IRDS: Data Mining Process
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(many figures used from Murphy. Machine Learning: A Probabilistic Perspective.)

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“Data Science”

• Our working definition
  • Data science is the study of the computational principles, methods, and systems for extracting knowledge from data.
• A relatively new term. A lot of current hype…
  • “If you have to put ‘science’ in the name…”
• Component areas have a long history
  • machine learning  • natural language processing
  • databases  • computer vision
  • statistics  • speech processing
  • optimization  • applications to science, business, health….
• Difficult to find another term for this intersection

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The term “data mining”

Data mining is the analysis of (often large) observational data sets to find unsuspected relationships and to summarise the data in novel ways that are both understandable and useful to the data owner. — Hand, Mannila, Smyth, 2001

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Many “easy” patterns already known
e.g., pregnant example from association rule mining

Tradeoff between
• predictive performance
• human interpretability
Ex: neural networks vs decision trees

Before I get too far ahead of myself…

What problem am I trying to solve?
Problem Types

- Visualization
- Prediction: Learn a map $x \rightarrow y$
  - Classification: Predict categorical value
  - Regression: Predict a real value
- Others
  - Collaborative filtering
  - Learning to rank
  - Structured prediction
- Description
  - Clustering
  - Dimensionality reduction
  - Density estimation
  - Finding patterns
    - Association rule mining
    - Detecting anomalies / outliers

Prediction Examples

- Classification
  - Advertising
    - Ex: Given the text of an online advertisement and a search engine query, predict whether a user will click on the ad
  - Document classification
    - Ex: Spam filtering
  - Object detection
    - Ex: Given an image patch, does it contain a face?
- Regression
  - Predict the final vote in an election (or referendum) from polls
  - Predict the temperature tomorrow given the previous few days
- Sometimes augmented with other structure / information
  - Structured prediction
    - Spatial data, Time series data
    - Ex: Predicting coding regions in DNA
  - Collaborative filtering (Amazon, Netflix)
  - Semi-supervised learning

Description Examples

- Clustering
  - Assign data into groups with high intra-group similarity
    - (like classification, except without examples of “correct” group assignments)
  - Ex: Cluster users into groups, based on behaviour
    - Social network analysis
  - Autoclass system (Cheeseman et al. 1988) discovered a new type of star,
- Dimensionality reduction
  - Eigenfaces
  - Topic modelling
- Discovering graph structure
  - Ex: Transcription networks
  - Ex: JamBayes for Seattle traffic jams
- Association rule mining
  - Market basket data
  - Computer security

Dimensionality reduction

General problem

Application to Images

Data

Basis
In the next few weeks, we’ll talk about
- Visualization
- Feature extraction
- Evaluation and debugging

But to talk about these, we still need to understand **representation** behind the algorithms

1. Given input, what goes in the feature vector?
Two Representation Problems

1. What features to use
2. What is the space of possible models

- In this course, we discuss features.
- Model —> IAML, PMR, MLPR
- But: To pick features, must understand model.
- So: Whirlwind tour of models, leaving out learning algorithms

Linear regression

Let $\mathbf{x} \in \mathbb{R}^d$ denote the feature vector. Trying to predict $y \in \mathbb{R}$

Simplest choice a linear function. Define parameters $\mathbf{w} \in \mathbb{R}^d$

$$\hat{y} = f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \mathbf{x} = \sum_{j=1}^{d} w_j x_j$$

(to keep notation simple assume that always $x_d = 1$)

Given a data set

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

find the best parameters

$$\min_{\mathbf{w}} \sum_{i=1}^{N} (y^{(i)} - \mathbf{w}^T x^{(i)})^2$$

which can be solved easily (but I won’t say how)

Nonlinear regression

What if we want to learn a nonlinear function?

Trick: Define new features, e.g., for scalar $x$, define $\phi(x) = (1, x, x^2)^T$

$$\hat{y} = f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \phi(\mathbf{x})$$

this is still linear in $\mathbf{w}$

To find parameters, the minimisation problem is now

$$\min_{\mathbf{w}} \sum_{i=1}^{N} \left( \hat{y}^{(i)} - \mathbf{w}^T \phi(x^{(i)}) \right)^2$$

exactly the same form as before (because $\mathbf{x}$ is fixed)
so still just as easy
Logistic regression
(a classification method, despite the name)

Linear regression was easy.
Can we do linear classification too?

Define a discriminant function
\[ f(x, w) = w^T x \]
Then predict using
\[ y = \begin{cases} 1 & \text{if } f(x, w) \geq 0 \\ 0 & \text{otherwise} \end{cases} \]
yields linear decision boundary

Can get class probabilities from this idea, using logistic regression:
\[ p(y = 1 | x) = \frac{1}{1 + \exp(-w^T x)} \]
(to show decision boundaries same, compute log odds \( \log \frac{p(y = 1 | x)}{p(y = 0 | x)} \))

K-Nearest Neighbour
simple method for classification or regression

Define a distance function between feature vectors \( D(x, x') \)
To classify a new feature vector \( x \)
1. Look through your training set. Find the \( K \) closest points. Call them \( N_K(x) \) (this is memory-based learning.)
2. Return the majority vote.
3. If you want a probability, take the proportion
\[ p(y = c | x) = \frac{1}{K} \sum_{y' \in N_K(x)} I\{y' = c\} \]

(K-Nearest Neighbour
Decision boundaries can be highly nonlinear
The bigger the \( K \), the smoother the boundary
This is nonparametric: the complexity of the boundary varies depending on the amount of training data

K-means clustering
To split the data into \( k \) clusters, iterate:

Initialize cluster centroids randomly: \( \mu_1 \ldots \mu_K \)
Repeat
- For each data point \( i \)
  - Assign to closest cluster
    \[ k_i \leftarrow \arg \max_{k \in \{1 \ldots K\}} D(\mu_k, x^{(i)}) \]
- Move cluster centroids (average all points currently in cluster)
  For all \( k \) in \( 1, 2, \ldots K \)
    \[ \mu_k \leftarrow \frac{\sum_{i=1}^N x^{(i)} I\{k_i = k\}}{\sum_{i=1}^N I\{k_i = k\}} \]
Until converged
Results in “convex” clusters
Summary

• Different types of model structures
  1. Linear boundaries (for classification and regression)
  2. Nonlinear boundaries (but linear in a set of features)
  3. “Wavy” boundaries (nonparametric, piecewise linear)
  4. Convex boundaries (with respect to Euclidean distance)
• This will affect feature construction, soon.