CS-6404 (CRN 91132)
Advanced Topics in Mathematical Software:
Computational Data Assimilation –
Inverse Problems with Differential Equations
Fall 2022

Essential information.

Instructor  Adrian Sandu
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Office     2224 KnowledgeWorks II, 2202 Kraft Drive.
Lecture    Tue-Thu, 2:00PM–3:15PM, 209 McBryde Hall
Office hours by appointment
Web Page   http://www.cs.vt.edu/~asandu/Courses/CS6404/CS6404.html
Prerequisites  Graduate standing.
Exam section 14T, December 13, 2022, 2:05PM–4:05PM

Prerequisites.
Graduate standing; graduate coursework in numerical methods; instructor approval.

Overview.

Computer/mathematical models encapsulate the physical laws that govern the evolution of a real
system, and allow us to predict the evolution of that system.

- The forward problem consists of using the model (with prescribed values of system parameters)
to simulate the evolution of the physical system. (As a useful example, consider a pendulum
of known length $L$. For a prescribed mass $m$ of the pendulum the model can predict the
period of small oscillations).

- The inverse problem consists of using data from measurements of reality to infer the values of
the parameters that characterize the system. (In this case one measures the period of small
oscillations; based on this data, and using the model equations, one infers the mass of the
pendulum).

Inverse problems are tremendously important in many fields from biology to nuclear engineering
to numerical weather prediction. They are also highly challenging, and special methodologies are
required for their solution.

This class introduces different computational methods for solving inverse and data assimilation
problems, including ensemble Kalman filters, variational methods, and nonlinear and non-Gaussian
techniques. We will build a strong background in inverse problems by covering topics such as
statistical estimation theory, ill-conditioning and regularization techniques, differential equations
and adjoint modeling, and numerical optimization.
Textbook.

The instructor will hand in typeset course notes to registered students. There is no single textbook that covers all the material discussed; nevertheless, the following texts may prove useful.


Topics.

This class will introduce different computational methods for solving inverse problems. Topics discussed during the course include:

1. Review of probability theory, statistical estimation theory, minimum variance, maximum likelihood, Bayesian approach.
2. The Kalman filter and Kalman smoother.
3. Ensemble-based (Monte Carlo) inversion methods:
   - Sampling,
   - Ensemble Kalman filters, and
   - Ensemble Kalman smoothers.
4. Particle filters and smoothers:
   - Classical (sequential importance with resampling – SIR) approach,
   - Inference based on optimal transform maps,
   - Variational Fokker-Planck approach based on particle flows.
5. Maximum likelihood estimation:
   - Three-dimensional variational filtering (3D-Var),
   - Four-dimensional variational smoothing (4D-Var),
   - Gradient computation. Direct and adjoint sensitivity analysis for ordinary and partial differential equations.
   - Numerical optimization.
6. Hybrid methods:
   - Optimization over ensemble spaces (4D-EnVar),
• Ensembles of four-dimensional variational smoothing (En-4DVar),

7. Robust estimation, $L_1$ and Huber norm assumptions.

• Optimization over ensemble spaces (4D-EnVar),
• Ensembles of four-dimensional variational smoothing (En-4DVar),

8. Speeding up computations: reduced order models, data assimilation using inexpensive surrogates in place of full order dynamical models.

**Grading.**

There will be no in-class midterm or final examinations. The grade will be based on homework problems and projects. For those topics for which lecture notes are not available one student may be designated, by rotation, to take notes in class. You are responsible for typesetting them in LaTeX, making sure they are error-free (after consulting with your colleagues), and handing them to the instructor *no later than one week after the lecture*. Any figures drawn on the table during the lecture will be reproduced using any appropriate drawing software. The LaTeX notes will be distributed to the entire class when ready.

**Disclaimer.**

The information given to you in class will supersede the information in this syllabus.

**Student Complaints and Academic Misconduct.**

The Honor Code guides student conduct in the class. If you have any problems, the first step is to discuss with me directly. Should you need to speak with the Chair of the C.S. Department, you can make an appointment by speaking with the Departmental Secretary in KWII.

**Disabilities.**

Please let me know if you have a disability which requires special arrangements.