Last Lecture

Advanced Machine Learning
Data Mining &
Artificial Intelligence
CSCI E-82
Fall 2018

Peter V. Henstock



Aggressive agenda tonight

- Eliud: perspective on NIPS
- HW6 discussion
- Brief intro to RL
 - Last two topic presentations on RL
 - Gerald Pho's application of RL to neurosci
- 1 final presentation
- Course wrap-up
 - Peter's Top 10 List for what's next in Al
 - Course survey
 - Conclusion

Types of Machine Learning

- Unsupervised
 - · Clustering, PCA, etc.
 - Provide data without labels
- Supervised
 - Classification, regression
 - Provide data with labels
- Semi-Supervised
 - Classification but leverage clusters or distributions of unlabeled data
 - Provide data with some labels
- Reinforcement Learning
 - Choose best actions but find your own labels

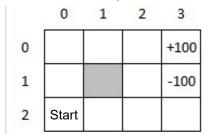
Reinforcement Learning

- 1) Deterministic Search
- 2) Markov Decision Process
- 3) Reinforcement Learning

1) [Deterministic] Search

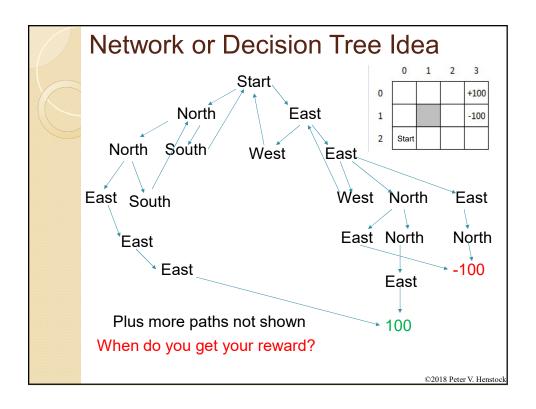
Example: "Grid World" Maze problem

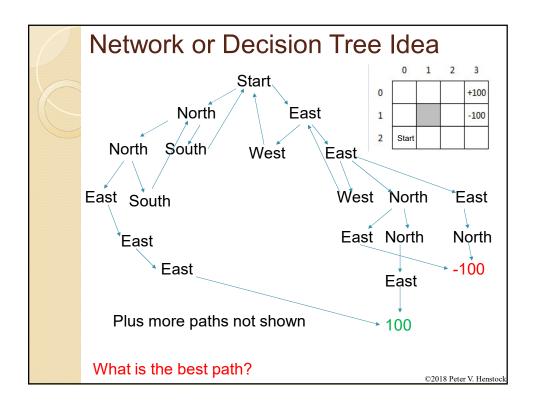
- Find the path to maximize reward
- Run multiple approaches = search
- Answer: shortest path & max reward

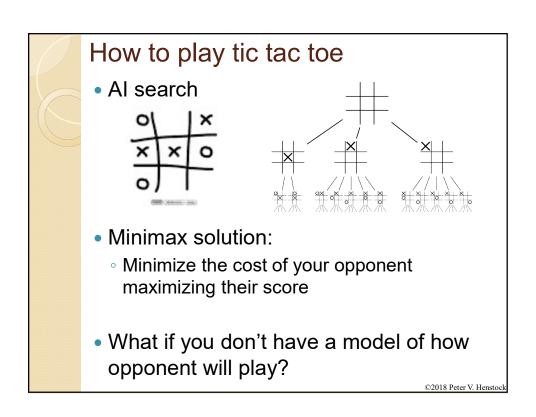


- How would you solve this?
- What would a solution look like? #steps?

https://galweejit.wordpress.com/2010/12/16/ai-class-implementation-of-mdp-grid-world-from-week-5-unit-9/











Solution for Traditional Al

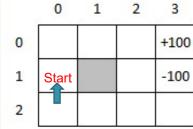
- Define heuristic measures
 - Create a quantitative score that encourages the algorithm to make good choices
 - 2 in a row → 10
 - Blocking 3 in a row → 20
 - Block 3 in a row and getting 2 in a row 30
 - Middle edge → 5
 - · Corner → 7
- Use search to find efficient algorithms
 - A* heuristic search
 - AO* heuristic search

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[Deterministic] Search

Example: "Grid World" Maze problem

- Find the path to maximize reward
- Run multiple approaches = search
- Answer: shortest path & max reward



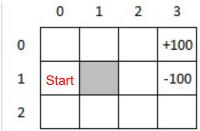
https://galweejit.wordpress.com/2010/12/16/ai-class-implementation-of-mdp-grid-world-from-week-5-unit-9/

• How would it change the problem?

[Deterministic] Search

Example: "Grid World" Maze problem

- Find the path to maximize reward
- Run multiple approaches = search
- Answer: shortest path & max reward



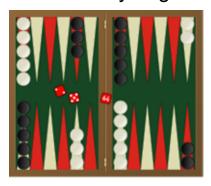
https://galweejit.wordpress.com/2010/12/16/ai-class-implementation-of-mdp-grid-world-from-week-5-unit-9/

- Add -5 reward per step
- How would it change the problem?

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Timing of the Rewards

• When do you get the rewards?

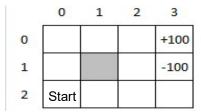




- Which is worth more:
 - 3% bond due in 5 years
 - 3% bond due in 25 years
- Discounted future rewards

2) Non-Deterministic Search

- Same input → different behaviors
- Standard: probabilistic algorithm
- Example: "Grid World" Maze problem
 - 80% of time action as expected (N,S,E,W)
 - 10% of time: 90° clockwise of target
 - 10% of time: 90° counter-clockwise of target



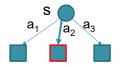
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Process of switching states

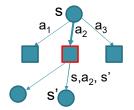
Q-state is

State is





- Start in state s
- Choose an action a₂ that takes you to a "Q-state"
- Randomness shows transition to state s'



• (s,a₂,s') is a "move"

Markov Decision Process

- · Framework using probabilities to optimize
- Take allowed actions from state s → s'
- Get a reward for taking certain actions
- Set of states $s \in S$
- Set of actions a ∈ A
- Reward function R(s, a, s')
 - Utility = Σ rewards
- Transition function T(s, a, s')
 - Model of the world or probability
- Why is it a Markov Decision Process?

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Markov Decision Process

- Why is it a Markov Decision Process?
 - s' depends only on previous state s and action a and not all earlier states/actions

$$P(s' | s, a) =$$

$$= P(S_{t+1} = s_{t+1}' | S_t = s_t, A_t = a_{t,}$$

$$S_{t-1} = s_{t-1}, A_{t-1} = a_{t-1,}$$

$$S_{t-2} = s_{t-2}, A_{t-2} = a_{t-2,...}$$

Because it's Markov…

=
$$P(S_{t+1} = s_{t+1})' | S_t = s_t, A_t = a_t)$$

Solving MDP problems

Several related problems as solutions

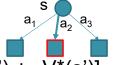
- Assess value of being in a given state based on future rewards
- Assess the future [discounted] rewards from taking a given action from a given state
- Finding optimal actions or policies

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Recursive Optimization

$$V^*(s) = max_a Q^*(s,a)$$

∘ q-state is **g** state is **d**

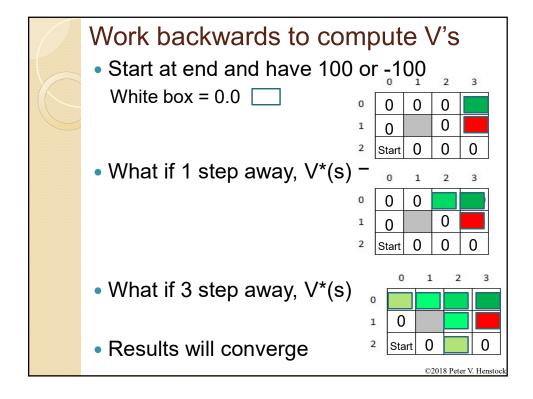


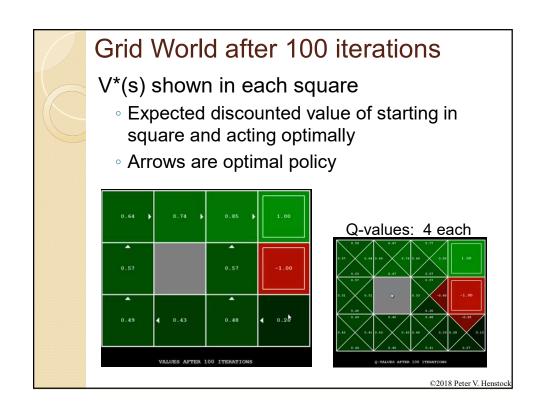
$$Q^*(s,a) = \Sigma_{s'}T(s,a,s')[R(s,a,s') + \gamma V^*(s')]$$

- Average over all children s'
- Prob of given s' = Transition function

Start off $V^*(s) = 0 \& iterate$

 $V^*(s) = \max_{a} \sum_{s'} T(s,a,s') [R(s,a,s') + \gamma V^*(s')]$ $V_{k+1}(s) = \max_{a} \sum_{s'} T(s,a,s') [R(s,a,s') + \gamma V_{k}(s')]$





MDP ideas

- Started off with an MDP game rule with the stochastic process
 - Compute Value of each state
 - Compute policies of each state
- What if don't know what the transition probabilities are?
- What if don't know reward function?
 - We'd have to learn these
- How would you learn these?

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Reinforcement Learning



- Environment has states s ∈ S
- Agent makes actions a ∈ A
- Rewards r ∈ R possibly for each action
- Markov assumption P(s_{t+1} | s_t, a_t)
 - Next state depends only on previous state and the action from that state to next
- Don't know T or R but do exist as MDP

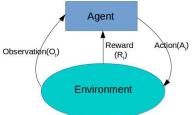
Parts of Reinforcement Learning

- Observations
- Observations
- Agent

Action

Feedback

Gender, age, disease, etc.



- Example:
- Web page, ad, treatments
- Show which ads to which users
 - Goal: maximize profit
- Treat patients using different medicines
 - · Maximize patient quality of life

https://becominghuman.ai/components-of-an-rl-agent-and-its-application-on-snake-1b3b6c8e1de5

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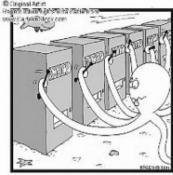
iRobot Roomba Bedford, MA



- Goal = clean my house
- Explore: doesn't know how many rooms
- Exploit: has to clean the full space
- Constraint: limited power → recharge

N-Armed Bandit Problem

- Goal is maximize \$
- 1000 actions
- Slot with N levers
- Maximize return



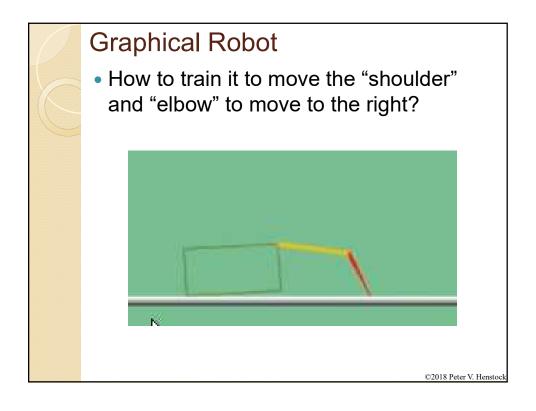
http://www.socsci.uci.edu/~szhang/pics/gamble.ips

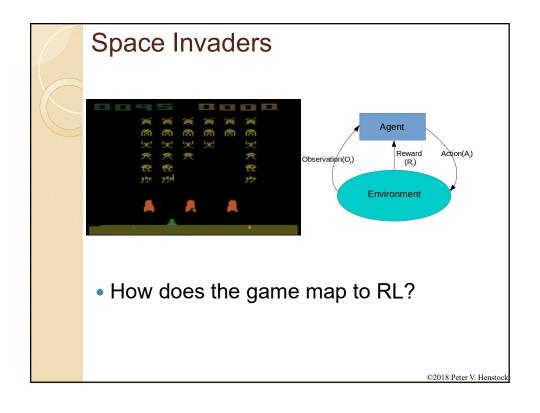
- Doctor has sick patients
- Doctor has multiple treatment options
- Reward is successful treatment or survival of patients

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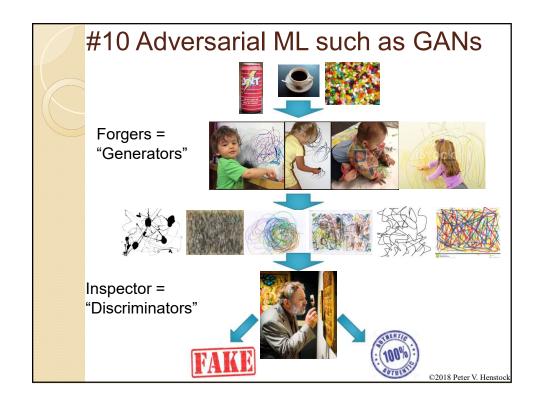
Concept of Reinforcement Learning

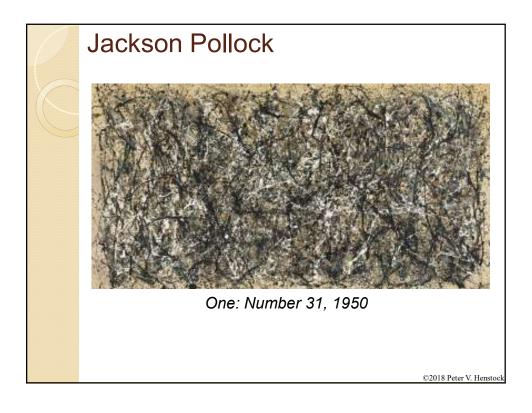
- Builds a model of its environment
 - May choose many bad paths in the process
 - Learns the transition state probabilities
 - Learns rewards
- Strategies in play (Q-learning)
 - Exploration (small probability)
 - Exploitation (large probability)
- Advantage:
 - Gathers own data and teaches itself

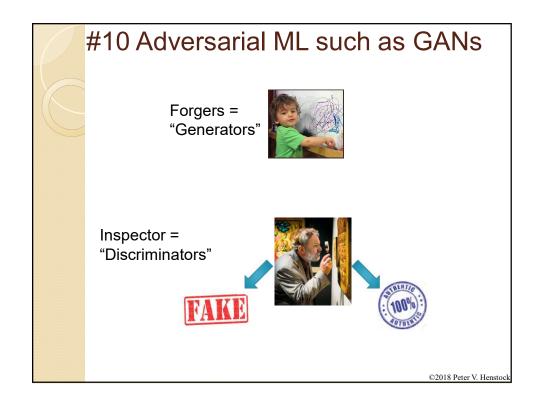


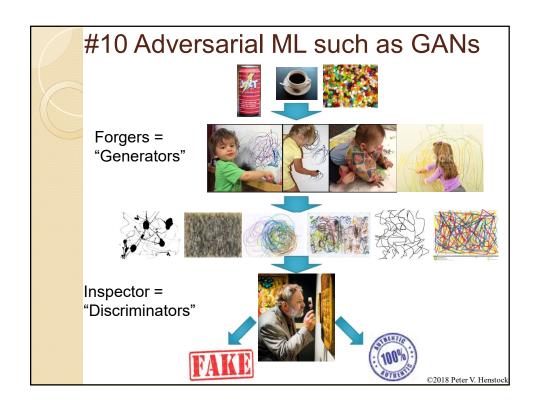








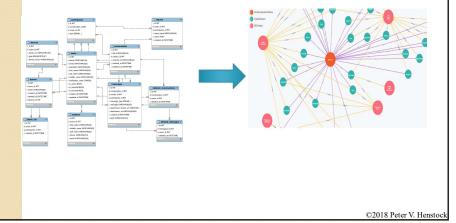






Peter's Upcoming ML/DM/AI Trends

- 10) Further adversarial networks
- 9) Reinforcement Learning on the rise
- 8) Graphs & more flexible data models



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- 7) Push for both open-source & IP

Open-Source

- High quality open-source tools for machine learning & data mining
- Google, Facebook and universities release all their solutions
- Al vendors incorporate the latest tools
 - RapidMiner, H2O, Datalku, Weka
 - DataBricks, Hadoop, etc.
 - IBM

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Who Owns the Intellectual Property?

- Small companies are not leading
- Google, Microsoft, Uber, Baidu, Facebook, Didi are leading
 - Hiring the top talent
 - Collaborating with top universities
 - Patenting the latest scalable technologies
- Difficult to maintain talent
- Difficult to compete against giants
- Multitude of problems to solve

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- 5) Interpretability & Accuracy

Cassandra

- Apollo gave her ability to create prophecies in order to seduce her
- She refused
- Apollo cursed her so that no one would ever believe her
- ML/Al has this problem



Cassandra by Evelyn De Morgan (1898, London);

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Rule of 5

- Set of rules for predicting bioavailability of small molecules in humans from few thousand drug candidates
- Poor viability if:
 - Molecular Weight > 500
 - More than 5 H-bond donors
 - More than 10 H-bond acceptors
 - ∘ cLogP > 5
- What do you think of this model?

10 year Risk Coronary Heart Disease http://www.qrisk.org/ Age (25-84): 64 Male Female Sex: White or not stated ▼ Ethnicity: UK postcode: leave blank if unknown Postcode: Smoking status: non-smoker Diabetes status: none ▼ Angina or heart attack in a 1st degree relative < 60? Chronic kidney disease (stage 4 or 5)? Atrial fibrillation? On blood pressure treatment? Rheumatoid arthritis? Leave blank if unknown Cholesterol/HDL ratio: Systolic blood pressure (mmHg): -Body mass index-Height (cm): Weight (kg): Calculate risk over 10 ▼ vears. Calculate risk ©2018 Peter V. Henstock

Emergency Room Protocol

- 10 year risk of coronary heart disease
- Ask patients 5 questions
- Count up scores and get a decision
- Two possibilities:
 - Model came from doctors
 - Model came from machine learning
- Which would you prefer?

Case Study

Intelligible Models for HealthCare: Predicting Pneumonia Risk and Hospital 30-day Readmission

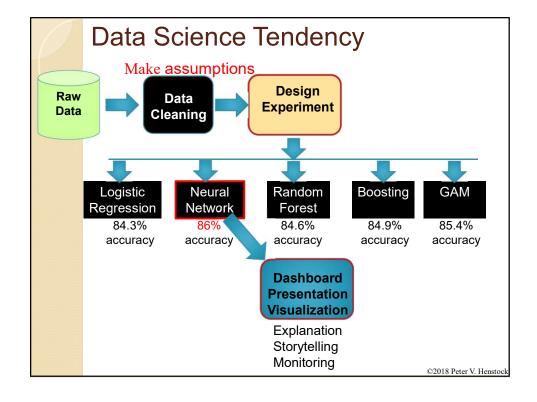
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Paul Koch
Microsoft Research
Paulkoch@microsoft.com

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Noémie Elhadad Columbia University noemie.elhadad@columbia.edu

- Goal: To predict probability of death for patients with pneumonia
 - Use machine learning to identify risk
 - Admit high-risk patients to hospital
 - Treat low-risk patients as outpatient
- 9847 patient training set, 4352 test set
- 46 features: age, gender, heart rate, BP..

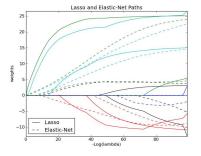


Findings Asthma patients → lower risk of death??? Chronic lung disease→lower risk of death??1 Chest pain history → lower risk of death??? Risk by Age 0.8 0.6 0.4 0.2 -0.250 60 70 80 30 40 90 age ©2018 Peter V. Henstock



Don't we have that already?

- Decision trees are most widely used mostly due to their interpretability
 - ID3
 - CART
 - o C5.0
- Lasso
 - Regression method
 - Regularization



http://jaquesgrobler.github.io/Online-Scikit-Learn-stat-tut/ images/plot lasso coordinate descent path 11.png

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Bayesian Rule List

- http://web.mit.edu/rudin/www/LethamRuMcMa12.pdf
- Probabilistic Classifier like CART
- User can specify: Number of rules
 - Conditions per rule
 - Priors of the output labels
- Steps
 - Mine data to come up with rules:
 - Apriori, FP Growth, decision tree, etc. if X → Y
 - Sample decision rule length~ Poisson(lambda)
 - Conditions ~ Poisson(eta)
 - Sample from rules that apply for conditions
 - Predict using first rule that applies from list Pater V. Henstock

Opposite Trends

- Deep Learning
 - State of the art algorithms
 - Training data added up to the limits of GPU and training time
 - Better decisions that no one can understand
- Trend toward Simplicity
 - Rule of 5 (Lipinski)
 - Emergency Room Protocol: Risk of heart disease
 - · Doctors: Ask 5 questions and count score
 - ML/AI: Ask questions and enter values to compute a correct interpretation

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- 5) Interpretability & Accuracy
- 4) Privacy, bias, and legal aspects

Data

- Currently every web site tracks us
 - How much longer do we allow this?
 - Who keeps our medical records? Blockchain
- Are our results biased?
 - Data collection methods are biased
 - How do we acknowledge, leverage & fix?
- Legal aspects of Al
 - If robots replace us, will they pay taxes?
 - Technology is not limiting self-driving cars
 - What does war look like with AI? Preventable?

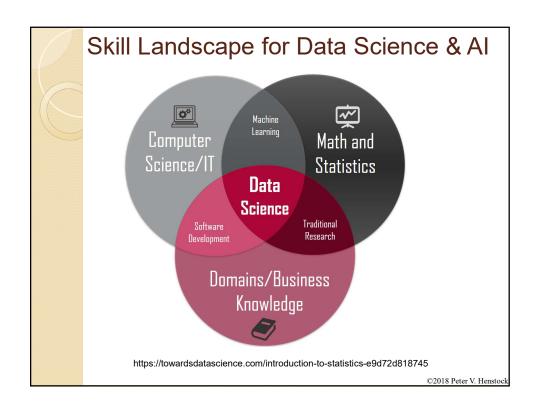
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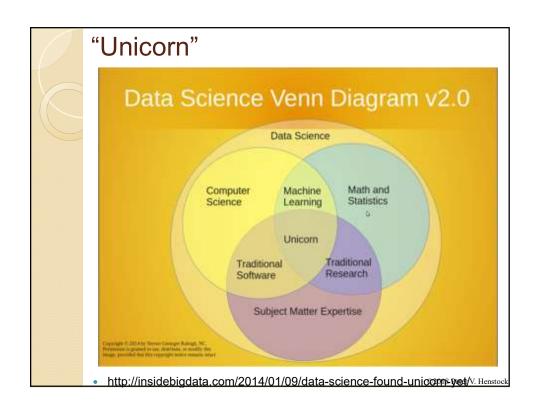
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- 4) Privacy, bias, and legal aspects
- 3) Shortage of Al talent in US









Strong Shift of Al Talent to Tech Industry

- "Tech giants are paying huge salaries for scarce Al Talent" -- NYT October 22, 2017
- "Carnegie Mellon reels after Uber lures away researchers" -- wsj November 21, 2018

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Scarcity of Talent

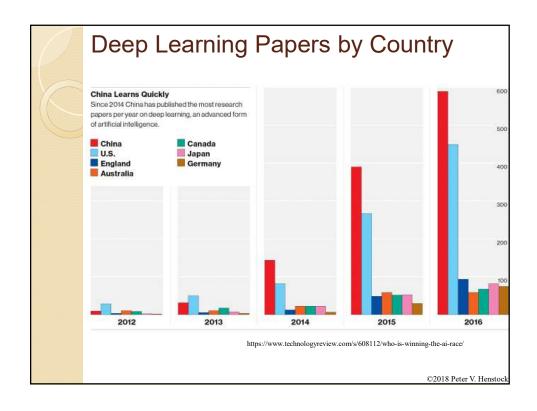
80% of machine learning engineers with PhDs are scooped up by Google and Facebook, especially if they have a patent.

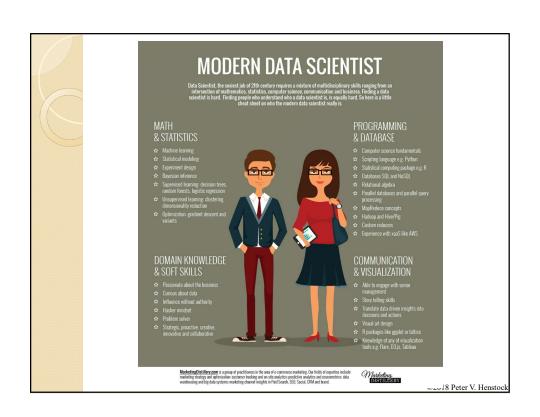
Forbes post: Gal Almog Feb 9, 2018

LinkedIn Jobs report:

6.5x growth in data science jobs from 2012-2017

https://www.kdnuggets.com/2018/09/how-many-data-scientists-are-there.html





Needed Skills

- What do you do when it doesn't work?
 - Machine learning
- Is machine learning the right approach?
 - Statistics can often provide a better method
- How do you avoid resolving it again?
 - Software engineering
 - Shortage of SWE who can do data science
 - Holding the field back
- Business knowledge

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Current need: data science

- Need in 2020 will be machine learning
- Data science algorithms have become quite accessible to everyone
 - ∘ Available on Oracle, python, R, Java, etc.
 - Many can push data through algorithms
- Competitive advantage of ML
 - How to go beyond the standard algorithms
 - What to do when the results are OK
 - How to achieve superior results

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- 2) Integration of approaches

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Pedro Domingos: U Washington 5 Tribes of Machine Learning (ACM) Where Does Knowledge Come From? Evolution Experience Culture Computers

5 Tribes of Machine Learning

- 1) Symbolists
- 2) Connectionists
- 3) Evolutionaries
- 4) Bayesians
- 5) Analogizers

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5 Tribes of Machine Learning

Tribe	Origins	Master Algorithm
Symbolists	Logic, philosophy	Inverse deduction
Connectionists	Neuroscience	Backpropagation
Evolutionaries	Evolutionary biology	Genetic programming
Bayesians	Statistics	Probabilistic inference
Analogizers	Psychology	Kernel machines

5 Tribes of Machine Learning

- 1) Symbolists: Use logic
 - Decision trees
- 2) Connectionists: model the brain
 - Neural networks
- 3) Evolutionaries: Nature's optimizations
 - Genetic algorithms/programming
- 4) Bayesians: Statistical inference
 - Naïve Bayes
 - Bayesian networks
 - Causal reasoning
- 5) Analogizers: Kernel machines
 - SVM as well as recommender systems, tenstock

5 tribes of machine learning

- So what?
- Currently each tribe is doing its own research independently
- Opportunity is for tribes to converge

State of the Art (Domingos)

- Representation
 - Probabilistic logic
 - First order logic ←→ graphical models
 - Markov logic networks attach weights to logic
 - Weighted formula: distribution over states
- Evaluation
 - Posterior probability
 - User-defined objective function
- Optimization
 - Formula discovery (genetic programming)
 - Weighted learning (backpropagation)

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- 1) Auto-ML

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- 7) Push for both open-source & IP
- 6) New deep learning architectures 5 yrs
- 5) Interpretability & Accuracy
- 4) Privacy, bias, and legal aspects
- 3) Shortage of AI talent
- 2) Integration of approaches
- 1) Auto-ML
- 0) Al everywhere

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IBM Commercials

- Watson predicts the weather
- Watson helps make our Olympians
- Watson cures cancer
- Watson solves education problems
- Watson learned to read and we sent it to medical school
- Watson designed this dress
- Watson raised the awareness of what Al can bring to the overall community

What area is next for AI?

- Al for data-driven decision making
 - When are you most efficient? What to do?
 - Scientific directions
 - Financial decisions
 - Political decisions
 - Legal decisions
 - Personal automated data-driven decision making

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What area is next for AI?

Your opinions?

What area is next for AI?

- Your opinions?
- Decision making
 - When are you most efficiencies? What to do?
 - Scientific directions
 - Financial decisions
 - Political decisions
 - Legal decisions
 - Personal automated data-driven decision making
 - Where does this leave your boss?

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Currently Data Science is hot

- Standard functionality
 - Can you move data and call functions?
 - Can you interpret the results?
- Better than nothing, but high school skill
- Can Al replace data science? AutoML
 - Data Robot, H2O.ai feature eng., Auto-sklearn
- Data science vs. Machine learning
 - "Machine learning is part of data science"
 - Sure, try to do data science w/o it

Course in Review

How do you measure a course?

- 600 email threads 850 emails
- Piazza:
 - 1057 total contributions
 - 221 instructor responses; 28 by students
 - 12 min. avg. response time
- 240 homework/exams/projects
- 37 paper summaries
- 17 student presentations + code sets
- 1866 lecture slides
- 12 quality section notebooks



Top 10 Data Mining Algorithms

- http://www.cs.uvm.edu/~icdm/algorithms/index.shtml
- Nice review paper: http://www.cs.uvm.edu/~icdm/algorithms/10Algorithms-08.pdf
- 2006 IEEE Data Mining Conference
- 1) C4.5
- 2) K-Means
- 3) Support Vector Machines
- 4) APRIORI
- 5) Expectation Maximization
- 6) PageRank
- 7) AdaBoost
- 8) K-Nearest Neighbors
- 9) Naïve Bayes
- 10) Classification and Regression Tree (CART)

	•		OVE		Johns Hopk							Courses		
Course Areas	Udacity	Udacity	Udacity	Udacity	coursera	Cluster		Text			Stanford		Harvard	Harvard
Course Areas			reinforcement		practical JH						Min Mass		CSCI E-181	
decision trees	x	unsupervised	remiorcement	X	X	Allalysis	Discovery	Netrievai	IVIL	ivedialive	X	X	C3C1 E-101	X
regression	X			X	×				x		^	^	x	^
classification	×			^	^				^			x	^	
neural networks	×									×		^	х	
instance based learning	×								^	^			^	
ensemble b&b	X											x		x
kernel methods and sym	×			x							x	^	x	×
computational learning theory	×			^					^		^	x	^	^
VC dimensions	x											x		
Bayesian learning	×													×
Bayesian inference	x											×		1.0
Naïve bayes	x											x		
clustering		×		x		×			x		x	x	x	
feature scaling		Y Y		x	x									
text learning				x								×		
feature selection		×		x										
pca				×					x	x	x		x	
evaluation metrics				×	×									
markov decision			x										x	
reinforcement			x										x	
game theory			x											
randomized optimization									x					
information theory		x										x		
boosting					×									
regularized					×								x	
EM						x						x	x	
sequential patterns							x							
linear algebra									х	x				x
logistic regression									x					
outliers									x					
convolution networks										x				
boltzman										x				
pagerank											x			
ISH											×			
nearest neighbor											x	x		
recommender systems											x			
нмм													x	
deep learning												x		x
rule-based												Y		

Your achievements

- PCA, eigenvectors, t-SNE, visualization
- Word2vec, topics, trend detection
- Regression & time series modeling
- Clustering and classification
- Deep learning with CNNs
- Text mining
- Recommender systems
- Network analysis
- Outlier analysis

Great Topic Presentations + Code

- Ensembles, XGBoost, GANs, SMOTE
- Density clustering
- Sentiment analysis
- ICA & dynamic PCA, UMAP
- Local outlier factor
- Time series change, clusters & MVA
- Network clustering
- Collaborative Filtering
- REINFORCE and Deep RL

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Machine Learning Journal Sept.

- ALR accelerated logistic regression
- Fast and scale Lasso
- Factorizing LambdaMart for cold start recommendations
- Topological insight into deep learning
- Adaptive trajectory analysis of ... clustering
- On need for structure modeling in sequence prediction
- Cost sensitive boosting algorithms

• . . .

KDD 2017 Conference Sections

- Networks & graphs
- Intelligent systems & data science
- Methodology
- Novel applications
- Representations
- Matrices
- Clustering
- Recommendations
- Supervised Learning
- Humans & crowds
- Medical data
- Deep learning
- · Anomaly Detection
- Kernels and Sketches
- Temporal Analysis

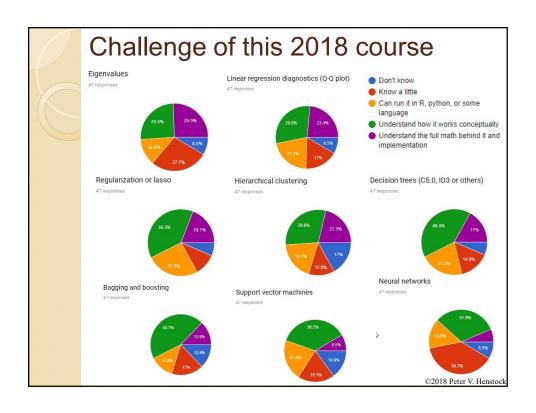
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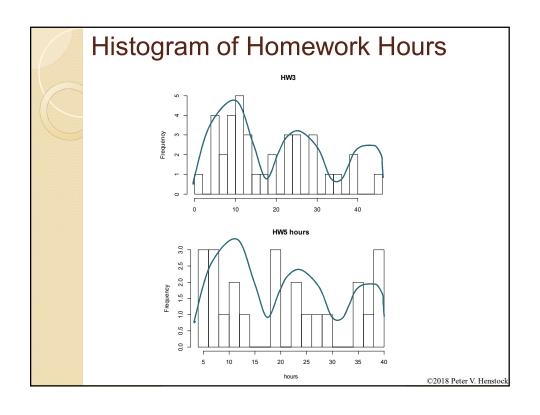
Not just the ML/DM/Al areas

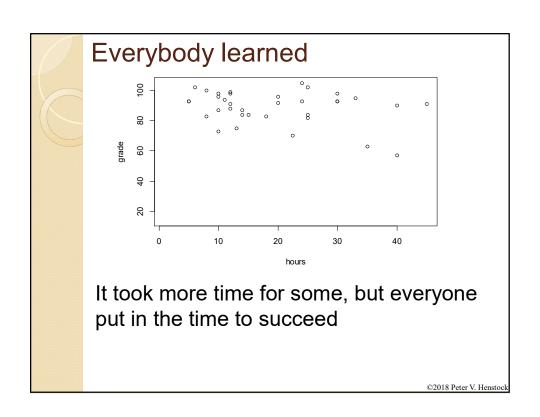
- Bioinformatics Journal
 - DepQA: Improving estimation of single protein model quality with deep belief networks
- JCIM (Computational Chemistry)
 - Boosting docking-based virtual screening with deep learning
- Agriculture
 - Combo of fuzzy logic and analytical hierarchical process techniques to assess K saturation in soils....
- Journal of Politics
 - Strategic retirements of elected & appointed justices: Hazards model approach
- Economics
 - Tariffs, Trade & Productivity, Quantitative Evaluation of Heterogeneous Firm Models

Goals

- Learn core ML/DM techniques at a moderate level so you can quickly go into more depth later
 - Statistics & time series, DTW
 - Unsupervised: Clustering, PCA, visualization
 - Supervised: classifiers, deep learning
 - Applications: text, freq. pattern, recommenders, networks, outliers, images, time series
 - Common methods: matrix, eigenvalue, optimization, entropy, EM
- Gain hands-on XP with state of art tools & applications
 - Used main python libraries scikit-learn & others
 - Deep learning, text mining, img. proc., classifiers, Kaggle, etc.
 - Keras, XGBoost, Scikit-Learn, AWS, Dask
- Leverage resources:
 - Present on recent research & read papers
 - Section/Exploratory notebooks = resources for you
- Apply skills: final project







Conclusion

Personal Ideas

- Differentiate your skill set
 - Difficult to be the best ML expert
 - Difficult to be the best programmer
 - Difficult to be the best anything
 - Combinations have massive opportunities
- Data science is the manifestation of this

3 Types of ML/DM/AI jobs

- Solver of all problems
 - Technical wizard to solve any problem
 - Solve different problems each week
 - Sometimes exploit knowledge from one to work on another
 - Frequently working alone
- Solver of one problem
 - Improve "revenue" or "predictions"
 - Basis of the business model
 - Every increment → \$
 - Frequently teams of people
- Implementer

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Recommendations

- Become more fluent in python or R
- Choose 1-2 favorite classifiers
- Choose 1-2 clustering methods
- Choose 1-2 higher dimensionality visualization approaches
- Learn the space where you apply them
- Be able to interpret results

Problem Solutions

- Visualize your data
- Try your favorite methods
- Start with solutions out of the box
- Identify a metric to assess results
 - Try multiple solutions
 - Adapt solutions based on:
 - Knowledge of the problem (visualize issues)
 - Research papers
 - Watch out for the bias-variance trade-off
- Communicate well: needs, results and insight to domain experts (not ML folks)

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What are good next steps?

- ML & Stat: core of most non-obvious analyses
 - Use and maintain these skills in your toolbox
- Need more experience applying the tools
- Need a wider range of problems to push your envelopes into new areas
- Take on new project at work
- Let's research a problem together for a paper
- Work in the field: 6.4% raises in 2017 (Forbes)

Want more skills?

- Statistics & math (linear algebra)
- Graph analysis (social networks)
- Visualization
- Databases
- Text mining/linguistics/NLP
- Big Data
- Better coding: scripting & software eng.
- Don't forget domain expertise

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Thanks to our Awesome TAs

Dave & Rashmi





Thanks to our Awesome TAs

- Created fabulous notebooks each week
- Assembled examples of all the python concepts in first weeks
- Provided hands-on examples of how to convert lecture concepts into python
- Dove into sometime unfamiliar areas like Deep Learning, XGBoost, Spark
 - Dave's Deep Learning lecture
- Graded and provided great feedback

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- Hope to offer this class next Fall
- Need TAs in the future
- Teaching will increase your knowledge
- Also might need TA for Spring Software Engineering Capstone if you are an experienced developer

Thanks to You

- Great group of people
- Challenged our ideas
- Presented new concepts
- Worked very hard all semester
- Contributed professionally
- Shared feedback to help us

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Where are you now?

- Machine learning is core knowledge
 - Have exposure and moderate understanding across all the main sub-fields of the field
 - Can easily go deeper for a particular task
- Data science is the implementation
- You have more knowledge than most "data scientists" working in the field
- You have proven you can implement a wide range of solutions in many domains

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Final thoughts...

- I'd like to keep in touch with you
- Let me know if I can do anything for you now or in the future
- Go make the world better....

