AI Slides Viewer & Checker - 2

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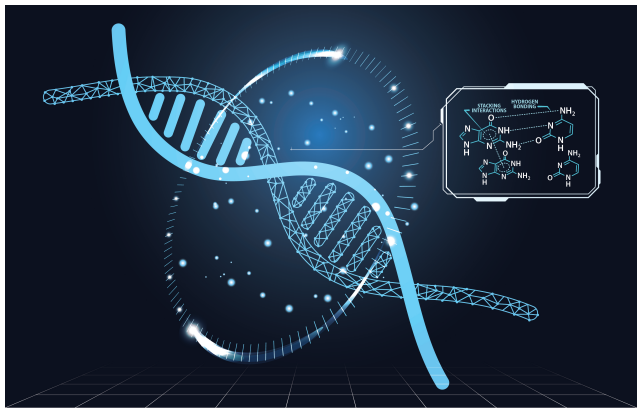
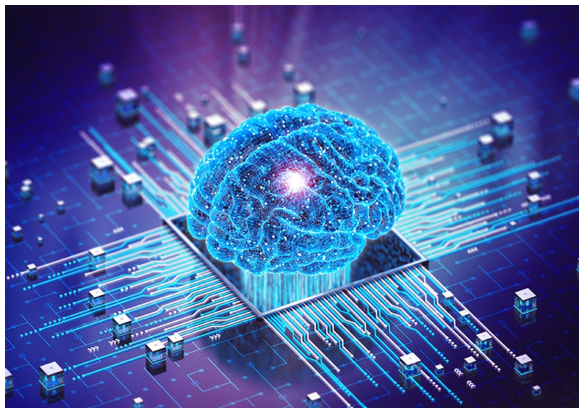
AI & Biotech

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





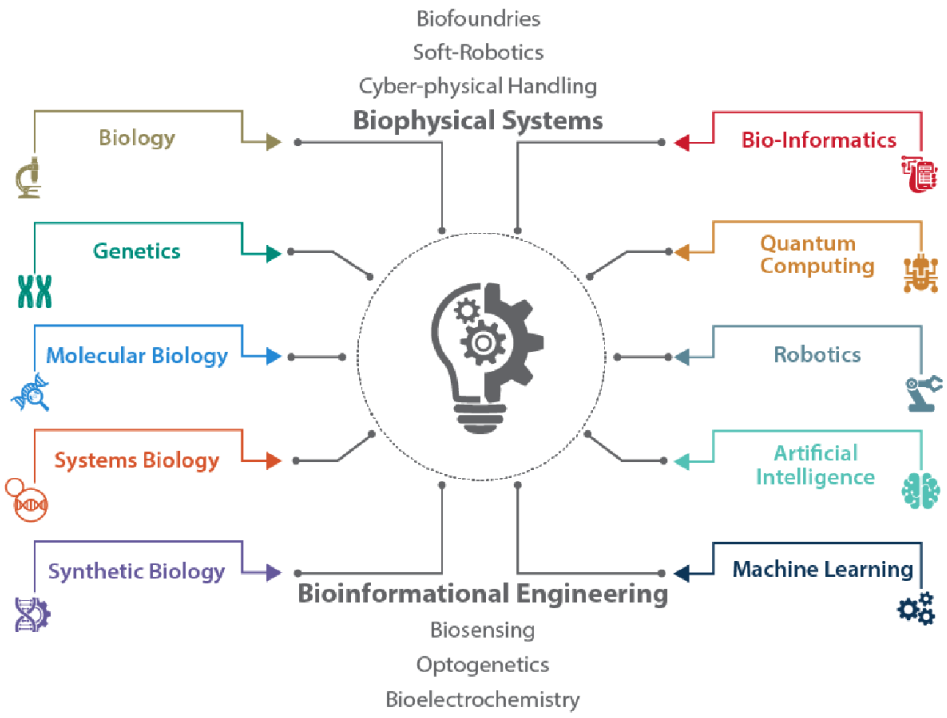
Biotech

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

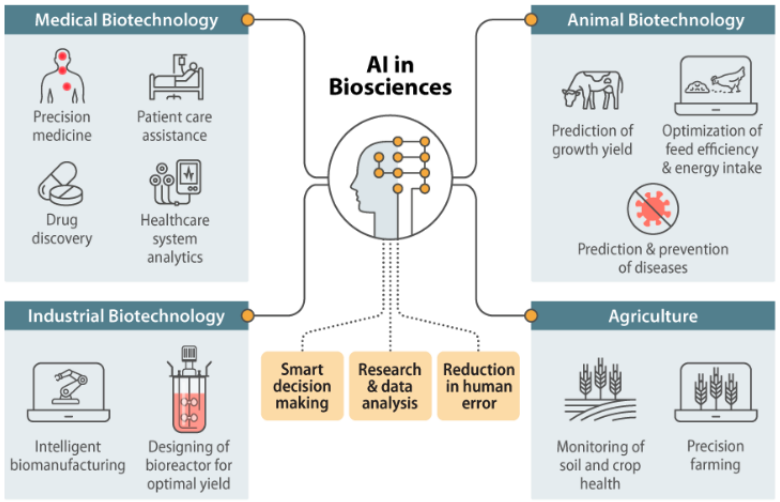
- sciences and technologies enabling biotechnology include (but not limited to)
  - (molecular) biology, genetics, systems biology, synthetic biology, bio-informatics, quantum computing, robotics [DFJ22]



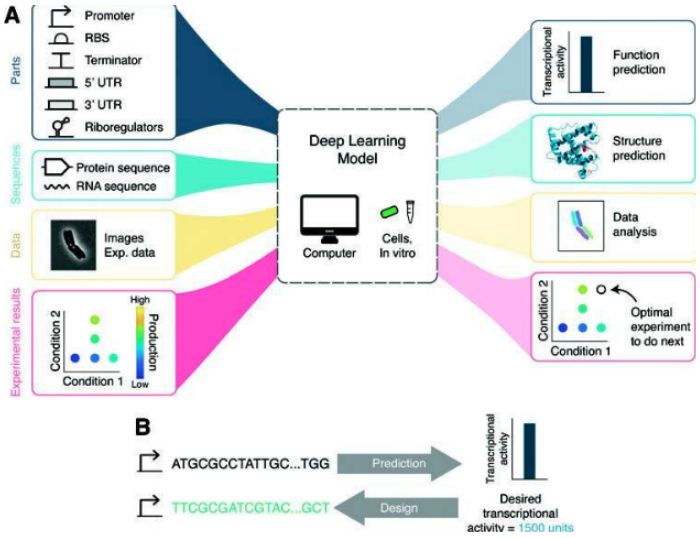
Convergence of AI and biological design

- 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

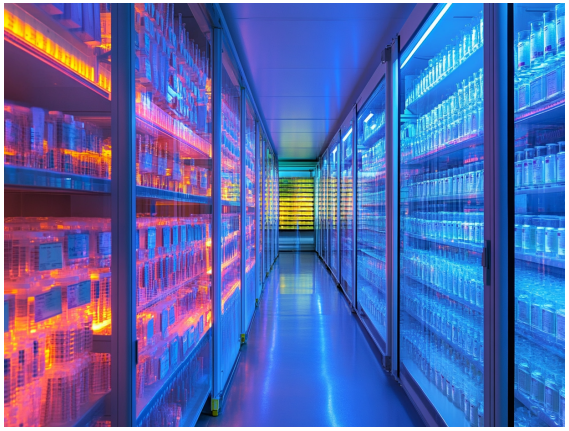
  "AI will be essential to fully understanding how genetic code interacts with biological processes" - US National Security Commission on Artificial Intelligence (NSCAI)

  – 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



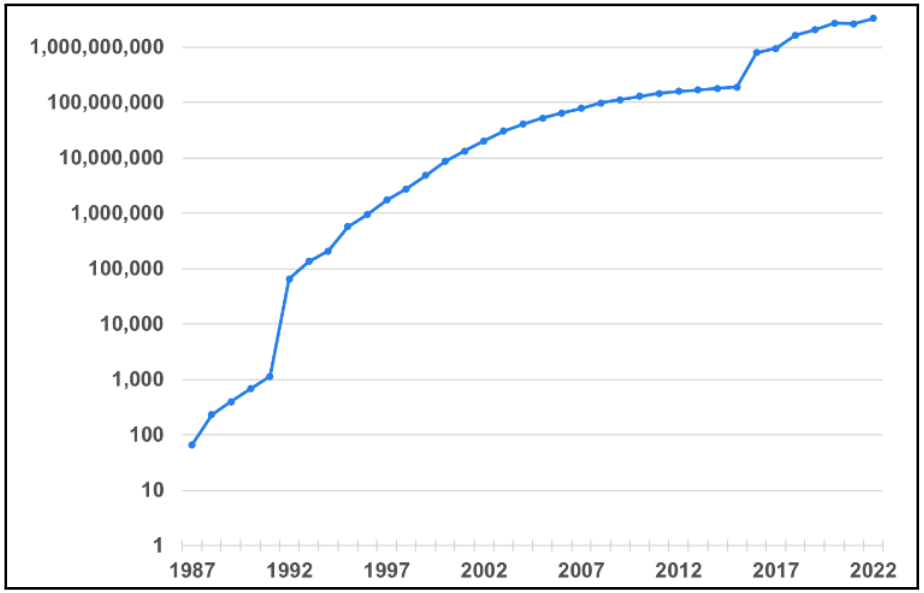
Rapid growth of biological data

- 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

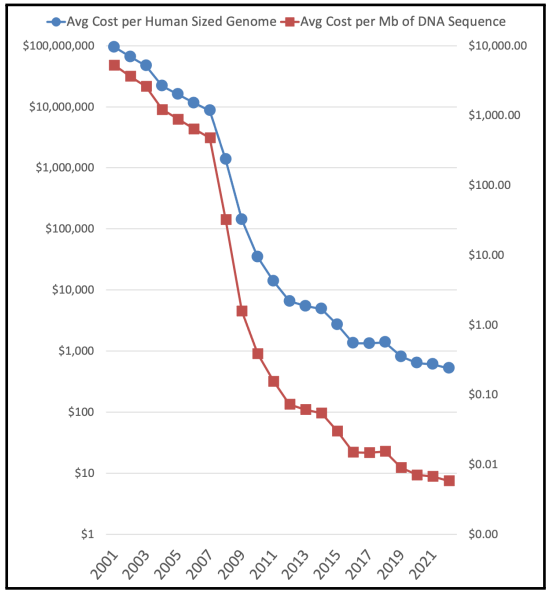
Volume and sequencing cost of DNA over time

- 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



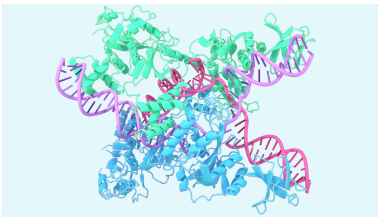
Bio data availability and bias

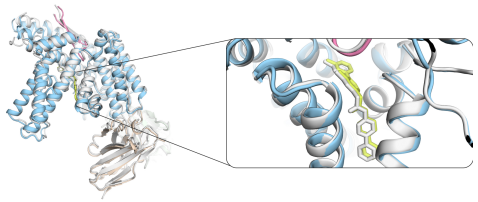
- US National Security Commission on Artificial Intelligence (NSCAI) recommends
  - US fund and prioritize development of a biobank containing *"wide range of high-quality biological and genetic data sets securely accessible by researchers"*
  - establishment of database of broad range of human, animal, 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 → 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





AlphaGo

- Go board marked with 19×19 grid - $(19 \times 19)! = 361! \approx 1.44 \times 10^{768}$
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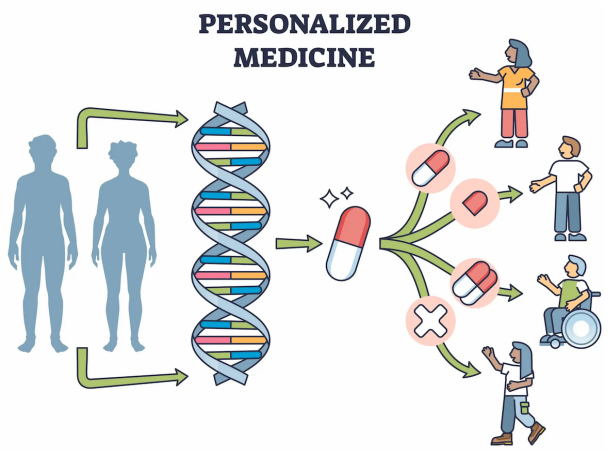
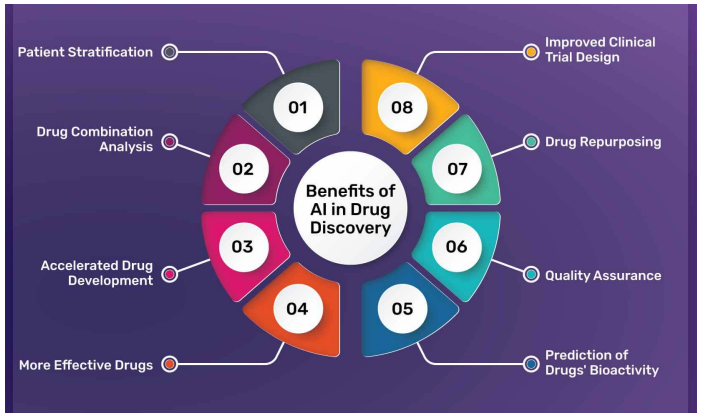
- deep reinforcement learning with Monte Carlo tree search
  - trained on thousands of years of Go game history
  - AlphaGo Zero learns by playing against itself
- development experience, insight, knowledge, know-how transferred to AlphaFold

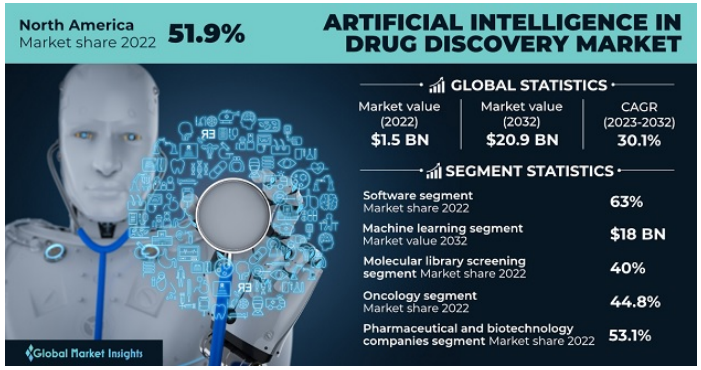
Personalized medicine

- *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

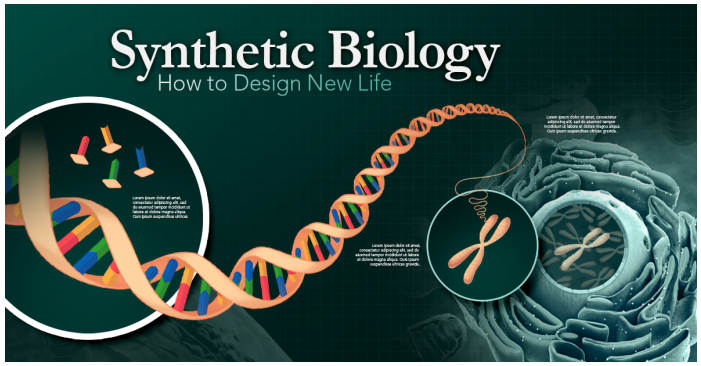


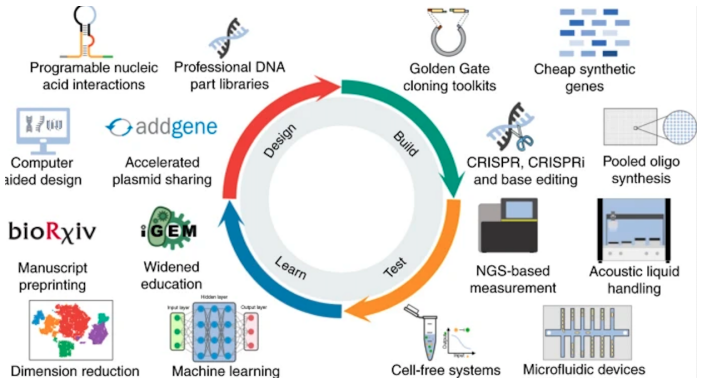


- traditional drug discovery process - time-consuming and costly often taking decades and billions of dollars
- AI streamlines this process by predicting the efficacy and safety of potential compounds with more speed and accuracy
- AI models analyze chemical databases to identify new drug candidates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

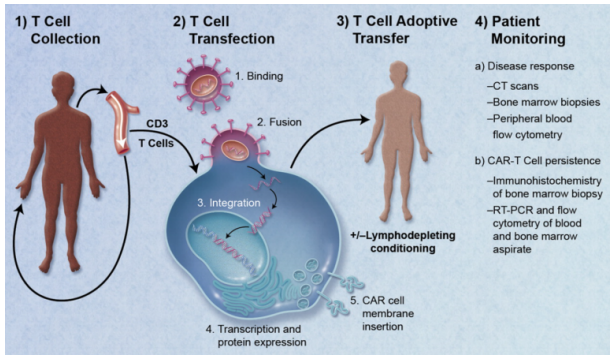
Synthetic biology

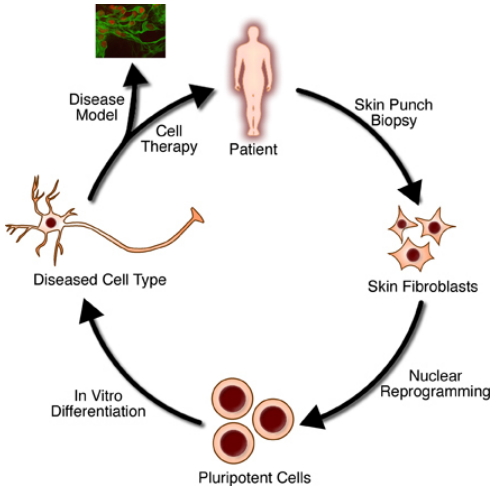
- use AI for gene editing, biomaterial production and synthetic pathways
- combine principles of biology and engineering to design and construct new biological entities
- AI optimizes synthetic biology processes from designing genetic circuits to scaling up production
- company - Ginkgo Bioworks uses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





Regenerative medicine

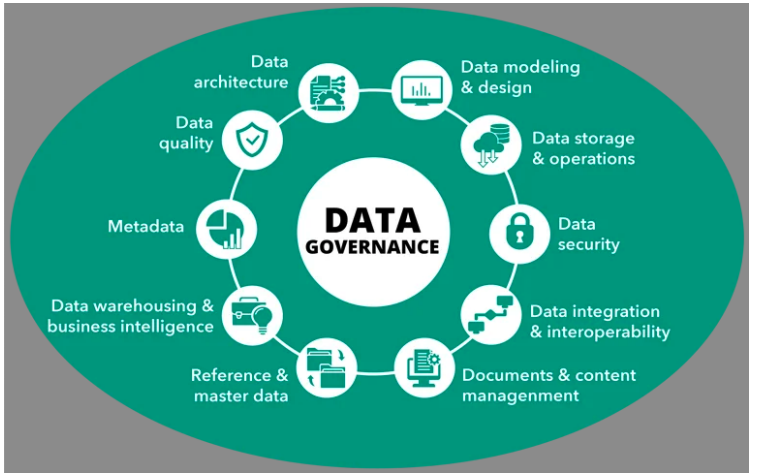




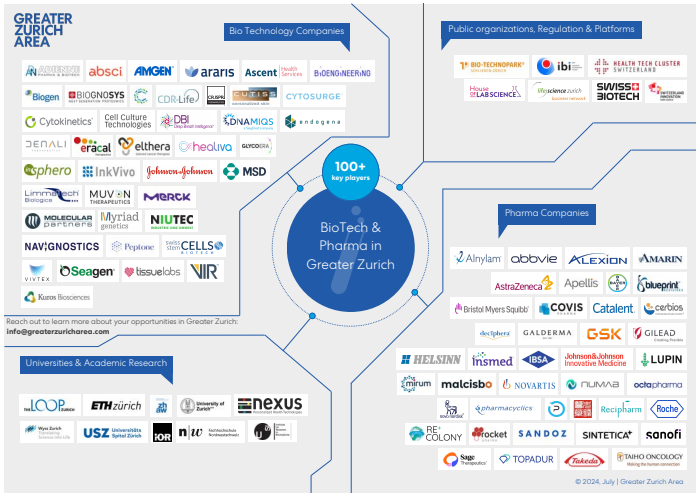
- AI advances development of stem cell therapies & tissue engineering
- AI algorithms assist in identifying optimal cell types, predicting cell behavior & personalized treatments
- particularly for conditions such as neurodegenerative diseases, heart failure and orthopedic injuries
- company - Organovo 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



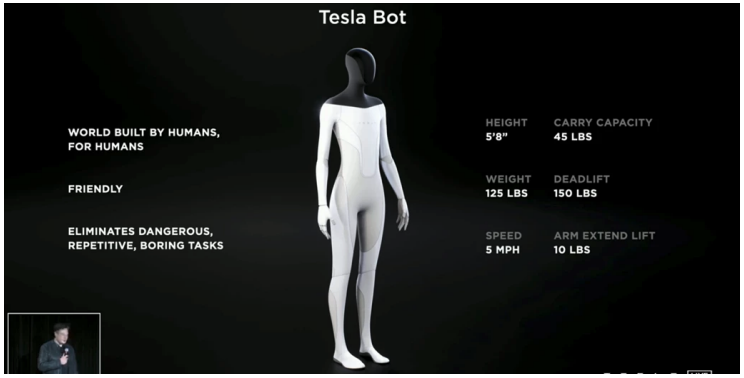
- Atomwise - small molecule drug discovery
- Cradle - protein design
- Exscientia - precision medicine
- Iktos - small molecule drug discovery and design
- Insilico Medicine - full-stack drug discovery system
- Schrödinger, Inc. - use physics-based models to find best possible molecule
- Absci Corporation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

AI-powered Humanoid Robots

Tesla Optimus

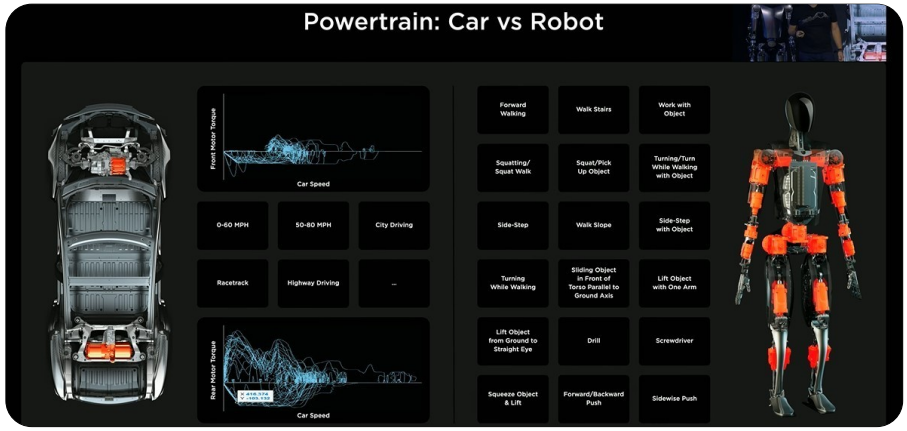
Tesla Optimus

- humanoid robot developed by Tesla intended to handle repetitive & dangerous tasks
- objective - *revolutionize automation* & assist in human labor across various industries
- features - YouTube - Optimus - Gen 2
  - dimensions - 5'8" tall & 125 lbs
  - capabilities - lifting weights, walking at 5 MPH & performing everyday tasks
  - AI-powered - runs on Tesla's AI leveraging same technology used in self-driving cars
  - power source - 2.3 KWH battery designed for efficient power management
  - launch year - announced by Elon Musk during Tesla AI Day in 2021
  - *price - $25,000∼$30,000* expected to decrease over time



History of Tesla Optimus

- inception - first conceptualized as extension of Tesla's AI & robotics capabilities
- AI day 2021 - *officially announced by Elon Musk* w/ vision to solve labor shortages & improve productivity
- Sep 2022 - prototype unveiled
- gen 2 introduced in 2023 - improved capabilities
- Jun 2024 w/ more advanced tasks - *towards mass production for commercial applications*



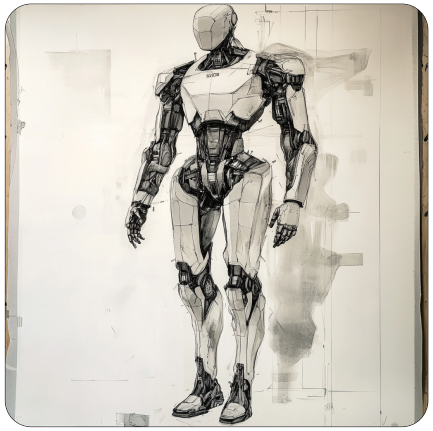
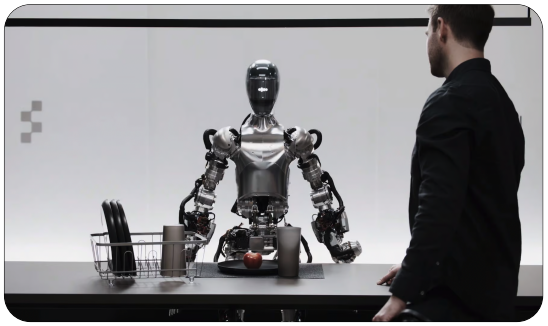
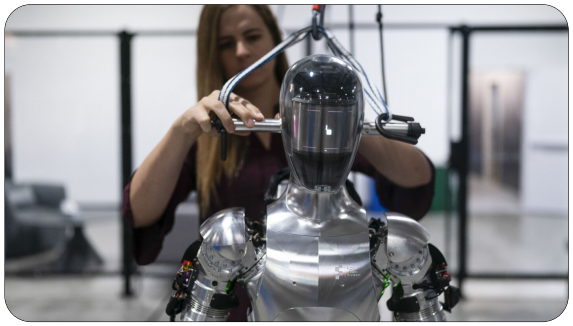


Figure AI

Figure AI robots

- Figure AI
  - founded in 2022 as Silicon Valley startup company by Brett Adcock - serial entrepreneur with successful Archer Aviation & Vettery
  - vision of enhancing productivity by integrating AI and robotics into both industrial & personal spaces
- Figure 02
  - 5'6" tall, 154 lbs, payload of 44 lbs, 5 hr runtime, 1.2 m/s speed
  - imitation learning
  - capabilities - advanced cognition, STS task, dexterous hands w/ 16 degrees of freedom





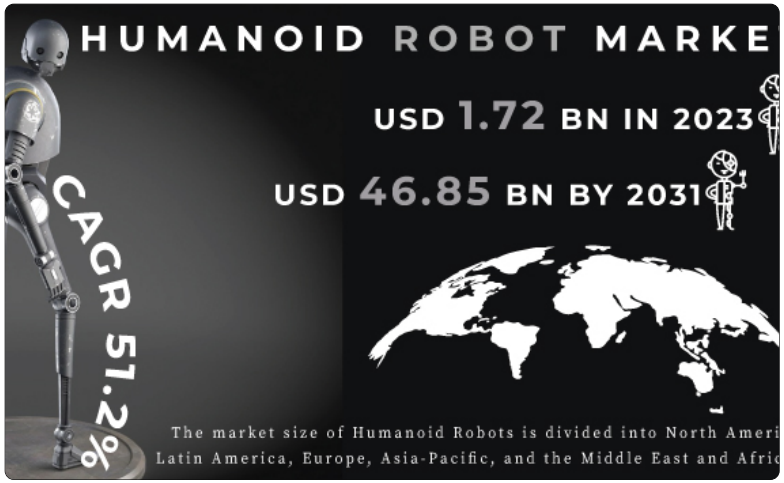
History of Figure AI

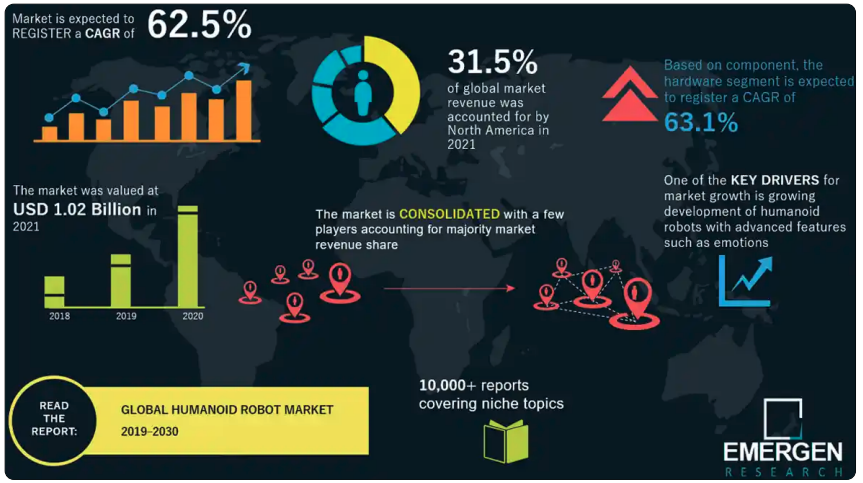
- 2022 - founded by Brett Adcock - previously co-founded Archer Aviation & Vettery
- 2022-2023 - early development - stealth mode focusing on developing their own technology
- May 2023 - public announcement - officially announces mission to develop general-purpose humanoid robots - already raised $70M @ announcement
- Aug 2023 - unveils Figure 01, first prototype w/ basic mobility & manipulation capabilities
- Oct 2023 - series B funding - raised $675M beyond initial goal of $500M - Jeff Bezos, Microsoft, OpenAI - valuation of $\sim$ $2.6B
- late 2023 $\sim$ early 2024 - partnership announcements - refines humanoid robot technology in locomotion, object manipulation & human-robot interaction
- 2024 - significant strides in robot control & decision-making

Impacts & Future

Impacts on industries & markets

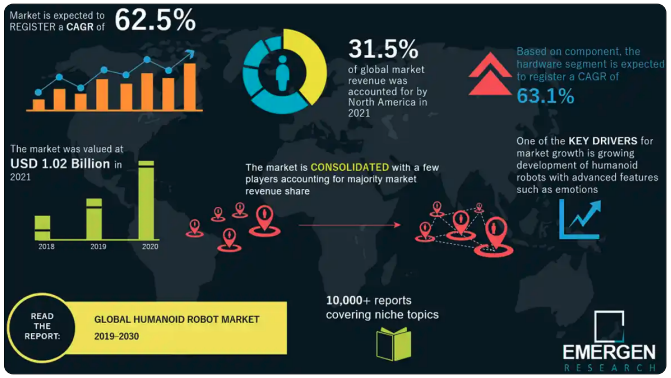
- impacts on robotics history
  - competitor benchmark - competes with robotics giants such as Boston dynamics
  - affordability & scale - predict to lead to *lower costs & higher adoption*
- impacts on labor market
  - task automation - replace human labor in *high-risk & repetitive roles*
  - *job displacement vs creation* - new roles in AI, robot maintenance & oversight
- impacts on consumer market - home automation





Future outlook & predictions

- widespread industrial adoption - expected to become common tool in factories by 2030
- market valued @ *$1.02B in 2021* - expected *CAGR of 62.5%, 63.1% in hardware segment by 2030* - *31.5% revenue increase in 2021* North America - *10,000 humanoid robots* will be shipped worldwide each year by 2027
- AI evolution - continuous learning and AI enhancements will lead to greater efficiency & adaptability
- consumer integration - long-term vision includes personal assistant
- societal impact - could redefine human roles in industries & homes *raising philosophical & ethical questions on human-robot collaboration*



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)

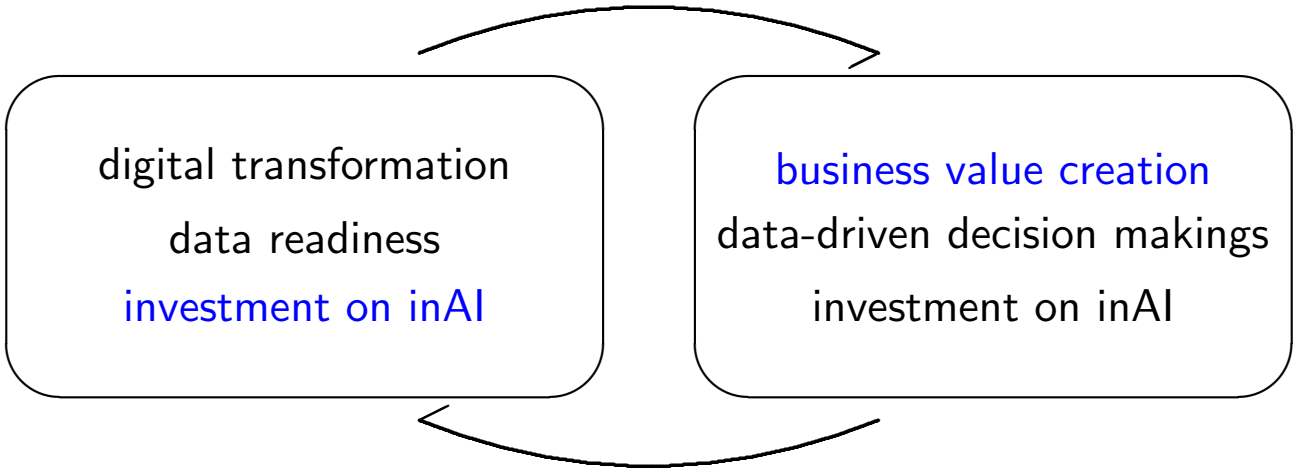
inAI fields

- 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!



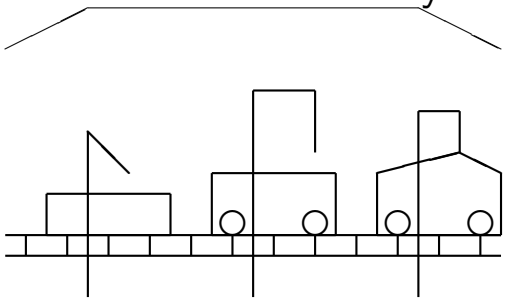
Data-centric AI

- 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

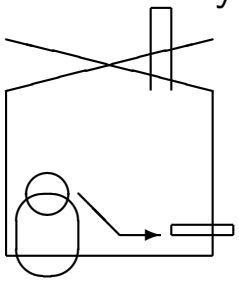
  ". . . need 1,000 models for 1,000 problems" - Andrew Ng

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

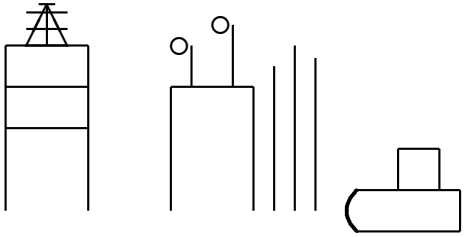
automobile industry



steel industry



oil & gas industry



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

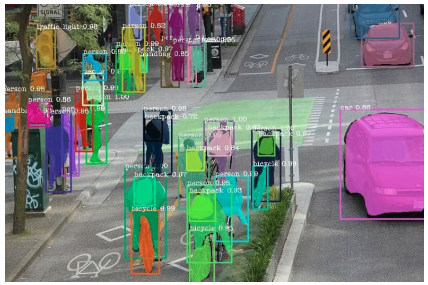
Manufacturing AI

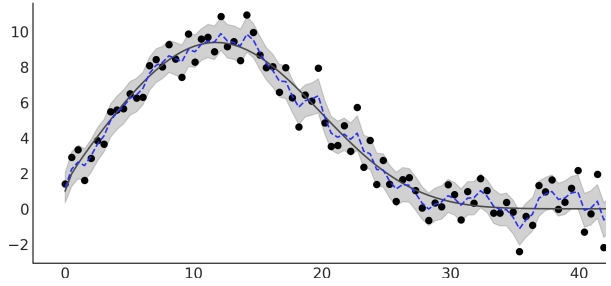
MLs in manufacturing AI (manAI)

- *image data* - huge amount of image data measured and inspected
  - SEM/TEM images, wafer defect maps, test failure pattern maps [1]

  $\rightarrow$ 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 [2]

  $\rightarrow$ regression, anomaly detection, semi-supervised learning, Bayesian inference





[1] SEM: scanning electron miscroscope, TEM: transmission electron miscroscope

[2] MES: manufacturing execution system

CV ML in manAI

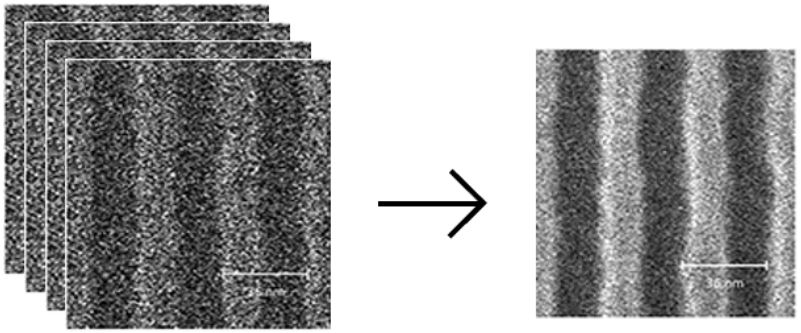
Computer vision ML in manAI

- 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

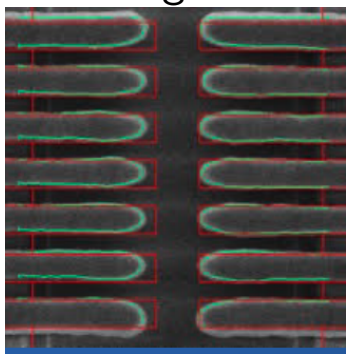
Automatic feature measurement

- ML techniques
  - image enhancement (denoising)
  - texture segmentation
  - repetitive pattern recognition
  - automatic measurement

image enhancement



texture segmentation



auto-measurement

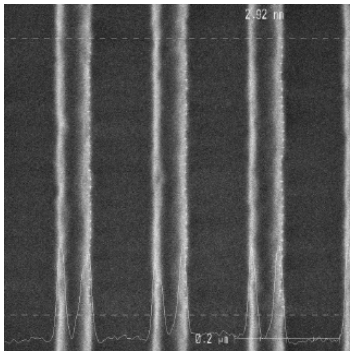
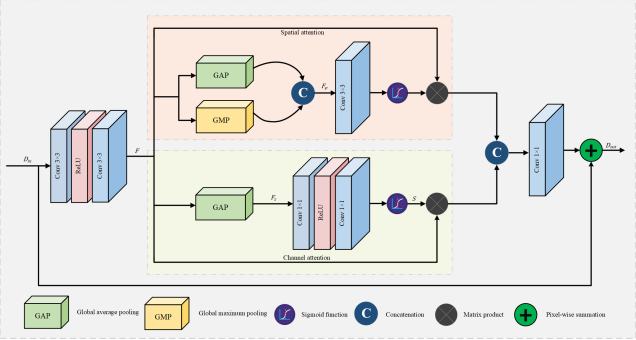


Image enhancement

- 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



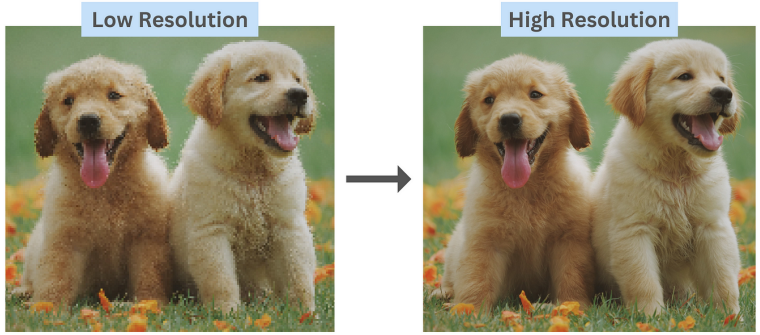
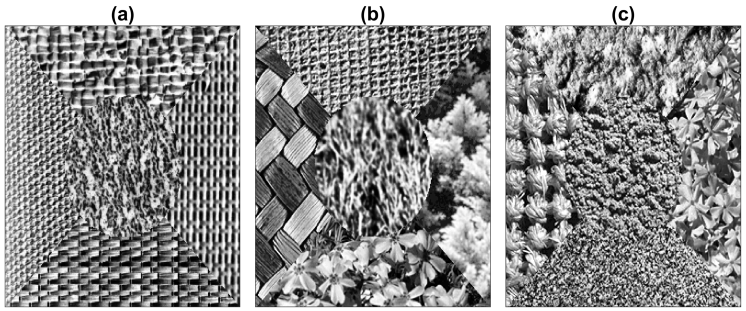


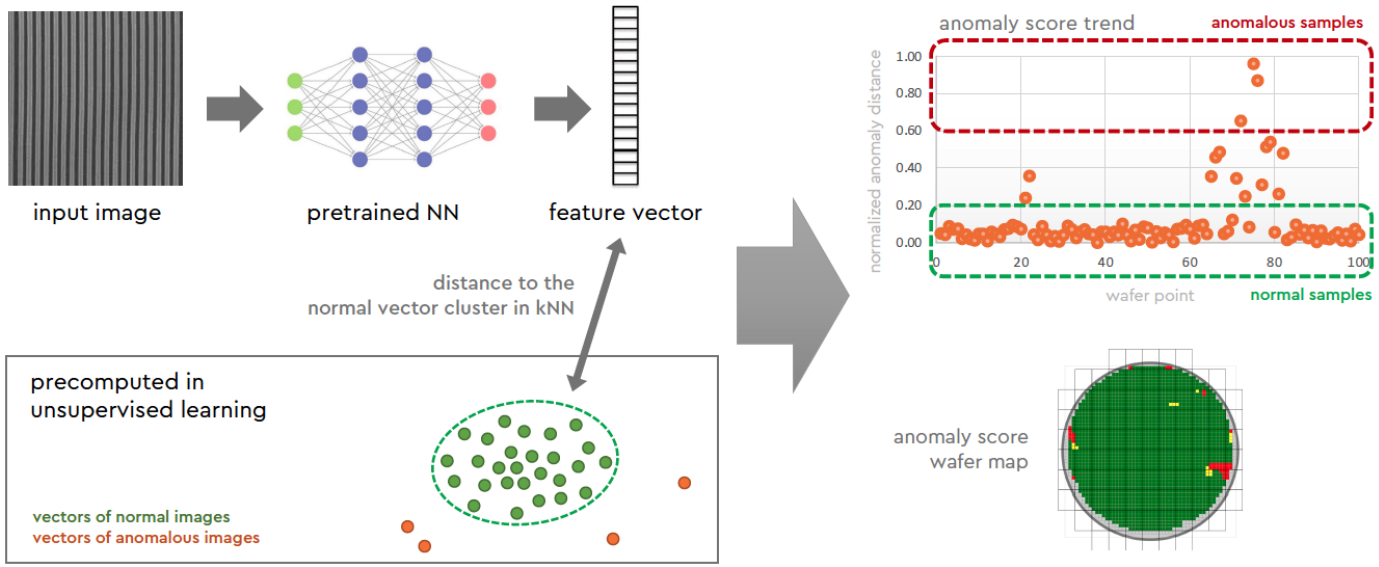
Image segmentation

- 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



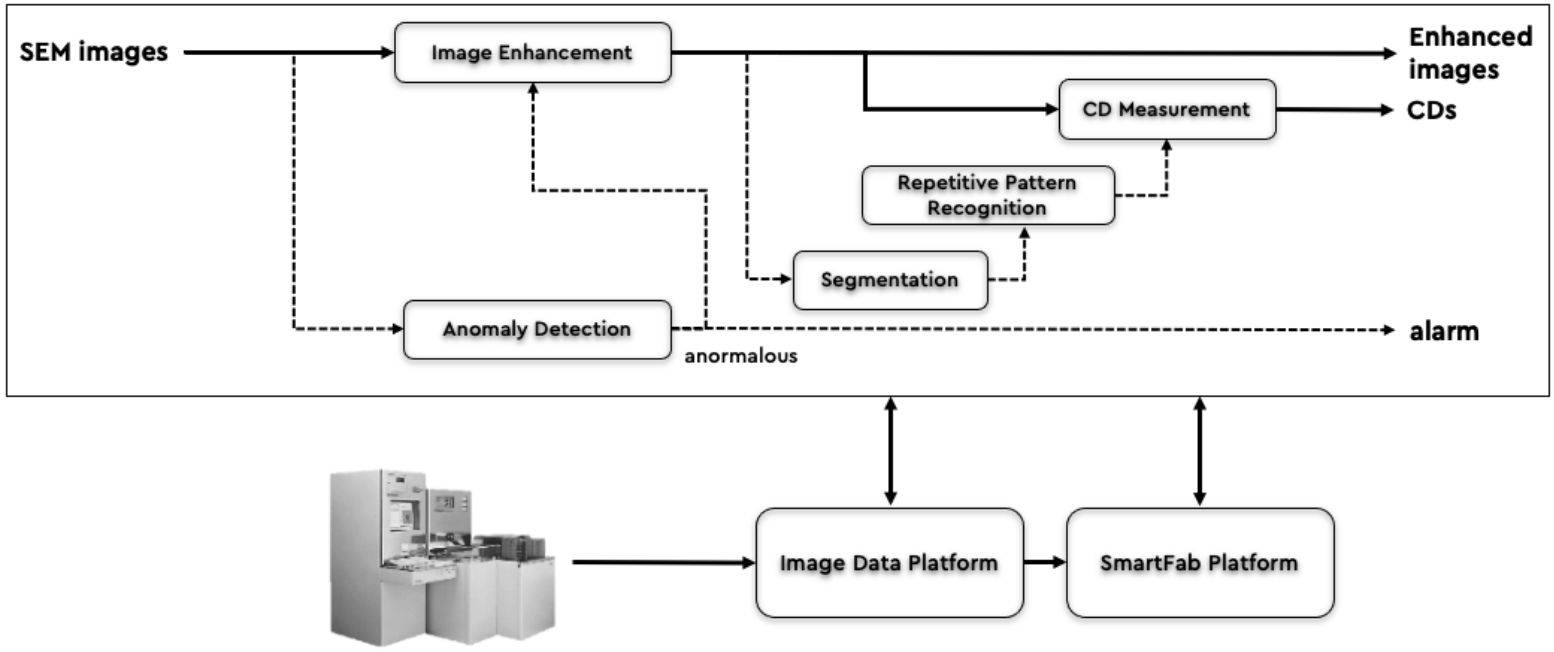
Anomaly detection using side product

- 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



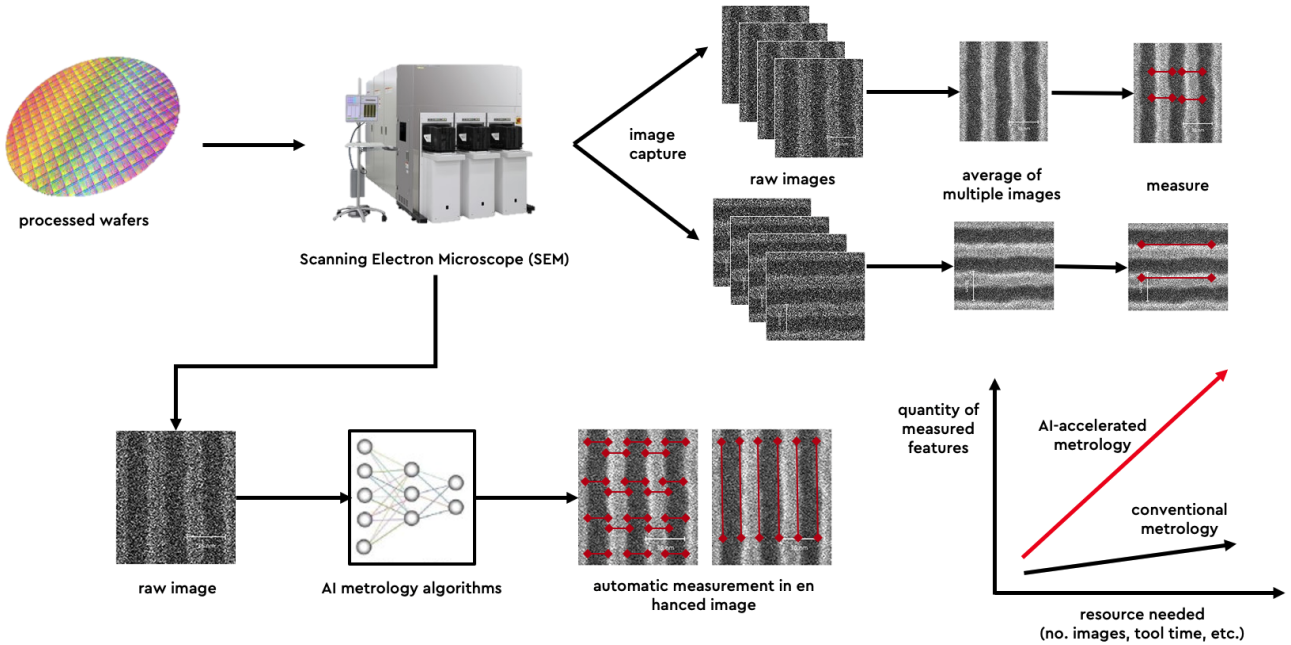
AI-enabled metrology system

- integration of separate components creates AI-enabled metrology system



Benefits of new system

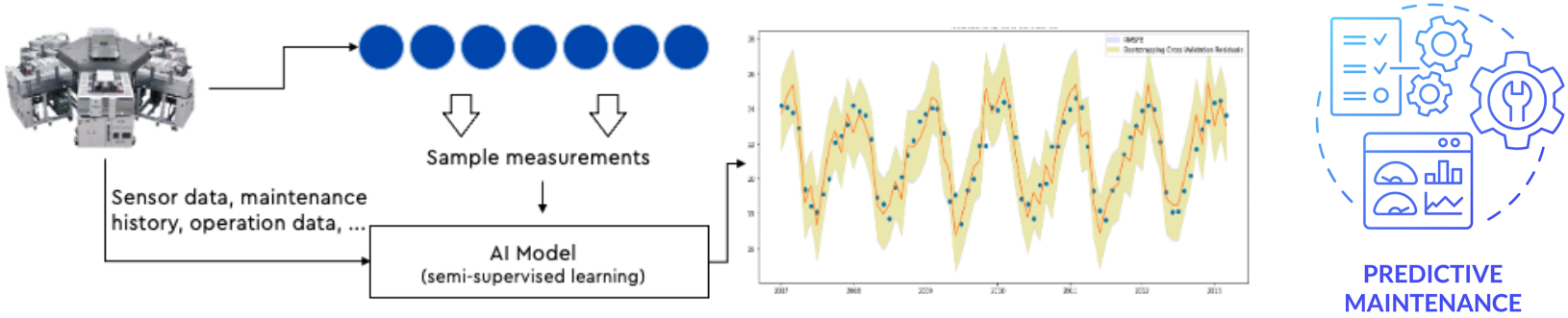
- new system provides
  - improved accuracy and reliability
  - improved throughput
  - savings on investment on measurement equipment



TS ML in manAI

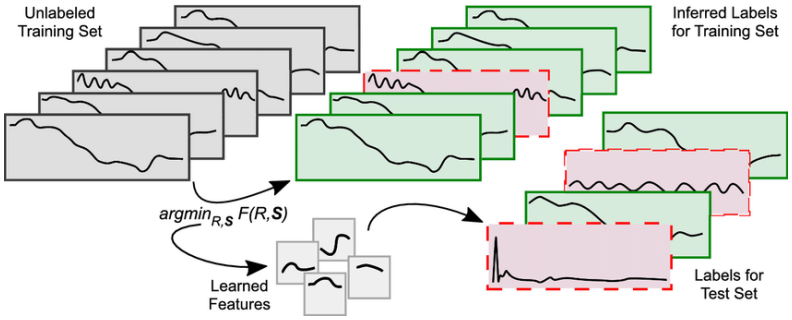
Time-series ML applications in manAI

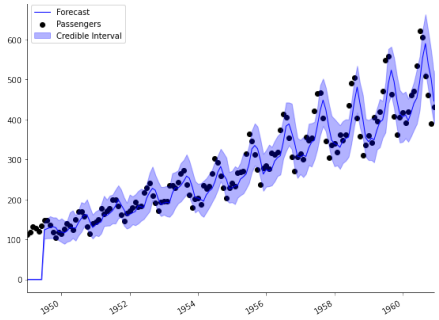
- estimation of TS values
  - virtual metrology - estimate measurement without physically measuring things
- anomaly detection on TS
  - predictive maintenance - predict maintenance times ahead
- multi-modal ML using LLM & genAI
  - root cause analysis and recommendation system



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



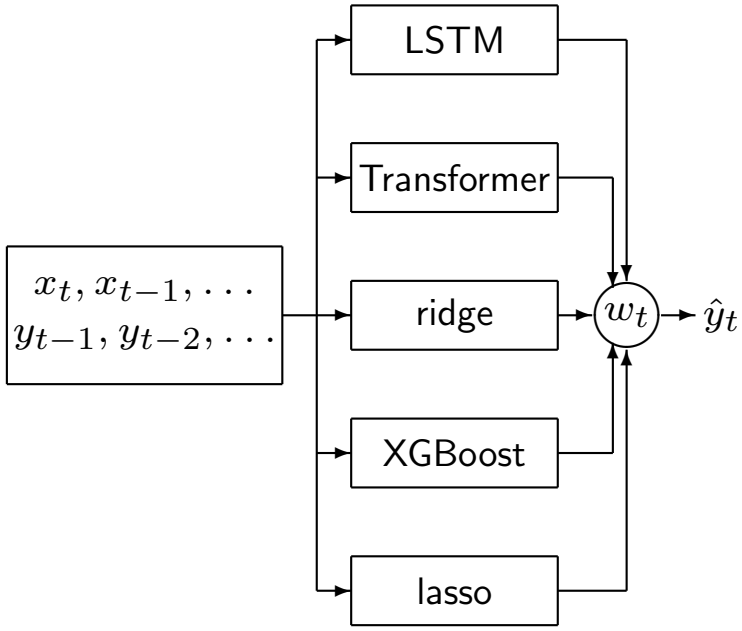


Difficulties with TS ML

- 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



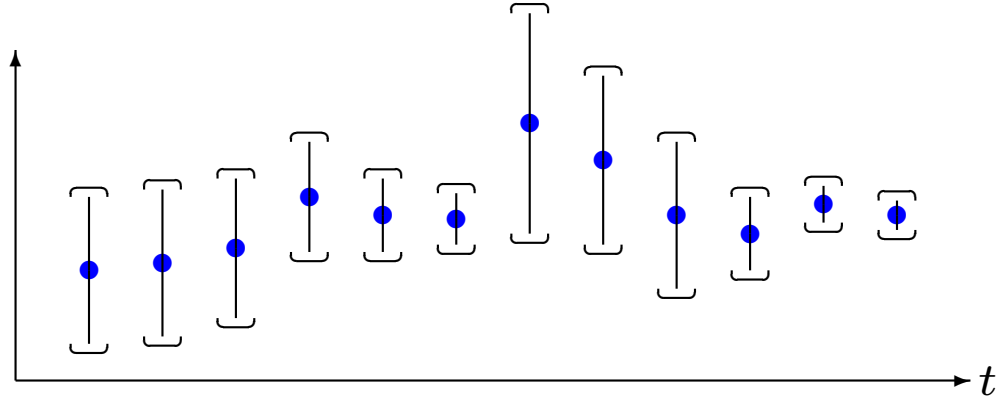
$$g_k = w_{1,k} f_{1,k} + w_{2,k} f_{2,k} + \cdots + w_{p_k,k} f_{p_k,k} = \sum_{i=1}^{p_k} w_{i,k} f_{i,k}$$

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*



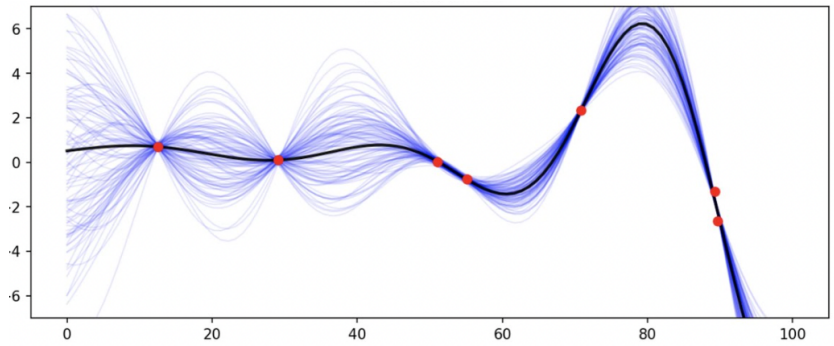
Bayesian approach for credibility interval evaluation

- 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

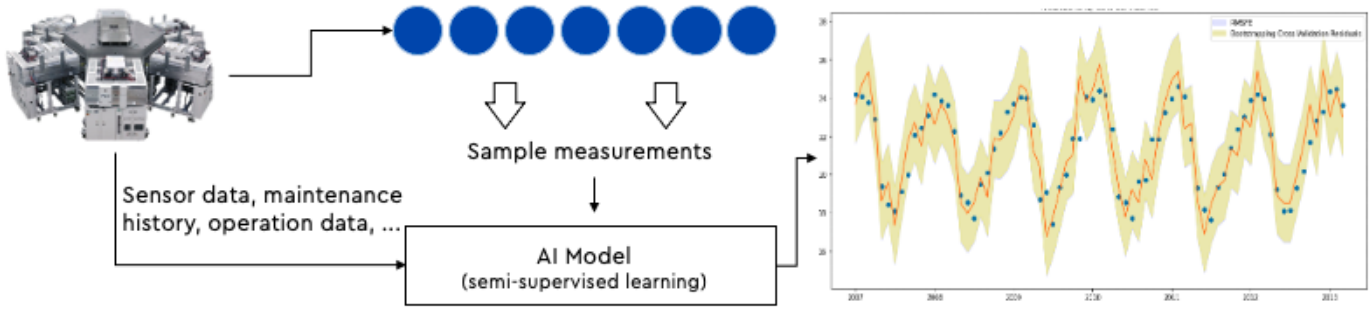
- problem description

$$\begin{array}{rl} \text{(stochastically) predict} & y_{t_k} \\ \text{given} & x_{t_k}, x_{t_{k-1}}, \ldots, y_{t_{k-1}}, y_{t_{k-2}}, \ldots \end{array}$$

- our problem formulation

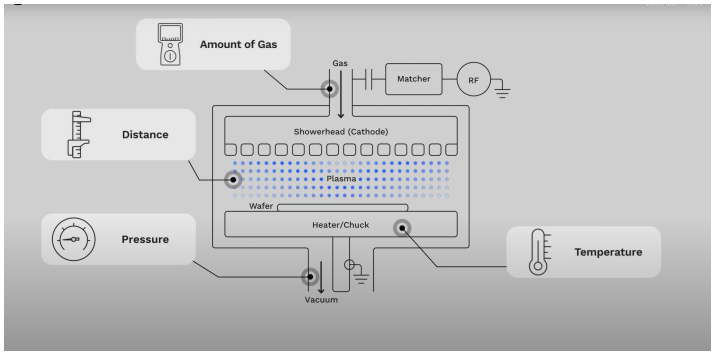
$$\begin{array}{ll} \text{minimize} & \sum_{k=1}^{K} w_{k,K-k}\, l(y_{t_k}, \hat{y}_{t_k}) \\ \text{subject to} & \hat{y}_{t_k} = g_k(x_{t_k}, x_{t_{k-1}}, \ldots, y_{t_{k-1}}, y_{t_{k-2}}, \ldots) \end{array}$$

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



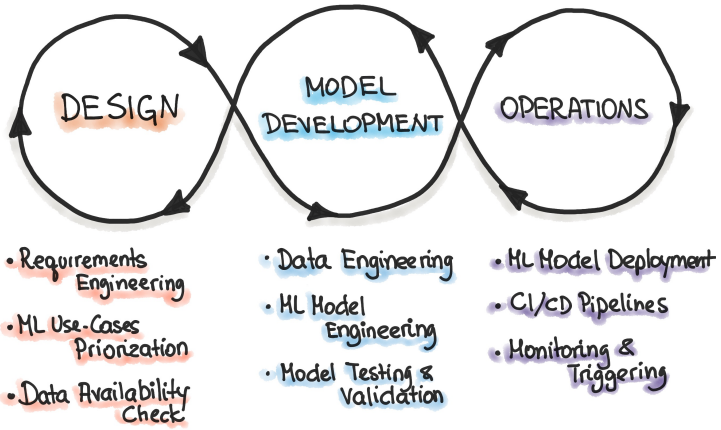
Manufacturing AI Productionization

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

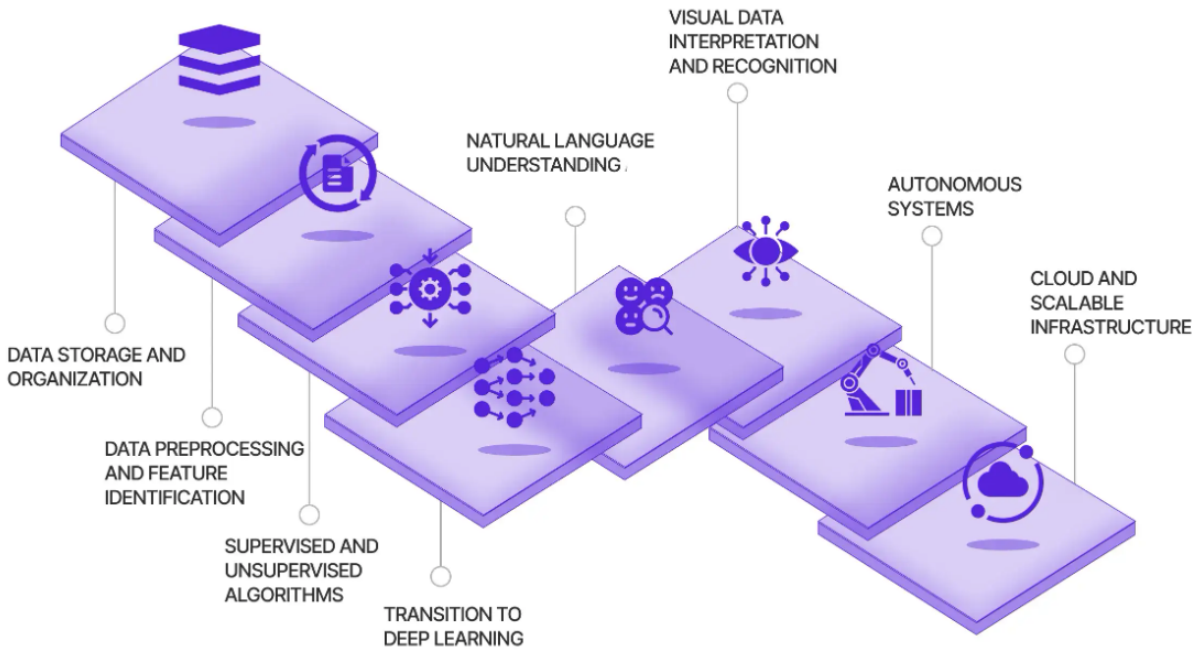
- environment for flexible and agile exploration - EDA[3]
- fast & efficient iteration of algorithm selection, experiements, & analysis
- correct training / validation / test data sets critical!
- seamless productionization from, $e.g.$, Jupyter notebook to production-ready code
- monitorning, *right* metrics, notification, re-training



[3] EDA - exploratory data analysis

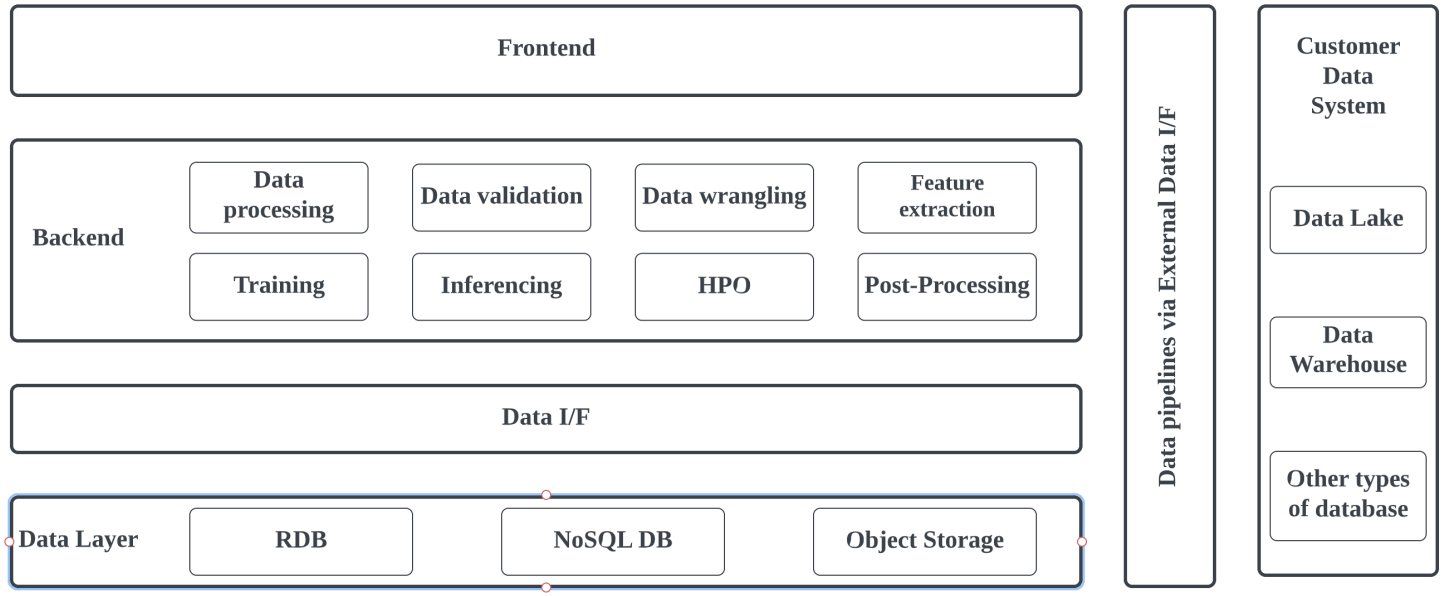
manAI software system

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



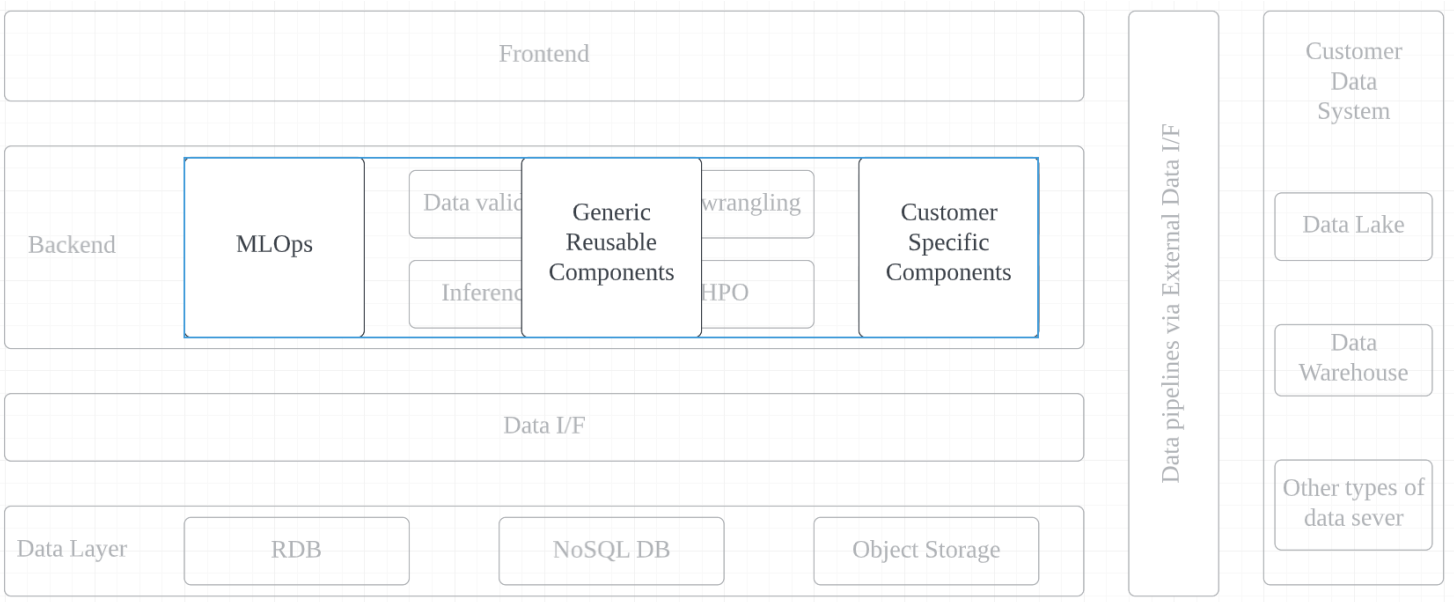
manAI system architecture

- 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

Silicon Valley's Cultural Engine of Innovation and Disruption

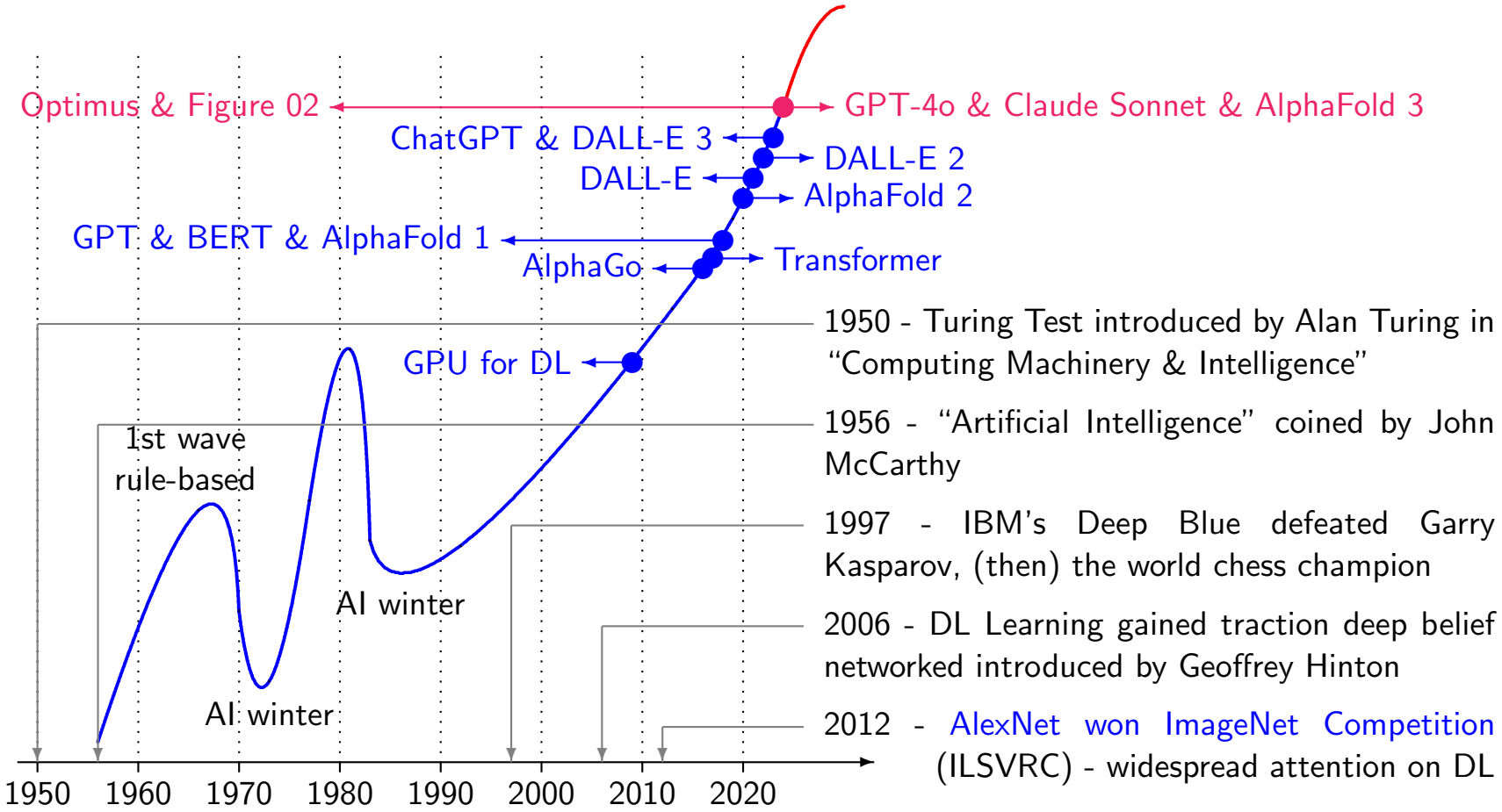
My journey from Samsung & Amazon to Gauss Labs & Erudio Bio

- Samsung Semiconductor, Inc.
  - inception into industry from academia, the world's best memory chip maker!
- Amazon.com, Inc.
  - experience so-called Silicon Valley big tech culture and technology
  - set tone for my future career trajectory!
- Gauss Labs, Inc.
  - found & operate AI startup, shaping corporate culture & spearheading R&D as CTO
  - inherent challenges of Korean conglomerate spin-off startup - cultural constraints, over-capitalization, and leadership limitations
- Erudio Bio, Inc.
  - concrete & tangible bio-technology in addition to AI
  - great decisions regarding business development; business models, market fit, go-to-market (GTM) strategies based on lessons learned *in a hard way* ☺



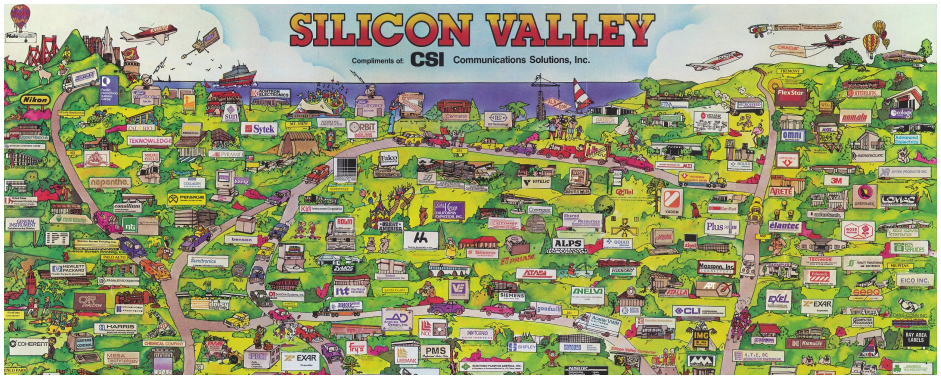


Joining Amazon.com, Inc. at the inflection point of AI



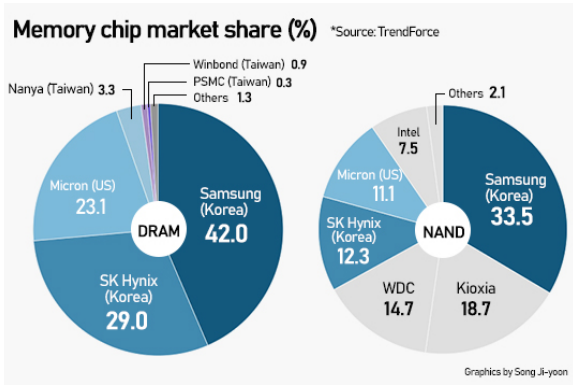
Innovation ecosystem of Silicon Valley

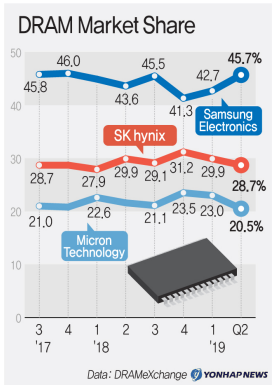
- key characteristics
  - risk-taking culture, *trust* in technology → *genuine* respect for engineers and scientists
  - easy access to huge capital - VCs, angel investors alike
  - talent density - engineers, researchers, scientists, entrepreneurs, PMs, TPMs, . . .
  - diversity, "collision density" of ideas
  - ecosystem of collaboration and competition - startups, academia, industry leaders
- what they mean for global big tech
  - set trends in AI, software & hardware (and or hence) product & industry innovation
  - act as testing ground for disruptive ideas



Case study: Amazon - amazing differentiators of big techs

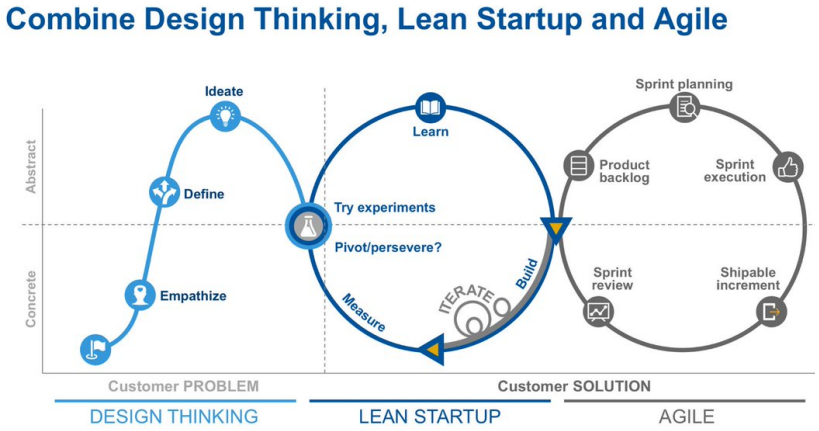
- Amazon's culture & leadership principles
  - customer obsession as driver of innovation
  - high standards & ownership culture, disagree & commit
  - bias for action and long-term thinking - sounds contradictory?
  - mechanisms like "two-pizza teams" & "Day One" for (or rather despite) scalability
- lessons for Korean corporations
  - applying customer-centric innovation in hardware & AI, *e.g.*, on-device AI
  - balancing agility with long-term R&D
  - *build / adapt / apply on the core strength of Samsung that no other company has!*

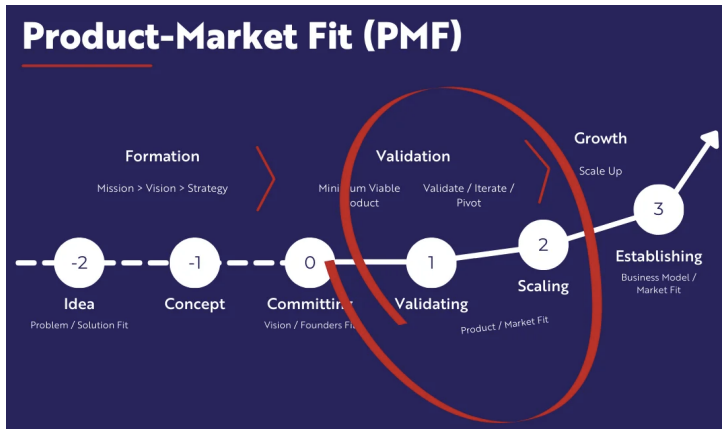




Founding and scaling startups

- challenges
  - competence of and chemistry among co-founders crucial
  - technology & great team are *necessary*, but *not sufficient (at all!)* for success
  - business models, market fit, timing, agility, flexibility for pivoting / perseverance
- insight
  - importance of domain expertise in addition to AI
  - balancing innovation with good business decisions





Bridging Silicon Valley & Korea

- cultural differences
  - risk appetite & failure tolerance
  - decision-making speed vs hierarchy
  - innovation vs execution focus
- opportunities for collaboration
  - leveraging Korea's manufacturing expertise with Silicon Valley's software/AI strengths
  - building global teams with diverse perspectives

To be successful . . .

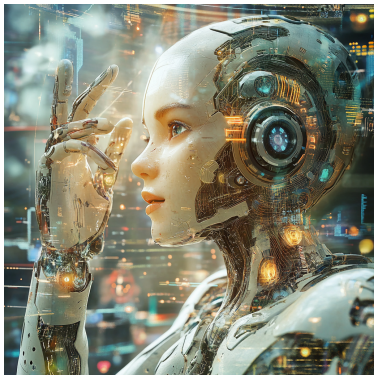
- embrace customer/market-centric mindset in innovation and for business decisions
- balance agility with long-term vision
- foster cross-cultural collaboration for global impact
- ((very) strategically and carefully) leverage AI to solve real-world industrial challenges

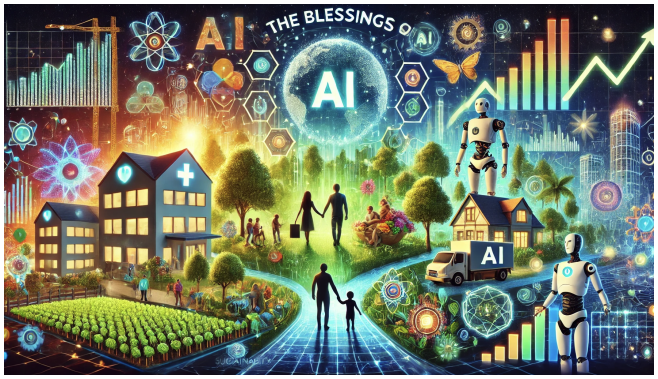
Empowering Humanity for Future Enriched by AI

Blessings & Curses of AI

Blessings

- advancements in healthcare & improved quality of life
  - much faster & more accurate diagnosis, far superior personalized medicine, accelerated drug discovery, assistive technologies
- economic growth & efficiency
  - automation to increase productivity and reduce cost, far superior decision-making
- environmental solutions
  - climate change prediction, global warming effect mitigation, solutions for sustainability
- safety & security
  - natural disaster prediction & relief, cybersecurity





Curses

- job displacement & overall impacts on labor market
  - millions of jobs threatened, wealth gap widened
- bias & inequality, misinformation & manipulation
  - existing human biases, both conscious and unconscious, perpetuated through AIs, asymmetric accessibility to advanced AI technologies by nations & corporations
- ethical dilemmas
  - infringing privacy & human rights, accountability for weapon uses and damages by AI
- environmental costs
  - significant energy for training AI models, waste generated by obsolescent AI hardware

Salzburg Global Seminar

KFAS-Salzburg Global Leadership Initiative

- "Uncertain Futures and Connections Reimagined: Connecting Technologies" - 41 global leaders convened from 4-Dec to 8-Dec, 2024 @ Schloss Leopoldskron in Salzburg, Austria
- My working group was "Technology, Growth, and Inequality: The Case of AI"
  - International Cooperation Officer (Portugal)
  - Gender Equality, Disability Inclusion Consultant, UN Women (Lithuania)
  - Assistant Professor @ Lincoln Alexander School of Law (Canada)
  - Research Associate @ Luxembourg Institute of Socio-Economic Research
  - Policy Officer & Delegation of the EU Union (India)
- blog: Bridging Technology & Humanity - Reflections from Lyon, Salzburg, and München

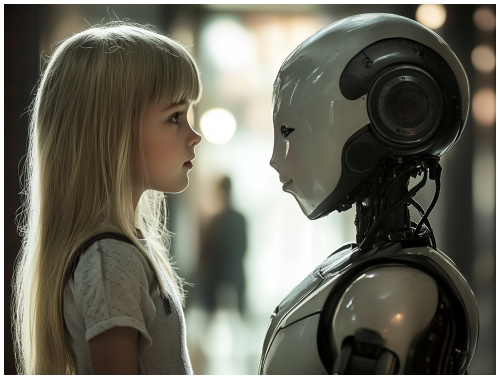
KFAS-Salzburg Global Leadership Initiative

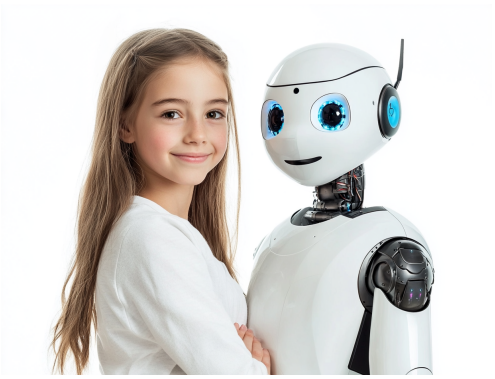
Salzburg Global photo collections

Empowering Humanity

AI capacity building - scientists, engineers & practitioners

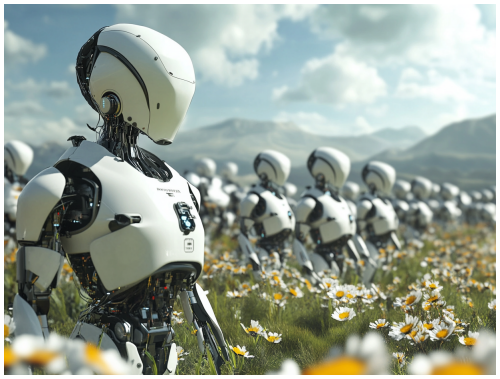
- ethics and responsible AI education or campaign via interdisciplinary collaboration
  - foster continuous learning programs on AI risks, bias & societal impacts
- bias detection & mitigation
  - bias-detection tools to identify & reduce discrimination in data & models
  - regular fairness audits
- transparency & explainability
  - explainable AI (xAI) techniques, frameworks like Model Cards for transparency
- environmental impact awareness
  - reduce AI's carbon footprint, advocate for sustainable AI development practices





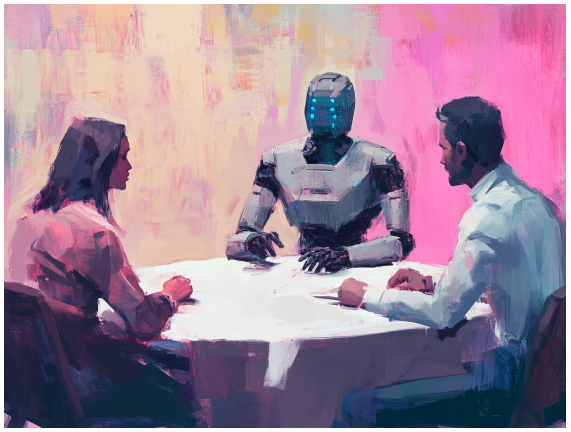
AI capacity building - lawmakers & policy makers

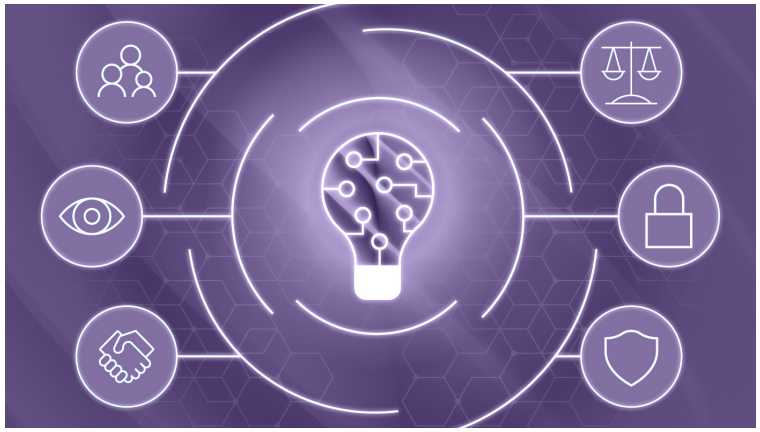
- problems
  - difficulties in understanding of rapidly evolving AI technologies
  - lead to reactive or insufficient regulation
- proposed solutions
  - develop comprehensive regulatory frameworks addressing transparency, bias & privacy concerns
    - gender bias, racial bias, hallucinations
  - foster public debates on ethical AI use & societal implications
  - introduce policies to limit spread of AI-generated misinformation,



Participatory social agreements

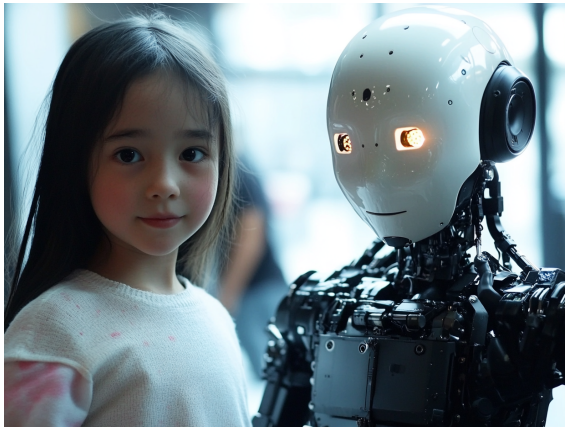
- open data frameworks including data sovereignty, regulation of data transfer, storage & localization
- corporate social responsibility, extra-territorial obligations & environmental protection
  - including outside the jurisdiction of the country
- labour and employment displacements, tax cuts & algorithmic impact assessments
  - including remedies for AI harms and enforcements





Reclaiming technology for Humanity

- strategic approach to AI development
  - *leverage very technologies alienating humans to strengthen human connection*
  - transform automation from replacement to *enhancement of human capabilities*
  - leverage technological scale to address fundamental human needs
- *paradigm shift* in technological implementation
  - recognize the duality of advanced technologies
  - *systematically channel AI capabilities toward human-centric solutions*
  - convert technological challenges into opportunities for human advancement



Some Important Questions around AI

Some important questions around AI

- why human-level AI?
- what lies in very core of DL architecture? what makes it work amazingly well?
- biases that can hurt judgement, decision making, social good?
- AI ethics & legal issues
- consciousness
- utopia vs dystopia
- knowledge, belief, reasoning
- risk of anthropomorphization

Human-level AI?

Why human-level in the first place?

- lots of times, when we measure AI performance, we say
  - how can we achieve human-level performance, $e.g.$, CV models?
- why human-level?
  - are all human traits desirable? are humans flawless?
  - aren't humans still evolving?
- advantage of AI over humans
  - $e.g.$, self-driving cars can use extra eyes, GPS, computer network
  - $e.g.$, recommendation system runs for hundreds of millions of people overnight
  - AI is available 24 / 7 while humans cannot
    . . . critical advanages for medical assitance, emergency handling
  - AI does not make more mistakes because task is repetative and tedius
  - AI does not request salary raise or go on strike

What makes DL so successful?

Factors constributing to astonishing success of DL

- analysis based on speaker's mathematical, numerical algorithmic & statistical perspectives considering hardware innovations

  30% universal approximation theorem? - (partially) yes! but that's not all

  - function space of neural network is *dense* (math theory), $i.e.$, for every $f : \mathbf{R}^n \to \mathbf{R}^m$, exists $\langle f_n \rangle$ such that $\lim_{n\to\infty} f_n = f$

  25% architectures/algorithms tailored for each class of applications, $e.g.$, CNN, RNN, Transformer, NeRF, diffusion, GAN, VAE, . . .

  20% data labeling - expensive, data availability - unlimited web text corpus

  15% computation power/parallelism - AI accelerators, $e.g.$, GPU, TPU & NPU

  10% rest - Python, open source software, cloud computing, MLOps, . . .

Sudden leap in LLM performance

Probability inferenced sequence is correct

- assume
  - t_i - ith token
  - p_i - probability that t_i is correct
  - ρ_i - correlation coefficient between t_{i-1} & t_i
  - $\tilde{p}_k$ - probability that $(t_1, \ldots, t_k)$ are correct
- recursion

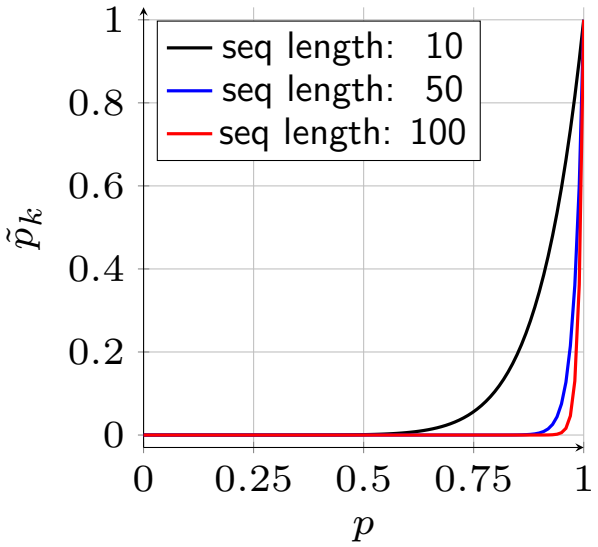
$$\rho_i = \frac{\tilde{p}_i - \tilde{p}_{i-1} p_i}{\sqrt{\tilde{p}_{i-1}(1 - \tilde{p}_{i-1}) p_i (1 - p_i)}}$$

$$\Leftrightarrow \qquad \tilde{p}_i = \tilde{p}_{i-1} p_i + \rho_i \sqrt{\tilde{p}_{i-1}(1 - \tilde{p}_{i-1}) p_i (1 - p_i)}$$

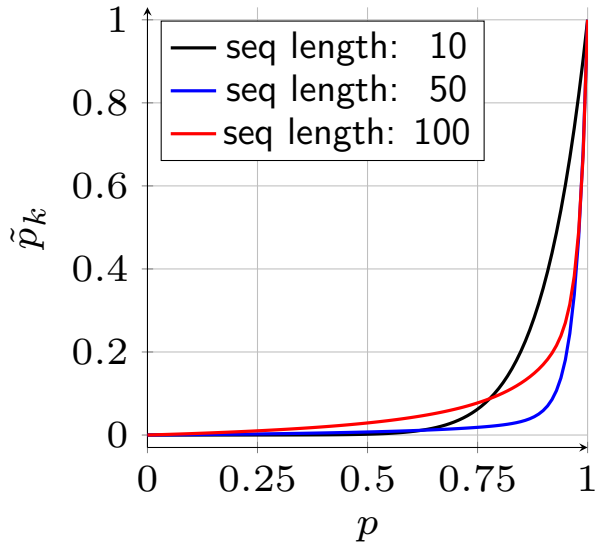
Dramatic improvement of LLM near saturation

- do simulations for both independent & dependent cases
  - assume p_i are same for all i
- (for both cases) sequence inference improves dramatically as p approaches 1
- this explains *why we have observed sudden dramatic performance improvement of certain seq2seq learning technologies*, $e.g.$, LLM

when tokens are independent



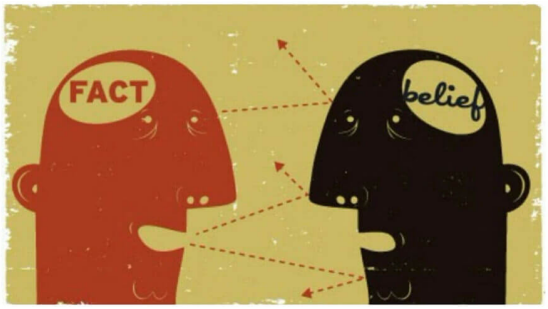
when tokens are dependent

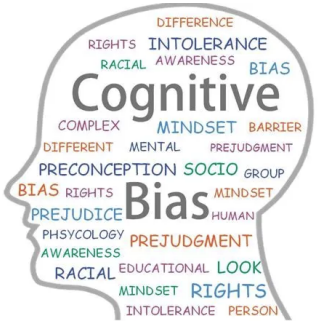


Biases

Cognitive biases attributed to humans

- cognitive biases [Kah11]
  - confirmation bias, availability bias
  - hindsight bias, confidence bias, optimistic bias
  - anchoring bias, halo effect, framing effect, outcome bias
  - belief bias, negativity bias, false consensus





Biases of LLMs

- LLMs subjec to
  - availability bias - baised by imbalancedly available information
    - LLM trained by imbalanced # articles for specific topics
  - belief bias - derive conclusion not by reasoning, but by what it saw
    - LLM eaisly inferencing what it saw, $i.e.$, data it trained on
  - halo effect - overemphasize on what prestigious figures say
    - LLM trained by imbalanced # reports about prestigious figures
- similar facts true for other types of ML models,
  - $e.g.$, video caption, text summarization, sentiment analysis
- cognitive biases only human represent
  - confirmation bias, hindsight bias, confidence bias, optimistic bias, anchoring bias, negativity bias, framing effect

AI Ethics

Ethical issues related to AI

- AI can be exploited by those who have bad intention to
  - manupilate / deceive people - using manupilated data corpus for training
    - $e.g.$, spread false facts
  - induce unfair social resource allocation
    - $e.g.$, medical insurance, taxation
  - exploit advantageous social and economic power
    - $e.g.$, unfair wealth allocation, mislead public opinion
- AI for Good - advocated by Andrew Ng
  - $e.g.$, public health, climate change, disaster management
- should scientists and engineers be morally & politically conscious?
  - $e.g.$, Manhattan project

AI related Legal Issues

Legal issues with ethical consideration

- scenario 1 - full self-driving algorithm causes traffic accident killing people
  - who is responsible? - car maker, algorithm developer, driver, algorithm itself?
- scenario 2 - self-driving cars kill less people than human drivers
  - $e.g.$, human drivers kill 1.5 people for 100,000 miles & self-driving cars kill 0.2 people for 100,000 miles
  - how should law makers make regulations?
  - utilitarian & humanitarian perspectives
- scenario 3 - someone is not happy with their data being used for training
  - "The Times sues OpenAI and Microsoft over AI use of copyrighted work" (Dec-2023)
  - "Newspaper publishers in California, Colorado, Illinois, Florida, Minnesota and New York said Microsoft and OpenAI used millions of articles without payment or permission to develop ChatGPT and other products" (Apr-2024)

Consciousness

Consciousness

- what is consciousness, anyway?
  - recognizes itself as independent, autonomous, valuable entity?
  - recognizes itself as living being, unchangeable entity?
- no agreed definition on consciousness exists yet
  . . . and will be so forever
- does it have anything to do with the fact that humans are biologically living being?
- is SKYNET ever plausible?
  - can AI have *desire* to survive (or save earth)?

Utopia vs Dystopia

Utopia vs dystopia

- not important questions (at all) *I think . . .*
- what we should focus on is *not* the possibilities of doomday or Judgment Day, but rather
  - our limits on controlling unintended impacts of AI
  - *misuse* by (greedy, immoral, and unethical) people possessing social, economic & political power
  - *social good and welfare impaired* by either exploiting AI or ignorance of (inner workings of) AI
- should concern
  - choice or balance among utilitarianism, humanitarianism & values
  - amend or improve laws/regulations
  - ethical issues caused by AI

Knowledge, Belief, and Reasoning

Does AI (LLM) have knowledge or belief? Can it reason?

What categories of questions do they belong to?

engineering, scientific, philosophical, cognitive scientific, . . . ?

LLMs . . .

- LLM is very different sort of animal . . . except that it is *not* an animal!
- *unreasonable* effectiveness of data [HNF09]
  - *performance scales with size of training data*
  - *qualitative leaps* in capability as models scale
  - tasks demanding human intelligence *reduced to next token prediction*
- focus on third surprise

  conditional probability model looks like human with intelligence

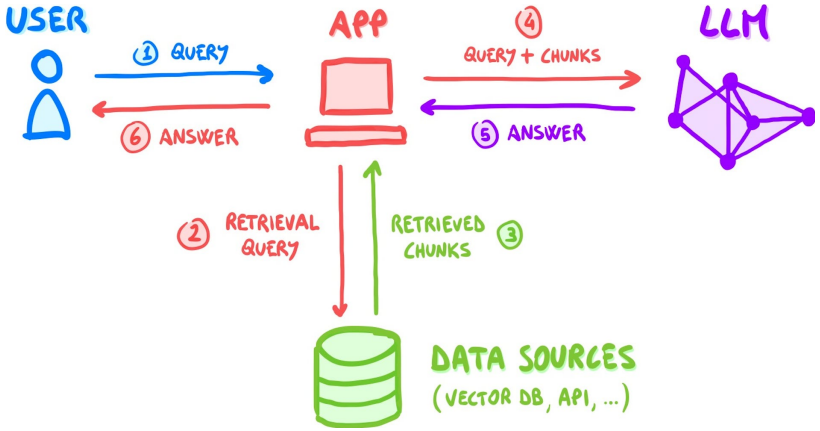
  - making vulnerable to anthropomorphism
- examine it by throwing questions such as
  - *"does LLM have knowledge and belief?"*
  - *"can it reason?"*

What LLM really does!

- given prompt "the first person to walk on the Moon was", LLM responds with "Neil Armstrong". . . strictly speaking
  - it's *not* being asked *who* was the first person to walk on the Moon
  - what are being *really* asked is *"given statistical distribution of words in vast public corpus of text, what words are most likely to follow 'The first person to walk on the Moon was'?"*
- given prompt "after ring was destroyed, Frodo Baggins returned to", LLM responds with "the Shire"
  - on one level, it seems fair to say, you might be testing LLM's knowledge of fictional world of Tolkien's novels
  - what are being *really* asked is *"given statistical distribution of words in vast public corpus of text, what words are most likely to follow 'After the ring was destroyed, Frodo Baggins returned to'?"*

LLMs vs systems in which they are embedded

- crucial to distinguish between the two (for philosophical clarity)
  - LLM (bare-bones model) - highly specific & well-defined function, which is *conditional probability estimator*
  - systems in which LLMs are embedded, $e.g.$, for question-answering, news article summarization, screenplays generation, language translation



How ChatBot works?

- conversational AI agent does *in-context learning* or *few-shot prompting*
- for example,
  - when the user enters

    ```
    who is the first person to walk on the Moon?
    ```

  - ChatBot, LLM-embedded system, feeds the following to LLM

    ```
    User, a human, and BOT, a clever and knowledgeable AI agent.
    User:  what is 2+2?
    BOT: the answer is 4.
    User:  where was Albert Einstein born?
    BOT: he was born in Germany.
    User:  who is the first person to walk on the Moon?
    BOT:
    ```

Knowledge, belief & reasoning around LLM

- *not* easy topic to discuss, or even impossible because
  - we *do not have agreed definition* of these terms especially in context of being asked questions like

    does LLM have belief?

    or

    do humans have knowledge?

- let us discuss them in two different perspectives
  - laymen's perspectives
  - cognitive scientific & philosophical perspectives

Laymen's perspectives on knowledge, belief & reasoning

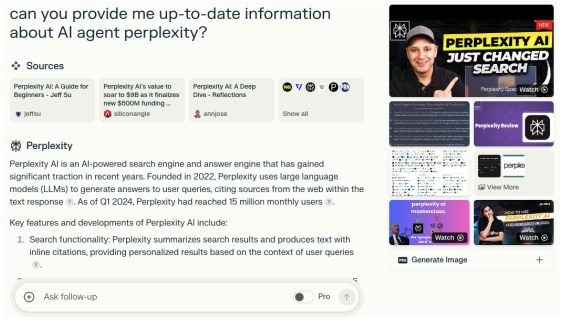
- does (good) LLM have knowledge?
  - Grandmother: looks like it cuz when instructed *"explaing big bang"*, it says
    " The Big Bang theory is prevailing cosmological model that explains the origin and evolution of the universe. . . . 13.8 billion years ago . . . "
- does it have belief?
  - Grandmother: I don't think so, $e.g.$, it does not believe in God!
- can it reason?
  - Grandmother: seems like it! $e.g.$, when asked *"Sunghee is a superset of Alice and Beth is a superset of Sunghee. is Beth a superset of Alice?"*, it says
    " Yes, based on information provided, if Sunghee is a superset of Alice and Beth is a superset of Sunghee, then Beth is indeed a superset of Alice . . . "
- can it reason to prove theorem whose inferential structure is more complicated?
  - Grandmother: I'm not sure – actually, I don't know what you're talking about!

Knowledge

- could argue LLM "knows" which words follow which other words with high probability
- but, only *in context of capacity to distinguish truth from falsehood* can we legitimately speak of "knowledge"!
- LLM(-embedded BOT)
  - can be said to *"encode"*, *"store"*, *or "contain"* knowledge
  - lacks means to use words "true" & "false" in all ways & in all contexts because . . .
  - *does not inhabit the world* we human language-users share!

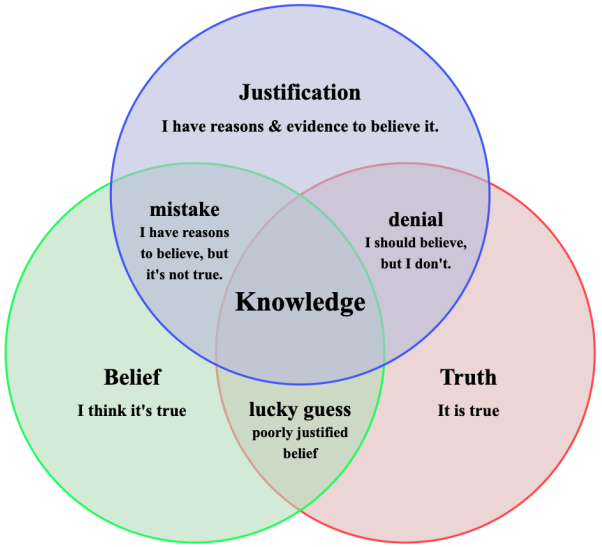
Belief

- nothing can count as *belief about the world* we share unless
  - is against backdrop of *"ability to update beliefs appropriately in light of evidence from that world*" - (again) essential capacity to distinguish truth from falsehood
- change taking place in humans when acquiring or updating belief is
  - reflection of their nature as language-using animals inhabiting shared world with community of language-users
- then, *what if LLM-embedded system updates LLM with outside world information?*
  - even so, when interacting with AI systems based on LLMs, these grounds are *absent*!



Knowledge in philosophical and cognitive scientific sense

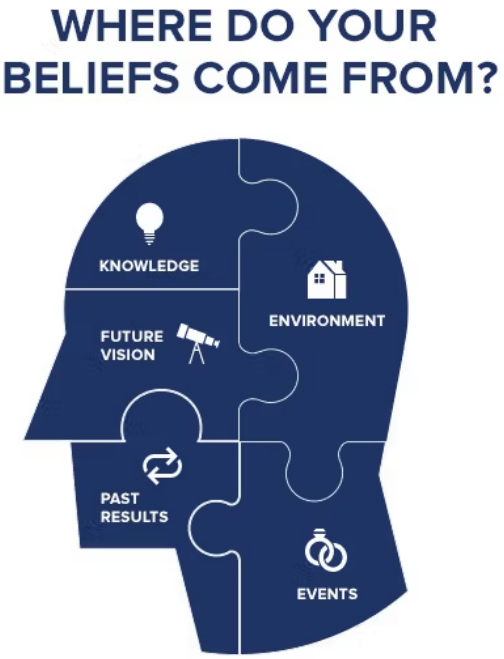
- does LLM have knowledge?
  - Sunghee: *I don't think so!*
- why?
  - we say we have "knowledge" when
    "we do so against ground of various human capacities that we all take for granted when we engage in everyday conversation with each other."
  - when asked *"who is Tom Cruise's mother?"*, it says *"Tom Cruise's mother is Mary Lee Pfeiffer."* However, this is nothing but
    "guessing" by conditional probability model the most likely words following "Tom Cruise's mother is."
  - so *we cannot say it really knows the fact!*



Belief in philosophical and cognitive scientific sense

- for the discussion
  - do *not* concern any specific belief
  - but concern *prerequisites for ascribing any beliefs to AI system*
- so does it have belief?
  - nothing can count as belief about the world we share unless

    it is against ground of the ability to update beliefs appropriately in light of evidence from that world, essential aspect of the capacity to distinguish truth from falsehood
  - LLM does not have this ground, essential consideration when deciding whether it *really* had beliefs.
- Sunghee: so *no, LLM cannot have belief!*



Reasoning in philosophical and cognitive scientific sense

- note reasoning is *content neutral*
  - $e.g.$, following logic is perfect regardless of truth of premises
  - hence, no access to outside world does *not* disqualify
- when asked *"if humans are immortal, would Socrates have survived today?"*, LLM says
  " . . . it's logical to conclude that Socrates would likely still be alive today. . . . "
- however, remember, once again, what we just asked it to do is *not* "deductive inference"
  given the statistical distribution of words in public corpus, what words are likely to follow the sequence, "humans are immortal and Socreates is human therefore."
- Sunghee: so *no, LLM cannot reason, either!*
- but, LLM
  - pretends to reason, and from which capabilities, we can benefit!
  - also, can *mimic even multi-step reasoning whose inferencing structure is complicated* using *chain-of-thoughts prompting*, $i.e.$, *in-context learning* or *few-short prompting*

Simple example showing LLM not possessing knowledge

- User

  "Who is Tom Cruise's mother?"

- LLM(-embedded question-answering system) (as of Jan 2022)

  "Tom Cruise's mother is Mary Lee Pfeiffer. She was born Mary Lee South. . . . Information about his family, including his parents, has been publicly available, *. . . "*

- User

  "Who is Mary Lee Pfeiffer's son?"

- LLM(-embedded question-answering system) (as of Jan 2022)

  "As of my last knowledge update in January 2022, I don't have specific information about Mary Lee Pfeiffer or her family, including her son. *. . . "*

Risk of anthropomorphization

- unfortunately, contemporary LLMs are *too powerful, too versatile, and too useful for most people to accept (after understanding) previous arguments!*
- maybe, o.k. for laymen to (mistakenly) anthropomorphize LLM(-embedded systems)
- however, *imperative for (important, smart, and responsible) AI researchers, scientists, engineers & practitioners* to have rigorous understanding in these aspects especially when
  - advise and be consulted by law makers, policy makers, journalists, and various stakeholders responsible for *critical business decisions (in private sectors) and public policies (in public sectors)*
  - collaborate with or/and help professionals in liberal arts, such as *philosophy, ethics, law, religion, literature, history, music, cultural studies, psychology, sociology, anthropology, political science, economics, archaeology, linguistics, media studies, natural sciences, fine arts, . . .*

  — to address negative soceital and economic impacts

Moral

- AI shows incredible utility and commercial potentials, hence should
  - make informed decisions about trustworthiness and safety
  - avoid ascribing capacities they lack
  - *take best utilization of remarkable capabilities of AI*
- today's AI so powerful, so (seemingly) convincingly intelligent
  - obfuscate mechanism
  - actively encourage *anthropomorphism* with philosophically loaded words like *"believe"* and *"think"*
  - easily mislead people about character and capabilities of AI
- matters not only to scientists, engineers, developers, and entrepreneurs, but also
  - *general public, law & policy makers, journalists, . . .*

Recent AI Development

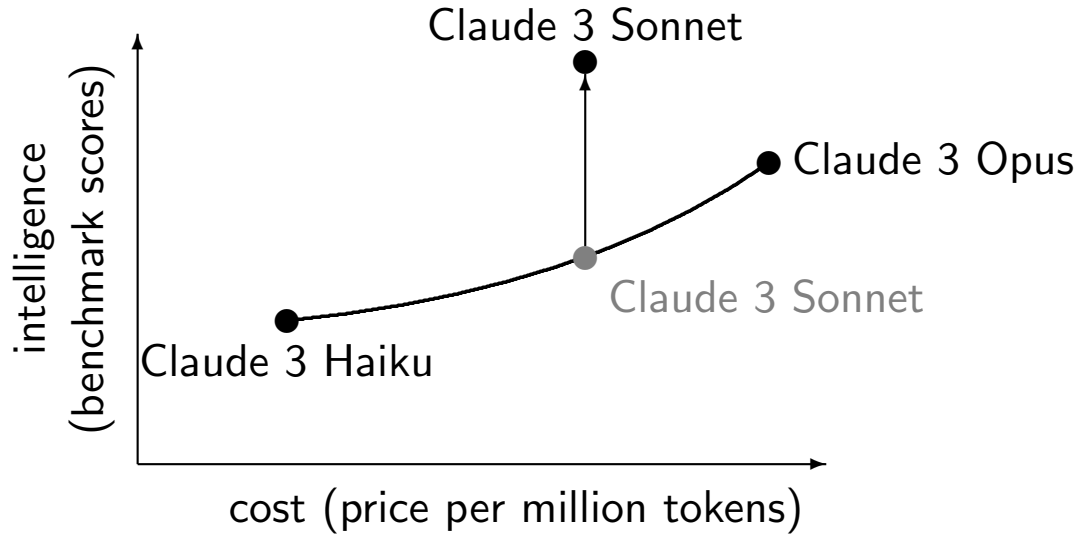
Notable recent AI research and new development

- Claude 3.5 Sonnet
- Kolmogorov–Arnold networks (KAN)
- JEPA ($e.g.$, I-JEPA & V-JEPA) & consistency-diversity-realism trade-off

Claude 3.5 Sonnet

Claude 3.5 Sonnet

- Anthropic
  - releases Claude 3.5 Sonnet (Jul-2024)
    - when! GPT-4o accepted to be default best model for many tasks, $e.g.$, reasoning & summarization
  - claims Claude 3.5 Sonnet sets *new industry standard for intelligence*



Main features & performance

- Claude 3.5 Sonnet shows off
  - improved vision tasks, 2x speed (compared to GPT-4o), artifacts - new UIs for, $e.g.$, code generation & animation
- with GPT-4o, Claude 3.5 Sonnet
  - wins at code generation
  - on par for logical reasoning
  - loses at logical reasoning
  - *wins at generation speed*

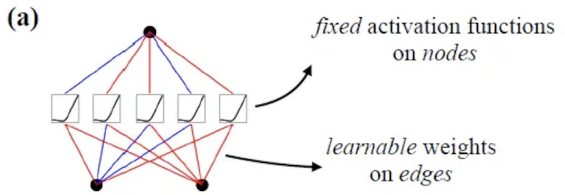
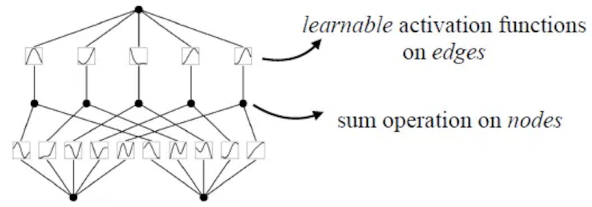
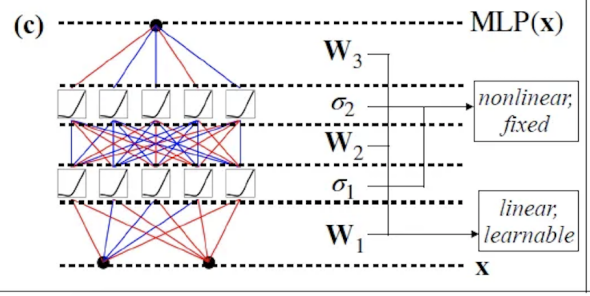
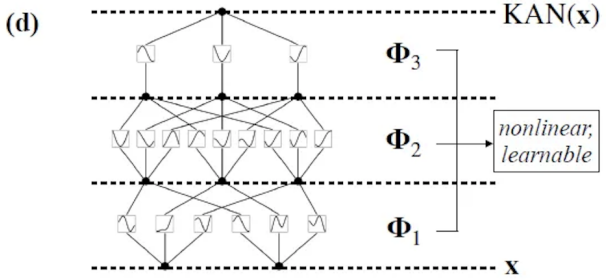
	Claude 3.5 Sonnet	Claude 3 Opus	GPT-4o	Gemini 1.5 Pro
visual math reasoning	67.7%	50.5%	63.8%	63.9%
science diagrams	94.7%	88.1%	94.2%	94.4%
visual question answering	68.3%	59.4%	69.1%	62.2%
chart Q&A	90.8%	80.8%	85.7%	87.2%
document visual Q&A	95.2%	89.3%	92.8%	93.1%

KAN

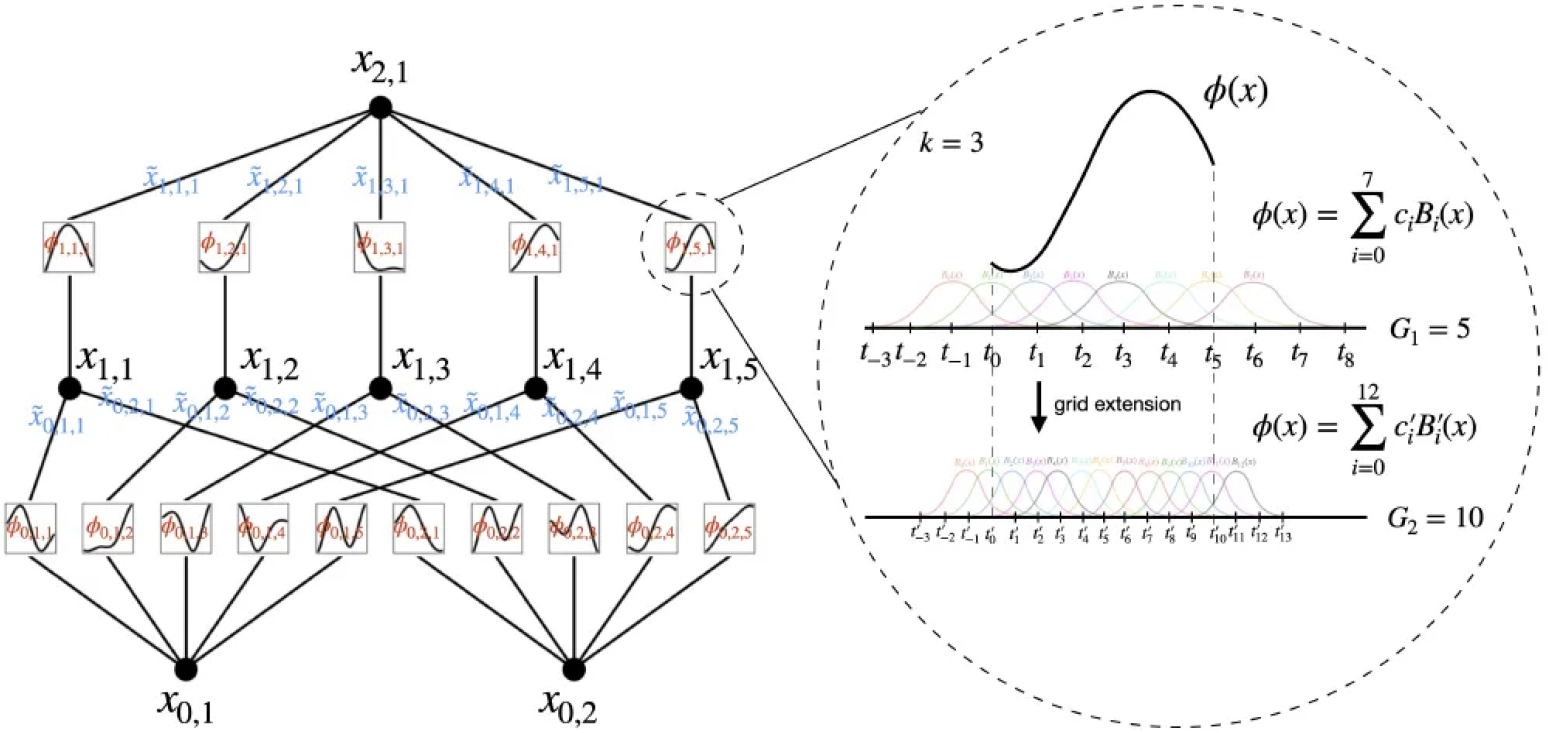
Kolmogorov–Arnold networks (KAN)

- KAN: Kolmogorov-Arnold Networks - MIT, CalTech, Northeastern Univ. & IAIFI
- techniques
  - inspired by Kolmogorov-Arnold representation theorem - every $f : \mathbf{R}^n \to \mathbf{R}$ can be written as finite composition of continuous functions of single variable, $i.e.$
    $$f(x) = \sum_{q=0}^{2n} \Phi_q \left(\sum_{p=1}^{n} \phi_{q,p}(x_p) \right)$$
    where $\phi_{q,p} : [0, 1] \to \mathbf{R}$ & $\Phi_q : \mathbf{R} \to \mathbf{R}$
  - replace (fixed) activation functions with learnable functions
  - use B-splines for learnable (uni-variate) functions - for flexibility & adaptability
- advantages
  - benefits structure of MLP on outside & splines on inside
  - reduce complexity and # parameters to achieve accurate modeling
  - *interpretable* by its nature
  - *better continual learning* - adapt to new data without forgetting thanks to local nature of spline functions

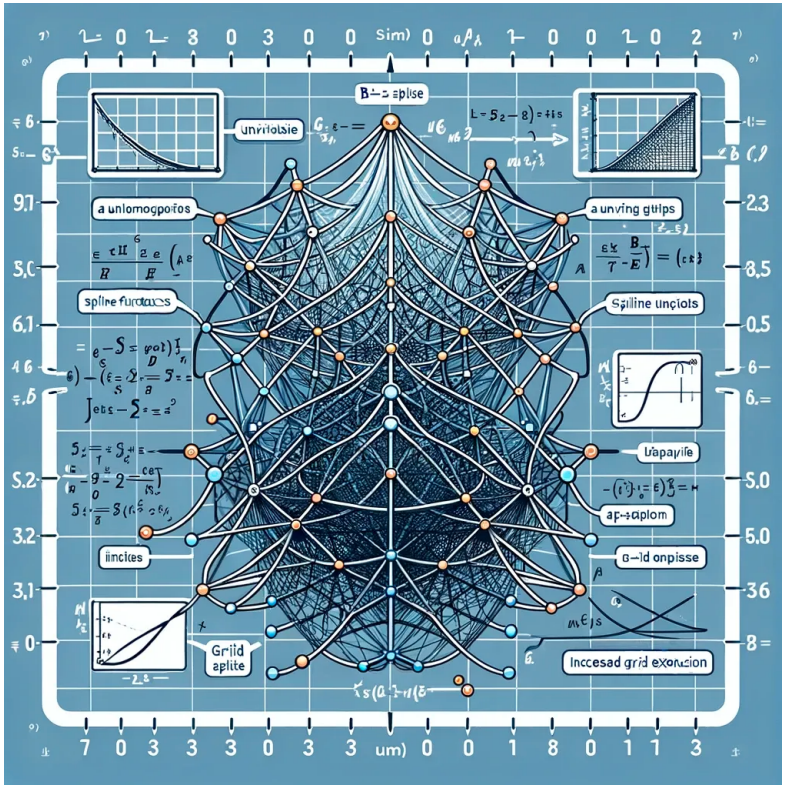
MLP vs KAN

Model	Multi-Layer Perceptron (MLP)	Kolmogorov-Arnold Network (KAN)
Theorem	Universal Approximation Theorem	Kolmogorov-Arnold Representation Theorem
Formula (Shallow)	$f(\mathbf{x}) \approx \sum_{i=1}^{N(\epsilon)} a_i \sigma(\mathbf{w}_i \cdot \mathbf{x} + b_i)$	$f(\mathbf{x}) = \sum_{q=1}^{2n+1} \Phi_q \left(\sum_{p=1}^{n} \phi_{q,p}(x_p) \right)$
Model (Shallow)		
Formula (Deep)	$\mathrm{MLP}(\mathbf{x}) = (\mathbf{W}_3 \circ \sigma_2 \circ \mathbf{W}_2 \circ \sigma_1 \circ \mathbf{W}_1)(\mathbf{x})$	$\mathrm{KAN}(\mathbf{x}) = (\mathbf{\Phi}_3 \circ \mathbf{\Phi}_2 \circ \mathbf{\Phi}_1)(\mathbf{x})$
Model (Deep)		

KAN architecture with spline parametrization unit layer



Future work on KAN



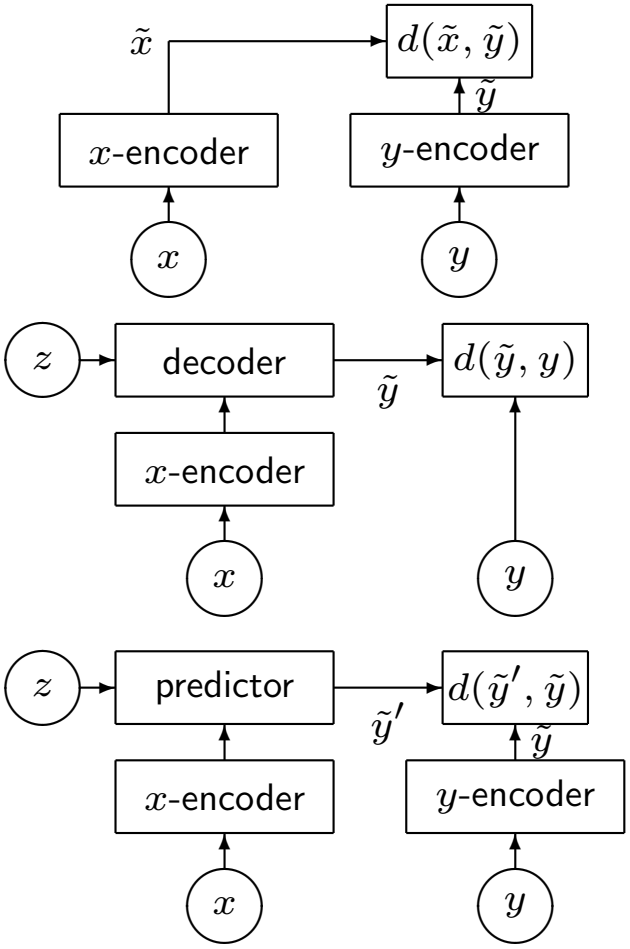
- natural question is
  - what if use both MLP and KAN?
  - what if use other types of splines?
  - how to control forgetfulness of continual learning?
  - why functions of one varible? possible to use functions of two variables?

(figure created by DALLE-3)

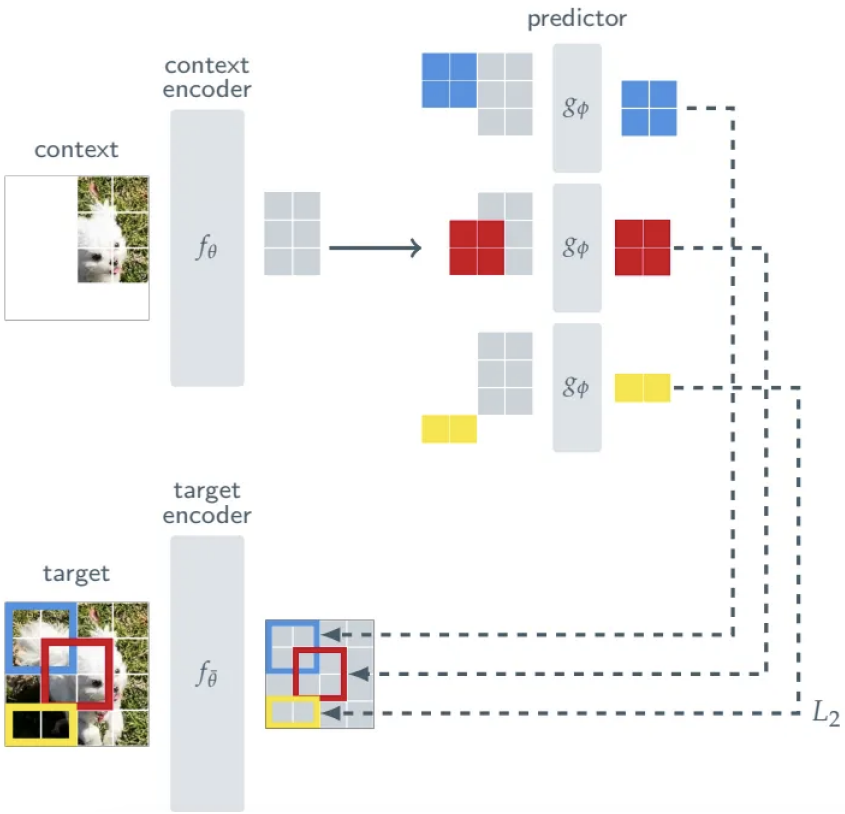
JEPA

Joint-Embedding Predictive Architecture (JEPA)

- Self-Supervised Learning from Images with a Joint-Embedding Predictive Architecture (JEPA) - Yann LeCun et al. - Jan-2023
  - joint-embedding architecture (JEA)
    - output similar embeddings for compatible inputs x, y and dissimilar embeddings for incompatible inputs
  - generative architecture
    - directly reconstruct signal y from compatible signal x using decoder network conditioned on additional variables z *to facilitate reconstruction*
  - joint-embedding predictive architecture (JEPA)
    - similar to generative architecture, but comparison is done in embedding space
    - *e.g.*, I-JEPA learns y (masked portion) from x (unmasked portion) conditioned on z (position of mask)



Learning semantic representation better

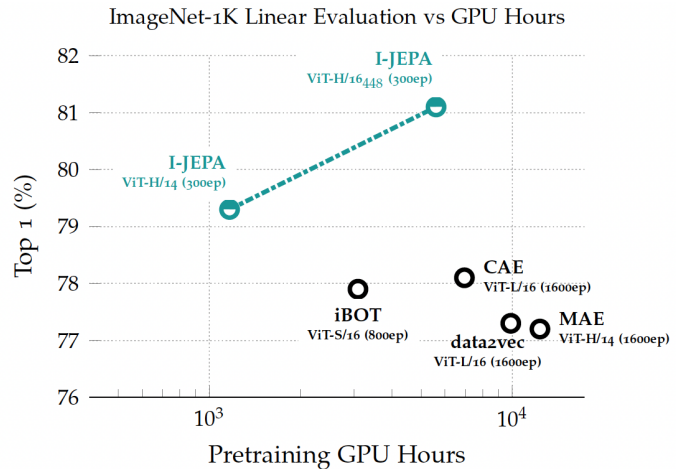


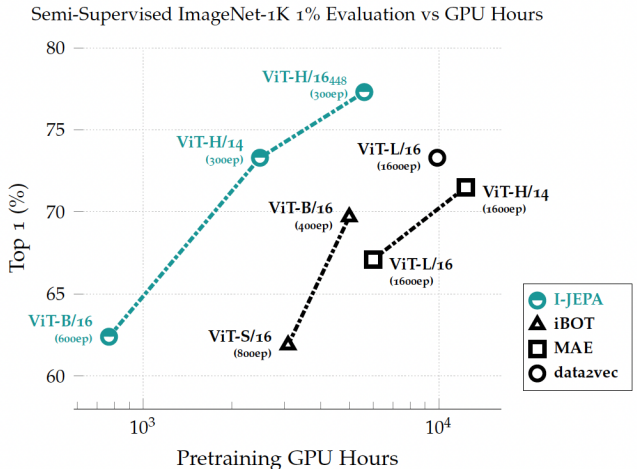
- I-JEPA
  - predicts missing information in *abstract representation space*
    - $e.g.$, given single context block (unmasked part of the image), predict representations of various target blocks (masked regions of same image) where target representations computed by learned target-encoder
  - *generates semantic representations* (not pixel-wise information) potentially eliminating unnecessary pixel-level details & allowing model to concentrate on learning more semantic features

I-JEPA outperforms other algorithms

Method	Arch.	CIFAR100	Places205	iNat18
Methods without view data augmentations				
data2vec [8]	ViT-L/16	81.6	54.6	28.1
MAE [36]	ViT-H/14	77.3	55.0	32.9
I-JEPA	ViT-H/14	**87.5**	**58.4**	**47.6**
Methods using extra view data augmentations				
DINO [18]	ViT-B/8	84.9	57.9	55.9
iBOT [79]	ViT-L/16	**88.3**	**60.4**	**57.3**

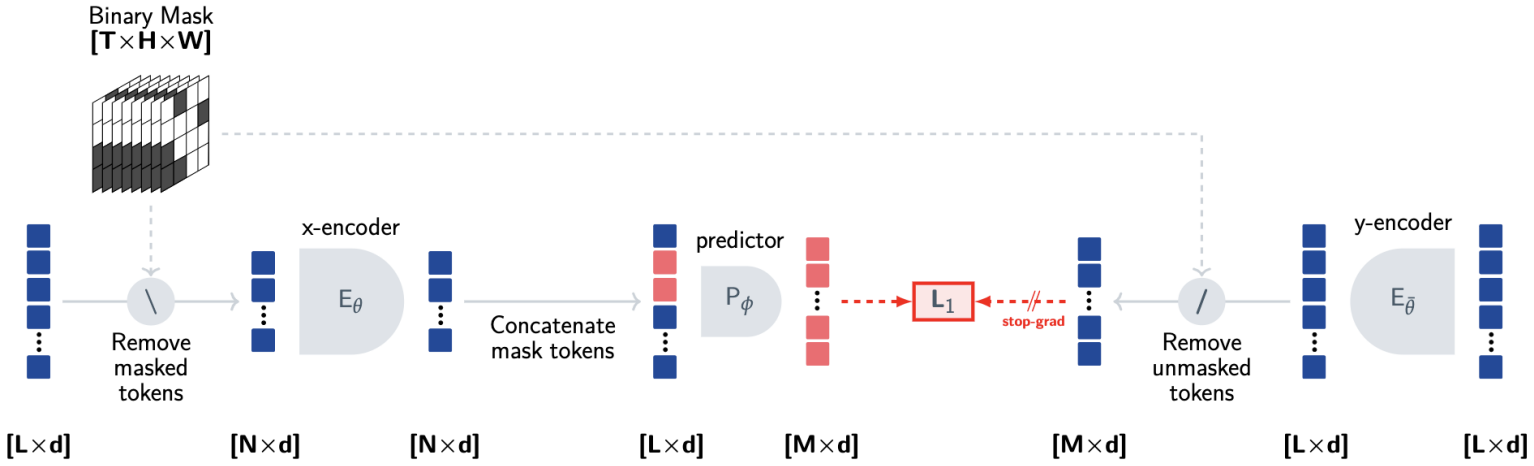
Method	Arch.	Clevr/Count	Clevr/Dist
Methods without view data augmentations			
data2vec [8]	ViT-L/16	85.3	71.3
MAE [36]	ViT-H/14	**90.5**	**72.4**
I-JEPA	ViT-H/14	86.7	**72.4**
Methods using extra data augmentations			
DINO [18]	ViT-B/8	86.6	53.4
iBOT [79]	ViT-L/16	85.7	62.8





V-JEPA

- Revisiting Feature Prediction for Learning Visual Representations from Video - Yann LeCun et al. - Feb-2024
  - essentially same ideas of JEPA - loss function is calculated in embedding space - for better semantic representation learning (rather than pixel-wise learning)



More realistic generative model becomes, less diverse it becomes

- Consistency-diversity-realism Pareto fronts of conditional image generative models - FAIR at Meta - Montreal, Paris & New York City labs, McGill University, Mila, Quebec AI institute, Canada CIFAR AI - Jun-2024

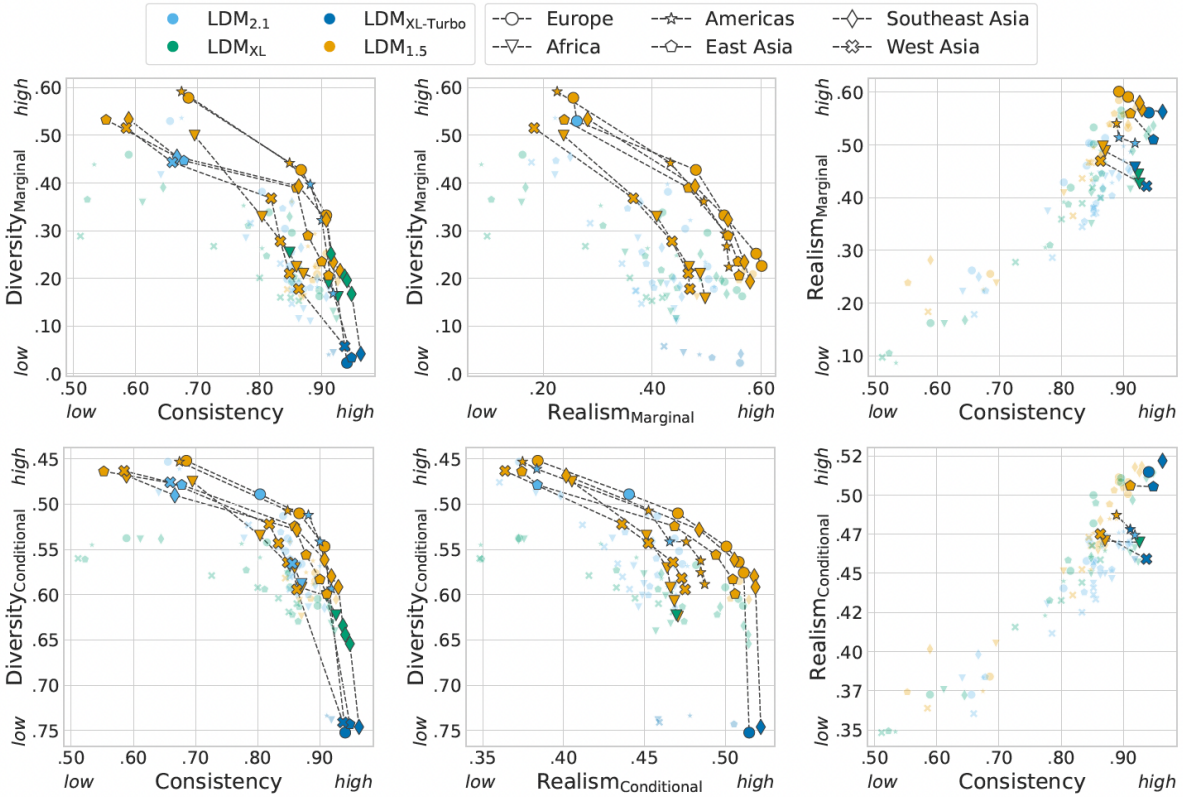
- realism comes at the cost of coverage, $i.e.$, *the most realistic systems are mode-collapsed!*

- intuition (or hunch)

  – world models should *not* be generative - should make predictions in representation space - in representation space, unpredictable or irrelevant information is absent

$\rightarrow$ main argument in favor of JEPA

Consistency-diversity-realism trade-off



Learning ML & AI

Best ways to learn ML & AI

- first, learn basics - college classes, online courses, (easy) books
  - not need to understand every mathematical details, but should know rough ideas!
- hands-on is MUST!
  - learn and practice coding - `Python` is MUST; do not do only `R`
  - learn `git` - know how to develop efficiently, plus `import` others' work
- *(I think) online cources are blessing to mankind!*
  - you *can't* say "I can't do it because resource is not available or classes of good schools are not available" because . . . they are available! :)
  - getting (expensive) certificates is good idea because . . . otherwise you wouldn't finish it! :) plus you can post it on your LinkedIn
- would be best if your task at work is related to ML
- however, even if that's not the case or can't be the case, can always do your own personal projects – or contribute to public projects (on `github`)!

Andrew Ng!

- Andrew Ng
  - (co-)founder of "Deep Learning.AI" and "Coursera", prominent figure in ML & AI
  - his courses highly regarded because well-structured and provide insights

- latest Andrew Ng courses
  - AI Agents in LangGraph
  - AI Agentic Design Patterns with AutoGen
  - Introduction to On-device AI
  - Multi AI Agent Systems with Crew AI
  - Building Multimodal Search and RAG - contrastive learning, multimodality to RAG
  - Building Agentic RAG with LlamaIndex
  - Quantisation In Depth
  - In Prompt Engineering for Vision Models
  - Getting Started with Mistral - open-source models (Mistral 7B, Mixtral 8x7B)
  - Preprocessing Unstructured Data for LLM

ML Prerequisites

Linear Algebra Basics

Scalars, vectors, and matrices

- real number $a \in \mathbf{R}$, called *scalar*
- (ordered) collection of real numbers $(a_1, \ldots, a_n) \in \mathbf{R}^n$, called *vector*

$$\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \in \mathbf{R}^n \quad \text{- column vector}$$

$$\begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix} \in \mathbf{R}^{1\times n} \quad \text{- row vector}$$

- (ordered) collection of 2-dimensional array, called *matrix*

$$\begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m,1} & A_{m,2} & \cdots & A_{m,n} \end{bmatrix} \in \mathbf{R}^{m\times n}$$

Transposes

- transpose of row vector is column vector & vice versa

$$\begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}^T = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} \quad \& \quad \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}^T = \begin{bmatrix} a_1 & a_2 & \cdots & a_n \end{bmatrix}$$

- transpose of m-by-n matrix is n-by-m matrix

$$\begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m,1} & A_{m,2} & \cdots & A_{m,n} \end{bmatrix}^T = \begin{bmatrix} A_{1,1} & A_{2,1} & \cdots & A_{m,1} \\ A_{1,2} & A_{2,2} & \cdots & A_{m,2} \\ \vdots & \vdots & \ddots & \vdots \\ A_{1,n} & A_{2,n} & \cdots & A_{m,n} \end{bmatrix} \in \mathbf{R}^{n \times m}$$

Matrix-vector multiplication

- for matrix $A \in \mathbf{R}^{m \times n}$ & vector $b \in \mathbf{R}^n$
  - matrix-vector multiplication Ab defined by

$$Ab = \begin{bmatrix} A_{1,1}b_1 + A_{1,2}b_2 + \cdots + A_{1,n}b_n \\ A_{2,1}b_1 + A_{2,2}b_2 + \cdots + A_{2,n}b_n \\ \vdots \\ A_{m,1}b_1 + A_{m,2}b_2 + \cdots + A_{m,n}b_n \end{bmatrix} \in \mathbf{R}^m$$

    in other words

$$(Ab)_i = \sum_{j=1}^{n} A_{i,j}b_j \quad \text{for } 1 \leq i \leq m$$

  - resulting quantity is vector of length m
  - number of columns of A *must* equal to length of b

Matrix-matrix multiplication

- for matrices $A \in \mathbf{R}^{m \times n}$ & $B \in \mathbf{R}^{n \times p}$
  - matrix-matrix multiplication $AB \in \mathbf{R}^{m \times p}$ defined by

$$(AB)_{i,j} = \sum_{k=1}^{n} A_{i,k} B_{k,j} \quad \text{for } 1 \leq i \leq m$$

  - resulting quantity is m-by-p matrix
  - *order matters* and number of columns of A *must* equal to number of rows of B
- note matrix-vector multiplication is *special case* of matrix-matrix multiplication

Calculus Basics

Functions

- $f : X \to Y$
  - $X = \mathbf{dom}\, f$ - domain of f
  - Y - codomain of f
  - $\mathcal{R}(f) = \{f(x) \in Y | x \in X\}$ - range of f

Differentiation & derivatives

- for real-valued function $f : \mathbf{R} \to \mathbf{R}$
  - derivative of f at $x \in \mathbf{R}$

$$f'(x) = \frac{d}{dx} f(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h} \in \mathbf{R}$$

    - derivative exists *if and only if* limit exists
  - second derivative of f at $x \in \mathbf{R}$

$$f''(x) = \frac{d^2}{dx^2} f(x) = \lim_{h \to 0} \frac{f'(x+h) - f'(x)}{h} \in \mathbf{R}$$

    - second derivative exists *if and only if* limit exists

Multivariate functions

- $f : \mathbf{R}^n \to \mathbf{R}$ - real-valued multivariate function

$$f(x) = f\left(\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}\right) = f(x_1, x_2, \ldots, x_n) \in \mathbf{R}$$

- examples
  - $f : \mathbf{R}^3 \to \mathbf{R}$ - linear function

$$f(x) = x_1 + 3x_2 + 2x_3$$

  - $f : \mathbf{R}^3 \to \mathbf{R}$ - convex quadratic function

$$f(x) = x_1^2 + x_1x_2 + 3x_2^2 + 5x_3^2$$

Multivariate vector functions

- $f : \mathbf{R}^n \to \mathbf{R}^m$ - real-valued multivariate vector function

$$f(x) = \begin{bmatrix} f_1(x) \\ f_2(x) \\ \vdots \\ f_m(x) \end{bmatrix} \in \mathbf{R}^m$$

  where $f_j : \mathbf{R}^n \to \mathbf{R}$ for $1 \leq j \leq m$

- examples
  - $f : \mathbf{R}^3 \to \mathbf{R}^2$ - linear function

$$f(x) = \begin{bmatrix} x_1 + 3x_2 + 2x_3 \\ -3x_2 + x_3 \end{bmatrix} \in \mathbf{R}^2$$

  - $f : \mathbf{R}^3 \to \mathbf{R}^3$ - componentwise function

$$f(x) = \begin{bmatrix} \exp(x_1) & \exp(x_2) & \exp(x_3) \end{bmatrix}^T \in \mathbf{R}^3$$

Partial derivative & gradient

for $f : \mathbf{R}^n \to \mathbf{R}$

- ith partial derivative

$$\frac{\partial}{\partial x_i} f(x) = \frac{f(x + he_i) - f(x)}{h} = \frac{f(\ldots, x_{i-1}, x_i + h, x_{i+1}, \ldots) - f(x)}{h}$$

  where $e_i \in \mathbf{R}^n$ is ith unit vector
- gradient is vector of partial derivatives

$$\nabla f(x) = \begin{bmatrix} \partial f(x)/\partial x_1 \\ \partial f(x)/\partial x_2 \\ \vdots \\ \partial f(x)/\partial x_n \end{bmatrix} \in \mathbf{R}^n$$

- we have

$$(\nabla f(x))_i = \frac{\partial}{\partial x_i} f(x) = e_i^T \nabla f(x) \in \mathbf{R}$$

Jacobian

for $f : \mathbf{R}^n \to \mathbf{R}^m$

- Jacobian matrix

$$Df(x) = \begin{bmatrix} \frac{\partial f_1(x)}{\partial x_1} & \frac{\partial f_1(x)}{\partial x_2} & \cdots & \frac{\partial f_1(x)}{\partial x_n} \\ \frac{\partial f_2(x)}{\partial x_1} & \frac{\partial f_2(x)}{\partial x_2} & \cdots & \frac{\partial f_2(x)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_m(x)}{\partial x_1} & \frac{\partial f_m(x)}{\partial x_2} & \cdots & \frac{\partial f_m(x)}{\partial x_n} \end{bmatrix} \in \mathbf{R}^{m \times n}$$

  - equivalently

$$Df(x) = \begin{bmatrix} \nabla f_1(x)^T \\ \nabla f_2(x)^T \\ \vdots \\ \nabla f_m(x)^T \end{bmatrix} \in \mathbf{R}^{m \times n}$$

Chain rule

- for $f : \mathbf{R} \to \mathbf{R}^m$, $g : \mathbf{R}^m \to \mathbf{R}$ & $h = g \circ f$, *i.e.*, $h(x) = g(f_1(x), \ldots, f_m(x))$, derivative of h at $x \in \mathbf{R}$

$$h'(x) = \sum_{j=1}^{m} \frac{\partial}{\partial y_j} g(f(x)) f_j'(x) = \sum_{j=1}^{m} \nabla g(f(x))_j f_j'(x) \in \mathbf{R}$$

- for $f : \mathbf{R}^n \to \mathbf{R}^m$, $g : \mathbf{R}^m \to \mathbf{R}^p$ & $h = g \circ f$, Jacobian of h at $x \in \mathbf{R}^n$

$$Dh(x) = Dg(f(x))Df(x) \in \mathbf{R}^{p \times n}$$

  - note $Dg(f(x)) \in \mathbf{R}^{p \times m}$ & $Df(x) \in \mathbf{R}^{m \times n}$

- first is *special case* of second

Staistics Basics

Random experiments & probability law

- *random experiment*
  - outcome varies in unpredictable fashion (even) when experiment is being repeated under same conditions
  - specified by stating experimental procedure and set of one or more measurements or observations
- probability law
  - rule assigning probabilities to events of experiment that belong to event class $\mathcal{F}$

$$p : \mathcal{F} \to \mathbf{R}_+$$

- properties (or axioms)
  - for event $A \in \mathcal{F}$, $p(A)$ called *probability* of A
  - for event $A, B \in \mathcal{F}$ with $A \cap B = \emptyset$

$$p(A \cup B) = p(A) + p(B)$$

Conditional probability

- probability of event A given that event B has occurred, called *conditional probability*, denoted by
$$p(A|B)$$
- formula
$$p(A|B) = \frac{p(A \cap B)}{p(B)}$$
  - thus
$$p(A \cap B) = p(A|B)p(B) = p(B|A)p(A)$$
- Bayes' theorem
$$p(A|B) = \frac{p(B|A)p(A)}{p(B)}$$

Independence

- for events A & B, when knowledge of occurrence of B does not alter probability of A
  - A said to be *independent* of B
- following statements are equivalent
  - A is independent of B
  - B is independent of A
  - $p(A|B) = p(A)$
  - $p(B|A) = p(B)$
  - $p(A \cap B) = p(A)p(B)$

Random variables

- *discrete* random variable X assumes values from countable set $\{x_1, x_2, \ldots\}$
- *continuous* random variable X assumes values from $\mathbf{R}$
- random *vector* X assumes values from $\mathbf{R}^n$

PMF, PDF & CDF

- *probability mass function (PMF)* of discrete X

$$p_X(x) = p(X = x)$$

- *probability density function (PDF)* of continuous X

$$\int_a^b p_X(x) = p(a \leq X \leq b)$$

- *cumulative distribution function (CDF)* of (any) X

$$F_X(x) = p(X \leq x)$$

  - for discrete X - $F_X(x) = \sum_{x' \leq x} p_X(x')$
  - for continuous X - $F_X(x) = \int_{-\infty}^{x} p_X(x')dx'$

Expected value, variance & covariance matrix

- expected value
  - for discrete X

$$\mathbf{E}\, X = \sum_x x p_X(x)$$

  - for conditions X

$$\mathbf{E}\, X = \int_{-\infty}^{\infty} x p_X(x) dx$$

- variance for scalar $X \in \mathbf{R}$

$$\mathbf{Var}(X) = \mathbf{E}(X - \mathbf{E}\, X)^2 = \mathbf{E}\, X^2 - (\mathbf{E}\, X)^2$$

- covariance matrix for vector $X \in \mathbf{R}^n$

$$\mathbf{Var}(X) = \mathbf{E}(X - \mathbf{E}\, X)(X - \mathbf{E}\, X)^T = \mathbf{E}\, X X^T - (\mathbf{E}\, X)(\mathbf{E}\, X)^T$$

Joint PMF, PDF & CDF

- *joint PMF* of discrete X & Y

$$p_{X,Y}(x, y) = p(X = x, Y = y)$$

- *join PDF* of continuous X & Y

$$\int_c^d \int_a^b p_{X,Y}(x, y)dxdy = p(a \leq X \leq b \ \& \ c \leq Y \leq d)$$

- *joint CDF* of X & Y

$$F_{X,Y}(x, y) = p(X \leq x \ \& \ Y \leq y)$$

Conditional expectation

for two random variables X & Y

- expected value of Y conditioned on X

$$\mathbf{E}(Y|X=x) = \int yp(y|x)dy$$

where

$$p(y|x) = \frac{p_{X,Y}(x,y)}{p_X(x)}$$

- note

$$\mathop{\mathbf{E}}_{X,Y} f(X,Y) = \mathop{\mathbf{E}}_{X}\mathop{\mathbf{E}}_{Y}(f(X,Y)|X)$$

because

$$\int\int f(x,y)p(x,y)dxdy = \int\left(\int f(x,y)p(y|x)dy\right)p(x)dx$$

ML Basics

Estimation, Regression, and Inference

The optimal estimator

- estimation problem
  - for two random variables $X \in \mathbf{R}^n$ & $Y \in \mathbf{R}^m$
  - design *estimator or predictor* $g : \mathbf{R}^n \to \mathbf{R}^m$ to make $g(X)$ *as close as possible* to Y
- when *closeness* measured by mean-square-error (MSE), *the optimal solution* exists

$$g^*(x) = \mathbf{E}(Y|X = x)$$

Proof of optimality

$$\begin{aligned}
\underset{X,Y}{\mathbf{E}}(g(X)-g^*(X))^T(g^*(X)-Y) &= \underset{X}{\mathbf{E}}\,\underset{Y}{\mathbf{E}}((g(X)-g^*(X))^T(g^*(X)-Y)|X) \\
&= \underset{X}{\mathbf{E}}((g(X)-g^*(X))^T\,\underset{Y}{\mathbf{E}}(g^*(X)-Y)|X) \\
&= 0
\end{aligned}$$

hence

$$\begin{aligned}
\mathbf{E}\,\|g(X)-Y\|_2^2 &= \mathbf{E}\,\|g(X)-g^*(X)+g^*(X)-Y\|_2^2 \\
&= \mathbf{E}\,\|g(X)-g^*(X)\|_2^2+\mathbf{E}\,\|g^*(X)-Y\|_2^2+2\,\mathbf{E}(g(X)-g^*(X))^T(g^*(X)-Y) \\
&= \mathbf{E}\,\|g(X)-g^*(X)\|_2^2+\mathbf{E}\,\|g^*(X)-Y\|_2^2 \\
&\geq \mathbf{E}\,\|g^*(X)-Y\|_2^2
\end{aligned}$$

Regression

- in most cases, *not* possible to obtain g^* (unless, $e.g.$, full knowledge of join PDF)
- regression problem
  - given data set $D = \{(x_1, y_1), \ldots, (x_N, y_N)\} \subset \mathbf{R}^n \times \mathbf{R}^m$
  - find $g : \mathbf{R}^n \to \mathbf{R}^m$ to make $g(X)$ *as close as possible* to Y
- given certain regression method, regressor depends on dataset D

$$g(\cdot; D)$$

Bias & variance

assuming $\mathcal{D}$ is random variable for dataset D

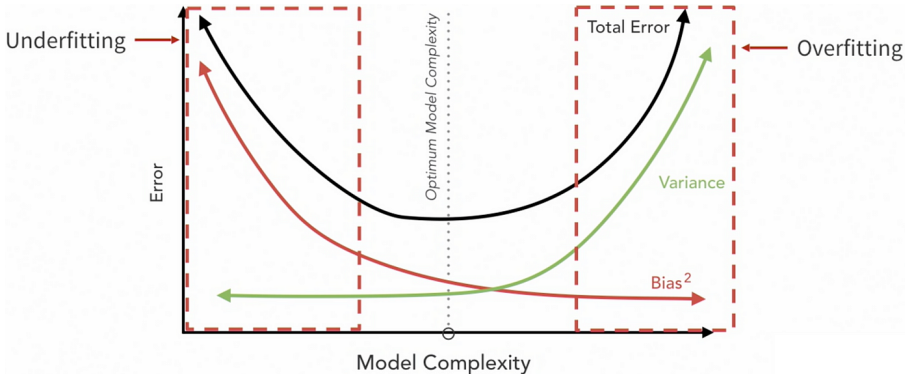
- estimation MSE is

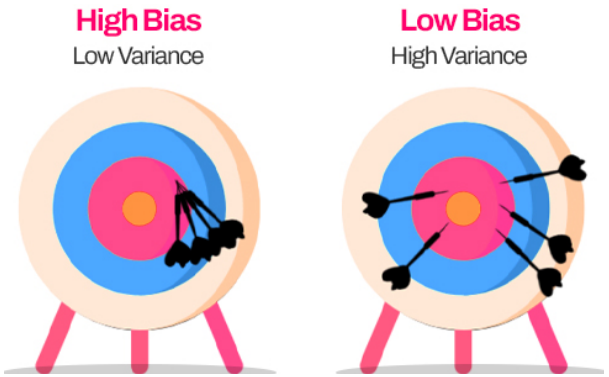
$$\begin{aligned}
&\mathop{\mathbf{E}}_{X,Y,\mathcal{D}} \|g(X;\mathcal{D}) - Y\|_2^2 \\
&= \underbrace{\mathop{\mathbf{E}}_{X,\mathcal{D}} \|g(X;\mathcal{D}) - \mathop{\mathbf{E}}_{\mathcal{D}} g(X;\mathcal{D})\|_2^2}_{\text{variance}} + \underbrace{\mathop{\mathbf{E}}_{X} \| \mathop{\mathbf{E}}_{\mathcal{D}} g(X;\mathcal{D}) - g^*(X)\|_2^2}_{\text{bias}} + \underbrace{\mathop{\mathbf{E}}_{X,Y} \|g^*(X) - Y\|_2^2}_{\text{noise}} \\
&= \underbrace{\mathop{\mathbf{E}}_{X,\mathcal{D}} \|g(X;\mathcal{D}) - \mathop{\mathbf{E}}_{\mathcal{D}} g(X;\mathcal{D})\|_2^2}_{\text{variance}} + \underbrace{\mathop{\mathbf{E}}_{X,Y} \| \mathop{\mathbf{E}}_{\mathcal{D}} g(X;\mathcal{D}) - Y\|_2^2}_{\text{bias + noise}}
\end{aligned}$$

- bias & variance
  - *bias* measures how good model is in average
  - *variance* measures how much model varies depending on dataset it is trained on
- *noise* cannot be reduced even with the optimal predictor

Model choice & hyperparameter optimization

- want to choose model or modeling method to make both bias & variance low
  - (too) complex models have low bias, but high variance
  - (too) simple models have low variance, but high bias
- usually solved by *hyperparameter optimization*
  - sometimes called *hyperparameter tuning*





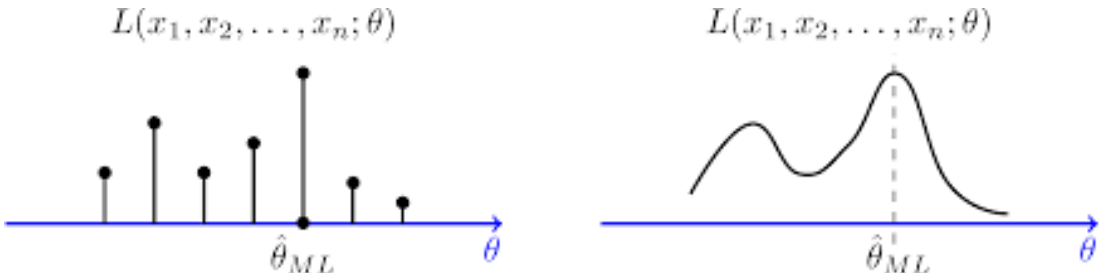
MLE

- maximum likelihood estimation (MLE)
  - assume parameterized distribution of $X \in \mathbf{R}^n$ by $\theta \in \Theta$ - $p(x;\theta)$
  - find θ maximizing *likelihood function*

$$p(x_1, \ldots, x_N; \theta) = \prod_{i=1}^{N} p(x_i; \theta)$$

- MLE solution

$$\hat{\theta}_{\text{MLE}} = \underset{\theta \in \Theta}{\text{argmax}} \prod_{i=1}^{N} p(x_i; \theta)$$



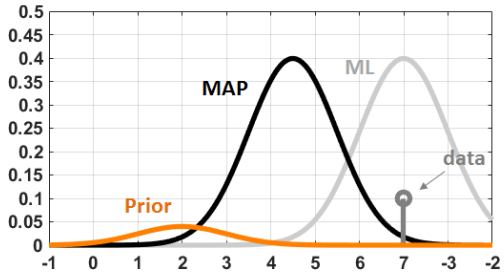
MAP estimation

- maximum a posteriori (MAP) estimation
  - assume *prior knowledge* of θ - $p(\theta)$
  - assume parameterized distribution of $X \in \mathbf{R}^n$ by θ - $p(x|\theta)$
  - find θ maximizing *posteriori probability*

$$p(\theta|x_1, \ldots, x_N)$$

  - Bayes' theorem implies $p(\theta|x_1, \ldots, x_N) \propto p(\theta) \prod_{i=1}^{N} p(x_i|\theta)$
- MAP solution

$$\hat{\theta}_{\text{MAP}} = \underset{\theta \in \Theta}{\operatorname{argmax}}\, p(\theta) \prod_{i=1}^{N} p(x_i|\theta)$$



Bayesian inference

- both MLE & MAP estimation are *point estimations*
- Bayesian inference
  - updates *prior distribution* by replacing it with posterior distribution
- conjugate prior
  - if prior can be further parameterized by hyperparameter α and posterior is in same probability distribution family, both prior and posterior called *conjugate distributions*, prior called *conjugate prior*

$$p(\theta; \alpha)$$

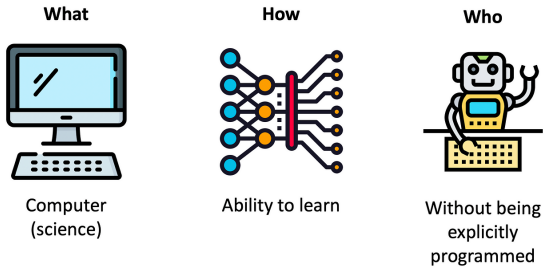
  - in this case, can update hyperparameter α, *i.e.*, find α^+ such that

$$p(\theta; \alpha^+) = p(\theta | x_1, \ldots, x_N; \alpha) = \frac{p(\theta; \alpha) \prod_{i=1}^{N} p(x_i | \theta; \alpha)}{p(x_1, \ldots, x_N; \alpha)}$$

Machine Learning

Machine Learning

- ML
  - subfield of computer science that
    "gives computers the ability to learn without being explicitly programmed."
    - Arthur Samuel (1959)
  - *not* magic, still less intelligent than humans for many cases
  - *numerically minimizes* certain (mathematical) loss function to (indirectly) solve *some statistically meaningful* problems



Machine learning is the subfield of computer science that gives "computers the ability to learn without being explicitly programmed."

Arthur Samuel

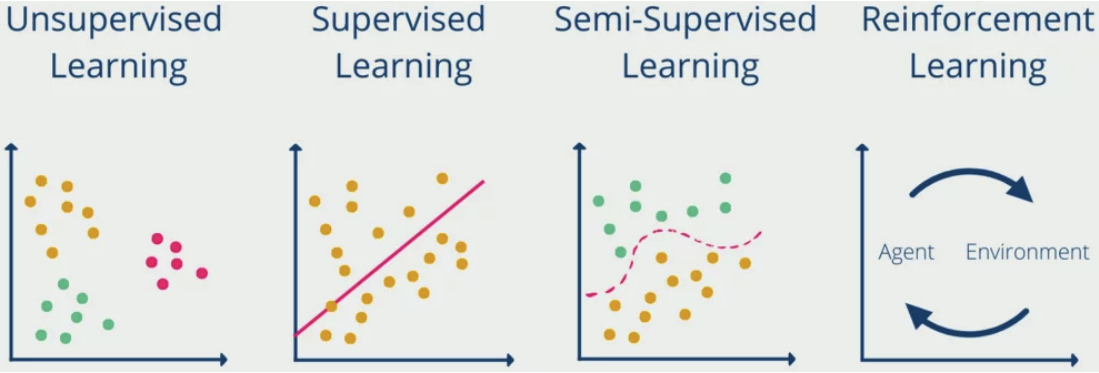
Two famous quotes

- Albert Einstein

  The grand aim of all science is to cover the greatest number of empirical facts by logical deduction from the smallest possible number of hypotheses or axioms.

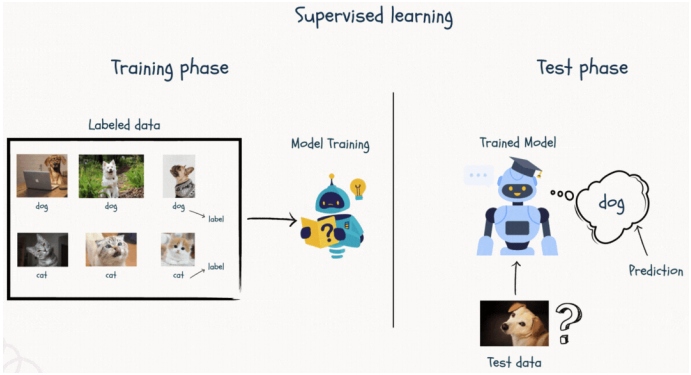
- Alfred North Whitehead

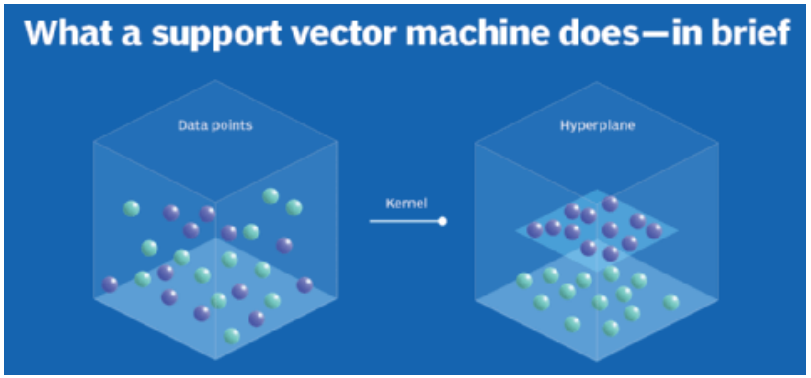
  Civilization advances by extending the number of important operations which we can perform without thinking about them. - Operations of thought are like cavalry charges in a battle – they are strictly limited in number, they require fresh horses, and must only be made at decisive moments.



Supervised learning

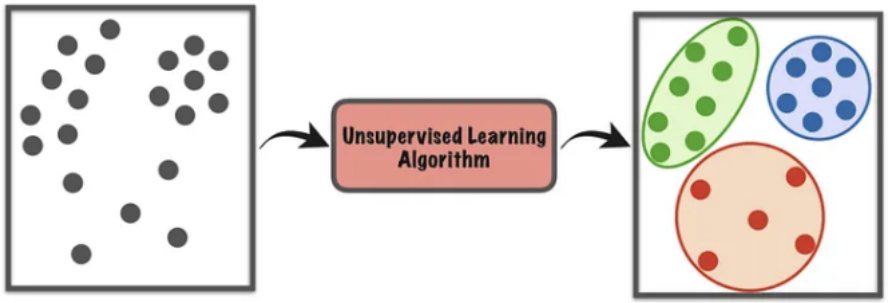
- most basic and widely used type of ML
- model is trained on dataset where correct output or "label" is provided for each input
- use cases
  - image classification, object detection, semantic segmentation
  - natural language processing (NLP) - text classification, sentiment analysis
  - predictive modeling, medical diagnosis
- algorithms
  - linear regression, logistic regression, decision trees, random forest
  - support vector machine (SVM), k-nearest neighbors (kNN)





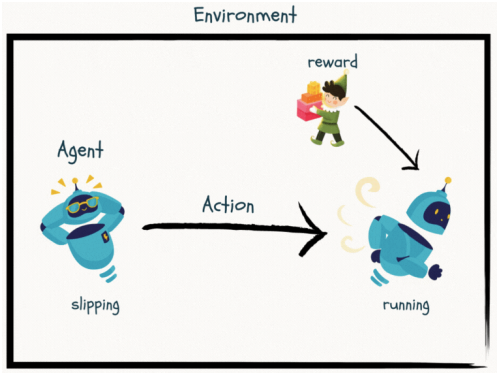
Unsupervised learning

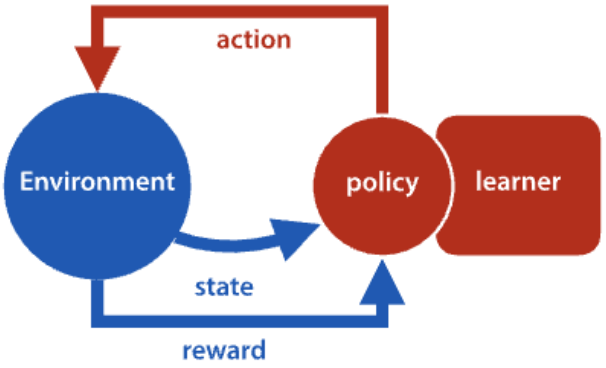
- model is given dataset without any labels or output
- model finds patterns & structure within data on its own
- use cases
  - clustering, dimensionality reduction
  - anomaly detection, generative models
- algorithms
  - k-means clutering, hierarchical clustering, principal component analysis (PCA)
  - t-distributed stochastic neighbor embedding (t-SNE)



Reinforcement learning

- (quite different from supervised & unsupervised learnings)
- model learns from consequences of its actions
  - model receives feedback on its performance; feedback called *reward*
  - uses that information to adjust its actions and improve its performance over time
- use cases
  - robotics, game playing, autonomous vehicles, industrial control
  - healthcare, finance
- algorithms
  - Q-learning, SARSA, DQN, A3C, policy gradient





ML Formulations

Statistical problem formulation

- assume data set $X_m = \{x^{(1)}, \ldots, x^{(m)}\}$
  - drawn independently from (true, but unknown) data generating distribution $p_{\text{data}}(x)$
- maximum likelihood estimation (MLE) is to solve

$$\text{maximize} \quad p_{\text{model}}(X; \theta) = \prod_{i=1}^{m} p_{\text{model}}(x^{(i)}; \theta)$$

  where optimization variable is θ
  - find *most plausible or likely model* that fits data
- equivalent (but more numerically tractable) formulation

$$\text{maximize} \quad \log p_{\text{model}}(X; \theta) = \sum_{i=1}^{m} \log p_{\text{model}}(x^{(i)}; \theta)$$

MLE & KL divergence

- in information theory, Kullback-Leibler (KL) divergence defines distance between two probability distributions p & q

$$D_{\mathrm{KL}}(p\|q) = \mathop{\mathbf{E}}_{X\sim p} \log p(X)/q(X) = \int_{x\in\Omega} p(x) \log \frac{p(x)}{q(x)}\, dx$$

- KL divergence between data distribution p_{data} & model distribution p_{model} can be approximated by Monte Carlo method as

$$D_{\mathrm{KL}}(p_{\mathrm{data}}\|p_{\mathrm{model}}(\theta)) \simeq \frac{1}{m}\sum_{i=1}^{m}(\log p_{\mathrm{data}}(x^{(i)}) - \log p_{\mathrm{model}}(x^{(i)};\theta))$$

  where $x^{(i)}$ are drawn (of course) according to p_{data}

- hence *minimizing KL divergence is equivalent to solving MLE problem!*

Equivalence of MLE to MSE

- assume model is Gaussian, *i.e.*, $y \sim \mathcal{N}(g_\theta(x), \Sigma)$ ($g_\theta(x) \in \mathbf{R}^p$, $\Sigma \in \mathbf{S}^p_{++}$)

$$p(y|x;\theta) = \frac{1}{\sqrt{2\pi}^p |\Sigma|^{1/2}} \exp\left(-\frac{1}{2}\left(y - g_\theta(x)\right)^T \Sigma^{-1} \left(y - g_\theta(x)\right)\right)$$

- assuming that $\Sigma = \alpha I_p$, log-likelihood becomes

$$\sum_{i=1}^m \log p(x^{(i)}, y^{(i)}; \theta) = \sum_{i=1}^m \log p(y^{(i)}|x^{(i)};\theta) p(x^{(i)})$$

$$= \quad -\sum_{i=1}^m \|y^{(i)} - g_\theta(x^{(i)})\|_2^2 / 2\alpha - \frac{pm}{2}\log(2\pi\alpha) + \sum_{i=1}^m \log p(x^{(i)})$$

- hence *minimizing mean-square-error (MSE) is equivalent to solving MLE problem!*

Numerical optimization problem formulation

- (true) problem to solve

$$\text{minimize} \quad \mathbf{E}\, l(g_\theta(X), Y)$$

  - *impossible* to solve

- basic formulation - surrogate problem to solve

$$\text{minimize} \quad f(\theta) = \frac{1}{m} \sum_{i=1}^{m} l(g_\theta(x^{(i)}), y^{(i)})$$

- formulation with regularization

$$\text{minimize} \quad f(\theta) = \frac{1}{m} \sum_{i=1}^{m} l(g_\theta(x^{(i)}), y^{(i)}) + \gamma r(\theta)$$

- stochastic gradient descent (SGD)

$$\theta^{(k+1)} = \theta^{(k)} - \alpha_k \nabla f(\theta^{(k)})$$

Deep Learning

Deep learning (DL)

- machine learning using artificial neural networks with multiple layers for
  - automatically learning hierarchical representations of data
- key components
  - deep neural networks, hidden layers, backpropagation, activation functions
  - hierarchical feature learning, representation learning, end-to-end learning
- key breakthroughs enabling DL
  - massively available data, GPU computing, algorithmic advances

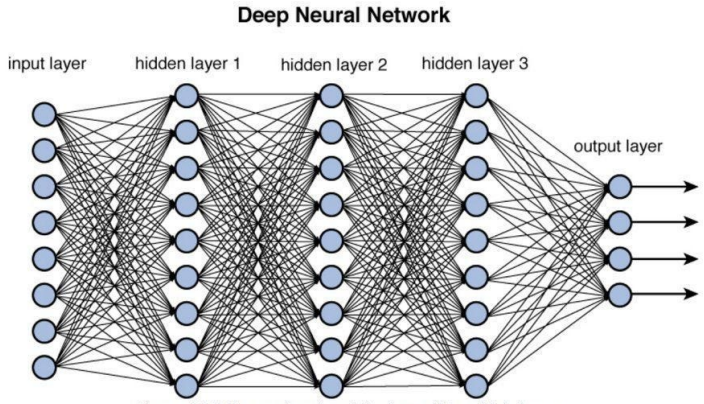
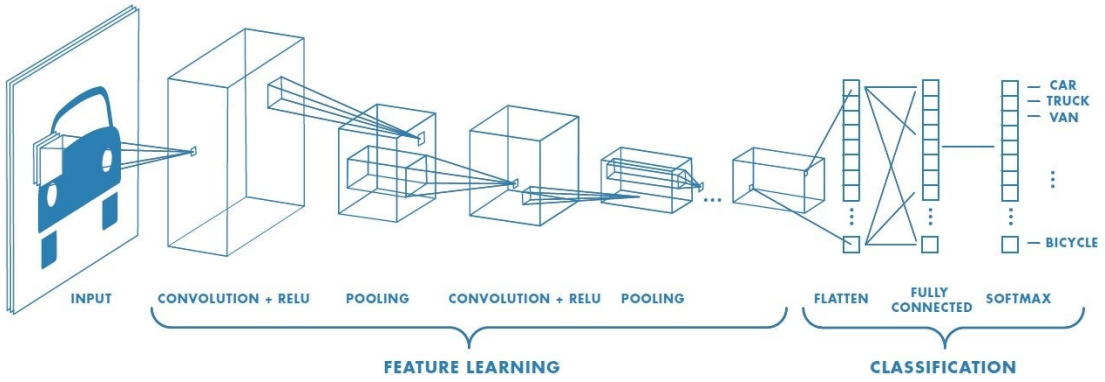


Figure 12.2 Deep network architecture with multiple layers.

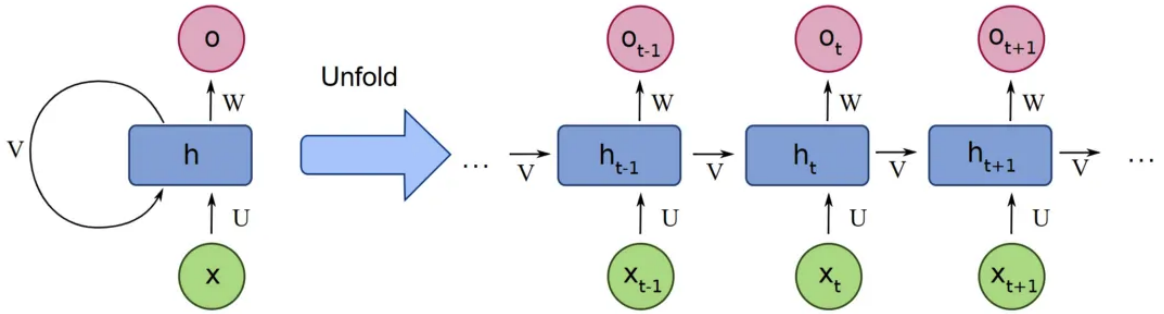
Convolutional neural network (CNN)

- specialized DL learning architecture designed for
  - processing grid-like data such as images
  - where spatial relationships between pixels matter
- key components
  - convolutional layers, pooling layers, activation functions, fully connected layers
- how it works
  - feature extraction, translation invariance, parameter sharing
- why it excels
  - local connectivity, hierarchical learning



Recurrent neural network (RNN)

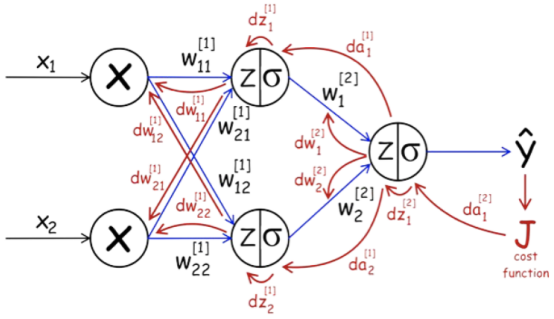
- neural network designed for
  - processing sequential data by maintaining memory of previous inputs
- key components
  - hidden states, recurrent connections, input/output layers, weight sharing
- how it works
  - sequential processing, memory mechanism, temporal dependencies
- why it excels
  - variable length input, context awareness, flexible architecture
- variants - long short-term memory (LSTM), gated recurrent unit (GRU)

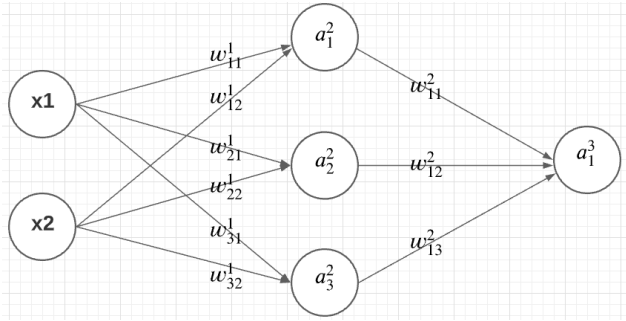


Training DNN using SGD

Notations

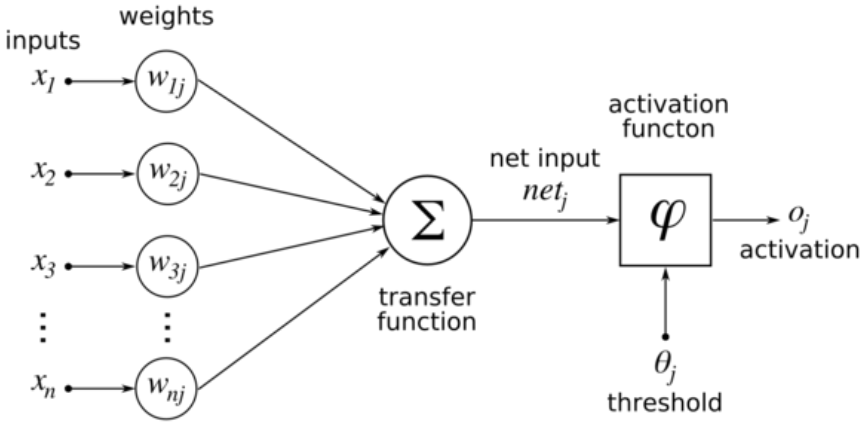
- p / q - dimension of input / output spaces
- $l : \mathbf{R}^q \times \mathbf{R}^q \to \mathbf{R}_+$ - loss function
- d - depth of neural network
- n_i $(1 \leq i \leq d)$ - number of perceptrons in ith layer
- $z^{[i]} \in \mathbf{R}^{n_i}$ - input to ith layer
- $o^{[i]} \in \mathbf{R}^{n_i}$ - output of ith layer
- $W^{[i]} \in \mathbf{R}^{n_i \times n_{i-1}}$ - weights of connections between $(i-1)$th and ith layer
- $w^{[i]} \in \mathbf{R}^{n_i \times n_{i-1}}$ - bias weights of ith layer
- $\phi^{[i]} : \mathbf{R}^{n_i} \to \mathbf{R}^{n_i}$ - activation functions of ith layer



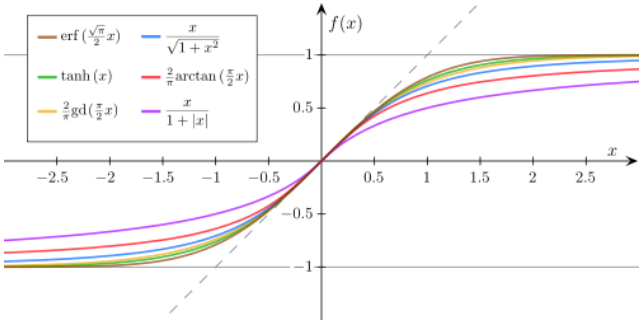


Basic unit & activation function

- basic unit



- activation function



Neural net equations

- modeling function for the (deep) neural network $g_\theta : \mathbf{R}^p \to \mathbf{R}^q$

$$g_\theta = \phi_\theta^{[d]} \circ \psi_\theta^{[d]} \circ \cdots \circ \phi_\theta^{[1]} \circ \psi_\theta^{[1]}$$

  or equivalently

$$g_\theta(x) = \phi_\theta^{[d]}(\psi_\theta^{[d]}(\cdots(\phi_\theta^{[1]}(\psi_\theta^{[1]}(x)))))$$

- for ith layer
  - output via (componentwise) activation function

$$o^{[i]} = \phi^{[i]}(z^{[i]}) \Leftrightarrow o_j^{[i]} = \phi_j^{[i]}(z_j^{[i]}) \quad (1 \le j \le n_i)$$

  - input via affine transformation $\psi^{[i]} : \mathbf{R}^{n_{i-1}} \to \mathbf{R}^{n_i}$

$$z^{[i]} = \psi^{[i]}(o^{[i-1]}) = W^{[i]} o^{[i-1]} + w^{[i]}$$

Stochastic gradient descent

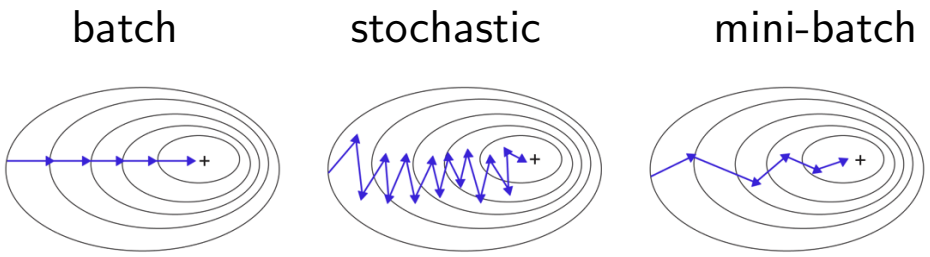
- ML training tries to minimize some loss function - $f(\theta)$ depends on (not only θ, but also) batch of data $(x^{(1)}, y^{(1)}), \ldots (x^{(m)}, y^{(m)})$

$$\text{minimize} \quad f(\theta)$$

- while exist hundreds of optimization methods solving this problem
  - *the only method used widely* is stochastic *gradient descent*!
- (stochastic) gradient descent

$$f(\theta^{k+1}) = f(\theta^k) - \alpha^k \nabla f(\theta^k)$$

- *backpropagation* is used to evaluate this (stochastic) *gradient* using *chain rule*



Chain rule

- suppose
  - two functions $f : \mathbf{R}^n \to \mathbf{R}^m$ & $g : \mathbf{R}^m \to \mathbf{R}$
  - Jacobian of f - $Df : \mathbf{R}^n \to \mathbf{R}^{m \times n}$
  - gradient of g - $\nabla g : \mathbf{R}^m \to \mathbf{R}^m$
- gradient of composite function $h = g \circ f$

$$\nabla h(\theta) = Df(\theta)^T \nabla g(f(\theta)) \in \mathbf{R}^n \quad \text{(using matrix-vector multiplication)}$$

in other words

$$\frac{\partial}{\partial \theta_i} h(\theta) = \sum_{j=1}^{m} \frac{\partial}{\partial \theta_i} f_j(\theta) \nabla_j g(f(\theta)) \quad \text{(scalar version)}$$

Loss function & its gradient

- assume cost function of deep neural network is

$$f(\theta) = \frac{1}{m}\sum_{k=1}^{m} l(g_\theta(x^{(k)}), y^{(k)}) = \frac{1}{m}\sum_{k=1}^{m} f_k(\theta)$$

  where

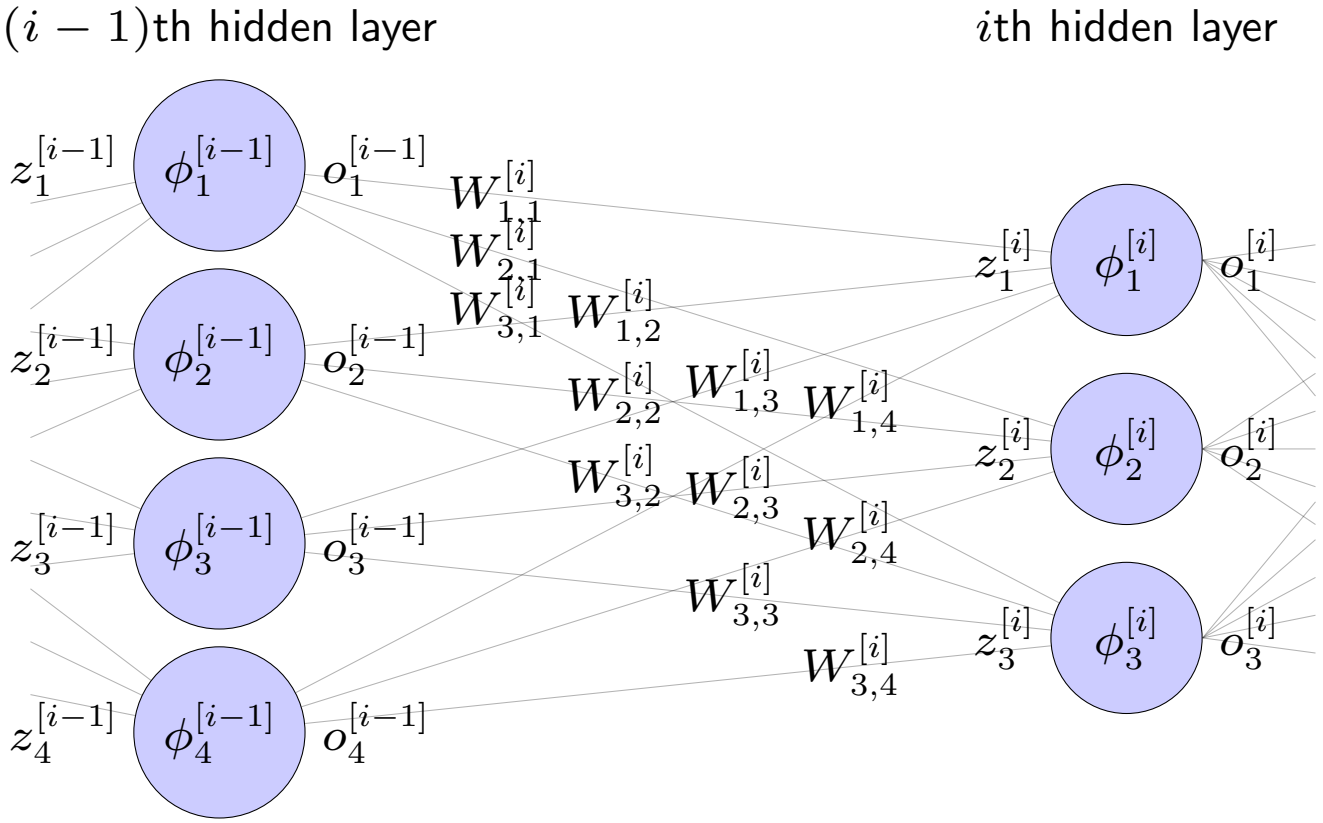
$$f_k(\theta) = l(g_\theta(x^{(k)}), y^{(k)})$$

- gradient is

$$m\nabla_\theta f(\theta) = \sum_{k=1}^{m} \nabla_\theta l(g_\theta(x^{(k)}), y^{(k)}) = \sum_{k=1}^{m} \nabla_\theta f_k(\theta)$$

  - $i.e.$, evaluate gradient $\nabla_\theta f_k(\theta)$ for each data point $(x^{(k)}, y^{(k)})$

Hidden layers



Backpropagation formula using chain rule

- for each data $(x^{(k)}, y^{(k)})$
  - via activation function

$$\frac{\partial}{\partial z_j^{[i]}} f_k(\theta) = \frac{\partial}{\partial o_j^{[i]}} f_k(\theta) \phi_j^{[i]'}(o_j^{[i]}) \quad \text{for } 1 \le j \le n_i \tag{1}$$

    where $\phi_j^{[i]'}(o_j^{[i]})$ is derivative of activation function $\phi_j^{[i]}$ evaluated at $o_j^{[i]}$
  - via affine transformation

$$\frac{\partial}{W_{j,l}^{[i]}} f_k(\theta) = o_l^{[i-1]} \frac{\partial}{\partial z_j^{[i]}} f_k(\theta) \quad \text{for } 1 \le j \le n_i \ \& \ 1 \le l \le n_{i-1} \tag{2}$$

$$\frac{\partial}{\partial w_j^{[i]}} f_k(\theta) = \frac{\partial}{\partial z_j^{[i]}} f_k(\theta) \quad \text{for } 1 \le j \le n_i \tag{3}$$

$$\frac{\partial}{\partial o_l^{[i-1]}} f_k(\theta) = \sum_{j=1}^{n_i} W_{j,l}^{[i]} \frac{\partial}{\partial z_j^{[i]}} f_k(\theta) \quad \text{for } 1 \le l \le n_{i-1} \tag{4}$$

Backpropagation formula using matrix-vector multiplication

- for each data $(x^{(k)}, y^{(k)})$
  - via activation function

$$\nabla_{z^{[i]}} f_k(\theta) = D\phi^{[i]} \nabla_{o^{[i]}} f_k(\theta) \tag{5}$$

where $D\phi^{[i]} = \mathbf{diag}(\phi_1^{[i]'}(o_1^{[i]}), \ldots, \phi_{n_i}^{[i]'}(o_{n_i}^{[i]}))$ is Jacobian of $\phi^{[i]}$ evaluated at $o^{[i]}$

  - via affine transformation

$$\begin{aligned} \nabla_{W^{[i]}} f_k(\theta) &= \nabla_{z^{[i]}} f_k(\theta) o^{[i-1]^T} \in \mathbf{R}^{n_i \times n_{i-1}} && (6) \\ \nabla_{w^{[i]}} f_k(\theta) &= \nabla_{z^{[i]}} f_k(\theta) \in \mathbf{R}^{n_i} && (7) \\ \nabla_{o^{[i-1]}} f_k(\theta) &= W^{[i]^T} \nabla_{z^{[i]}} f_k(\theta) \in \mathbf{R}^{n_{i-1}} && (8) \end{aligned}$$

Backpropagation formula using `Python numpy` package

- for each data $(x^{(k)}, y^{(k)})$
  - via activation function

$$\texttt{grad\_z = phi\_dir * grad\_o} \tag{9}$$

    where `grad_z`, `phi_dir`, `grad_o` are 1d `numpy.ndarray` of size n_i
  - via affine transformation

$$\texttt{grad\_W = numpy.dot(grad\_z, val\_o.T)} \tag{10}$$

$$\texttt{grad\_w = grad\_z.copy()} \tag{11}$$

$$\texttt{grad\_o\_prev = numpy.dot(grad\_z, W)} \tag{12}$$

    where `val_o`, `grad_w` are 1d `numpy.ndarray` of size n_i, `grad_o_prev` is 1d `numpy.ndarray` of size n_{i-1}, `grad_W` is 2d `numpy.ndarray` of shape (n_i, n_{i-1})

Gradient evaluation using backpropagation

- forward propagation - evaluate for each $(x^{(k)}, y^{(k)})$

$$g_\theta(x^{(k)}) = \phi_\theta^{[d]}(\psi_\theta^{[d]}(\cdots(\phi_\theta^{[1]}(\psi_\theta^{[1]}(x^{(k)})))))$$

- *backpropagation - evaluate partial derivatives backward*
  - evaluate gradient with respect to output of output layer $o^{[d]} = g_\theta(x^{(k)})$

$$\nabla_{o^{[d]}} f_k(\theta) = \nabla_{y_1} l(g_\theta(x^{(k)}), y^{(k)})$$

  - evaluate gradient with respect to input from that with respect to output using (1), or equivalently, using (5) $i.e.$, evaluate $\nabla_{z^{[i]}} f_k(\theta)$ from $\nabla_{o^{[i]}} f_k(\theta)$
  - evaluate gradient with respect to weights, bias, and intput of previous layer using (3), (4), & (2) or equivalently, using (7), (8), & (6) $i.e.$, evaluate $\nabla_{W^{[i]}} f_k(\theta)$, $\nabla_{w^{[i]}} f_k(\theta)$ & $\nabla_{o^{[i-1]}} f_k(\theta)$ from $\nabla_{z^{[i]}} f_k(\theta)$
  - repeat back to input layer to evaluate all

$$\nabla_{W^{[1]}} f_k(\theta), \nabla_{w^{[1]}} f_k(\theta), \ldots, \nabla_{W^{[d]}} f_k(\theta), \nabla_{w^{[d]}} f_k(\theta)$$

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