Machine Learning: Overview

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Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Elad Hazan, Tom Dietterich, and Pedro Domingos.

Goals for the lecture

- define the supervised and unsupervised learning tasks
- consider how to represent instances as fixed-length feature vectors
- understand the concepts
  - instance (example)
  - feature (attribute)
  - feature space
  - feature types
  - model (hypothesis)
  - training set

  - supervised learning
  - classification (concept learning) vs. regression
  - batch vs. online learning
  - i.i.d. assumption
  - generalization

Goals for the lecture (continued)

- understand the concepts
  - unsupervised learning
  - clustering
  - anomaly detection
  - dimensionality reduction

Can I eat this mushroom?

I don’t know what type it is – I’ve never seen it before. Is it edible or poisonous?

Can I eat this mushroom?

suppose we're given examples of edible and poisonous mushrooms
(we'll refer to these as *training examples* or *training instances*)

edible

poisonous

can we learn a model that can be used to classify other mushrooms?

Representing instances using feature vectors

- we need some way to represent each instance
- one common way to do this: use a fixed-length vector to represent *features* (a.k.a. *attributes*) of each instance
- also represent *class label* of each instance

	cap-shape	cap-surface	cap-color	bruises	odor			class
$\mathbf{x}^{(1)} = \langle$	bell,	fibrous,	gray,	false,	foul,	$\ldots\rangle$	$y^{(1)} =$	edible
$\mathbf{x}^{(2)} = \langle$	convex,	scaly,	purple,	false,	musty,	$\ldots\rangle$	$y^{(2)} =$	poisonous
$\mathbf{x}^{(3)} = \langle$	bell,	smooth,	red,	true,	musty,	$\ldots\rangle$	$y^{(3)} =$	edible
		$\vdots$						$\vdots$

Standard feature types

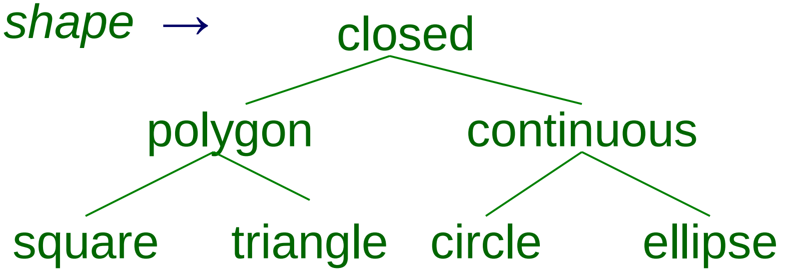
- *nominal* (including Boolean)
  - no ordering among possible values
    e.g. *color* $\in$ {*red*, *blue*, *green*}   (vs. *color = 1000* Hertz)

- *ordinal*
  - possible values of the feature are totally ordered
    e.g. *size* $\in$ {*small, medium, large*}

- *numeric (continuous)*
  weight $\in$ [0…500]

- *hierarchical*
  - possible values are partially *ordered* in a hierarchy

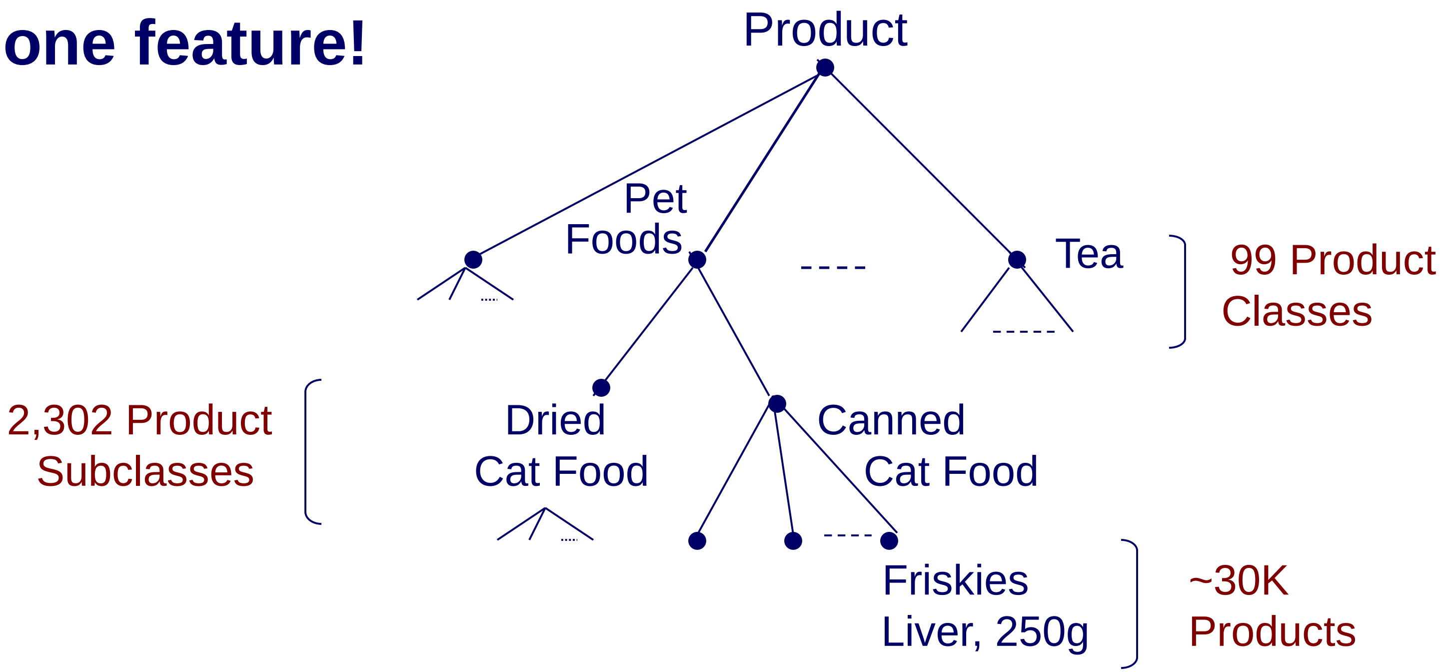
e.g. *shape* $\rightarrow$



Feature hierarchy example

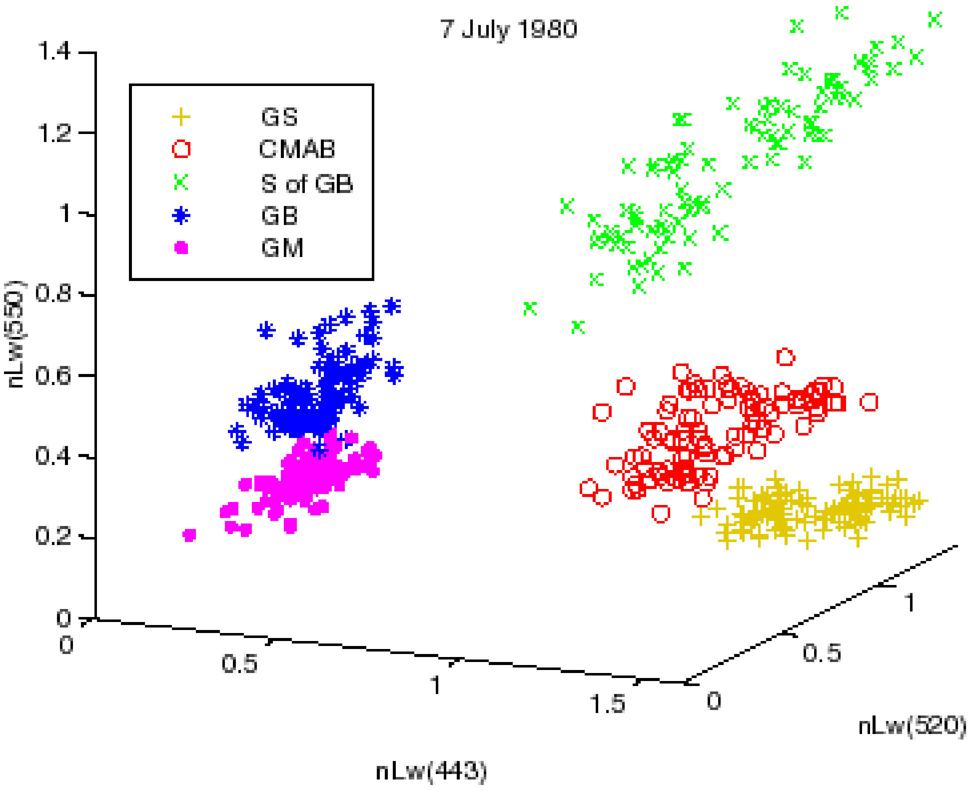
Lawrence et al., *Data Mining and Knowledge Discovery* 5(1-2), 2001

Structure of one feature!



Feature space

we can think of each instance as representing a point in a d-dimensional 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]

Another view of the feature-vector representation: a single database table

	feature 1	feature 2	. . .	feature d	class
instance 1	0.0	small		red	true
instance 2	9.3	medium		red	false
instance 3	8.2	small		blue	false
. . .					
instance n	5.7	medium		green	true

The supervised learning task

problem setting

- set of possible instances: X
- unknown *target function*: $f : X \rightarrow Y$
- set of *models* (a.k.a. *hypotheses*): $H = \{h \mid h : X \rightarrow Y\}$

given

- *training set* of instances of unknown target function f

$$\left(\mathbf{x}^{(1)}, y^{(1)}\right), \left(\mathbf{x}^{(2)}, y^{(2)}\right) \ \ldots \ \left(\mathbf{x}^{(m)}, y^{(m)}\right)$$

output

- model $h \in H$ that best approximates target function

The supervised learning task

- when y is discrete, we term this a *classification* task (or *concept learning*)
- when y is continuous, it is a *regression* task
- there are also tasks in which each y is more structured object like a *sequence* of discrete labels (as in e.g. image segmentation, machine translation)

Batch vs. online learning

In batch learning, the learner is given the training set as a batch (i.e. all at once)

$$\left(\mathbf{x}^{(1)}, y^{(1)}\right), \left(\mathbf{x}^{(2)}, y^{(2)}\right) \ldots \left(\mathbf{x}^{(m)}, y^{(m)}\right)$$

In online learning, the learner receives instances sequentially, and updates the model after each (for some tasks it might have to classify/make a prediction for each $\mathbf{x}^{(i)}$ before seeing $y^{(i)}$)

$$\left(\mathbf{x}^{(1)}, y^{(1)}\right) \qquad \left(\mathbf{x}^{(2)}, y^{(2)}\right) \qquad \left(\mathbf{x}^{(i)}, y^{(i)}\right)$$

time

i.i.d. instances

- we often assume that training instances are *independent and identically distributed* (i.i.d.) – sampled independently from the same unknown distribution

- there are also cases where this assumption does not hold
  - cases where sets of instances have dependencies
    - instances sampled from the same medical image
    - instances from time series
    - etc.
  - cases where the learner can select which instances are labeled for training
    - *active learning*
  - the target function changes over time (*concept drift*)

Generalization

- The primary objective in supervised learning is to find a model that *generalizes* – one that accurately predicts y for previously unseen $\boldsymbol{x}$

Can I eat this mushroom that **was not** in my training set?

Model representations

throughout the semester, we will consider a broad range of representations for learned models, including

- decision trees
- neural networks
- support vector machines
- Bayesian networks
- ensembles of the above
- etc.

Mushroom features (from the UCI Machine Learning Repository)

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

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

A learned decision tree

```
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)
```

if odor=almond, predict edible

if odor=none $\wedge$
spore-print-color=white $\wedge$
gill-size=narrow $\wedge$
gill-spacing=crowded,
predict poisonous

Classification with a learned decision tree

once we have a learned model, we can use it to classify previously unseen instances

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

```
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)
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|   spore-print-color = k: e (1296.0)
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|   spore-print-color = o: e (48.0)
|   spore-print-color = r: p (72.0)
|   spore-print-color = u: e (0.0)
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|   |   gill-size = n
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|   |   |   |   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)
```

$y =$ edible or poisonous?

Unsupervised learning

in unsupervised learning, we're given a set of instances, without y's

$$\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \ \ldots \ \mathbf{x}^{(m)}$$

goal: discover interesting regularities/structures/patterns that characterize the instances

common unsupervised learning tasks

- *clustering*
- *anomaly detection*
- *dimensionality reduction*

Clustering

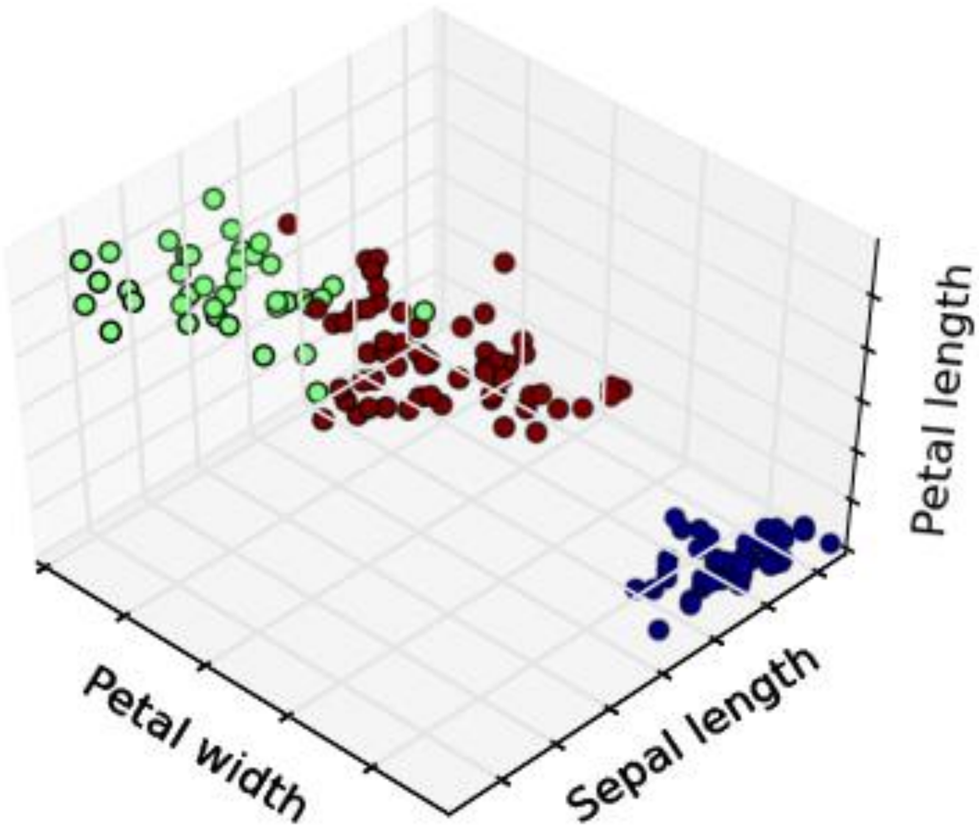
given

- training set of instances $\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \ \ldots \ \mathbf{x}^{(m)}$

output

- model $h \in H$ that divides the training set into clusters such that there is intra-cluster similarity and inter-cluster dissimilarity

Clustering example



Clustering irises using three different features (the colors represent clusters identified by the algorithm, not y's provided as input)

Anomaly detection

learning task

given

- training set of instances $\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \ldots \mathbf{x}^{(m)}$

output

- model $h \in H$ that represents "normal" $\boldsymbol{x}$

performance task

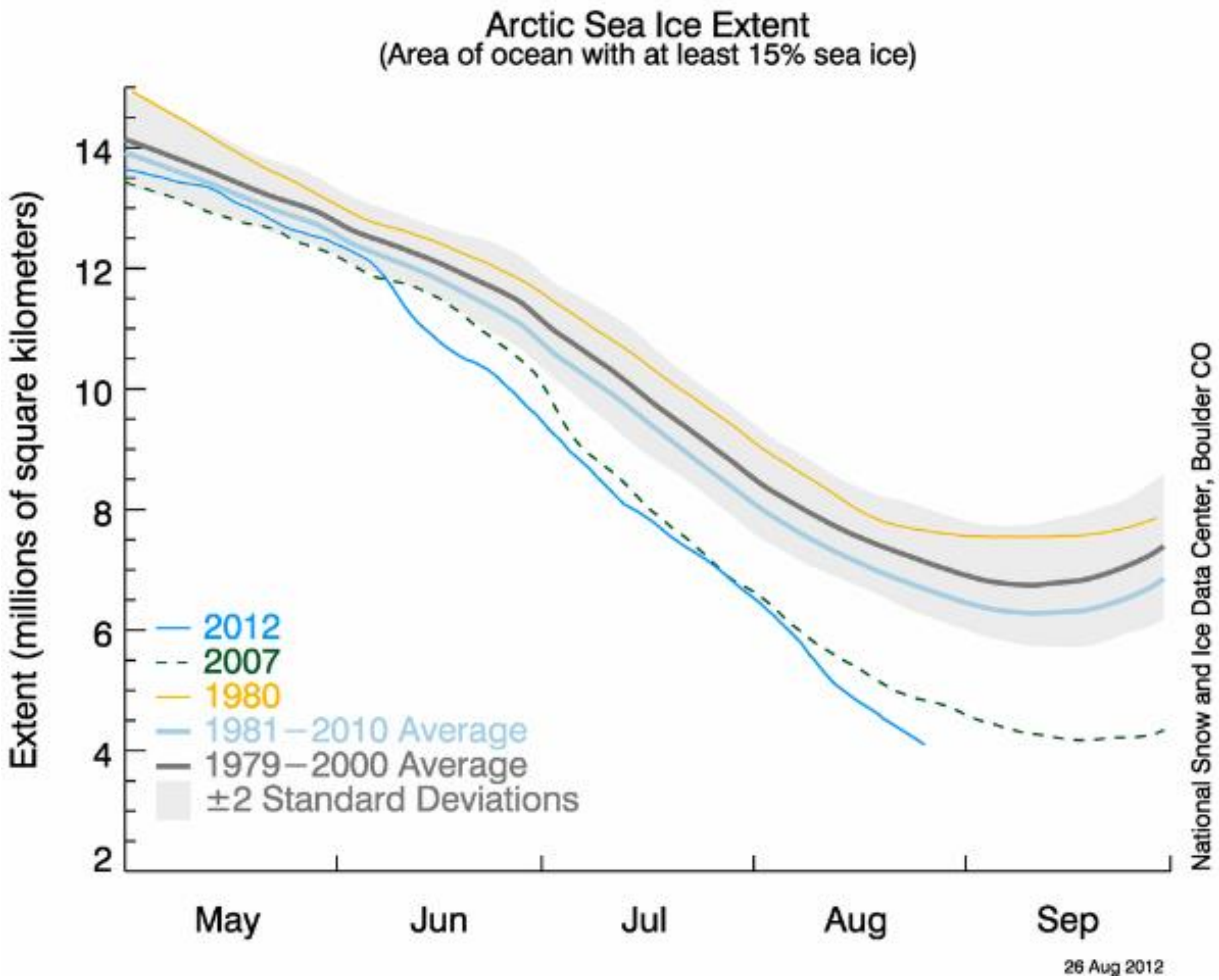
given

- a previously unseen $\boldsymbol{x}$

determine

- if $\boldsymbol{x}$ looks normal or anomalous

Anomaly detection example



Let's say our model is represented by: 1979-2000 average, ±2 stddev

Does the data for 2012 look anomalous?

Dimensionality reduction

given

- training set of instances $\mathbf{x}^{(1)}, \mathbf{x}^{(2)} \ldots \mathbf{x}^{(m)}$

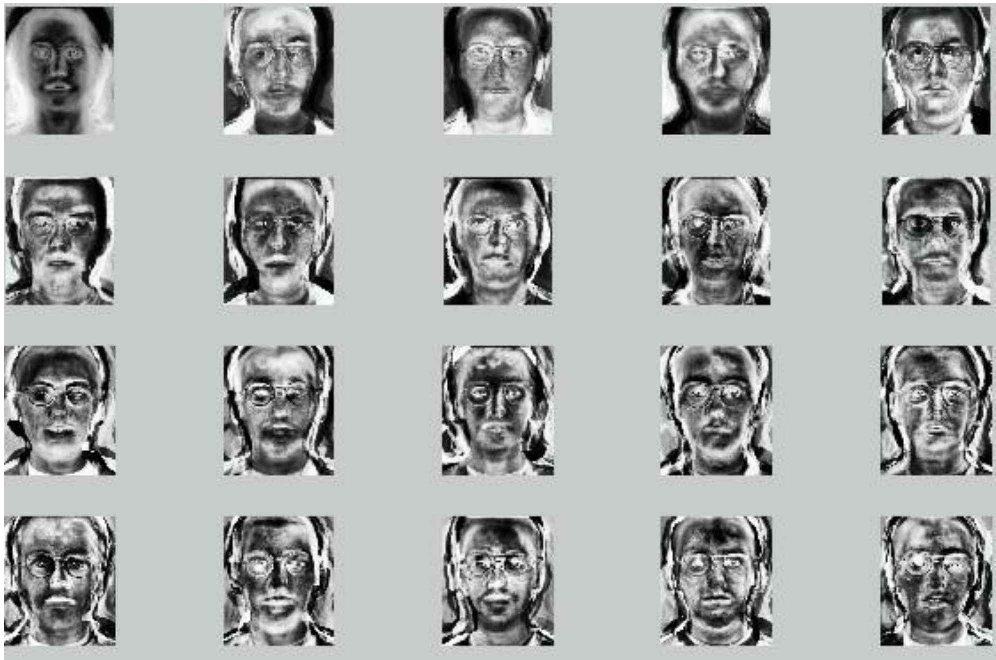
output

- model $h \in H$ that represents each $\boldsymbol{x}$ with a lower-dimension feature vector while still preserving key properties of the data

Dimensionality reduction example

We can represent a face using all of the pixels in a given image

More effective method (for many tasks): represent each face as a linear combination of *eigenfaces*



Dimensionality reduction example

represent each face as a linear combination of *eigenfaces*

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

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

 $= a_1^{(2)}$ ´  $+ a_2^{(2)}$ ´  $+ \ldots + \alpha_{20}^{(2)} \times$ 

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

# of features is now 20 instead of # of pixels in images

Other learning tasks

later in the semester we'll cover other learning tasks that are not strictly supervised or unsupervised

- *reinforcement learning*
- *semi-supervised learning*
- *etc.*