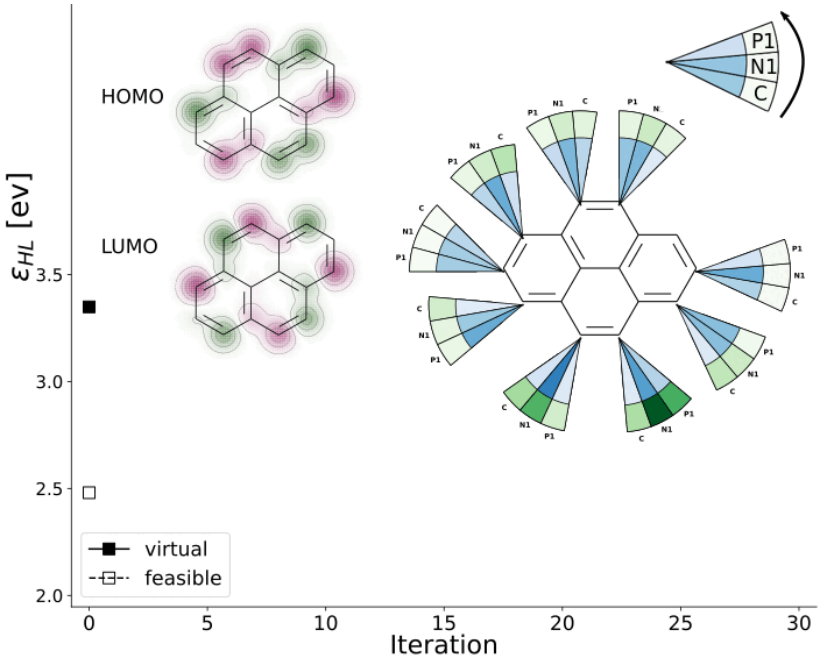

CHEM-4PB3 (2022)

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# Chemistry + Computer Science
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Goal

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Do NOT be afraid of coding
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Oscar Méndez Lucio @omendezlucio · 15 jun. 2018
#RSC_AIChem quotes:

“Artificial Intelligence will not replace chemists.

But chemists who don’t use AI will be replace by those who do”

Willem Van Hoorn

Evaluation

1. **Final project**
    i. Oral presentation $\rightarrow$ 20 to 30 min
    ii. Online tutorial $\rightarrow$ code or data set for reproducibility
    iii. Two written reports:
        a. Midterm report (maximum 2 pages, deadline: week after reading break)
        b. Final report (maximum 6 pages)
2. **Tutorials & coding exercises**
    -To help you develop the skills needed for your final project

Final project

Examples,

1. Reproduce some results of a published paper
2. Data analysis for a lab project
3. Theoretical study:
    i. pontential energy urface for a reaction
    ii. transition state search
    iii. ...
4. Parameter fitting for model

Outline

1. Introduction to programming (**Python**)
2. Linear algebra and calculus (**refresh**)
3. **Machine learning***
    i. Regression models
    ii. Classification models
    iii. Optimization algorithms
4. **Computational Chemistry***
    i. Hartree-Fock
    ii. Density Functional Theory
    iii. Molecular Dynamics

Final report

1. Section 1: Introduction, literature review and problem statement (**midterm report**)
2. Section 2: Hypothesis (**midterm report**)
3. Section 3: Describe your data/model or chemical system (**midterm report**)
4. Section 4: Results
5. Section 5: Summary
6. Section 6: Future work
7. Section 8: References (not included in the page limit)

4 to 6 page limit

Final presentation

Time limit:

20 to 30 min included questions and a go-through the working demo.

Colab demo:

Colab demo that explains and displays the model/data used for the problem of interest.
(**example**) https://github.com/RodrigoAVargasHdz/steady_state_jax

Software

1. **Machine Learning**
    i. Scikit learn
    ii. Jax ecosystem
    iii. PyTorch
2. **Data science**
    i. Numpy
    ii. Matplotlib (or Seaborn)
    iii. SciPy
    iv. Pandas

Software

3. **Computational Chemistry**
    i. PySCF (**or others**)
    ii. RDKit
    iii. **Molecular Dynamics**: JaxMD, TorchMD, openMD
    iv. **Visualization**

What do you want to learn?

- This course is for you!

VA

What are the most relevant skills for a computational chemistry now a days?

In computational chemistry, some of the most relevant skills include:

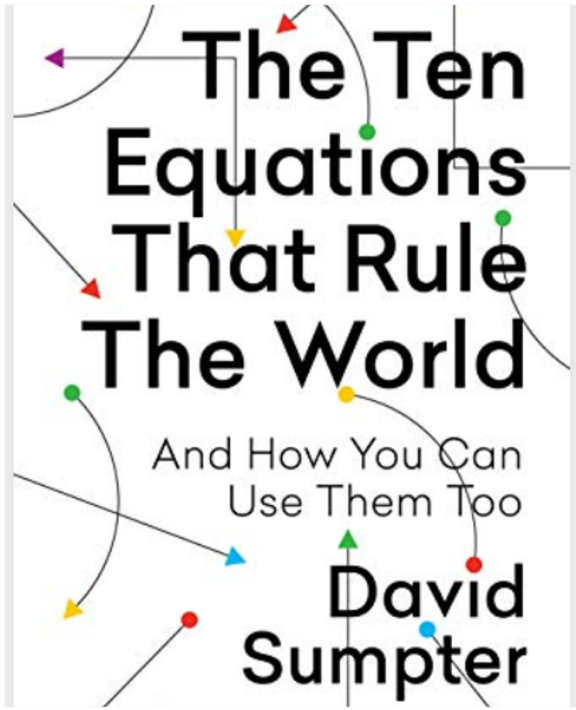
1. Familiarity with quantum chemistry methods: These methods are used to model the electronic structure of molecules and predict their properties.
2. Experience with molecular modeling software: These programs are used to build and analyze chemical systems.
3. Programming skills: Many computational chemistry tasks involve automating tasks or analyzing large datasets, so being able to program can be very useful.
4. Knowledge of statistical analysis: This can be helpful for analyzing and interpreting the results of computational chemistry simulations.
5. Familiarity with drug design: Many computational chemists work on developing new drugs, so understanding the principles of drug design can be important.
6. Good communication skills: Computational chemistry often involves collaborating with researchers from other disciplines, so being able to clearly communicate your work is important.

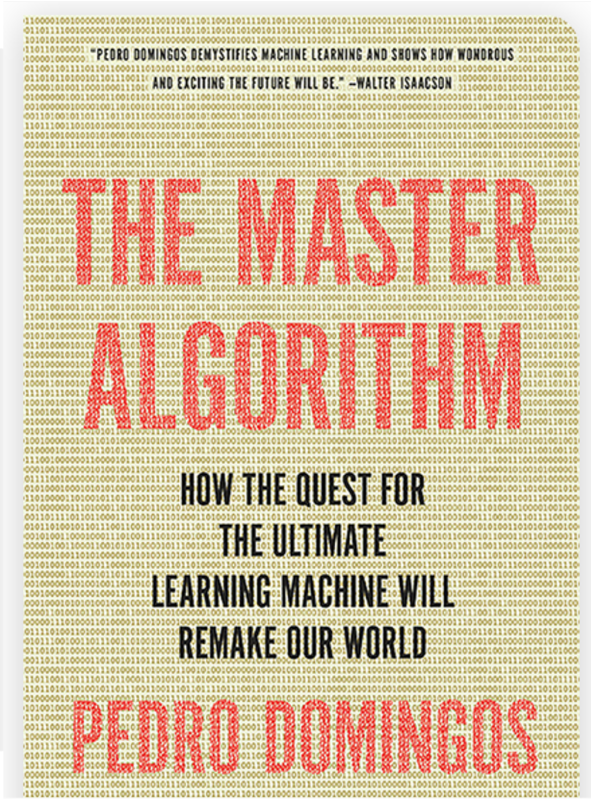
VA

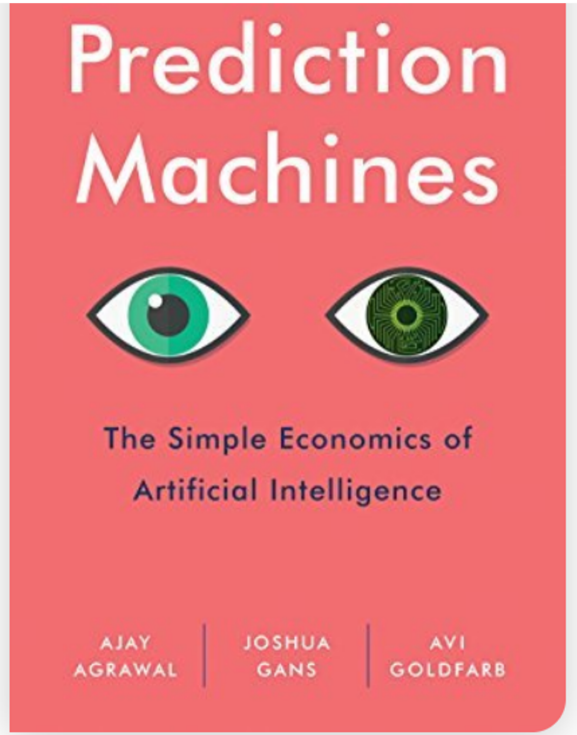
What are the most relevant topics for a modern computational chemistry course?

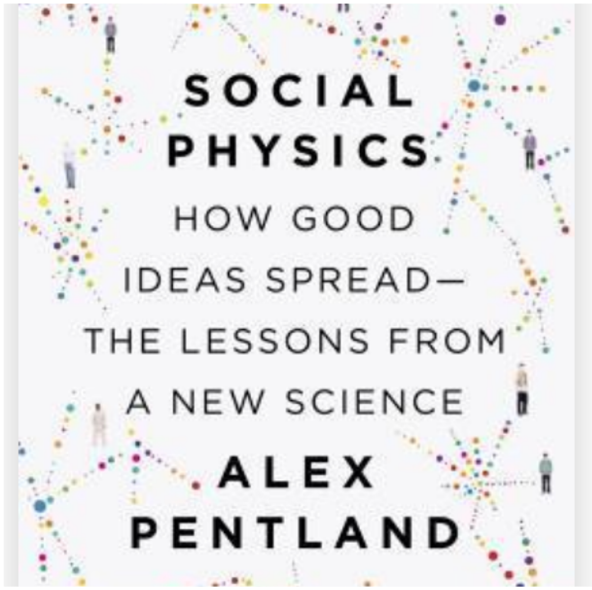
Here are some topics that might be covered in a modern computational chemistry course:

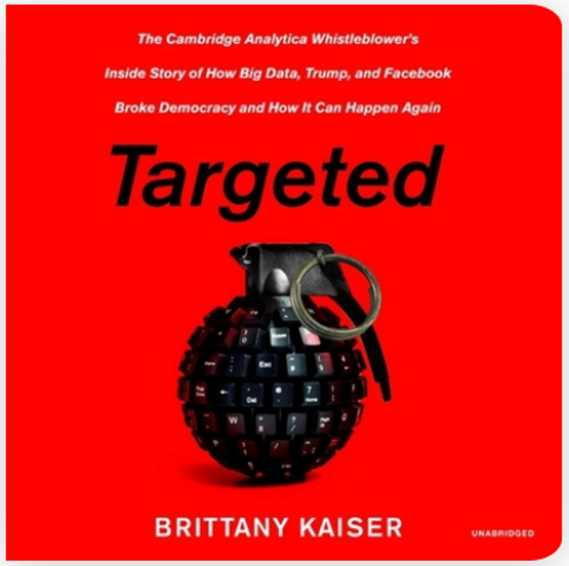
1. Quantum chemistry methods: This could include topics such as Hartree-Fock theory, density functional theory, and wavefunction-based methods.
2. Molecular mechanics: This includes classical methods for modeling the behavior of molecules, such as molecular dynamics and Monte Carlo simulations.
3. Molecular dynamics simulations: This involves using computational methods to model the movement of atoms and molecules over time.
4. Drug design: This could include topics such as virtual screening, docking, and pharmacophore modeling.
5. Materials modeling: This could include topics such as predicting the properties of solid materials or modeling the behavior of surfaces.
6. Statistical analysis: This could include topics such as hypothesis testing, regression analysis, and machine learning.
7. High-performance computing: This could include topics such as parallel computing and optimization for running simulations on supercomputers.
8. Data analysis: This could include topics such as visualizing and interpreting the results of computational simulations.

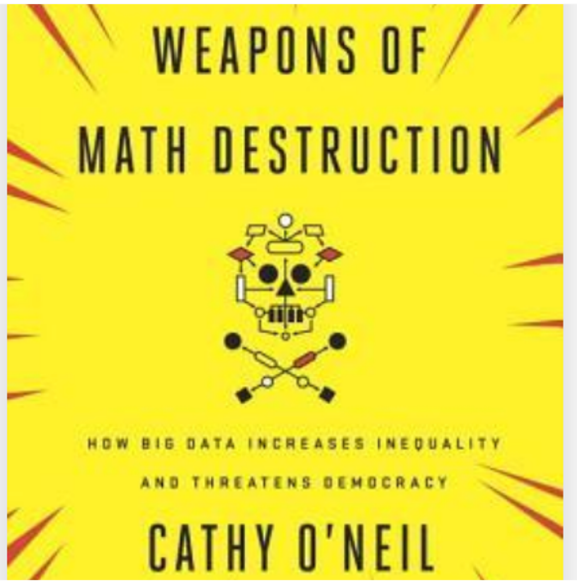

The Ten Equations That Rule The World
And How You Can Use Them Too
David Sumpter


"PEDRO DOMINGOS DEMYSTIFIES MACHINE LEARNING AND SHOWS HOW WONDROUS AND EXCITING THE FUTURE WILL BE." –WALTER ISAACSON
THE MASTER ALGORITHM
HOW THE QUEST FOR THE ULTIMATE LEARNING MACHINE WILL REMAKE OUR WORLD
PEDRO DOMINGOS


Prediction Machines
The Simple Economics of Artificial Intelligence
AJAY AGRAWAL
JOSHUA GANS
AVI GOLDFARB


SOCIAL PHYSICS
HOW GOOD IDEAS SPREAD—THE LESSONS FROM A NEW SCIENCE
ALEX PENTLAND


The Cambridge Analytica Whistleblower's Inside Story of How Big Data, Trump, and Facebook Broke Democracy and How It Can Happen Again
Targeted
BRITTANY KAISER
UNABRIDGED


WEAPONS OF MATH DESTRUCTION
HOW BIG DATA INCREASES INEQUALITY AND THREATENS DEMOCRACY
CATHY O'NEIL