

# AM 207

ADVANCED SCIENTIFIC COMPUTING: MONTE CARLO  
METHODS FOR INFERENCE AND DATA ANALYSIS, AND  
STOCHASTIC OPTIMIZATION

---

Verena Kaynig-Fittkau

[vkaynig@seas.harvard.edu](mailto:vkaynig@seas.harvard.edu)

NW 235.1 or B164

# All About Randomness

- Solve your problems using random numbers and uncertainty.



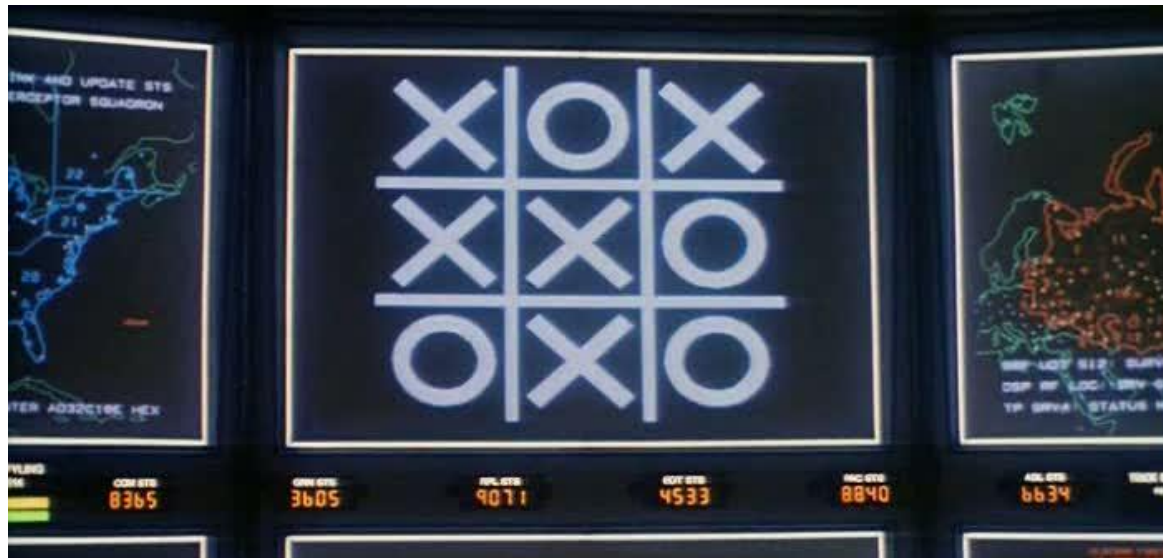
# Outline

- Why care about this course
- What is the course about
- Who is helping you learn the material
- How will we learn it



# Why

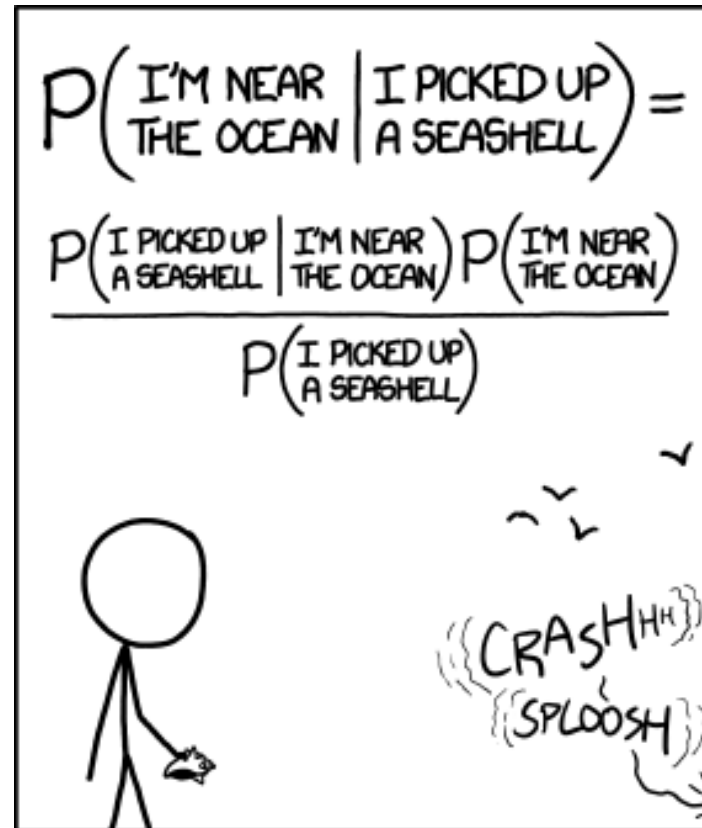
- Sometimes defining your problem in a deterministic way is very hard / infeasible
- But computers nowadays are fast
- It is easier and faster to let the Computer run for a day than think for a week



# Why – Numerical Integration

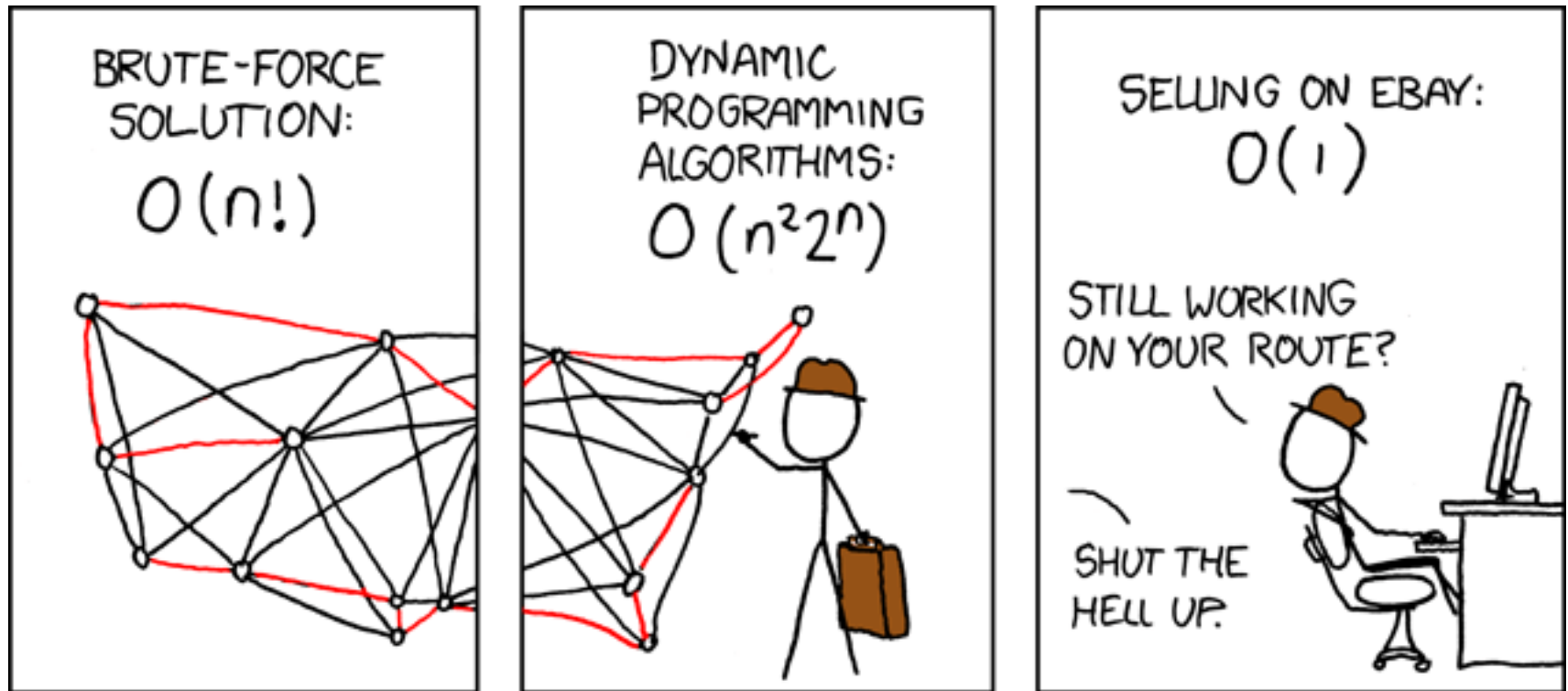
$$\int \frac{[\cos^{-1}x \{ \sqrt{1-x^2} \}]^{-1}}{\log_e \left\{ 1 + \left( \frac{\sin (2x\sqrt{1-x^2})}{\pi} \right) \right\}} dx$$

# Why – Bayesian Inference

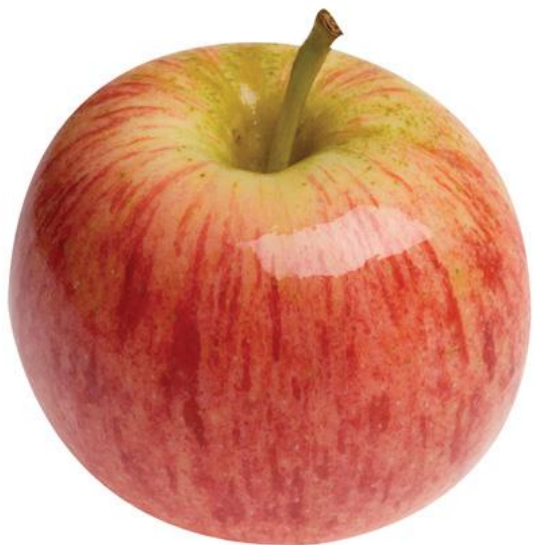


STATISTICALLY SPEAKING, IF YOU PICK UP A SEASHELL AND DON'T HOLD IT TO YOUR EAR, YOU CAN PROBABLY HEAR THE OCEAN.

# Why – Stochastic Optimization

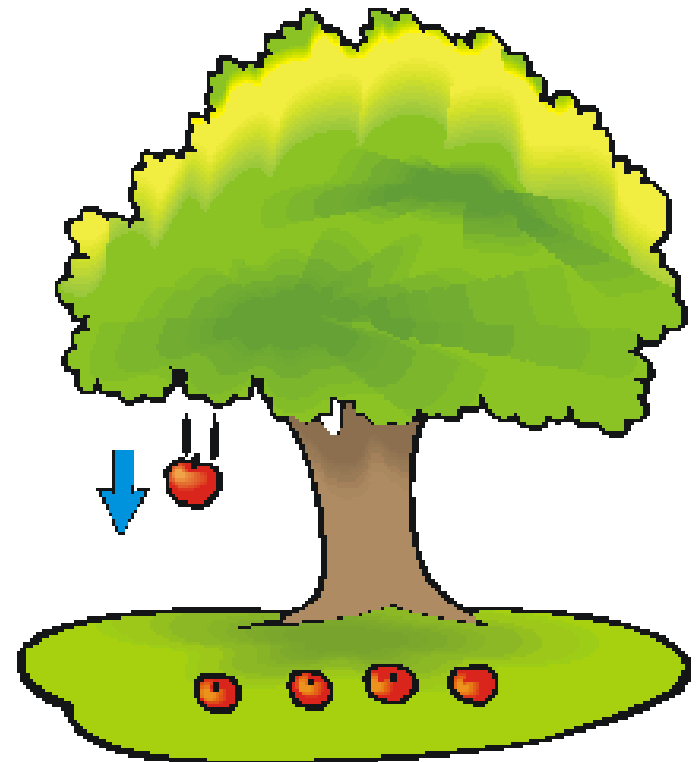
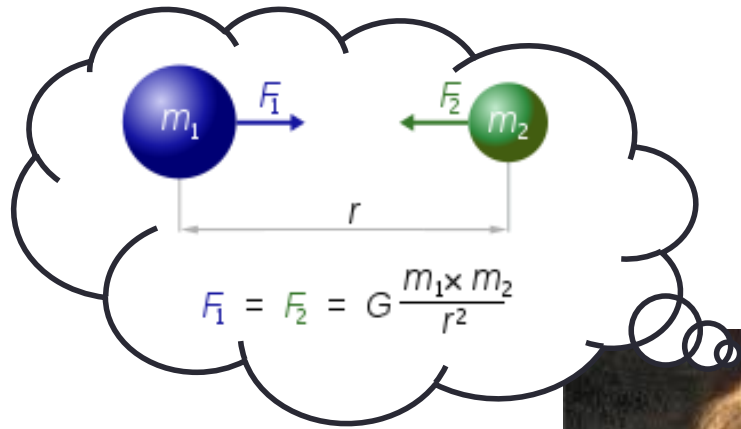


# Apples to Cards

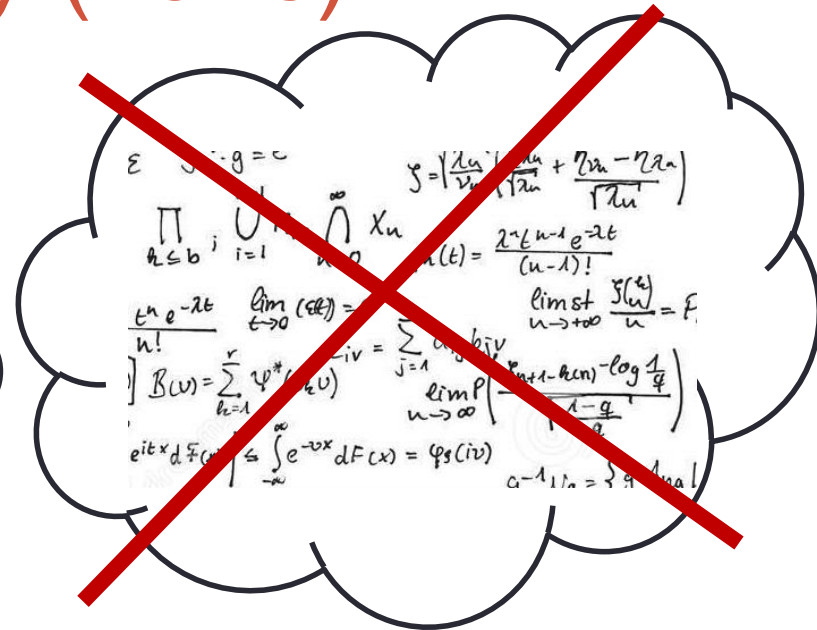




# Deterministic Modeling



# The Monte Carlo Way (1946)



# The Monte Carlo Way



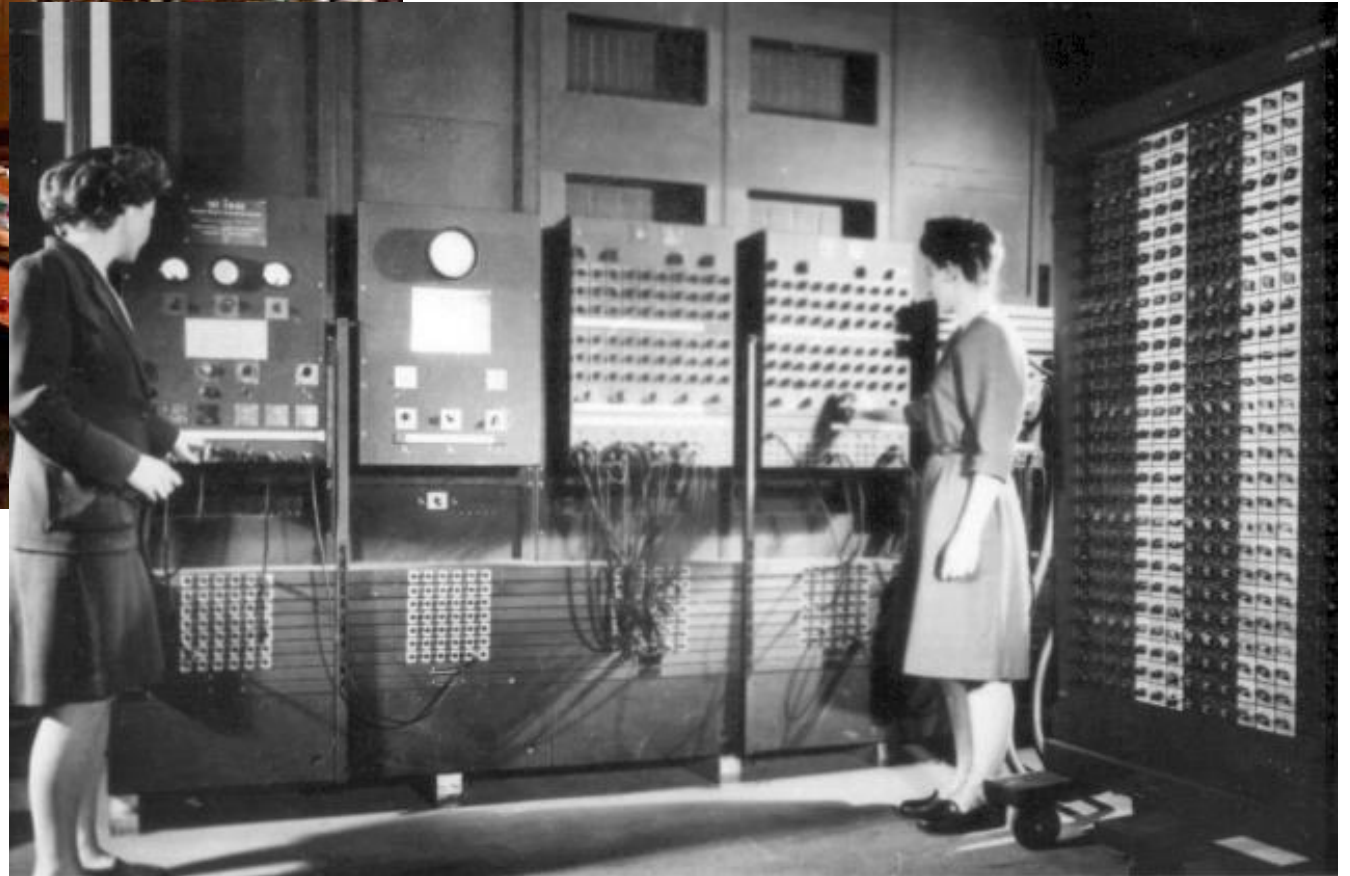
Just do it!

# The Isaac Newton of Monte Carlo



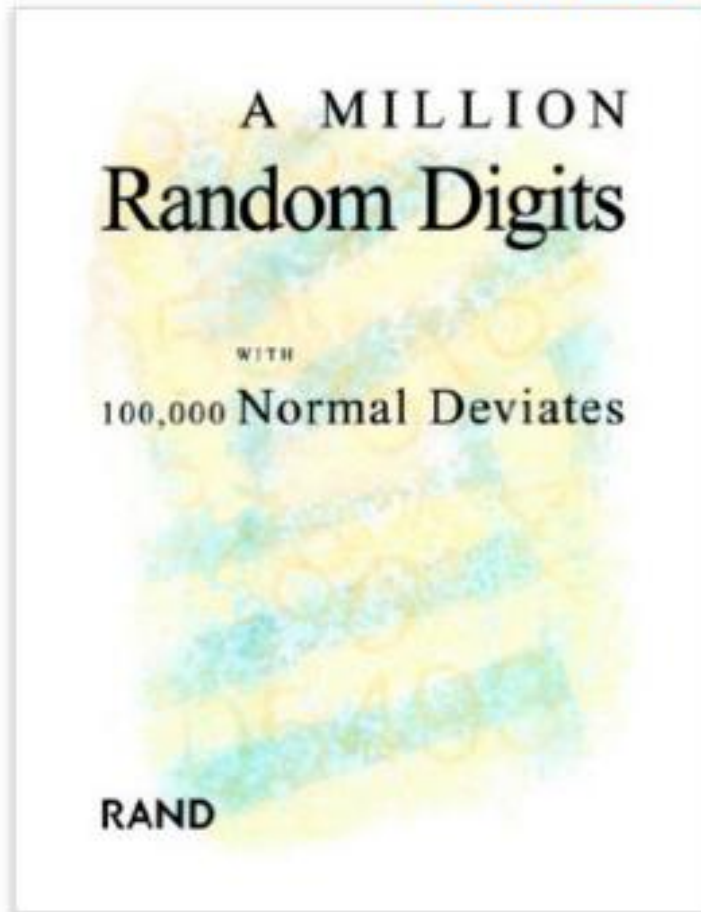
- Stanislaw Ulam
- 13 April 1909 – 13 May 1984
- Polish-American mathematician
- Spend 1936-1939 in Harvard  
working on ergodic theory
- Worked later on Manhattan Project
- Teller-Ulam design is the basis for  
all thermonuclear weapons

# Code Name Monte Carlo



# Valuable Random Numbers

Look inside ↴





# Valuable Random Numbers

LOOK INSIDE!

Kindle Book

Print Book

Zoom - Zoom +



A Million Random Digits  
with 100,000 Normal D...  
(Paperback)  
by The RAND  
Corporation

★★★★☆ (632)

Paperback **\$51.38**

Add to Cart

24 used & new from **\$51.38**

Book sections

Front Cover

Copyright

Table of Contents

First Pages

Back Cover

Surprise Me!

Search Inside This Book



Sample searches in this book:

digit table

normal deviates

random digits

00047 11884 43883 52079 84827 59381 71539 09973 33440 88461 23356  
00048 48324 77928 31249 64710 02295 36870 32307 57546 15020 09994  
00049 69074 94138 87637 91976 35584 04401 10518 21615 01848 76938

Copyrighted Material

Copyrighted Material

2

TABLE OF RANDOM DIGITS

00050	09188	20097	32825	39527	04220	86304	83389	87374	64278	58044
00051	90045	85497	51981	50654	94938	81997	91870	76150	68476	64659
00052	73189	50207	47677	26269	62290	64464	27124	67018	41361	82760
00053	75768	76490	20971	87749	90429	12272	95375	05871	93823	43178
00054	54016	44056	66281	31003	00682	27398	20714	53295	07706	17813
00055	08358	69910	78542	42785	13661	58873	04618	97553	31223	08420
00056	28306	03264	81333	10591	40510	07893	32604	60475	94119	01840
00057	53840	86233	81594	13628	51215	90290	28466	68795	77762	20791
00058	91757	53741	61613	62269	50263	90212	55781	76514	83483	47055
00059	89415	92694	00397	58391	12607	17646	48949	72306	94541	37408
00060	77513	03820	86864	29901	68414	82774	51908	13980	72893	55507
00061	19502	37174	69979	20288	55210	29773	74287	75251	65344	67415
00062	21818	59313	93278	81757	05686	73156	07082	85046	31853	38452
00063	51474	66499	68107	23621	94049	91345	42836	09191	08007	45449
00064	99559	68331	62535	24170	69777	12830	74819	78142	43860	72834
00065	33713	48007	93584	72869	51926	64721	58303	29822	93174	93972
00066	85274	66893	11303	22970	28834	34137	73515	90400	71148	43643
00067	84133	89640	44035	52166	73852	70091	61222	60561	62327	18423
00068	56732	16234	17395	96131	10123	91622	85496	57560	81604	18880
00069	65138	56806	87648	85261	34313	65861	45875	21069	85644	47277
00070	38001	02176	81719	11711	71602	92937	74219	64049	65584	49698
00071	37402	96397	01304	77586	56271	10086	47324	62605	40030	37438
00072	97125	40348	87083	31417	21815	39250	75237	62047	15501	29578
00073	21826	41134	47143	34072	64638	85902	49139	06441	03856	54552
00074	73135	42742	95719	09035	85794	74296	08789	88156	64691	19202
00075	07638	77929	03061	18072	96207	44156	23821	99538	04713	66994
00076	60528	83441	07954	19814	59175	20695	05533	52139	61212	06455
00077	83596	35655	06958	92983	05128	09719	77433	53783	92301	50498
00078	10850	62746	99599	10507	13499	06319	53075	71839	06410	19362
00079	39820	98952	43622	63147	64421	80814	43800	09351	31024	73167
00080	59580	06478	75569	78800	88835	54486	23768	06156	04111	08408
00081	38508	07341	23793	48763	90822	87022	17719	04207	95954	49953
00082	30692	70668	94688	16127	56196	80091	82067	63400	05462	69200
00083	65443	95659	18288	27437	49632	24041	08337	65676	36299	90836
00084	27767	50264	13192	72294	07477	44606	17985	48911	97341	30358

# Valuable Random Numbers

## Most Helpful Customer Reviews

1,687 of 1,726 people found the following review helpful

★★★★☆ **almost perfect**

By [a curious reader](#) on October 26, 2006

Format: Paperback

Such a terrific reference work! But with so many terrific random digits, it's a shame they didn't sort them, to make it easier to find the one you're looking for.

[40 Comments](#) | Was this review helpful to you?   [Report abuse](#)

734 of 750 people found the following review helpful

★★★★☆ **Wait for the audiobook version**

By [R. Rosini](#) on October 19, 2006

Format: Paperback

While the printed version is good, I would have expected the publisher to have an audiobook version as well. A perfect companion for one's Ipod.

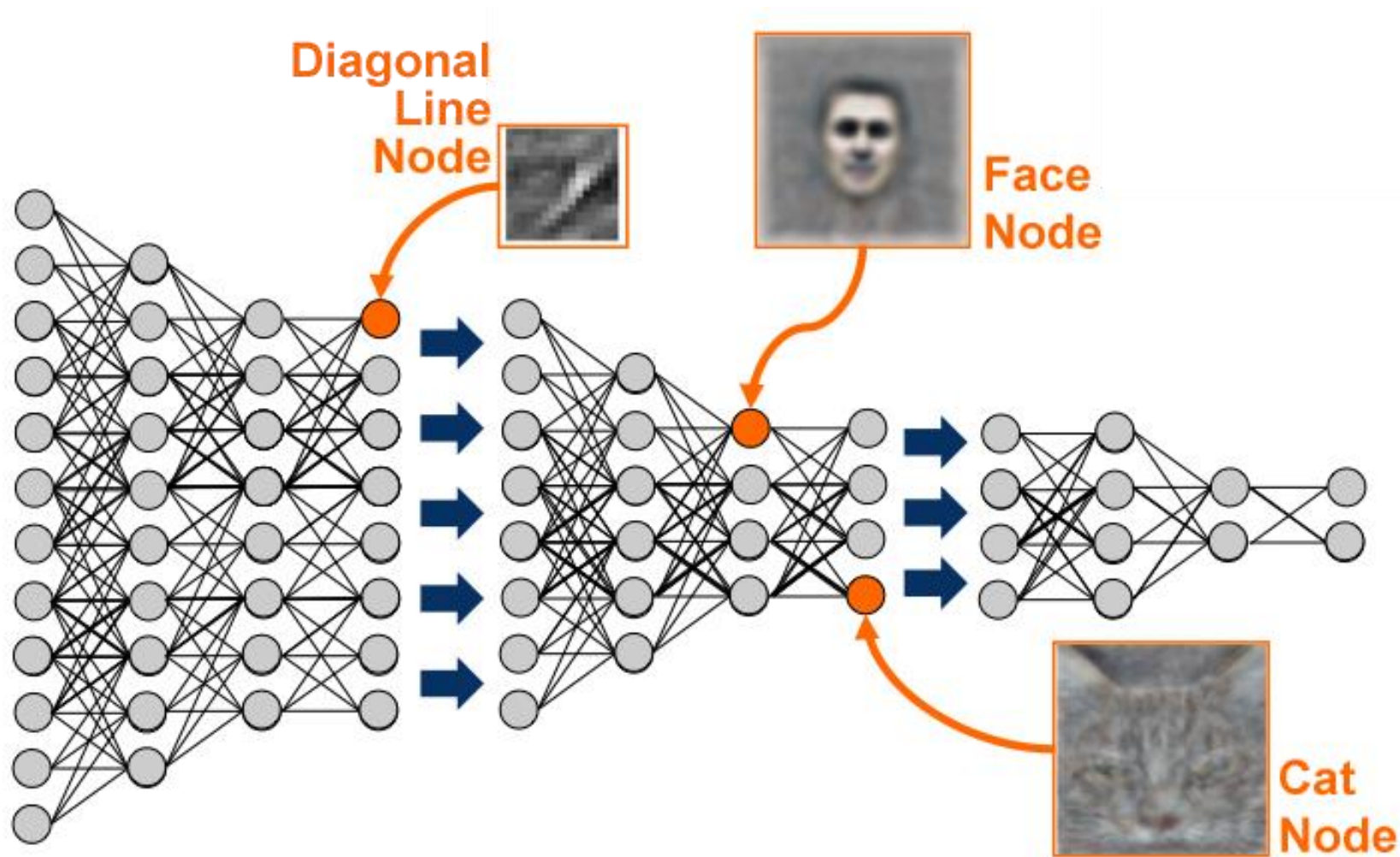
[4 Comments](#) | Was this review helpful to you?   [Report abuse](#)



# Monte Carlo Applications

- Model evolution of galaxies
- Weather forecasting
- Predict energy output of a wind farm
- Wireless network panning
- Computational biology (Bayesian inference in phylogeny)
- Computer graphics: 3D rendering by random ray tracing
- Game AIs (Monte Carlo tree search)

# Stochastic Optimization - Deep Learning



# What - Course Schedule

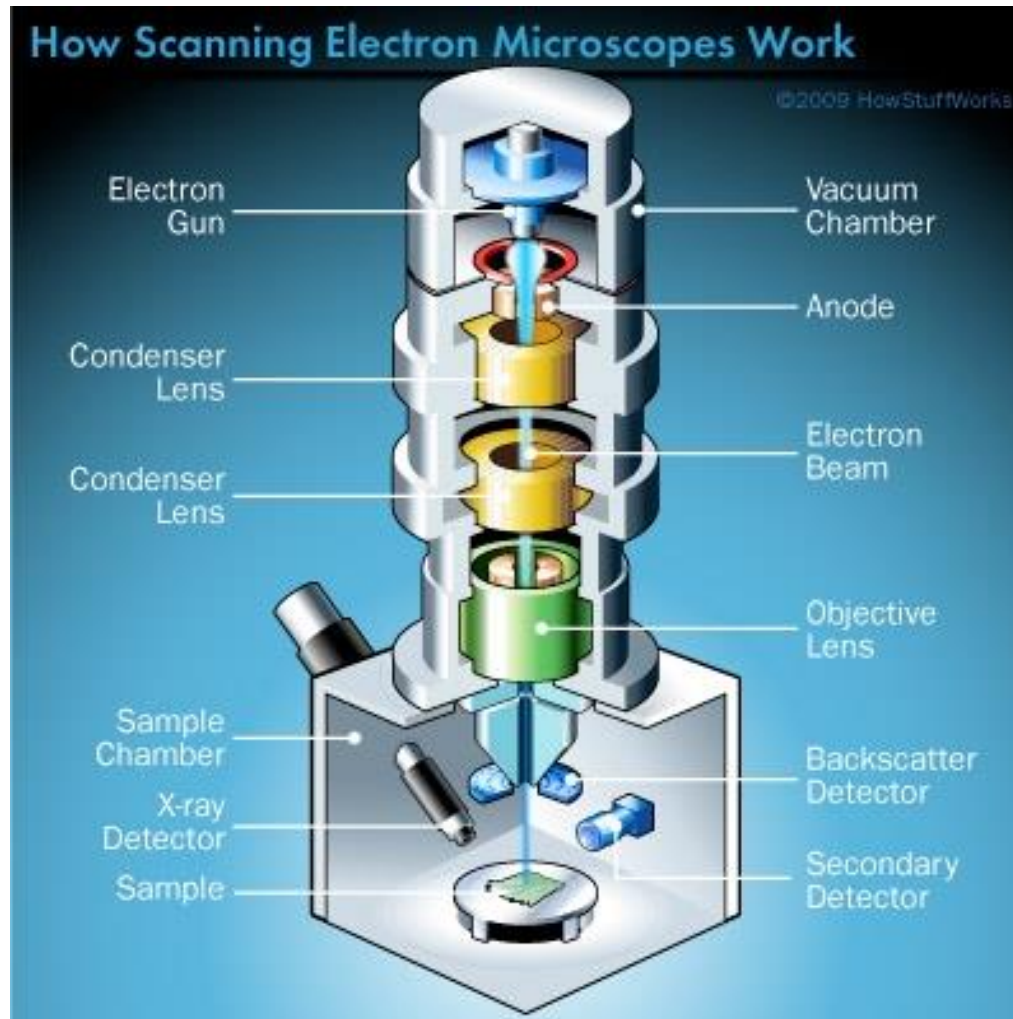
## Five Modules:

- Monte Carlo integration and variance reduction
- Bayesian inference
- Stochastic optimization
- Time series
- Advanced methods

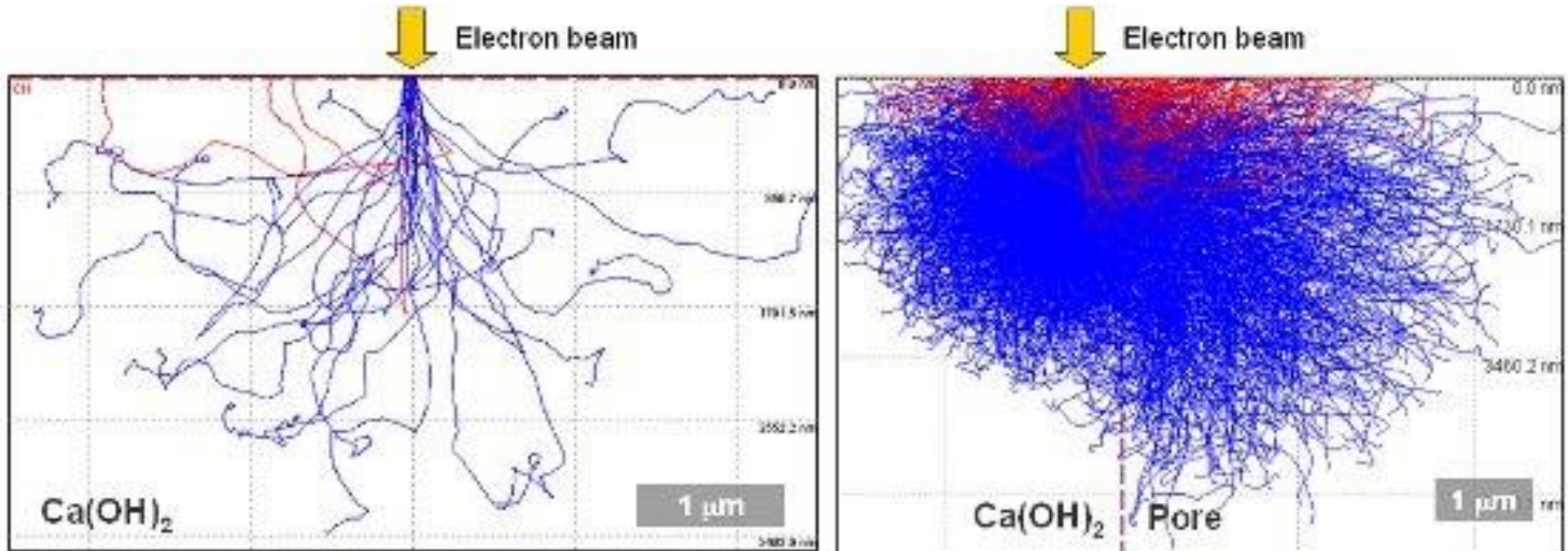
# Course Schedule

- <http://am207.github.io/2016/pages/schedule.html>

# Scanning Electron Microscope



# Electron Beam – Sample Interaction



Monte-Carlo simulation of electron-sample interaction in a solid phase and across a pore boundary. Each electron is followed until it is either backscattered (red) or loses all of its energy (blue)

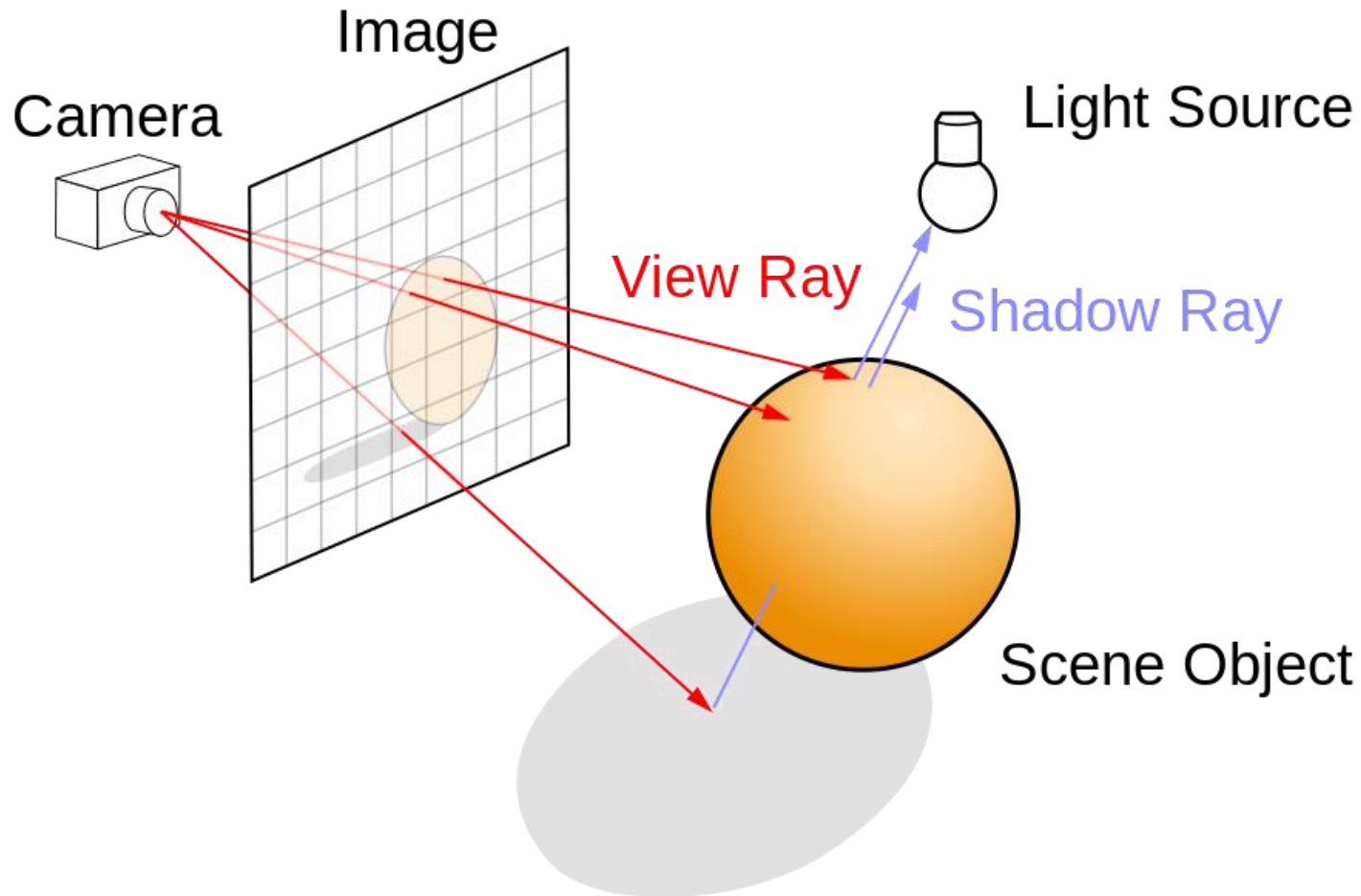
<http://www3.imperial.ac.uk/portal/page/portallive/concretedurability/researchprojects/porestructureanalysis>



# Monte Carlo Integration – Ray tracing



# Ray Tracing





# Importance Sampling



ray\_tracing\_importance\_sampling.mp4

<https://www.youtube.com/watch?v=mYMkAnm-PWw>

# Bayesian Inference

USS *Scorpion* (SSN-589)



[https://en.wikipedia.org/wiki/USS\\_Scorpion\\_\(SSN-589\)](https://en.wikipedia.org/wiki/USS_Scorpion_(SSN-589))

# Bayesian Inference



Bayesian\_search.mp4

<https://www.youtube.com/watch?v=U9-G-noZrwc>

# Stochastic Optimization



Traveling\_salesman.mp4

<https://www.youtube.com/watch?v=SC5CX8drAtU>

# Gaussian Process Inpainting



GP\_inpainting.mp4

<https://www.youtube.com/watch?v=8vIZnWKV8zw>

# Who

- Verena Kaynig-Fittkau
- Pavlos Protopapas
- Wei Dai
- Rafael Martinez Galarza
- Giri Gopalan
- Alexander Isakov
- Richard Kim
- Steve Klosterman
- Xide Xia

# Verena Kaynig-Fittkau

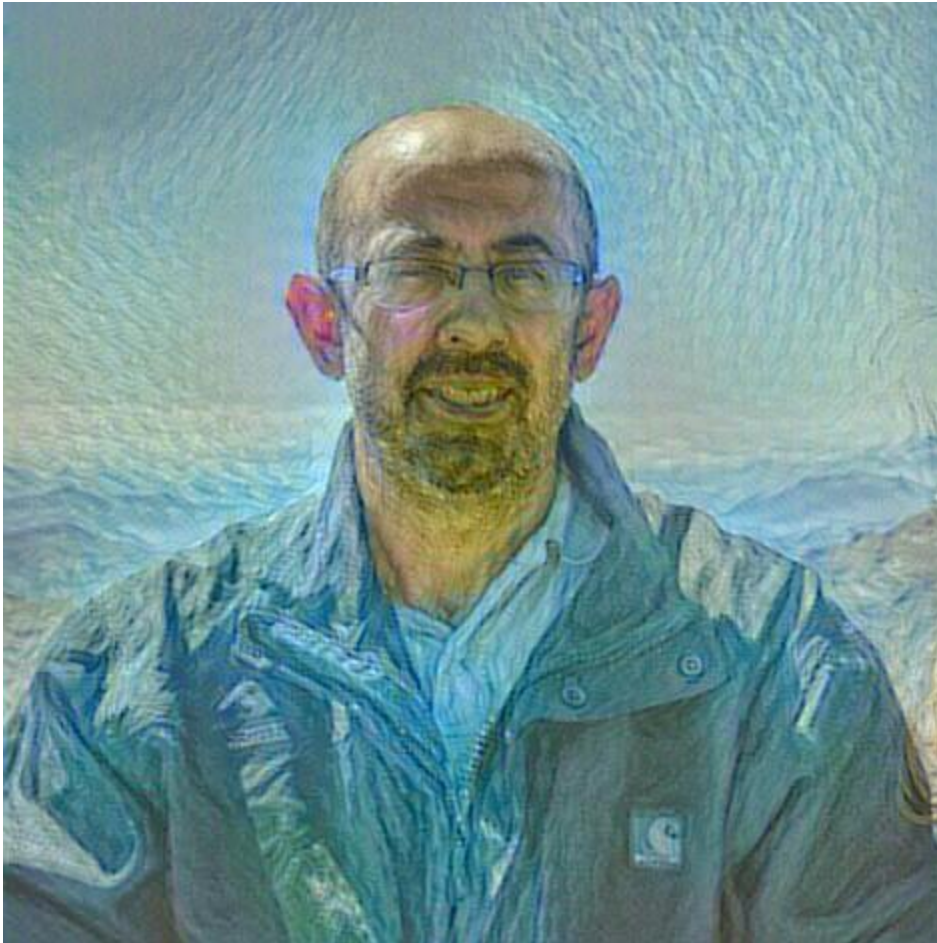


Lecturer and research scientist  
at IACS

NW B164 or 235.1

[vkaynig@seas.harvard.edu](mailto:vkaynig@seas.harvard.edu)

# Pavlos Protopapas



Scientific Program Director  
and Lecturer at IACS

NW B155

[pavlos@seas.harvard.edu](mailto:pavlos@seas.harvard.edu)



# Rafael Martinez Galarza



Postdoctoral fellow at the Harvard-Smithsonian Center for Astrophysics.

Research interest: infrared studies of galactic and extra-galactic star-forming regions, stochastic optimization.

He likes to sail on the Charles and is also interested in artificial intelligence. He is a volunteer for the Future of Life Institute.

# Wei Dai



G2 master student in Computational Science and Engineering

Master Thesis on High Frequency Market Beta Using HMM Model

I Love Mexican food.

# Giri Gopalan



Giri is a researcher interested in applications of Monte Carlo to science and engineering with a background in applied and computational mathematics and statistics.

# Alexander Isakov



Alexander Isakov is a 5<sup>th</sup> year PhD student in the Department of Physics. His work focuses mainly on behavior on networks, including synchronization or cooperation on networks. He has reached frequently for some of the tools in the toolbox AM207 provides (especially the optimization component), and hopes you enjoy the course!



# Richard Kim



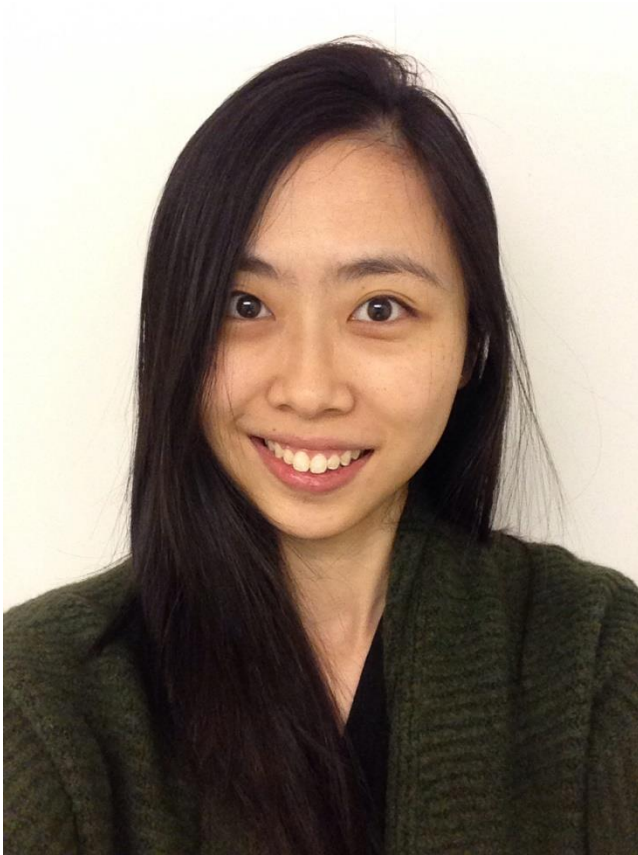
- - I am a Harvard Extension School graduate student pursuing the master's degree in Information Technology with concentration in Mathematics & Computations.
- - Prior to coming back to school, I worked as an investment banking analyst and equity research analyst for approximately 6 years. I am also a Chartered Financial Analyst (CFA).
- - I went to work in Tokyo, Japan for 3 years after graduating from UCLA with BA in Economics.

# Steve Klosterman



Steve is a 5th year PhD student in Organismic and Evolutionary Biology. His research focuses on the interaction between plant life cycle events and climate change.

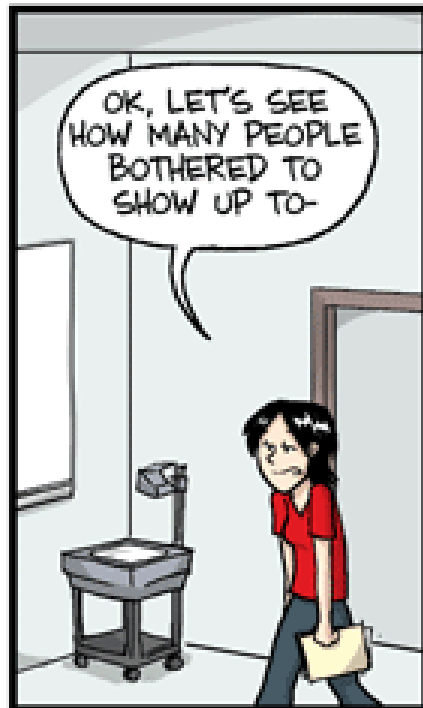
# Xide Xia



Hi! My name is Xide Xia. I am a second-year ME student in the Computational Science and Engineering program at Harvard. My academic interests broadly include machine learning, artificial intelligence, and data science. AM207 is a great course and you will love it. Looking forward to working with you all!

# How

- Lecture
- Lab
- Homework
- Office hours
- Piazza
- Final project





# Lab

- Fridays 2-4 pm
- Cruft 309
- Homework comes out on Thursdays
- This is your large office hour before the weekend!
- Meant to give you a good start

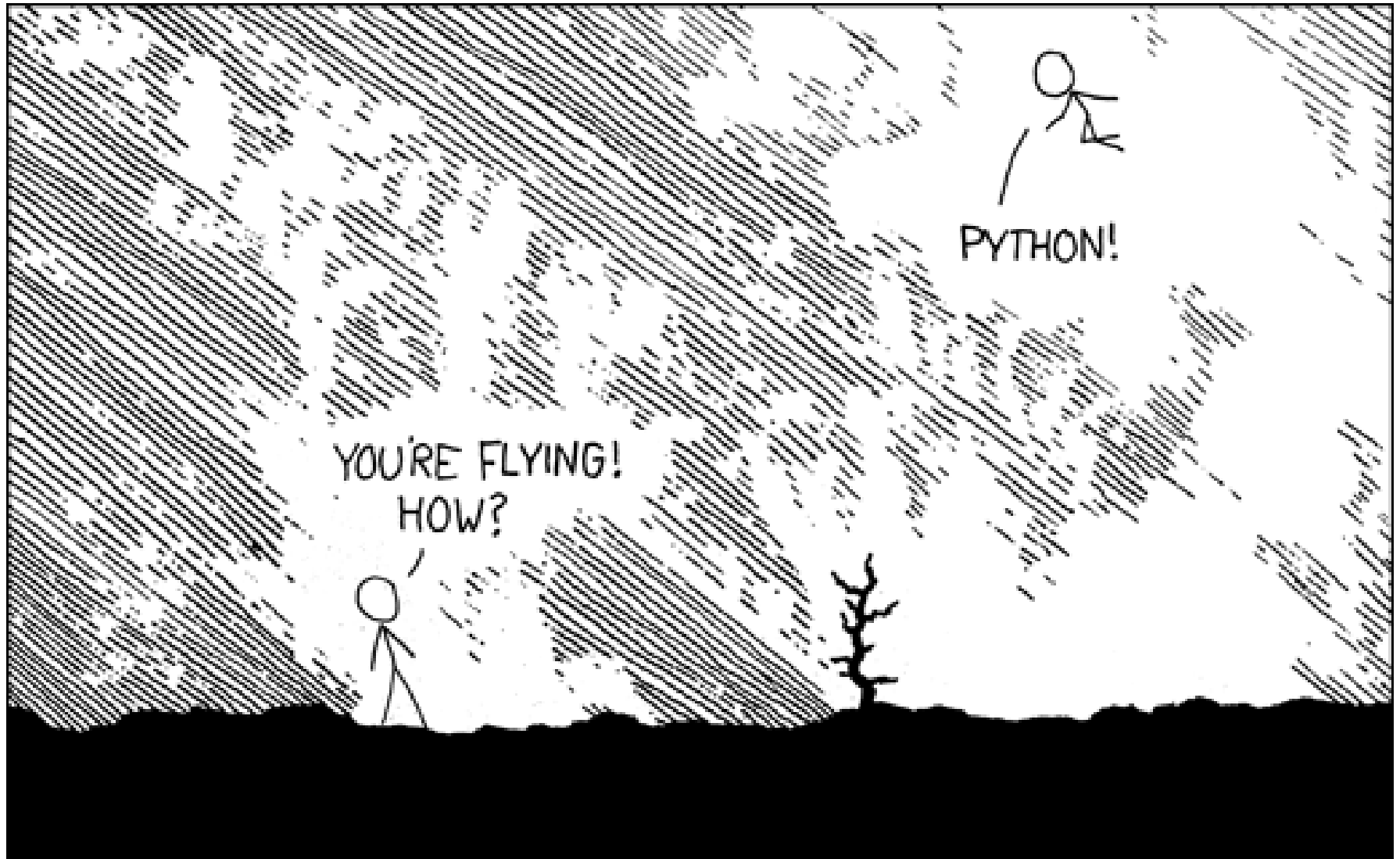
# Homework

- 5 assignments
- Out: Thursday evening
- Due: Two weeks later on Thursday
- Late days:
  - May use up to 2 per assignment
  - Not more than 6 total
  - Otherwise we deduct points
- Canvas:
  - Folders are timed
  - Might close few minutes early
  - **It is your responsibility to be on time!**

# Homework

- 55% of your grade
- Work you submit must be your own! Discuss in groups, program / write on your own
- Please see also guidelines on the webpage
- Jupyter notebooks
- **Treat them as reports, not only as code!**
- **HW0 comes out today**, not graded, but do submit!
- We want to make sure everything works for you

# Python



# Python Resources

- Google is your best friend
- Really.. try googling: length of a list in python
- Stackoverflow
- Enthought training in python with academic license:
- <https://training.enthought.com/courses>

# Grading

5 = Exceptional / above and beyond

4 = Solid / no mistakes (or really minor)

3 = Good / some mistakes

2 = Fair / some major conceptual errors

1 = Poor / did not finish?

0 = Did not participate / did not hand in

Grading is holistic, not subtract half a point here, half a point there, its about the learning process.

# Piazza

- This is a very valuable resource, ask, and save time, answer and show off!
- Let's apply Stackoverflow rules
- Counts as participation
- Participation is 5% of your final grade





# Final Project

- Your chance to show off what you learned
- 3-4 person teams!
- Hand-ins:
  - written paper ( $\leq 6$  pages)
  - screencast
  - poster
- 40% of your grade

# Is This Course For Me?

- Fond of math and statistics
- Basic statistical knowledge
- There is going to be magic and beauty!
- Basic background in programming
- Python knowledge helps
- Willing to learn new software and tools
- Read online documentation
- This can be time consuming



Be constructive

Be proactive

Be patient




# HWO

- Out this afternoon
- Not graded, but you should submit!
- General Python setup
- Make sure all works!
- Some first exercises




# Github

- All materials are in the github repository
- <https://github.com/AM207/2016>
- Just pull to get lecture notes, extra material, and homework assignments
- If you don't feel comfortable with git you can also download them from the webpage.

# Github

 This repository Search

Pull requests Issues Gist

AM207 / 2016

Unwatch 4 Star 0 Fork 0



<> Code Issues 0 Pull requests 0 Wiki Pulse Graphs Settings


No description or website provided. — Edit



3 commits 2 branches 0 releases 1 contributor

Branch: master New pull request

New file Find file HTTPS https://github.com/AM207/

  Download ZIP

 vkaynig readme Latest commit 2c6c7be on Nov 16, 2015

 _site	readme	2 months ago
 README.md	Updated readme	2 months ago

README.md

## AM207 2016

You find all public material for AM207 in this GitHub repository.

# Office Hours

Xide	Mon 10am-11am
Steve	Mon 3pm - 4pm
Giri	Monday 7-8pm
Rafael	Tuesday 2pm-3pm
Richard	Thur 4pm-5pm
Wei	Friday 11am-noon
Alex	Friday 6pm-7pm

**Also Lab starts this Friday!**



# Next Steps

- Register for Piazza
- Follow setup instructions in HW0
- Run HW0 notebook on your machine
- Solve what you would like to solve
- Submit HW0

# Questions?