

Software libraries: Eigen

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1. Linear algebra

- Linear algebra is very important in science
- You're not the first person to need linear algebra software
- \Rightarrow many libraries in existence
- many old libraries in Fortran, C

2. Eigen library

```
1 // eigen/matvec.cpp
2 #include <Eigen/Dense>
3 using namespace Eigen;
```

- Eigen library: idiomatic C++
- Many common operations
- High performance

Linear algebra objects

3. Dense matrices and vectors

- Matrix size as template parameter:

```
1 // eigen/matvec.cpp
2 const int siz=5;
3 Matrix<double,siz,siz> A;
4 Vector<double,siz> true_solution,rhs,tmp;
```

- Dynamic definition:

```
1 // eigen/matvec.cpp
2 Matrix<float,Dynamic,Dynamic> Af(20,20);
3 // or: MatrixXf Af(20,20);
```

(last character: use 'f' for float, 'i' for `int`, and 'd' for `double`)

4. Elementary operations

- Indexing with parentheses: $A(i,j)*v(j)$
- Methods `rows`, `cols`, `size`
- Range over vector, output:

```
1 // eigen/matvec.cpp
2 for ( auto& v : rhs )
3     v = 1.;
4 cout << rhs << '\n';
```

- `seq(f,t)` is the sequence $f, f+1, \dots, t$:

```
1 A( seq(0,5), seq(3,10) );
```

- Subblock of size $p \times q$ starting at (i,j) :

```
1 A.block(i,j,p,q);
```

Exercise 1: Matrix vector product

Code the matrix-vector product with a matrix A and vector x .
Compare the result to writing

```
1 y = A*x;
```

5. Jacobi method

Matrix-vector product with x unknown:

$$Ax = f \Leftrightarrow \forall_i: \sum_j a_{ij}x_j = f_i$$

repeatedly solve:

$$x_i^{(n+1)} = (f_i - \sum_{j \neq i} a_{ij}x_j^{(n)}) / a_{ii}$$

Speed of convergence depends on matrix sizes and diagonal dominance:

$$\forall_i: a_{ii} > \sum_{j \neq i} |a_{ij}|$$

Exercise 2: Jacobi method

- Code the jacobi; iterate a few steps
- Write a second version using `seq` or `block` compare to the first for correctness
- Optionally, can you write a version using ranges?

(Use the `matvec` skeleton in the repository.)

- Since you know the exact solution, iterate until a certain precision.
- How does the number of iterations depend on matrix size and amount of diagonal dominance?

Operations

6. Solving $Ax = b$

Multiply by inverse: $x = A^{-1}b$:

```
1 // eigen/invert.cpp
2 auto sol1 = A.inverse() * rhs;
```

Use Gaussian elimination:

$$A = LU, \quad Ly = f, \quad Ux = y$$

```
1 // eigen/invert.cpp
2 PartialPivLU<MatrixXd> LU(A);
3 auto sol2 = LU.solve(rhs);
```

Exercise 3: System solving

Diagonal dominance:

$$\forall_i: a_{ii} > \sum_{j \neq i} |a_{ij}|$$

- Solve the linear system by both methods above. How accurate is the solution?
- Experiment with different matrix sizes and amounts of diagonal dominance.

Exercise 4: Vandermonde matrix

$$a_{ij} = x_i^j$$

where $\{x_i\}_i$ sequence without duplicates

- Again solve the system both ways. Observations?

7. Singular values

```
1 // eigen/invert.cpp
2 JacobiSVD<MatrixXd> svd(A);
3 VectorXd sigmas = svd.singularValues();
```

- Singular values are a little like eigenvalues
- The spread in singular values indicates how 'difficult' the matrix is
- \Rightarrow 'condition number': largest divided by smallest eigenvalue

8. Example: Generalized Inverse

- Regression / curve fitting:

$$Ax = b$$

with A rectangular.

- Solution:

$$x = A^+ b = (A^t A)^{-1} A^t b$$

Generalized inverse / Moore-penrose inverse

```
1 // eigen/penrose.cpp
2 auto gen_inverse = ( A.transpose() * A ).inverse() * A.transpose();
3 x = gen_inverse * b;
```

Exercise 5: Commandline options

Use commandline options to:

- set the size of the matrix
- switch between diagonal dominant and vandermonde matrix
- for the former case set the diagonal dominance

9. Parallelism

Some operations support multi-thread parallelism,
for instance through OpenMPI

- Compile with OpenMP: `-fopenmp`
- Set number of threads: `Eigen::setNbThreads(4)`

10. Discovery

Through pkg-config:

```
1 $ pkg-config --cflags eigen3
2 -I/somewhere/installation-eigen-3.4.0/include/eigen3
```

As Cmake module:

```
1 find_package( Eigen3 REQUIRED )
2 target_link_libraries( ${PROJECTNAME} PUBLIC Eigen3::Eigen )
```