[Institut Pasteur AI Special Lecture]
Silicon Valley AI Innovation - Silicon Valley Insights on Technology Transfer from Semiconductor & E-Commerce to AI-Powered Biotech

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 $\sim$ 2020

- Principal Engineer @ Software R&D Center, DS Division, Samsung, Korea $\sim$ 2017

- Principal Engineer @ Strategic Marketing & Sales Team, Samsung, Korea $\sim$ 2016

- Principal Engineer @ DT Team, DRAM Development Lab, Samsung, Korea $\sim$ 2015

- Senior Engineer @ CAE Team, Samsung, Korea $\sim$ 2012

- PhD - Electrical Engineering @ Stanford University, CA, USA $\sim$ 2004

- Development Engineer @ Voyan, Santa Clara, CA, USA $\sim$ 2001

- MS - Electrical Engineering @ Stanford University, CA, USA $\sim$ 1999

- BS - Electrical & Computer Engineering @ Seoul National University   1994 $\sim$ 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 AIs - anomaly detection, deep RL, and recommender system

  – Bezos's project - drove *$200M* in additional sales 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.
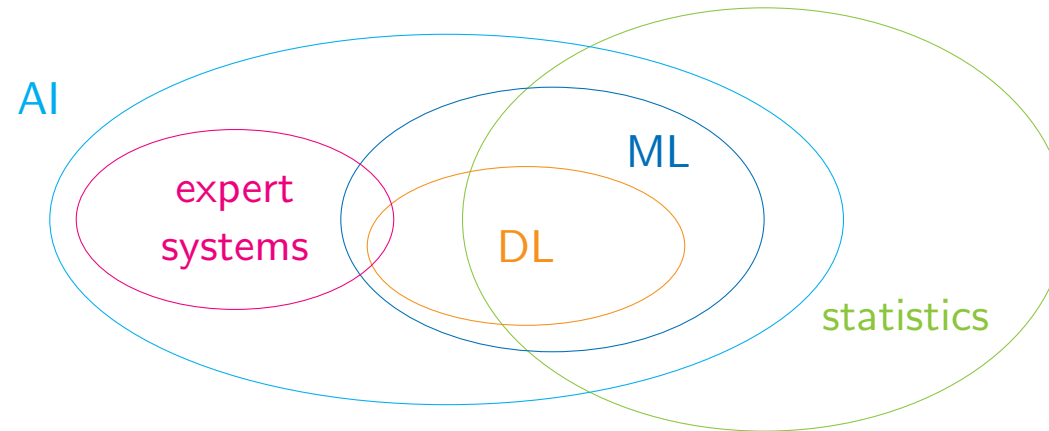
Today

Artificial Intelligence
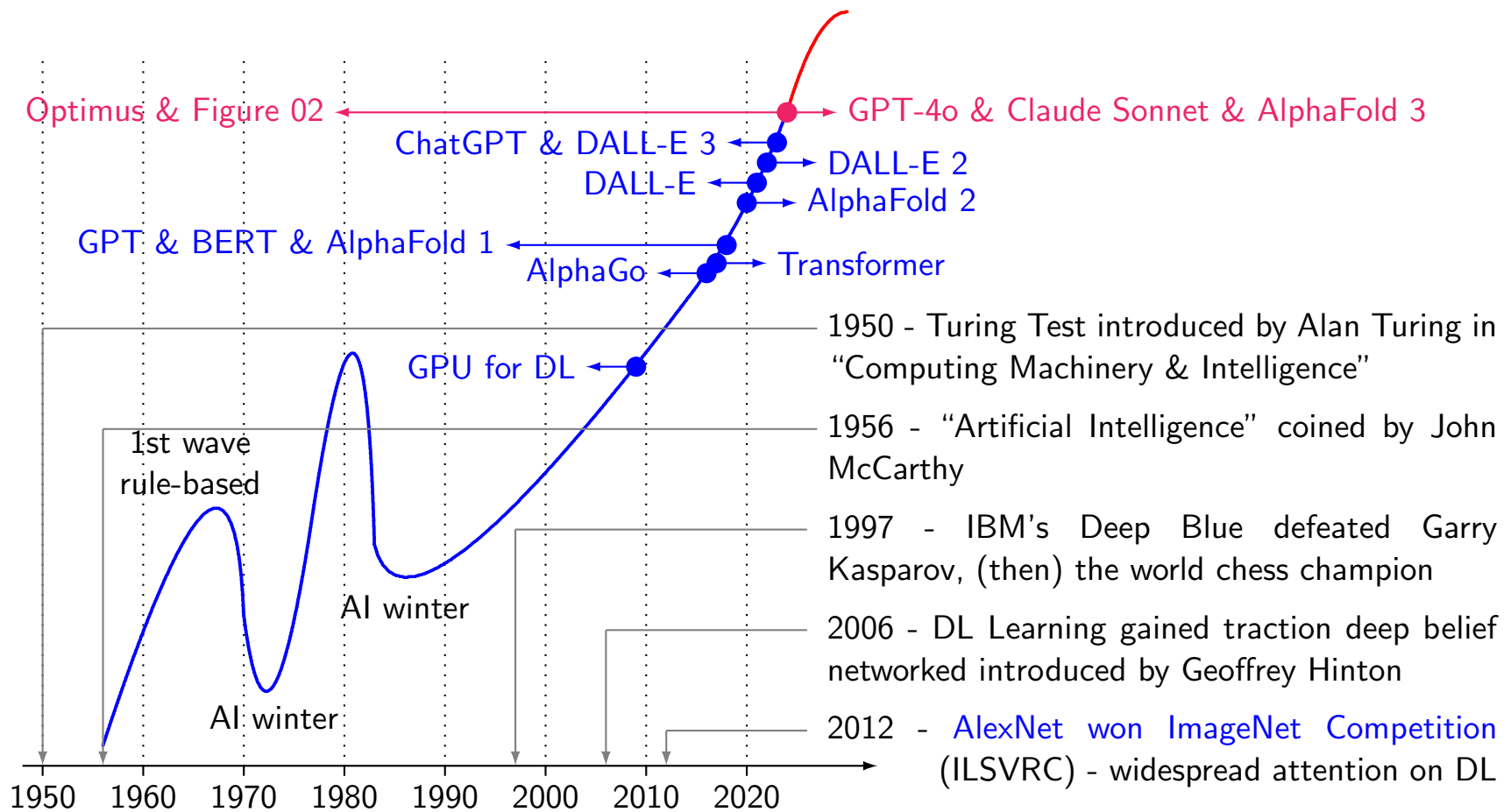
Definition and History

Definition & relation to other technologies

- AI

  - is technology doing tasks requiring human intelligence, such as learning, problem-solving, decision-making & language understanding

  - encompasses *range of technologies, methodologies, applications & products*

- AI, ML, DL, statistics & expert system[1] [HGH[+]22]

---

[1]ML: machine learning & DL: deep learning

History

Optimus & Figure 02 ←——————————————————→ GPT-4o & Claude Sonnet & AlphaFold 3

ChatGPT & DALL-E 3 ←

DALL-E → DALL-E 2

AlphaFold 2

GPT & BERT & AlphaFold 1 ←

AlphaGo ← Transformer

1st wave
rule-based

GPU for DL ←

AI winter

AI winter

1950 - Turing Test introduced by Alan Turing in "Computing Machinery & Intelligence"

1956 - "Artificial Intelligence" coined by John McCarthy

1997 - IBM's Deep Blue defeated Garry Kasparov, (then) the world chess champion

2006 - DL Learning gained traction deep belief networked introduced by Geoffrey Hinton

2012 - AlexNet won ImageNet Competition (ILSVRC) - widespread attention on DL

1950 1960 1970 1980 1990 2000 2010 2020

Birth of AI - early foundations & precursor technologies

- 1950s ~ 1970s

  - Alan Turing - concept of *"thinking machine" & Turing test* to evaluate machine intelligence (1950s)

  - *symbolists* (as opposed to connectionists) - early AI focused on symbolic reasoning, logic & problem-solving - Dartmouth Conference in 1956 by *John McCarthy, Marvin Minsky, Allen Newell & Herbert A. Simon*

  - precursor technologies - genetic algorithms (GAs), Markov chains & *hidden Markov models (HMMs)* - laying foundation for generative processes (1970s ~)
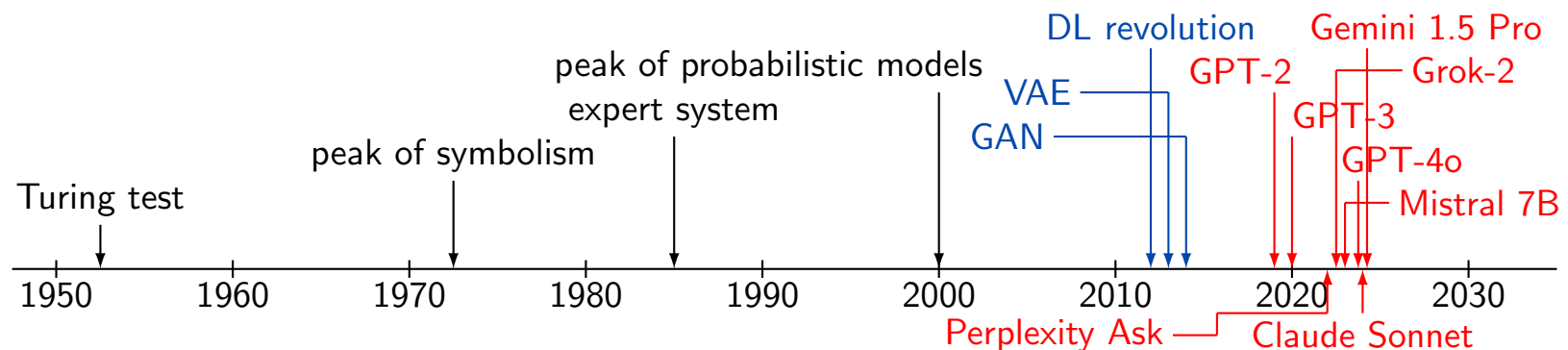
Rule-based systems & probabilistic models

- 1980s ∼ early 2000s

  - *expert systems* (1980s) - AI systems designed to mimic human decision-making in specific domains

  - development of neural networks (NN) w/ backpropagation *training multi-layered networks* - setting stage for way more complex generative models

  - *probabilistic models* (including network models, *i.e.*, Bayesian networks) & Markov models - laying groundwork for data generation & pattern prediction
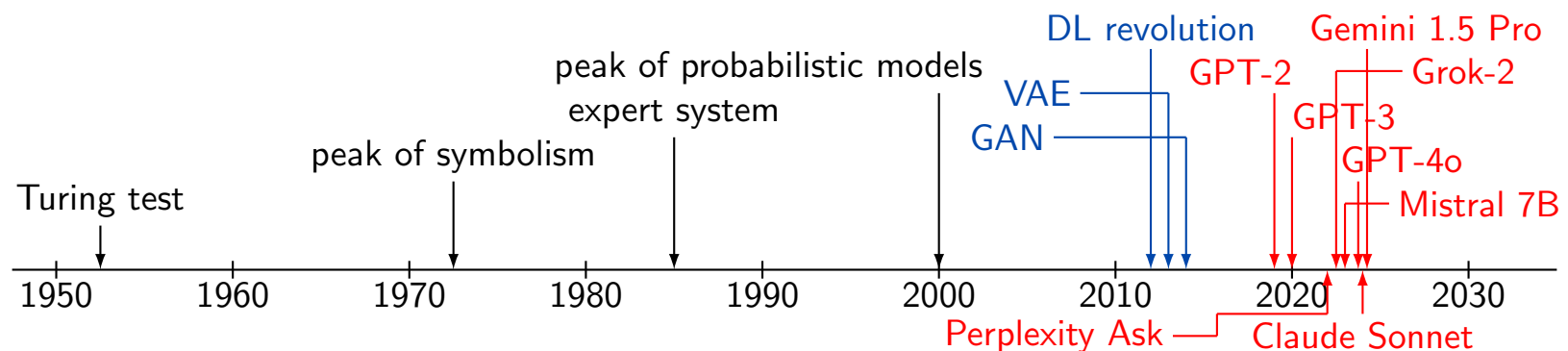
Rise of deep learning & generative models

- 2010s - breakthrough in genAI
  - *deep learning (DL) revolution* - advances in GPU computing and data availability led to the rapid development of deep neural networks.
  - *variational autoencoder (VAE)* (2013) - by Kingma and Welling - learns mappings between input and latent spaces
  - *generative adversarial network (GAN)* (2014) - by Ian Goodfellow - game-changer in generative modeling where two NNs compete each other to create realistic data
    - widely used in image generation & creative tasks
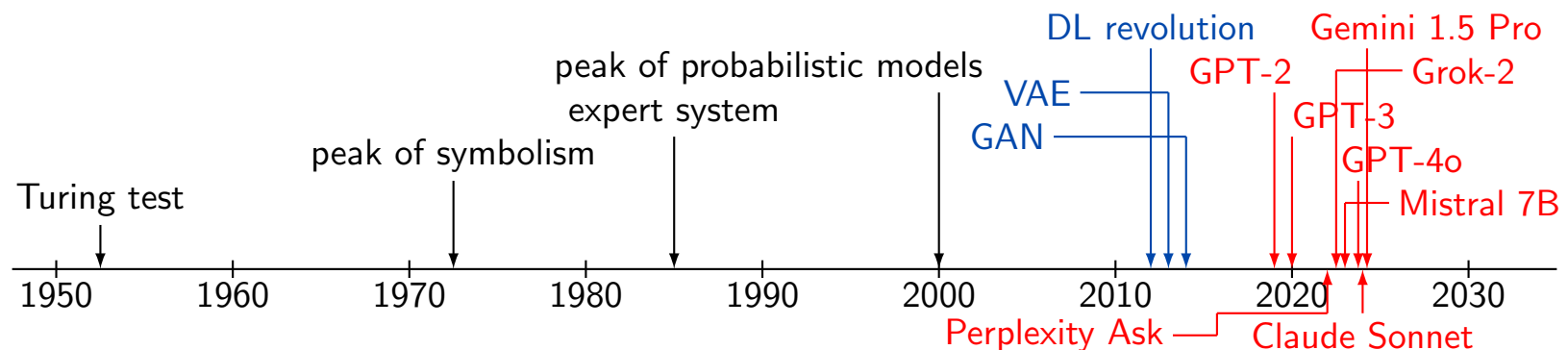
Transformer models & multimodal AI

- late 2010s $\sim$ Present
  - Transformer architecture (2017) - by Vaswani et al.
    - *revolutionized NLP, e.g.*, LLM & various genAI models
  - GPT series - generative pre-trained transformer
    - GPT-2 (2019) - generating human-like texts - *marking leap in language models*
    - GPT-3 (2020) - 175B params - set *new standards for LLM*
  - multimodal systems - DALL-E & CLIP (2021) - *linking text and visual data*
  - emergence of diffusion models (2020s) - new approach for generating high-quality images - progressively "denoising" random noise (DALL-E 2 & Stable Diffusion)
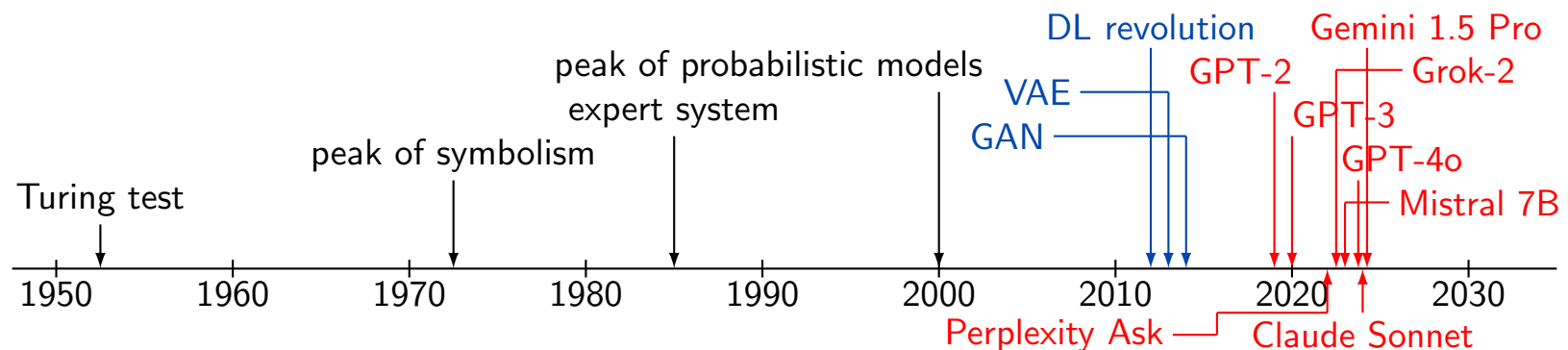
Significant AI Achievements - 2014 – 2025

Deep learning revolution

- 2012 – 2015 - DL revolution[2]
  - 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 - AI's potential in solving complex & strategic problems

---

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

Transformer changes everything

- 2017 – 2018 - Transformers & NLP breakthroughs[3]
  - *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

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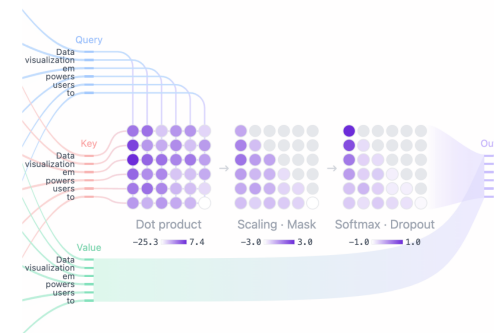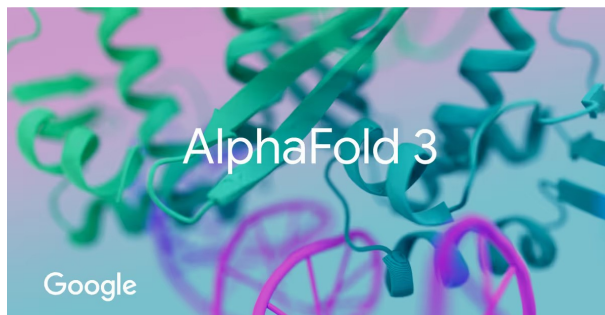
[3]NLP: natural language processing, GPT: generative pre-trained transformer

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*
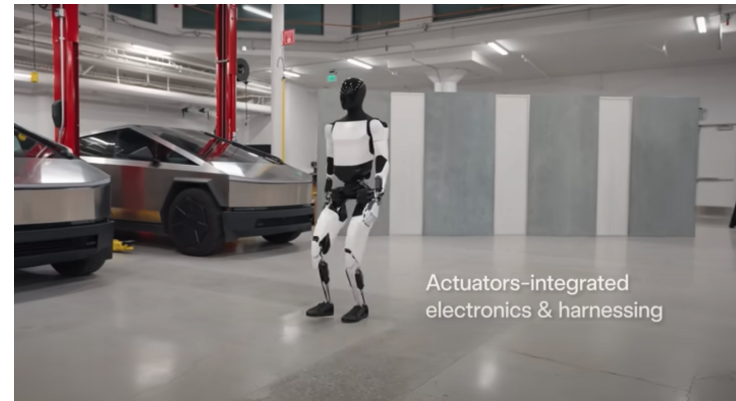
Major AI Breakthroughs in 2025

- 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
- AI-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
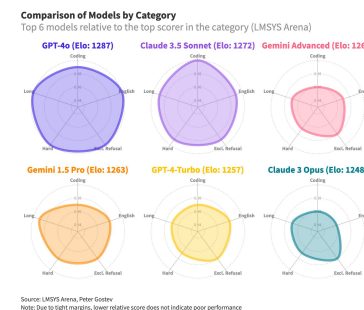
## Transformative impact of AI - reshaping industries, work & society

- accelerating human-AI collaboration
  - not only reshaping industries but *altering how humans interact with technology*
  - AI's role as collaborator and augmentor redefines productivity, creativity, the way we address global challenges, $e.g.$, *sustainability & healthcare*
- AI-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*
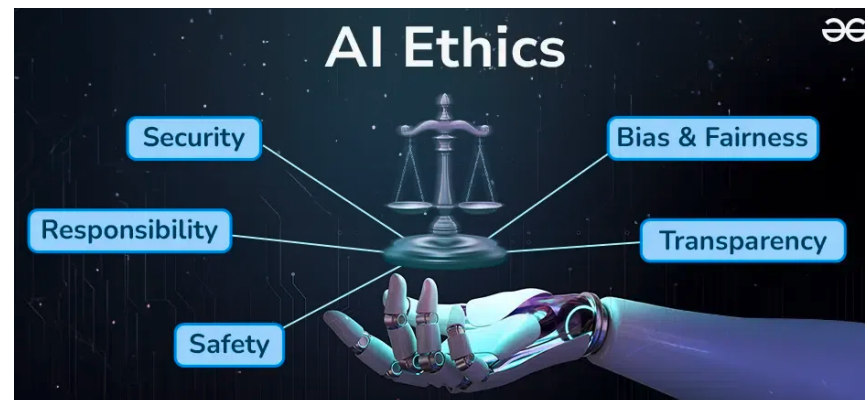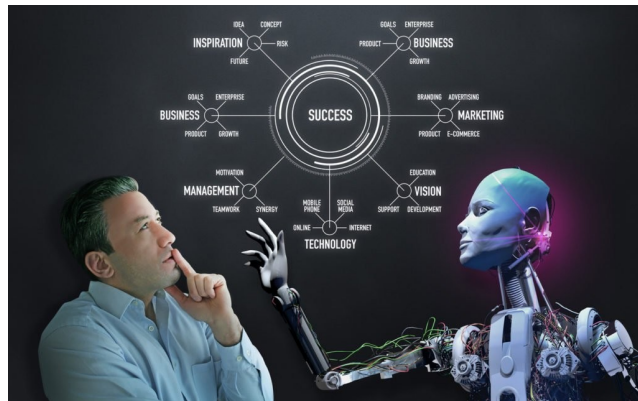
Measuring AI's Ascent

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

% US technology adoption
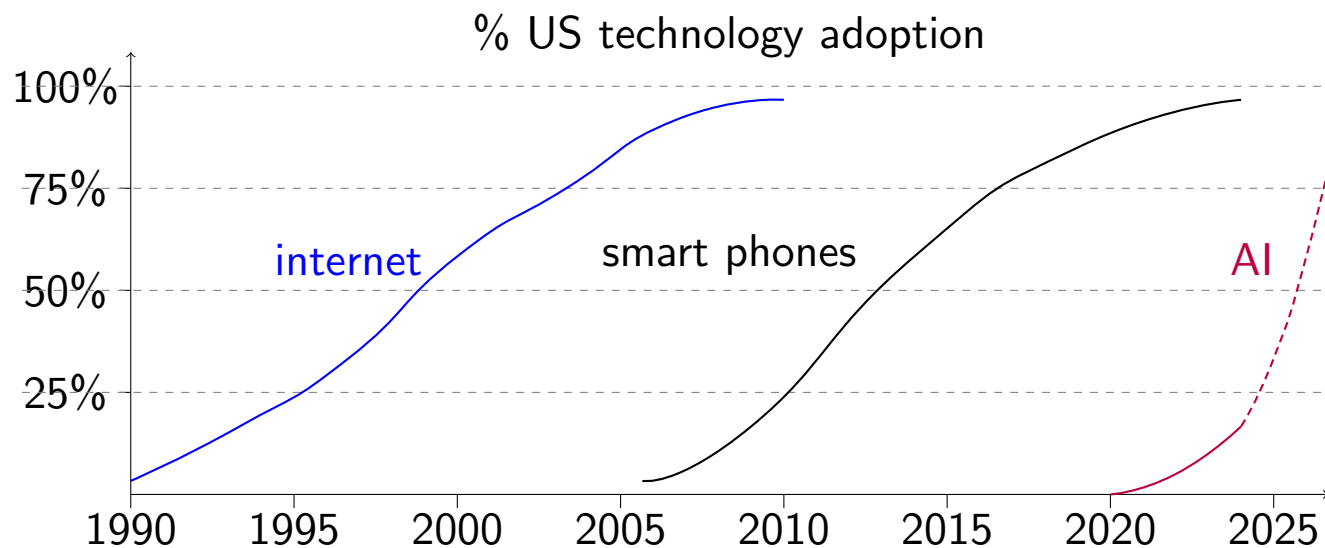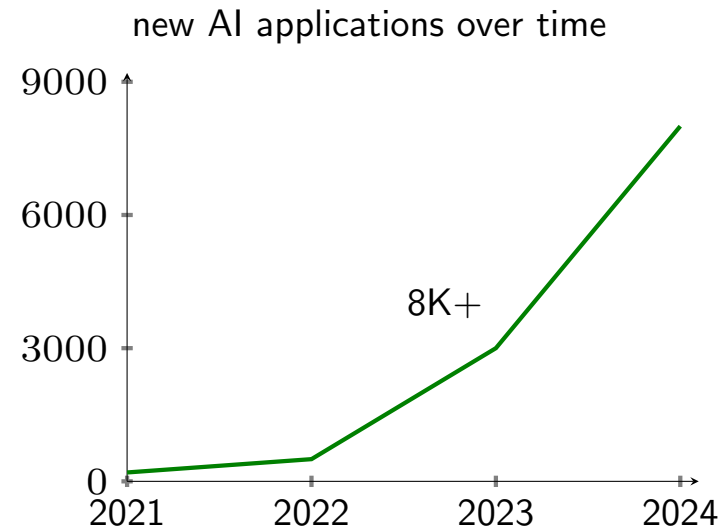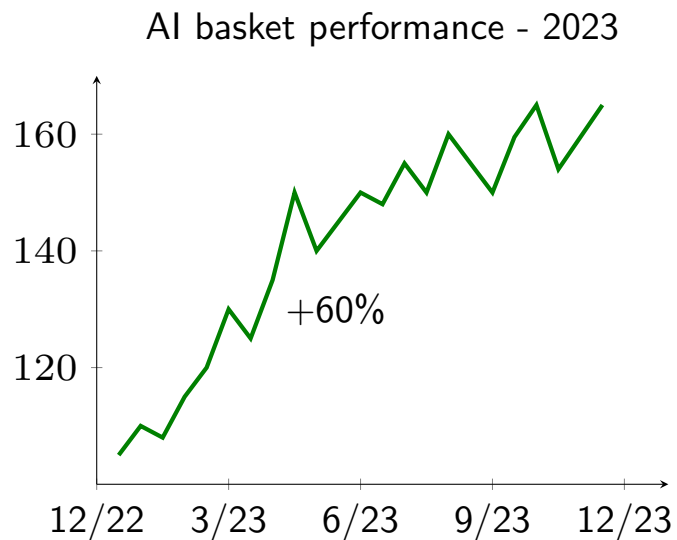
Explosion of AI ecosystems - ChatGPT & NVIDIA

- 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 year[4]

ChatGPT weekly unique visits

NVDA 2023-2Q earning
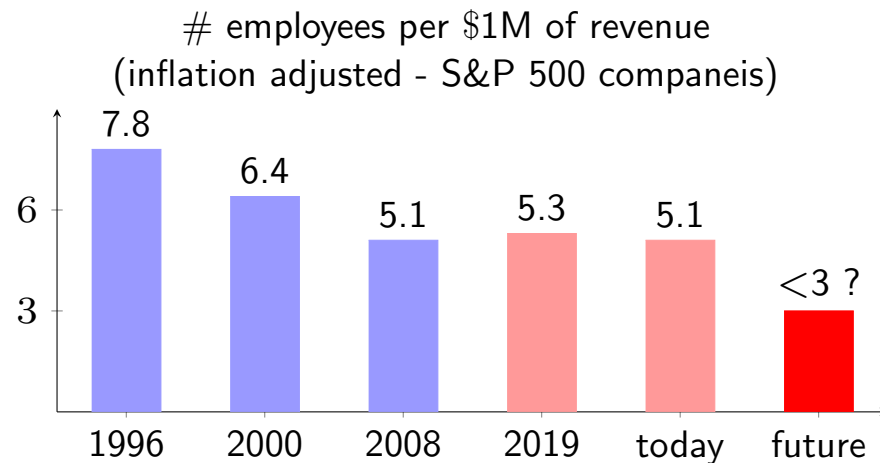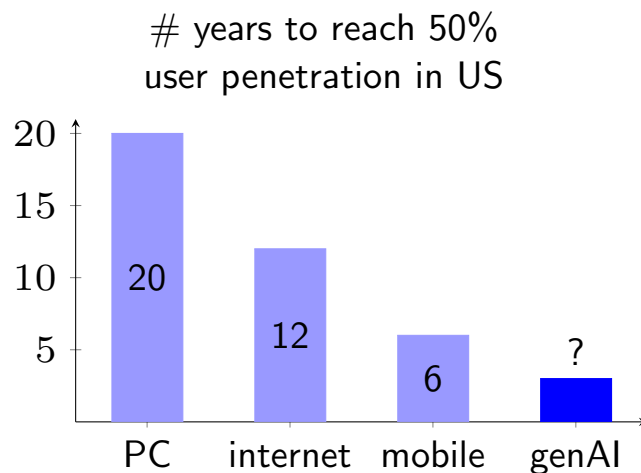
---
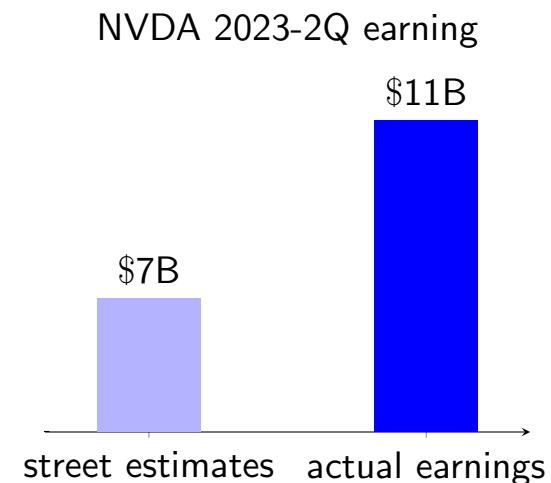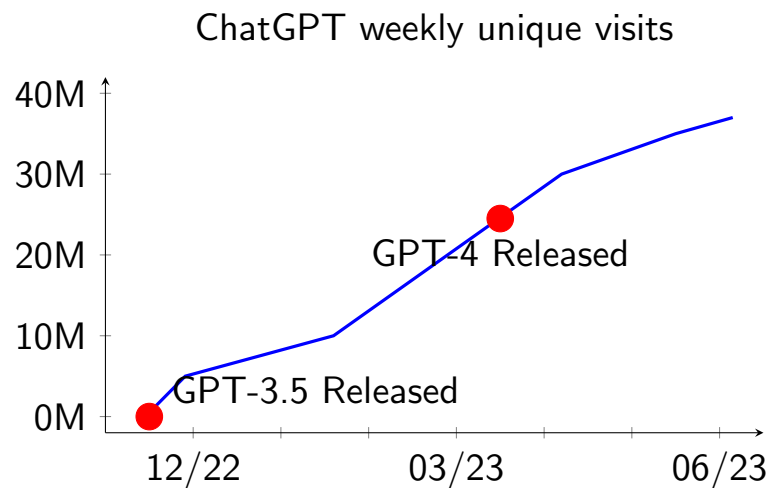
[4]source - Bloomberg

Explosion of AI ecosystems - AI stock market

- *AI investment surge in 2023 - portfolio performance soars by 60%*

    – AI-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

AI basket performance - 2023

new AI applications over time

+60%

8K+

12/22   3/23   6/23   9/23   12/23

2021   2022   2023   2024

AI'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
- AI'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

years to reach 50% user penetration in US

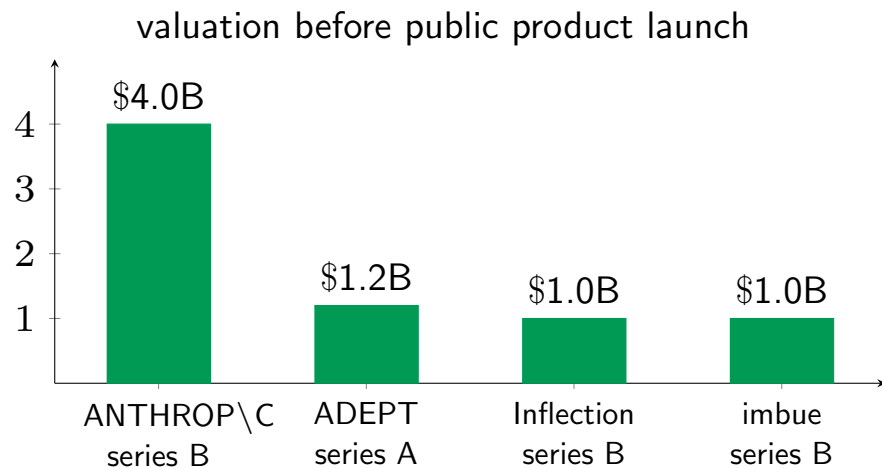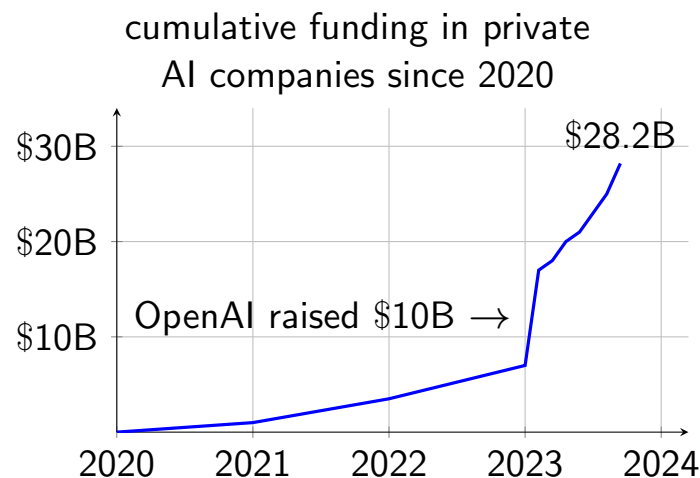# employees per $1M of revenue (inflation adjusted - S&P 500 companeis)

AI 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
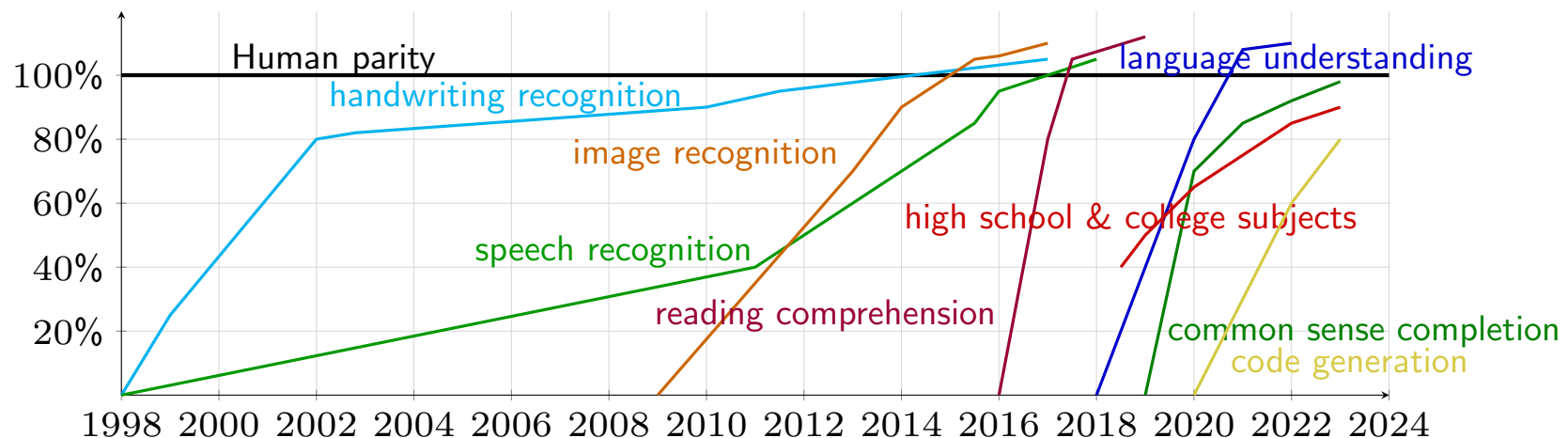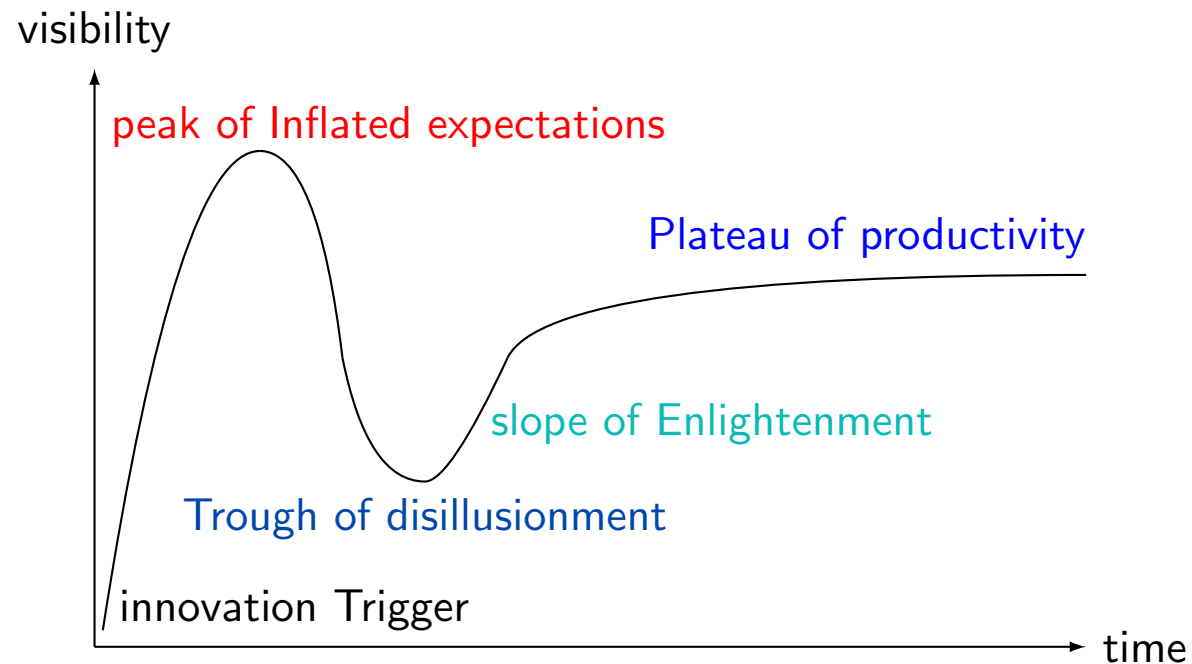
Massive investment in AI

- *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

cumulative funding in private
AI companies since 2020

$30B

$20B

OpenAI raised $10B →

$10B

$28.2B

2020   2021   2022   2023   2024

valuation before public product launch

$4.0B

4

3

2

$1.2B

$1.0B

$1.0B

1

ANTHROP\C   ADEPT   Inflection   imbue
series B   series A   series B   series B

Is AI hype?

Technology hype cycle

visibility

peak of Inflated expectations

Plateau of productivity

slope of Enlightenment

Trough of disillusionment

innovation Trigger

time

- 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

[Institut Pasteur AI Special Lecture] Silicon Valley AI Innovation - Artificial Intelligence - Is AI hype?

27

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

Yes & No

| characteristics of hype cycles	speaker's views
value accrual misaligned with investment	• OpenAI still operating at a loss; business model *still* not clear • gradual value creation across broad range of industries and technologies (*e.g.*, CV, LLMs, RL) unlike fiber optic bubble in 1990s
overestimating timeline & capabilities of technology	• 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
lack of widespread utility due to technology maturity	• AI already providing significant utility across various domains • vs quantum computing remains promising in theory but lacks widespread practical utility

AI Agents

AI progress in 21st century in keywords

- 2010 ∼ Big Data

- 2012 ∼ Deep Learning

- 2017 ∼ Transformer - Attention is All you need!

- 2022 ∼ LLM & genAI

- 2024 ∼ AI Agent (Agentic AI)
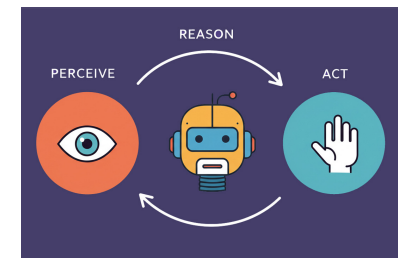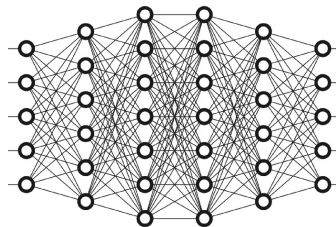
Multimodal learning

- 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)
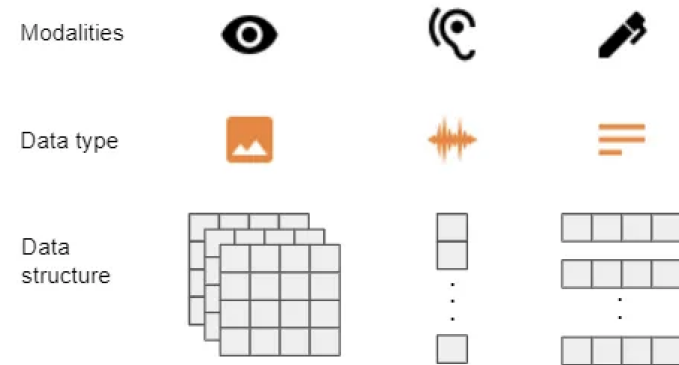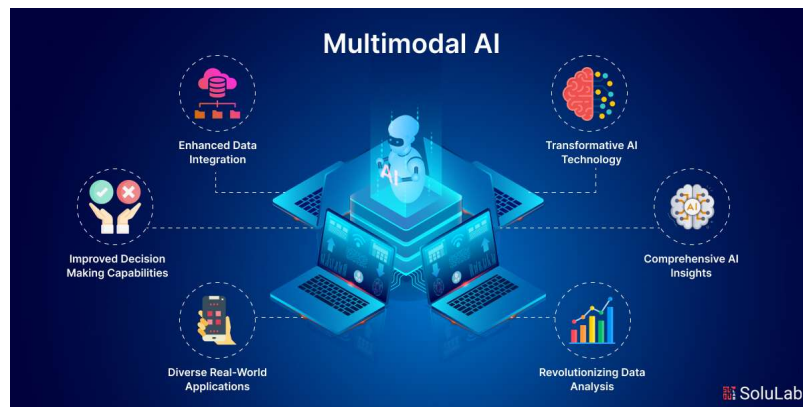
Implications of success of LLMs

- many researchers change gears towards LLM
  - from computer vision (CV), speech, 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)*
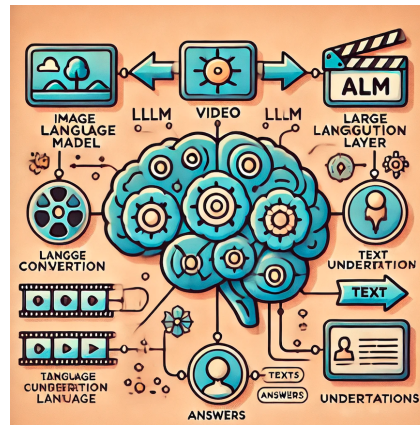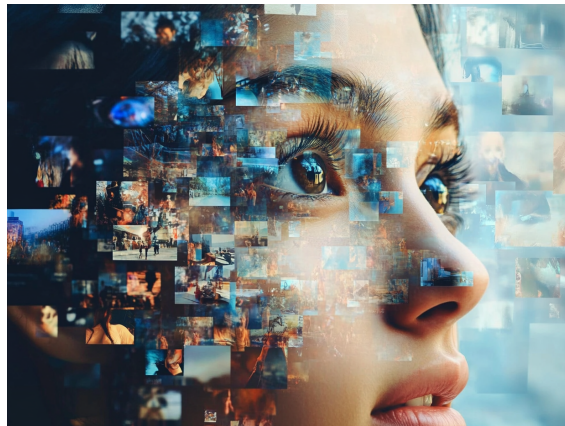
Multimodal AI (mmAI)

- 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
- mmAI *mimics human cognitive ability* to interpret and integrate information from various sources, leading to holistic decision-making
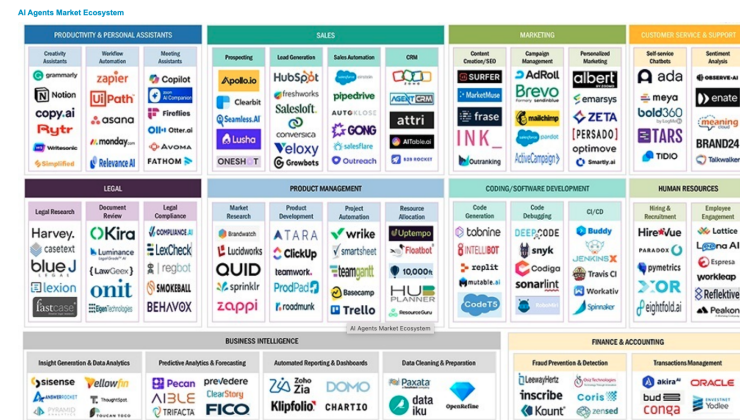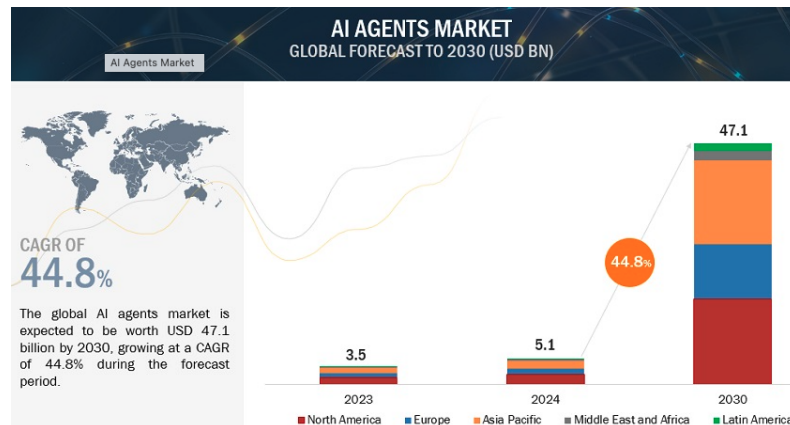
mmAI Technology

- 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

AI 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
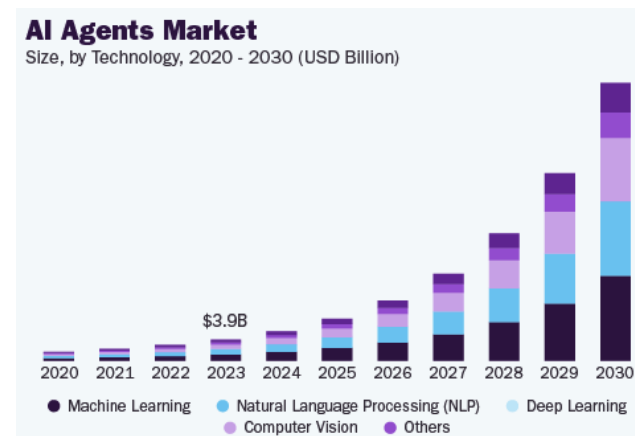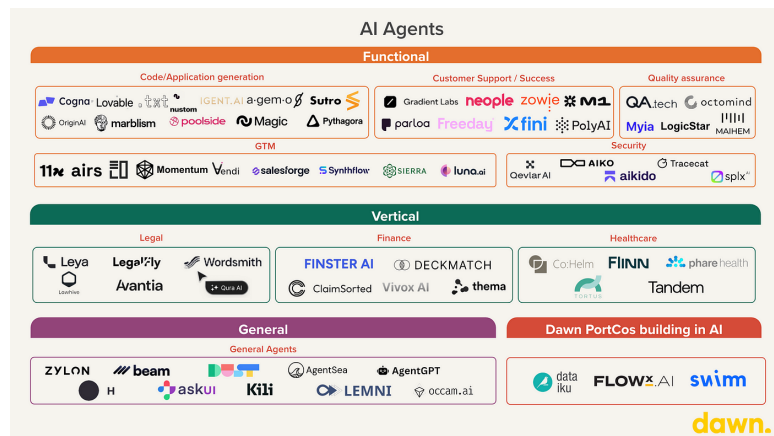
AI agents - Present & Future

- 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

AI in biology

- AI has been used in biological sciences, and science in general
- AI'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
- AI increases human ability to make direct changes at cellular level and create novel genetic material ($e.g.$, DNA and RNA) to obtain specific functions
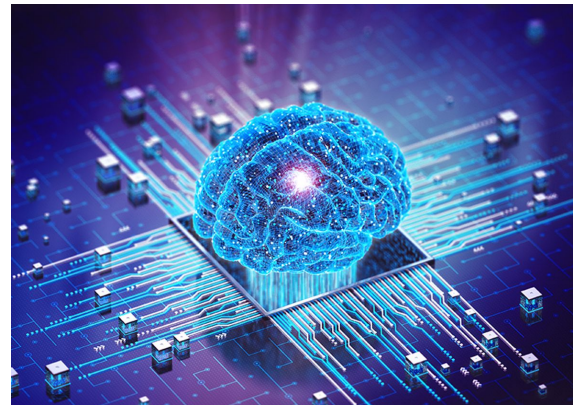
Biotech

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)

Biotech - multidisciplinary field

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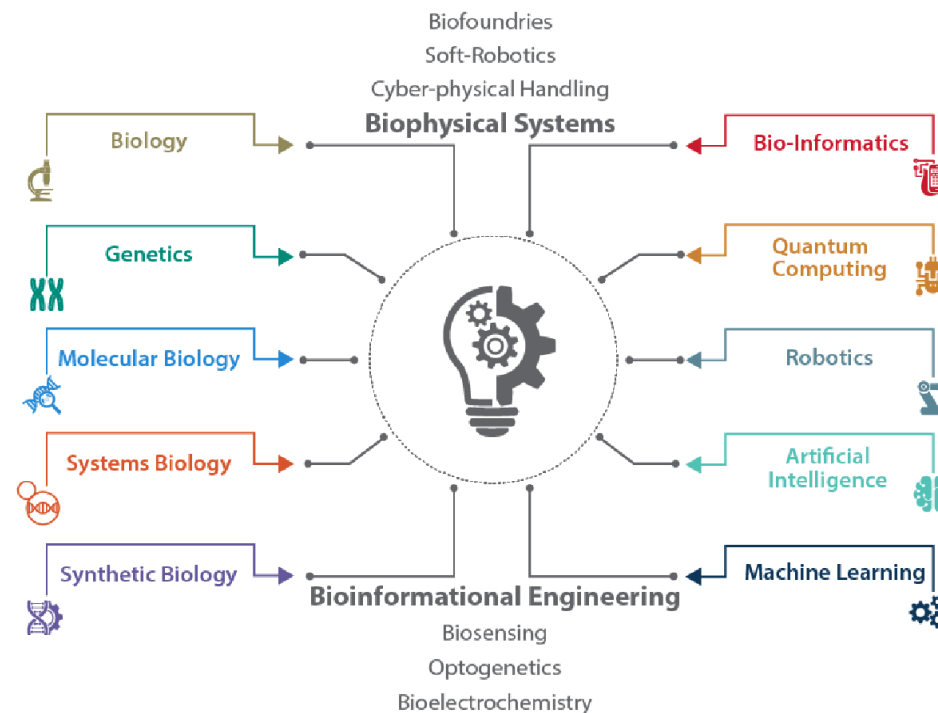
Convergence of AI and biological design

- 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 AI!*"

- 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*
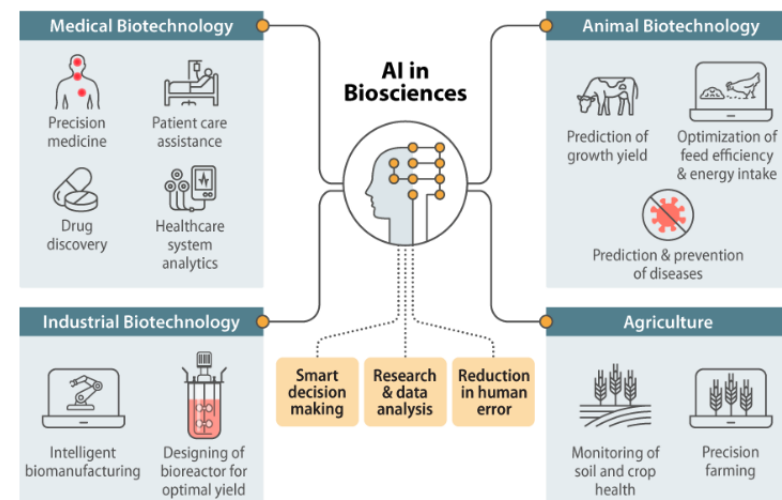
Multi-source genetic sequence data
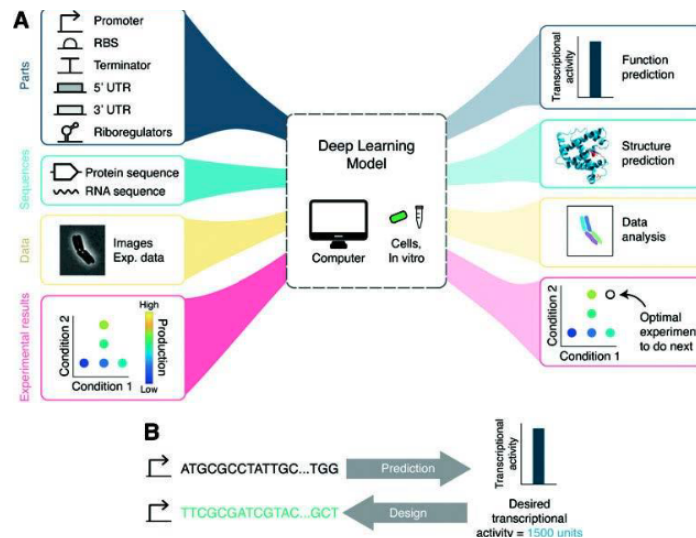
- AI, essential to analyzing exponential growth of genetic sequence data

  "AI 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
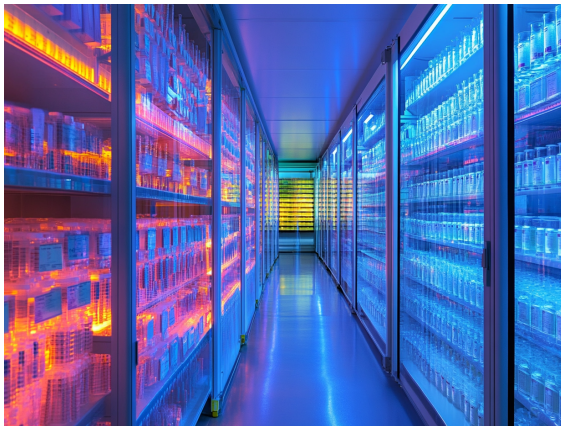
Rapid growth of biological data

- 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 three-dimensional 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
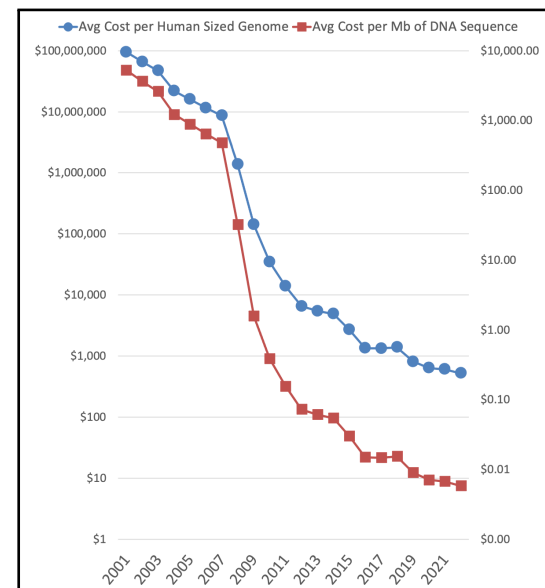
Volume and sequencing cost of DNA over time

- 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!*

sequences in INSDC
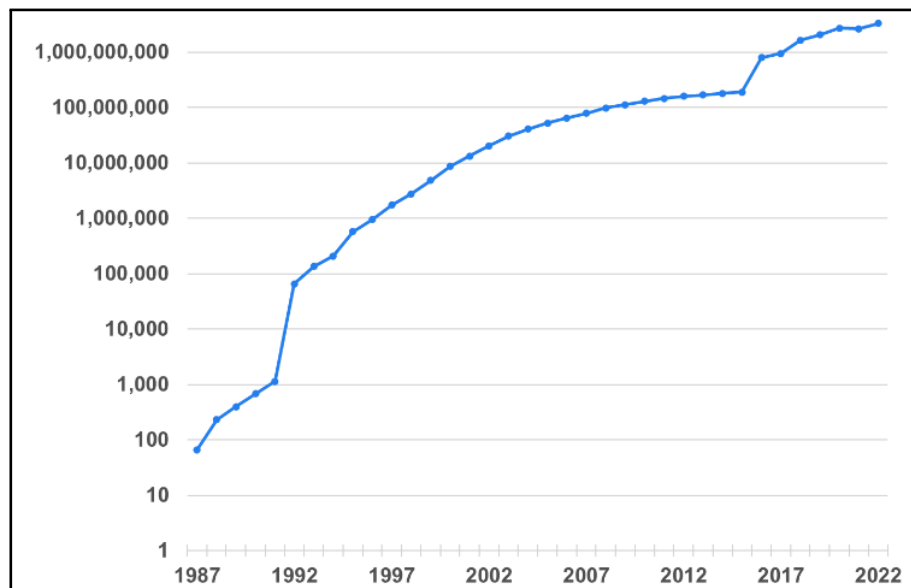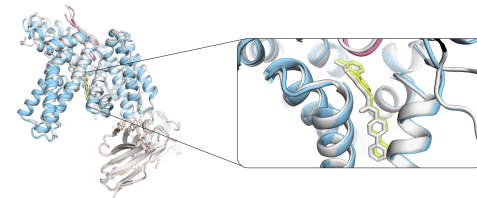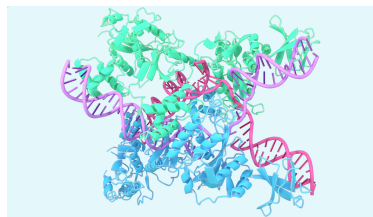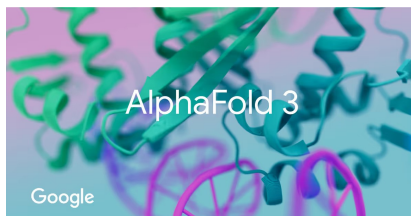

DNA sequencing cost

Bio data availability and bias

- 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 $\rightarrow$ AlphaFold 2 (2020) - attention-based NN solving protein folding "in principle" $\rightarrow$ 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

AlphaGo

- Go board marked with 19×19 grid - $(19 \times 19)! = 361! \approx 1.44 \times 10^{768}$

  1437923258884890654832362511499863354754907538644755876127282765299227795534389618856841908003141196
  0714137944348905859683839682333043216077138088370565578796691924861827097800358990211005794501073330
  5079262777172275041226808677528136885057526541812043502150623466302643442673632627092764643302557772
  2695595343233942204301825548143785112222186834487969871267194205609533306413935710635197200721473378
  7338269803085351043174203653673779887217565513450041291061650506154496265581102824241428406627054585
  5623101563752892899924857388316647687165212001536218913733713768261861456295440900774337589490771443
  9917299937133680728459000034496420337066440853337001284286412654394495050773954560000000000000000000
  000000000000000000000000000000000000000000000000000000000000000000000000

- 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

Personalized medicine

- *shift from one-size-fits-all approach to tailored treatments*

- based on individual genetic profiles, lifestyles & environments

- AI 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.*
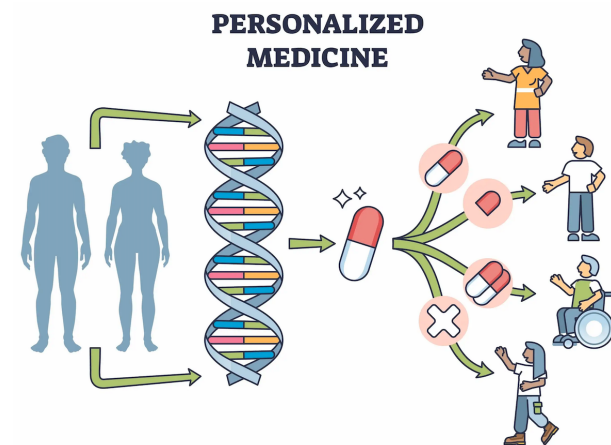
# AI-driven drug discovery
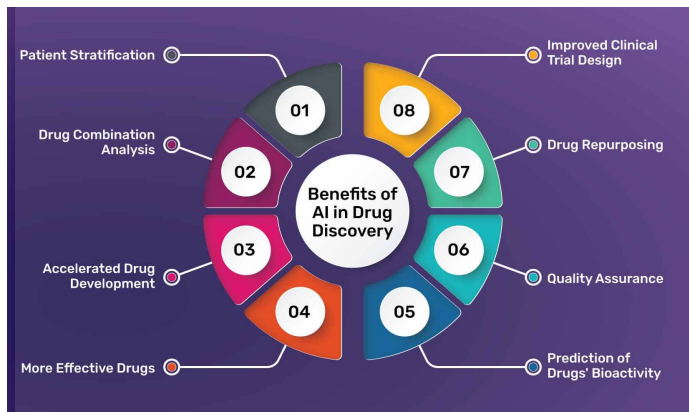
- traditional drug discovery process - time-consuming and costly often taking decades and billions of dollars

- AI streamlines this process by predicting the efficacy and safety of potential compounds with more speed and accuracy

- AI models analyze chemical databases to identify new drug candidates or repurpose existing drugs for new therapeutic uses

- companies - Insilco Medicine, Atomwise.
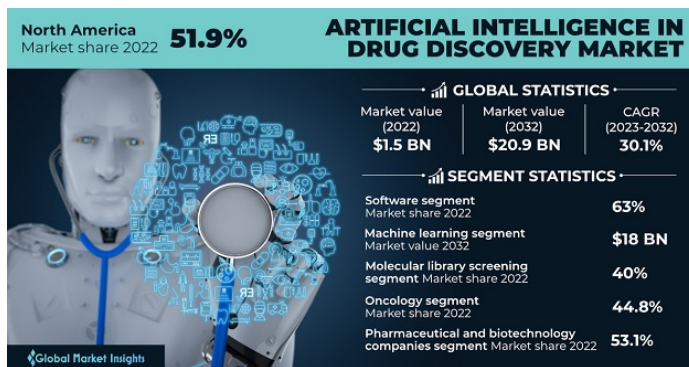
Synthetic biology

- use AI for gene editing, biomaterial production and synthetic pathways

- combine principles of biology and engineering to design and construct new biological entities

- AI 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
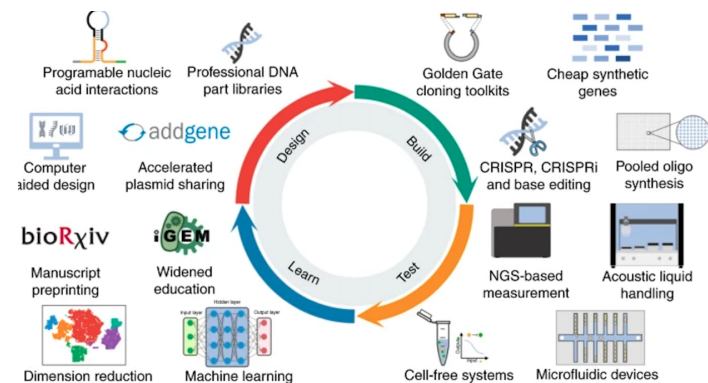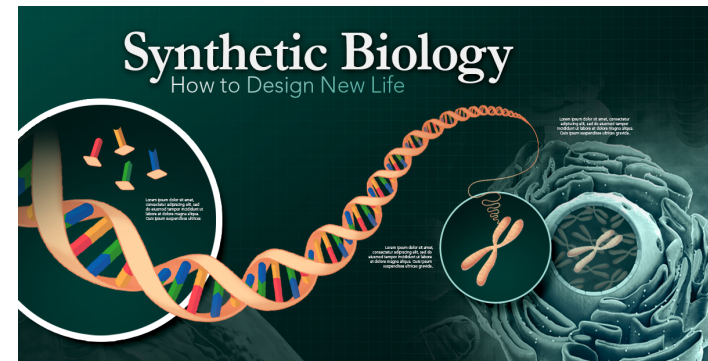
Regenerative medicine
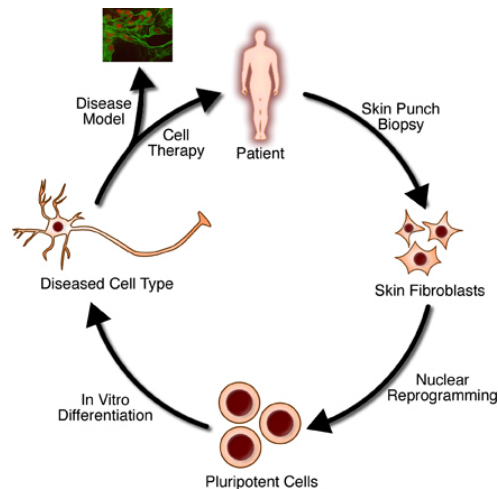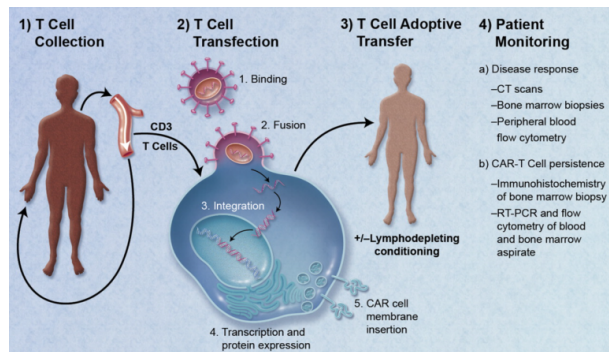
- AI advances development of stem cell therapies & tissue engineering

- AI 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
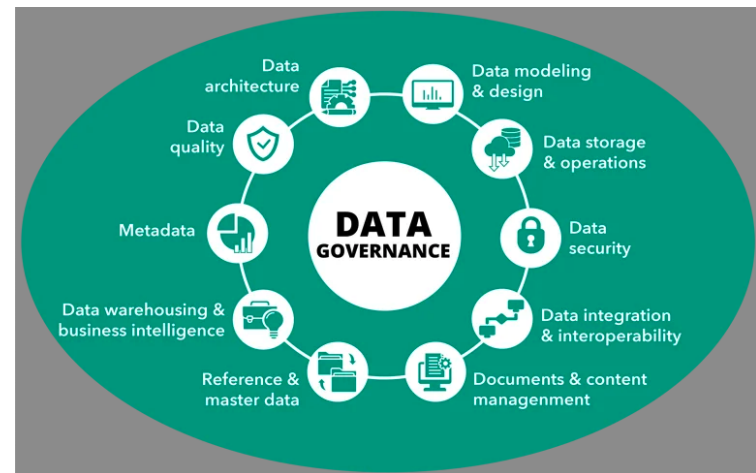
Biotech companies

- 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
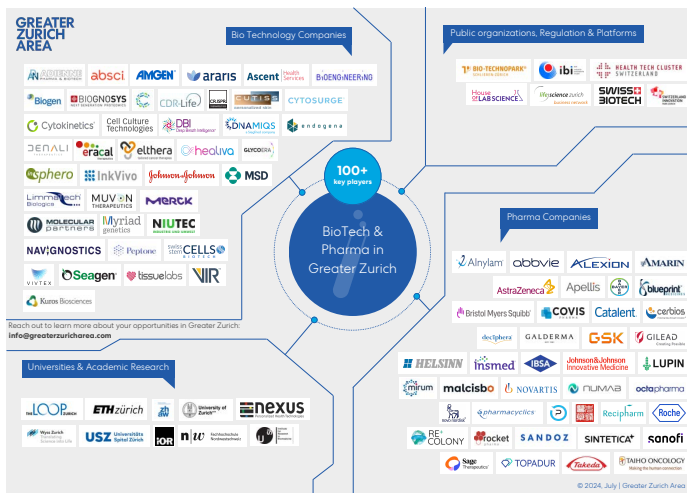
Industrial AI

Industrial AI (inAI)

- inAI (collectively) refers to AI technology & software and their products developed for
  - *customer values creation, productivity improvement, cost reduction, production optimization, predictive analysis, insight discovery*

  in industries such as
  - *semiconductor, steel, oil & gas, cement, and other various manufacturing industries*

  (unlike general AI, which is frontier research discipline striving to achieve human-level intelligence)

inAI fields

- product
  - product design & innovation, adaptability & advancement, product quality & validation, design for reusability & recyclability, performance optimization

- production process

  - *production quality,* process management, inter-process relations, process routing & scheduling, process design & innovation, *traceability, predictive process control*

- machinery & equipment

  - *predictive maintenance, monitoring & diagnosis,* component development, *ramp-up optimization,* material consumption prediction

- supply chain

  - supply chain monitoring, material requirements planning, customer management, supplier management, logistics, reusability & recyclability
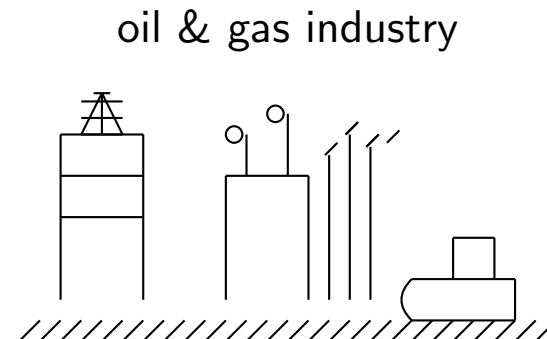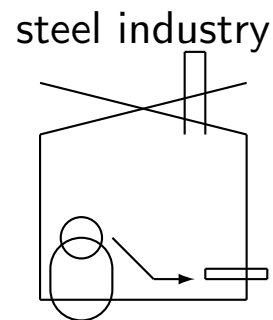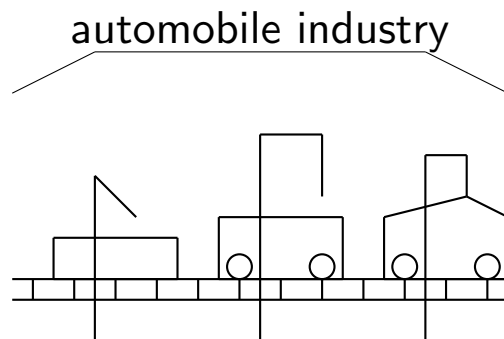
Characteristics of inAI

Vicious (or virtuous) cycle

- integration of inAI with customers' business creates monetary values and encourages data-driven decisions

- however, to do so, digital transformation with data-readiness is MUST-have

- created values, in turn, can be invested into infrastructure required for digital transformation and success of inAI!
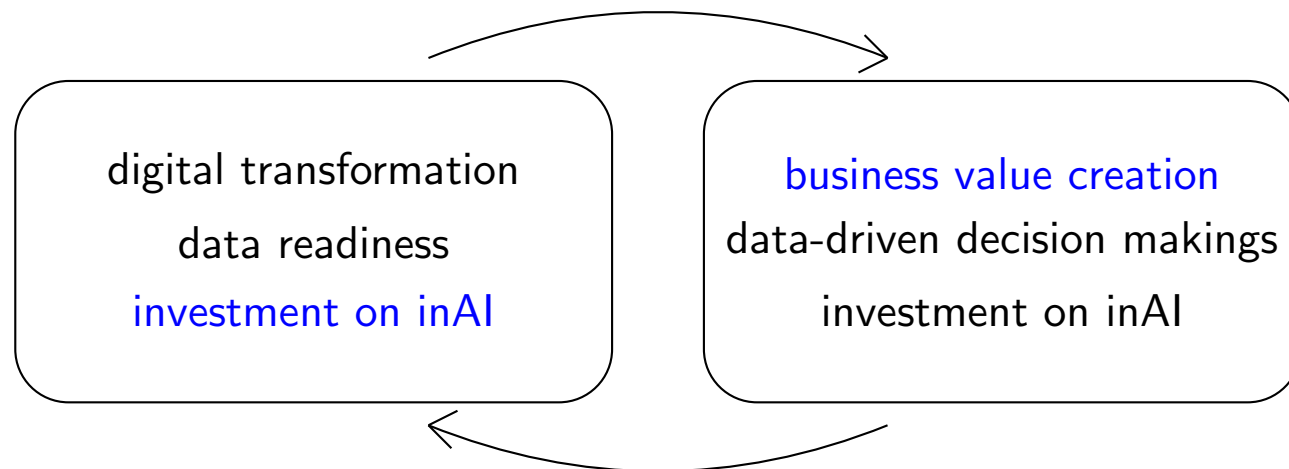
Data-centric AI

- unlike many ML disciplines where foundation models do generic representation learning, $i.e.$, learn universal features

- each equipment has (gradually) different data characteristics, hence need data-centric AI

    ". . . need 1,000 models for 1,000 problems" - Andrew Ng

    – data-centric AI - discipline of systematically engineering the data used to build AI system

# Challenging data characteristics

- huge volume

- data multi-modality

- high velocity requirement

- very fat data

- sever data shift & drift (in many cases)

- label imbalance

- data quality

Manufacturing AI

MLs in manufacturing AI (manAI)

- *image data* - huge amount of image data measured and inspected
  - SEM/TEM images, wafer defect maps, test failure pattern maps [5]
  $\rightarrow$ semantic segmentation, defect inspection, anomaly detection

- *time-series (TS) data* - *all the data* coming out of manufacturing is TS
  - equipment sensor data, process times, various measurements, MES data [6]
  $\rightarrow$ regression, anomaly detection, semi-supervised learning, Bayesian inference
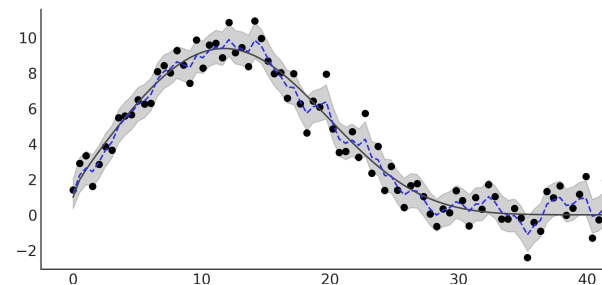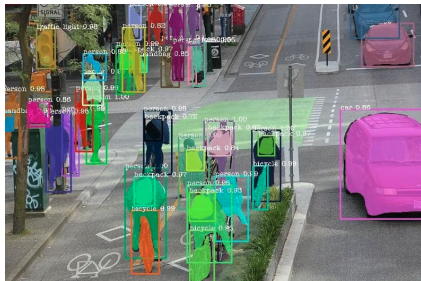
[5]SEM: scanning electron miscroscope, TEM: transmission electron miscroscope
[6]MES: manufacturing execution system

CV ML in manAI

Computer vision ML in manAI

- measurement and inspection (MI)

  – metrology - measurement of critical features

  – inspection - defect inspection, defect localization, defect classification

  – failure pattern analysis

- applications

  – automatic feature measurement

  – anomaly detection

  – defect inspection

Automatic feature measurement

- ML techniques

  - image enhancement (denoising)

  - texture segmentation

  - repetitive pattern recognition

  - automatic measurement

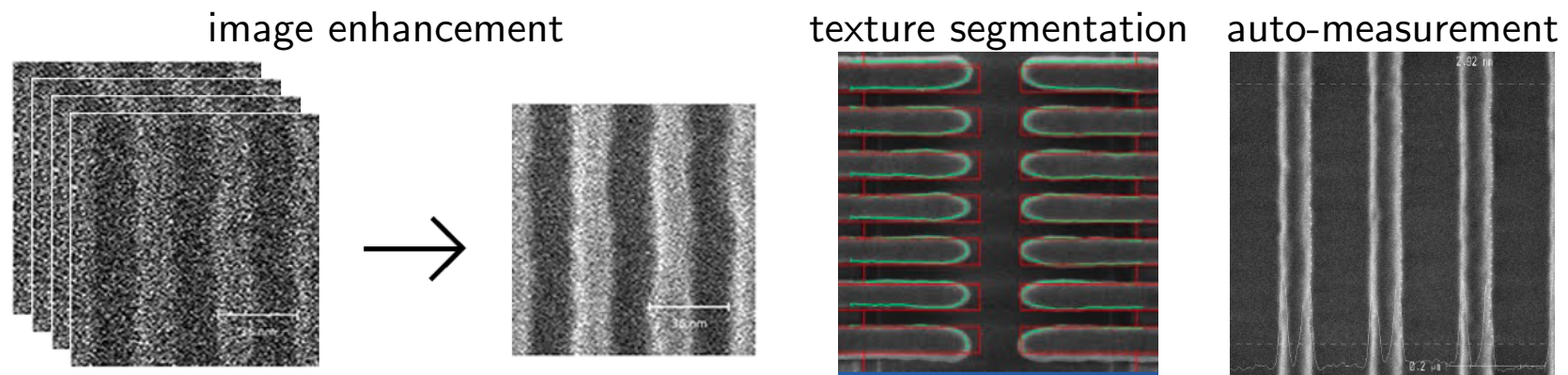image enhancement · · · texture segmentation · · · auto-measurement

Image enhancement

- image enhancement techniques

  - general supervised denoising using DL

  - blind denoising using DL - remove noise without prior knowledge of noise adapting to various noise types

  - super-resolution - upscale low-resolution images, add realistic details for sharper & higher-quality images
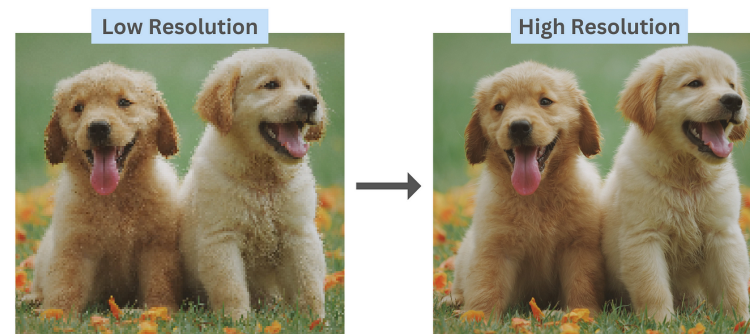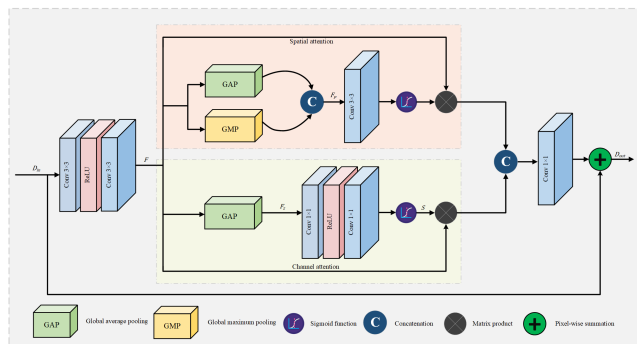
Image segmentation

- texture segmentation

  - distinguish areas based on texture patterns - identifying regions with similar textural features - used for material classification, surface defect detection, medical imaging
  - methods - Gabor filters, wavelet transforms, DL

- semantic segmentation

  - assign class labels to every pixel - enabling precise object and region identification - used for autonomous driving, scene understanding, medical diagnostics
 - methods - fully convolutional network (FCN), U-net, DeepLab
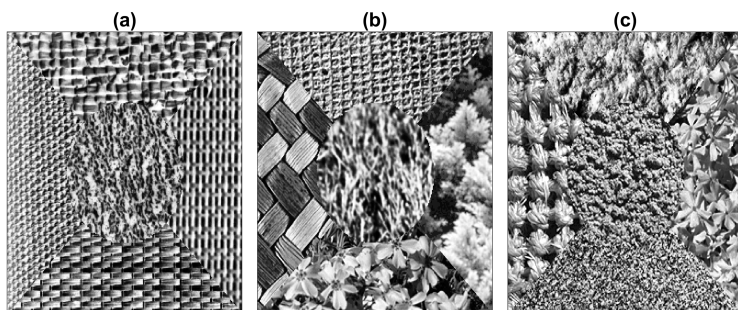
Anomaly detection using side product

- representation in embedding space obtained as side product from previous processes

- distance from normal clusters used for anomaly detection

- can be used for yield drop prediction and analysis
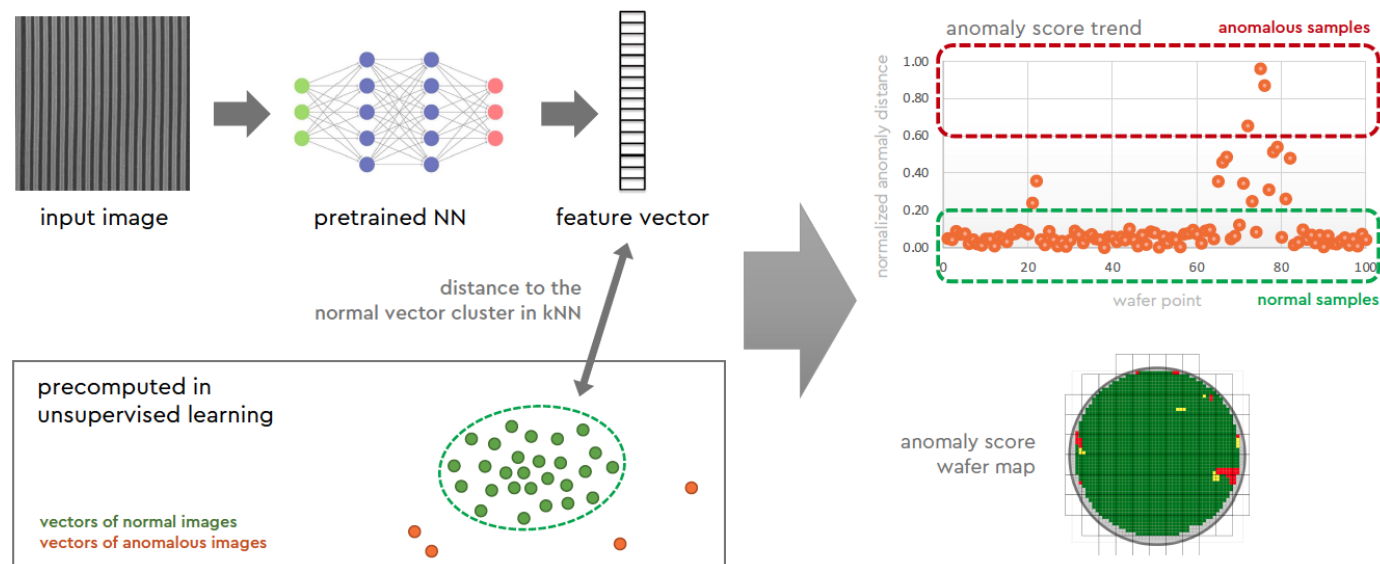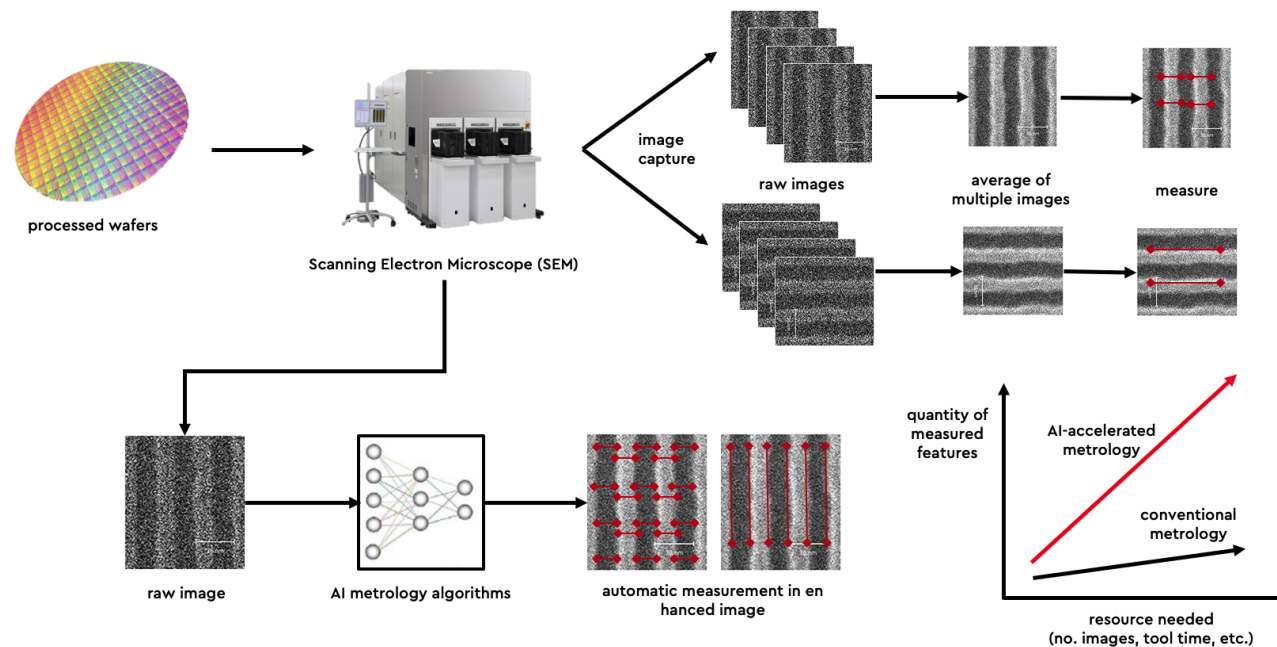
AI-enabled metrology system

- integration of separate components creates AI-enabled metrology system
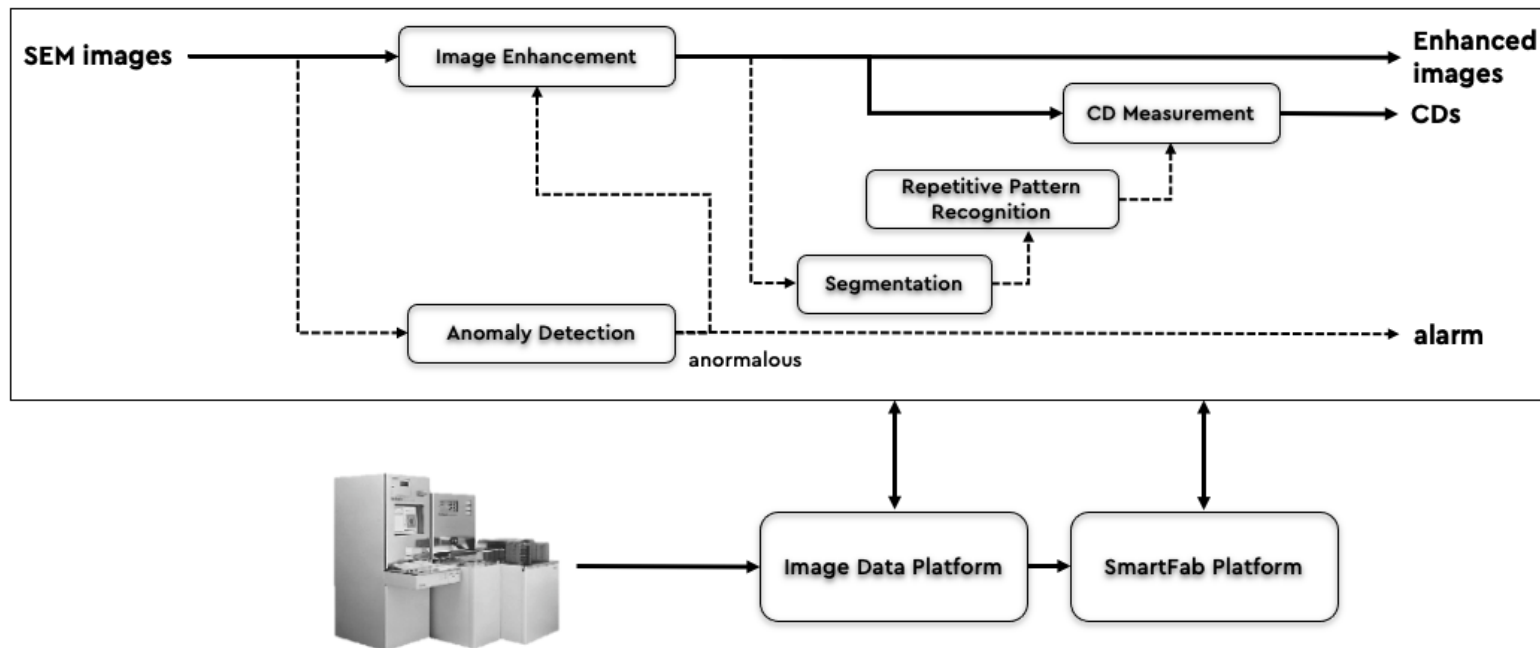
Benefits of new system

- new system provides
  - improved accuracy and reliability
  - improved throughput
  - savings on investment on measurement equipment

TS ML in manAI

Time-series ML applications in manAI

- estimation of TS values

  – virtual metrology - estimate measurement without physically measuring things

- anomaly detection on TS

  – predictive maintenance - predict maintenance times ahead

- multi-modal ML using LLM & genAI

  – root cause analysis and recommendation system
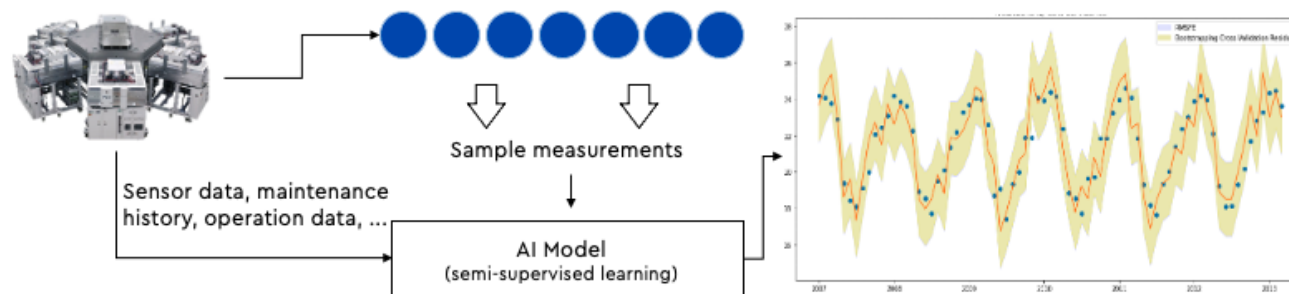
TS MLs in manAI

- TS regression/prediction/estimation
  - LSTM, GRU, attention-based models, Transformer-based architecture for capturing long-term dependencies and patterns

- anomaly detection
  - isolation forest, autoencoders, one-class SVM

- TS regression providing credibility intervals
  - Bayesian-based approaches offering uncertainty estimation alongside predictions
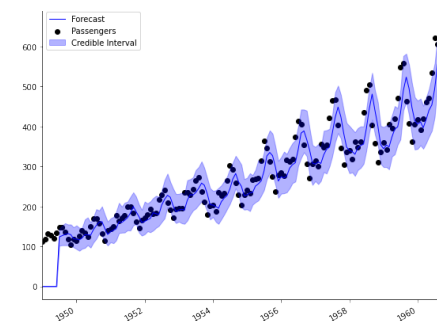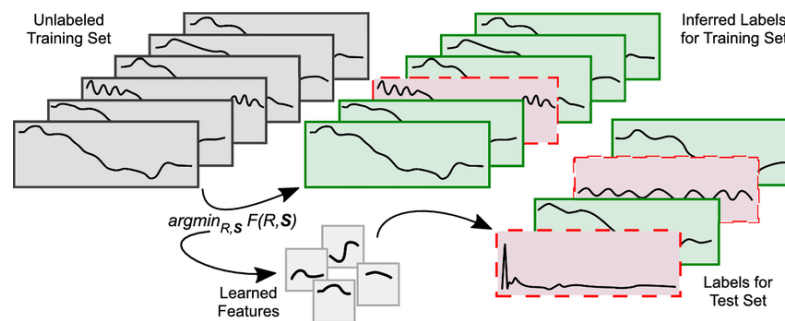
Difficulties with TS ML

- no definition exists for general TS data

- data drift & shift

  - $p(x_{t_k}, x_{t_{k-1}}, \ldots)$ changes over time

  - $p(y_{t_k} | x_{t_k}, x_{t_{k-1}}, \ldots, y_{t_{k-1}}, y_{t_{k-2}}, \ldots)$ changes over time

- (extremely) fat data, poor data quality, huge volume of data to process

- not many research results available

- none of algorithms in academic papers work / no off-the-shelf algorithms work

Online learning for TS regression

- use multiplie experts - $f_{1,k}, \ldots, f_{p_k,k}$ for each time step $t = t_k$ where $f_{i,k}$ can be any of following

  – seq2seq models ($e.g.$, LSTM, Transformer-based models)

  – non-DL statistical learning models ($e.g.$, online ridge regression)

- model predictor for t_k, $g_k : \mathbf{R}^n \to \mathbf{R}^m$ as weighted sum of experts
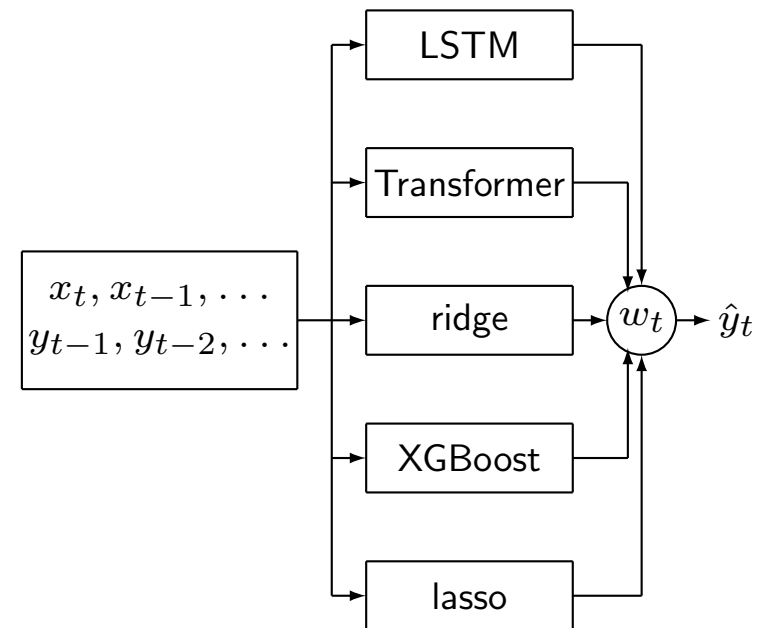
$$g_k = w_{1,k}f_{1,k} + w_{2,k}f_{2,k} + \cdots + w_{p_k,k}f_{p_k,k} = \sum_{i=1}^{p_k} w_{i,k}f_{i,k}$$

Credibility intervals

- every point prediction is wrong, $i.e.$

$$\mathbf{Prob}(\hat{y}_t = y_t) = 0$$

- reliability of prediction matters, however, *none* literature deals with this (properly)
- critical for our customers, $i.e.$, *such information is critical for downstream applications*
  - $e.g.$, when used for feedback control, need to know how reliable prediction resuilts are
  - sometimes *more crucial than algorithm accuracy*
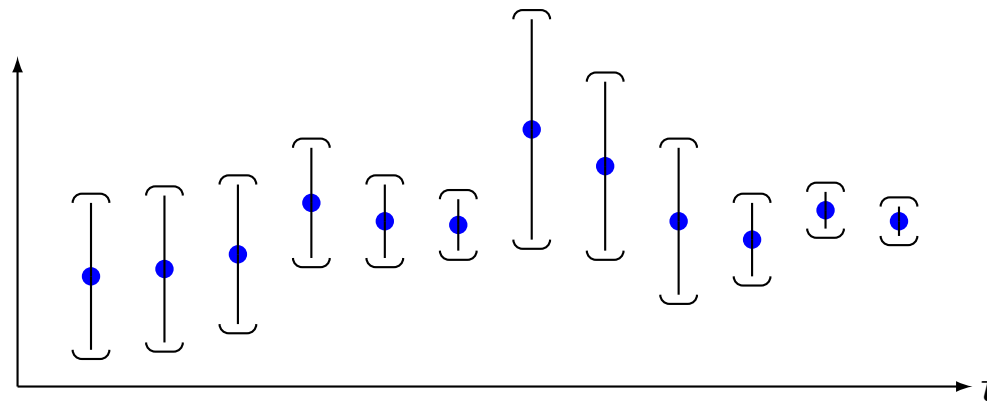
Bayesian approach for credibility interval evaluation

- assume conditional distribution ith predictor parameterized by $\theta_{i,k} \in \Theta$

$$p_{i,k}(y(t_k)|x_{t_k}, x_{t_{k-1}}, \ldots, y(t_{k-1}), y(t_{k-2}), \ldots) = p_{i,k}(y(t_k); x_{t_k}, \theta_{i,k})$$

  – depends on prior & current input, $i.e.$, $\theta_{i,k}$ & x_{t_k}
- update $\theta_{i,k+1}$ from $\theta_{i,k}$ after observing true $y(t_k)$ using Bayesian rule

$$p(w; \theta_{i,k+1}) := p(w|y(t_k); x_{t_k}, \theta_{i,k}) = \frac{p(y(t_k)|w, x_{t_k})p(w; \theta_{i,k})}{\int p(y(t_k)|w, x_{t_k})p(w; \theta_{i,k})dw}$$
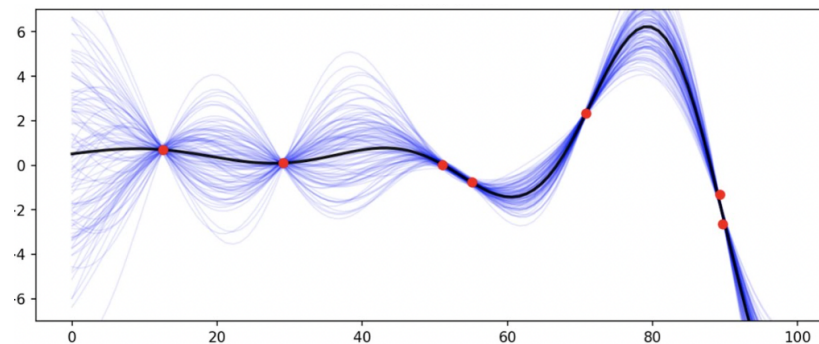
Virtual Metrology

VM

- background

  – every process engineer wants to (so badly) measure every material processed - make sure process done as desired

    - *e.g.*, in semiconductor manufacturing, photolithography engineer wants to make sure diameter of holes or line spacing on wafers done correctly to satisfy specification for GPU or memory chips

  – however, various constraints prevent them from doing it, *e.g.*, in semiconductor manufacturing

    - measurement equipment requires investment

    - incur intolerable throughput

    - fab space does not allow

- GOAL - *measure every processed material without physically measuring them*

VM - problem formulation

- problem description

$$\text{(stochastically) predict} \quad y_{t_k}$$
$$\text{given} \quad x_{t_k}, x_{t_{k-1}}, \ldots, y_{t_{k-1}}, y_{t_{k-2}}, \ldots$$

- our problem formulation

$$\begin{aligned}
\text{minimize} \quad & \sum_{k=1}^{K} w_{k,K-k}\, l(y_{t_k}, \hat{y}_{t_k}) \\
\text{subject to} \quad & \hat{y}_{t_k} = g_k(x_{t_k}, x_{t_{k-1}}, \ldots, y_{t_{k-1}}, y_{t_{k-2}}, \ldots)
\end{aligned}$$

where optimization variables - $g_1, g_2, \ldots : \mathcal{D} \to \mathbf{R}^m$
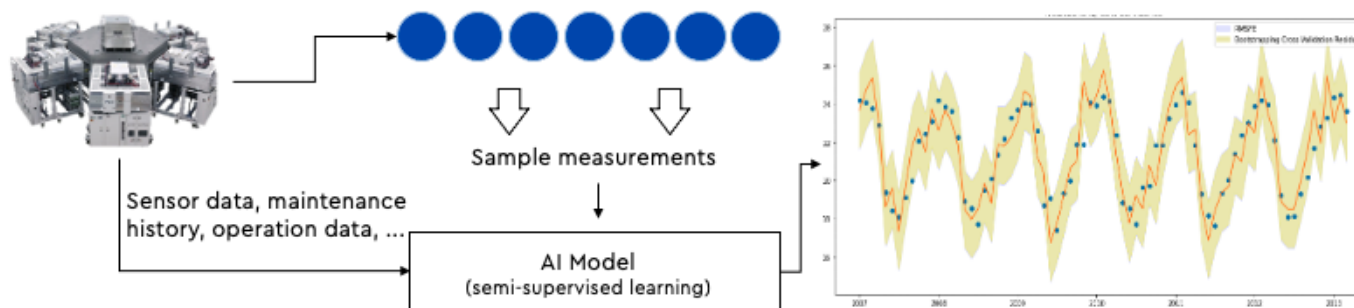
VM - Gauss Labs' inAI success story

- Gauss Labs' ML solution & AI product
  - fully home-grown online TS adpative ensemble learning method
  - outperform competitors and customer inhouse tools, *e.g.*, *Samsung, Intel, Lam Research*
  - published & patented in US, Europe, and Korea
- business impacts
  - improve process quality - reduction of process variation by tens of percents
  - (indirectly) contribute to better product quality and yield
  - Gauss Labs' main revenue source
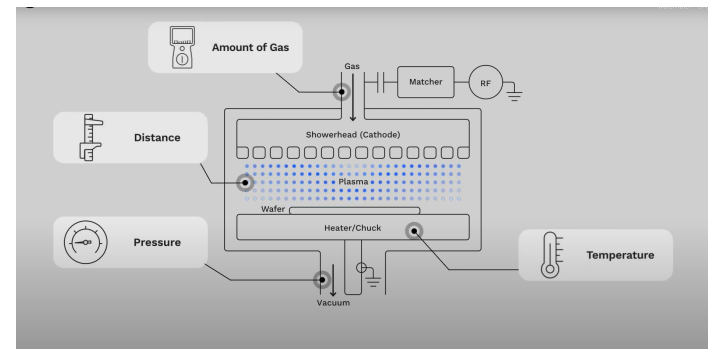
Manufacturing AI Productionization

Minimally required efforts for manAI

- MLOps - for CI/CD

- data preprocessing - missing values, inconsistent names, difference among different systems

- feature extraction & selection

- monitoring & retraining

- notification, via messengers or emails

- mainline merge approvals by humans

- data latency, data reliability, & data availability

MLOps for manAI

- environment for flexible and agile exploration - EDA[7]

- fast & efficient iteration of algorithm selection, experiements, & analysis

- correct training / validation / test data sets critical!

- seamless productionization from, $e.g.$, Jupyter notebook to production-ready code

- monitorning, *right* metrics, notification, re-training

---
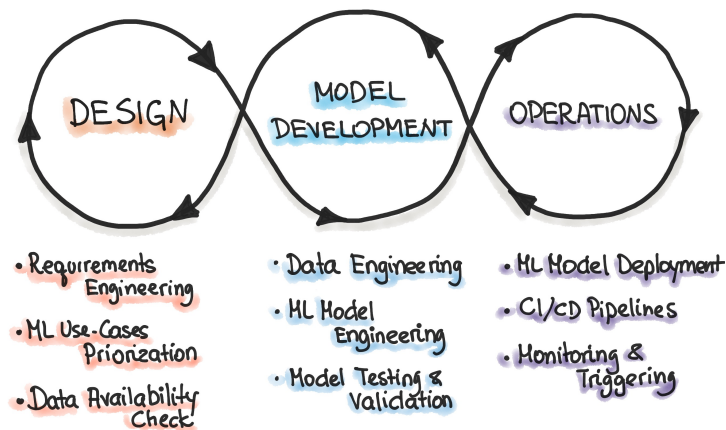
[7]EDA - exploratory data analysis

manAI software system

- data, data, data! – store, persist, retrieve, data quality
- seamless pipeline for development, testing, running deployed services
- development envinroment should be built separately
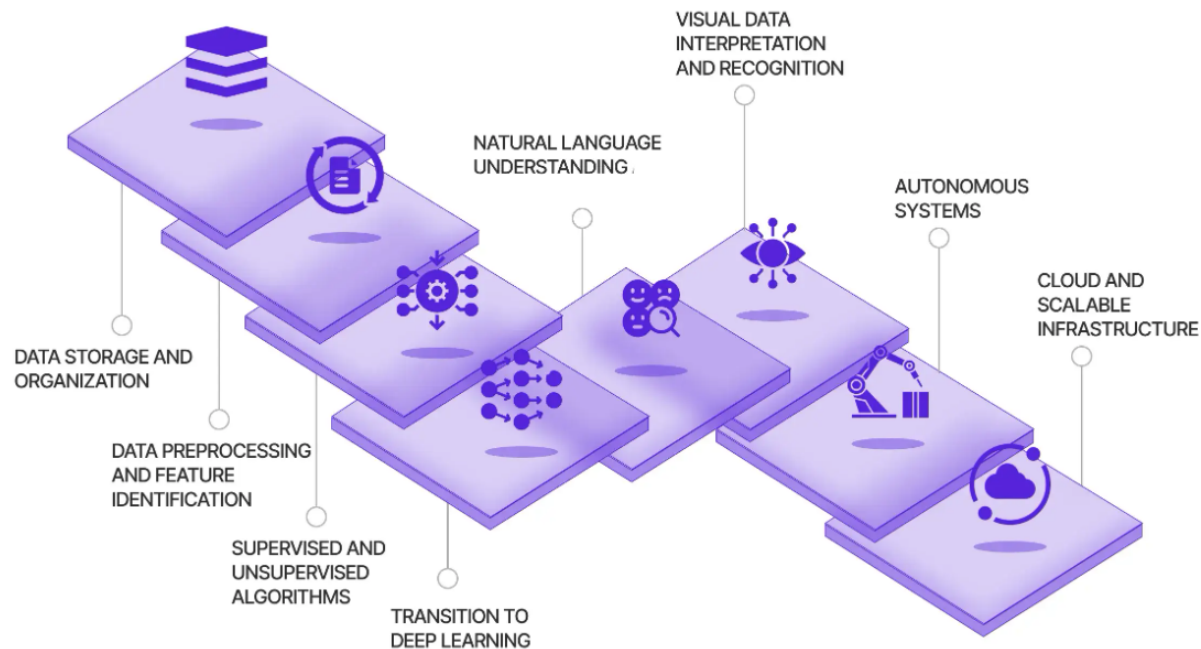
manAI system architecture

- frontend / backend / data I/F / data layer

- efficient and effective MLOps in backend or development environment
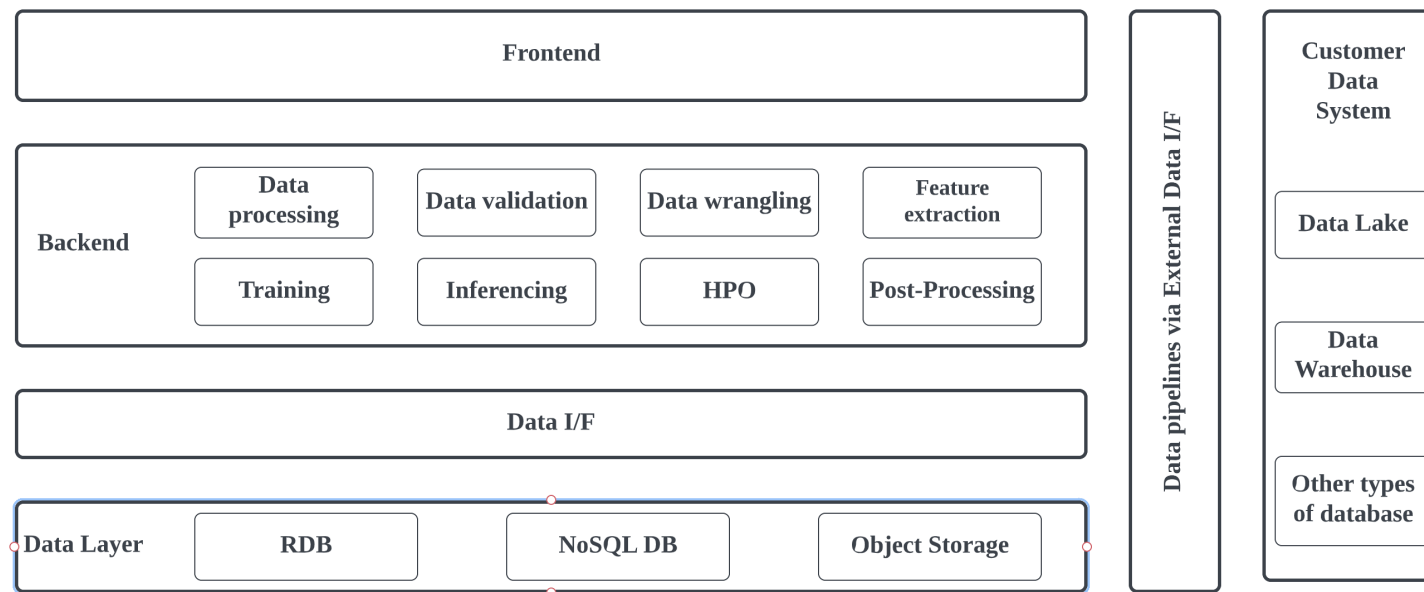
Reusuable components vs customer specific components

- make sure to build two components separate - generic reusable and customer specific

- generic models should be tuned for each use case

- generic model library grows as interacting with more and more customers
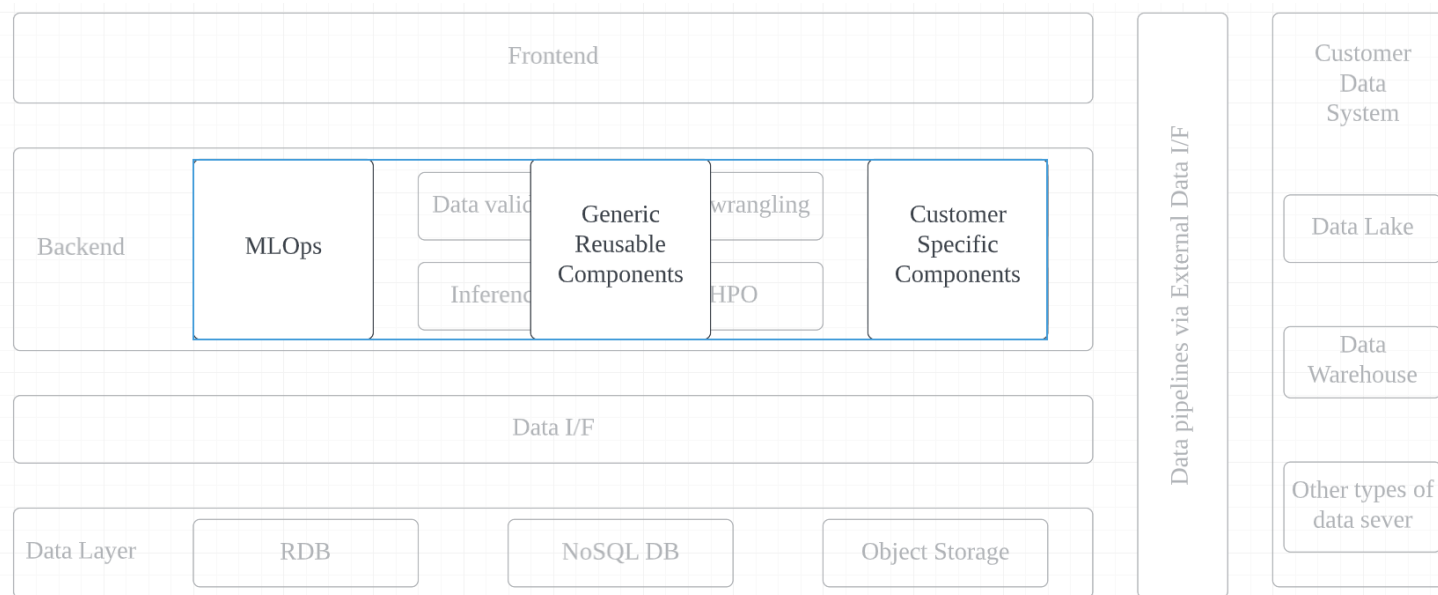
My Two Cents

Recommendations for maximum impact via inAI

- concrete goals of projects

  – north star – yield improvement, process quality, making engineers' lives easier

  – hard problem – scheduling and optimization

- be strategic!

  – learn from others – lots of successes & failures of inAI

  – ball park estimation for ROI cricial – efforts, time, expertise, data

  – utilities vs technical excellency / uniqueness vs common technology

  – home-grown vs off-the-shelf

Remember . . .

- data, data, data! – readiness, quality, procurement, pre-processing, DB

- *never* underestimate domain knowledge & expertise – data do NOT tell you everything

- EDA

- do *not* over-optimize your algorithms – ML is all about trials-&-errors

- overfitting, generalization, concept drift/shift - way more important than you could ever imagine

- devOps, MLOps, agile dev, software development & engineering

Conclusion

Conclusion

- various CV MLs used for inAI applications

- TS ML applications found in every place in manufacturing

- drift/shift & data noise make TS MLs very challenging, but working solutions found

- in reality, crucial bottlenecks are

  – data quality, prepocessing, monitoring, notification, and retraining

  – data latency, avaiability, and reliability

  – excellency in software platform design and development using cloud services

Selected References & Sources

Selected references & sources

- Robert H. Kane "Quest for Meaning: Values, Ethics, and the Modern Experience" 2013

- Michael J. Sandel "Justice: What's the Right Thing to Do?"   2009

- Daniel Kahneman "Thinking, Fast and Slow"   2011

- Yuval Noah Harari "Sapiens: A Brief History of Humankind"   2014

- M. Shanahan "Talking About Large Language Models"   2022

- A.Y. Halevry, P. Norvig, and F. Pereira "Unreasonable Effectiveness of Data"   2009

- A. Vaswani, et al. "Attention is all you need" @ NeurIPS   2017

- S. Yin, et. al. "A Survey on Multimodal LLMs"   2023

- Chris Miller "Chip War: The Fight for the World's Most Critical Technology"   2022

- CEOs, CTOs, CFOs, COOs, CMOs & CCOs @ startup companies in Silicon Valley

- VCs on Sand Hill Road - Palo Alto, Menlo Park, Woodside in California, USA

References

References

[BKP22]   Abhaya Bhardwaj, Shristi Kishore, and Dhananjay K. Pandey. Artificial intelligence in biological sciences. *Life*, 12(1430), 2022.

[DFJ22]   Thomas A. Dixon, Paul S. Freemont, and Richard A. Johnson. A global forum on synthetic biology: The need for international engagement. *Nature Communications*, 13(3516), 2022.

[GPAM$^+$14] Ian J. Goodfellow, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio. Generative adversarial networks, 2014.

[HGH$^+$22] Sue Ellen Haupt, David John Gagne, William W. Hsieh, Vladimir Krasnopolsky, Amy McGovern, Caren Marzban, William Moninger, Valliappa Lakshmanan, Philippe Tissot, and John K. Williams. The history and practice of AI in the environmental sciences. *Bulletin of the American Meteorological Society*, 103(5):E1351 − E1370, 2022.

[HM24]   Guadalupe Hayes-Mota. Emerging trends in AI in biotech. *Forbes*, June 2024.

[Kui23]   Todd Kuiken. Artificial intelligence in the biological sciences: Uses, safety, security, and oversight. *Congressional Research Service*, Nov 2023.

[KW19]   Diederik P. Kingma and Max Welling. An introduction to variational autoencoders. *Foundations and Trends in Machine Learning*, 12(4):307–392, 2019.

[MLZ22]   Louis-Philippe Morency, Paul Pu Liang, and Amir Zadeh. Tutorial on multimodal machine learning. In Miguel Ballesteros, Yulia Tsvetkov, and Cecilia O. Alm, editors, *Proceedings of the 2022 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies: Tutorial Abstracts*, pages 33–38, Seattle, United States, July 2022. Association for Computational Linguistics.

[RAB$^+$23]   Ziaur Rahman, Muhammad Aamir, Jameel Ahmed Bhutto, Zhihua Hu, and Yurong Guan. Innovative dual-stage blind noise reduction in real-world images using multi-scale convolutions and dual attention mechanisms. *Symmetry*, 15(11), 2023.

[Say21]   Kelley M. Sayler. Defense primer: Emerging technologies. *Congressional Research Service*, 2021.

[Toe23]   Rob Toews. The next frontier for large language models is biology. *Forbes*, July 2023.

[VSP$^+$17]   Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need. In *Proceedings of 31st Conference on Neural Information Processing Systems (NIPS)*, 2017.

[Wet23]   Kris A. Wetterstrand. Dna sequencing costs: Data, 2023.

[YFZ$^+$24]   Shukang Yin, Chaoyou Fu, Sirui Zhao, Ke Li, Xing Sun, Tong Xu, and Enhong Chen. A survey on multimodal large language models, 2024.

Thank You