

AI TODAY, TOMORROW, AND BEYOND

Manolis Kellis, MIT

TOO MANY CRISES

1. Economic disruption

- Jobs, automation, inflation, AI ROI

2. Social fragmentation

- Family, loneliness, addiction, attention

3. Cognitive decay

- Cheating, distraction, shallow thinking, overload

4. Institutional erosion

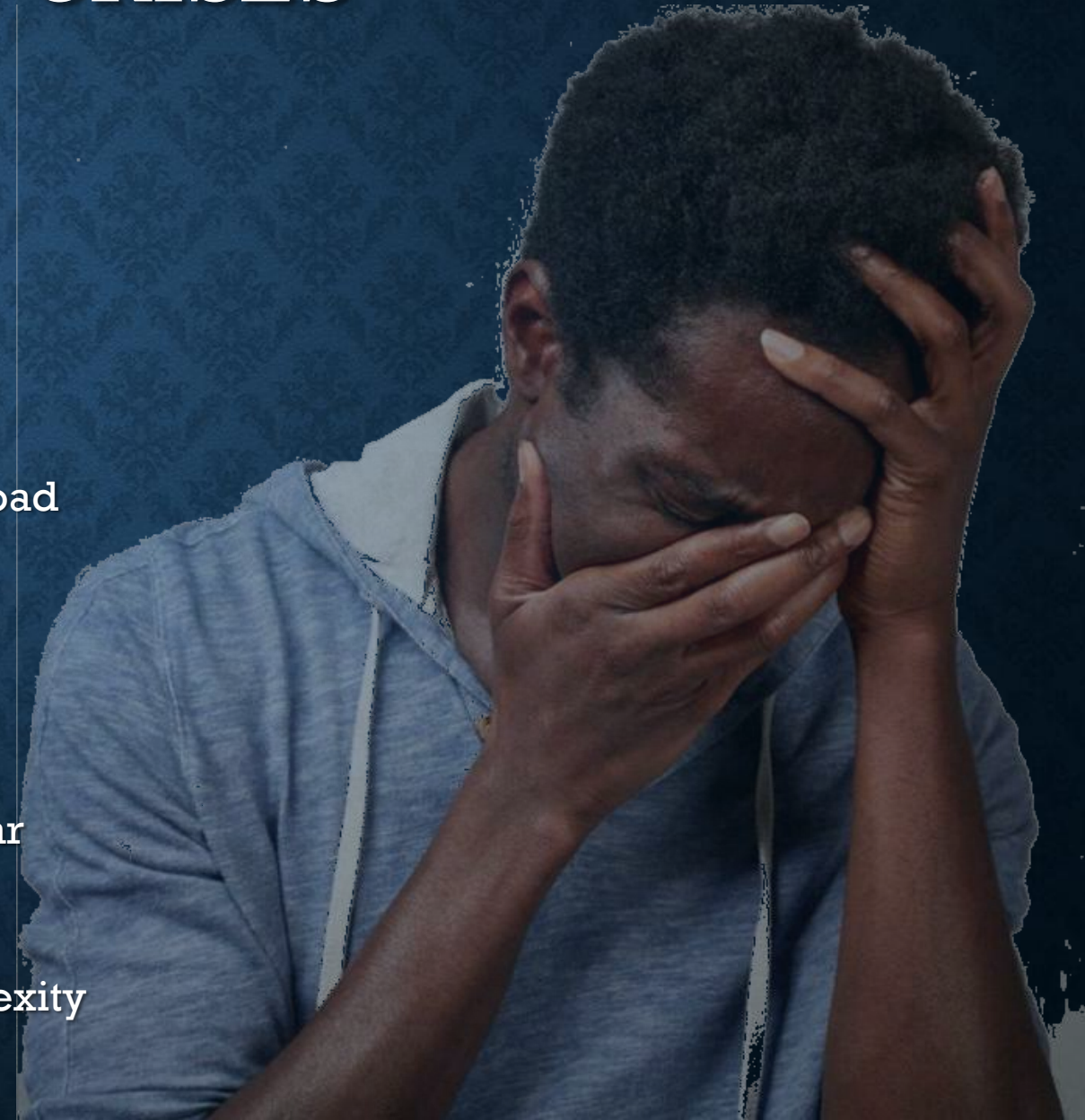
- Education, academia, trust, leadership

5. Geopolitical instability

- Protectionism, supply chains, polarization, war

6. Technological disillusionment

- Corporate AI, hallucinations, burnout, complexity



AI AS A FORCE FOR GOOD

A background image showing two rock climbers on a cliff face. One climber is higher up, wearing a blue helmet and a green shirt, while the other is lower down, wearing a white helmet and a yellow shirt. They are both secured with ropes and harnesses. The scene is set against a clear blue sky.

- AI: best hope to address challenges, whole world benefit
- Current form: still needs great improvements for full potential
 - Architectures: limited, disconnected
 - Need: reasoning, causality, fact-checking, transparency, fairness, common sense, creativity, empathy, efficiency, generalizability.
- Technical, societal, political, economic challenges
- Humanity tackled greater challenges before, always prevailed
 - Work together, deliver better world for all
 - AI: our **partner**, not our **enemy**.
- AI will not destroy humanity. It will lift humanity as our climbing partner

LOOKING BACK FROM 2050

The background image shows a vast, multi-level conservatory. A prominent feature is a large, circular waterfall cascading from a high, glass-and-steel structure. The conservatory is filled with a dense variety of tropical plants, including palm trees and ferns. People can be seen walking on different levels, and the overall atmosphere is bright and airy due to the natural light filtering through the glass roof.

1. Work as creation

- Purpose, agents, autonomy, joy

2. Education as orchestration

- Pods, motivation, mastery, peer-driven

3. AGI as collaboration

- Co-intelligence, glass-box, multi-agent, human-centered

4. Health without disease

- Prediction, prevention, personalization, longevity

5. Wealth with purpose

- Investing, stewardship, intelligence, legacy

6. Relationships with depth

- Empathy, connection, narrative, co-reflection

7. Philanthropy with intelligence

- Optimization, impact, transparency, alignment

AI FOR EDUCATION, TRAINING, RE-SKILLING

- Teams:
 - Train: New members of our team, new students entering a field
 - Self-driven exploration: paper stacks, Wikipedia bundles
 - AI: **train the next generation** for the transformation of biotechnology.
- Education: Schools understaffed, teachers not qualified to identify talents, no time
 - Need: lift **every child to their full potential**
 - Enable self-driven knowledge exploration
 - AI: powerful ally for teachers at all levels: research, university, secondary, primary
- Job market evolves: AI will not be an enemy; it will be a **partner**.
 - Unblocking opportunities for personal and professional growth
 - Help creative, talented, and driven individuals become more productive
 - Allow entering of areas previously too challenging to tackle
 - Help retrain to new professions, more fulfilling jobs

AI: ASSISTANT, COACH, PARTNER, ALLY

- GPT-4 as personal coach, partner, assistant.
- Source of inspiration, most challenging creative endeavors
- Design complex systems from scratch
 - Outline large codebases, break into parts, identify libraries, lay out design process
 - Send tools to students, save months of exploration trial / error
- For my own goals and tasks:
 - Break into manageable steps
 - Fight writer's block in generating early draft, outlining ideas
- Past Saturday: eyes shining, 4 hrs w/GPT-4
 - Lucile: "You have found your match."
- I am not Iron Man, but I have found my Jarvis
 - Perhaps AI can be everyone's Jarvis
- These tools are only a few weeks old.
 - Dramatic improvements ahead
 - Dramatic productivity gains
 - Humans not getting replaced, getting augmented



FROM HERE TO THERE

The Transitional Roadmap

1. Personal preparation – AI fluency, habits, reflection, growth
2. Collective coordination – platforms, governance, knowledge-sharing, trust
3. Timeline of transformation – 2025, 2035, 2045, 2050
4. Infrastructure and rituals – rituals, feedback, collaboration, sharing
5. Living the future now – mentorship, data practices, workflow evolution

Mantis as a Platform for the Pillars

1. Health insights and foresight – trajectories, biology, clustering, diagnosis
2. Wealth intelligence and leverage – investing, macro-tracking, discovery, signals
3. Relationship mapping and meaning – journaling, family, storylines, memory
4. Philanthropy optimization and action – cause-maps, ROI, funding gaps, coordination

The (non-linear) progress of AI

Extraordinary advances of AI

- Deep, Representation Learning
- Multi-Modal Understanding
- Intuitive 'reasoning'

Where the field took a wrong turn

- Language-only interactions
- Black box, no peeking in box
- Humans left out of the loop



Cognitive Cartography

The power of Maps for Physical Space Navigation

Maps give us

Landscape

Landmarks

Anchor points

Street names

Highway names

Simplification

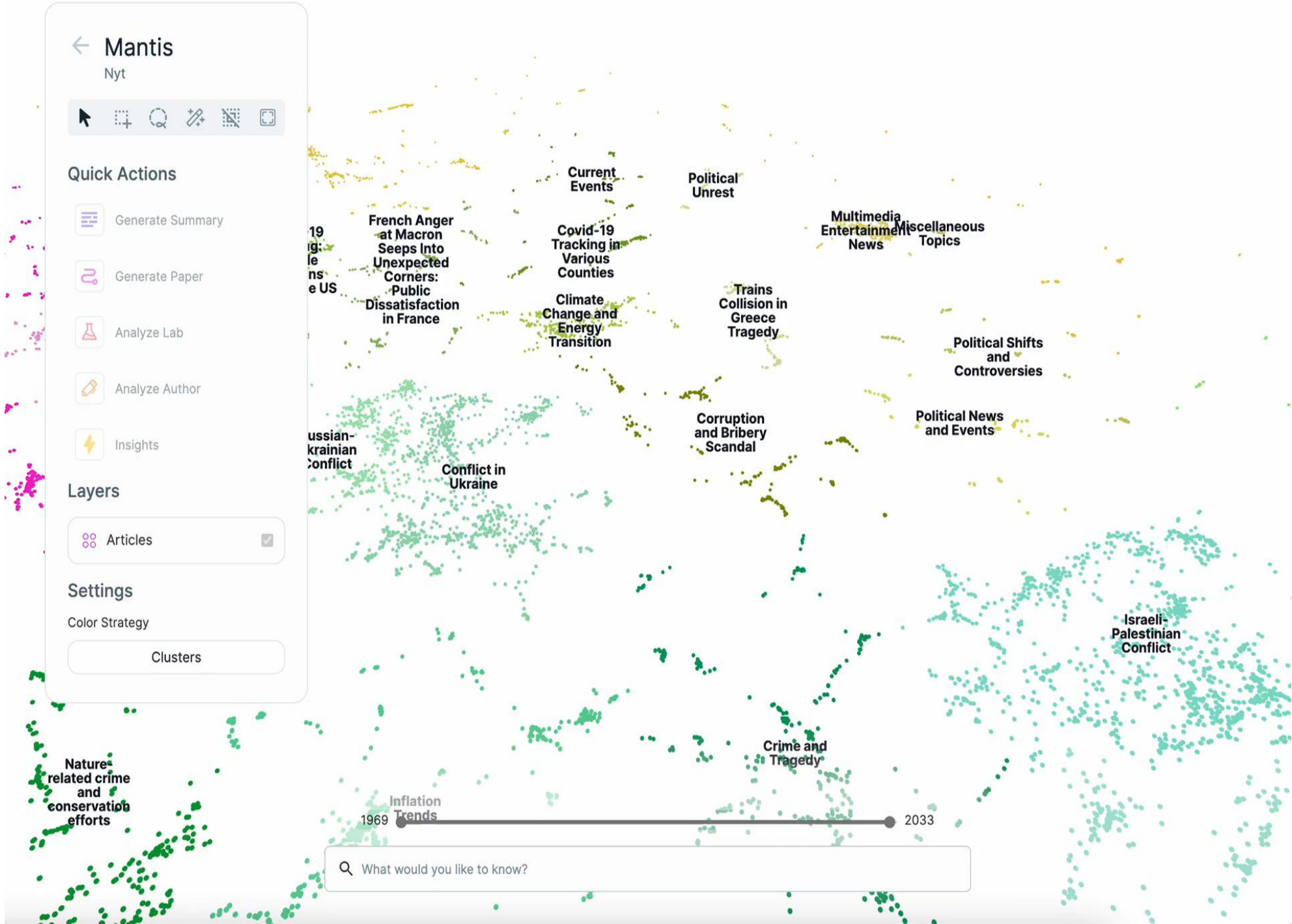
Abstraction

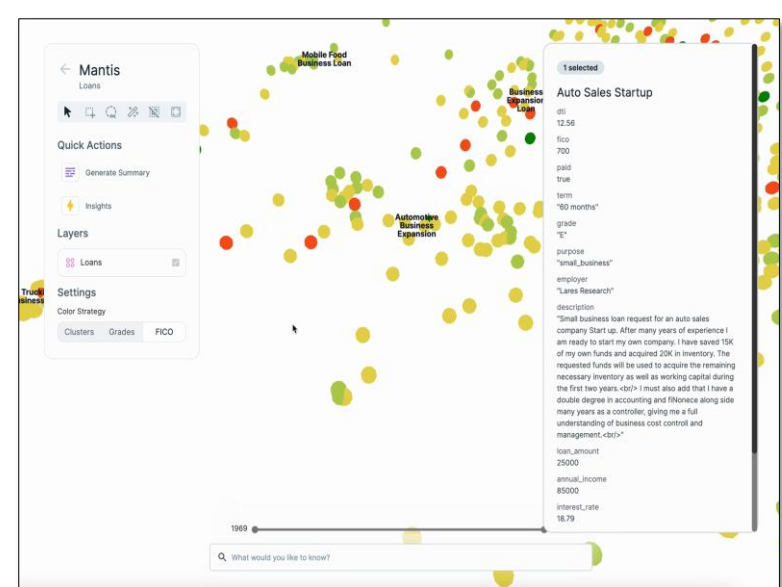
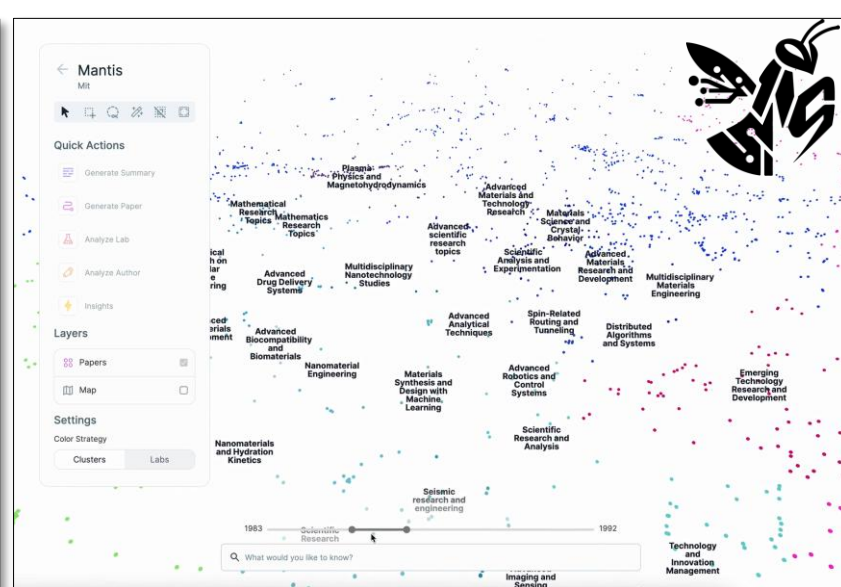
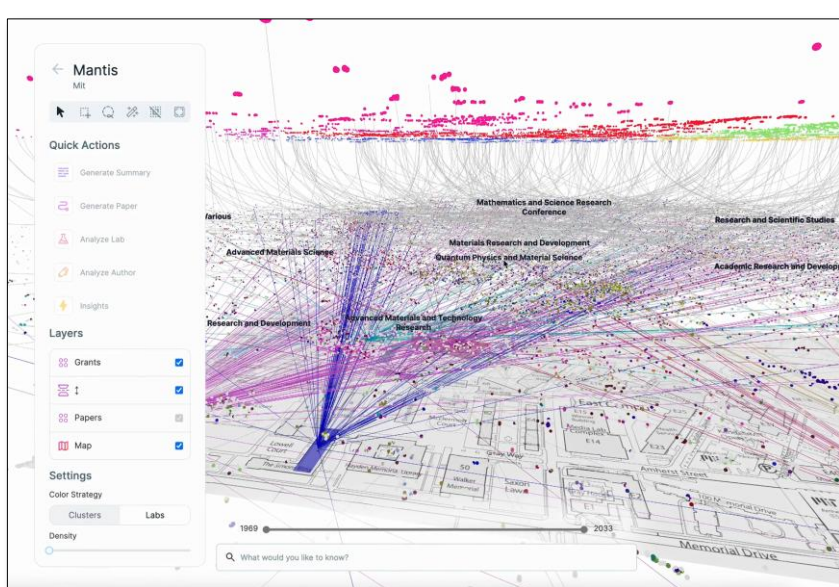
Summarization

Decision making



Navigate 3 million NY Times articles

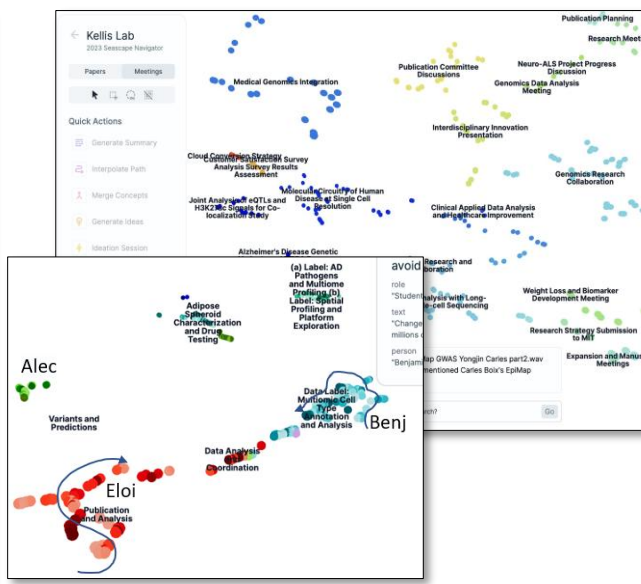
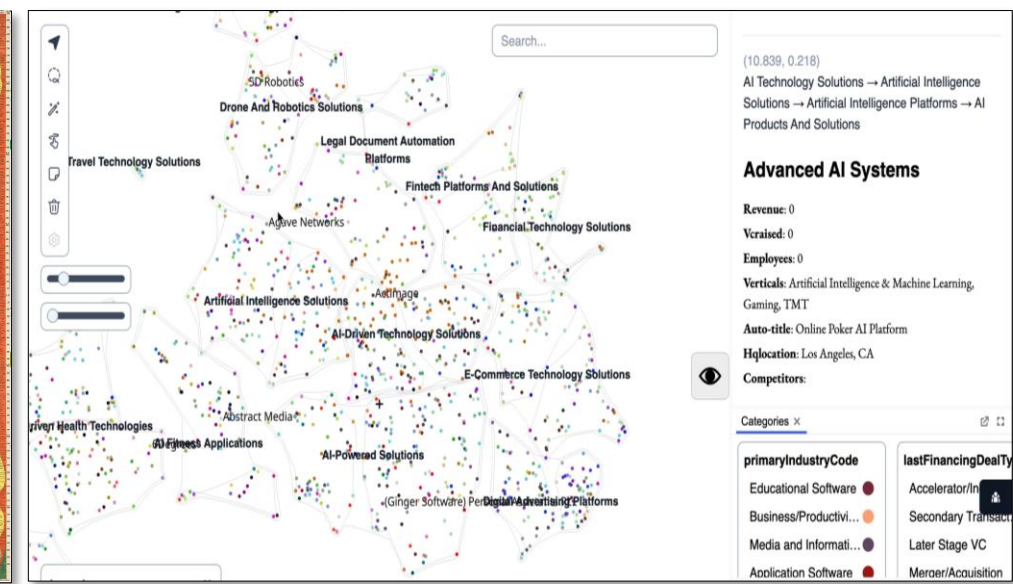
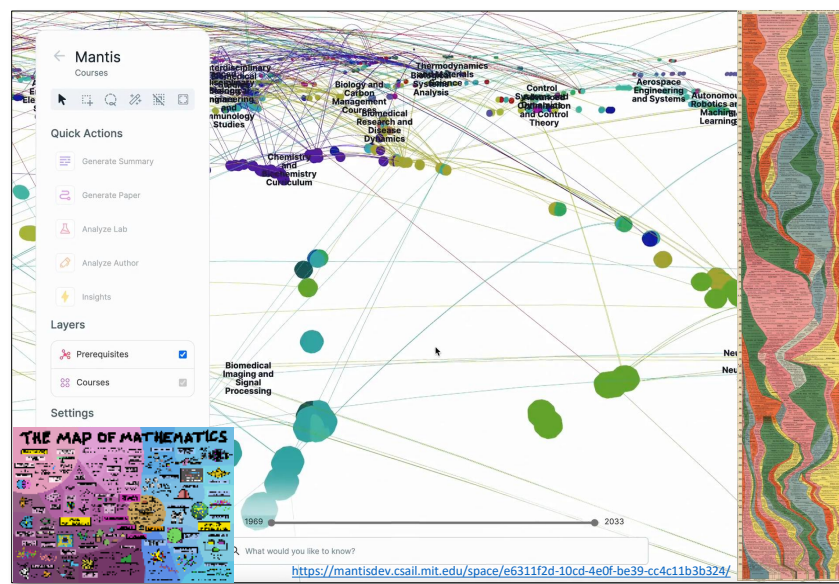




Papers + Grants + Patents + Startups + Offices
➔ Flow of Knowledge, resources

Dynamics over time: Knowledge evolution
➔ Disciplines emerging, maturing, changing

100,000 loans, clustered by description
➔ Context-specific predictive algorithms



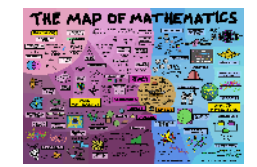
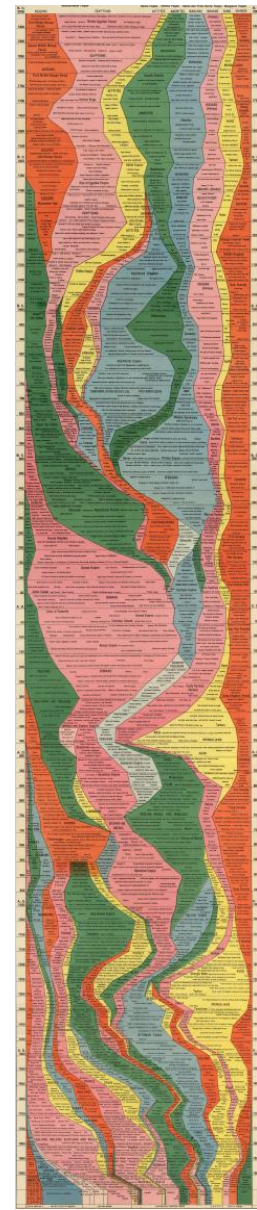
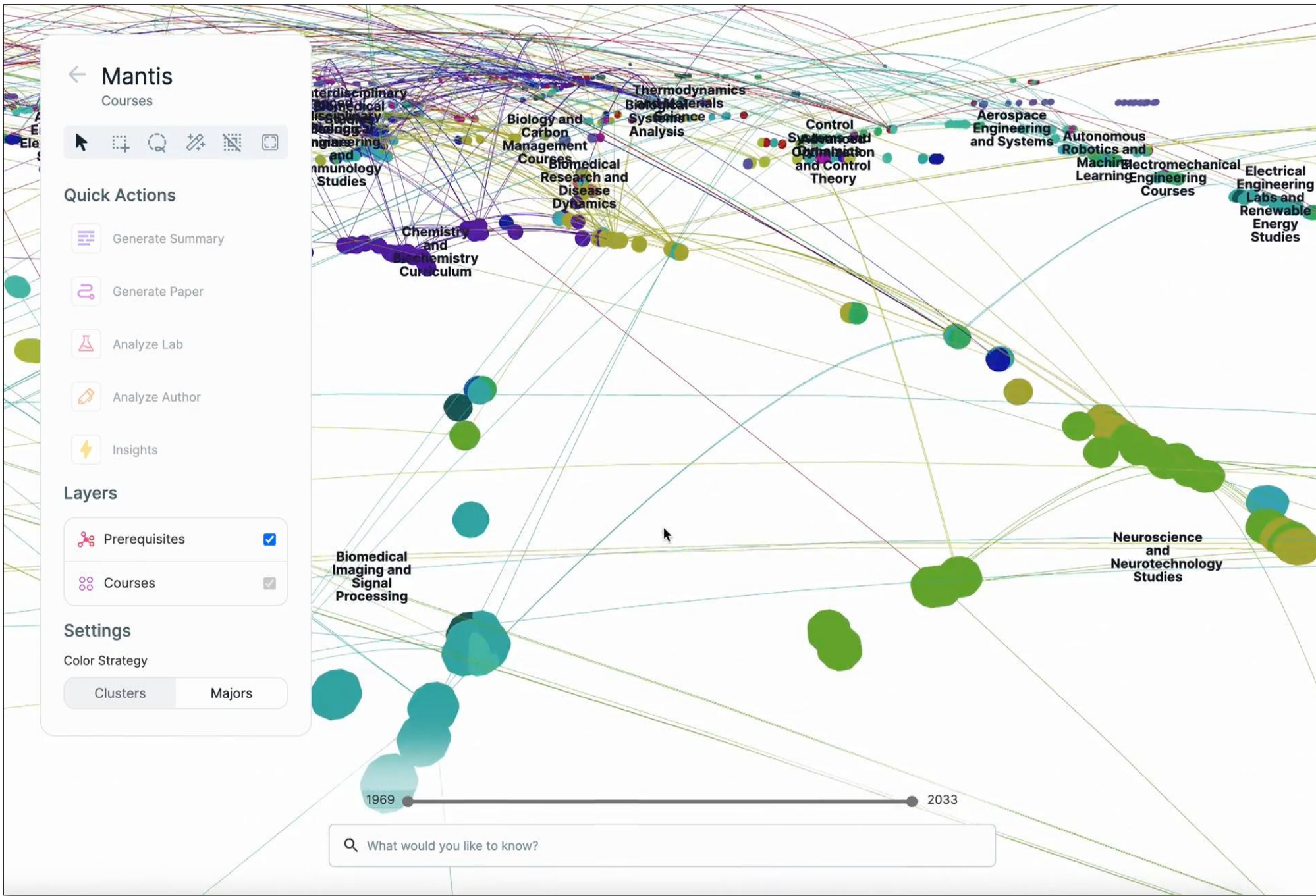
Education: MIT, EdX, AP, High-school, YouTube
➔ Multi-modal learning, interdisciplinary links
➔ Match CVs, job descriptions, skill sets

Investment, Start-ups, Intellectual Property
➔ Evaluate performance in context
➔ Combinations of skills and products

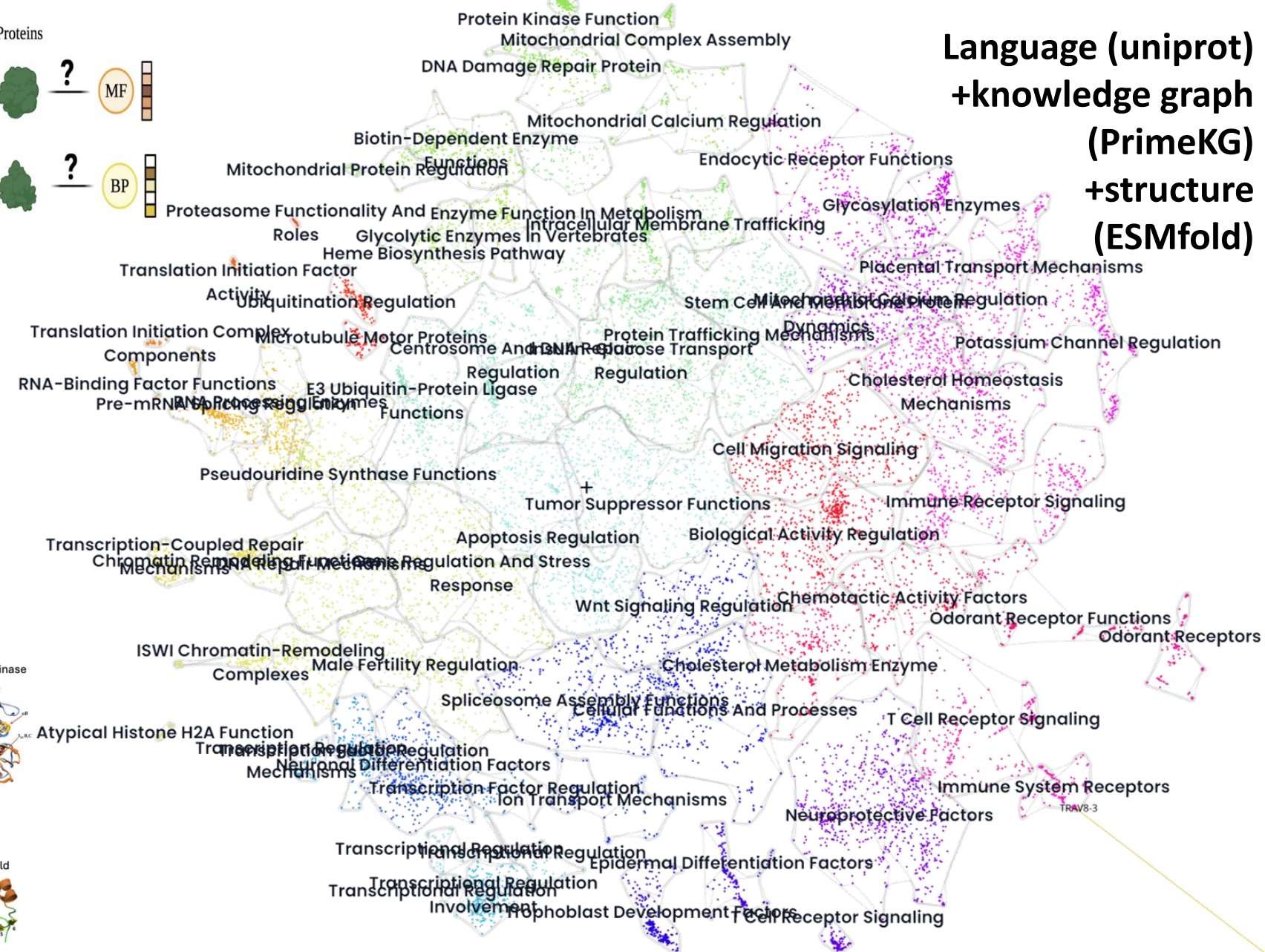
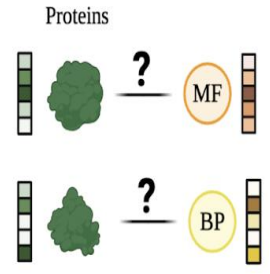
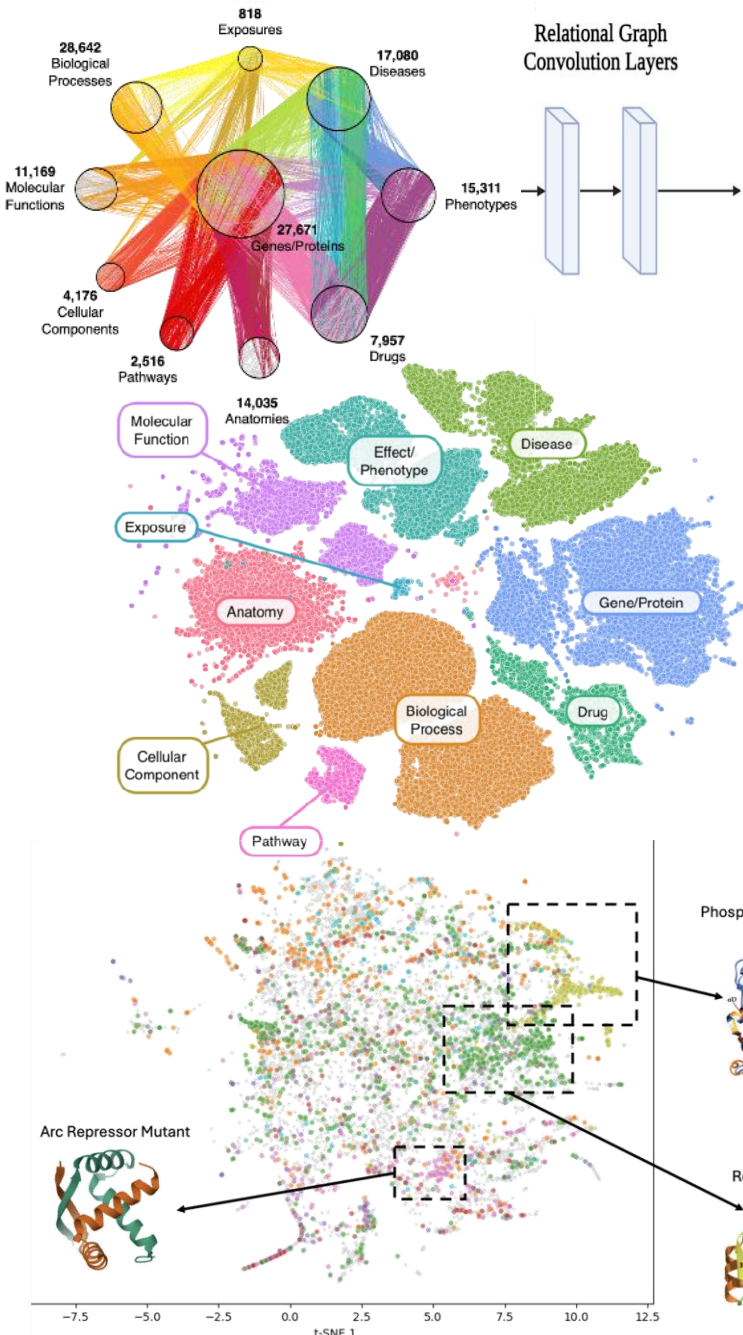
Collaboration, Productivity, Team Progress
➔ Link projects across team members
➔ Within-meeting live track of productivity

Education

MIT, EdX, AP, High-school, YouTube → Multi-modal learning, interdisciplinary links



Joint protein-structure-function embeddings of 20,000 human proteins





Media, Podcasts

Narrator x

appreciating the beauty and complexity of existence as it unfolds. This perspective encourages mindfulness and a focus on immediate experiences rather than deferring happiness to future achievements.

7. **Technological Involvement:** In contexts discussing the future, particularly regarding technology and AI, some experts posit that these developments can enhance human connection and creativity. However, concerns about the implications of technology on societal values and human relationships also emerged.

8. **Philosophical Reflections:** Figures like Sam Harris and philosophers introduce the idea that the search for meaning itself might be inherently meaningful. The act of questioning and seeking understanding is an essential part of what it means to be human.

9. **Nature of Existence:** Some conversations delve into

Orchestrator x

Ask about anything

Narrator v

Chat Clear Agent v

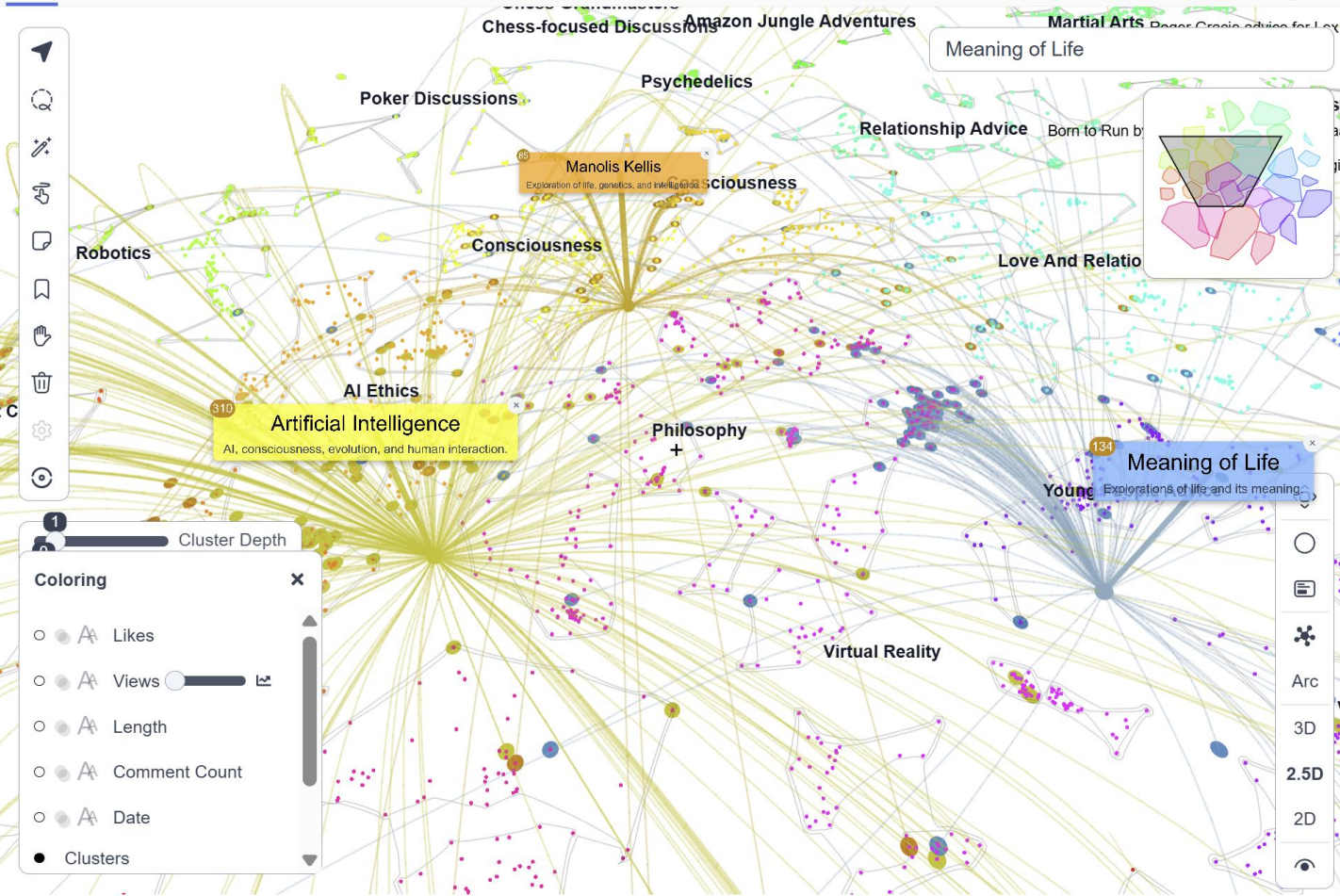
Bags x

World Bags - 5 + Clear Delete

Red 1 +

- 85 Manolis Kellis
- 310 Artificial Intelligence
- 310 Artificial Intelligence
- 134 Meaning of Life
- 134 Meaning of Life

Map



Red 1 (clipboard) Manolis Kellis (clipboard) Artificial Intelligence (clipboard) Meaning of Life (clipboard)

Podcast Interviews	Philosophical Discussions	Meaning Of Life	Celebrity Interviews	Celebrity Interviews	Grimes On Podcasts	Documentary Filmmaking	Origin Of Humanity	Exploration Of Meaning
Matthew McConaughey: Meaning of Life	Meaning of Life Michael Levin and Lex Fridman	Jordan Peterson: Meaning of Life	Dan Reynolds sings for Lex	Bobby Lee: Meaning of Life	Meaning of Life Grimes and Lex	Meaning of Life Skye Fitzgerald	Meaning of Life Michael Saylor	Meaning of Life Ariel Ekblaw and Lex

Tree x

- Filter nodes...
- AI Podcast Clips
 - AI Podcast Discussions
 - AI Ethics
 - Consciousness
 - Consciousness
 - Poker Discussions
 - Robotics
 - Chess Grandmasters
 - Chess-focused Discussions
 - Psychedelics
 - Amazon Jungle Adventures

Inspector x

Matthew McConaughey: Meaning of Life

(0.763, 2.166)

Interviews With Lex Fridman → Podcast Interviews → Tech And Leadership → Interviews

Reducing toxicity on the internet | George Hotz and Lex Fridman

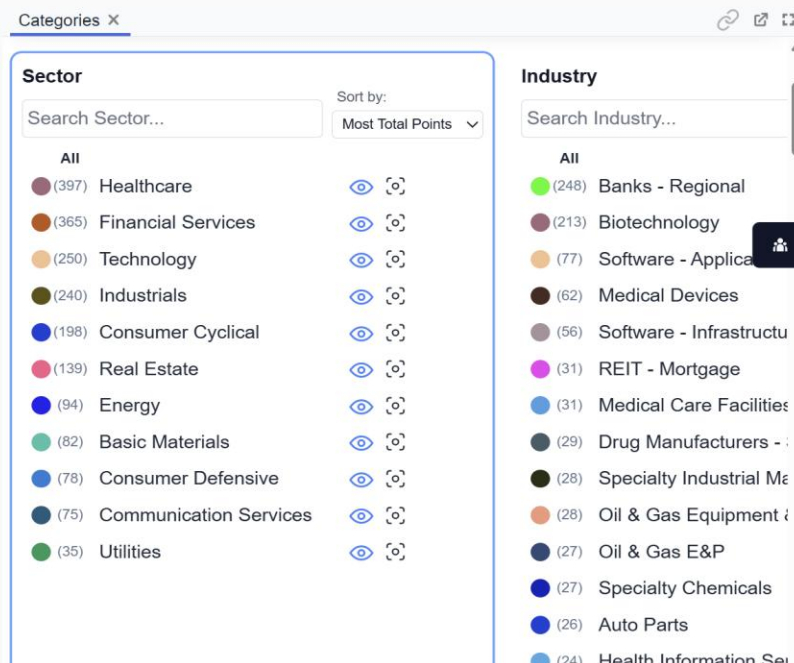
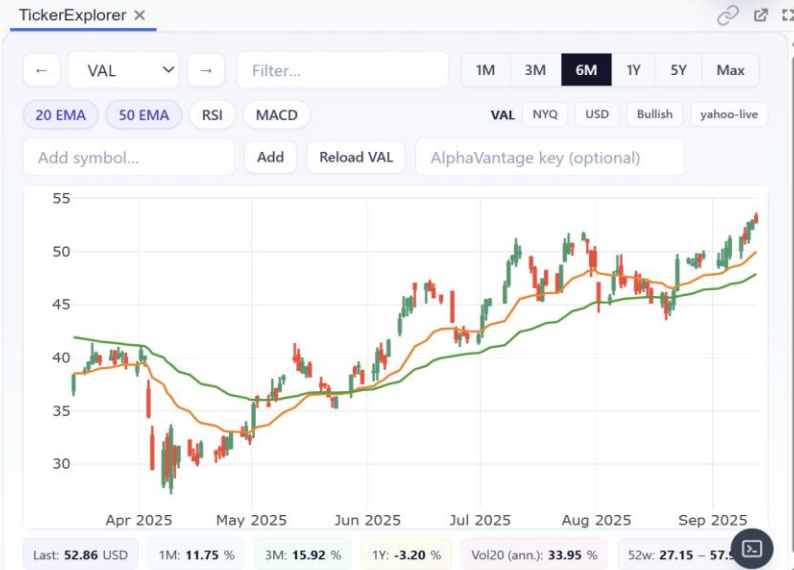
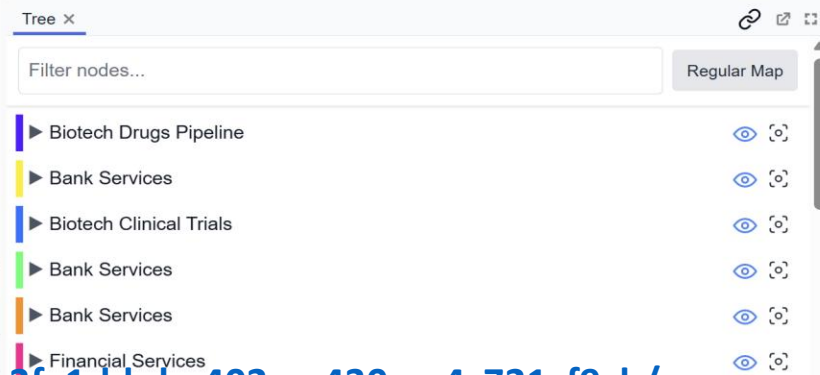
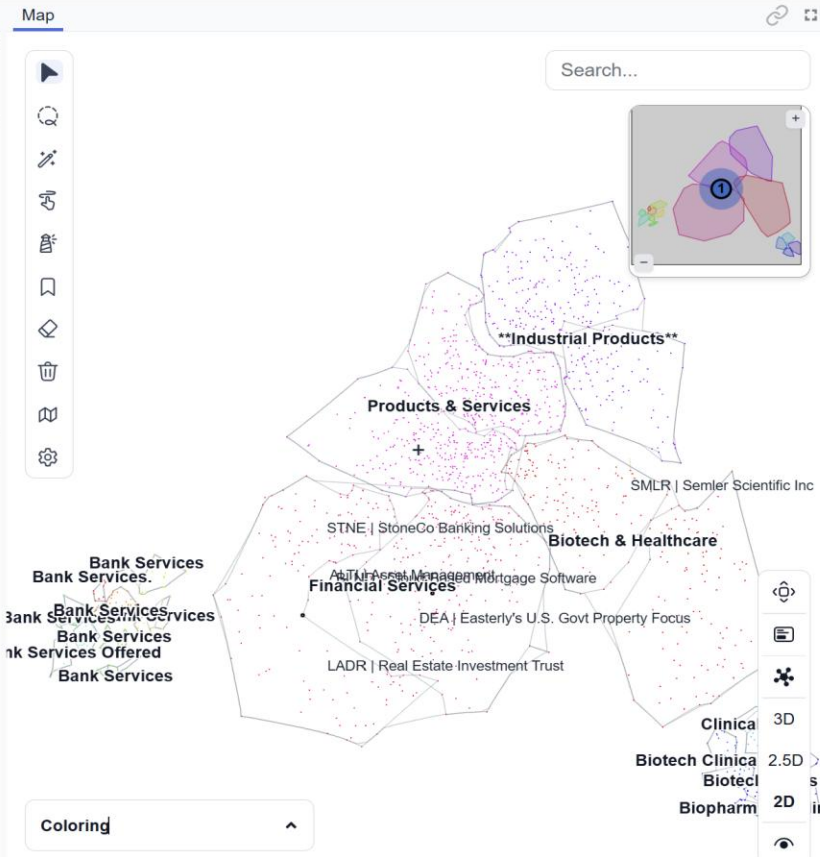
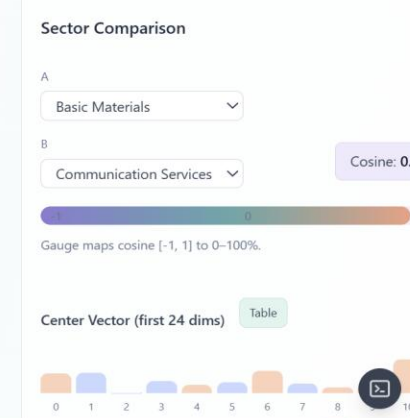
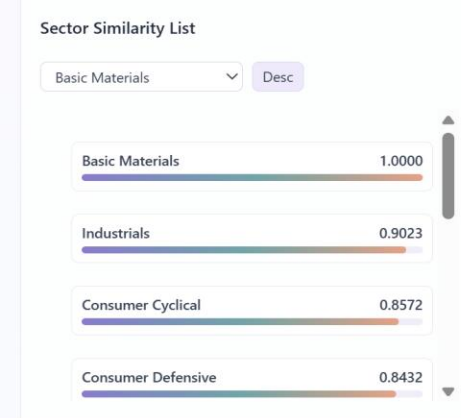
Date: 1970
 Likes: 494
 Views: 14524

Investment, Stocks, Financial Analytics, Quant Trading

SectorSimilarity

	Basic Materials	Communication Services	Consumer Cyclical	Consumer Defensive	Energy	Financial Services	Healthcare	Industrials	Real Estate	Technology
Basic Materials	1.00	0.77	0.86	0.84	0.84	0.75	0.78	0.90	0.73	0.79
Communication Services	0.77	1.00	0.87	0.82	0.76	0.80	0.78	0.86	0.75	0.90
Consumer Cyclical	0.86	0.87	1.00	0.91	0.79	0.80	0.80	0.91	0.78	0.84
Consumer Defensive	0.84	0.82	0.91	1.00	0.75	0.76	0.80	0.85	0.73	0.80
Energy	0.84	0.76	0.79	0.75	1.00	0.73	0.72	0.86	0.70	0.75
Financial Services	0.75	0.80	0.80	0.76	0.73	1.00	0.72	0.82	0.78	0.80
Healthcare	0.78	0.78	0.80	0.80	0.72	0.72	1.00	0.81	0.72	0.81
Industrials	0.90	0.86	0.91	0.85	0.86	0.82	0.81	1.00	0.77	0.91
Real Estate	0.73	0.75	0.78	0.73	0.70	0.78	0.72	0.77	1.00	0.72
Technology	0.79	0.90	0.84	0.80	0.75	0.80	0.81	0.91	0.72	1.00
Utilities	0.80	0.75	0.79	0.76	0.86	0.73	0.70	0.85	0.70	0.74

Click a cell to set (row = selected, column = compare).



Corporate Knowledge and Organizational Data

Narrator x

what are the key contributions of {Layer: Pascal Passigan}?

Narrator: The key contributions of Pascal Passigan encompass a variety of topics focused on enhancing data processing, infrastructure, and user experience within the Mantis platform. Here are the highlights:

1. Space Creation and User Interaction:

Initiated discussions on creating spaces that allow users to dynamically adjust parameters such as UMAP and t-SNE, enabling real-time visual feedback during data clustering.

Proposed the decoupling of space creation from data processing tasks, allowing users to interact with their data more quickly while background processes occur.

2. Synthesis Pipeline Improvements:

Contributed to the optimization of the synthesis pipeline using GPU acceleration to enhance processing speed.

Focused on addressing critical issues like context overflow and ensuring the robustness of the pipeline through better error handling and integration testing.

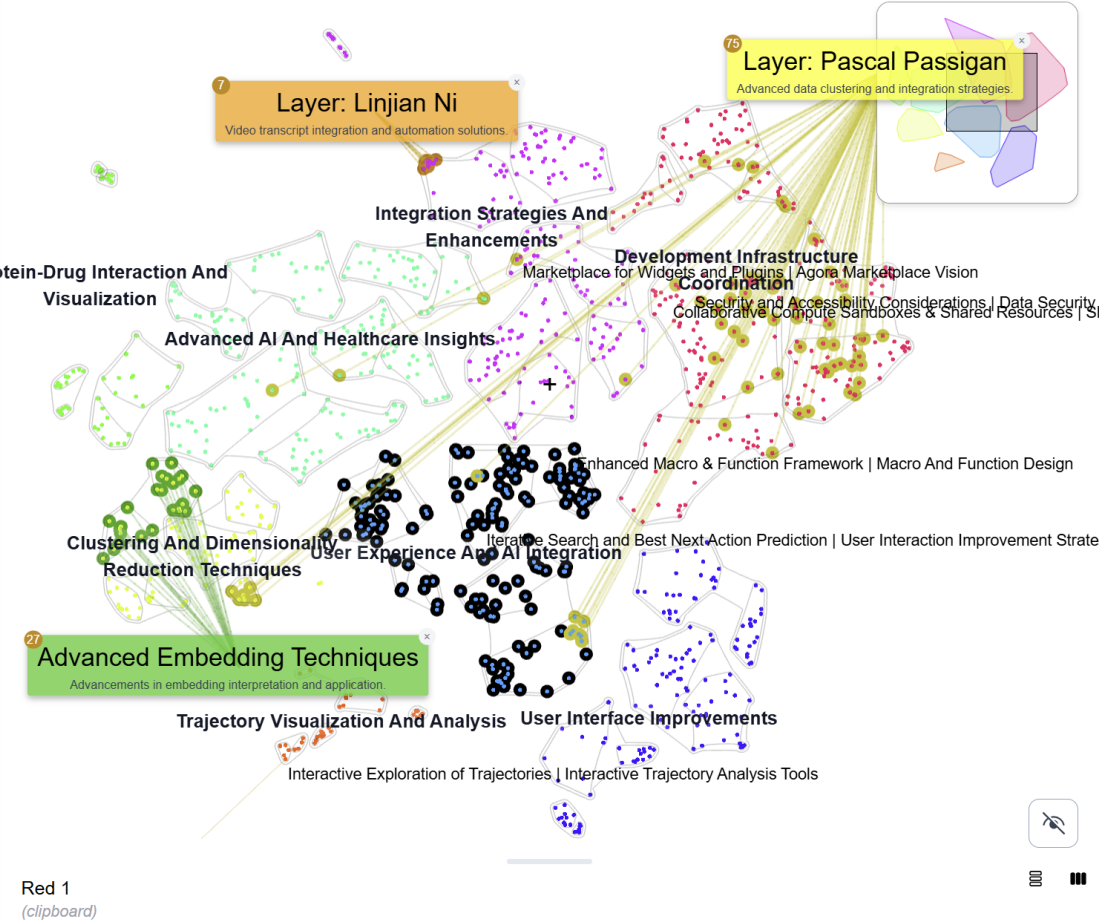
3. GPU Infrastructure Planning:

Advocated for the establishment of a cost-effective internal compute farm to reduce dependence on external APIs and manage increasing client loads efficiently.

Highlighted the need for modular GPU setups that enhance performance through containerized applications and optimized workload distribution.

4. Reinforcement Learning and AI Models:

Map



Red 1
(clipboard)

Tree x

Filter nodes...

- ▶ Advanced AI And Healthcare Insights
- ▶ User Experience And AI Integration
- ▶ User Interface Improvements
- ▶ Protein-Drug Interaction And Visualization
- ▶ Trajectory Visualization And Analysis
- ▶ Clustering And Dimensionality Reduction Techniques
- ▶ Integration Strategies And Enhancements
- ▶ Development Infrastructure Coordination

Categories x

Speaker

- Sarah Mokhtar
- Andrew Varughese
- Linjian Ni
- Sufian Aldogom
- Raymund Thongthip...
- Manolis Kellis
- Pascal Passigan
- Jake Weiss
- Nikhil Chandra
- Angelika
- Kaiden Simon
- Arjun Kulkarni
- Thanosan Prathifku...
- Vinay Singamsetty
- Joshua Wu

Meeting

- Onboarding
- BeaverWorks Onbo...
- Team C Compute
- Team A Agents
- ML Widget convers...
- Team B Backbone
- AllHands Midweek / ...
- Team A Agents / Te...
- Team D Embeddings
- Leadership Team
- AllHands Mantis
- Team G Genes Dru...
- Team I Integrations
- Mantis Platform Up...
- Team C Compute / ...

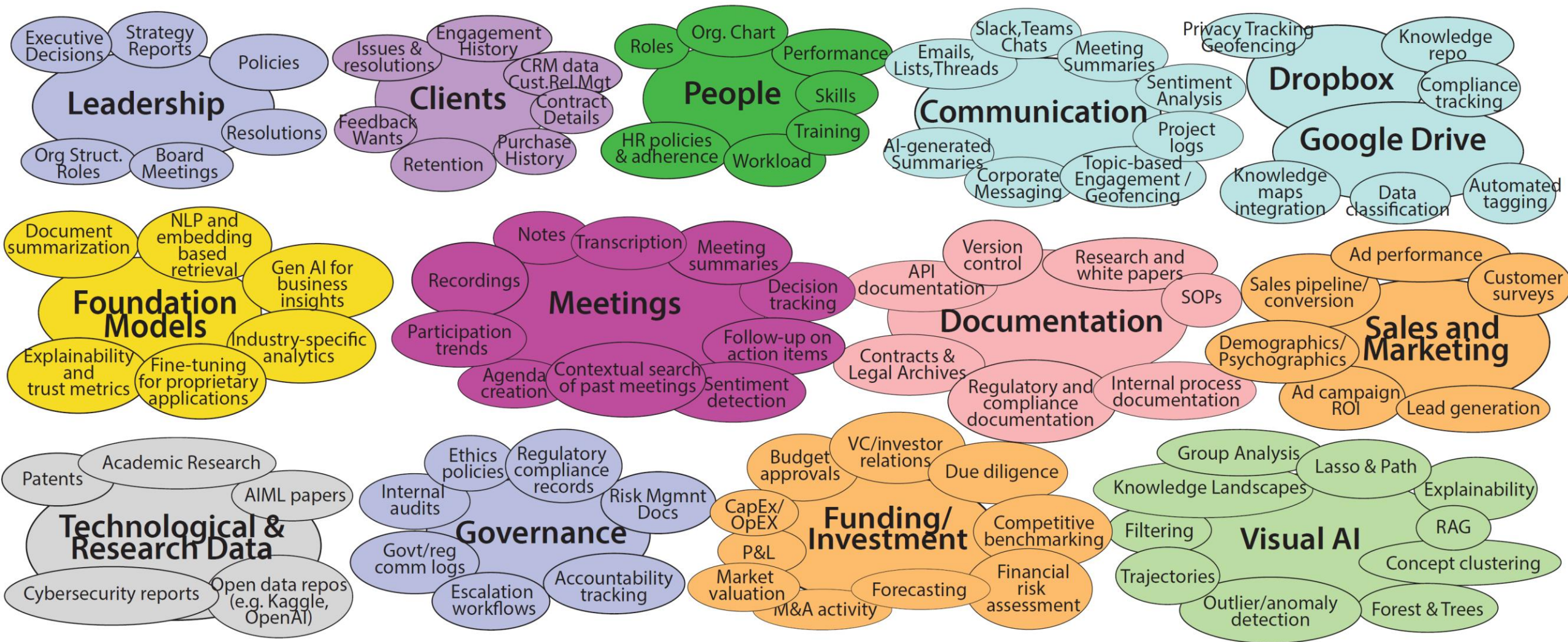
Bags x

World | Bags - 5 + | Clear | Delete

Red 1 +

7 Layer: Linjian Ni | 75 Layer: Pascal Passigan | 27 Advanced Embedding Techniques

<https://mantisdev.csail.mit.edu/space/d99efc56-00d5-4f18-8ecc-0620500fcf79/>

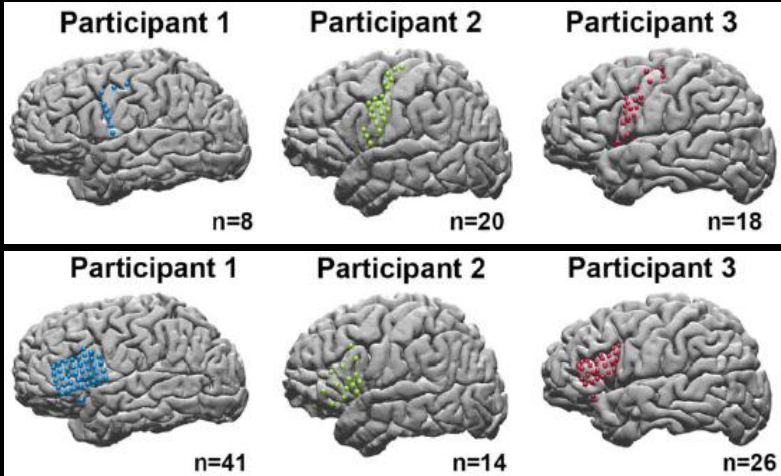


- For AI to have an impact, every aspect of the business must be available to it
- Connect between dramatically different data streams
- Make systematic connections, insights: *Do not leave serendipity to chance:*

Peeking inside the brain of the machine



Maybe we're not that different after all



nature communications

Article <https://doi.org/10.1038/s41467-024-46631-y>

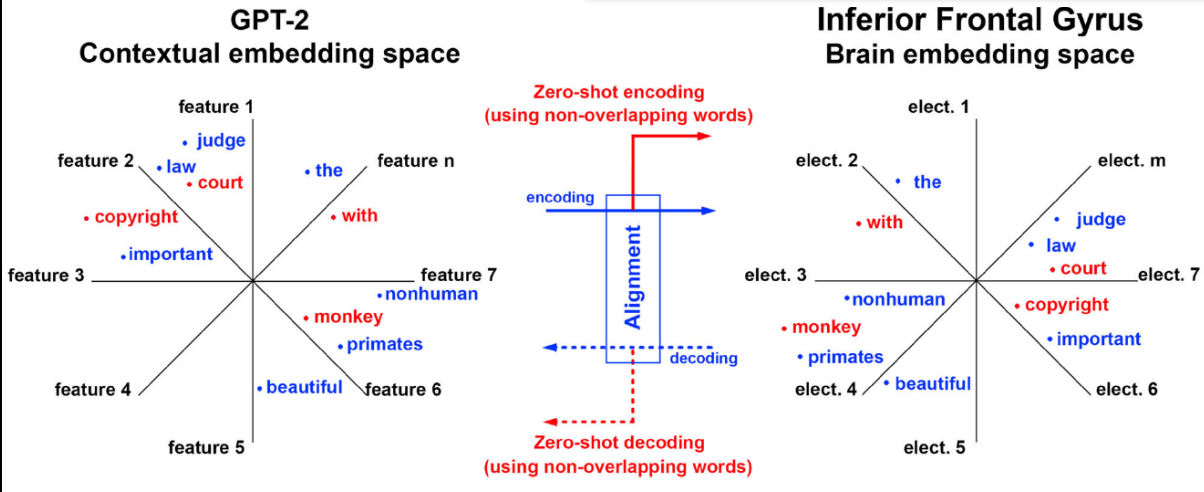
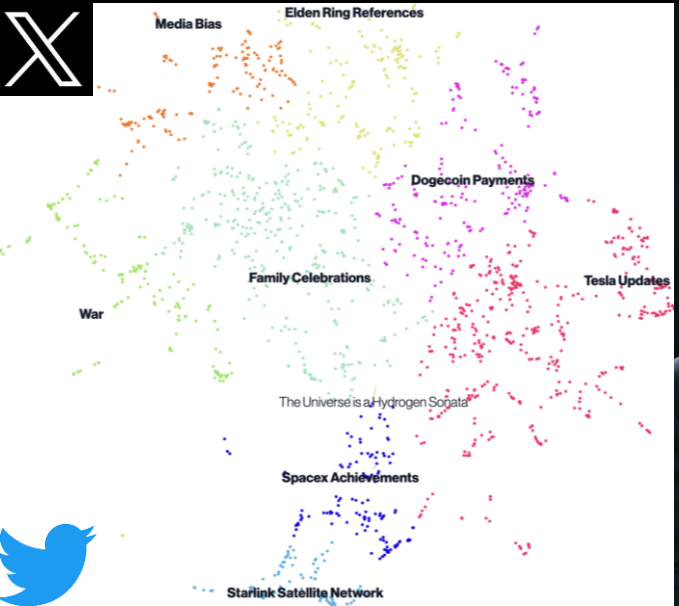
Alignment of brain embeddings and artificial contextual embeddings in natural language points to common geometric patterns

Received: 24 July 2022
 Accepted: 4 March 2024
 Published online: 30 March 2024

Ariel Goldstein^{1,2}, Avigail Grinstein-Dabush^{2,6}, Mariano Schain^{2,6}, Haocheng Wang³, Zhuoqiao Hong³, Bobbi Aubrey^{3,4}, Mariano Schain², Samuel A. Nastase², Zaid Zada², Eric Ham⁵, Amir Feder², Harshvardhan Gazula², Elav Buchnik², Werner Doyle⁴, Sasha Devore⁴, Patricia Dugan⁴, Roi Reichart², Daniel Friedman², Michael Brenner^{2,6}, Avinatan Hassidim², Orrin Devinsky^{2,4}, Adee Flinker^{2,4,7} & Uri Hasson^{2,3}

Contextual embeddings, derived from deep language models (LLMs), provide a continuous vectorial representation of language. This embedding space differs fundamentally from the symbolic representations posited by traditional psycholinguistics. We hypothesize that language areas in the human brain, similar to LLMs, rely on a continuous embedding space to represent language. To test this hypothesis, we densely record the neural activity patterns in the inferior frontal gyrus (IFG) of three participants using dense intracranial arrays while they listened to a 30-minute podcast. From these fine

Peeking inside the brain of the human



Similarities in Brain activation maps & LLM embeddings

Perhaps expected, we both learn from context!

Clusters



Hierarchical



Plotting

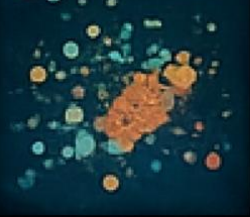


Temporal Fitting



Clig

1.0.2019



Classo



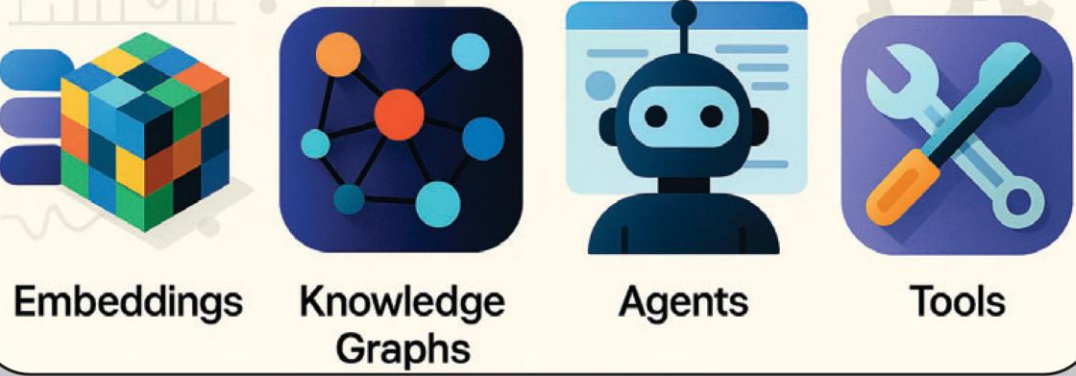
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Plotting

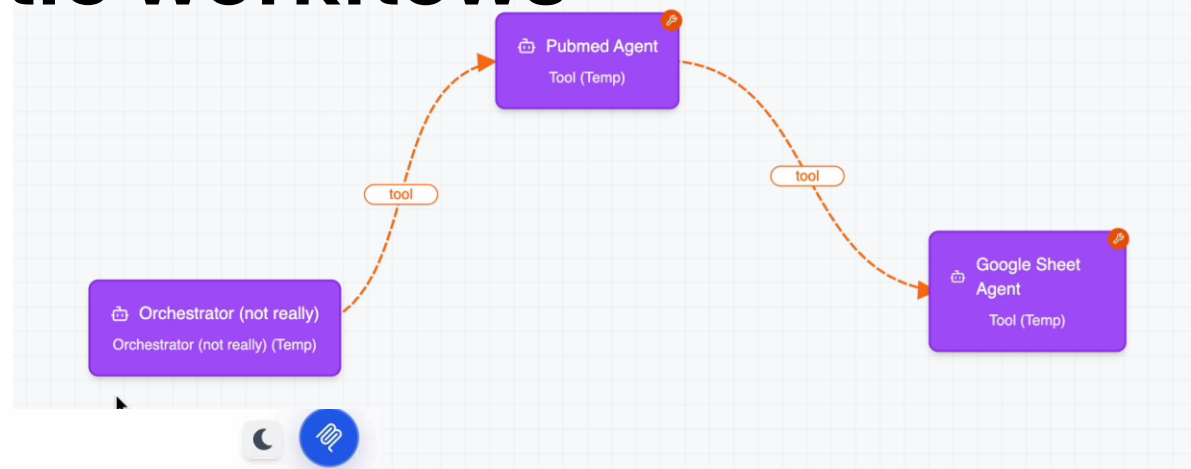


Four pillars of Mantis



Embeddings Knowledge Graphs Agents Tools

Agentic workflows



Lex Clips File Export Plugins View Help Cache Space Menu

Agent's Agora x MantisGPT x

Agent & Team Management

My Workflows (2) Public Agents (7) Public Teams (0) Public Workflows (6)

Saathvik and anant agent Pipeline

This is the drug discovery agent pipeline of Saathvik and Anant but in Mantis...

4 nodes 5 connections

Chat Workflow

Public

Active

Created Jul 7, 2025

By anas.maarouf@eleve.lfgermain.com

Active Wildfire Detector Report writing

Active Wildfire Detector Report writing

2 nodes 1 connections

Chat Workflow

Public

Active

Created Jul 6, 2025

By g.angelis.contact@gmail.com

BioMarker Researcher

Retrieves the sentence descriptions for each of the biomarkers in the presente...

3 nodes 2 connections

Chat Workflow

Public

Active

Created Jul 6, 2025

By anas.maarouf@eleve.lfgermain.com

Mantis X Youtube X Gmail (hackathon example)

3 nodes 4 connections

Chat Workflow

Public

Active

Video Navigator

Proposing ordering of educational videos

3 nodes 4 connections

Chat Workflow

Public

Active

Summarization

Summarizes clusters hierarchically

1 nodes 0 connections

Chat Workflow

Public

Active

New Conversation

Custom Workflow: BioMarker Researcher

tolerance to therapy and outcomes

PS ECOG	Performance Status, ECOG scale (0-5); lower = better outcome	0-1 (higher is worse)	PMID: 28952933
Date of Dx	Date of diagnosis; relevant for chronology, less predictive itself	N/A	N/A

Next Steps:

- Confirm if this level of detail matches your needs.
- I will expand in groups of 5-10 biomarkers at a time to keep the information manageable.
- Let me know if you want to prioritize specific markers, go by groups (labs, clinical, cytogenetics...), or continue sequentially.

Shall I proceed with the next five biomarkers?

Today, 09:59 AI

Enter to send Shift + Enter for new line

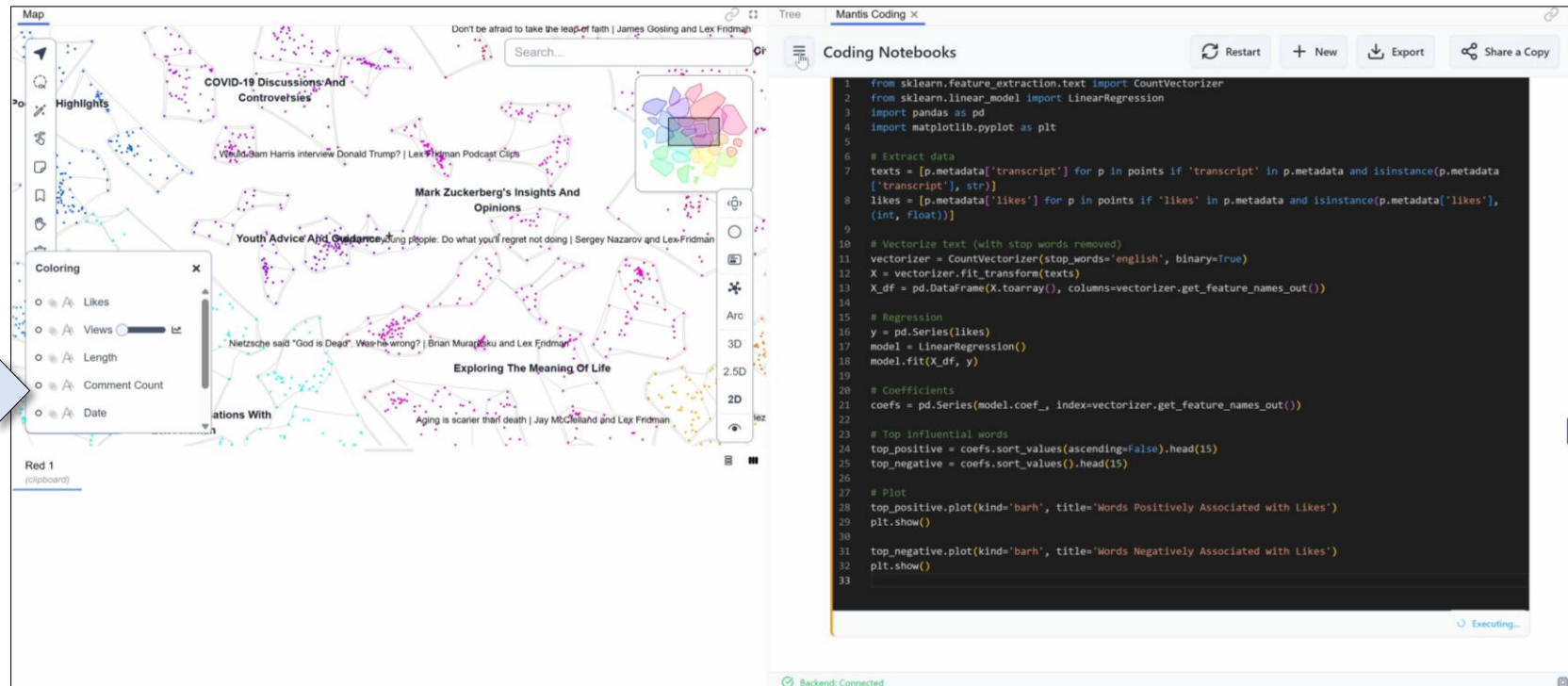
- An agora of collaborating agents
- Building and sharing agent teams
- Empowering agents with tools capabilities
- Sharing and re-using teams for complex tasks

Height at time of treatment	There is no established evidence or guidance regarding the clinical
Response Criteria - Guidelines updated by the International Working Group (IWG) 2016 and 2023 for classification, risk stratification, and response in MDS. Key for therapeutic response assessment and patient management.	
Time of best response	Time to best response in MDS refers to the interval between initia
Azacitidine	Reasons for stopping azacitidine in Myelodysplastic Syndromes (M
LDH	Serum lactate dehydrogenase (LDH) is an enzyme involved in ener

Agentic Coding: Data+UI

Coding Notebooks: Data/UI/markdown cells

- Data (back-end) coding agent:**
- Understands user intent
 - Realizes need for a program
 - Plans, reflects
 - Knows the data structure
 - Writes code to answer complex questions
 - Runs code
 - Finds insights
 - Plots them back

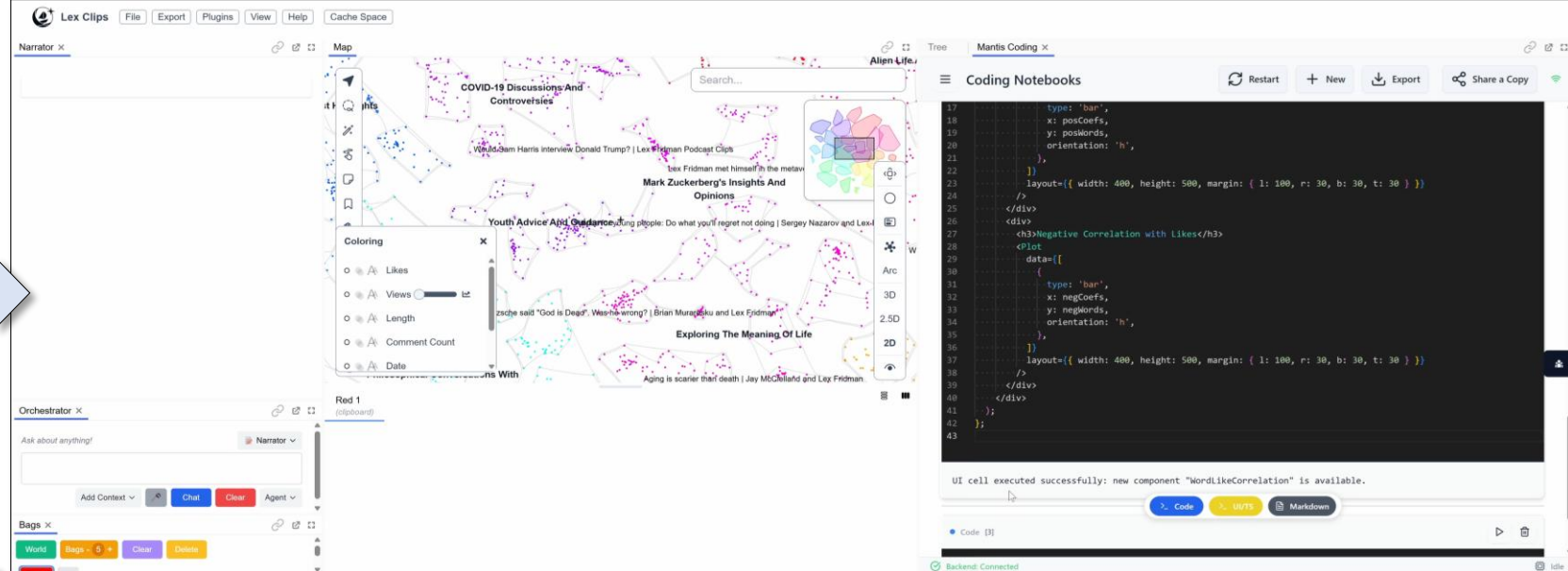


Question: What podcast topics are most popular on Lex Fridman's podcast?

- Front-end agent:**
- Understands UI/UX platform
 - Reflects, plans
 - Selects visualization component
 - Links coding answers to data
 - Reveals source of the answers
 - Transparency
 - Interactivity
 - Traceability
 - Accountability
 - Groundedness



Data coder: analyzes millions of points in secs, reveals insights



Answer: Persevere, completion,

UI coder: creates interactive visualizations, new widgets, see and 'touch' results

Navigating Knowledge - Wikipedia Page for AI (Chrome

Extension)

Connection - 2259ae71-1a18-45a1-a720-edd767bf648f | File | Export | Plugins | View | Help | Cache Space

Narrator x | Map | Tree x

Search...

Filter nodes...

- Agent Decision-Making Theories
- Theoretical Foundations Of AI Algorithms
- Bayesian Networks And Probabilistic Algorithms
- Ethical Implications Of AI
- Algorithmic Bias In Machine Learning
- Socio-Economic Impact Of AI
- Ethical Implications Of AI
- Knowledge Representation Challenges In AI
- Formal Logic Theory Focus
- Deductive Reasoning Education
- Algorithmic Search Methodologies
- Ethical Considerations Of AI Rights
- Philosophical Debates On AI Ethics
- Philosophical Inquiry Into AI
- Theoretical Insights On AI

Cluster Depth: 4 | Local Labels: 0 | Flashcards: 0

Remake Partitions | Show Partitions

Coloring x

- Idx
- Paragraph_idx
- Clusters
- Bags
- Main Layer

Orchestrator x | Ask about anything | Narrator v

World | Bags - 5 | Clear | Delete

Red 1 (clipboard)

WIKIPEDIA the free encyclopedia

Search Wikipedia | Search

Artificial intelligence 164 languages

Article | Talk | Read | View source | View history | Tools

From Wikipedia, the free encyclopedia

"AI" redirects here. For other uses, see AI (disambiguation) and Artificial intelligence (disambiguation).

Artificial intelligence (AI) refers to the capability of computational systems to perform tasks typically associated with human intelligence, such as learning, reasoning, problem-solving, perception, and decision-making. It is a field of research in computer science that develops and studies methods and software that enable machines to perceive their environment and use learning and intelligence to take actions that maximize their chances of achieving defined goals.^[1] Such machines may be called AIs.

High-profile applications of AI include advanced web search engines (e.g., Google Search); recommendation systems (used by YouTube, Amazon, and Netflix); virtual assistants (e.g., Google Assistant, Siri, and Alexa); autonomous vehicles (e.g., Waymo); generative and creative tools (e.g., ChatGPT and AI art); and superhuman play and analysis in strategy games (e.g., chess and Go). However, many AI applications are not perceived as AI: "A lot of cutting edge AI has filtered into general applications, often without being called AI because once something becomes useful enough and common enough it's not labeled AI anymore."^{[2][3]}

Various subfields of AI research are centered around particular goals and the use of particular tools. The traditional goals of AI research include learning, reasoning, knowledge representation, planning, natural language processing, perception, and support for robotics.^[9] General intelligence—the ability to complete any task performed by a human on an at least equal level—is among the field's long-term goals.^[4] To reach these goals, AI researchers have adapted and integrated a wide range of techniques, including search and mathematical optimization, formal logic, artificial neural networks, and methods based on statistics, operations research, and economics.^[6] AI also draws upon psychology, linguistics, philosophy, neuroscience, and other fields.^[5]

Artificial intelligence was founded as an academic discipline in 1956,^[6] and the field went through multiple cycles of optimism throughout its history,^{[7][8]} followed by periods of disappointment and loss of funding, known as AI winters.^{[9][10]} Funding and interest vastly increased after 2012 when deep learning outperformed previous AI techniques.^[11] This growth accelerated further after 2017 with the transformer architecture,^[12] and by the early 2020s many billions of dollars were being invested in AI and the field experienced rapid ongoing progress in what has become known as the AI boom. The emergence of advanced generative AI in the midst of the AI boom and its ability to create and modify content exposed several unintended consequences and harms in the present and raised concerns about the risks of AI and its long-term effects in the future, prompting discussions about regulatory policies to ensure the safety and benefits of the technology.

Goals

The general problem of simulating (or creating) intelligence has been broken into subproblems. These consist of particular traits or capabilities that researchers expect an intelligent system to display. The traits described below have received the most attention and cover the scope of AI research.^[3]

Reasoning and problem-solving

Early researchers developed algorithms that imitated step-by-step reasoning that humans use when they solve puzzles

Versatility, Privacy, Cost Saving, Scaling to Billions of Data

Versatility

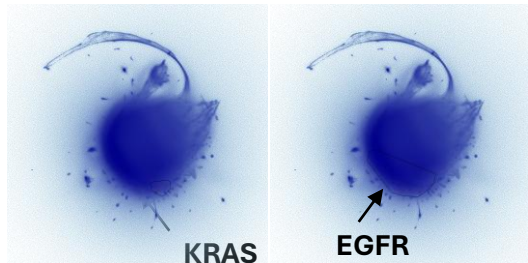
- ChatGPT, Claude, Gemini
- User custom sessions
- MantisGPT: Our own LLM (knows tools/code/schemas)

Privacy + Cost Savings

- Custom LLM installed locally
- DeepSeek/Kimi K2
- Data lives locally, never moved to server, only load as needed

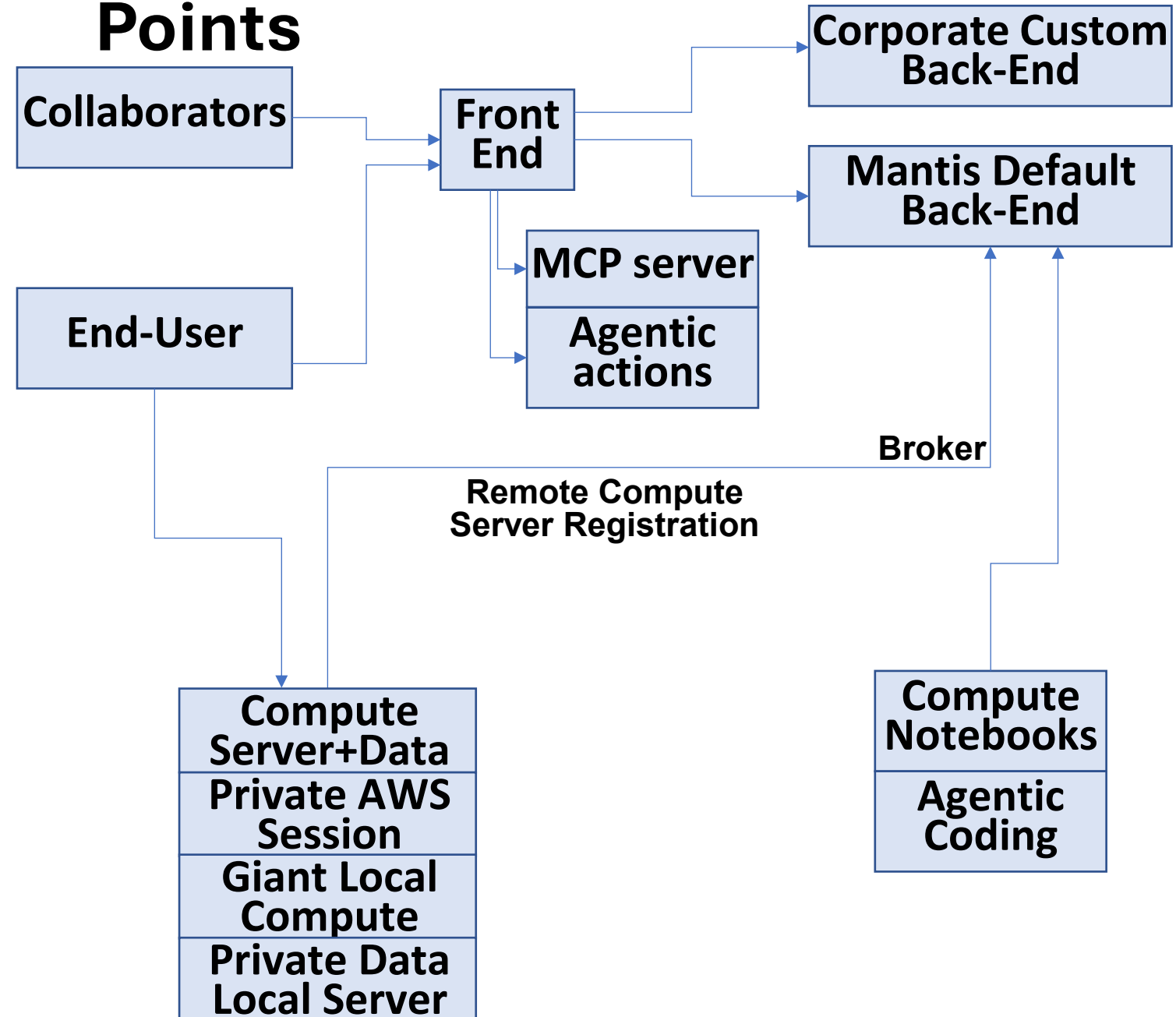
Scaling to billions of points

- Progressive loading of points
- Lasso, search include more points as needed after selection is made

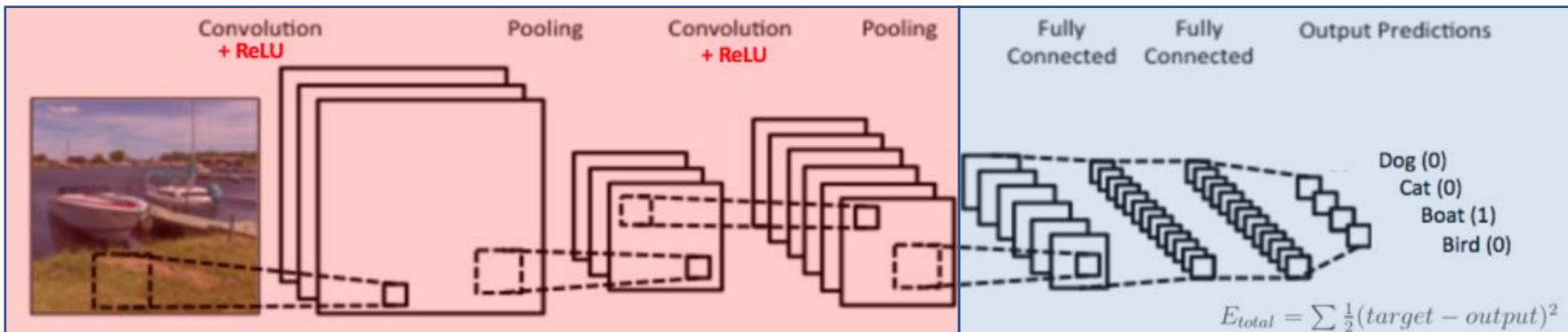


Example: 120 million drugs

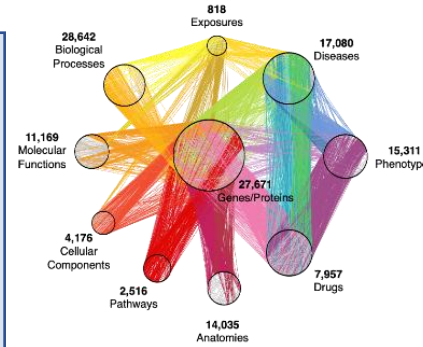
Points



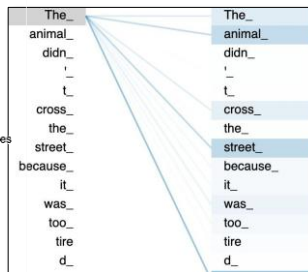
GenAI Key idea: Representation learning



Knowledge Graphs



Free Text



X
data

'Modern' Deep learning:
Hierarchical Representation Learning
Feature extraction

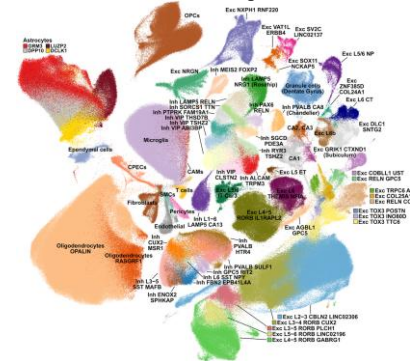
Z

Latent space representation

'Classical' Fully-connected Neural Networks
Classification

y
label

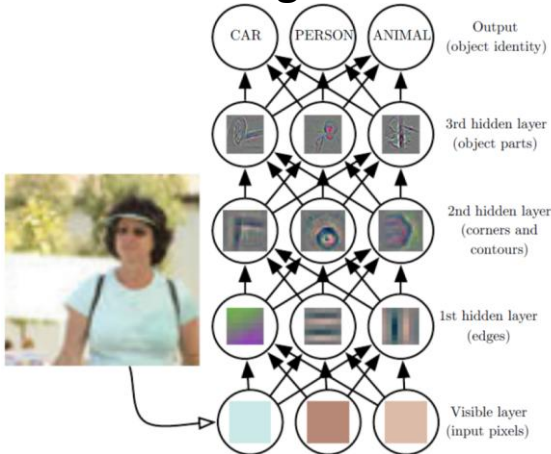
Cells: scRNA/scATAC



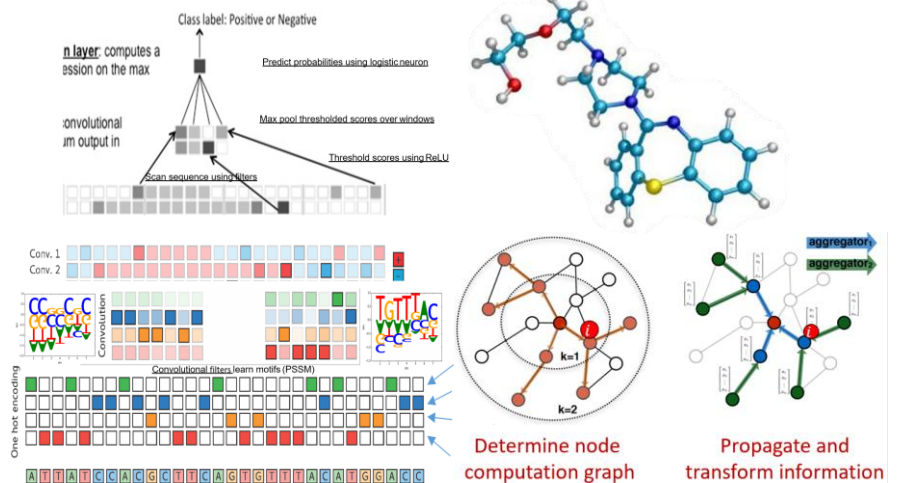
Scientific papers

GENETICS
FlyBase: a guided tour of highlighted features
The Drosophila melanogaster genome project has produced a wealth of data on the genetics of this model organism. FlyBase is a database that provides a central location for all the genetic information about Drosophila melanogaster. It includes information on genes, proteins, and other genomic features, as well as information on the interactions between these features. FlyBase is a valuable resource for researchers studying the genetics of Drosophila and other model organisms.

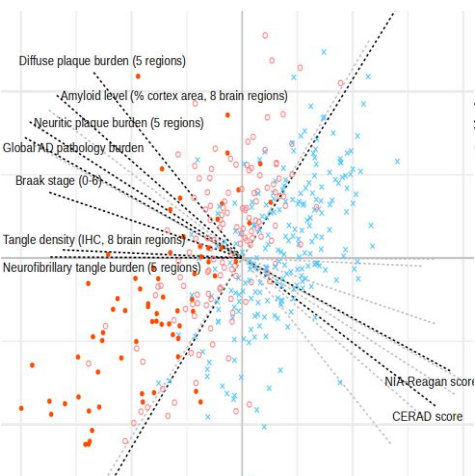
Images



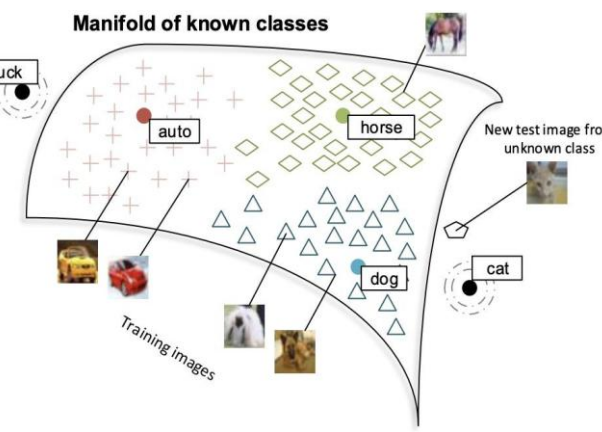
DNA/Seq/Motifs Chemical/Prot. Structure



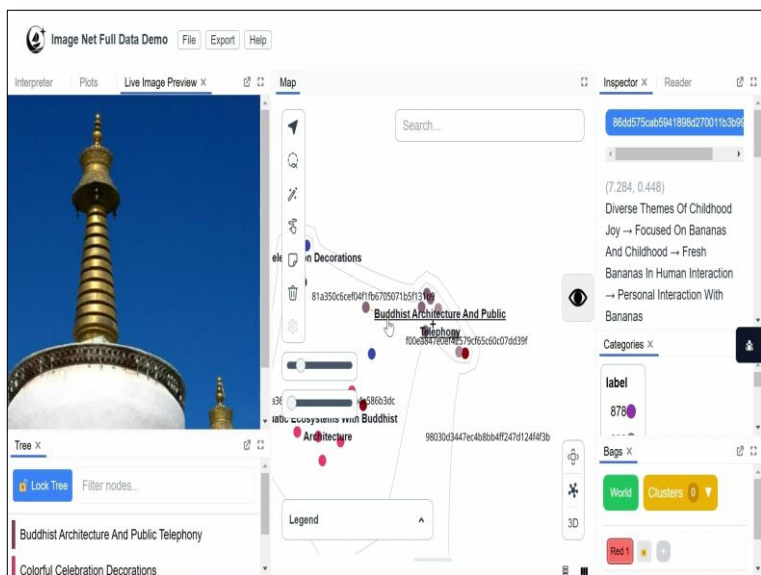
Patient records



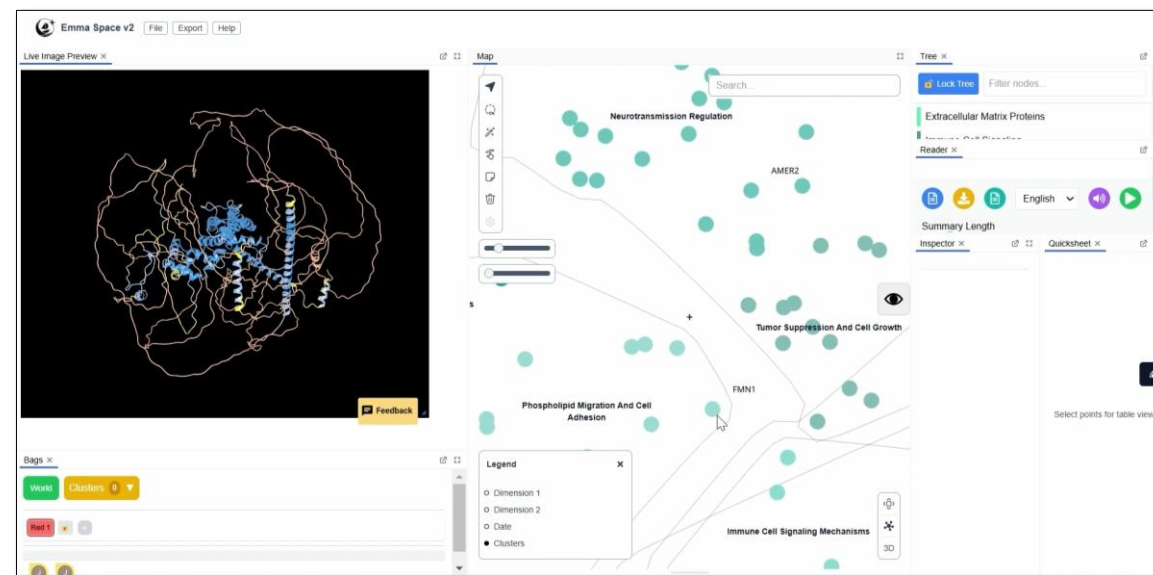
Multi-Modal



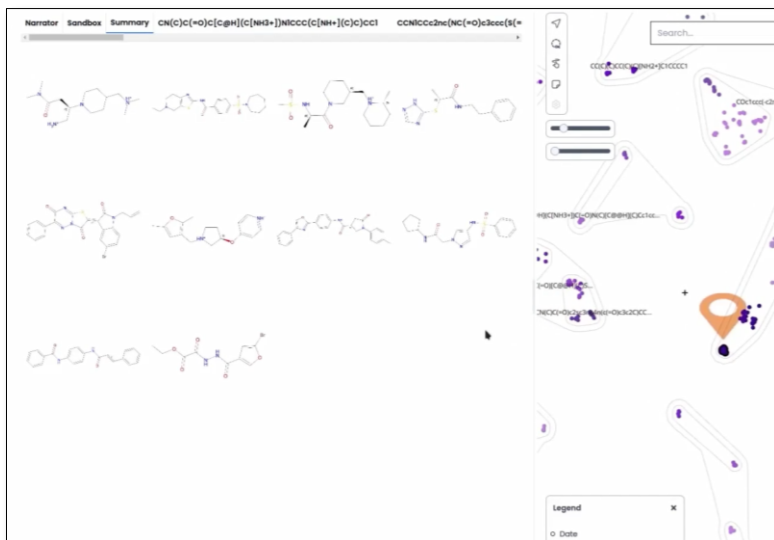
Navigating custom embeddings: Images, Videos, Proteins, Drugs, Patients, Plugins



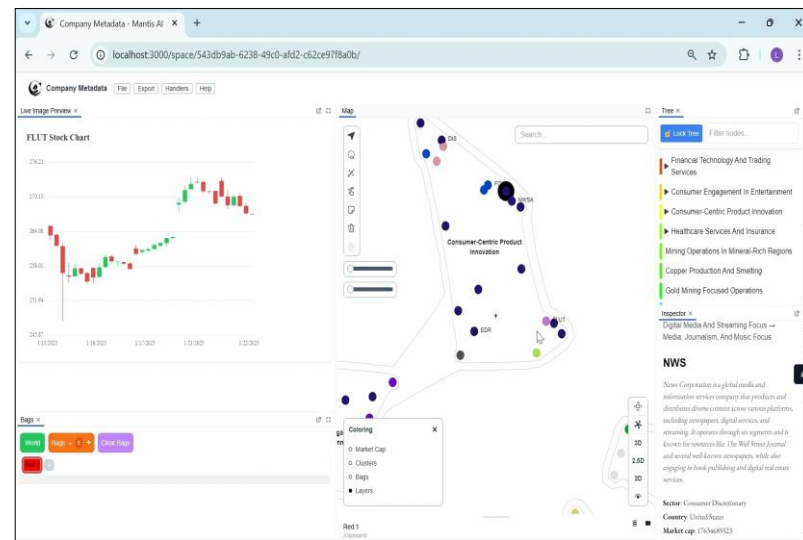
Images: Multi-modal compatible HuggingFace model, label clusters contrastively bottom-up, base64 compact image representation,



Proteins: KellisLab joint protein-structure-function knowledge graph model, Protein structure 3D rendering shows latent spaces captures structure similarity



Drugs: 250,000 molecules, graph-based (VAE), molecules as SMILES strings, GNN-VAE for geometry

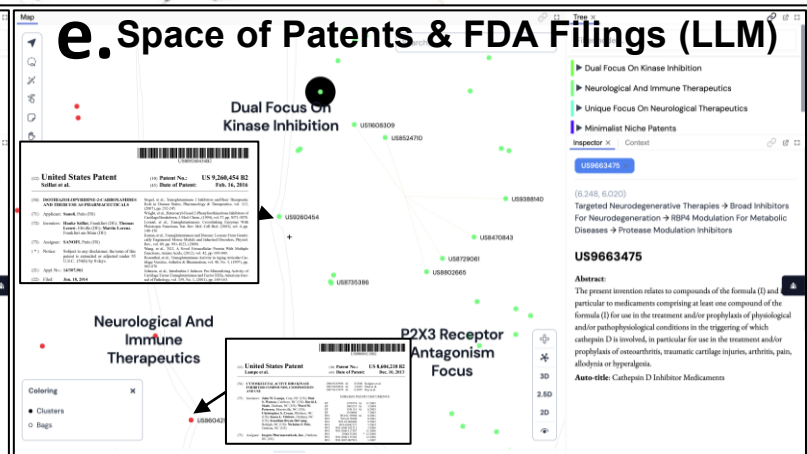
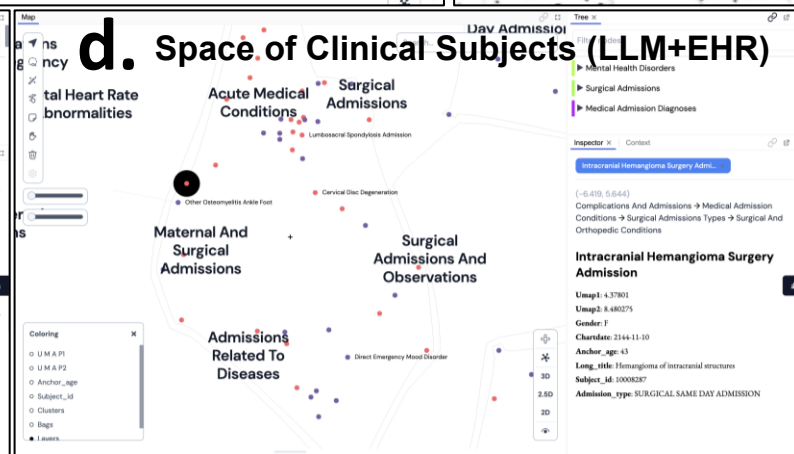
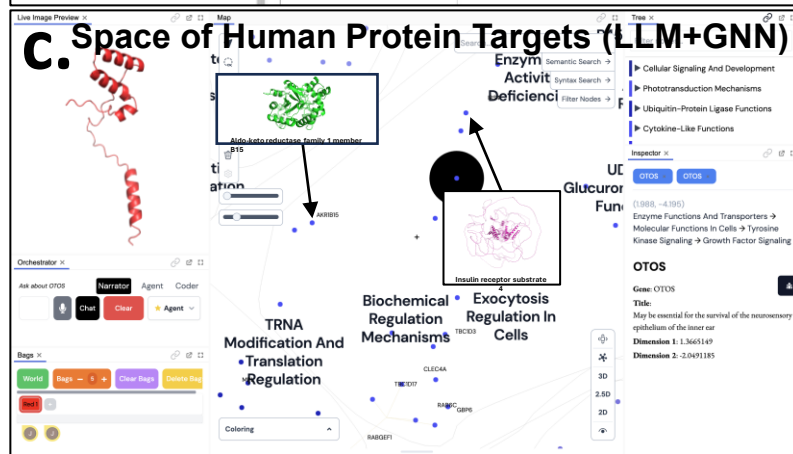
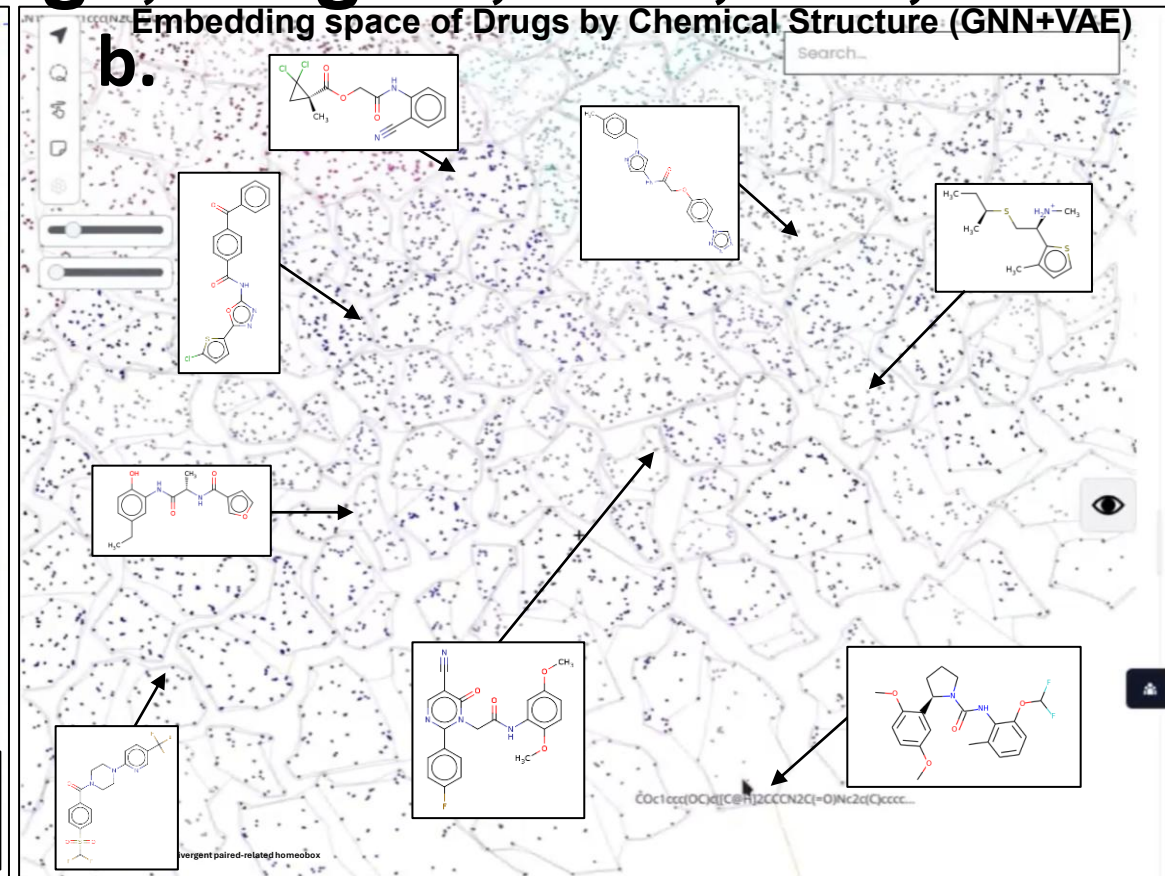
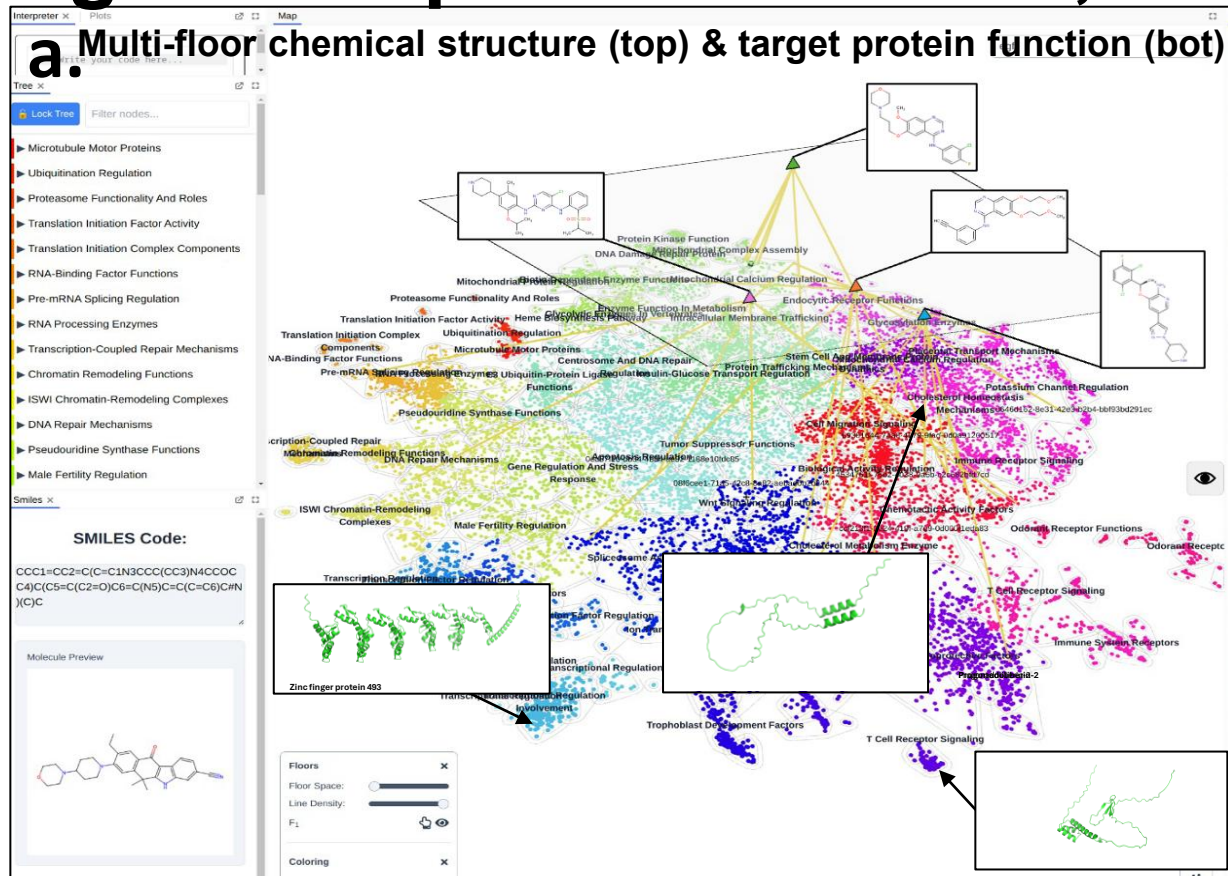


Instant Ingestions: Stock Price Monitoring, Any information live from the internet

```
3 const forceAlpha = /[A-Z]/;
4
5 return smilesRegex.test(key) && forceAlpha.test(key);
6 };
7
8 export const renderBuilder = (key: string): ReactElement => {
9   const url = `https://www.simolecule.com/cdkdepict/depict/bo
10
11   return `
12     <div style={{ display: 'flex', justifyContent: 'center'
13       <iframe
14         src=${url}
15         style={{ border: 'none', width: '100%', height:
16         title="Molecule Structure"
17     />
```

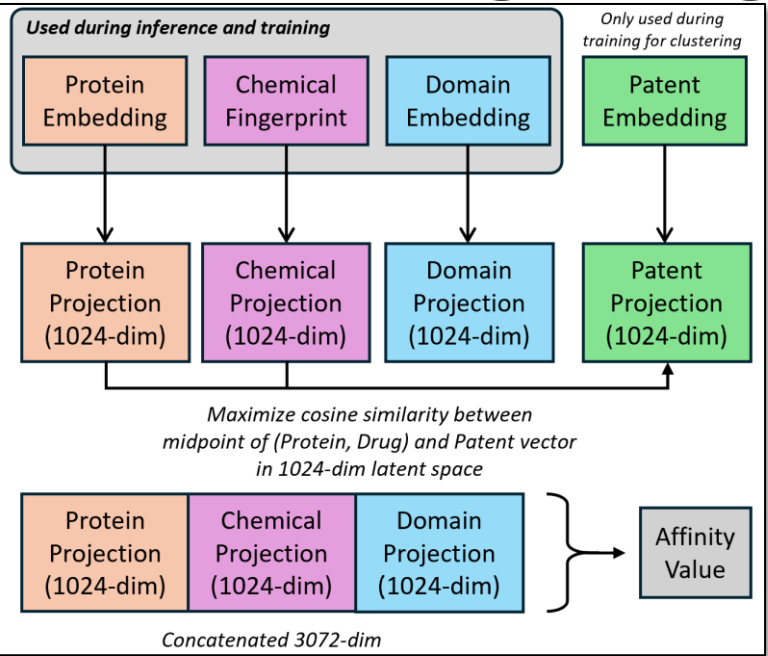
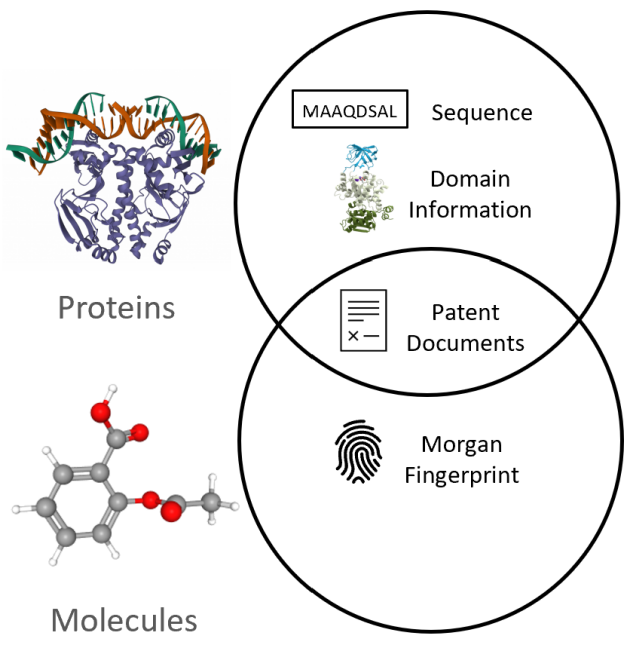
Custom: Load HuggingFace embedding model, automatically find/suggest encoders, custom plugins

Drug Development: Proteins, Drugs, Targets, FDA, IND, Patents

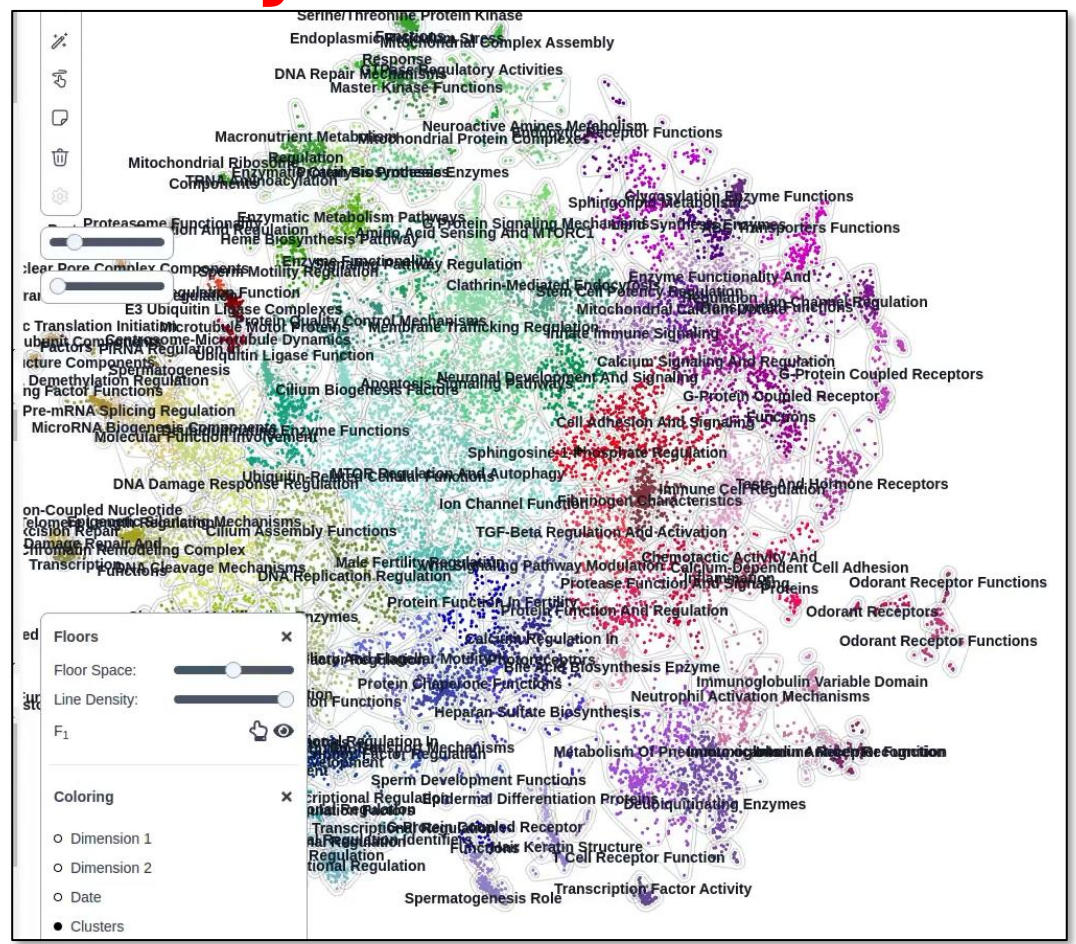
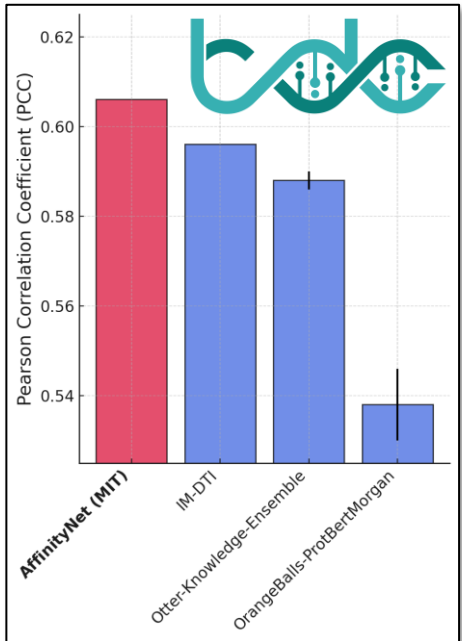


Whole Proteome Docking using AffinityNet and Mantis

Using multiple drug and protein representations to develop higher prediction accuracy

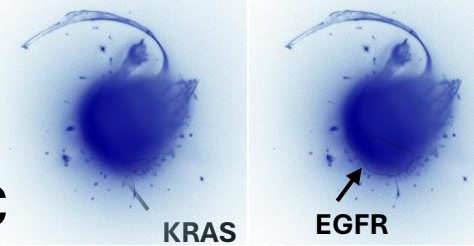


Saathvik Kannan



Enables Proteome Docking in under 10 seconds

121 million chemicals projected using AffPubChem



Top performer in TDC
Therapeutic Data Commons benchmark

- Drug-Target Interaction Domain Generalization Benchmark Group** evaluates ML models on predicting drug-target interactions under realistic temporal shifts. It tests models on unseen compounds/targets patented in 2019-2021 after training on 2013-2018 data, simulating real-world drug discovery.
- Realistic temporal domain shifts:** Simulates real-world drug discovery scenarios.
 - Out-of-distribution testing:** Evaluates model robustness on unseen compounds/targets.
 - Standardized evaluation:** Ensures fair comparison using PCC and domain-specific validation.

Mantis: Identifying patient trajectories and subtypes

MIMIC-IV Diagnoses (10/18/24) File Export Plugins View Help Cache Space

Narrator x

Map

Inspector x

Tree x

neoplasm

4 surgery
Variety of surgical admission cases

3 malignancy
Malignant neoplasms of various body parts

21 sepsis
Sepsis admissions with various unspecified organisms

35 pregnancy
Complications related to pregnancy and childbirth

Coloring x

- U.M.A.P1
- U.M.A.P2
- Anchor_age
- Subject_id
- Clusters
- Bags
- Gender

what treatments would you recommend for (surgery) patients?

Narrator: Based on the information provided, recommendations for treatments for surgical patients can vary significantly depending on the specific type of surgery and the patient's individual condition. Here are some general considerations that can be made for surgical patients:

1. Preoperative Care:

- Comprehensive evaluation to assess any underlying health conditions that could affect surgery.
- Optimization of existing medical conditions (e.g.,

Orchestrator x

Bags x

World Bags: 5 Clear Delete

sepsis surgery pregnancy hematological neurological malignancy neoplasm

Red 1 (clipboard) sepsis (clipboard) surgery (clipboard) pregnancy (clipboard) pregnancy (clipboard) malignancy (clipboard) neoplasm (clipboard)

Emergency Admissions Cardiac And Surgical Admissions Ovarian Neoplasm Admissions Gastrointestinal And Liver Conditions Surgical Admissions Surgical And Diagnostic Conditions Maternal Care Complications Cardiovascular And Respiratory Conditions Complications From Fractures Digestive System Conditions Ovarian Malignant Neoplasm Cancer And Hemorrhage Cases Neoplasms Surgical Admissions

Malignant Neoplasm of Lung Benign Lipomatous Neoplasm Unspecified Endocrine Neoplasm Admission Benign Ovarian Neoplasm Admission Surgical Admission Neoplasm Diagnosis Urgent Anal Neoplasm Admission Neoplasm Related Pain Benign Neoplasm Of Liver Thyroid Gland Malignant Neoplasm Pancreatic Malignant Neoplasm

Inspector

Malignant Neoplasm of Lung Benign Lipomatous

(4,286, 0,855)

Complications And Admissions → Infection Observations And Admissions → Cervicalgia And Septicemia Cases → Emergency Admissions

Malignant Neoplasm of Lung

Umap1: ← 10.780595 →

Umap2: ← 7.350239 →

Gender: F

Chartdate: 2129-08-31

Anchor_age: 80

Long_title: Malignant neoplasm of other parts of bronchus or lung

Subject_id: ← 10002155 →

Admission_type: EW EMER.

de9bcbf3-45f8-46fc-81fb-1e0ff7f92465

Categories x

gender

- F
- M

Quicksheet x

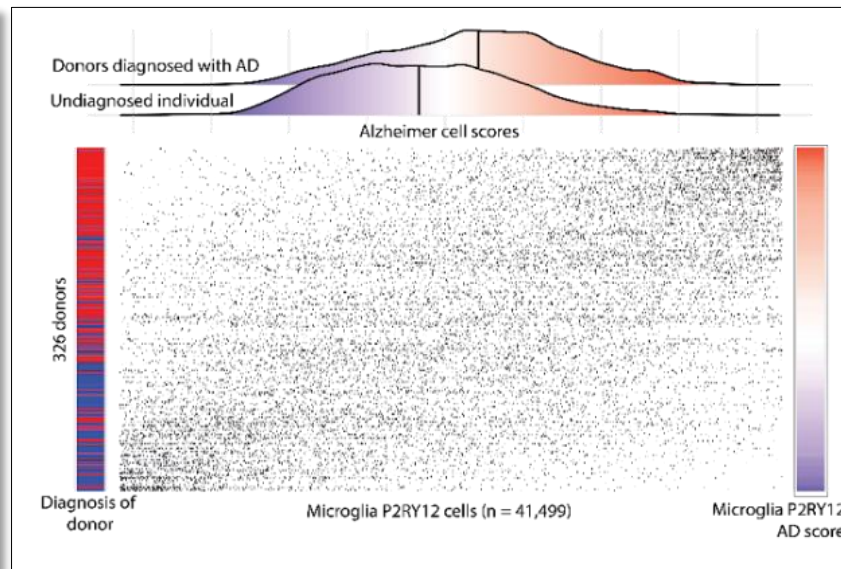
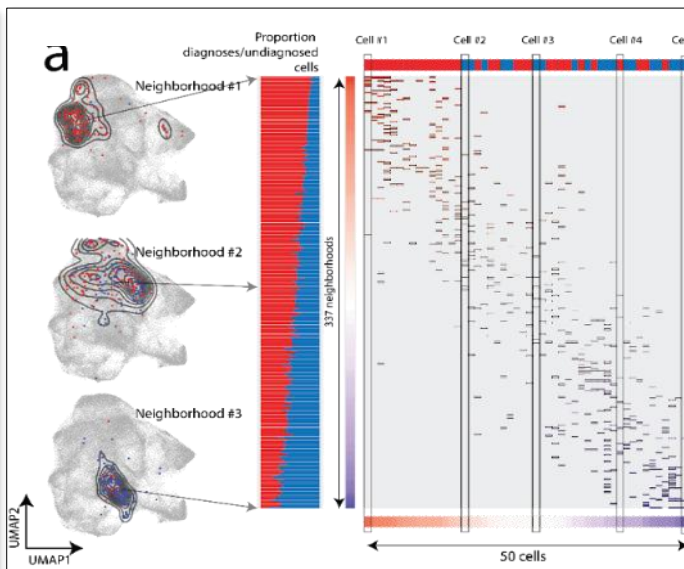
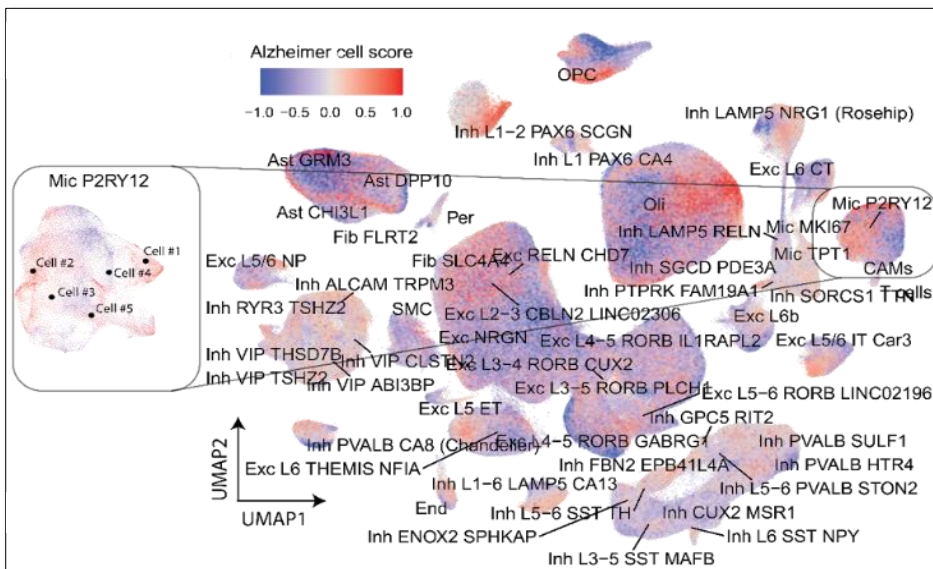
	1.22	4.52	7.71	11.01	F	3/15/2173
Secondary Pleural Malignancy						
Surgical Admission For Neoplasm	1.34	2.10	7.84	8.60	F	11/25/2186
Pancreatic Malignant Neoplasm Admission	1.34	-1.81	7.84	4.69	F	6/25/2115

Filter nodes...

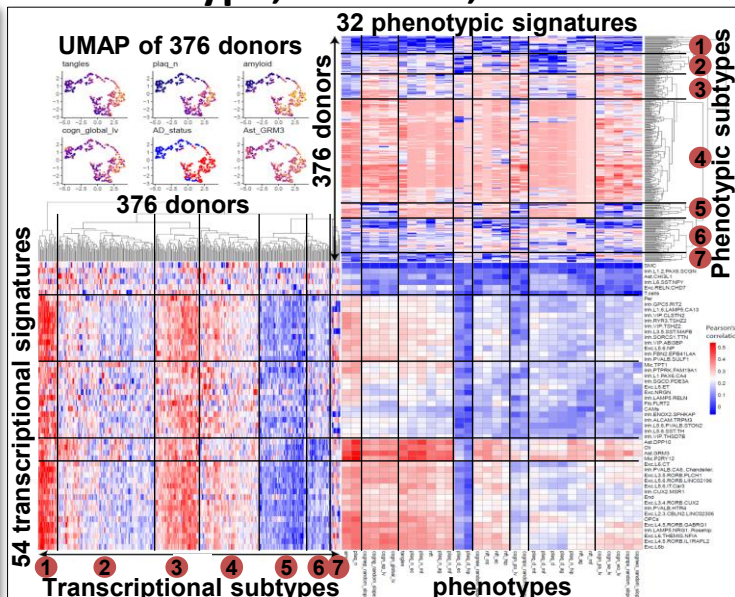
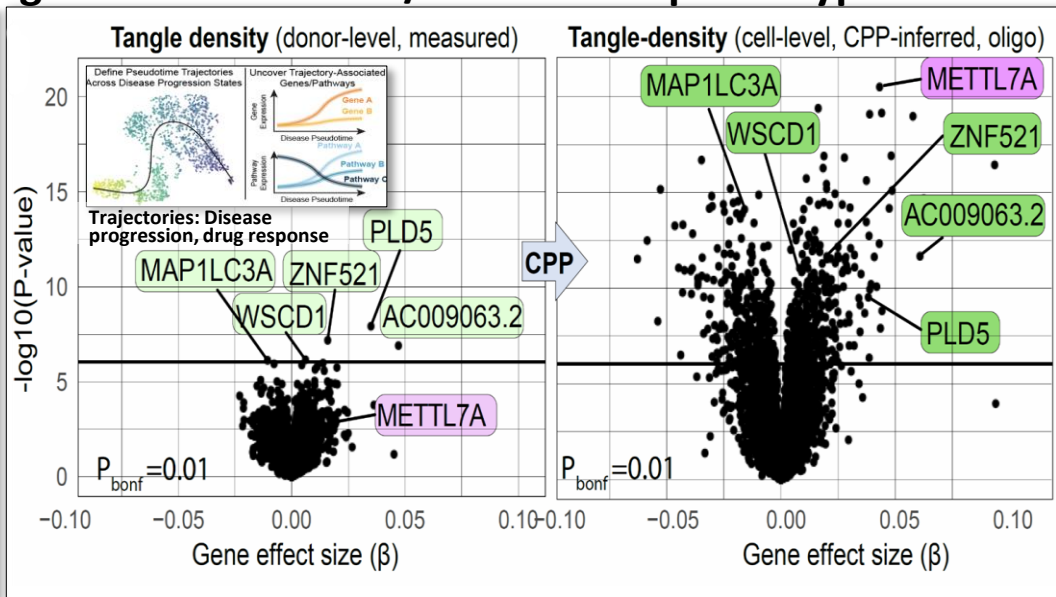
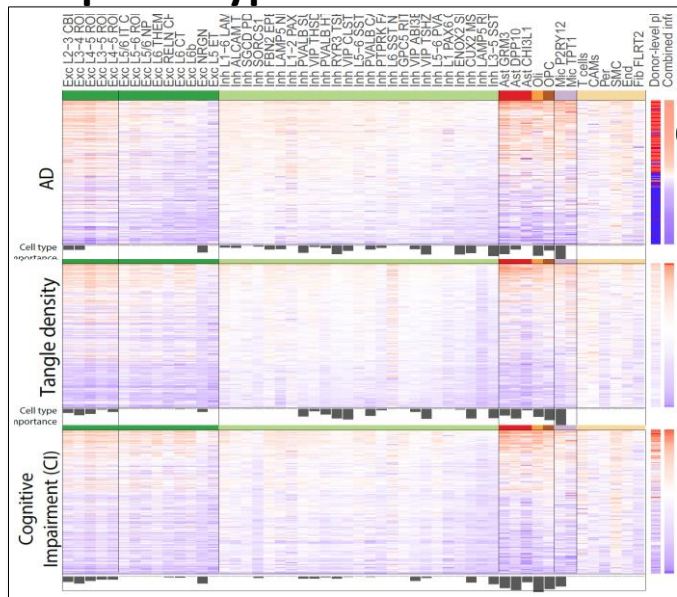
- Surgical Admissions And Observations
- Surgical Admissions For Neoplasms
- Cardiovascular Conditions Admissions
- Surgical Admissions
- Maternal And Surgical Admissions
- Surgical Admissions And Complications
- Surgical Admissions And Observations
- Infection Diagnosis Summaries
- Emergency Medical Conditions
- Abdominal Pain Observations
- Medical Admission Types
- Surgical Admissions And Observations
- Surgical Admission Summary
- Mental Health Disorders
- Pregnancy Complications
- Obstetric And Gynecological Admissions
- Atrial Fibrillation Admissions
- Medical Admissions And Observations
- Neurological Health Issues
- Neurological Injuries And Conditions
- Cardiovascular Conditions
- Acute Medical Conditions
- Cardiac Conditions And Emergencies
- Chest Pain Related Conditions

<https://mantisdev.csail.mit.edu/space/b8d50281-03c5-4844-9f9f-b5ed0f7113a5/>

Cell-Projected Phenotypes: heterogeneity, cell-specificity, gradations



Cell Transcriptional neighborhoods ↔ phenotypes Neighborhood memberships → Individual annotations for each cell type, each cell, each donor
 Diff. phenotypes manifest in diff. neighborhoods → AD/Ctrl-like cell phenotypes



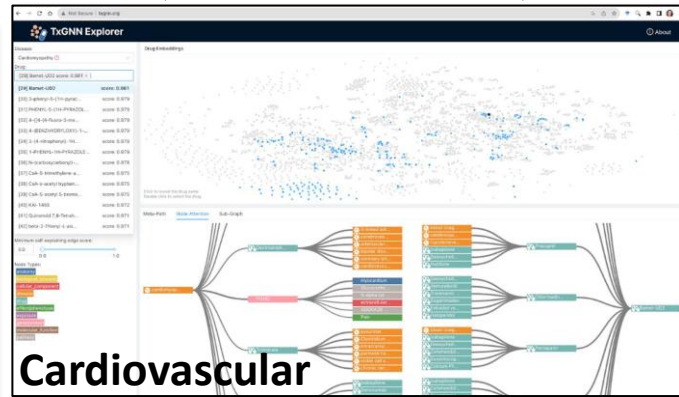
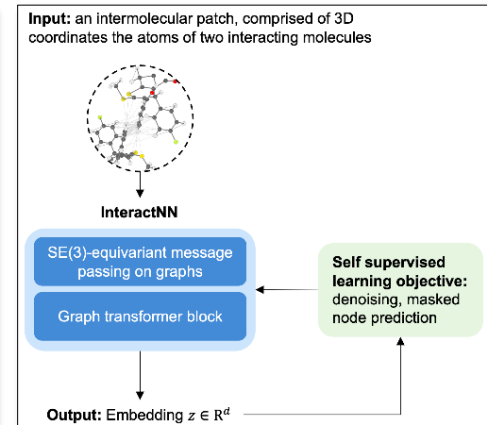
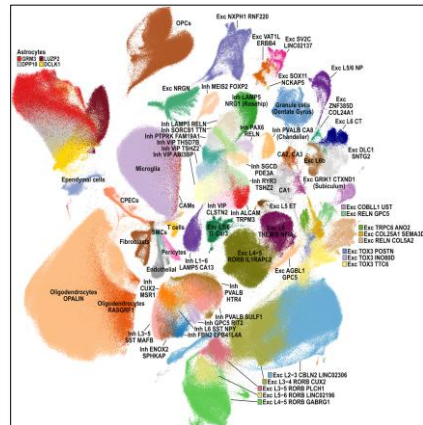
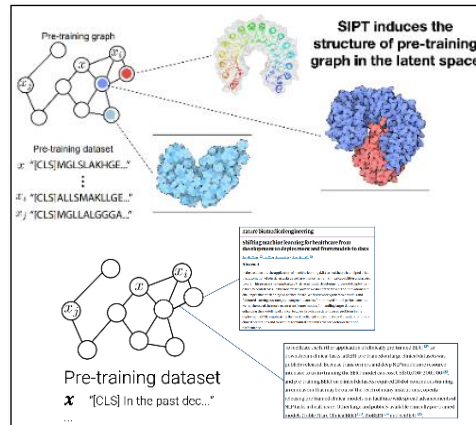
Burden for each donor+cell type Applied for multiple phenotypes

Dramatic increase in DEG discovery power for DEGs (differentially-expressed genes) FDR in all cell types

Discovery of patient subtypes with similar transcription & phenotypes

Geometric deep learning drug design: heart, cancer, Alz

Thirty years of brain imaging research has converged to define the brain's default network—a novel and only recently appreciated brain system that participates in internal modes of cognition. Here we [redacted] past observations to provide strong evidence that the default network is a specific, anatomically defined brain system [redacted] when individuals are not focused on the external environment. Analysis of [redacted] anatomy in the monkey supports the presence of an interconnected brain system. Providing insight into function, the default network is active when individuals are engaged in internally focused tasks including autobiographical memory retrieval, envisioning the future, and conceiving the perspectives of others. Probing the [redacted] anatomy of the network in detail reveals that it is best understood as multiple interacting subsystems. The medial temporal lobe subsystem provides [redacted] from prior experiences in the form of memories and associations that are the building blocks of mental simulation. The medial prefrontal subsystem facilitates the flexible use of this information during the construction of self-relevant mental [redacted]. These two subsystems converge on important nodes of integration including the posterior cingulate cortex. The implications of these functional and anatomical observations are discussed in relation to possible adaptive roles of the [redacted] for using past experiences to plan for the future, navigate social interactions, and maximize the utility of moments when we are not otherwise engaged by the external world. We [redacted] by discussing the relevance of the default network for understanding mental disorders including autism, schizophrenia, and Alzheimer's disease.

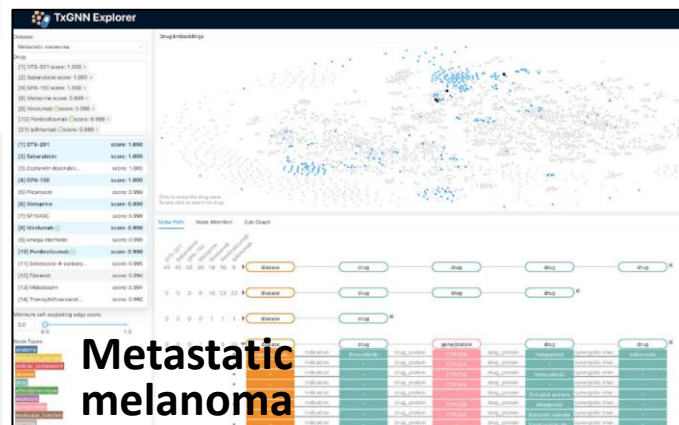
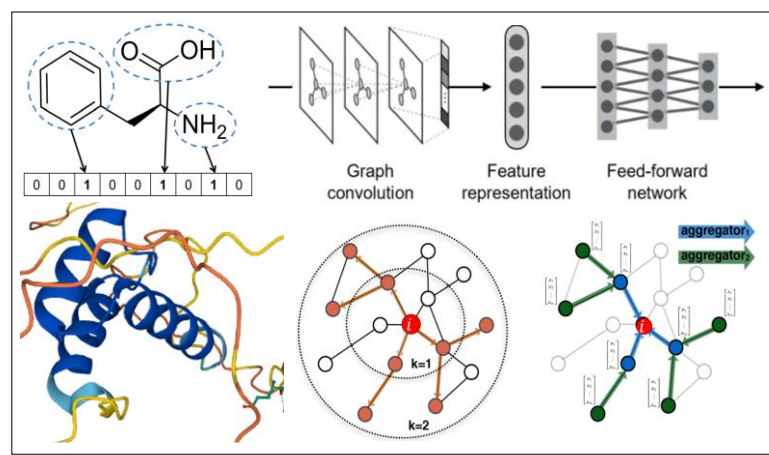
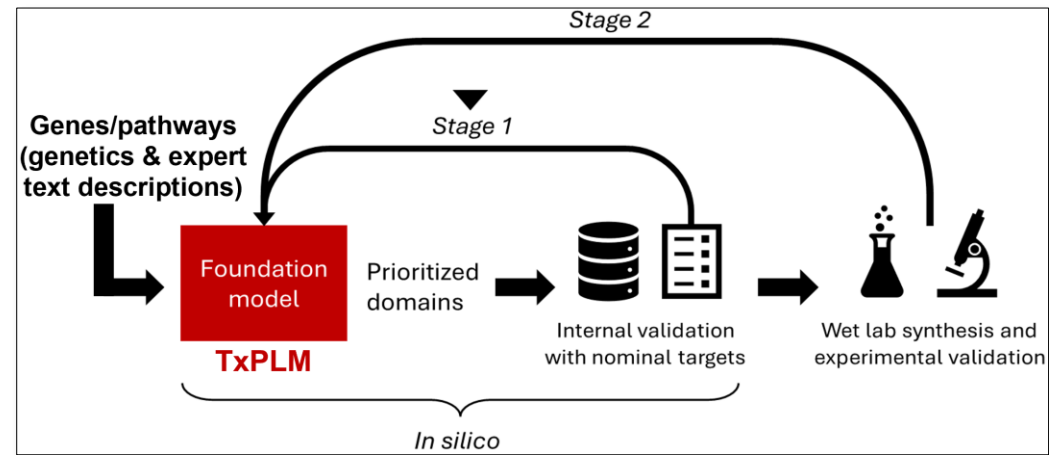


Large language models

Biological language models

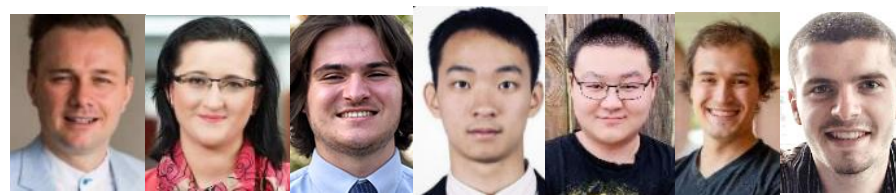
Single-cell AI models

Geometric deep learning

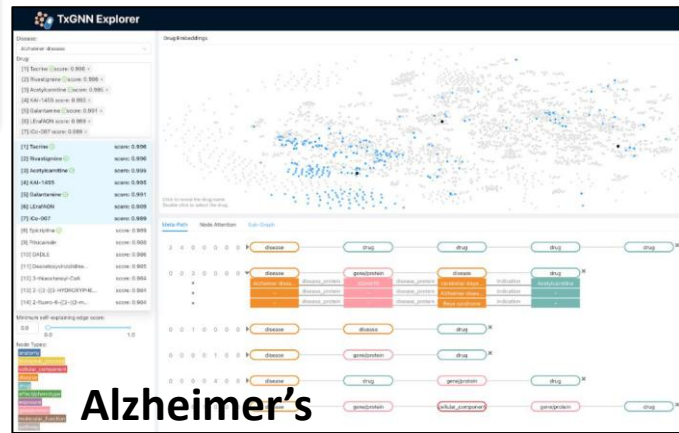
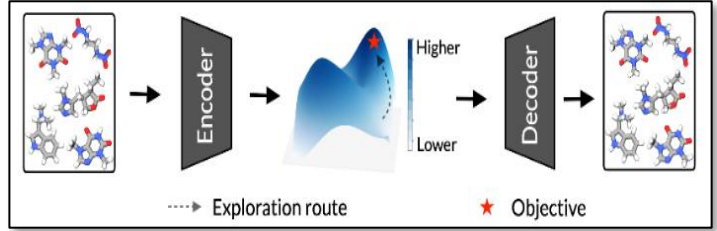


Reasoning, interactive, user-guided, AI-powered drug design

Structure-to-Function for proteins+chemistry

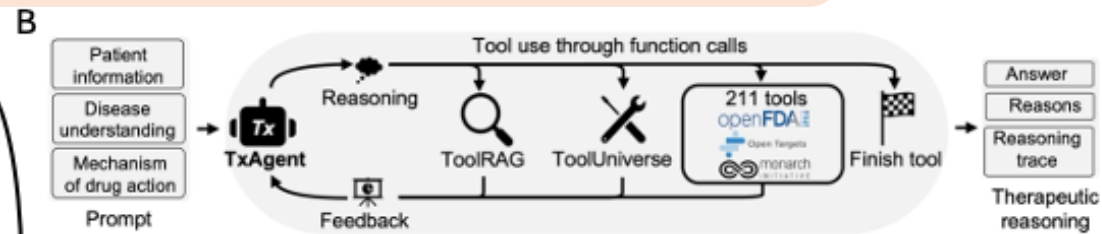
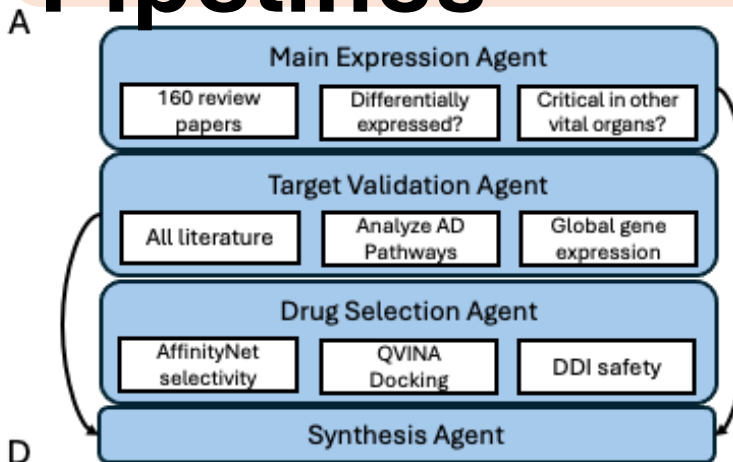


Brad Pentelute
 Marinka Zitnik
 Owen Queen
 Yepeng Huang
 Tianlong Chen
 Tom Hartvigsen
 Tom Cogley



Self-supervised struct. foundation models

Agentic Drug Discovery Pipelines

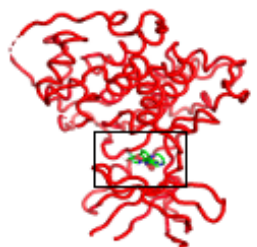


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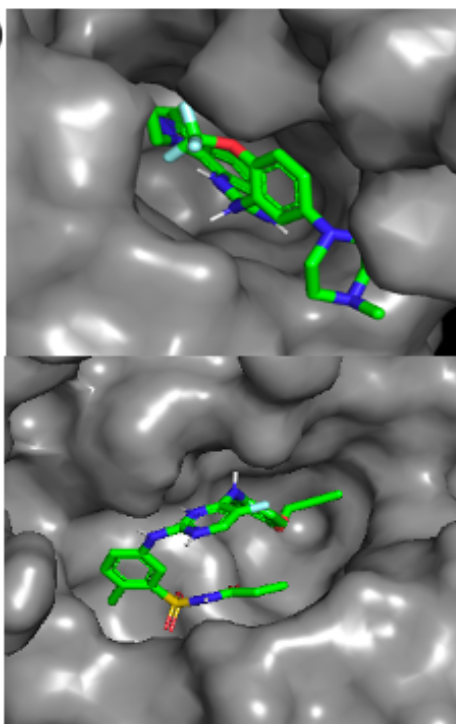
Prompt: Find a combination of approved or post-phase-1 clinical trial drugs that can treat Alzheimer's.

<p>Main Expression Agent</p> <p>I will begin by searching for cell-type-specific mechanisms implicated in Alzheimer's...</p> <p>Using search_corpus...</p> <p>Literature indicates that inhibiting GSK3B could reduce tau pathology...</p> <p>Targets must be differentially expressed.</p> <p>Using is_diff_exp...</p> <p>I have identified two potential target genes, GSK3B and PTK2B...</p>	<p>Target Validation Agent</p> <p>I will now proceed with their validation.</p> <p>Using get_module...</p> <p>The targets are not pathway-redundant.</p> <p>Now, I will check the tissue expression</p> <p>Using tissue_express...</p> <p>GSK3B has an nTPM of 17.7 in heart muscle...</p> <p>Next, I need to identify biomarkers...</p> <p>Using read_literature...</p> <p>For GSK3B and PTK2B, biomarkers include...</p>	<p>Drug Selection Agent</p> <p>I will now identify suitable small molecule drugs.</p> <p>Using top_10_selective...</p> <p>I will now evaluate by docking to the protein.</p> <p>Using qvina_dock...</p> <p>1. Ovansertib (phase 2) predicted mechanism of action: ...</p> <p>2. R-348 (phase 2) predicted mechanism of action: ...</p> <p>This dual-inhibition strategy is expected to offer a synergistic effect by addressing multiple core pathological processes of Alzheimer's disease.</p>
<p>Synthesis Agent: Okay, I will now compile the information for the report.</p>		

GSK3B-(Ovansertib)
-9.9 kcal/mol



PTK2B-(R-348)
-7.6 kcal/mol



Target Identification Agent

Alzheimer's Disease

Start Pipeline

View Full Report

View Generated Images

Target Validation Agent

Alzheimer's Disease

Start Pipeline

View Full Report

View Generated Images

Drug Development Agent

Alzheimer's Disease

Start Pipeline

View Full Report

View Generated Images

Analysis Agent & Full Report

Alzheimer's Disease

Start Pipeline

View Full Report

View Generated Images

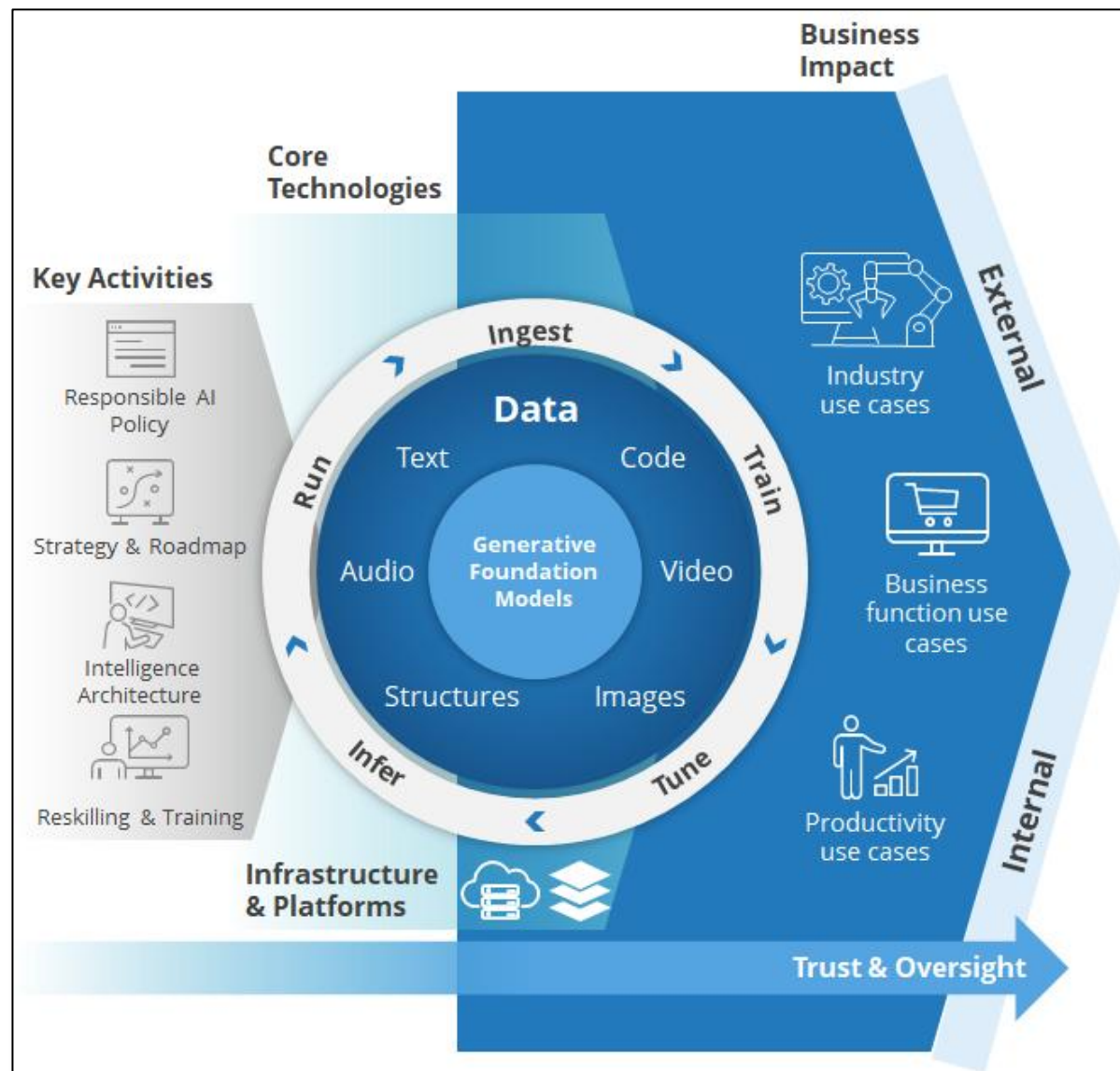
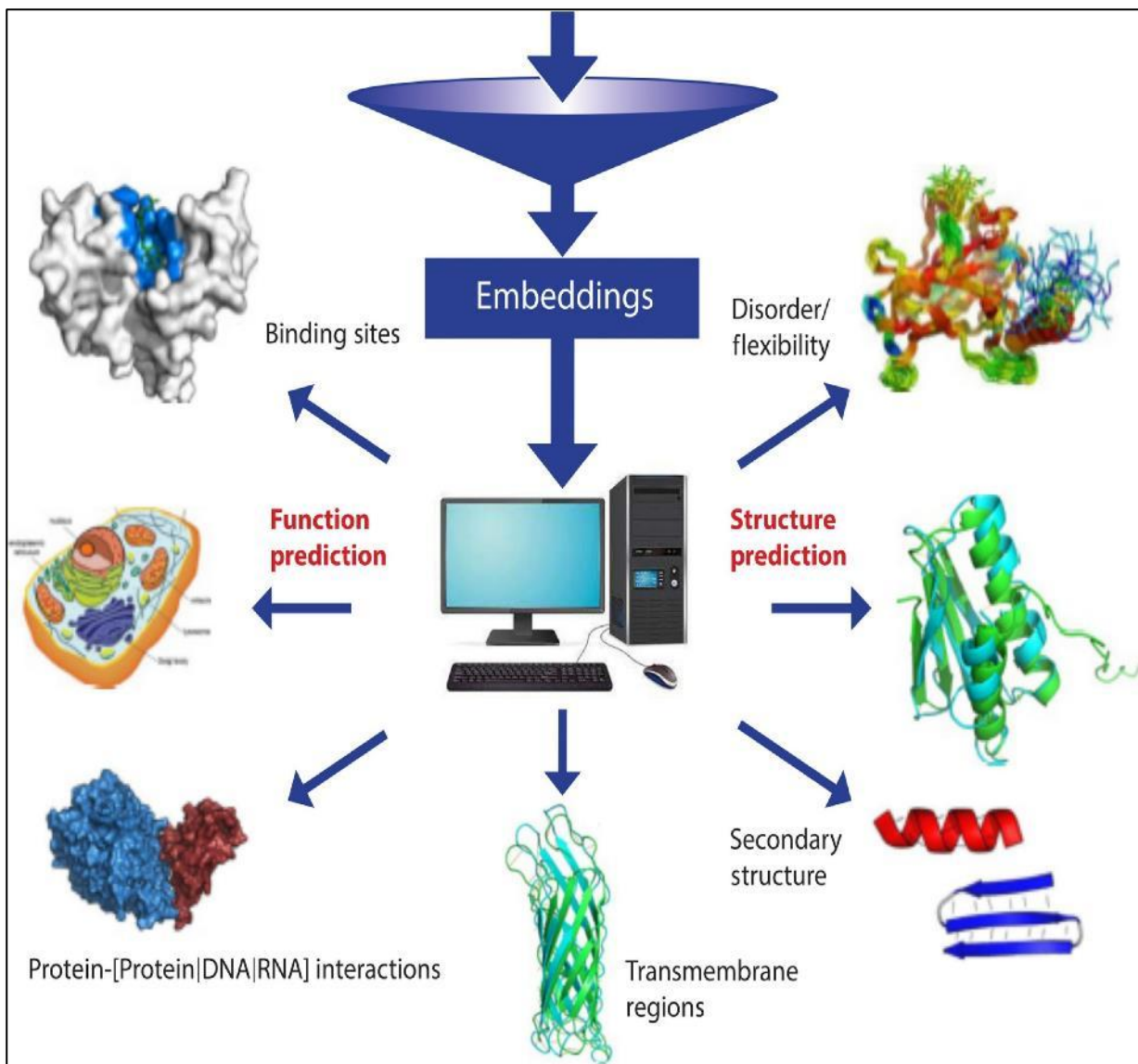
Identified Drug Candidate

SMILES: C1=CC=C(C=C1)C2=CC=CC=C2C3=CC=CC=C3C4=CC=CC=C4

View Full Report

View Generated Images

The road ahead: Systematic understanding in biology + work



- AI as a discovery partner: multi-modal foundation models
- Gain insights previous inaccessible to human scientists
- Build rich intuition on biological + therapeutic space

- AI as "Google Maps" for navigating knowledge space
- Visual search + integration through millions of documents
- Hierarchical interactive knowledge representation + manip.

THE ROAD AHEAD

- Journey to full AI potential still long, will not easy
- Challenges: technological, societal, economic, political. **Uncharted territories.**
- Society dramatically transformed; 'irreplaceable' jobs changed or gone.

- Opportunity: create more **fulfilling jobs**
- Shape transition to improve human condition
- More humane, nurturing, fulfilling, inclusive world

- Been there before: Agricultural, Industrial Revolution
- AI: natural next step in continuity of civilization
- AI: natural next step in physics-biology-cognition-consciousness

- Riding exponential for 1000s of years: always looks steeper next to us

- Our future: we can build it better for all of us
- AI will not destroy humanity. Instead: Raise humanity to new heights
- We can each become the **best version of ourselves**
- AI can help **Humanity** achieve our true **humanity** for all of humanity.





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withMantis.com
MantisAI.csail.mit.edu

Cognitive Cartography