Inspiration

Technology in Healthcare is Transforming Lives. Mobility is important as software can remove barriers, improve accessibility, and save lives. For instance, in rural communities where doctors are far away, they can't travel long distances. The global artificial intelligence in drug discovery market size was estimated at USD 897.6 million in 2021 and is expected to reach USD 1.1 billion in 2022 accelerated by telemedicine during COVID19 pandemic. If someone was suffering from a rare disease (like Mila from MilaSen), they would have difficulty accessing healthcare resources with long wait times. Telemedicine can speed up connections to specialists such as genetic counselors and oncologists. Advanced analytics can identify patterns in misdiagnosis and guide better decision making. And patient-centered innovations can promote community and agency among rare disease patients. In the current state of our world, there has never been a greater need to build tools that benefit public health. Healthcare needs disruptive innovation like telemedicine accelerated by the Covid 19 pandemic

Problem Statement: From bench to bedside, on averages $2.6B over 10 years with a 90% clinical trial failure rate to create a new drug with FDA approval. Basic research starts with over 10,000 compounds, before it narrows down to 1 FDA approved drug. Alternatives like X-ray crystallography costs $120,000 and takes over one year just for one picture are also very pricey. The clinical trial process involving phase 1/2/3 involves tens of thouands of volunteers (humans!) which increases the time and costs. The entire process from target identification, to invirtro studies, and phase 1/2/3, trials is slow, expensive, and flawed.

What it does

Solution: Genesis's AI-Powered Drug Discovery on the Blockchain

Introducing Genesis... Genesis is a one-of-a-kind non-intrusive AI powered drug discovery platform for healthcare providers. This helps to cut costs, and enable healthcare organizations to ensure the patient has access to drugs.The quality drugs your patients deserve at a price they can afford. Genesis can be used commercial for computational approaches to identify new drugs for COVID-19 reduce admission rates to the hospitals / reduce costs to test centers, assist healthcare providers and improving the lives of people everywhere. Cutting-edge technology leverages big data and analytics to improve the drug discovery process with 24/7 access – anyne can use the Genesis anytime, anywhere. Genesis's web Inclusive Human-Centered Design UI/UX unlocks collaboration among patients, scientists, and health care providers to improve patient outcomes with blockchain technology. With considerations for healthcare proximity to the community, and embodies and addresses diversity, equity, and inclusion. For example, less than 3% of the participants in published, genome-wide association studies are of African or Hispanic or Latin American ancestries, and 86% of clinical trial participants are white. The lack of diversity in research and clinical

studies is not the only problem. For underserved rare disease communities, individuals can face important barriers and obstacles to care often before they even enter the healthcare system.

Data: Amino Acid Sequence to a 3D Structure. Amino acids are basic building blocks of life (21 of them). Every protein is made up of a sequence of amino acids bonded together and fold up on larger scales. These amino acids interact locally to form shapes like helices and sheets to form 3D protein structure where proteins are chains of amino acids. Gensis of living organisms (structure providers, movers, reaction catalysts, etc) which can interact with other proteins via signalling or transcribing DNA. Simplified Molecular Input Line Entry System (SMILE). SMILE Specification in the form of a line notation for describing the structure of chemical species using short ASCII strings. SMILES strings can be imported by most molecule editors for conversion back into two-dimensional drawings or three-dimensional models of the molecules. This data 3D structure determines its function. Annontation of protein domains (functional part of a protein). Conversion to 3D representation with energy-minimization allows Genesis to predict 3D structure given amino acid sequence. In Genesis's open sourced github, this data is found in GENESIS -> SRC -> DATA -> .CSV.

Uniqueness of Personalized health information – health drugs are personal to each person's unique health profile. Genesis's sequence maps dataset 200 million proteins which are Representations of a chemical drug entity. 170,000 protein 3D structures (PFAM has 54 million protein sequences) 1-to-1 to a 3D structure with millions of possible combinations. Genesis expliots these conformational diversity from molecular simulation to make predictions via molecular simulations. Fingerprints like GM9 Sample Data and MolCAN QED Sample Data Protein family from sequence simularity (MSA). 3D structure determines its function. Annontation of protein domains (functional part of a protein). Example: Given 10^143 way to fold in Levinthal's paradox where a disease is from misfolded proteinsGenesis's docking scores for binding energies can output the top predicted drugs in clinincal trials. This takes advantage of MD simulations of the complex stability of atomic interactions. The AI-powered docking simulation allows us to train millions of possible matches - example ftrying to find a drug on a trained model for Covid 19 trrget protein complex.

Artifical Intelligence: Graph Neural Network :

According to the mHealth App Economics 2017 study, 61% of decision makers and experts of digital health see Artificial Intelligence as the most disruptive technology shaping the digital health sector. Genesis Unnatural Selection is an Artifiical intelligence powered molecular simulations with SMILE data can accelerate drug discovery with access to new biology, improved or novel chemistry, and better success rates. Genesis uses graph link predictions where the nodes== drugs and proteins, and the edges == interactions. AI generated protein structures to solve protein folding with spatial graphs. Nodes == amino acides in a protein sequences, edges == proximinity between these amino acides via residues (MSA embedding).The SMILE data (MCF, pIC50, or

MCE-18) is encoded to a vector and used to create a molecular graph. This is then used for Electron Path Predictions in the chemical space. The parameter optomization of the generative model with the SMILE data loops to a predictive graph model. A gradient decent is applied on the protein-specific potentnial for the distance and torsion distrbution predictions which outputs a reward and can be quantified via a confidence score or the pairwise distanes between the sequence-residue edges. Options include specific Kinase SOM, general Kinase SOM, and trending SOM. Genesis occurs due to evolutionary related protein sequences being used (MSA) instead of just normal feature engineering. GAN Generative Adversarial Network - GANs are a model from 2016 which uses real sample data from SMILE latent space can be introduced to Genesis. Then a generator create fake samples that are compared with a discriminator - to see if it is correct. Accuracy percentage of Genesis benchmarked by AlphaGo 80% as a key metric for benchmarking.

How we built it

Genesis Requires:

click Sphinx coverage awscli flake8 python-dotenv>=0.5.1 numpy pandas scipy torch molsets

Genesis Directory ├── LICENSE ├── Makefile <- Makefile with commands like `make data` or `make train` ├── README.md <- The top-level README for developers using this project. ├── data | ├── external <- Data from third party sources. | ├── interim <- Intermediate data that has been transformed. | ├── processed <- The final, canonical data sets for modeling. | └── raw <- The original, immutable data dump. | ├── docs <- A default Sphinx project; see sphinx-doc.org for details | ├── models <- Trained and serialized models, model predictions, or model summaries | ├── notebooks <- Jupyter notebooks. Naming convention is a number (for ordering), | the creator's initials, and a short `-` delimited description, e.g. | `1.0-jqp-initial-data-exploration`. | ├── references <- Data dictionaries, manuals, and all other explanatory materials. | ├── reports <- Generated analysis as HTML, PDF, LaTeX, etc. | └── figures <- Generated graphics and figures to be used in reporting | ├── requirements.txt <- The requirements file for reproducing the analysis environment, e.g. | generated with `pip freeze > requirements.txt` | ├── setup.py <- makes project pip installable (pip install -e .) so src can be imported ├── src <- Source code for use in this project. | ├── init.py <- Makes src a Python module | | | ├── data <- Scripts to download or generate data | | | └── make_dataset.py | | | ├── features <- Scripts to turn raw data into features for modeling | | | └── build_features.py | | | ├── models <- Scripts to train models and then use trained models to make | | | predictions | | ├── predict_model.py | | | └── train_model.py | | | └── visualization <- Scripts

to create exploratory and results oriented visualizations | └── visualize.py | └── tox.ini <- tox file with settings for running tox; see tox.readthedocs.io

Healthcare Security

Auth0 features like social sign-in, Multi-Factor Authentication, and passwordless log-in and authentication for social networks with what is called token-based authentication - allow for doctors to spend more time saving lives and less time worrying about cybersecurity. This is done with temporary encrypted security tokens when users verify their identity, preventing cookies, and data breaches. Protecting user information is vital to your company's reputation and the well-being of those who use your application. This is important since we are talking about HIPPA compliance and Client PHI - private healthcare information. Auth0 has also recently introduced push notifications that immediately alert users if their passwords have been compromised. Users can immediately change their passwords to protect their information. Genesis's security of healthcare data accessing electronic health records on the go. Auth0 also helpswith scalability and performance and works well with enterprise-level applications for our B2B platform. Auth0 Analytics can be used by Genesis's sales and marketing team (refer to business model canvas slide) to increase leads and conversions throughout the buyer journey. For commercialization, and as a potential startup idea - this is great for building funnels, track retention, and capture and measure specific events with key metrics like the number of new users, in-app login activity per year, new registrations per day.

Hedera is a next generation blockchain technology that allows anyone anywhere to pay for Genesis's drug discovery platform given a Hedera account ID and private key with HBAR tokens in addition to fiat currency. Decentralized healthcare technology allows for direct access to the native speed, security, and fair ordering guarantees of the hashgraph consensus algorithm.The use of hedera.hashgraph.sdk improves accessibility of payments via crypto by connecting the user's public key to Hedera mainnet with Atomic Wallet, BRD, or Exodus. In the future, Genesis wants successfully scanning QR codes, ScheduleSign transactions for Genesis's subscription model, secure messages to subscribe to the topic via a Hedera mirror node, and signed the healthcare transaction with the treasury key. We are looking to store medical data on Hedera Token Service - a secure platform. Medical data will be anonymized and can only be linked back to personal data using a unique key. Genesis's information architecture follows the security-by-design principle, implementing strict data separation and encryption of moving data and data at rest. for NFTs to improve security allowing doctors to provide better care for their patients by associating User Accounts with the NFT. Blockchain encryption on Genesis with it's Treasury Key allows for data privacy and endpoint security. Considerations made for cybersecurity, compliance, connectivity while leveraging cloud technologies. Since the healthcare data is immutable as transactions to a Hedera network with receipts - Genesis will have the full trust of the Hedera ledger. Paitent's' information will be stored for as long

as you have an active account with Genesis such that when they delete their account, all their personal information will be deleted too.

Challenges we ran into

Payments via Hedera Crypto for Subscription Model not easy to digest the AI-information that is presented especially in a 48 hr hackathon due to high information density Physician Usefulness - not sure how physician integrate Genesis's front-end it into their legacy healthcare systems.

Accomplishments that we're proud of

1. Sign up to the website with Auth0
2. Super easy to use UI/UX

What we learned

Healthcare providers like travelling nurses, doctors, and governments.Top market manufacturers are Atomwise Inc, BenevolentAI, Bio age, Cloud Pharmaceuticals Inc, Exscientia Ltd, Insilico Medicine Inc, Numerate Inc, Envisagenics Inc and others. AI is helping to accelerate the efficiency and cost-effectiveness of drug discovery as Genesis AI can lead to lower drug development costs. Subscription based model that scales depending on the drug produced (commercial v.s. individual)

MilaSen, Google AlphaFold, and Insilico are super inspiration to see people already successful in this space. AI companies' model is analogous to that of a typical biotech, either repurposing old drugs in new indications or designing new -Manual FDA approval of drugs takes 10 years Insilico Medicine raised $255 million in Series C financing.

https://www.forbes.com/sites/alexknapp/2019/09/02/this-startup-used-ai-to-design-a-drug-in-21-days/?sh=42dea08f2594

What's next for Genesis: Unnatural Selection

1 Year: In one year we will have several additional users in different countries and based on our estimate we would have ~10000 people in Genesis's databases. In the meantime, we will also be working to generate data-packs drug discoveries (confidential data) which based on the previous calculation should give us the opportunity to serve ~50000 people

5 Years: In five years we are aiming to have a world leading product used in more than 100 countries and a total close to 50000 patients in Genesis's database (these would include ~1000 patients from ethnic minorities that would have received our free-of-

charge service as results of this project). In addition, we would work to produce a portfolio of at least 15 data-packs (confidential data) which based on the previous calculation should give us the opportunity to serve ~5 million of people.

- •Multi-drug side effects feature
- •Implement quality proteomics 3D data
- •Detection of various diagnostic/vaccine markers
- •team wide clinical collaboration, sharing data, esalating a call, secure communication : find and reach the right person at the right time
- •secure facility messaging with voice and touch activation -Human post-translational modifications -making important decisions - put computers into all EMS vechicles - to transport the health data
- •personalized genomic services
- •Alteration of selective expression protein patterns
- •seek emotional support -Blockchain epigenome records
- •look for subject matter experts to audit idea and create a Patient Advocacy and Engagement Advisory Board
- •legal audit to ensure we comply with industry regulations and standards TEST APP WITH hospital run HEALTH PILOT PROGRAMS -Direct marketing, social media, ads, partnerships with healthcare providers like travelling nurses, doctors, and governments.

Built With

- awscli
- click
- coverage
- flake8
- juypter
- molsets
- numpy
- pandas
- python-dotenv>=0.5.1
- rdkit
- scipy
- sphinx
- torch