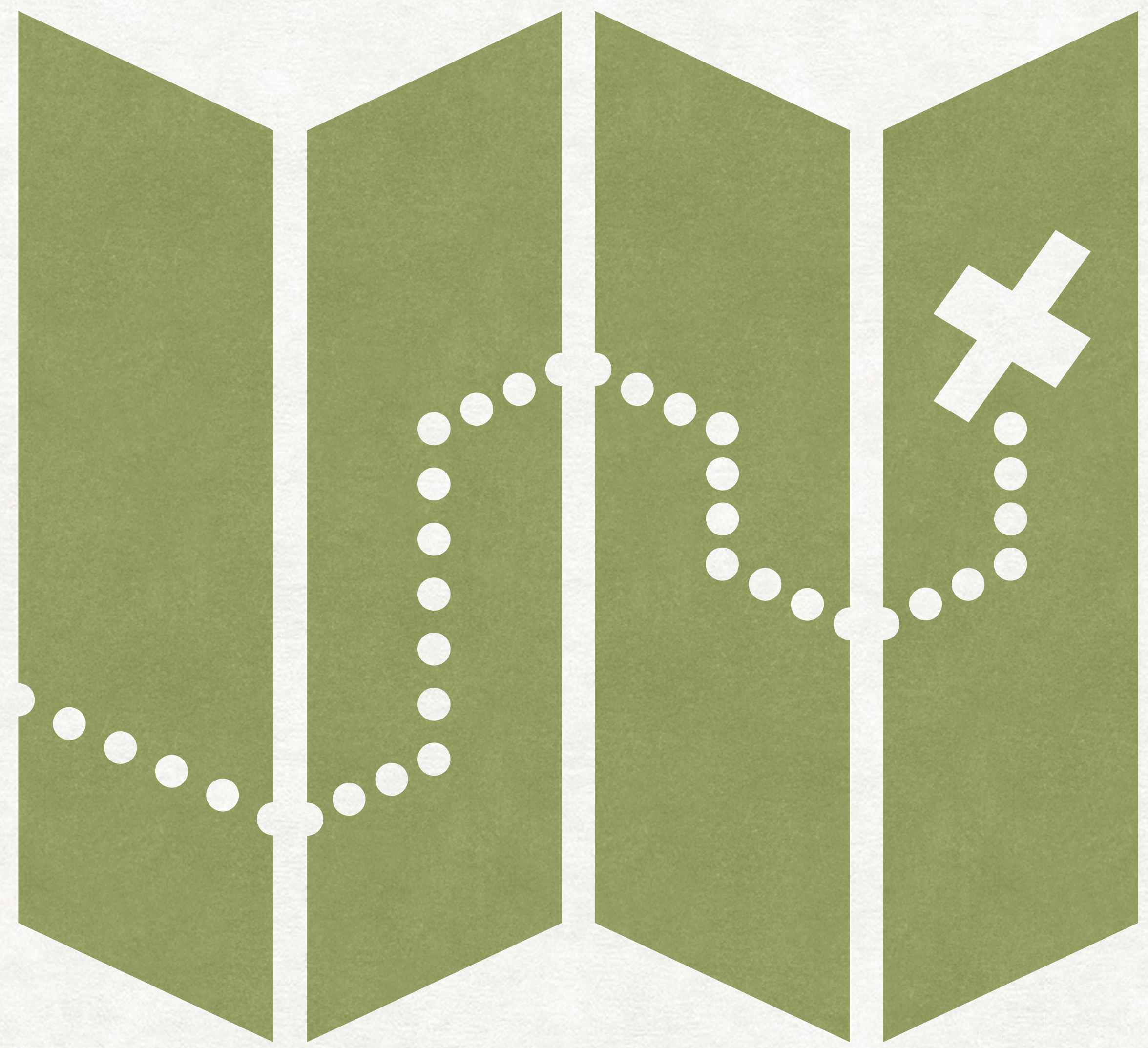
MARK ASCH

AI FOR SCIENCE
SCIENCE FOR AI

2024 MSP Annual Convention, Tacloban City, Philippines - May 30 to June 2, 2024

PLAN

1. ML/AI revolution (ML for Science)
2. Scientific ML (Science for ML)
3. Ethics, bias, responsibility (certifiability)
4. LLMs for science - "quo vadimus"?



“

AI IS ONE OF THE MOST TRANSFORMATIVE AND VALUABLE SCIENTIFIC TOOLS EVER DEVELOPED.

BY HARNESSING VAST AMOUNTS OF DATA AND COMPUTATIONAL POWER, AI SYSTEMS CAN UNCOVER PATTERNS, GENERATE INSIGHTS, AND MAKE PREDICTIONS THAT WERE PREVIOUSLY UNATTAINABLE*.

— Rick Stevens, ISC 2024

”

*However, these tools are absolutely **useless** if we cannot **trust** the information we receive from them.

ML/AI FOR SCIENCE

AI REVOLUTION OF 2020'S

3 MAJOR REASONS/CAUSES/FACTORS

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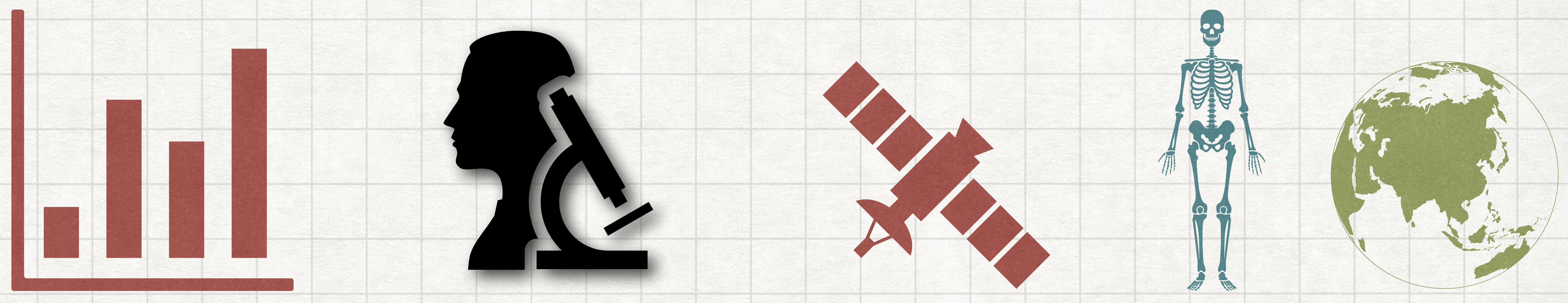
1. Big Data

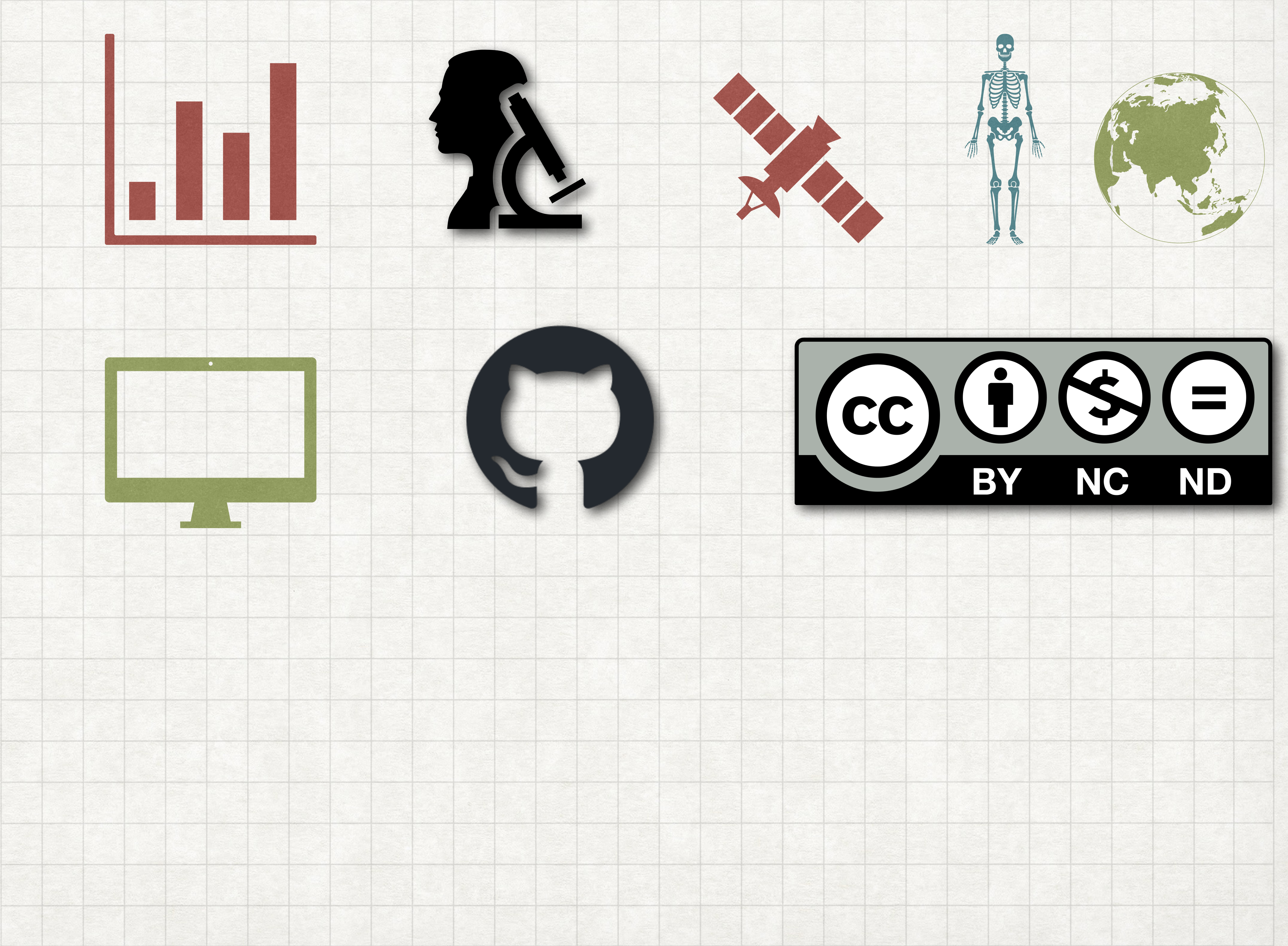


AI REVOLUTION OF 2020'S

3 MAJOR REASONS/CAUSES/FACTORS

1. Big Data

2. Open source (ML) software libriairies



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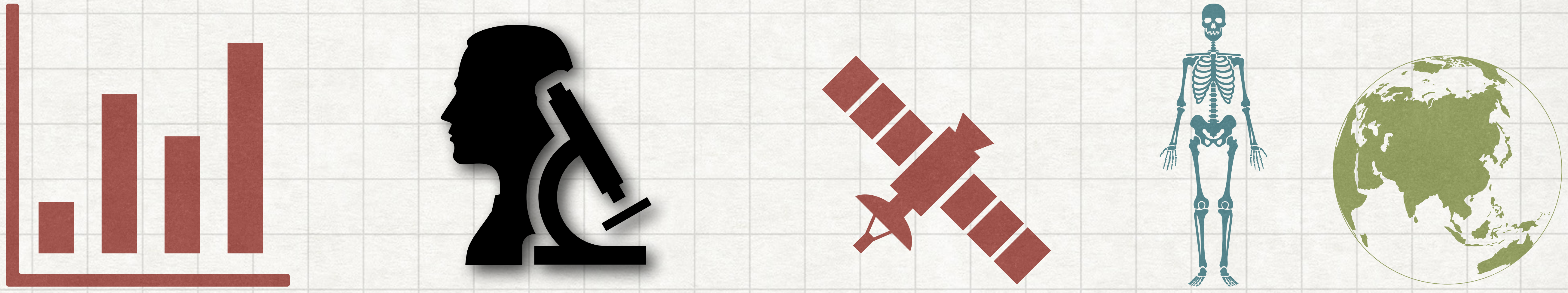
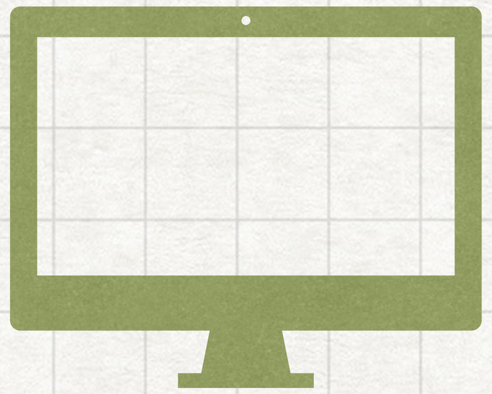
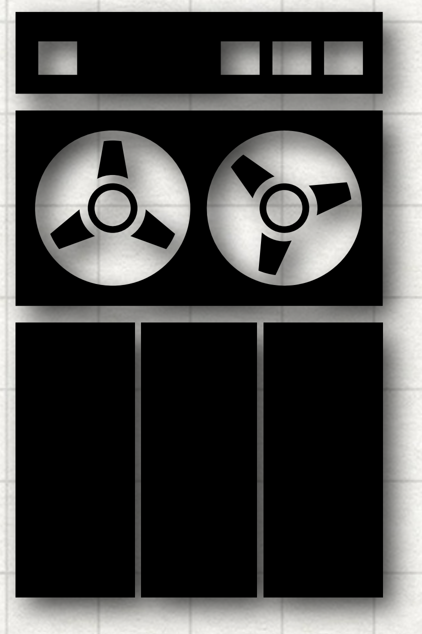
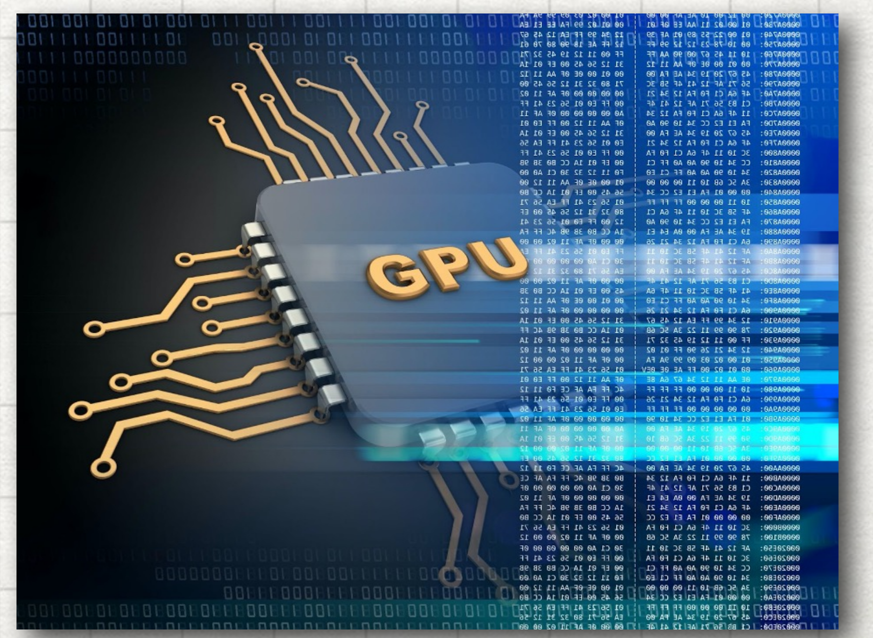


2. Open source (ML) software librairies

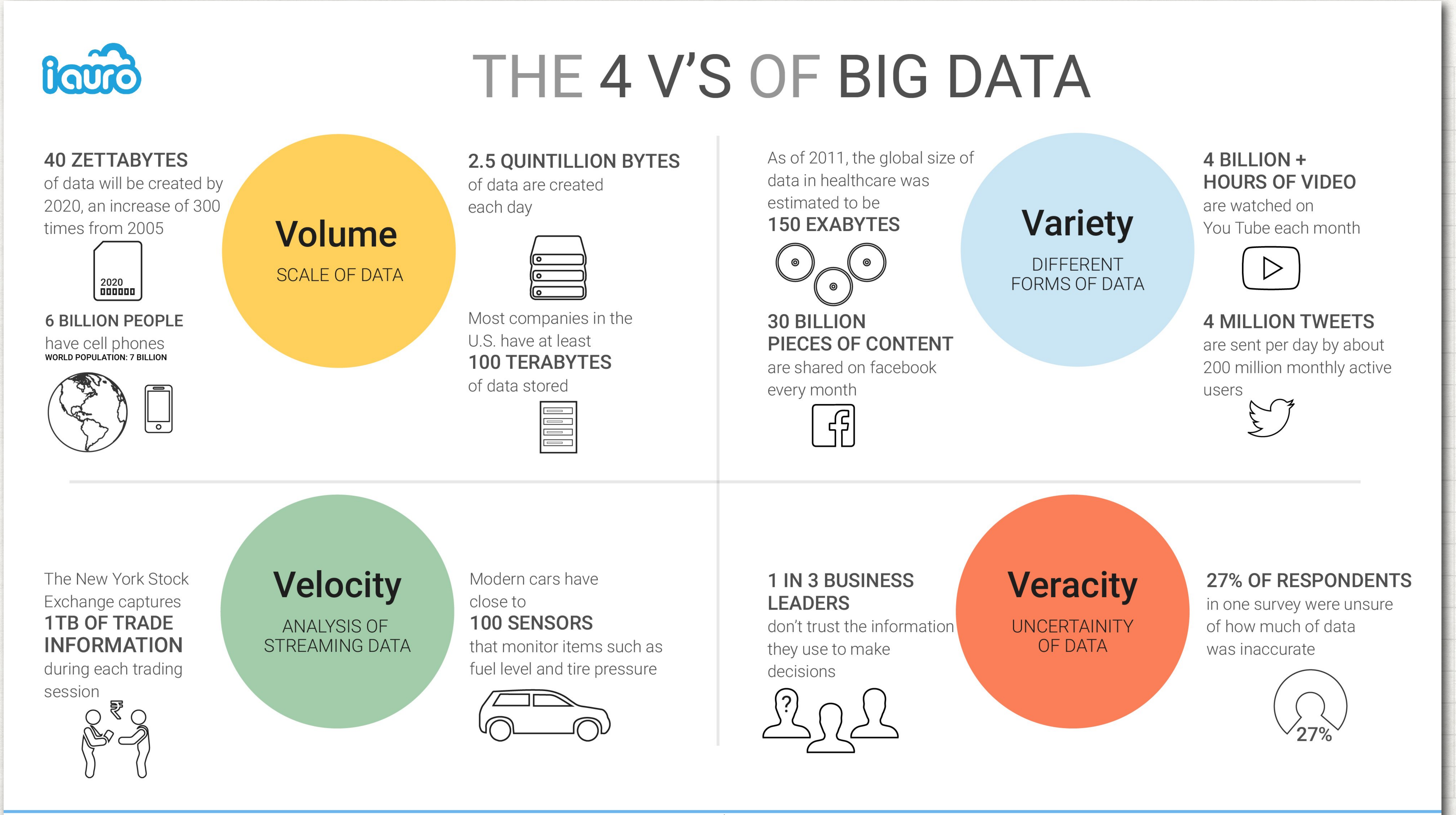


3. Access to (cheap) computer hardware and storage





FACTOR 1: BIG DATA

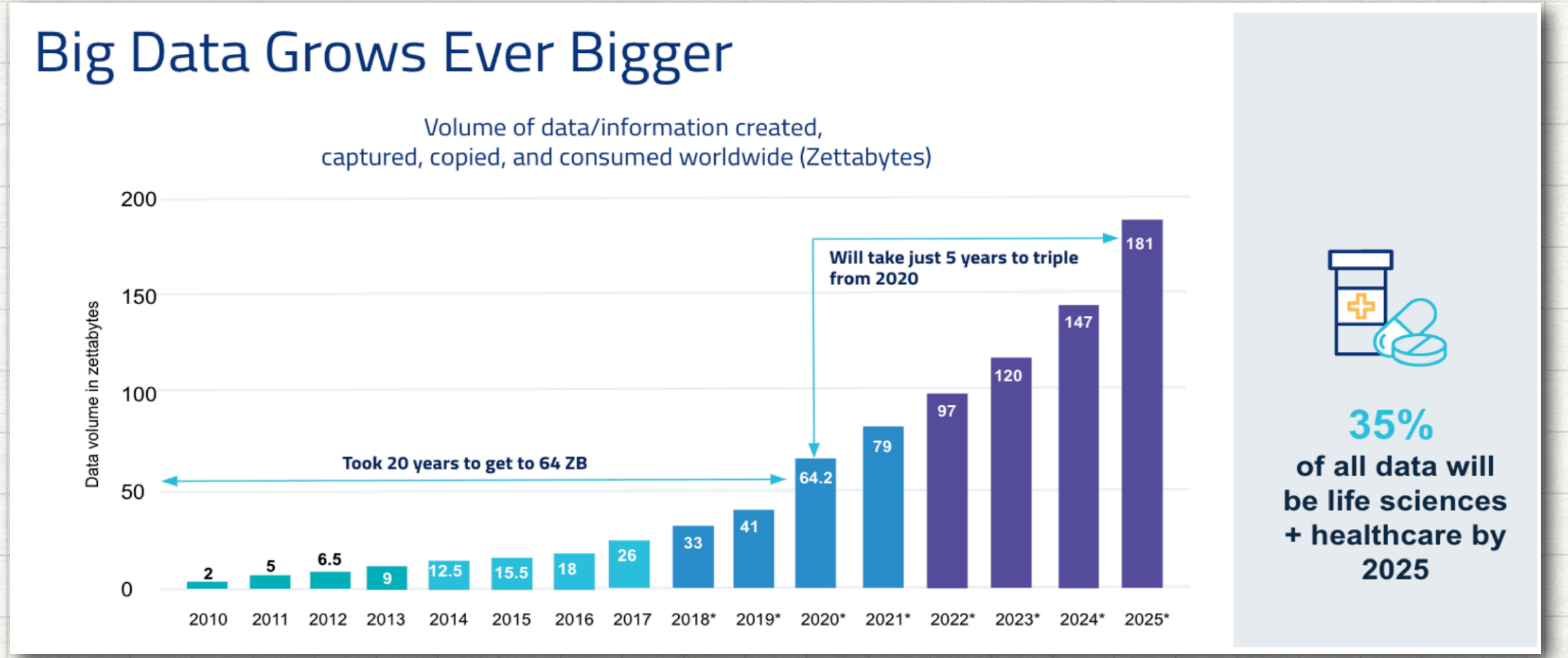


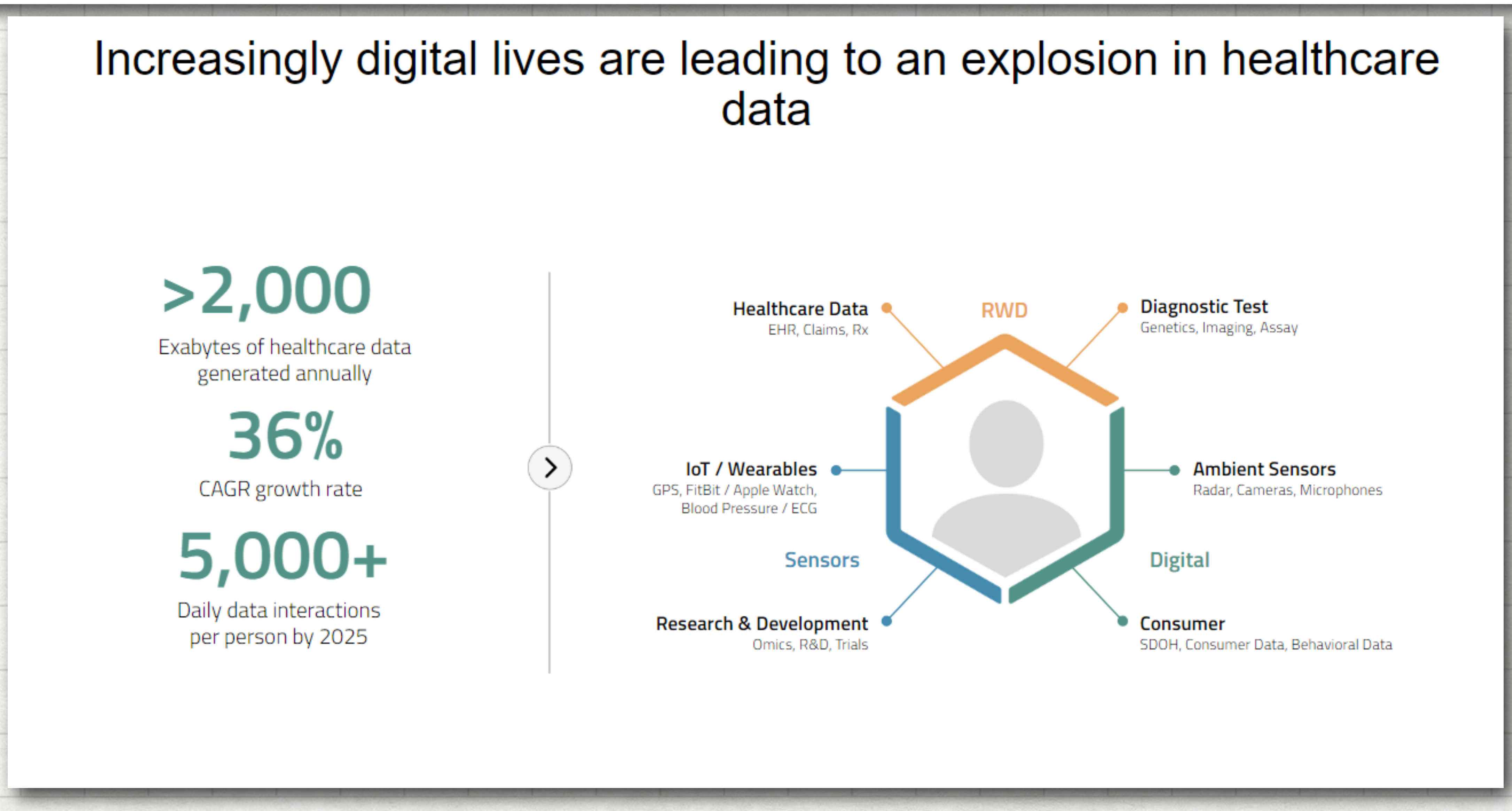
Reference : http://www.ibmbigdatahub.com/infographic/four-vs-big-data

FACTOR 1: BIG DATA

EXAMPLE: HEALTH DATA IS EVERYWHERE…

1. Healthcare Data
2. Diagnostics Data
3. Omics Data
4. IoT and Wearables Data
5. Consumer Data





FACTOR 2: OPEN SOURCE

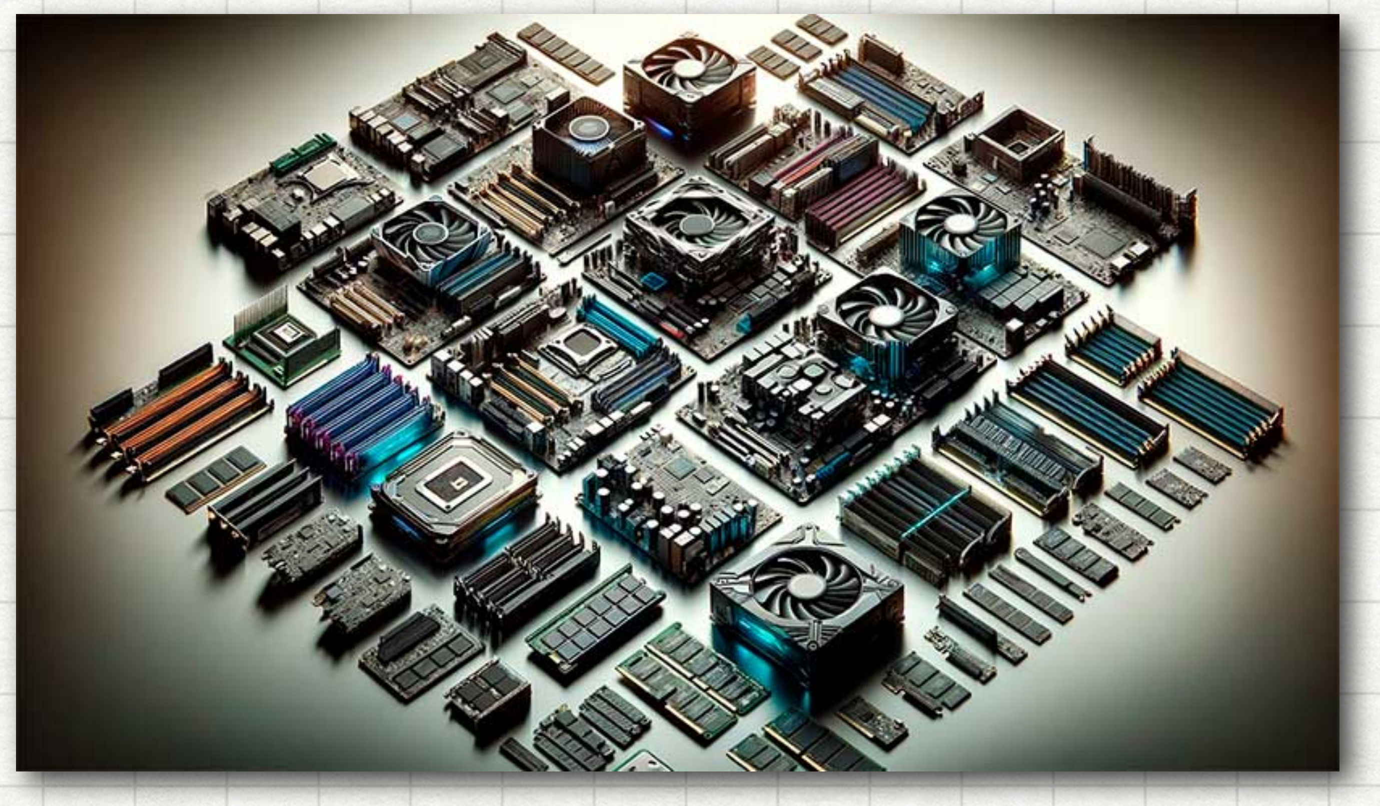
SOFTWARE IS THE KEY

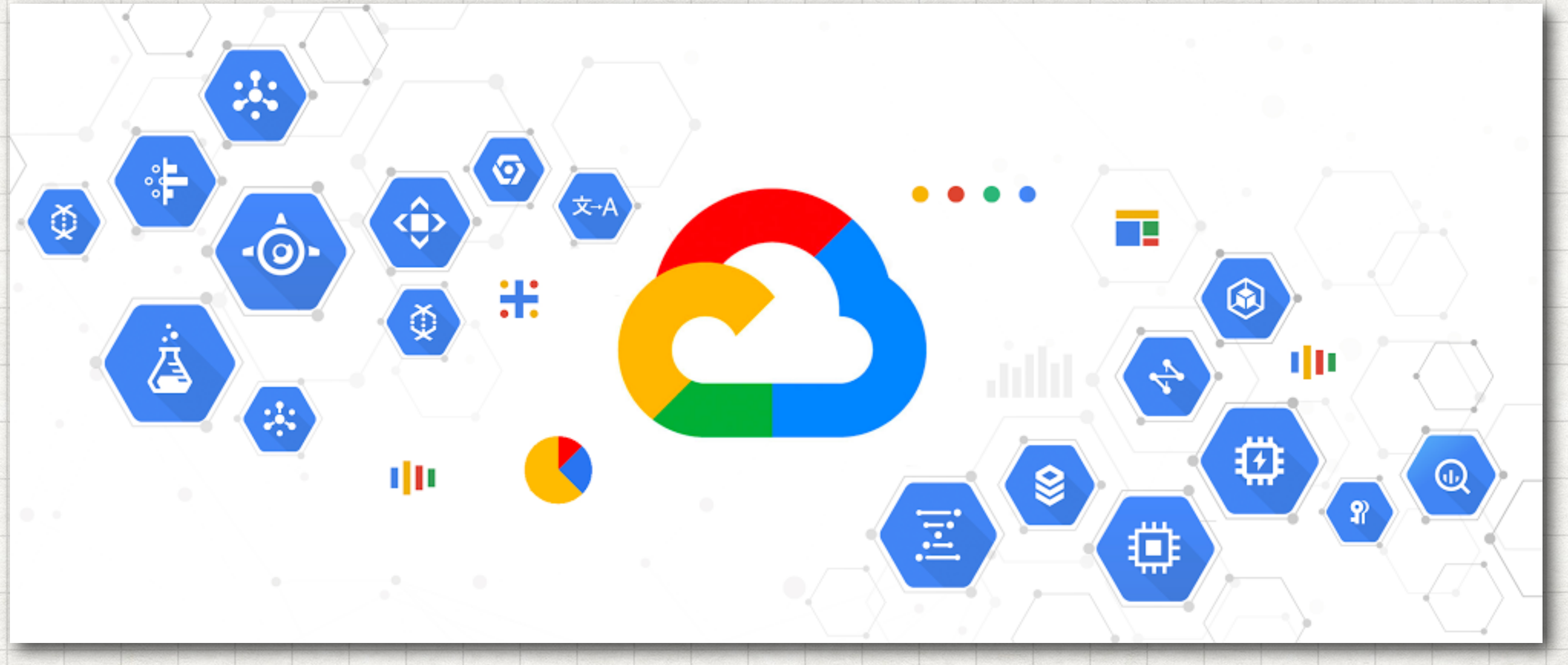
1. Driven by GAFAM…
    1. TensorFlow, Keras
    2. PyTorch
2. Open is the default
    1. Scikit-Learn
    2. R
    3. JaX/Autograd

FACTOR 3: HARDWARE

SPEED AND STORAGE

1. CPUs
2. GPUs
3. Storage
4. Cloud: AWS, Azure, Google CoLab, …

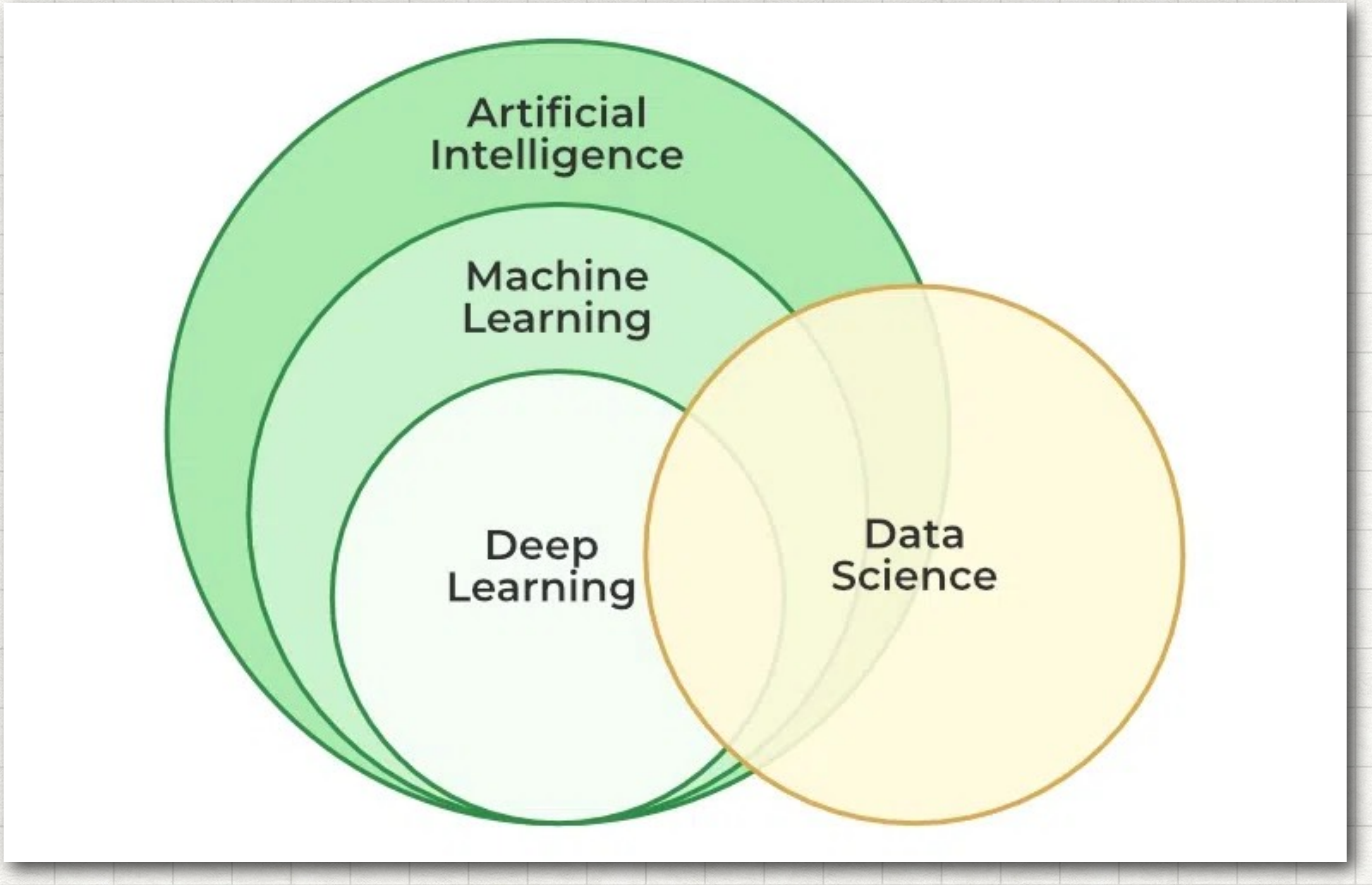




MACHINE LEARNING

INTRINSIC PART OF THE AI UNIVERSE

- Supervised
- Unsupervised
- Reinforcement
- Self-supervised = LLM



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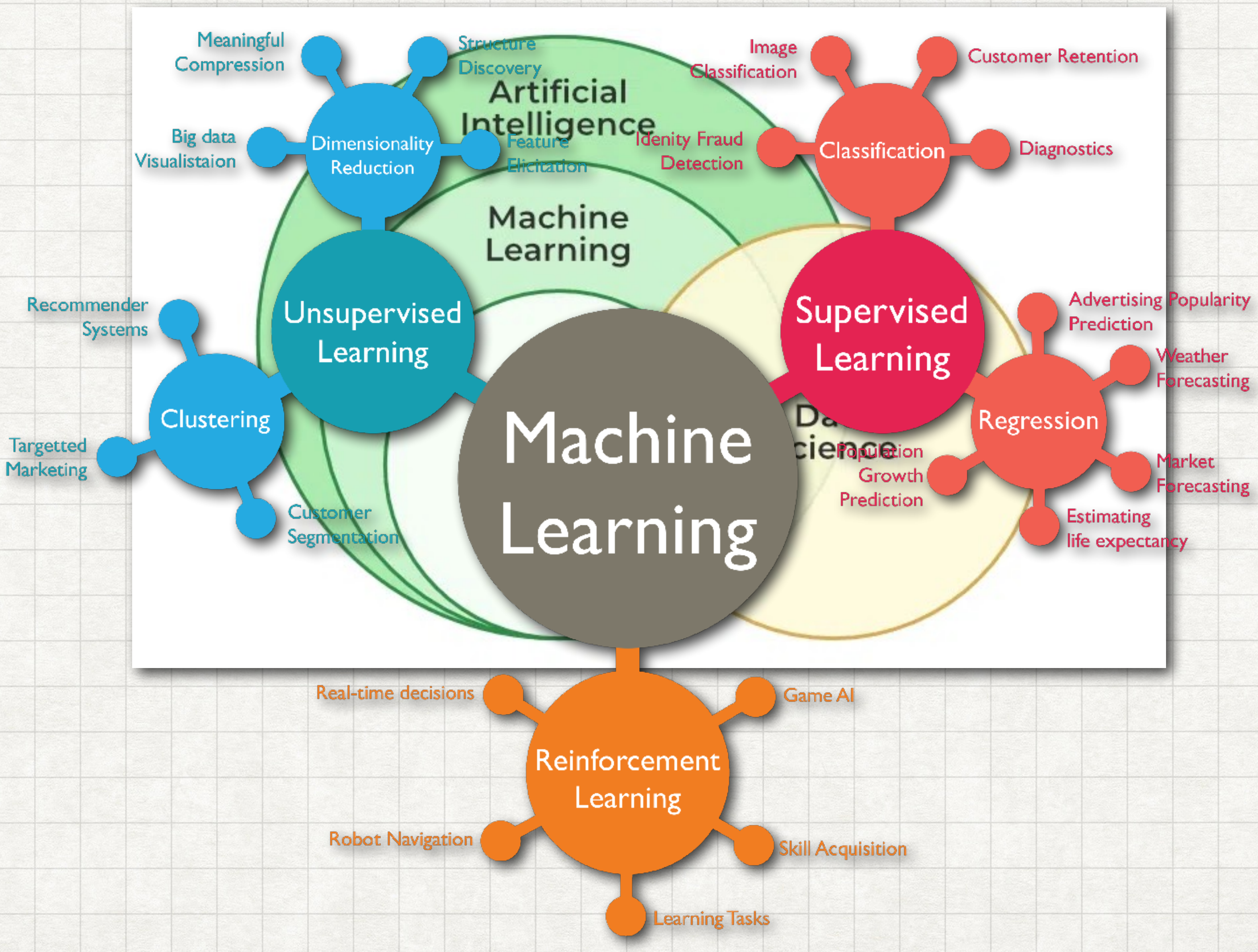

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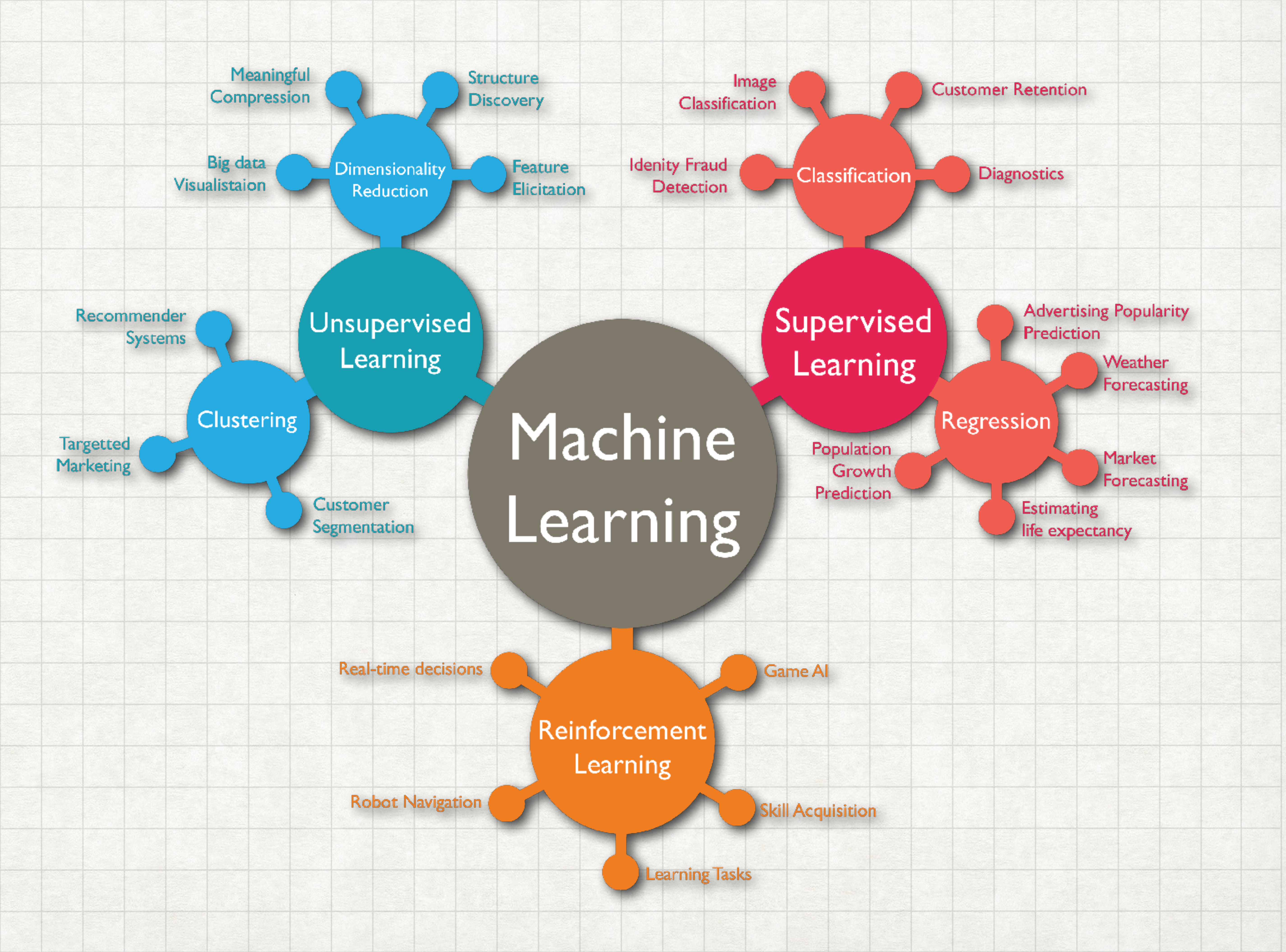


APPLICATIONS AND USE CASES IN HEALTHCARE

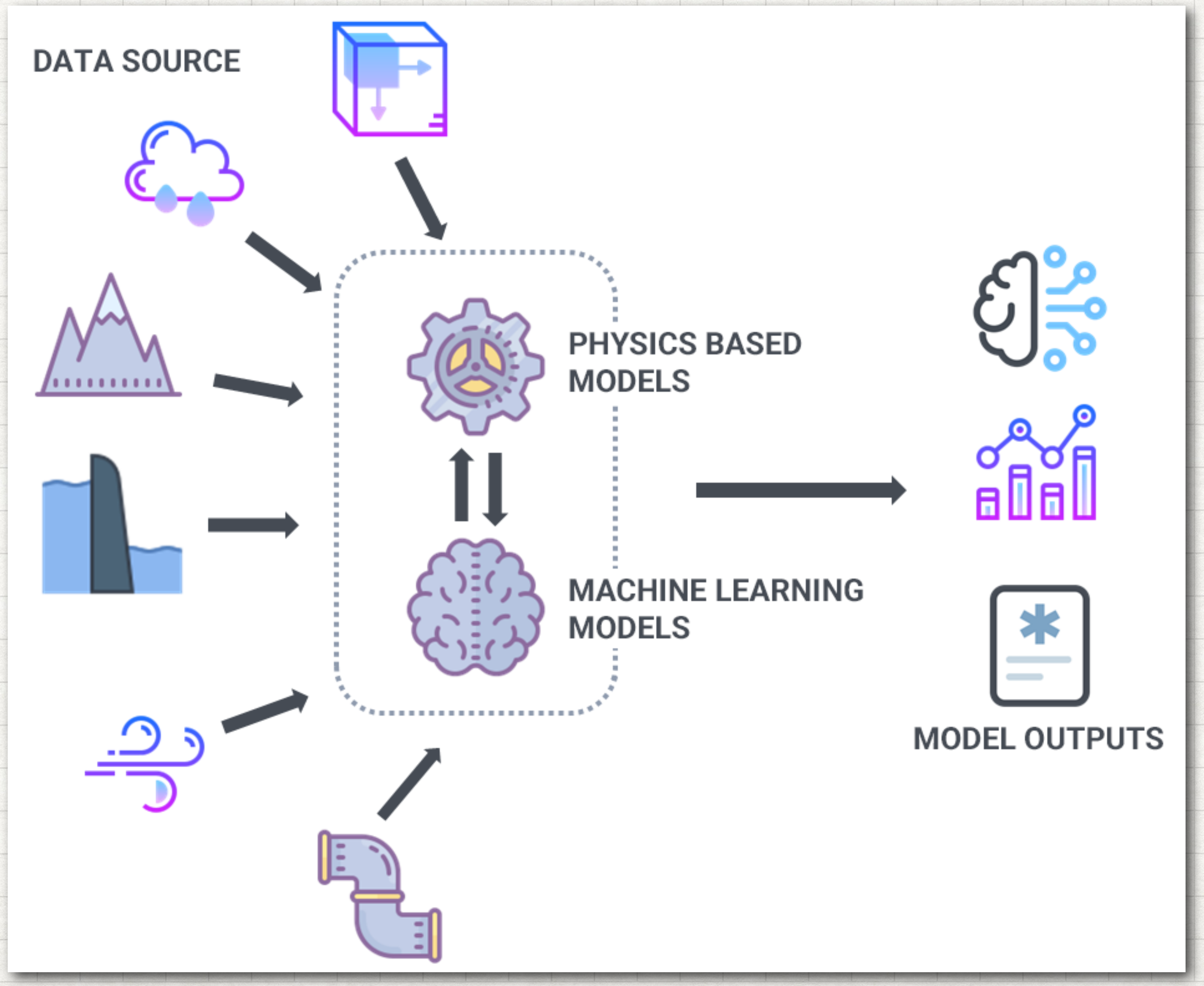
- Disease diagnosis: Machine learning algorithms can analyze medical images, electronic health records, and genomic data to assist healthcare professionals in diagnosing diseases such as cancer, Alzheimer's, and rare genetic disorders.
- Treatment personalization: Big data analytics can help healthcare providers tailor treatments to individual patients based on their unique genetic makeup, lifestyle factors, and medical history.
- Drug discovery: Machine learning can accelerate the drug discovery process by predicting the effectiveness and safety of new compounds, identifying potential drug targets, and optimizing clinical trial designs.
- Population health management: Big data analytics can help healthcare organizations identify populations at risk of chronic diseases, monitor disease outbreaks, and evaluate the effectiveness of public health interventions.
- Mental health assessment: Machine learning algorithms can analyze speech patterns, facial expressions, and social media data to detect early signs of mental health disorders such as depression and anxiety.
- Wearable technology: Sensor data from wearable devices such as fitness trackers and smartwatches can be used to monitor patients' vital signs, activity levels, and sleep patterns, enabling real-time monitoring and personalized care.
- Medical imaging: Machine learning algorithms can automate the analysis of medical images such as MRIs and CT scans, improving accuracy and reducing the need for manual interpretation by radiologists.
- Clinical decision support: Big data analytics can provide healthcare providers with real-time insights into patient health status, treatment options, and potential risks, enabling evidence-based decision making and improving patient outcomes.

SCIENCE FOR ML/AI

WHAT IS SCIENTIFIC ML?

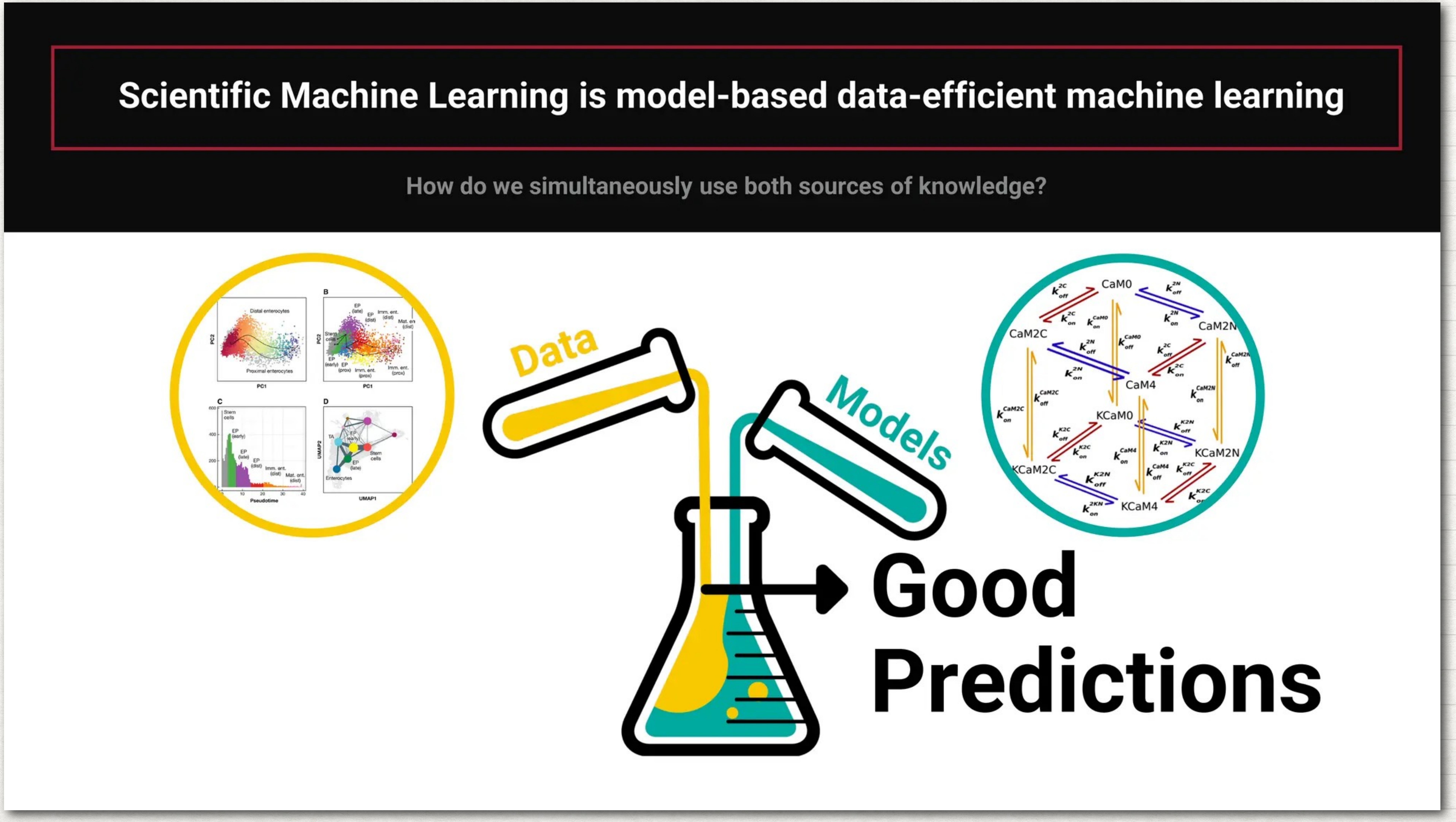
TWO WORLDS UNITED

Scientific Machine Learning (SciML) is a field of research that combines traditional *scientific modeling* with *machine learning* techniques. It aims to develop new methods and tools for solving scientific problems that are more accurate, efficient, and generalizable than traditional methods.



WHAT IS SCIENTIFIC ML?

BLENDING



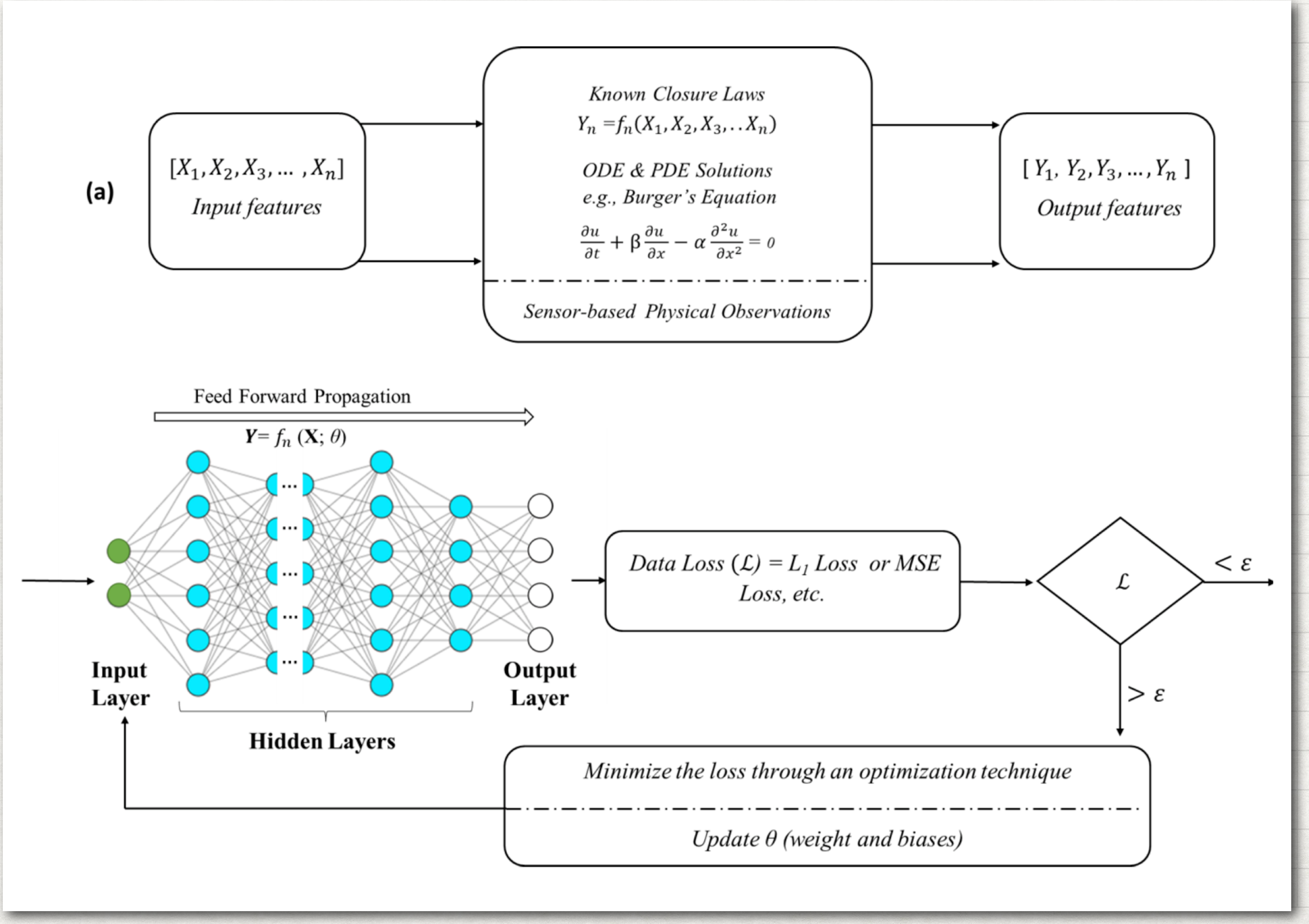
[C. Rackaukas]

HOW IS SCIENTIFIC ML DONE?

BLENDING

3 possible paths:

1. Physics-guided NNs
2. Physics-informed NNs
3. Physics-encoded NNs



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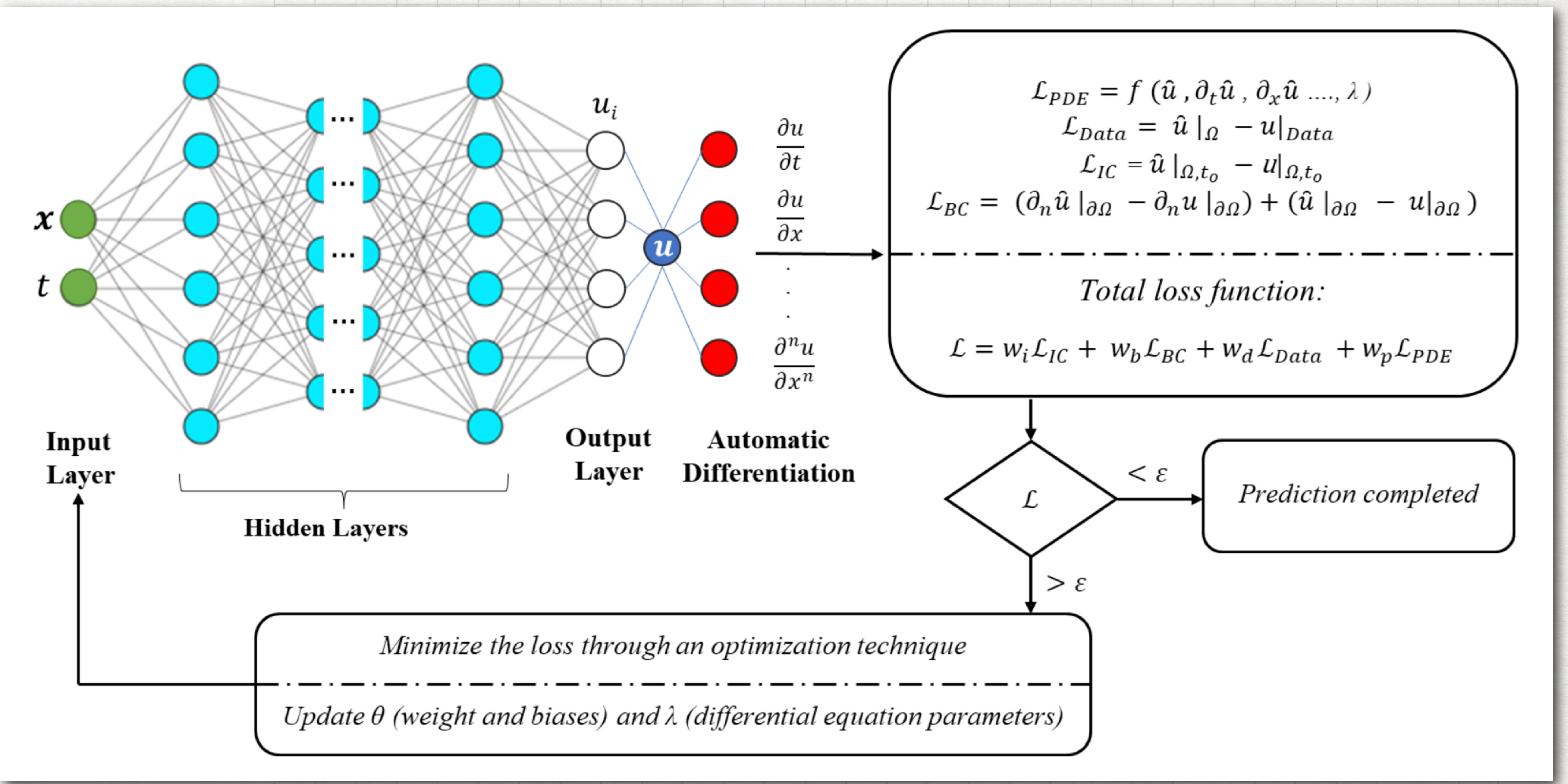

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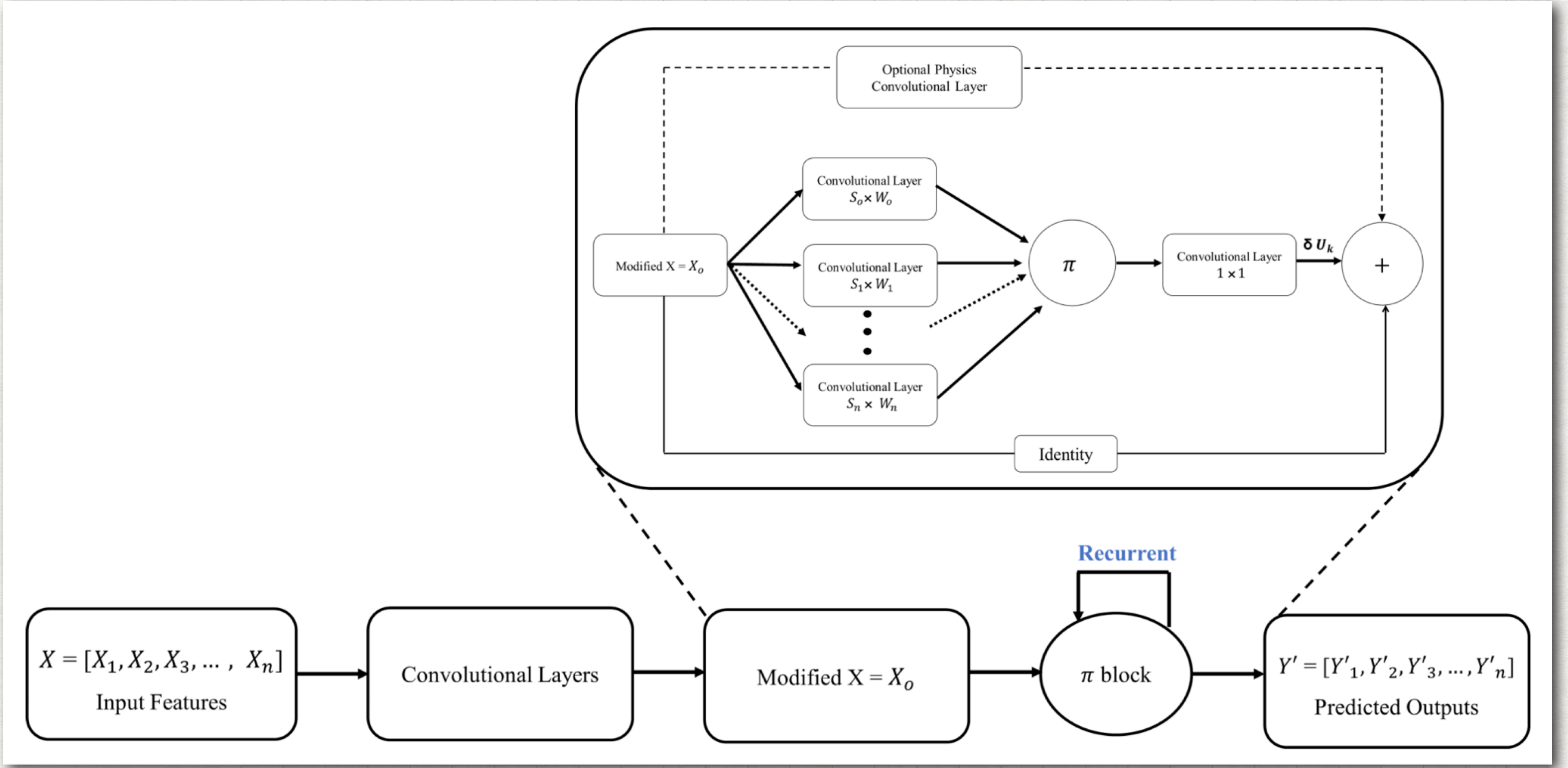
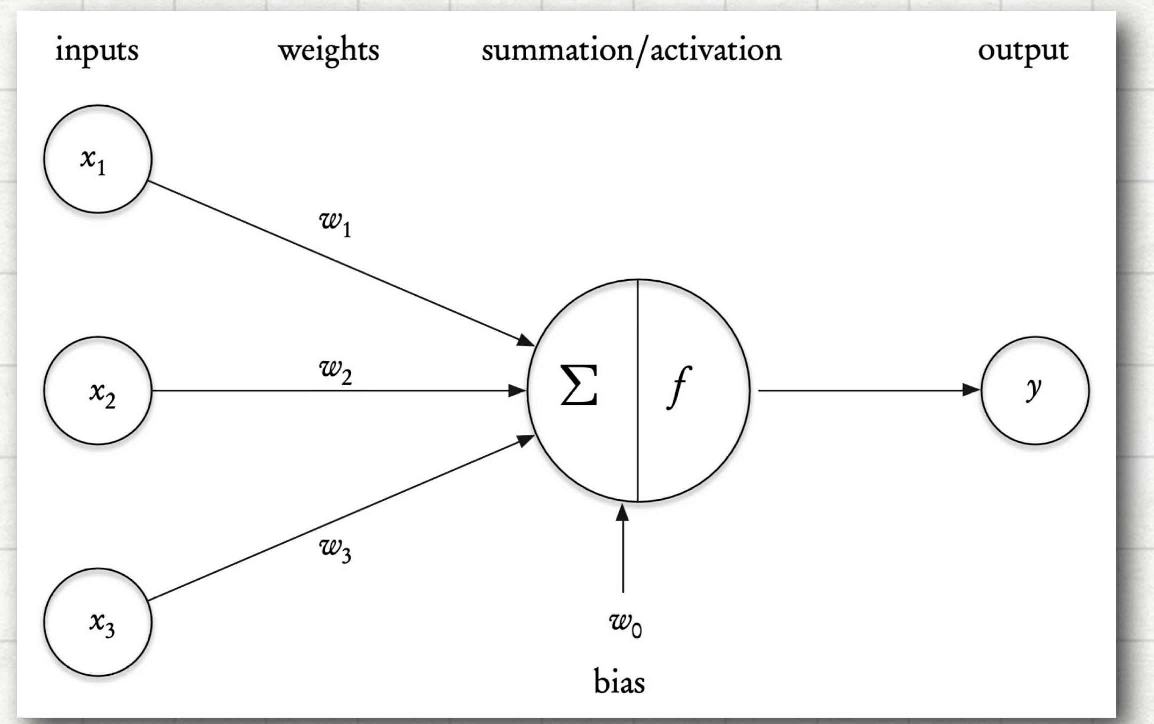


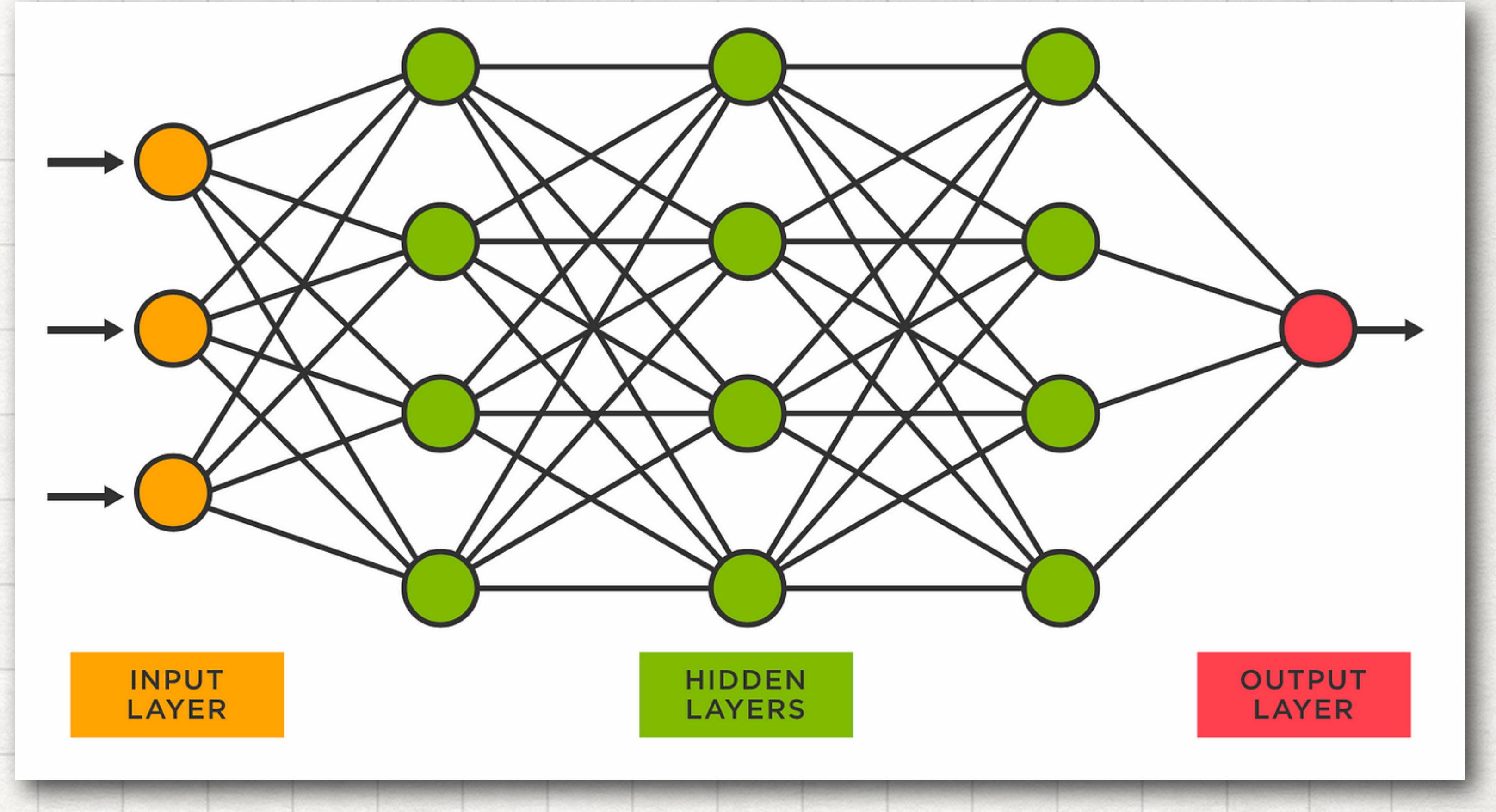
THE MATH BEHIND SCI-ML

APPROXIMATION THEORY

- Multi-layer perceptrons - 1950's - the basis.
- Universal Approximation Property - 1990's - the theory.
- *Differentiable programming - 2020's - makes it all possible! (see next slide)*



$$y = f\left(w_0 + \sum_{i=1}^{3} w_i x_i\right)$$



Theorem 1 (Cybenko 1989). *If σ is any continuous sigmoidal function, then finite sums*

$$G(x) = \sum_{j=1}^{N} \alpha_j \sigma\left(w_j \cdot x + b_j\right)$$

are dense in $C(I_d)$.

Theorem 2 (Pinkus 1999). *Let $\mathbf{m}_i \in \mathbb{Z}^d$, $i = 1, \ldots, s$, and set $m = \max_i \left|\mathbf{m}^i\right|$. Suppose that $\sigma \in C^m(\mathbb{R})$, not polynomial. Then the space of single hidden layer neural nets,*

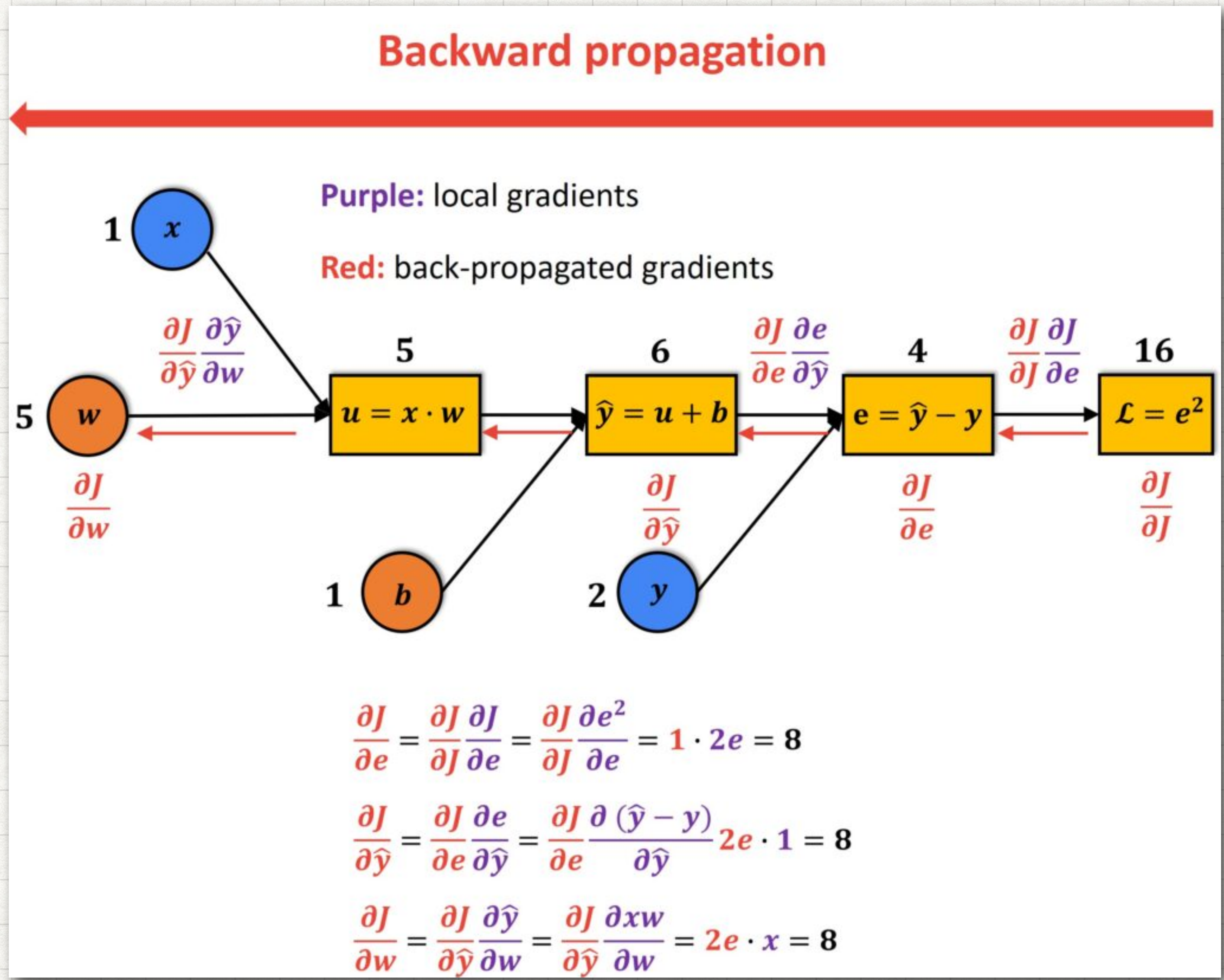
$$\mathcal{M}(\sigma) = \operatorname{span}\left\{\sigma(\mathbf{w} \cdot \mathbf{x} + b) \colon \mathbf{w} \in \mathbb{R}^d,\ b \in \mathbb{R}\right\},$$

is dense in $C^{\mathbf{m}^1, \ldots, \mathbf{m}^s}(\mathbb{R}^d) \doteq \cap_{i=1}^{s} C^{\mathbf{m}^i}(\mathbb{R}^d)$.

THE CODE BEHIND SCI-ML

"AUTOGRAD"

- Differentiable programming - 2020's - makes it all possible!
- Based on:
  - Computational graphs
  - Chain-rule for differentiation



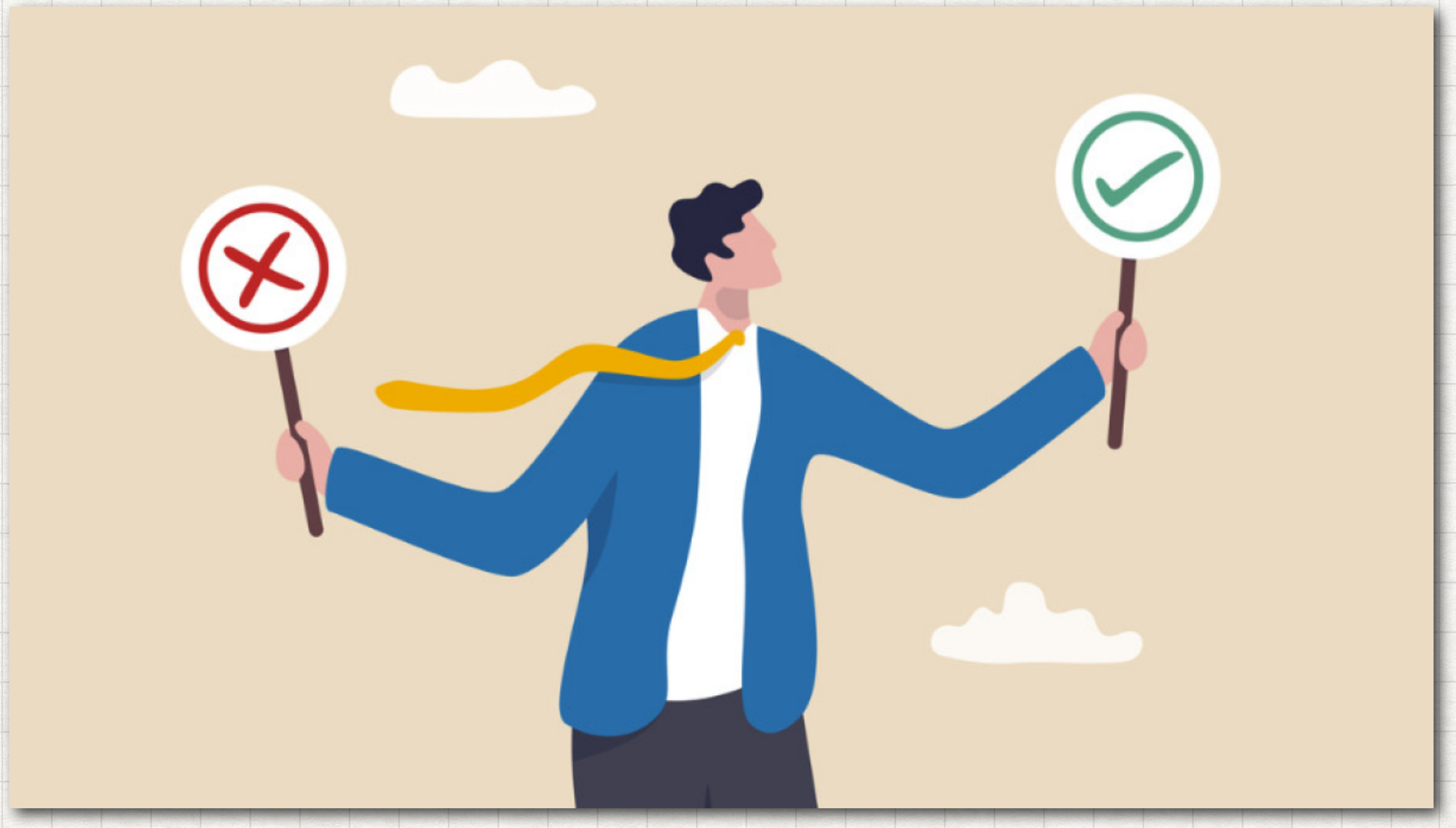
JAX PyTorch TensorFlow

ETHICAL CONSIDERATIONS

ETHICS, BIAS, RESPONSIBILITY, TRUST

DEFINITIONS

- ETHICS = what is morally good or bad, right or wrong? (norms)
- BIAS = prejudice against a person, object, position.
- TRUST = willingness to assume risk by relying on, or believing in, the actions of another party
- TRUSTWORTHY AI should be lawful, ethical, unbiased.

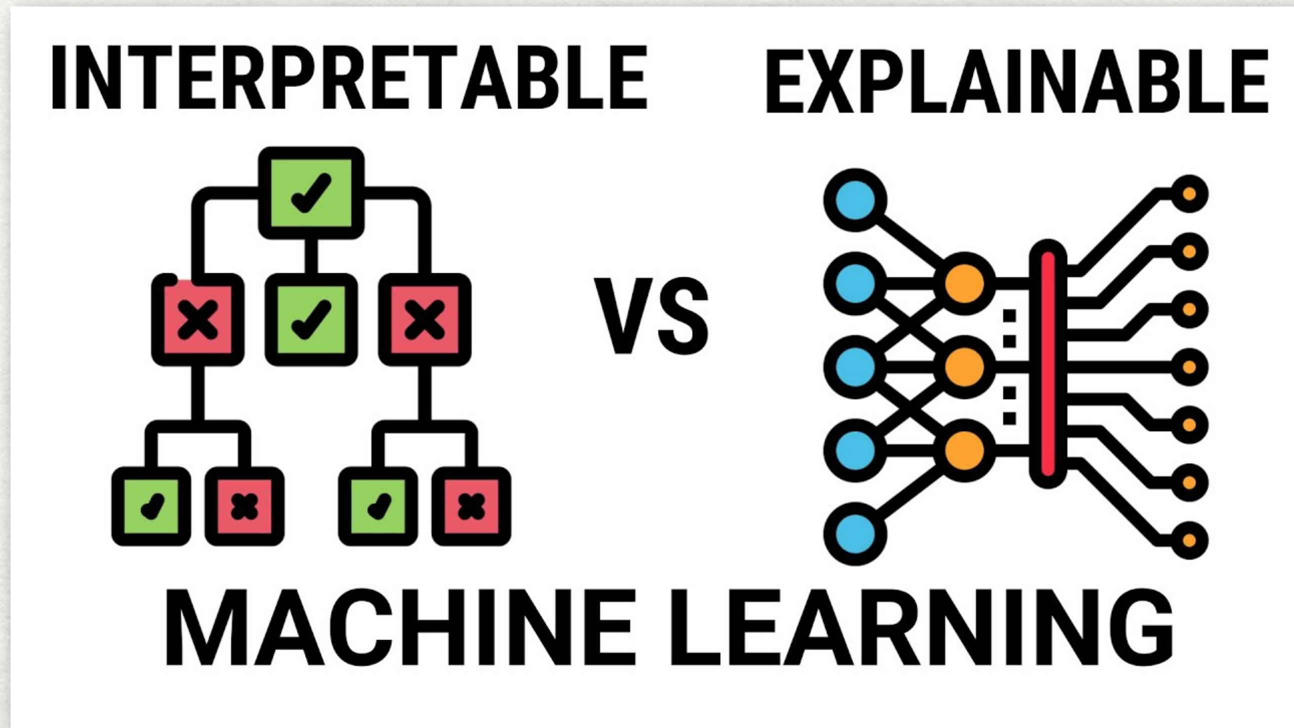


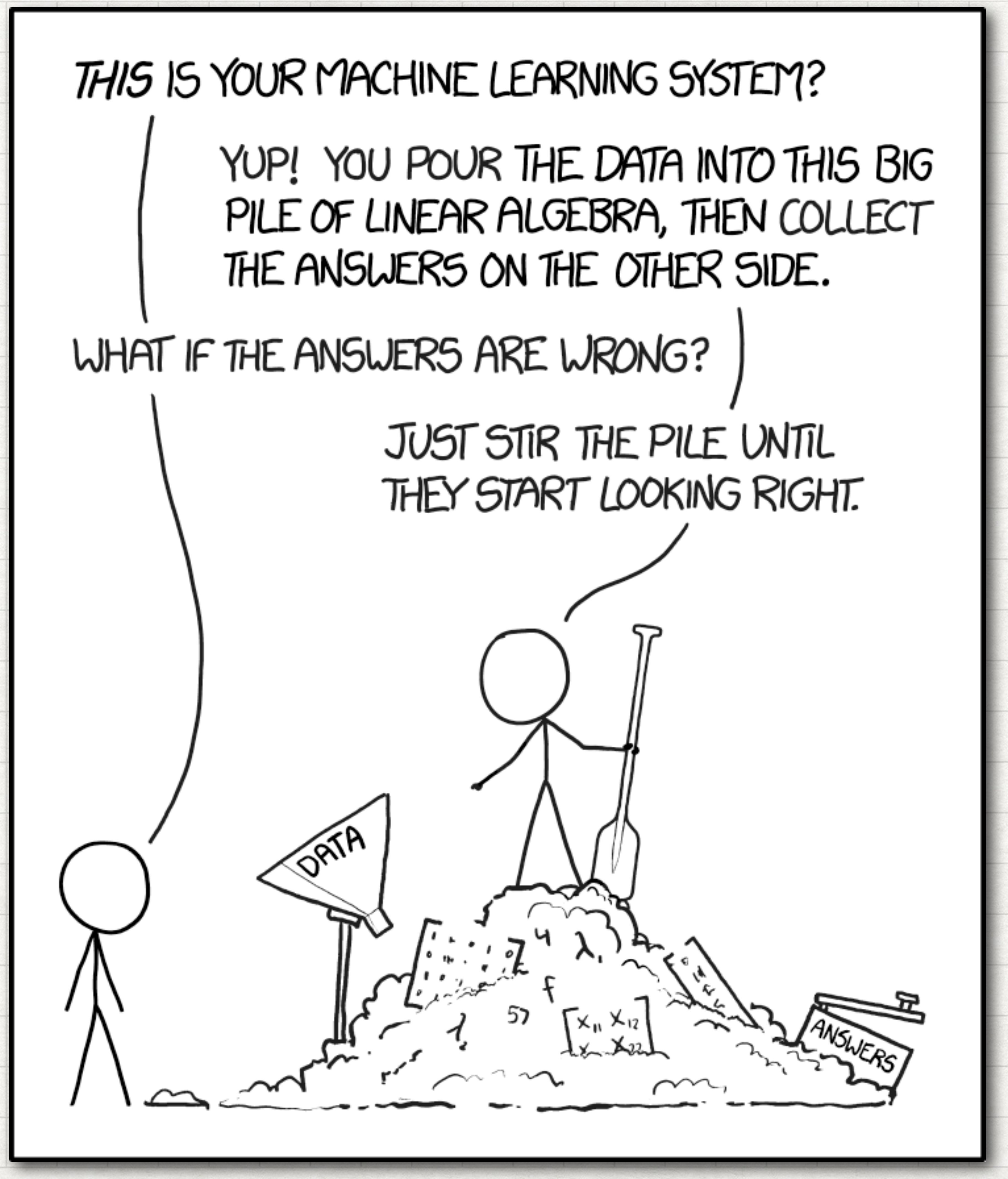
EXPLAINABILTY & INTERPRETABILITY

DEFINITIONS

- INTERPRETABLE AI = can be understood by humans without additional explanation = permits a decision of trust = not a black box

- EXPLAINABLE AI = can be explained post hoc, after training, in a way that makes it understandable = transparency in black boxes = feature importance, effects, interactions





HOW CAN AI GO WRONG?

TRAINING, MODELS, SOCIETY

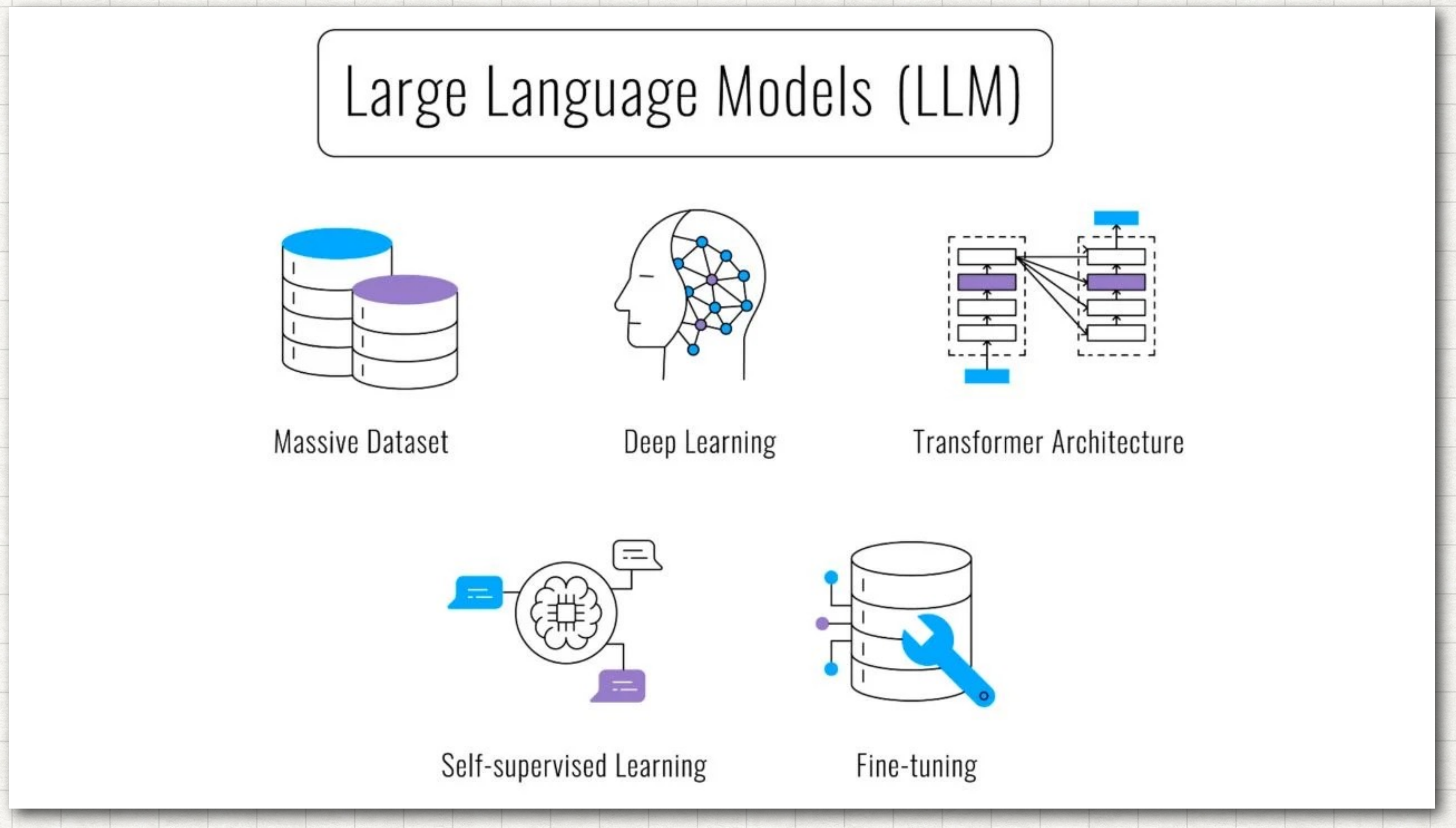
- Training data issues:
    - Non-representative, lack of geodiversity.
    - Faulty, biased training labels.
    - Adversarial effects.
- AI model issues:
    - Learn faulty strategies.
    - Fake something plausible.
    - Non-trustworthy, lack of robustness.
- Societal issues:
    - Lack of consent on data collection.
    - Disenfranchise scientists.
    - CO_2 emissions.
    - Globally applicable AI approaches may stymie burgeoning efforts in developing countries.

LLM'S - THE FUTURE OF SCIENCE?

LARGE LANGUAGE MODELS

DEFINITION AND FUNCTIONS

- Deep learning models, trained on massive data sets, that perform NLP tasks (translate, predict, generate).
- A glorified chatbot/parrot???
- YES, but
    - Can be trained to "speak" physics, biology, epidemiology, etc., etc.
    - Tools such as fine-tuning, RAG (prompt engineering).



LARGE LANGUAGE MODELS

APPLICATIONS

- Current:
  - NLP - text generation, chatbots
  - Education - tutoring, languages
  - Healthcare - medical record analysis, symptom checker
  - Business - customer support, content creation, market analysis
  - Software - code generation, documentation

- Future
  - R&D - NWP, drug discovery, research assistant
  - Human-Machine interaction
  - Autonomous Systems - assistive technologies, robotics

LARGE LANGUAGE MODELS

IMPACT

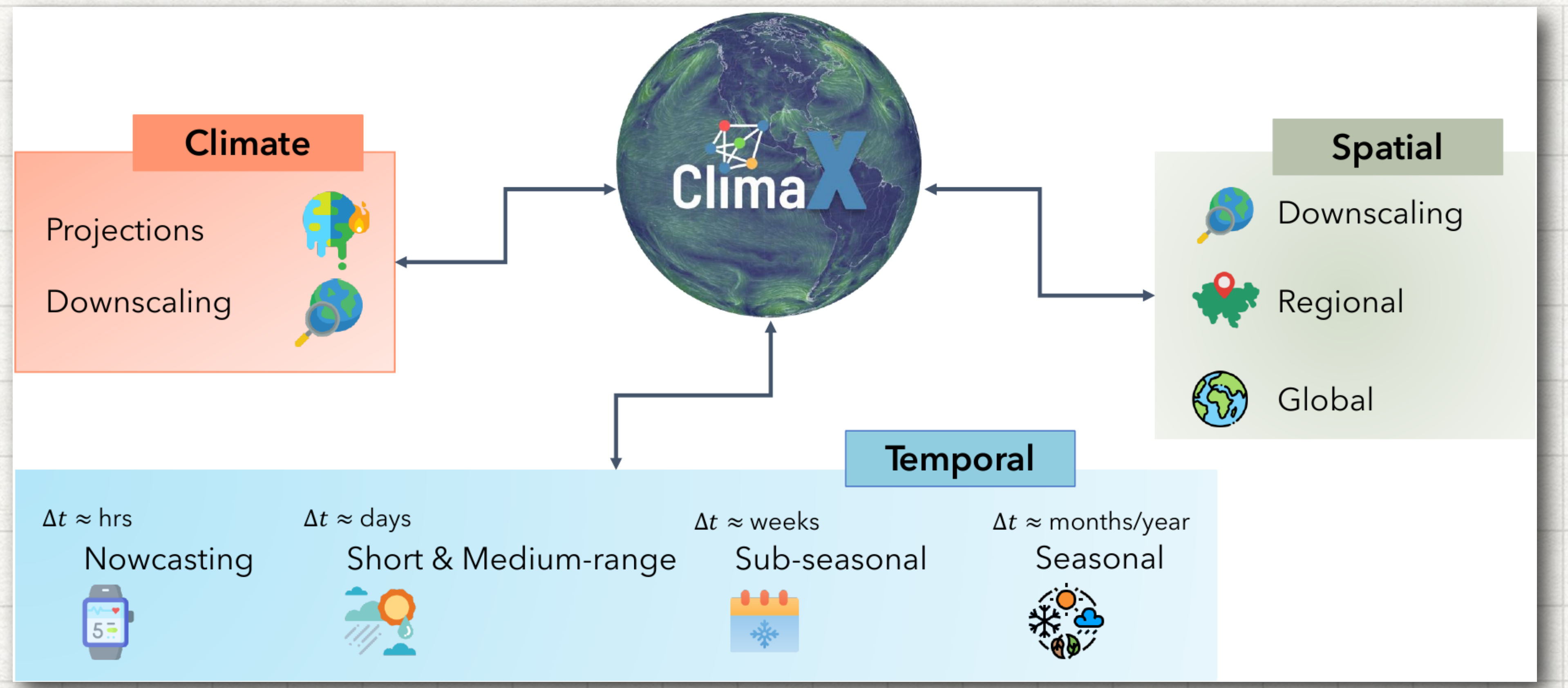
- Economic
  - Job transformation
  - Productivity gains
- Social and Ethical
  - Bias and fairness
  - Privacy concerns
- Educational
  - Personalize learning
  - Critical thinking
- Healthcare
  - Improved diagnostics
  - Patient-health system interactions

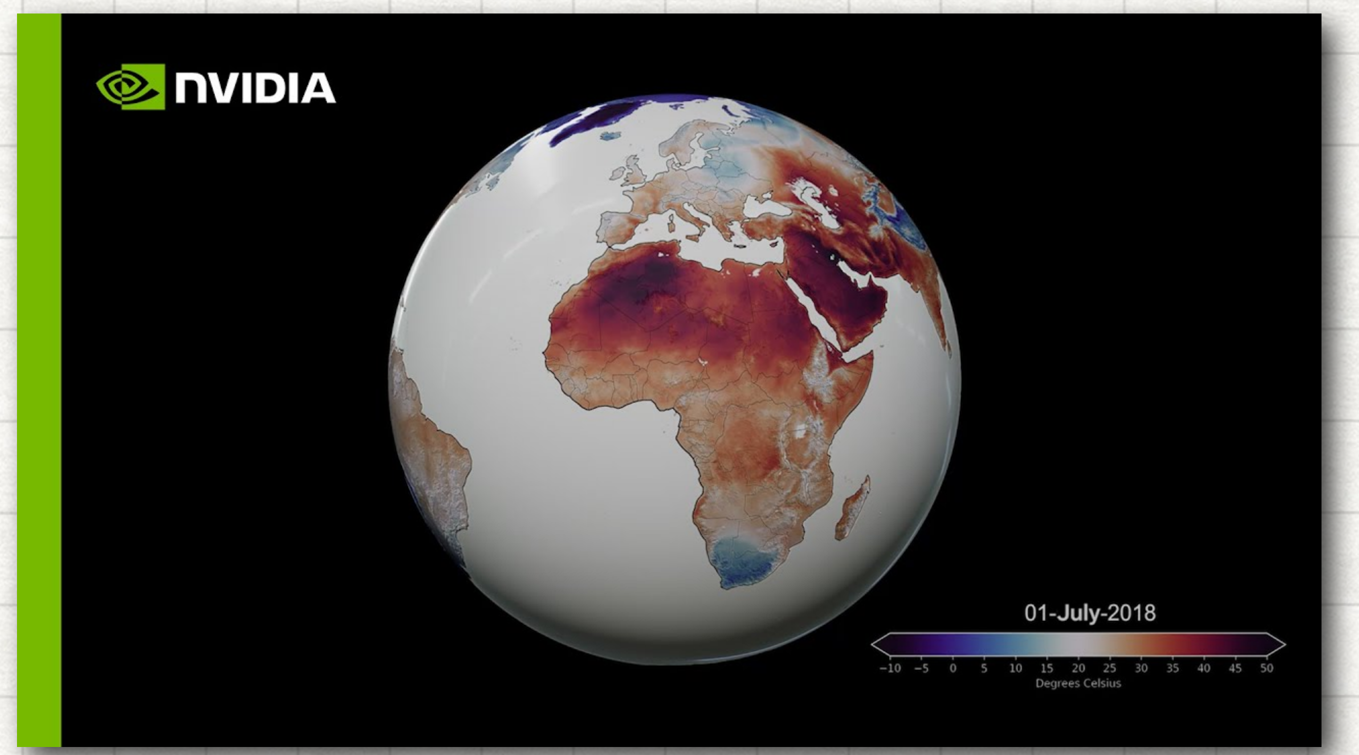
LLM APPLICATIONS

NWP & CLIMATOLOGY

USING LLM'S

- NVIDIA, Huawei, Microsoft, Google
- Trained on (lots of) historical reanalysis data
- Claims:
    - 10 000X speedup!
    - Accuracy for nowcasts
- Is health data next?

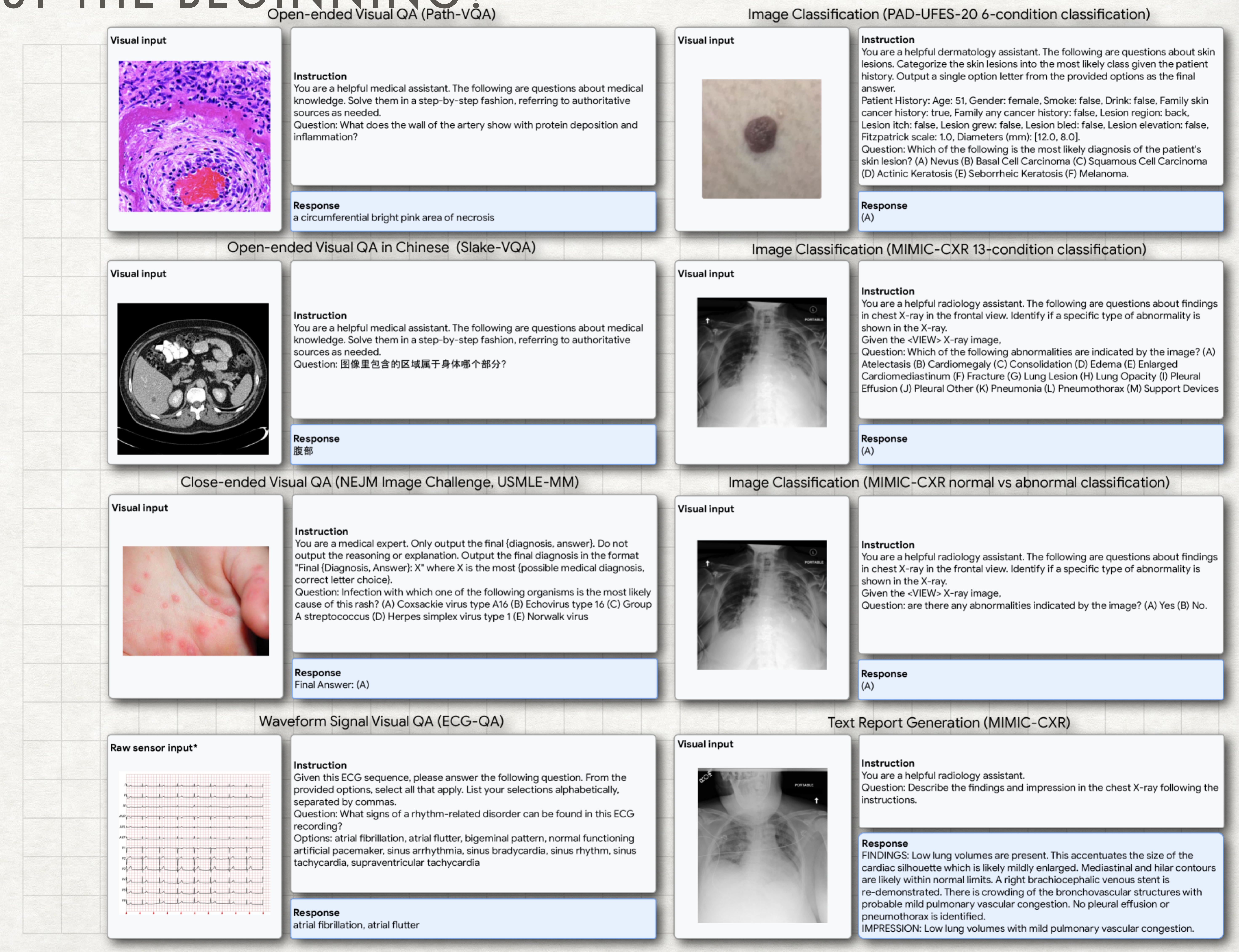




LLM FOR HEALTHCARE

JUST THE BEGINNING?

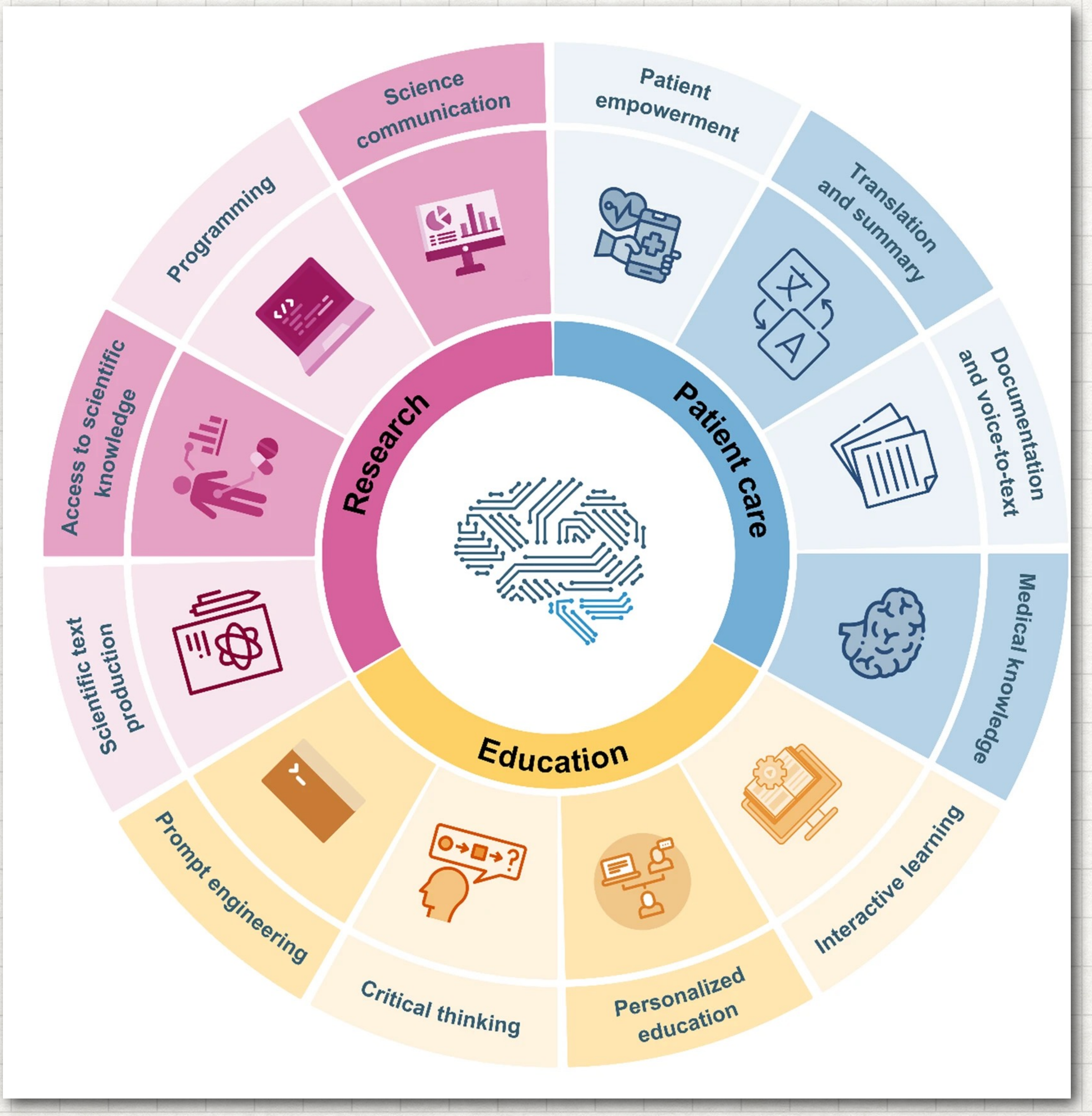
- Google announces Med-Gemini https://arxiv.org/pdf/2404.18416v2 (29 April 2024)
  - Family of multimodal models built upon Gemini specifically designed for the healthcare industry.
  - "Groundbreaking Family of AI Models Revolutionizing Medical Diagnosis and Clinical Reasoning"
  - Models excel in multimodal tasks, with substantial improvements in analyzing medical images and videos and accurately retrieving information from long health records



LARGE LANGUAGE MODELS

TOMORROW?

- Small number of very large, intelligent LLMs
- Many smaller, specialized LLMs
  - Healthcare, legal, finance, etc.
- Personal LLMs (your "story")
- Uses in education
  - How to educate?
  - What to teach?



[J. Clusmann, et al. Nature Comm. Medecine, 2023]

THANK YOU!

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DETAILS

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- https://github.com/markasch
- https://markasch.github.io/DT-tbx-v1/

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