Introduction to data mining and machine learning

Data Mining—CS 530 Spring 2021 Chapman University

Instructor: Uri Maoz TAs: Dehua (Andy) Liang Caitlyn Chavez Elnaz Lashgari Machine learning

 Machine learning pervasive in academia, in industry, and in every-day life



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Focus of course | Hearing | Construence | C

Focus of course

- Data mining & machine-learning extremely strong tools. But if (as too often) used incorrectly, do more harm than good
- While application-centered, course will give intuition & insight, & often delve into math behind methods

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What this course is & is not

Course is not

- Hand-wavy intro to deep-learning (& other cool, fashionable concepts)
- · Theory-only introduction to machine-learning
- Easy, entertaining undergraduate course

What this course is & is not

Course is

- Broad, Practical intro to machine-learning
- Dive into math & theory as needed
- Discussion of intuition & insights into material
- Wide-ranging final project
 Typically Work on real data
- Teach concepts crucial for advanced machinelearning courses & continuing on your own

What this course is & is not

- · This is a graduate course
- Expect that everyone here is specifically interested in course material
- Everyone willing to work hard to master material
 - Material we do not finish in class will be left for home
- · Backgrounds diverse
 - Some more math & science
 - Some more programming
 - Some with other backgrounds

What you need to know for this course

- Course programming language: Python (3.8)
- Math we will be using
 - Linear algebra (matrix & vector algebra)
 - Calculus
 - Probability



 $e^{i\pi} + 1 = 0$

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More about course

- Later classes build upon information disseminated in earlier classes
- Online classes will be recorded & slides distributed for students to revisit material as needed



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- Pace is fast, but feel free to ask questions if something is not clear



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More about course

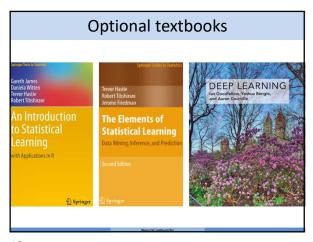
- Later classes build upon information disseminated in earlier classes
 - If you must miss a class—highly not recommended make very sure you read though material & understand it completely. Talk to colleagues, TAs, or me
- Pace is fast, but feel free to ask questions if something is not clear
- Math involved in course not trivial. We will try to give intuition so that even if math not completely clear, its motivation & meaning will be
 - Again, feel free to ask questions

TA recitation classes

Recitation classes will

- · Cover more technical material
 - Example: Python in a nutshell
- Work through step-by-step examples of material from class, including coding examples
- Go over solutions to homework exercises & quizzes

Neural networks



Bureaucracy CS530

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On Canvas

https://canvas.chapman.edu/

SP215 CS-530-01
Data Mining SP215 CS-530-01
Spring 2021

Display SP215 CS-530-01
Spring 2021

Topics

- 1. Regression, resampling, & regularization
 - Simple linear-regression
 - Multiple regression
 - Resampling methods
 - Regularization

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Topics

- 2. Unsupervised learning
 - K-Means
 - PCA/LDA
 - ICA (if there is time)

Topics

- 3. Classification
 - Logistic regression
 - Naive Bayes
 - Tree-based methods
 - Support-vector machines

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Topics

- 4. Neural networks & deep learning
 - Single neurons (biological & models)
 - Feed-forward neural networks (fixed weight & learning)

 - Gradient descent & Back Propagation in multi-layer feedforward neural networks
 - Other architectures (convolutional layers, autoencoders, recurrent neural networks)
 - Regularization, data augmentation, & optimization in neural networks

Grading

· Grade breakdown **Total points** Homework 25 points - Typically, every week (worst 2 dropped) 10 points Quizzes - Typically, take-home Final project 30 points In groups (individual grading) Final exam 20 points

• Participation (not attendance) 15 points

 Overall 100 points

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Grading

- Homework & quizzes track comprehension continuously
 - What do you & don't you understand?
 - Homework typically given early in the week for submission by Sunday at 11:59pm
- Final project
 - Work on actual dataset using all material learned in class

Grading

- Participation (more than just attendance)
 - Class discussions, TA recitation class, office hours
 - Exit surveys

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- Group work (also judged by peers)
- Camera on during entire class (while online)
- Quality of participation matters more than quantity

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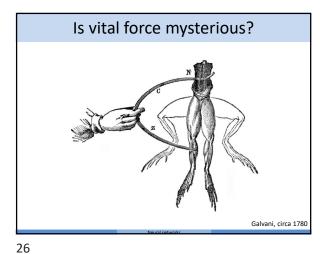
Exit surveys (part of participation)

Typically made up of two questions

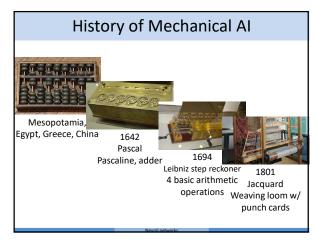
- 1. Please list two things that you learned in class today
- 2. Please list two things that were unclear to you in class today

Introduction to Machine-Learning, Deep Learning & Artificial Intelligence (AI)



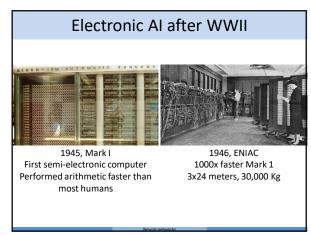


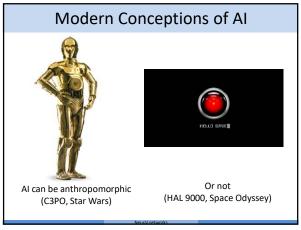
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Software: Algorithmic advances

- 1952 first checkers learning program (Samuel, IBM)
- 1957 Perceptron, simplest neural network (Rosenblatt)
- 1967 Nearest neighbor for pattern recognition
- 1981 Explanation-based learning of rules from examples
- 1990's ML formalized: applied to data mining, adaptive software, ...
- 2000's ML everywhere: used in technology, science, engineering, ...

Artificial intelligence (AI)

- Term AI coined in 1956 conference at Dartmouth
- Initial optimism: "within a generation... the problem of creating 'artificial intelligence" will substantially be solved" (Minsky, 1967)
- Attempts to make general artificial intelligence failed. Rule-based programs successful in specific fields: word problems in math, proving geometry theorems, ...

Data-processing pipeline

ANALYTICAL PROCESSING

RUILDING

RUUDING

FEEDBACK (OPTIONAL)

OUTPUT

FOR ANALYST

DATA PREPROCESSING

FEEDBACK (OPTIONAL)

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DATA

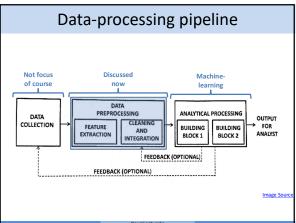
COLLECTION

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Introduction to Data Mining

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Data processing: feature extraction

Select features of dataset for further analysis

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Data processing: feature extraction

- Select features of dataset for further analysis
- Sometimes data needs combining into features

Data processing: feature extraction

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Data processing: Data cleaning

Almost all data types contain errors (or at least inaccuracies)

	Date	RegionName	InventorySeasonallyAdjusted	MedianListingPricePerSqft	
2346125	10/31/10	acworthcobbga	119	3	85.705263
2363168	11/30/10	acworthcobbga	118	3	84.719280
2380867	12/31/10	acworthcobbga	117	9	82.703214
2398571	1/31/11	acworthcobbga	118	2	81.462677
2416287	2/28/11	acworthcobbga	120	1	79.934225

Data processing: Data cleaning

Almost all data types contain errors (or at least inaccuracies)

	Date	RegionName	InventorySeasonallyAdjusted	MedianListingPricePerSqft
2346125	10/31/10	acworthcobbga	1193	85.705263
2363168	11/30/10	acworthcobbga	1183	847.19280
2380867	12/31/10	acworthcobbga	1179	82.703214
2398571	1/31/11	acworthcobbga	1182	81.462677
2416287	2/28/11	acworthcobbga	1204	79.934225

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Data processing: Data cleaning Handling missing entries

1. Eliminating record

	Date	RegionName	InventorySeasonallyAdjusted	MedianListingPricePerSqft	
2346125	10/31/10	acworthcobbga	1193		85.705263
2363168	11/30/10	acworthcobbga	1183		NaN
2380867	12/31/10	acworthcobbga	1179		82.703214
2398571	1/31/11	acworthcobbga	1182		81.462677
2416287	2/28/11	acworthcobbga	1204		79.934225

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Data processing: Data cleaning Handling missing entries

1. Eliminating record: problematic when many entries have NaNs

	Date	RegionName	InventorySeasonallyAdjusted	MedianListingPricePerSqft	
2346125	10/31/10	acworthcobbga	1193	85.7052	63
2363168	11/30/10	acworthcobbga	1183	Na Na	N
2380867	12/31/10	acworthcobbga	1179	82.7032	14
2398571	1/31/11	acworthcobbga	1182	81.4626	77
2416287	2/28/11	acworthcobbga	1204	79.9342	25

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Data processing: Data cleaning Handling missing entries

2. Estimating missing value (from other values)

	Date	RegionName	InventorySeasonallyAdjusted	MedianListingPricePerSqft	
2346125	10/31/10	acworthcobbga	1193		85.705263
2363168	11/30/10	acworthcobbga	1183)
2380867	12/31/10	acworthcobbga	1179		82.70321
2398571	1/31/11	acworthcobbga	1182		81.46267
2416287	2/28/11	acworthcobbga	1204		79.934225

(85.705263+82.703214+81.462677+79.934225)/4= 82.451345

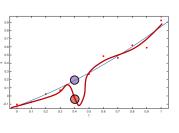
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Data processing: Data cleaning Handling missing entries 2. Estimating missing value (from other values)

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Data processing: Data cleaning Handling missing entries

2. Estimating missing value assumes: underlying model



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Data processing: Data cleaning Missing entries

3. Designing analytics to work with missing data: not always works, especially when using off-the-shelf code (increasingly common)

	Date	RegionName	InventorySeasonallyAdjusted	MedianListingPricePerSqft	
2346125	10/31/10	acworthcobbga	1193		85.70526
2363168	11/30/10	acworthcobbga	1183		NaN
2380867	12/31/10	acworthcobbga	1179		82.70321
2398571	1/31/11	acworthcobbga	1182		81.46267
2/16297	2/29/11	acworthcohhaa	1204		70 02/22

numpy.nanmean, numpy.std, ...

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Data processing: Data cleaning Outlier detection

Definition of outlier: "An observation that deviates so much from the other observations as to arouse suspicions that it was generated by a different mechanism" (Hawkins, 1980)

	Date	RegionName	InventorySeasonallyAdjusted	MedianListingPricePerSqft
2346125	10/31/10	acworthcobbga	1193	85.705263
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2416287	2/28/11	acworthcobbga	1204	79.934225

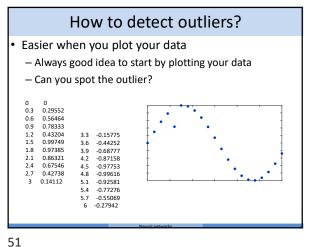
Data processing: Data cleaning Outlier detection

- Outliers might arise from
 - noise
 - human error
 - · sensor error
 - · communication error
 - etc. - malicious activity,
- rare event

Detecting outliers necessitates model for normal data



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How to detect outliers? Easier when you plot your data - Always good idea to start by plotting your data

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Data processing: Data cleaning Outlier detection **Detecting outliers** necessitates model for regular data Without reasonable model, outlier detection is illdefined problem

Dealing with bimodal distributions How to handle missing values with bi modal distribution? Cannot replace them with median - Can separate into 2 distributions and handle separately

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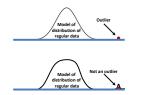
Data processing: Data cleaning **Outlier detection** Often better to calculate probability of sample being outlier-outlier scorethan to make binary decision

Data processing: Data cleaning **Outlier detection** Outlier detection & removal large, non-trivial topic Various methods exist Extreme-value Probabilistic Clustering Distance-based Density-based - Information-theory - Component independence

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Recap of Data Mining

- No silver bullet to dealing with missing data
 - Removing it decreases available data
 - Interpolating requires some model
- Similarly, defining outliers requires some assumptions about underlying distribution



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General Mathematical Framework of Machine-Learning

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Goal of machine learning

Machine learning focuses on the problem of **prediction**.

Given a training set

 $\{(\vec{x}_1,y_1),\ldots,(\vec{x}_n,y_n)\}\in\mathbb{R}^p\times\mathbb{R},$ we learn a predictor function

$$h_n:\mathbb{R}^p\to\mathbb{R}$$

that predicts label y for some $\vec{x} \notin \{\vec{x}_1,...,\vec{x}_n\}$ —i.e., for \vec{x} that was not in the training set.



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Goal of machine learning The predictor h_n is typically chosen from some function class \mathcal{H} . \mathcal{H} could be • A set of linear regression functions • A random forest with hyperparameters in some subspace • Neural networks of certain architecture, depth, and width • ...

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Goal of machine learning

For some training set $\{(\vec{x}_1,y_1),...,(\vec{x}_n,y_n)\},h_n$ could be chosen using empirical-risk minimization (ERM):

Here, an $h \in \mathcal{H}$ is chosen such that

$$h = \operatorname{argmin} \frac{1}{n} \sum_{i=1}^{n} \ell(h(\vec{x}_i), y_i)$$

where ℓ is a loss function. So, for ERM, h is chosen such that it minimizes the loss on the training set.

The loss function, ℓ , can be:

- Regression (squared loss): $\ell(y', y) = (y' y)^2$
- Classification (0-1 loss): $\ell(y',y) = \begin{cases} 0, & y' = y \\ 1, & y' \neq y \end{cases}$

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The goal of machine learning is to find h_n with a small loss on data (\vec{x}, y) not in the training set—i.e., to find h_n that generalizes well to unseen data. We typically assume that the training set is drawn from some (unknown) probability distribution D over $\mathbb{R}^p \times \mathbb{R}$. And we evaluate h_n on test sample (\vec{x}, y) independently drawn from the same probability distribution D.

Group exercise



In breakout rooms, we will now work on the following google doc:

https://docs.google.com/document/d/1Kn PD10ETqpDFK18wBuJzb13U_IsDac8BE2fFk z-UHYM/edit?usp=sharing

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General machine-learning problem

- Machine-learning is about function approximation
- The data $\overrightarrow{x} = \begin{bmatrix} x_{1,1} & \cdots & x_{p,1} \\ \vdots & \ddots & \vdots \\ x_{1,n} & \cdots & x_{p,n} \end{bmatrix}$ is assumed to be n samples of p dimensions each.

	name	mfr	type	calories	protein	fat	sodium	fiber	carbo	sugars	potass	vitamins	shelf	weight	cup
0	100%_Bran	N	С	70	4	1	130	10.0	5.0	6	290	25	3	1.00	0.33
1	100% Natural Bran	٥	С	120	3	5	15	2.0	8.0	8	135	0	3	1.00	1.00
2	All-Bran	ĸ	c	70	4	1	260	9.0	7.0	5	320	25	3	1.00	0.33
3	All-Bran_with_Extra_Fiber	к	С	50	4	0	140	14.0	8.0	0	330	25	3	1.00	0.50
4	Almond_Delight	R	С	110	2	2	200	1.0	14.0	8	-1	25	3	1.00	0.75
5	Apple_Cinnamon_Cheerios	G	С	110	2	2	190	1.5	10.5	10	70	25	1	1.00	0.75
6	Apple_Jacks	ĸ	С	110	2	0	125	1.0	11.0	14	30	25	2	1.00	1.00
7	Basic_4	G	С	130	3	2	210	2.0	18.0	8	100	25	3	1.33	0.75
8	Bran_Chex	R	С	90	2	1	200	4.0	15.0	6	125	25	1	1.00	0.67
9	Bran Flakes	Р	С	90	3	0	210	5.0	13.0	5	190	25	3	1.00	0.67

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General machine-learning problem

• The input data \vec{x} , is typically associated with an output, \vec{y} , such that $\vec{y} = f(\vec{x})$ for some unknown f (or h) that we want to learn.

$$\vec{y} = f \begin{pmatrix} \begin{bmatrix} x_{1,1} & \cdots & x_{p,1} \\ \vdots & \ddots & \vdots \\ x_{1,n} & \cdots & x_{p,n} \end{bmatrix} \end{pmatrix}$$

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General machine-learning problem

- Machine-learning can be boiled down to function approximation
- The data $\overrightarrow{x} = \begin{bmatrix} x_{1,1} & \cdots & x_{p,1} \\ \vdots & \ddots & \vdots \\ x_{1,n} & \cdots & x_{p,n} \end{bmatrix}$ is typically n samples of n dimensions each
- The labels are typically one dimensional for each sample. So, \vec{y} is (n x 1)
- So $\vec{y} = f(\vec{x})$ is the machine-learning problem, and the function to approximate is f

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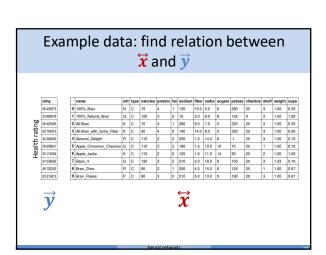
General machine-learning problem

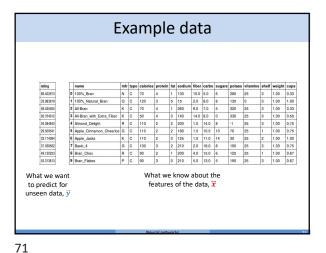
We want to learn

relationship between $\overrightarrow{x} = \begin{bmatrix} x_{1,1} & \cdots & x_{p,1} \\ \vdots & \ddots & \vdots \\ x_{1,n} & \cdots & x_{p,n} \end{bmatrix}$

 $\vec{y} = f(\vec{x})$ is the general machine-learning problem

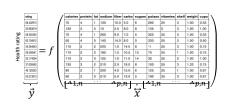
- Hence, function we want approximate is f when given \vec{x} and \vec{y} .
- After computing \hat{f} , we can find $\overrightarrow{\hat{y'}} = \hat{f}\left(\overrightarrow{x'}\right)$





General machine-learning problem

• The input data $,\vec{x}$, is typically associated with an output, \vec{y} , such that $\vec{y} = f(\vec{x})$ for some unknown f that we want to approximate (learn).



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Supervised Machine-Learning

- Given a set of samples where $\vec{y} = f(\vec{x})$ for some unknown f, supervised machine-learning strives to learn a good approximation of f, \hat{f} . The goal is for the approximation \hat{f} to be a good approximation of f such that it could well predict $\hat{\vec{y'}} = \hat{f}\left(\vec{x'}\right)$ for some $\hat{x'}$ different than \hat{x} .
 - Regression problem: \vec{y} is continuous
 - Classification problem: \vec{y} is categorical
 - \vec{y} are typically termed *labels* in this case

General <u>supervised</u> machine-learning problem

$$\vec{y} = f \begin{pmatrix} x_{1,1} & \cdots & x_{p,1} \\ \vdots & \ddots & \vdots \\ x_{1,n} & \cdots & x_{p,n} \end{pmatrix}$$

What we want to predict for unseen data, \vec{y}

What we know about the features of the data, \vec{x}

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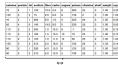
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Unsupervised Machine-Learning

- Only the data, \vec{x} , is given—without labels, \vec{y} .
- The goal is to model \overrightarrow{x} differently—or find another representation for \overrightarrow{x} or find structure in \overrightarrow{x} —under some assumptions
 - Clustering: discover the inherent groupings in the data samples (under some assumed metric)
 - Dimensionality reduction: find lower-dimensional representation of data (under some assumed metric) change feature-space

General <u>unsupervised</u> machine-learning problem





Find latent relations within $\stackrel{\leftrightarrow}{x}$

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Supervised vs. unsupervised learning

Supervised learning

Unsupervised learning



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Supervised vs. Unsupervised Learning

- Many problems in machine learning can be thought of as supervised or unsupervised
- But many other problems are in between
 - A lot of data, only some of it has labels
 - Under some assumption (e.g., smoothness) unlabeled samples can learn labeling from labeled ones
 - Example: Photo archive where only some data is labeled

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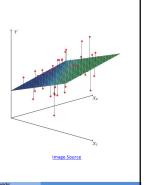
Example: Linear Regression

In general (multiple) linearregression, we have input data \vec{x} and output \vec{y} and we assume

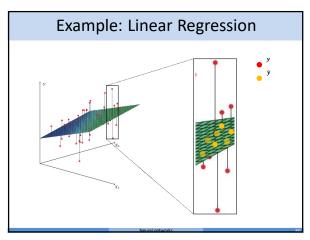
$$\vec{y} = \vec{x} \, \vec{\beta} + \vec{\varepsilon}.$$

So, we approximate using $\vec{\beta}$:

$$\hat{\vec{y}} = \vec{x} \, \hat{\vec{\beta}}.$$



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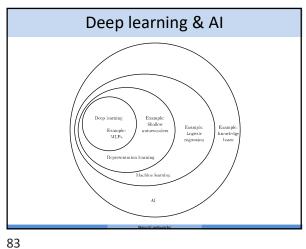
Artificial Intelligence & machine learning

Rule-based vs. learning from examples

- Rule-based learning: try to understand logical foundation of problems & teach computers to follow those rules
- Limited success in specific domains
- Learning from examples: expose computer to examples & let computer learn rule from examples
 - Much more successful generally
 - This is what machine-learning is all about

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Types of AI	Rule-Based	Example-Based
Given Representation	Classic Al	Classic Machine Learning
Learn Representation		Deep Learning

