MA3227 Numerical Analysis II

Topics for Final Exam

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Topics for Final Exam

Midterm topics

- All topics covered in the midterm can also be tested in the final.

Banach fixed point theorem

- Not part of the exam.

Ordinary differential equations

- You should be familiar with the basic theory for ODEs, but I will not explicitly test this in the exam. Topics in this category include:
  - Meaning of $\dot{y} = f(y)$.
  - Picard-Lindelöf theorem
  - Gronwall's inequality.
  - Stability with respect to initial conditions.
- You should know how to write $\ddot{x} = g(x, \dot{x})$ or $\dot{x} = g(x, t)$ in the form $\dot{y} = f(y)$.

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Runge-Kutta methods

Example questions (see lab 5 and assignment 3):

- Translate Butcher tableau into one-step equation or vice versa.
- Perform by hand a few steps of a Runge-Kutta method given in the form of either a Butcher tableau or a one-step equation.
- Determine the order of consistency of a given scheme.
- Determine the stability function of a given scheme.

Remarks:

- You can practice the above questions using the schemes from `https://en.wikipedia.org/wiki/List_of_Runge-Kutta_methods`.
  You can test your answers using the `convergence()` and `stability()` functions from assignment 3.
- Showing consistency of order $p + 1 > 3$ is tedious and not required to demonstrate understanding of the theory. I will not ask for this.
- Unlike in assignment 3, I may also ask you to determine the order of consistency of an implicit method.
- Recall that there are two ways for determining the stability functions, and one may be much easier to execute than the other.

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Runge-Kutta methods (continued)

Other things which you should know:

- Lipschitz-continuity of $f(y)$ and $(p+1)$th-order consistency imply pth-order convergence.
- A Runge-Kutta scheme applied to an ODE $\dot{y} = f(y)$ with fixed point y_F may exhibit spurious exponential blow-up if $|R(\lambda\,\Delta t)| > 1$ for some eigenvalue λ of $\nabla f(y_F)$.
- The one and only advantage of implicit Runge-Kutta methods is that they allow for $R(z)$ to be bounded for $|z| \to \infty$.

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Adaptive time-stepping

Facts you should know:

- Accuracy of Runge-Kutta methods depends on curvature of solution.
- Errors can be estimated by comparing the numerical results for different step-sizes Δt or Runge-Kutta schemes of different orders.
- There are two algorithms for choosing the "effort parameter" n such that the error $e(n)$ satisfies $e(n) \lesssim \varepsilon$:
  - Double n until converged. This takes at most two times longer than running the algorithm only once with the "correct" n.
  - Extrapolate convergence,

$$e(n) \approx C\, n^{-p} \quad \longrightarrow \quad n_{\text{ideal}} = n_{\text{trial}} \left(\frac{e(n_{\text{trial}})}{\varepsilon} \right)^{1/p}.$$

    Pro: close to no overhead compared to using the "correct" n.
    Con: n_{ideal} can be wrong if $e(n) \approx C\, n^{-p}$ is not satisfied.
    If this happens, then this is likely because n_{trial} is too small.

  Both of these methods can also be used for choosing the step size Δt.

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Time-dependent PDEs

Things you should know:

- Time-dependent PDEs can be solved by using finite differences in space to convert the PDE to a system of ODEs, and then using a Runge-Kutta scheme to solve the ODE.
- The resulting system of ODEs is stiff and should be solved using an implicit Runge-Kutta scheme.

Things I do not expect you to know:

- Convergence theory for finite differences + Runge Kutta.

Trajectory of Cannonball

Things you should know:

- Derivatives of $y(t)$ with respect to the initial conditions y_0 can be computed by solving

$$\tfrac{d}{dt}\tfrac{\partial y}{\partial y_0} = \nabla f(y)\,\tfrac{\partial y}{\partial y_0}, \qquad \tfrac{dy}{dy_0}(0) = 1.$$

  See also the shooting method in lab 7.

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Molecular dynamics

Things you should know:

- Newton's equations of motion conserve the total energy.
- Most Runge-Kutta methods lead to a drift in the total energy.
- This drift can be avoided by using a symplectic integrator.

Things I do not expect you to know:

- Anything about molecular dynamics or symplectic integrators not explicitly mentioned above.

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Probability theory

You should be familiar with the following definitions and results from probability theory.

- Probability space, random variables (RVs), distributions of RVs.
- Representations of distributions: PDF / PMF, CDF.
- Expectation: $\begin{cases} \mathbb{E}[f(X)] = \int_{\Xi} f(x)\, p(x)\, dx \\ \mathbb{E}[aX + bY] = a\,\mathbb{E}[X] + b\,\mathbb{E}[Y] \end{cases}$
- Variance: $\begin{cases} \mathrm{Var}[X] = \mathbb{E}\big[(X - \mathbb{E}[X])^2\big] = \mathbb{E}[X^2] - \mathbb{E}[X]^2 \\ \mathrm{Var}[aX + b] = a^2\,\mathrm{Var}[X] \end{cases}$
- Independence: $p(x_1, \dots, x_n) = p_1(x_1)\,\dots\,p_n(x_n)$.

$p(x)$ denotes the PDF / PMF of X in the above formulae.

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Monte Carlo sampling

Things you should know:

- Monte Carlo estimator $\tilde{\mathbb{E}}_N[X] = \frac{1}{N}\sum_{k=1}^{N} X_k$.
- Error estimation using central limit theorem. In particular:
  - The two interpretations of the central limit theorem regarding expected error and likelihood of outliers.
  - How to estimate $\mathrm{Var}[X]$ using the X_k computed for the Monte Carlo estimator $\tilde{\mathbb{E}}_N[X]$ (see Lecture 24).

Simulation of random variables

Things you should know:

- pRNGs: what they are and why we use them.
- Transformation sampling theorem.
- Rejection sampling theorem.
- Importance sampling theorem.

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The above is a complete list of all exam-relevant topics for this module. If you have any questions about it, please do not hesitate to ask.

The remaining slides contain:

- A one-page list of topics of particular importance for the exam. The idea of this list is to help you focus your study efforts on topics which guarantee a decent passing grade. Obviously, if you want an outstanding grade then you should master all of the above topics.
- An overview of the module which is intended to help you organise the various topics in this module in a unified framework.

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Key exam topics

Some key techniques to master for the exam:

- Application of fill path theorem (practise using Q1 in lab 2).
- Root-finding algorithms by hand (practise using codes in Lect. 12 & 13).
- Runge-Kutta methods by hand (see slide 3 for practice material).
- Determining the order of consistency and stability function of Runge-Kutta methods (see slide 3 for practice material).
- Application of transformation, rejection and importance sampling. (see assignment 4 and lab 9 for practice material).

Furthermore, make sure you are aware of the following facts:

- Krylov methods:
  - Cost of k Krylov iterations:
  $$k \text{ matvecs} + \begin{cases} \mathcal{O}(nk^2) \text{ other operations for GMRES} \\ \mathcal{O}(nk) \text{ other operations for CG and MinRes} \end{cases}$$
  - k distinct eigenvalues $\implies$ convergence in at most k iterations.
  - Eigenvalues in $[a, b]$ $\implies$ $\mathcal{O}\big(|\log(\varepsilon)|\sqrt{b/a}\big)$ required for error ε.
- Jacobi-type methods:
  - Error analysis amounts to determining the error recurrence $x_{k+1} - x = R\,(x_k - x)$ and determining the eigenvalues $\hat{\lambda}$ of R.

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Module overview

Numerical algorithms discussed in this module, grouped by the type of problem that they solve.

- Poisson equation (or more generally, PDEs)
  - Finite difference discretisation
- Linear systems of equations
  - Sparse LU factorisation
  - Krylov subspace methods
  - Jacobi and multigrid iteration
- Nonlinear equations and systems of equations
  - Bisection and false position
  - Newton's method
  - Secant and Broyden's method
  - Steepest descent / gradient descent
- Ordinary differential equations
  - Explicit and implicit Runge-Kutta methods
- High-dimensional problems
  - Monte Carlo methods

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Module overview (continued)

For each problem type listed above, make sure you can comment on the following:

- Precise problem formulation
- Existence and uniqueness
  - Poisson equation: not discussed in this module.
  - Linear equations: A nonsingular.
  - Nonlinear equations: convexity, fixed-point theorems. (Only briefly mentioned in this module.)
  - ODEs: Picard-Lindelöf theorem.
  - High-dim : usually not an issue since we have explicit formulae.
- Conditioning / stability / sensitivity
  - Poisson equation: not discussed in this module.
  - Linear equations: condition number $\kappa(A) = \|A\| \, \|A^{-1}\|$.
  - Nonlinear equations: not discussed in this module
  - ODEs: Gronwall inequality and the stability corollary.
  - High-dim: not discussed in this module.

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Module overview (continued)

For each algorithm, make sure you can comment on the following:

- Runtime & algorithmic details.
- Is the algorithm exact up to rounding errors?

  Answer is no for all algorithms except LU factorisation.
- If no, which result guarantees convergence?
  - Finite differences: stability & consistency $\implies$ convergence theorem.
  - Krylov methods: equivalence to polynomial minimisation problems.
  - Jacobi, multigrid, Newton, secant: error recursion $e_{k+1} = f(e_k)$.
  - Bisection & false position: shrinking bracketing intervals.
  - Runge-Kutta methods: consistency and Lipschitz continuity theorem.
  - Monte Carlo: central limit theorem.
- How do we estimate the error?
  - PDEs: not discussed in this module.
  - Linear equations: residual $\|A\tilde{x} - b\|$.
  - Nonlinear equations: either residual $\|f(x)\|$ or progress $\|x_{k+1} - x_k\|$.
  - ODEs: compare results for different orders or step sizes.
  - Monte Carlo: estimate $\mathrm{Var}[X]$.