ETH Lecture 401-0663-00L Numerical Methods for CSE

Numerical Methods for Computational Science and Engineering

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URL: http://www.sam.math.ethz.ch/~hiptmair/tmp/NumCSE/NumCSE15.pdf

Introduction

- Use the study center HG E 41, Mon from 18:00
- A toolbox course → many different topics, that are only loosely related

[toolbox contains hammer, screwdriver, duct tape]

I. Computing with Matrices and Vectors

(some aspects of $\underbrace{\text{numerical linear algebra}}_{\text{foundation of all numerical codes}}$)

I.1. Fundamentals

I.1.1. Notations:

Vector $\underline{v} = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix} \in \mathbb{K}^n$, $\mathbb{K} = \mathbb{R}, \mathbb{C}$ (default: column vector)

Matrix $A = \begin{bmatrix} a_{1,1} & \cdots & a_{1,n} \\ \vdots & & \vdots \\ a_{m,1} & \cdots & a_{m,n} \end{bmatrix} \in \mathbb{K}^{m,n}$

row vector $v^T = [v_1 \cdots v_n]$

↳ just special matrices $\in \mathbb{K}^{1,n}$

Components/entries: $(v)_i := v_i$, $(A)_{i,j} := a_{ij}$

sub-vector/matrix blocks: $(v)_{k:\ell} = \begin{bmatrix} v_k \\ \vdots \\ v_\ell \end{bmatrix}$, $1 \leq k \leq \ell \leq n$

$(A)_{k:\ell, r:s} \in \mathbb{K}^{\ell-k+1, s-r+1}$

$\mathbf{A} := \begin{bmatrix} a_{11} & \dots & a_{1m} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nm} \end{bmatrix}$

→ entry $(\mathbf{A})_{i,j} = a_{ij}$, $1 \leq i \leq n, 1 \leq j \leq m$,

→ i-th row, $1 \leq i \leq n$: $a_{i,:} = (\mathbf{A})_{i,:}$,

→ j-th column, $1 \leq j \leq m$: $a_{i,:} = (\mathbf{A})_{:,j}$,

→ matrix block (sub-matrix) $(a_{ij})_{\substack{i=k,\dots,l \\ j=r,\dots,s}} = (\mathbf{A})_{k:l,r:s}$, $1 \leq k \leq l \leq n$, $1 \leq r \leq s \leq m$.

1.2. Software and Libraries

→ Always rely on them for numerical linear algebra

1.2.1. MATLAB

↳ IDE for numerical computation (numerical engine, libraries, editor, debugger, profiler, help)

"In MATLAB everything is a matrix"

(Fundamental "data type" in MATLAB = matrix of complex numbers)

↳ non-typed language

[m,n] = size(A) → request dimensions of matrix

A(i,j), v(i) → entry access

Initialization of matrix:

, ⟺ horizontal
; ⟺ vertical
} concatenation

Example:

```
% Caution: matrices are dynamically
  expanded when
% out of range entries are accessed
M = [1,2,3;4,5,6]; M(4,6) = 1.0; M,
```

Output: M=

1	2	3	0	0	0
4	5	6	0	0	0
0	0	0	0	0	0
0	0	0	0	0	1

"loop index vectors" $v = (a:s:b)$

```
>> v = (3:-0.5:-0.3)
v =   3.0000    2.5000    2.0000    1.5000    1.0000    0.5000         0
>> v = (1:2.5:-13)
v = Empty matrix: 1-by-0
```

⇒ loop: for $i = (a:s:b)$

```
% MATLAB loop over columns of a matrix
M = [1,2,3;4,5,6];
for i = M; i, end
```

Output:

```
i = 1    i = 2    i = 3
    4        5        6
```

1.2.2. Eigen

= Header-only C++ library for numerical algebra,
→ template metaprogramming
→ expression templates

Fundamental data type : matrix

```
Matrix<typename Scalar, int RowsAtCompileTime, int
    ColsAtCompileTime>
```

for specifying small fixed size matrices

Special data types : MatrixX*, $* \in \{i, f, d, cd\}$

```
#include <Eigen/Dense >

template<typename Scalar>
void eigenTypeDemo(unsigned int dim)
{
  using dynMat_t =
     Eigen::Matrix<Scalar,Eigen::Dynamic,Eigen::Dynamic>;
  using dynColVec_t = Eigen::Matrix<Scalar,Eigen::Dynamic,1>;
  using dynRowVec_t = Eigen::Matrix<Scalar,1,Eigen::Dynamic>;
  using index_t = typename dynMat_t::Index;
  using entry_t = typename dynMat_t::Scalar;

  dynColVec_t colvec(dim);
  dynRowVec_t rowvec(dim);
  for(index_t i=0; i< colvec.size(); ++i) colvec(i) = (Scalar)i;
  for(index_t i=0; i< rowvec.size(); ++i) rowvec(i) =
     (Scalar)1/(i+1);
  dynMat_t vecprod = colvec*rowvec;  ← matrix product
  const int nrows = vecprod.rows();
  const int ncols = vecprod.cols();
}
```

Initialization of matrices :

```
#include <Eigen/Dense >
// Just allocate space for matrix, no initialisation
Eigen::MatrixXd A(rows,cols);  ← reserve space
// Zero matrix.  Similar to matlab command zeros(rows, cols);
Eigen::MatrixXd B = MatrixXd::Zero(rows, cols);
// Ones matrix.  Similar to matlab command ones(rows, cols);
Eigen::MatrixXd C = MatrixXd::Ones(rows, cols);
// Matrix with all entries same as value.
Eigen::MatrixXd D = MatrixXd::Constant(rows, cols, value);
// Random matrix, entries uniformly distributed in [0,1]
Eigen::MatrixXd E = MatrixXd::Random(rows, cols);
// (Generalized) identity matrix, 1 on main diagonal
Eigen::MatrixXd I = MatrixXd::Identity(rows,cols);
std::cout << "size of A = (" << A.rows() << ',' << A.cols() << ')'
   << std::endl;
```

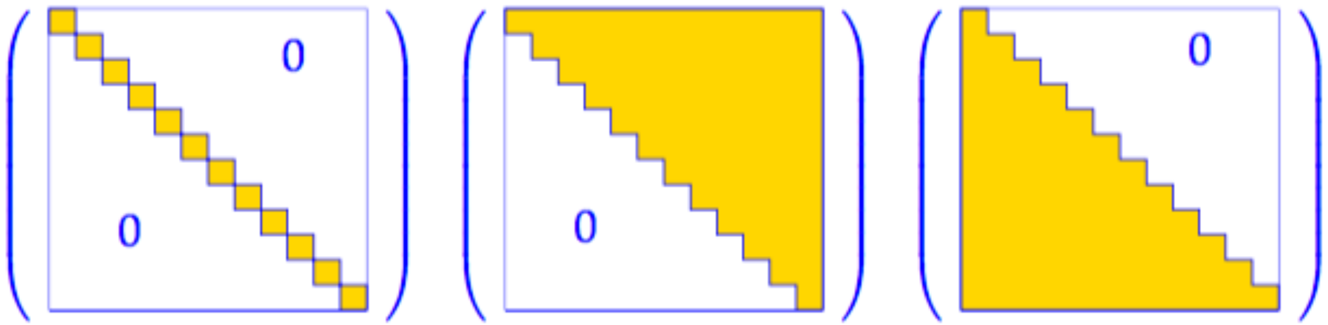
Addressing sub-matrices :

```
template<typename MatType> void
  blockAccess(Eigen::MatrixBase<MatType> &M)
{
  using index_t = typename Eigen::MatrixBase<MatType>::Index;
  using entry_t = typename Eigen::MatrixBase<MatType>::Scalar;
  const index_t nrows(M.rows()); % No. of rows
  const index_t ncols(M.cols()); % No. of columns

  cout << "Matrix M = " endl << M << endl; // Print matrix
  // Block size half the size of the matrix
  index_t p = nrows/2,q = ncols/2;
  // Output submatrix with left upper entry at position (i,i)
  for(index_t i=0; i < min(p,q); i++)
    cout << "Block (" << i << ',' << i << ',' << p << ',' << q
         << ") = " << M.block(i,i,p,q) << endl;
  // l-value access: modify sub-matrix by adding a constant
  M.block(1,1,p,q) += MatrixXd::Constant(p,q,1.0);
  cout << "M = " endl << M << endl;
  // r-value access: extract sub-matrix
  MatrixXd B(M.block(1,1,p,q));
  cout << "Isolated modified block = " endl << B << endl;
  // Special sub-matrices
  cout << p << " top rows of m = " << M.topRows(p) << endl;
  cout << p << " bottom rows of m = " << M.bottomRows(p) << endl;
  cout << q << " left cols of m = " << M.leftCols(q) << endl;
  cout << q << " right cols of m = " << M.rightCols(p) << endl;
  // r-value access to upper triangular part
  const MatrixXd T = M.template triangularView<Upper>(); //
  cout << "Upper triangular part = " << endl << T << endl;
  // l-value access to upper triangular part
  M.template triangularView<Lower>() *= -1.5; //
  cout << "Matrix M = " << endl << M << endl;
}
```

In Eigen : indexing from 0 !

Triangular matrices :



diagonal matrix   upper triangular   lower triangular

1.2.3. Matrix storage formats

→ Matrix stored in linearized form (as a vector)

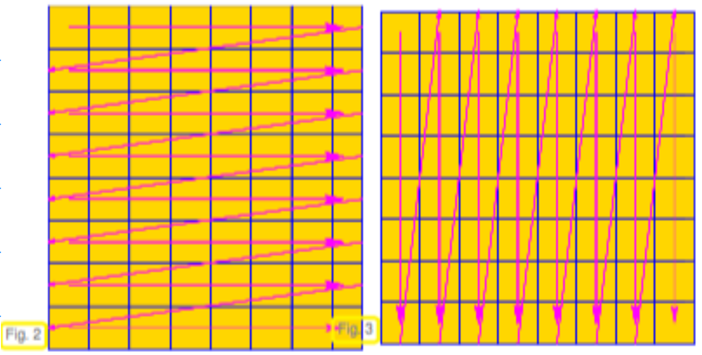
$$\mathbf{A} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{pmatrix}$$

Row major (C-arrays, bitmaps, Python):

A_arr	1	2	3	4	5	6	7	8	9

Column major (Fortran, MATLAB, EIGEN):

A_arr	1	4	7	2	5	8	3	6	9



row major   column major

Index mappings $A \in \mathbb{K}^{n,m}$

r.m. : $(i,j) \leftrightarrow m(i-1)+j$

```
// Template parameter ColMajor selects column major data layout
Matrix<double,Dynamic,Dynamic,ColMajor> mcm(nrows,ncols);
```
→ default

```
// Template parameter RowMajor selects row major data layout
Matrix<double,Dynamic,Dynamic,RowMajor> mrm(nrows,ncols);
```

Why care ? → Calling library functions

Exp.: Impact of storage format on runtime

1.2.20

Matlab : Column major

```
A = randn(n,n);
for j = 1:n-1,
  A(:,j+1) = A(:,j+1) - A(:,j);
end
```
column oriented access

↓

faster, because contiguous access to memory

```
A = randn(n,n);
for i = 1:n-1,
  A(i+1,:) = A(i+1,:) - A(i,:);
end
```
row oriented access

↓

many cache misses