GCE SOLUTIONS

*Derive Value from Excellence …*

# Opportunities for Artificial Intelligence and Machine Learning in Life Sciences to Achieve Quality and Automation

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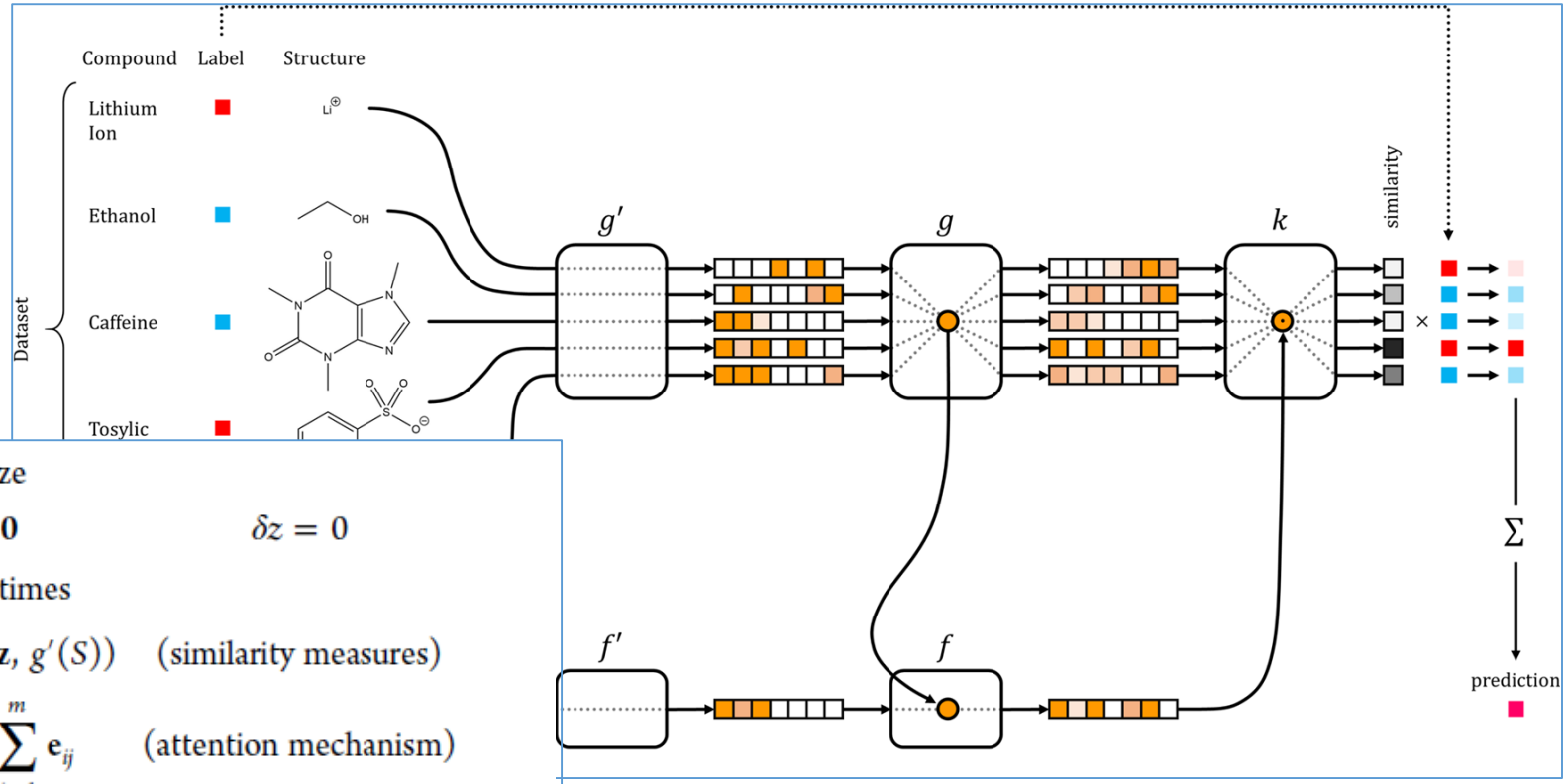



Initialize

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

Repeat L times

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

$a_j = e_j / \sum_{j=1}^{m} e_{ij}$ $\quad \mathbf{A}_{ij} = \mathbf{e}_{ij} / \sum_{j=1}^{m} \mathbf{e}_{ij}$ $\quad$ (attention mechanism)

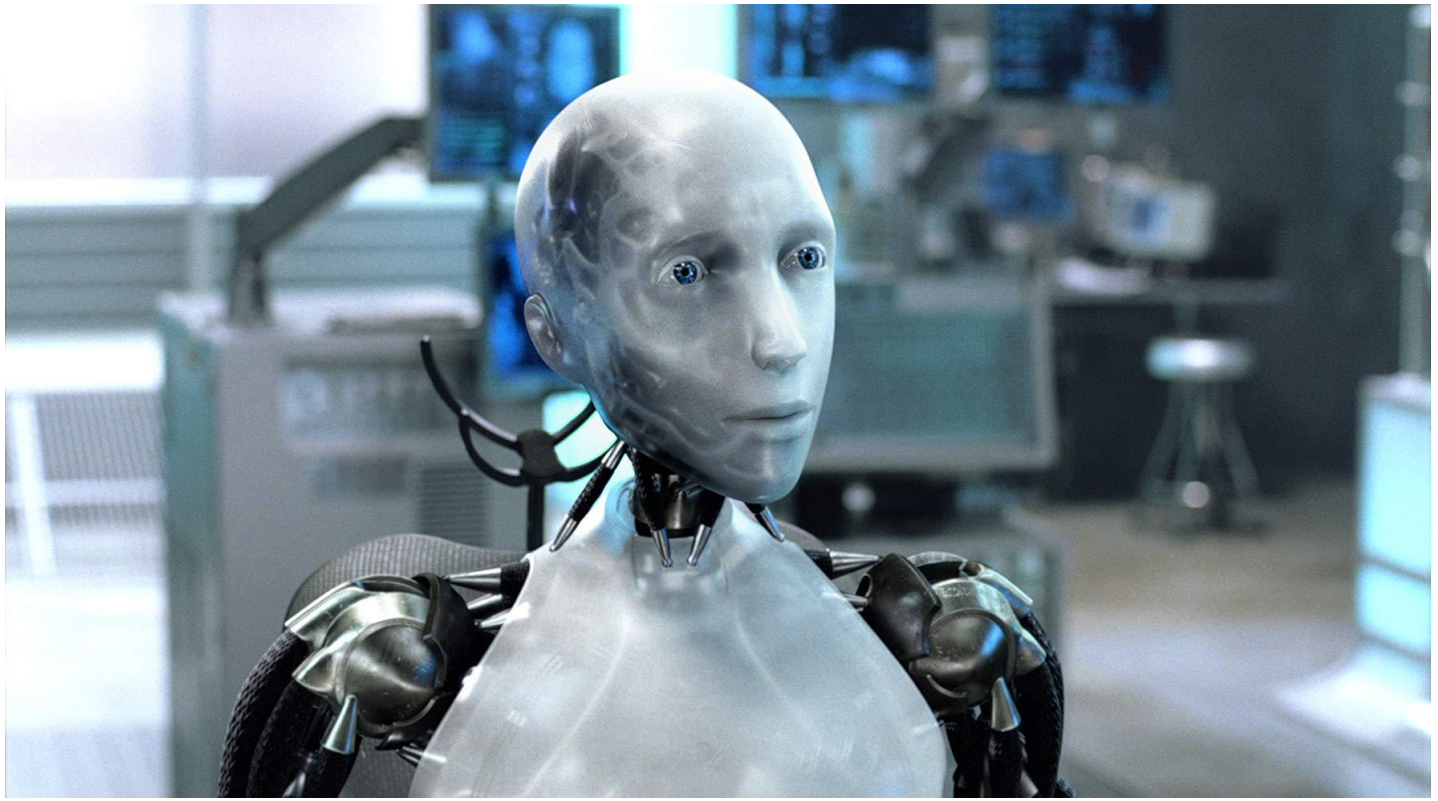
$r = a^{\mathrm{T}}\mathbf{r}$ $\quad \mathbf{r} = \mathbf{A}g'(\mathbf{S})$ $\quad$ (expected feature map)

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

Return

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

Altae-Tran, 2017



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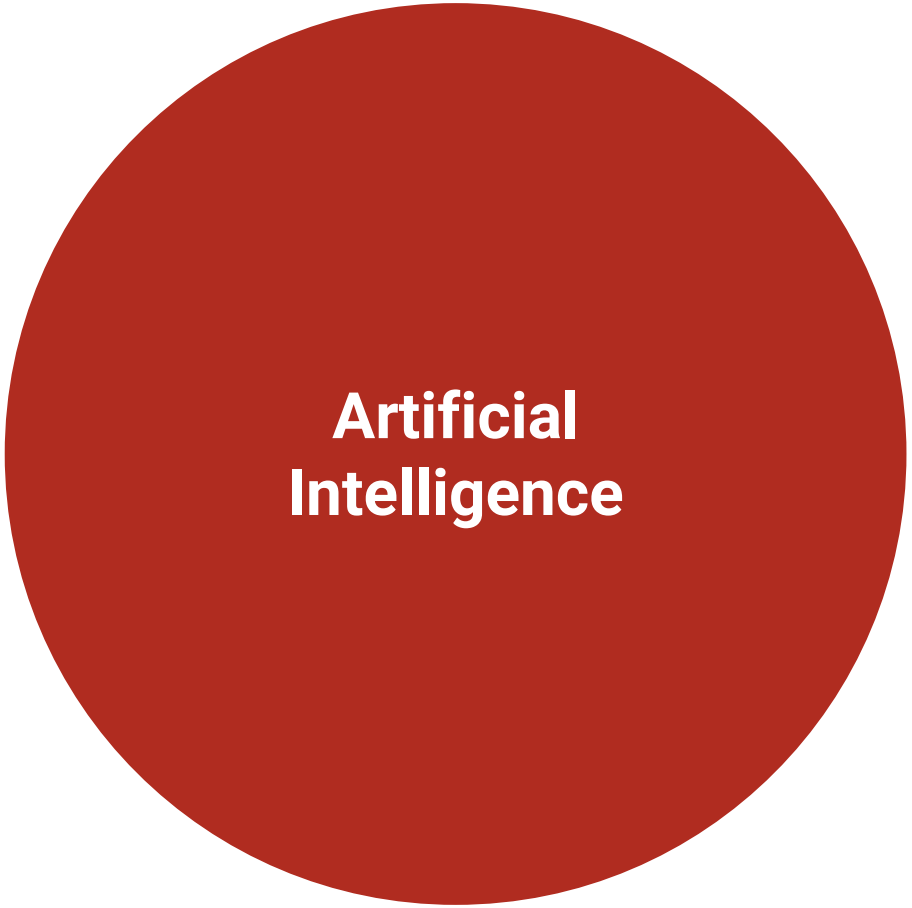
# What We'll Cover...

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

# Overview: AI, ML and NLP…

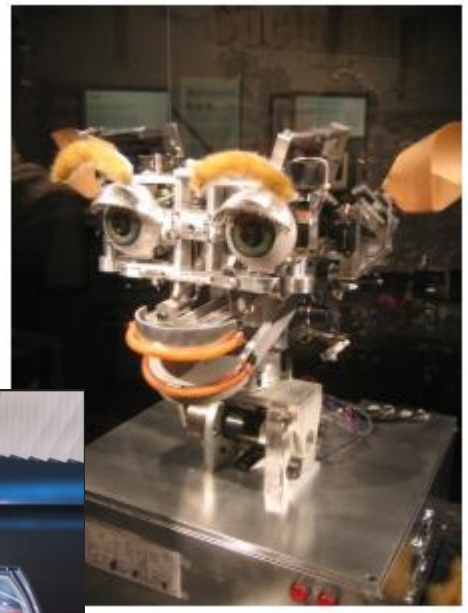



## Artificial Intelligence:

A branch of computational science involving any device that perceives its environment and takes actions that maximize its chance of successfully achieving its goals. This includes

- 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)



## Levels of complexity:

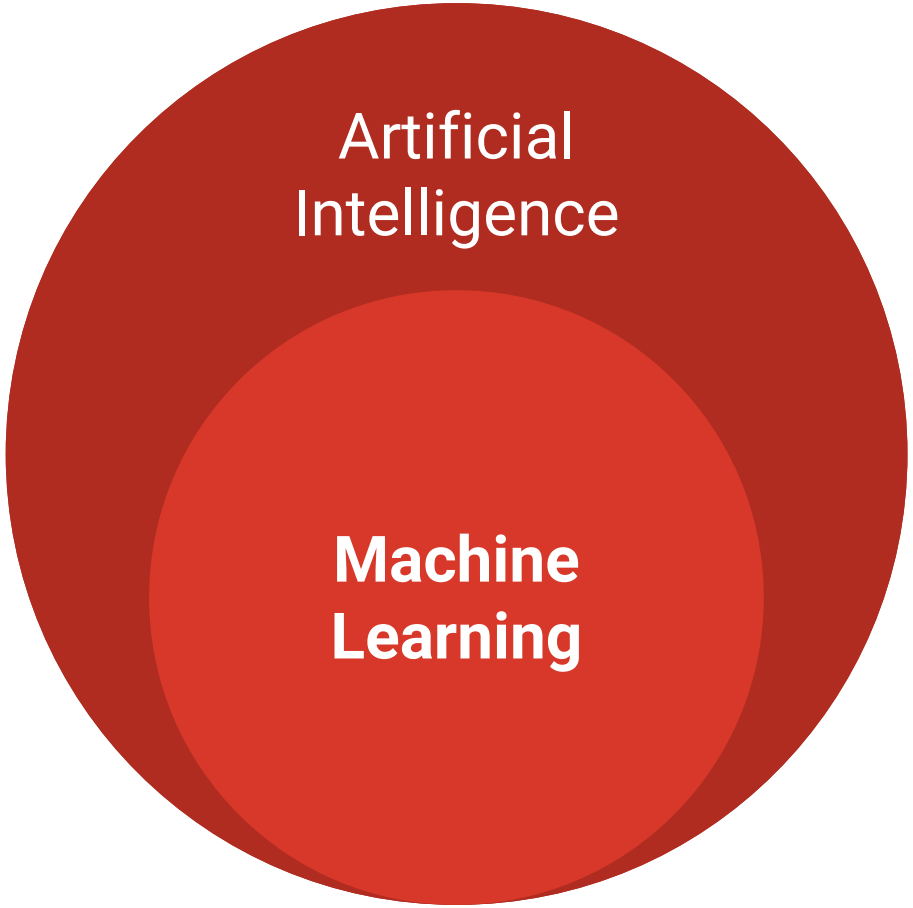
**Reactive machines** eg, chess opponent

**Limited memory** eg, self driving cars

**Theory of mind** Robots that simulate human emotional response

**Self awareness** Currently limited to science fiction

# Overview: AI, ML and NLP…(cont'd)

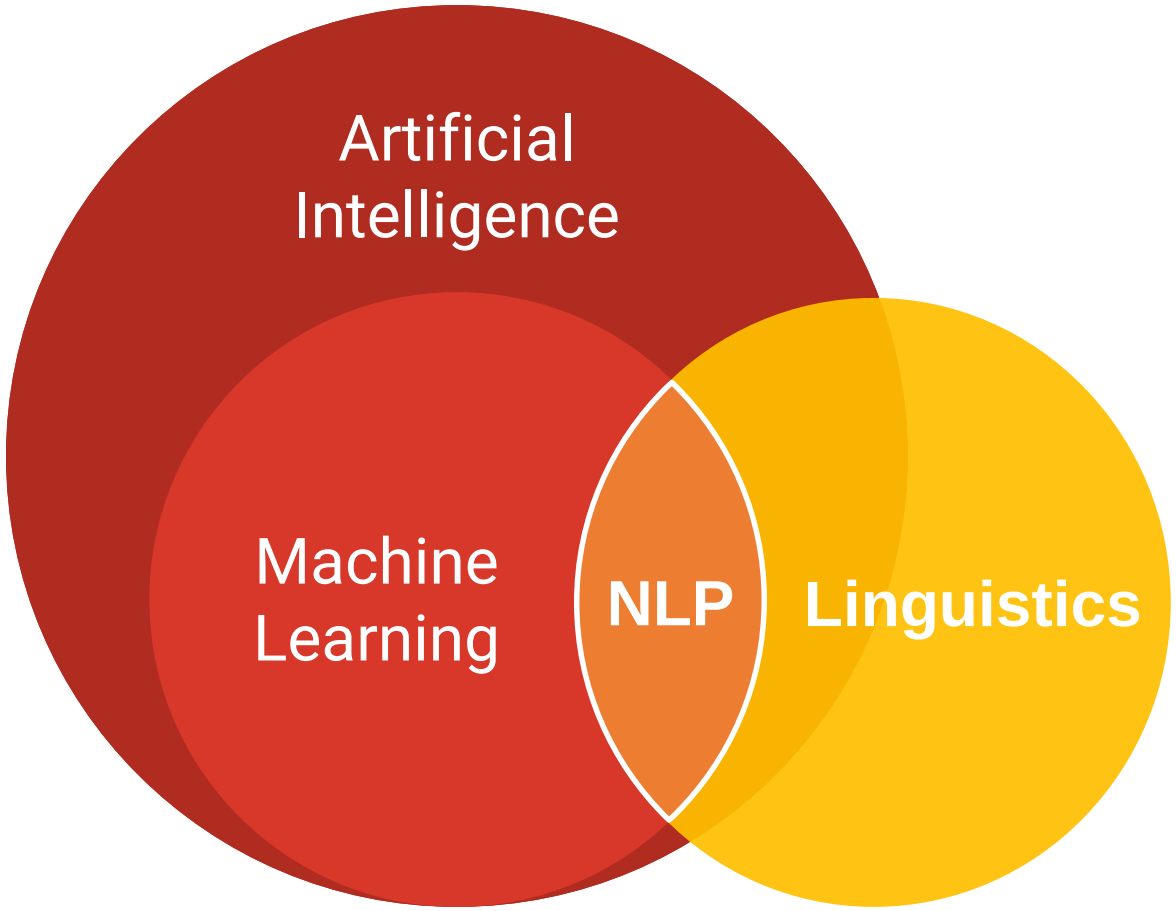



**Machine Learning:**

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)



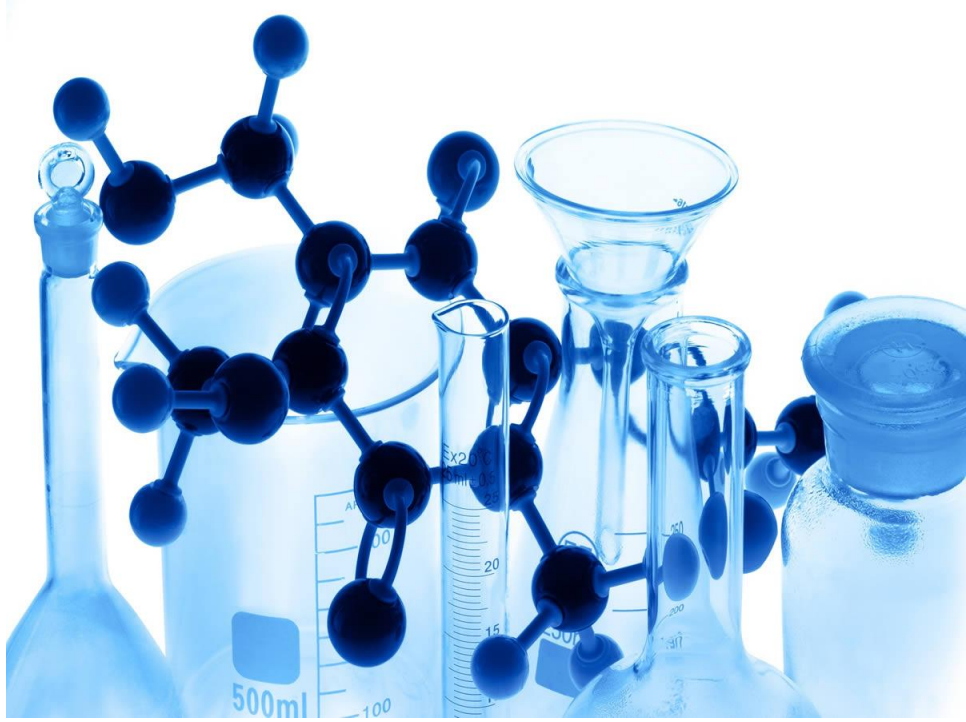

**Natural Language Processing (NLP):**

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…
  - 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

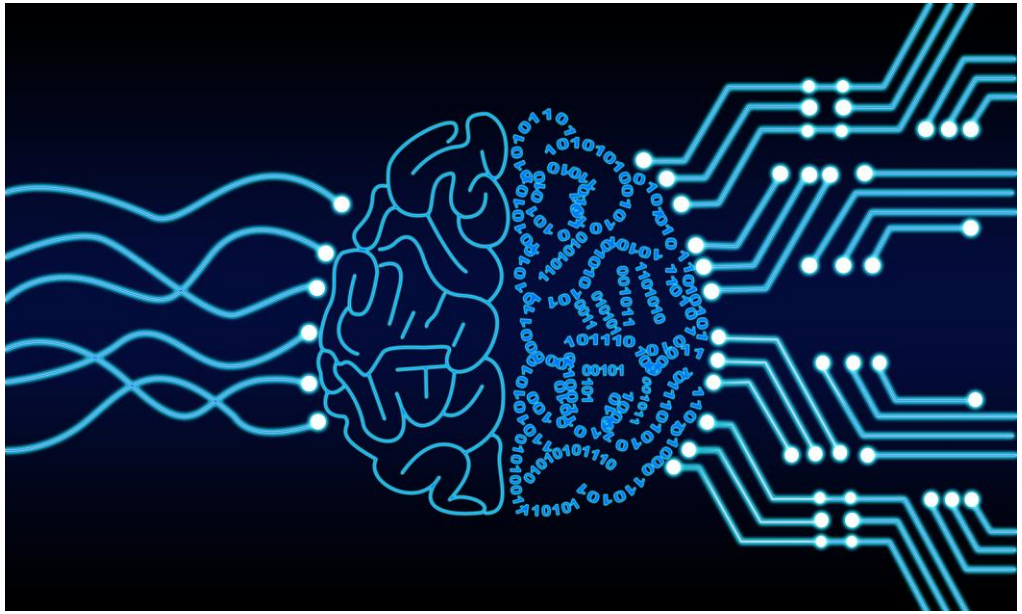



Rosso. How Artificial Intelligence is accelerating Life Sciences. Psychology Today

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

- AI is also being adopted in the data management and biometrics areas...

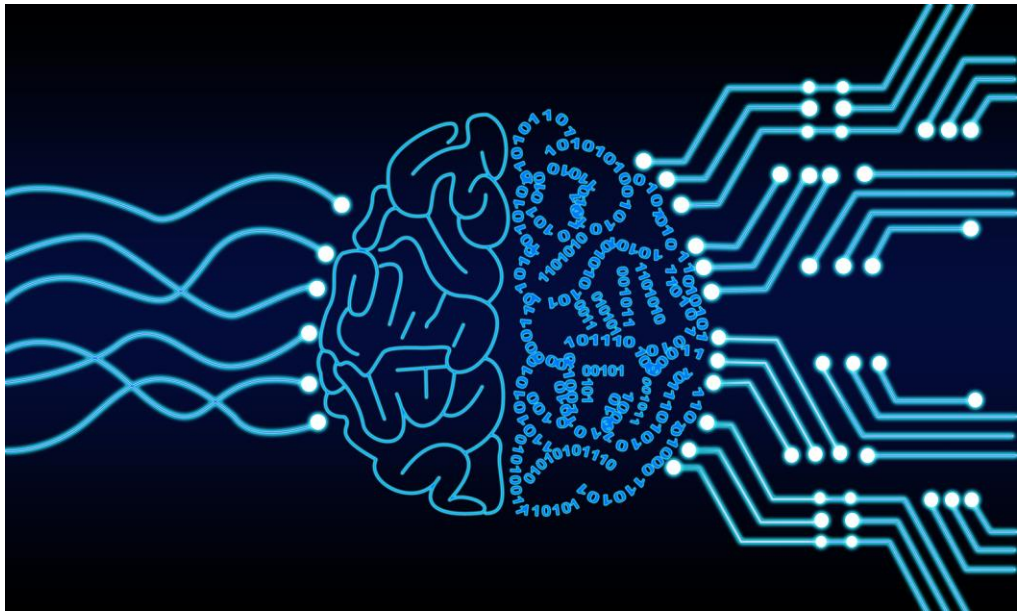
  - **Generation of standard datasets**
  - **Outlier Detection**
  - **QC of documents**
  - **Anonymization**



# How AI/ML has been implemented in….

…….**Generation of standard datasets** with ability to detect transformations based on metadata

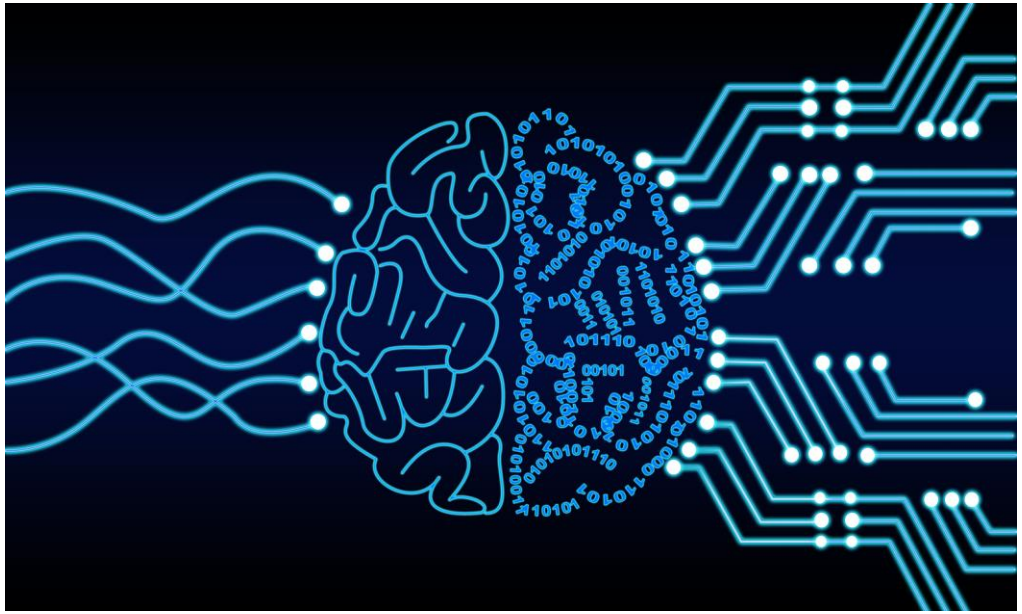
- Metadata-driven generation
- Project definition/attribute matching
- Domain/field recognition/recommendations



# How AI/ML has been implemented in…

…..**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.

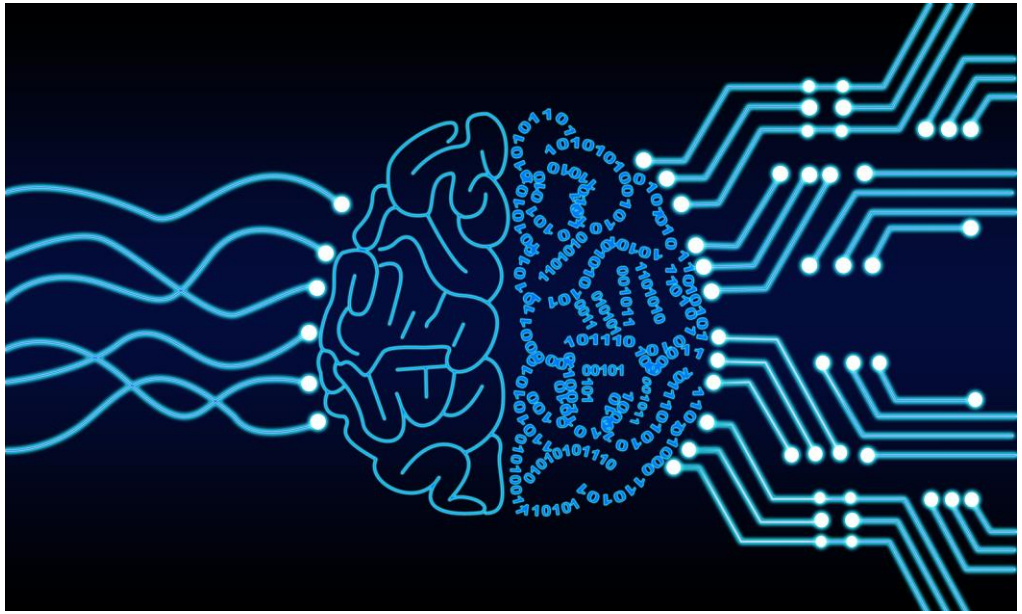
- Project definition/attribute matching
- Data-driven determination of most appropriate detection models to use



# How AI/ML has been implemented in…

**…QC of documents** (e.g., CSR) against results using an automated tool to avoid human error

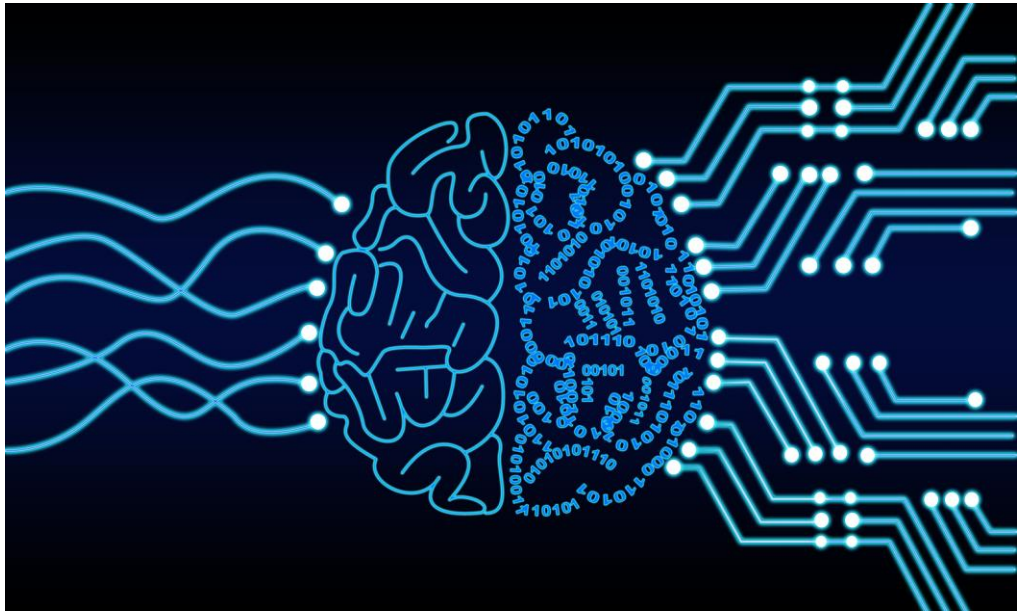
- Use of business rules as metadata to perform normally complicated and time-intensive checks on unstructured data



# How AI/ML has been implemented in…

**…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 heading…


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.

# 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 for achieving quality and automation
- 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

# Acknowledgements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