DSAA 5002: Knowledge Discovery and Data Mining in Data Science

Acknowledgement: Slides modified by Dr. Lei Chen based on the slides provided by Jiawei Han, Micheline Kamber, and Jian Pei

Course Description

- Data Mining and Knowledge Discovery
- Topics:
  - Introduction
  - Getting to Know Your Data
  - Data Preprocessing
  - Data Warehouse and OLAP Technology: An Introduction
  - Advanced Data Cube Technology
  - Mining Frequent Patterns & Association: Basic Concepts
  - Mining Frequent Patterns & Association: Advanced Methods
  - Classification: Basic Concepts
  - Classification: Advanced Methods
  - Cluster Analysis: Basic Concepts
  - Cluster Analysis: Advanced Methods
  - Outlier Analysis:

Important Sites

- Instructor Web Site
  - http://www.cse.ust.hk/~leichen/courses/DSAA5002/
- TA:
- Assignment Hand-in: online
- Course Discussion Site:
  - Check out the web site

Prerequisites

- Statistics and Probability would help,
  - but not necessary
- Pattern Recognition would help,
  - but not necessary
- Databases
  - Knowledge of SQL and relational algebra
  - But not necessary
- One programming language
  - One of Java, C++, Perl, Matlab, etc.
  - Will need to read Java Library

Grading

- Grade Distribution:
  - Assignments 30%
  - Project 30%
  - Exams 40%
    - Midterm 15%
    - Final 25%

Introduction

- Why Data Mining?
- What Is Data Mining?
- A Multi-Dimensional View of Data Mining
- What Kinds of Data Can Be Mined?
- What Kinds of Patterns Can Be Mined?
- What Kinds of Technologies Are Used?
- What Kinds of Applications Are Targeted?
- Major Issues in Data Mining
- A Brief History of Data Mining and Data Mining Society
- Summary

Background: DL applications are ubiquitous

- DL has made a huge *success* over the past years.

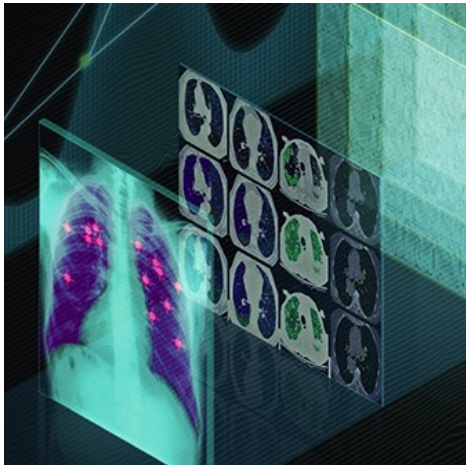
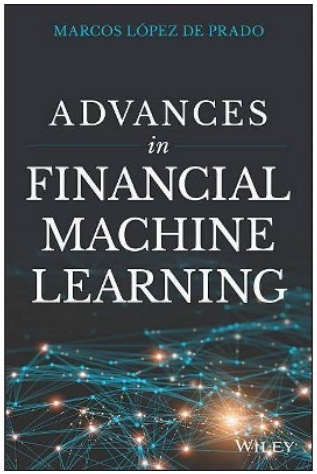


Image Recognition

Natural Language Processing

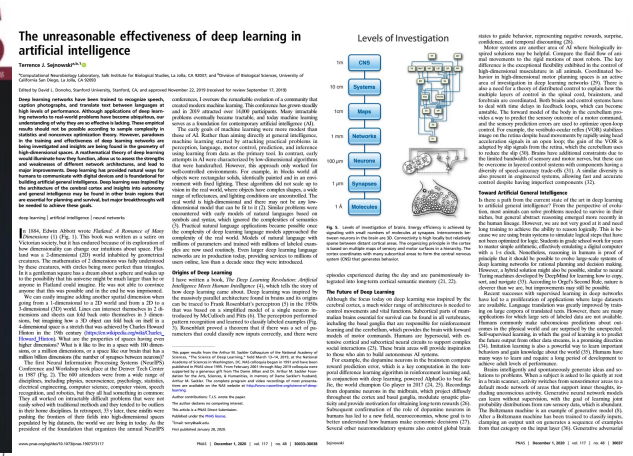


Smart Finance

Intelligent Transportation

Background: Data is the new oil

- The first secret of DL's success: *big data*


The unreasonable effectiveness of deep learning in artificial intelligence

Terrence J. Sejnowski

Levels of Investigation

"The world's *most valuable resource* is no longer oil, but data". -- The Economist, 2017

"*Recent successes* in deep networks have led to a proliferation of applications where *large datasets are available*". -- Terrence J. Sejnowski, in PNAS 2020

Motivation: Why data management for DL?

: related to data management

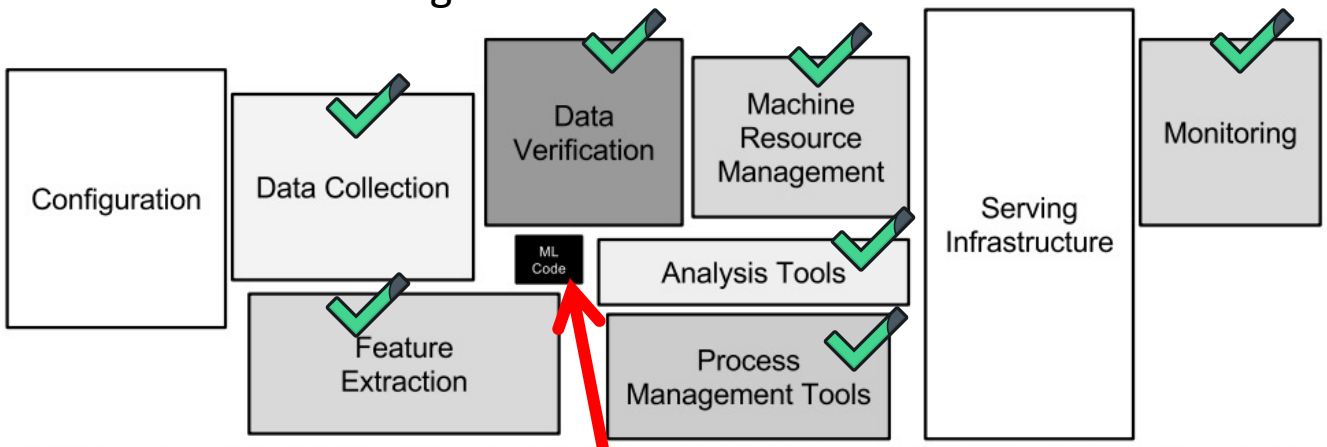
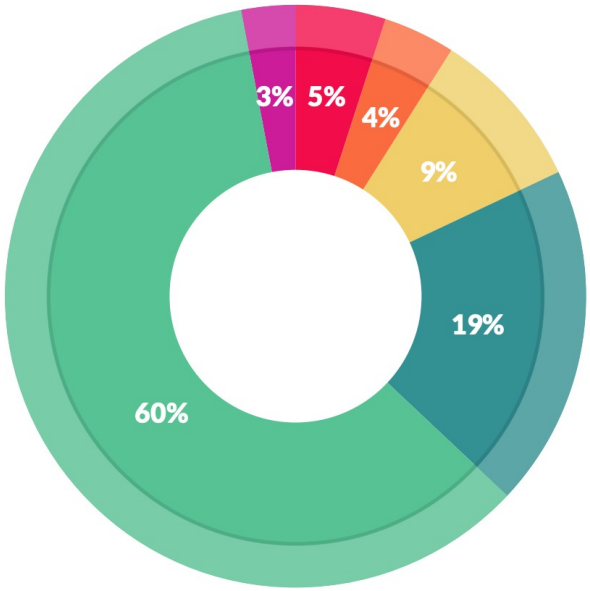


Figure 1: Only a small fraction of real-world ML systems is composed of the ML code, as shown by the small black box in the middle. The required surrounding infrastructure is vast and complex.

Google

"In Google, only a tiny fraction of the code in many ML systems is actually devoted to learning."

Motivation: Why data management for DL?



What data scientists spend the most time doing

- *Building training sets: 3%*
- *Cleaning and organizing data: 60%*
- *Collecting data sets; 19%*
- *Mining data for patterns: 9%*
- *Refining algorithms: 4%*
- *Other: 5%*

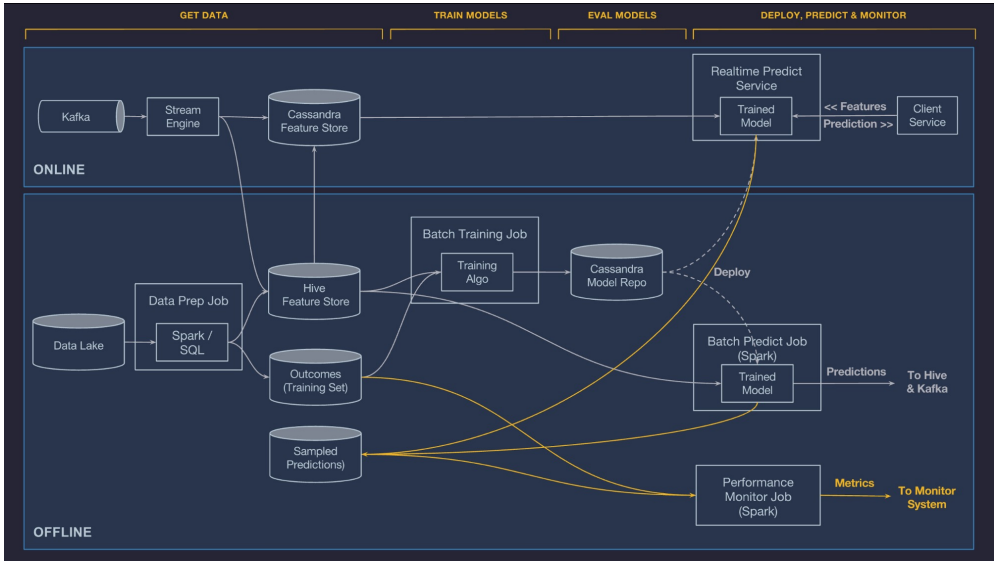
"80% of ML users' time/effort (often more) spent on data issues!"

Motivation: Why data management for DL?

Meet Michelangelo: Uber's Machine Learning Platform

Jeremy Hermann and Mike Del Balso

September 5, 2017



Uber

"Building and managing data pipelines is typically one of the most costly pieces of a complete machine learning solution."

Benefits of data management for DL

Key concerns in DL:

- Accuracy
- Runtime efficiency (sometimes)

Additional key *practical* concerns in DL systems:

- Scalability (and efficiency at scale)
- Usability
- Manageability
- Developability

Can often trade off accuracy a bit to gain on the rest!

Long-standing concerns in the DB systems world!

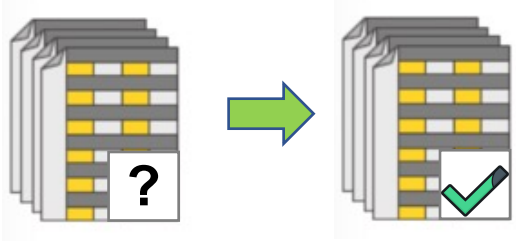
Challenges: data management for DL

- "Data management …": How to organize, query, scale, and manage the analysis of large and complex datasets?
- "… for DL": *three fundamental challenges* in our proposal.
  - Data preparation for DL
  - Optimized training in DL
  - Result Validation and Explanation in DL

Challenge 1: Data preparation for DL

- Why *data preparation for DL* is important? Data preparation aims to collect enough qualified data for training.
- There are two steps in data preparation for DL:
  - Data extraction and integration
  - Semi-automatic Data Labeling

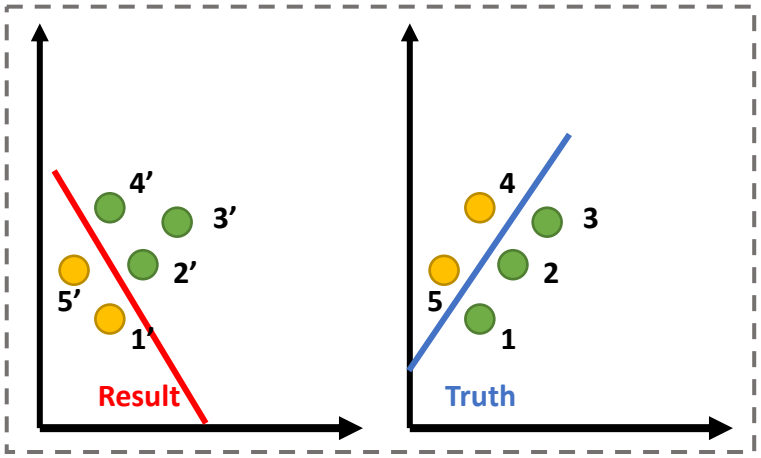
1.1 Data Extraction and Integration



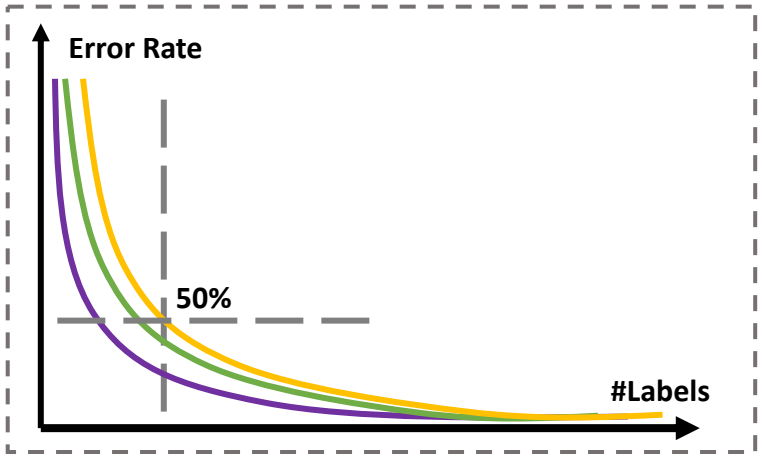
1.2 Semi-automatic Data Labeling

Challenge 1: Data preparation for DL

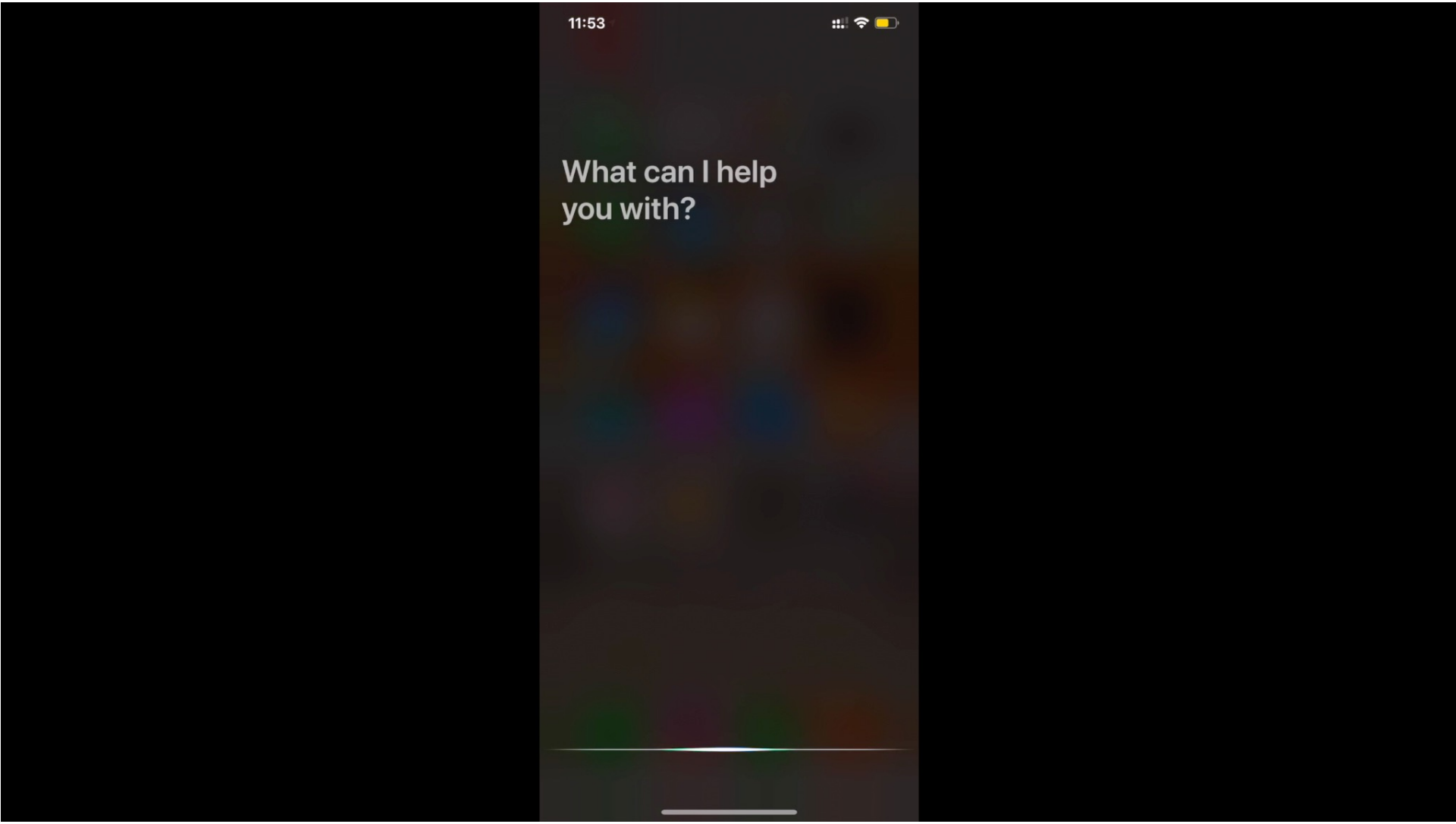
- What will happen in DL when the data preparation is bad?
  - Eg, noised data, insufficient, etc.



Noised data can result in low accuracy

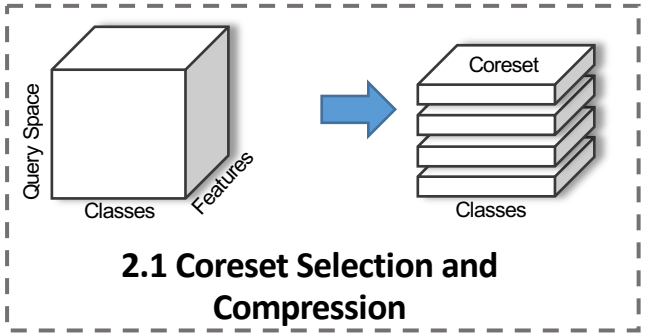


Insufficient data can result in low accuracy

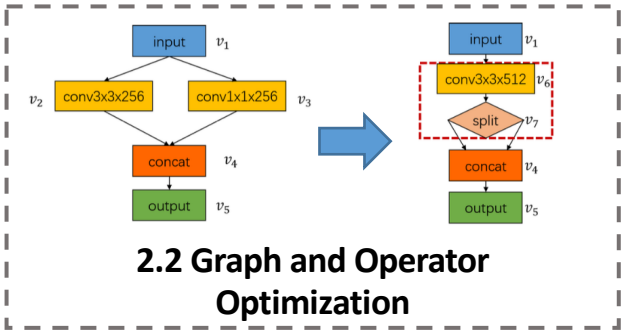

11:53
What can I help you with?

Challenge 2: Optimized Training in DL

- Why *optimized training in DL* is important? Optimized training achieves a better balance between efficiency and accuracy.
- There are two ways to optimize training in DL:
  - Coreset Selection and Data Compression
  - Graph and Operator Optimization



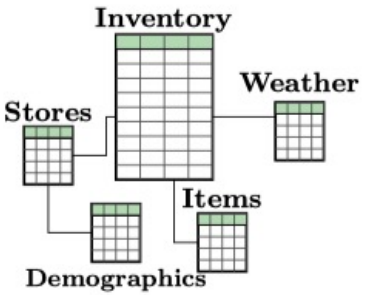
2.1 Coreset Selection and Compression



2.2 Graph and Operator Optimization

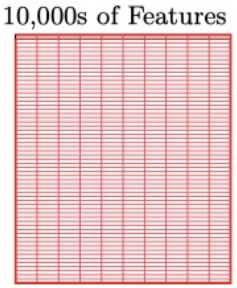
Challenge 2: Optimized Training in DL

- What will happen in DL when the amount of input data is too huge?



Relational Data

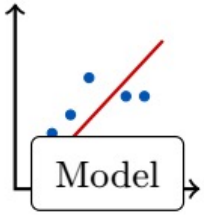
Inventory⋈Stores⋈ …⋈Demographics



Training Data

TensorFlow

PyTorch



Models

Relation	Cardinality/Attrs	CSV Size
Inventory	84,055,817 / 4	2 GB
Items	5,618 / 5	129 KB
Stores	1,317 / 15	139 KB
Demogr.	1,302 / 16	161 KB
Weather	1,159,457 / 8	33 MB
Join	84,055,817 / 44	23GB

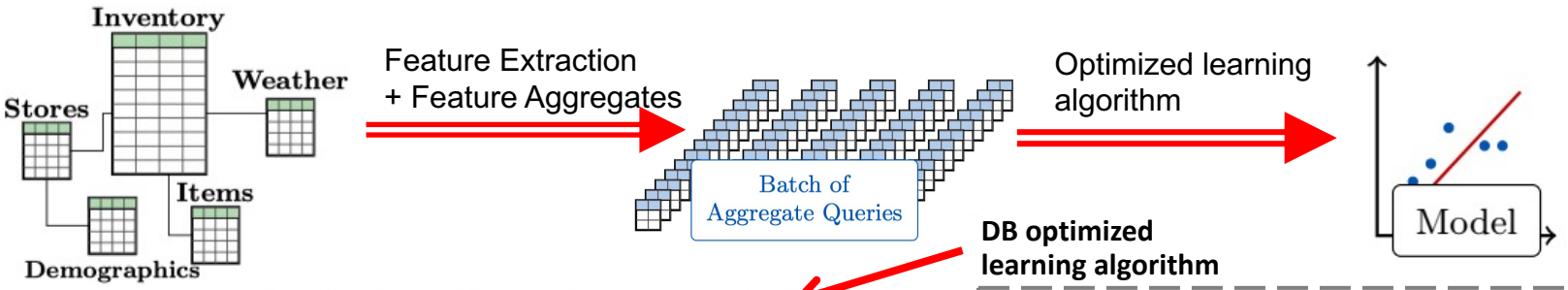
When tables are joined, data gets larger.

	PostgreSQL+TensorFlow Time	CSV Size
Database	–	2.1 GB
Join	152.06 secs	23 GB
Export	351.76 secs	23 GB
Shuffling	5,488.73 secs	23 GB
Query batch	–	–
Grad Descent	7,249.58 secs	–
Total time	13,242.13 secs	

High Training time

Challenge 2: Optimized Training in DL

- What will happen in DL when the amount of input data is too huge?



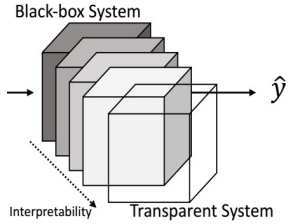
	PostgreSQL+TensorFlow		LMFAO	
	Time	CSV Size	Time	CSV Size
Database	–	2.1 GB	–	2.1 GB
Join	152.06 secs	23 GB	–	–
Export	351.76 secs	23 GB	–	–
Shuffling	5,488.73 secs	23 GB	–	–
Query batch	–	–	6.08 secs	37 KB
Grad Descent	7,249.58 secs	–	0.05 secs	–
Total time	13,242.13 secs		6.13 secs	

- *2,160× faster while being more accurate (RMSE on 2% test data)*
- *TensorFlow trains one model. Our approach takes < 0.1 sec for any extra model over a subset of the given feature set.*

Challenge 3: Result Validation and Explanation in DL

- Why *Result validation and explanation in DL* is important?
  Result validation ensures the effectiveness of the DL model.
  Result explanation improves the transparency of the DL model.
- There are two things we can work on:
  - Result validation
  - Explanation in DL

3.1 Result Validation



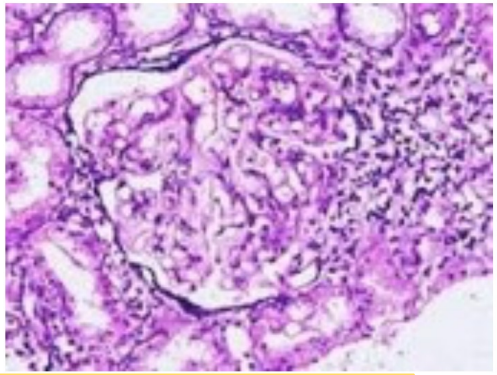
3.2 Result Explanation

Challenge 3: Result Validation and Explanation in DL

- What will happen when DL model is a blackbox?
  - Wrong decision can be dangerous for critical systems.

"Autonomous car crashes, because it wrongly recognizes …"

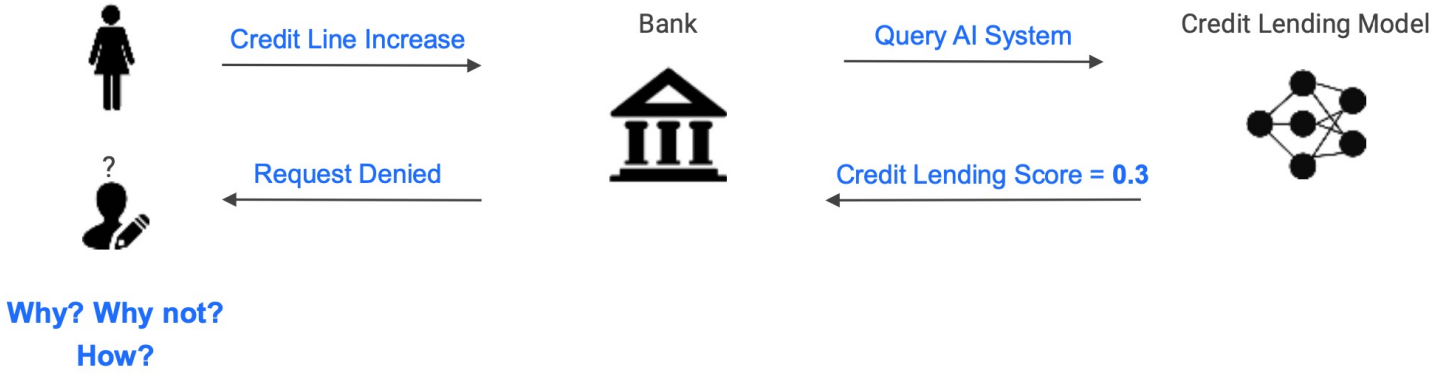
"AI medical diagnosis system misclassifies patient's disease …"



[Samek et al., 2018] Wojciech Samek and Alexander Binder. Tutorial on Interpretable Machine Learning. MICCAI 2018.

Challenge 3: Result Validation and Explanation in DL

- What will happen when DL model is a blackbox?
  - Client can't trust your model in banking.



[Geyik et al., 2019] Sahin Cem Geyik, Krishnaram Kenthapadi, Varun Mithal, Krishna Gade and Ankur Taly . Explainable AI in Industry. KDD 2019.

Why Data Mining?

- The Explosive Growth of Data: from terabytes to petabytes
  - Data collection and data availability
    - Automated data collection tools, database systems, Web, computerized society
  - Major sources of abundant data
    - Business: Web, e-commerce, transactions, stocks, …
    - Science: Remote sensing, bioinformatics, scientific simulation, …
    - Society and everyone: news, digital cameras, YouTube
- We are drowning in data, but starving for knowledge!
- "Necessity is the mother of invention"—Data mining—Automated analysis of massive data sets

Evolution of Sciences: New Data Science Era

- Before 1600: **Empirical science**
- 1600-1950s: **Theoretical science**
  - Each discipline has grown a *theoretical* component. Theoretical models often motivate experiments and generalize our understanding.
- 1950s-1990s: **Computational science**
  - Over the last 50 years, most disciplines have grown a third, *computational* branch (e.g. empirical, theoretical, and computational ecology, or physics, or linguistics.)
  - Computational Science traditionally meant simulation. It grew out of our inability to find closed-form solutions for complex mathematical models.
- 1990-now: **Data science**
  - The flood of data from new scientific instruments and simulations
  - The ability to economically store and manage petabytes of data online
  - The Internet and computing Grid that makes all these archives universally accessible
  - Scientific info. management, acquisition, organization, query, and visualization tasks scale almost linearly with data volumes
  - Data mining is a major new challenge!
- Jim Gray and Alex Szalay, *The World Wide Telescope: An Archetype for Online Science*, Comm. ACM, 45(11): 50-54, Nov. 2002

Chapter 1. Introduction

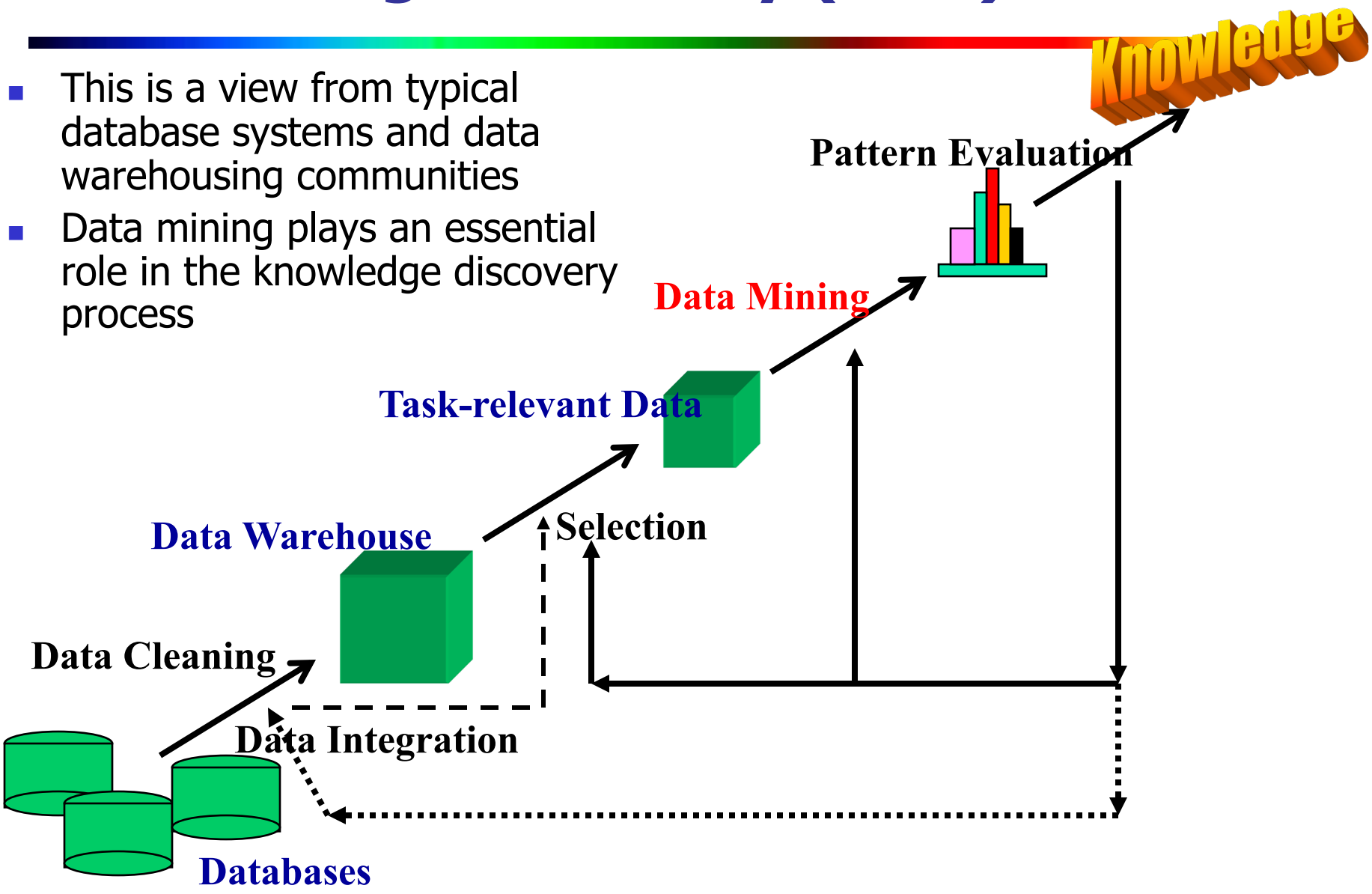
- Why Data Mining?
- What Is Data Mining?
- A Multi-Dimensional View of Data Mining
- What Kinds of Data Can Be Mined?
- What Kinds of Patterns Can Be Mined?
- What Kinds of Technologies Are Used?
- What Kinds of Applications Are Targeted?
- Major Issues in Data Mining
- A Brief History of Data Mining and Data Mining Society
- Summary

What Is Data Mining?

- Data mining (knowledge discovery from data)
  - Extraction of interesting (non-trivial, implicit, previously unknown and potentially useful) patterns or knowledge from huge amount of data
  - Data mining: a misnomer?
- Alternative names
  - Knowledge discovery (mining) in databases (KDD), knowledge extraction, data/pattern analysis, data archeology, data dredging, information harvesting, business intelligence, etc.
- Watch out: Is everything "data mining"?
  - Simple search and query processing
  - (Deductive) expert systems

Knowledge Discovery (KDD) Process

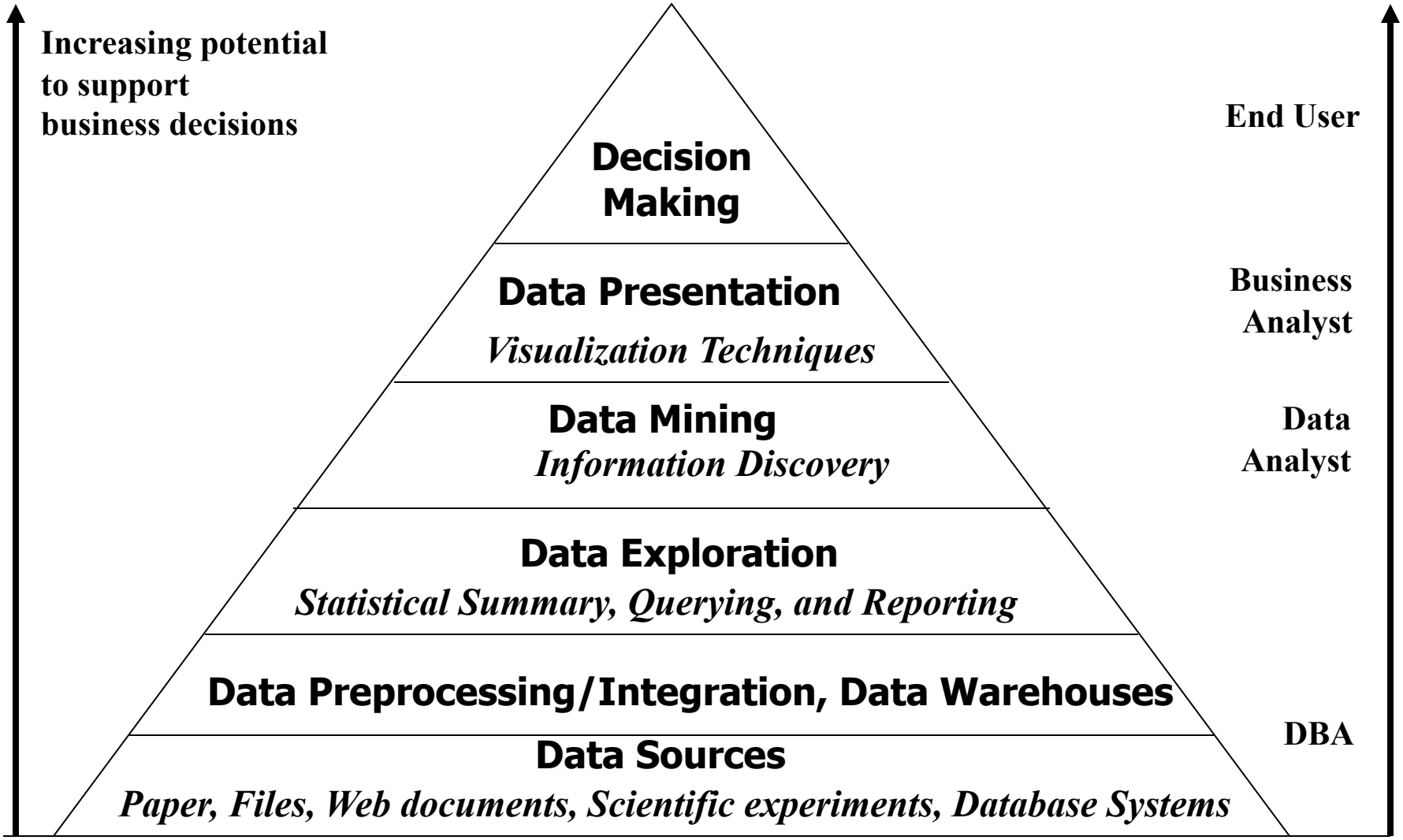
- This is a view from typical database systems and data warehousing communities
- Data mining plays an essential role in the knowledge discovery process



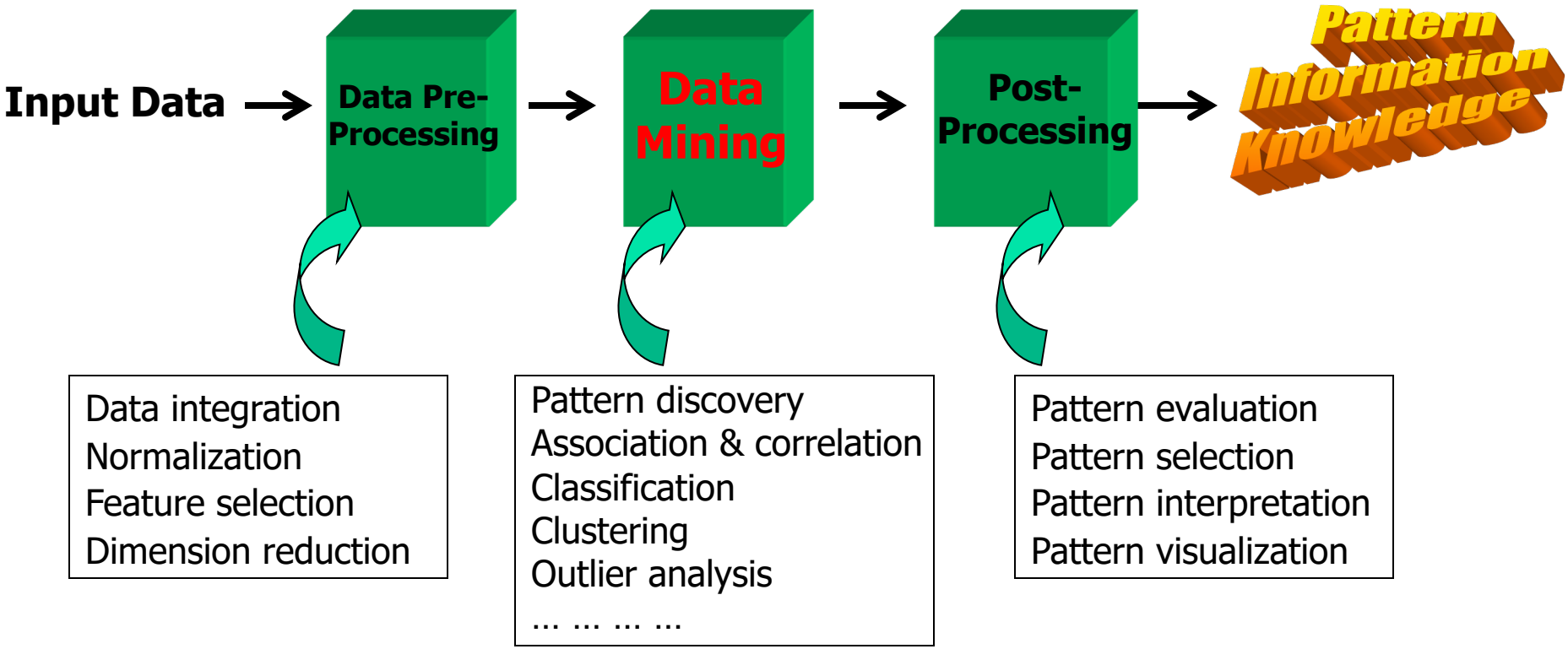
Example: A Web Mining Framework

- Web mining usually involves
  - Data cleaning
  - Data integration from multiple sources
  - Warehousing the data
  - Data cube construction
  - Data selection for data mining
  - Data mining
  - Presentation of the mining results
  - Patterns and knowledge to be used or stored into knowledge-base

Data Mining in Business Intelligence



KDD Process: A Typical View from ML and Statistics



- This is a view from typical machine learning and statistics communities

Which View Do You Prefer?

- Which view do you prefer?
  - KDD vs. ML/Stat. vs. Business Intelligence
  - Depending on the data, applications, and your focus
- Data Mining vs. Data Exploration
  - Business intelligence view
    - Warehouse, data cube, reporting but not much mining
  - Business objects vs. data mining tools
  - Supply chain example: mining vs. OLAP vs. presentation tools
  - Data presentation vs. data exploration

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Multi-Dimensional View of Data Mining

- **Data to be mined**
  - Database data (extended-relational, object-oriented, heterogeneous, legacy), data warehouse, transactional data, stream, spatiotemporal, time-series, sequence, text and web, multi-media, graphs & social and information networks
- **Knowledge to be mined (or: Data mining functions)**
  - Characterization, discrimination, association, classification, clustering, trend/deviation, outlier analysis, etc.
  - Descriptive vs. predictive data mining
  - Multiple/integrated functions and mining at multiple levels
- **Techniques utilized**
  - Data-intensive, data warehouse (OLAP), machine learning, statistics, pattern recognition, visualization, high-performance, etc.
- **Applications adapted**
  - Retail, telecommunication, banking, fraud analysis, bio-data mining, stock market analysis, text mining, Web mining, etc.

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Data Mining: On What Kinds of Data?

- Database-oriented data sets and applications
  - Relational database, data warehouse, transactional database
- Advanced data sets and advanced applications
  - Data streams and sensor data
  - Time-series data, temporal data, sequence data (incl. bio-sequences)
  - Structure data, graphs, social networks and multi-linked data
  - Object-relational databases
  - Heterogeneous databases and legacy databases
  - Spatial data and spatiotemporal data
  - Multimedia database
  - Text databases
  - The World-Wide Web

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Data Mining Function: (1) Generalization

- Information integration and data warehouse construction
  - Data cleaning, transformation, integration, and multidimensional data model
- Data cube technology
  - Scalable methods for computing (i.e., materializing) multidimensional aggregates
  - OLAP (online analytical processing)
- Multidimensional concept description: Characterization and discrimination
  - Generalize, summarize, and contrast data characteristics, e.g., dry vs. wet region

Data Mining Function: (2) Association and Correlation Analysis

- Frequent patterns (or frequent itemsets)
  - What items are frequently purchased together in your Walmart?
- Association, correlation vs. causality
  - A typical association rule
    - Diaper → Beer [0.5%, 75%] (support, confidence)
  - Are strongly associated items also strongly correlated?
- How to mine such patterns and rules efficiently in large datasets?
- How to use such patterns for classification, clustering, and other applications?

Data Mining Function: (3) Classification

- Classification and label prediction
  - Construct models (functions) based on some training examples
  - Describe and distinguish classes or concepts for future prediction
    - E.g., classify countries based on (climate), or classify cars based on (gas mileage)
  - Predict some unknown class labels
- Typical methods
  - Decision trees, naïve Bayesian classification, support vector machines, neural networks, rule-based classification, pattern-based classification, logistic regression, …
- Typical applications:
  - Credit card fraud detection, direct marketing, classifying stars, diseases, web-pages, …

Data Mining Function: (4) Cluster Analysis

- Unsupervised learning (i.e., Class label is unknown)
- Group data to form new categories (i.e., clusters), e.g., cluster houses to find distribution patterns
- Principle: Maximizing intra-class similarity & minimizing interclass similarity
- Many methods and applications

Data Mining Function: (5) Outlier Analysis

- Outlier analysis
  - Outlier: A data object that does not comply with the general behavior of the data
  - Noise or exception? — One person's garbage could be another person's treasure
  - Methods: by product of clustering or regression analysis, …
  - Useful in fraud detection, rare events analysis

Time and Ordering: Sequential Pattern, Trend and Evolution Analysis

- Sequence, trend and evolution analysis
  - Trend, time-series, and deviation analysis: e.g., regression and value prediction
  - Sequential pattern mining
    - e.g., first buy digital camera, then buy large SD memory cards
  - Periodicity analysis
  - Motifs and biological sequence analysis
    - Approximate and consecutive motifs
  - Similarity-based analysis
- Mining data streams
  - Ordered, time-varying, potentially infinite, data streams

Structure and Network Analysis

- Graph mining
  - Finding frequent subgraphs (e.g., chemical compounds), trees (XML), substructures (web fragments)
- Information network analysis
  - Social networks: actors (objects, nodes) and relationships (edges)
    - e.g., author networks in CS, terrorist networks
  - Multiple heterogeneous networks
    - A person could be multiple information networks: friends, family, classmates, …
  - Links carry a lot of semantic information: Link mining
- Web mining
  - Web is a big information network: from PageRank to Google
  - Analysis of Web information networks
    - Web community discovery, opinion mining, usage mining, …

Evaluation of Knowledge

- Are all mined knowledge interesting?
  - One can mine tremendous amount of "patterns" and knowledge
  - Some may fit only certain dimension space (time, location, …)
  - Some may not be representative, may be transient, …
- Evaluation of mined knowledge → directly mine only interesting knowledge?
  - Descriptive vs. predictive
  - Coverage
  - Typicality vs. novelty
  - Accuracy
  - Timeliness
  - …

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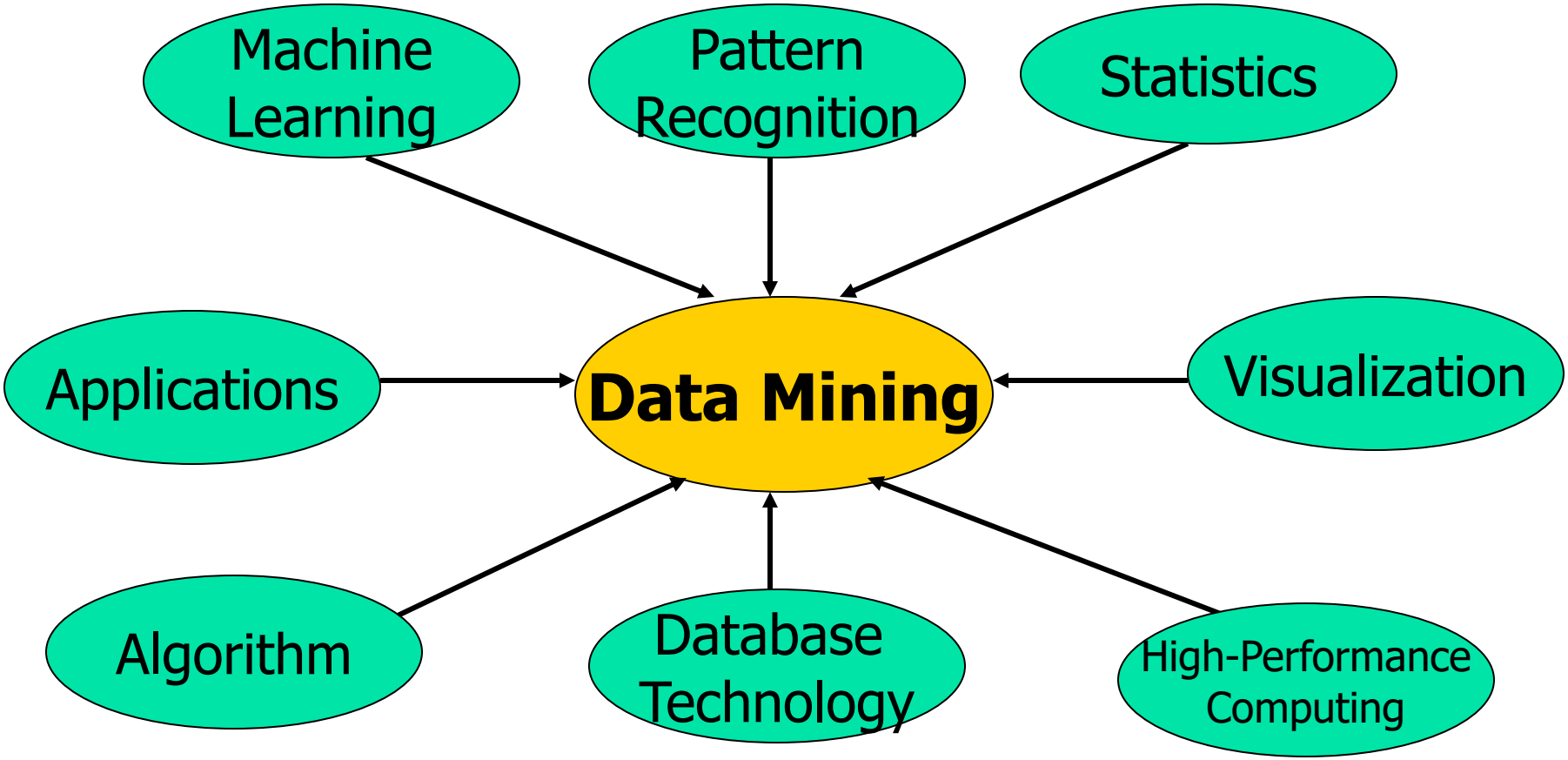
Data Mining: Confluence of Multiple Disciplines



Why Confluence of Multiple Disciplines?

- Tremendous amount of data
  - Algorithms must be highly scalable to handle such as tera-bytes of data
- High-dimensionality of data
  - Micro-array may have tens of thousands of dimensions
- High complexity of data
  - Data streams and sensor data
  - Time-series data, temporal data, sequence data
  - Structure data, graphs, social networks and multi-linked data
  - Heterogeneous databases and legacy databases
  - Spatial, spatiotemporal, multimedia, text and Web data
  - Software programs, scientific simulations
- New and sophisticated applications

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- Why Data Mining?
- What Is Data Mining?
- A Multi-Dimensional View of Data Mining
- What Kinds of Data Can Be Mined?
- What Kinds of Patterns Can Be Mined?
- What Kinds of Technologies Are Used?
- What Kinds of Applications Are Targeted?
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Applications of Data Mining

- Web page analysis: from web page classification, clustering to PageRank & HITS algorithms
- Collaborative analysis & recommender systems
- Basket data analysis to targeted marketing
- Biological and medical data analysis: classification, cluster analysis (microarray data analysis), biological sequence analysis, biological network analysis
- Data mining and software engineering (e.g., IEEE Computer, Aug. 2009 issue)
- From major dedicated data mining systems/tools (e.g., SAS, MS SQL-Server Analysis Manager, Oracle Data Mining Tools) to invisible data mining

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Major Issues in Data Mining (1)

- Mining Methodology
  - Mining various and new kinds of knowledge
  - Mining knowledge in multi-dimensional space
  - Data mining: An interdisciplinary effort
  - Boosting the power of discovery in a networked environment
  - Handling noise, uncertainty, and incompleteness of data
  - Pattern evaluation and pattern- or constraint-guided mining
- User Interaction
  - Interactive mining
  - Incorporation of background knowledge
  - Presentation and visualization of data mining results

Major Issues in Data Mining (2)

- Efficiency and Scalability
  - Efficiency and scalability of data mining algorithms
  - Parallel, distributed, stream, and incremental mining methods
- Diversity of data types
  - Handling complex types of data
  - Mining dynamic, networked, and global data repositories
- Data mining and society
  - Social impacts of data mining
  - Privacy-preserving data mining
  - Invisible data mining

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A Brief History of Data Mining Society

- 1989 IJCAI Workshop on Knowledge Discovery in Databases
  - Knowledge Discovery in Databases (G. Piatetsky-Shapiro and W. Frawley, 1991)
- 1991-1994 Workshops on Knowledge Discovery in Databases
  - Advances in Knowledge Discovery and Data Mining (U. Fayyad, G. Piatetsky-Shapiro, P. Smyth, and R. Uthurusamy, 1996)
- 1995-1998 International Conferences on Knowledge Discovery in Databases and Data Mining (KDD'95-98)
  - Journal of Data Mining and Knowledge Discovery (1997)
- ACM SIGKDD conferences since 1998 and SIGKDD Explorations
- More conferences on data mining
  - PAKDD (1997), PKDD (1997), SIAM-Data Mining (2001), (IEEE) ICDM (2001), WSDM (2008), etc.
- ACM Transactions on KDD (2007)

Conferences and Journals on Data Mining

- KDD Conferences
  - ACM SIGKDD Int. Conf. on Knowledge Discovery in Databases and Data Mining (KDD)
  - SIAM Data Mining Conf. (SDM)
  - (IEEE) Int. Conf. on Data Mining (ICDM)
  - European Conf. on Machine Learning and Principles and practices of Knowledge Discovery and Data Mining (ECML-PKDD)
  - Pacific-Asia Conf. on Knowledge Discovery and Data Mining (PAKDD)
  - Int. Conf. on Web Search and Data Mining (WSDM)
- Other related conferences
  - DB conferences: ACM SIGMOD, VLDB, ICDE, EDBT, ICDT, …
  - Web and IR conferences: WWW, SIGIR, WSDM
  - ML conferences: ICML, NIPS
  - PR conferences: CVPR,
- Journals
  - Data Mining and Knowledge Discovery (DAMI or DMKD)
  - IEEE Trans. On Knowledge and Data Eng. (TKDE)
  - KDD Explorations
  - ACM Trans. on KDD

Where to Find References? DBLP, CiteSeer, Google

- Data mining and KDD (SIGKDD: CDROM)
  - Conferences: ACM-SIGKDD, IEEE-ICDM, SIAM-DM, PKDD, PAKDD, etc.
  - Journal: Data Mining and Knowledge Discovery, KDD Explorations, ACM TKDD
- Database systems (SIGMOD: ACM SIGMOD Anthology—CD ROM)
  - Conferences: ACM-SIGMOD, ACM-PODS, VLDB, IEEE-ICDE, EDBT, ICDT, DASFAA
  - Journals: IEEE-TKDE, ACM-TODS/TOIS, JIIS, J. ACM, VLDB J., Info. Sys., etc.
- AI & Machine Learning
  - Conferences: Machine learning (ML), AAAI, IJCAI, COLT (Learning Theory), CVPR, NIPS, etc.
  - Journals: Machine Learning, Artificial Intelligence, Knowledge and Information Systems, IEEE-PAMI, etc.
- Web and IR
  - Conferences: SIGIR, WWW, CIKM, etc.
  - Journals: WWW: Internet and Web Information Systems,
- Statistics
  - Conferences: Joint Stat. Meeting, etc.
  - Journals: Annals of statistics, etc.
- Visualization
  - Conference proceedings: CHI, ACM-SIGGraph, etc.
  - Journals: IEEE Trans. visualization and computer graphics, etc.

Recommended Reference Books

- E. Alpaydin. Introduction to Machine Learning, 2nd ed., MIT Press, 2011
- S. Chakrabarti. Mining the Web: Statistical Analysis of Hypertex and Semi-Structured Data. Morgan Kaufmann, 2002
- R. O. Duda, P. E. Hart, and D. G. Stork, Pattern Classification, 2ed., Wiley-Interscience, 2000
- T. Dasu and T. Johnson. Exploratory Data Mining and Data Cleaning. John Wiley & Sons, 2003
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- U. Fayyad, G. Grinstein, and A. Wierse, Information Visualization in Data Mining and Knowledge Discovery, Morgan Kaufmann, 2001
- J. Han, M. Kamber, and J. Pei, Data Mining: Concepts and Techniques. Morgan Kaufmann, 3rd ed. , 2011
- T. Hastie, R. Tibshirani, and J. Friedman, The Elements of Statistical Learning: Data Mining, Inference, and Prediction, 2nd ed., Springer, 2009
- B. Liu, Web Data Mining, Springer 2006
- T. M. Mitchell, Machine Learning, McGraw Hill, 1997
- Y. Sun and J. Han, Mining Heterogeneous Information Networks, Morgan & Claypool, 2012
- P.-N. Tan, M. Steinbach and V. Kumar, Introduction to Data Mining, Wiley, 2005
- S. M. Weiss and N. Indurkhya, Predictive Data Mining, Morgan Kaufmann, 1998
- I. H. Witten and E. Frank, Data Mining: Practical Machine Learning Tools and Techniques with Java Implementations, Morgan Kaufmann, 2nd ed. 2005

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- Data mining: Discovering interesting patterns and knowledge from massive amount of data
- A natural evolution of science and information technology, in great demand, with wide applications
- A KDD process includes data cleaning, data integration, data selection, transformation, data mining, pattern evaluation, and knowledge presentation
- Mining can be performed in a variety of data
- Data mining functionalities: characterization, discrimination, association, classification, clustering, trend and outlier analysis, etc.
- Data mining technologies and applications
- Major issues in data mining