ETH Zürich D-MATH

Numerical Methods for CSE

Problem Sheet 1

You should try to your best to do the core problems. If time permits, try and do the rest as well.

Problem 1. Arrow matrix-vector multiplication (core problem)

Consider the multiplication of the two "arrow matrices" A with a vector x, implemented as a function arrowmatvec (d, a, x) in the following MATLAB script

Listing 1: multiplying a vector with the product of two "arrow matrices"

```
function y = arrowmatvec(d,a,x)

% Multiplying a vector with the product of two ``arrow
    matrices''

% Arrow matrix is specified by passing two column
    vectors a and d

fi (length(d) = length(a)), error ('size mismatch'); end

% Build arrow matrix using the MATLAB function diag()

% A = [diag(d(1:end-1)),a(1:end-1);(a(1:end-1))',d(end)];

y = A*A*x;
```

(1a) • For general vectors $d = (d_1, \dots, d_n)^{\mathsf{T}}$ and $a = (a_1, \dots, a_n)^{\mathsf{T}}$, sketch the matrix A created in line 6 of Listing 1.

HINT: This MATLAB script is provided as file arrowmatvec.m.

(1b) ☐ The tic-toc timing results for arrowmatvec.m are available in Figure 1. Give a detailed explanation of the results.

HINT: This MATLAB created figure is provided as file arrowmatvectiming. {eps, jpg}.

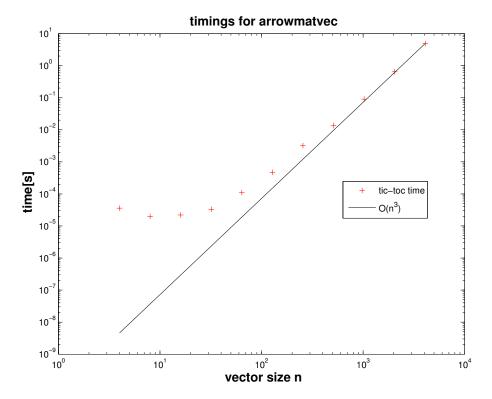


Figure 1: timings for arrowmatvec (d, a, x)

(1c) Write an *efficient* MATLAB function

function
$$y = arrowmatvec2(d,a,x)$$

that computes the same multiplication as in code 1 but with optimal asymptotic complexity with respect to n. Here d passes the vector $(d_1, \ldots, d_n)^T$ and a passes the vector $(a_1, \ldots, a_n)^T$.

- (1d) \odot What is the complexity of your algorithm from sub-problem (1c) (with respect to problem size n)?
- (1e) \Box Compare the runtime of your implementation and the implementation given in code 1 for $n=2^{5,6,\dots,12}$. Use the routines tic and toc as explained in example [1, Ex. 1.4.10] of the Lecture Slides.
- (1f) Write the EIGEN codes corresponding to the functions arrowmatvec and arrowmatvec2.

Problem 2. Avoiding cancellation (core problem)

In [1, Section 1.5.4] we saw that the so-called *cancellation phenomenon* is a major cause of numerical instability, *cf.* [1, § 1.5.38]. Cancellation is the massive amplification of *relative errors* when subtracting two real numbers of about the same value.

Fortunately, expressions vulnerable to cancellation can often be recast in a mathematically equivalent form that is no longer affected by cancellation, see [1, § 1.5.43]. There we studied several examples, and this problem gives some more,

(2a) • We consider the function

$$f_1(x_0, h) := \sin(x_0 + h) - \sin(x_0)$$
 (1)

It can the transformed into another form, $f_2(x_0, h)$, using the trigonometric identity

$$\sin(\varphi) - \sin(\psi) = 2\cos\left(\frac{\varphi + \psi}{2}\right)\sin\left(\frac{\varphi - \psi}{2}\right).$$

Thus, f_1 and f_2 give the same values, in exact arithmetic, for any given argument values x_0 and h.

- 1. Derive $f_2(x_0, h)$, which does no longer involve the difference of return values of trigonometric functions.
- 2. Suggest a formula that avoids cancellation errors for computing the approximation $(f(x_0 + h) f(x_0))/h$) of the derivative of $f(x) := \sin(x)$ at $x = x_0$. Write a MATLAB program that implements your formula and computes an approximation of f'(1.2), for $h = 1 \cdot 10^{-20}, 1 \cdot 10^{-19}, \dots, 1$.

HINT: For background information refer to [1, Ex. 1.5.40].

- 3. Plot the error (in doubly logarithmic scale using MATLAB's loglog plotting function) of the derivative computed with the suggested formula and with the naive implementation using f_1 .
- 4. Explain the observed behaviour of the error.
- (2b) Using a trick applied in [1, Ex. 1.5.48] show that

$$\ln(x - \sqrt{x^2 - 1}) = -\ln(x + \sqrt{x^2 - 1}).$$

Which of the two formulas is more suitable for numerical computation? Explain why, and provide a numerical example in which the difference in accuracy is evident.

(2c) • For the following expressions, state the numerical difficulties that may occur, and rewrite the formulas in a way that is more suitable for numerical computation.

1.
$$\sqrt{x+\frac{1}{x}} - \sqrt{x-\frac{1}{x}}$$
, where $x \gg 1$.

2.
$$\sqrt{\frac{1}{a^2} + \frac{1}{b^2}}$$
, where $a \approx 0, b \approx 1$.

Problem 3. Kronecker product

In [1, Def. 1.4.16] we learned about the so-called Kronecker product, available in MATLAB through the command kron. In this problem we revisit the discussion of [1, Ex. 1.4.17]. Please refresh yourself on this example and study [1, Code 1.4.18] again.

As in [1, Ex. 1.4.17], the starting point is the line of MATLAB code

$$y = kron(A, B) * x, (2)$$

where the arguments are $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n,n}, \mathbf{x} \in \mathbb{R}^{n \cdot n}$.

- (3a) Obtain further information about the kron command from MATLAB help issuing doc kron in the MATLAB command window.
- (3b) Explicitly write Eq. (2) in the form y = Mx (i.e. write down M), for $A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$ and $B = \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix}$.
- (3c) \odot What is the asymptotic complexity (\rightarrow [1, Def. 1.4.3]) of the MATLAB code (2)? Use the Landau symbol from [1, Def. 1.4.4] to state your answer.
- (3d) \odot Measure the runtime of (2) for $n=2^{3,4,5,6}$ and random matrices. Use the MATLAB functions tic and toc as explained in example [1, Ex. 1.4.10] of the Lecture Slides.
- (3e) Explain in detail, why (2) can be replaced with the single line of MATLAB code

$$y = reshape(B * reshape(x,n,n) * A', n*n, 1);$$
 (3)

and compare the execution times of (2) and (3) for random matrices of size $n = 2^{3,4,5,6}$.

(3f) \Box Based on the EIGEN numerical library (\rightarrow [1, Section 1.2.2]) implement a C++ function

```
template <class Matrix>
void kron(const Matrix & A, const Matrix & B, Matrix &
   C) {
   // Your code here
}
```

returns the Kronecker product of the argument matrices A and B in the matrix C.

HINT: Feel free (but not forced) to use the partial codes provided in kron.cpp as well as the CMake file CMakeLists.txt (including cmake-modules) and the timing header file timer.h.

(3g) Devise an implementation of the MATLAB code (2) in C++according to the function definition

```
template <class Matrix, class Vector>
void kron_mv(const Matrix & A, const Matrix & B, const
   Vector & x, Vector & y);
```

The meaning of the arguments should be self-explanatory.

(3h) Now, using a function definition similar to that of the previous sub-problem, implement the C++ equivalent of (3) in the function kron_mv_fast.

HINT: Study [1, Rem. 1.2.18] about "reshaping" matrices in EIGEN.

(3i) • Compare the runtimes of your two implementations as you did for the MATLAB implementations in sub-problem (3e).

Problem 4. Structured matrix-vector product

In [1, Ex. 1.4.14] we saw how the particular structure of a matrix can be exploited to compute a matrix-vector product with substantially reduced computational effort. This problem presents a similar case.

Consider the real $n \times n$ matrix A defined by $(A)_{i,j} = a_{i,j} = \min\{i,j\}$, for $i,j = 1,\ldots,n$. The matrix-vector product y = Ax can be implemented in MATLAB as

$$y = min(ones(n, 1) * (1:n), (1:n)' * ones(1,n)) * x;$$
 (4)

(4a) \odot What is the asymptotic complexity (for $n \to \infty$) of the evaluation of the MATLAB command displayed above, with respect to the problem size parameter n?

```
function y = multAmin(x)
```

that computes the same multiplication as (4) but with a better asymptotic complexity with respect to n.

HINT: you can test your implementation by comparing the returned values with the ones obtained with code (4).

- (4c) \odot What is the asymptotic complexity (in terms of problem size parameter n) of your function multAmin?
- (4d) \Box Compare the runtime of your implementation and the implementation given in (4) for $n = 2^{5,6,...,12}$. Use the routines tic and toc as explained in example [1, Ex. 1.4.10] of the Lecture Slides.
- **(4e)** Can you solve task (4b) without using any for- or while-loop? Implement it in the function

```
function y = multAmin2(x)
```

HINT: you may use the MATLABbuilt-in command cumsum.

(4f) • Consider the following MATLABscript multAB.m:

Listing 2: MATLABscript calling multAmin

Sketch the matrix B created in line 3 of multAB.m.

HINT: this MATLABScript is provided as file multAB.m.

(4g) ☐ Run the code of Listing 2 several times and conjecture a relationship between the matrices A and B from the output. Prove your conjecture.

HINT: You must take into account that computers inevitably commit round-off errors, see [1, Section 1.5].

(4h) Implement a C++ function with declaration

```
template <class Vector>
void minmatmv(const Vector &x, Vector &y);
```

that realizes the efficient version of the MATLAB line of code (4). Test your function by comparing with output from the equivalent MATLAB functions.

Problem 5. Matrix powers

(5a) Implement a MATLAB function

that, using only basic linear algebra operations (including matrix-vector or matrix-matrix multiplications), computes efficiently the k^{th} power of the $n \times n$ matrix \mathbf{A} .

HINT: use the MATLAB operator \wedge to test your implementation on random matrices **A**.

HINT: use the MATLAB functions de2bi to extract the "binary digits" of an integer.

- (5b) \odot Find the asymptotic complexity in k (and n) taking into account that in MATLAB a matrix-matrix multiplication requires a $O(n^3)$ effort.
- (5c) \odot Plot the runtime of the built-in MATLAB power (\land) function and find out the complexity. Compare it with the function Pow from (5a). Use the matrix

$$A_{j,k} = \frac{1}{\sqrt{n}} \exp\left(\frac{2\pi i \ jk}{n}\right)$$

to test the two functions.

(5d) Using EIGEN, devise a C++ function with the calling sequence

```
template <class Matrix>
void matPow(const Matrix &A, unsigned int k);
```

that computes the k^{th} power of the square matrix **A** (passed in the argument A). Of course, your implementation should be as efficient as the MATLAB version from sub-problem (5a).

HINT: matrix multiplication suffers no aliasing issues (you can safely write A = A * A).

HINT: feel free to use the provided matPow.cpp.

HINT: you may want to use log and ceil.

HINT: EIGEN implementation of power (A.pow(k)) can be found in:

#include <unsupported/Eigen/MatrixFunctions>

Problem 6. Complexity of a MATLAB function

In this problem we recall a concept from linear algebra, the diagonalization of a square matrix. Unless you can still define what this means, please look up the chapter on "eigenvalues" in your linear algebra lecture notes. This problem also has a subtle relationship with Problem 5.

We consider the MATLAB function defined in getit.m (cf. Listing 3)

Listing 3: MATLABimplementation of getit for Problem 6...

```
function y = getit(A, x, k)
[S,D] = eig(A);
y = S*diag(diag(D).^k)* (S\x);
end
```

HINT: Give the command doc eig in MATLAB to understand what eig does.

HINT: You may use that eig applied to an $n \times n$ -matrix requires an asymptotic computational effort of $O(n^3)$ for $n \to \infty$.

HINT: in MATLAB, the function $\operatorname{diag}(x)$ for $\mathbf{x} \in \mathbb{R}^n$, builds a diagonal, $n \times n$ matrix with \mathbf{x} as diagonal. If \mathbf{M} is a $n \times n$ matrix, $\operatorname{diag}(M)$ returns (extracts) the diagonal of \mathbf{M} as a vector in \mathbb{R}^n .

HINT: the operator $v \cdot \hat{k}$ for $v \in \mathbb{R}^n$ and $k \in \mathbb{N} \setminus \{0\}$ returns the vector with components v_i^k (i.e. component-wise exponent)

- **(6a)** What is the output of getit, when A is a diagonalizable $n \times n$ matrix, $x \in \mathbb{R}^n$ and $k \in \mathbb{N}$?
- **(6b)** \Box Fix $k \in \mathbb{N}$. Discuss (in detail) the asymptotic complexity of getit $n \to \infty$.

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References

[1] R. Hiptmair. *Lecture slides for course "Numerical Methods for CSE"*. http://www.sam.math.ethz.ch/~hiptmair/tmp/NumCSE/NumCSE15.pdf. 2015.