

AutoPrognosis 2.0: Democratising Diagnostic and Prognostic Modelling in Healthcare with Automated and Interpretable Machine Learning

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\ LAB**

vanderschaar-lab.com



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mihaela-van-der-schaar/](https://linkedin.com/in/mihaela-van-der-schaar/)

Our research team

☆ = joined us in 2022

<https://www.vanderschaar-lab.com/>
→ Research Team



Fergus Imrie



Alan Jeffares



Alex Chan



Alicia Curth



Alihan Hüyük



Boris van Breugel



Dan Jarrett



Hao Sun



Jeroen Berrevoets



Jonathan Crabbé



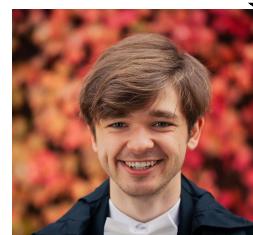
Krzysztof Kacprzyk



Nicolas Huynh



Nabeel Seedat



Paulius Rauba



Sam Holt



Tennison Liu



Yangming Li



Yuchao Qin



Zhaozhi Qian



Bogdan Cebere



Evgeny Saveliev

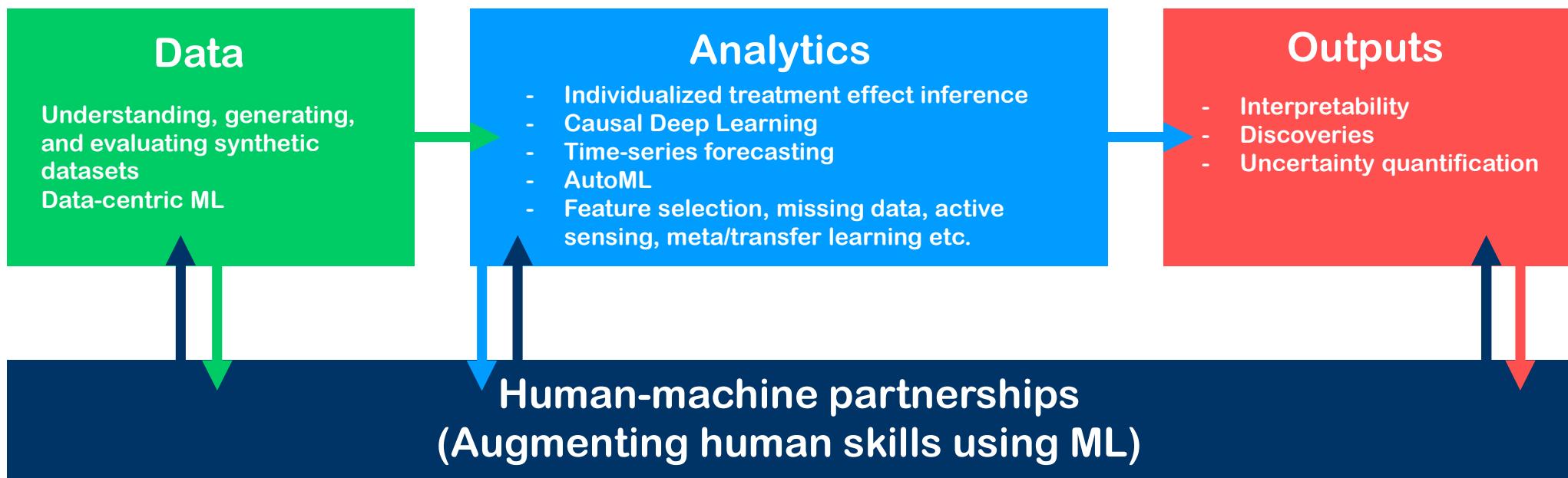


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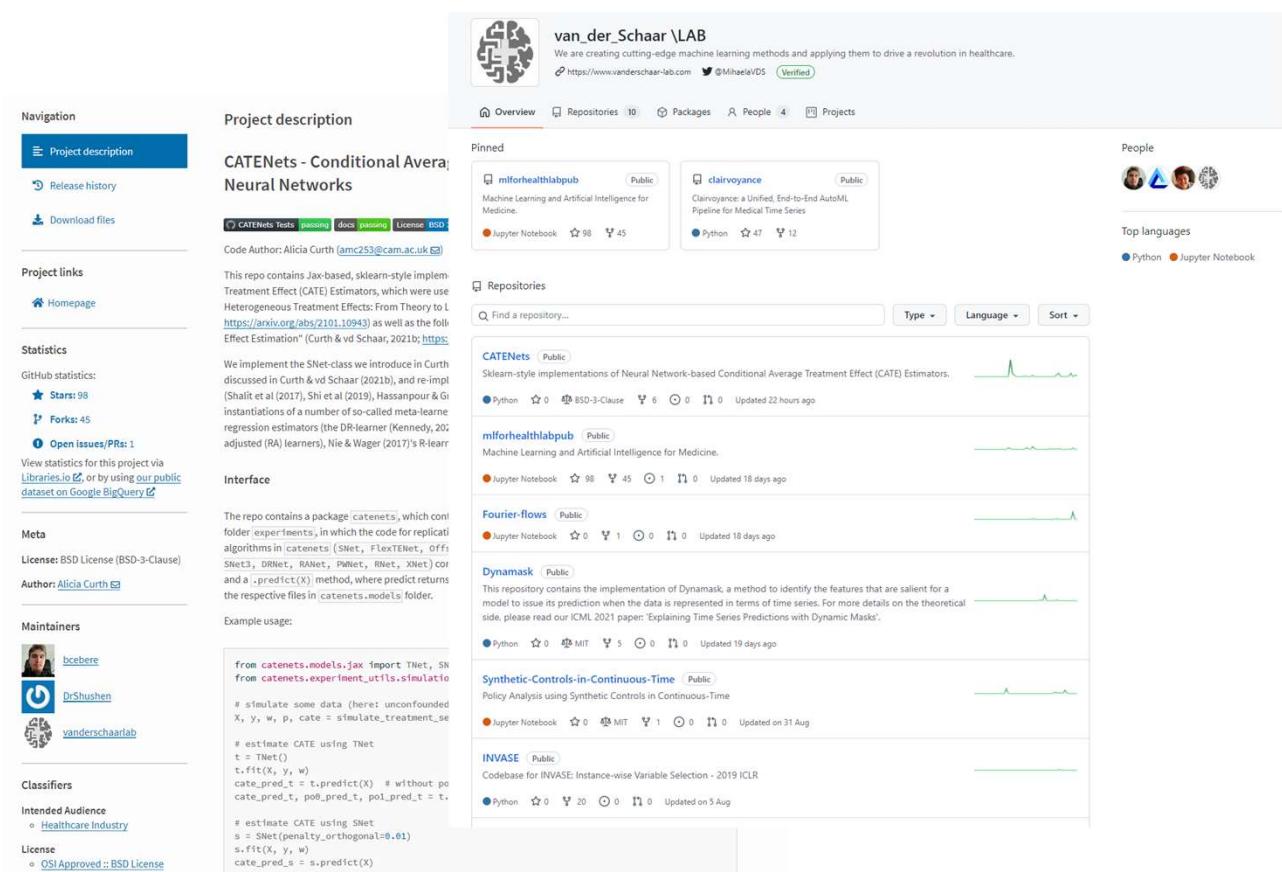
We develop cutting-edge ML needed to address these opportunities



Bringing papers to life through software

<https://www.vanderschaar-lab.com/>
→ Software

<https://github.com/vanderschaarlab/>
<https://pypi.org/user/vanderschaarlab/>

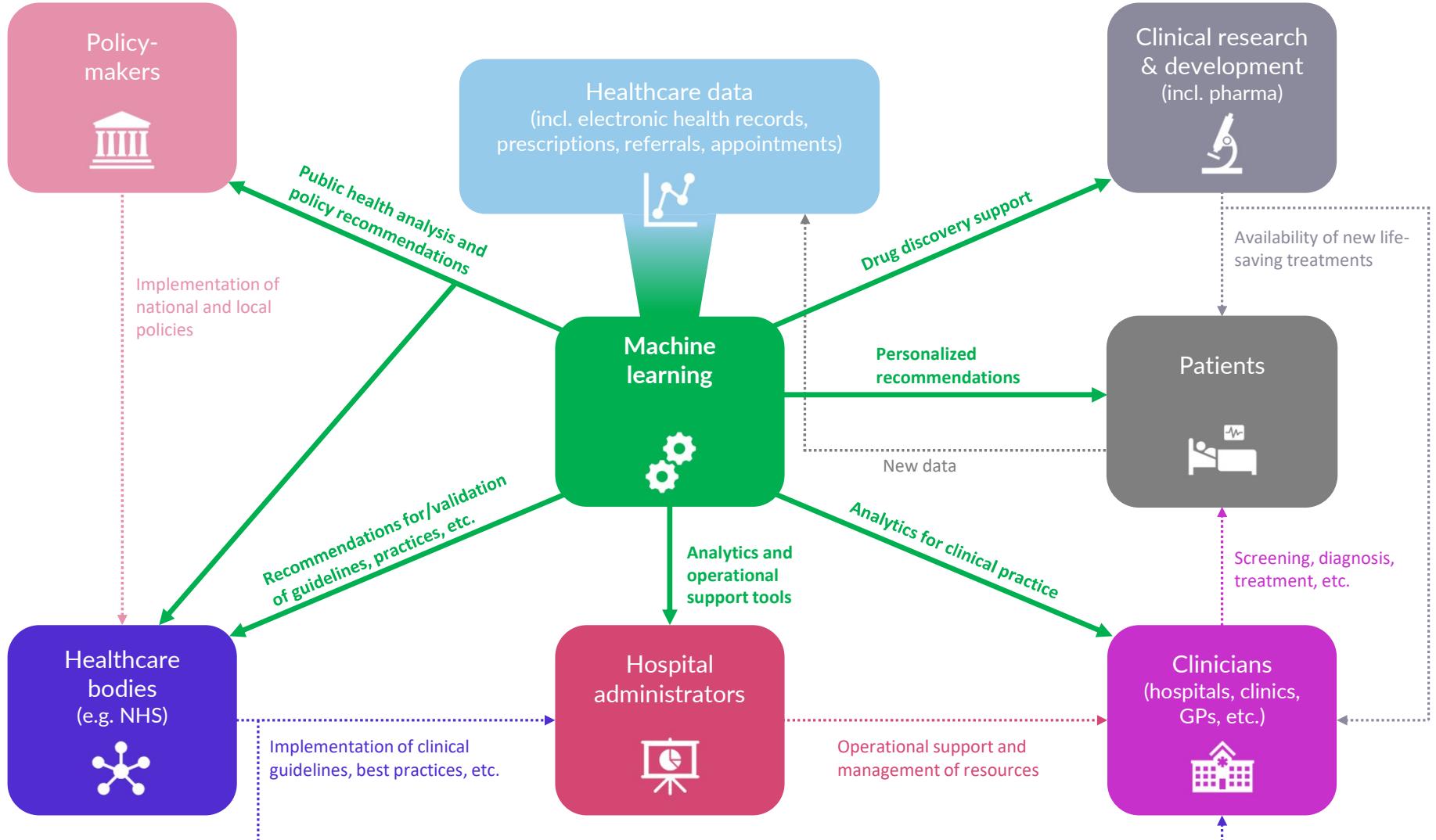


The screenshot shows the GitHub organization page for `van_der_Schaar \LAB`. The main navigation bar includes links for Overview, Repositories (10), Packages, People (4), and Projects. The `CATEGNets - Conditional Average Neural Networks` project is highlighted. It has a green "passing" status for tests and documentation. The code author is Alicia Curth (`amc253@cam.ac.uk`). The repository description mentions Jax-based, sklearn-style implementations of Treatment Effect (CATE) Estimators. Below the repository are sections for Pinned, Repositories, and a search bar. Other pinned projects include `miforhealthlabpub`, `clairvoyance`, `Fourier-flows`, `Dynamask`, `Synthetic-Controls-in-Continuous-Time`, and `INVASE`.



vanderschaar-lab.com





How to democratize Machine Learning?

Challenges

- Many ML models available, their performance can drastically vary
Different models work better for different datasets and different tasks!
- ML models often require state-of-the-art knowledge to train effectively
- ML models may need to be repeatedly updated as more data is collected
- ML need to be transparent and easy to debug and understand
- ML needs to remain state-of-the-art – enable easy addition of new methods
- Reproducible ML results and analytics are essential

ML in healthcare should be free!

How to democratize Machine Learning?

How to address
these
challenges?

Make
Machine Learning
DO the Crafting

Automated and Interpretable Machine Learning

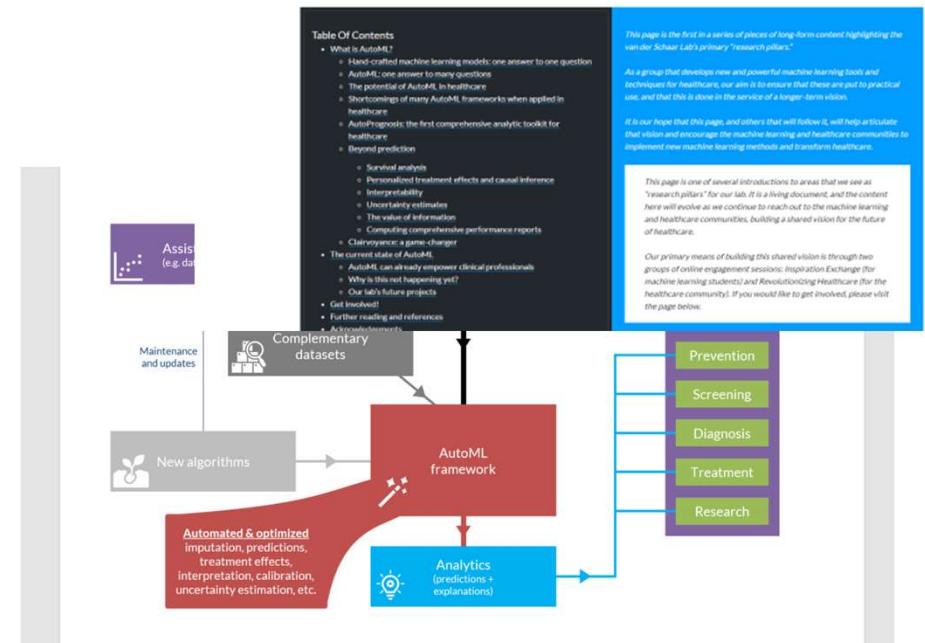
Our work: Automated Machine Learning for Healthcare

High-level overview

Explains the importance of/need for automated machine learning in and beyond healthcare

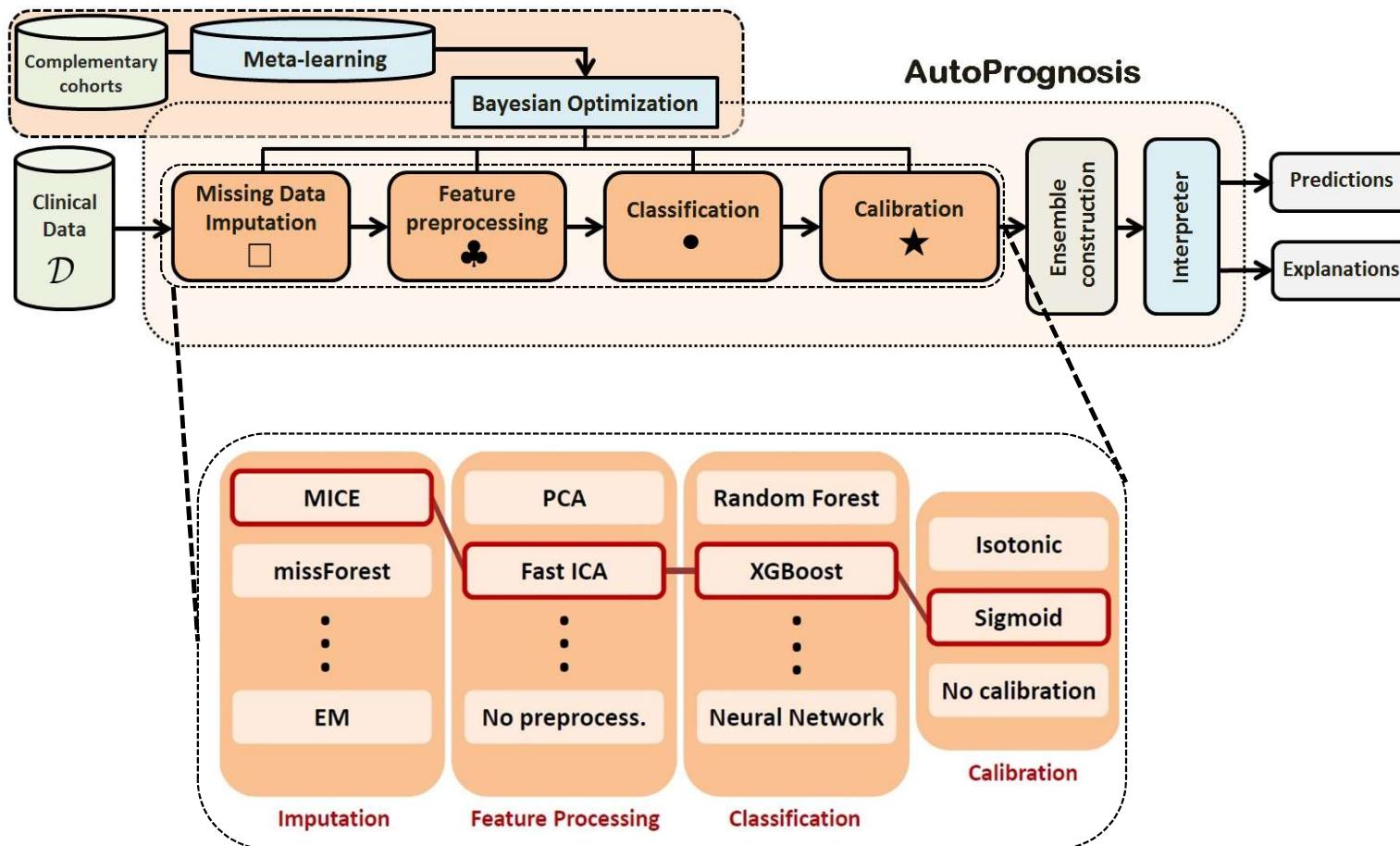
Describes some of our lab's pioneering work in the area

vanderschaar-lab.com/
→ Research pillars
→ Automated machine learning

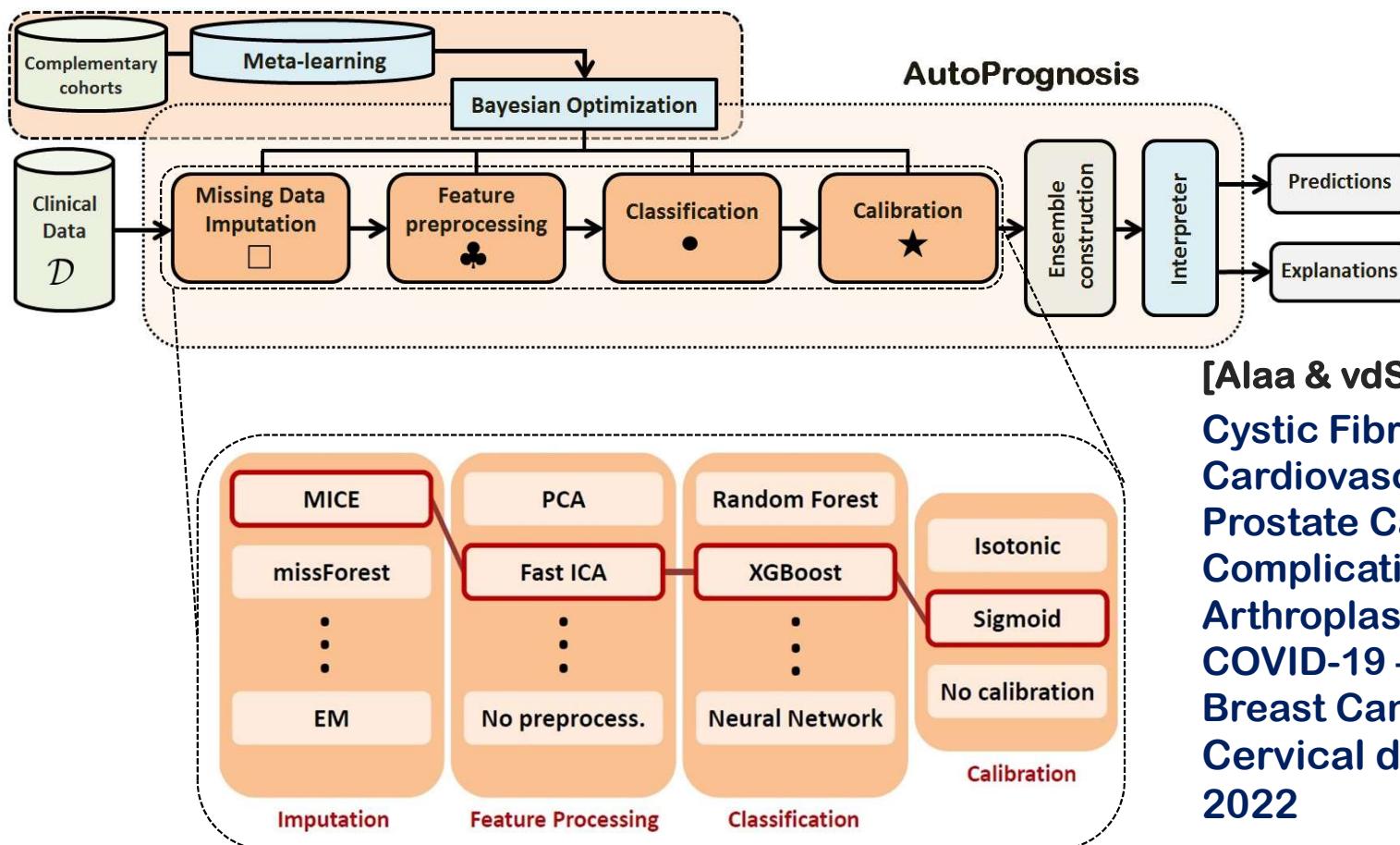


AutoPrognosis: A tool for crafting Clinical Scores

[Ahmed Alaa & Mihaela van der Schaar, ICML 2018]



AutoPrognosis in Practice



[Alaa & vdS, ICML 2018]

Cystic Fibrosis - 2018
Cardiovascular - 2019
Prostate Cancer – 2020
Complication After Hip Arthroplasty - 2020
COVID-19 – 2020
Breast Cancer – 2021
Cervical discectomy and fusion - 2022

<https://www.vanderschaar-lab.com/covid-19/>



Digital

NHS Digital > News and events

News

Trials begin of machine learning system to help hospitals plan and manage COVID-19 treatment resources developed by NHS Digital and University of Cambridge

Trials have begun of a system that will use machine learning to help predict the upcoming demand for intensive care (ICU) beds and ventilators needed to treat patients with COVID-19 at individual hospitals and across regions in England.

Date: 20 April 2020

AutoPrognosis 2.0



<https://arxiv.org/abs/2210.12090>

AutoPrognosis 2.0: Democratizing Diagnostic and Prognostic Modeling in Healthcare with Automated Machine Learning

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^dThe Alan Turing Institute, London, UK

Abstract

Diagnostic and prognostic models are increasingly important in medicine and inform many clinical decisions. Recently, machine learning approaches have shown improvement over conventional modeling techniques by better capturing complex interactions between patient covariates in a data-driven manner. However, the use of machine learning introduces a number of technical and practical challenges that have thus far restricted widespread adoption of such techniques in clinical settings. To address these challenges and empower healthcare professionals, we present a machine learning framework, AutoPrognosis 2.0, to develop diagnostic and prognostic models. AutoPrognosis leverages state-of-the-art advances in automated machine learning to develop optimized machine learning pipelines, incorporates model explainability tools, and enables deployment of clinical demonstrators, *without* requiring significant technical expertise. Our framework eliminates the major technical obstacles to predictive modeling with machine learning that currently impede clinical adoption. To demonstrate AutoPrognosis 2.0, we provide an illustrative application where we construct a prognostic risk score for diabetes using the UK Biobank, a prospective study of 502,467 individuals. The models produced by our automated framework achieve greater discrimination for diabetes than expert clinical risk scores. Our risk score has been

Preprint

2022

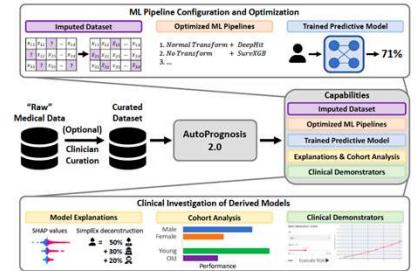


Figure 1: Overview of the AutoPrognosis 2.0 framework. AutoPrognosis takes either raw or curated medical datasets and provides an imputed dataset, a report detailing the optimized machine learning pipelines, a diagnostic or prognostic model, explanations, and a web-based interface for clinicians to interact with and use the derived model.

capabilities and can unlock the potential of ML in healthcare for clinical researchers *without* the requirement for extensive technical capabilities.

AutoPrognosis 2.0 empowers healthcare professionals with the following capabilities:

1. Build highly performant ML pipelines for classification, regression and time-to-event analysis, optimized specifically for the data at hand.
2. Understand when ML provides benefits over traditional regression models, and thus when ML is valuable.
3. Enable principled selection of variables and allow users to understand the value of information.
4. Explain and debug ML models using diverse interpretability methods.
5. Update systems whenever the available data changes to ensure the best possible clinical models.
6. Provide confidence in the reproducibility of models.

AutoPrognosis 2.0



AutoPrognosis 2.0

Democratising Diagnostic and Prognostic Modelling in Healthcare with Automated Machine Learning

The next big step in machine learning and Healthcare

On this page, we are introducing **AutoPrognosis 2.0** - the van den Schaer Lab's newest framework offering the healthcare community a tool that utilises the power of **AutoML** in a flexible and interpretable way. By erasing the need for significant technical expertise, we **democratise diagnostic and prognostic modelling**, making it accessible for a wide array of healthcare practitioners.



About AutoPrognosis 2.0

written by Andreas Bedorf and Mihaela van der Schaar

Expert Voices

The van den Schaer lab has been developing AutoPrognosis, a cutting-edge framework and associated open-source package which enables easy creation of new risk scores, personalised diagnostics, and prognostics using state-of-the-art machine learning methods.

By erasing the need for significant technical expertise, we democratise predictive modeling, making it accessible via a wide array of expert and non-expert clinicians, healthcare researchers, industrial developers as well as anyone interested in building a risk score for a disease or predicting anything of interest.

AutoPrognosis provides not only predictions and forecasts, but also a wide-range of interpretability methods that enable users with the ability to understand and debug the resulting machine learning models.

Mihaela van der Schaar

"We have built AutoPrognosis, a tool aimed at democratising machine learning for anyone interested in developing new risk scores, personalised diagnostics, and prognostics using state-of-the-art, interpretable machine learning techniques. We hope that, irrespective of their knowledge of machine learning, numerous clinicians, researchers, and healthcare professionals will use AutoPrognosis to build powerful analytics that will empower them to better support patients."

Eoin McKinney

"Machine learning has great potential to change how we practise medicine. However that potential cannot be realised unless cutting edge algorithms are used to address important questions posed by those with clinical knowledge. AutoPrognosis makes this possible, allowing clinical experts to access powerful tools in a robust, reproducible way that has not so far been feasible without substantial technical know-how."

Thomas Callender

"AutoPrognosis is the first comprehensive, low-code framework for developing and deploying clinical risk prediction tools. With a straightforward interface, AutoPrognosis brings the power of state-of-the-art methods to machine learning experts and non-experts alike, freeing the healthcare community to focus on building the tools you co-plot."

Find out more

van der Schaer Lab

AutoPrognosis 2.0 on Github

Our Paper

For Clinicians: Revolutionizing Healthcare Engagement Sessions on 24 October and 21 December dedicated to AutoPrognosis

For Clinicians in Cambridge: CCAIM AI Clinic on 10 November

For ML Researchers: Inspiration Exchange Session on 22 November

<https://www.autoprognosis.vanderschaar-lab.com/>



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AutoPrognosis 2.0 – Summary

Goal: democratizing machine learning for *anyone* interested in developing new risk scores, personalized diagnostics, and prognostics

Solution: AutoPrognosis 2.0 – an open-source, easy-to-use, state-of-the-art, interpretable machine learning package

Users: Expert and non-expert users – including clinicians, researchers, and healthcare professionals...and hopefully many others

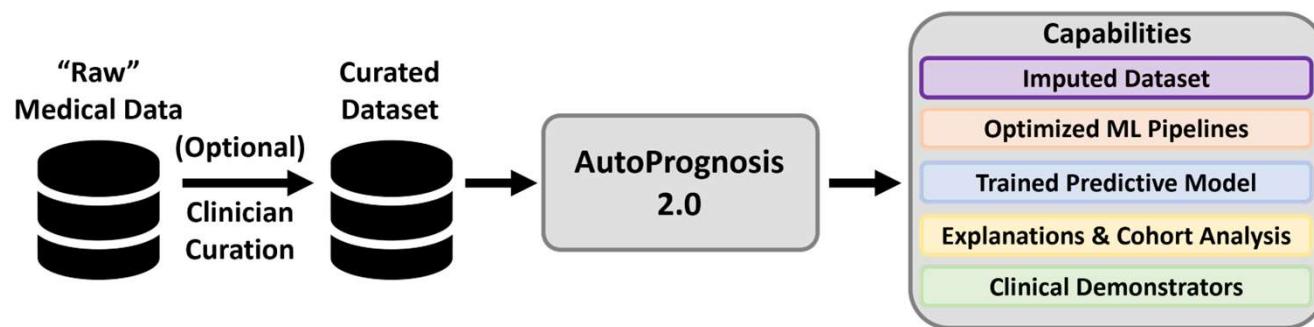


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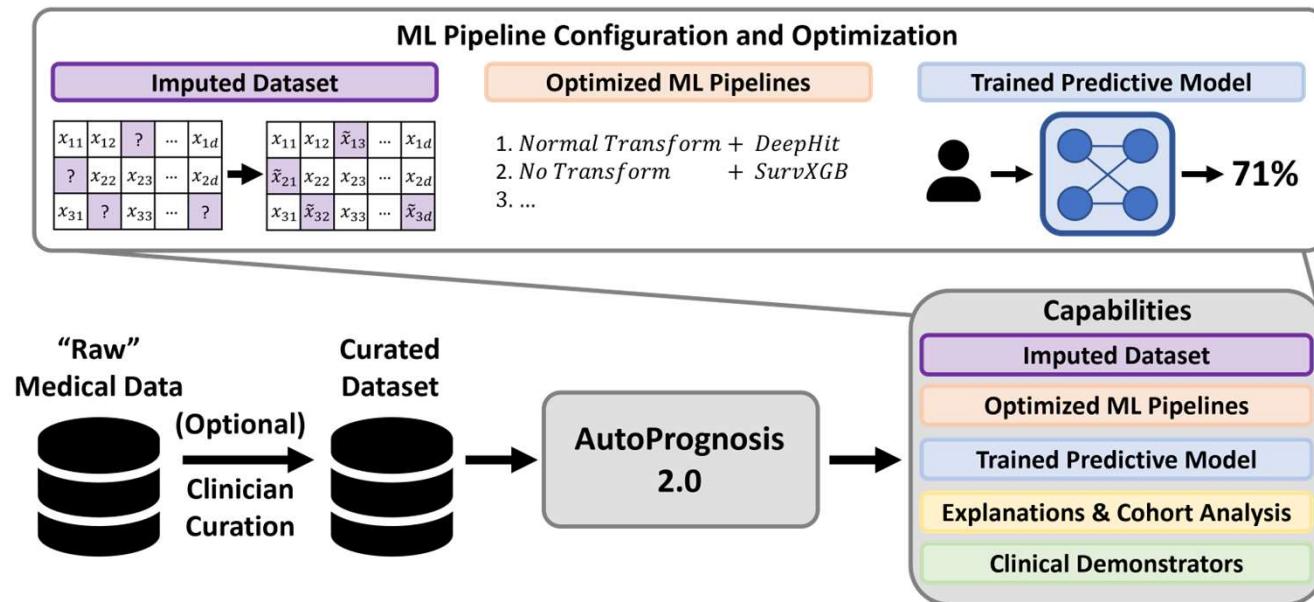
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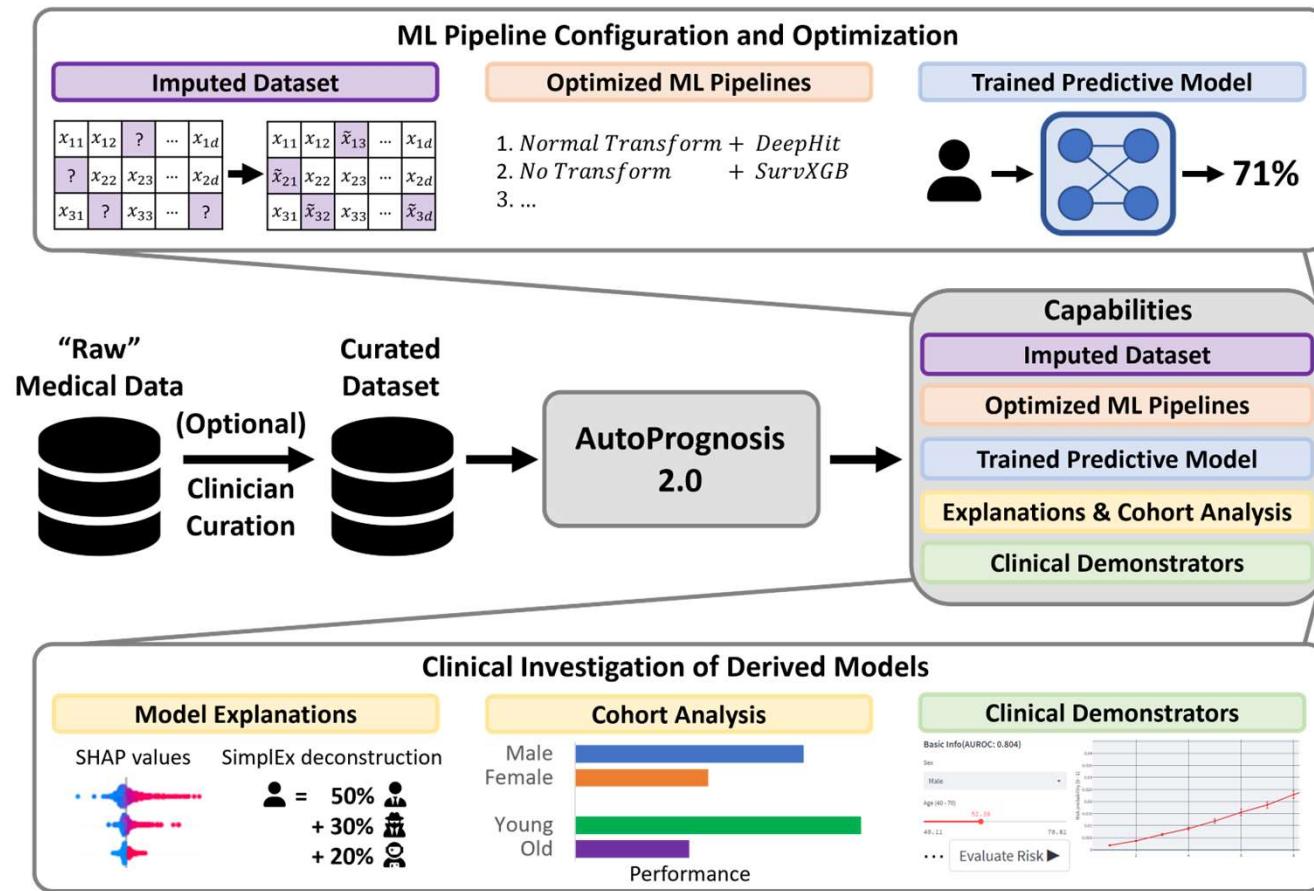
AutoPrognosis 2.0



AutoPrognosis 2.0



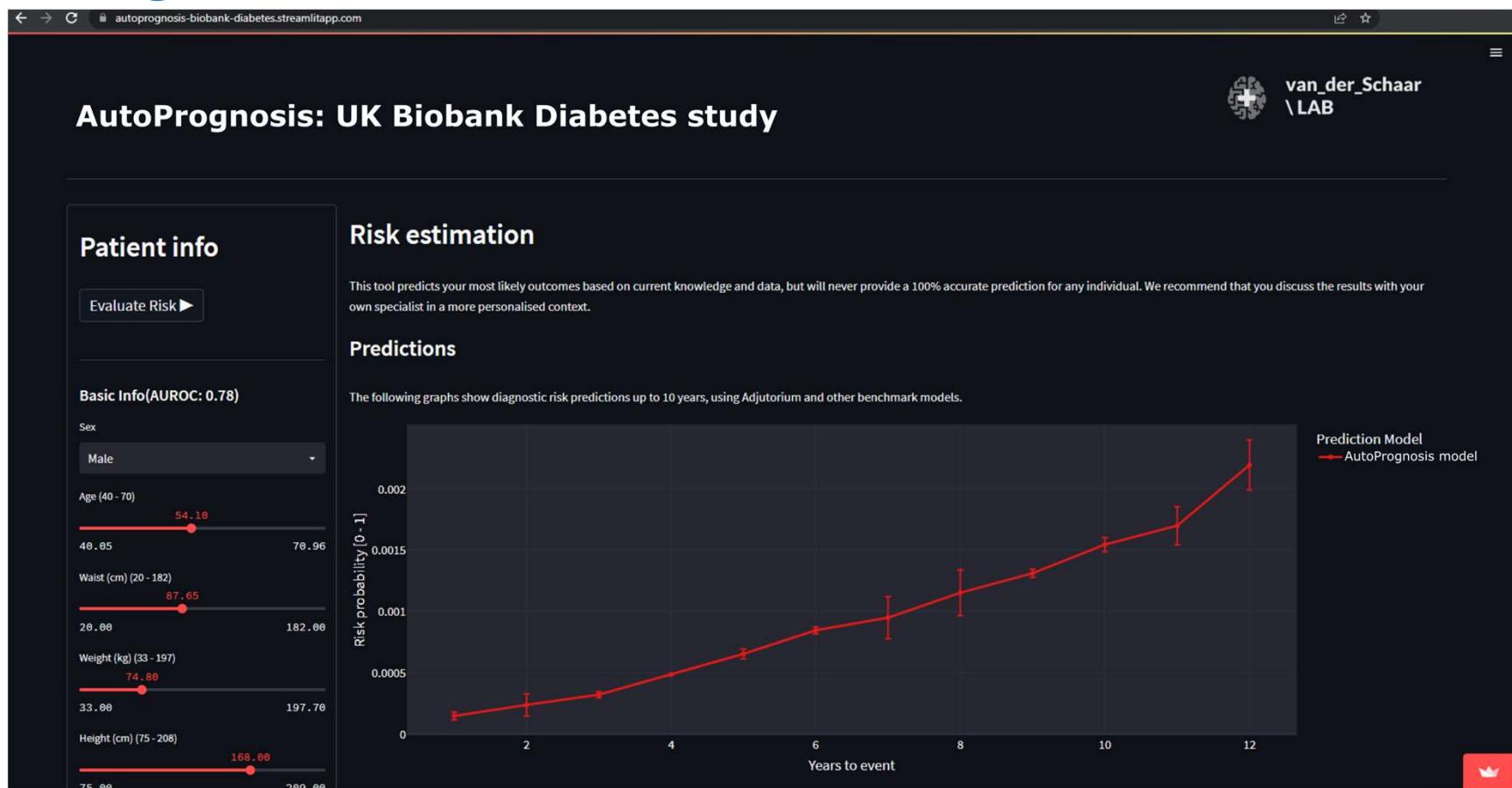
AutoPrognosis 2.0



AutoPrognosis 2.0

Pipeline Stage	Algorithm (No. Hyperparameters Optimized by AutoPrognosis)				
Imputation	HyperImpute (M)ICE (0)	Mean (0) SoftImpute (2)	Median (0) EM (1)	Most-Frequent (0) Sinkhorn (6)	MissForest (2) None (0)
Dimensionality Reduction	Fast ICA (1)	Feat. Agg. (1)	Gauss. Rand. Proj. (1)	PCA (1)	Var. Thresh. (0)
Feature Scaling	L2 Norm. (0) Unif. Trans. (0)	Max (0) None (0)	MinMax (0)	Normal Trans. (0)	Quant. Trans. (0)
Classification	ADABoost (3) ExtraTree (1) LDA (0) Neural Net. (6) TabNet (8)	Bagging (4) Gauss. NB (0) Light GBM (6) Perceptron (2) XGBoost (11)	Bernoulli NB (1) Grad. Boost. (3) Linear SVM (1) QDA (0)	CatBoost (2) Hist. Grad. Boost. (2) Log. Reg. (4) Random Forest (5)	Decision Tree (1) KNN (4) Multi. NB (1) Ridge Class. (1)
Regression	Bayesian RR (1) TabNet (8)	CatBoost (2) XGBoost (2)	Linear (0)	MLP (0)	Neural Net. (6)
Survival Analysis	Cox PH (2) Surv. XGB (4)	CoxNet (6) Weibull AFT (2)	DeepHit (7)	LogLogistic AFT (1)	LogNorm. AFT (2)
Interpretability	INVASE SimplEx	KernelSHAP Symb. Pursuit	LIME	Effect Size	Shap Permutation

AutoPrognosis 2.0



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Software slide



The screenshot shows the GitHub repository page for `vanderschaarlab/autoprognosis`. The repository is public and has 42 commits. The main branch is `main`. The repository has 0 stars and 0 forks. It includes sections for `About`, `Sample Usage`, and `Code`. The `About` section describes the system as "A system for automating the design of predictive modeling pipelines tailored for clinical prognosis". The `Sample Usage` section provides code examples for survival analysis and classifier studies. The `Code` section shows the repository's structure and recent commits.

About

A system for automating the design of predictive modeling pipelines tailored for clinical prognosis.

Sample Usage

More advanced use cases can be found on our [tutorials](#) section.

List the available classifiers

```
from autoprognosis.plugins.prediction.classifiers import Classifiers
print(Classifiers().list_available())
```

Create a study for classifiers

```
from pathlib import Path
from sklearn.datasets import load_breast_cancer

from autoprognosis.studies.classifiers import ClassifierStudy
from autoprognosis.utils.serialization import load_model_from_file
from autoprognosis.utils.tester import evaluate_estimator

X, Y = load_breast_cancer(return_X_y=True, as_frame=True)

df = X.copy()
df["target"] = Y

workspace = Path("workspace")
study_name = "example"
```

<https://github.com/vanderschaarlab/AutoPrognosis>



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Engagement sessions: Revolutionizing Healthcare

Revolutionizing Healthcare is a series of engagement sessions aiming to share ideas and discuss topics that will define the future of machine learning in healthcare. These events target the healthcare community and focus on challenges and opportunities in clinical application of machine learning. We now have roughly 400 clinicians from around the world registered to participate in these sessions.

As a lab, our purpose is to create new and powerful machine learning techniques and methods that can revolutionize healthcare. This doesn't happen in a vacuum. At inception, we are inspired by ideas and discussions. In implementation, we need connections, trust, and partnership to make a real difference.

While you can learn about our work at major conferences in machine learning or in our papers, we think it's a better idea to create a community and keep these conversations going. We're also aware that many people—both in healthcare and machine learning—have questions about what we do, and how they can contribute.

For more information about Revolutionizing Healthcare—and to sign up to join in—please have a look at the sections below, and keep checking for new updates.

Revolutionizing Healthcare

Themed discussion sessions specifically for healthcare professionals (primarily clinicians).

We would like to:

- introduce machine learning concepts as they relate to healthcare
- spark new projects and collaborations
- demonstrate the real-world impact of machine learning in clinical settings
- discuss institutional barriers preventing wider adoption
- develop a shared vision for the future of machine learning in healthcare.

Standard session format:

- brief introductory presentation
- roundtable discussion featuring clinicians
- open Q&A



The top half shows a video conference with four participants: Michaela van der Schaar, Carsten Niemann, Eoin McKinney, and Lucas Fleuren. The bottom half shows a dashboard titled 'Aduitorium' with sections for 'Feature selection', 'Prediction results', and 'Model Selection'. The 'Prediction results' section includes a graph of 'Model accuracy (%)' vs 'Days after diagnosis' and a table of 'Performance metrics'.

<https://www.vanderschaar-lab.com/>
→ Engagement sessions
→ Revolutionizing Healthcare

A vertical list of recorded video sessions from the Revolutionizing Healthcare series, each with a thumbnail, title, and timestamp. The sessions include:

- Revolutionizing Healthcare - getting ML-powered tools in the hands of clinicians (1:18:58)
- Revolutionizing Healthcare - Roundtable on AI/ML decision-support tools (1:06:20)
- Revolutionizing Healthcare - roundtable on personalized therapeutics (1:04:53)
- Revolutionizing Healthcare - second roundtable on interpretability in ML/AI for healthcare (1:08:25)
- Revolutionizing Healthcare - roundtable on interpretability in ML/AI for healthcare (1:08:02)
- Revolutionizing Healthcare - ML tools for cancer (post-diagnosis care) (1:10:53)
- Revolutionizing Healthcare - ML tools for cancer (risks, screening, diagnosis) (1:14:21)
- Revolutionizing Healthcare - tools for acute care (1:09:04)
- Revolutionizing Healthcare - a framework for ML for healthcare (1:10:49)
- Revolutionizing Healthcare - what machine learning can offer healthcare (1:06:52)

Engagement sessions: Inspiration Exchange

Online engagement sessions for
ML researchers in healthcare;
themed presentations & Q&A

<https://www.vanderschaar-lab.com/>
→ Engagement sessions
→ Inspiration Exchange

Session dedicated to
AutoPrognosis -
November 22, 4pm UK



Inspiration Exchange is a series of engagement sessions aiming to share ideas and discuss topics that will define the future of machine learning in healthcare. These events will target machine learning students, and will emphasize sharing of new ideas and development of new methods, approaches, and techniques.

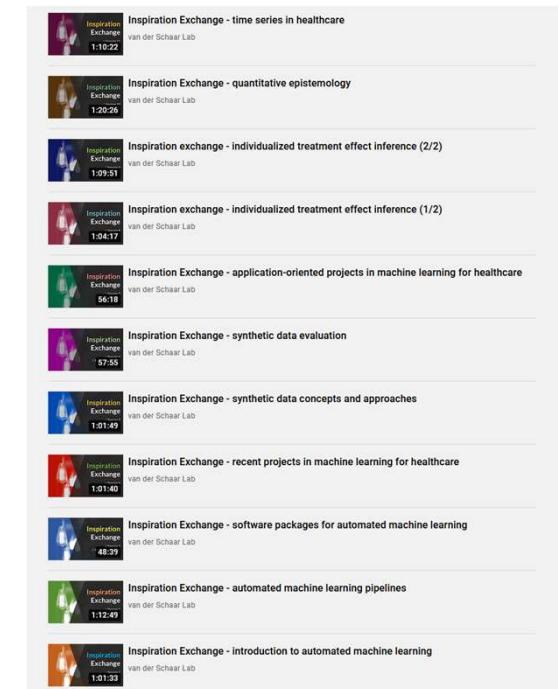
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For more information about Inspiration Exchange—and to sign up to join in—please have a look at the sections below, and keep checking for new updates.



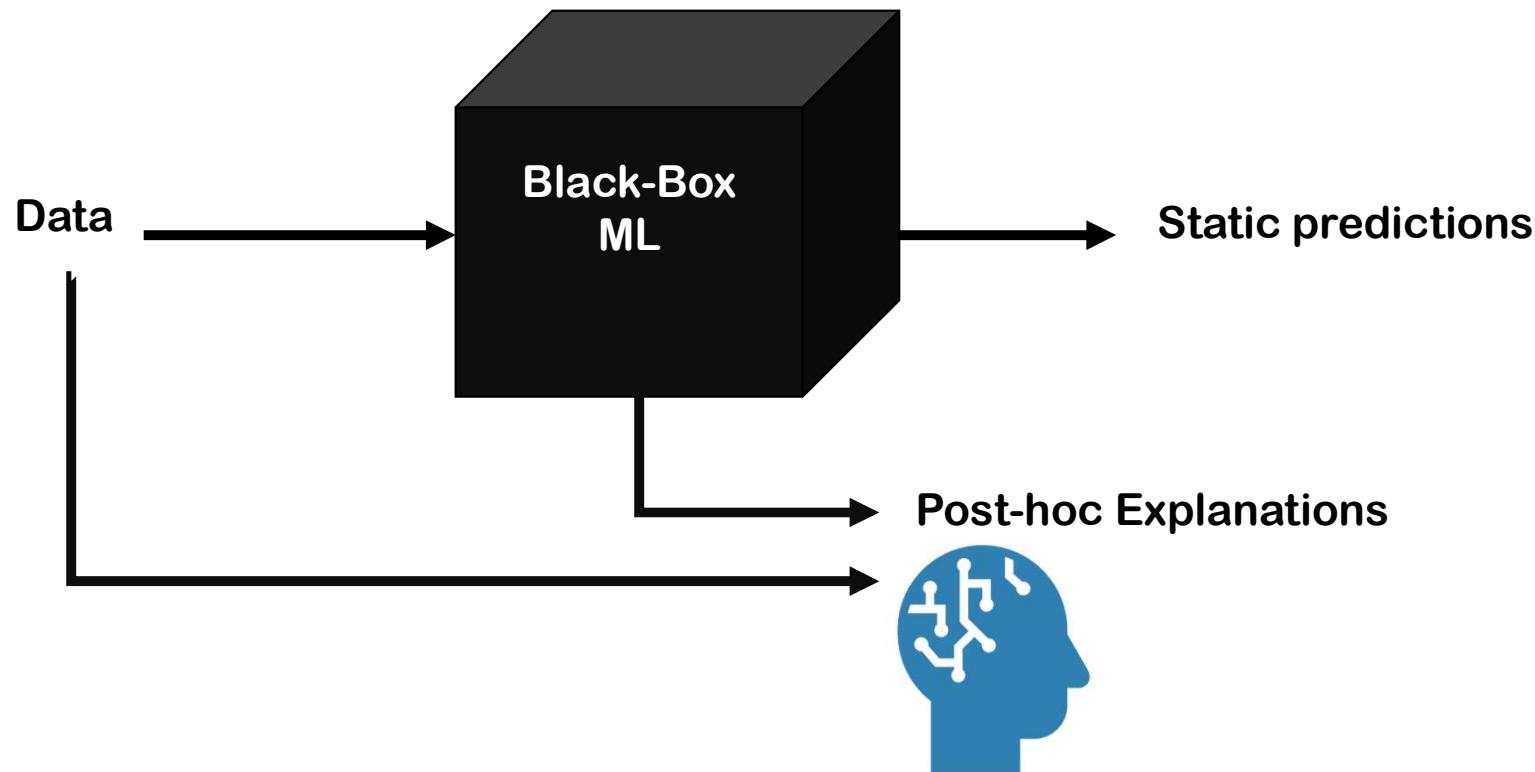
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AutoPrognosis 2.0

Pipeline Stage	Algorithm (No. Hyperparameters Optimized by AutoPrognosis)				
Imputation	HyperImpute (M)ICE (0)	Mean (0) SoftImpute (2)	Median (0) EM (1)	Most-Frequent (0) Sinkhorn (6)	MissForest (2) None (0)
Dimensionality Reduction	Fast ICA (1)	Feat. Agg. (1)	Gauss. Rand. Proj. (1)	PCA (1)	Var. Thresh. (0)
Feature Scaling	L2 Norm. (0) Unif. Trans. (0)	Max (0) None (0)	MinMax (0)	Normal Trans. (0)	Quant. Trans. (0)
Classification	ADABoost (3) ExtraTree (1) LDA (0) Neural Net. (6) TabNet (8)	Bagging (4) Gauss. NB (0) Light GBM (6) Perceptron (2) XGBoost (11)	Bernoulli NB (1) Grad. Boost. (3) Linear SVM (1) QDA (0)	CatBoost (2) Hist. Grad. Boost. (2) Log. Reg. (4) Random Forest (5)	Decision Tree (1) KNN (4) Multi. NB (1) Ridge Class. (1)
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Interpretability	INVASE SimplEx	KernelSHAP Symb. Pursuit	LIME	Effect Size	Shap Permutation

Turning black-boxes into white boxes



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Our Resources



Our Papers

vanderschaar-lab.com/interpretable-machine-learning/

Our Code

github.com/vanderschaarlab/Interpretability

Desiderata: Explanations which clinicians find useful

1. What is the ML model looking at?

Explanatory patient features

2. Which examples explain the prediction issued?

Personalized explanations with reference to particular examples

3. Which explicit risk formulae has the ML model learned?

Provide explicit formulae for the ML model's predictions

Discover hypotheses/laws



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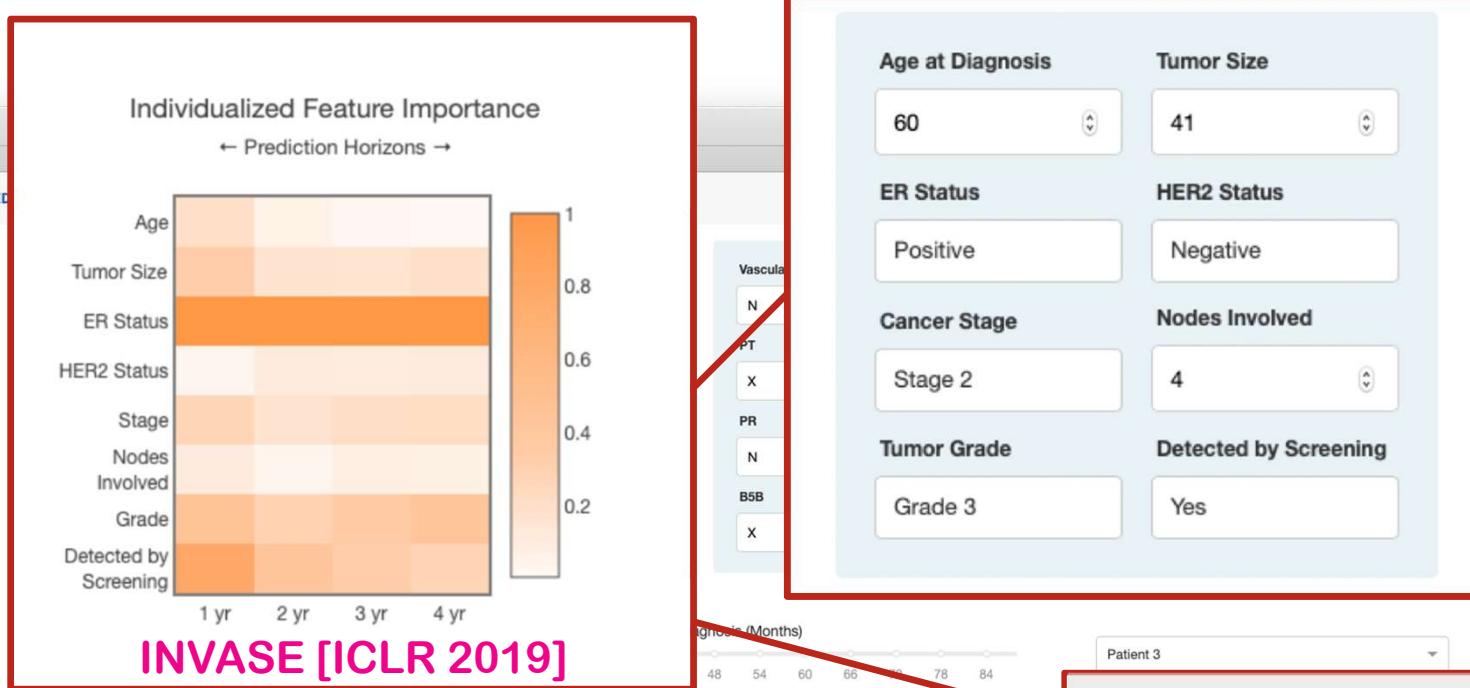
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ML interpretability: type 1

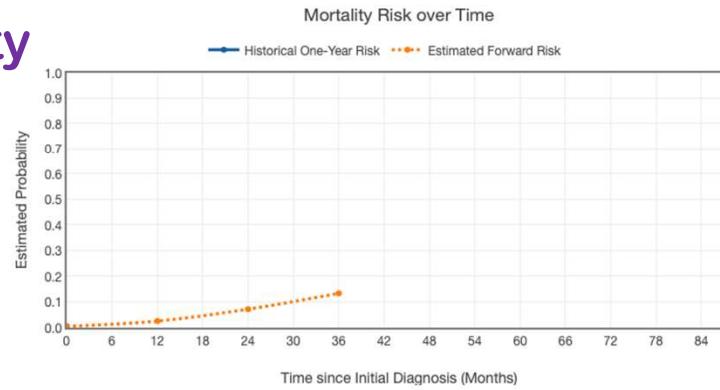
Explanatory patient features

Identify those patient-specific features the ML model has considered when issuing a prediction for a patient

Global & individualized feature importance

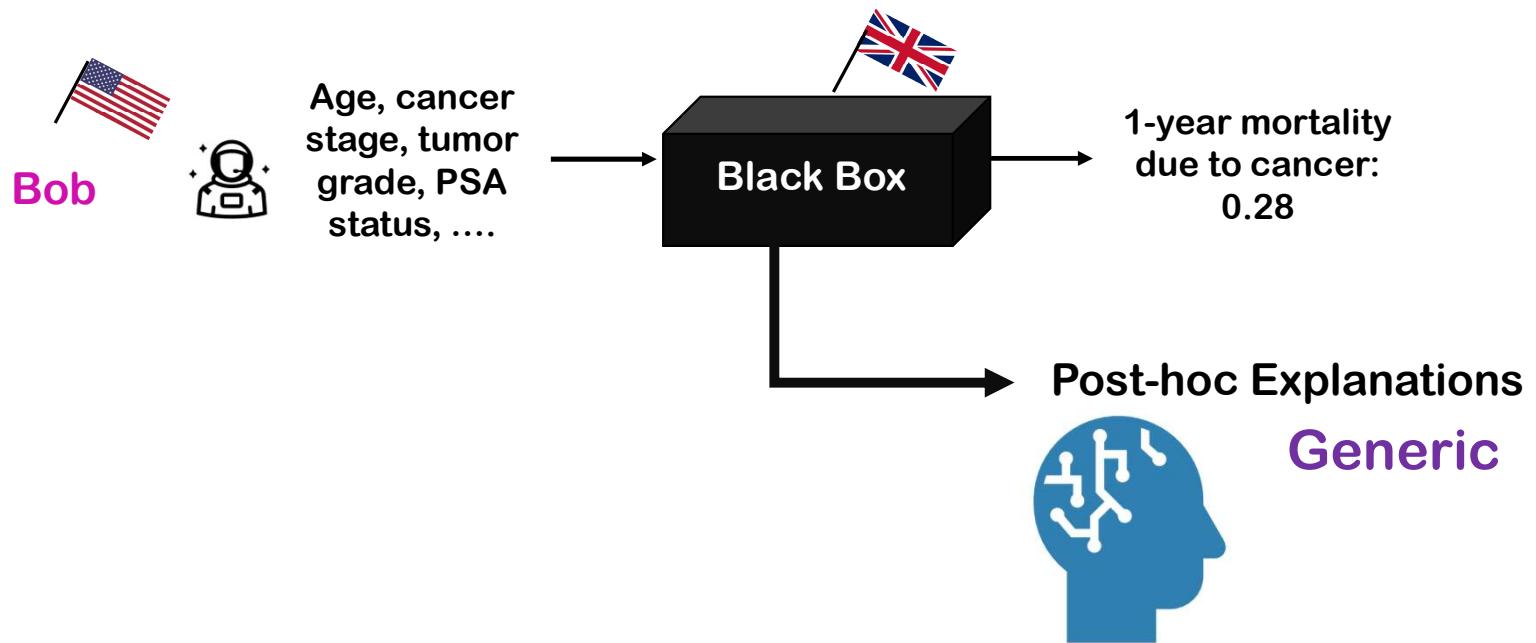


Interpretability

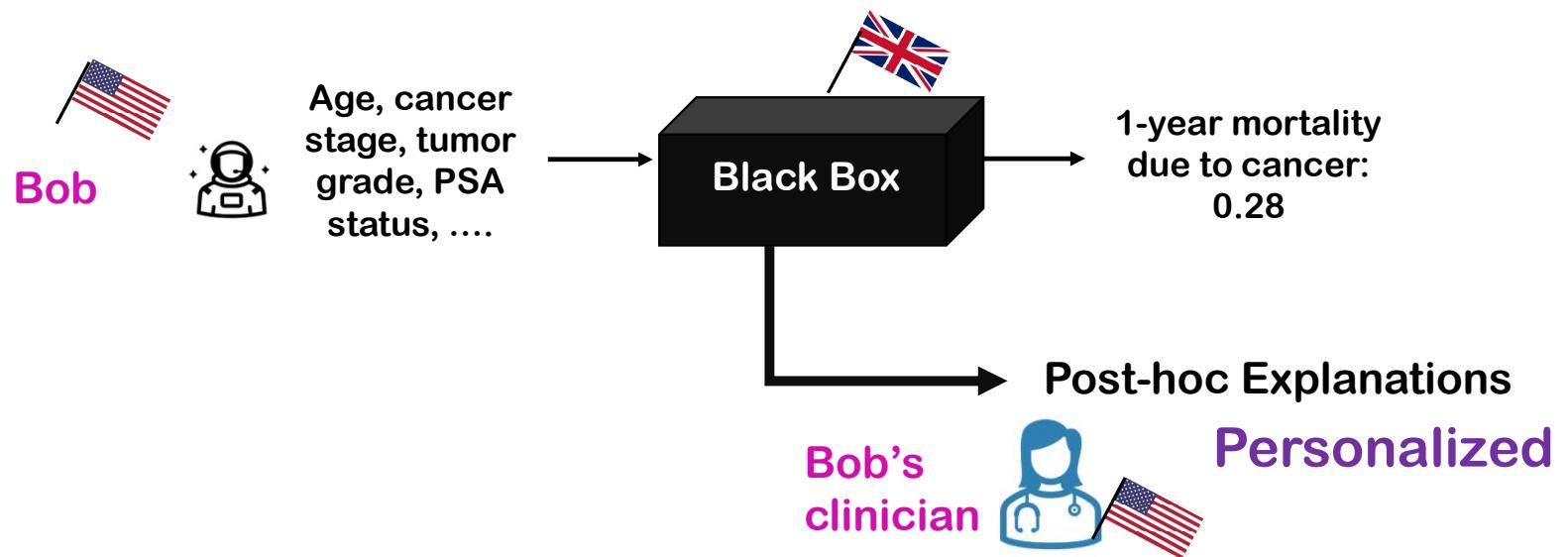


ML interpretability: type 2

Personalized explanations – Beyond “one-size-fits-all” example explanations



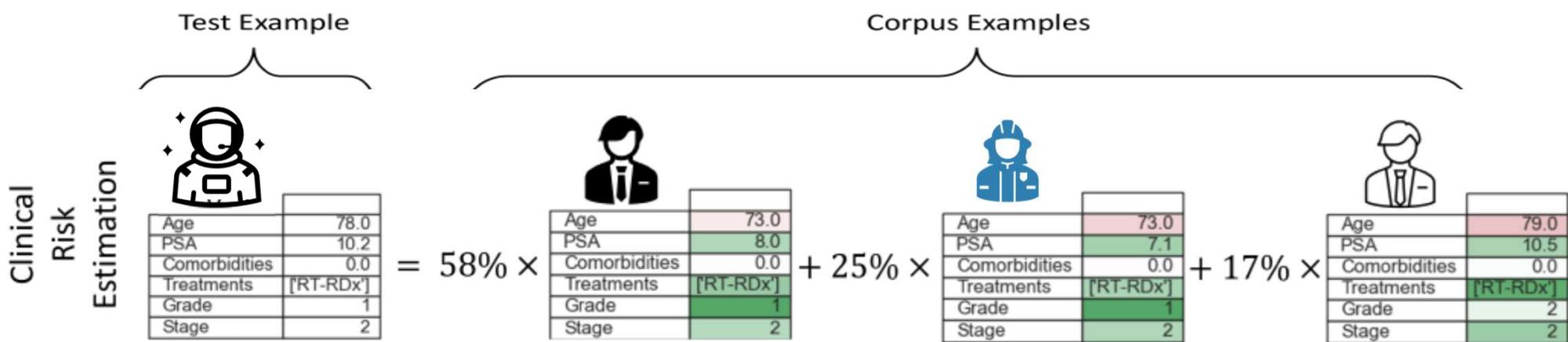
Personalized explanations – Beyond “one-size-fits-all” example explanations



Desiderata

Personalized explanations with reference to a “corpus” (a selected set of examples)

- ✓ Which corpus examples explain the prediction issued for a given test example?
- ✓ What features of these corpus examples are relevant for the model to relate them to the test example?



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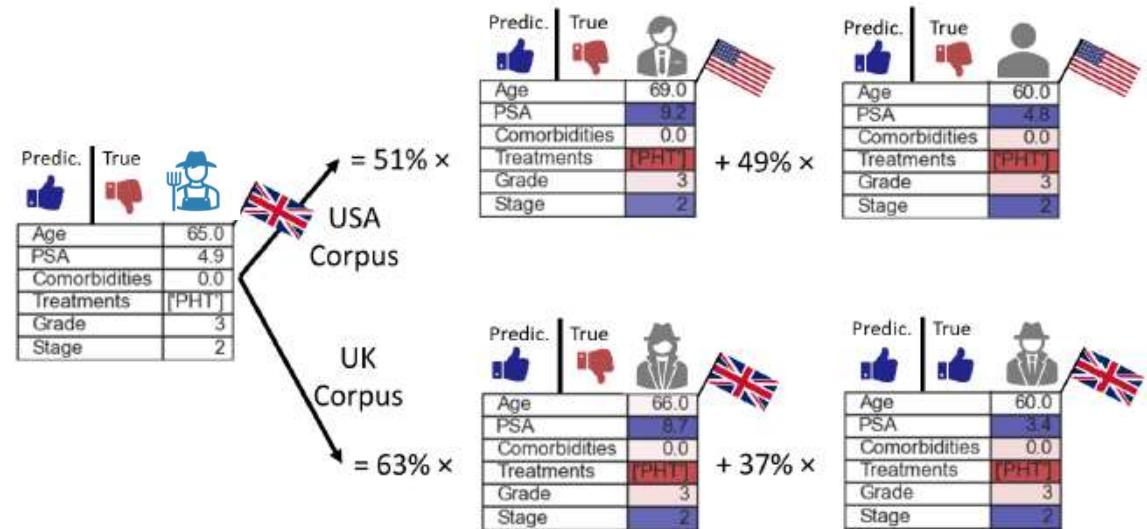
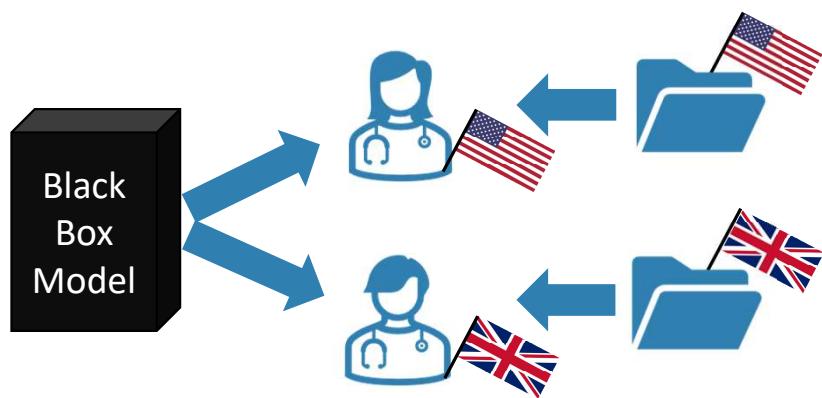


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Our solution: SimplEx [Crabbe, Qian, Imrie, vdS, NeurIPS 2021]

- ✓ SimplEx – able to reconstruct the test latent representation as a mixture of corpus latent representations
- ✓ Novel approach (**Integrated Jacobian**) allows SimplEx to make explicit the contribution of each corpus feature in the mixture
 - ✓ Bridge between feature importance & example-based explanations
- ✓ SimplEx gives the user freedom to choose the corpus of examples to explain model predictions in a user-centric way
- ✓ SimplEx provides user-centric explanations for any ML methods on diverse data (tabular, imaging, time-series, multi-modal)

SimplEx Explanations: Personalized



- Debug the ML models

Present examples for which the model **extrapolates**

ML interpretability: type 3



Regressions – explicit risk formulae

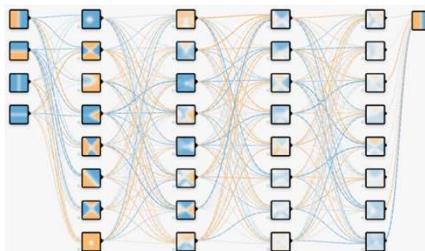
Which explicit risk formulae has the ML model learned?

Provide explicit formulae for the ML model's predictions –
Same level of transparency as regressions!!

Building transparent risk equations of black-box ML

[Alaa & vdS, NeurIPS 2019] [Crabbe, Zhang, vdS, NeurIPS 2020]

Black-box ML model



$$f(\mathbf{x})$$

Symbolic
Metamodelling
 $g(\mathbf{x}) = G(\mathbf{x}; \theta^*)$

$$\theta^* = \arg \min_{\theta \in \Theta} \ell(f(\mathbf{x}), G(\mathbf{x}; \theta))$$

Explicit function

$$\alpha_1 X_1 + \alpha_2 X_2^2 + \alpha_3 X_1 X_2$$

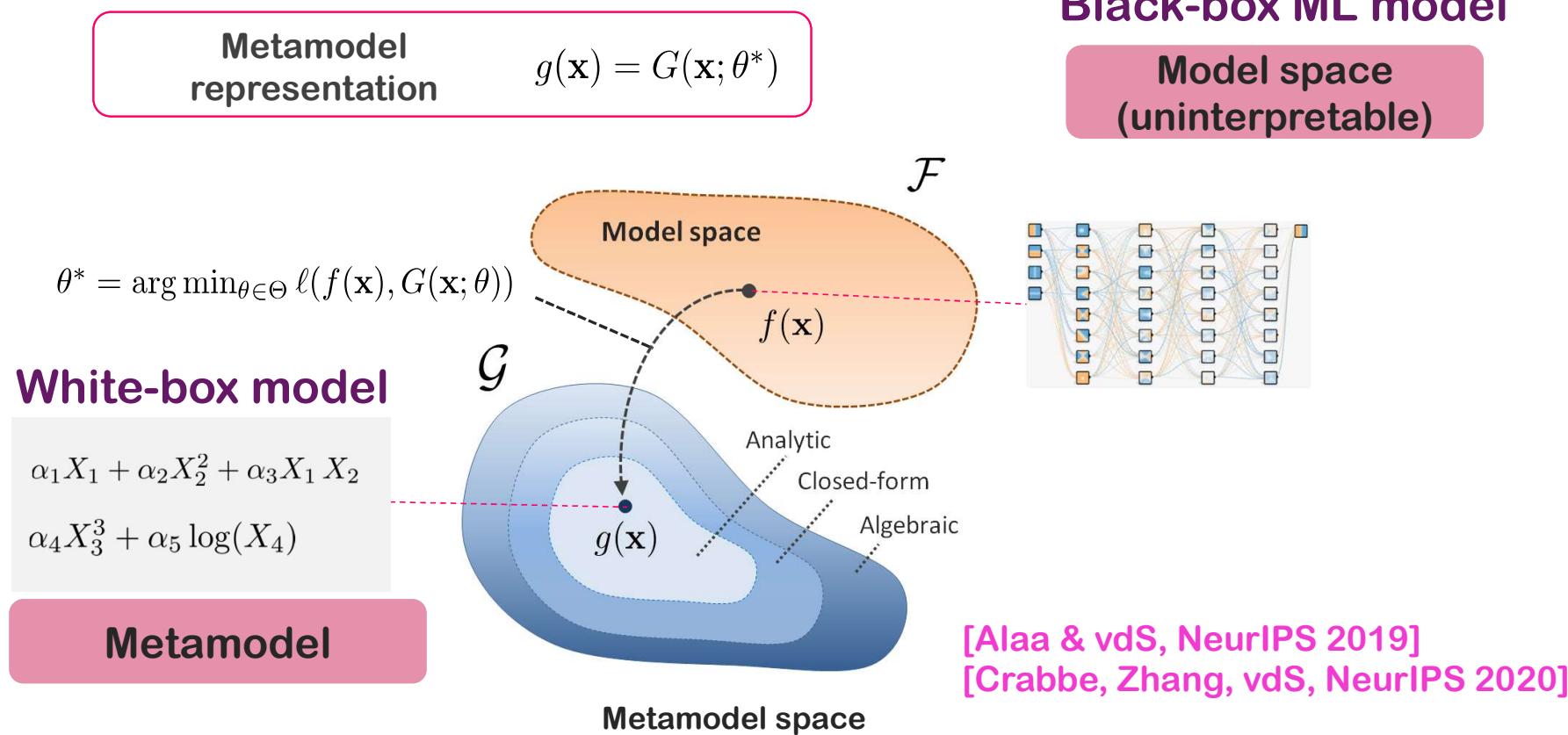
$$\alpha_4 X_3^3 + \alpha_5 \log(X_4)$$

$$g(\mathbf{x})$$

Metamodels

Operates on a **trained machine learning** model and outputs a symbolic formula describing the model's prediction surface

Building transparent risk equations of black-box ML



Interpretability using symbolic metamodeling in practice

[Alaa, Gurdasani, Harris, Rashbass & vdS, Nature MI, 2021]

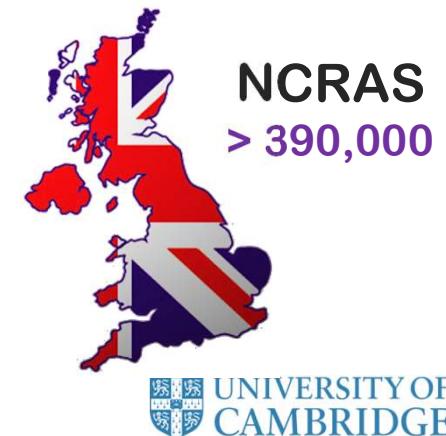
Example: Predicting breast cancer risk survival (5 years)



Nearly 1 million patients involved in the analysis.



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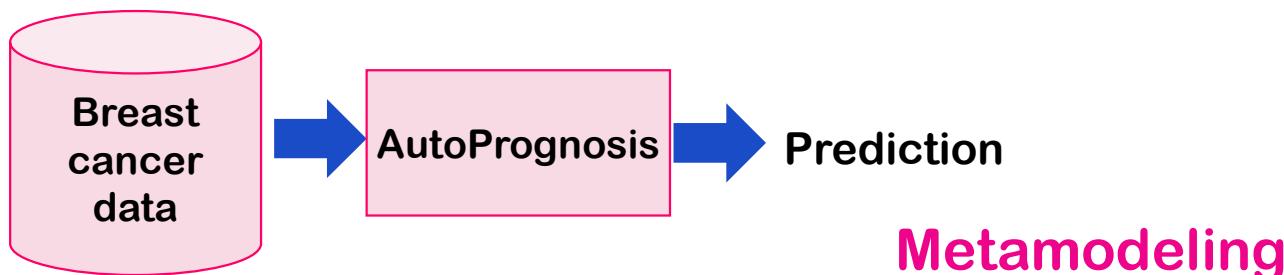


NCRAS
> 390,000

Interpretability using symbolic metamodeling in practice

[Alaa, Gurdasani, Harris, Rashbass & vdS, Nature MI, 2021]

Example: Predicting breast cancer risk survival (5 years)

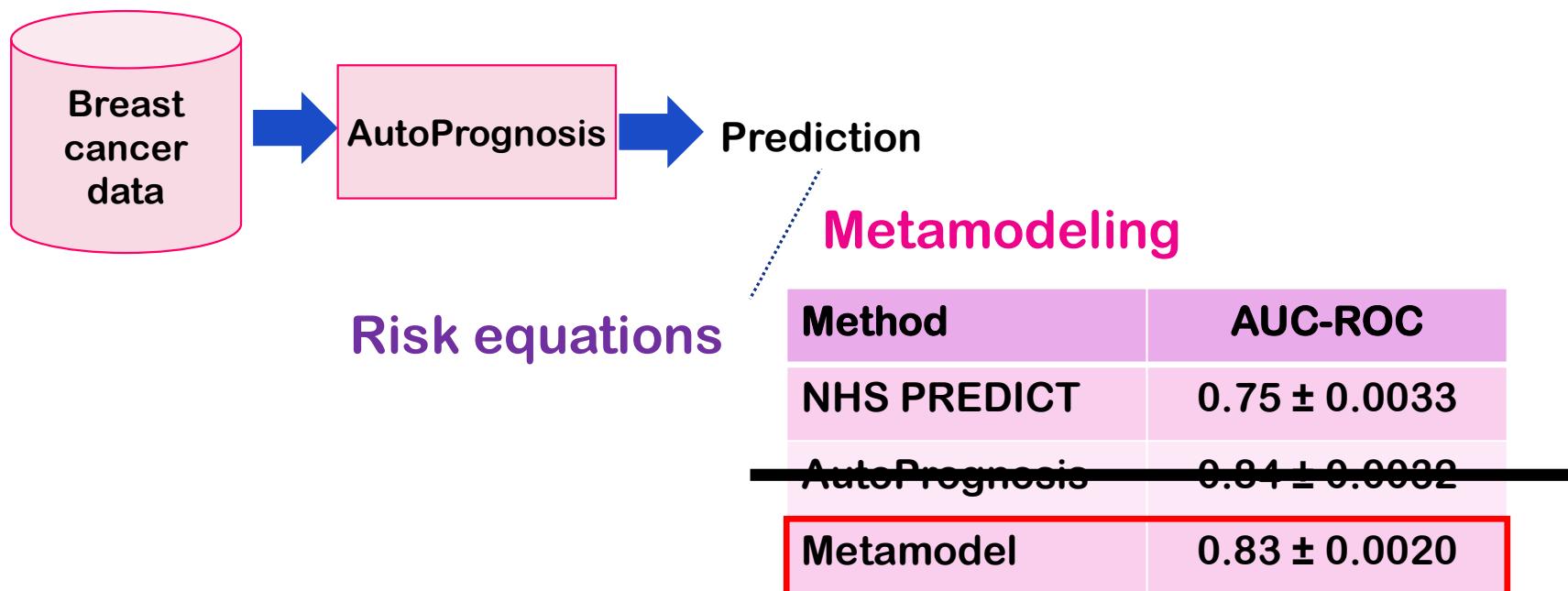


Method	AUC-ROC
NHS PREDICT	0.75 ± 0.0033
AutoPrognosis	0.84 ± 0.0032

Interpretability using symbolic metamodeling in practice

[Alaa, Gurdasani, Harris, Rashbass & vdS, Nature MI, 2021]

Example: Predicting breast cancer risk survival (5 years)



Medicine – We need to go beyond interpretability of static predictions

Patient trajectories

Time-series forecasting - Dynamask [ICML 2021]

Patient phenotyping

Unsupervised learning methods – Label-free explainability [ICML 2022]

Personalized actions (therapeutics for each patient)

Heterogeneous effects estimation – ITEGRABILITY [NeurIPS 2022]

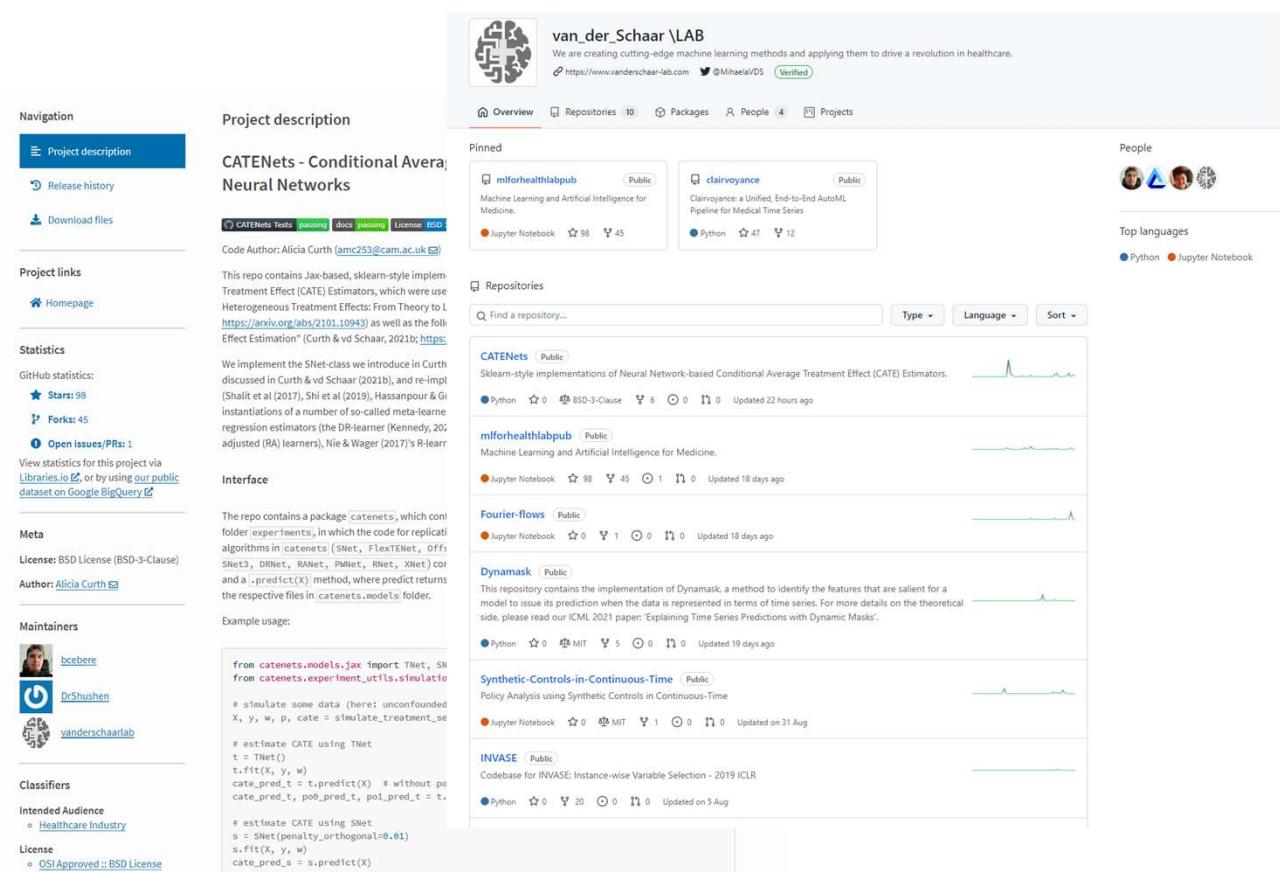
Discover new (clinical) concepts

Generalized framework for concept based explanations – Concept activation regions [NeurIPS 2022]

Bringing papers to life through software

<https://www.vanderschaar-lab.com/>
→ Software

<https://github.com/vanderschaarlab/>
<https://pypi.org/user/vanderschaarlab/>



The screenshot shows the GitHub organization page for `van_der_Schaar \LAB`. The main navigation bar includes links for Overview, Repositories (10), Packages, People (4), and Projects. The `CATEGNets - Conditional Average Neural Networks` project is highlighted. It has a green "passing" status for tests and documentation. The code author is Alicia Curth (`amc253@cam.ac.uk`). The repository description mentions Jax-based, sklearn-style implementations of Treatment Effect (CATE) Estimators. Below the repository are sections for Pinned, Repositories, and a search bar. Other pinned projects include `miforhealthlabpub`, `clairvoyance`, `Fourier-flows`, `Dynamask`, `Synthetic-Controls-in-Continuous-Time`, and `INVASE`.



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Engagement sessions: Inspiration Exchange

Online engagement sessions for
ML researchers in healthcare;
themed presentations & Q&A

<https://www.vanderschaar-lab.com/>
→ Engagement sessions
→ Inspiration Exchange

Session dedicated to
AutoPrognosis -
November 22, 4pm UK



Inspiration Exchange is a series of engagement sessions aiming to share ideas and discuss topics that will define the future of machine learning in healthcare. These events will target machine learning students, and will emphasize sharing of new ideas and development of new methods, approaches, and techniques.

As a lab, our purpose is to create new and powerful machine learning techniques and methods that can revolutionize healthcare. This doesn't happen in a vacuum. At inception, we are inspired by ideas and discussions; in implementation, we need connections, trust, and partnership to make a real difference.

While you can learn about our work at major conferences in machine learning or in our papers, we think it's a better idea to create a community and keep these conversations going. We're also aware that many people—both in healthcare and machine learning—have questions about what we do, and how they can contribute.

For more information about Inspiration Exchange—and to sign up to join in—please have a look at the sections below, and keep checking for new updates.



vanderschaar-lab.com

