CS 760: Machine Learning
ML Overview

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Announcements

- **Enrollment:**
  - Some of you should have been able to enroll last week.
  - Undergraduates: email me (if you haven’t in the last 1-2 weeks)

- **Recordings**
  - Not set up yet. Will try and resolve this by next week.

Announcements

- **Background knowledge:**
  - We will assume knowledge of calculus, linear algebra, prob/stat etc.
  - If you consider yourself to be mathematically inclined, you should be fine.
  - Some programming experience is necessary.
    - We will use Python, Numpy, and relevant libraries but you don't need specific experience in any of them.

- **Homework 1**
  - Due on Wednesday at 10

Outline

- **Review from last time**
  - Supervised vs. unsupervised learning
- **Supervised learning concepts**
  - Features, models, training, other terminology
- **Unsupervised learning concepts**
  - Clustering, anomaly detection, dimensionality reduction

Outline

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Review: ML Overview: Definition

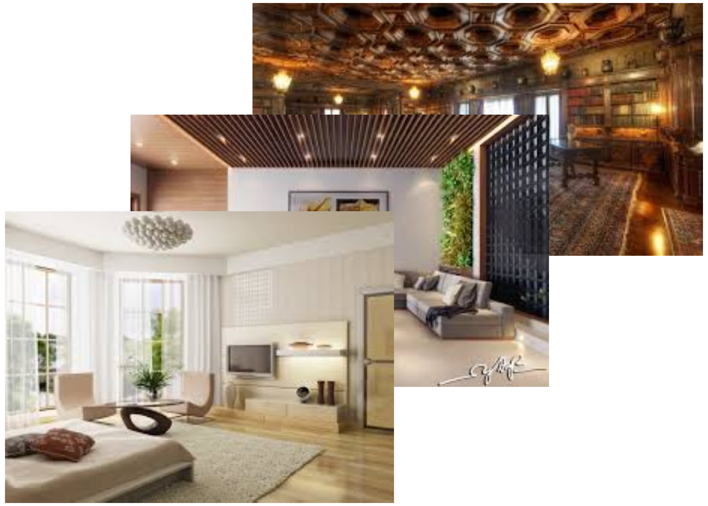
What is machine learning?

“A computer program is said to learn from experience **E** with respect to some class of tasks **T** and performance measure **P**, if its performance at tasks in **T** as measured by **P**, improves with experience **E**.” *Machine Learning*, Tom Mitchell, 1997

ML Overview: Flavors

Supervised Learning

- Learning from examples, as above
- **Workflow**:
  - Collect a set of examples {data, labels}: **training set**
  - “**Train**” a model to match these examples
  - ”**Test**” it on new data
- **Image classification**:



indoor

outdoor

ML Overview: Flavors

Supervised Learning

- **Example: Image classification**
- Recall **T**ask/**P**erformance measure/**E**xperience definition
  - **T**ask: distinguish **indoor** vs **outdoor**
  - **P**erformance measure: probability of misclassifying
  - **E**xperience: labeled examples

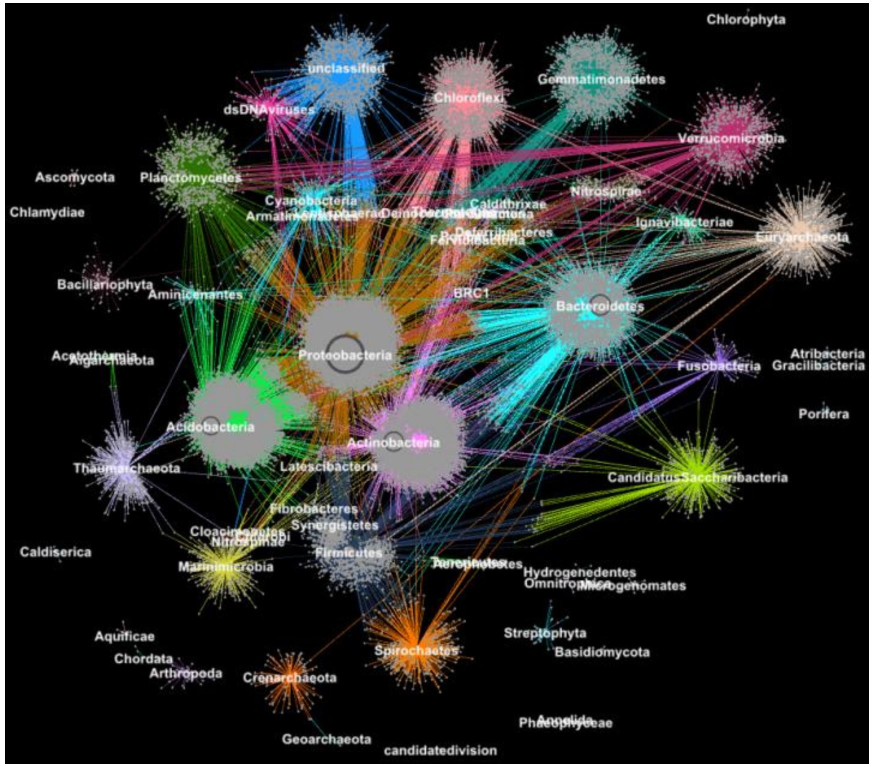
indoor

outdoor

ML Overview: Flavors

Unsupervised Learning

- Data, but no labels. No input/output.
- Goal: get “something”: structure, hidden information, more
- **Workflow**:
  - Collect a set {data}
  - Perform some algorithm on it

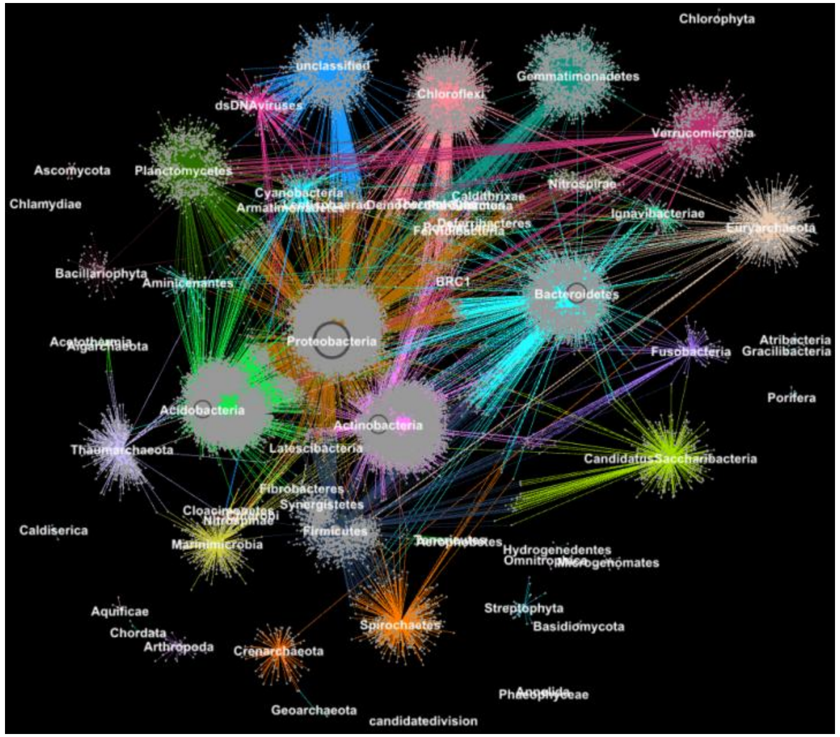


- **Clustering**: reveal hidden structure

ML Overview: Flavors

Unsupervised Learning

- **Example: Clustering**
  - **T**ask: produce distinct clusters for a set of data
  - **P**erformance measure: closeness to underlying structure
  - **E**xperience: available datapoints



ML Overview: Flavors

Reinforcement Learning

- Agent interacting with the world; gets rewards for actions
- Goal: learn to perform some activity
- **Workflow**:
  - Create an environment, reward, agent
  - **Train**: modify policy to maximize rewards
  - **Deploy** in new environment

- **Controlling aircraft**: learn to fly

ML Overview: Flavors

Reinforcement Learning

- **Example: Controlling aircraft**
  - **T**ask: keep the aircraft in the air, steer towards a desired goal
  - **P**erformance measure: reward for reaching goal quickly
  - **E**xperience: data (state/action/reward) from previous flights

Break & Quiz

Q1-1: Which of the following is generally NOT a supervised learning task?

1. Binary classification
2. Email spam detection
3. Handwriting recognition
4. Eigenvalue calculation

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Supervised Learning

- Can I eat this?

- Safe or poisonous?
  - **Never seen it before**

- How to decide?

Supervised Learning: Training Instances

- I know about other mushrooms:

safe



poisonous




- Training set of **examples/instances/labeled data**

Supervised Learning: Formal Setup

Problem setting

- Set of possible instances $\mathcal{X}$
- Unknown *target function* $f : \mathcal{X} \rightarrow \mathcal{Y}$
- Set of *models* (a.k.a. *hypotheses*): $\mathcal{H} = \{h | h : \mathcal{X} \rightarrow \mathcal{Y}\}$

Get

- Training set of instances for unknown target function, where $y^{(i)} \approx f(x^{(i)})$

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})$$


safe


poisonous


safe

Supervised Learning: Formal Setup

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Get

- Training set of instances for unknown target function *f*,

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})$$

Goal: model *h* that best approximates *f*

Supervised Learning: Objects

Three types of sets

- Input space, output space, hypothesis class

$$\mathcal{X}, \mathcal{Y}, \mathcal{H}$$

- **Examples**:
  - Input space: feature vectors $\mathcal{X} \subseteq \mathbb{R}^d$

  - Output space:
    - **Binary classification** $\mathcal{Y} = \{-1, +1\}$ safe poisonous
    - **Continuous** $\mathcal{Y} \subseteq \mathbb{R}$ $13.23°$

Input Space: Feature Vectors

- Need a way to represent instance information:

cap-shape, cap-surface, cap-color, bruises, odor

$$\mathbf{x}^{(1)} = \langle \text{bell}, \quad \text{fibrous}, \ \text{gray}, \quad \text{false}, \ \text{foul}, \ldots \rangle$$

safe

- For each instance, store features as a vector.
  - What kinds of features can we have?

Input Space: Feature Types

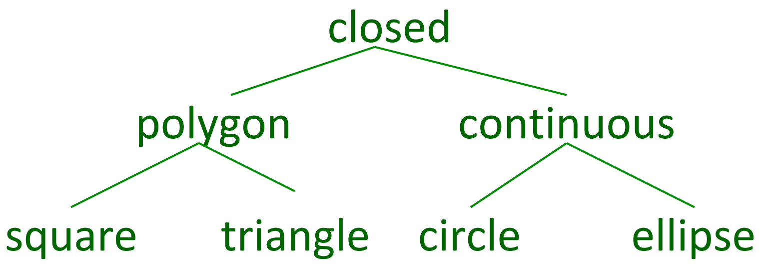
- *nominal* (including Boolean)
  - no ordering among values (e.g. *color* ∈ {*red*, *blue*, *green*}   (vs. *color = 1000* Hertz))

- *ordinal*
  - values of the feature are totally ordered (e.g. *size* ∈ {*small, medium, large*})

- *numeric (*continuous*)*

  height ∈ [0, 100] inches

- *hierarchical*
  - possible values are partially *ordered* in a hierarchy, e.g. *shape*



Input Space: Features Example

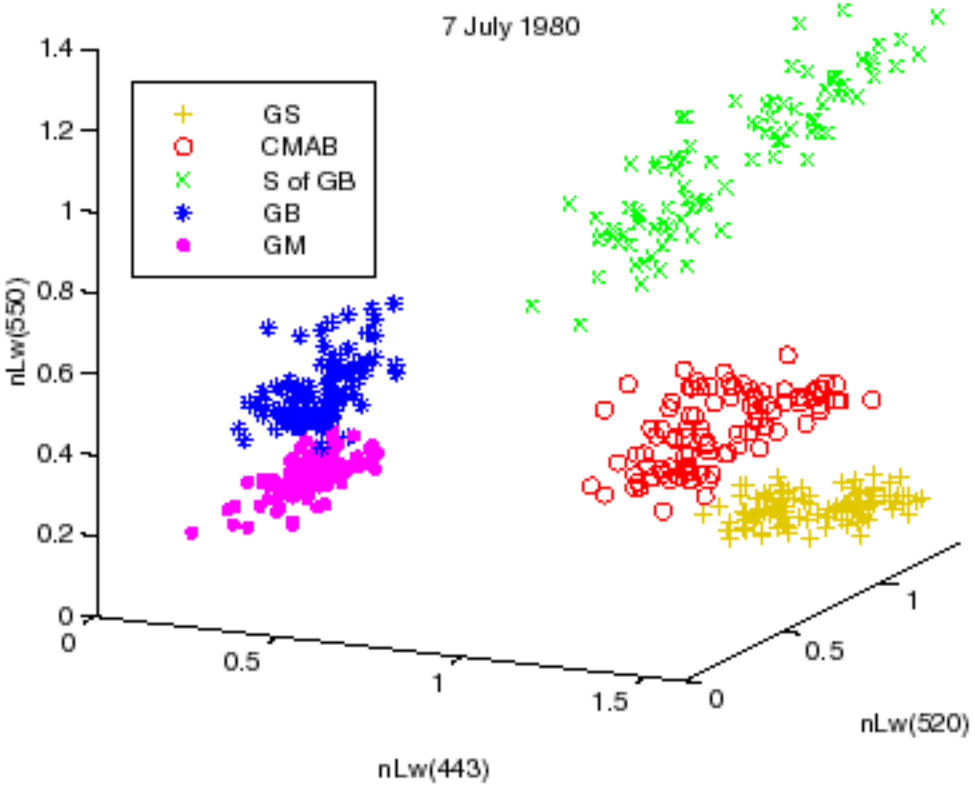
sunken **is one possible value of the *cap-shape* feature**

Mushroom features (UCI Repository)

cap-shape: bell=b,conical=c,convex=x,flat=f, knobbed=k,sunken=s
cap-surface: fibrous=f,grooves=g,scaly=y,smooth=s
cap-color: brown=n,buff=b,cinnamon=c,gray=g,green=r, pink=p,purple=u,red=e,white=w,yellow=y
bruises?: bruises=t,no=f
odor: almond=a,anise=l,creosote=c,fishy=y,foul=f, musty=m,none=n,pungent=p,spicy=s
gill-attachment: attached=a,descending=d,free=f,notched=n
gill-spacing: close=c,crowded=w,distant=d
gill-size: broad=b,narrow=n
gill-color: black=k,brown=n,buff=b,chocolate=h,gray=g, green=r,orange=o,pink=p,purple=u,red=e, white=w,yellow=y
stalk-shape: enlarging=e,tapering=t
stalk-root: bulbous=b,club=c,cup=u,equal=e, rhizomorphs=z,rooted=r,missing=?
stalk-surface-above-ring: fibrous=f,scaly=y,silky=k,smooth=s
stalk-surface-below-ring: fibrous=f,scaly=y,silky=k,smooth=s
stalk-color-above-ring: brown=n,buff=b,cinnamon=c,gray=g,orange=o, pink=p,red=e,white=w,yellow=y
stalk-color-below-ring: brown=n,buff=b,cinnamon=c,gray=g,orange=o, pink=p,red=e,white=w,yellow=y
veil-type: partial=p,universal=u
veil-color: brown=n,orange=o,white=w,yellow=y
ring-number: none=n,one=o,two=t
ring-type: cobwebby=c,evanescent=e,flaring=f,large=l, none=n,pendant=p,sheathing=s,zone=z
spore-print-color: black=k,brown=n,buff=b,chocolate=h,green=r, orange=o,purple=u,white=w,yellow=y
population: abundant=a,clustered=c,numerous=n, scattered=s,several=v,solitary=y
habitat: grasses=g,leaves=l,meadows=m,paths=p, urban=u,waste=w,woods=d

Input Space: Feature Spaces

- *If all features are numeric*, we can think of each instance as a point in a d-dimensional Euclidean feature space where d is the number of features



- **Example**: optical properties of oceans in three spectral bands

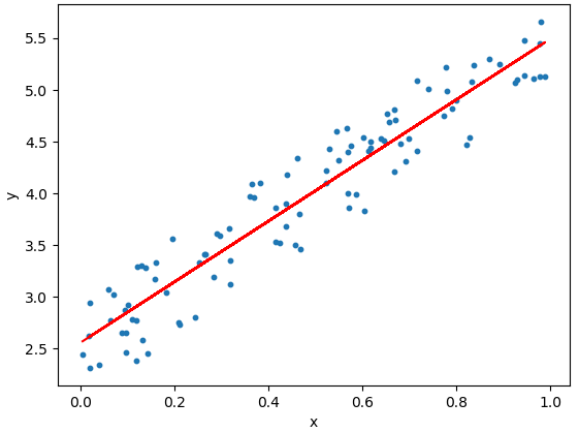
[Traykovski and Sosik, *Ocean Optics XIV Conference Proceedings*, 1998]

Output space: Classification vs. Regression

Choices of $\mathcal{Y}$ have special names:

- Discrete: "**classification**". The elements of $\mathcal{Y}$ are **classes**
  - Note: does not have to be binary

- Continuous: "**regression**"
  - Example: linear regression



- There are other types…

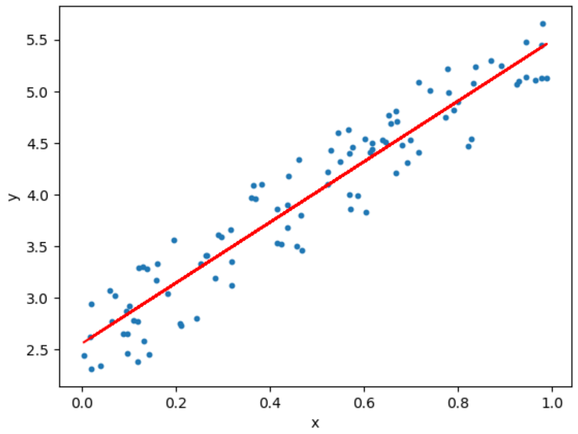
Hypothesis class

We talked about $\mathcal{X}, \mathcal{Y}$ what about $\mathcal{H}$?

- Recall: hypothesis class / model space.
  - Theoretically, could be all maps from $\mathcal{X}$ to $\mathcal{Y}$
  - Does not work! We'll see why later.

- Pick specific class of models. E.g. linear models:

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d$$



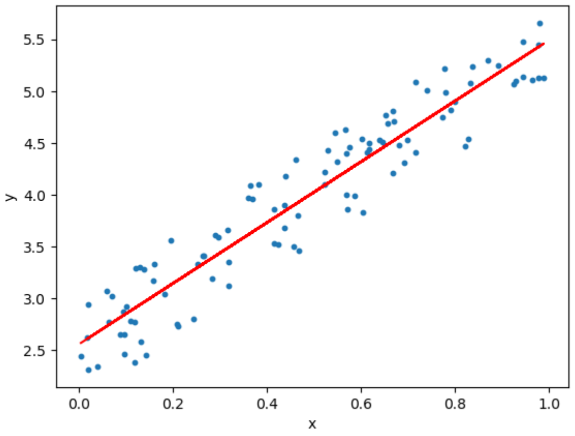
Hypothesis class: Linear Functions

- **Example** class of models: linear models

$$h_\theta(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d$$

Parameters (weights) — $\theta_0, \theta_1, \theta_2, \ldots, \theta_d$

Features — $x_1, x_2, \ldots, x_d$

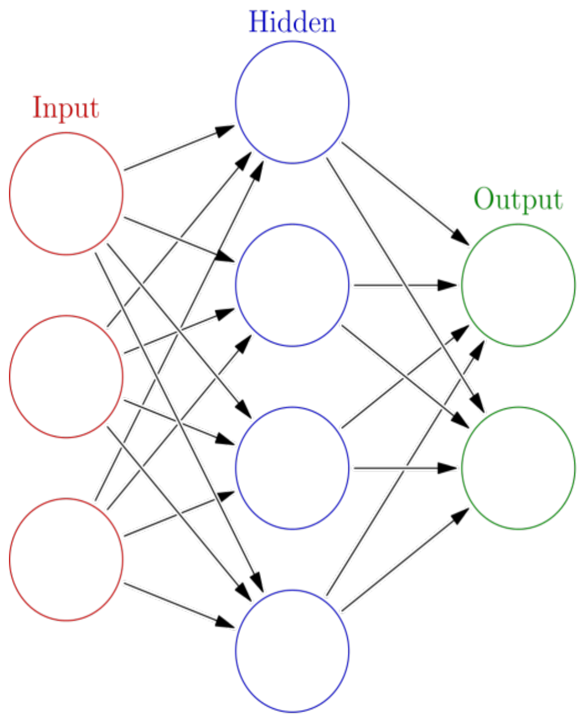


- How many linear functions are there?
  - Can any function be fit by a linear model?

Hypothesis class: Other Examples

Example classes of models: neural networks

$$f^{(k)}(x) = \sigma(W_k^T f^{(k-1)}(x)))$$



Wikipedia

Feedforward network

- Each layer:
  - linear transformation
  - Non-linearity

  - What are the parameters here?

Back to Formal Setup

Problem setting

- Set of possible instances $\mathcal{X}$ ✔
- Unknown *target function* $f : \mathcal{X} \rightarrow \mathcal{Y}$ ✔
- Set of *models* (a.k.a. *hypotheses*) $\mathcal{H} = \{h | h : \mathcal{X} \rightarrow \mathcal{Y}\}$ ✔

Get

- Training set of instances for unknown target function *f*,

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})$$ ✔

Goal: model *h* that best approximates *f*

Supervised Learning: Training

Goal: model *h* that best approximates *f*

- One way: empirical risk minimization (ERM)

$$\hat{f} = \arg\min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)}))$$

Model prediction

Hypothesis Class

Loss function: how far is the prediction from the label)?

Batch vs. Online Learning

- **Batch learning**: get all your instances at once

$$(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})$$

- **Online learning**: get them sequentially
  - Train a model on initial group, then update

$$\{(x^{(1)}, y^{(1)}), \ldots, (x^{(m)}, y^{(m)})\} \qquad \{(x^{(m+1)}, y^{(m+1)})\}$$

Supervised Learning: Predicting

Now that we have our learned model, we can use it for predictions.

$\mathbf{x} = \langle \text{bell}, \text{fibrous}, \text{brown}, \text{false}, \text{foul}, \ldots \rangle$

```
odor = a: e (400.0)
odor = c: p (192.0)
odor = f: p (2160.0)
odor = l: e (400.0)
odor = m: p (36.0)
odor = n
|   spore-print-color = b: e (48.0)
|   spore-print-color = h: e (48.0)
|   spore-print-color = k: e (1296.0)
|   spore-print-color = n: e (1344.0)
|   spore-print-color = o: e (48.0)
|   spore-print-color = r: p (72.0)
|   spore-print-color = u: e (0.0)
|   spore-print-color = w
|   |   gill-size = b: e (528.0)
|   |   gill-size = n
|   |   |   gill-spacing = c: p (32.0)
|   |   |   gill-spacing = d: e (0.0)
|   |   |   gill-spacing = w
|   |   |   |   population = a: e (0.0)
|   |   |   |   population = c: p (16.0)
|   |   |   |   population = n: e (0.0)
|   |   |   |   population = s: e (0.0)
|   |   |   |   population = v: e (48.0)
|   |   |   |   population = y: e (0.0)
|   spore-print-color = y: e (48.0)
odor = p: p (256.0)
odor = s: p (576.0)
odor = y: p (576.0)
```

safe or **poisonous**

Recall supervised learning workflow

- Collect a set of examples {data, labels}: **training set** ✓
- "**Train**" a model to match these examples ✓
  - E.g. Choose a hypothesis class and perform ERM
- "**Test**" it on new data ✓

Recall supervised learning workflow

- Collect a set of examples {data, labels}: **training set** ✓
- "**Train**" a model to match these examples ✓
  - E.g. Choose a hypothesis class and perform ERM

$$\hat{f} = \arg\min_{h \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} \ell(h(x^{(i)}), y^{(i)}))$$

Model prediction

Hypothesis Class

Loss function

- "**Test**" it on new data ✓

From linear to polynomial regression

Another class of models: polynomials:

$$h_\theta(x) = \theta_d x^d + \theta_{d-1} x^{d-1} + \ldots + \theta_1 x + \theta_0$$

- We can get a perfect fit by setting d to be very large.
  - E.g. In 1D, set d = n-1

- So, are we done?
  - How sensitive to noise?
  - How will they **extrapolate**?

Generalization

Fitting data isn't the only task, we want to **generalize**

- Apply learned model to unseen data:
  - For $(x, y) \sim \mathcal{D}$,

$$\mathbb{E}_{\mathcal{D}}[\ell(\hat{f}(x), y)]$$

- Can study theoretically or empirically
  - For theory: need assumptions, ie, training instances are iid
  - Not always the case!
    - Sequential data

Break & Quiz

Q2-1: Which of the following is a NOMINAL feature as introduced in the lecture?

1. Cost $\in [0, 100]$
2. Awarded $\in \{True, False\}$
3. Steak $\in \{Rare, Medium\ Rare, Medium, Medium\ Well, Well\ Done\}$
4. Attitude $\in \{strongly\ disagree, disagree, neutral, agree, strongly\ agree\}$

Q2-2: What is the dimension of the following feature space?

The CIFAR-10 dataset contains 60,000 32x32 **color** images in 10 different classes.
(convert each data to a vector)

1. 10
2. 60,000
3. 3072
4. 1024

Q2-3: Are these statements true or false?
(A) Instances from time series are independent and identically distributed.
(B) The primary objective of supervised learning is to find a model that achieves the highest accuracy on the training data.

1. True, True
2. True, False
3. False, True
4. False, False

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- **Unsupervised learning concepts**
  - Clustering, anomaly detection, dimensionality reduction

Unsupervised Learning: Setup

- Given instances $\{x^{(1)}, x^{(2)}, \ldots, x^{(n)}\}$

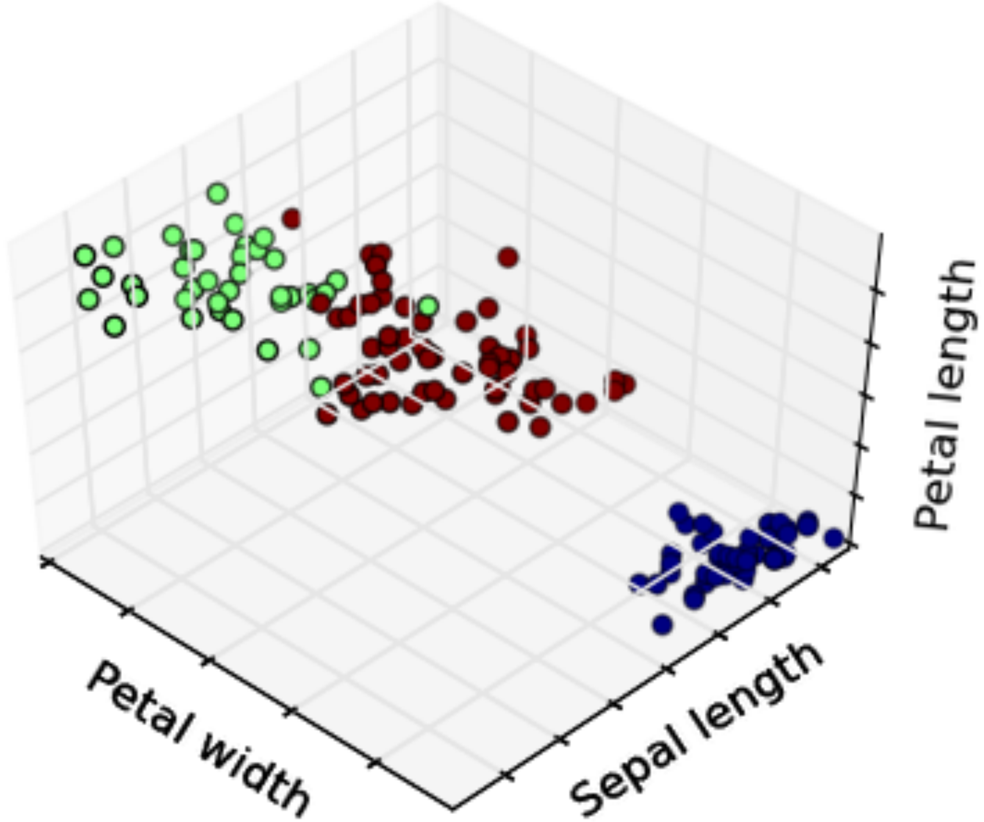
- **Goal**: discover interesting regularities/structures/patterns that characterize the instances. For example:
  - clustering
  - anomaly detection
  - dimensionality reduction

Clustering: Setup

- Given instances $\{x^{(1)}, x^{(2)}, \ldots, x^{(n)}\}$

- **Goal**: model *h* divides the training set into clusters with
  - intra-cluster similarity
  - inter-cluster dissimilarity

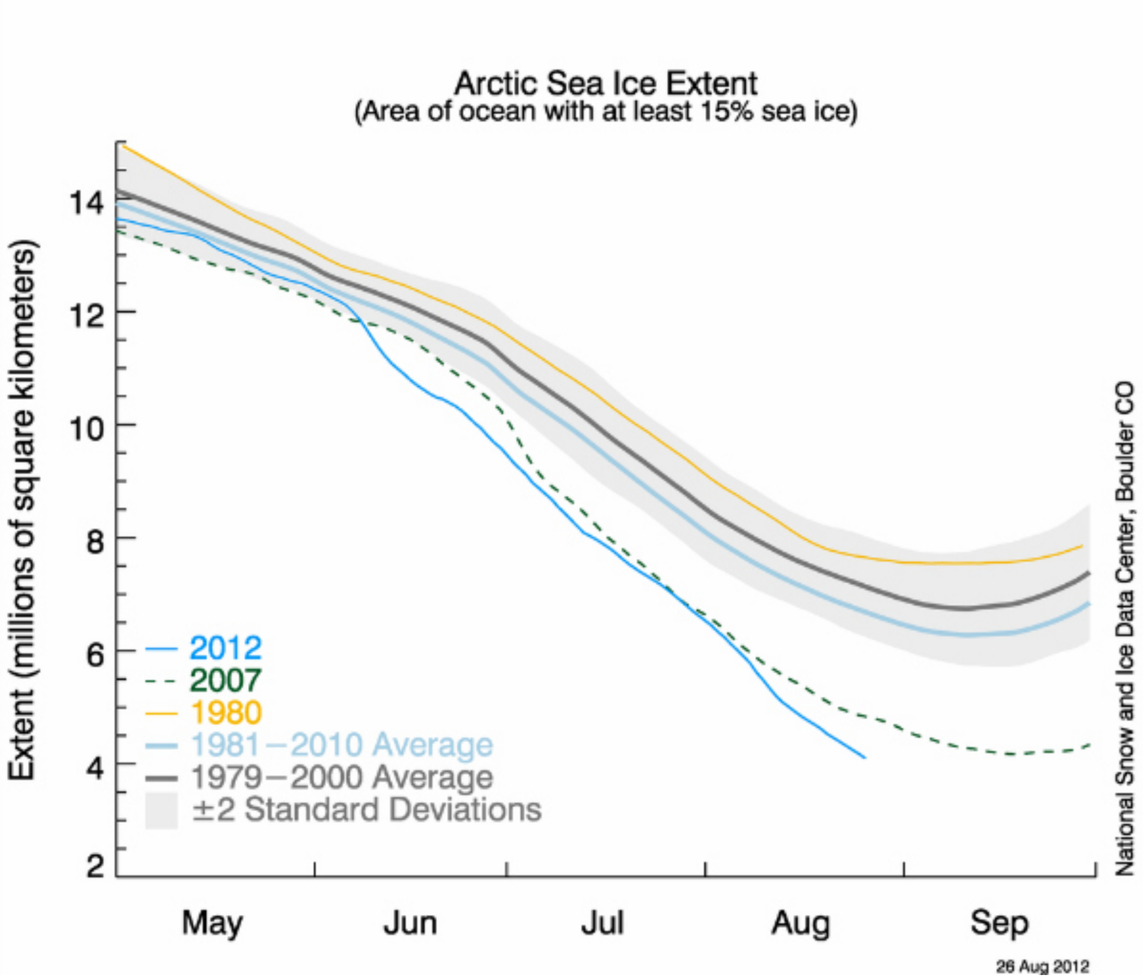
- Clustering *irises*:



Anomaly Detection: Setup

- Given instances $\{x^{(1)}, x^{(2)}, \ldots, x^{(n)}\}$

- **Goal**: model *h* that represents "normal" *x*
  - Can apply to new data to find anomalies



Let's say our model is represented by:

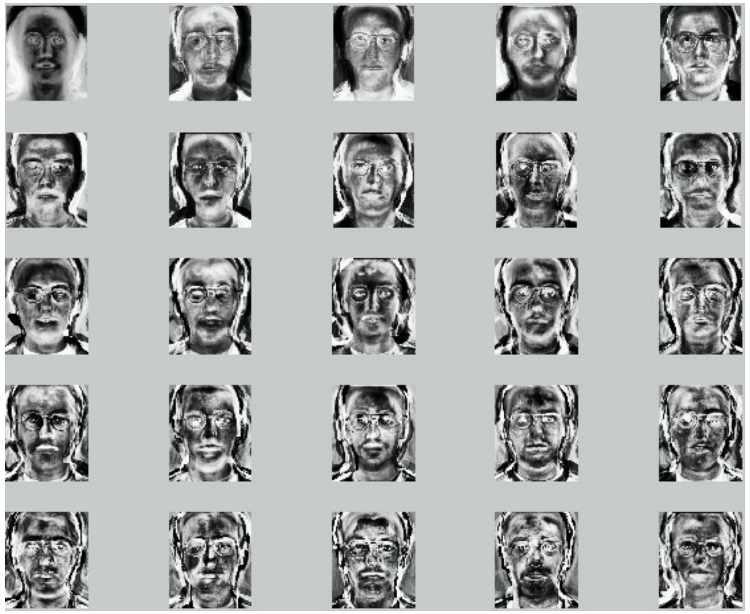
1979-2000 average, ±2 stddev

Does the data for 2012 look anomalous?

Dimensionality Reduction: Setup

- Given instances $\{x^{(1)}, x^{(2)}, \ldots, x^{(n)}\}$

- **Goal**: model *h* that represents *x* with
  - lower-dim. feature vectors
  - preserving information
- Example: Eigenfaces



Dimensionality Reduction: Setup

Example: Eigenfaces

 $= \alpha_1^{(1)} \times$  $+ \alpha_2^{(1)} \times$  $+ \ldots + \alpha_{20}^{(1)} \times$ 

$$x^{(1)} = \langle \alpha_1^{(1)}, \alpha_2^{(1)}, \ldots, \alpha_{20}^{(1)} \rangle$$

 $= \alpha_1^{(2)} \times$  $+ \alpha_2^{(2)} \times$  $+ \ldots + \alpha_{20}^{(2)} \times$ 

$$x^{(1)} = \langle \alpha_1^{(2)}, \alpha_2^{(2)}, \ldots, \alpha_{20}^{(2)} \rangle$$

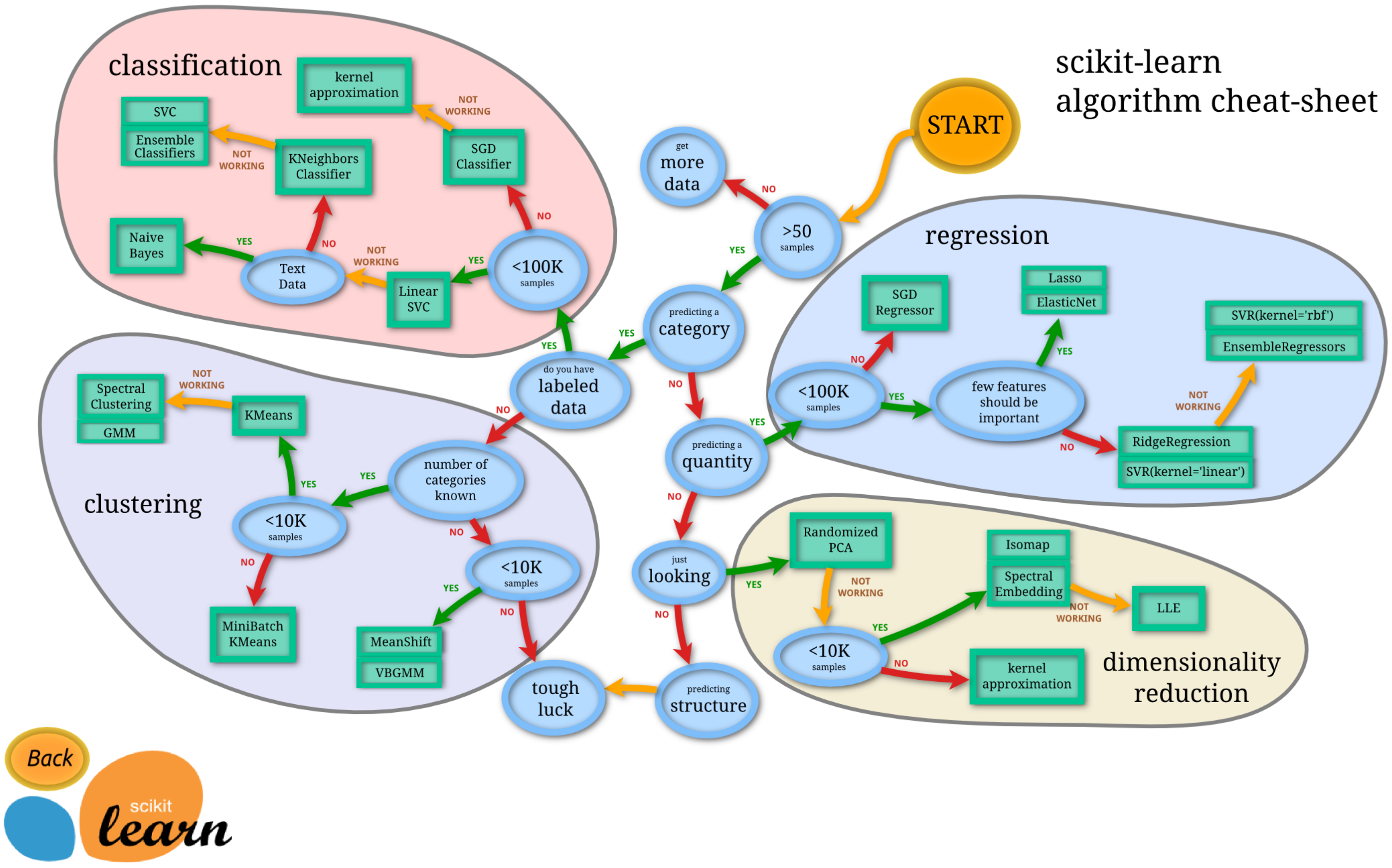
What dimension are we using now?

Q3-1: Which generally is NOT an unsupervised learning task?

1. Principal component analysis
2. Fraud detection
3. CIFAR-10 image classification
4. Community detection

Model Zoo

Lots of models!



Thanks Everyone!

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