L * U,
       where P is a permutation matrix, L is unit lower triangular, and U is upper triangular.
       The factored form of A is then used to solve the system of equations A * X = B.

ARGUMENTS
      N       (input) INTEGER
              The number of linear equations, i.e., the order of the matrix A.  N >= 0.

      NRHS    (input) INTEGER
              The number of right hand sides, i.e., the number of columns of the matrix B.
```

LAPACK Example: DGESV (Solve A x = b)

```cpp
// dgesvex.cpp
#include <print>
#include <lapacke.h>
#include <rarray>
int main() {
   const int N=3, NRHS=2, LDA=N, LDB=NRHS;
   rvector<int> ipiv(N);
   int info;
   rmatrix<double> A(N, N);
   A.fill({{6.80, -6.05, -0.45},
           {-2.11, -3.30,  2.58},
           {5.66,  5.36, -2.70}});
   rmatrix<double> b(N,NRHS);
   b.fill({{4.02, -1.56},
           {6.19,  4.00},
           {-8.22, -8.67}});
   info = LAPACKE_dgesv(LAPACK_ROW_MAJOR, N, NRHS,
                        &A[0,0], A.extent(1), &ipiv[0], &b[0,0], b.extent(1));
   std::println("Solutions x: {}", b);
   std::println("Details of LU factorization: {}", A);
   std::println("Pivot indices: {}", ipiv);
}
```

LAPACK Example: DGESV (Solve A x = b)

```
$ g++ -std=c++23 dgesvex.cpp -o dgesvex -lopenblas
$ ./dgesvex
```

```
Solutions x: {
{-0.0517981,-0.892398},
{-0.819976,-0.736171},
{1.30806,-0.121056}
}
Details of LU factorization: {
{6.8,-6.05,-0.45},
{0.832353,10.3957,-2.32544},
{-0.310294,-0.49802,1.28225}
}
Pivot indices: {1,3,3}
```

What about non-dense matrices?

E.g.:

$$\begin{pmatrix}
-2 & 1 & & & & & \\
1 & -2 & 4 & & & & \\
 & 4 & -2 & 4 & & & \\
 & & 4 & -2 & 4 & & \\
 & & & 4 & -2 & 4 & \\
 & & & & & \ddots & \\
 & & & & 4 & -2 & 1 \\
 & & & & & 1 & -2
\end{pmatrix}$$

For different types, use different functions

- Banded: `DGBSV`
- Tri-diagonal: `DGTSV`
- Symmetric positive definite: `DPOSV`

LAPACK Example: DGTSV (Solve Ax=b)

```cpp
// dgtsvex.cpp
#include <print>
#include <lapacke.h>
#include <rarray>
int main() {
    const int N=5, NRHS=3;
    rvector<double> dl(N-1); dl.fill({1, 4, 4, 1});
    rvector<double> dc(N);   dc.fill({-2, -2 ,-2 ,-2, -2});
    rvector<double> du(N-1); du.fill({1, 4, 4, 1});
    rmatrix<double> b(N, NRHS);
    b.fill({{3, -1.56,  9.81},
            {5,  4.00, -4.09},
            {5, -8.67, -4.57},
            {5,  1.75, -8.61},
            {3,  2.86,  8.99}});
    int info = LAPACKE_dgtsv(LAPACK_ROW_MAJOR, N, NRHS,
                             &dl[0], &dc[0], &du[0], &b[0,0], b.extent(1));
    std::print("Solutions x: {}", b);
    return info;
}
```

LAPACK Example: DGTSV (Solve Ax=b)

```
$ g++ -std=c++23 dgtsvex.cpp -o dgtsvex -lopenblas
$ ./dgtsvex
```

```
Solutions x:
{
{-0.931034,0.285747,-6.09874},
{1.13793,-0.988506,-2.38747},
{2.05172,0.43431,-0.691552},
{1.13793,-0.961839,0.899195},
{-0.931034,-1.91092,-4.0454}
}
```

Sparse BLAS ?

Unfortunately there is not just one mature, standard sparse matrix BLAS library.

Some potential options:

- "Official'' Sparse BLAS: a reference implementation is not yet available
  https://www.netlib.org/blas/blast-forum
- NIST Sparse BLAS: An alternative BLAS system; a reference implementation is available
  https://math.nist.gov/spblas
- MKL sparse linear algebra routines:

  https://www.intel.com/content/www/us/en/docs/onemkl/developer-reference-c/2025-2/inspector-executor-sparse-blas-routines.html
- AMD sparse linear algebra routines:

  https://www.amd.com/en/developer/aocl/sparse.html
- Various linear algebra packages may offer support for sparse matrices.

LAPACK References

- https://www.netlib.org/lapack
- LAPACK Internet Interface and Search Engine
  https://www.cs.colorado.edu/~jessup/lapack
- https://web.cs.ucdavis.edu/~bai/publications/baidemmeletal06.pdf