Reality-Centric AI

Mihaela van der Schaar

John Humphrey Plummer Professor of Machine Learning, Artificial Intelligence and Medicine, University of Cambridge // Director, Cambridge Center for AI in Medicine // Turing Faculty Fellow, The Alan Turing Institute

van_der_Schaar
\ LAB

vanderschaar-lab.com

UNIVERSITY OF CAMBRIDGE

mv472@cam.ac.uk

@MihaelaVDS

linkedin.com/in/
mihaela-van-der-schaar/

A complex world

- Enormous leaps in AI (NLP/ChatGPT, computer vision, robotics, etc.)

- And yet…
  - Deliver personalized medicine?
  - Transform healthcare systems?
  - Traffic control?
  - Solve the energy crisis?
  - Transform education?

A complex world

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- And yet…
  - Deliver personalized medicine?
  - Transform healthcare systems?
  - Traffic control?
  - Solve the energy crisis?
  - Transform education?

Not just a few breakthroughs away…..
Because of the complexity of the real-world – a different AI/ML paradigm

A complex world – our lab's work for the past 20 years

Smart Cities

Finance

Transportation

Networks of Experts

Economics

Networks
Communication Systems
Internet of Things

Energy/Smart Grids

Medicine &
Healthcare

Education

Solving these complex human-centric problems is our biggest task as AI researchers!

A fundamentally new paradigm is needed for AI

- **Reality-centric AI aims to reorientate AI towards the complexities of the real world**

https://www.vanderschaar-lab.com/the-case-for-reality-centric-ai/

What is Reality-centric AI?

- AI which can operate effectively, reliably, and accountably *in the real world*

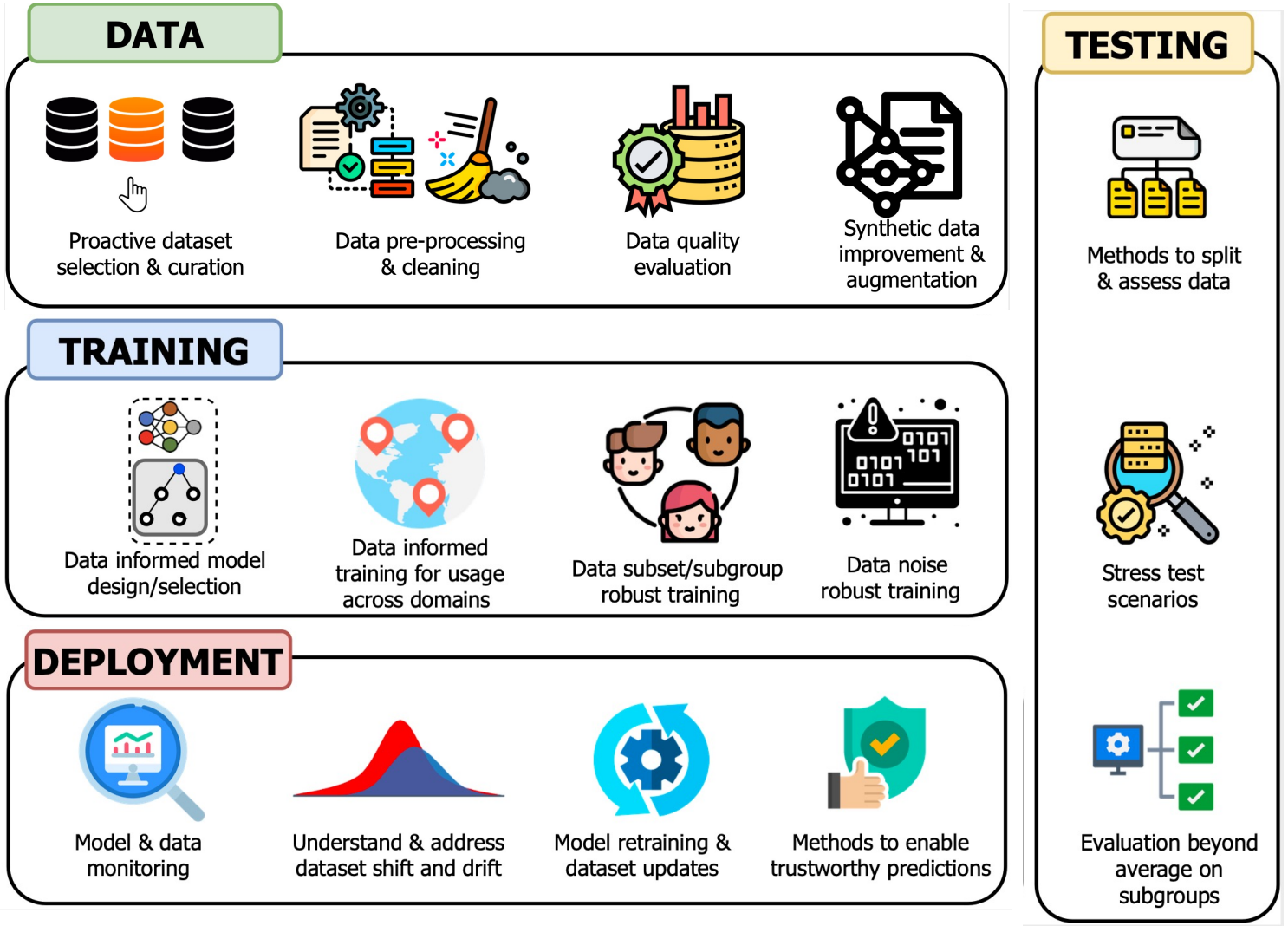
- Focuses on inherent and unavoidable complexity of the real world at the heart of designing, training, testing, and deploying AI models.

Reality-centric AI – Use of Real-world Data

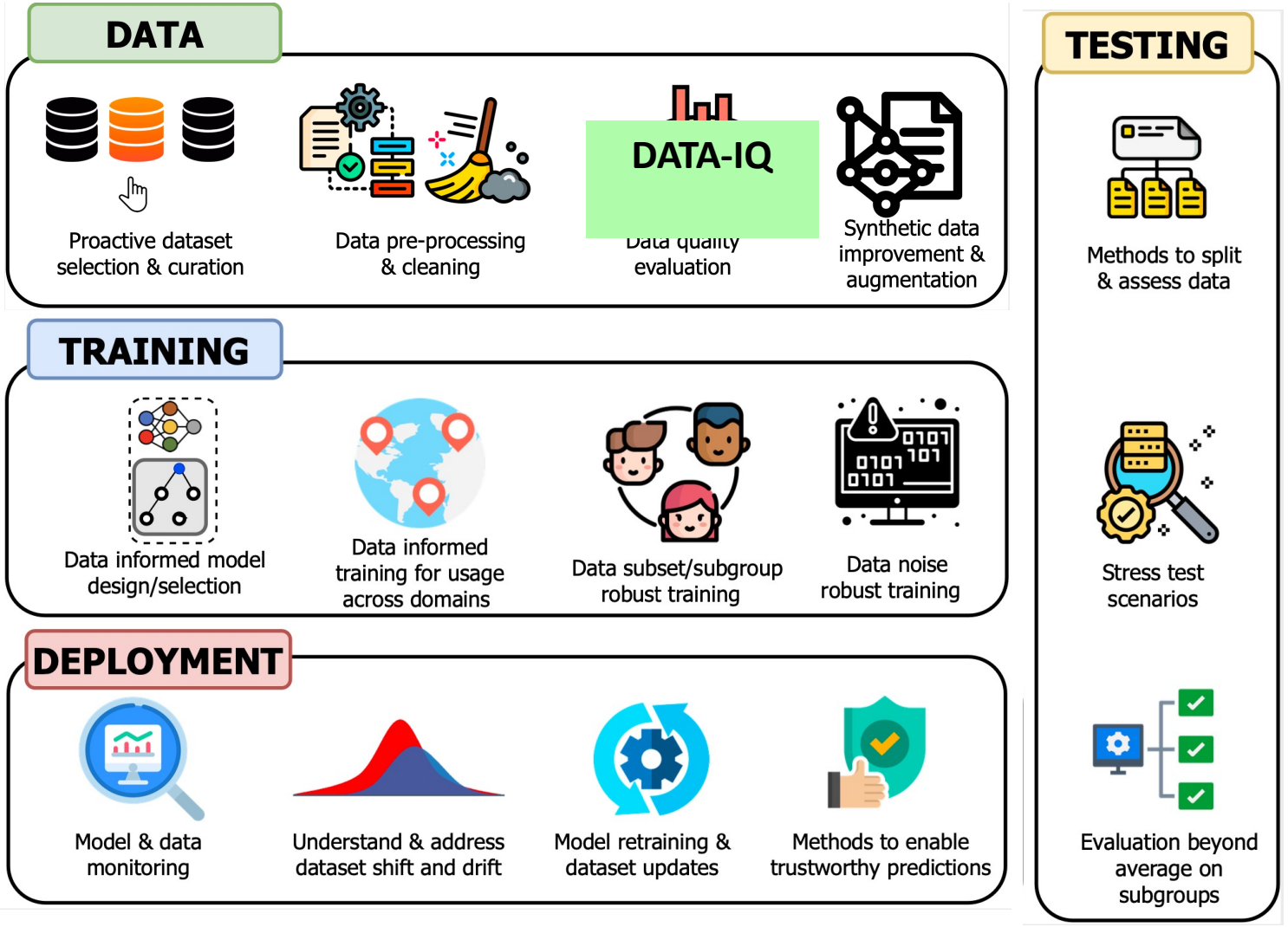
- messy, biased, noisy, erroneous
- costly to acquire
- limited
- incomplete
- changes over time

Construct Reality-Centric ML pipelines with Real-world data

Construct Reality-Centric ML pipelines with Real-world data



Construct Reality-Centric ML pipelines with Real-world data



vanderschaar-lab.com/ → dc-check

DC-Check provides online & offline tools to actionably engage with data-centric considerations in ML development

Nabeel Seedat

Fergus Imrie

Data-IQ: Characterizing heterogeneous subgroups in tabular data

NeurIPS 2022

Nabeel Seedat, Jonathan Crabbé, Ioana Bica & Mihaela van der Schaar

Focus: Characterize the data to create higher quality training datasets!

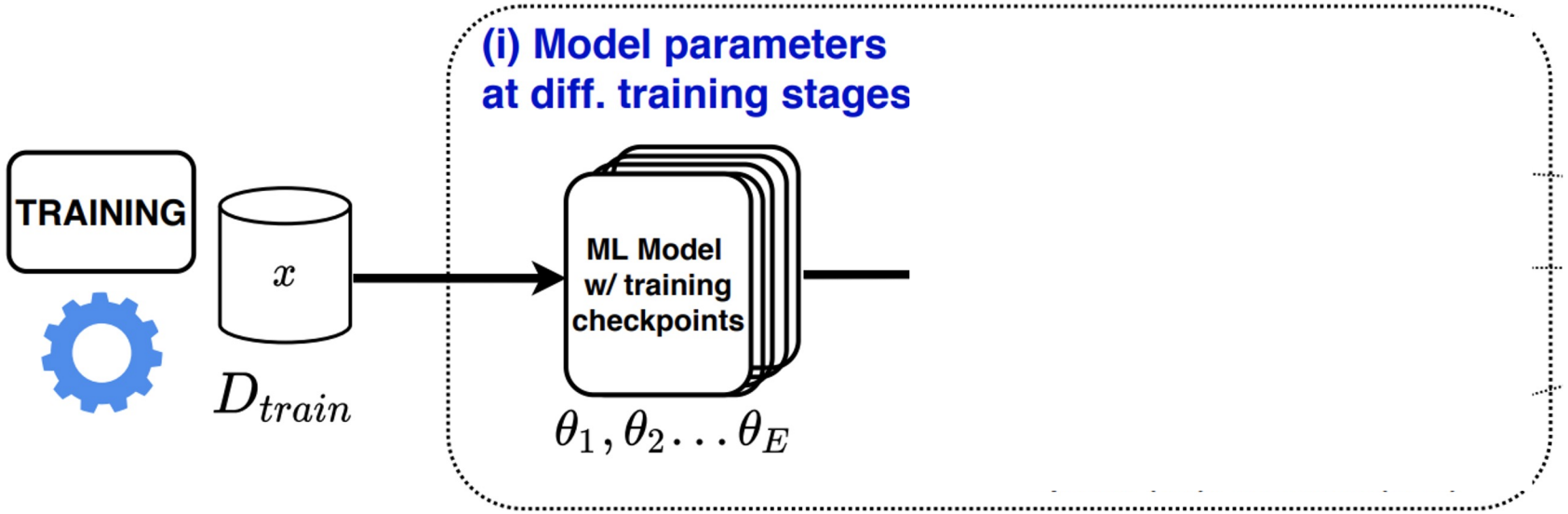
Auditing datasets

Auditing datasets at scale is hard & time-consuming!

Contributions of Data-IQ

- Data-IQ can characterize samples into subgroups based on the inherent uncertainty in data
- Useful tool for practitioners: understand quality of data, guide feature acquisition and/or help judiciously sculpt datasets
- Useful for many data modalities: our focus is on tabular data, however, DataIQ also work for other data modalities – including images and text (see our paper)

Data-IQ pipeline



Two types of uncertainty

Data-IQ

$$v_{\text{al}} = \mathbb{E}_{\vartheta}[\mathbb{V}_{\tilde{Y}|X,\vartheta}[\tilde{Y}|X = x, \vartheta]]$$

Variability due to inherent inability to predict with certainty (linked to the **data**)

Aleatoric uncertainty

Data maps [23]

$$v_{\text{ep}} = \mathbb{V}_{\vartheta}[\mathbb{E}_{\tilde{Y}|X,\vartheta}[\tilde{Y}|X = x, \vartheta]]$$

Variability due to change in predictions via parameters (linked to the **model**)

Epistemic uncertainty

Data-IQ assesses uncertainty over training

Data-IQ

$$v_{\text{al}} = \mathbb{E}_{\vartheta}\left[\mathbb{V}_{\tilde{Y}|X,\vartheta}\left[\tilde{Y}|X=x,\vartheta\right]\right]$$

Variability due to inherent inability to predict with certainty (linked to the **data**)

EASY: PREDICTED CORRECTLY, WITH HIGH CONFIDENCE

HARD: PREDICTED INCORRECTLY, WITH HIGH CONFIDENCE

AMBIGUOUS: INHERENT AMBIGUITY,
CURRENT FEATURES INSUFFICIENT TO DISTINGUISH,
NO MATTER THE MODEL

Two types of uncertainty

Data-IQ

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Variability due to change in predictions via parameters (linked to the **model**)

Epistemic uncertainty

Stratification based on data uncertainty

Differences between Data-IQ & Data Maps:
Type of uncertainty matters!

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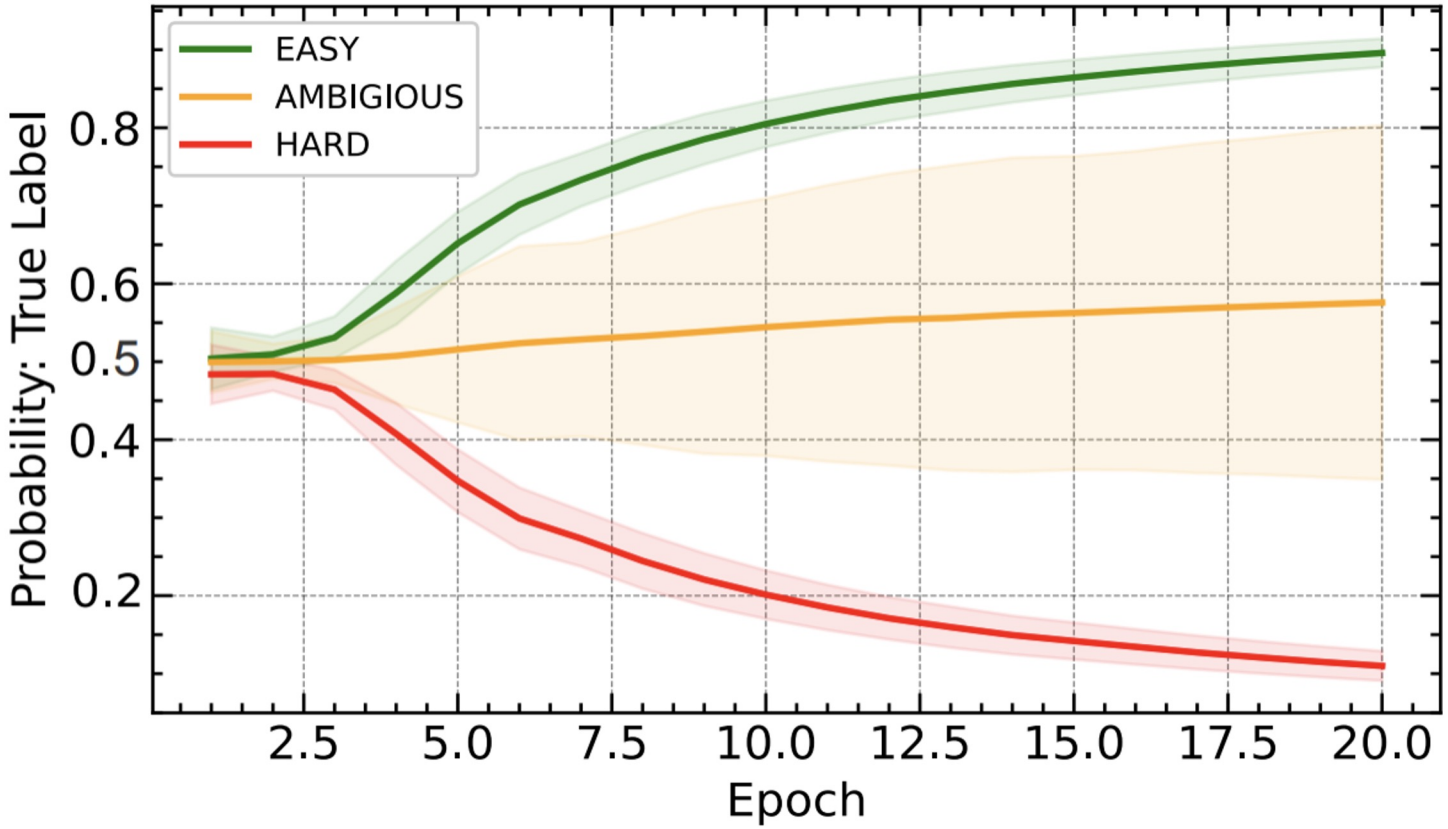
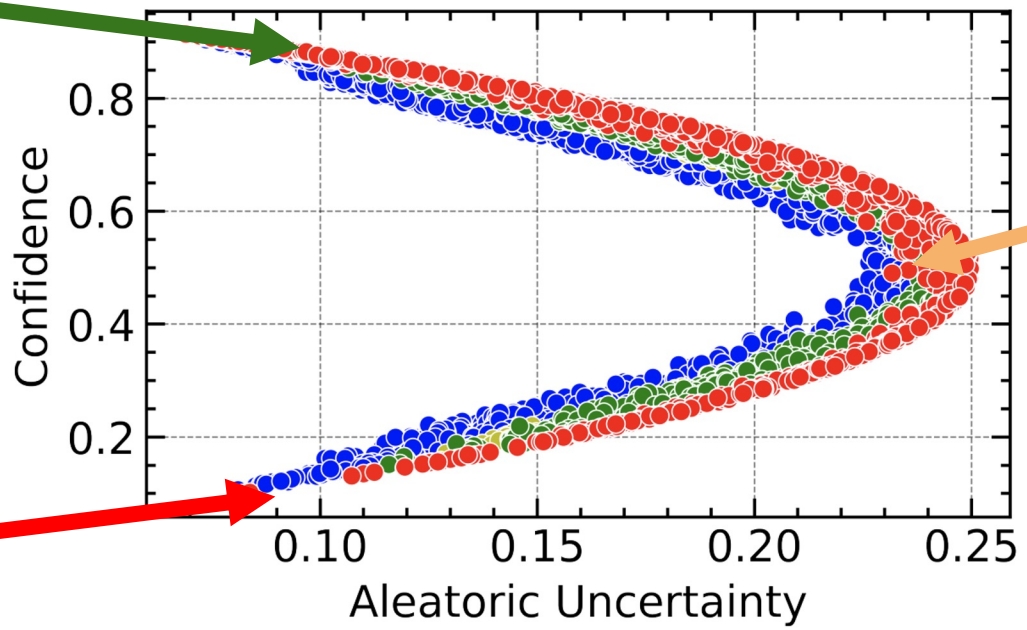
Type of uncertainty matters!



Differences between Data-IQ & Data Maps:
Type of uncertainty matters!

EASY



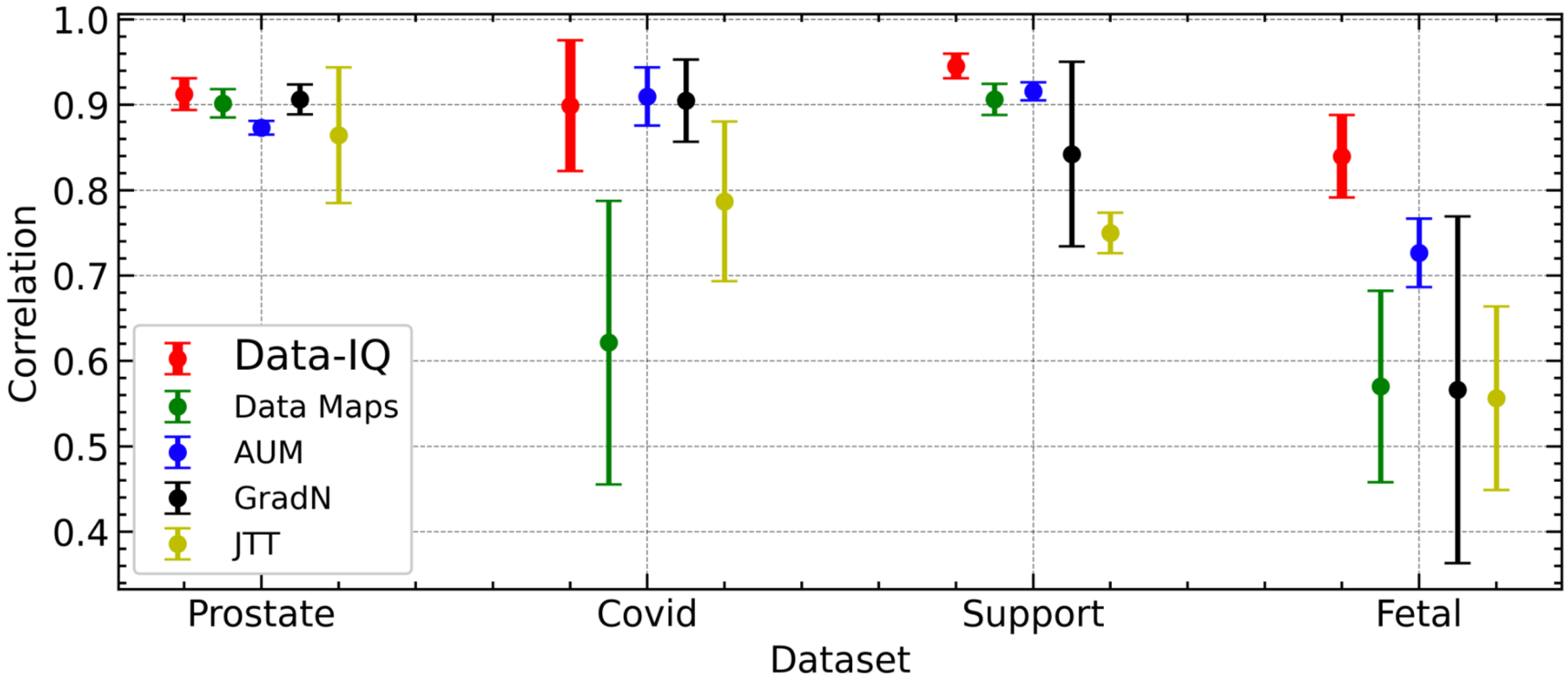
AMBIGUOUS

HARD

Data-IQ: Impact

ROBUST DATA CHARACTERIZATION

Aleatoric (data) uncertainty: consistent sample characterization for similar performing models



Data-IQ: Impact

ROBUST DATA CHARACTERIZATION

Aleatoric (data) uncertainty: consistent sample characterization

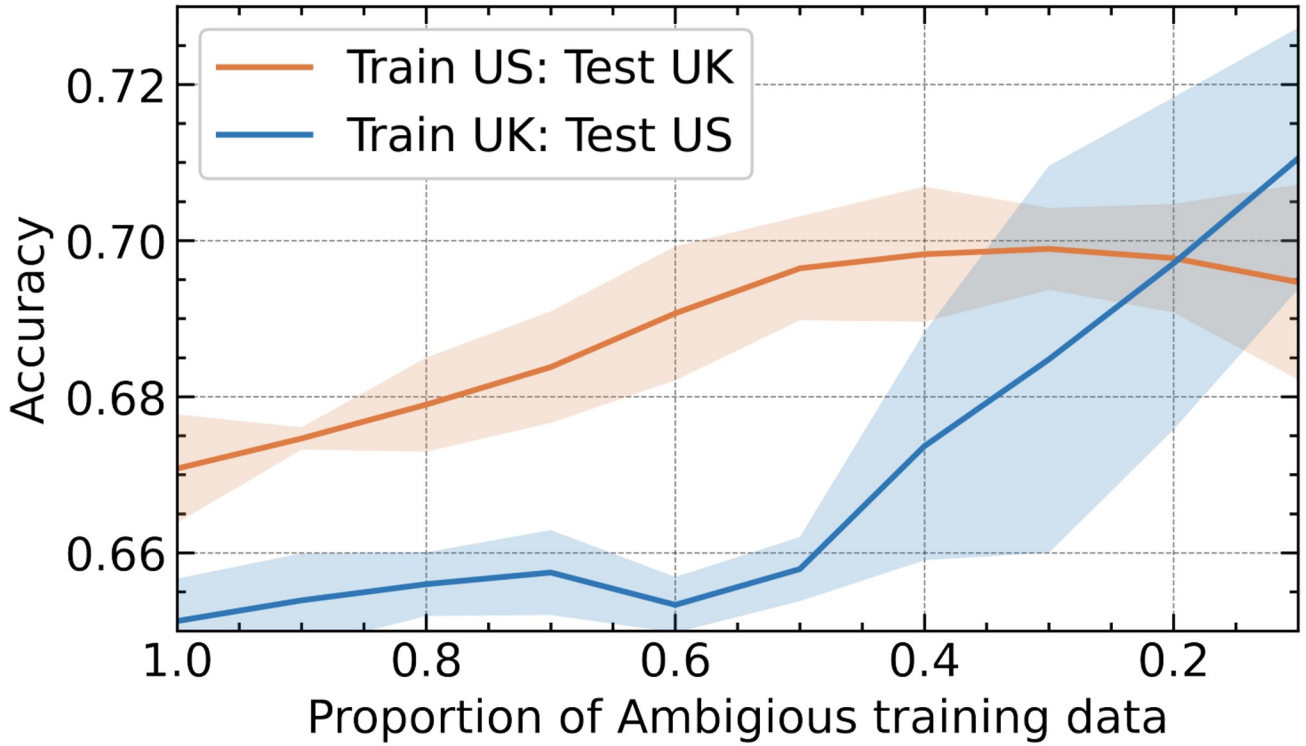
Principled data collection

Utility for feature acquisition & dataset selection

Data-IQ: Impact

Reliable model deployment

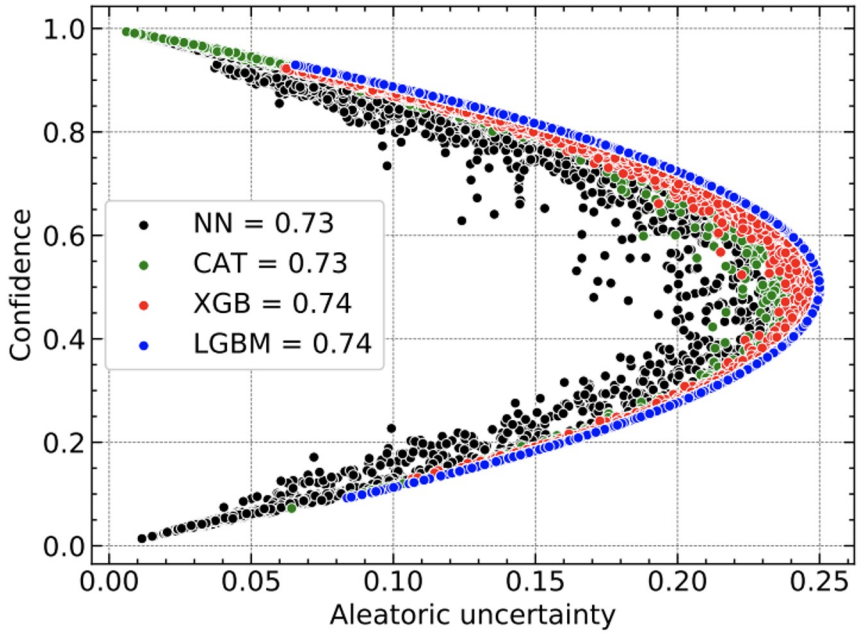
Guide sculpting of datasets for more reliable deployment of models (improved generalization)



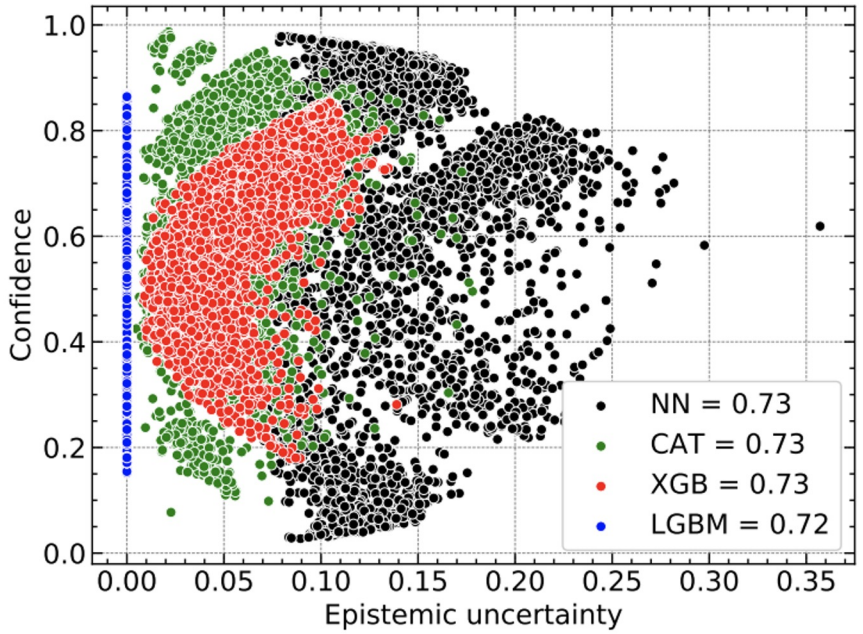
Data-IQ: Impact

Plug & Play

Data-IQ is usable with any model trained iteratively: neural nets, XGBoost etc



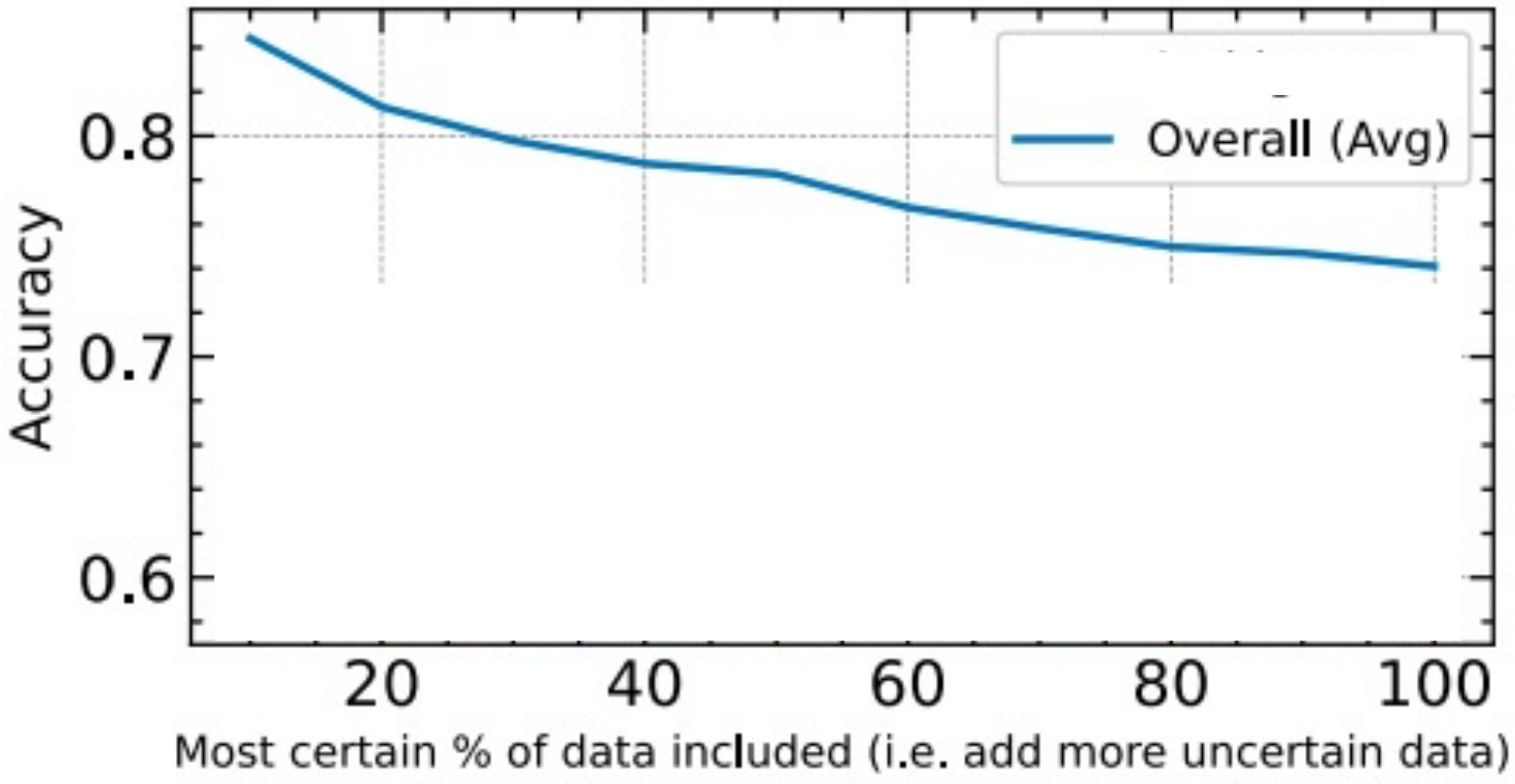
(a) Data-IQ



(b) Data Maps

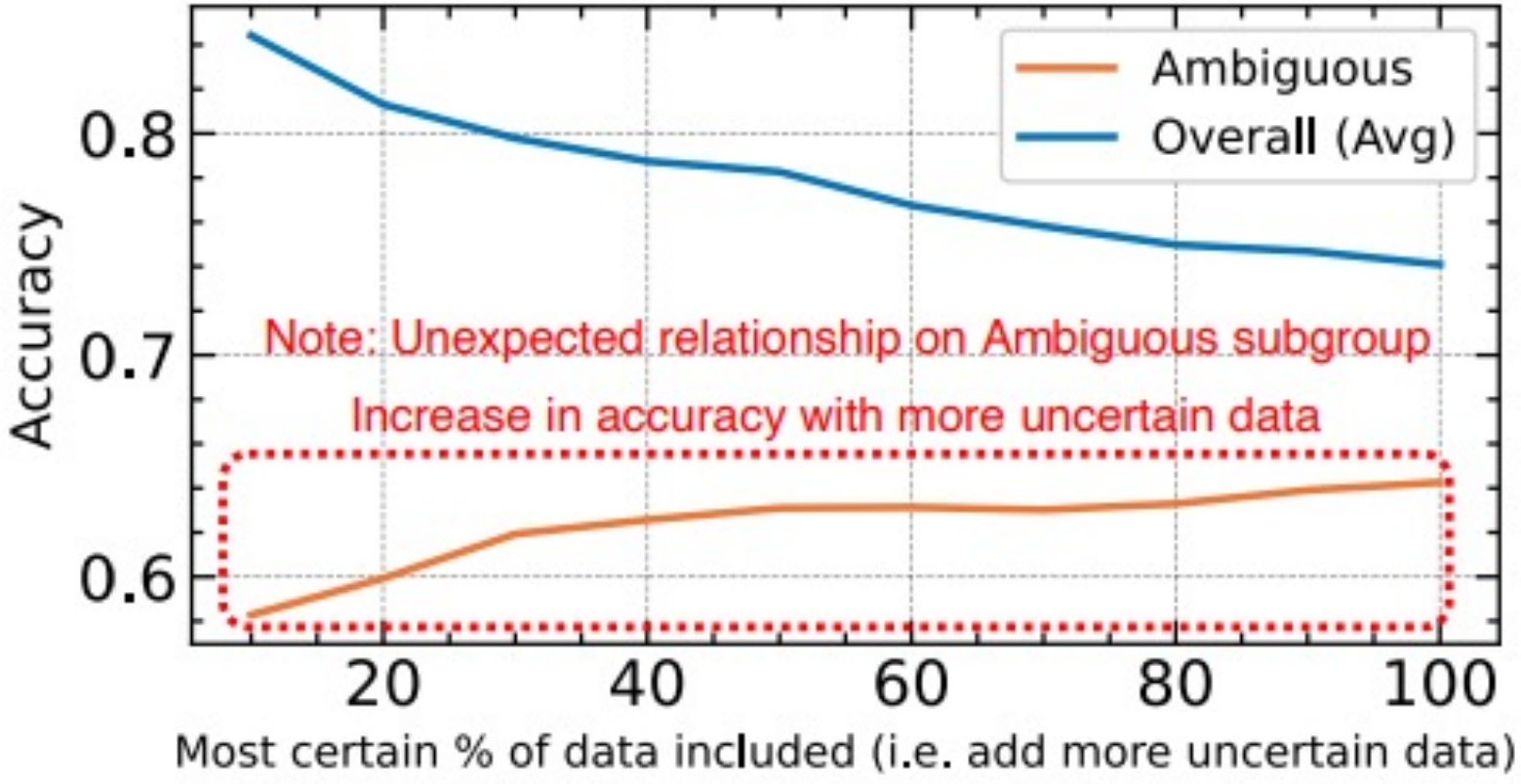
Data-IQ: Impact

Subgroup-informed usage of uncertainty estimation

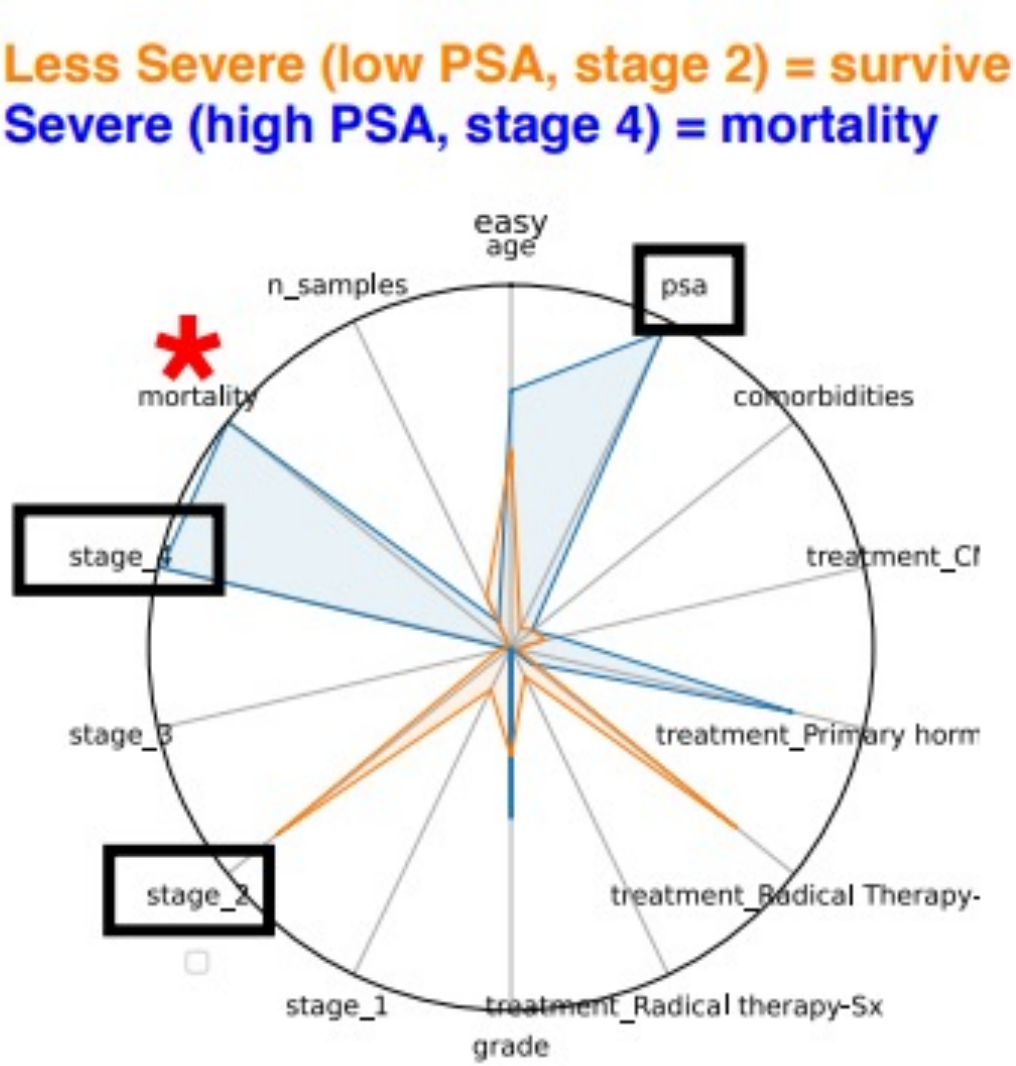


Data-IQ: Impact

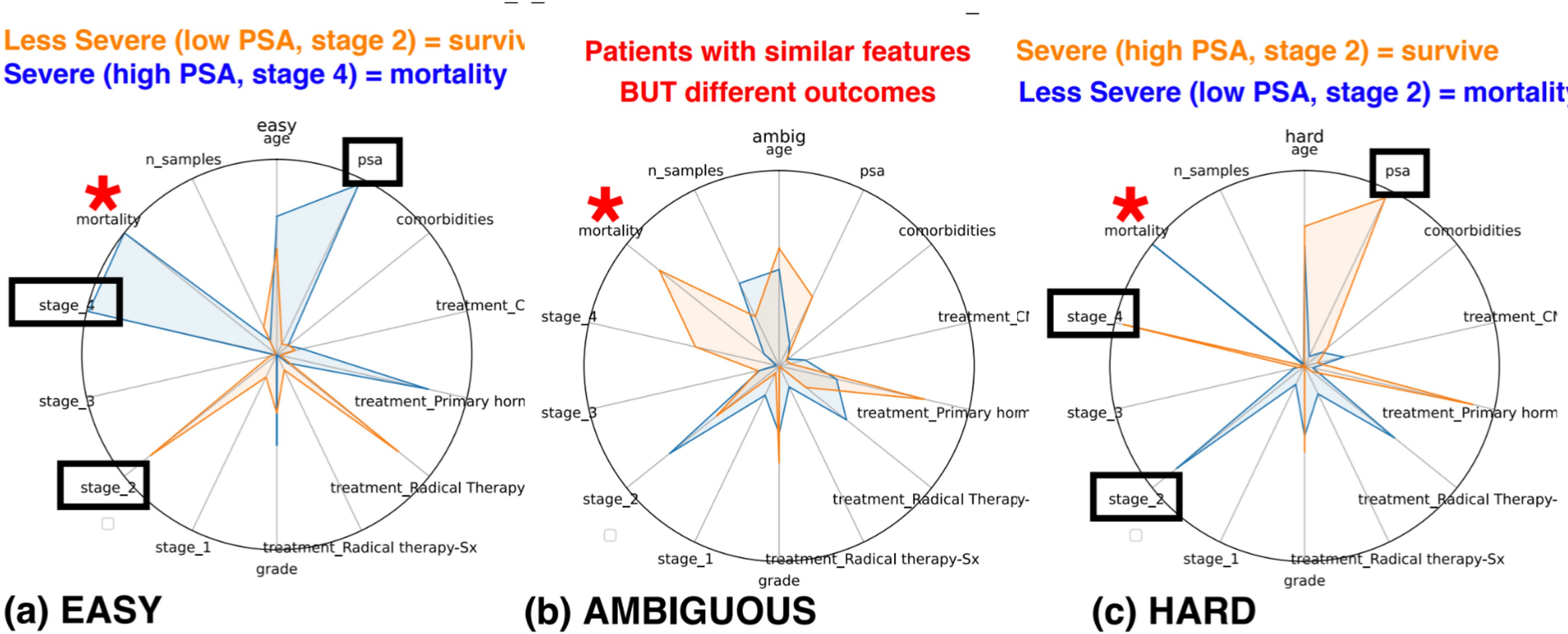
Subgroup-informed usage of uncertainty estimation



Data-IQ: Insights



Data-IQ: Insights



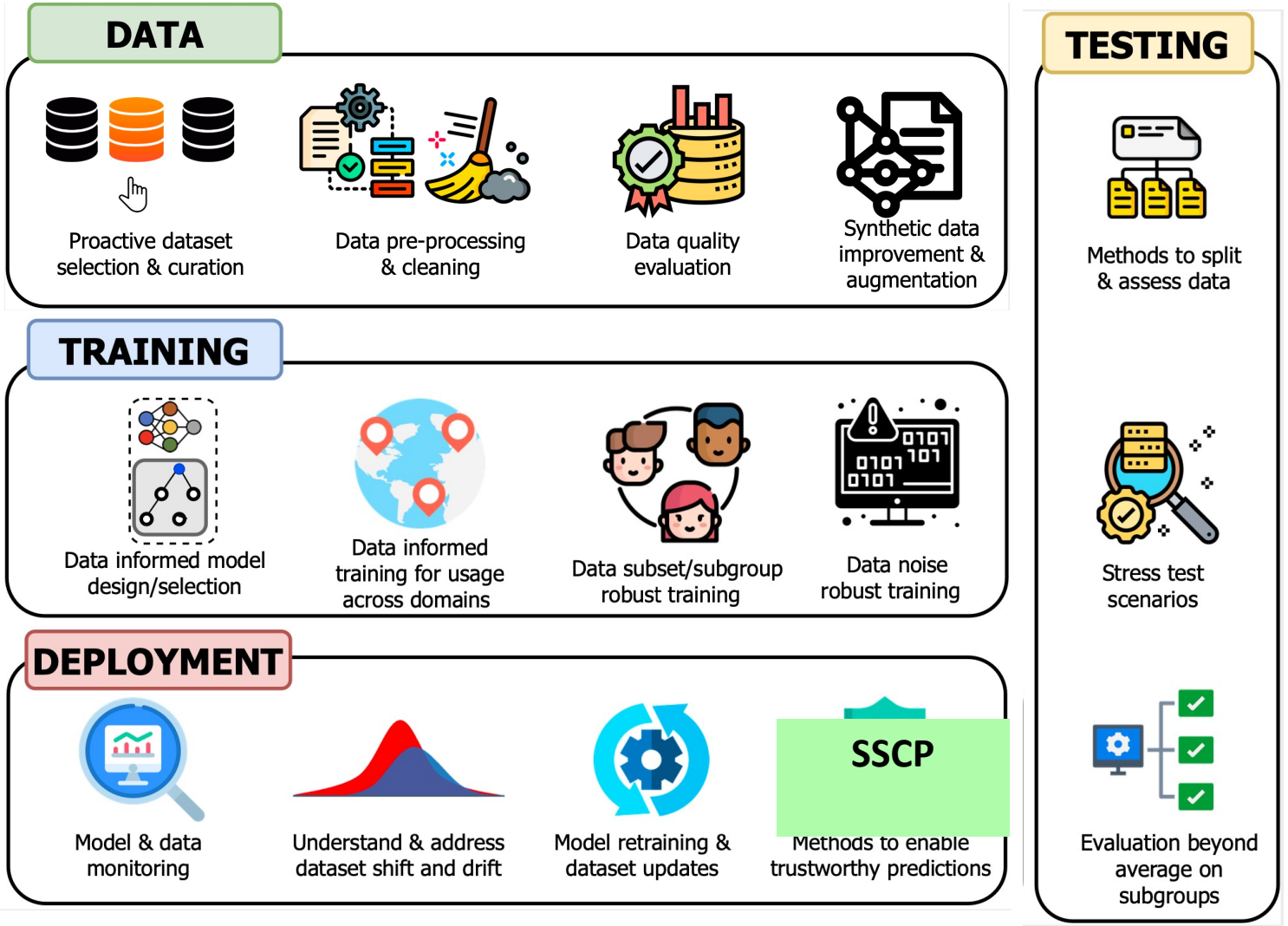
Using Data-IQ on your own data

Easily applied in your existing model training loops

Just 2 extra lines of code!

Plug-ins for Pytorch, Tensorflow & Sklearn

Construct Reality-Centric ML pipelines



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Improving Adaptive Conformal Prediction Using Self-Supervised Learning

AISTATS 2023

Nabeel Seedat*, Alan Jeffares*, Fergus Imrie & Mihaela van der Schaar

Self- and Semi-Supervised Learning for tabular data

VIME (NeurIPS 2020)

First self- and semi-supervised method for tabular data

Self-supervised pretext tasks:

- **Feature vector estimation**
- **Mask vector estimation**

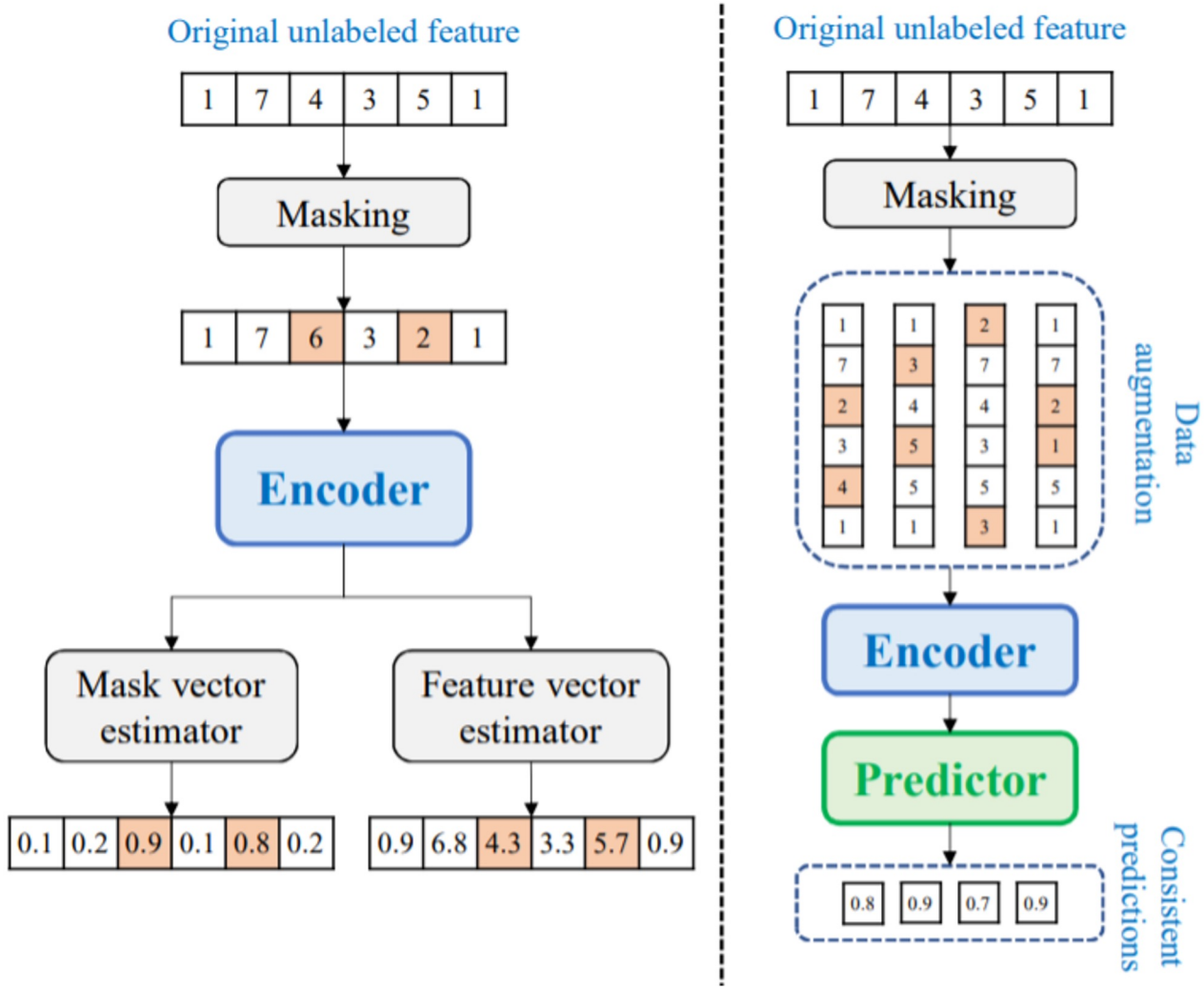
Masking process can be used for semi-supervised learning

SEFS (ICLR 2022)

Improvements to masking process

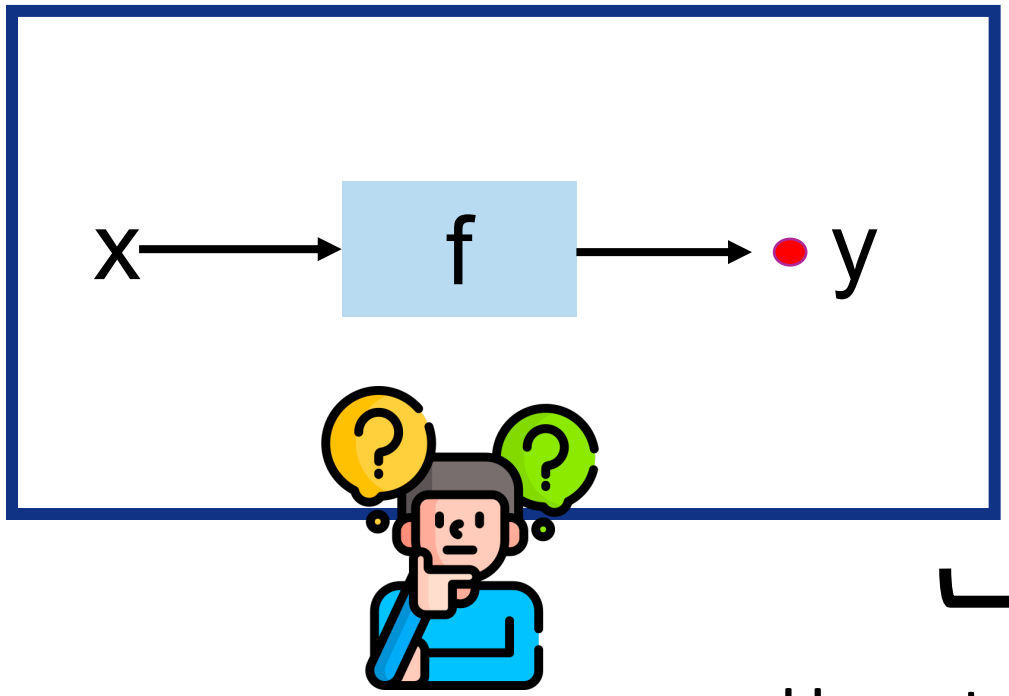
→ Independent vs. Correlated masking

Extension to feature selection

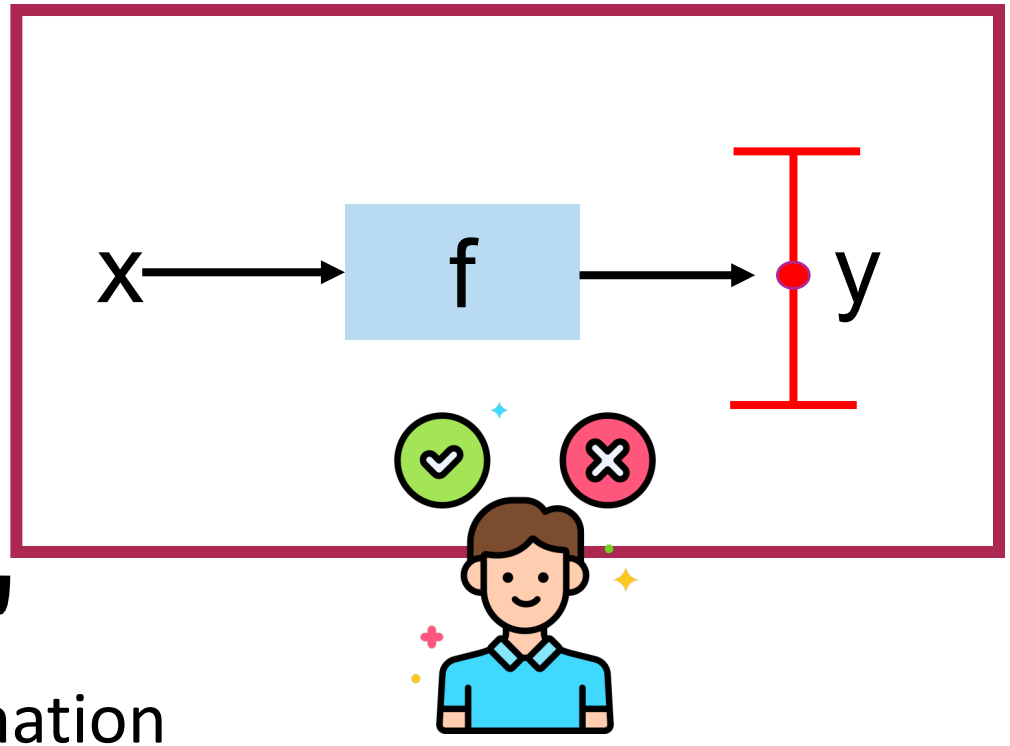


Trustworthy ML

Typical ML: Point Estimates



Trustworthy ML: Point Estimates + Uncertainty



Uncertainty estimation

This work: Conformal Prediction

Conformal Prediction (CP) – Vovk et al (2005)

Prediction Intervals, with guarantees on coverage

i.e. true value will be contained within the interval with a specified probability

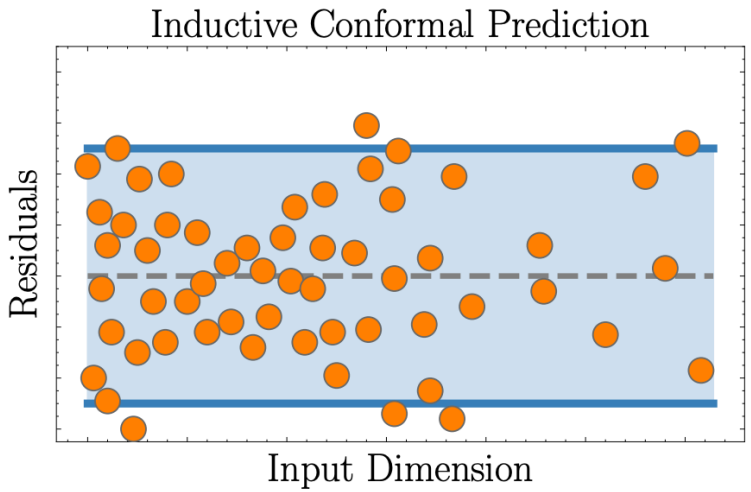
$$\mathbb{P}\{Y \in \hat{C}(X)\} \geq 1 - \alpha.$$

Powerful: Model-agnostic & distribution-free assumptions

Paradigms of Conformal Prediction

Inductive CP:

Constant width intervals



Paradigms of Conformal Prediction

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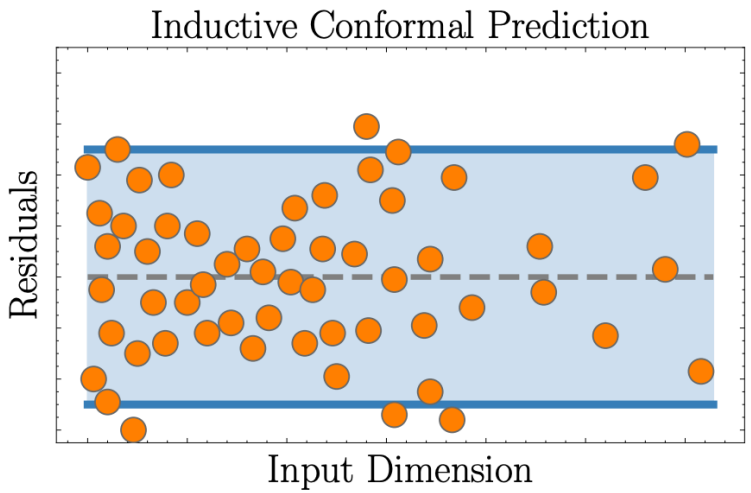
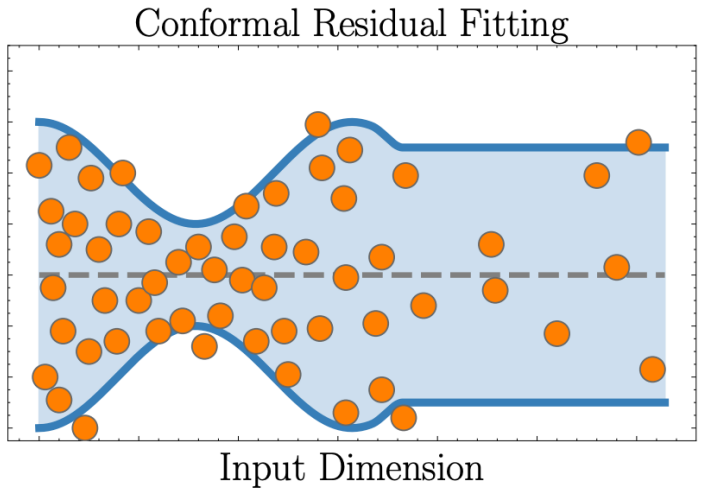


Conformal Residual Fitting:
Adaptive but inefficient
in some regions



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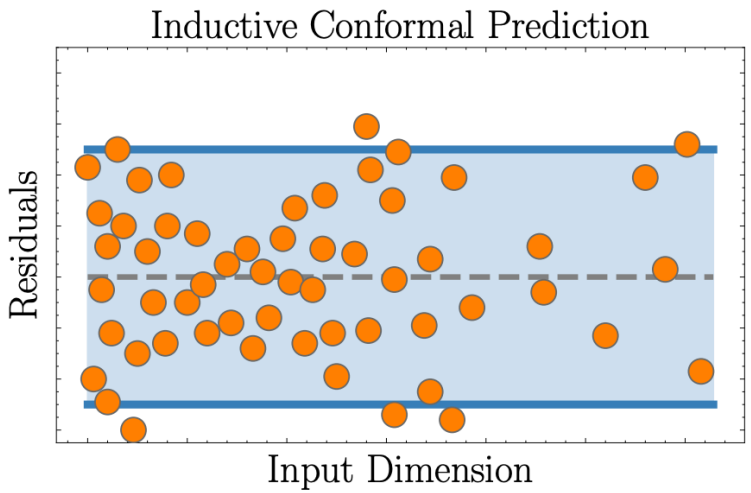

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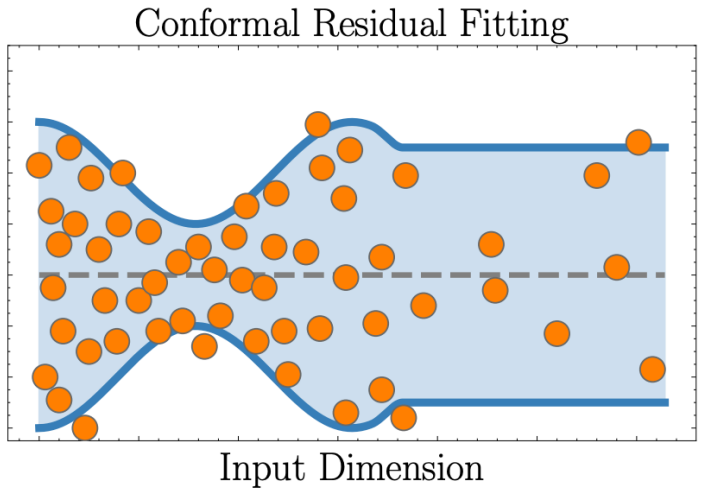
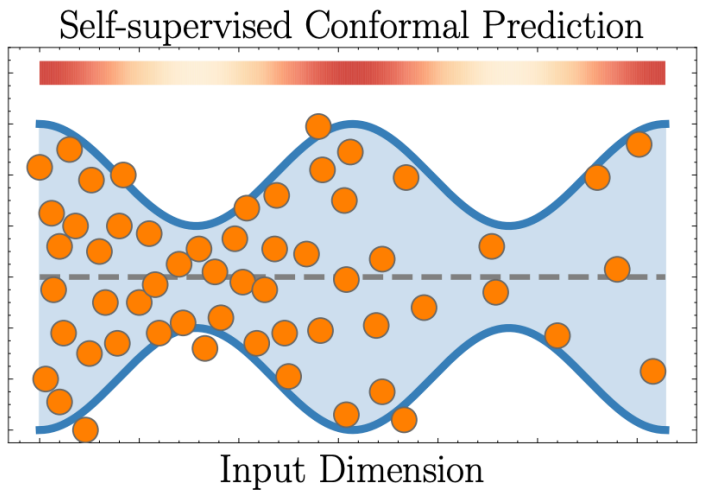
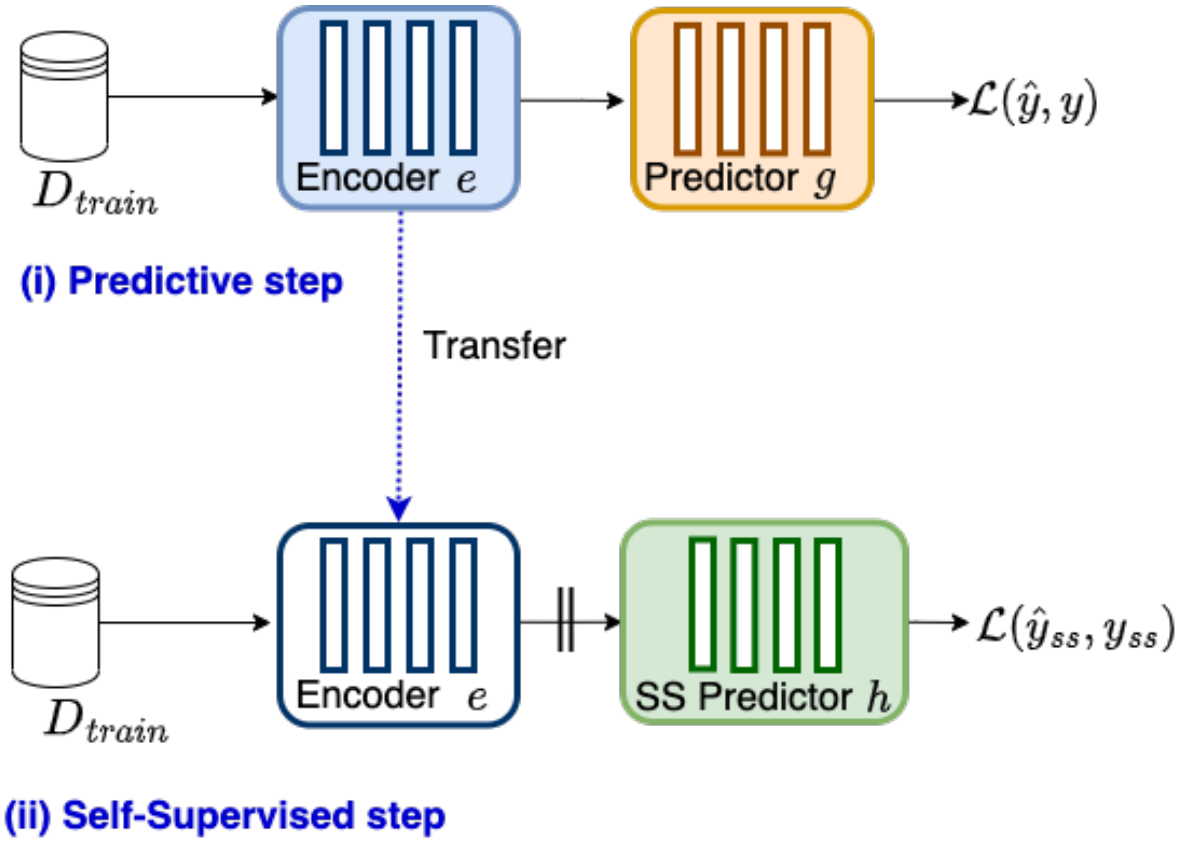


Self-supervised CP (SSCP):
Improved efficiency,
particularly for sparser regions



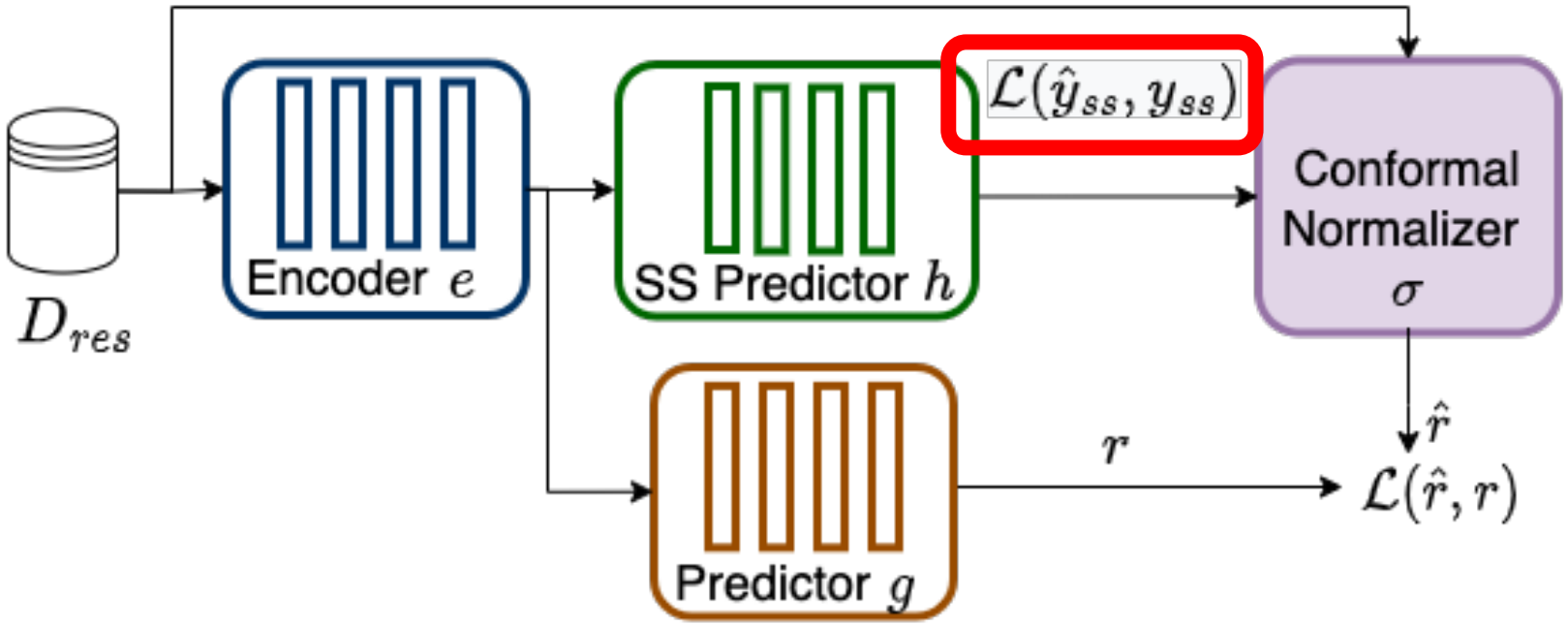
SSCP: Predictive & Self-Supervised phase

- Train predictor *f = e o g*
- Transfer encoder *e* for self-supervised task
- Train self-supervised predictor *h*



SSCP: Conformal Normalized Phase

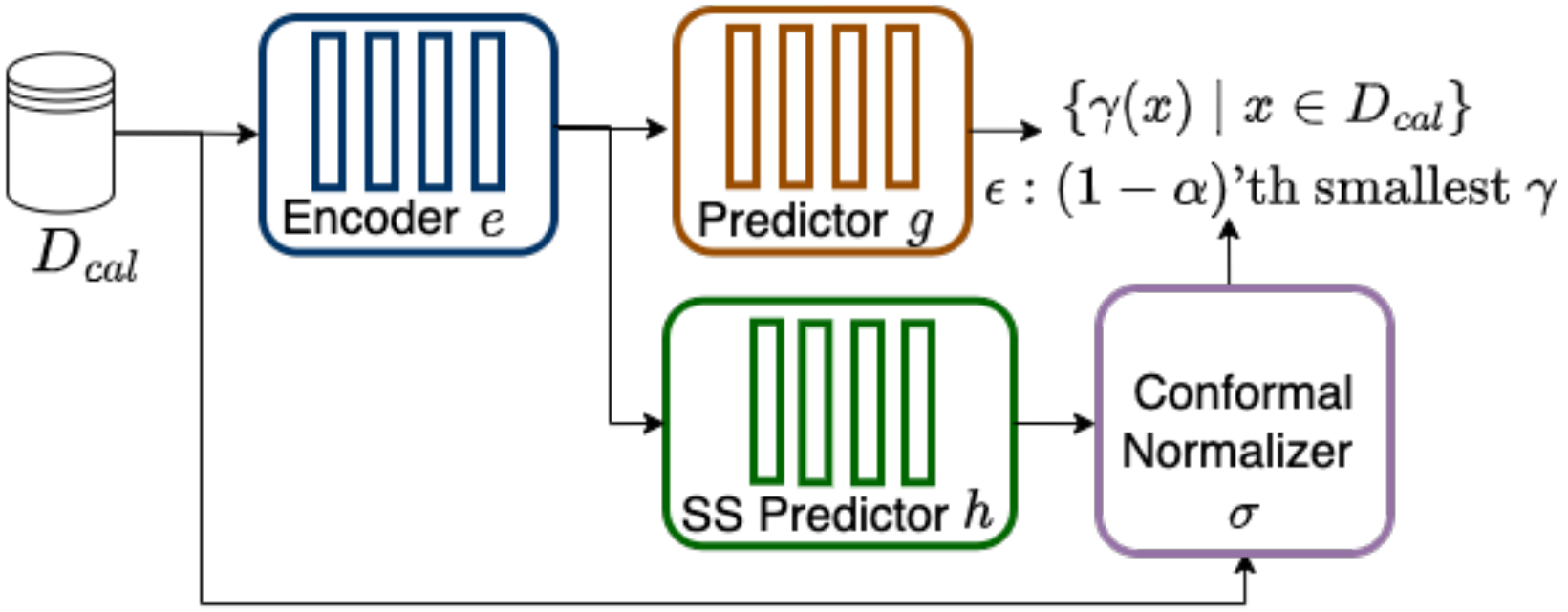
- Augment with self-supervised input x



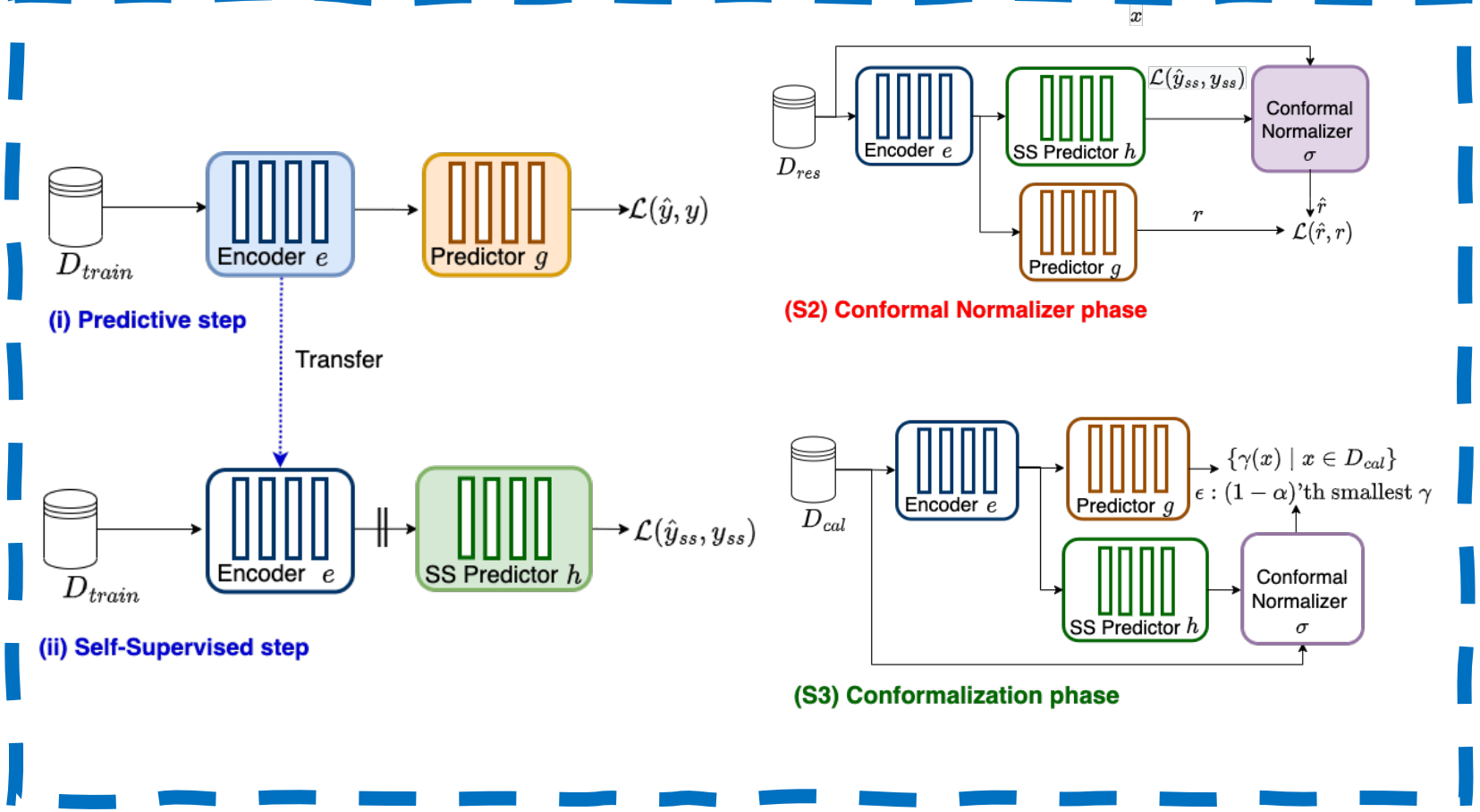
(S2) Conformal Normalizer phase

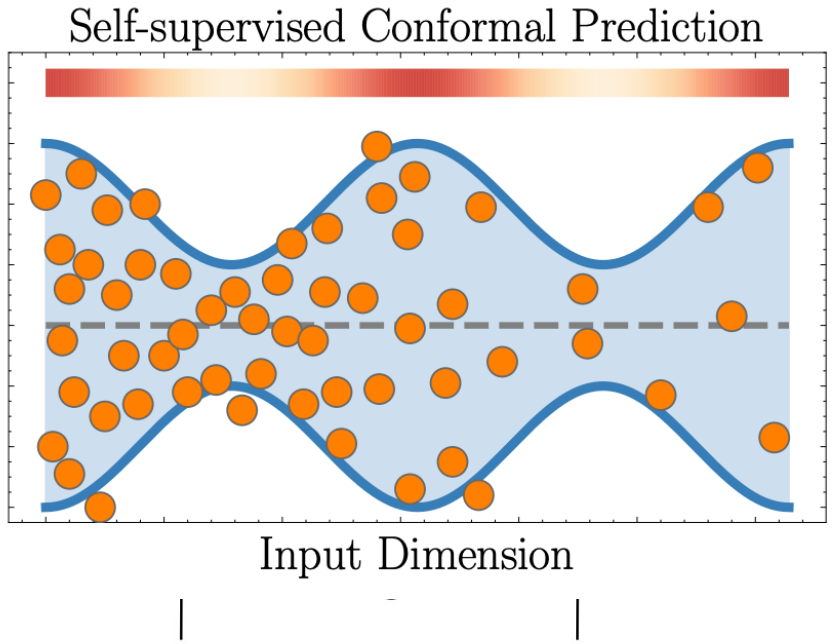
SSCP: Conformalization phase

- Conformalize using the calibration set



SSCP produces Adaptive Intervals

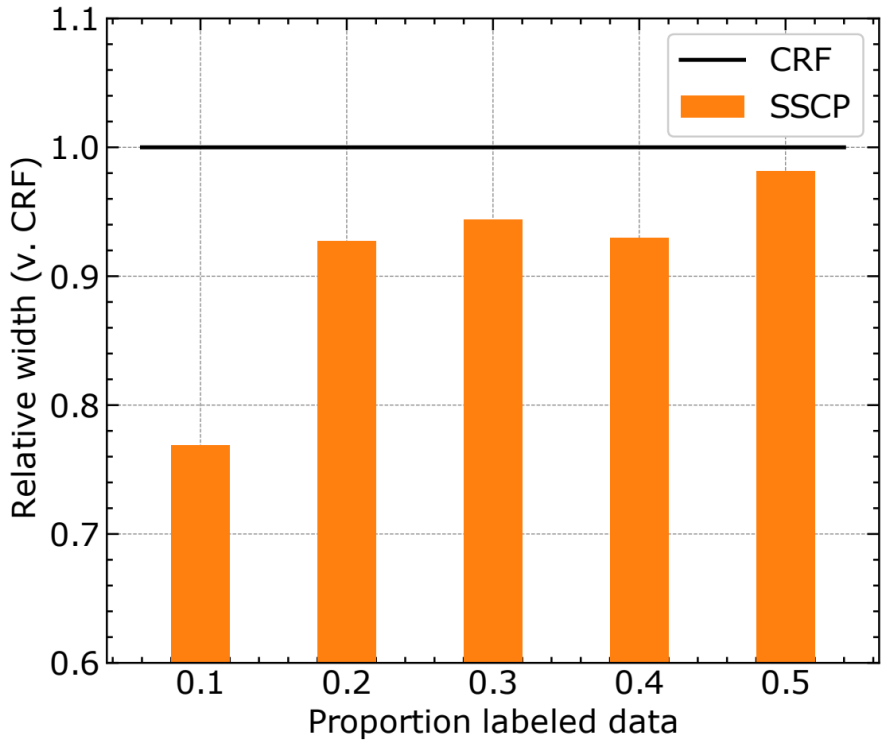




Adaptive conformal prediction intervals

SSCP produces more Adaptive Intervals

UNLABELED DATA*

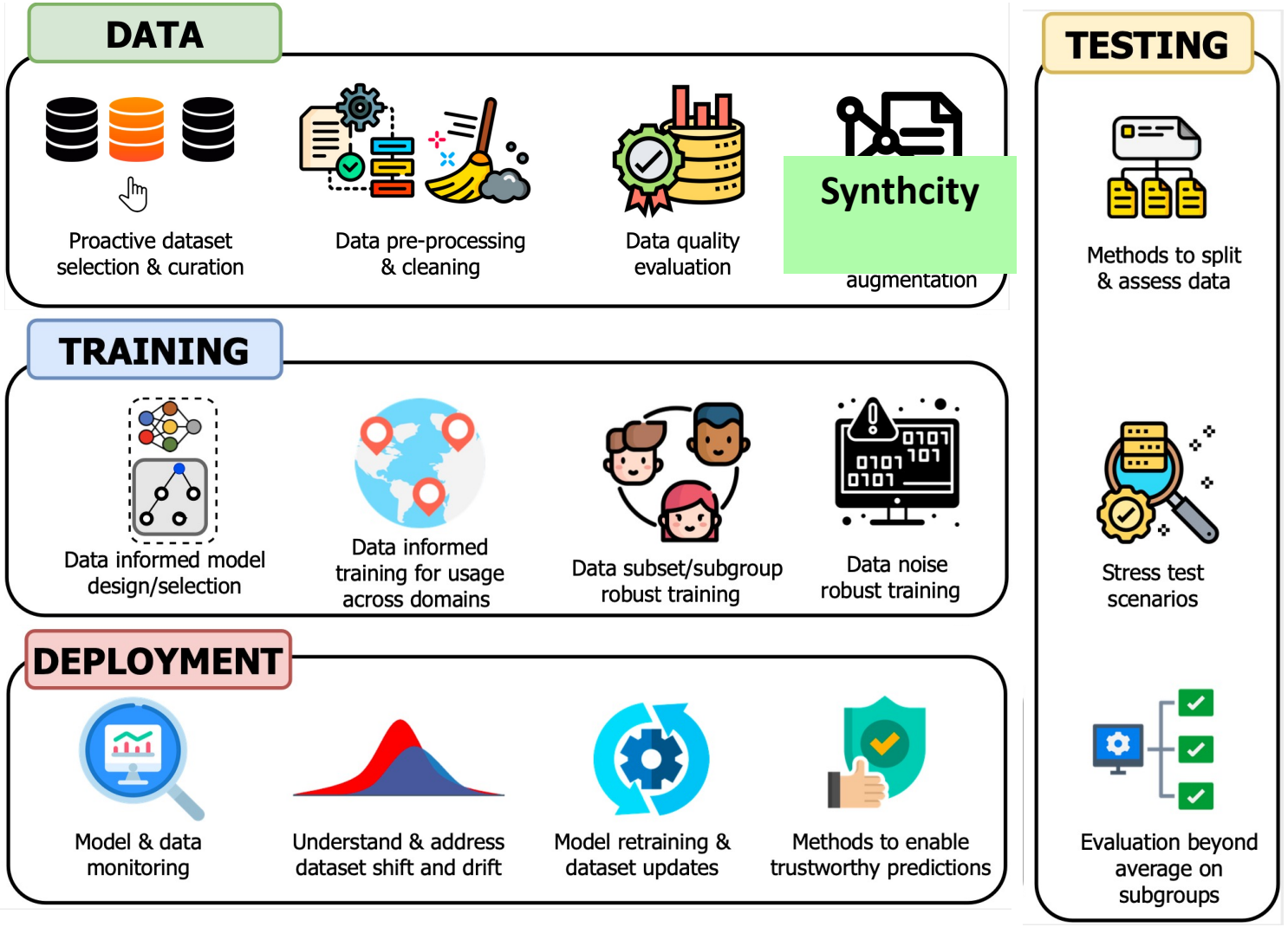


LABELED DATA*

Dataset	Metric	CRF	SSCP
concrete (n=1030)	Avg.Width	0.768	**0.743**
	Avg.Deficit	0.099	**0.098**
	Avg.Excess	0.263	**0.253**
community (n=1994)	Avg.Width	2.602	**2.462**
	Avg.Deficit	0.355	**0.361**
	Avg.Excess	1.030	**0.967**
star (n=2161)	Avg.Width	0.293	**0.263**
	Avg.Deficit	0.036	**0.031**
	Avg.Excess	0.120	**0.100**
bike (n=10886)	Avg.Width	0.720	**0.690**
	Avg.Deficit	0.164	**0.161**
	Avg.Excess	0.244	**0.232**
Blog data (n=52397)	Avg.Width	3.474	**3.360**
	Avg.Deficit	**3.084**	3.155
	Avg.Excess	1.292	**1.227**
Facebook (n=81311)	Avg.Width	1.917	**1.860**
	Avg.Deficit	**1.956**	1.998
	Avg.Excess	0.584	**0.554**

**** SSCP improves both Conformal Residual Fitting (CRF) & Conformalized Quantile Regression (CQR)***

Construct Reality-Centric ML pipelines



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DC-Check provides online & offline tools to actionably engage with data-centric considerations in ML development

Why is my data not good enough?

Relevancy – is my data fit for purpose?

- Dataset does not contain all relevant variables
- Dataset does not faithfully represent the population of interest
- Historical data may not be future-proof

Quality – how accurate is my data?

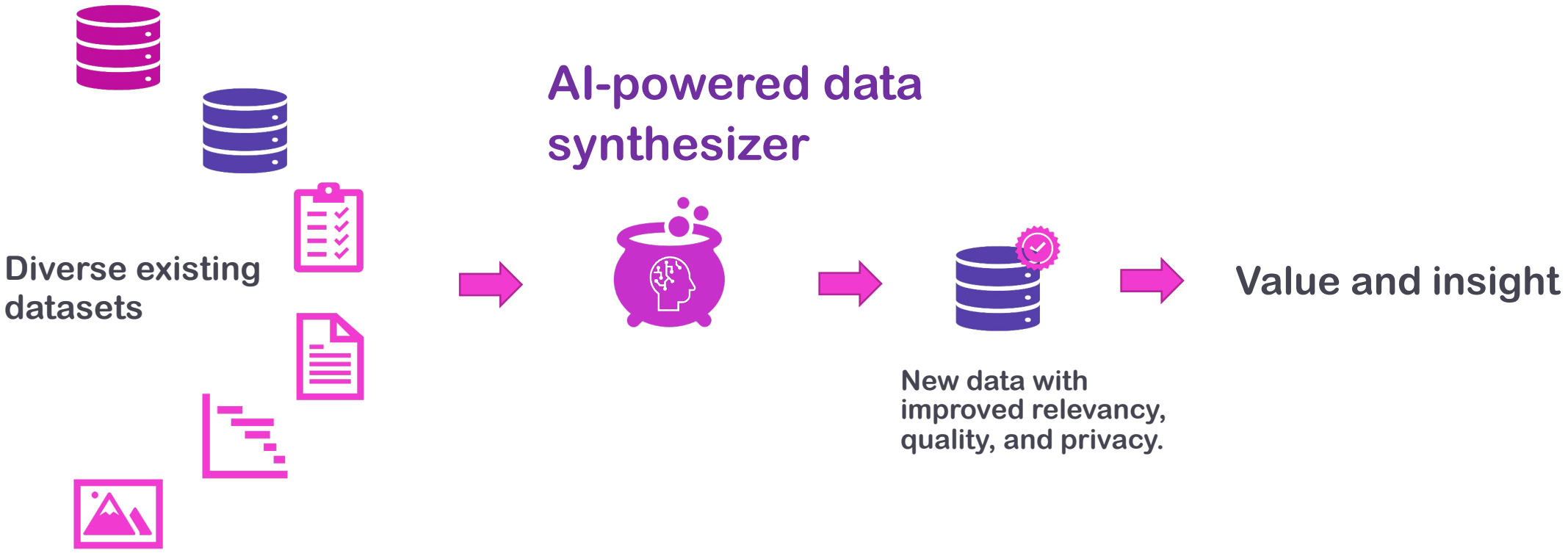
- Measurement, recording, and linking errors
- Missing values (not at random)
- Bias (unfair data)

Privacy – can I easily access or share the data?

- Personal identifiable and sensitive information

Data synthesis promises to bridge the data gap

Turns the data you have into the data you need!



Synthetic Data: Introduced the idea in 2017

Synthetic data tutorial – ICML 2021

"Synthetic Healthcare Data Generation and Assessment: Challenges, Methods, and Impact on Machine Learning"

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→ Tutorials
→ ICML 2021 tutorial: Synthetic healthcare data generation and assessment

Synthetic data tutorial – AAAI 2023

"Innovative Uses of Synthetic Data Tutorial"

Synthetic data fixes the issues with real data

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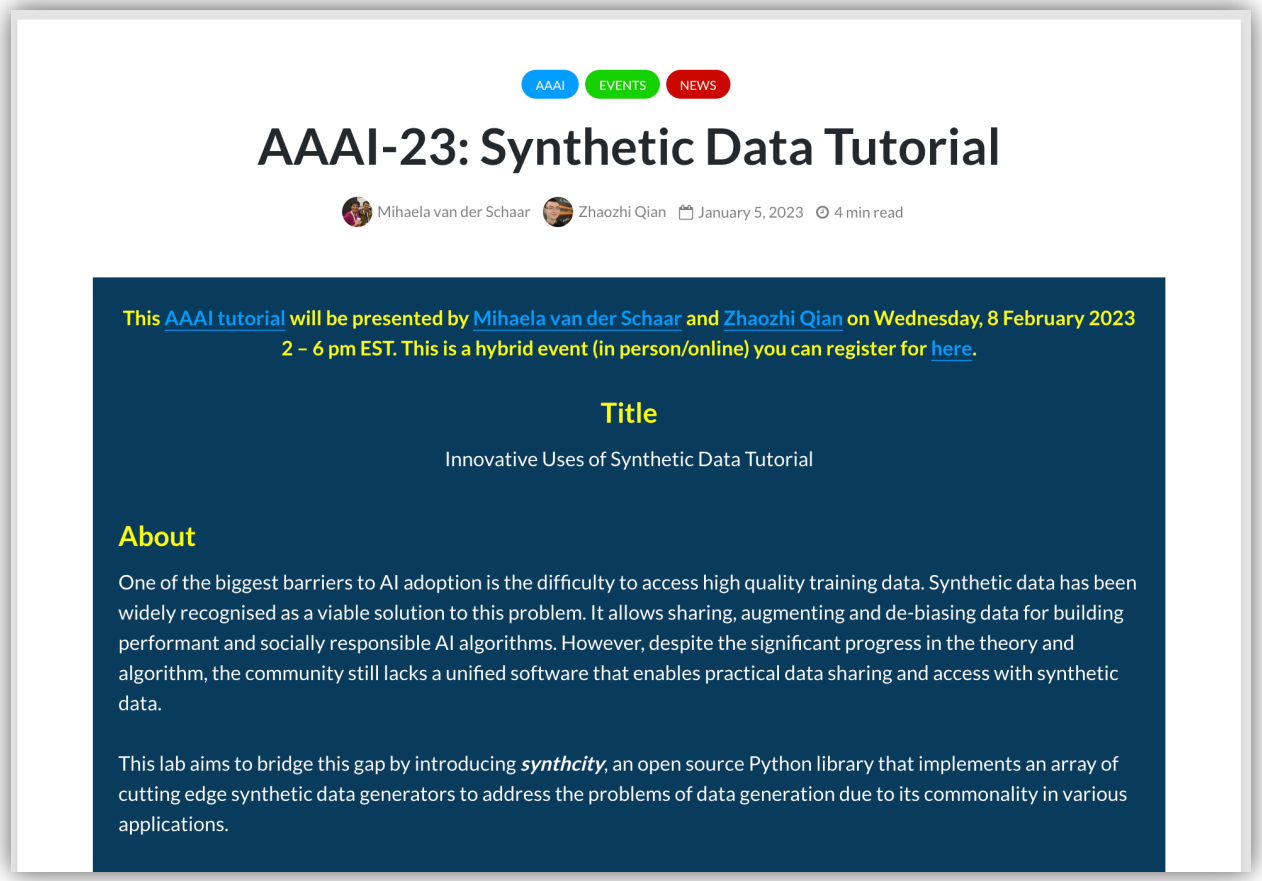
→ AAAI-23: Synthetic Data Tutorial



AAAI EVENTS NEWS

AAAI-23: Synthetic Data Tutorial

Mihaela van der Schaar Zhaozhi Qian January 5, 2023 4 min read

This AAAI tutorial will be presented by Mihaela van der Schaar and Zhaozhi Qian on Wednesday, 8 February 2023 2 – 6 pm EST. This is a hybrid event (in person/online) you can register for here.

Title

Innovative Uses of Synthetic Data Tutorial

About

One of the biggest barriers to AI adoption is the difficulty to access high quality training data. Synthetic data has been widely recognised as a viable solution to this problem. It allows sharing, augmenting and de-biasing data for building performant and socially responsible AI algorithms. However, despite the significant progress in the theory and algorithm, the community still lacks a unified software that enables practical data sharing and access with synthetic data.

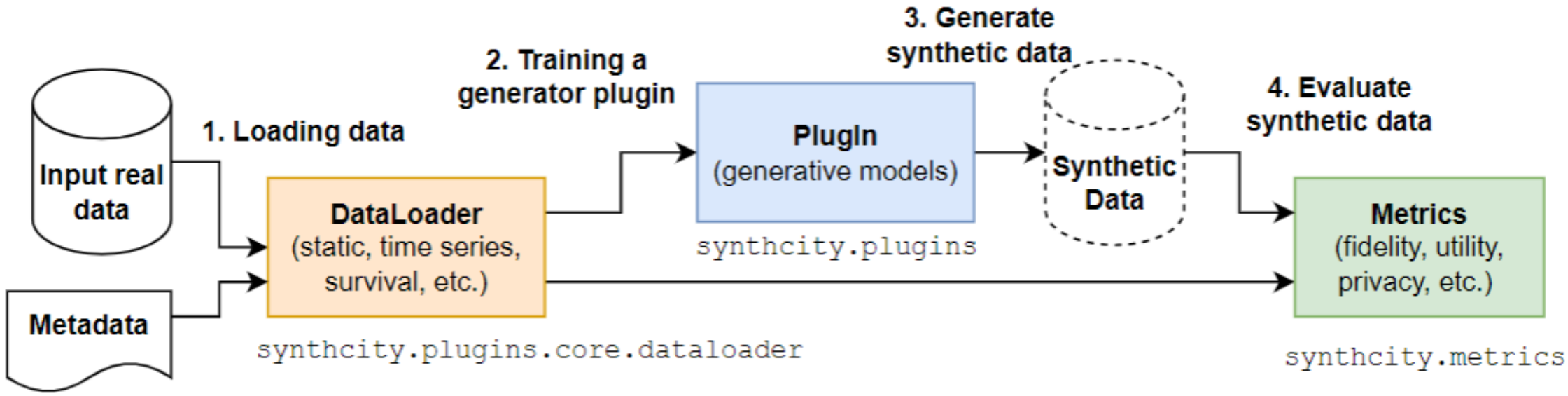
This lab aims to bridge this gap by introducing ***synthcity***, an open source Python library that implements an array of cutting edge synthetic data generators to address the problems of data generation due to its commonality in various applications.

Synthetic data fixes the issues with real data

Synthetic data is a unified way to address various issues with real data

Contains preexisting bias	→	Creating debiased synthetic data
Small sample size	→	Augmenting with synthetic data
Collected from different domains	→	Transfer and domain adaptation with synthetic data
Future-proof	→	Forward looking data and future scenarios

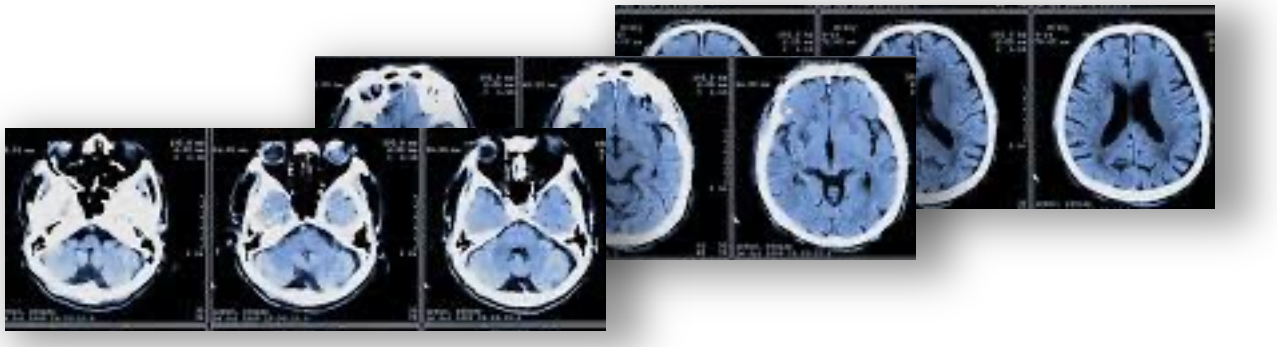
Synthcity:
the most comprehensive open-source synthetic data generation and evaluation library – focused on tabular data



https://www.vanderschaar-lab.com/synthcity-and-using-synthetic-data/

Synthcity: Contains metrics for measuring the quality of generative models/synthetic data?

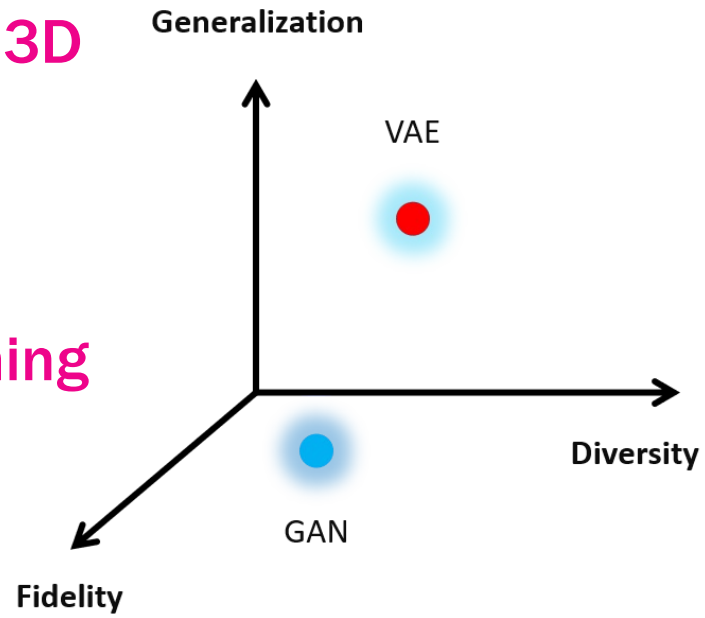
- **We have followed the recipe and generated the desired synthetic data…**



- **How do we know if the synthetic data is of a high quality? What does "quality" mean?**
  - Inspect individual samples? We may have generated millions!
  - Train on synthetic, test on real? Does not tell us the full picture…
- **What makes a good synthetic dataset? How do we define "quality"?**

Different ways in which a generative model may fail

- A single-dimensional metric is not enough…
- Every model's performance can be viewed as a point in a 3D space
  - **Fidelity:** How "good" the synthetic samples are?
  - **Diversity:** How much of the real data is covered?
  - **Generalization:** How often does the model copy training data?
- **Need probabilistic, interpretable, multi-dimensional quantities**



A. Alaa, B. van Breugel, E. Saveliev, vdS,
How Faithful is your Synthetic Data? Sample-level Metrics for Evaluating and Auditing Generative Models, ICML 2022, (in archive since 2021)

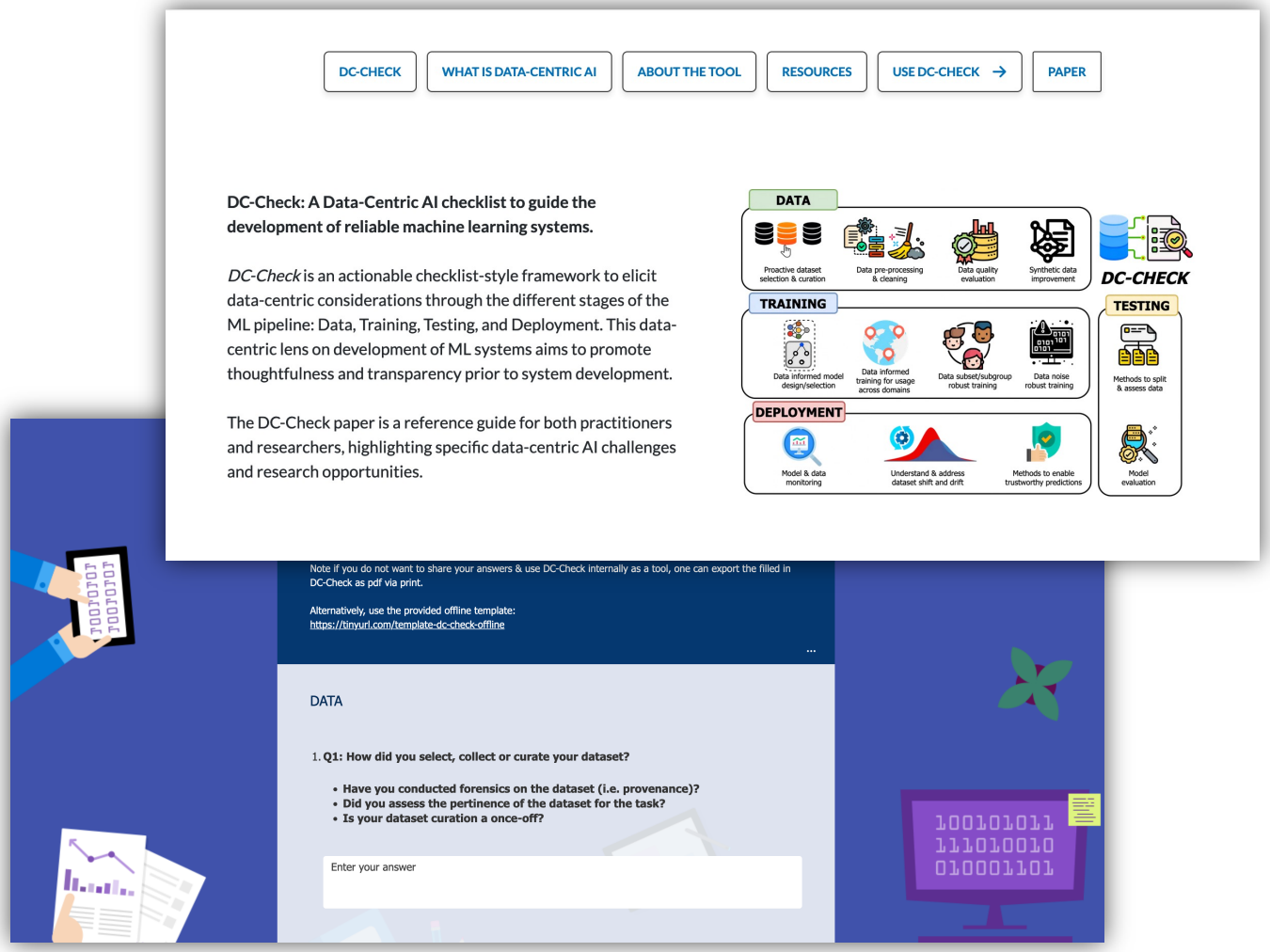
Reality-centric AI – Use of Real-world Data

- messy, biased, noisy, erroneous
- costly to acquire
- limited
- incomplete
- changes over time

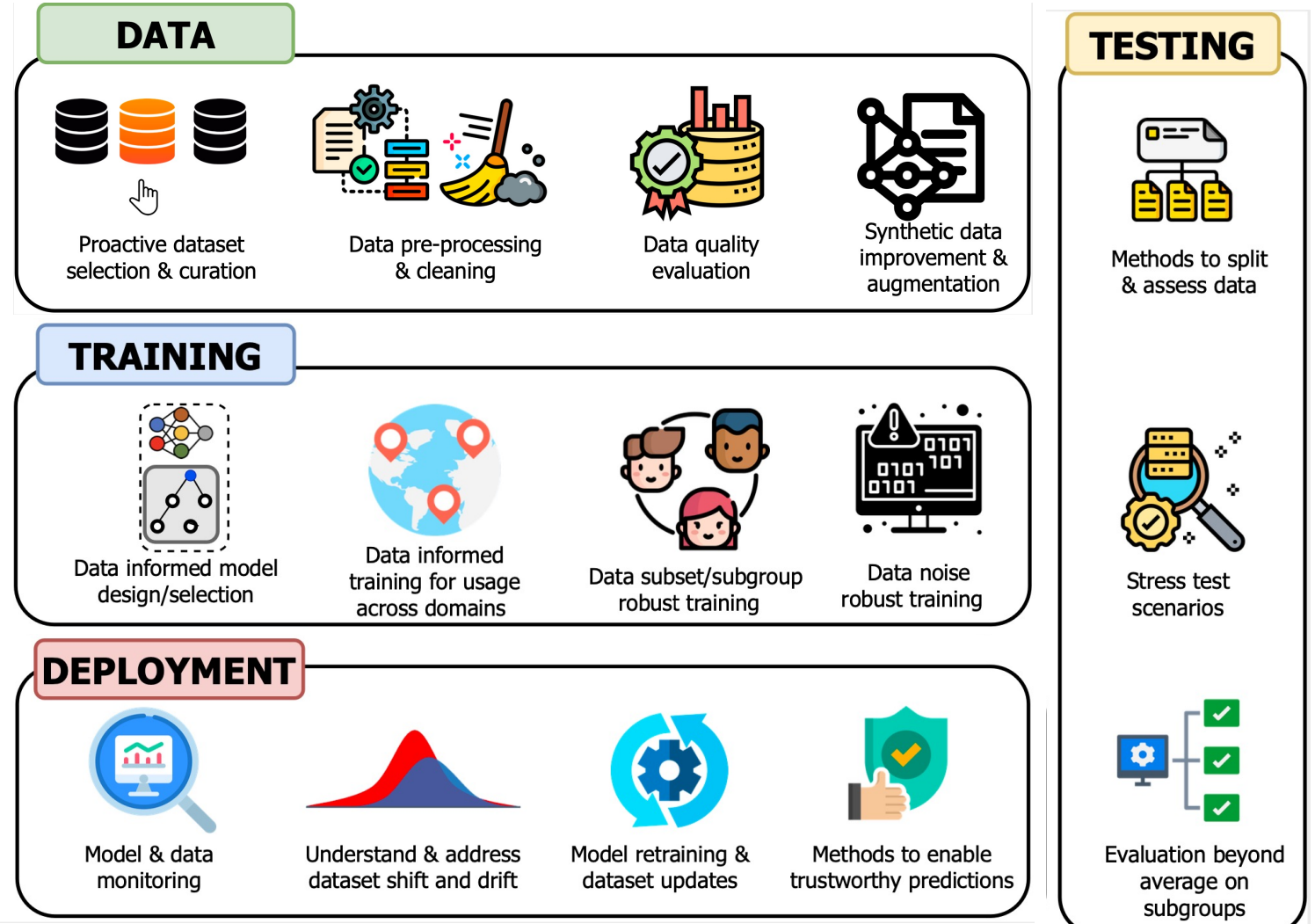
Construct Reality-Centric ML pipelines with Real-world data

Data-Centric AI: Resources

vanderschaar-lab.com/
→ data-centric-ai



Construct Reality-Centric ML pipelines



DC-Check: “Making ML work” to “Making ML real”

Find out more & engage with DC-Check resources @
https://www.vanderschaar-lab.com/dc-check

An actionable & standardized process to design data-centric AI

For BOTH researchers & practitioners

A recommendation tool for enabling transparency & accountability

Join us in doing Reality-Centric AI!

- **Reality-centric AI aims to reorientate AI towards the complexities of the real world**

https://www.vanderschaar-lab.com/the-case-for-reality-centric-ai/