CHE 599: machine learning primer

## what is machine learning?

i.e. if ... then ... else ...

machine learning is the study of algorithms and statistical/mathematical models that allow computers to perform tasks without being programmed with explicit instructions.

- instead, we construct a mathematical model & tune it using training examples (data)
- this model is then used to make predictions / decisions or to gain insights into the structure of our data set

## supervised learning

distinction: training examples are labeled

goal: learn a function that maps an input $\vec{x}$ (feature vector) to an output $\vec{y}$ (target or response vector, dependent variable) $\vec{x} \mapsto \vec{y}$, from training examples

training examples: data $D := \{(\mathbf{x}_1, \mathbf{y}_1), ..., (\mathbf{x}_i, \mathbf{y}_i), ..., (\mathbf{x}_n, \mathbf{y}_n)\}$ example input/output pairs

$n$ examples

feature vector for example $i$

target vector

*example*

$\mathbf{x}$: vector representation of a patient

$y$: has Celiac disease ($y = 1$) or not ($y = 0$)

} D consists of $n$ "labeled" patients

$$\mathbf{x} = \begin{bmatrix} \text{concentration of IgG antibody in blood} \\ \text{has HLA-DQ2 gene} \\ \text{appetite (low, medium, high)} \end{bmatrix}$$

} stack features of a patient into a vector

model parameters

goal: use training examples to train a discriminative model $P(y = 1|\mathbf{x}; \boldsymbol{\alpha})$

"given the features of a patient, what is probability they have Celiac disease?" $P(y=1|\vec{x})$

"train" $\implies$ tuning model parameters $\vec{\alpha}$ to fit the training data

*Three types of variables:*

e.g.

- x[1] quantitative, (approximately) continuous : quantitative variables that obey notions of order, distance
- x[2] categorical/discrete : qualitative variables (categories) without a natural order
- x[3] categorical *and* ordinal : categorical variables with a notion of order but not distance

above.

## classification vs. regression

In classification, the target variables are categorical

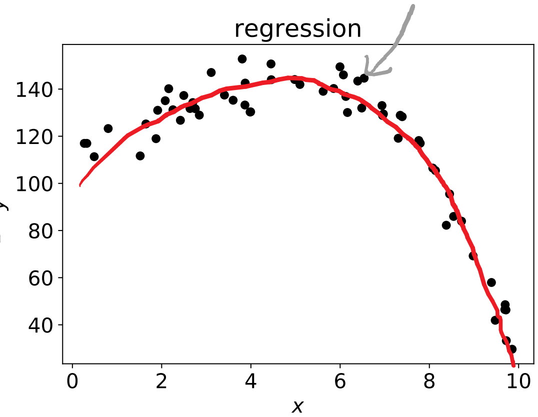
In regression, the target variables are quantitative

↳ e.g. same $\vec{x}$ above except $y :=$ concentration of C reactive protein in blood.

conceptually, ML aims to automatically learn, from the training examples, the response surface (regression) or decision boundary (classification)

↑ manifold in feature space that separates the classes

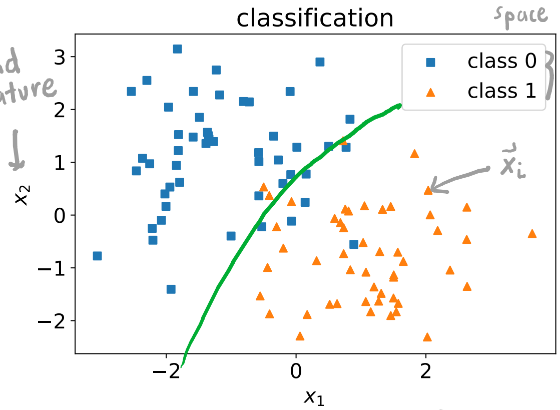
$(x_i, y_i)$




target var.

← 1-D feature vector

2nd feature




target var. depicted by color/symbol

$\vec{x}_i$

← first feature

## unsupervised learning

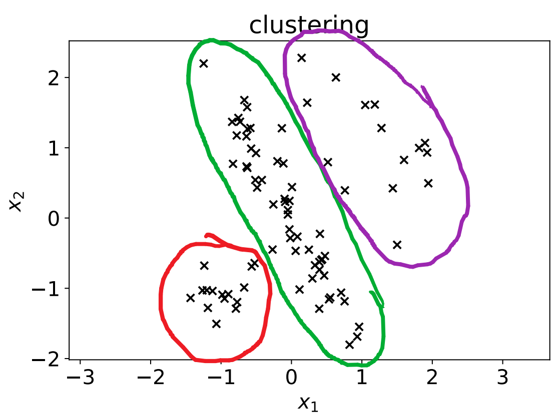
distinction: training examples are unlabeled

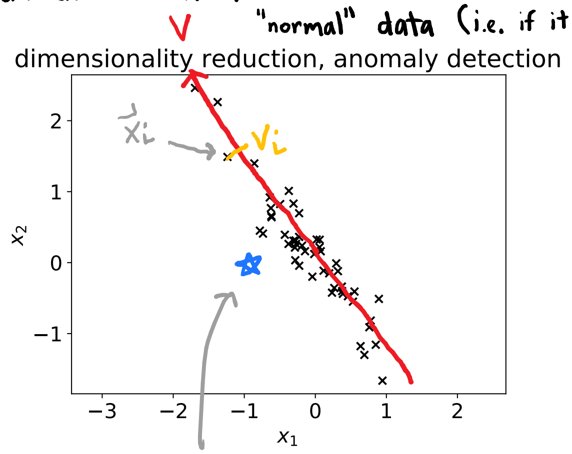
goal: find patterns/structure in data or identify groups/clusters in data (can be exploratory)

training examples: data $D := \{\mathbf{x}_1, ..., \mathbf{x}_i, ..., \mathbf{x}_n\}$ no target values associated with examples! (e.g. too costly to label)

↑ feature vector for example $i$

- clustering : automatically group together "similar" data points
- dimensionality reduction : extract the most salient features of data, compression
- anomaly detection : if we learn the "structure" of D, assumed to consist of "normal" data, when a new data pt. comes, we can determine if it falls outside the structure of the "normal" data (i.e. if it is anomalous) e.g. credit card fraud detection




new data point.

$x_1, x_2$ on their own not too extreme.

but clearly ☆ falls outside the structure of the "normal" data points (x's)

☆ does not conform to normal behavior.

now, imagine learning the response surface, decision boundary, or "primary axis" in much higher dimensions! (can't make a plot!)