[KASBP AI-biotech Seminar] Beyond AlphaFold – Building AI-Powered Biomarker Platforms for the Next Generation of Drug Discovery

Sunghee Yun

Co-Founder & CTO - AI Technology & Biz Dev @ Erudio Bio, Inc. Advisor & Evangelist - Biz Dev @ CryptoLab, Inc. Adjunct Professor & Advisory Professor @ Sogang Univ. & DGIST

About Speaker

- Co-Founder & CTO @ Erudio Bio, San Jose & Novato, CA, USA
- Advisor & Evangelist @ CryptoLab, Inc., San Jose, CA, USA
- Chief Business Development Officer @ WeStory.ai, Cupertino, CA, USA
- Advisory Professor, Electrical Engineering and Computer Science @ DGIST, Korea
- Adjunct Professor, Electronic Engineering Department @ Sogang University, Korea
- Global Advisory Board Member @ Innovative Future Brain-Inspired Intelligence System Semiconductor of Sogang University, Korea
- KFAS-Salzburg Global Leadership Initiative Fellow @ Salzburg Global Seminar, Salzburg, Austria
- Technology Consultant @ Gerson Lehrman Gruop (GLG), NY, USA
- Co-Founder & CTO / Head of Global R&D & Chief Applied Scientist / Senior Fellow @ Gauss Labs, Inc., Palo Alto, CA, USA 2020 – 2023

 Senior Applied Scientist @ Amazon.com, Inc., Vancouver, BC, Canada 	- 2020
• Principal Engineer @ Software R&D Center, DS Division, Samsung, Korea	- 2017
• Principal Engineer @ Strategic Marketing & Sales Team, Samsung, Korea	- 2016
• Principal Engineer @ DT Team, DRAM Development Lab, Samsung, Kore	ea – 2015
 Senior Engineer @ CAE Team, Samsung, Korea 	- 2012
 PhD - Electrical Engineering @ Stanford University, CA, USA 	- 2004
 Development Engineer @ Voyan, Santa Clara, CA, USA 	- 2001
 MS - Electrical Engineering @ Stanford University, CA, USA 	- 1999
• BS - Electrical & Computer Engineering @ Seoul National University	1994 – 1998

Highlight of Career Journey

- BS in EE @ SNU, MS & PhD in EE @ Stanford University
 - Convex Optimization Theory, Algorithms & Software
 - advised by Prof. Stephen P. Boyd
- Principal Engineer @ Samsung Semiconductor, Inc.
 - AI & Convex Optimization
 - collaboration with DRAM/NAND Design/Manufacturing/Test Teams
- Senior Applied Scientist @ Amazon.com, Inc.
 - e-Commerce Als anomaly detection, deep RL, and recommender system
 - Jeff Bezos's project boosted up sales by \$200M via Amazon Mobile Shopping App
- Co-Founder & CTO / Global R&D Head & Chief Applied Scientist @ Gauss Labs, Inc.
- Co-Founder & CTO AI Technology & Business Development @ Erudio Bio, Inc.

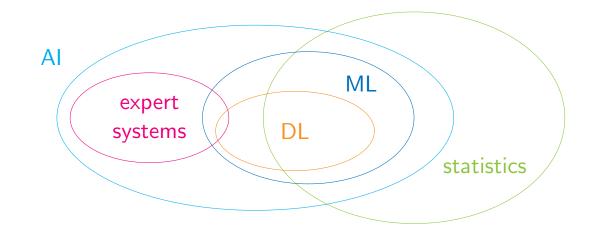
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Artificial Intelligence

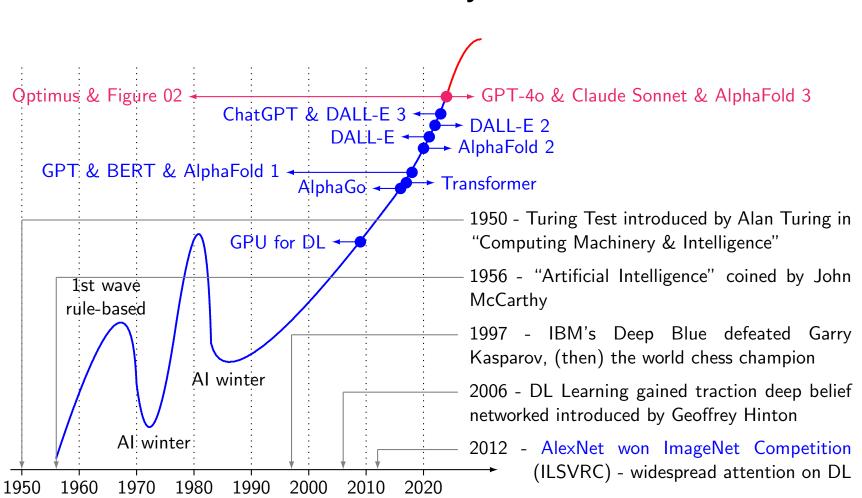
Definition and History

Definition & relation to other technologies

- Al
 - is technology doing tasks requiring human intelligence, such as learning, problemsolving, decision-making & language understanding
 - encompasses range of technologies, methodologies, applications & products
- AI, ML, DL, statistics & expert system¹ [HGH⁺22]



¹ML: machine learning & DL: deep learning



History

[KASBP AI-biotech Seminar] Beyond AlphaFold - Artificial Intelligence - Definition and History

Significant AI Achievements - 2014 - 2025

Deep learning revolution

- 2012 2015 DL revolution²
 - CNNs demonstrated exceptional performance in image recognition, *e.g.*, *AlexNet's* victory in ImageNet competition
 - widespread adoption of DL learning in CV transforming industries
- 2016 AlphaGo defeats human Go champion
 - DeepMind's AlphaGo defeated world champion in Go, extremely complex game believed to be beyond AI's reach
 - significant milestone in RL Al's potential in solving complex & strategic problems



 2 CV: computer vision, NN: neural network, CNN: convolutional NN, RL: reinforcement learning

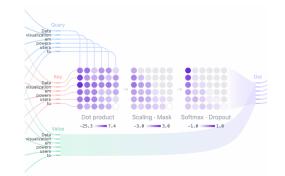
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Transformer changes everything

- 2017 2018 Transformers & NLP breakthroughs³
 - Transformer (e.g., BERT & GPT) revolutionized NLP
 - major advancements in, e.g., machine translation & chatbots
- 2020 AI in healthcare AlphaFold & beyond
 - DeepMind's AlphaFold solves 50-year-old protein folding problem predicting 3D protein structures with remarkable accuracy
 - accelerates drug discovery and personalized medicine offering new insights into diseases and potential treatments





³NLP: natural language processing, GPT: generative pre-trained transformer

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Lots of breakthroughs in AI technology and applications in 2024

- proliferation of advanced AI models
 - GPT-4o, Claude Sonnet, Claude 3 series, Llama 3, Sora, Gemini
 - transforming industries such as content creation, customer service, education, etc.
- breakthroughs in specialized AI applications
 - Figure 02, Optimus, AlphaFold 3
 - driving unprecedented advancements in automation, drug discovery, scientific understanding - profoundly affecting healthcare, manufacturing, scientific research





Major AI Breakthroughs in 2025

- next-generation foundation models
 - GPT-5 and Claude 4 demonstrate emergent reasoning abilities
 - open-source models achieving parity with leading commercial systems from 2024
- hardware innovations
 - NVIDIA's Blackwell successor architecture delivering 3-4x performance improvement
 - AMD's MI350 accelerators challenging NVIDIA's market dominance
- Al-human collaboration systems
 - seamless multimodal interfaces enabling natural human-AI collaboration
 - AI systems effectively explaining reasoning and recommendations
 - augmented reality interfaces providing real-time AI assistance in professional contexts

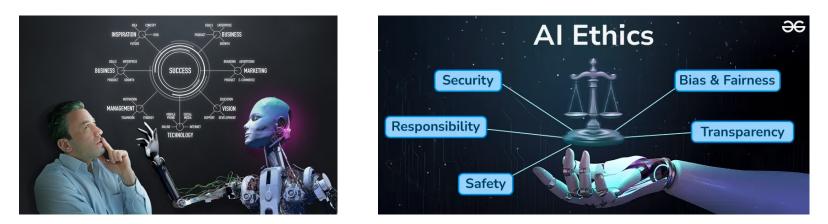


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Transformative impact of AI - reshaping industries, work & society

- accelerating human-AI collaboration
 - not only reshaping industries but altering how humans interact with technology
 - Al's role as collaborator and augmentor redefines productivity, creativity, the way we address global challenges, *e.g.*, *sustainability & healthcare*
- Al-driven automation *transforms workforce dynamics* creating new opportunities while challenging traditional job roles
- *ethical AI considerations* becoming central not only to business strategy, but to society as a whole *influencing regulations, corporate responsibility & public trust*

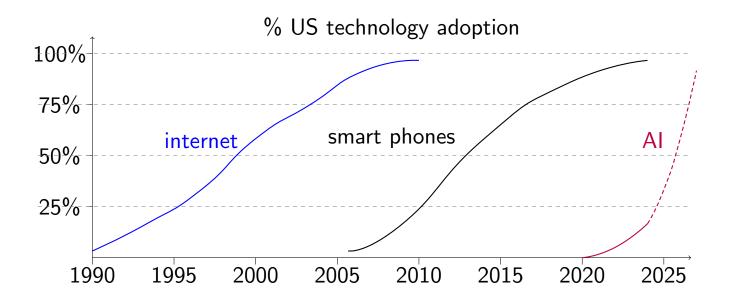


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Measuring Al's Ascent

Where are we in AI today?

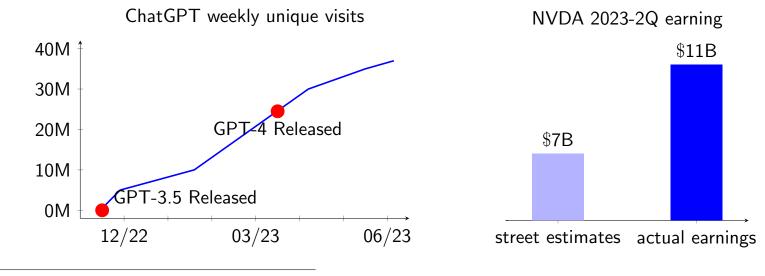
- sunrise phase currently experiencing dawn of AI era with significant advancements and increasing adoption across various industries
- early adoption in early stages of AI lifecycle with widespread adoption and innovation across sectors marking significant shift in technology's role in society



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Explosion of AI ecosystems - ChatGPT & NVIDIA

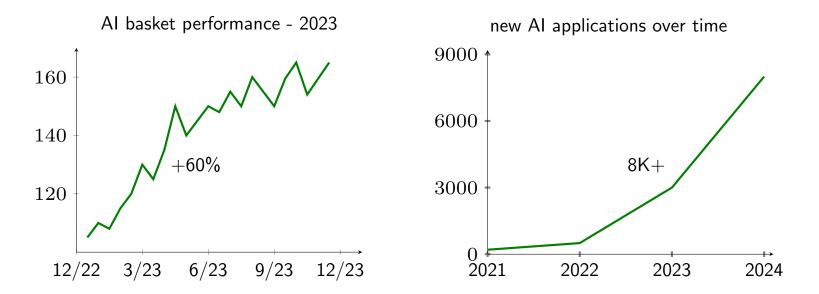
- took only 5 months for ChatGPT users to reach 35M
- NVDIA 2023 Q2 earning exceeds market expectation by big margin \$7B vs \$13.5B
 - surprisingly, 101% year-to-year growth
 - even more surprisingly gross margin was 71.2% up from 43.5% in previous year⁴



⁴source - Bloomberg

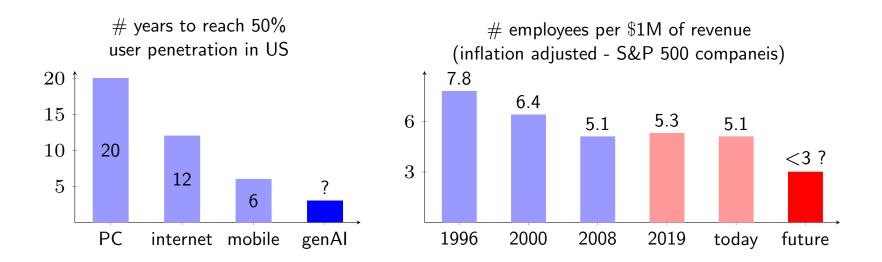
Explosion of AI ecosystems - AI stock market

- Al investment surge in 2023 portfolio performance soars by 60%
 - Al-focused stocks significantly outpaced traditional market indices
- over 8,000 new AI applications developed in last 3 years
 - applications span from healthcare and finance to manufacturing and entertainment



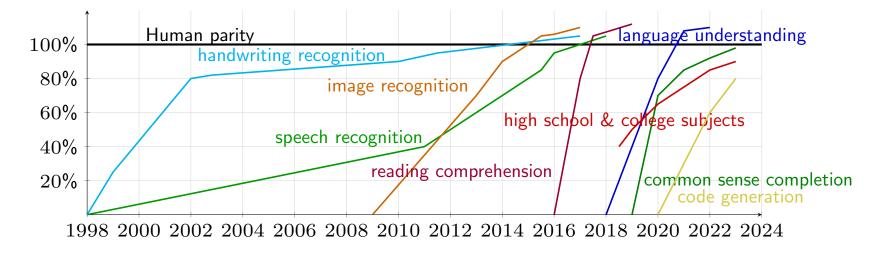
Al's transformative impact - adoption speed & economic potential

- adoption has been twice as fast with platform shifts suggesting
 - increasing demand and readiness for new technology improved user experience & accessibility
- Al's potential to drive economy for years to come
 - 35% improvement in productivity driven by introduction of PCs and internet
 - greater gains expected with AI proliferation



Al getting more & more faster

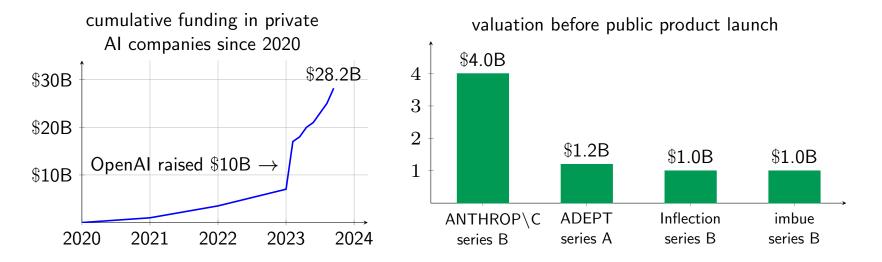
- steep upward slopes of AI capabilities highlight accelerating pace of AI development
 - period of exponential growth with AI potentially mastering new skills and surpassing human capabilities at ever-increasing rate
- closing gap to human parity some capabilities approaching or arguably reached human parity, while others having still way to go
 - achieving truly human-like capabilities in broad range remains a challenge



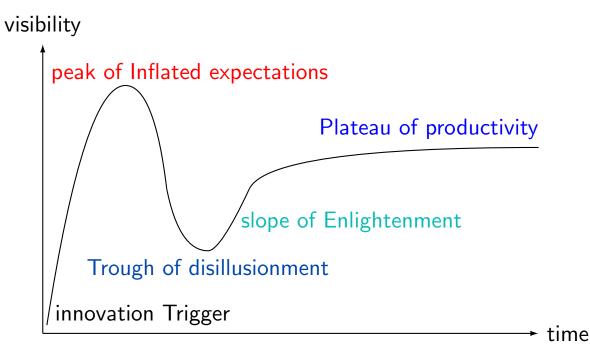
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Massive investment in AI

- explosive growth cumulative funding skyrocketed reaching staggering \$28.2B
- OpenAI significant fundraising (=\$10B) fueled rapid growth
- *valuation surge* substantial valuations even before public products for stella companies
- *fierce competition for capital* among AI startups driving innovation & accelerating development
- massive investment indicates *strong belief in & optimistic outlook for potential of AI* to revolutionize industries & drive economic growth



Is AI hype?



- innovation trigger technology breakthrough kicks things off
- peak of inflated expectations early publicity induces many successes followed by even more
- trough of disillusionment expectations wane as technology producers shake out or fail
- slope of enlightenment benefit enterprise, technology better understood, more enterprises fund pilots

Fiber vs cloud infrastructure

- fiber infrastructure 1990s
 - Telco Co's raised \$1.6T of equity & \$600B of debt
 - bandwidth costs decreased 90% within 4 years
 - companies Covage, NothStart, Telligent, Electric Lightwave, 360 networks, Nextlink, Broadwind, UUNET, NFS Communications, Global Crossing, Level 3 Communications
 - became *public good*

- cloud infrastructure 2010s
 - entirely new computing paradigm
 - mostly public companeis with data centers
 - big 4 hyperscalers generate \$150B
 + annual revenue



[KASBP AI-biotech Seminar] Beyond AlphaFold - Artificial Intelligence - Is AI hype?

Yes	&	No
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speaker's views
 OpenAl still operating at a loss; business model still not clear
 gradual value creation across broad range of industries and technologies (<i>e.g.</i>, CV, LLMs, RL) unlike fiber optic bubble in 1990s
 self-driving cars delayed for over 15 years, with limited hope for achieving level 5 autonomy AI, however, has proven useful within a shorter 5-year span, with enterprises eagerly adopting
 Al already providing significant utility across various domains vs quantum computing remains promising in theory but lacks widespread practical utility

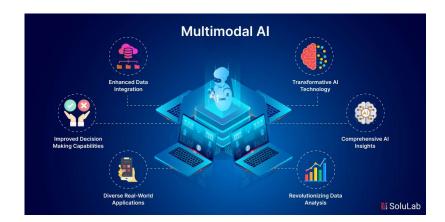
AI Agents

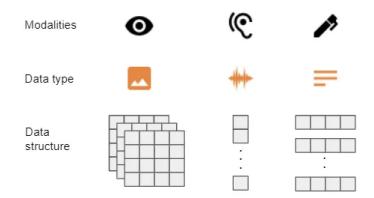
- 2010 \sim Big Data
- 2012 \sim Deep Learning
- 2017 \sim Transformer Attention is All you need!
- 2022 \sim LLM & genAl
- 2024 \sim AI Agent (Agentic AI)



Multimodal learning

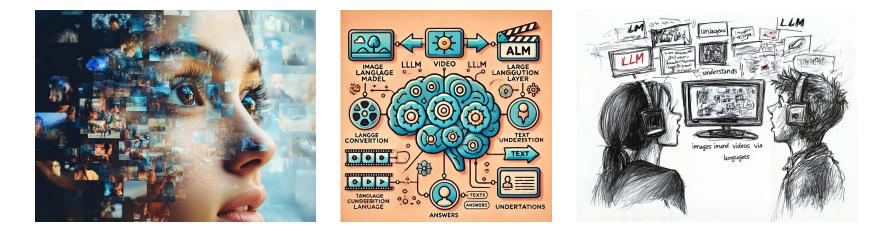
- understand information from multiple modalities, e.g., text, images, audio, video
- representation learning methods
 - combine multiple representations or learn multimodal representations simultaneously
- applications
 - images from text prompt, videos with narration, musics with lyrics
- collaboration among different modalities
 - understand image world (open system) using language (closed system)





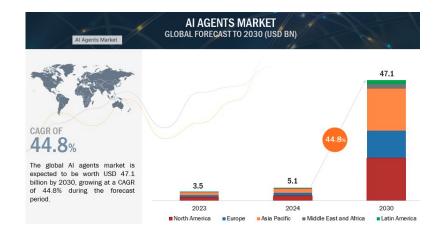
Implications of success of LLMs

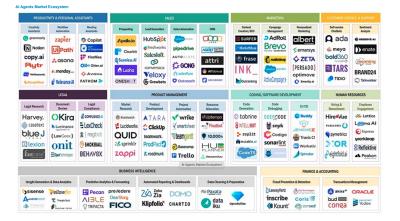
- many researchers change gears towards LLM
 - from computer vision (CV), speach, music, video, even reinforcement learning
- LLM is not only about NLP . . . humans have . . .
 - evolved to optimize natural language structures for eons
 - handed down knowledge using this natural languages for thousands of years
 - internal structure (or equivalently, representation) of natural languages optimized via thousands of generation by evolution
- LLM connects non-linguistic world (open system) via natural languages (closed system)



Multimodal AI (mmAI)

- mmAI systems processing & integrating data from multiple sources & modalities, to generate unified response / decision
- 1990s 2000s early systems initial research combining basic text & image data
- 2010s CNNs & RNNs enabling more sophisticated handling of multimodality
- 2020s modern multimodal models Transformer-based architectures handling complex multi-source data at highly advanced level
- mmAl *mimics human cognitive ability* to interpret and integrate information from various sources, leading to holistic decision-making





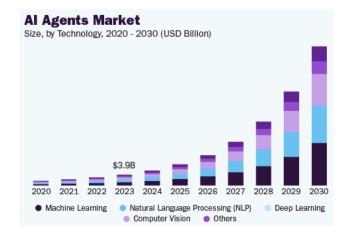
mmAI Technology

- core components
 - data preprocessing images, text, audio & video
 - architectures unified Transformer-based (e.g., ViT) & cross-attention mechanisms / hybrid architectures (e.g., CNNs + LLMs)
 - integration layers fusion methods for combining data representations from different modalities
- technical challenges
 - data alignment accurate alignment of multimodal data
 - computational demand high-resource requirements for training and inferencing
 - diverse data quality manage variations in data quality across modalities
- advancements
 - multimodal embeddings shared feature spaces interaction between modalities
 - self-supervised learning leverage unlabeled data to learn representations across modalities

Al agents powered by multimodal LLMs

- foundation
 - integrate multimodal AI capabilities for enhanced interaction & decision-making
- components
 - perceive environment through multiple modalities (visual, audio, text), process using LLM technology, generate contextual responses & take actions
- capabilities
 - understand complex environments, reason across modalities, engage in natural interactions, adapt behavior based on context & feedback

AI Agents				
Functional				
Code/Application generation	Customer	Support / Success Quality assurance		
Cogna: Lovable . txt . IGENT. AI a-gen orginal @ marblism & poolside O Mag		eople zowie ⋇мユ ay Xfini ≋PolyAI Myia LogicStar MaiHEM		
GTM		Security		
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Vertical				
Legal	Finance	Healthcare		
Leya Lega // Wordsmith	FINSTER AI (1) DECKMAT	CH Co:Helm Flinn 🤽 phare health		
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O Avantia	ClaimSorted Vivox AI	hema 🦰 🥂 Tandem		
Learning Avantia	ClaimSorted Vivox Al	hema Tandem		
Contraction Avantia	ClaimSorted Vivox Al	hema Tandem		



Al agents - Present & Future

- emerging applications
 - scientific research agents analyzing & running experiments & generating hypotheses
 - creative collaboration AI partners in design & art combining multiple mediums
 - environmental monitoring processing satellite sensor data for climate analysis
 - healthcare enhanced diagnostic combining imaging, e.g., MRI, with patient history
 - customer experience virtual assistants understanding spoken language & visual cues
 - autonomous vehicles integration of visual, radar & audio data
- future
 - ubiquitous AI agents seamless integration into everyday devices
 - highly tailored personalized experience in education, entertainment & healthcare



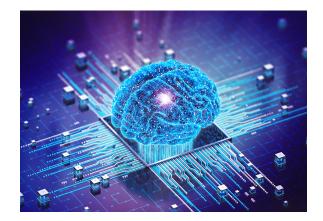


AI & Biotech

Al in biology

- Al has been used in biological sciences, and science in general
- Al's ability to process large amounts of raw, unstructured data (*e.g.*, DNA sequence data)
 - reduces time and cost to conduct experiments in biology
 - enables others types of experiments that previously were unattainable
 - contributes to broader field of engineering biology or biotechnology
- Al increases human ability to make direct changes at cellular level and create novel genetic material (*e.g.*, DNA and RNA) to obtain specific functions





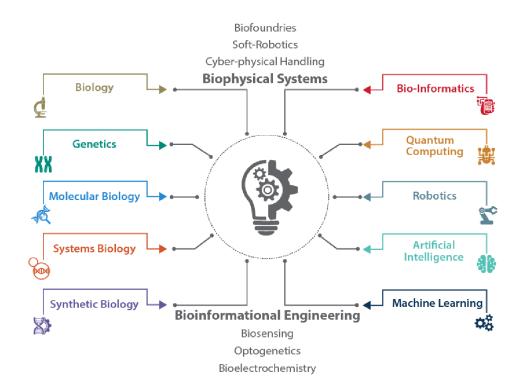
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Biotech

Biotech

- biotechnology
 - is multidisciplinary field leveraging broad set of sciences and technologies
 - relies on and builds upon advances in other fields such as nanotechnology & robotics, and, increasingly, AI
 - enables researchers to read and write DNA
 - sequencing technologies "read" DNA while gene synthesis technologies take sequence data and "write" DNA turning data into physical material
- 2018 National Defense Strategy & Senior US Defense and Intelligence Officials identified emerging technologies that could have disruptive impact on US national security [Say21]
 - AI, lethal autonomous weapons, hypersonic weapons, directed energy weapons, biotechnology, quantum technology
- other names for biotechnology are engineering biology, synthetic biology, biological science (when discussed in context of AI)

- sciences and technologies enabling biotechnology include (but not limited to)
 - (molecular) biology, genetics, systems biology, synthetic biology, bio-informatics, quantum computing, robotics [DFJ22]

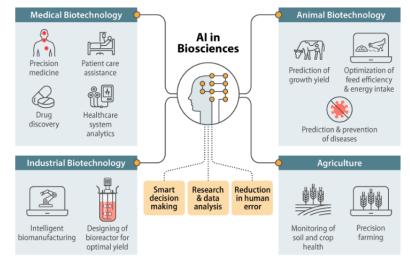


Convergence of AI and biological design

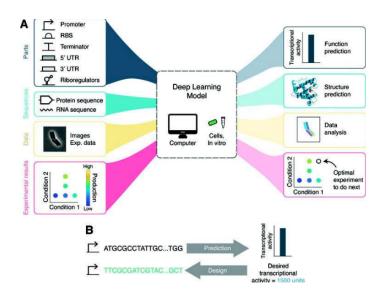
- AI & biological sciences converging [BKP22]
 - each building upon the other's capabilities for new research and development across multiple areas
- Demis Hassabis, CEO & cofounder of DeepMind, said of biology [Toe23]

". . . biology can be thought of as information processing system, albeit extraordinarily complex and dynamic one . . . just as mathematics turned out to be the right description language for physics, biology may turn out to be *the perfect type of regime for the application of Al!*"

- both AI & biotech rely on and build upon advances in other scientific disciplines and technology fields, such as nanotechnology, robotics, and increasingly big data (*e.g.*, genetic sequence data)
 - each of these fields itself convergence of multiple sciences and technologies
- so their impacts can combine to create new capabilities



Multi-source genetic sequence data



- Al, essential to analyzing exponential growth of genetic sequence data
 - "Al will be essential to fully understanding how genetic code interacts with biological processes" - US National Security Commission on Artificial Intelligence (NSCAI)
 - process huge amounts of biological data, *e.g.*, genetic sequence data, coming from different biological sources for understanding complex biological systems
 - sequence data, molecular structure data, image data, time-series, omics data
- *e.g.*, analyze genomic data sets to determine the genetic basis of particular trait and potentially uncover genetic markers linked with that trait

Quality & quantity of biological data

- limiting factor, however, is *quality and quantity* of biological data, *e.g.*, DNA sequences, that AI is trained on
 - e.g., accurate identification of particular species based on DNA requires reference sequences of sufficient quality to exist and be available
- databases have varying standards access, type, and quality of information
- design, management, quality standards, and data protocols for reference databases can affect utility of particular DNA sequence

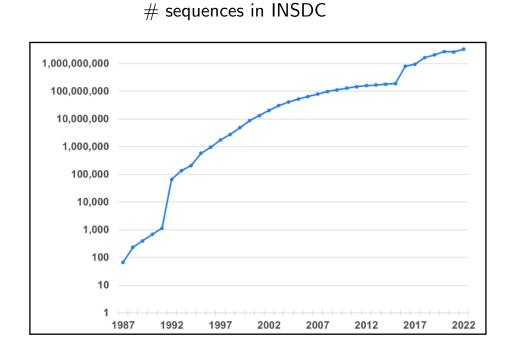


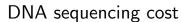


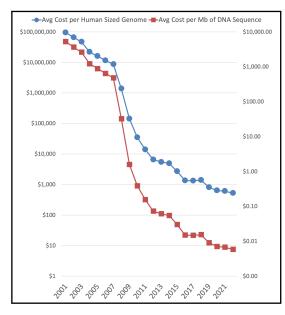
- volume of genetic sequence data grown exponentially as sequencing technology evolved
- more than 1,700 databases incorporating data on genomics, protein sequences, protein structures, plants, metabolic pathways, *etc.*, *e.g.*
 - open-source public database
 - Protein Data Bank, US-funded data center more than *terabyte of threedimensional structure data* for biological molecules, *e.g.*, proteins, DNA, RNA
 - proprietary database
 - Gingko Bioworks more than 2B protein sequences
 - public research groups
 - Broad Institute produces roughly 500 terabases of genomic data per month
- great potential value in aggregate volume of genetic datasets that can be collectively mined to discover and characterize relationships among genes

Volume and sequencing cost of DNA over time

- volume of DNA sequences & DNA sequencing cost
 - data source: National Human Genome Research Institute (NHGRI) [Wet23] & International Nucleotide Sequence Database Collaboration (INSDC)
- more dramatic than Moore's law!







- US National Security Commission on Artificial Intelligence (NSCAI) recommends
 - US fund and prioritize development of a biobank containing *"wide range of high-quality biological and genetic data sets securely accessible by researchers"*
 - establishment of database of broad range of human, animal, and plant genomes would
 - enhance and democratize biotechnology innovations
 - facilitate new levels of AI-enabled analysis of genetic data
- bias availability of genetic data & decisions about selection of genetic data can introduce bias, e.g.
 - training AI model on datasets emphasizing or omitting certain genetic traits can affect how information is used and types of applications developed - *potentially privileging or disadvantaging certain populations*
 - access to data and to AI models themselves may impact communities of differing socioeconomic status or other factors unequally

Emerging Trends in Biotech

AlphaFold

- solving 50-year-old protein folding problem, "one of biology's grand challenges"
 - definition given amino acid sequence, predict how it folds into a 3D structure
 - proteins fold in microseconds, but predicting computationally nearly impossible
- AlphaFold 1 (2018) DL + physics-based energy functions → AlphaFold 2 (2020)
 attention-based NN solving protein folding "in principle" → AlphaFold 3 (2024) diffusion-based DL, drug-protein interactions, protein complexes
- AlphaFold protein structure database
 - >200MM protein structures nearly every known protein, used by >2MM researchers
- Applications & implications
 - drug discovery target identification, lead optimization, side effect prediction
 - enzyme engineering, agriculture, environmental, vaccine development



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AlphaGo

- deep reinforcement learning with Monte Carlo tree search
 - trained on thousands of years of Go game history
 - AlphaGo Zero learns by playing against itself
- development experience, insight, knowledge, know-how transferred to AlphaFold



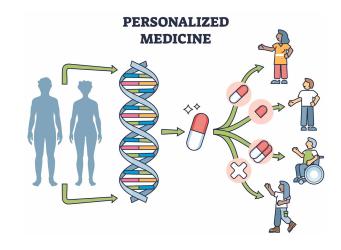




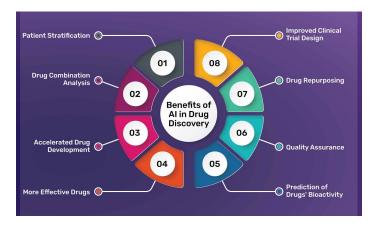
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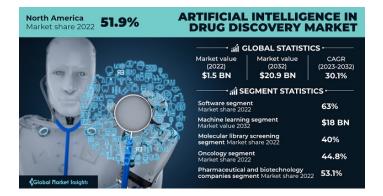
Personalized medicine

- shift from one-size-fits-all approach to tailored treatments
- based on individual genetic profiles, lifestyles & environments
- Al enables analysis of vast data to predict patient responses to treatments, thus enhancing efficacy and reducing adverse effects
- *e.g.*
 - custom cancer therapies
 - personalized treatment plans for rare diseases
 - precision pharmacogenomics
- companies Tempus, Foundation Medicine, *etc.*



Al-driven drug discovery



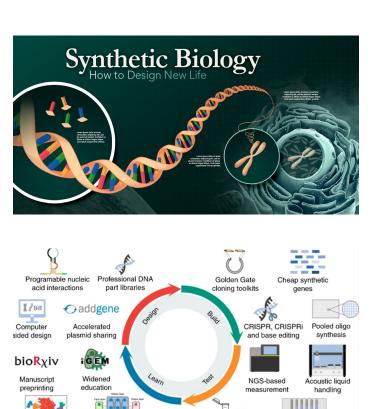


- traditional drug discovery process timeconsuming and costly often taking decades and billions of dollars
- Al streamlines this process by predicting the efficacy and safety of potential compounds with more speed and accuracy
- Al models analyze chemical databases to identify new drug candidates or repurpose existing drugs for new therapeutic uses
- companies Insilco Medicine, Atomwise.

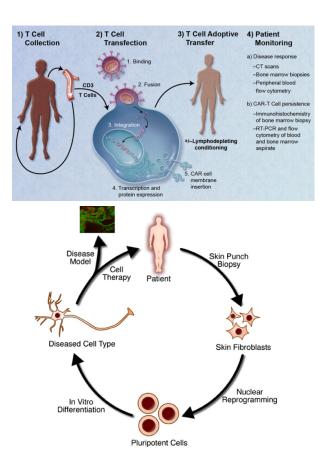
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Synthetic biology

- use AI for gene editing, biomaterial production and synthetic pathways
- combine principles of biology and engineering to design and construct new biological entities
- Al optimizes synthetic biology processes from designing genetic circuits to scaling up production
- company Ginkgo Bioworks uses AI to design custom microorganisms for applications ranging from pharmaceuticals to industrial chemicals



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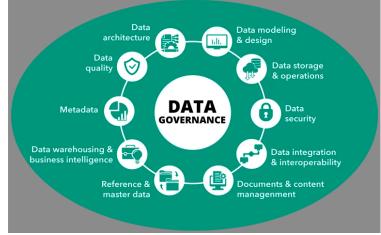


Regenerative medicine

- Al advances development of stem cell therapies & tissue engineering
- Al algorithms assist in identifying optimal cell types, predicting cell behavior & personalized treatments
- particularly for conditions such as neurodegenerative diseases, heart failure and orthopedic injuries
- company Organovo leverages AI to potentially improve the efficacy and scalability of regenerative therapies, developing next-generation treatments

Bio data integration

- integration of disparate data sources, including genomic, proteomic & clinical data - one of biggest challenges in biotech & healthcare
- AI delivers meaningful insights only when seamless data integration and interoperability realized
- developing platforms facilitating comprehensive, longitudinal patient data analysis - vital enablers of AI in biotech
- company Flatiron Health working on integrating diverse datasets to provide holistic view of patient health



- Atomwise small molecule drug discovery
- Cradle protein design
- Exscientia precision medicine
- Iktos small molecule drug discovery and design
- Insilico Medicine full-stack drug discovery system
- Schrödinger, Inc. use physics-based models to find best possible molecule
- Absci Corporation antibody design, creating new from scratch antibodies, *i.e.*, "de novo antibodies", and testing them in laboratories



Serendipities around Als

Serendipity or inevitability?

- What if Geoffrey Hinton had not been a persistent researcher?
- What if symbolists won AI race over connectionists?
- What if attention mechanism did not perform well?
- What if Transformer architecture did not perform super well?
- What if OpenAI had not been successful with ChatGPT in 2022?
- What if Jensen Huang had not been crazy about making hardware for professional gamers?
- Is it like Alexander Fleming's Penicillin?
- Or more like Inevitability?

Selected References & Sources

Selected references & sources

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Thank You