

CS 6824: AI-powered Molecular Modeling

Website: <https://people.cs.vt.edu/dbhattacharya/courses/cs6824/>

Canvas: <https://canvas.vt.edu/courses/196265>

This week

- **What is the field about?**
 - Why should we care?
- **What is this class about?**
 - What to expect?
 - Logistics

Welcome!

- **Introductions**

- What is your year / background / research interests?
- What do you want to learn from this class?
- Fun fact?

- **About me**

- Debswapna Bhattacharya - CS@VT Assoc. Prof.
- Second time teaching this class — as always, feedback is welcome!
- Interested in developing new machine learning and optimization algorithms for addressing fundamental structural biology problems
 - We will explore this new research area, its various subfields and connections to other topics in CS throughout this semester

Course Design

- **Goals of this course:**
 - Learn about machine learning methods applied to problems in molecular modeling
 - Learn how to critically read and evaluate papers
 - Learn how to pose research problems and practice oral and written scientific communication skills
- **What to expect:**
 - This is an advanced, interdisciplinary class.
 - You should have exposure/working knowledge of machine learning concepts and deep learning architectures.
 - I will provide supplementary reading/online resources
 - No prior knowledge of biology is required, however, students should expect to develop a sufficient understanding of each application area to evaluate new developments.
- **Prerequisite:**
 - Interest in achieving a deep understanding of **both** ML algorithms and molecular modeling problems
 - Interested in "AI for science"? A key ability is to be able to read and understand papers from both communities
 - This course is appropriate for graduate students in computer science, computational biology, bioinformatics, and statistics. Familiarity with fundamental concepts in machine learning, statistics, probability and algorithms is expected.

Course Information

- **Course website**
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Todo: before next class

Go through the course webpage at:

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...and ask any questions in the next class.