SciML + DA - Syllabus

Mark Asch - IMU/VLP/CSU

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Course Outline for Scientific Machine Learning and Data Assimilation

1. Introduction to scientific machine learning:
   (a) What is scientific machine learning?
   (b) Why use scientific machine learning?
   (c) Examples of scientific machine learning.
   (d) The role of mathematics in scientific machine learning.
   (e) The role of computer science in scientific machine learning.

2. Brief recall of the mathematical foundations of scientific machine learning:
   (a) Linear algebra.
   (b) Calculus.
   (c) Differential equations.
   (d) Optimization.
   (e) Probability theory.

3. Machine learning techniques for scientific applications (see Basic Course for details):
   (a) Supervised learning:
      i. Regression.
      ii. Classification.
   (b) Unsupervised learning:
      i. Clustering.
      ii. Trees.
   (c) Surrogate models and dimensionality reduction.
   (d) The use of machine learning in scientific applications.
   (e) The challenges of applying machine learning to scientific applications.

4. Probabilistic programming for scientific machine learning:
   (a) Bayesian inference.
   (b) Markov chain Monte Carlo.
   (c) Bayesian optimization.
   (d) The use of probabilistic programming in scientific applications.
   (e) The challenges of applying probabilistic programming to scientific applications.

5. Automatic differentiation for scientific machine learning:
   (a) Differentiable programming with autograd and PyTorch.
   (b) Gradients, adjoints, backpropagation and inverse problems.
   (c) Neural networks for scientific machine learning.
   (d) Physics-informed neural networks.
   (e) The use of automatic differentiation in scientific machine learning.
   (f) The challenges of applying automatic differentiation to scientific applications.

6. Applications of scientific machine learning:
   (a) Fluid dynamics.
   (b) Materials science.
   (c) Biology.
   (d) Medicine.
   (e) The challenges of applying scientific machine learning to different scientific domains.

7. Case studies in scientific machine learning:

(a) Solving partial differential equations with neural networks.
(b) Predicting protein structures with deep learning.
(c) Diagnosing diseases with machine learning.
(d) Epidemiology with machine learning.
(e) The use of case studies to illustrate the power of scientific machine learning.
(f) The challenges of applying scientific machine learning to real-world problems.

8. Ethics and responsible use of scientific machine learning:

(a) Inference Cycle
(b) SSL and LLMs
(c) Bias in machine learning models.
(d) Fairness in machine learning.
(e) Transparency in machine learning.
(f) Trustworthiness, explainability.
(g) The ethical challenges of using scientific machine learning.
(h) The responsible use of scientific machine learning.

9. Advanced Data Assimilation

(a) Variational DA
(b) Statistical DA
(c) Hybrid DA
(d) DA and ML

10. Project work:

    (a) Students will work on a project that applies scientific machine learning and/or data assimilation to a real-world problem.
    (b) The project will be supervised by the instructor.
    (c) The project will be presented to the class at the end of the course.

11. Presentation of project work:

    (a) Students will present their project work to the class.
    (b) The presentations will be an opportunity for students to share their work with the class and get feedback from the instructor and other students.

References

1. M. Asch. *Digital Twins: from Model-Based to Data-Driven.* SIAM, 2022.

2. J. Nocedal, S. Wright. *Numerical Optimization.* Springer, 2006.

3. G. Strang. *Linear Algebra and Learning from Data.* Wellesley-Cambridge Press, 2019.