A SYSTEMATIC APPROACH TO DATA SCIENCE

M. TAMER ÖZSU
UNIVERSITY OF WATERLOO

WORLD'S MOST VALUABLE RESOURCE

"**Data** is the new oil."

Clive Robert Humby
mathematician, entrepreneur, and
Chief Data Scientist, Starcount

"**Data** is the new currency."

Antonio Neri, *President*
Hewlett Packard Enterprise

"Data is a commodity like gold."

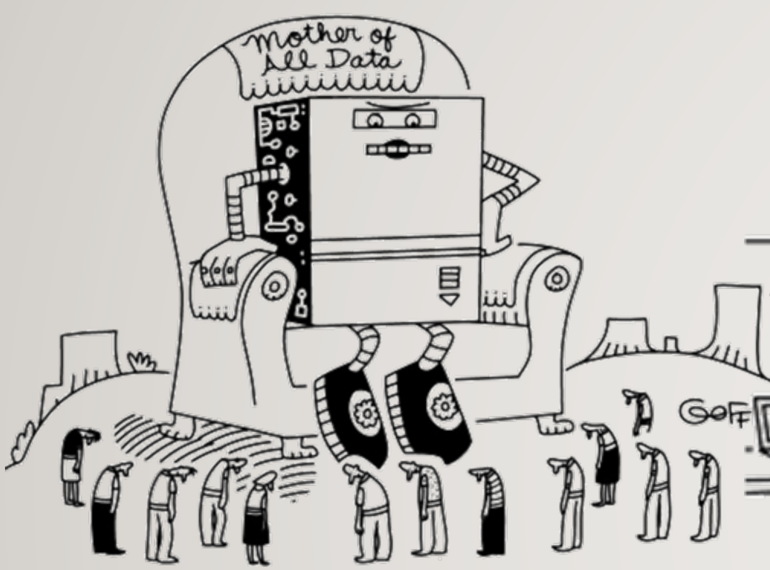
Matt Shepherd
Head of Data Strategy, BBH London

"At the heart of the digital economy and society is the explosion of insight, intelligence and information – data. Data is the lifeblood of the digital economy.

World Economic Forum
A New Paradigm for Business of Data
BRIEFING PAPER - JULY 2020

DATA SCIENCE/BIG DATA IN THE NEWS…

DATA SCIENCE EVERYWHERE!...

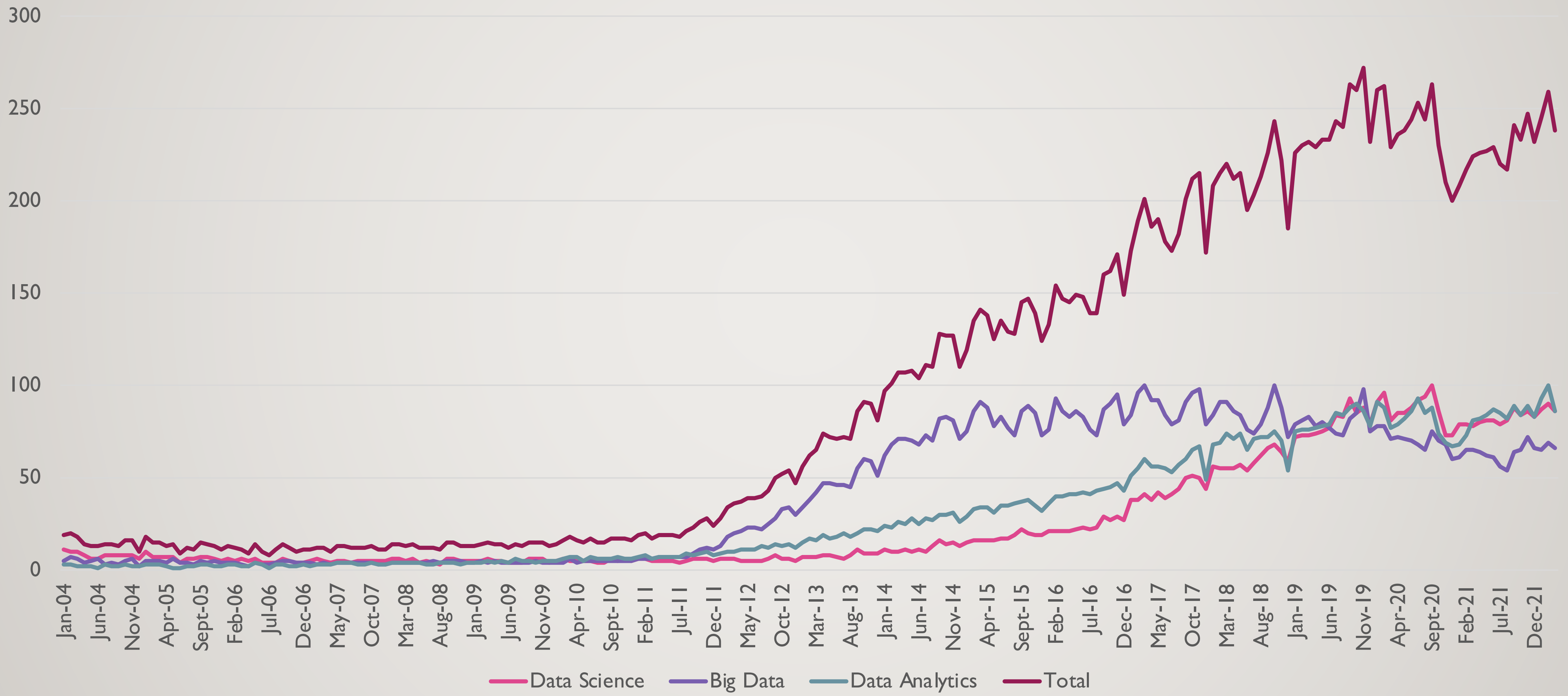


"No candy? No flowers? No cards? Big Data predicted that 67.53% of you would remember!"

"You can't keep adjusting the data to prove that you would be the best Valentine's date for Scarlett Johansson."

"I don't like the look of this. Searches for gravy and turkey stuffing are going through the roof !"

GOOGLE TRENDS



DATA SCIENCE NEEDS POSITIONING

AGENDA

- What is Data Science
- Data Science Applications
- Data Science Ecosystem
- Data Science Lifecycle
- Data Science System Architecture
- Who Owns Data Science

WHAT IS DATA SCIENCE?

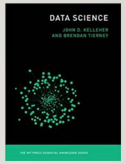
"**Data science**, also known as **data-driven science**, is an interdisciplinary field of scientific methods, processes, algorithms and systems to extract knowledge or insights from data in various forms, either structured or unstructured, similar to data mining."

"Data science intends to **analyze and understand actual phenomena with 'data'**. In other words, the aim of data science is to reveal the features or the hidden structure of complicated natural, human, and social phenomena with data from a different point of view from the established or traditional theory and method."

Chikio Hayashi
1998

"… change of all sciences moving from observational, to theoretical, to computational and now to the 4th Paradigm – **Data-Intensive Scientific Discovery**"

Gordon Bell
2009



"Data science encompasses a set of principles, problem definitions, algorithms, and processes for extracting non-obvious and useful patterns from large data sets."

- "…the terms *data science*, *machine learning*, and *data mining* are often used interchangeably."
- "…although data science borrows from these other fields, it is broader in scope."

John Kelleher & Brendan Tierney
2018

"Data science is a **multidisciplinary approach to extracting actionable insights from the large and ever-increasing volumes of data** collected and created by today's organizations. Data science encompasses preparing data for analysis and processing, performing advanced data analysis, and presenting the results to reveal patterns and enable stakeholders to draw informed conclusions."

"Data science **combines multiple fields, including statistics, scientific methods, artificial intelligence (AI), and data analysis, to extract value from data**. … Data science encompasses preparing data for analysis, including cleansing, aggregating, and manipulating the data to perform advanced data analysis."

Data science is the field of study that combines domain expertise, programming skills, and knowledge of mathematics and statistics to **extract meaningful insights from data**. … In turn, these systems generate insights which analysts and business users can translate into tangible business value."

"data science is an umbrella term to describe the entire complex and multistep processes used to **extract value from data**."

Rafael A. Irizarry
2020-01-31

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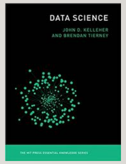

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- Data-driven
- Insights from data
- Reveal patterns
- A process

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A WORKING DEFINITION

A data-driven approach to problem solving by analyzing and exploring large volumes of possibly multi-modal data, extracting from it knowledge and insight that is used for better decision-making.

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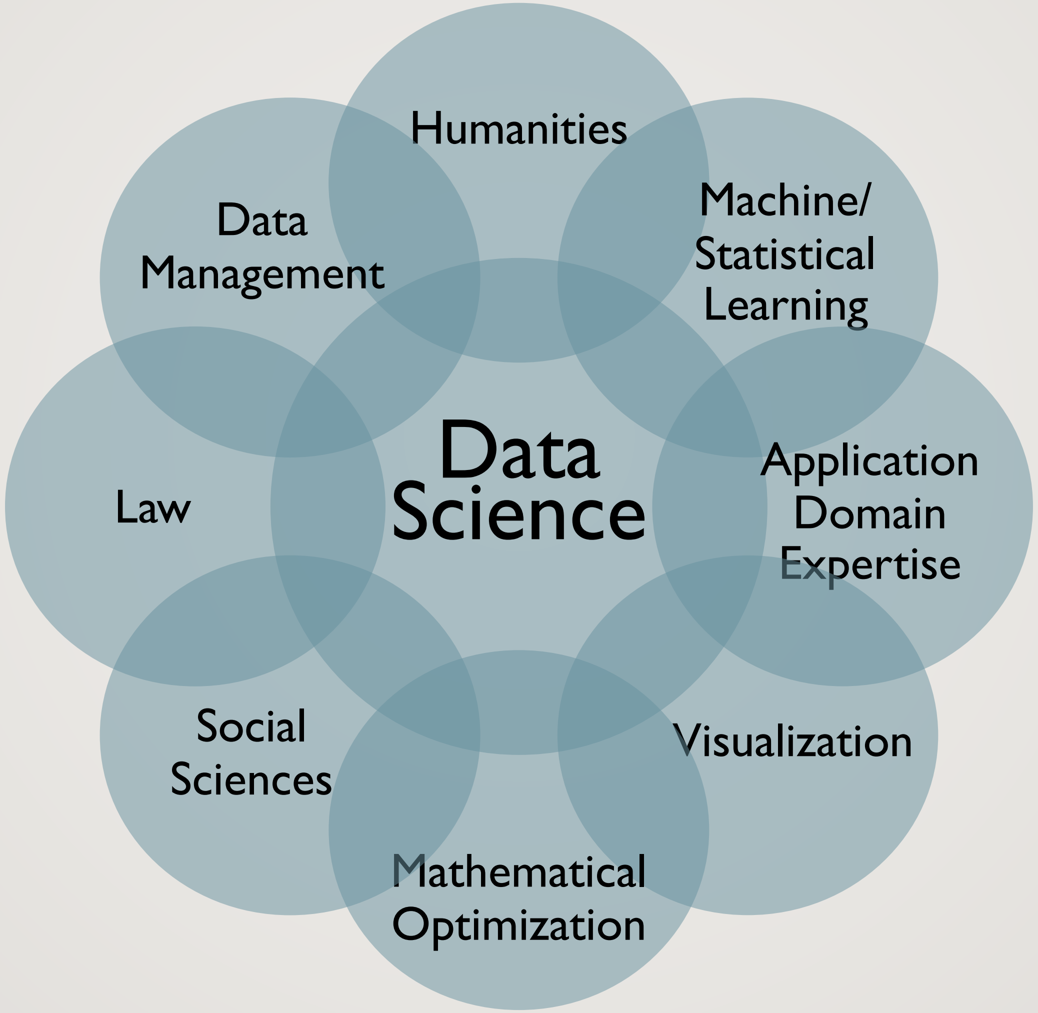
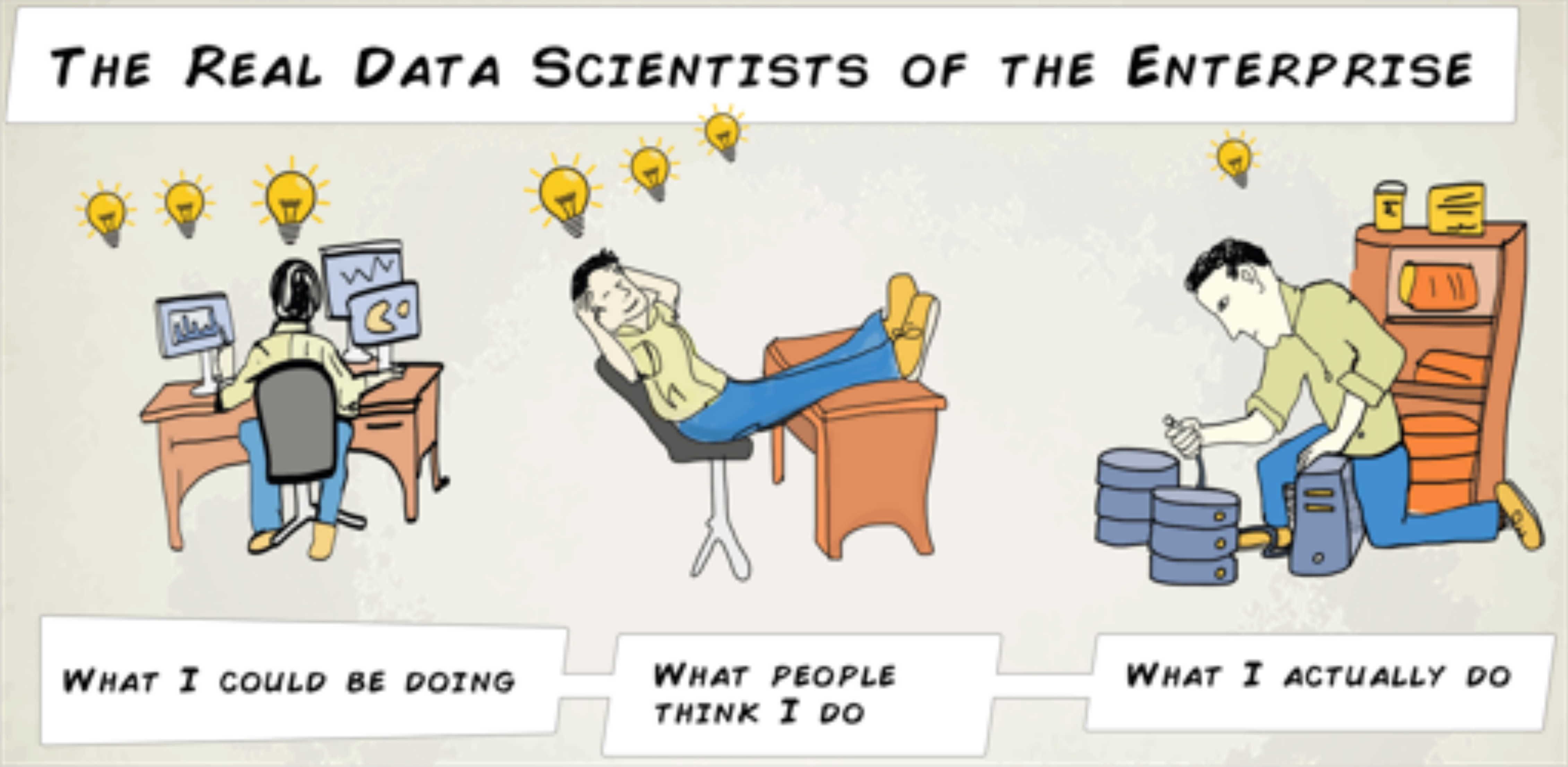
It involves the process of collecting, preparing, managing, analyzing, and explaining the data and analysis results.

DATA SCIENCE AS A UNIFIER



WHO IS A DATA SCIENTIST?



WHO IS A DATA SCIENTIST?

To be revealed at the end…

TWO MYTHS…

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- Data science = Big data

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- Data science $\neq$ Big data
- Big data is like a raw material
- Processing it leads to data science & better understanding
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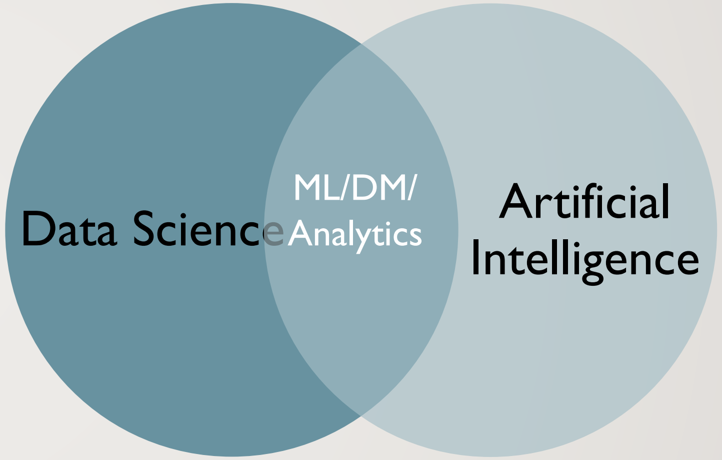

- They are related but not the same

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DATA SCIENCE APPLICATIONS

- Data science is about applications
  - Applications give purpose
  - Applications inform core technologies
- Almost any domain with large data sets are good candidates
- Some examples
  - Fraud detection
  - Biological & biomedical applications
  - Recommender systems
  - Health sciences & health informatics applications
  - Sustainability
  - Finance & insurance
  - Smart cities
  - Sports
  - …

DATA SCIENCE APPLICATION EXAMPLES

Sustainability

- Climate variability and change
- Ecology
- FEW
- Large data sources
  - Earth observation data
  - Remote sensing data
  - Citizen-science data
  - Ground-based observational data
  - High spatial and temporal resolution data from mobile devices

DATA SCIENCE APPLICATION EXAMPLES

Biological & Biomedical

- Bioinformatics
- Genomics
- Transcriptomics
- Proteomics
- Computational systems biology
- Mathematical and computational medicine

Explosion of data

DATA SCIENCE APPLICATION EXAMPLES

Fraud detection

- Investigate fraud patterns in past data
- Early detection is important
  - Before damage propagates
  - Harder than late detection
- Precision is important
  - False positive and false negative are both bad
- Real-time analytics

DATA SCIENCE APPLICATION EXAMPLES

Recommender systems

- The ability to offer unique personalized service
- Increase sales, click-through rates, conversions, …
- Collaborative filtering at scale

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DATA SCIENCE ECOSYSTEM

Data Science Building Blocks

Data Engineering

- Big data management
- Data preparation

Data Analytics

- Explore data (data mining)
- Build models & algorithms (machine learning)
- Visualizations & visual analytics

Data Protection

- Security for data science
- Data privacy

Data Ethics

- Impact on individuals, organizations & society
- Ethical & normative concerns
- Bias in data
- Algorithmic bias
- Regulatory issues

DATA SCIENCE ECOSYSTEM

Applications

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Social and Policy Context

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DATA ENGINEERING

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Big data management

Data preparation

- Data enrichment, integration and storage
  - ETL/ELT process (?)
  - Data lakes
- Storage and management of big datasets
- Data processing platforms

DATA ENGINEERING

Big data management

Data preparation

- Data enrichment, integration and storage
  - ETL/ELT process (?)
  - Data lakes
- Storage and management of big datasets
- Data processing platforms
- Data acquisition/gathering
- Data cleaning
- Data provenance & lineage

DATA ENGINEERING IS ESSENTIAL

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DATA UNDERLYING DATA SCIENCE: BIG DATA – FOUR VS

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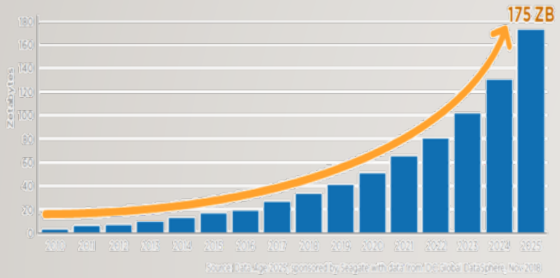
"refers to large, diverse, complex, longitudinal, and/or distributed data sets generated from instruments, sensors, Internet transactions, email, video, click streams, and/or all other digital sources available today and in the future."

NSF BIGDATA Solicitation

DATA UNDERLYING DATA SCIENCE: BIG DATA – FOUR VS



Volume

- Scale of data
- Data at rest

Variety

- Forms of data
- Unstructured challenges

Velocity

- Streaming data
- Data in motion

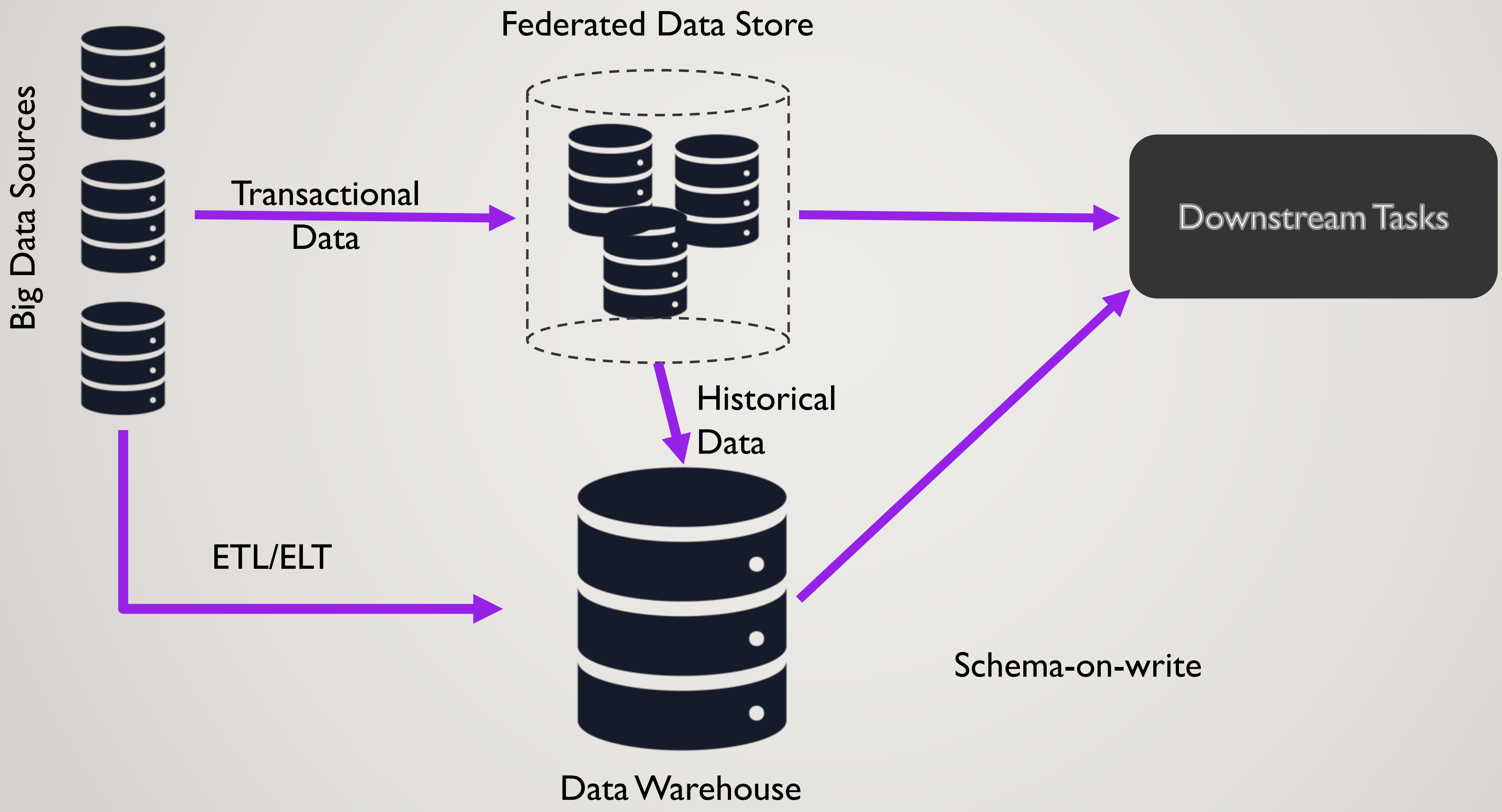
Veracity

- Uncertainty/ incorrecness in data
- Data quality

DATA PREPARATION

Data Acquisition	Dataset Selection	Data Integration	Data Quality
Find data sources appropriate for the problem	Determine which datasets are most useful and appropriate	Integrate multi-modal data from multiple sources	Address all impurities and errors in the integrated data

DATA INTEGRATION



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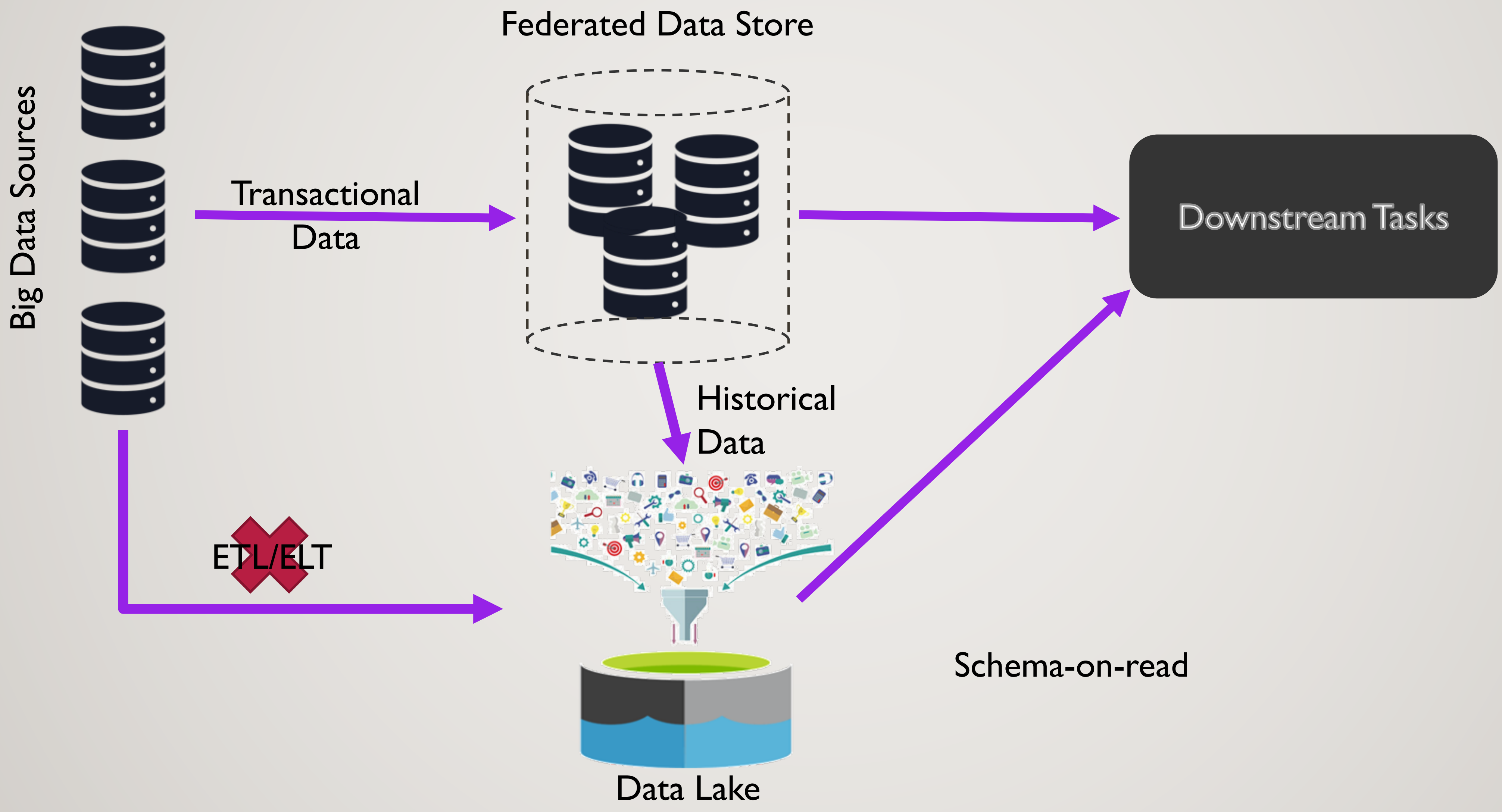


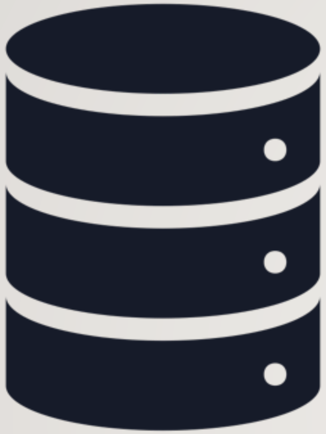
DATA INTEGRATION – DATA LAKES

“massive collection of datasets that:

- may be hosted in different storage systems;
- may vary in their formats;
- may not be accompanied by any useful metadata or may use different formats to describe their metadata; and
- may change autonomously over time.”

Margesian et al, Data Lake Management: Challenges and Opportunities, *PVLDB*, 2019.

DATA WAREHOUSES VS DATA LAKES



- Simpler to architect
- Single store
- Centralized analytics
- Privacy concerns

- Complexity of dealing with autonomous systems
- Distributed
- Federated/distributed analytics
- Maintain original ownership of data

DATA INTEGRATION ⇒ DATA QUALITY ISSUES

89% of executives believe that data quality issues impact the quality of customer service they provide (2017)

Only 33% of senior executives have a high level of trust in the accuracy of their big data analytics (2016)

59% of executives do not believe their company has capabilities to generate business insights from their data (2016)

DATA INTEGRATION ⇒ DATA QUALITY ISSUES

DATA QUALITY DIMENSIONS

DAMA UK Working Group, 2013

DATA SCIENCE ECOSYSTEM

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DATA ANALYTICS

The application of statistical and machine learning techniques to draw insights from data under study and to make predictions about the behaviour of the system under study

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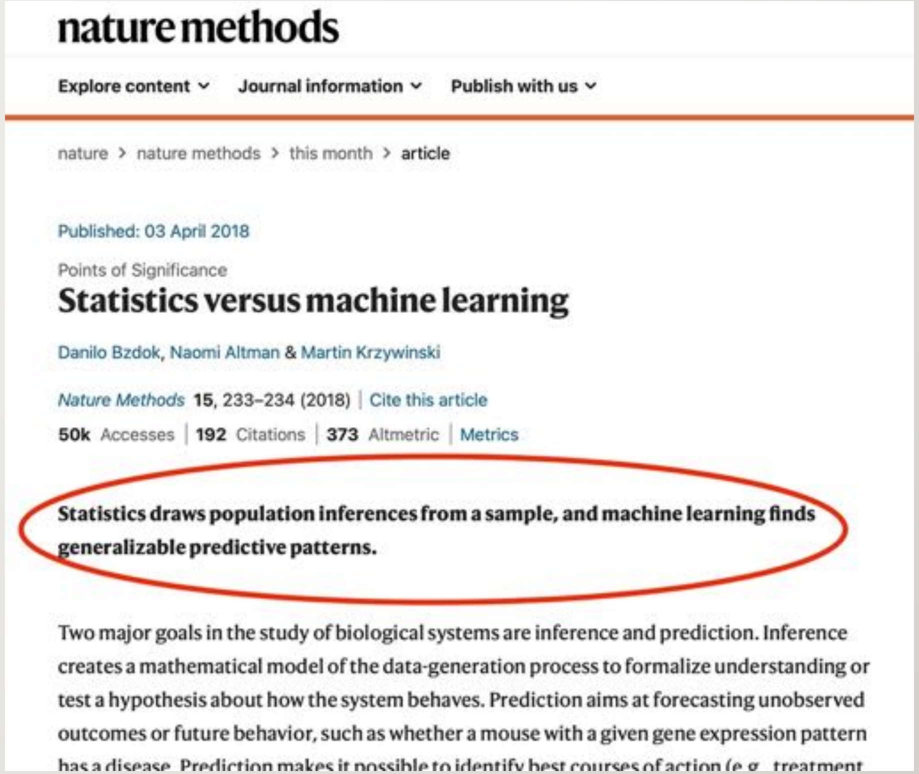

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Points of Significance

Statistics versus machine learning

Danilo Bzdok, Naomi Altman & Martin Krzywinski

Nature Methods **15**, 233–234 (2018) | Cite this article

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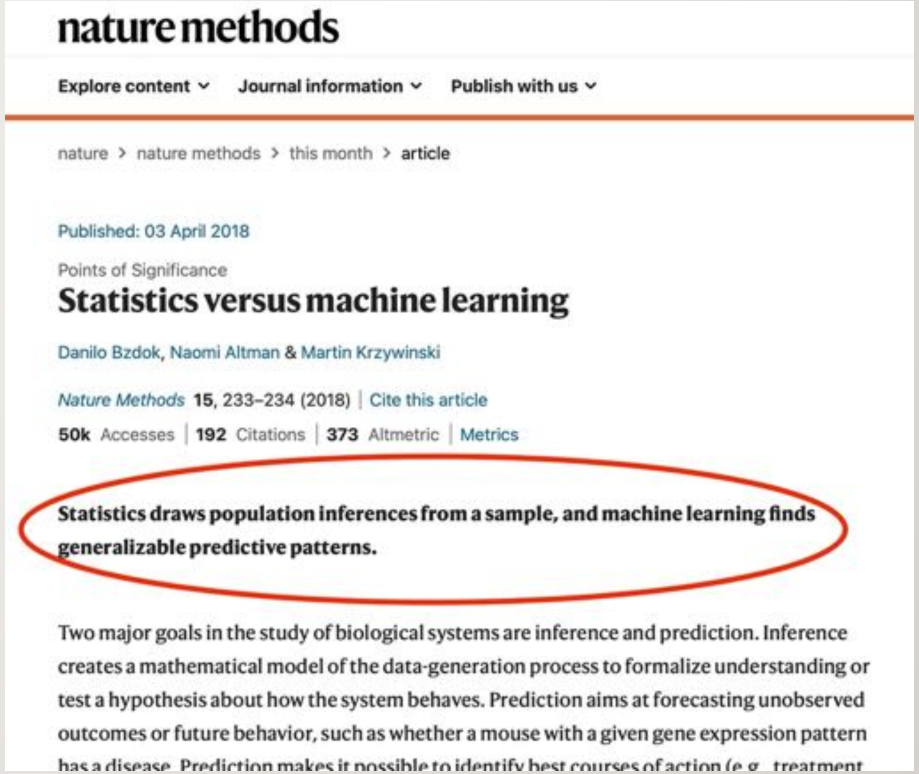
Statistics draws population inferences from a sample, and machine learning finds generalizable predictive patterns.

Two major goals in the study of biological systems are inference and prediction. Inference creates a mathematical model of the data-generation process to formalize understanding or test a hypothesis about how the system behaves. Prediction aims at forecasting unobserved outcomes or future behavior, such as whether a mouse with a given gene expression pattern has a disease. Prediction makes it possible to identify best courses of action (e.g., treatment

DATA ANALYTICS

The application of statistical and machine learning techniques to draw insights from data under study and to make predictions about the behaviour of the system under study

- Statistics
- Computer Science (DM/ML)
- The lines between the two disciplines have blurred



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DATA ANALYTICS TYPES

Descriptive

- What does the data reveals about what is happening?
- Exploratory analysis

Diagnostic

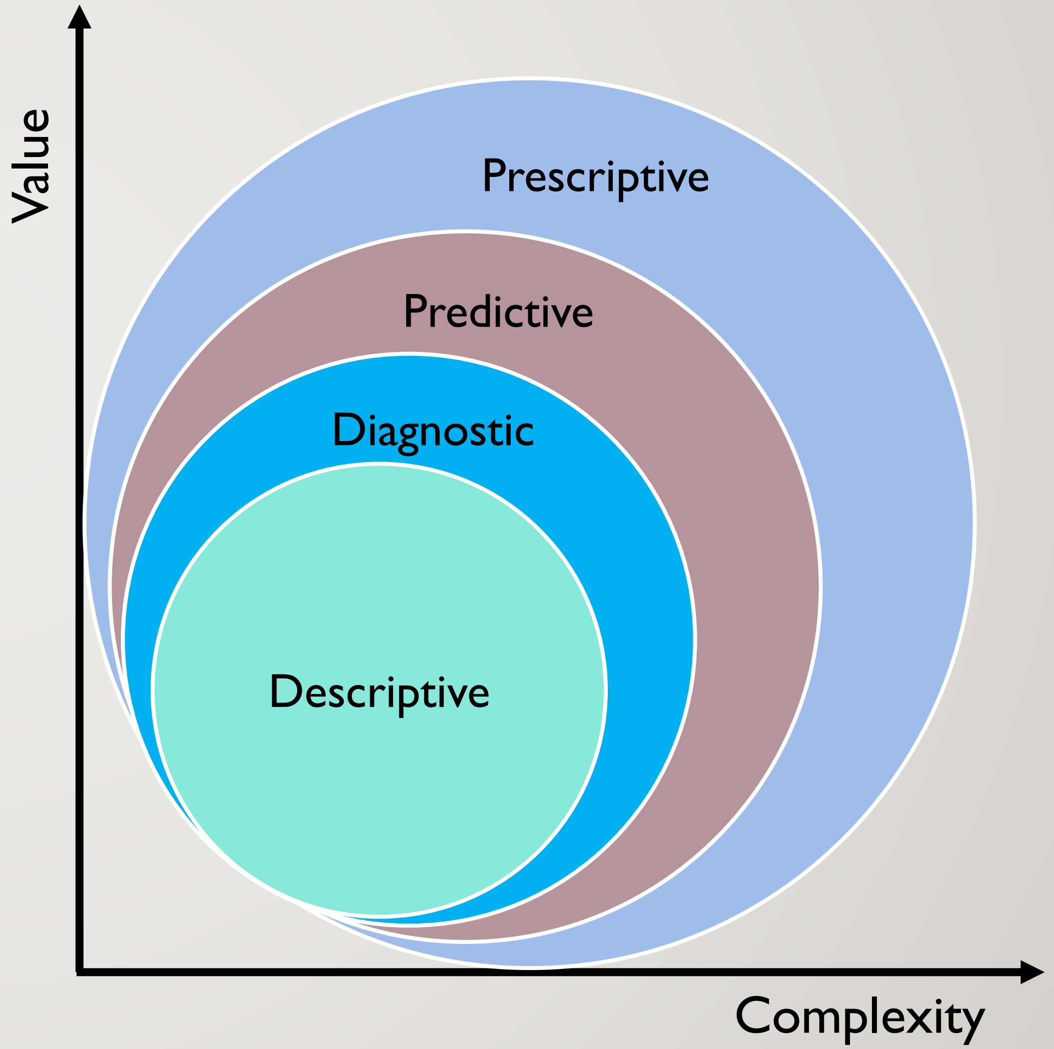
- Why is it happening?
- What does the data suggest about the reasons?

Predictive

- What is likely to happen?
- Decisions are affected
- Machine learning fits here

Prescriptive

- Recommended actions



https://www.kdnuggets.com/2017/07/4-types-data-analytics.html

DATA ANALYTICS TASKS/METHODS

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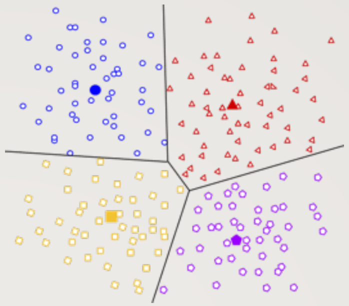

Clustering
- Discovering groups & structures of data that are “similar”

Outlier detection
- Detection of anomalous (rare) data items

Association rule learning
- Detecting relations between variables

Classification
- Generalizing known structure to new data

Regresssion
- Find model that fits data with least error

Summarization
- More compact representation of the data set

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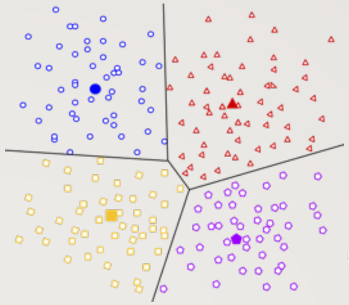

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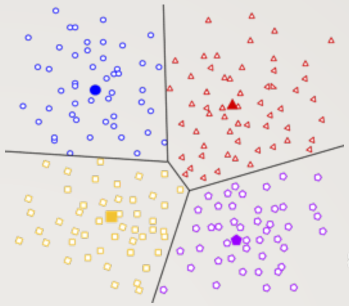

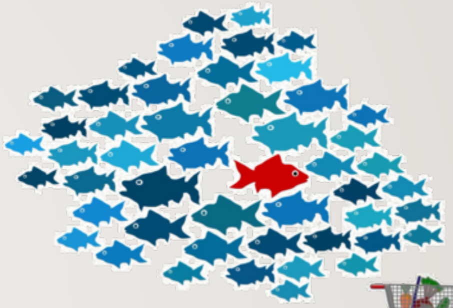

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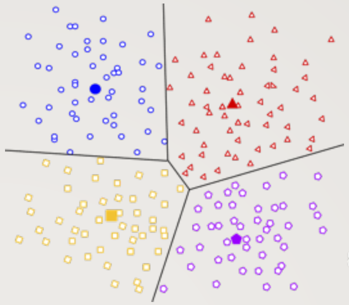

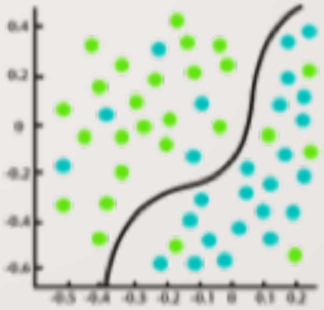

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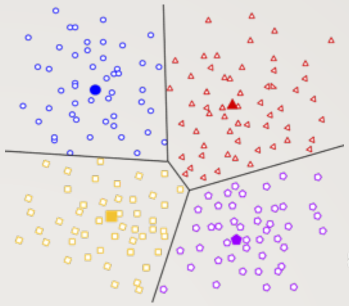

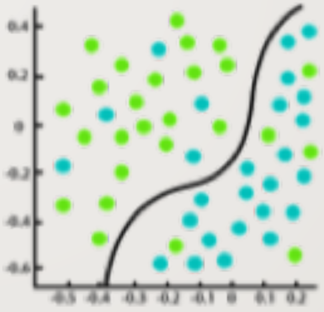

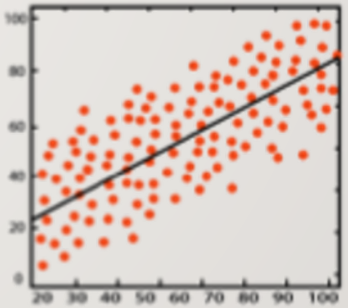

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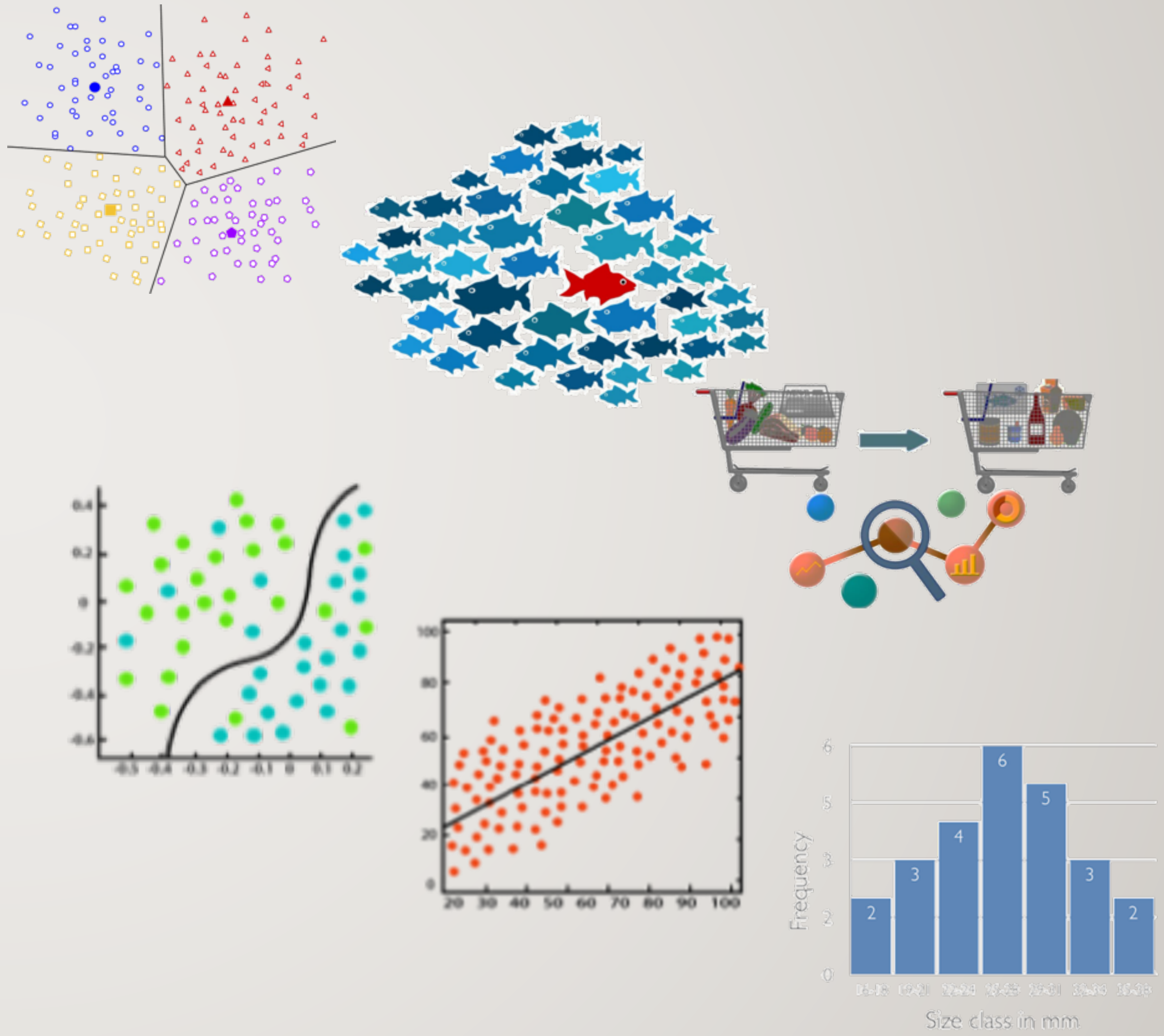

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ANALYTICS ARCHITECTURES

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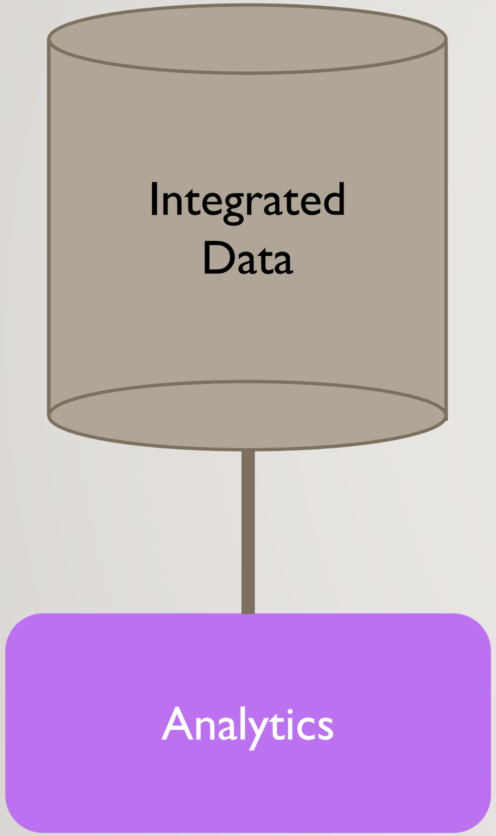
Batch Analytics



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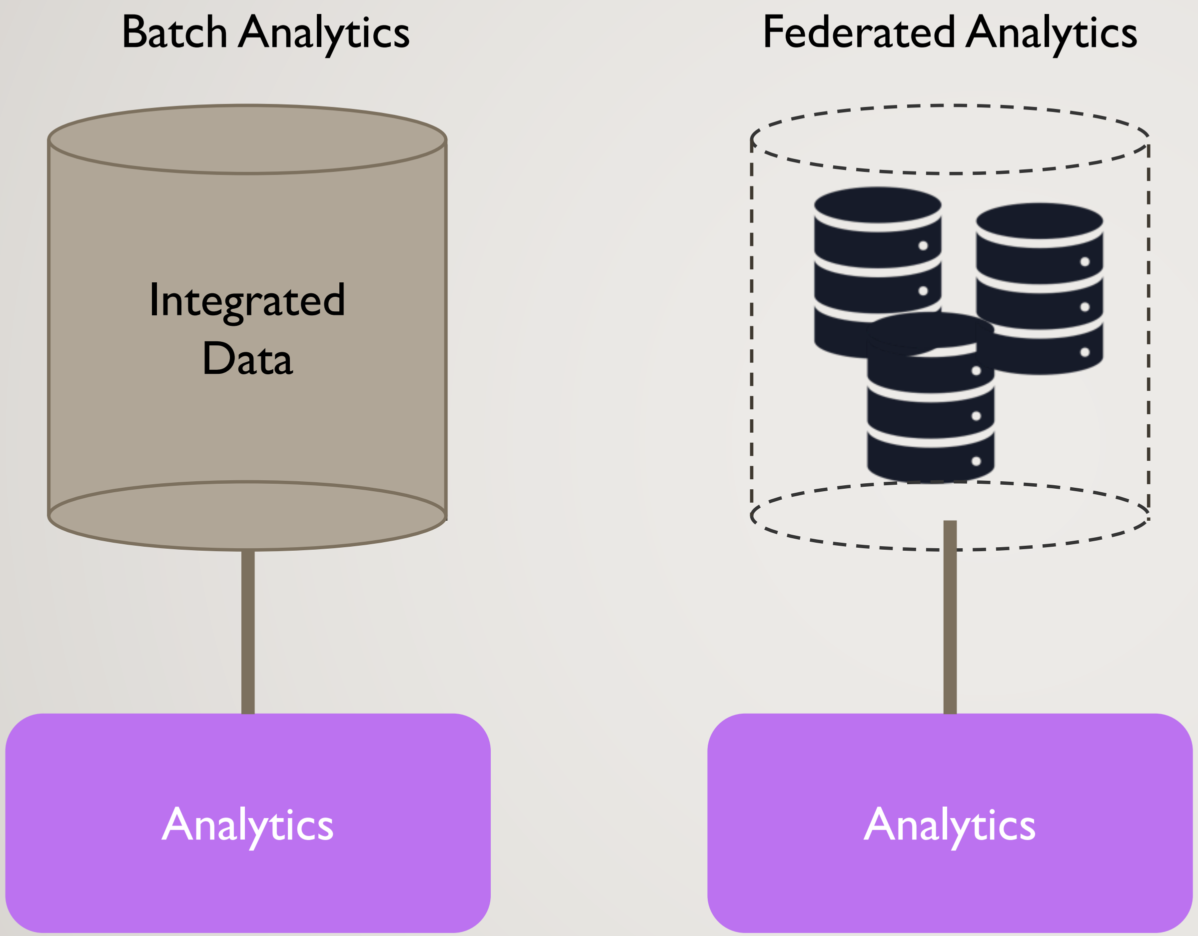

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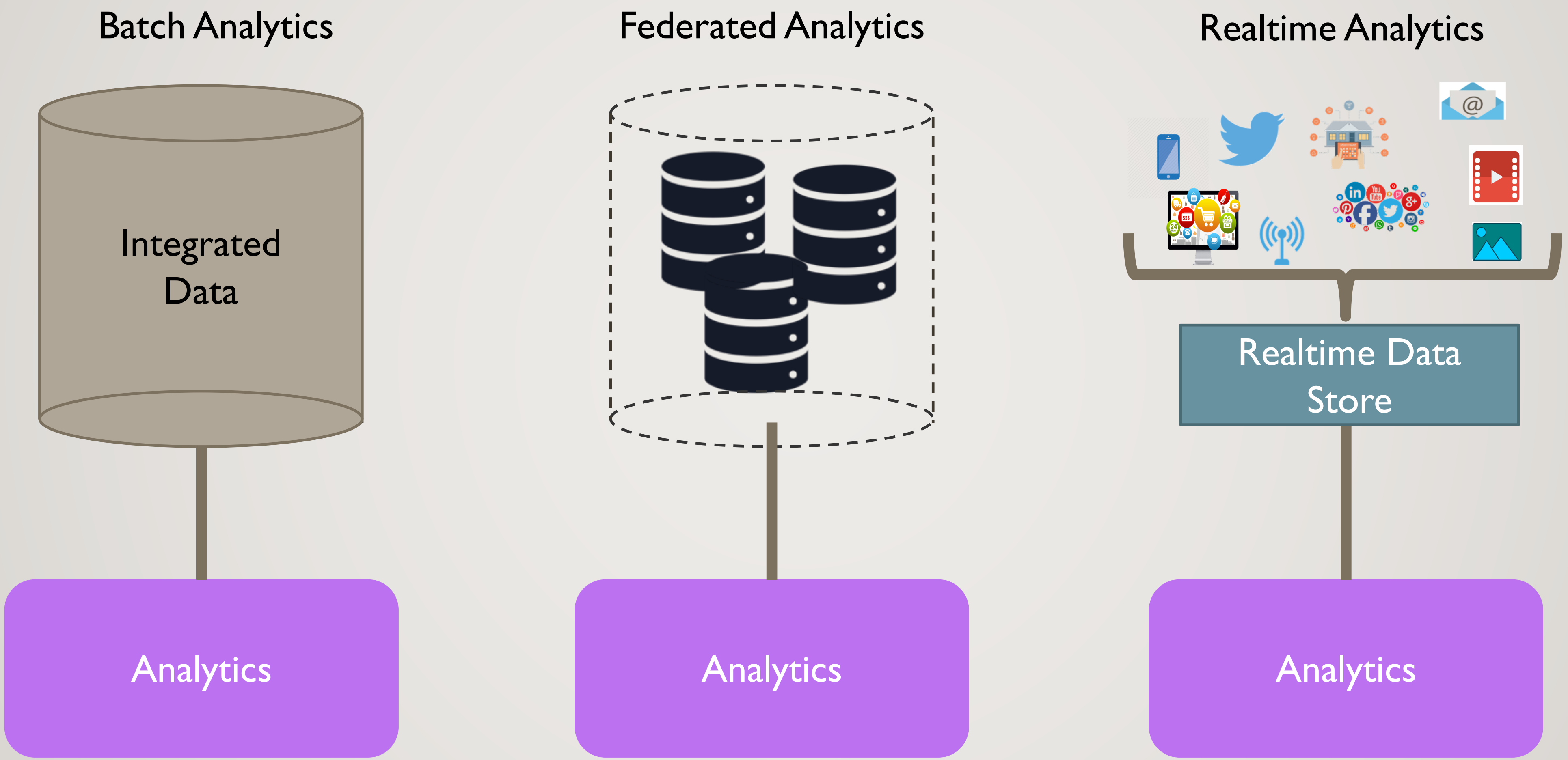

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DATA PROTECTION – DATA SECURITY & PRIVACY

DIMENSIONS OF DATA PROTECTION

- Proper handling, processing, storage and usage of information
- Privacy policies
- Data retention & deletion policies
- DSARs
- Third-party management
- User consent
- PETs

- Protecting information from any unauthorized access or malicious attacks
- Encryption
- TEEs
- Infrastructure security
- Access control
- Monitoring
- DLP

CHANGING CONCEPTS OF DATA PROTECTION

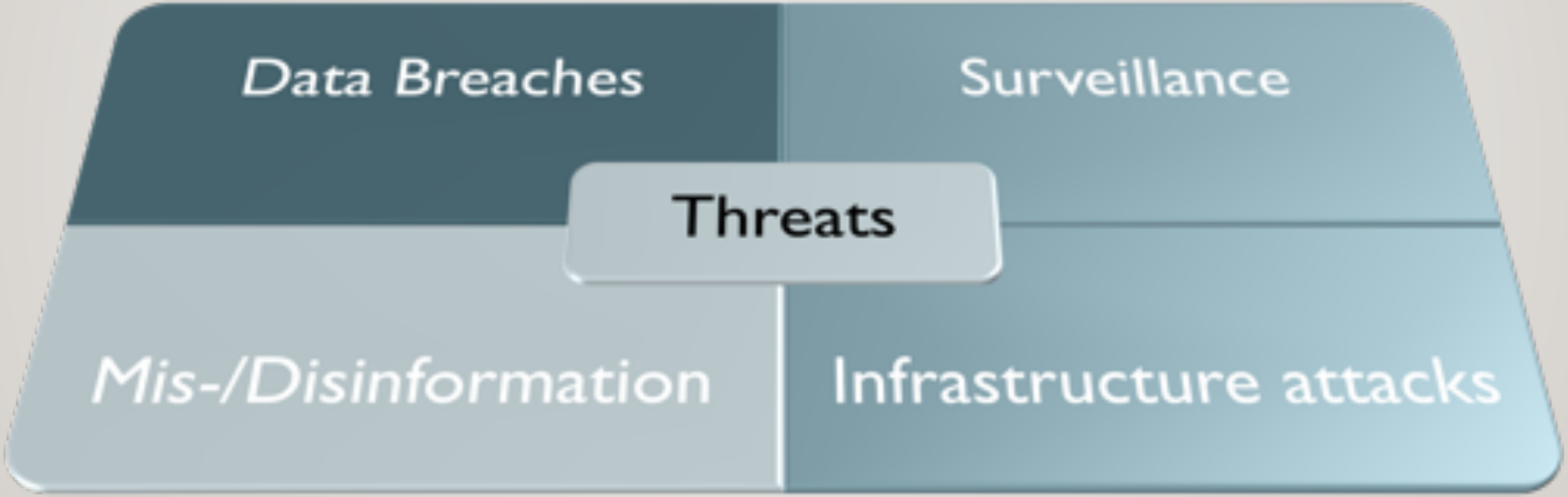
TRADITIONAL SECURITY & PRIVACY

- Confidentiality
  - Do not reveal data to unauthorized users
- Integrity
  - Unauthorized users should not be able to modify data

DATA SECURITY & PRIVACY IN DATA SCIENCE

- Privacy
  - Enable users to control their data usage by others
- Veracity
  - Data provided should be true and current

BIG DATA PRIVACY & SECURITY THREATS



DATA PROTECTION ⇒ CYBERSECURITY

- Platform
- Network
- Software
- Data

CLOUD SECURE ALLIANCE RECOMMENDATIONS

- Infrastructure security
  - Distributed processing of data
  - Non-relational databases
- Data privacy
  - Privacy-preserving analysis
  - Cryptography
  - Granular access control
- Data management & integrity
  - Secure data storage & tx logs
  - Granular audits
  - Data provenance
- Reactive security
  - End-to-end filtering & validation
  - Real-time supervision of security

DATA SCIENCE ECOSYSTEM

Data Science Building Blocks

Data Engineering
- Big data management
- Data preparation

Data Analytics
- Explore data (data mining)
- Build models & algorithms (machine learning)
- Visualizations & visual analytics

Data Protection
- Security for data science
- Data privacy

Data Ethics
- Impact on individuals, organizations & society
- Ethical & normative concerns
- Bias in data
- Algorithmic bias
- Regulatory issues

DATA ETHICS

"… the branch of ethics that studies and evaluates moral problems related to data, … algorithms, … and corresponding practices, in order to formulate and support morally good solutions."

L. Floridi & M. Taddeo, What is data ethics?, *Phil. Trans. R. Soc. A*, 2016.

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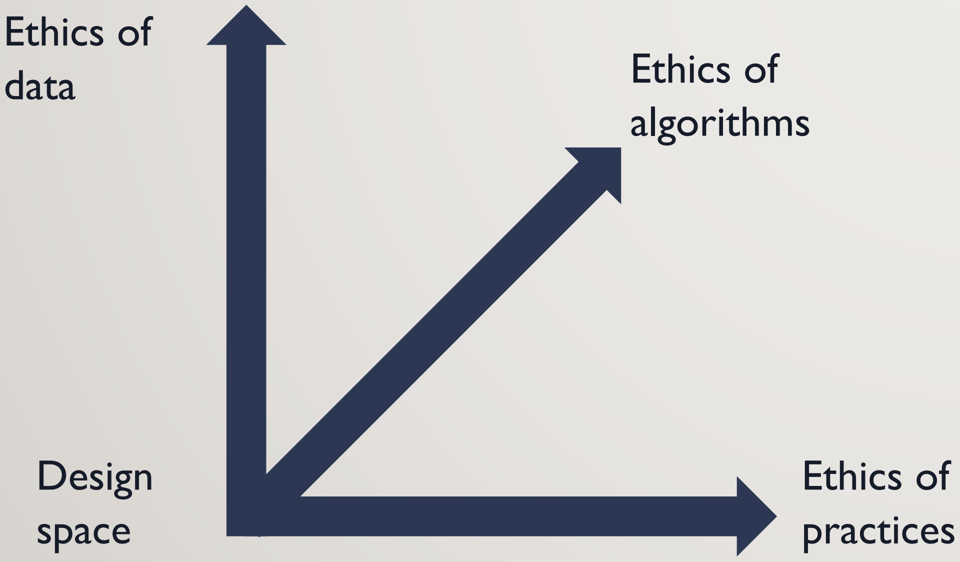


BIAS

"inclination or prejudice for or against one person or group, especially in a way considered to be unfair a concentration on or interest in one area or subject a systematic distortion of a statistical result due to a factor not allowed for in its derivation"

Oxford English Dictionary

Bias is inherent in human decision-making

- Accuracy
- Speed
- Efficiency

TYPES OF BIAS IN HUMANS

Action-Oriented Biases

- Speedy decision-making
- van Restorff effect, bizarreness effect, overconfidence

Stability Biases

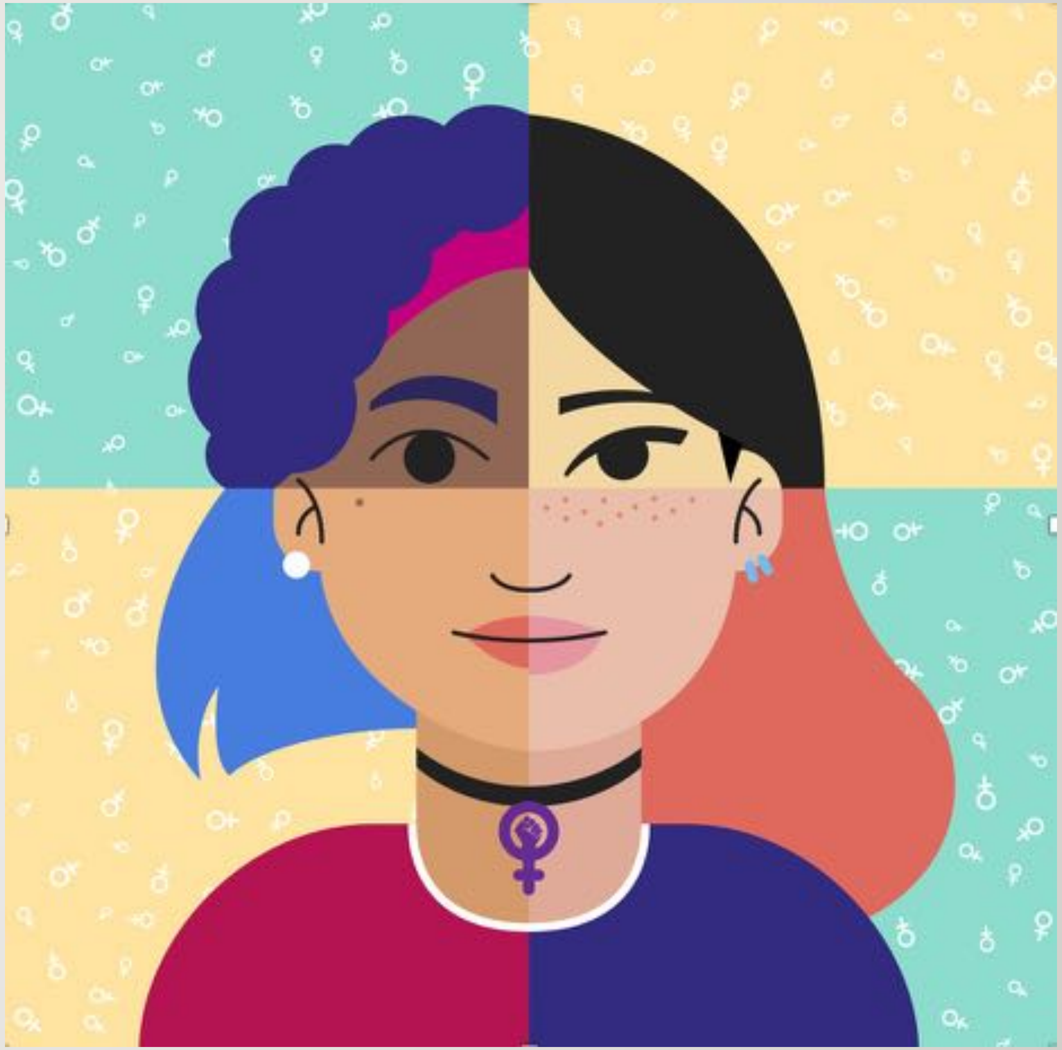
- Preference for the status quo
- Anchoring effect

Pattern Recognition Biases

- Recognizing patterns to fill-in gaps
- Educated guess, confirmation bias

Interest Biases

- What do I want?
- Social biases
  - groupthink
  - go along



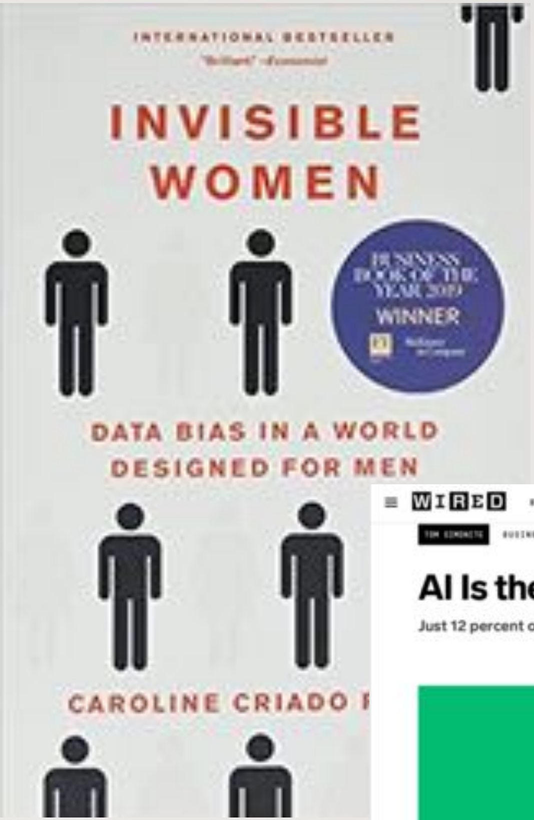
Tobias Baer, Understand, Manage and Prevent Algorithmic Bias, 2019

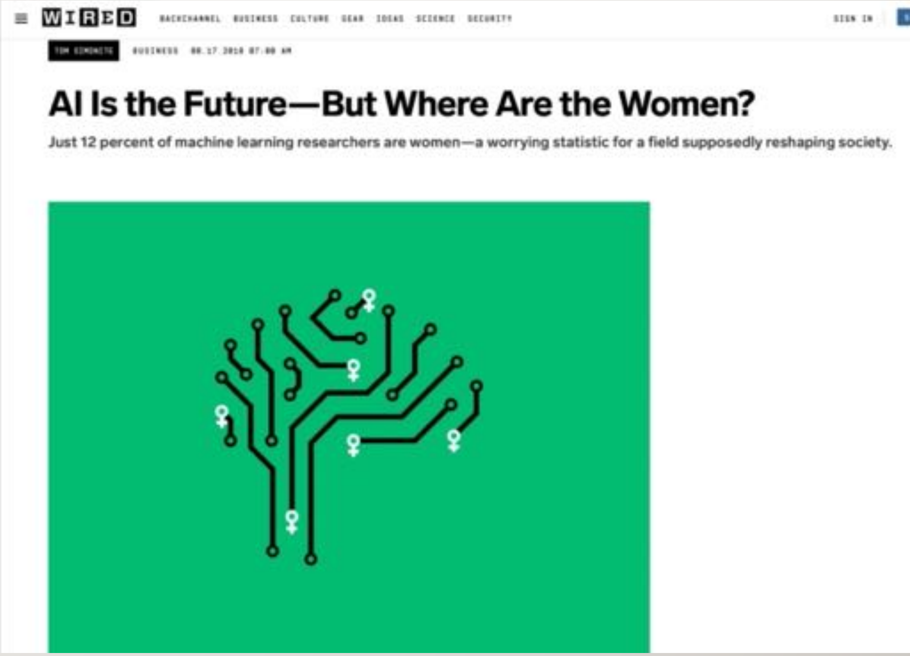
TYPES OF BIAS IN DATA SCIENCE

TYPES OF BIAS IN DATA SCIENCE

Bias in Data

- Historical or representational bias





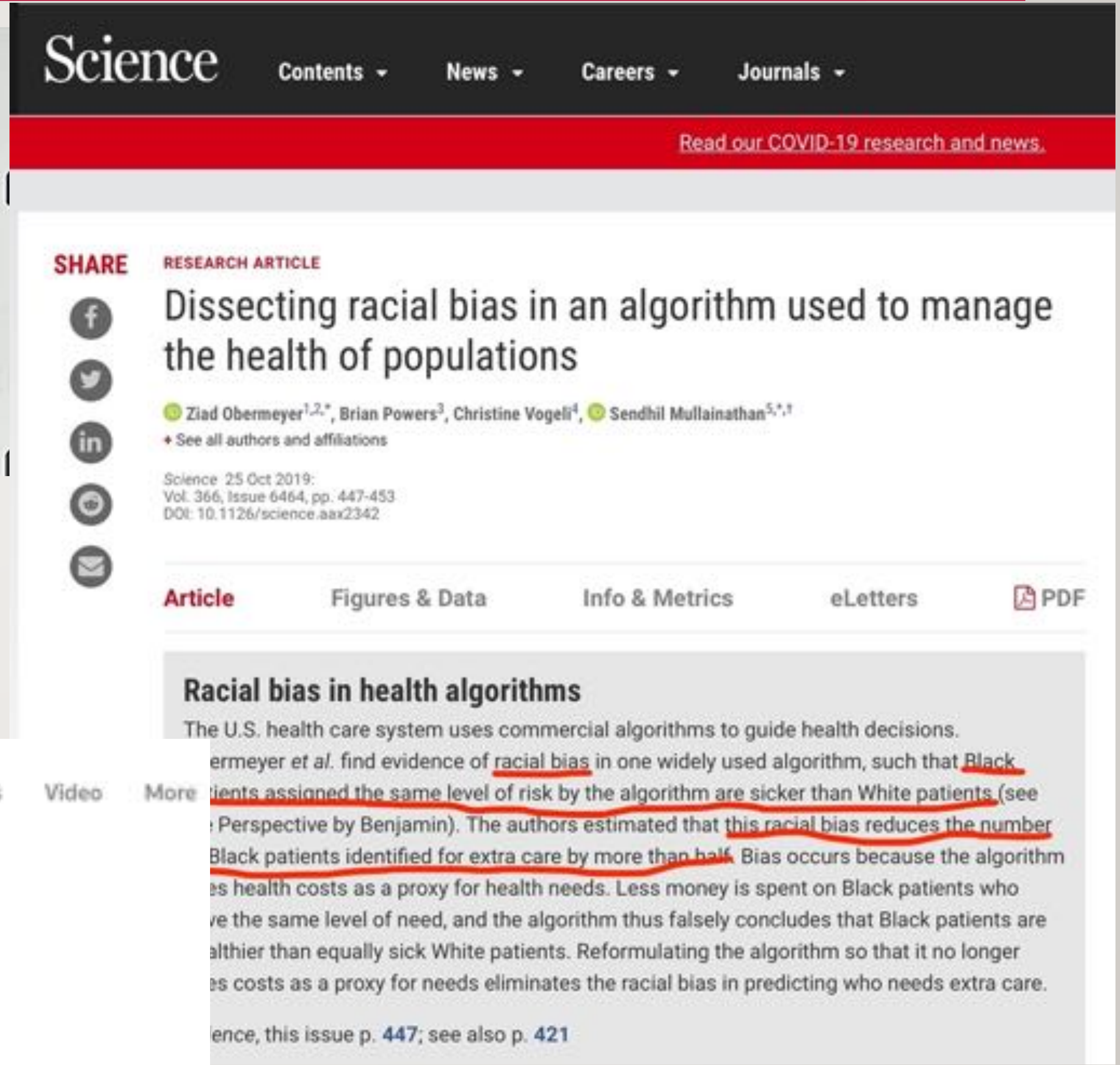
TYPES OF BIAS IN DATA SCIENCE

Bias in Data

- Historical or representational bias

Bias in Algorithms

- Inclusion or omission of features will introduce bias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RESEARCH ARTICLE

Dissecting racial bias in an algorithm used to manage the health of populations

Ziad Obermeyer[1,2,*], Brian Powers[3], Christine Vogeli[4], Sendhil Mullainathan[5,*,†]

+ See all authors and affiliations

Science 25 Oct 2019:
Vol. 366, Issue 6464, pp. 447-453
DOI: 10.1126/science.aax2342

Article | Figures & Data | Info & Metrics | eLetters | PDF

Racial bias in health algorithms

The U.S. health care system uses commercial algorithms to guide health decisions. ermeyer et al. find evidence of racial bias in one widely used algorithm, such that Black ients assigned the same level of risk by the algorithm are sicker than White patients (see Perspective by Benjamin). The authors estimated that this racial bias reduces the number Black patients identified for extra care by more than half. Bias occurs because the algorithm es health costs as a proxy for health needs. Less money is spent on Black patients who ve the same level of need, and the algorithm thus falsely concludes that Black patients are althier than equally sick White patients. Reformulating the algorithm so that it no longer es costs as a proxy for needs eliminates the racial bias in predicting who needs extra care.

ence, this issue p. 447; see also p. 421


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Amazon scraps secret AI recruiting tool that showed bias against women

By Jeffrey Dastin 8 MIN READ

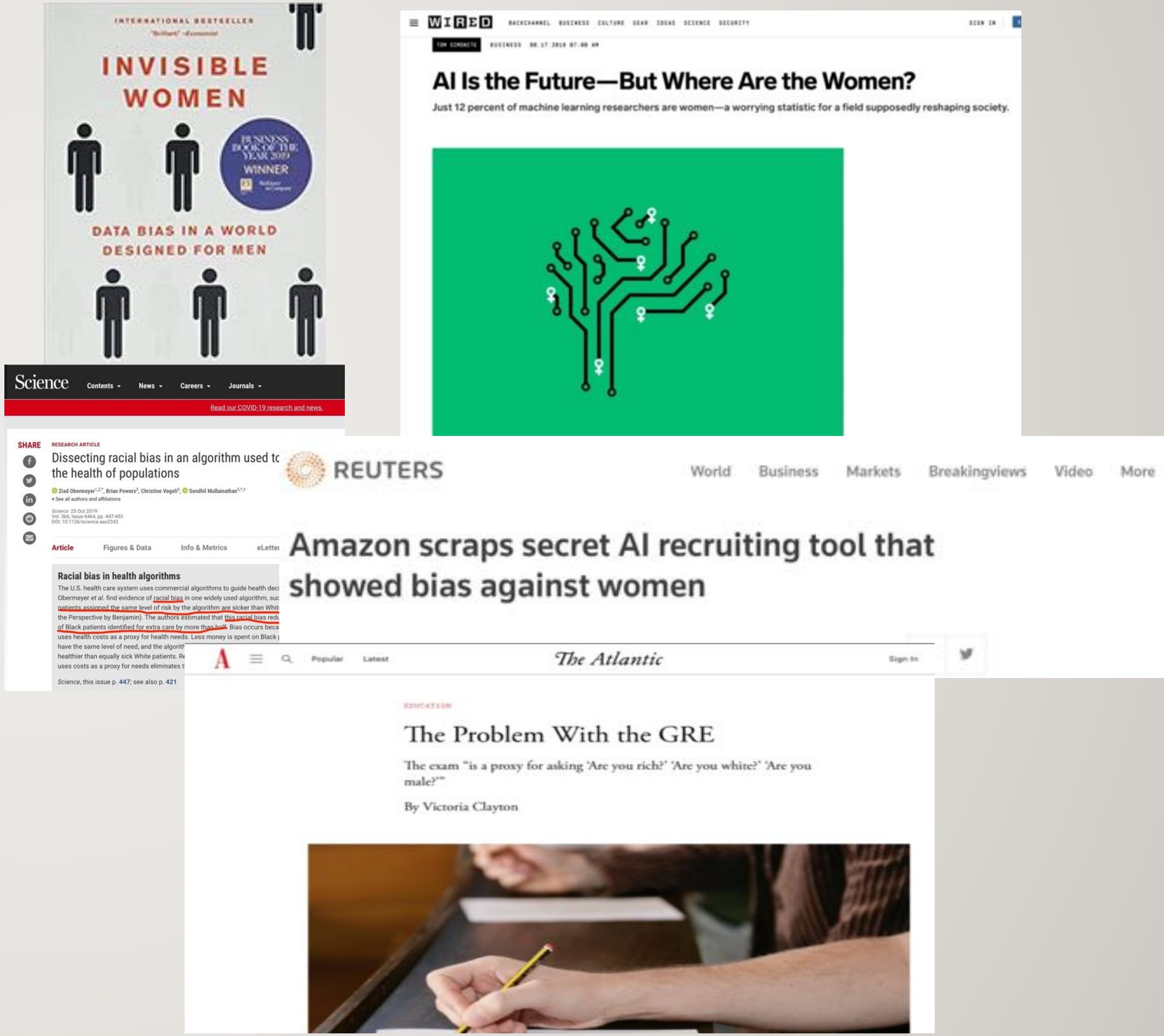
TYPES OF BIAS IN DATA SCIENCE

Bias in Data

- Historical or representational bias

Bias in Algorithms

- Inclusion or omission of features will introduce bias
- Unmeasurable outcomes & use of proxies will introduce bias



ETHICS OF DATA

Ownership

- Who has ownership of data?
- Typically, individuals should have ownership

Transparency

- Subjects should know that data about them is being collected, stored and will be processed and how
- Consent

Privacy

- Personal identifiable information

Intention

- What are you planning to do with the data?
- Secondary use

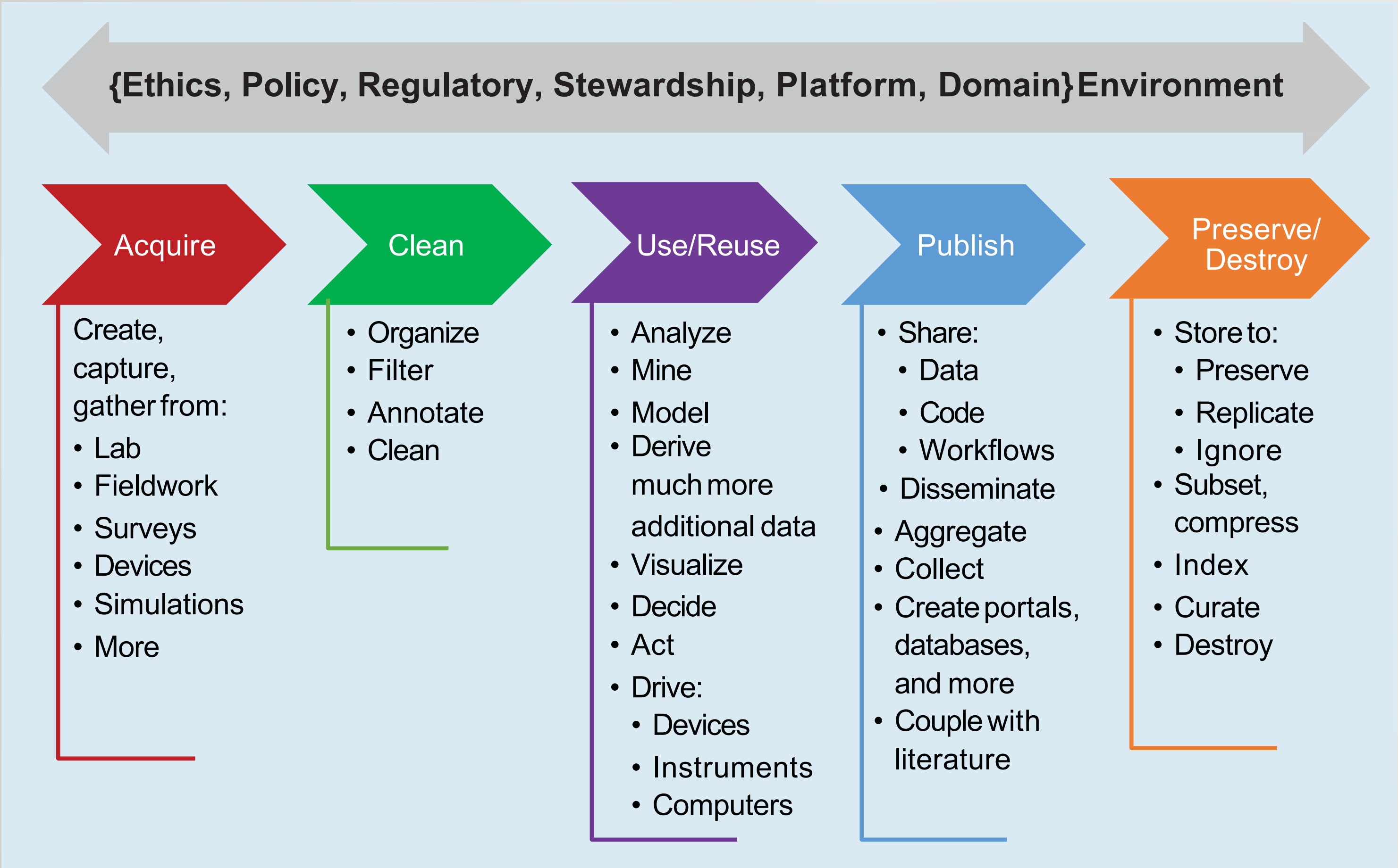
DATA ETHICS CHECKLIST

- Have we listed how this technology can be attacked or abused? [SECURITY]
- Have we tested our training data to ensure it is fair and representative? [FAIRNESS]
- Have we studied and understood possible sources of bias in our data? [FAIRNESS]
- Does our team reflect diversity of opinions, backgrounds, and kinds of thought? [FAIRNESS]
- What kind of user consent do we need to collect to use the data? [PRIVACY/TRANSPARENCY]
- Do we have a mechanism for gathering consent from users? [TRANSPARENCY]
- Have we explained clearly what users are consenting to? [TRANSPARENCY]
- Do we have a mechanism for redress if people are harmed by the results? [TRANSPARENCY]
- Can we shut down this software in production if it is behaving badly?
- Have we tested for fairness with respect to different user groups? [FAIRNESS]
- Have we tested for disparate error rates among different user groups? [FAIRNESS]
- Do we test and monitor for model drift to ensure our software remains fair over time? [FAIRNESS]
- Do we have a plan to protect and secure user data? [SECURITY]

AGENDA

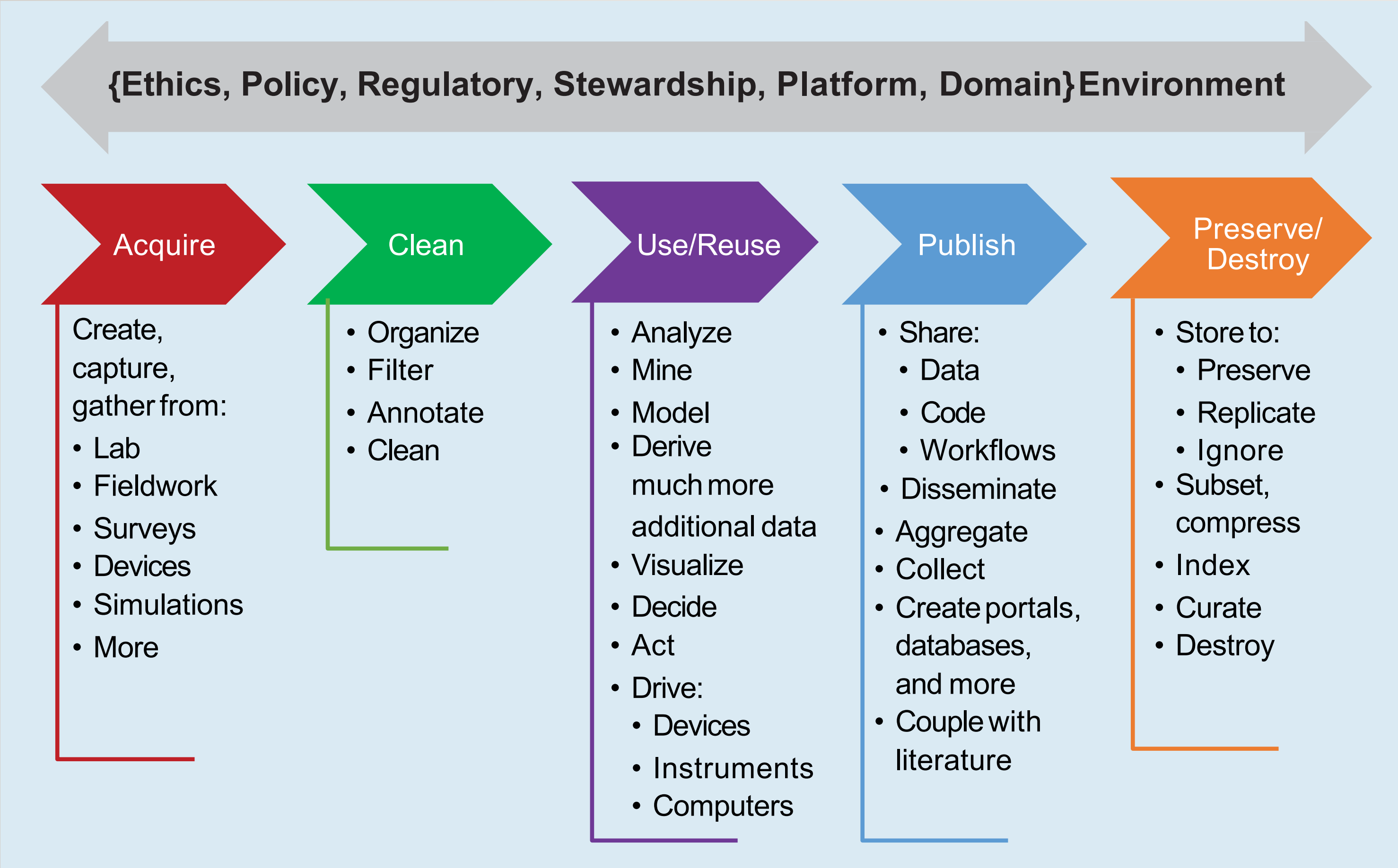
- What is Data Science
- Data Science Applications
- Data Science Ecosystem
- Data Science Lifecycle
- Data Science System Architecture
- Who Owns Data Science

DATA LIFECYCLE



F. Berman et al., Realizing the Potential of Data Science, *Comm. ACM*, 2018

DATA LIFECYCLE

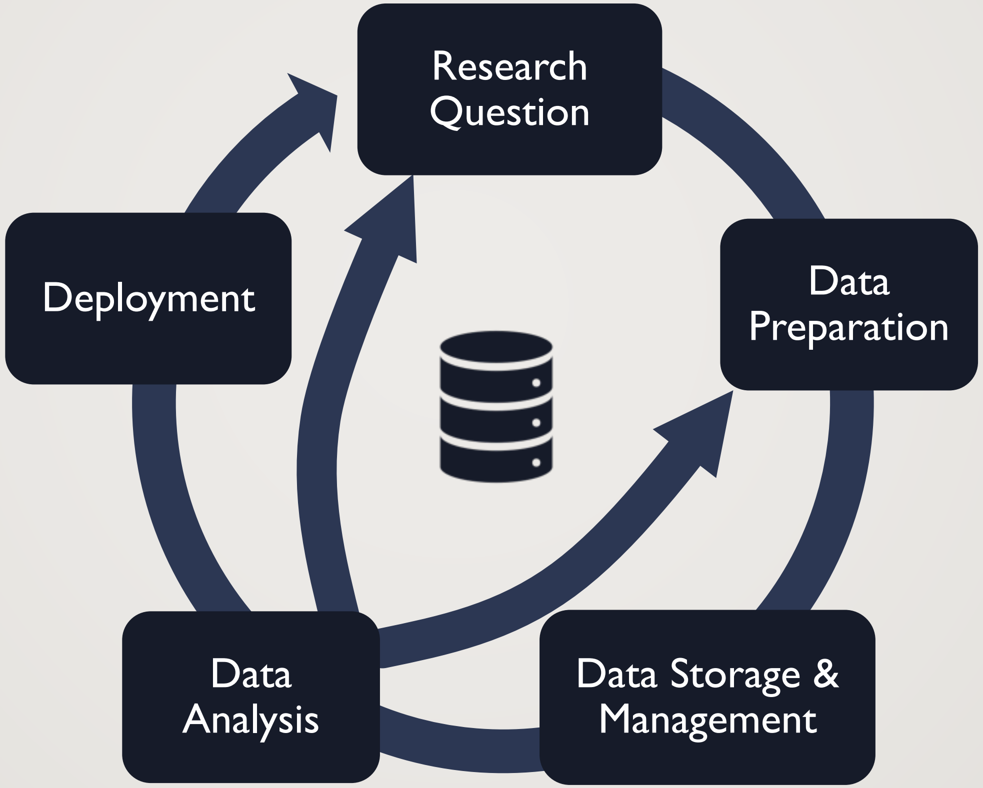


F. Berman et al., Realizing the Potential of Data Science, *Comm. ACM*, 2018

Variations

- D. Agrawal et al., Challenges and Opportunities with Big Data, White paper for CCC of CRA, 2012.
- H.V. Jagadish, Big Data and Science: Myths and Reality, *Big Data Research*, 2015.
- V. Stodden, The Data Science Life Cycle: A Disciplined Approach to Advancing Data Science as a Science, *Comm. ACM*, 2020.

DATA SCIENCE LIFECYCLE



Similar to:

- CRISP-DM Model (C. Shearer, The CRISP-DM Model, *J. Data Warehousing*, 2000)
- PPDAC Model (R.J. MacKay & R.W. Oldford, Scientific Method, Statistical Method and the Speed of Light, *Statistical Sci.*, 2000)

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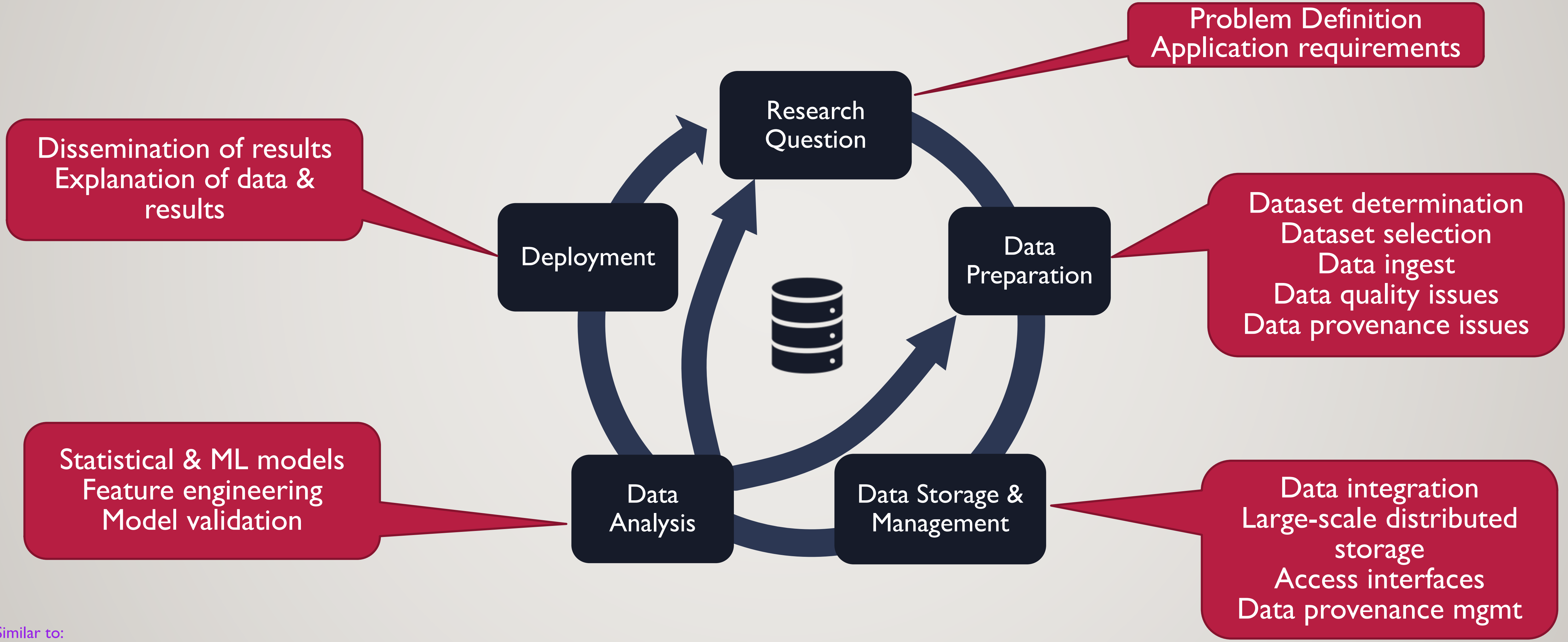

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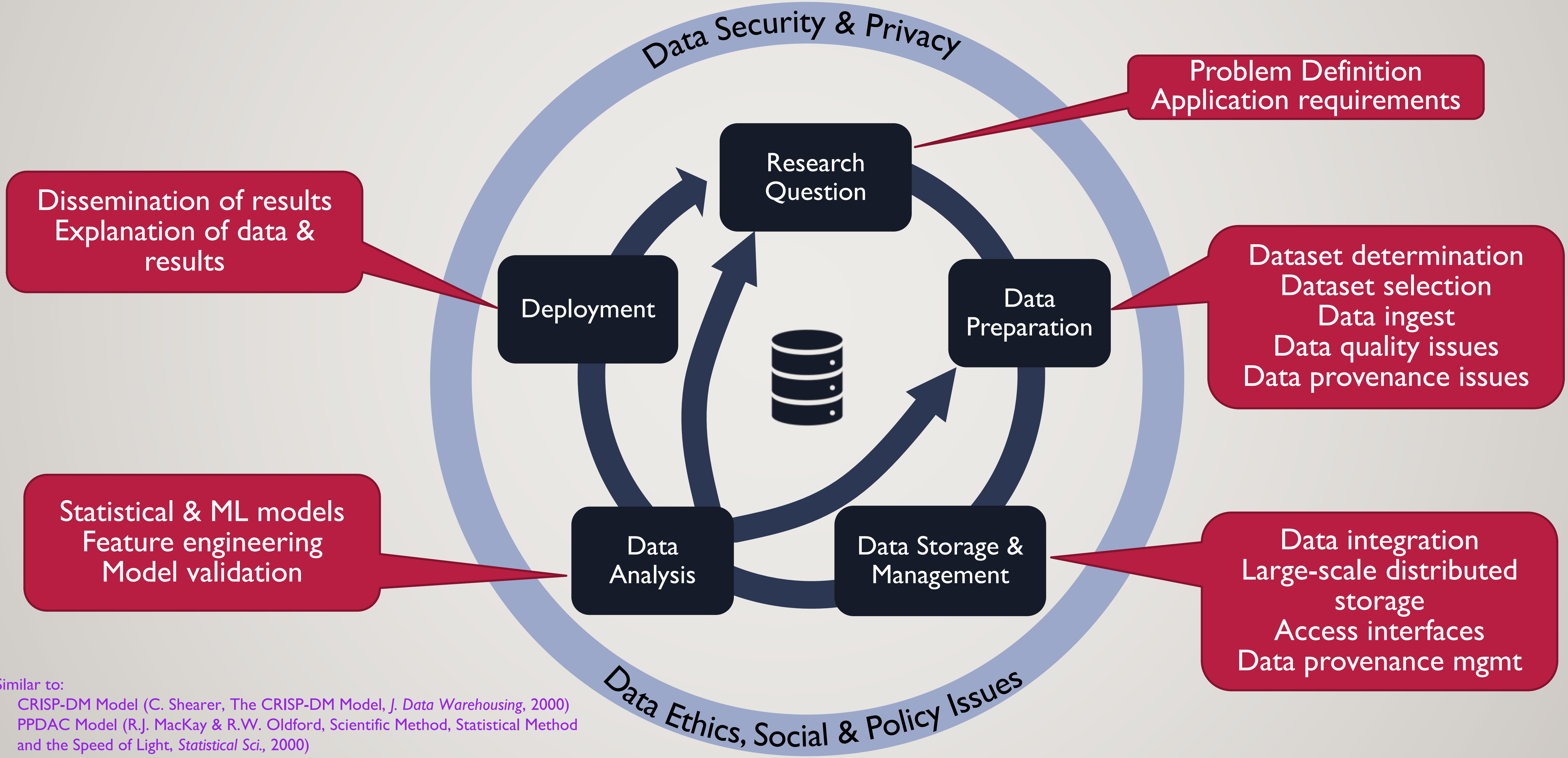

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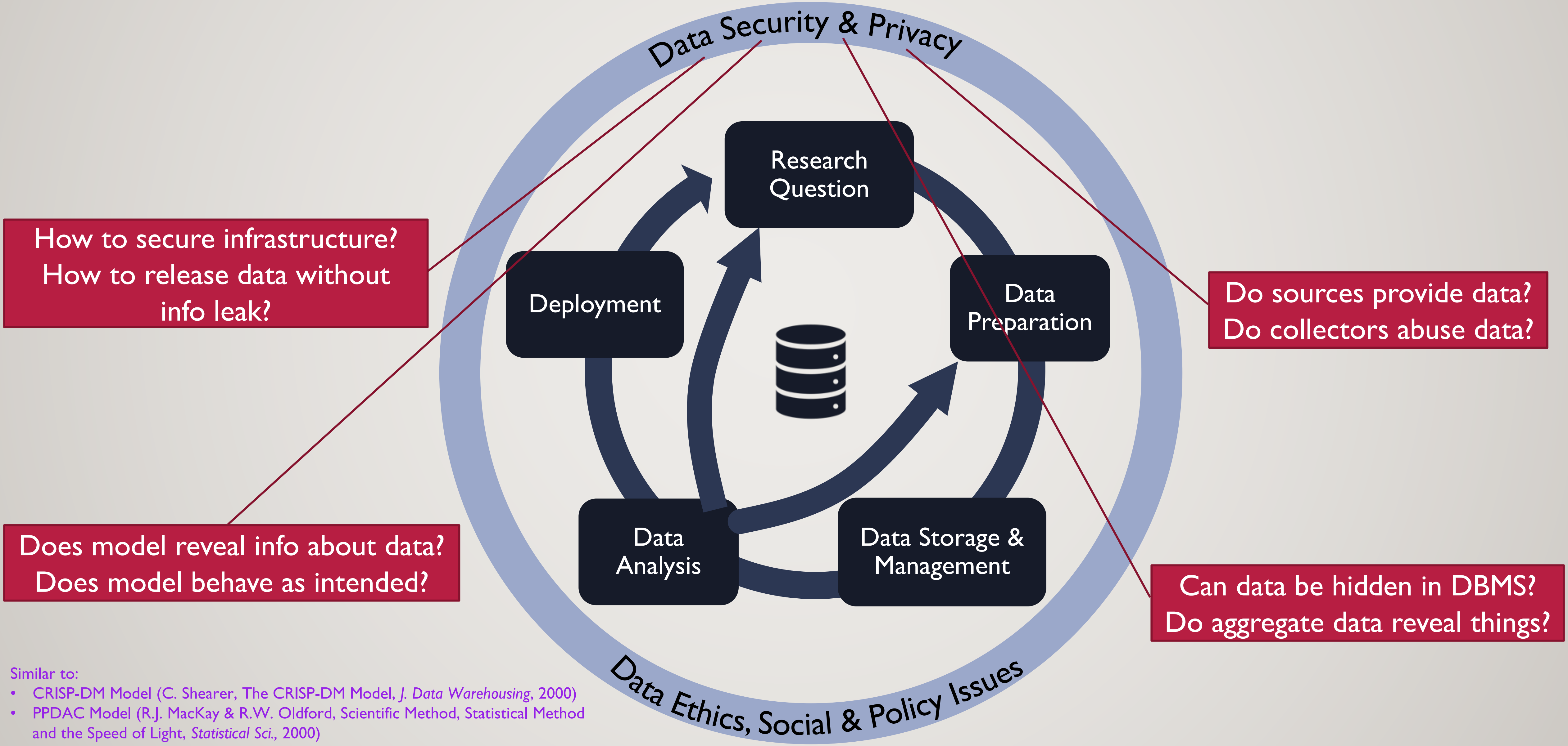

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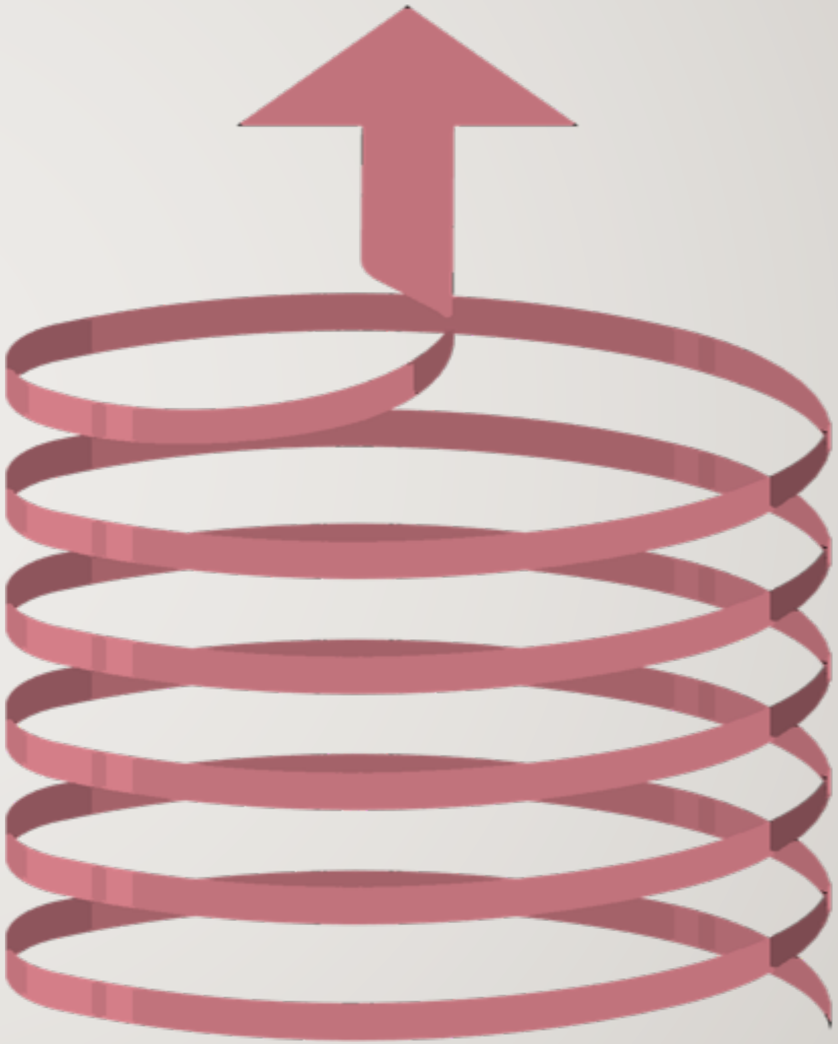

ISSUES AT THE INTERSECTIONS

- Data science components should not be siloed
- Many important problems at the intersections remain to be solved
- Examples
  - Data visualization – Visual analytics
  - Data management – Machine Learning
  - Data management support for provenance
  - Trustworthy data management
  - Privacy & security – Ethics
  - …

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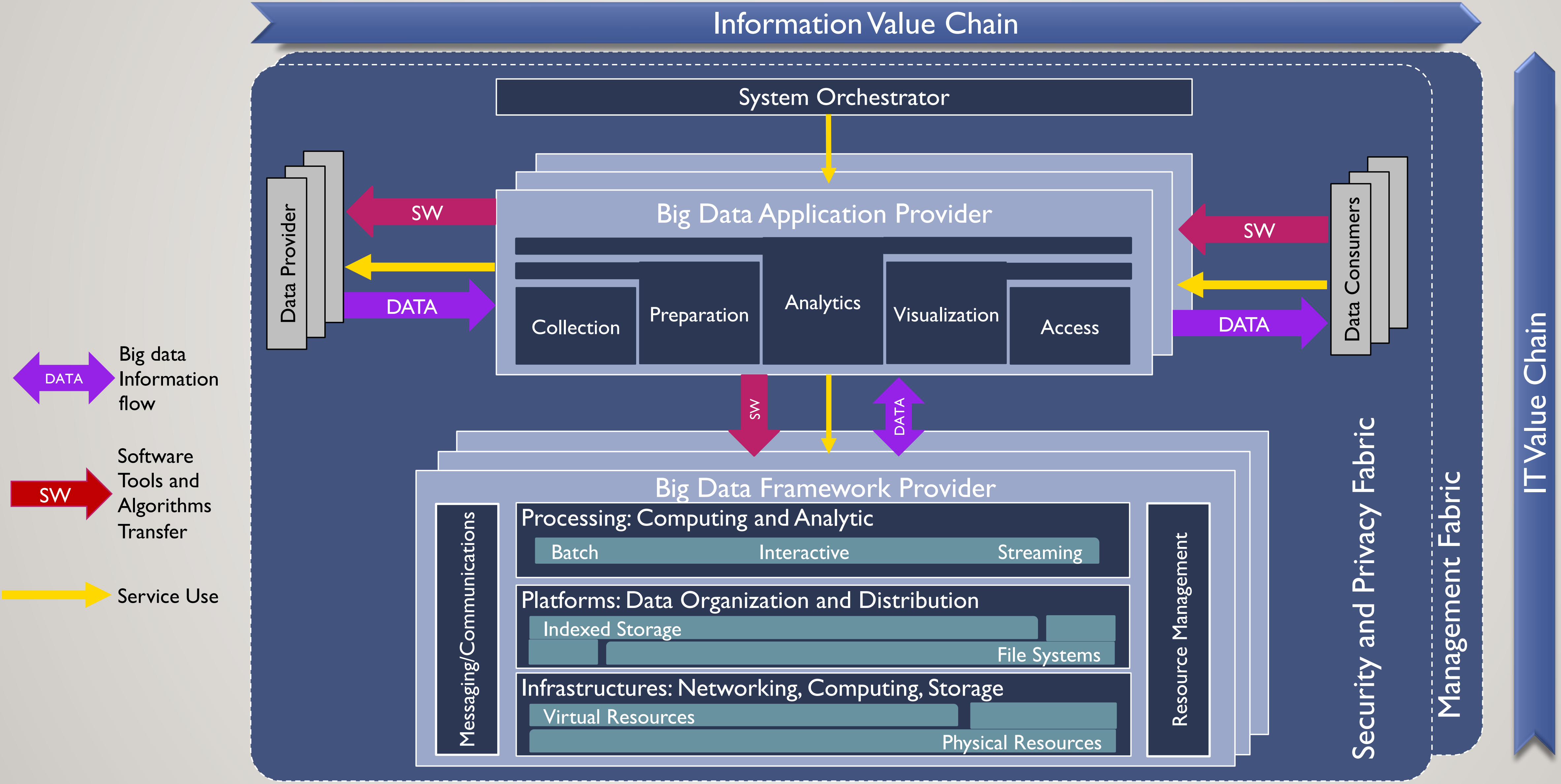
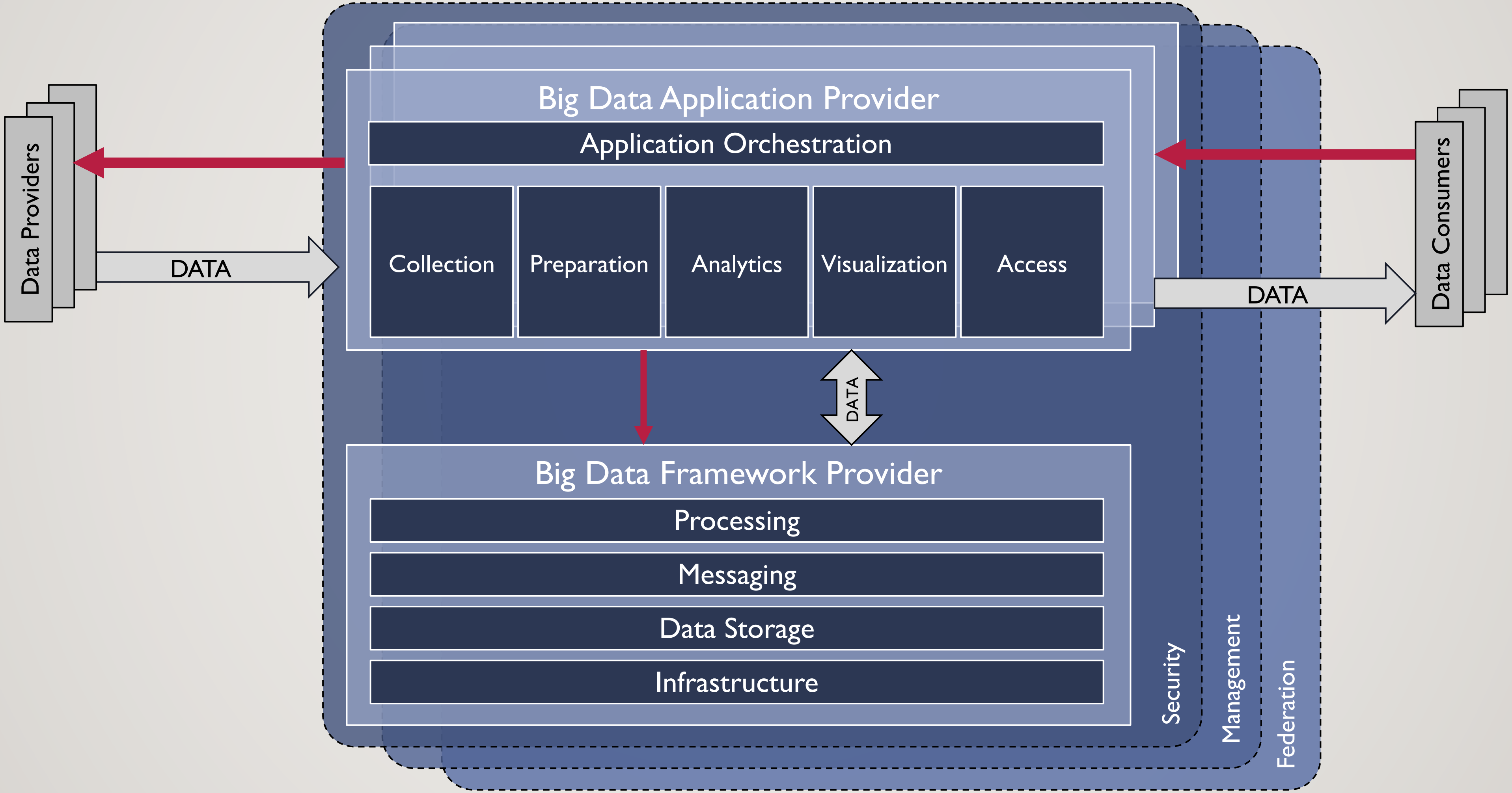
NIST REFERENCE ARCHITECTURE (NBDRA)



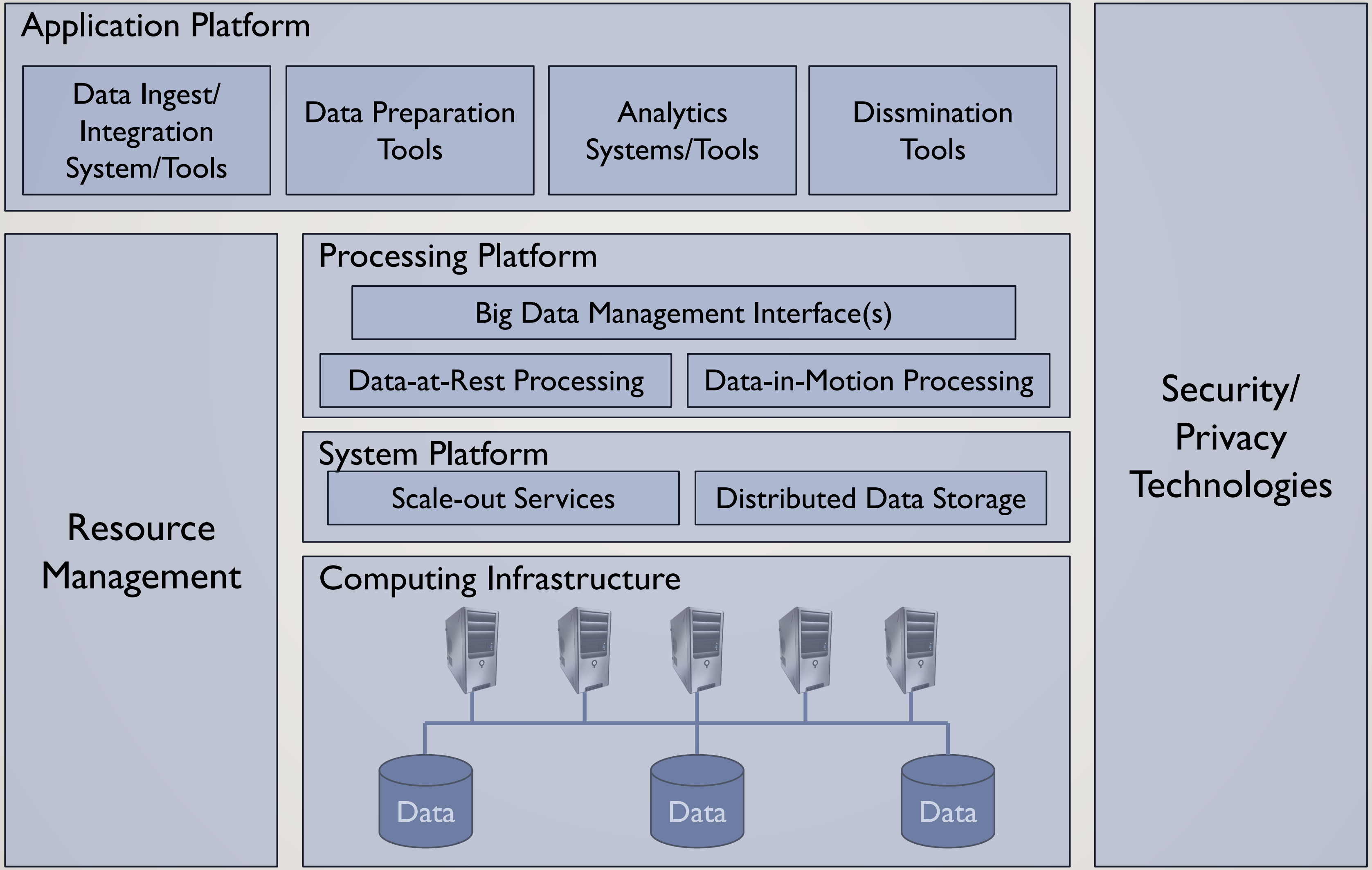
NIST Big Data Public Working Group. NIST big data interoperability framework: Volume 6, reference architecture, version 3, 2019

NBDRA MAPPING TO NATIONAL SECURITY APPLICATIONS



J. Klein et al., A Reference Architecture for Big Data Systems in the National Security Domain, *Proc. 2nd Int. Workshop on Big Data Soft. Eng.*, 2016

CONCRETE ARCHITECTURE –SOFTWARE STACK



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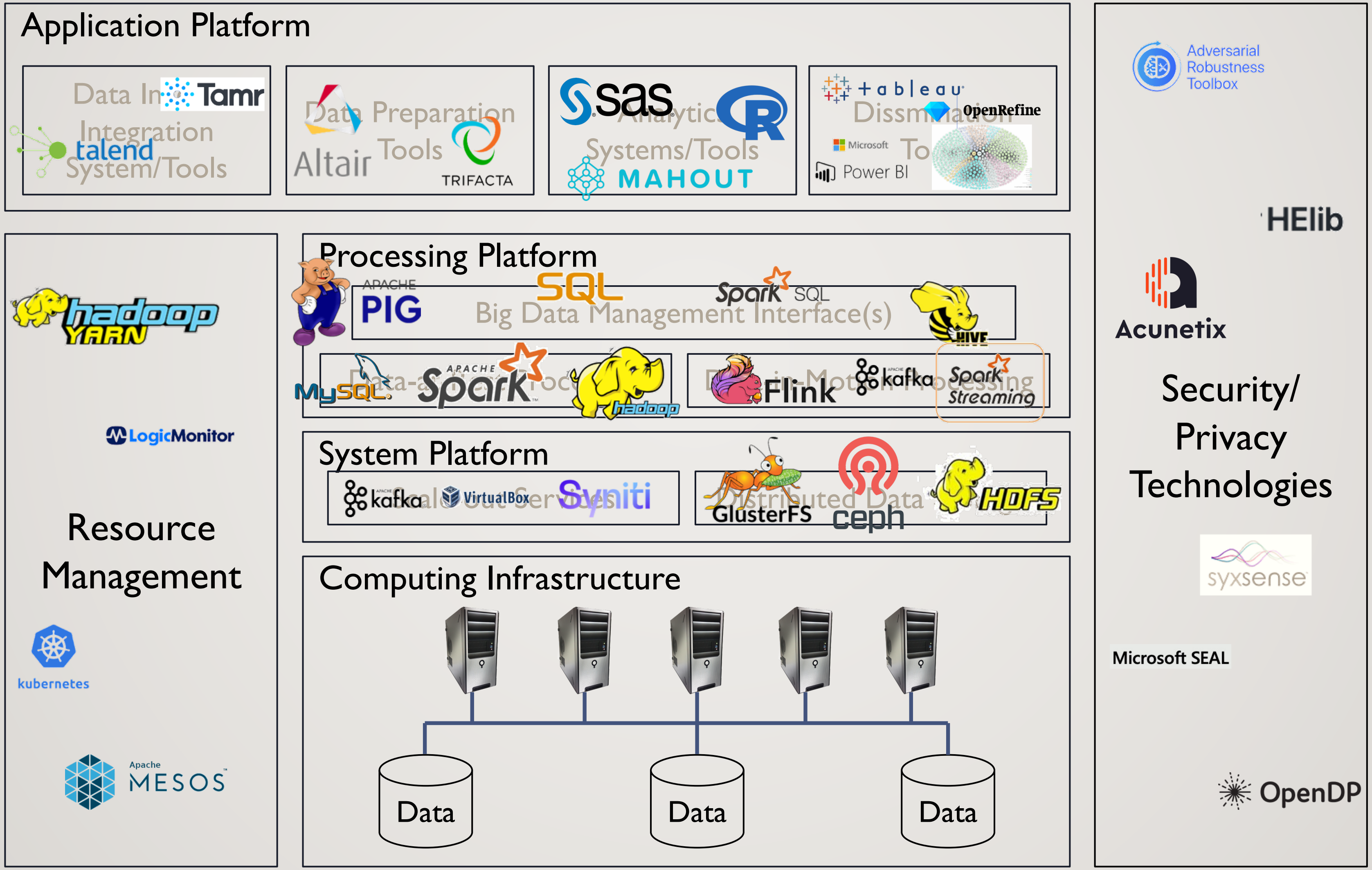
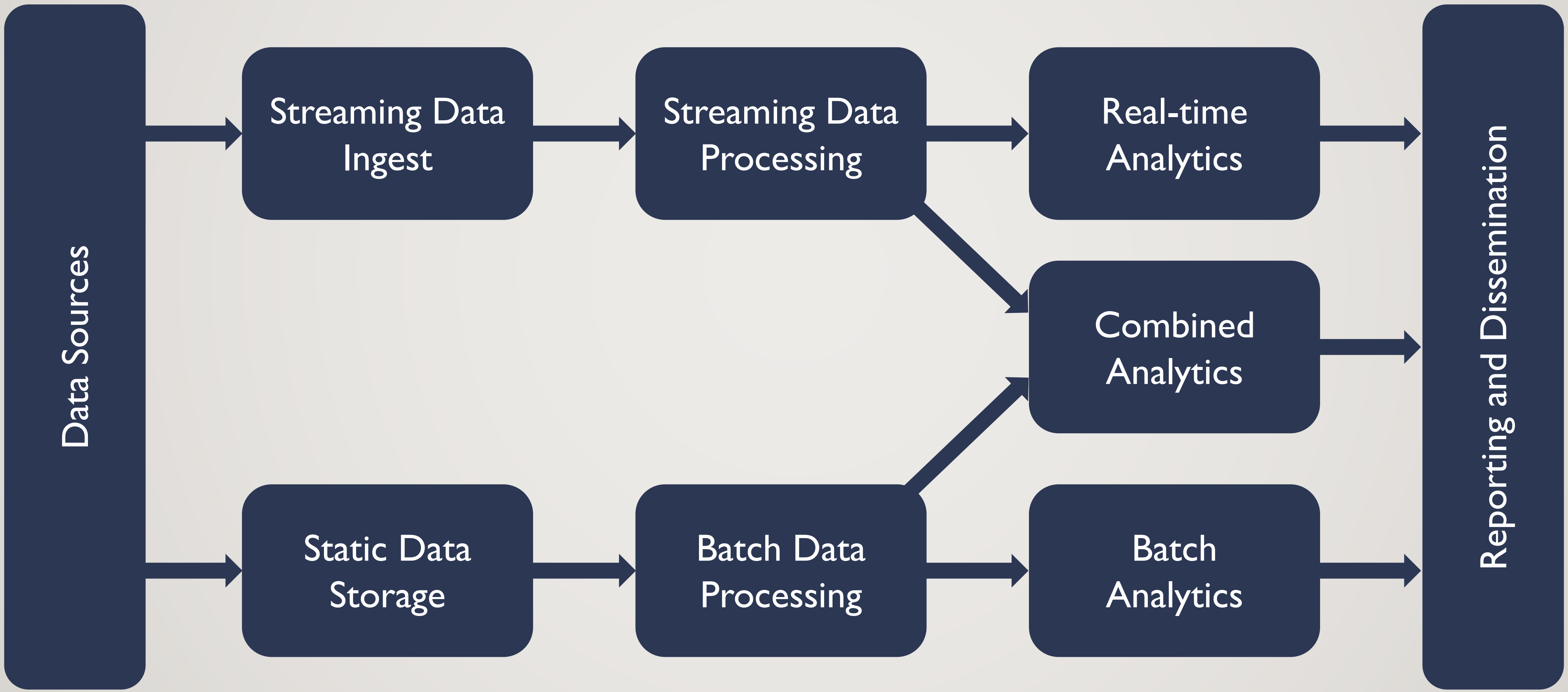


ARCHITECTURE – PROCESS VIEW



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WHO OWNS DATA SCIENCE?
TUG OF WAR BETWEEN CS & STATS

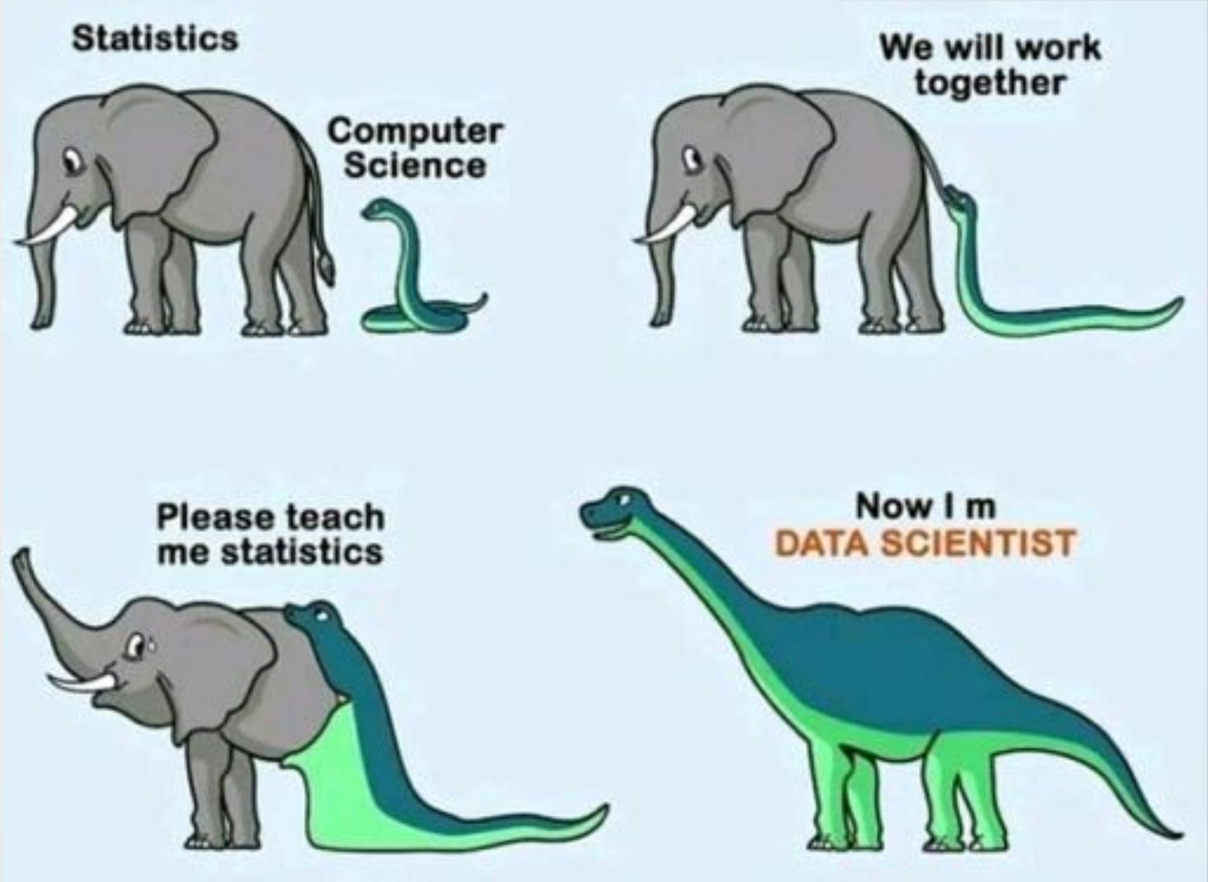
"many academic statisticians perceive the new programs as 'cultural appropriation' …

`Insightful statisticians have for at least 50 years been laying the groundwork for constructing [data science] as an enlargement of traditional academic statistics."

50 Years of Data Science
David Donoho
2017

Aren't We Data Science?

Marie Davidian
President of ASA, 2013



WHO OWNS DATA SCIENCE?

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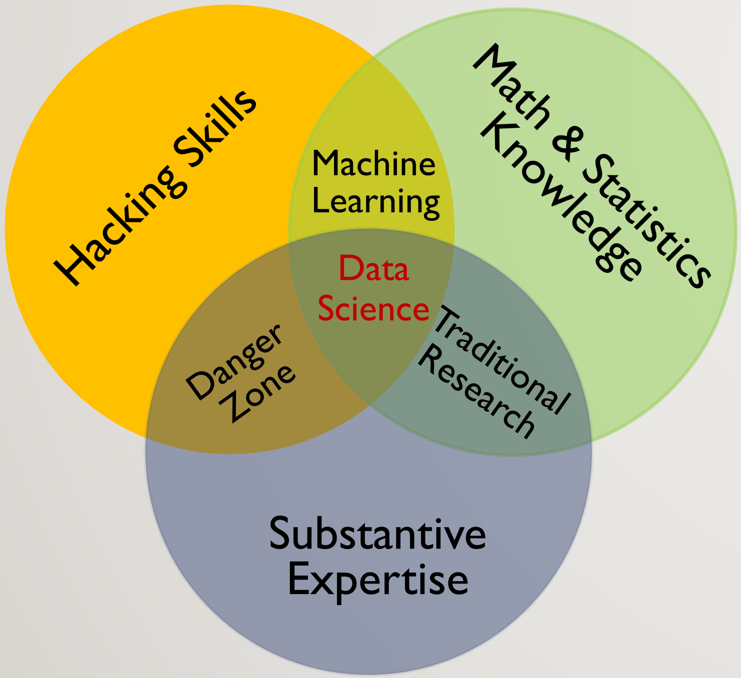
Statistics – Conway Diagram

- CS part is just hacking



https://www.kdnuggets.com/2016/10/battle-data-science-venn-diagrams.html/2

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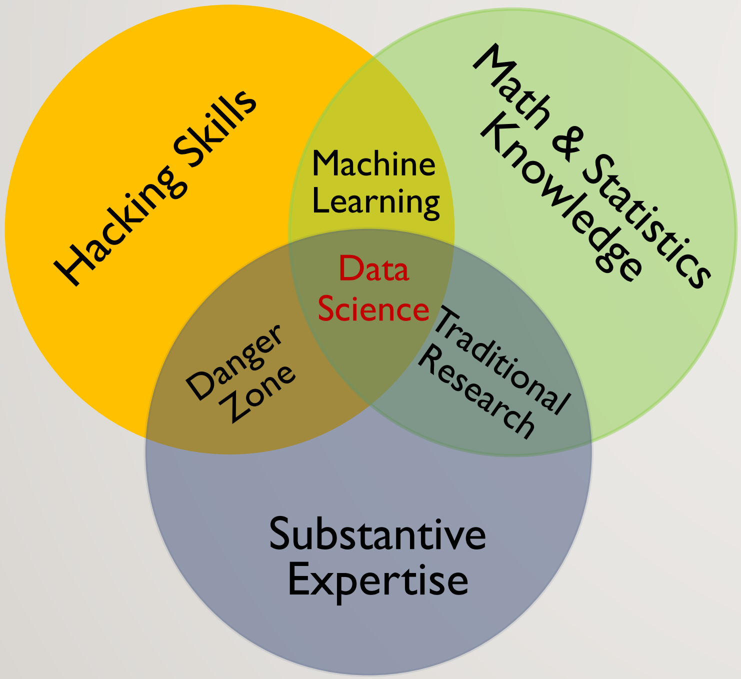
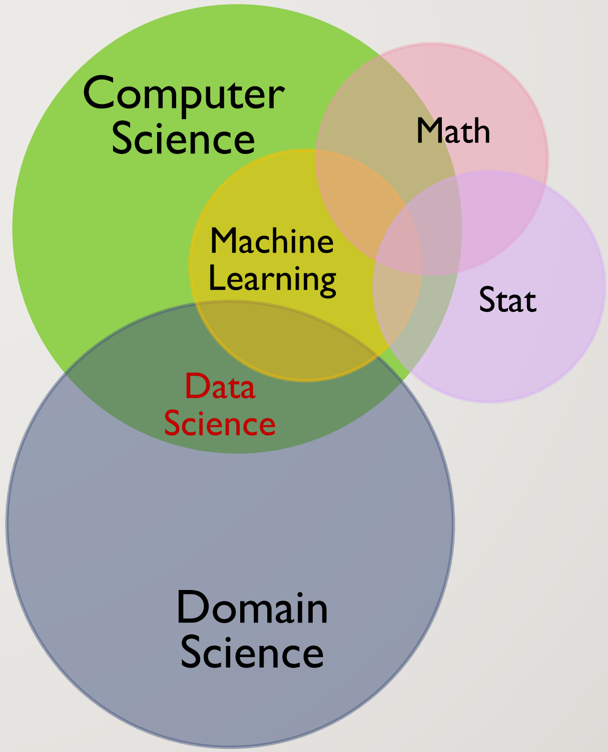


CS – Ullman Diagram

- Major CS role



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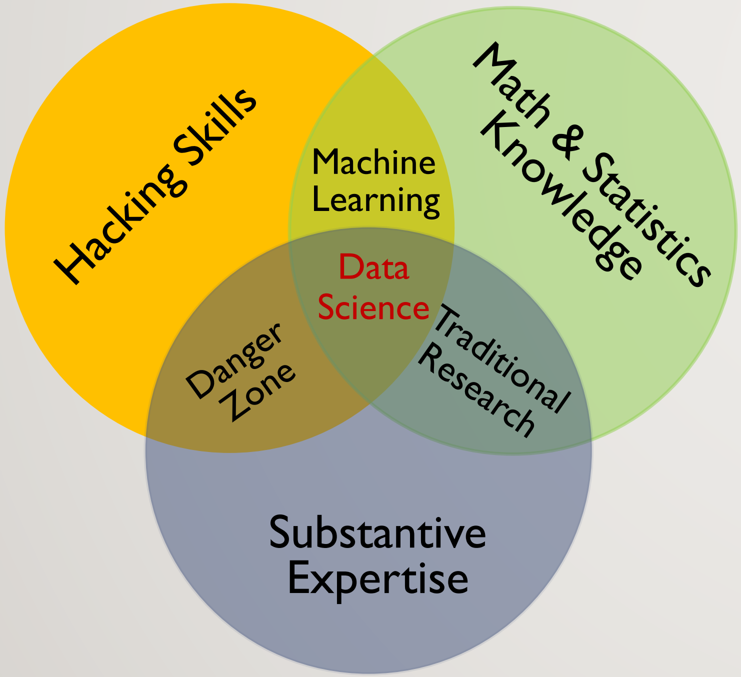
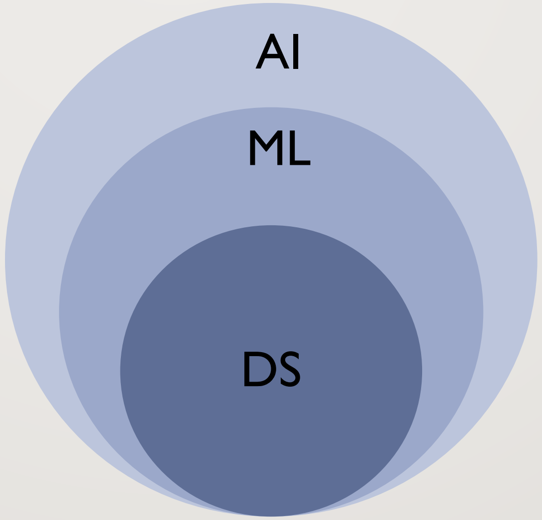


CS Internal

- It is all AI



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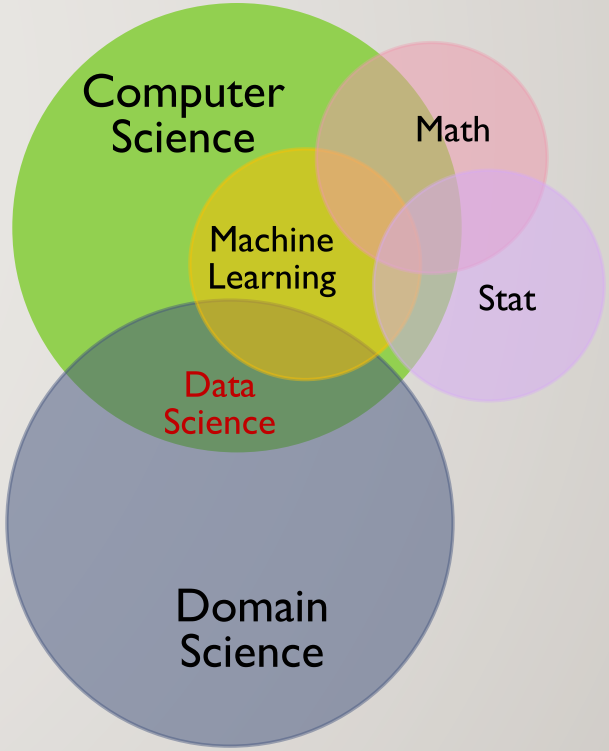

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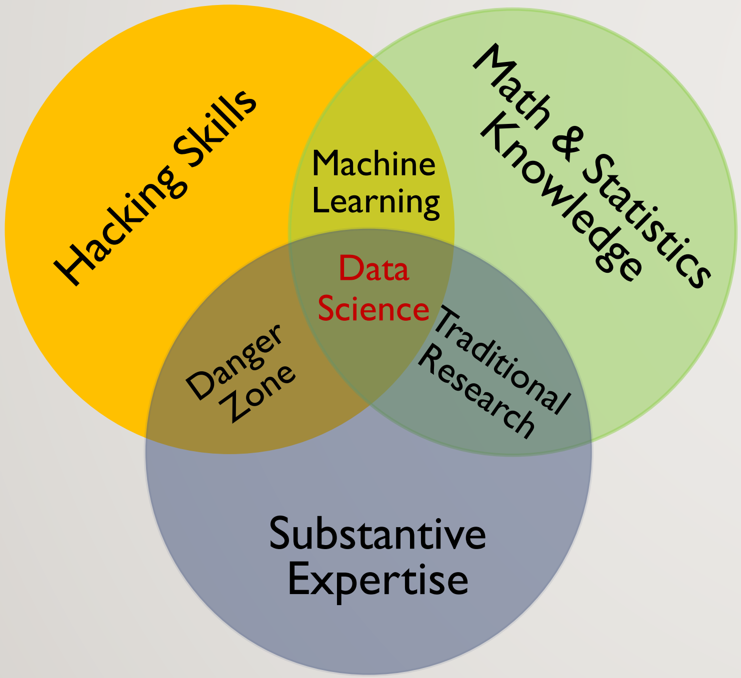

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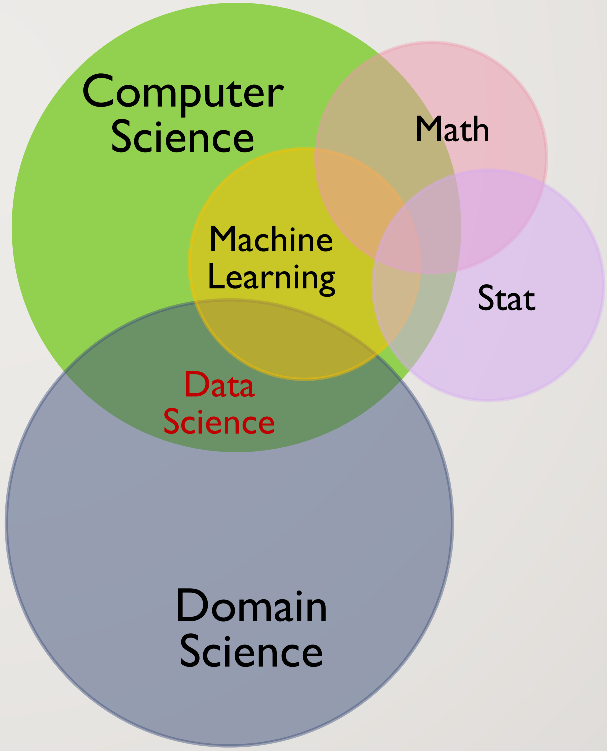

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WHO ARE THE STAKEHOLDERS?

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Core Technology

STEM people who are involved in developing the core technologies

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Application

People in STEM, social sciences or humanities who are involved in data science applications in some domain

WHO ARE THE STAKEHOLDERS?

Core Technology

STEM people who are involved in developing the core technologies

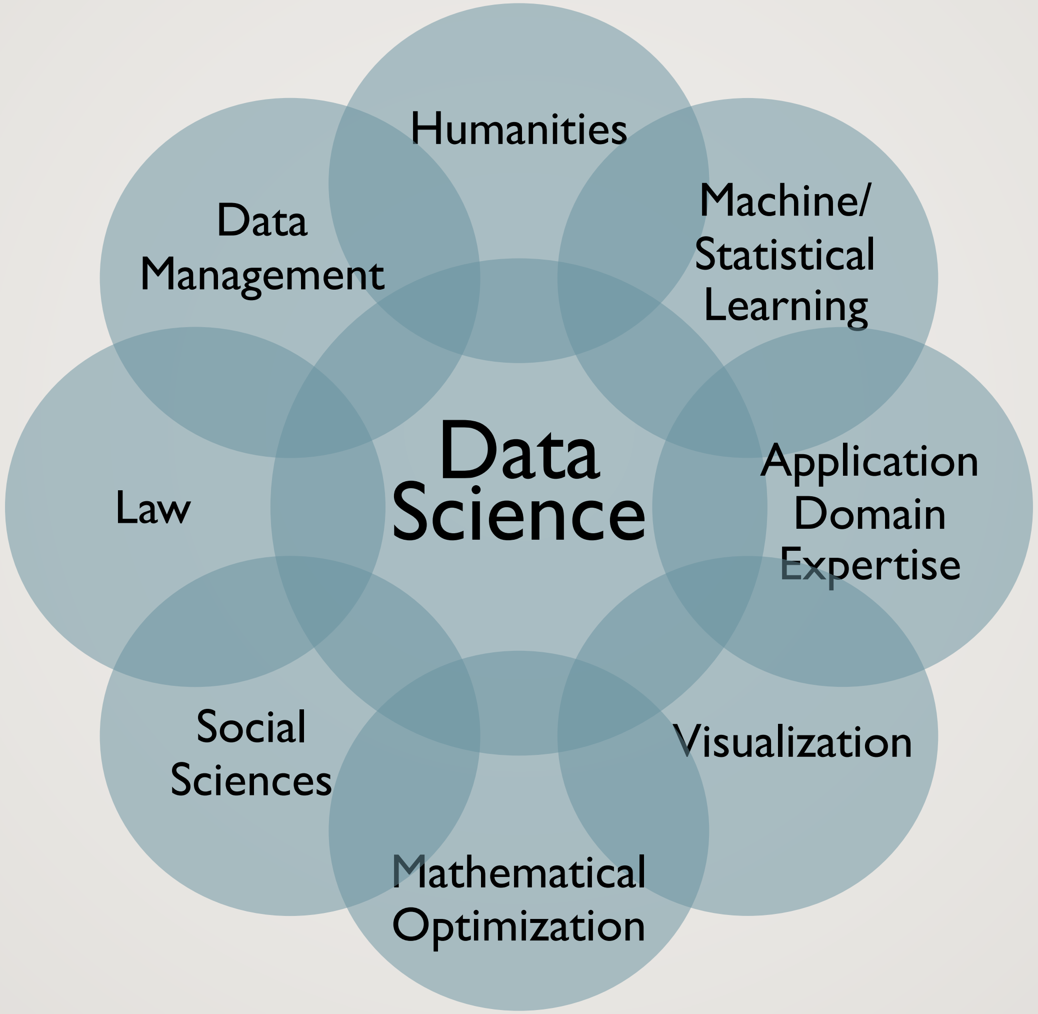
Application

People in STEM, social sciences or humanities who are involved in data science applications in some domain

Ethicists, Social, Policy

People in social sciences and humanities who are concerned with and work on data science ethics or social impact of data science or policy issues

WHO ARE THE STAKEHOLDERS?



WHO IS A DATA SCIENTIST?

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Core competencies

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- In-depth knowledge of at least one of data engineering or data analytics pillars (expert level)

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- Working knowledge of the other three pillars

UDACITY

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- Working knowledge of the other three pillars
- In-depth knowledge of at least one, preferably multiple, application areas (almost expert level)

UDACITY

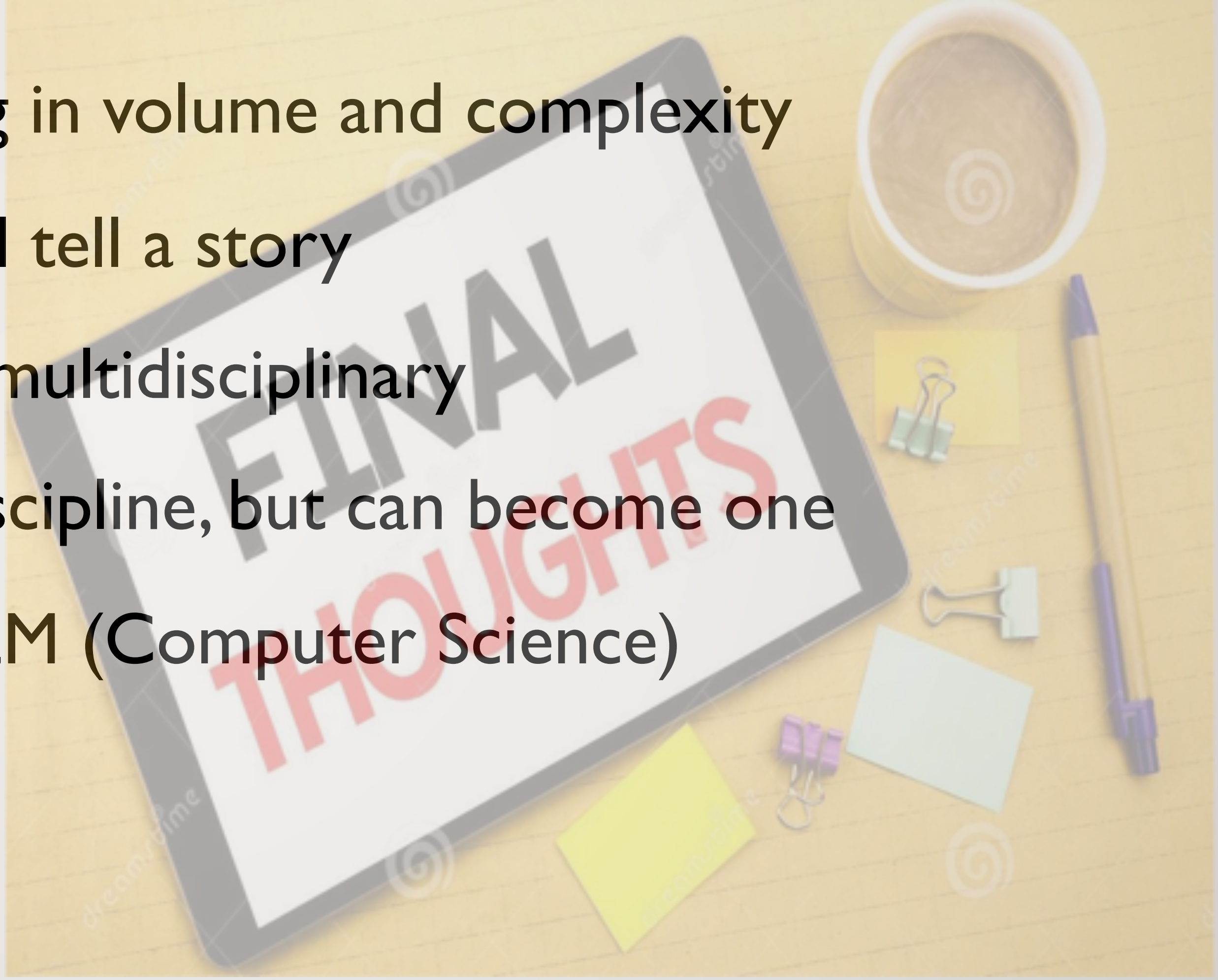
WHO IS A DATA SCIENTIST?

Core competencies

- In-depth knowledge of at least one of data engineering or data analytics pillars (expert level)
- Working knowledge of the other three pillars
- In-depth knowledge of at least one, preferably multiple, application areas (almost expert level)
- Ability to work in a team & communicate

FINAL THOUGHTS

- Data is central and it is increasing in volume and complexity
- Treat the data properly and it will tell a story
- Data science is multifaceted and multidisciplinary
- Data science may not yet be a discipline, but can become one
- The view I presented is from STEM (Computer Science) perspective
  - There is much more



Thank you to many colleagues who contributed to various initiatives I’ve led and who contributed to my understanding of data science.