ETH Lectures 401-0663-00L Numerical Methods for Computer Science
401-2673-00L Numerical Methods for CSE

Numerical Methods for Computational Science and Engineering

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(with contributions from Prof. P. Arbenz and Dr. V. Gradinaru)

Autumn Term 2024, Version of December 16, 2024

Link to the current version of this lecture document

Always under construction!

The online version will always be work in progress and subject to change.

(Nevertheless, structure and main contents can be expected to be stable)

Do not print before the end of term!

Chapter 0

Introduction

0.1 Course Fundamentals

0.1.1 Focus of this Course

Emphasis is put

▷ on **algorithms** (principles, computational cost, scope, and limitations),

▷ on (efficient and stable) **implementation** in **C++** based on the numerical linear algebra template library EIGEN, a **D**omain **S**pecific **L**anguage (DSL) embedded into C++.

▷ on **numerical experiments** (design and interpretation).

§0.1.1.1 (Aspects outside the scope of this course) No emphasis will be put on

- theory and proofs (unless essential for derivation and understanding of algorithms).

  ☞ 401-3651-00L Numerical Methods for Elliptic and Parabolic Partial Differential Equations
  401-3652-00L Numerical Methods for Hyperbolic Partial Differential Equations
  (both courses offered in BSc Mathematics)

- hardware aware implementation (cache hierarchies, CPU pipelining, vectorization, etc.)

  ☞ 263-0007-00L Advanced System Lab (How To Write Fast Numerical Code, Prof. M. Püschel, D-INFK)

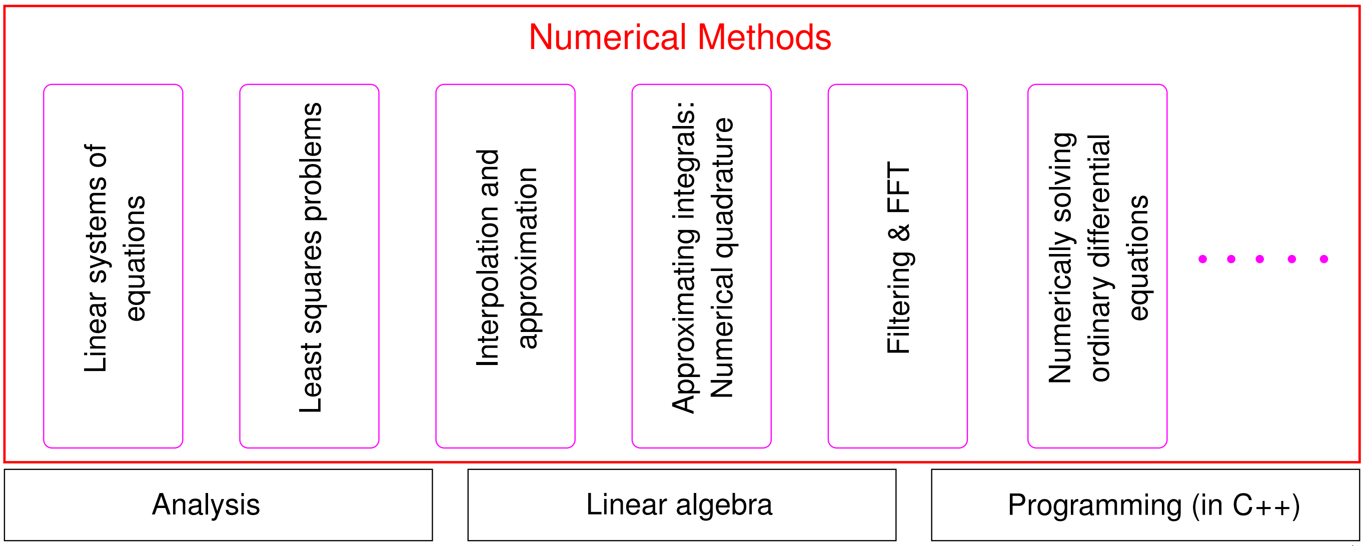
- issues of high-performance computing (HPC, shard and distributed memory parallelisation, vectorization)

  ☞ 151-0107-20L High Performance Computing for Science and Engineering (HPCSE, Prof. P. Koumoutsakos, D-MAVT)
  263-2800-00L Design of Parallel and High-Performance Computing (Prof. T. Höfler, D-INFK)

However, note that these other courses partly rely on knowledge of elementary numerical methods, which is covered in this course. ⌟

Contents

§0.1.1.2 (Prequisites) This course will take for granted basic knowledge of linear algebra, calculus, and programming, that you should have acquired during your first year at ETH.



§0.1.1.3 (Numerical methods: A motley toolbox)

This course discusses **elementary numerical methods and techniques**

They are vastly different in terms of ideas, design, analysis, and scope of application. They are the items in a **toolbox**, some only loosely related by the common purpose of being building blocks for codes for numerical simulation.

Do not expect much coherence between the chapters of this course!

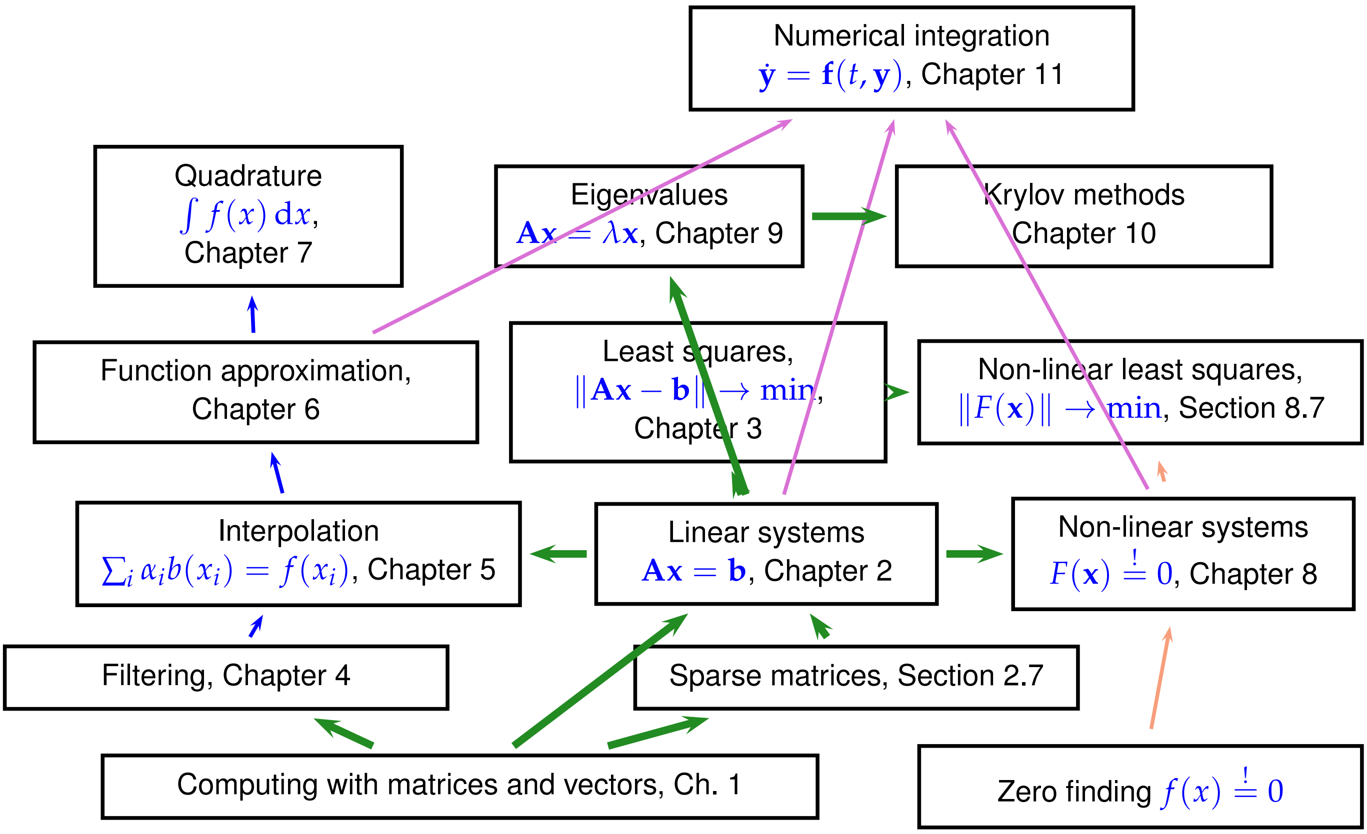
Fig. 1

A purpose-oriented notion of "Numerical methods for CSE":

A: "Stop putting a hammer, a level, and duct tape in one box! They have nothing to do with each other!"

B: "I might need any of these tools when fixing something about the house"

§0.1.1.4 (Dependencies of topics) Despite the diverse nature of the individual topics covered in this course, some depend on others for providing essential building blocks. The following directed graph tries to capture these relationships. The arrows have to be read as "uses results or algorithms of".



Any one-semester course "Numerical methods for CSE" will cover only selected chapters and sections of this document. Only topics addressed in **class** or in **homework problems** will be relevant for exams!

§0.1.1.5 (Relevance of this course) I am a student of computer science. After the exam, may I safely forget everything I have learned in this mandatory "numerical methods" course? **No**, because it is highly likely that other courses or projects will rely on the contents of this course:

singular value decomposition least squares	▶	Computational statistics, machine learning
function approximation numerical quadrature numerical integration	▶	machine learning, Numerical methods for PDEs
interpolation least squares	▶	Computer graphics
eigensolvers sparse linear systems	▶	Graph theoretic algorithms
numerical integration	▶	Computer animation, robotics

and many more applications of fundamental numerical methods . . ..

Hardly anyone will need everything covered in this course, but *most of you will need something*.

0.1.2 Goals

This course is meant to impart

- knowledge of some fundamental algorithms forming the basis of numerical simulations,
- familiarity with essential terms in numerical mathematics and the techniques used for the analysis of numerical algorithms
- the skill to choose the appropriate numerical methods for concrete problems,
- the ability to interpret numerical results,
- proficiency in implementing numerical algorithms efficiently in C++, using numerical libraries.

Indispensable: Learning by doing (➔ exercises)

0.1.3 Literature

Parts of the following textbooks may be used as supplementary reading for this course. References to relevant sections will be provided in the course material.

Studying extra literature is not important for following this course!

- [AG11] U. Ascher and C. Greif, *A First Course in Numerical Methods*, SIAM, Philadelphia, 2011.

  Comprehensive introduction to numerical methods with an algorithmic focus based on MATLAB. (Target audience: students of engineering subjects)

- [DR08] W. Dahmen and A. Reusken, *Numerik für Ingenieure und Naturwissenschaftler*, Springer, Heidelberg, 2006.

  Good reference for large parts of this course; provides a lot of simple examples and lucid explanations, but also rigorous mathematical treatment.
  (Target audience: undergraduate students in science and engineering)
  Available for download as PDF

- [Han02] M. Hanke-Bourgeois, *Grundlagen der Numerischen Mathematik und des Wissenschaftlichen Rechnens*, Mathematische Leitfäden, B.G. Teubner, Stuttgart, 2002.

  Gives detailed description and mathematical analysis of algorithms and relies on MATLAB. Profound treatment of theory way beyond the scope of this course. (Target audience: undergraduates in mathematics)

- [QSS00] A. Quarteroni, R. Sacco, and F. Saleri, *Numerical mathematics*, vol. 37 of Texts in Applied Mathematics, Springer, New York, 2000.

Classical introductory numerical analysis text with many examples and detailed discussion of algorithms. (Target audience: undergraduates in mathematics and engineering)
Can be obtained from website.

- [DH03] P. DEUFLHARD AND A. HOHMANN, *Numerische Mathematik. Eine algorithmisch orientierte Einführung*, DeGruyter, Berlin, 1 ed., 1991.

  Modern discussion of numerical methods with profound treatment of theoretical aspects (Target audience: undergraduate students in mathematics).

- [GGK14]: W.. GANDER, M.J. GANDER, AND F. KWOK, *Scientific Computing*, Text in Computational Science and Engineering, springer, 2014.

  Comprehensive treatment of elementary numerical methods with an algorithmic focus.

D-INFK maintains a webpage with links to some of these books.

Essential prerequisite for this course is a solid knowledge in linear algebra and calculus. Familiarity with the topics covered in the first semester courses is taken for granted, see

- [NS02] K. NIPP AND D. STOFFER, *Lineare Algebra*, vdf Hochschulverlag, Zürich, 5 ed., 2002.
- [Gut09] M. GUTKNECHT, *Lineare algebra*, lecture notes, SAM, ETH Zürich, 2009, available online.
- [Str09] M. STRUWE, *Analysis für Informatiker*. Lecture notes, ETH Zürich, 2009, available online.

0.2 Teaching Style and Model

0.2.1 Flipped Classroom

This course will depart from the usual academic teaching arrangement centering around classes taught by a lecturer addressing an audience in a lecture hall.

A flipped-classroom course

This course will follow the **flipped-classroom** paradigm:

Learning by **self-study** guided by

instruction videos tablet notes	lecture notes	interactive Q&A sessions	homeworks tutorial classes

All the course material will be published online through the course Moodle Page. All notes jotted down by the lecturer during the creation of videos or during the Q&A sessions will be made available as PDF.

0.2.1.1 Course Videos

In the flipped-classroom teaching model regular lectures will be replaced with pre-recorded videos. These videos are not commercial-grade clips, but resemble video recordings from a standard classroom setting; they convey the development of the material on a tablet accompanied by the lecturer's voice.

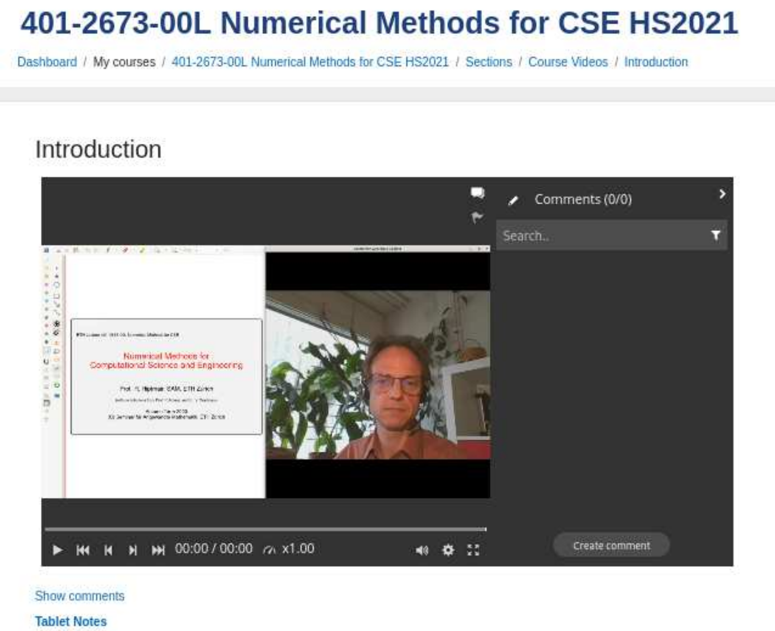


Fig. 2

The Videos will be published through

1. the course Moodle Page (see beside),
2. and as `.mp4`-files on PolyBox (password required).

Every video comes with a PDF containing the tablet notes taken during the creation of the video. However, the PDF may have been *corrected, updated, or supplemented* later.

§0.2.1.2 ("Pause" and "fast forward") Videos have *two big advantages*:

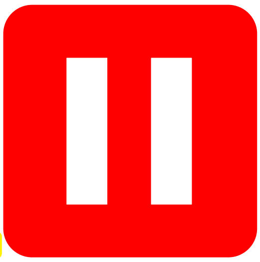


Fig. 3

You can stop a video at any time, whenever

- you need more time to think,
- you want to look up related information,
- you want to work for yourself.

Make use of this possibility!

The video portal also allows you to play the videos at *1.5× speed*. This can be useful, if the current topic is very clear to you. You can also *skip* entire *parts* using the scroll bar. The same functionality (fast playing and skipping) is offered by most video players, for instance the VLC media player. ⌟

§0.2.1.3 (Review questions) Most lecture units (corresponding to a video) are accompanied with a list of review questions. You should try to answer them off the top of your head *without consulting any written material* shortly after you have finished studying the unit .

In case you are utterly clueless about how to approach a review question, you probably need to refresh some of the unit's topics.

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§0.2.1.4 (List of available tutorial videos) This is the list of available video tutorials as of December 16, 2024:

1. Video tutorial for Chapter 0 "Introduction": (16 minutes) Download link, tablet notes
2. Video tutorial for Section 1.1.1 "Notations and Classes of Matrices": (7 minutes) Download link, tablet notes

   → review questions 1.1.2.9
3. Video tutorial for Section 1.2.1 "EIGEN ": (11 minutes) Download link, tablet notes

→ review questions 1.2.1.14

4. Video tutorial for Section 1.2.3 "(Dense) Matrix Storage Formats": (10 minutes) Download link, tablet notes

→ review questions 1.2.3.11

5. Video tutorial for Section 1.4 "Computational Effort": (29 minutes) Download link, tablet notes

→ review questions 1.4.3.11

6. Video tutorial for Section 1.5 "Machine Arithmetic and Consequences": (16 minutes) Download link, tablet notes

→ review questions 1.5.3.18

7. Video tutorial for Section 1.5.4 "Cancellation": (22 minutes) Download link, tablet notes

→ review questions 1.5.4.33

8. Video tutorial for Section 1.5.5 "Numerical Stability": (17 minutes) Download link, tablet notes

→ review questions 1.5.5.23

9. Video tutorial for Section 2.1 & Section 2.2.1 "Introduction and Theory: Linear Systems of Equations (LSEs)": (6 minutes) Download link, tablet notes

→ review questions 2.2.1.7

10. Video tutorial for Ex. 2.1.0.3 "Nodal Analysis of Linear Electric Circuits": (8 minutes) Download link, tablet notes

→ review questions 2.1.0.8

11. Video tutorial for Section 2.2.2 "Sensitivity of Linear Systems": (15 minutes) Download link, tablet notes

→ review questions 2.2.2.12

12. Video tutorial for Section 2.3 & Section 2.5 "Gaussian Elimination": (17 minutes) Download link, tablet notes

→ review questions 2.3.2.21

13. Video tutorial for Section 2.6 "Exploiting Structure when Solving Linear Systems": (17 minutes) Download link, tablet notes

→ review questions 2.6.0.25

14. Video tutorial for Section 2.7.1 "Sparse Matrix Storage Formats": (10 minutes) Download link, tablet notes

→ review questions 2.7.1.5

15. Video tutorial for Section 2.7.2 "Sparse Matrices in EIGEN ": (6 minutes) Download link, tablet notes

→ review questions 2.7.2.17

16. Video tutorial for Section 2.7.3 "Direct Solution of Sparse Linear Systems of Equations": (10 minutes) Download link, tablet notes

→ review questions>2.7.3.7

17. Video tutorial for Section 3.0.1 "Overdetermined Linear Systems of Equations: Examples": (12 minutes) Download link, tablet notes

→ review questions 3.0.1.11

18. Video tutorial for Section 3.1.1 "Least Squares Solutions": (9 minutes) Download link, tablet notes

→ review questions 3.1.1.14

19. Video tutorial for Section 3.1.2 "Normal Equations": (16 minutes) Download link, tablet notes

→ review questions 3.1.2.23

20. Video tutorial for Section 3.1.3 "Moore-Penrose Pseudoinverse": (8 minutes) Download link, tablet notes

→ review questions 3.1.3.8

21. Video tutorial for Section 3.2 "Normal Equation Methods": (12 minutes) Download link, tablet notes

→ review questions 3.2.0.11

22. Video tutorial for Section 3.3 "Orthogonal Transformation Methods": (10 minutes) Download link, tablet notes

→ review questions 3.3.2.3

23. Video tutorial for Section 3.3.3.1 "QR-Decomposition: Theory": (11 minutes) Download link, tablet notes

→ review questions 3.3.3.8

24. Video tutorial for Section 3.3.3.2 & Section 3.3.3.4 "Computation of QR-Decomposition, QR-Decomposition in EIGEN ": (32 minutes) Download link, tablet notes

→ review questions 3.3.3.29

25. Video tutorial for Section 3.3.4 "QR-Based Solver for Linear Least Squares Problems": (9 minutes) Download link, tablet notes

→ review questions 3.3.4.8

26. Video tutorial for Section 3.3.5 "Modification Techniques for QR-Decomposition": (25 minutes) Download link, tablet notes

→ review questions 3.3.5.7

27. Video tutorial for Section 3.4.1 "Singular Value Decomposition: Definition and Theory": (13 minutes) Download link, tablet notes

→ review questions 3.4.1.15

28. Video tutorial for Section 3.4.2 "SVD in EIGEN ": (9 minutes) Download link, tablet notes

→ review questions 3.4.2.10

29. Video tutorial for Section 3.4.3 "Solving General Least-Squares Problems by SVD": (14 minutes) Download link, tablet notes

→ review questions 3.4.3.17

30. Video tutorial for Section 3.4.4.1 "Norm-Constrained Extrema of Quadratic Forms": (11 minutes) Download link, tablet notes

→ review questions 3.4.4.13

31. Video tutorial for Section 3.4.4.2 "Best Low-Rank Approximation": (13 minutes) Download link, tablet notes

→ review questions 3.4.4.25

32. Video tutorial for Section 3.4.4.3 "Principal Component Data Analysis (PCA)": (28 minutes) Download link, tablet notes

→ review questions 3.4.4.51

33. Video tutorial for Section 3.6 "Constrained Least Squares": (23 minutes) Download link, tablet notes

→ review questions 3.6.2.1

34. Video tutorial for Section 4.1.1 "Discrete Finite Linear Time-Invariant Causal Channels/Filters": (11 minutes) Download link, tablet notes

→ review questions 4.1.1.13

35. Video tutorial for Section 4.1.2 "LT-FIR Linear Mappings": (12 minutes) Download link, tablet notes

→ review questions 4.1.2.10

36. Video tutorial for Section 4.1.3 "Discrete Convolutions": (9 minutes) Download link, tablet notes

→ review questions 4.1.3.11

37. Video tutorial for Section 4.1.4 "Periodic Convolutions": (12 minutes) Download link, tablet notes

→ review questions 4.1.4.19

38. Video tutorial for Section 4.2.1 "Diagonalizing Circulant Matrices": (17 minutes) Download link, tablet notes

→ review questions 4.2.1.23

39. Video tutorial for Section 4.2.2 "Discrete Convolution via DFT": (7 minutes) Download link, tablet notes

→ review questions 4.2.2.6

40. Video tutorial for Section 4.2.3 "Frequency filtering via DFT": (20 minutes) Download link, tablet notes

→ review questions 4.2.3.11

41. Video tutorial for Section 4.2.5 "Two-Dimensional DFT": (20 minutes) Download link, tablet notes

→ review questions 4.2.5.23

42. Video tutorial for Section 4.3 "Fast Fourier Transform (FFT)": (16 minutes) Download link, tablet notes

→ review questions 4.3.0.13

43. Video tutorial for Section 4.5 "Toeplitz Matrix Techniques": (20 minutes) Download link, tablet notes

→ review questions 4.5.3.8

44. Video tutorial for Section 5.1 "Abstract Interpolation": (16 minutes) Download link, tablet notes

→ review questions 5.1.0.27

45. Video tutorial for Section 5.2.1 "Uni-Variate Polynomials": (7 minutes) Download link, tablet notes

→ review questions 5.2.1.8

46. Video tutorial for Section 5.2.2 "Polynomial Interpolation: Theory": (6 minutes) Download link, tablet notes

→ review questions 5.2.2.19

47. Video tutorial for Section 5.2.3 "Polynomial Interpolation: Algorithms": (18 minutes) Download link, tablet notes

→ review questions 5.2.3.14

48. Video tutorial for Section 5.2.3.3 "Extrapolation to Zero": (12 minutes) Download link, tablet notes

→ review questions 5.2.3.20

49. Video tutorial for Section 5.2.3.4 "Newton Basis and Divided Differences": (17 minutes) Download link, tablet notes

→ review questions 5.2.3.39

50. Video tutorial for Section 5.2.4 "Polynomial Interpolation: Sensitivity": (13 minutes) Download link, tablet notes

→ review questions 5.2.4.16

51. Video tutorial for Section 5.3 "Shape-Preserving Interpolation": (23 minutes) Download link, tablet notes

→ review questions 5.3.3.19

52. Video tutorial for Section 5.4.1 "Spline Function Spaces": (9 minutes) Download link, tablet notes

→ review questions 5.4.1.5

53. Video tutorial for Section 5.4.2 "Cubic Spline Interpolation": (14 minutes) Download link, tablet notes

→ review questions 5.4.2.16

54. Video tutorial for Section 5.4.3 "Structural Properties of Cubic Spline Interpolants": (12 minutes) Download link, tablet notes

→ review questions 5.4.3.11

55. Video tutorial for Section 5.6 "Trigonometric Interpolation": (14 minutes) Download link, tablet notes

→ review questions 5.6.3.10

56. Video tutorial for Section 5.7 "Least Squares Data Fitting": (13 minutes) Download link, tablet notes

→ review questions 5.7.0.31

57. Video tutorial for Section 6.1 "Approximation of Functions in 1D: Introduction": (7 minutes) Download link, tablet notes

→ review questions 6.1.0.9

58. Video tutorial for Section 6.2 "Polynomial Approximation: Theory": (13 minutes) Download link, tablet notes

→ review questions 6.2.1.28

59. Video tutorial for Section 6.2.2 "Error Estimates for Polynomial Interpolation": (12 minutes) Download link, tablet notes

→ review questions 6.2.2.14

60. Video tutorial for Section 6.2.2.2 "Error Estimates for Polynomial Interpolation: Interpolands of Finite Smoothness": (17 minutes) Download link, tablet notes

→ review questions 6.2.2.34

61. Video tutorial for Section 6.2.2.3 "Error Estimates for Polynomial Interpolation: Analytic Interpolands": (27 minutes) Download link, tablet notes

→ review questions 6.2.2.69

62. Video tutorial for Section 6.2.3.1 "Chebychev Interpolation: Motivation and Definition": (21 minutes) Download link, tablet notes

→ review questions 6.2.3.13

63. Video tutorial for Section 6.2.3.2 "Chebychev Interpolation Error Estimates": (14 minutes) Download link, tablet notes

→ review questions 6.2.3.30

64. Video tutorial for Section 6.2.3.3 "Chebychev Interpolation: Computational Aspects": (11 minutes) Download link, tablet notes

→ review questions 6.2.3.44

65. Video tutorial for Section 6.5.1 "Approximation by Trigonometric Interpolation": (5 minutes) Download link, tablet notes

→ review questions 6.5.1.6

66. Video tutorial for Section 6.5.2 "Trigonometric Interpolation Error Estimates": (14 minutes) Download link, tablet notes

→ review questions 6.5.2.26

67. Video tutorial for Section 6.5.3 "Trigonometric Interpolation of Analytic Periodic Functions": (16 minutes) Download link, tablet notes

→ review questions 6.5.3.18

68. Video tutorial for Section 6.6.1 "Piecewise Polynomial Lagrange Interpolation": (17 minutes) Download link, tablet notes

69. Video tutorial for Section 6.6.2 "Cubic Hermite and Spline Interpolation: Error Estimates": (10 minutes) Download link, tablet notes

70. Video tutorial for Section 7.1 "Numerical Quadrature: Introduction": (4 minutes) Download link, tablet notes

→ review questions 7.1.0.5

71. Video tutorial for Section 7.2 "Quadrature Formulas/Rules": (13 minutes) Download link, tablet notes

→ review questions 7.2.0.15

72. Video tutorial for Section 7.3 "Polynomial Quadrature Formulas": (9 minutes) Download link, tablet notes

→ review questions 7.3.0.12

73. Video tutorial for Section 7.4.1 "Order of a Quadrature Rule": (9 minutes) Download link, tablet notes

→ review questions 7.4.1.12

74. Video tutorial for Section 7.4.2 "Maximal-Order Quadrature Rules": (16 minutes) Download link, tablet notes

→ review questions 7.4.2.27

75. Video tutorial for Section 7.4.3 "(Gauss-Legendre) Quadrature Error Estimates": (18 minutes) Download link, tablet notes

→ review questions 7.4.3.16

76. Video tutorial for Section 7.5 "Composite Quadrature": (18 minutes) Download link, tablet notes

→ review questions 7.5.0.26

77. Video tutorial for Section 7.6 "Adaptive Quadrature": (13 minutes) Download link, tablet notes

→ review questions 7.6.0.20

78. Video tutorial for Section 8.1 "Iterative Methods for Non-Linear Systems of Equations: Introduction": (6 minutes) Download link, tablet notes

→ review questions 8.1.0.6

79. Video tutorial for Section 8.2.1 "Iterative Methods: Fundamental Concepts": (6 minutes) Download link, tablet notes

→ review questions 8.2.1.11

80. Video tutorial for Section 8.2.2 "Iterative Methods: Speed of Convergence": (15 minutes) Download link, tablet notes

→ review questions 8.2.2.16

81. Video tutorial for Section 8.2.3 "Iterative Methods: Termination Criteria/Stopping Rules": (14 minutes) Download link, tablet notes

→ review questions 8.2.3.10

82. Video tutorial for Section 8.3 "Fixed-Point Iterations": (12 minutes) Download link, tablet notes

→ review questions 8.3.2.21

83. Video tutorial for Section 8.4.1 "Finding Zeros of Scalar Functions: Bisection": (7 minutes) Download link, tablet notes

→ review questions 8.4.1.4

84. Video tutorial for Section 8.4.2.1 "Newton Method in the Scalar Case": (20 minutes) Download link, tablet notes

→ review questions 8.4.2.16

85. Video tutorial for Section 8.4.2.3 "Multi-Point Methods": (12 minutes) Download link, tablet notes

→ review questions 8.4.2.41

86. Video tutorial for Section 8.4.3 "Asymptotic Efficiency of Iterative Methods for Zero Finding": (10 minutes) Download link, tablet notes

→ review questions 8.4.3.15

87. Video tutorial for Section 8.5.1 "The Newton Iteration in $\mathbb{R}^n$ (I)": (10 minutes) Download link, tablet notes

→ review questions 8.5.1.46

88. Video tutorial for § 8.5.1.15 "Multi-dimensional Differentiation": (20 minutes) Download link, tablet notes

89. Video tutorial for Section 8.5.1 "The Newton Iteration in $\mathbb{R}^n$ (II)": (15 minutes) Download link, tablet notes

90. Video tutorial for Section 8.5.2 "Convergence of Newton's Method": (9 minutes) Download link, tablet notes

→ review questions 8.5.2.8

91. Video tutorial for Section 8.5.3 "Termination of Newton Iteration": (7 minutes) Download link, tablet notes

→ review questions 8.5.3.9

92. Video tutorial for Section 8.5.4 "Damped Newton Method": (11 minutes) Download link, tablet notes

→ review questions 8.5.4.8

93. Video tutorial for Section 8.6 "Quasi-Newton Method": (15 minutes) Download link, tablet notes

→ review questions 8.6.0.22

94. Video tutorial for Section 8.7 "Non-linear Least Squares": (7 minutes) Download link, tablet notes

→ review questions 8.7.0.10

95. Video tutorial for Section 8.7.1 "Non-linear Least Squares: (Damped) Newton Method": (13 minutes) Download link, tablet notes

→ review questions 8.7.1.9

96. Video tutorial for Section 8.7.2 "(Trust-region) Gauss-Newton Method": (13 minutes) Download link, tablet notes

→ review questions 8.7.3.3

97. Video tutorial for Section 11.1: Initial-Value Problems (IVPs) for Ordinary Differential Equations (ODEs): (35 minutes) Download link, tablet notes

→ review questions 11.1.4.8

98. Video tutorial for Section 11.2: Introduction: Polygonal Approximation Methods: (17 minutes) Download link, tablet notes

→ review questions 11.2.3.4

99. Video tutorial for Section 11.3: General Single-Step Methods: (14 minutes) Download link, tablet notes

→ review questions 11.3.1.17

100. Video tutorial for Section 11.3.2:(Asymptotic) Convergence of Single-Step Methods: (20 minutes) Download link, tablet notes

→ review questions 11.3.2.34

101. Video tutorial for Section 11.4: Explicit Runge-Kutta Single-Step Methods (RKSSMs): (27 minutes) Download link, tablet notes

→ review questions 11.4.0.20

102. Video tutorial for Section 11.5: Adaptive Stepsize Control: (32 minutes) Download link, tablet notes

→ review questions 11.5.3.10

103. Video tutorial for Section 12.1:Model Problem Analysis: (40 minutes) Download link, tablet notes

→ review questions 12.1.0.54

104. Video tutorial for Section 12.2: Stiff Initial-Value Problems: (24 minutes) Download link, tablet notes

→ review questions 12.2.0.17

105. Video tutorial for Section 12.3: Implicit Runge-Kutta Single-Step Methods: (50 minutes) Download link, tablet notes

→ review questions 12.3.4.23

106. Video tutorial for Section 12.4: Semi-Implicit Runge-Kutta Methods: (13 minutes) Download link, tablet notes

→ review questions 12.4.0.10

107. Video tutorial for Section 12.5: Splitting Methods: (21 minutes) Download link, tablet notes

→ review questions 12.5.0.14

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Necessary corrections and updates of the lecture document will sometimes lead to changes in the numbering of paragraphs and formulas, which, of course, cannot be applied to the recorded videos.
However, these changes will be taken into account into the tablet notes supplied for every video.

0.2.1.2 Following the Course

Weekly study assignments

- For every week there is a list of course units and associated videos published on the course Moodle Page.
- The corresponding contents **must** be studied in that same week.

§0.2.1.6 (How to organize your learning)

☛ **Develop a routine**: Plan *fixed slots*, with a total duration of *four hours*, for studying for the course material in your weekly calendar. This does not include homework.

☛ **Choose a stable setting**, in which you can really concentrate (quiet area, headphones, coffee, etc.)

☛ **Take breaks**, when concentration is declining, usually after 20 to 45 minutes, but *avoid online distractions* during breaks.

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You must not procrastinate!

Do not put off studying for this course. Dependencies between the topics will make it very hard to catch up.

§0.2.1.7 ("Personalized learning") The flipped classroom model allows students to pursue their preferred ways of studying. The following approaches can be tried.

- **Traditional**: You watch the assigned videos similar to attending a conventional classroom lecture. Afterwards digest the material based on the tablet notes and/or the lecture document. Finally, answer the review questions and look up more information in the lecture document.
- **Reading-centered**: You work through the unit reading the tablet notes, and, sometimes, related sections of the lecture document. You occasionally watch parts of the videos, in case some considerations and arguments have not become clear to you already.

Fig. 4

Collaborative studying is encouraged:

- You may watch course videos together with classmates.
- You may meet to discuss course units.
- You may solve homework problems in a group assigning different parts to different members.

☛ Explaining to others is a great way to deepen understanding.

☛ It is easy to sustain motivation and avoid distraction in a peer study group.

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§0.2.1.8 (Question and Answer (Q&A) sessions) The lecturer will offer a two-hour so-called **Q&A session** almost every week during the teaching period, but not in the weeks in which term exams will be held. These Q&A sessions will be devoted to

- discussing and answering questions asked by the participants of the course,
- presenting solutions of review questions, and
- offering additional explanations for some parts of the course.

Questions can be asked right during the Q&A session, but participants of the course are encouraged to submit general or specific questions of comments beforehand.

Questions/comments can be posted in dedicated DISCUNA chat channels (folder "Q&A Channels", community "NumCSE Autumn <YEAR>"), which will be set up for each week in which a regular Q&A session will take place.

It is highly desirable that questions are *submitted* at least a few hours *before* the start of the Q&A session so that the lecturer has the opportunity to structure his or her answer.

Tablet notes of the Q&A sessions will be made available for download. ⌟

0.2.2 Clarifications and Frank Words

§0.2.2.1 ("Lecture notes")

The PDF you are reading is referred to as lecture document and is an important source of information, but

this course document is neither a textbook nor comprehensive lecture notes.
They are meant to supplement and be supplemented by explanations given in the videos.

Some pieces of advice:

✦ The lecture document is only partly designed to be self-contained and can/should be studied *in parts* in addition to attending to watching the course videos and/or reading the tablet notes.

✦ This text is not meant for mere reading, but for working with,

✦ Turn pages all the time and follow the numerous cross-references,

✦ study the relevant section of the course material when doing homework problems,

✦ You may study referenced literature to refresh prerequisite knowledge and for alternative presentation of the material (from a different angle, maybe), but be careful about not getting confused or distracted by information overload.

⌟

§0.2.2.2 (Comprehension is a process ...)

✦ This course will require

hard work – perseverance – patience

✦ Do **not** expect to understand everything at once. Most students will

- understand about one third of the material when watching videos and studying the course material
- understand another third when making a *serious effort* to solve the homework problems,

- hopefully understand the remaining third when studying for the main examination after the end of the course.

Perseverance will be rewarded!

§0.2.2.3 (Expected workload)

(I) You are a student in the BSc/MSc programme of Computational Science and Engineering (CSE) or others. Then you are taking the *full version* of the course (401-2673-*), which is endowed with **9 ECTS credits**, which roughly corresponds to a total workload of 270 hours:

$$270\text{ hours} = \underbrace{180\text{ hours}}_{\text{during term}} + \underbrace{90\text{ hours}}_{\text{exam preparation}} ,$$

which amounts to a massive

$$\text{average workload} \quad \approx \quad 10-14 \ \text{ hours per week.}$$

(II) If you are a student in the BSc Computer Science you are offered a *trimmed version* of the course, which is worth **7 ECTS credits**. Though a very loose relationship, this roughly indicates a total workload of 180 hours:

$$180\text{ hours} = \underbrace{110\text{ hours}}_{\text{during term}} + \underbrace{70\text{ hours}}_{\text{exam preparation}} .$$

This indicates that you should brace for an

$$\text{average workload} \quad \approx \quad 7-9 \ \text{ hours per week.}$$

For both versions of the course your efforts have to be split between

- watching videos and/or studying the course material,
- and solving homework problems,
- attending Q&A sessions and tutorials.

where homework may keep you busy for $5-7$ hours every week for the full version.

Of course, all these are averages and the workload may vary between different weeks.

0.2.3 Requests

The lecturers very much welcome and, putting it even more strongly, rather depend on feedback and suggestions of the students taking the course for continuous improvement of the course contents and presentation. Therefore all participants are strongly encouraged to get involved actively and contribute in the following ways:

§0.2.3.1 (Reporting errors) As the documents for this course will always be in a state of flux, they will inevitably and invariably teem with small errors, mainly typos and omissions.

discuna

For error reporting we use the DISCUNA online collaboration platform that runs in the browser.

DISCUNA allows to attach various types of annotations to shared PDF documents, see instruction video.

Please report errors in the lecture material through the DISCUNA NumCSE Community to which various course-related documents have already been uploaded.

In the beginning of the teaching period you receive a join link of the form `https://app.discuna.com/<JOIN CODE>`. Open the link in a web browser and it will take you to the DISCUNA community page.

To report an error,

1. select the corresponding PDF document (chapter of the lecture document of homework problem) in the left sidebar,
2. press the prominent white-on-blue **+**-button in the right sidebar,
3. click on the displayed PDF where the error is located,
4. then in the pop-up window choose the “Error” category,
5. and add a title and,
6. if the title does not tell everything, a short description.

In case you cannot or do not want to link an error to a particular point in the PDF, you may just click on the title page of the respective chapter. Then, please precisely specify the concerned section and the number of the paragraph, remark, equation etc. *Do not give page numbers* as they may change with updates to the documents.

Note that chapter PDFs and homework problem files will gradually be added to the DISCUNA NumCSE community. Hence, the final chapters will not be accessible in the beginning of the course. ⌟

§0.2.3.2 (Pointing out technical problems) The DISCUNA NumCSE Community is equipped with a **chat channel “Technical Problems”**. In case you encounter a problem affecting the videos, the course web pages, or the PDF documents supplied online, say, severely distorted or missing audio tracks or a faulty link, instantly post a comment to this channel with a short description of the problem. You can do this after clicking on the channel name in the left sidebar in the community ⌟

§0.2.3.3 (Providing comments and suggestions) The **chat channel “General Comments”** of the DISCUNA NumCSE Community is meant for letting the lecturer know about weaknesses of the contents, structure, and presentation of the course and how they can be remedied. Your statements should be constructive and address specific parts or aspects of the course.

Regularly, students attending the course remark that they have found online resources like instruction videos that they think present some of the course material in a much clearer and better structured way. It is important that you tell the lecturer about those online resources so that he can include pointers to them and get inspiration. Use the “General Comments” channel also for this purpose. State clearly, which part of the course you are referring to, and briefly explain why the online resource is superior or a valuable supplement. ⌟

§0.2.3.4 (Asking/posting questions) Whenever a question comes up while you are studying for the course or trying to solve homework problems and that question lingers, it is probably connected to an issue that also bothers other students. What to do, in case you are not able to attend the Q&A session?

Please post arising question to the DISCUNA Q&A channels even if you do not attend the Q&A session! See also § 0.2.1.8

This has the benefit of

- initiating a discussion of the question that may also be relevant for other students, and
- will make it possible for you to find an answer in the Q&A tablet notes.

Tongue in cheek:

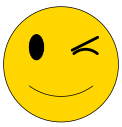
There is no question too stupid to be worth asking!

The most stupid practice is to hesitate to ask questions!

0.2.4 Assignments

A steady and persistent effort spent on homework problems is essential for success in this course.

You should expect to spend 3-5 hours per week on trying to solve the homework problems. Since many involve small coding projects, the time it will take an individual student to arrive at a solution is hard to predict.



For the sake of efficiency:
Avoid coding errors (bugs) in your homework coding projects!

The problems are published online together with plenty of hints. A master solution will also be made available, but it is foolish to read the master solution parallel to working on a problem sheet, because *trying to find the solution on one's own is essential for developing problem solving skills*, though it may occasionally be frustrating.

§0.2.4.1 (Homeworks and tutors' corrections)

- ✦ The weekly assignments will be a few problems from the **NCSE Problem Collection** available online as PDF, see course Moodle page for the link. The particular problems to be solved will be communicated through that Moodle page every week.

  Please note that this problem collection is being extended throughout the semester. Thus, make sure that you obtain the most current version every week. A polybox link will also be distributed; if you install the Polybox Client the most current version of all course documents will always be uploaded to your machine.

- ✦ Some or all of the problems of an assignment sheet will be discussed in the tutorial classes at least one week after the problems have been assigned.

- ✦ Your tutors are happy to examine your solutions and give you feedback : You may either hand them your solution papers during the tutorial session (put your name on every sheet and clearly mark the problems you want to be inspected) or upload a scan/photo through the CODEEXPERT upload interface, see § 0.2.4.2 below. You are encouraged to hand in incomplete and wrong solutions, so that you can receive valuable feedback even on incomplete or failed attempts.

- ✦ Your tutors will automatically have access to all your homework codes, see § 0.2.4.2 below.

§0.2.4.2 (CODEEXPERT C++ online IDE and testing evironment)

[code]expert

CODEEXPERT has been developed at ETH as on online IDE for small programming assignment and coding homeworks. It will be used in this course for all C++ homework problems.

Please study the documentation!

CODEEXPERT also offers the possibility of uploading any files to a private area (connected with a homework problem) that, beside you, only the tutor in charge of your exercise group can access. This is the preferred option for sharing (scans/photos of) your solutions of homework problem with your tutor.

> Note that CODEEXPERT will also be using for the coding problems of the main examination.

§0.2.4.4 (CODEEXPERT synchronization with local folder) If you prefer to use your own editor locally on your computer, synchronization between the online CODEEXPERT repository and your local folder is available via Code Expert Sync tool. Follow the instruction here.

The working pipeline is:

> Sync from CODEEXPERT platform $\longrightarrow$ Edit locally $\longrightarrow$ Sync with CODEEXPERT and run/test $\longrightarrow$ continue editting locally ...

0.2.5 Information on Examinations

0.2.5.1 For the Course 401-2673-00L Numerical Methods for CSE (BSc CSE)

§0.2.5.1 (Examinations during the teaching period) From the ETH course directory:

> An optional 30-minutes **mid-term exam** and an optional 30-minutes **end-term exam** will be held during the teaching period. The grades of these interim examinations will be taken into account through a *BONUS* of up to 30% for the final grade.

The term exams will be conducted as *closed book* examinations *on paper*. The dates of the exams will be communicated in the beginning of the term and published on the course webpage. The term exams can neither be repeated nor be taken remotely.

The final grade is computed according to the formula

$$G := 0.25 \cdot \lceil 4 \cdot \max\{G_s, 0.85G_s + 0.15g_m, 0.85G_s + 0.15g_e, 0.7G_s + 0.15g_m + 0.15g_e\} \rceil \ , \tag{0.2.5.2}$$

$G_s \hat{=}$ grade in main exam, $g_m \hat{=}$ mid-term grade, $g_e \hat{=}$ end-term grade,

where $\lceil x \rceil$ designates the smallest integer $\geq x$.

§0.2.5.3 (Main examination during exam session)

- Three-hour written examination involving coding problems to be done at the computer. The date of the exam will be set and communicated by the ETH exam office, and will also be published on the course webpage.
- The coding part of the exam has to be done using CODEEXPERT.
- Subjects of examination:

- All topics that have been addressed in a video listed on the course Moodle page or in any assigned homework problem

The lecture document contains much more material than covered in class. All these extra topics are not relevant for the exam.

✦ Lecture document (as PDF), the EIGEN documentation, and the online C++ REFERENCE PAGES will be available PDF during the examination. The corresponding final version of the lecture document will be made available at least two weeks before the exam.

✦ No other materials may be used during the exam.

✦ The homework problem collection cannot be accessed during the exam.

✦ The exam questions will be asked in English.

✦ In case you come to the conclusion that you have too little time to prepare for the main exam a few weeks before the exam, contemplate withdrawing in order not to squander an attempt.

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§0.2.5.4 (Repeating the main exam)

- Bonus points earned in term exams in last year's course can be taken into account for this course's main exam.
- If you want to take this option, please declare this intention by email to the course organizers before the mid-term exam. Otherwise, your bonus will be based on the results of this year's term exams.

┘

0.2.5.2 For the Course 401-0663-00L Numerical Methods for CS (BSc Informatik)

§0.2.5.5 (Homework bonus) During the teaching period every week quizzes and exercices similar to those that will appear in the final exam are published on the moodle page of the lecture. These are open for answers for about one week and students are expected to answer them within this time. Answering them later is not possible. Correct answers are awarded "**semester points**" that are defined for each questions. Hence, each student has the possibility to accumulate such points during the semester.

Grade bonus

The grade achieved in the final exam will be raised by 0.25 for all students who have earned at least 75% of the "semester points".

┘

§0.2.5.7 (Main (session) examination)

- Most of the exam questions are quizzes and exercices simmilar to those assigned as homework.
- The exam will mainly comprise either multiple choice tasks or tasks where you have to type the answer in an answer box.
- The exam may contain questions addressing coding. You may be asked to find and correct errors in code snippets or supplement missing parts of a code.
- Some tasks may require programming in order to be answered, though these codes will NOT be checked, but only the correctness of the final result will matter.

- Visual code studio can be used as an editor during the exam, but only the codes submitted through CODEEXPERT will be saved during the exam and taken into account for grading.

┘

0.3 Programming in C++

C++20 is the *current* ANSI/ISO standard for the programming language C++. On the one hand, it offers a wealth of features and possibilities. On the other hand, this can be confusing and even be prone to inconsistencies. A major cause of inconsistent design is the requirement with backward compatibility with the C programming language and the earlier standard C++ 98.

However, C++ has become the main language in computational science and engineering and high performance computing. Therefore this course relies on C++ to discuss the implementation of numerical methods.

In fact C++ is a blend of different programming paradigms:

- an object oriented core providing classes, inheritance, and runtime polymorphism,
- a powerful template mechanism for parametric types and partial specialization, enabling *template meta-programming* and compile-time polymorphism,
- a collection of abstract data containers and basic algorithms provided by the Standard Template Libary (STL).

Supplementary literature. A popular book for learning C++ that has been upgraded to include the C++11 standard is [LLM12].

The book [Jos12] gives a comprehensive presentation of the new features of C++11 compared to earlier versions of C++.

There are plenty of online reference pages for C++, for instance `http://en.cppreference.com` and `http://www.cplusplus.com/`.

The following sections highlight a few particular aspects of C++ that may be important for code development in this course.

> The version of the course for BSc students of Computer Science includes a two-week introduction to C++ in the beginning of the course.

0.3.1 Function Arguments and Overloading

§0.3.1.1 (Function overloading, [LLM12, Sect. 6.4]) Argument types are an integral part of a function declaration in C++. Hence the following functions are different

```
int* f(int);      // use this in the case of a single numeric argument
double f(int *); // use only, if pointer to a integer is given
void f(const MyClass &);  // use when called for a MyClass object
```

and the compiler selects the function to be used depending on the type of the arguments following rather sophisticated rules, refer to overload resolution rules. Complications arise, because implicit type conversions have to be taken into account. In case of ambiguity a compile-time error will be triggered. Functions cannot be distinguished by return type!

For member functions (methods) of classes an additional distinction can be introduced by the **const** specifier:

```
struct MyClass {
  double f(double);       // use for a mutable object of type MyClass
  double f(double) const; // use this version for a constant object
  ...
};
```

The second version of the method `f` is invoked for *constant objects* of type **MyClass**. ⌟

§0.3.1.2 (Operator overloading [LLM12, Chapter 14]) In C++ unary and binary operators like `=`, `==`, `+`, `-`, `*`, `/`, `+=`, `-=`, `*=`, `/=`, `%`, `&&`, `||`, «, », etc. are regarded as functions with a fixed number of arguments (one or two). For built-in numeric and logic types they are defined already. They can be extended to any other type, for instance

```
MyClass operator +(const MyClass &,const MyClass &);
MyClass operator +(const MyClass &,double);
MyClass operator +(const MyClass &);   // unary + !
```

The same selection rules as for function overloading apply. Of course, operators can also be introduced as class member functions.

C++ gives complete freedom to overload operators. However, the semantics of the new operators should be close to the customary use of the operator. ⌟

§0.3.1.3 (Passing arguments by value and by reference [LLM12, Sect. 6.2]) Consider a generic function declared as follows:

```
void f(MyClass x); // Argument x passed by value.
```

When `f` is invoked, a *temporary copy* of the argument is created through the copy constructor or the move constructor of **MyClass**. The new temporary object is a *local variable* inside the function body.

When a function is declared as follows

```
void f(MyClass &x); // Argument x passed by reference.
```

then the argument is passed to the scope of the function and can be changed inside the function. *No copies* are created. If one wants to avoid the creation of temporary objects, which may be costly, but also wants to indicate that the argument will not be modified inside `f`, then the declaration should read

```
void f(const MyClass &x); // Argument x passed by constant referene.
```

New in C++11 is move semantics, enabled in the following definition

```
void f(const MyClass &&x); // Optional shallow copy
```

In this case, if the scope of the object passed as the argument is merely the function or **std::move**() tags it as disposable, the move constructor of **MyClass** is invoked, which will usually do a *shallow copy* only. Refer to Code 0.3.5.10 for an example. ⌟

0.3.2 Templates

§0.3.2.1 (Function templates) The template mechanism supports parameterization of definitions of classes and functions by type. An example of a function templates is

```
template <typename ScalarType,typename VectorType>
VectorType saxpy(ScalarType alpha,const VectorType &x,const
   VectorType &y)
  { return(alpha*x+y); }
```

Depending on the concrete type of the arguments the compiler will instantiate particular versions of this function, for instance `saxpy<float,double>`, when `alpha` is of type `float` and both `x` and `y` are of type `double`. In this case the return type will be **double**.

For the above example the compiler will be able to deduce the types `ScalarType` and `VectorType` from the arguments. The programmer can also specify the types directly through the `< >`-syntax as in

```
saxpy<double,double>(a,x,y);
```

If an instantiation for all arguments of type `double` is desired. In case, the arguments do not supply enough information about the type parameters, specifying (some of) them through `< >` is mandatory. ⌟

§0.3.2.2 (Class templates) A class template defines a class depending on one or more type parameters, for instance

```
template <typename T>
class MyClsTempl {
public:
  using parm_t = T;          // T-dependent type
  MyClsTempl(void);          // Default constructor
  MyClsTempl(const T&);      // Constructor with an argument
  template <typename U>
  T memfn(const T&,const U&) const; // Templated member function
private:
  T *ptr;   // Data member, T-pointer
};
```

Types **MyClsTempl<T>** for a concrete choice of **T** are instantiated when a corresponding object is declared, for instance via

```
double x = 3.14;
MyClass myobj; // Default construction of an object
MyClsTempl<double> tinstd; // Instantiation for T = double
MyClsTempl<MyClass> mytinst(myobj); // Instantiation for T = MyClass
MyClass ret = mytinst.memfn(myobj,x); // Instantiation of member
   function for U = double, automatic type deduction
```

The types spawned by a template for different parameter types have nothing to do with each other. ⌟

> **Requirements on parameter types**
>
> The parameter types for a template have to provide all type definitions, member functions, operators, and data to make possible the instantiation ("compilation") of the class of function template.

0.3.3 Function Objects and Lambda Functions

A function object is an object of a type that provides an overloaded "function call" **operator** `()`. Function objects can be implemented in two different ways:

(I) through special classes like the following that realizes a function $\mathbb{R} \mapsto \mathbb{R}$

```
class MyFun {
public:
  ...
  double operator (double x) const; // Evaluation operator
  ...
};
```

The evaluation operator can take more than one argument and need not be declared `const`.

(II) through lambda functions, an "anonymous function" defined as

```
[<capture list>] (<arguments>) -> <return type> { body; }
```

where
- <capture list> is a list of variables from the local scope to be passed to the lambda function; an `&` indicates passing by reference,
- <arguments> is a comma separated list of function arguments complete with types,
- <return type> is an *optional* return type; often the compiler will be able to deduce the return type from the definition of the function.

Function classes should be used, when the function is needed in different places, whereas lambda functions for short functions intended for single use.

C++ code 0.3.3.1: Demonstration of use of lambda function ➜ GITLAB

```
int main() {
  // initialize a vector from an initializer list
  std::vector<double> v({1.2,2.3,3.4,4.5,5.6,6.7,7.8});
  // A vector of the same length
  std::vector<double> w(v.size());
  // Do cumulative summation of v and store result in w
  double sum = 0;
  std::transform(v.begin(),v.end(),w.begin(),
                 [&sum] (double x) { sum += x; return sum;});
  cout << "sum = " << sum << ", w = [ ";
  for(auto x: w) cout << x << ' '; cout << ']' << endl;
  return(0);
};
```

In this code the lambda function captures the local variable `sum` by reference, which enables the lambda function to change its value in the surrounding scope.

§0.3.3.2 (Function type wrappers) The special class **std**::`function` provides types for general polymorphic function wrappers.

```
std::function<return type(arg types)>
```

C++ code 0.3.3.3: Use of std::function ➜ GITLAB

```
double binop(double arg1,double arg2) { return (arg1/arg2); }

void stdfunctiontest(void) {
  // Vector of objects of a particular signature
```

```cpp
  std::vector<std::function<double(double,double)>> fnvec;
  // Store reference to a regular function
  fnvec.push_back(binop);
  // Store a lambda function
  fnvec.push_back([] (double x,double y)  -> double { return y/x; });
  for (auto fn : fnvec) { std::cout << fn(3,2) << std::endl; }
}
```

In this example an object of type **std::**`function<`**double**`(`**double, double**`)>` can hold a regular function taking two **double** arguments and returning another **double** or a lambda function with the same signature. Guess the output of `stdfunctiontest`! ┘

§0.3.3.4 (Recorder objects) In the case of routines that perform some numerical computations we are often interested in the final result only. Occasionally we may also want to screen intermediate results. The following example demonstrates the use of an optional object for collecting information while the function is being executed. If no such object is supplied, an idle lambda function is passed, which incurs absolutely no runtime overhead.

C++ code 0.3.3.5: An example of a function taking a recorder object. ➺ GITLAB

```cpp
template <typename RECORDER = std::function<void(int, int)>>
unsigned int myloopfunction(
    unsigned int n, unsigned int val = 1,
    RECORDER &&rec = [](int, int) -> void {}) {
  for (unsigned int i = 0; i < n; ++i) {
    rec(i, val); // Removed by the compiler for the default argument
    if (val % 2 == 0) {
      val /= 2;
    } else {
      val *= 3;
      val++;
    }
  }
  rec(n, val);
  return val;
}
```

C++ code 0.3.3.6: Calling `myloopfunction()` ➺ GITLAB

```cpp
  std::cout << "myloopfunction(10, 1) = " << myloopfunction(10, 1) << std::endl;
  // Run with recorder
  std::vector<std::pair<int, int>> store{};
  std::cout << "myloopfunction(10, 1) = "
            << myloopfunction(10, 1,
                              [&store](int n, int val) -> void {
                                store.emplace_back(n, val);
                              })
            << std::endl;
  std::cout << "History:" << std::endl;
  for (const auto& i : store) {
    std::cout << i.first << " -> " << i.second << std::endl;
  }
```

┘

§0.3.3.7 (Captures of lambda functions)

- Putting the name of a variable in the current scope in a lambda's capture list, makes that variable accessible inside the lambda's body as a *const reference*. The variables are *immutable* inside the lambda's body.
- Capturing a local variable as *non-const reference* prepend the variable name with `&`. That variable's value can be changed by the lambda.
- The capture list `[=]` captures all local variables as const references.
- Conversely, the capture list `[&]` means that all variables in the local scope are captured by non-const reference and can be changed by the lambda function.

┘

§0.3.3.8 (Lambda functions inside member functions) To access class methods or class variables in a lambda function inside a member function of a class you have to capture the current object as *const reference* by putting **this** or $\star$**this** in the capture list.

C++ code 0.3.3.9: A lambda function inside a member function. ➺ GITLAB

```cpp
struct X {
  explicit X(int N) : N_(N) {}
  [[nodiscard]] unsigned int mod(unsigned int n) const { return N_ % n; }
  bool modmatch(const std::vector<int> &nums, unsigned int n);
  private:
    int N_;
};

bool X::modmatch(const std::vector<int> &nums, unsigned int n) {
  auto it = std::find_if(nums.begin(), nums.end(), [this, n](int k) -> bool {
    N_++; return (N_ != 0) and ((k % n) == mod(n));
  });
  return (it != nums.end());
}
```

┘

§0.3.3.10 (Recursions based on lambda functions) Lambda functions offer an elegant way to implment recursive algorithms locally inside a function. Note that

- you have to capture the lambda function itself by reference,
- and that you cannot use **auto** for automatic compile-time type deduction of that lambda function!

C++ code 0.3.3.11: Recursively calling a lambda function ➺ GITLAB

```cpp
int main() {
  int n_calls = 0;
  std::function<int(int)> factorial = [&factorial, &n_calls](int n) -> int {
    n_calls++;
    if (n == 0) {
      return 1;
    }
    return n * factorial(n - 1);
};
  std::cout << "10! = " << factorial(10) << std::endl;
  return 0;
}
```

┘

0.3.4 Multiple Return Values

In PYTHON it is customary to return several variables from a function call, which, in fact, amounts to returning a tuple of mixed-type objects:

```python
def f(a, b):
    return min(a, b), max(a, b), (a+b)/2
x, y, z = f(1, 2)
```

In C++ this is also possible by using the tuple utility. For instance, the following function computes the mimimal and maximal element of a vector and also returns its cumulative sum. It returns all these values.

C++ code 0.3.4.1: Function with multiple return values ➺ GITLAB

```cpp
template<typename T>
std::tuple<T,T,std::vector<T>> extcumsum(const std::vector<T> &v) {
  // Local summation variable captured by reference by lambda function
  T sum{};
  // temporary vector for returning cumulative sum
  std::vector<T> w{};
  // cumulative summation
  std::transform(v.cbegin(),v.cend(),back_inserter(w),
           [&sum] (T x) { sum += x; return(sum); });
  return (std::make_tuple(*std::min_element(v.cbegin(), v.cend()),
                          *std::max_element(v.cbegin(), v.cend()),
                          std::move(w)));
}
```

This code snippet shows how to extract the individual components of the tuple returned by the previous function.

C++ code 0.3.4.2: Calling a function with multiple return values ➺ GITLAB

```cpp
int main () {
  // initialize a vector from an initializer list
  std::vector<double> v({1.2,2.3,3.4,4.5,5.6,6.7,7.8});
  // Variables for return values
  double minv,maxv;  // Extremal elements
  std::vector<double> cs; // Cumulative sums
  std::tie(minv,maxv,cs) = extcumsum(v);
  cout << "min = " << minv << ", max = " << maxv << endl;
  cout << "cs = [ "; for(double x: cs) cout << x << ' '; cout << "]" << endl;
  return(0);
}
```

Be careful: many temporary objects might be created! A demonstration of this hidden cost is given in Exp. 0.3.5.27. From C++17 a more compact syntax is available:

C++ code 0.3.4.3: Calling a function with multiple return values ➺ GITLAB

```cpp
int main () {
  // initialize a vector from an initializer list
  std::vector<double> v({1.2,2.3,3.4,4.5,5.6,6.7,7.8});
  // Definition of variables and assignment of return values all at once
  auto [minv, maxv, cs] = extcumsum(v);
```

```
  cout << "min = " << minv << ", max = " << maxv << endl;
  cout << "cs = [ "; for(double x: cs) cout << x << ' '; cout << "]" << endl;
  return(0);
}
```

Remark 0.3.4.4 ("auto" considered harmful) C++ is a strongly typed programming language and every variable must have a precise type. However, the developer of templated classes and functions may not know the type of some variables in advance, because it can be deduced only after instantiation through the compiler. The **auto** keyword has been introduced to handle this situation.

There is a temptation to use **auto** profligately, because it is convenient, in particular when *using* templated data types. However, this denies a major benefit of types, consistency checking at compile time and, as a developer, one may eventually lose track of the types completely, which can lead to errors that are hard to detect.

Thus, the use of **auto** should be avoided, unless in the following situations:

- for variables inside templated functions or classes, whose precise type will only become clear during instantiation,
- for lambda functions, see Section 0.3.3,
- for return values of templated library (member) functions, whose type is "impossible to deduce" by the user. An example is expression templates in EIGEN, refer to Rem. 1.2.1.11 below.

┘

0.3.5 A Vector Class

Since C++ is an object oriented programming language, datatypes defined by classes play a pivotal role in every C++ program. Here, we demonstrate the main ingredients of a class definition and other important facilities of C++ for the class **MyVector** meant for objects representing vectors from $\mathbb{R}^n$. The codes can be found in ⇢ GITLAB. A similar vector class is presented in [Fri19, Ch. 6].

C++ 11 class 0.3.5.1: Definition of a simple vector class MyVector ⇢ GITLAB

```
namespace myvec {
class MyVector {
public:
  using value_t = double;
  // Constructor creating constant vector, also default constructor
  explicit MyVector(std::size_t n = 0,double val = 0.0);
  // Constructor: initialization from an STL container
  template <typename Container> MyVector(const Container &v);
  // Constructor: initialization from an STL iterator range
  template <typename Iterator> MyVector(Iterator first,Iterator last);
  // Copy constructor, computational cost O(n)
  MyVector(const MyVector &mv);
  // Move constructor, computational cost O(1)
  MyVector(MyVector &&mv);
  // Copy assignment operator, computational cost O(n)
  MyVector &operator = (const MyVector &mv);
  // Move assignment operator, computational cost O(1)
  MyVector &operator = (MyVector &&mv);
  // Destructor
  virtual ~MyVector(void);
  // Type conversion to STL vector
```

```
22   operator std::vector<double> () const;
23 
24   // Returns length of vector
25   std::size_t size(void) const { return n; }
26   // Access operators: rvalue & lvalue, with range check
27   double operator [] (std::size_t i) const;
28   double &operator [] (std::size_t i);
29   // Comparison operators
30   bool operator == (const MyVector &mv) const;
31   bool operator != (const MyVector &mv) const;
32   // Transformation of a vector by a function ℝ → ℝ
33   template <typename Functor>
34   MyVector &transform(Functor &&f);
35 
36   // Overloaded arithmetic operators
37   // In place vector addition: x += y;
38   MyVector &operator +=(const MyVector &mv);
39   // In place vector subtraction: x-= y;
40   MyVector &operator -=(const MyVector &mv);
41   // In place scalar multiplication: x *= a;
42   MyVector &operator *=(double alpha);
43   // In place scalar division: x /= a;
44   MyVector &operator /=(double alpha);
45   // Vector addition
46   MyVector operator + (MyVector mv) const;
47   // Vector subtraction
48   MyVector operator - (const MyVector &mv) const;
49   // Scalar multiplication from right and left: x = a*y; x = y*a
50   MyVector operator * (double alpha) const;
51   friend MyVector operator * (double alpha,const MyVector &);
52   // Scalar divsion: x = y/a;
53   MyVector operator / (double alpha) const;
54 
55   // Euclidean norm
56   [[nodiscard]] double norm(void) const;
57   // Euclidean inner product
58   double operator *(const MyVector &) const;
59   // Output operator
60   friend std::ostream &
61   operator << (std::ostream &,const MyVector &mv);
62 
63   static bool dbg; // Flag for verbose output
64   // Non-const static class variables deprecated by C++ core guidelines!
65 private:
66   std::size_t n {0}; // Length of vector
67   double *data {nullptr}; // data array (standard C array)
68 };
69 } // namespace myvec
```

Note the use of a public static data member `dbg` in Line 63 that can be used to control debugging output by setting `MyVector::dbg = ` **true** or `MyVector::dbg = ` **false**.

Remark 0.3.5.2 (Contiguous arrays in C++) The class **MyVector** uses a C-style array and dynamic memory management with **new** and **delete** to store the vector components. This is for demonstration purposes only and not recommended.

Arrays in C++

In C++ use the STL container **std::vector<T>** for storing data in contiguous memory locations.
Exception: use **std::array<T>**, if the number of elements is known at compile time.

┘

§0.3.5.4 (Member and friend functions of MyVector ⇝ GITLAB)

C++ code 0.3.5.5: Constructor for constant vector, also default constructor, see Line 6 in Code 0.3.5.1 ⇝ GITLAB

```cpp
MyVector::MyVector(std::size_t _n,double _a):n(_n),data(nullptr) {
  if (dbg) cout << "{Constructor MyVector(" << _n
                << ") called" << '}' << endl;
  if (n > 0) data = new double [_n];
  for (std::size_t l=0;l<n;++l) data[l] = _a;
}
```

This constructor can also serve as default constructor (a constructor that can be invoked without any argument), because defaults are supplied for all its arguments.

The following two constructors initialize a vector from sequential containers according to the conventions of the STL.

C++ code 0.3.5.6: Templated constructors copying vector entries from an STL container ⇝ GITLAB

```cpp
1 template <typename Container>
2 MyVector::MyVector(const Container &v):n(v.size()),data(nullptr) {
3   if (dbg) cout << "{MyVector(length " << n
4                 << ") constructed from container" << '}' << endl;
5   if (n > 0) {
6     double *tmp = (data = new double [n]);
7     for(auto i: v) *tmp++ = i; // foreach loop
8   }
9 }
```

Note the use of the new C++ 11 facility of a "foreach loop" iterating through a container in Line 7.

C++ code 0.3.5.7: Constructor initializing vector from STL iterator range ⇝ GITLAB

```cpp
template <typename Iterator>
MyVector::MyVector(Iterator first,Iterator last):n(0),data(nullptr) {
  n = std::distance(first,last);
  if (dbg) cout << "{MyVector(length " << n
                << ") constructed from range" << '}' << endl;
  if (n > 0) {
    data = new double [n];
    std::copy(first,last,data);
  }
}
```

The use of these constructors is demonstrated in the following code

C++ code 0.3.5.8: Initialization of a MyVector object from an STL vector ⇝ GITLAB

```
int main() {
  myvec::MyVector::dbg = true;
  std::vector<int> ivec = { 1,2,3,5,7,11,13 }; // initializer list
  myvec::MyVector v1(ivec.cbegin(),ivec.cend());
  myvec::MyVector v2(ivec);
  myvec::MyVector vr(ivec.crbegin(),ivec.crend());
  cout << "v1 = " << v1 << endl;
  cout << "v2 = " << v2 << endl;
  cout << "vr = " << vr << endl;
  return(0);
}
```

The following output is produced:

```
{MyVector(length 7) constructed from range}
{MyVector(length 7) constructed from container}
{MyVector(length 7) constructed from range}
v1 = [ 1,2,3,5,7,11,13 ]
v2 = [ 1,2,3,5,7,11,13 ]
vr = [ 13,11,7,5,3,2,1 ]
{Destructor for MyVector(length = 7)}
{Destructor for MyVector(length = 7)}
{Destructor for MyVector(length = 7)}
```

The copy constructor listed next relies on the *STL algorithm* **std::**`copy` to copy the elements of an existing object into a newly created object. This takes n operations.

C++ code 0.3.5.9: Copy constructor ⇝ GITLAB

```
MyVector::MyVector(const MyVector &mv):n(mv.n),data(nullptr) {
   if (dbg) cout << "{Copy construction of MyVector(length "
                 << n << ")" << '}' << endl;
   if (n > 0) {
     data = new double[n];
     std::copy_n(mv.data,n,data);
   }
}
```

An important new feature of C++11 is move semantics which helps avoid expensive copy operations. The following implementation just performs a shallow copy of pointers and, thus, for large n is much cheaper than a call to the copy constructor from Code 0.3.5.9. The source vector is left in an empty vector state.

C++ code 0.3.5.10: Move constructor ⇝ GITLAB

```
MyVector::MyVector(MyVector &&mv):n(mv.n),data(mv.data) {
   if (dbg) cout << "{Move construction of MyVector(length "
                 << n << ")" << '}' << endl;
   mv.data = nullptr; mv.n = 0; // Reset victim of data theft
}
```

The following code demonstrates the use of **std::move**() to mark a vector object as disposable and allow the compiler the use of the move constructor. The code also uses left multiplication with a scalar, see Code 0.3.5.23.

C++ code 0.3.5.11: Invocation of copy and move constructors ➺ GITLAB

```cpp
int main() {
  myvec::MyVector::dbg = true;
  myvec::MyVector v1(std::vector<double>(
    {1.2,2.3,3.4,4.5,5.6,6.7,7.8,8.9}));
  myvec::MyVector v2(2.0*v1); // Scalar multiplication
  myvec::MyVector v3(std::move(v1));
  cout << "v1 = " << v1 << endl;
  cout << "v2 = " << v2 << endl;
  cout << "v3 = " << v3 << endl;
  return (0);
}
```

This code produces the following output. We observe that `v1` is empty after its data have been "stolen" by `v2`.

```
{MyVector(length 8) constructed from container}
{operator a*, MyVector of length 8}
{Copy construction of MyVector(length 8)}
{operator *=, MyVector of length 8}
{Move construction of MyVector(length 8)}
{Destructor for MyVector(length = 0)}
{Move construction of MyVector(length 8)}
v1 = [ ]
v2 = [ 2.4,4.6,6.8,9,11.2,13.4,15.6,17.8 ]
v3 = [ 1.2,2.3,3.4,4.5,5.6,6.7,7.8,8.9 ]
{Destructor for MyVector(length = 8)}
{Destructor for MyVector(length = 8)}
{Destructor for MyVector(length = 0)}
```

We observe that the object `v1` is reset after having been moved to `v3`.

⚠ Use `std::move` only for special purposes like above and only if an object has a move constructor. Otherwise a 'move' will trigger a plain copy operation. In particular, do not use `std::move` on objects at the end of their scope, e.g., within `return` statements.

The next operator effects copy assignment of an rvalue **MyVector** object to an lvalue **MyVector**. This involves $O(n)$ operations.

C++ code 0.3.5.12: Copy assignment operator ➺ GITLAB

```cpp
MyVector &MyVector::operator = (const MyVector &mv) {
  if (dbg) cout << "{Copy assignment of MyVector(length "
                << n << "<-" << mv.n << ")"<< '}' << endl;
  if (this == &mv) return(*this);
  if (n != mv.n) {
    n = mv.n;
    if (data != nullptr) delete [] data;
    if (n > 0) data = new double [n]; else data = nullptr;
  }
  if (n > 0) std::copy_n(mv.data,n,data);
  return(*this);
}
```

The move semantics is realized by an assignment operator relying on shallow copying.

C++ code 0.3.5.13: Move assignment operator ➺ GITLAB

```
MyVector &MyVector::operator = (MyVector &&mv) {
  if (dbg) cout << "{Move assignment of MyVector(length "
                << n << "<-" << mv.n << ")"<< '}' << endl;
   if (data != nullptr) delete [] data;
  n = mv.n; data = mv.data;
  mv.n = 0; mv.data = nullptr;
  return(*this);
}
```

The destructor releases memory allocated by **new** during construction or assignment.

C++ code 0.3.5.14: Destructor: releases allocated memory ➺ GITLAB

```
MyVector::~MyVector(void) {
  if (dbg) cout << "{Destructor for MyVector(length = "
                << n << ")" << '}' << endl;
  if (data != nullptr) delete [] data;
}
```

The **operator** keyword is also use to define implicit type conversions.

C++ code 0.3.5.15: Type conversion operator: copies contents of vector into STL vector ➺ GITLAB

```
MyVector::operator std::vector<double> () const {
  if (dbg) cout << "{Conversion to std::vector, length = " << n << '}' << endl;
  return std::vector<double>(data,data+n);
}
```

The bracket operator `[]` can be used to fetch and set vector components. Note that index range checking is performed; an *exception* is thrown for invalid indices. The following code also gives an example of operator overloading as discussed in § 0.3.1.2.

C++ code 0.3.5.16: rvalue and lvalue access operators ➺ GITLAB

```
double MyVector::operator [] (std::size_t i) const {
  if (i >= n) throw(std::logic_error("[] out of range"));
  return data[i];
}

double &MyVector::operator [] (std::size_t i) {
  if (i >= n) throw(std::logic_error("[] out of range"));
  return data[i];
}
```

Componentwise direct comparison of vectors. Can be dangerous in numerical codes,*cf.* Rem. 1.5.3.15.

C++ code 0.3.5.17: Comparison operators ➺ GITLAB

```
bool MyVector::operator == (const MyVector &mv) const
{
  if (dbg) cout << "{Comparison ==: " << n << " <-> " << mv.n << '}' << endl;
  if (n != mv.n) return(false);
  else {
```

```
    for(std::size_t l=0;l<n;++l)
      if (data[l] != mv.data[l]) return(false);
  }
  return(true);
}

bool MyVector::operator != (const MyVector &mv) const {
  return !(*this == mv);
}
```

The `transform` method applies a function to every vector component and overwrites it with the value returned by the function. The function is passed as an object of a type providing a `()`-operator that accepts a single argument convertible to `double` and returns a value convertible to `double`.

C++ code 0.3.5.18: Transformation of a vector through a functor `double` → `double` ➺ GITLAB

```
template <typename Functor>
MyVector &MyVector::transform(Functor &&f) {
  for(std::size_t l=0;l<n;++l) data[l] = f(data[l]);
  return(*this);
}
```

The following code demonstrates the use of the `transform` method in combination with

1. a function object of the following type

   C++ code 0.3.5.19: A functor type

```
struct SimpleFunction {
  SimpleFunction(double _a = 1.0):cnt(0),a(_a) {}
  double operator () (double x) { cnt++; return(x+a); }
  int cnt;          // internal counter
  const double a;  // increment value
};
```

2. a lambda function defined directly inside the call to `transform`.

C++ code 0.3.5.20: transformation of a vector via a functor object

```
int main() {
  myvec::MyVector::dbg = false;
  double a = 2.0; // increment
  int cnt = 0;    // external counter used by lambda function
  myvec::MyVector mv(std::vector<double>(
    {1.2,2.3,3.4,4.5,5.6,6.7,7.8,8.9}));
  mv.transform([a,&cnt] (double x) { cnt++; return(x+a); });
  cout << cnt << " operations, mv transformed = " << mv << endl;
  SimpleFunction trf(a); mv.transform(trf);
  cout << trf.cnt << " operations, mv transformed = " << mv << endl;
  mv.transform(SimpleFunction(-4.0));
  cout << "Final vector = " << mv << endl;
  return(0);
}
```

The output is

```
8 operations, mv transformed = [ 3.2,4.3,5.4,6.5,7.6,8.7,9.8,10.9 ]
8 operations, mv transformed = [ 5.2,6.3,7.4,8.5,9.6,10.7,11.8,12.9 ]
Final vector = [ 1.2,2.3,3.4,4.5,5.6,6.7,7.8,8.9 ]
```

Operator overloading provides the "natural" vector operations in $\mathbb{R}^n$ both in place and with a new vector created for the result.

C++ code 0.3.5.21: In place arithmetic operations (one argumnt) ➺ GITLAB

```cpp
MyVector &MyVector::operator +=(const MyVector &mv) {
  if (dbg) cout << "{operator +=, MyVector of length "
                << n << '}' << endl;
  if (n != mv.n) throw(std::logic_error("+=: vector size mismatch"));
  for(std::size_t l=0;l<n;++l) data[l] += mv.data[l];
  return(*this);
}

MyVector &MyVector::operator -=(const MyVector &mv) {
  if (dbg) cout << "{operator -=, MyVector of length "
                << n << '}' << endl;
  if (n != mv.n) throw(std::logic_error("-=: vector size mismatch"));
  for(std::size_t l=0;l<n;++l) data[l] -= mv.data[l];
  return(*this);
}

MyVector &MyVector::operator *=(double alpha) {
  if (dbg) cout << "{operator *=, MyVector of length "
                << n << '}' << endl;
  for(std::size_t l=0;l<n;++l) data[l] *= alpha;
  return(*this);
}

MyVector &MyVector::operator /=(double alpha) {
  if (dbg) cout << "{operator /=, MyVector of length "
                << n << '}' << endl;
  for(std::size_t l=0;l<n;++l) data[l] /= alpha;
  return(*this);
}
```

C++ code 0.3.5.22: Binary arithmetic operators (two arguments) ➺ GITLAB

```cpp
MyVector MyVector::operator + (MyVector mv) const {
  if (dbg) cout << "{operator +, MyVector of length "
                << n << '}' << endl;
  if (n != mv.n) throw(std::logic_error("+: vector size mismatch"));
  mv += *this;
  return(mv);
}

MyVector MyVector::operator - (const MyVector &mv) const {
  if (dbg) cout << "{operator -, MyVector of length "
                << n << '}' << endl;
  if (n != mv.n) throw(std::logic_error("+: vector size mismatch"));
  MyVector tmp(*this); tmp -= mv;
  return(tmp);
}

MyVector MyVector::operator * (double alpha) const {
  if (dbg) cout << "{operator *a, MyVector of length "
```

```
                 << n << '}' << endl;
  MyVector tmp(*this); tmp *= alpha;
  return(tmp);
}

MyVector MyVector::operator / (double alpha) const {
  if (dbg) cout << "{operator /, MyVector of length " << n << '}' << endl;
  MyVector tmp(*this); tmp /= alpha;
  return(tmp);
}
```

C++ code 0.3.5.23: Non-member function for left multiplication with a scalar ➺ GITLAB

```
MyVector operator * (double alpha,const MyVector &mv) {
  if (MyVector::dbg) cout << "{operator a*, MyVector of length "
                         << mv.n << '}' << endl;
  MyVector tmp(mv); tmp *= alpha;
  return(tmp);
}
```

C++ code 0.3.5.24: Euclidean norm ➺ GITLAB

```
double MyVector::norm(void) const {
  if (dbg) cout << "{norm: MyVector of length " << n << '}' << endl;
  double s = 0;
  for(std::size_t l=0;l<n;++l) s += (data[l]*data[l]);
  return(std::sqrt(s));
}
```

Adopting the notation in some linear algebra texts, the operator $\star$ has been chosen to designate the Euclidean inner product:

C++ code 0.3.5.25: Euclidean inner product ➺ GITLAB

```
double MyVector::operator *(const MyVector &mv) const {
  if (dbg) cout << "{dot *, MyVector of length " << n << '}' << endl;
  if (n != mv.n) throw(std::logic_error("dot: vector size mismatch"));
  double s = 0;
  for(std::size_t l=0;l<n;++l) s += (data[l]*mv.data[l]);
  return(s);
}
```

At least for debugging purposes every reasonably complex class should be equipped with output functionality.

C++ code 0.3.5.26: Non-member function output operator ➺ GITLAB

```
std::ostream &operator << (std::ostream &o,const MyVector &mv) {
  o << "[ ";
  for(std::size_t l=0;l<mv.n;++l)
    o << mv.data[l] << (l==mv.n-1?' ':',');
  return(o << "]");
}
```

┘

EXPERIMENT 0.3.5.27 ("Behind the scenes" of MyVector arithmetic) The following code highlights the use of operator overloading to obtain readable and compact expressions for vector arithmetic.

C++ code 0.3.5.28:

```cpp
int main() {
  myvec::MyVector::dbg = true;
  myvec::MyVector x(std::vector<double>({1.2,2.3,3.4,4.5,5.6,6.7,7.8,8.9}));
  myvec::MyVector y(std::vector<double>({2.1,3.2,4.3,5.4,6.5,7.6,8.7,9.8}));
  auto z = x+(x*y)*x+2.0*y/(x-y).norm();
}
```

We run the code and trace calls. This is printed to the console:

```
{MyVector(length 8) constructed from container}
{MyVector(length 8) constructed from container}
{dot *, MyVector of length 8}
{operator a*, MyVector of length 8}
{Copy construction of MyVector(length 8)}
{operator *=, MyVector of length 8}
{operator +, MyVector of length 8}
{operator +=, MyVector of length 8}
{Move construction of MyVector(length 8)}
{operator a*, MyVector of length 8}
{Copy construction of MyVector(length 8)}
{operator *=, MyVector of length 8}
{operator -, MyVector of length 8}
{Copy construction of MyVector(length 8)}
{operator -=, MyVector of length 8}
{norm: MyVector of length 8}
{operator /, MyVector of length 8}
{Copy construction of MyVector(length 8)}
{operator /=, MyVector of length 8}
{operator +, MyVector of length 8}
{operator +=, MyVector of length 8}
{Move construction of MyVector(length 8)}
{Destructor for MyVector(length = 0)}
{Destructor for MyVector(length = 8)}
{Destructor for MyVector(length = 8)}
{Destructor for MyVector(length = 8)}
{Destructor for MyVector(length = 0)}
{Destructor for MyVector(length = 8)}
{Destructor for MyVector(length = 8)}
{Destructor for MyVector(length = 8)}
```

Several temporary objects are created and destroyed and quite a few *copy operations* take place. The situation would be worse unless move semantics was available; if we had not supplied a move constructor, a few more copy operations would have been triggered. Even worse, the frequent copying of data runs a high risk of cache misses. This is certainly not an efficient way to do elementary vector operations though it looks elegant at first glance. ⌟

EXAMPLE 0.3.5.29 (Gram-Schmidt orthonormalization based on MyVector implementation) Gram-Schmidt orthonormalization has been taught in linear algebra and its theory will be revisited in § 1.5.1.1.

Here we use this simple algorithm from linear algebra to demonstrate the use of the vector class **MyVector** defined in Code 0.3.5.1.

The templated function `gramschmidt` takes a sequence of vectors stored in a **std::vector** object. The actual vector type is passed as a template parameter. It has to supply `size()` and `norm()` member functions as well as in place arithmetic operations $-=$, $/$ and $=$. Note the use of the highlighted methods of the **std::vector** class.

C++ code 0.3.5.30: templated function for Gram-Schmidt orthonormalization ⇝ GITLAB

```cpp
template <typename Vec>
std::vector<Vec> gramschmidt(const std::vector<Vec> &A,double eps=1E-14) {
  const int k = A.size();   // no. of vectors to orthogonalize
  const int n = A[0].size(); // length of vectors
  cout << "gramschmidt orthogonalization for " << k << ' ' << n << "-vectors" <<
      endl;
  std::vector<Vec> Q({A[0]/A[0].norm()}); // output vectors
  for(int j=1;(j<k) && (j<n);++j) {
    Q.push_back(A[j]);
    for(int l=0;l<j;++l) Q.back() -= (A[j]*Q[l])*Q[l];
    if (Q.back().norm() < eps*A[j].norm()) { // premature termination ?
      Q.pop_back(); break;
    }
    Q.back() /= Q.back().norm(); // normalization
  }
  return (Q); // return at end of local scope
}
```

This driver program calls a function that initializes a sequence of vectors and then orthonormalizes them by means of the Gram-Schmidt algorithm. Eventually orthonormality of the computed vectors is tested. Please pay attention to

- the use of auto to avoid cumbersome type declarations,
- the for loops following the “foreach” syntax.
- automatic indirect template type deduction for the templated function `gramschmidt` from its argument. In Line 6 the function gramschmidt<MyVector> is instantiated.

C++ code 0.3.5.31: Driver code for Gram-Schmidt orthonormalization

```cpp
1  int main() {
2    myvec::MyVector::dbg = false;
3    const int n = 7; const int k = 7;
4    auto A(initvectors(n,k,[] (int i,int j)
5            { return std::min(i+1,j+1); }));
6    auto Q(gramschmidt(A)); // instantiate template for MyVector
7    cout << "Set of vectors to be orthonormalized:" << endl;
8    for (const auto &a: A) { cout << a << endl; }
9    cout << "Output of Gram-Schmidt orthonormalization: " << endl;
10   for (const auto &q: Q) { cout << q << endl; }
11   cout << "Testing orthogonality:" << endl;
12   for (const auto &qi: Q) {
13     for (const auto &qj: Q)
14       cout << std::setprecision(3) << std::setw(9) << qi*qj << ' ';
15     cout << endl; }
16   return(0);
17 }
```

This initialization function takes a functor argument as discussed in Section 0.3.3.

C++ code 0.3.5.32: Initialization of a set of vectors through a functor with two arguments

```
template<typename Functor>
  std::vector<myvec::MyVector>
    initvectors(std::size_t n,std::size_t k,Functor &&f) {
  std::vector<MyVector> A{};
  for(int j=0;j<k;++j) {
    A.push_back(MyVector(n));
    for(int i=0;i<n;++i)
      (A.back())[i] = f(i,j);
    }
  return(A);
}
```

┘

0.3.6 Complex numbers in C++

§0.3.6.1 (Data types for complex numbers) The fundamental data type for complex numbers is

```
using complex = std::complex<T>;
```

where the template argument `T` must be a floating point type like **double** or **float**. Then he type **complex**

- t supports all basic arithmetic operations $+, -, *, /$,
- provides the member functions `real()` and `imag()` for extracting real and imaginary parts,
- and can be passed to `std::abs()` and `std::arg()` to get the modulus $|z|$ and the argument $\varphi \in [-\pi, \pi]$ of the complex number $z = |z| \exp(i\varphi)$.

Complex conjugation can be done by calling `std::conj()` for a complex number. ┘

§0.3.6.2 (Initialization of complex numbers) The value of a variable of type **std::complex<double>** can be initialized

- by calling the standard constructor and supplying real and imaginary part: `x = std::complex<double>(x,y)`, where `x,y` are of a numeric type that can be converted to **double**. If the second argument is omitted, the imaginary part is set to zero.
- by providing a **complex literal**, `x = 1.0+1.0i`. This entails the directive `using namespace std::complex_literals`.
- by specifying the modulus $r \geq 0$ and argument $\varphi \in \mathbb{R}$ and calling `std::polar()`: `x = std::polar(r,phi)`. Arguments are always given in radians.

┘

§0.3.6.3 (Functions with complex arguments) All standard mathematical functions like $\exp$, $\sin$, $\cos$, $\sinh$, and $\cosh$ can be supplied with complex arguments.

Note that the definition of $\log$ and of square roots for complex argument entails specifying a **branch cut**. The default choice for the built-in functions is the negative real line. For instance this means that `std::sqrt(z)` for a complex number z will always have non-negative real part. ┘

The following code demonstrates the handling of complex numbers.

C++ code 0.3.6.4: Data types and operations for complex numbers ⇝ GITLAB

```cpp
#include <complex>
#include <iostream>
#include <numbers>
using complex = std::complex<double>;
using namespace std::complex_literals;
int main(int /*argc*/, char** /*argv*/) {
  std::cout << "Demo: Complex numbers in C++" << std::endl;
  // This initialization requires std::complex_literals
  complex z = 0.5; // Std constructor, real part only
  z += 0.5 + 1.0i;
  // Various elementary operations, see
  // https://en.cppreference.com/w/cpp/numeric/complex
  std::cout << "z = " << z << ", Re(z) = " << z.real()
            << ", Im(z) = " << z.imag() << "| z | = " << std::abs(z)
            << ", arg(z) = " << std::arg(z) << ", conj(z) = " << std::conj(z)
            << std::endl;
  complex w = std::polar(1.0, std::numbers::pi / 4.0);
  std::cout << "w = " << w << std::endl;
  std::cout << "exp(z) = " << std::exp(z)
            << ", abs(exp(z)) = " << std::abs(std::exp(z)) << " = "
            << std::exp(z.real()) << std::endl;
  std::cout << "sqrt(z) = " << std::sqrt(z)
            << ", arg(sqrt(z)) = " << std::arg(std::sqrt(z)) << std::endl;

  return 0;
}
```

Terminal output:

```
Demo: Complex numbers in C++
z = (1,1), Re(z) = 1, Im(z) = 1| z | = 1.41421, arg(z) = 0.785398, conj(z)
  = (1,-1)
w = (0.707107,0.707107)
exp(z) = (1.46869,2.28736), abs(exp(z)) = 2.71828 = 2.71828
sqrt(z) = (1.09868,0.45509), arg(sqrt(z)) = 0.392699
```

0.4 Prerequisite Mathematical Knowledge

0.4.1 Basics

In school you should have learned basic facts of real analysis of one variable, in particular, about differentiation, integration, and fundamental special functions.

§0.4.1.1 (Power functions and roots)

$$x^0 := 1\,,\quad x^{m+n} = x^m x^n\,,\quad x^{-n} = \frac{1}{x^n}\quad \forall x \in \mathbb{R}\setminus\{0\}\,,\quad m,n \in \mathbb{Z}\,, \tag{0.4.1.2}$$

$$x^{a+b} = x^a x^b\,,\quad x^{ab} = (x^a)^b\quad \forall x > 0\,,\quad a,b \in \mathbb{R}\,, \tag{0.4.1.3}$$

$$\frac{d}{dx}\{x \mapsto x^n\} = nx^{n-1}\,,\quad x \neq 0,\ n \in \mathbb{N}\quad,\quad \frac{d}{dx}\{x \mapsto x^a\} = ax^{a-1}\,,\quad x > 0,\ a \in \mathbb{R}\,, \tag{0.4.1.4}$$

$$\int x^a\,\mathrm{d}x = \frac{x^{a+1}}{a+1} + C\,,\quad a \in \mathbb{R}\setminus\{-1\}\,, \tag{0.4.1.5}$$

where the last integral can only cover subsets of $\mathbb{R}^+$ unless $a \in \mathbb{N}$. The notation in (0.4.1.5) expresses that $x \mapsto \frac{x^{a+1}}{a+1}$ in the principal (ger.: Stammfunktion) of $x \mapsto x^a$. ┘

§0.4.1.6 (Exponential functions and logarithms) In this course $\log$ always stands for the logarithm with respect to basis $e = 2.71828\ldots$.

$$\exp(x) = e^x\,, \quad x \in \mathbb{R} \quad, \quad \log(\exp(x)) = x \quad \forall x \in \mathbb{R} \quad, \quad a^x := \exp(x\log(a))\,, \quad x \in \mathbb{R},\ a > 0\,.\,. \tag{0.4.1.7}$$

Calculus of exponential functions and logarithms:

$$\exp(x+y) = \exp(x)\exp(y)\,, \quad \exp(-x) = \frac{1}{\exp(x)} \quad \forall x,y \in \mathbb{R}\,, \tag{0.4.1.8}$$

$$\log(xy) = \log(x) + \log(y)\,, \quad \log({}^x/_y)\log(x) - \log(y) \quad \forall x,y > 0\,,$$

$$\exp(nx) = \exp(x)^n\,, \quad \exp(ax) = \exp(x)^a \quad \forall x \in \mathbb{R},\ n \in \mathbb{Z},\ a > 0\,. \tag{0.4.1.9}$$

Differentiation and integration:

$$\frac{d}{dx}\{x \mapsto \exp(x)\} = \exp(x)\,, \quad x \in \mathbb{R} \quad, \quad \frac{d}{dx}\{x \mapsto \log(x)\} = \frac{1}{x}\,, \quad x > 0\,, \tag{0.4.1.10}$$

$$\int \exp(x)\,\mathrm{d}x = \exp(x) + C \quad, \quad \int \log(x)\,\mathrm{d}x = x\log(x) - x + C\,, \tag{0.4.1.11}$$

where, of course, the logarithm can only be integrated over subsets of $\mathbb{R}^+$. ┘

§0.4.1.12 (Rules for differentiation and integration) Assuming sufficient smoothness of the involved functions $f : I \subset \mathbb{R} \to \mathbb{R}$ and $g : D \subset \mathbb{R} \to \mathbb{R}$ and that products and compositions are well-defined, we have, writing $f'(x) := \frac{df}{dx}(x)$, $g'(x) := \frac{dg}{dx}(x)$,

1D product rule: $$\frac{d}{dx}\{x \mapsto f(x)g(x)\} = f'(x)g(x) + f(x)g'(x)\,, \tag{0.4.1.13}$$

1D chain rule: $$\frac{d}{dx}\{x \mapsto f(g(x))\} = f'(g(x))g(x)\,. \tag{0.4.1.14}$$

This implies the following standard integration techniques:

Integration by substituion: $$\int_a^b f(g(x))g'(x)\,\mathrm{d}x = \int_{g(a)}^{g(b)} f(y)\mathrm{d}y\,, \tag{0.4.1.15}$$

integration by parts: $$\int f(x)g'(x)\,\mathrm{d}x = -\int f'(x)g(x)\,\mathrm{d}x + f(x)g(x)\,. \tag{0.4.1.16}$$

Taylor expansion formula in one dimension for a function that is $m+1$ times continuously differentiable in a neighborhood of x_0

$$f(x_0+h) = \sum_{k=0}^{m} \frac{1}{k!} f^{(k)}(x_0)h^k + R_m(x_0,h)\,, \quad R_m(x_0,h) = \frac{1}{(m+1)!} f^{(m+1)}(\xi)h^{m+1}\,, \tag{1.5.4.28}$$

for some $\xi \in [\min\{x_0, x_0+h\}, \max\{x_0, x_0+h\}]$, and for all sufficiently small $|h|$. ┘

0.4.2 Complex Numbers

We write $\imath$ for the imaginary unit: $\operatorname{Re}\imath = 0$, $\operatorname{Im}\imath = 1$, $\imath^2 = -1$. Then every complex number $z \in \mathbb{C}$ can be identified with a pair $(x, y) \in \mathbb{R}^2$ of real numbers via $z = x + \imath y$.

$$\begin{aligned}
\text{Multiplication:}\quad & (x+\imath y)(u+\imath v) = (xu - yv) + \imath(xv + yu) \quad \forall x,y,u,v \in \mathbb{R}\,,\\
\text{Complex conjugation:}\quad & \overline{x+\imath y} = x - \imath y \quad \forall x,y \in \mathbb{R}\,,\\
\text{Modulus:}\quad & |z|^2 := \operatorname{Re}\{z\bar{z}\}\,,\quad |Z| = |z||w| \quad \forall z,w \in \mathbb{C}\,,\\
\text{Division:}\quad & \frac{w}{z} = \frac{w\bar{z}}{|z|^2} \quad \forall w,z \in \mathbb{C},\ z \neq 0\,.
\end{aligned}$$

Many mathematical functions can be extended to complex arguments and many calculus rules will remain valid for them, in particular the formulas involving the functions $\exp$, $\sin$, $\cos$.

$$\text{Euler's formula:}\qquad \exp(\imath t) = \cos(t) + \imath\sin(t) \quad \forall t \in \mathbb{R}\,. \tag{0.4.2.1}$$

Some parts of this course will rely on sophisticated results from complex analysis, that is, the field of mathematics studying functions $\mathbb{C} \to \mathbb{C}$. This results will be recalled when needed.

0.4.3 Trigonometric Functions

Trigonometric functions can be defined via the complex exponential function:

$$\cos(z) = \tfrac{1}{2}(\exp(\imath z) + \exp(-\imath z)) \quad,\quad \sin(z) = \tfrac{1}{2\imath}(\exp(\imath z) - \exp(-\imath z))\,,\quad z \in \mathbb{C}\,. \tag{0.4.3.1}$$

This implies

$$\sin^2 z + \cos^2 z = 1 \quad \forall z \in \mathbb{C} \quad,\quad 1 + \tan^2 z = \frac{1}{\sin^2 z} \quad \forall z \in \mathbb{C} \setminus \pi\mathbb{Z}\,.$$

Addition formulas:

$$\sin(z \pm w) = \sin z \cos w \pm \cos z \sin w \quad,\quad \cos(z \pm w) = \cos z \cos w \mp \sin z \sin w \quad \forall z,w \in \mathbb{C}\,,$$

and, whenever defined

$$\tan(z \pm w) = \frac{\tan z \pm \tan w}{1 \mp \tan z \tan w} \quad,\quad \arctan z \pm \arctan w = \arctan\left(\frac{z \pm w}{1 \mp zw}\right)\,.$$

0.4.4 Linear Algebra and Analysis

This course takes for granted that participants have been educated in the foundations of linear algebra by attending corresponding first-year introductory courses, for instance

- 401-0151-00L Lineare Algebra
- 401-0231-10L Analysis 1
- 401-0232-10L Analysis 2

Quite a few concepts and techniques introduced in those courses will be needed for and *will be taken for granted* in the current course.

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