An Introduction to Artificial Intelligence in Pharmacy & Biomedicine

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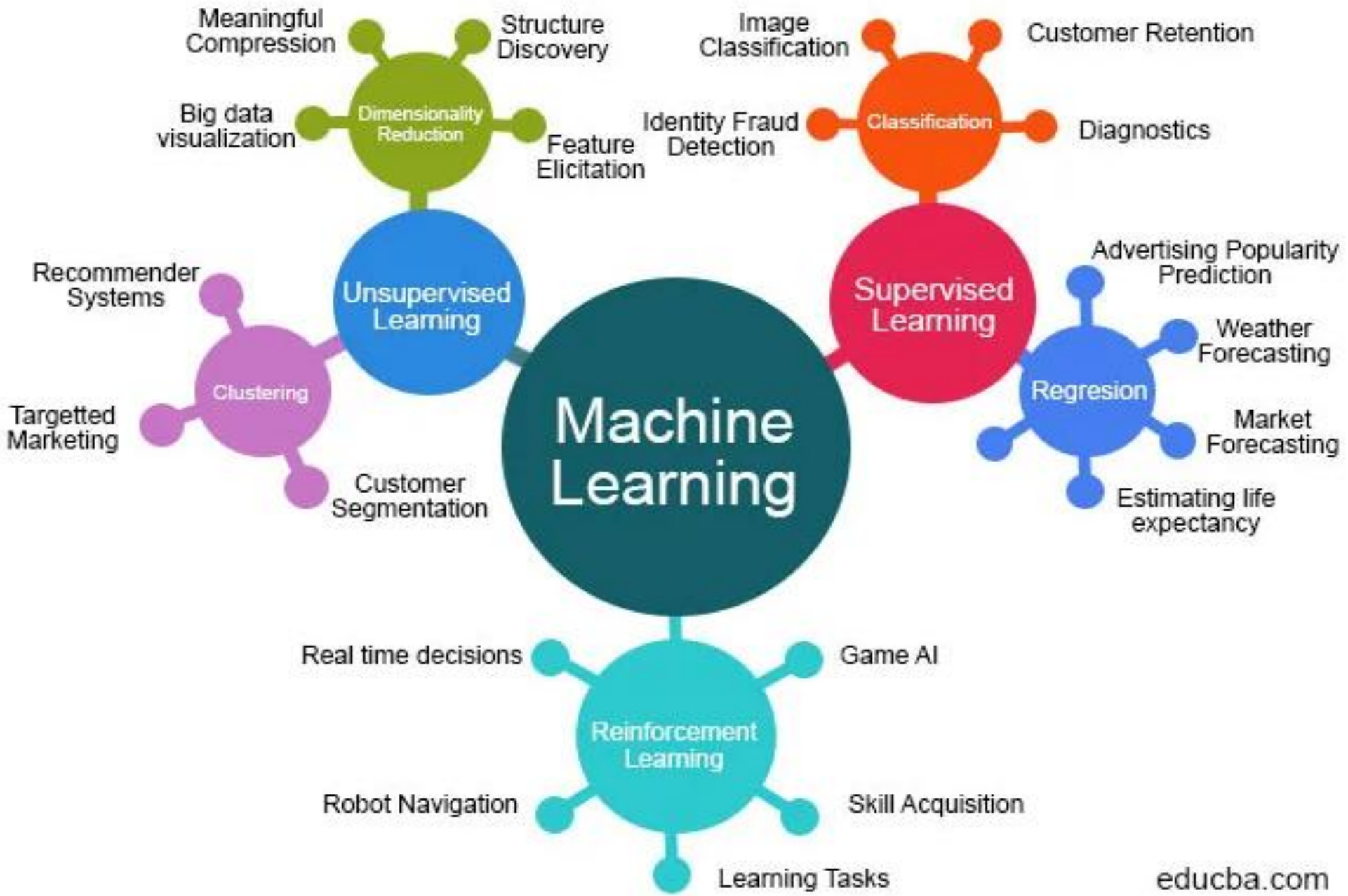
2023


Machine Learning
Unsupervised Learning
Supervised Learning
Reinforcement Learning
Dimensionality Reduction
Clustering
Classification
Regresion
Meaningful Compression
Structure Discovery
Big data visualization
Feature Elicitation
Recommender Systems
Targetted Marketing
Customer Segmentation
Image Classification
Customer Retention
Identity Fraud Detection
Diagnostics
Advertising Popularity Prediction
Weather Forecasting
Market Forecasting
Estimating life expectancy
Real time decisions
Game AI
Robot Navigation
Skill Acquisition
Learning Tasks
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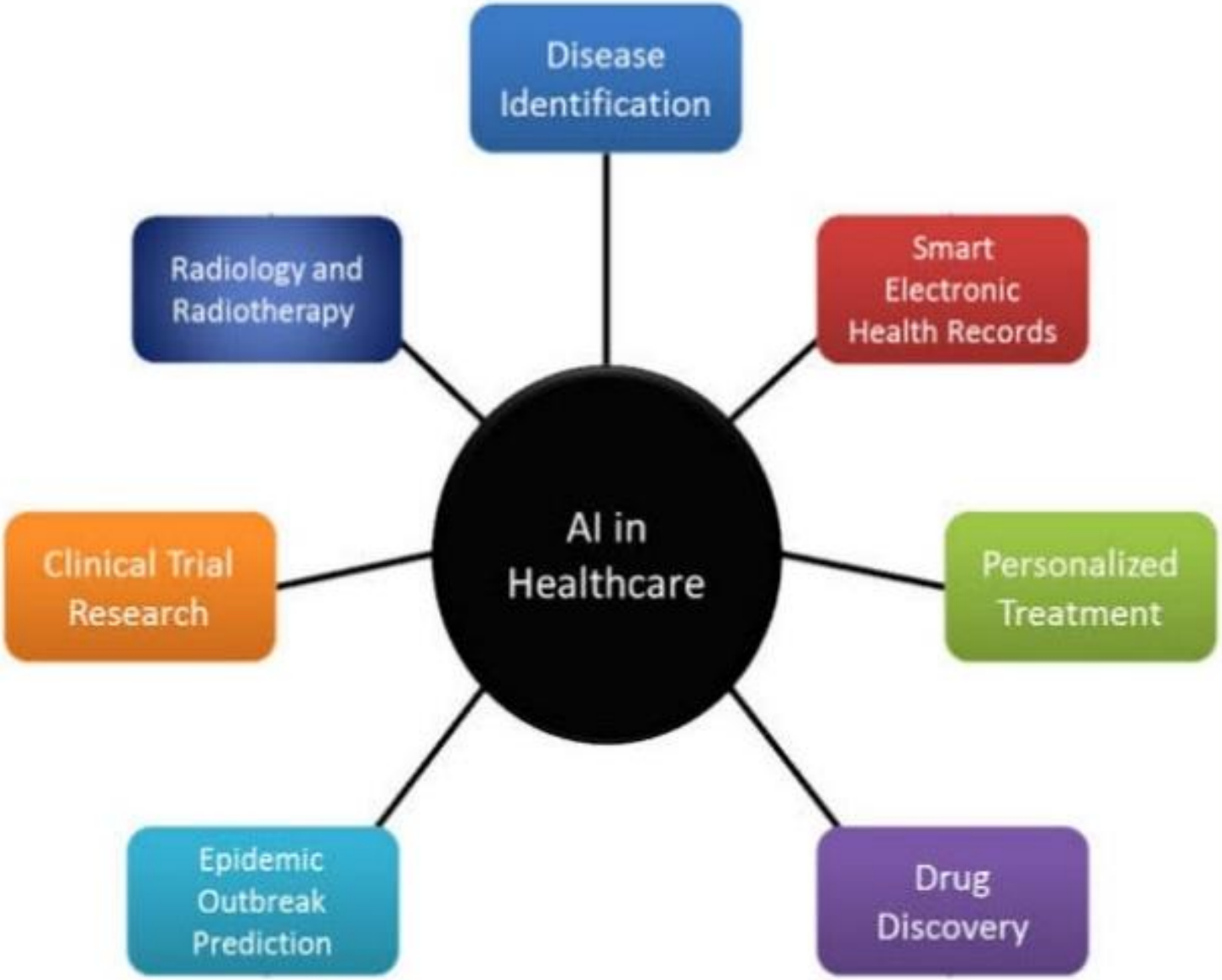

AI in Healthcare
Disease Identification
Smart Electronic Health Records
Personalized Treatment
Drug Discovery
Epidemic Outbreak Prediction
Clinical Trial Research
Radiology and Radiotherapy

Augmented Intelligence

AI as a powerful tool and partner

Man + machine = enhanced human capabilities (AMA, 2018)

AI can help human

- Unlock the power of big data and gain insight into patients
- Support evidence-based decision making, improving quality, safety, and efficiency
- Coordinate care and foster communication
- Improve patient experience and outcomes
- Deliver value and reduce costs
- Improve health system performance & optimization

THE LANCET
Digital Health

COMMENT | VOLUME 1, ISSUE 1, PE35-E37, MAY 01, 2019

Artificial intelligence for diabetic retinopathy screening in Africa

Wanjiku Ciku Mathenge

Published: May, 2019 DOI: https://doi.org/10.1016/S2589-7500(19)30009-5

Artificial intelligence for diabetic retinopathy screening in Africa

Blindness from diabetic retinopathy has become another addition to the myriad of demands on eye health systems in low-resource countries. This is driven by the rising number of people living with diabetes all over the world, with the largest increases projected in Asia and Africa.[1]

Despite screening for diabetic retinopathy in the their diabetic retinopathy status without waiting for feedback from reading centres, which often necessitates an extra journey for them. The Article describes a tested methodology using convolutional neural networks and its effectiveness in reading images from African patients. Although Bellemo and colleagues' final ensemble model

See Articles page e35

Using AI for digital retinopathy screening will allow non-clinicians to be trained on retinal imaging, obtaining interpretation of the images within minutes and thus giving patients instant feedback.

PLOS ONE

RESEARCH ARTICLE

A data-driven artificial intelligence model for remote triage in the prehospital environment

Dohyun Kim[1☯], Sungmin You[2☯], Soonwon So[2], Jongshill Lee[2], Sunhyun Yook[2], Dong Pyo Jang[2], In Young Kim[2], Eunkyoung Park[3], Kyeongwon Cho[3], Won Chul Cha[4,5], Dong Wook Shin[5,6], Baek Hwan Cho[3,7]*, Hoon-Ki Park[8]*

1 Convergence Research Center for Diagnosis, Treatment, and Care of Dementia, Korea Institute of Science and Technology, Seoul, South Korea, 2 Department of Biomedical Engineering, Hanyang University, Seoul, South Korea, 3 Smart Healthcare & Device Research Center, Samsung Medical Center, Sungkyunkwan University School of Medicine, Seoul, South Korea, 4 Department of Emergency Medicine, Samsung Medical Center, Sungkyunkwan University School of Medicine, Seoul, South Korea, 5 Department of Digital Health,

In todays world health emergencies are numerous and medical personnel are limited. This study has designed a consciousness index to substitute the factor by manpower and improved the classification accuracy (triage) by applying a machine learning algorithm.

DP, et al. (2018) A data-driven artificial intelligence model for remote triage in the prehospital environment. PLoS ONE 13(10): e0206006. https://doi.org/10.1371/journal.pone.0206006

Editor: Wajid Mumtaz, University Technology Petronas, MALAYSIA

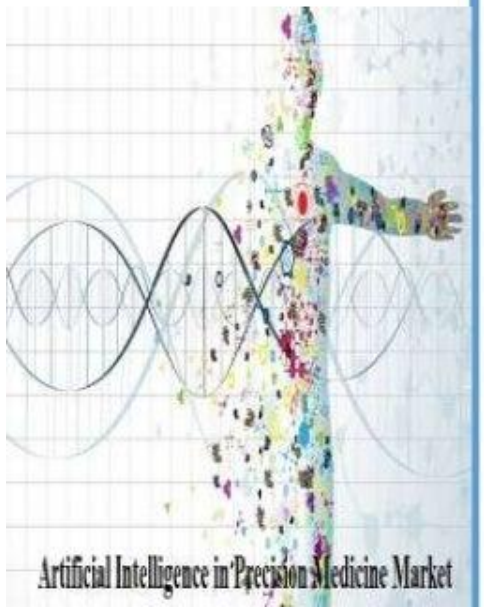
Received: August 28, 2018

In a mass casualty incident, the factors that determine the survival rate of injured patients are diverse, but one of the key factors is the time for triage. Additionally, the main factor that determines the time of triage is the number of medical personnel. However, when relying on a small number of medical personnel, the ability to increase survivability is limited. Therefore, developing a classification model for survival prediction that can quickly and precisely triage via wearable devices without medical personnel is important. In this study, we

Role of AI in Health

Treatment Design

Artificial intelligence systems have been created to analyze data – notes and reports from a patient's file, external research, and clinical expertise – to help select the correct, individually customized treatment path.

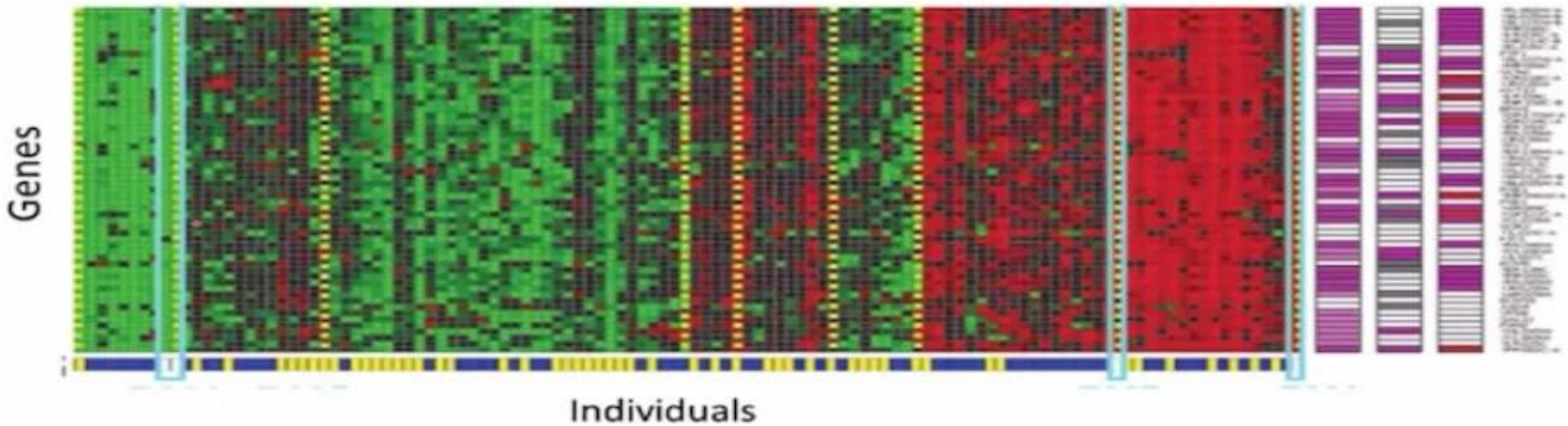


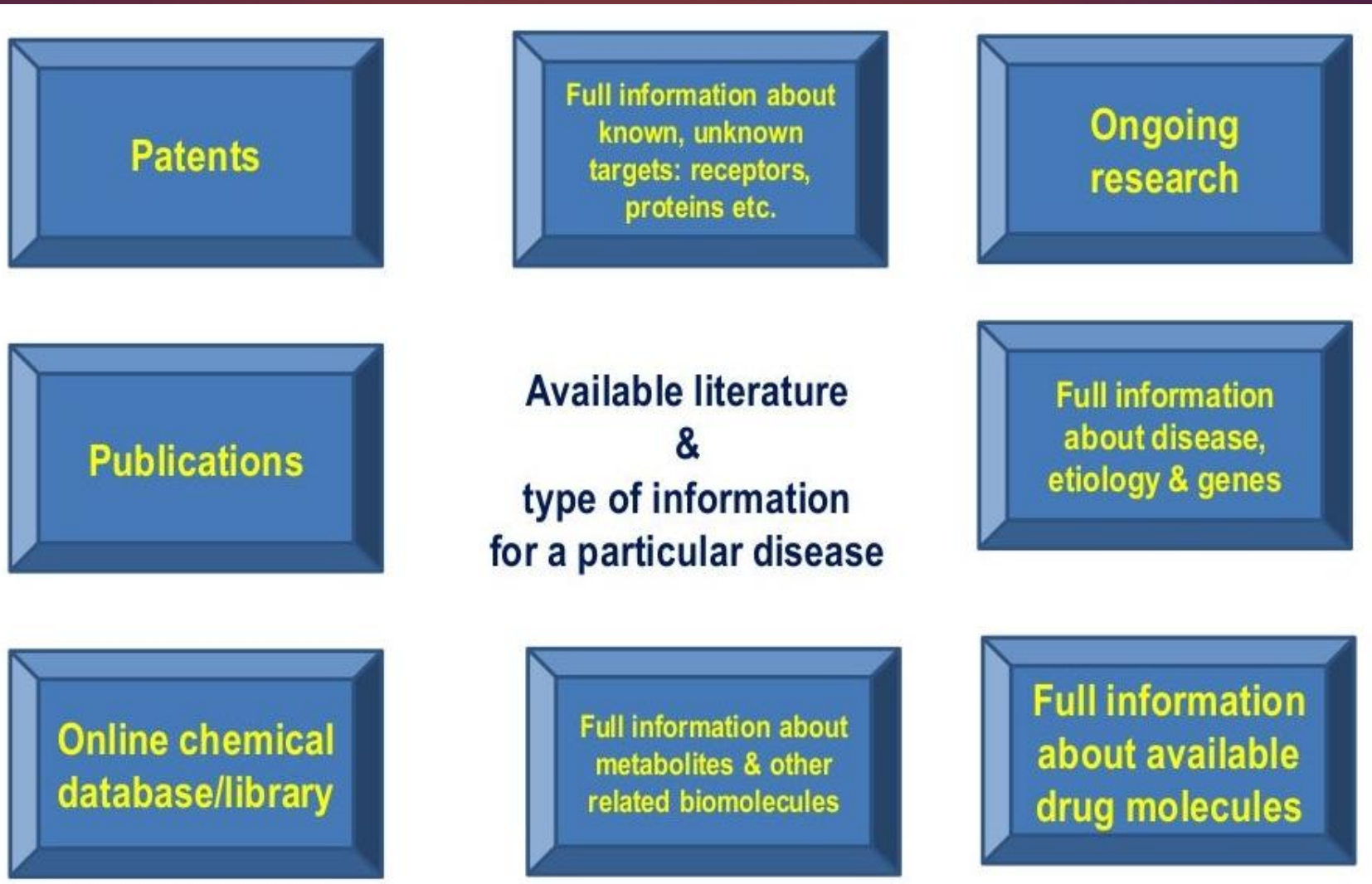
Precision Medicine

Instead of developing treatments for populations and making the same medical decisions based on a few similar physical characteristics among patients, medicine has shifted toward prevention, personalization, and precision.

Genetics and genomics look for mutations and links to disease from the information in DNA. With the help of AI, body scar spot cancer and vascular diseases early and predict the health issues people might face based on their genetics.

Unsupervised learning: Pattern recognition in genomics




Patents
Full information about known, unknown targets: receptors, proteins etc.
Ongoing research
Publications
Available literature & type of information for a particular disease
Full information about disease, etiology & genes
Online chemical database/library
Full information about metabolites & other related biomolecules
Full information about available drug molecules

Healthcare is "*dying of thirst in an ocean of data*"

90% of the world's data was created in the **last two years**

80% of data in the world is **unstructured** making decisions more complex

200% data growth, in the next two years fed by 1T connected devices

1 in 5 diagnoses are estimated to be inaccurate or incomplete

---

2X

medical information is doubling **every 4 years**

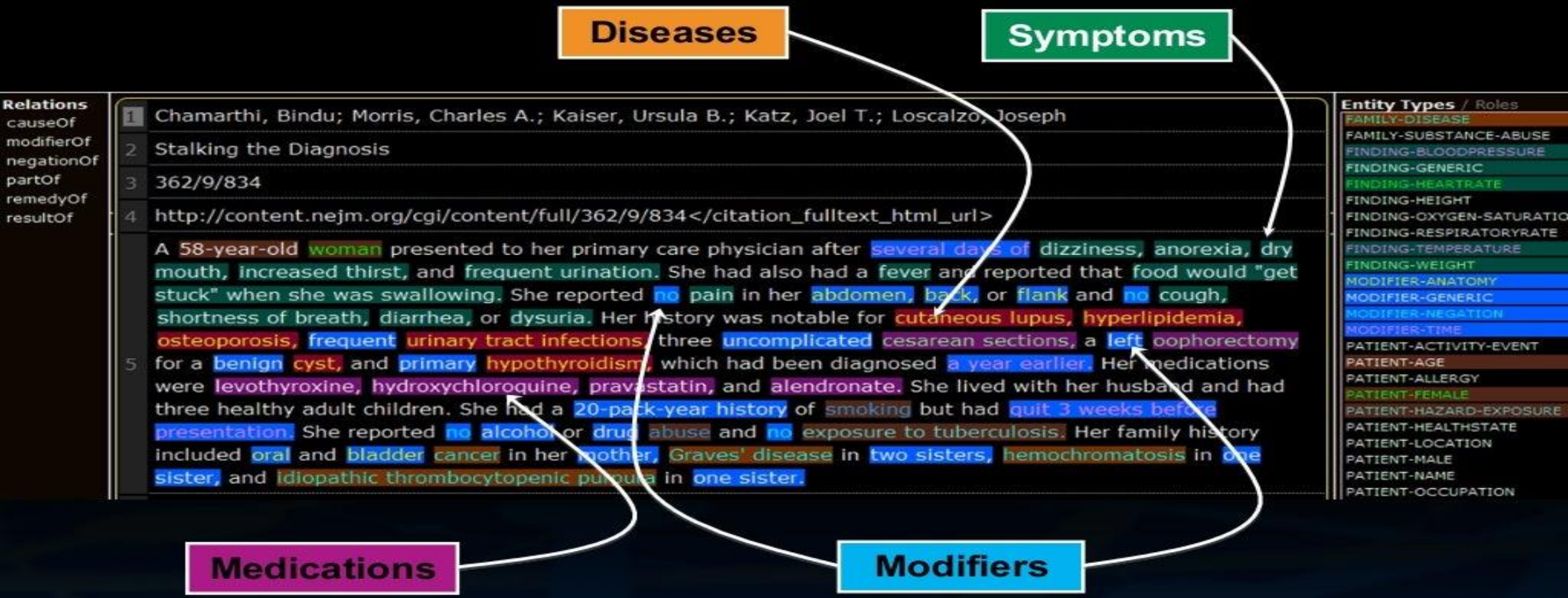
75

new clinical trials start **every day** in the US alone

$750B

or 30 cents of every dollar spent on healthcare in the US is **wasted**

Medical journal concept annotations



Challenges for using AI in Healthcare

- Inadequate understanding about what a particular type of AI technology can or can't do
- Lack of good implementation strategies
- Incompatibility with legacy technologies and data
- Shortage of trained workforce
- Pre-existing corporate biases

AI Ethics

- Privacy and data security

  protecting patient privacy and ensuring the security of sensitive health data when using AI in medical education and practice

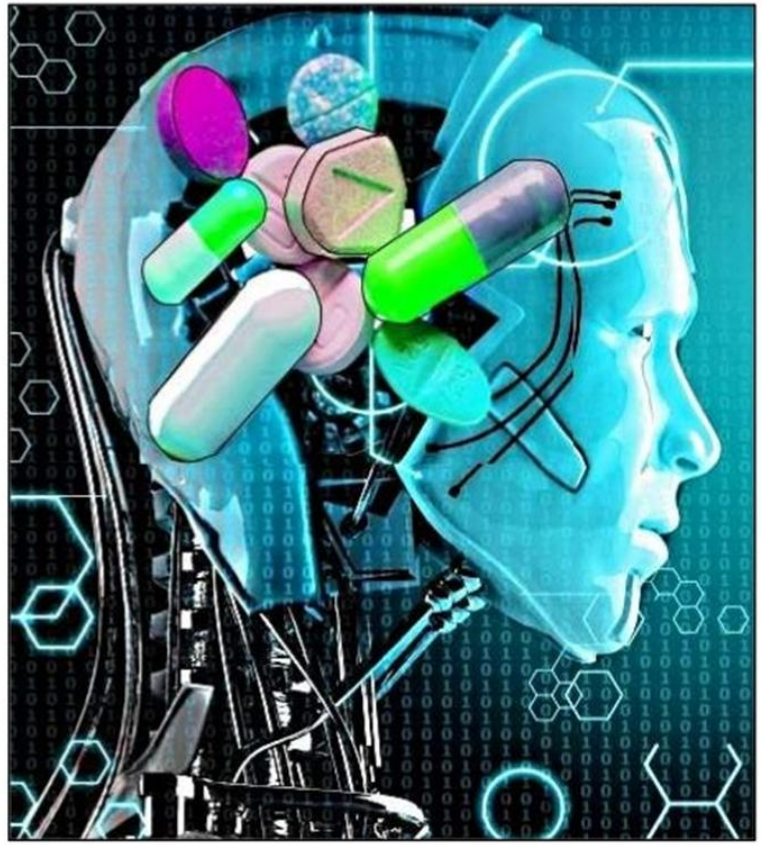
  AI can be used to protect patient privacy and data security by data anonymization and encryption

- Transparency and explainability in AI systems are of prime importance particularly in the context of medical decision-making
- Accountability and responsibility

- Ethical and legal responsibilities of those who develop and deploy AI systems and the need for accountability and oversight
- Establishing clear guidelines and standards for AI development and deployment

In almost all the steps involved in drug discovery and development, may have its say/inputs

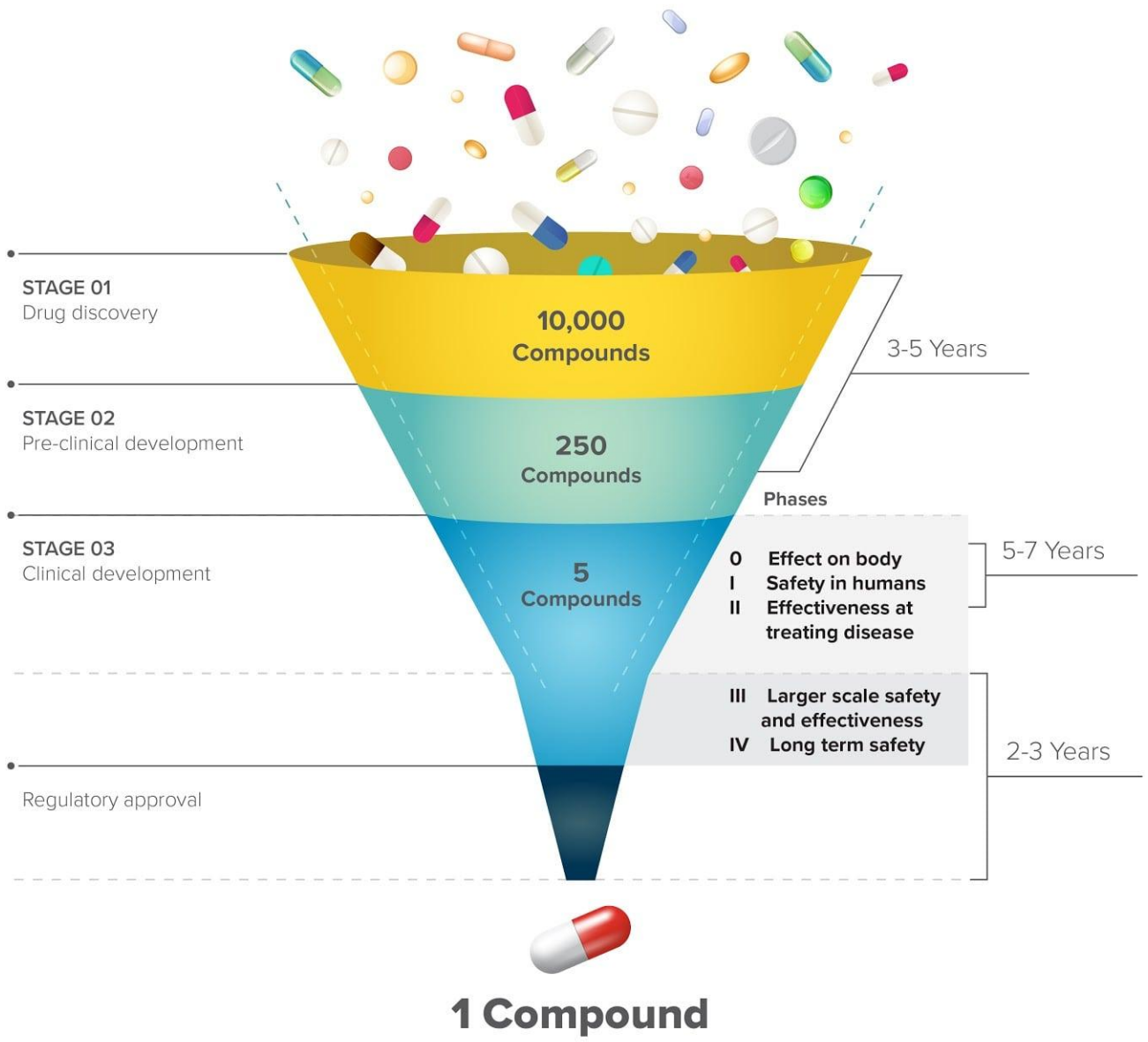
- Target discovery/identification
- Discovery and screening
- Lead optimization
- ADMET
- Development
- Registration
- Marketing



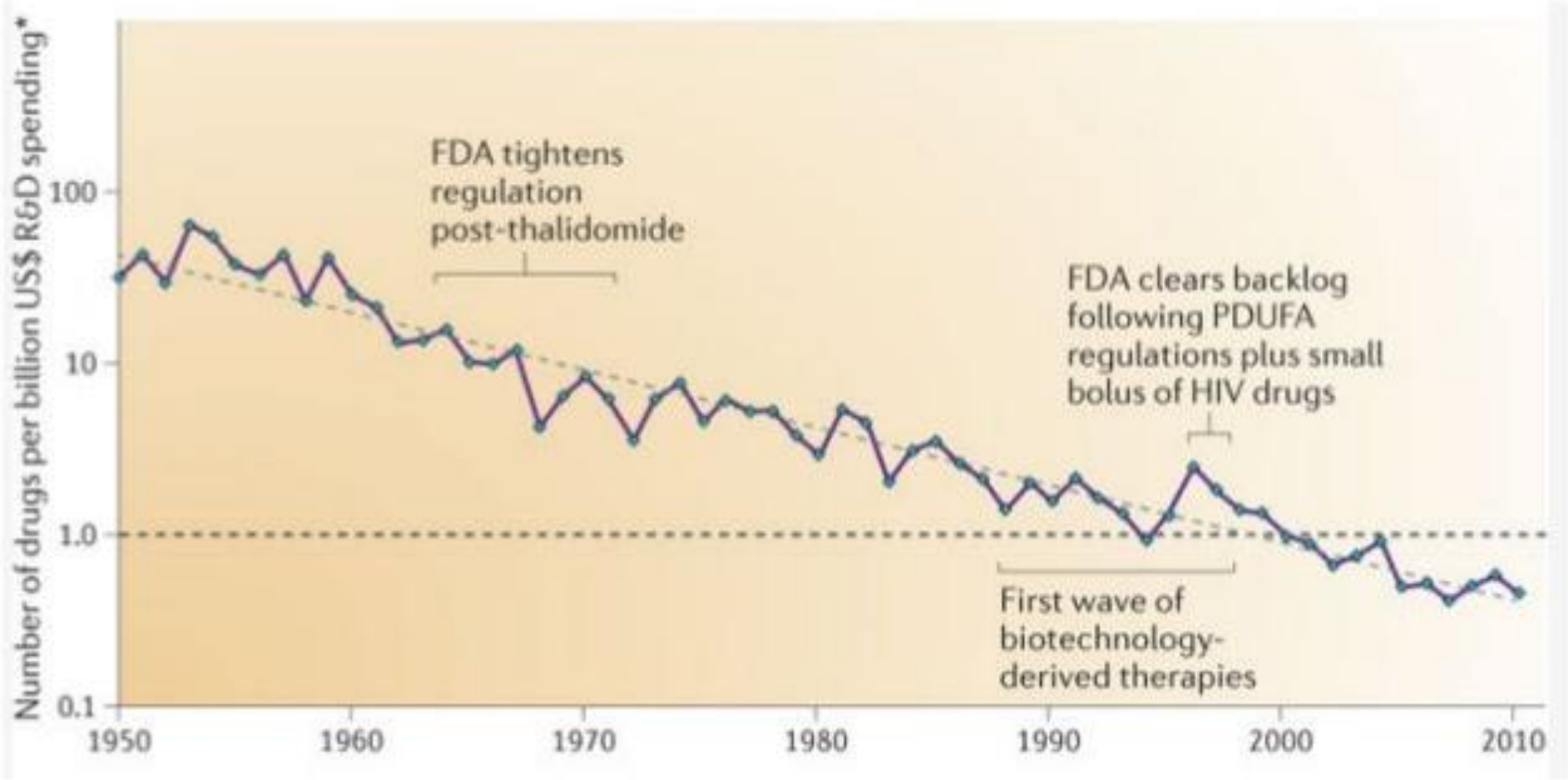
AI tools are being used to

1. Aggregate and synthesize information
2. Understand mechanisms of disease
3. Establish biomarkers
4. Generate data and models
5. Repurpose existing drugs
6. Generate novel drug candidates
7. Validate and optimize drug candidates
8. Design drugs
9. Design preclinical experiments
10. Run preclinical experiments
11. Design clinical trials
12. Recruit for clinical trials
13. Optimize clinical trials
14. Publish data
15. Analyze real world evidence

Drug discovery and development timeline



Pharma R&D Cost



Drug Discovery

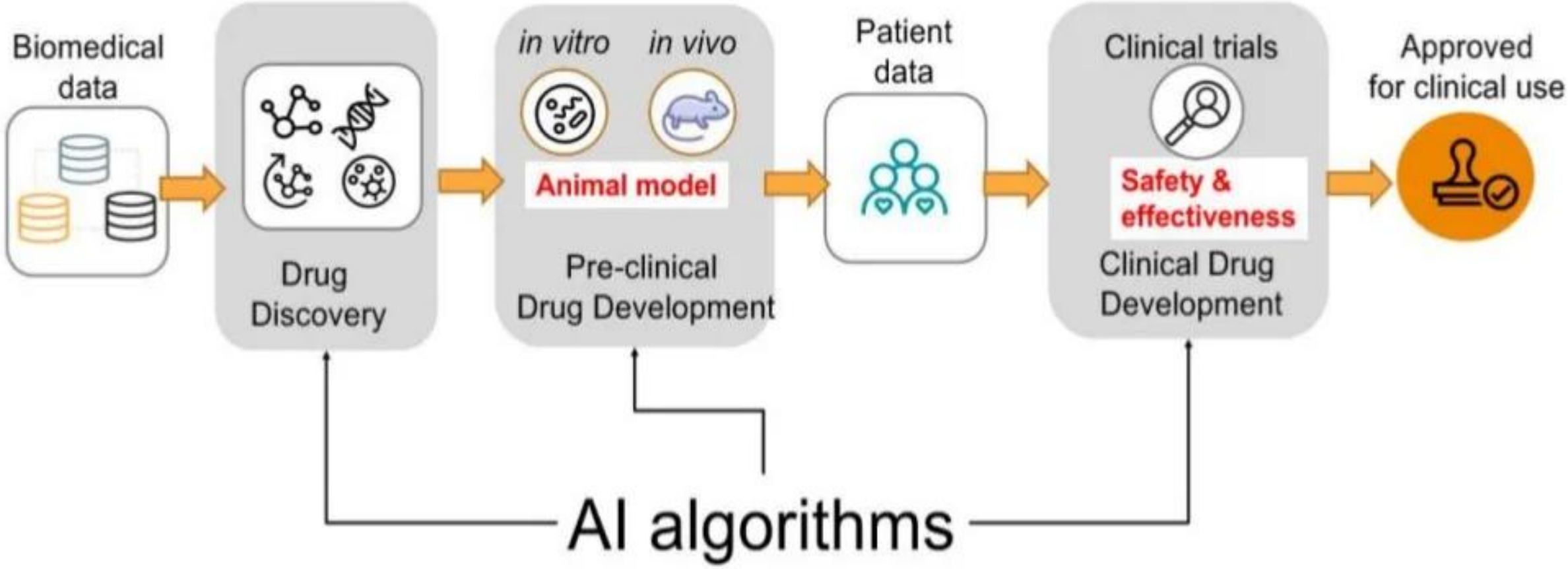
The main idea behind applying machine learning in drug discovery is to **automate the prioritization of molecules with desired properties** for downstream experimental verification

- In silico modeling of medicine means direct use of computational methods in drug discovery and development. Machine learning & data mining methods have become an fundamental part of in silico modeling.

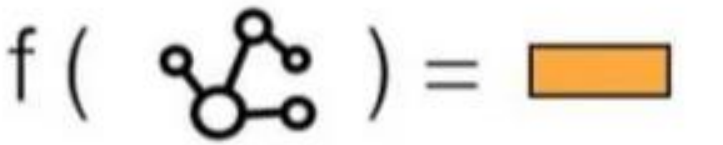
Classical approach Vs Modern approach

LOOKING FOR A NEEDLE IN A HAYSTACK

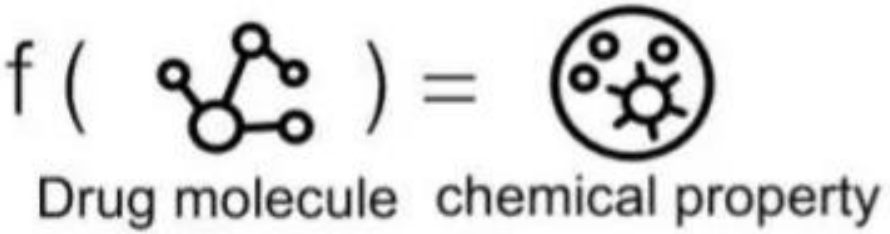
GENERATE PERFECT NEEDLES


Biomedical data
Drug Discovery
in vitro
in vivo
Animal model
Pre-clinical Drug Development
Patient data
Clinical trials
Safety & effectiveness
Clinical Drug Development
Approved for clinical use
AI algorithms

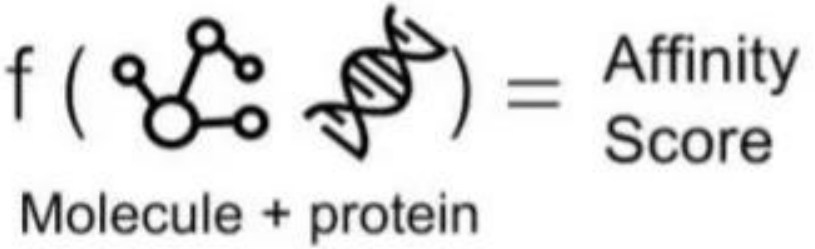
0. Molecular Representation Learning



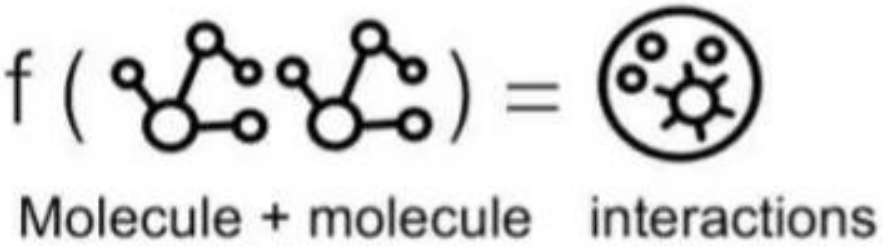
1. Molecule Property Prediction



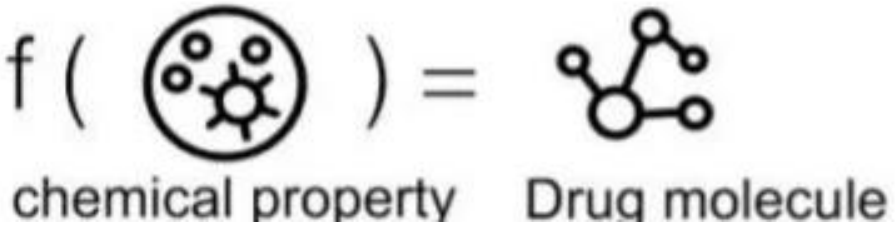
2. Drug repositioning



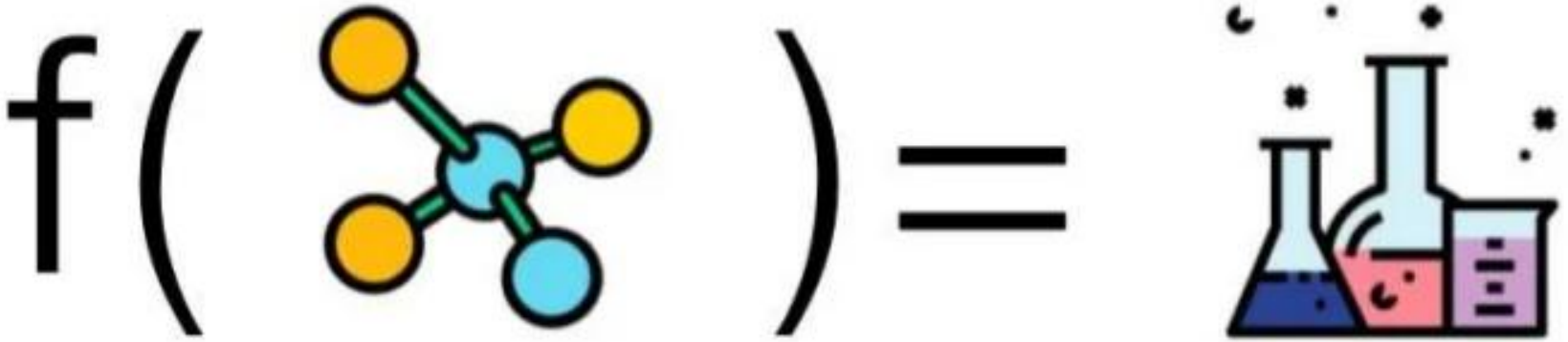
3. Adverse drug Reaction/interaction



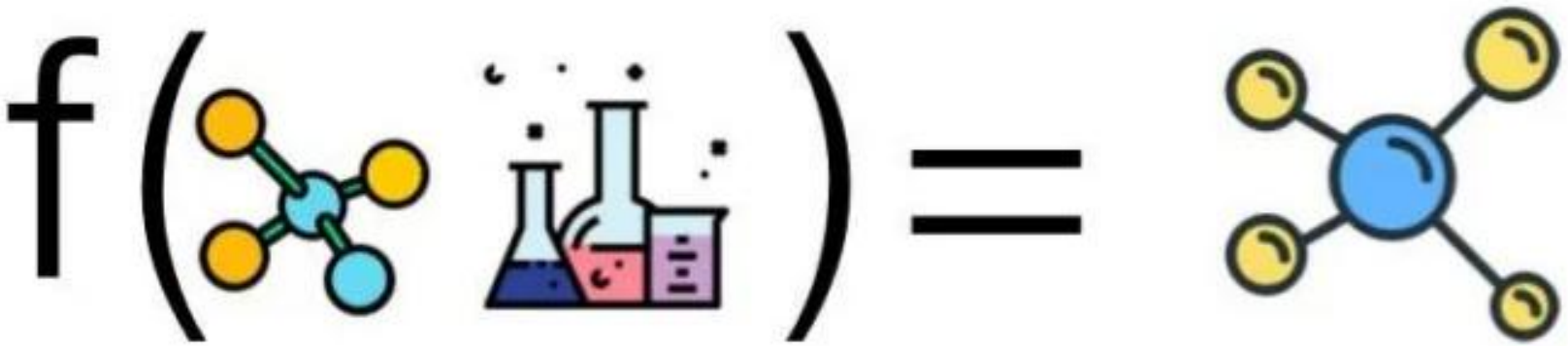
4. De *Novo* Design



QSAR: given the molecular descriptors, predict the chemical property.



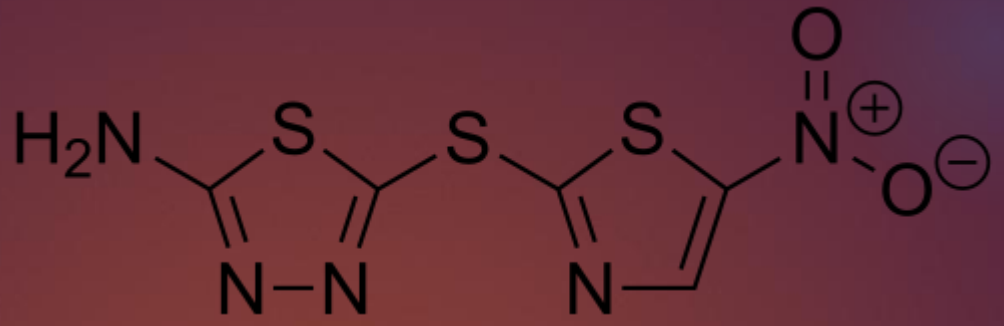
De novo: want a molecule with certain property.



Deep/Machine Learning Reports of New Drugs

Type of Drug	Efficacy Endpoint	Virtual Screening	Special Notes	Reference
Antifibrotic (DDR1 kinase)	In vivo mice	30,000 structures, use of GANs	46 days from target selection to in vivo efficacy	Zhavoronkov A, Nature Biotech August 2019
Copper transport (Wilson's disease)	In vitro	Database of >100,000 pathogenic mutations	18 months from target selection	Merico D, bioRxiv, Sept 2019 (on mutation only)
5-HT1a agonist (OCD)	In vitro	"Tens of millions" to 350 candidates, use of GANs	Entering Phase 1 clinical trial in 12 months	Murgia M, Financial Times, 30 Jan 2020
Antibiotic (Halicin)	In vivo mice	ZINC 15 database >1.5 billion molecules	From Drug Repurposing Hub	Stokes JM, Cell, Feb 20, 2020

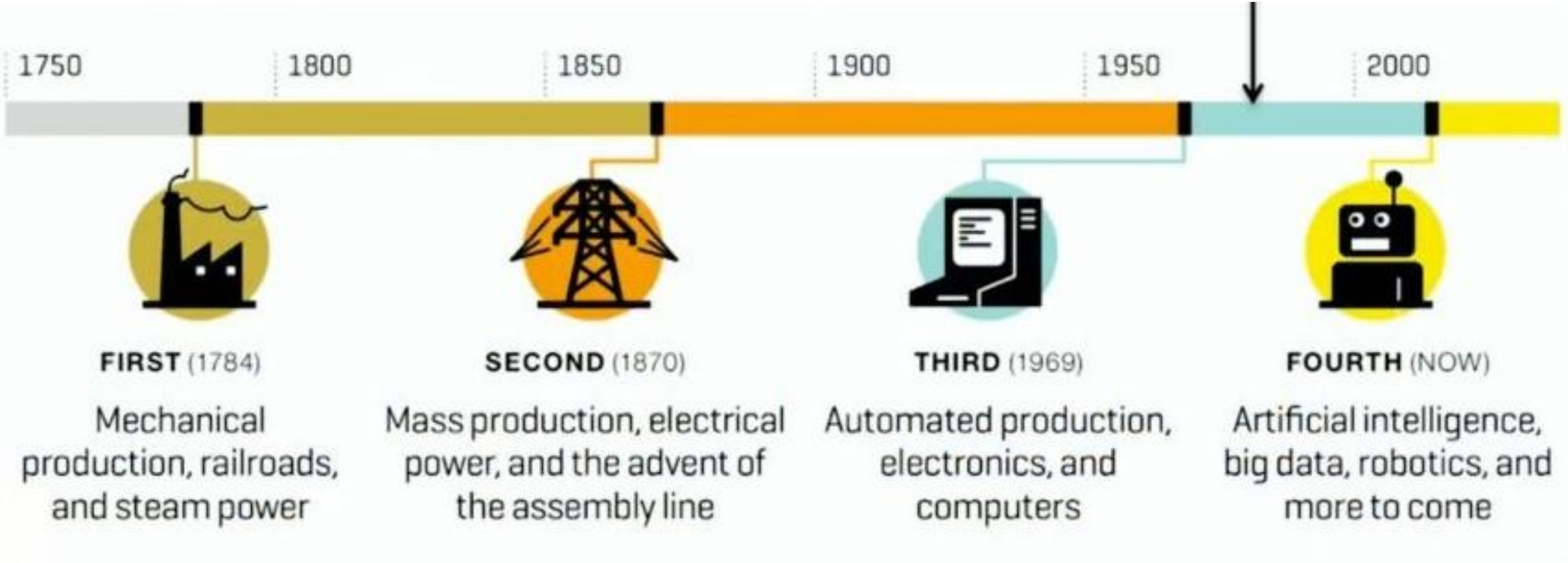
Halicin



- A new under investigation antibiotic “Halicin” has been identified using AI by MIT team.
- The team used a deep learning neural network to recognize a molecule which is different from most known antibiotics. The researchers trained its neural network to find molecules that inhibit the growth of the bacterium Escherichia coli, using a around 2,335 molecules with already proven antibacterial activity. This includes a library of about 300 approved antibiotics, as well as 800 natural products from plant, animal and microbial sources.
- The algorithm learns to predict molecular function without any assumptions about how drugs work and without chemical groups being labelled (like human experts). “As a result, the model can learn new patterns unknown to human experts.”

Fourth Industrial Revolution

Industry 4.0


1750
1800
1850
1900
1950
2000
FIRST (1784)
Mechanical production, railroads, and steam power
SECOND (1870)
Mass production, electrical power, and the advent of the assembly line
THIRD (1969)
Automated production, electronics, and computers
FOURTH (NOW)
Artificial intelligence, big data, robotics, and more to come