# On the Democratization of AI:

## Bridging the Gap with AutoML


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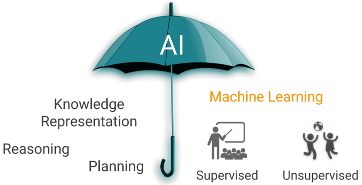
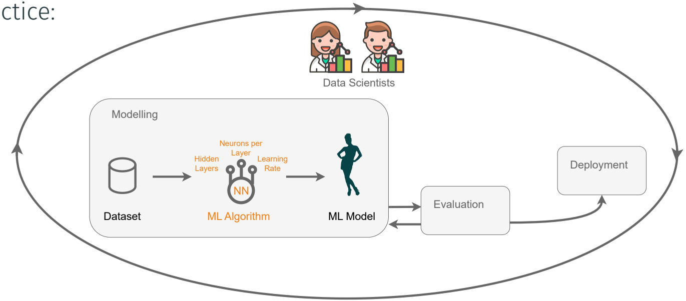
# What Do We Mean By AI?

Machine Learning[1]

A **computer program** is said to learn in some class of **tasks**, with respect to a **performance measure**, if it improves with **experience**.




In practice:

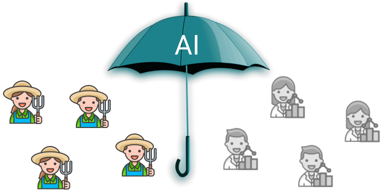



[1] Mitchell, T. M. 1997. Machine Learning.

# Bridging the Gap with AutoML

## Democratization of AI[2]

Making AI **accessible to a broader audience**, allowing domain experts to apply it in their own fields.

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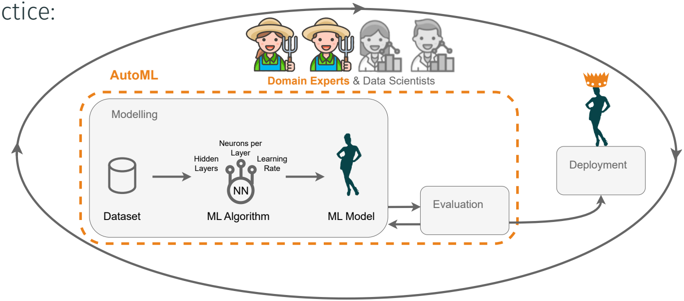
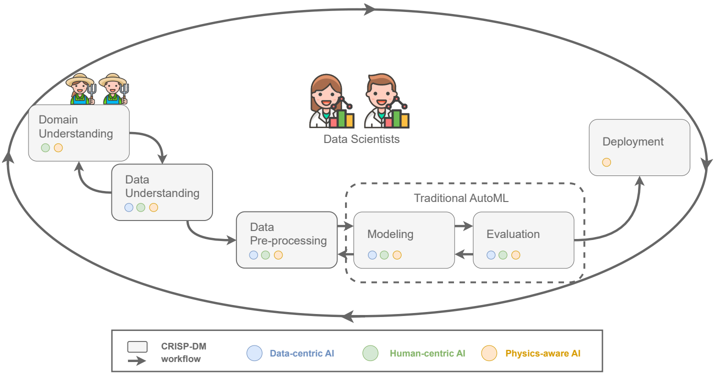



[2] Thornton, C. et al. 2013. Auto-WEKA: Combined selection and hyperparameter optimization of classification algorithms. In Proceedings of ACM SIGKDD.

**Cross-Industry Standard Process for Data Mining (CRISP-DM)**
is a process model for dealing with problem complexity.




## Data-centric AI

systematically engineers data used to build an AI system.

# Real-case problem scenarios

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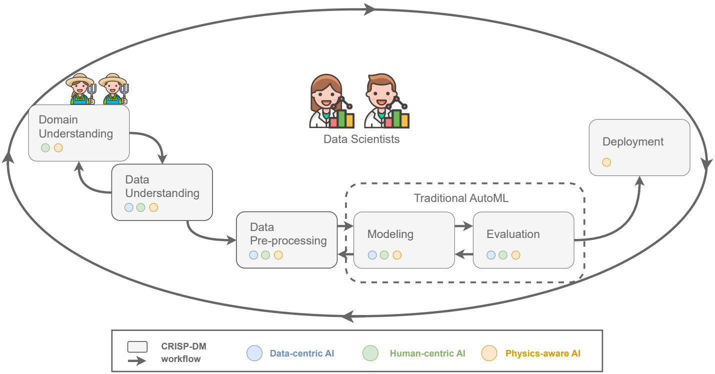


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aims at complementing, instead of replacing, human intelligence.

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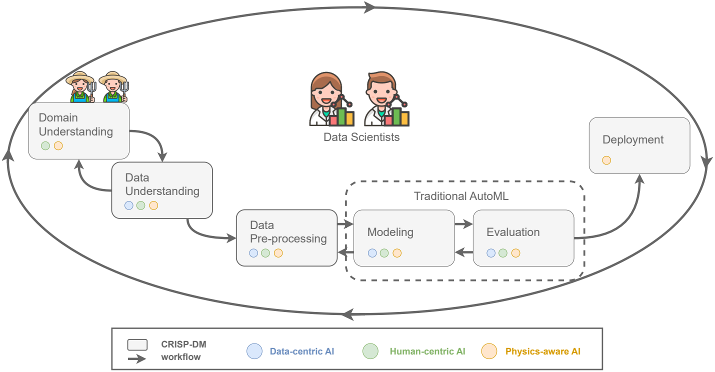


## Physics-aware AI

focuses on coupling and enhancing physical simulators with AI.

# Contribution Overview

## Data-centric AI

1. Effective Data Pre-processing Pipelines in Supervised Learning

$$\mathcal{D} = \{(x_i, y_i)\}_{i=0}^{N} \in \mathbb{D} \subset \mathcal{X} \times \mathcal{Y}$$

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3. Human-centric AutoML via Logic and Argumentat.

$$\boldsymbol{\lambda}^{\star} \in argmin_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \mathcal{L}(A_{\boldsymbol{\lambda}}(\mathcal{D}_{train}), \mathcal{D}_{val})$$

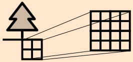
4. Interactive HPO via Preference Learning

$$\mathcal{L}_1, \ldots, \mathcal{L}_m$$

5. AutoML in the Age of the Large Language Models

## Physics-aware AI

6. Multi-sensor Profiling for Soil-Moisture Monitoring



7. Enhancing Process-Based Models for Soil Moisture Forecasting

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**1. Effective Data Pre-processing Pipelines in Supervised Learning [3,4]**

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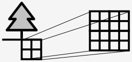

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[3] Giovanelli J., Bilalli B., and Abelló A. (2022). Data pre-processing pipeline generation for AutoETL. Information Systems 108 (2022): 101957..

[4] Giovanelli J., Bilalli B., and Abelló A., et al. (2023). Reproducible experiments for generating pre-processing pipelines for AutoETL. Information Systems (2023): 102314.

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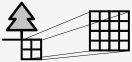

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[5] Francia M., Giovanelli J., and Golfarelli M. (2024). **AutoClues: Exploring Clustering Pipelines via AutoML and Diversification**. In Proceedings of Pacific-Asia Conference on Knowledge Discovery and Data Mining (PAKDD). Springer Nature Singapore.

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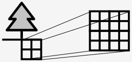

7. Enhancing Process-Based Models for Soil Moisture Forecasting

[6] Francia M., Giovanelli J., and Pisano G. (2022). **HAMLET: A framework for Human-centered AutoML via Structured Argumentation**. Future Generation Computer Systems 142 (2023): 182-194.

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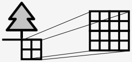

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[7] Giovanelli J., Tornede A., Tornede T., and Lindauer M. (2024). **Interactive hyperparameter optimization in multi-objective problems via preference learning**. In Proceedings of the AAAI Conference on Artificial Intelligence. Vol. 38. No. 11. 2024.

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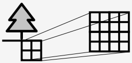

7. Enhancing Process-Based Models for Soil Moisture Forecasting

[8] Tornede A., Difan D., Giovanelli J., Mohan A., Ruhkopf T., Segel S., Theodorakopoulos D., Tornede T., Wachsmuth H., and Lindauer M. (2024). Automl in the age of large language models: Current challenges, future opportunities and risks. Transaction on Machine Learning Research. ISSN 2835-8856 2024.

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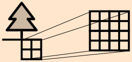

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[9] Francia M., Giovanelli J., and Golfarelli M. (2022). Multi-sensor profiling for precision soil-moisture monitoring. Computers and Electronics in Agriculture. 197 (2022): 106924.

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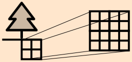

7. **Enhancing Process-Based Models for Soil Moisture Forecasting** [10]

[10] Bitelli M., Francia M., Giovanelli J., Golfarelli M., and Tomei F. **An Auto-Tuning Three-Dimensional Numerical Model Coupled with Data Assimilation from a Sensor Grid to Forecast Irrigation Demand in Kiwifruit**. Submitted to Computers and Electronics in Agriculture.

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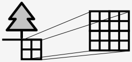

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# Interactive Hyperparameter Optimization via Preference Learning in Multi-Objective Problems

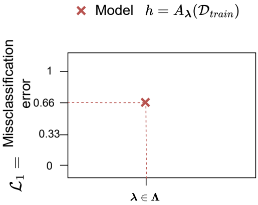
HPO Problem. Given a machine learning (ML) algorithm $A$ and corresponding hyperparameter space of $\boldsymbol{\Lambda} = \Lambda_1 \times \cdots \times \Lambda_M$, the goal is to determine the configuration $\boldsymbol{\lambda}^\star \in \boldsymbol{\Lambda}$ with optimal loss function $\mathcal{L}$.

$$\boldsymbol{\lambda}^\star \in \operatorname*{arg\,min}_{\boldsymbol{\lambda} \in \boldsymbol{\Lambda}} \mathcal{L}(A_{\boldsymbol{\lambda}}(\mathcal{D}_{train}), \mathcal{D}_{val})$$

$\mathcal{L}$ quantifies how well the trained model $h = A_{\boldsymbol{\lambda}}(\mathcal{D}_{train})$ performs a disjoint split $\mathcal{D}_{val}$.

**Example** NN hyperparameter conf.

$$\boldsymbol{\lambda} \in \boldsymbol{\Lambda} = \begin{array}{ll} \texttt{learning rate:} & 0.05 \\ \texttt{hidden layers:} & 5 \\ \texttt{neurons per layer:} & 256 \end{array}$$




SOTA. **Bayesian Optimization (BO)**[11] drives the exploration toward new **promising configurations** via a surrogate trained on past evaluations.

[11] Brochu E., Vlad M. Cora, et al. **A tutorial on Bayesian optimization of expensive cost functions, with application to active user modeling and hierarchical reinforcement learning.** (2010).

# Hyperparameter Optimization (HPO)

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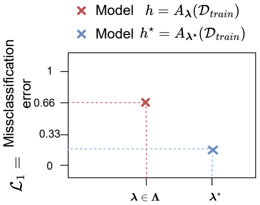
**Example** Best NN hyperparameter conf.

| | | |
|---|---|---|
| $\boldsymbol{\lambda}^\star \in \boldsymbol{\Lambda} =$ | `learning rate:` | 0.01 |
| | `hidden layers:` | 10 |
| | `neurons per layer:` | 256 |

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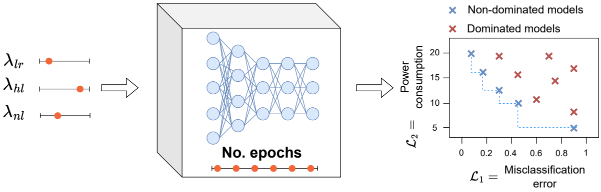
# Multi-Objective Machine Learning (MO-ML)

MO-ML algorithms. When optimizing multiple objectives $\mathcal{L}_1, \ldots, \mathcal{L}_M$, MO-ML algorithms $A_{\boldsymbol{\lambda}}(\mathcal{D}_{train})$ return a **Pareto front** $P_{\mathcal{D}_{val}}(\mathcal{H})$.



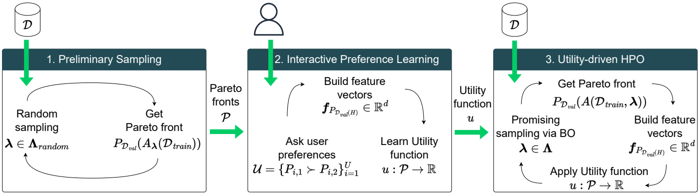

Quality Indicators. quantify the goodness of the Pareto front by measuring specific characteristics —**e.g., hypervolume (HV)**[13]**, maximum spread (MS)**[13]**, spacing (SP)**[14]**, closeness to reference point (R2)**[15].

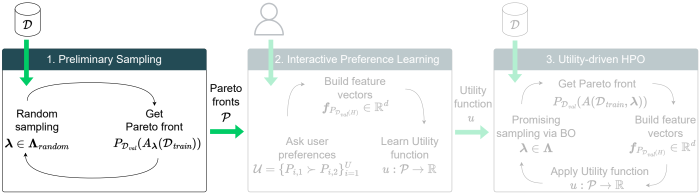
[13] Zitler E., Thiele L. **Multiobjective evolutionary algorithms: a comparative case study and the strength Pareto approach.** IEEE transactions on Evolutionary Computation, 1999.
[14] Schott J. R. **Fault tolerant design using single and multicriteria genetic algorithm optimization.** 1995. PhD Thesis. Massachusetts Institute of Technology.
[15] Hansen M. P., Jaszkiewicz A. **Evaluating the quality of approximations to the non-dominated set.** Copenhagen, Denmark: IMM, Technical University of Denmark, 1994.

Challenge. Choosing the **quality indicator** leading to a Pareto front which has a **desired shape** requires deep expert knowledge.

Approach. Learning a quality indicator via user preferences

1. **Preliminary Sampling**
   Collect Paretos $\mathcal{P} = \{P_i | P_i = P_{\mathcal{D}_{val}}(A_{\boldsymbol{\lambda}}(\mathcal{D}_{train})) : \boldsymbol{\lambda} \in \boldsymbol{\Lambda}\}$
2. **Interactive Preference Learning**
   a. Build preference dataset $\mathcal{U} = \{P_{i,1} \succ P_{i,2}\}_{i=1}^{U}$
   b. Learn utility function $u : \mathcal{P} \to \mathbb{R}$
3. **Utility-driven HPO**
   Solve HPO problem $\boldsymbol{\lambda}^{\star} \in \arg\min u(P_{\boldsymbol{\lambda}}) : P_{\boldsymbol{\lambda}} = A_{\boldsymbol{\lambda}}(\mathcal{D}_{val})$



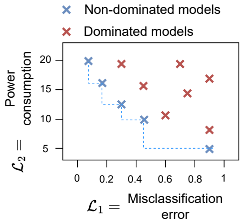



Example $\boldsymbol{\lambda}_1 \in \boldsymbol{\Lambda}$

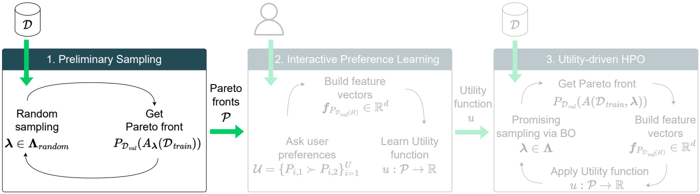
NN hyperparameter configuration:

| | |
|---|---|
| *learning rate:* | 0.01 |
| *hidden layers:* | 10 |
| *neurons per layer:* | 256 |

Example $P_{\mathcal{D}_{val}}(A_{\boldsymbol{\lambda}}(\mathcal{D}_{train}))$



# 1. Preliminary Sampling

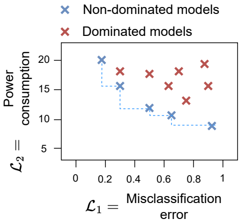



Example $\boldsymbol{\lambda}_2 \in \boldsymbol{\Lambda}$

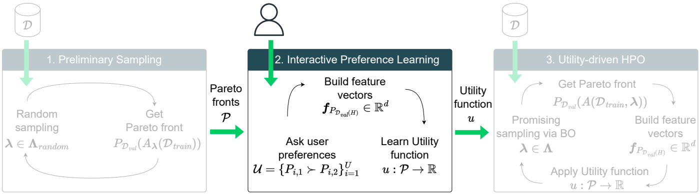
NN hyperparameter configuration:

| | |
|---|---|
| *learning rate:* | 0.05 |
| *hidden layers:* | 5 |
| *neurons per layer:* | 256 |

Example $P_{\mathcal{D}_{val}}(A_{\boldsymbol{\lambda}}(\mathcal{D}_{train}))$

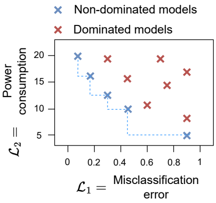


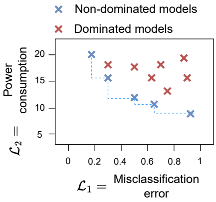
# 2. Interactive Preference Learning – Pairwise Preferences

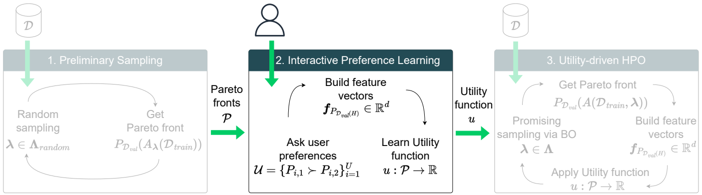



Example $\mathcal{U} = \{P_{i,1} \succ P_{i,2}\}_{i=1}^U$

$P_{i,1}$ $\succ$ $P_{i,2}$

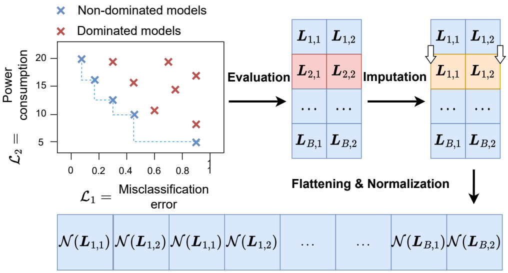


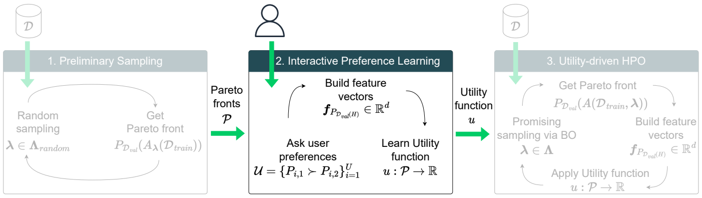






## Example

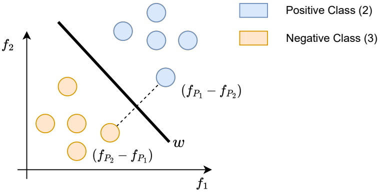
$f_{P_{\mathcal{D}_{val}(H)}} \in \mathbb{R}^d$



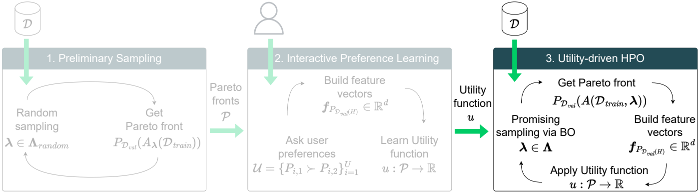



## **Example** Building $u : \mathcal{P} \to \mathbb{R}$ through RankSVM[16]

$$
\begin{aligned}
P_1 \succ P_2 &\Leftrightarrow \vec{w}^\intercal \vec{f}_{P_1} > \vec{w}^\intercal \vec{f}_{P_2} && (1)\\
&\Leftrightarrow \vec{w}^\intercal \left(\vec{f}_{P_1} - \vec{f}_{P_2}\right) > 0 && (2)\\
&\Leftrightarrow \vec{w}^\intercal \left(\vec{f}_{P_2} - \vec{f}_{P_1}\right) < 0\,. && (3)
\end{aligned}
$$




[16] Joachims T. **Optimizing search engines using clickthrough data.** Proceedings of the eighth ACM SIGKDD international conference on Knowledge discovery and data mining. (2002).

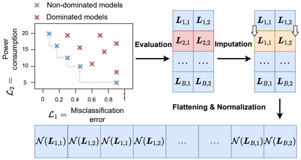



**Example.**
Promising sampling
$\boldsymbol{\lambda} \in \boldsymbol{\Lambda}$ $\longrightarrow$

**Example.**
Get Pareto and build feature vector
$P_{\mathcal{D}_{val}}(A(\mathcal{D}_{train}, \boldsymbol{\lambda}))$ $\longrightarrow$ $f_{P_{\mathcal{D}_{val}}}$ $\longrightarrow$

**Example.**
Apply utility
$u(f_{P_{\mathcal{D}_{val}}})$

| | |
|---|---|
| *learning rate:* | 0.001 |
| *hidden layers:* | 5 |
| *neurons layer:* | 256 |




$w^T \cdot f_{P_{\mathcal{D}_{val}}}(H, \boldsymbol{\lambda})$

# Evaluation – End-to-end Performance

**Preference-Based** (PB): HPO process driven by the utility function trained with the indicator in the row

**Indicator-Based** (IB): HPO process driven by the indicator in the column

LCBench[17]:

- funnel-shaped **MLP** from **Auto-pytorch**;
- 35 datasets from **OpenML CC-18** suite.

| PB\IB | *HV* | *SP* | *MS* | *R2* |
|---|---|---|---|---|
| *HV* | 98.70% | 146.15% | 146.15% | 98.70% |
| *SP* | 300.00% | 100.00% | 400.00% | 400.00% |
| *MS* | 321.05% | 321.05% | 93.85% | 265.22% |
| *R2* | 95.65% | 204.35% | 195.65% | 95.65% |

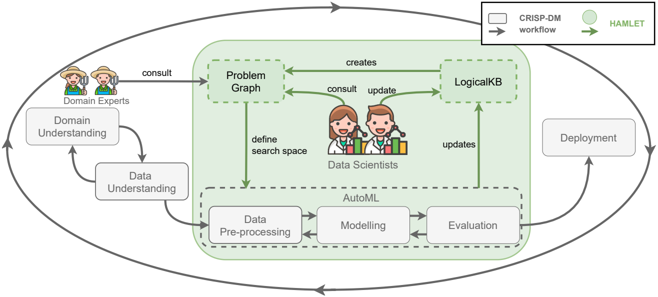
⟶ PB performs **better or equal** in 11/16 cases;

⟶ IB performs **slightly better** in only 5/16 cases.

[17] Zimmer L., Lindauer M, and Hutter F. **Auto-pytorch: Multi-fidelity metalearning for efficient and robust autodl.** IEEE transactions on pattern analysis and machine intelligence 43.9 (2021).

# Conclusions and Future Works

# Data-centric and Human-centric AI



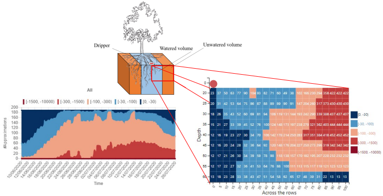

## Main Contributions

- Develop effective data pipelines for **supervised** and **unsupervised learning**.
- Propose a HAMLET: a human-centric AutoML framework allowing **explainability** and **interactive interventions**;

## Future Works

- Provide insight on data bias in pre-processing for **fairness** through HAMLET.
- Integrate HAMLET with **multi-objective** and **cross-cutting constraints** (e.g., ethical, legal) to allow fairness interventions.

# Physics-aware AI





## Main Contributions

- Integration of physical models with AI through AutoML for **monitoring** and **forecasting tasks**.
- During the whole campaign:
  Water saving: 44%
  Vine productivity: **unaffected**
  Fruit quality: **increased** (+1 brix)

## Future works:

- Integration of a smart-irrigation algorithm based on **control theory**, dynamically adjusting the water plan.
- Application of **transfer learning** with a pre-trained model to transfer the knowledge from different conditions, supporting a wider range of crops.

Thanks for the attention :)