Numerik Summary HS17

Tablet notes

Week 1

1. Computing with matrizes and vectors (1)
Fixed point / floating point representation (2)
Machine numbers, absolute & relative error (3/4)
Axiom of roundoff analysis (5)
Notations, Libraries, Dense matrix storage formats (7-9)
Computational effort, asymptotic complexity (10/11)
Cost of basic operations (12)
some tricks to reduce complexity (13)

Week 2

Hidden summation, Kronecker produkt (1-3)
Cancellation, roots, diff. quotient (4)
Numerical stability, backward/mixed stable (9)

2. Direct methods for solving LSE (12)
Gauss elimination (13)
LU-decomposition (14)
Block elimination (16)

Week 3

Low rank modifications (1)
sherman-Woodbury formula (2)
Sparse linear Systems (3)
Storage, COO/triplet (4)
Direct solution of sparse LSE (9)

3 Direct methods for linear least squares (11)
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kernel, range, normal equation, uniquness (15-16)
Generalized solution, uniquness (16)
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QR-decomposition, Gram-Schmidt (6)
QR-decomp. theorem, uniquness (10)
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SVD, singular values, rank/range/kernel (18)
SVD in Eigen (21)
Generalized solutions by SVD (22)
SVD Moore-Sherman pseudoinverse (23)

Week 5

SVD optimization: norm-constrained extrema (1)
best-low rank approx (2)
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Constrained least squares, Lagrange (10)
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4. Filtering (13)
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discrete convolution (18)

Week 6

discrete periodic convolution (1)
circulant matrix, disc conv → disc period conv (2)
DFT, EV/EW circulant matrix (4)
Inverse of Fourier matrix (6)
Diagonalization FM, DFT (7)
note on total least squares (8)
example on convolution (9)
disc conv via DFT, conv theorem, FFT (13-15)

Week 7

FFT (1)
Frequency filtering via DFT (3)
2D DFT, Filtering with 2D DFT (7)
2D convolution theorem (9)

Week 7 (continued)

- 5 Data interpolation in 1D (11)
- piecewise linear interpolation (13)
- hat functions, interpolant for p.l. interp (14)
- matrix representation (15)
- Global polynomial interpolation, horner scheme (17)
- Lagrange interpolation, existence & uniquness (18-19)

Week 8

- Lagrange, Complexity, matrix representation (1-2)
- Barycentric interpolation (2)
- Newton basis (3)
- Runge's phenomenon (5/6)
- Aitken-Neville scheme (6)
- Divided difference scheme + Horner scheme (8)

Week 9

- Splines, spline space (1)
- Cubic spline interpolation (2)

- 6. Approximation of functions in 1D (6)
- Global polynomials, Taylor approach (7)
- Bernstein approximation (8)

Week 10

- Jackson's theorem (2)
- Jackson's theorem on arbitrary intervals (3-4)
- Affine pullback, transformation under affine pullb. (4-5)
- Lagrangian approx scheme (7)
- algebraic, exponential convergence (8)
- representation of interpolation error (9)
- global L^∞ estimate (10)
- chebychev interpolation (11)
- chebychev polynomials (13)
- chebychev theorem, minimal polynomials, cheby. nodes (14-15)
- chebychev estimate (16)
- Lebesgue constant (18)
- implementation of chebychev interpolation (22)

Week 11

- implementation of Chebychev with Fourier (1)
- piece wise polynomial Lagrange interpolation (4)
- Continuous local Lagrange interpolants (5)
- error estimate (6)

- 7 Numerical quadrature (9)
- affine pullback (10)
- QF with Lagrange interpolation, Newton-Cotes (12)
- Gauss Quadrature (14)
- Sufficient order condition, maximal order (15-16)
- Legendre polynomials, Gauss-Legendre QF (20)

Week 12

- quadrature error for C^r-functions (2-3)
- increase of nodes (4)
- Composite Quadrature (6)

Week 13

- 8 Iterative methods (1)
- Bisection (2/3)
- Fixed point iterations (5)
- Order of convergence, linear convergence (6/7)
- quadratic conv: Newton iteration (8)
- Secant method for derivatives (11)
- Nonlinear systems of equations, equiv norms (13)
- local & global convergence (14)
- Fixed point iterations in $\mathbb{R}^n$, Banach, conditions (14/15)
- Newton's method in $\mathbb{R}^n$ (17)
- Failure examples (20)
- Damped Newton (21)

Week 14

- Unconstrained Optimization (1)
- Optimization with differentiable functions (3)
- Convex optimization (4)
- methods in 1D: Newton, Golden section search (5/6)
- Methods in ND: Gradient descent (8)
- Newton's method (11)
- BFGS method (quasi Newton) (12)

Code snippets

Lambda functions

```
auto func = [&globalVar] (int x) {return globalVar + x; };
```

Eval lamda functions

```
x.unaryExpr(func);
```

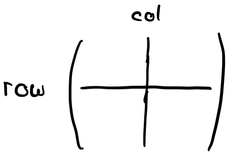
Iterate $2^0, 2^1, 2^2, \ldots$

```
for (int i=0; i≤N; ++i)  int n = 1 << i;
```

Matrix dimensions

A is $m \times n$

```
m = A.rows()
n = A.cols()
```



Solve $Ax = b$

we

```
FullPivLU<MatrixXd> B = A.fullPivLu();
PartialPivLU<MatrixXd> B = A.partialPivLu();      if A is invertible
ColPivHouseholder<MatrixXd> B = A.colPivHouseholderQr();
Full ..                                A.fullPiv...
TriangularView<MatrixXd, Upper> B = A.triangularView<Upper>();
                         Lower                           Lower

SparseLU<SparseMatrix<double>> B;                sparse
B.analyzePattern(A);   B.factorize(A);           matrices

VectorXd b = B.solve(b);
```

C++ vectors

```
std::vector<int> v;
v.push_back(42);
int m = v[0];
v.size();
std::sort(v.begin(), v.end());
v.pop_back();
(needs #include <algorithms>)
Map<VectorXd> myNewEigenVector(v.data(), v.size());
vector<double> v2(mat.data(), mat.data() + mat.rows() * mat.cols());
```

```
for (auto it = v.begin();
  it != v.end(); ++it) {
  cout << *it << endl;
}
for (auto t : v) {
  cout << t << endl;
}
```

Linspaced Vector

For $(0, 1, 2, \ldots, N)$: $(N+1,\ 0,\ N)$

```
VectorXd x = VectorXd::LinSpaced(len, from, to)
ArrayXd x = ArrayXd::LinSpaced(len, from, to)
```

Eps

(not :: denorm_min())

```
double eps = std::numeric_limits<double>::epsilon();
```

Pretty print

```
std::cout << std::scientific << std::setprecision(3) << std::setw(10)
  << out << std::endl;       #include <iomanip>
```

Triplets

```
         t.row()  t.col()  t.value()
Eigen::Triplet<double> t(3, 4, 42);
```

FFT

```
#include <unsupported/Eigen/FFT>
Eigen::FFT<double> fft;
VectorXcd v_fft = fft.fwd(v);
VectorXcd v_ffti = fft.inv(v_fft);
```

C++ constants and functions

```
pi: M_PI   (#include <cmath>)
sin(), exp(), cos(), abs()
```

Max coefficient + index

```
int index;      double max = v.maxCoeff(&index);
```

Sparse matrices

```
SparseMatrix<double> A(n,n);
std::vector<Triplet<double>> triplets;
triplets.reserve(n);
triplets.push_back(Triplet<double>(1, 2, 42))
A.setFromTriplets(triplets.begin(), triplets.end());
A.makeCompressed();
```

Code segments

```
backward_substitution (MatrixXd &A, VectorXd &b, VectorXd &x) {
  int n = A.cols();        x = VectorXd::zero(n);
  for (int i = n-1; i >= 0; --i) {
    x(i) = (b(i) - A.row(i) * x) / A(i,i);
  }
}        (for upper triangular matrices)
```

Householder QR-decomposition (economical)

```
  int m = A.rows();   int n = A.cols();
  HouseholderQR<MatrixXd> QR = A.householderQr();
  MatrixXd Q = QR.householderQ() * MatrixXd::Identity(m, n);
  MatrixXd R = MatrixXd::Identity(n, m) *
        QR.matrixQR().triangularView<Upper>();
```

CholeskyQR

```
  MatrixXd AtA = A.transpose() * A;
  LLT<MatrixXd> LLT = AtA.llt();
  MatrixXd R = LLT.matrixL().transpose();
  MatrixXd Q = R.transpose().triangularView<Lower>().
      solve(A.transpose()).transpose();
```

SVD / k-rank approximation

```
  JacobiSVD<MatrixXd> svd(A, ComputeThinU | ComputeThinV);
  U = svd.matrixU().leftCols(k);
  S = svd.singularValues().head(k).asDiagonal();
  V = svd.matrixV().leftCols(k);
  MatrixXd A_approx = U * S * V.transpose();
```

COO to CRS

```
  A.sort_byRow();          <------  std::sort(list.begin(), list.end(),
  int prevNotEmptyRow = -1;             [] (auto t1, auto t2) {
  auto &l = A.list;                       return t1.row() < t2.row();
                                        });
  for (int i=0; i<l.size(); i++) {
    while (prevNotEmptyRow < l[i].row()) {
      prevNotEmptyRow ++; row_ptr.push_back(i);
    }
    double currVal = l[i].value();
    while (i < l.size()-1 && l[i].col() = l[i+1].col() &&
           l[i].row() = l[i+1].row()) {
      currVal += l[i].value(); i++;
    }
    val.push_back(currVal); col_ind.push_back(l[i].col());
  }
  row_ptr.push_back(val.size());
```

Dense to CRS

```
  int nnz = 0; int prevNotEmptyRow = -1;
  for (int i = 0; i < A.rows(); i++) {
    for (int j = 0; j < A.cols(); j++) {
      if (A(i,j) =! 0) {
        while (prevNotEmptyRow < i) {
          row_ptr.push_back(nnz);
          prevNotEmptyRow ++;
        }
        nnz++;
        val.push_back(A(i,j));
        col_ind.push_back(j);
      }
    }
  }
  row_ptr.push_back(nnz);
```

COO efficient matrix multiplication

```
  if (&A1 == &A2) {
    MatrixCOO copyA2(A2.list); return mult_effic(A1, copyA2);
  }
  MatrixCOO result;
  vector<Triplet<double>> &l1 = A1.list;
  vector<Triplet<double>> &l2 = A2.list;
  vector<Triplet<double>> &lr = result.list;
  A1.sort_byCol();    A2.sort_byRow();
  vector<int> b1;   vector<int> b2;
  b1.push_back(0);  b2.push_back(0);
  for (int i = 0; i < l1.size()-1; i++)
    if (l1[i].col() != l1[i+1].col()) b1.push_back(i+1);
  b1.push_back(l1.size());
  for (int j = 0; j < l2.size()-1; j++)
    if (l2[j].row() != l2[j+1].row()) b2.push_back(j+1);
  b2.push_back(l2.size());
  int i = 0; int j = 0;
  while (i < b1.size()-1 && j < b2.size()-1) {
    if (l1[b1[i]].col() == l2[b2[j]].row()) {
      int c1, c2;
      for (c1 = b1[i]; c1 < b1[i+1]; c1++) {
        for (c2 = b2[j]; c2 < b2[j+1]; c2++) {
          Triplet<double> t(l1[c1].row(), l2[c2].col(),
             l1[c1].value() * l2[c2].value());
          lr.push_back(t);
        }
      } i++; j++;
    } else {
      if (l1[b1[i]].col() < l2[b2[j]].row()) i++;
      if (l1[b1[i]].col() > l2[b2[j]].row()) j++;
    }
  }
} return result;
```

Complexeties

Solve LSE

General $O(n^3)$

triangular $O(n^2)$

sparse system $O(nnz^{3/2})$ - $O(nnz^{5/2})$

low-rank modification $O(n^2)$

Sherman-Morrison factorization $O(nk^2)$

dot product $O(n)$

tensor product $O(mn)$

matrix product $O(mnk)$

Decompositions

SVD $O(n^3)$

thin SVD $O(mn^2)$

Householder QR $O(mn^2)$ for $A \in \mathbb{K}^{m,n}$, $m > n$

FFT $O(n \log n)$

Sparse shit

Insert element into CRS/CCS $O(nnz)$

Efficient initialization $O(n)$ if $nnz = O(n)$

Solve sparse LSE $O(nnz^{3/2})$ - $O(nnz^{5/2})$

Least squares

Normal equations $O(\underbrace{mn^2}_{C=A^TA} + \underbrace{nm}_{c=A^Tb} + \underbrace{n^3}_{Cx=c}) = O(n^3 + mn^2)$

Interpolation

Horner scheme $O(n)$

Monomial basis, evaluating N datasets $O(n^3 N)$

Lagrange, evaluating

L_i is $O(n)$, interpolant p is $O(n^2)$, N datasets $O(Nn^2)$

Barycentric interpolation,

computing $\lambda_0, \dots, \lambda_n$ $O(n^2)$, evaluating p $O(n)$

N datasets $O(n^2 + nN)$

Newton

building Vandermonde matrix $O(n^2)$, solving αs $O(n^2)$

N evaluations $O(n^2 N)$

Aitken-Neville, evaluating interpolant $O(n^2)$

Divided differences, evaluating interpolant $O(n)$,

adding new point $O(n)$

Other

Filter: causality is granted if $y_j = 0 \ \forall j < 0$

$\int_a^b f(t)\,dt \approx \sum_{j=1}^{n} \hat{\omega}_j f(\hat{c}_j)$ under affine pullback

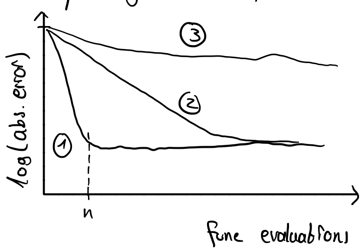
$\hat{c}_j = \frac{1}{2}(1 - c_j)a + \frac{1}{2}(1 + c_j)b$, $\quad \hat{\omega}_j = \frac{1}{2}(b-a)\omega_j$

Quadrature errorplot: linear trend in

lin-log plot $\rightarrow$ exponential convergence

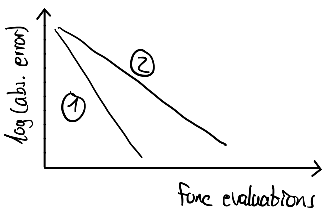
log-log plot $\rightarrow$ algebraic convergence

example global Gauss quadrature



1. $f \in \mathcal{P}_n$, QR exact up to $\sim n$ evaluations
2. $f \in C^\infty$, $f \notin \mathcal{P}_k \ \forall k \in \mathbb{N}$ exponential convergence
3. $f \in C^0$, $f \notin C^1$ algebraic convergence

other quadrature formulas



1. composite 2-point Gauss quadrat., because order ~ 4 (2x order of 2)
2. composite trapazoidal rule, order ~ 2

Estimates

Jackson's theorem for $f \in C^r([-1,1])$, $r \in \mathbb{N}$, for any polynomial degree $n \geq r$:

$$\inf_{p \in \mathcal{P}_n} \|f - p\|_{L^\infty([-1,1])} \leq \left(1 + \frac{\pi^2}{2}\right)^r \frac{(n-r)!}{n!} \|f^{(r)}\|_{L^\infty([-1,1])} = O(n^{-r})$$

$$\inf_{p \in \mathcal{P}_n} \|f - p\|_{L^\infty([a,b])} \leq \left(1 + \frac{\pi^2}{2}\right)^r \frac{(n-r)!}{n!} \left(\frac{b-a}{2}\right)^r \|f^{(r)}\|_{L^\infty([a,b])}$$

Lagrange for $f \in C^{n+1}(I)$ and equidistant nodeset $\mathcal{T} = \{t_0, \dots, t_n\} \subset I$

$$\|f - L_\mathcal{T} f\|_{L^\infty(I)} \leq \frac{\|f^{(n+1)}\|_{L^\infty(I)}}{(n+1)!} \max_{t \in I} |(t - t_0) \cdots (t - t_n)|$$

$$\|f - L_\mathcal{T} f\|_{L^2(I)} \leq \frac{2^{(n-1)/4} |I|^{n+1}}{\sqrt{n!(n+1)!}} \|f^{(n+1)}\|_{L^2(I)}$$

Chebychev for $f \in C^{n+1}(I)$, $I = [-1,1]$, $[a,b]$ and node set $\mathcal{T} = \{t_0, \dots, t_n\} \subset I$

$$\|f - I_\mathcal{T}(f)\|_{L^\infty([-1,1])} \leq \frac{2^{-n}}{(n+1)!} \|f^{(n+1)}\|_{L^\infty([-1,1])}$$

$$\|f - I_\mathcal{T}(f)\|_{L^\infty([a,b])} \leq \frac{2^{-2n-1}}{(n+1)!} |I|^{n+1} \|f^{(n+1)}\|_{L^\infty([a,b])}$$

Lebesgue constant

$$\|f - L_\mathcal{T} f\|_{L^\infty(I)} \leq (1 + \lambda_\mathcal{T}) \inf_{p \in \mathcal{P}_n} \|f - p\|_{L^\infty(I)} \quad \forall f \in C^0(I)$$

Chebychev + Lebesgue constant

$$\|f - L_\mathcal{T} f\|_{L^\infty([-1,1])} \leq \left(\frac{2}{\pi} \log(1+n) + 2\right)\left(1 + \frac{\pi^2}{2}\right)^r \frac{(n-r)!}{n!} \|f^{(r)}\|_{L^\infty([-1,1])}$$

Piecewise Lagrange

$$\|f - s\|_{L^\infty([x_0, x_m])} \leq h_\mathcal{M}^{n+1} \frac{1}{(n+1)!} \|f^{(n+1)}\|_{L^\infty([x_0, x_m])}$$

$$\|f - s\|_{L^2(I)} \leq h_\mathcal{M}^{n+1} \frac{2^{(n-1)/4}}{\sqrt{n!(n+1)!}} \|f^{(n+1)}\|_{L^2([x_0, x_m])}$$