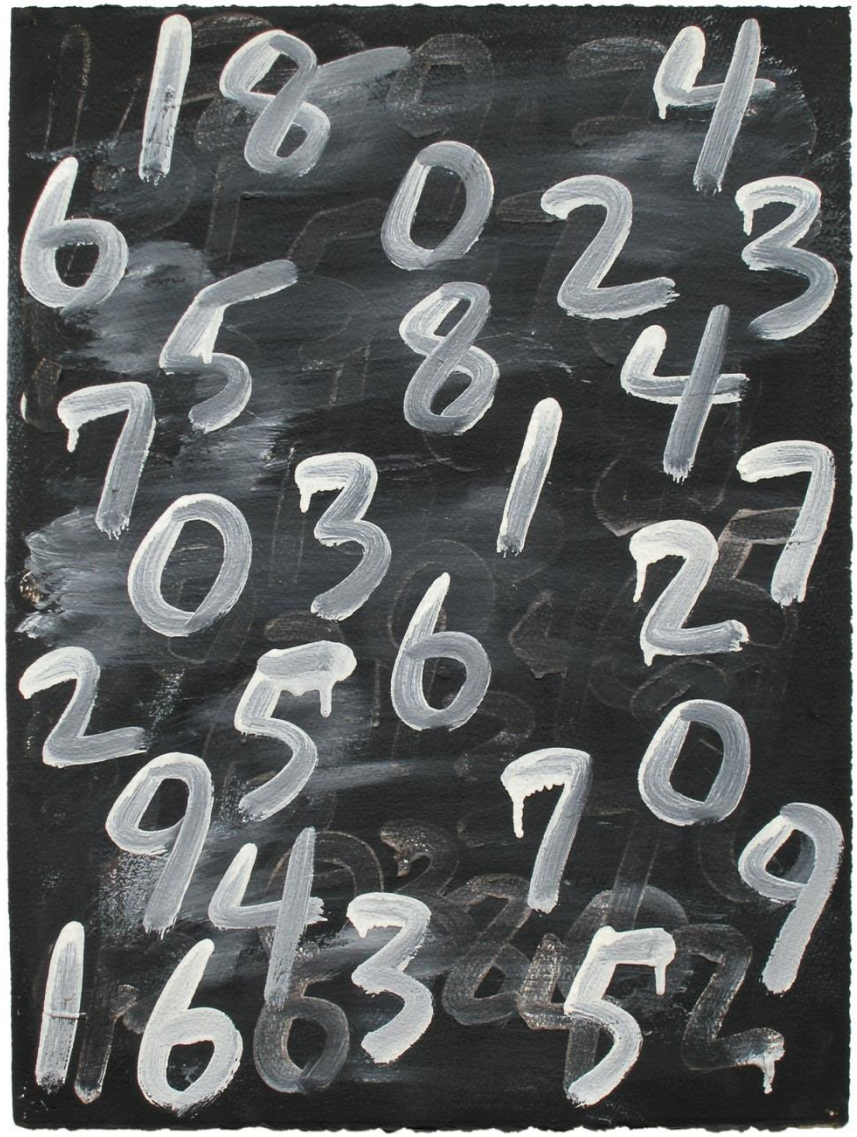
9. Linear Algebra Computation



Basic Linear Algebra Subprograms (BLAS)

- Routines that provide standard, low-level, building blocks for performing basic vector and matrix operations.

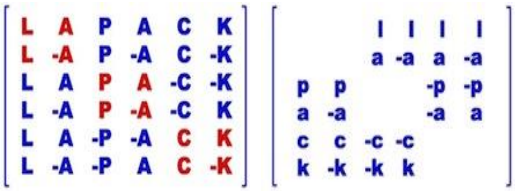
- Originally developed in 1979.
  Lawson, C.L., R.J. Hanson, D.R. Kincaid & F.T. Krogh, 1979, Basic Linear Algebra Subprograms for Fortran Usage, *ACM Trans. Math. Software*, *5*(3), 308-323

- Level-1 BLAS perform scalar, vector and vector-vector operations
  Level-2 BLAS perform matrix-vector operations
  Level-3 BLAS perform matrix-matrix operations

- Machine-specific optimized BLAS libraries are available for a variety of computer architectures. (provided by the computer or software vendor, e.g., Intel® Math Kernel Library)

- Because the BLAS are efficient, portable, and widely available, they are commonly used in the development of high quality linear algebra software, e.g., LAPACK (Linear Algebra PACKage).

- For source codes and documents see: www.netlib.org/blas



Example: matrix-matrix multiplication (Level-3 BLAS) www.netlib.org/blas/

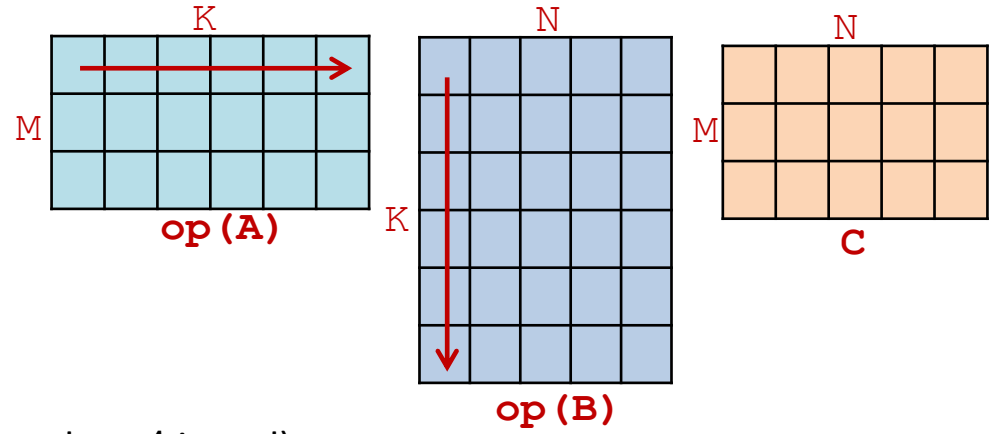
$$C \leftarrow \alpha \times op(A) \times op(B) + \beta \times C$$

```
SUBROUTINE SGEMM(TRANSA,TRANSB,M,N,K,ALPHA,A,LDA,B,LDB,BETA,C,LDC)
```

S: single precision

GE: general matrix

MM: matrix-matrix



TRANSA: the form of `op(A)` to be used

`'N' or 'n'`, `op(A)` = A

`'T' or 't'`, `op(A)` = A^T

`'C' or 'c'`, `op(A)` = A^T (transpose, when A is real)

A^H (conjugate transpose, when A is complex in `CGEMM`)

M: the number of rows of `op(A)` and `C`

N: the number of columns of `op(B)` and `C`

K: the number of columns of `op(A)` and the number of rows of `op(B)`

ALPHA, **BETA**: the scalar coefficients α and β

LDA, **LDB**, **LDC**: the first dimension of `A`, `B` and `C` as declared in the calling program

A: real array of dimension `(LDA,ka)`, where `ka` is `K` when `TRANSA='N'`, and is `M` otherwise

B: real array of dimension `(LDB,kb)`, where `kb` is `N` when `TRANSB='N'`, and is `K` otherwise

C: real array of dimension `(LDC,N)`

- To use BLAS and LAPACK:
  1. Download the zipped file `blas_lapack_lib.zip` containing the pre-built libraries.
  2. Unzip and put the four files `libblas.dll`, `libblas.lib`, `liblapack.dll` and `liblapack.lib` in the `GNU_emacs_Fortran` folder

- To link the BLAS library in compiling:

```
> gfortran -L. -lblas  my_program.f90
```

Example: using BLAS `sgemm` to re-do matrix multiplication exercise

```
> gfortran -L. -lblas example_blas.f90
```

```
program example_blas
implicit none
integer,parameter :: m=3, k=2, n=5
real :: a(m,k) = reshape((/1.3,3.6,3.05,2.5,-2.0,-0.03/),(/m,k/))
real :: b(k,n) = reshape((/2.0,12.4,-0.2,2.7,3.4,-7.1,38.9,1.2,23.9,2.4/),(/k,n/))
real :: c(m,n) = 0.0, c_blas(m,n) = 0.0, alpha, beta
integer :: i, j, ii, lda, ldb, ldc
!
do i = 1, m
do j = 1, n
  do ii = 1, k
    c(i,j) = c(i,j) + a(i,ii)*b(ii,j)
  end do
end do
end do
write(*,*) 'Hand crafted:', (c(i,i), i=1,min(m,n))
!
alpha = 1.0
beta = 0.0
lda = m
ldb = k
ldc = m
call sgemm('N','N',m,n,k,alpha,a,lda,b,ldb,beta,c_blas,ldc)
write(*,*) 'BLAS sgemm:  ', (c_blas(i,i), i=1,min(m,n))
!
write(*,*) 'Max error:', maxval(abs(c-c_blas))
end program
```

$$a = \begin{bmatrix} 1.3 & 2.5 \\ 3.6 & -2.0 \\ 3.05 & -0.03 \end{bmatrix}$$

$$b = \begin{bmatrix} 2.0 & -0.2 & 3.4 & 38.9 & 23.9 \\ 12.4 & 2.7 & -7.1 & 1.2 & 2.4 \end{bmatrix}$$

Example: A test driver for using BLAS `sgemm`; compare with intrinsic function `matmul`

```
> gfortran -L. -lblas t_blas.f90
```

```
program t_blas
implicit none
integer,parameter :: m=2000, k=1500, n=1000
integer :: lda=m, ldb=k, ldc=m
real :: random, t1, t2, t3, alpha, beta
real :: a(m,k), b(k,n), c(m,n), c_intr(m,n)
integer :: i, j, iseed
!
!-- Assign random values to a, b and c
iseed = 65432
do j = 1, k
do i = 1, m
  a(i,j) = random(iseed)
end do
end do
do j = 1, n
do i = 1, k
  b(i,j) = random(iseed)
end do
end do
do j = 1, n
do i = 1, m
  c(i,j) = random(iseed)
end do
end do
alpha = random(iseed)
beta = random(iseed)
```

>Continued on next page...

```fortran
!-- Compute alfa*a*b+beta*c using intrinsic function matmul and BLAS sgemm
call cpu_time(t1)
!
c_intr = alpha*matmul(a,b) +beta*c
!
call cpu_time(t2)
!
call sgemm('N','N',m,n,k,alpha,a,lda,b,ldb,beta,c,ldc)
!
call cpu_time(t3)
!
!-- Find the maximum error of abs(c-c_intr) using intrinsic function maxval
write(*,*) 'Max error: ', maxval(abs(c-c_intr))
write(*,*) 'Elapsed time of matmul:', t2-t1
write(*,*) 'Elapsed time of sgemm: ', t3-t2
!
end program
```

```
> gfortran -L. -lblas t_blas.f90 random.f90
> a.exe
> Max error:   1.23977661E-05
> Elapsed time of matmul:   3.5724230
> Elapsed time of sgemm:    25.474962
```

- The pre-built BLAS has *not* been optimized for GNU Fortran.

- But, using the optimized BALS of Intel math kernel library for Intel Fortran, the performance of BLAS becomes much better.

Using GNU gfortran and pre-built BLAS:

```
Max error:   1.23977661E-05
Elapsed time of matmul:   2.6832180
Elapsed time of sgemm:   23.712152
```

Using Intel Fortran and BLAS in Intel math kernel library:

```
Max error:   8.8214874E-06
Elapsed time of matmul:  1.007847
Elapsed time of sgemm:  0.3469471
```

Linear Algebra PACKage (LAPACK)

L	A	P	A	C	K
L	-A	P	-A	C	-K
L	A	P	A	-C	-K
L	-A	P	-A	-C	K
L	A	-P	-A	C	K
L	-A	-P	A	C	-K

- Solve systems of linear equations, linear least-squares problems, eigenvalue problems, and singular value problems.
- LAPACK can also handle many associated computations, such as matrix factorizations or estimating condition numbers.
- Written in Fortran and call level-3 BLAS as much as possible for the computation.
- Originally written in FORTRAN 77, but moved to Fortran 90 in version 3.2 (2008); The current version is 3.6.1 (06/2016).
- LAPACK can be seen as the successor to the linear equations and linear least-squares routines of LINPACK and the eigenvalue routines of EISPACK.

LINPACK is still being used as the benchmark for measuring the performance of top 500 supercomputers. (www.top500.org/project/linpack/)

- The original goal of the LAPACK project was to make the widely used EISPACK and LINPACK libraries run efficiently on shared-memory vector and parallel processors.

- For source codes and documents see: www.netlib.org/lapack

- LAPACK contains three levels of routines

  driver routines: for solving standard types of problems,
  typically calls a sequence of computational routines.

  computational routines: to perform a distinct computational task.

  auxiliary routines: to perform a certain subtask or common low-level computation.

- Both real and complex matrices are provided for in LAPACK.

- Dense and band matrices are provided for in LAPACK, but not general sparse matrices.

Example: solve a linear system with a general non-symmetric matrix

$$[A]\{x\} = \{B\}$$

```
subroutine SGESV(N,NRHS,A,LDA,IPIV,B,LDB,INFO)
```

S: single precision
GE: general non-symmetric matrix
SV: solve linear system

[in]	**N**	The number of linear equations, i.e., the order of the matrix `A`.
[in]	**NRHS**	The number of right hand sides, i.e., the number of columns of the matrix `B`.
[in,out]	**A(LDA,N)**	On entry, the `N x N` coefficient matrix `A`. On exit, the factors `L` and `U` from the factorization `A = P*L*U`.
[in]	**LDA**	The leading dimension of the array `A`.
[out]	**IPIV(N)**	The pivot indices that define the permutation matrix `P`.
[in,out]	**B(LDB,NRHS)**	On entry, the right-hand-side matrix `B`. On exit, if `INFO = 0`, the `N x NRHS` solution matrix `X`.
[in]	**LDB**	The leading dimension of the array `B`.
[out]	**INFO**	`INFO = 0`: successful exit. `INFO = -i`: unsuccessful exit, the i-th argument had an illegal value. `INFO = i`: unsuccessful exit, `U(i,i)` is exactly zero.

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  2. Unzip and put the four files `libblas.dll`, `libblas.lib`, `liblapack.dll` and `liblapack.lib` in the `GNU_emacs_Fortran` folder

- To link the LAPACK library in compiling:

```
> gfortran -L. -llapack  my_rogram.f90
```

Example: using LBLAS `sgesv` to solve a system of linear equations

$$\begin{aligned} x_1 + x_2 + x_3 &= 1. \\ 2x_1 + x_2 + x_3 &= 2. \\ x_1 + 3x_2 + 2x_3 &= 4. \end{aligned} \qquad \begin{aligned} x_1 &= 1. \\ x_2 &= 3. \\ x_3 &= -3. \end{aligned}$$

$$\begin{aligned} x_1 + x_2 + x_3 &= 0. \\ 2x_1 + x_2 + x_3 &= -1. \\ x_1 + 3x_2 + 2x_3 &= 1. \end{aligned} \qquad \begin{aligned} x_1 &= -1. \\ x_2 &= 0. \\ x_3 &= 1. \end{aligned}$$

```
> gfortran -L. -llapack example_lapack.f90
```

```
program example_lapack
implicit none
integer,parameter :: n=3, nrhs=2
integer,parameter :: lda=n, ldb=n
real :: a(lda,n) =
reshape((/1.0,2.0,1.0,1.0,1.0,3.0,1.0,1.0,2.0/),(/n,n/))
real :: b(ldb,nrhs) = reshape((/1.0,2.0,4.0,0.0,-1.0,1.0/),(/n,nrhs/))
integer :: ipiv(n), info, i, j
!
call sgesv(n,nrhs,a,lda,ipiv,b,ldb,info)
!
write(*,*) "info=",info
do i=1,n
 write(*,*) i,(b(i,j),j=1,nrhs),ipiv(i)
end do
!
end program
```

Exercise: Test driver for the subroutine of solution of system of linear equations

- A genetic method to test a solver for a linear system $[A]\times\{x\} = \{B\}$ is to invent a coefficient matrix $[A]$ and an "known" unknown vector $\{x\}$.

  The right-hand side of the equation $\{B\}$ can then be calculated by multiplying the two matrices $\{B\} = [A]\times\{x\}$.

  The vector $\{x\}$, which has been generated, is the known exact solution of the system of equations, and is denoted by $\{x\_exact\}$.

- Given $[A]$ and $\{B\}$, the subroutine of solution of system of linear equations (such as SGESV in LAPACK) is then called to solve the system of equations, and the result is denoted as $\{x\_solve\}$.

- Since we know the exact solution $\{x\_exact\}$, the numerical error when solving the equations, which is defined as the maximum of the absolute value of $(x\_exact_j - x\_solve_j)$, can be computed.

  If the system of equation has been solved correctly, the maximum error should be within the a limit determined by the precision of the computer.

Procedure:

- Generate matrix $[A]$
- Generate vector $\{x_{exact}\}$
- Compute vector $\{B\} = [A] \times \{x_{exact}\}$
- Solve $[A] \times \{x\} = \{B\}$ for $\{x\}$
- Find the maximum of $|\{x\} - \{x_{exact}\}|$

Write a test driver for SGESV in LAPACK. The program should contains the following components:

1. Input the dimension of the linear system, `ndim`.

2. Generate the elements of the matrix [*A*] and the vector {*x*_exact} using the random number generation function/subroutine. The values of the elements of [*A*] and {*x*} will be between 1 and -1.

3. Call the matrix-vector multiplication routine SGEMV in BLAS to compute {*B*} = [*A*]×{*x*_exact}. The values of the elements of [*B*] will also have the magnitude of order one.

4. Call the subroutine SGESV in LAPACK to solve the system of equations: [*A*]×{*x*_solve} = {*B*} for the solution {*x*_solve}.

5. Find the maximum error of the solved unknowns {*x*_solve} given the known solution {*x*_exact}, and output the result.

6. You need to link both libraries of Blas and Lapack in compiling the program:

```
> gfortran -L. -lblas –llapack my_program.f90
```