Scientists have developed a large library of numerical routines for linear algebra. These routines comprise the LAPACK package that can be obtained from http://www.netlib.org/lapack/.

The LAPACK routines build on (lower level) routines for basic linear algebra, denoted by BLAS (basic linear algebra subroutines).

These low-level routines represent the time-critical parts of a calculation and should be provided in a machine-specific version. This way the LAPACK code itself remains highly portable without losing performance. LAPACK comes with a default set of BLAS routines, and optimized replacement routines are available from:

- ATLAS (Automatically Tuned Linear Algebra Software), http://math-atlas.sourceforge.net/
- Intel Math Kernel Library (MKL), http://www.intel.com/
- AMD Core Math Library (ACML)
Arrays
Since LAPACK stems from old Fortran times, its conventions are Fortran-like: Arrays (and thus matrices) are stored column by column in memory. In contrast, C by default stores arrays row by row. To use the LAPACK routines from C/C++, matrices have to be stored in transposed form.

Function Names
Most LAPACK routines have a six-letter name of the form XYYZZZ with $X$ indicating the data type:
- s single
- d double
- c complex
- z double complex
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YY indicates the type of matrix:
- ge  general
- gt  general tridiagonal
- he  (complex) Hermitian
- sy  symmetric
  and many more.

ZZZ determines the actual task performed:
- trf  factorize
- tri  use factorization to compute inverse
- sv  simple driver that solves system of equations
- svx expert driver (checks condition number, computes error bounds)
- ev  compute the eigenvectors
  and many more.
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Linux man page of ("man dsyev") for a diagonalization routine:

DSYEV(1)

NAME
DSYEV - compute all eigenvalues and, optionally, eigenvectors of a real symmetric matrix A

SYNOPSIS
SUBROUTINE DSYEV( JOBZ, UPLO, N, A, LDA, W, WORK, LWORK, INFO )

CHARACTER JOBZ, UPLO
INTEGER INFO, LDA, LWORK, N
DOUBLE PRECISION A( LDA, * ), W( * ), WORK( * )

PURPOSE
DSYEV computes all eigenvalues and, optionally, eigenvectors of a real symmetric matrix A.

ARGUMENTS
JOBZ (input) CHARACTER*1
= 'N': Compute eigenvalues only;
= 'V': Compute eigenvalues and eigenvectors.

UPLO (input) CHARACTER*1
= 'U': Upper triangle of A is stored;
= 'L': Lower triangle of A is stored.

N (input) INTEGER
The order of the matrix A. N >= 0.

Harald O. Jeschke
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ITP, Uni Frankfurt
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A  (input/output) DOUBLE PRECISION array, dimension (LDA, N)
On entry, the symmetric matrix A. If UPLO = 'U', the leading N-by-N upper triangular part of
A contains the upper triangular part of the matrix A. If UPLO = 'L', the leading N-by-N lower
triangular part of A contains the lower triangular part of the matrix A. On exit, if
JOBZ = 'V', then if INFO = 0, A contains the orthonormal eigenvectors of the matrix A. If
JOBZ = 'N', then on exit the lower triangle (if UPLO='L') or the upper triangle (if UPLO='U')
of A, including the diagonal, is destroyed.

LDA  (input) INTEGER
The leading dimension of the array A. LDA >= max(1,N).

W  (output) DOUBLE PRECISION array, dimension (N)
If INFO = 0, the eigenvalues in ascending order.

WORK  (workspace/output) DOUBLE PRECISION array, dimension (LWORK)
On exit, if INFO = 0, WORK(1) returns the optimal LWORK.

LWORK  (input) INTEGER
The length of the array WORK. LWORK >= max(1,3*N-1). For optimal efficiency, LWORK >=
(NB+2)*N, where NB is the blocksize for DSYTRD returned by ILAENV.
If LWORK = -1, then a workspace query is assumed; the routine only calculates the optimal
size of the WORK array, returns this value as the first entry of the WORK array, and no error
message related to LWORK is issued by XERBLA.

INFO  (output) INTEGER
= 0: successful exit
< 0: if INFO = -i, the i-th argument had an illegal value
> 0: if INFO = i, the algorithm failed to converge; i off-diagonal elements of an intermedi-
ate tridiagonal form did not converge to zero.
Simple C++ program diagonalizing a $10 \times 10$ matrix and checking the result:

```cpp
#include <iostream>
#include <unistd.h>
#include <iomanip>
#include <math.h>
using namespace std;

#ifdef __cplusplus
extern "C" {
#endif
#ifdef USE_NAG
    extern void f06qff_(char* MATRIX, int* M, int* N, double* A,
                        int *LDA, double *B, int* LDB);
    extern void f02faf_(char* JOB, char* UPLO, int* N, double* A,
                        int* LDA, double* W, double* WORK, int* LWORK, int* IFAIL);
#else
    extern void dcopy_(int* N, double* DX, int* INCX, double* DY, int* INCY);
    extern void dsyev_(char* JOBZ, char* UPLO, int* N, double* A, int* LDA,
                        double* W, double* WORK, int* LWORK, int* INFO);
#endif
#ifdef __cplusplus
}
#endif

void calc_matrix(double* matrix, int matrix_size);
void diagonalize_matrix(double* matrix, double* eigenvalues, double* eigenvectors, int matrix_size);
```
int main() {
    int matrix_size = 10;
    double* eigenvectors = new double[matrix_size * matrix_size];
    double* matrix = new double[matrix_size * matrix_size];
    double* eigenvalues = new double[matrix_size];
    double sum, matelement;

calc_matrix(matrix, matrix_size);

    cout << setprecision(3) << "Real symmetric matrix:" << endl;
    for(int i=0;i<matrix_size;i++) {
        for(int j=0;j<matrix_size;j++) cout << matrix[i*matrix_size+j] << "\t";
        cout << endl;
    }
    
    diagonalize_matrix(matrix, eigenvalues, eigenvectors, matrix_size);

    cout << setprecision(15) << "Eigenvalue, <ev|mat|ev>, rel. error:" << endl;
    for(int evvec_i = 0; evvec_i < matrix_size; evvec_i++) {
        matelement = 0.0;
        for(int i=0;i<matrix_size;i++) {
            sum = 0.0;
            for(int j=0;j<matrix_size;j++)
                sum += eigenvectors[evvec_i*matrix_size+j] * matrix[i*matrix_size+j];
            matelement += sum * eigenvectors[evvec_i*matrix_size+i];
        }
        cout << evvec_i << " \t" << eigenvalues[evvec_i] << "\t" << matelement << "\t"
            << 100.0*fabs((eigenvalues[evvec_i] - matelement)/matelement) << endl;
    }
}

Harald O. Jeschke
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Some symmetric $10 \times 10$ matrix is calculated:

```c
void calc_matrix(double* matrix, int matrix_size) {
    double numvec[10] = {0.15, 0.37, 0.22, 0.58, 0.39, 0.21, 0.33, 0.095, 0.21, 0.93};
    for(int i=0;i<matrix_size;i++) {
        for(int j=i;j<matrix_size;j++) {
            matrix[j*matrix_size+i] = 0.0;
            matrix[i*matrix_size+j] = 0.0;
            for(int k=0;k<matrix_size;k++) {
                double koeff = ((double) k+2.0)/(10.0-(double) j);
                matrix[i*matrix_size+j] += numvec[i]*exp(-koeff*numvec[j]);
            }
            if(j>i) matrix[j*matrix_size+i] = matrix[i*matrix_size+j];
        }
    }
}
```
The diagonalization can be performed by NAG (if `USE_NAG` is defined at compile time) or by LAPACK. The Fortran specific variables are defined inside the scope of `do { ... } while(false)` in order to be forgotten right after use.

```c
void diagonalize_matrix(double* matrix, double* eigenvalues, double* eigenvectors, int matrix_size) {
    static double* work = new double[64*matrix_size];
    int iffail = 0;
    do {
        int B2 = matrix_size, B3 = matrix_size, B4 = matrix_size*matrix_size;
        int Bstep = 1, B6 = 64*matrix_size, B8 = iffail;
        char B9 = 'V', B10 = 'L';
        // in order to preserve matrix, matrix is copied into eigenvectors,
        // and then eigenvectors is diagonalized
        #ifdef USE_NAG
            f06qff_(&B10,&B3,&B3,matrix,&B3,eigenvectors,&B3);
            f02faf_(&B9, &B10, &B2, eigenvectors, &B3, eigenvalues, work, &B6, &B8);
            iffail = B8;
        #else
            dcopy_(&B4,matrix,&Bstep,eigenvectors,&Bstep);
            dsyev_(&B9,&B10,&B2,eigenvectors,&B3,eigenvalues,work,&B6,&B8);
            iffail = B8;
        #endif
    } while(false);
    if(iffail != 0) cout << "unexpected: diagonalisation failure ";
}
```
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Possibilities of compiling this code:

a) on linux, with liblapack.a installed in /usr/lib (you can use “locate liblapack.a” to find it):
   $ g++ diagonalize.cc -o diagonalize -llapack -lblas

b) with MKL lapack:
   $ icc diagonalize.cc -o diagonalize_mkl -lmkl_lapack -lmkl_core -lmkl_em64t -lguide -lpthread

c) with NAG (using RZ license):
   $ export NAG_KUSARI_FILE=orobas.rz.uni-frankfurt.de:
   $ g++ -DUSE_NAG diagonalize.cc -o diagonalize_nag -L/opt/NAG/fll6a22df1/lib -lnag_nag -lgfortran

Eigenvalue problems
Diagonalization library routines

LAPACK library XI

Program output:

```
$ ./diagonalize
Real symmetric matrix:
1.36  1.16  1.26  0.9   1  1.15  0.902  1.23  0.793  0.0386
1.16  2.85  3.1   2.22  2.47  2.84  2.23   3.02  1.96  0.0951
1.26  3.1   1.85  1.32  1.47  1.69  1.32   1.8   1.16  0.0566
0.9   2.22  1.32  3.48  3.87  4.45  3.49   4.74  3.07  0.149
1    2.47  1.47  3.87  2.6   2.99  2.35   3.19  2.06  0.1
1.15  2.84  1.69  4.45  2.99  1.61  1.26   1.72  1.11  0.054
0.902 2.23  1.32  3.49  2.35  1.26  1.98   2.7   1.74  0.0848
1.23  3.02  1.8   4.74  3.19  1.72  2.7   0.776  0.502  0.0244
0.793 1.96  1.16  3.07  2.06  1.11  1.74   0.502  1.11  0.054
0.0386 0.0951 0.0566 0.149  0.1  0.054  0.0848  0.0244  0.054  0.239

Eigenvalue, <ev|mat|ev>, rel. error:
0  -4.44362756263176  -4.44362756263176  1.99876881485112e-14
1  -1.46301700282751  -1.46301700282751  0
2  -0.881470789352469  -0.881470789352468  1.00760958891512e-13
3  -0.539773208392523  -0.539773208392525  6.17049720528806e-14
4   0.235630023754761   0.235630023754761  1.17793034916964e-14
5   0.566317297014242   0.566317297014241  1.56834034916964e-14
6   0.776590300395759   0.776590300395757  2.74626331891948e-14
7   0.888994640780154   0.888994640780153  7.49311395387622e-14
8   2.896957064929929    2.896957064929929  3.06590121908352e-14
9   19.8260174161067    19.8260174161067  3.5838904044832e-14
```