# MAS Data Science and Engineering Machine Learning

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Predictive Analytics Center of Excellence,

Director

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## WELCOME

## Logistics

- Check-in from 8:15am 9:00am
- Parking
- Restrooms
- Lunch

## Agenda

- Technical Sessions
- Hands-on Sessions
- Interactive format
- Assignments & Final
- TA Hours; Communication; Piazza





## Team

- Anwaya Aras aaras@eng.ucsd.edu
- Natasha Balac nbalac@ucsd.edu

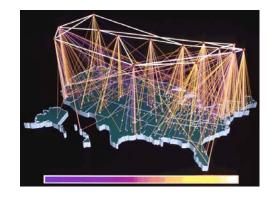




# **Brief History of SDSC**

- 1985-1997: NSF national supercomputer center; managed by General Atomics
- 1997-2007: NSF PACI program leadership center; managed by UCSD
  - PACI: Partnerships for Advanced Computational Infrastructure
- 2007-2009: Internal transition to support more diversified research computing
  - still NSF national "resource provider"
- 2009-future: Multi-constituency cyberinfrastructure (CI) center
  - provide data-intensive CI resources, services, and expertise for campus, state, and nation
- Approaching \$1B in lifetime contract and grant activity







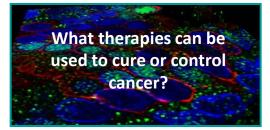


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Today's Information Technologies Drive 21st
Century Solutions

- Labs and Centers
  - Advanced Query Processing
  - Spatial Data Systems
  - Data-Driven High Performance Computing
  - Scientific Workflow Automation Technologies
  - Large-scale Data Systems
  - Predictive Analytics
  - Data Visualization
- We teach and mentor students
  - Graph Data Management
  - Semantic Web
  - Machine Learning and Analytics
  - GIS and Spatial Technologies
  - Information Integration
  - Text Analytics
  - Big Data technologies















- A "data-intensive" supercomputer based on SSD flash memory and virtual shared memory
  - Emphasizes MEM and IO over FLOPS
- A custom-designed system based on COTS to accelerate access to massive data bases being generated in all fields of science, engineering, medicine, and social science
- Designed specifically for data-intensive HPC applications





# Gordon Speeds and Feeds



L O	- 0		
INTEL SANDY BRIDGE COMPUTE NODE			
Sockets & Cores	2 & 16		
Clock speed	2.6 GHz		
DRAM capacity and speed	64 GB, 1,333 MHz		
INTEL710 eMLC FLASH I/O NODE			
NAND flash SSD drives	16		
SSD capacity per drive & per node	16 * 300 GB = 4.8 TB		
SMP SUPER-NODE (VIA VSMP)			
Compute nodes / I/O Nodes	32 / 2		
Addressable DRAM	2 TB		
Addressable memory including flash	11.6 TB		
GORDON (AGGREGATE)			
Compute Nodes	1,024		
Compute cores	16,384		
Peak performance	341 TF		
DRAM/SSD memory	64 TB DRAM; 300 TB SSD		
InfiniBand Int	ERCONNECT		
Architecture	Dual-Rail, 3D torus		
Link Bandwidth	QDR		
Vendor	Mellanox		
LUSTRE-BASED DISK I/O SUBSYSTEM (SHARED)			
Total storage: current/planned	4 PB/6 PB (raw)		
Total bandwidth	100 GB/s		





# SDSC Repertoire of Storage Systems



## Data Oasis (PFS)

- High-Performance Parallel File System for HPC Systems;
   Partitioned for Scratch and Medium-Term Parking Space
- Access: Lustre on HPC Systems (Gordon, Trestles, Triton)



## Project Storage

- Purpose: Typical Project / Home Directory / User File Server Storage Needs
- Access: NFS/CIFS, iSCI



#### SDSC Cloud

- Storage of Digital Data for Ubiquitous Access and High-Durability
- Access: Multi-platform web interface, S3-type interfaces, backup SW

DAIT DIEGO GOI ENGOINI GTEN GENTEN



# PACE Predictive Analytics Center of Excellence

# Closing the gap between Government, Industry and Academia





# PACE: Closing the gap between Government, Industry and Academia



**PACE** is a non-profit, public educational organization

- To promote, educate and innovate in the area of Predictive Analytics
- To leverage predictive analytics to improve the education and well being of the global population and economy
- To develop and promote a new, multi-level curriculum to broaden participation in the field of predictive analytics





# Foster Research and Collaboration



- Fraud Detection
- Modeling user behaviors
- Smart Grid Analytics
- Distributed Energy Generation
- Microgrid anomaly detection
- Battery Storage Analytics
- Sport Analytics
- Genomics



# CMS Fraud, Waste and Abuse Detection and Prediction

#### Descriptive Statistics

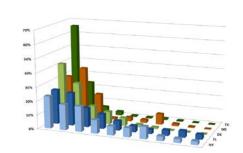
- Claims summary information
- History and trends
- Distributions across periods, transactions, etc.

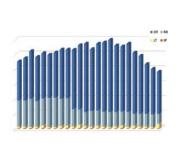
#### Exploratory Analysis

- Profiles of provider transactions
- Provider similarity according to profiles
- Visual summaries of large amounts of data
- Eligibility data link to provider billing

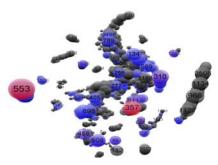
#### Predictive analytics

- Adjustments
- Equipment, Service Codes
- Long term vs. short term hospital stay
- Provider profiles









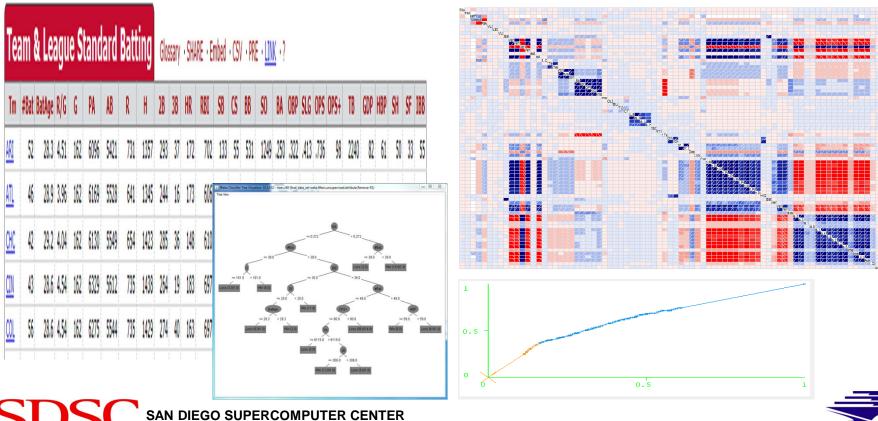




# Predictive Analytics In Action

#### **Sports Analytics**

#### Manufacturing





# **UCSD Smart Grid**

- UCSD Smart Grid sensor network data set
  - 45MW peak micro grid; daily population of over 54,000 people
  - Self-generate 92% of its own annual electricity load
- Smart Grid data over 100,000 measurements/sec
  - Sensor and environmental/weather data
    - Large amount of multivariate and heterogeneous data streaming from complex sensor networks
  - Predictive Analytics throughout the Microgrid







# Predictive Analytics for Discovering Energy Consumption Patterns

- The utility and the consumer both benefit from consumption analytics
- Forecasting the energy consumption patterns in the UCSD campus microgrid
- Different spatial and temporal granularities
- Novel Feature Engineering

Machine learning for demand response optimization





# Sustainable San Diego Partnership

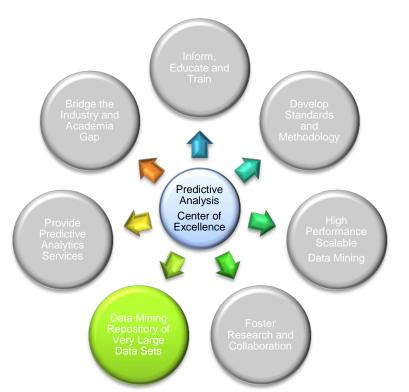
- Clean Tech San Diego, OSIsoft, SDG&E and UC San Diego Common data infrastructure connects physical assets: electrical, gas, water, waste, buildings, transportation &traffic
- Platform to securely transfer high volumes of Big Data from multiple, distributed measurement units
- Crowd-sourced Big Data in a cyber-secure, private cloud
- Predictive analytics on real-time time-series data



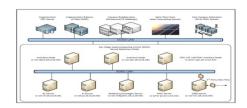


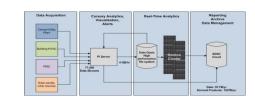


# Big Data



- Complexities introduced by the large amount of multivariate and heterogeneous data streaming from complex sensor networks
- Extremely large, complex sensor networks, enabling a novel feature reduction method that scales well

















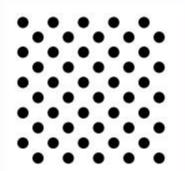




UCSD

# 4 V's of Big Data

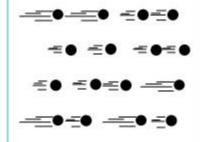
#### Volume



#### Data at Rest

Terabytes to exabytes of existing data to process

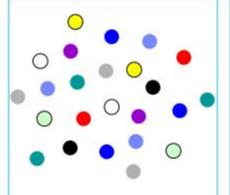
#### Velocity



#### Data in Motion

Streaming data, milliseconds to seconds to respond

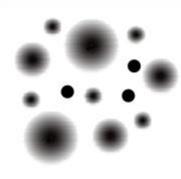
#### Variety



#### Data in Many Forms

Structured, unstructured, text, multimedia

#### Veracity\*



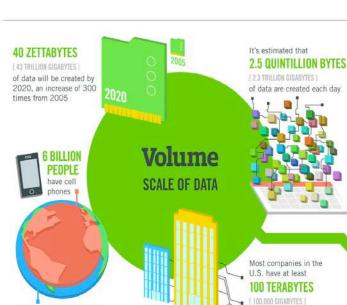
#### Data in Doubt

Uncertainty due to data inconsistency & incompleteness, ambiguities, latency, deception, model approximations

IBM, 2012







The New York Stock Exchange captures

WORLD POPULATION: 7 BILLION

#### 1 TB OF TRADE INFORMATION

during each trading session



ANALYSIS OF

By 2016, it is projected there will be

#### 18.9 BILLION NETWORK CONNECTIONS

- almost 2.5 connections per person on earth



of data stored

Modern cars have close to

that monitor items such as

fuel level and tire pressure

100 SENSORS

# The FOUR V's of Big Data

break big data into four dimensions: Volume. Velocity, Variety and Veracity

#### 4.4 MILLION IT JOBS



As of 2011, the global size of data in healthcare was estimated to be

#### 150 EXABYTES

[ 161 BILLION GIGABYTES ]



**Variety** DIFFERENT **FORMS OF DATA** 

there will be 420 MILLION WEARABLE, WIRELESS HEALTH MONITORS

By 2014, it's anticipated

#### 4 BILLION+ HOURS OF VIDEO

are watched on YouTube each month



#### 30 BILLION PIECES OF CONTENT

are shared on Facebook every month







are sent per day by about 200 million monthly active users

#### 1 IN 3 BUSINESS

don't trust the information they use to make decisions



Poor data quality costs the US economy around



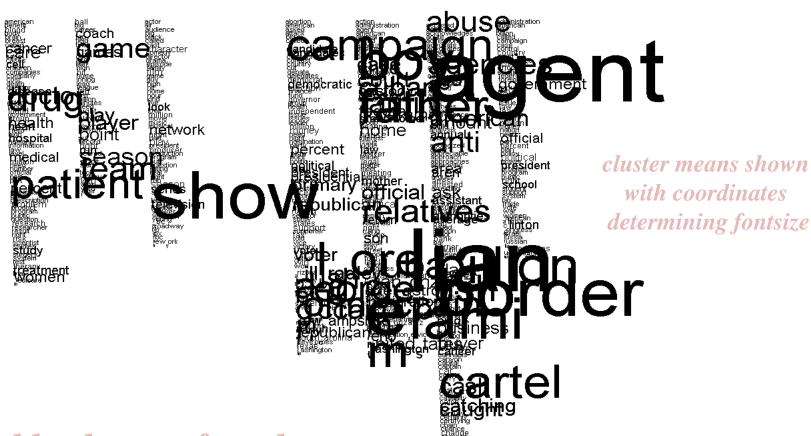
in one survey were unsure of how much of their data was inaccurate

#### Veracity

UNCERTAINTY OF DATA



# Kmeans Results from 10 million NYTimes articles



7 viable clusters found





# Big Data – Big Training

- "Data Scientist"
  - The "Hot new gig in town"
    - O'Reilly report
  - Data Scientist: The Sexiest Job of the 21st Century
    - Harvard Business Review, October 2012
    - The next sexy job in next 10 years will be statistician" Hal Varian, Google Chief Economist
    - Geek Chic Wall Street Journal new cool kids on campus
  - The future belongs to the companies and people that turn data into products
- "The human expertise to capture and analyze big data is both the most expensive and the most constraining factor for most organizations pursuing big data initiatives" – Thomas Davenport
- New curriculum Boot camps, Certificates, Data Science Institute, '14 MAS





# Big Data – Big Data Science

- "Data Scientist"
  - The "Hot new gig in town"
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  - Data Scientist: The Sexiest Job of the 21st Century
    - Harvard Business Review, October 2012
    - The next sexy job in next 10 years will be statistician" Hal Varian, Google Chief Economist
    - Geek Chic Wall Street Journal new cool kids on campus
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- "The human expertise to capture and analyze big data is both the most expensive and the most constraining factor for most organizations pursuing big data initiatives" – Thomas Davenport





# Data scientist: The hot new gig in tech

#### Article in Fortune

 "The unemployment rate in the U.S. continues to be abysmal (9.1% in July), but the tech world has spawned a new kind of highly skilled, nerdy-cool job that companies are scrambling to fill: data scientist"

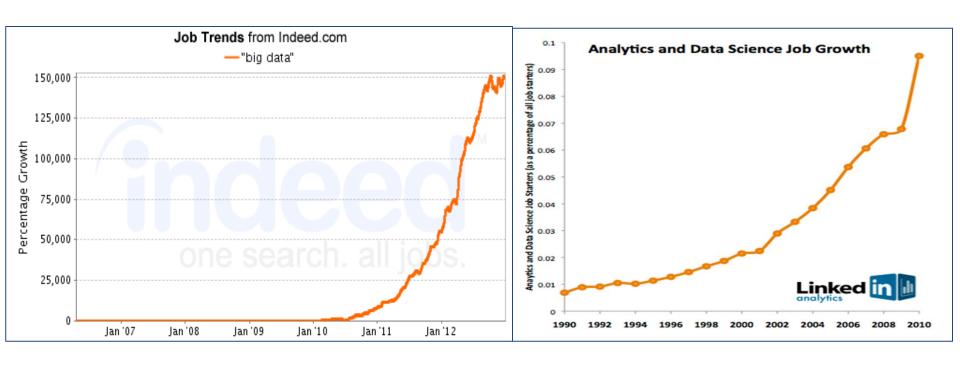
# McKinsey Global Institute "Big data Report"

 By 2018, the United States alone could face a shortage of 140,000 to 190,000 people with deep analytical skills as well as 1.5 million managers and analysts with the know-how to use the analysis of big data to make effective decisions





### Data Science Job Growth



# By 2018 shortage of 140-190,000 predictive analysts and 1.5M managers / analysts in the US

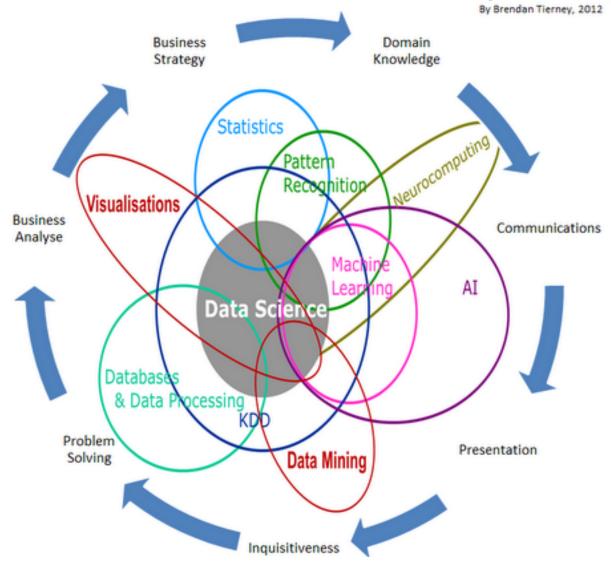




## Data Miners: Past and Present

- Traditional approaches have been for DM experts: "White-coat PhD statisticians"
  - DM tools also fairly expensive
- Today: approach is designed for those with some Database/Analytics skills
  - DM built into DB, easy to use GUI, Workflows
  - Many jobs available from Statistical analyst to Data Scientist!
- Data Science: The Art of mathematically sophisticated data engineers delivering insights from data into business decisions and systems

# Data Science Is Multidisciplinary







# Successful Data Scientist Characteristics

- Intellectual curiosity, Intuition
  - Find needle in a haystack
  - Ask the right questions value to the business
- Communication and engagements
- Presentation skills
  - Let the data speak but tell a story
  - Story teller drive business value not just data insights
- Creativity
  - Guide further investigation
- Business Savvy
  - Discovering patterns that identify risks and opportunities
  - Measure





# To Ph.D or NOT Ph.D? That is the Question!

#### LinkedIn Poll:

Do You Need a PhD to Analyze Big Data?

YES	NO
301 (12%)	2476 votes (87%)





# Data Scientist Self-ID

Data Developer	Developer	Engineer	
Data Researcher	Researcher	Scientist	Statistician
Data Creative	Jack of All Trades	Artist	Hacker
Data Businessperson	Leader	Businessperson	Entrepeneur

O'Reilly Strata Survey suggested Self-ID Group, along with the self-ID categories most strongly associated with each Group



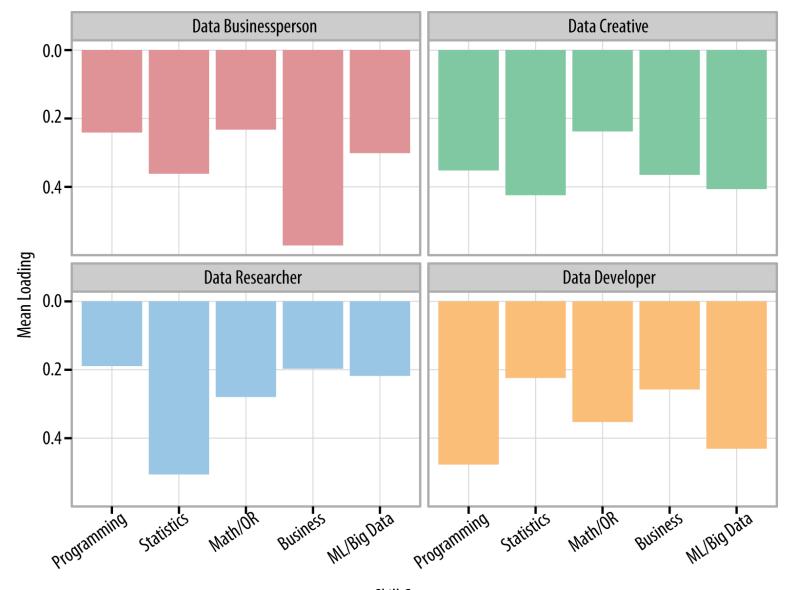


# **Strata Survey Skills**

Business	ML/Big Data	Math/OR	Programming	Statistics
Product Developement Business	Unstructured Data  Structured Data  Machine Learning  Big and Distributed Data	Optimization  Math  Graphical  Models  Bayesian /  Monte Carlo  Statistics  Algorithms	Systems Administration  Back End Programming  Front End Programming	Visualization  Temporal Statistics  Surveys and Marketing  Spatial Statistics  Science
		Simulation		Data Manipulation Classical Statistics









Skill Group

# Learning and Training Opportunities

- Many MS, MAS, Courses, Training, Workshops, Certificates, Boot camps, etc.
- Introduction to Data Science Example
  - Part 1: Data Manipulation at scale
    - Databases and the relational algebra
    - Parallel databases, parallel query processing, in-database analytics, MapReduce, Hadoop, relationship to databases, algorithms, extensions, languages
    - Key-value stores and NoSQL; Entity resolution, record linkage
  - Part 2: Analytics, Predictive Analytics, Text mining
  - Part 3: Communicating Results
    - Visualization, data products, visual data analytics
    - Provenance, privacy, ethics, governance SAN DIEGO SUPERCOMPUTER CENTER



# How long does it take for a beginner to become a good data scientist per Region?

Region (Count)	Avg Years to become a good data scientist
AU/NZ (9)	6.9 years
E. Europe (19)	5.9 years
US/Canada (143)	4.9 years
W. Europe (60)	4.9 years
Asia (25)	4.9 years
Africa/Middle East (9)	4.4 years
Latin America (12)	3.9 years





# INTRO TO MACHINE LEARNING DATA MINING PREDICTIVE ANALYTICS DATA SCIENCE





### **Necessity is the Mother of Invention**

#### Data explosion

Automated data collection tools and mature database technology lead to tremendous amounts of data stored in databases, data warehouses and other information repositories

"We are drowning in data, but starving for knowledge!" (John Naisbitt, 1982)





### **Necessity is the Mother of Invention**

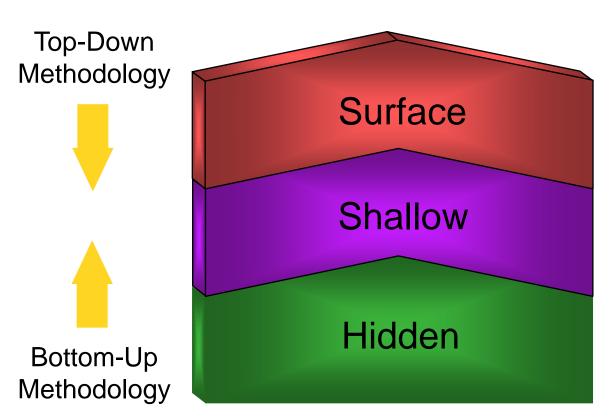
#### Solution

- Predictive Analytics or Data Mining
  - Extraction or "mining" of interesting knowledge (rules, regularities, patterns, constraints) from data in large databases
  - Data -driven discovery and modeling of hidden patterns in large volumes of data
  - Extraction of implicit, previously unknown and unexpected, potentially extremely useful information from data





#### **Predictive Analytics**



#### **Analytical Tools**

SQL tools for simple queries and reporting

Statistical & BI tools for summaries and analysis

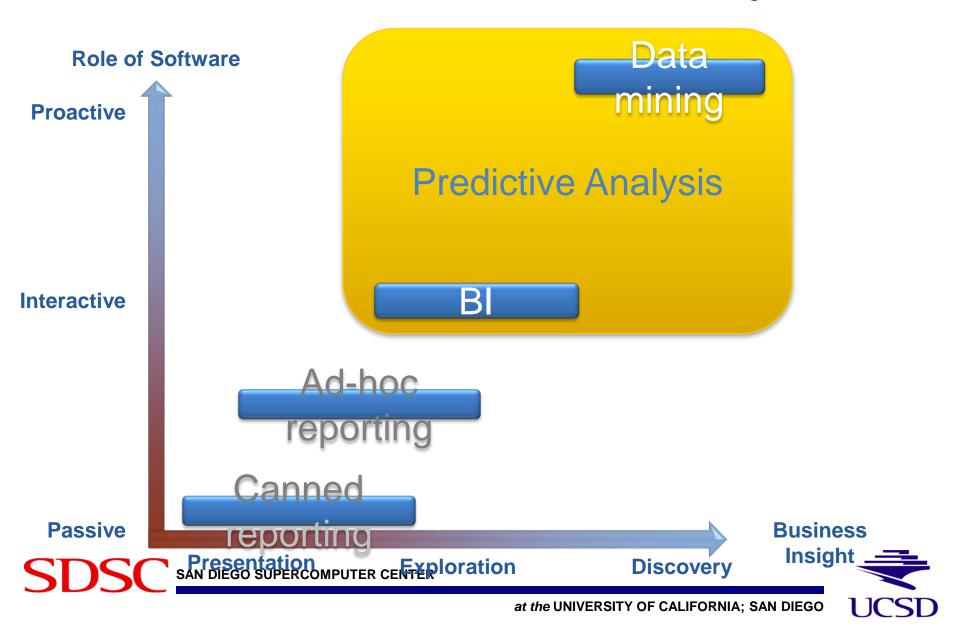
Data Mining methods for knowledge discovery





Query Reporting	BI	Data Mining
Extraction of data; detailed and/or summarized	Analysis, summaries, Trends	Discovery of hidden patterns, information, predicting future trends
Information	Analysis	Insight knowledge and prediction
Who purchased the product in the last 2 quarters?	What is an average income of the buyers per quarter by district?	Which customers are likely to buy a similar product in the future and why?

### DM Enables Predictive Analytics



#### What Is Data Mining?



- Combination of AI and statistical analysis to discover information that is "hidden" in the data
  - associations (e.g. linking purchase of pizza with beer)
  - sequences (e.g. tying events together: marriage and purchase of furniture)
  - classifications (e.g. recognizing patterns such as the attributes of employees that are most likely to quit)
  - forecasting (e.g. predicting buying habits of customers based on past patterns)



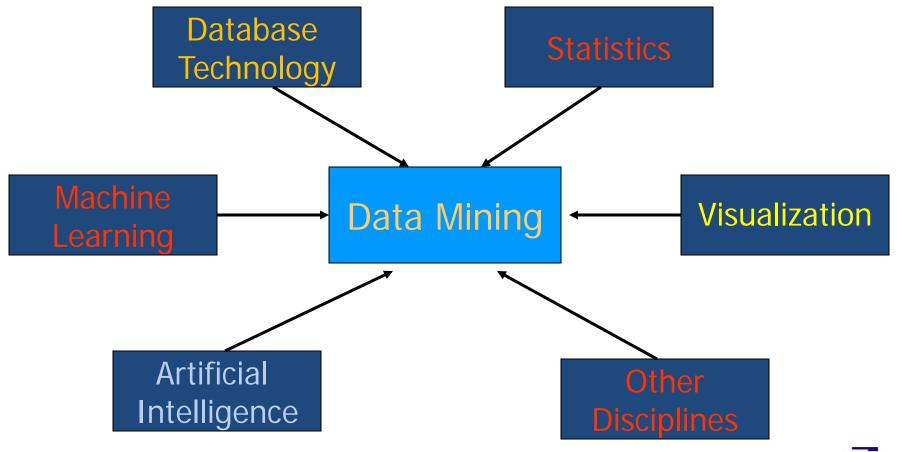
#### Data Mining is NOT...

- Data Warehousing
- (Deductive) query processing
  - SQL/ Reporting
- Software Agents
- Expert Systems
- Online Analytical Processing (OLAP)
- Statistical Analysis Tool
- Data visualization
- BI Business Intelligence





#### Multidisciplinary Field



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#### Data Mining is...

#### Multidisciplinary Field

- Database technology
- Artificial Intelligence
  - Machine Learning including Neural Networks
- Statistics
- Pattern recognition
- Knowledge-based systems/acquisition
- High-performance computing
- Data visualization
- Other Disciplines





### History of Data Mining





### **History**

- Emerged late 1980s
- Flourished –1990s
- Roots traced back along three family lines
  - Classical Statistics
  - Artificial Intelligence
  - Machine Learning





#### **Statistics**

- Foundation of most DM technologies
  - Regression analysis, standard distribution/deviation/variance, cluster analysis, confidence intervals
- Building blocks
- Significant role in today's data mining but alone is not powerful enough





### Artificial Intelligence

- Heuristics vs. Statistics
- Human-thought-like processing
- Requires vast computer processing power
- Supercomputers





### Machine Learning

- Union of statistics and Al
  - Blends AI heuristics with advanced statistical analysis
- Machine Learning let computer programs
  - learn about data they study make different decisions based on the quality of studied data
  - using statistics for fundamental concepts and adding more advanced AI heuristics and algorithms





### **Terminology**

- Gold Mining
- Knowledge mining from databases
- Knowledge extraction
- Data/pattern analysis
- Knowledge Discovery Databases or KDD
- Information harvesting
- Business intelligence
- Predictive Analytics
- Data Science





#### **TAXONOMY**

#### Predictive Methods

 Use some variables to predict some unknown or future values of other variables

#### Descriptive Methods

Find human –interpretable patterns that describe the data

#### Supervised vs. Unsupervised





#### What does Data Mining Do?

Explores
Your Data

Finds Patterns

Performs Predictions





#### What can we do with Data Mining?

- Exploratory Data Analysis
- Predictive Modeling: Classification and Regression
- Descriptive Modeling
  - Cluster analysis/segmentation
- Discovering Patterns and Rules
  - Association/Dependency rules
  - Sequential patterns
  - Temporal sequences
- Deviation detection





### Data Mining Applications

Science: Chemistry, Physics, Medicine, Energy

Biochemical analysis, remote sensors on a satellite, medical image analysis

Bioscience

Sequence-based analysis, protein structure and function prediction, protein family classification, microarray gene expression

• Pharmaceutical, Insurance, Health care, Medicine

Drug development, medical therapies, claims analysis, fraudulent behavior, medical diagnostics

Financial Industry, Banks, Businesses, E-commerce

Stock and investment analysis, identify loyal customers vs. risky customer, predict customer spending, risk management, sales forecasting

Market analysis and management

Target marketing, CRM, market basket analysis, cross selling, market segmentation

Risk analysis and management

Forecasting, customer retention, improved underwriting, quality control, competitive analysis

Sports and Entertainment

IBM Advanced Scout analyzed NBA game statistics (shots blocked, assists, and fouls) to gain competitive advantage for New York Knicks and Miami Heat



UCSD

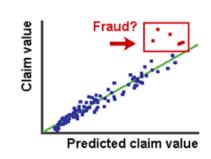
#### Data Mining Tasks

- Concept/Class description: Characterization and discrimination
  - Generalize, summarize, and contrast data characteristics, e.g., dry vs. wet regions; "normal" vs. fraudulent behavior
- Association (correlation and causality)
  - Multi-dimensional interactions and associations
     age(X, "20-29") ^ income(X, "60-90K") à buys(X, "TV")
     Hospital(area code) ^ procedure(X) ->claim (type) ^ claim(cost)





### Data Mining Tasks

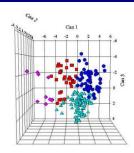


- Classification and Prediction
  - Finding models (functions) that describe and distinguish classes or concepts for future prediction
  - Example: classify countries based on climate, or classify cars based on gas mileage, fraud based on claims information, energy usage based on sensor data
  - Presentation:
    - If-THEN rules, decision-tree, classification rule, neural network
  - Prediction: Predict some unknown or missing numerical values





### Data Mining Tasks



#### Cluster analysis

- Class label is unknown: Group data to form new classes
- Clustering based on the principle: maximizing the intra-class similarity and minimizing the interclass similarity

#### Outlier analysis

- Data object that does not comply with the general behavior of the data
- Mostly considered as noise or exception, but is quite useful in fraud detection, rare events analysis

#### Trend and evolution analysis

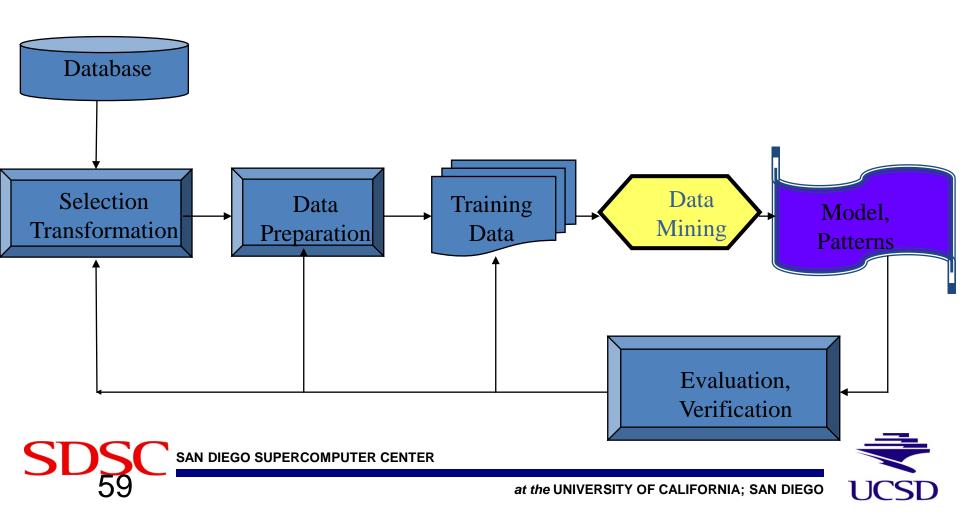
Trend and deviation: regression analysis





#### **KDD Process**





### **KDD Process Steps**

- Learning the application domain:
  - relevant prior knowledge and goals of application
- Creating a target data set: data selection
- Data cleaning and preprocessing: (may take 60% of effort!)
- Data reduction and transformation:
  - Find useful features, dimensionality/variable reduction, representation
- Choosing functions of data mining
  - summarization, classification, regression, association, clustering





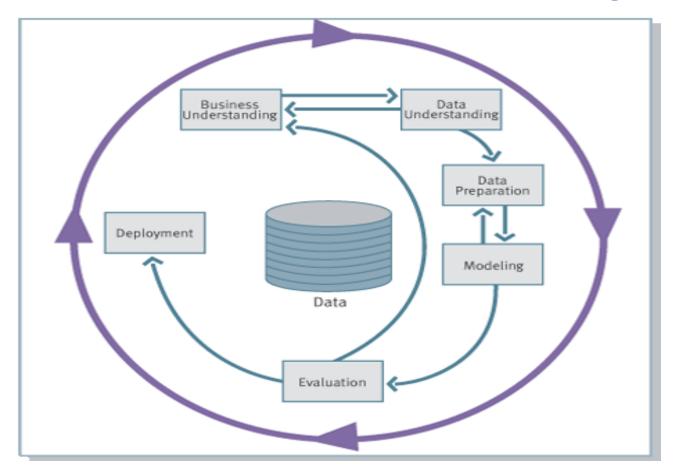
### **KDD Process Steps (2)**

- Choosing functions of data mining
  - summarization, classification, regression, association, clustering
- Choosing the mining algorithm(s)
- Data mining: search for patterns of interest
- Pattern evaluation and knowledge presentation
  - visualization, transformation, removing redundant patterns, etc.
- Use and integration of discovered knowledge





# CRISP-DM - Cross Industry Standard Process for Data Mining









### Learning and Modeling Methods

- Decision Tree Induction (C4.5, J48)
- Regression Tree Induction (CART, MP5)
- Multivariate Regression Tree (MARS)
- Clustering (K-means, EM, Cobweb)
- Artificial Neural Networks (Backpropagation, Recurrent)
- Support Vector Machines (SVM)
- Various other models





#### **Decision Tree Induction**

- Method for approximating discrete-valued functions
  - robust to noisy/missing data
  - can learn non-linear relationships
  - inductive bias towards shorter trees





#### **Decision Tree Induction**

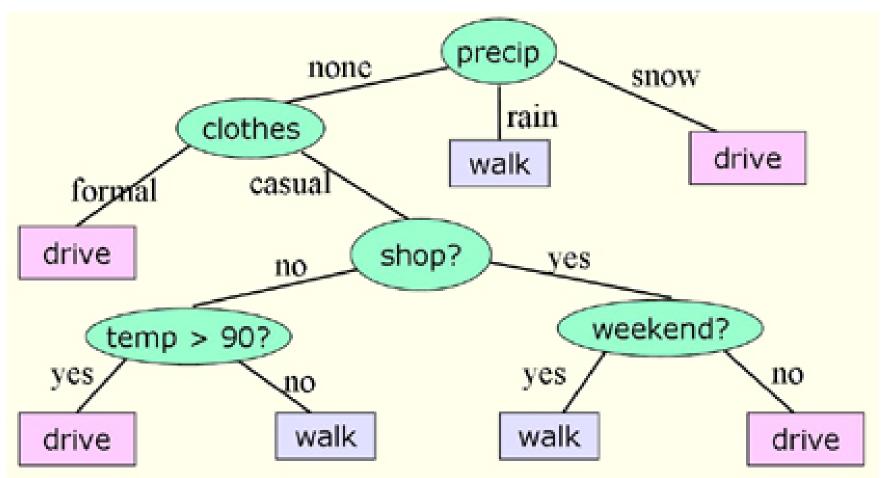
#### Applications:

- medical diagnosis ex. heart disease
- analysis of complex chemical compounds
- classifying equipment malfunction
- risk of loan applicants
- Boston housing project price prediction
- fraud detection





#### Decision Tree Example







#### Regression Tree Induction

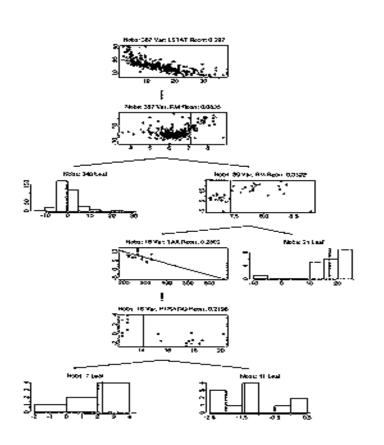
#### Why Regression tree?

- Ability to:
  - Predict continuous variable
  - Model conditional effects
  - Model uncertainty





#### Regression Trees



- Continuous goal variables
- Induction by means of an efficient recursive partitioning algorithm
- Uses linear regression to select internal nodes

Quinlan, 1992





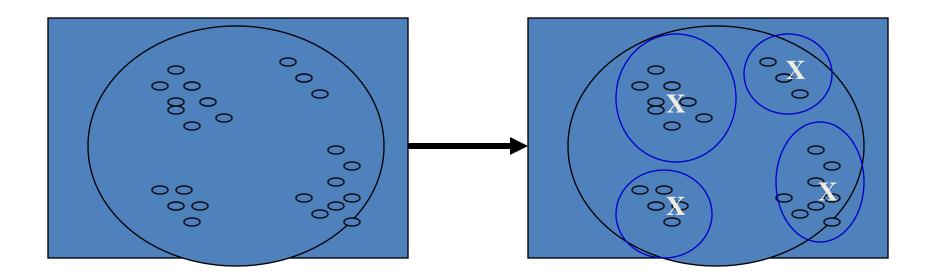
### Clustering

- Basic idea: Group similar things together
- Unsupervised Learning Useful when no other info is available
- K-means
  - Partitioning instances into <u>k</u> disjoint clusters
  - Measure of similarity





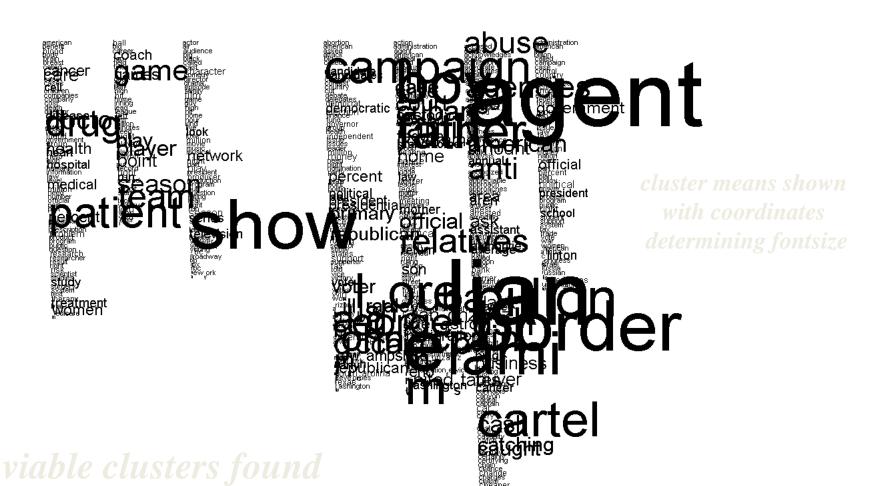
### Clustering







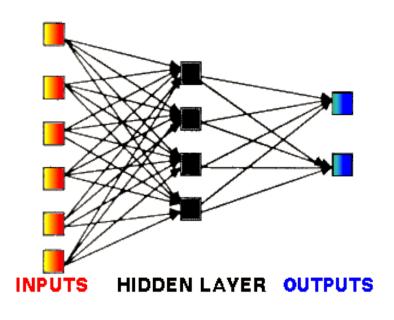
## Kmeans Results from 10 million NYTimes articles





UCSD

### Artificial Neural Networks (ANNs)



- Network of many simple units
- Main Components
  - Inputs
  - Hidden layers
  - Outputs
- Adjusting weights of connections
- Backpropagation





#### **Evaluation**

- Error on the training data vs. performance on future/unseen data
- Simple solution
  - Split data into training and test set
  - Re-substitution error
    - error rate obtained from the training data
- Three sets
  - training data, validation data, and test data





### Training and Testing

- Test set
  - set of independent instances that have not been used in formation of classifier in any way
  - Assumption
    - data contains representative samples of the underlying problem
- Example: classifiers built using customer data from two different towns A and B
  - To estimate performance of classifier from town in completely new town, test it on data from B





#### **Error Estimation Methods**

- Holdout
  - ½ training and ½ testing (2/3&1/3)
- Repeated Holdout Method
  - Random sampling repeated holdout
- Cross-validation
  - Partition in K disjoint clusters
  - Train k-1, test on remaining
- Leave-one-out Method
- Bootstrap
  - Sampling with replacement



### Data Mining Challenges

- Computationally expensive to investigate all possibilities
- Dealing with noise/missing information and errors in data
- Mining methodology and user interaction
  - Mining different kinds of knowledge in databases
  - Incorporation of background knowledge
  - Handling noise and incomplete data
  - Pattern evaluation: the interestingness problem
  - Expression and visualization of data mining results





### Data Mining Heuristics and Guide

- Choosing appropriate attributes/input representation
- Finding the minimal attribute space
- Finding adequate evaluation function(s)
- Extracting meaningful information
- Not overfitting





#### Available Data Mining Tools

#### COTs:

- **IBM Intelligent Miner**
- **SAS Enterprise Miner**
- Oracle ODM
- **■** Microstrategy
- **■** Microsoft DBMiner
- Pentaho
- Matlab
- Teradata

#### **Open Source:**

- **■** Python
- $\blacksquare R$
- **WEKA**
- **KNIME**
- Orange
- RapidMiner
- **■** Rattle
- **■** Mahout
- **■** MILib



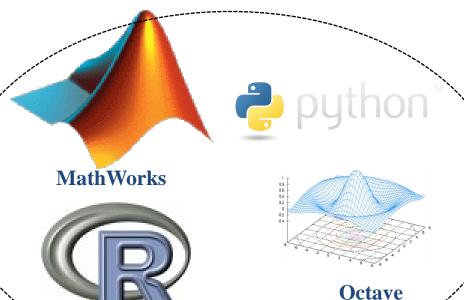


### Data mining applications at SDSC

**DM Suites** 







Computational Packages with DM tools

Others as Requested

Libraries for building tools

A library of Fundamental Algorithmic and Statistical Tools

**FASTlib** 



The Phoenix System for MapReduce SAN DIÈGO SUPERCOMPUTER CENTI Programming

at the UNIVERSITY OF CALIFORNIA; SAN DIEGO



### Summary

- Discovering interesting patterns from large amounts of data
- CRISP-DM Industry standard
- Learn from the past
  - High quality, evidence based decisions
- Predict for the future
  - Prevent future instances of fraud, waste & abuse
- React to changing circumstances
  - Current models, continuous learning





## Thank you!











#### **Questions?**





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