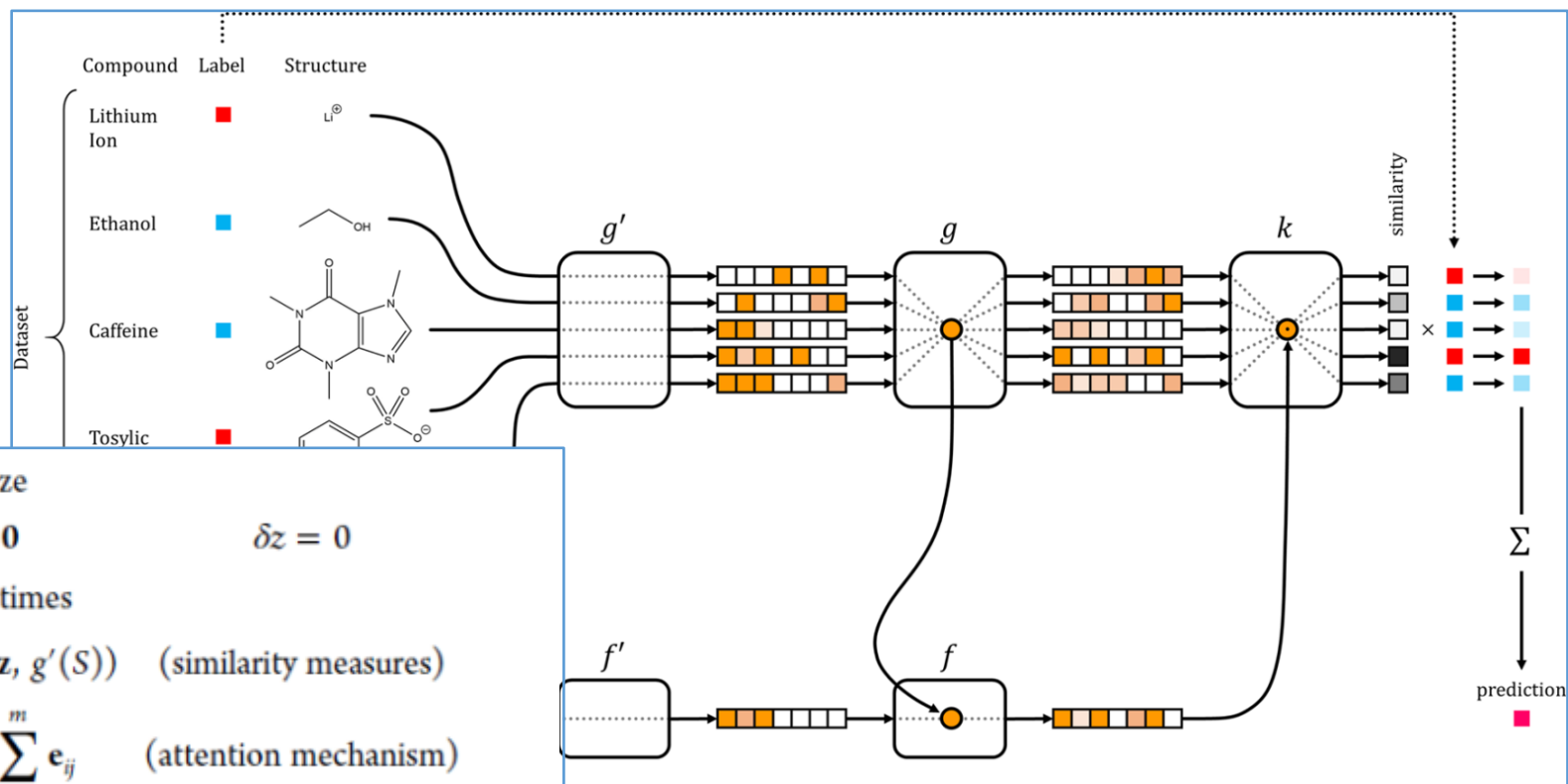




Derive Value From Excellence ...

Overview: Artificial Intelligence and Machine Learning in Life Sciences

Jeremy Wheeler
Director Biostatistics, GCE Solutions Ltd



Initialize

$\mathbf{r} = g'(S)$ $\delta \mathbf{z} = \mathbf{0}$ $\delta \mathbf{z} = \mathbf{0}$

Repeat L times

$\mathbf{e} = k(f'(x) + \delta \mathbf{z}, \mathbf{r})$ $\mathbf{e} = k(\mathbf{r} + \delta \mathbf{z}, g'(S))$ (similarity measures)

$a_j = e_j / \sum_{j=1}^m e_{ij}$ $A_{ij} = e_{ij} / \sum_{j=1}^m e_{ij}$ (attention mechanism)

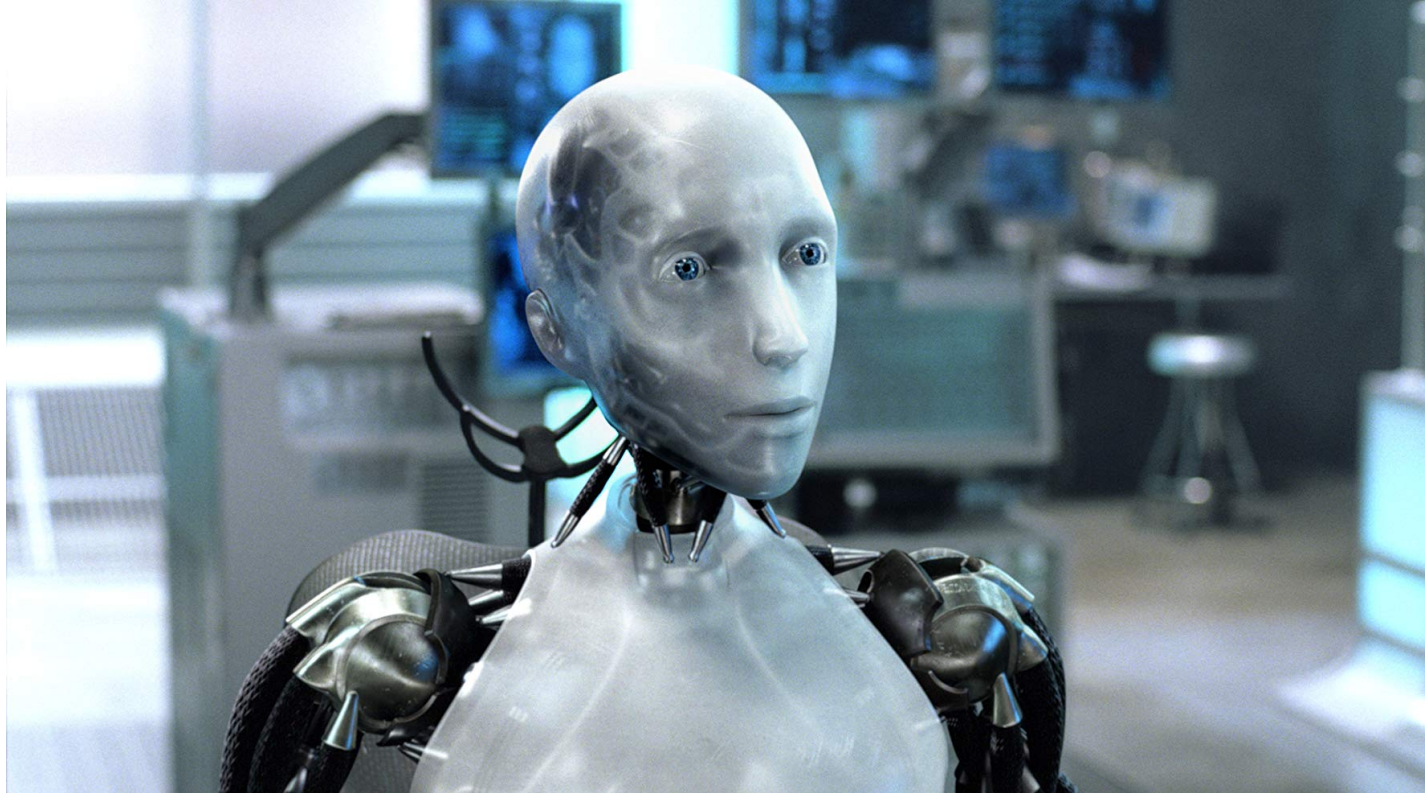
$\mathbf{r} = \mathbf{a}^T \mathbf{r}$ $\mathbf{r} = \mathbf{A} g'(S)$ (expected feature map)

$\delta \mathbf{z} = \text{LSTM}([\delta \mathbf{z}, \mathbf{r}])$ $\delta \mathbf{z} = \text{LSTM}([\delta \mathbf{z}, \mathbf{r}])$ (generate updates)

Return

$f(x) = f'(x) + \delta \mathbf{z}$ $g(S) = g'(S) + \delta \mathbf{z}$ (evolve embeddings)

Altae-Tran, 2017



© 20th Century Fox

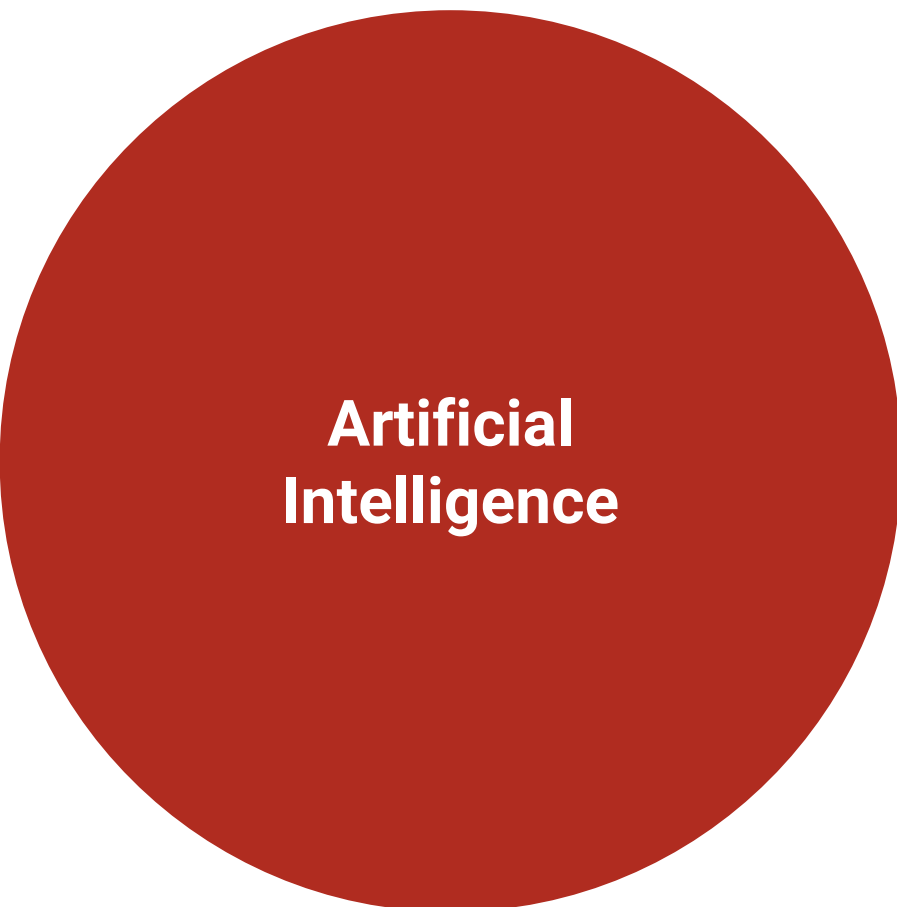


What We'll Cover...

- Overview of Artificial Intelligence (AI), Machine Learning (ML) and Natural Language Processing (NLP)
- Examples of AI/ML implementations in Life Sciences (LS)
- Where this appears to be headed



Overview: AI, ML and NLP...



Artificial Intelligence

Artificial Intelligence:

Subfield of computer science created in the 1950's concerned with solving tasks that are easy for humans but difficult for computers, e.g.:

- Planning
- Moving around in the world
- Recognizing objects and sounds
- Speaking and/or translating
- Creating art, music, poetry



Overview: AI, ML and NLP...(cont'd)



The 4 Types of AI:

1) Reactive Machines:

- Teaching computers to see and react
- But, computer has no concept of past or memory of what had happened previously and is focused on very specific tasks
- “Trustworthy”
- Examples:
 - IBM’s Deep Blue (Chess)
 - Google’s AlphaGo (Go)



Overview: AI, ML and NLP...(cont'd)



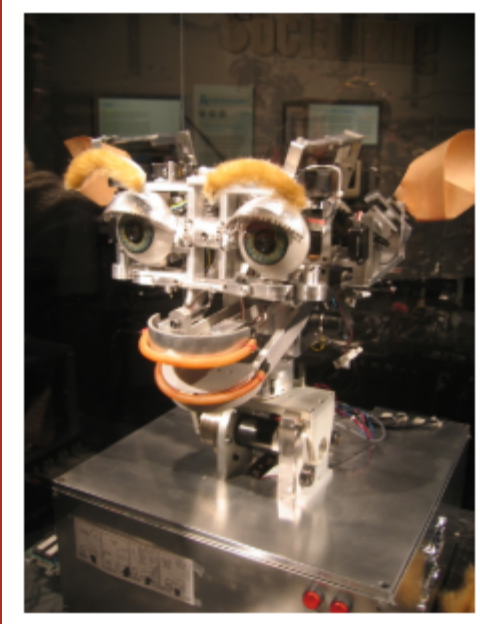
The 4 Types of AI (cont'd):

2) Limited Memory:

- Machines that can “look into the past”, i.e., make specific observations to compare to other conditions (programmed representations) and determine appropriate, predefined actions
- Information is transient, i.e., not able to be retained and used for inferences
- Example:
 - Self-driving cars



Overview: AI, ML and NLP...(cont'd)



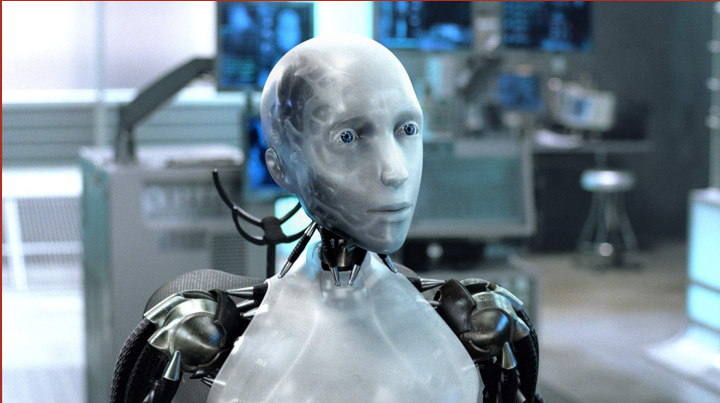
The 4 Types of AI (cont'd):

3) Theory of Mind:

- Machines of the future that can form their own representations of the world and other agents/entities in it
- Able to “understand” or even predict how others think/feel/act and adjust its own behavior/actions accordingly
- Example:
 - Kismet, a robot head made at MIT in the 90's that can mimic human emotions



Overview: AI, ML and NLP...(cont'd)



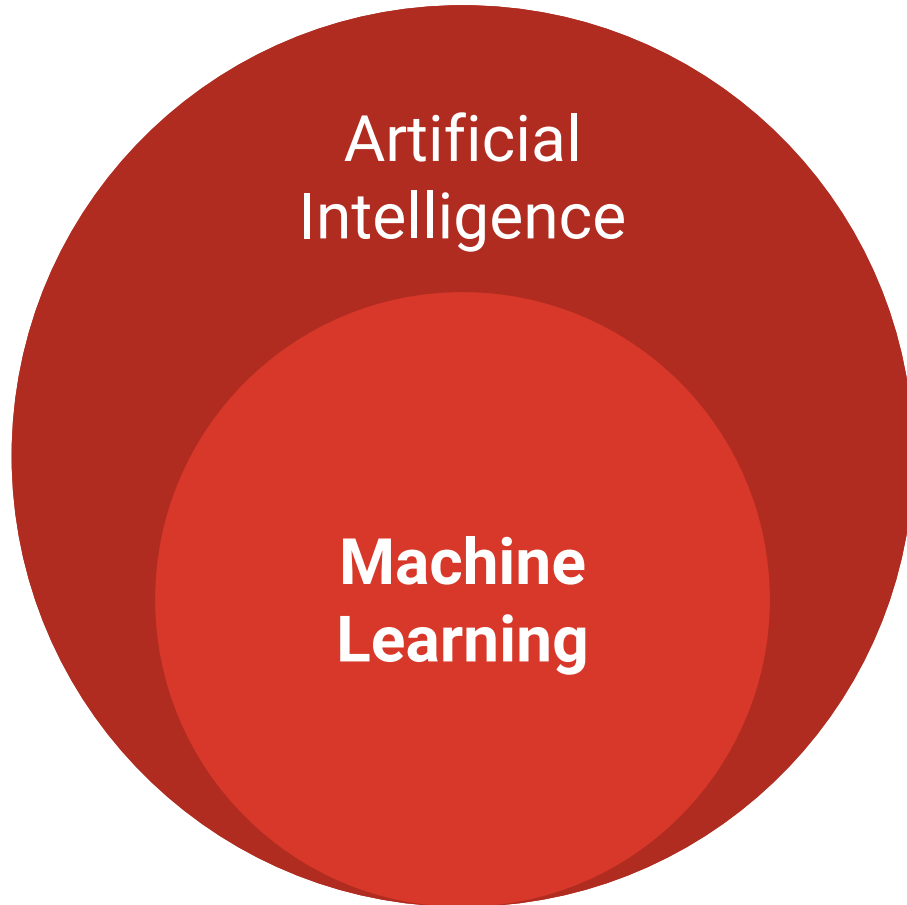
The 4 Types of AI (cont'd):

4) Self-Awareness:

- Most advanced type of AI where machines have consciousness and recognize it in other entities
- An extension of Theory of Mind AI where it (he/she?) is able to display self-driven reactions
- Example:
 - Nothing yet



Overview: AI, ML and NLP...(cont'd)



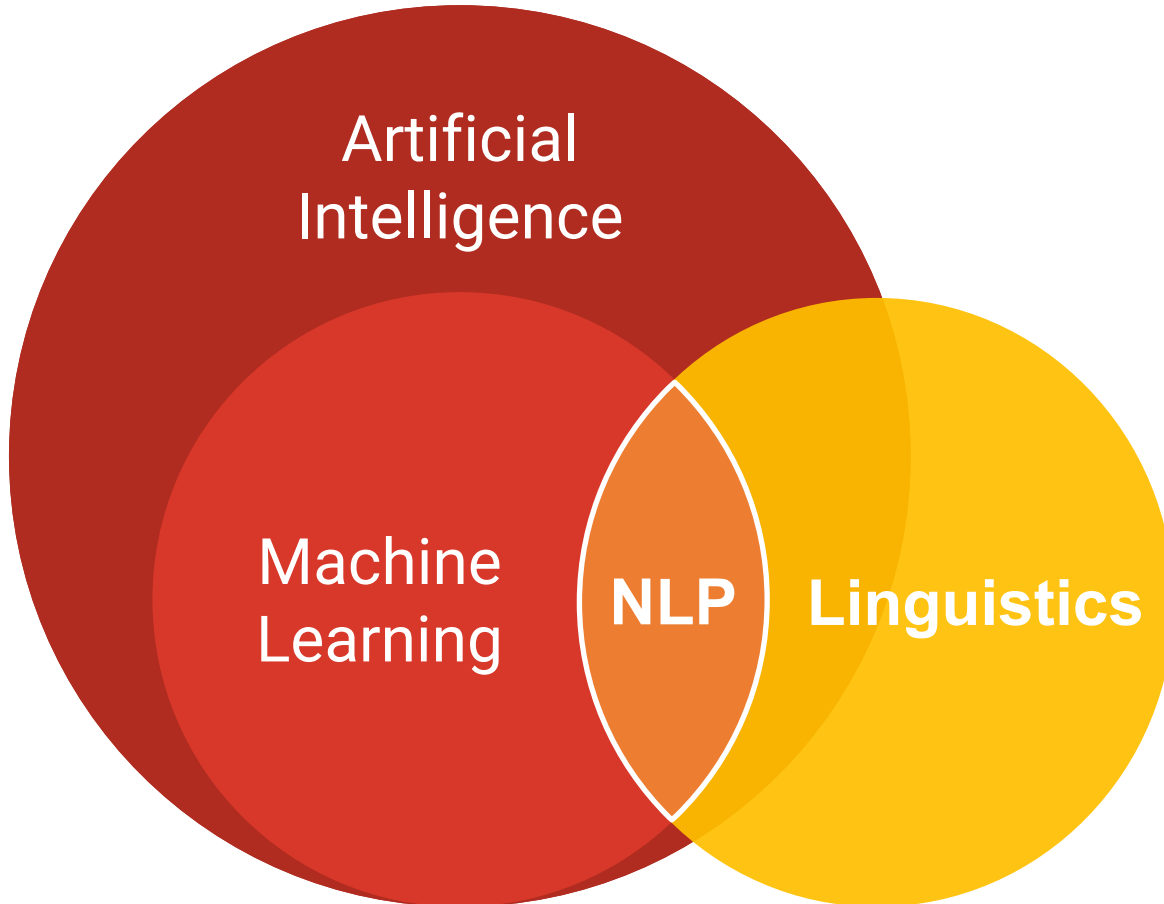
Machine Learning:

An application of AI to provide machines the ability to automatically learn and improve from data without having to be explicitly programmed. Three types of ML are:

- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning



Overview: AI, ML and NLP...(cont'd)



Natural Language Processing (NLP):

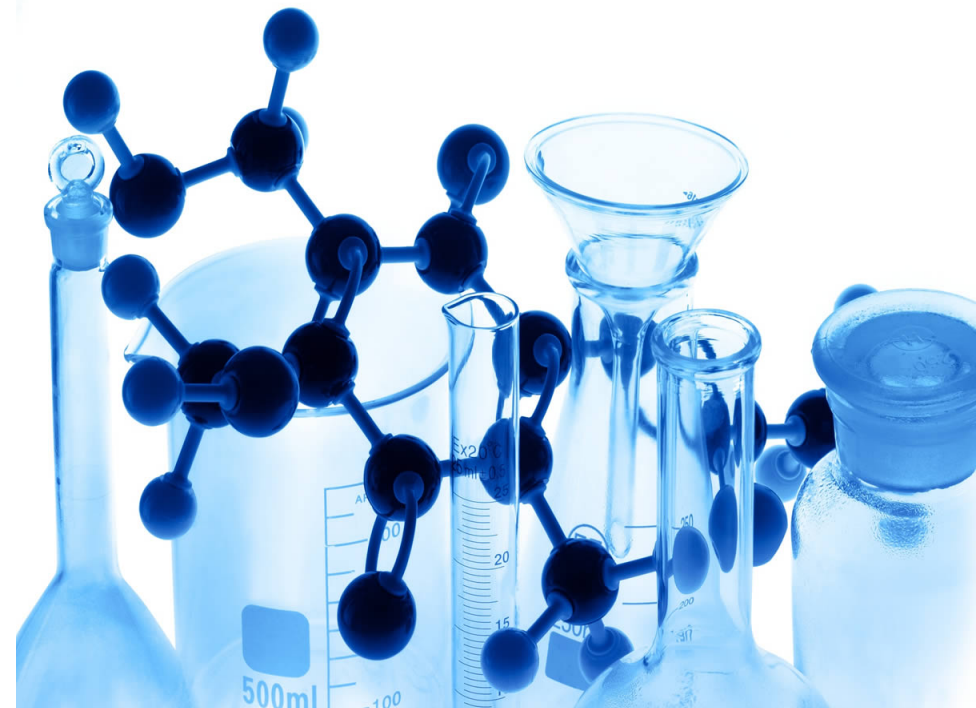
NLP is a confluence of AI and Linguistics giving machines the ability to read and understand human language

- Examples:
 - Autocomplete
 - Predictive Typing
 - Spell Checkers
 - Grammar Checkers
 - Siri/Alexa
 - Google Translate



How AI/ML has been implemented in LS...

- AI is already being used in drug discovery and development in a number of ways^[1]...
 - Computer-aided synthesis
 - Computer-assisted retrosynthesis based on molecular similarity
 - Organic synthesis and design
 - Scoring synthetic complexity
 - Automation of molecule design
 - Predicting organic reaction outcomes
 - Predict drug performance in testing
 - Discover off-label use
 - Predict toxicity prior to clinical trials
 - Personalized medicine



Rosso. How Artificial Intelligence is accelerating Life Sciences. Psychology Today



How AI/ML has been implemented in LS...(cont'd)

- AI is used in drug discovery and development in a number of ways^[1]...(cont'd)

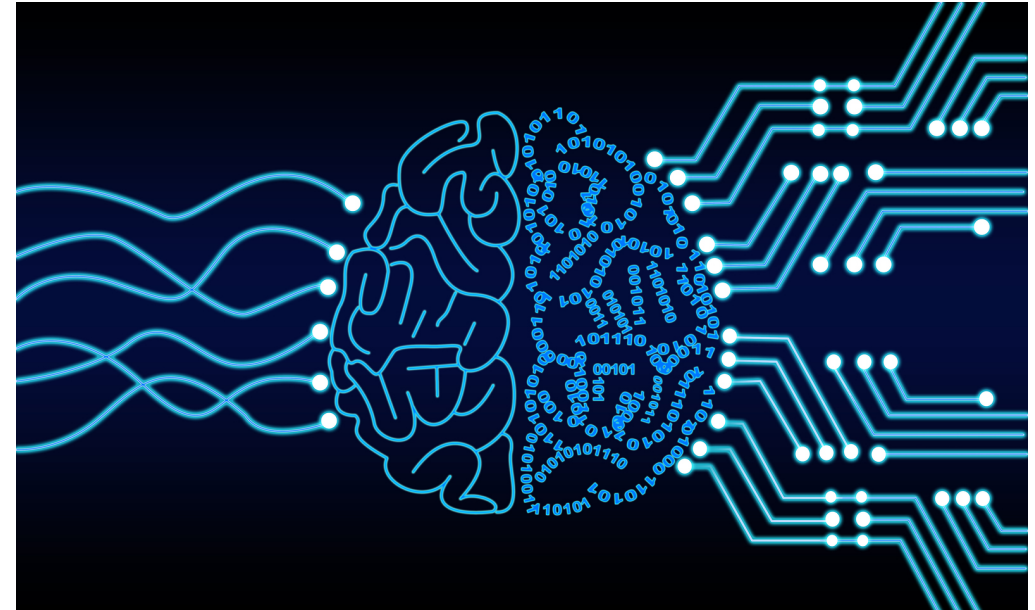


- **Neural networks** to predict the binding of small molecules to proteins, thereby accelerating the drug discovery process. Enables the analysis of 10 to 20 billion chemical compounds daily, reducing the time for discovery and optimization process from years to weeks.
- **Generative adversarial networks (GANs)** for new molecule drug discovery, biomarker development, and aging research
- **Long Short-term memory** combined with deep neural networks improves the learning of meaningful distance metrics



How AI/ML has been implemented in LS...(cont'd)

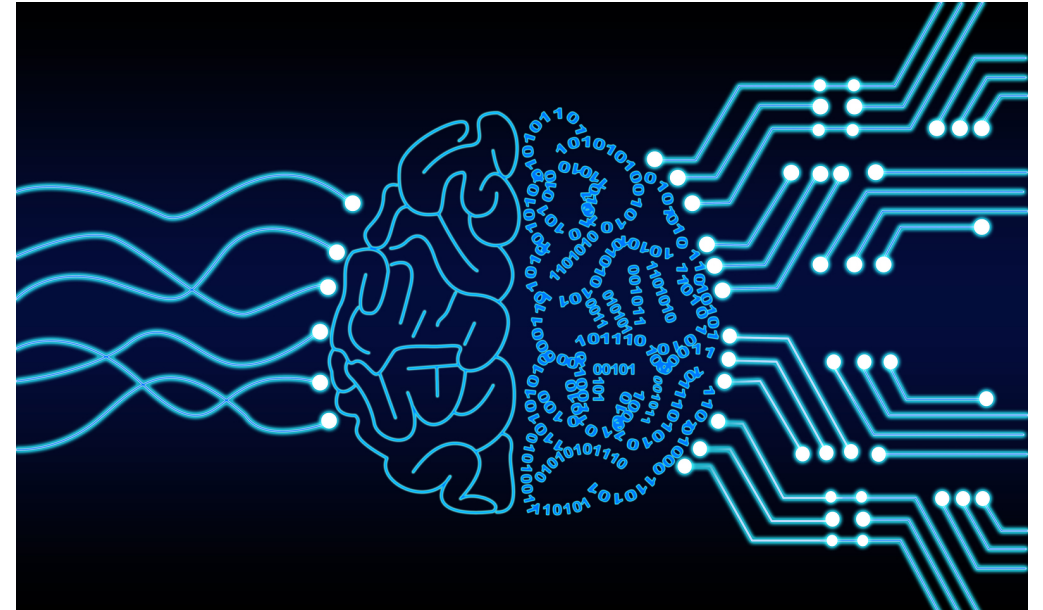
- AI is also being adopted in the data management and biometrics areas...
 - Generation of standard datasets with ability to detect transformations based on metadata
 - Outlier Detection based on combination of variables at the time of data collection at sites. Ability to detect odd/extreme values increases with increase in data passed through ML models.
 - QC of documents (e.g., CSR) against results using an automated tool to avoid human error
 - Anonymization of dataset and documents using pre-defined strategies and optimizing re-identification risk using ML





How AI/ML has been implemented in LS...(cont'd)

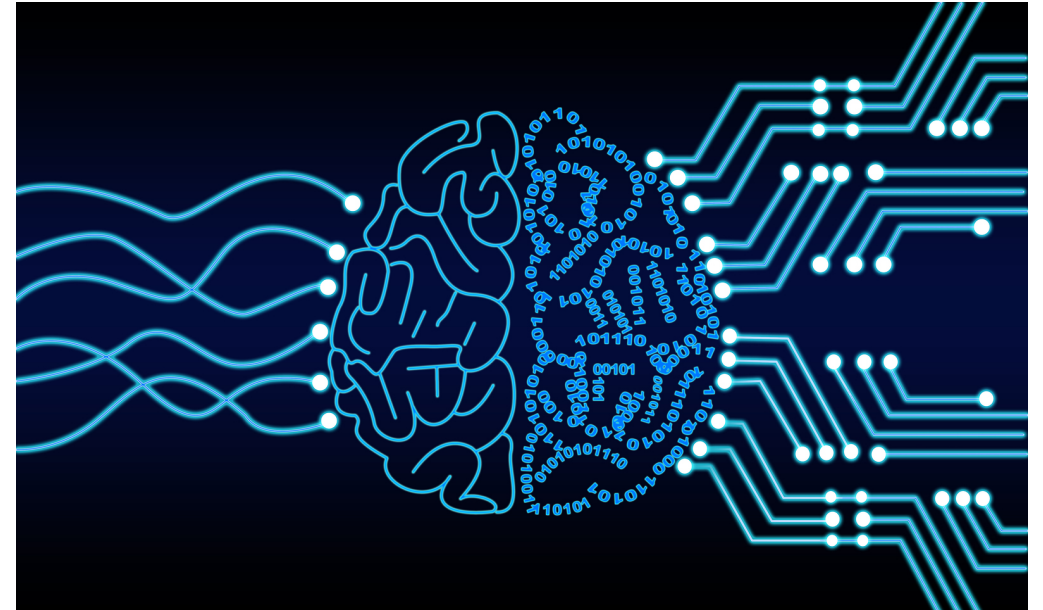
- AI is also being adopted in the data management and biometrics areas...
- Generation of standard datasets with ability to detect transformations based on metadata
 - Metadata-driven generation
 - Project definition/attribute matching
 - Domain/field recognition/recommendations





How AI/ML has been implemented in LS...(cont'd)

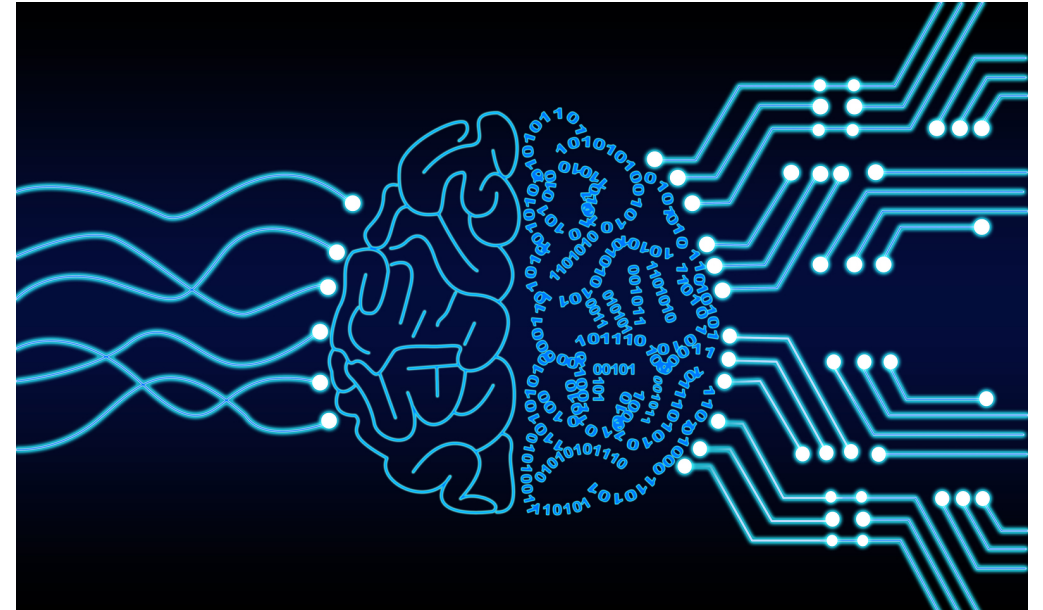
- AI is also being adopted in the data management and biometrics areas...
- Outlier Detection based on combination of variables at the time of data collection at sites. Ability to detect odd/extreme values increases with increase in data passed through ML models.
 - Project definition/attribute matching
 - Data-driven determination of most appropriate detection models to use





How AI/ML has been implemented in LS...(cont'd)

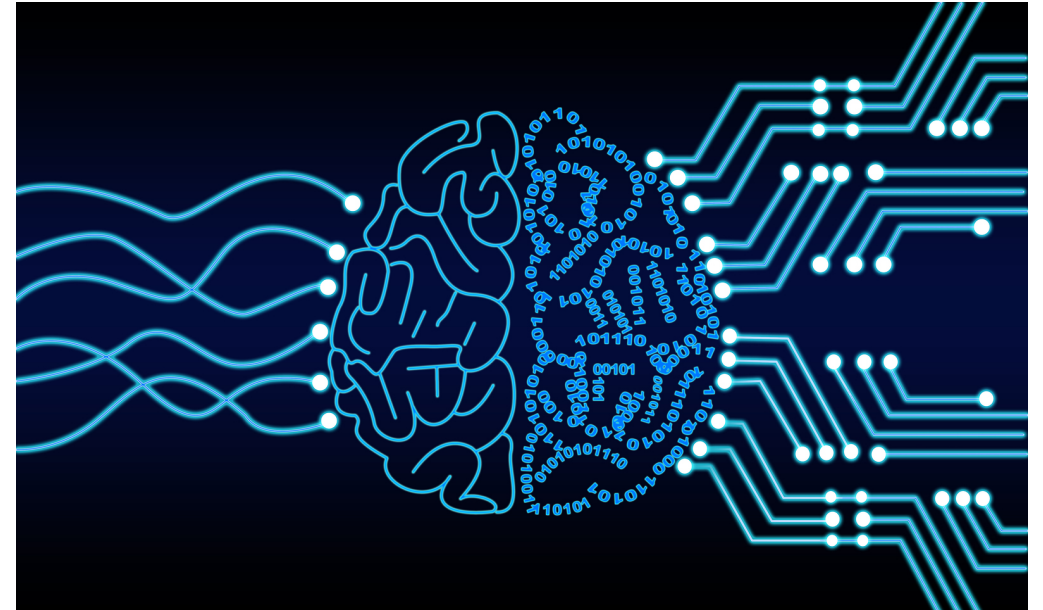
- AI is also being adopted in the data management and biometrics areas...
- QC of documents (e.g., CSR) against results using an automated tool to avoid human error
 - Use of business rules as metadata to perform normally complicated and time-intensive checks on unstructured data





How AI/ML has been implemented in LS...(cont'd)

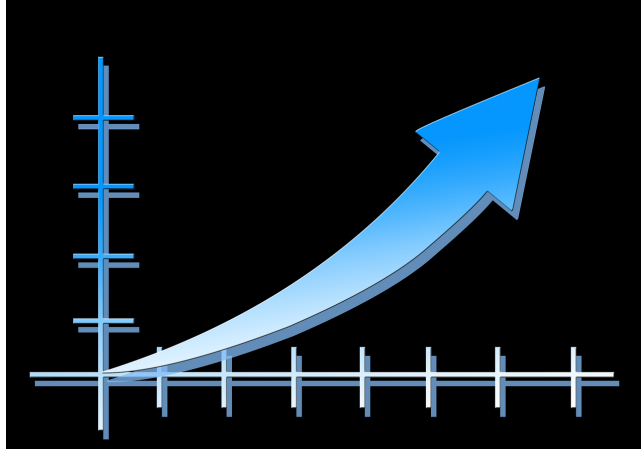
- AI is also being adopted in the data management and biometrics areas...
- Anonymization of dataset and documents using pre-defined strategies and optimizing re-identification risk using ML
 - Project definition/attribute matching
 - Workflow and “educated” parameterization leading users through the process





Where this is all headed...

In an online article, “AI in Life Sciences Trends and Terms that Executives Need to Know”, June 19, 2018 by Raghav Bharadwaj (<https://www.techemergence.com/ai-in-life-sciences-trends-and-terms/>), executives were asked to identify AI trends in the industry. Results were as follows:



- The time and associated costs of drug discovery and development has the pharma sector at the frontier of AI-integration
- Industry leaders are looking to AI technology to improve efficiency and save costs
- With uncertainty as to how to incorporate AI professionals into the LS workforce, startups are appearing and are either partnering or being acquired by bigger pharma companies
- AI adoption is a certainty, and those who use it most effectively will gain competitive advantage



Where this is all headed...(cont'd)

Large Pharma is investing in AI to help streamline processes and costs of new product development...



- Johnson & Johnson Innovation's life sciences has an incubator called JLABS. Its resident startups with AI technology include Analytics 4 Life [3], WinterLight Labs [4], A2A Pharmaceuticals, Envisagenics, Fited, Human Microbiology Institute, and Savor Health [5].
- Roche (Genentech) is collaborating with a precision medicine company, GNS Healthcare, to discover and validate new oncology drugs and patient response markers [6].
- Pfizer is collaborating with IBM Watson Health for Drug Discovery, to assist in immuno-oncological research and development [7]. IBM Watson Health for Drug Discovery is an AI solution that contains data from four million patents, 25 million Medline abstracts, and over a million full-text medical journal articles that are updated regularly.



Where this is all headed...(cont'd)



- Big Data, Data Lake, Data Mining and Visualization efforts have been exploring ways in which we can do more with our existing data. The vast amount of data requires AI/ML methods for automating the collection and management of this data. ^[1]



Summary...

- AI/ML is here and is gaining momentum
- Developing technologies require new types of data/data management, and will provide us with a greater range of tools/capabilities
- Our roles are changing as we work with these new tools
 - Adopting new approaches
 - Using the right/best tool for the job
 - “The best way to predict the future is to create it” - Abraham Lincoln





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