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ML Overview in CMS, HEP, and beyond

Outline

- I. Machine Learning beyond classification
- II. Geometric Deep Learning
- III. Machine Learning in CMS
- IV. Prospects of Deep Learning

Machine Learning beyond classification

control, reconstruction, simulation, …

AI in HEP

LHC Computing Grid 200k cores pledge to CMS over ~100 sites

CMS Detector 1PB/s CMS L1 & High-Level Triggers 50k cores, 1kHz Large Hadron Collider 40 MHz of collision CERN Tier-0 Computing Center 20k cores CERN Tier-0/Tier-1 Tape Storage 200PB total AI AI AI AI AI Up to date listing of references:

Role of AI: accelerator control, data acquisition, event triggering, anomaly detection, new physics scouting, event reconstruction, event generation, detector simulation, LHC grid control, analytics, signal extraction, likelihood free inference, background rejection, new physics searches, ...

Producing the Data

Opportunities in Machine Learning for Particle Accelerators [\[1811.03172\]](https://arxiv.org/abs/1811.03172) Machine learning for design optimization of storage ring nonlinear dynamics [\[1910.14220\]](https://arxiv.org/abs/1910.14220) Advanced Control Methods for Particle Accelerators (ACM4PA) 2019 Workshop Report [\[2001.05461\]](https://arxiv.org/abs/2001.05461) Machine learning for beam dynamics studies at the CERN Large Hadron Collider [\[2009.08109\]](https://arxiv.org/abs/2009.08109)

• Machine learning can be used to tune devices, control beams, perform analysis on accelerator parameters, etc.

…

A. Scheinker, C. Emma, A.L. Edelen, S. Gessner [\[2001.05461\]](https://arxiv.org/abs/2001.05461)

-
- Already successfully deployed on accelerator facilities.
- More promising R&D to increase beam time.
- Potential for detector control ?

More of the relevant works at: <https://iml-wg.github.io/HEPML-LivingReview/>

Compressing Data

Deep Auto-Encoders for compression in HEP <http://lup.lub.lu.se/student-papers/record/9004751> Make use of abstract semantic space for image compression.

Image compression can suffer

compression of image with

- Rich literature on data neural network.
-
- some loss of resolution.
- Saving on disk/tape cost.
- R&D needed to reach the

Potential in scouting strategies.

necessary level of fidelity.

More of the relevant works at: <https://iml-wg.github.io/HEPML-LivingReview/>

Cleaning Data

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Towards automation of data quality system for CERN CMS experiment [\[doi:10.1088/1742-6596/898/9/092041\]](https://doi.org/10.1088/1742-6596/898/9/092041) LHCb data quality monitoring [doi:10.1088/1742-6596/898/9/09202 Detector monitoring with artificial neural networks at the CMS experiment at the CERN Large Hadron Collider [\[1808.00911\]](https://arxiv.org/abs/1808.00911) Anomaly detection using Deep Autoencoders for the assessment of the quality of the data acquired by the CMS experiment [\[doi:10.1051/](https://doi.org/10.1051/epjconf/201921406008) [epjconf/201921406008\]](https://doi.org/10.1051/epjconf/201921406008) …

• Data quality is a person power intensive task, and crucial for swift delivery of Physics

• Machine learning can help

• Learning from operators,

-
- with automation.
- reducing workload.
- Continued R&D and experiment adoption.

A.A. Pol, G. Cerminara, C. Germain, M. Pierini, A. Seth [\[doi:10.1007/s41781-018-0020-1\]](https://doi.org/10.1007/s41781-018-0020-1)

Managing Data

- success of the LHC experiments.
- Complex ecosystem with dedicated operation teams.
- Person power demanding, and inefficient in some corner of the phase space.
- Potential for AI-aided operation.
- Lots of modeling and control challenges.
- R&D to increase operation efficiency.

Caching suggestions using Reinforcement Learning [LOD 2020](https://lod2020.icas.xyz/program/), in proceedings

• The LHC-grid is key to

More of the relevant works at: <https://iml-wg.github.io/HEPML-LivingReview/>

Detecting New Data

- Machine learning since long selected signatures.
- Further potential for reduction.
- Emerging opportunity for triggering on unknown
- More promising R&D and

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signatures : "a la Hotline".

deployed in the trigger for

background trigger rate

Use of variational auto-encoders directly on data to marginalize experiment adoption. outlier events, for anomalous event hotline operation. [\[doi:0.1007/JHEP05\(2019\)036\]](https://doi.org/10.1007/JHEP05(2019)036)

More of the relevant works at: <https://iml-wg.github.io/HEPML-LivingReview/>

Data Triggering and Scouting

Phase-2 upgrade of the CMS L1-Trigger [\[cds:2714892\]](https://cds.cern.ch/record/2714892)

- Trigger benefit from fast reconstruction algorithms
- L1 needs FPGA implementation. hls4ml-enabled algorithms.
- Quality of selection increases with refinement of object reconstruction
- Having the best reconstruction is particularly important in scouting
- Balance between speed and accuracy

Reconstructing Data

• Learn from the simulation, and/

• Image base methods evolving towards graph-based methods.

- techniques can help.
- or data.
- Learn from existing "slow ground truth.
- new detector design.
-
-

reconstruction" or simulation

• Automatically adapt algorithm to

• Accelerating R&D to exploit full

<https://iml-wg.github.io/HEPML-LivingReview/>

Simulating Data

simulators already in operation.

Generative models can provide multiple 1000x speed-up.

• Applicable at many levels : sampling, generator, detector model, analysis variable, etc

- computing intensive.
- Fast and approximate
-
-
- samples.
- starting.

• Careful study of statistical power of learned models over training

Many R&D, experiment adoption

More of the relevant works at: <https://iml-wg.github.io/HEPML-LivingReview/>

Generative Adversarial Networks for LHCb Fast Simulation [\[2003.09762\]](https://arxiv.org/abs/2003.09762)

Calibrating Data

• Energy regression is the most

obvious use case.

A deep neural network for simultaneous estimation of b jet energy and resolution [\[1912.06046\]](https://arxiv.org/abs/1912.06046) *More of the relevant works at:*

- Learning calibrating models from simulation and data.
- Parametrization of scale factors using neural networks.
- Reducing data/simulation dependency using domain adaptation.
- Continued R&D

<https://iml-wg.github.io/HEPML-LivingReview/>

Analyzing Data

infiltrated analysis for signal/bkg

- Machine learning has long classification.
- Increasing number of analysis with more complex DNN.
- Application to signal categorization, bkg modeling, kinematics reconstruction, decay product assignment, object identification, …
- Breadth of new model agnostic methods for NP searches.
- Continued R&D and experiment adoption initiated.

Use of masked autoregressive density estimator with normalizing flow as model-agnostic signal enhancement mechanism. [\[doi:10.1103/PhysRevD.101.075042\]](https://doi.org/10.1103/PhysRevD.101.075042)

More of the relevant works at: <https://iml-wg.github.io/HEPML-LivingReview/>

• Hypothesis testing is the core

Theory Behind the Data

• Intractable likelihood hinders solving the inverse problem.

• May involve probabilistic programming instrumentation

• Going beyond the standard approach using machine learning and additional information from the simulator.

- of HEP analysis.
-
-
-
- of HEP simulator.
- R&D to bring this in the experiment.

• More precise evaluation of the priors on theory's parameters.

More of the relevant works at: <https://iml-wg.github.io/HEPML-LivingReview/>

Graph Neural Network …

Geometric Deep Learning

Graph Representation

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Heterogenous data fits well in graph/set representation.

Graph Neural Networks for Particle Physics reconstruction [\[2007.13681\],](https://arxiv.org/abs/2007.13681) [\[2012.01249\]](https://arxiv.org/abs/2012.01249)

Multiple CMS ML Forum presentations on GNN applications [\[Sept 30, 2020\] ,](https://indico.cern.ch/event/952419/) [\[Oct 20,](https://indico.cern.ch/event/1051967/) [2021\]](https://indico.cern.ch/event/1051967/), [\[Nov 3, 2021\]](https://indico.cern.ch/event/1081541/) and reconstruction with ML [\[Feb 21, 2021\],](https://indico.cern.ch/event/1001993/) [\[Mar 10, 2021\].](https://indico.cern.ch/event/1001994/)

Forewords on Graph

A graph is composed of

- **Nodes** that can be represented as a vector.
- **Edges** that can be represented with the adjacency matrix.
- ➔ Flowing of information using matrix operations.
- ➔With machine learning on graphs, edges and nodes might acquire internal representations.

Graph Neural Networks Formalism

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Updated attributes

Updated attributes

Updated attributes

Lots of possibilities to operate on a graph. Most available architectures can be expressed with Φ and ρ.

> Readily software: https://github.com/deepmind/graph_nets https://github.com/rusty1s/pytorch_geometric …

Geometric Deep Learning (I)

Geometric Deep Learning (II)

 $\mathcal{T}^{(i)}$

 (b)

Jet tagging in the Lund plane, [\[2012.08526\]](https://arxiv.org/abs/2012.08526)

Geometric Deep Learning (III)

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Pileup mitigation using graph neural network and transformers

ECAL **superclustering** with machine learning

Geometric Deep Learning (IV)

E/G **energy regression** using dynamic reduction network, [\[2003.08013\]](https://arxiv.org/abs/2003.08013)

Geometric Deep Learning (V)

GCN-VAE_TriangularSNF **Best** $\vdash \Box$ GCN-VAE_PlanarFlow 2nd $3rd$ H GCN-VAE_OrthogonalSNF $4th$ ⊢∏∏ \Box 5th **GCN-VAE_IAF** \Box 6th ⊢∥ GCN-VAE_HouseholderSNF \Box 7th GCN-VAE_ConvFlow **GCN-VAE** 0.0 $0.5\,$ 1.010^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} 10^{-4} 10^{-3} 10^{-2} 10^{-1} 10^{0} AUC $\epsilon_S(\epsilon_B=10^{-3})$ $\epsilon_S(\epsilon_B=10^{-4})$ $\epsilon_S(\epsilon_B=10^{-2})$

Best models on all channels combined based on mean score

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Jet particle-based **simulation** with message passing GNN generative adversarial network, [\[2012.00173\]](https://arxiv.org/abs/2012.00173)

Anomalous jet detection using graph convolution network variational auto-encoder with normalizing flow in the latent space, [\[2110.08508\]](https://arxiv.org/abs/2110.08508)

GAN ARCHITECTURE Nodes in the graph learn via 'message passing' between their neighbours: $\mathbf{m}_{\nu}^{t+1} = \sum_{w \in \mathcal{N}_{\nu}} f_e^{t+1}(\mathbf{h}_{\nu}^t, \mathbf{h}_{w}^t, \mathbf{e}_{\nu w}^t)$ Generator ${\bf h}_v^{t+1} = f_n^{t+1}({\bf h}_v^t, {\bf m}_v^{t+1})$ \bigoplus Discriminator Aggregate θ FCN θ or Fale $0\frac{1}{0.0}$

a selected pick of recent results …

ML in CMS

di-photon Mass Regression

Learn the a/di-photon mass from the energy deposition at the Ecal surface. Unprecedented reach at low mass.

Ecal Regression

- [\[cds:2803235\]](https://cds.cern.ch/record/2803235)
- Graph-based model with self-attention trained to : ✓seed-cluster classification ✓super-cluster classification ✓super-cluster energy regression
- Promising work in progress for calorimeter reconstruction

Super-resolution Simulation

- Run GEANT4 with loose parameters as low-quality input
- Learn the full precision high-quality output with CNN
- Model able to "denoise" and approach full precision

- Combines jet features and particle-image features
- CNN model to classify hadronic tau
- Much reduced fake rate
- More hadronic taus in analysis

Hadronic Tau Identification

Vector-Like Lepton Pair Search

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- At least 3b jets and two third generation leptons in final state
- DeepTau [\[cds:2800114\]](https://cds.cern.ch/record/2800114) method used for tau identification.
- Attention-based graph model 2001.05311 working on final state objects acts as classifier used for signal categorization.
- State of the art deep-learning in state of the art NP search

Uses built-in dense matrix, reshape and scatter/gather operations in TF. Requires batch-mode graphs. No N² allocation or computation needed.

Particle-Flow Reconstruction

30000

Particle Reconstruction at HL-LHC

- High-Granularity Calorimeter (HGCAL) provides fine-grained description of energy deposition
- Graph-based models [\[2106.01832\]](https://arxiv.org/abs/2106.01832) using object condensation loss [\[2002.03605\]](https://arxiv.org/abs/2002.03605) trained to perform cell-to-particle association
- Stepping stone towards ML-based particle reconstruction in HGCAL

Vertexing at L1 at HL-LHC

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[\[cds:2801638\]](https://cds.cern.ch/record/2801638)

- Tracks reconstructed at L1 used in input
- Model regress position of primary vertex and track-PV assignment
- Quantized/pruned model can efficiently deploy on FPGA

a few words of wisdom …

Prospects for Deep Learning

Interpretability

Interplay between deep learning and science is key. Use Physics knowledge to produce better models. Use models to learn Physics knowledge.

Propagation and estimation of uncertainties are keys. Uncertainty-aware models. Uncertainty-predicting models. Uncertainty-improving models.

Uncertainty Quantification

Computational cost of Science is key. Adapt to heterogenous computing environment. Hardware-aware model optimization.

Computation Aspect

Publication Plans

Publishing in peer-reviewed journal is key. Importance of open-data samples. Flexibility in experiments to publish work in progress.

Summary

- ➡Modern machine learning a.k.a Deep Learning goes much beyond classification.
- ➡GDL is most promising for many applications.
- ➡Novel Deep Learning are being adopted in CMS. Many more upcoming results.
- ➡The future of AI4HEP is interpretable, quantifiable, runnable and publishable …

A Definition

"Giving computers the ability to learn without explicitly programming them" A. Samuel (1959).

Is fitting a straight line machine learning ? Models that have enough capacity to define its own internal representation of the data to accomplish a task : **learning from data.**

In practice : a statistical method that can extract information from the data, not obviously apparent to an observer.

➔ Most approach will involve a **mathematical model** and a cost/ reward function that needs to be **optimized.**

➔ The more **domain knowledge** is incorporated, the better.

Supervised Learning

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- Given a dataset of samples, a subset of features is qualified as **target**, and the rest as **input**
- Find a **mapping from input to target**
- \cdot The mapping should generalize to any extension of the given dataset, provided it is generated from the same mechanism

- Finite set of target values : ➔ **Classification**
- Target is a continuous variable :
	- ➔ **Regression**

$$
dataset = \{(x_i, y_i)\}.
$$

find function f s.t. $f(x_i) = y_i$

Unsupervised Learning

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- \cdot Given a dataset of samples, but there is no subset of feature that one would like to predict
- Find mapping of the samples to a lower dimension manifold
- \cdot The mapping should generalize to any extension of the given dataset, provided it is generated from the same mechanism

- \cdot Manifold is a finite set ➔ **Clusterization**
- Manifold is a lower dimension manifold :
	- ➔ **Dimensionality reduction, density estimator**

$$
dataset \equiv \{ (x_i) \}
$$

find f s.t. $f (x_i) = p_i$

Reinforcement Learning

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- Given an *environment* with multiple states, given a reward upon action being taken over a state
- Find an **action policy to drive** the environment toward maximum cumulative reward

$$
s_{t+1} = Env(s_t, a_t)
$$

\n
$$
r_t = Rew(s_t, a_t)
$$

\n
$$
\pi(a|s) = P(A_t = a|S_t = s)
$$

\nfind $\pi s.t.$ $\sum_t r_t$ is maximum

- **Biology inspired** analytical model, but **not bio-mimetic**
- Booming in recent decade thanks to large dataset, increased computational power and theoretical novelties
- Origin tied to logistic regression with change of data representation
- Part of any "deep learning" model nowadays
- Usually large number of parameters trained with stochastic gradient descent

Artificial Neural Network

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Neural Net Architectures

Deep Convolutional Inverse Graphics Network (DCIGN)

<http://www.asimovinstitute.org/neural-network-zoo>

➢ Does not cover it all : densenet, graph network, ...

ECHNOLOGY STACI OCTANE.AI howdy. MaluubA OpenAI Gym Kasisto GUTOr *b* semanticmachine: DataRobot *yhat* AYASDI tion Loop Cin reactive **Askumind WHYLIEN** LEXALYTICS SpaCy **CLUMINOS** LAYER 6 **ATASIFT** amaz DATALOGUE OTRIFACTA O pars Acerta $\frac{1}{2}$ **CNTK H2O DEEPLEARNING4J Ttorch** :ikit-learn <mark>← A</mark> AzureML <mark>∩ </mark>n DMTK Spark PaddlePaddle WEK **ELEMENT**

Machine Learning in Industry

Deep Learning Everywhere

MEDIA & ENTERTAINMENT

Speech Recognition

Language Translation

Language Processing

Sentiment Analysis Recommendation

MEDICINE & BIOLOGY

Cancer Cell Detection Diabetic Grading Drug Discovery

Video Captioning Video Search Real Time Translation

Face Detection Video Surveillance Satellite Imagery

& DEFENSE

SECURITY

AUTONOMOUS MACHINES Pedestrian Detection Lane Tracking

Recognize Traffic Sign

15 **SI DWIDIA**

<https://www.nvidia.com/en-us/deep-learning-ai/>

Rapidly Accelerating Use of Deep Learning at Google Used across products: Number of directories containing model description files 1500 1000 500 2013 2015 2012 2014

MACHINE INTELLIGENCE 3.0

<http://www.shivonzilis.com/machineintelligence>

Prominent skill in industry nowadays. Lots of data, lots of applications, lots of potential use cases, lots of money. Knowing machine learning can open significantly **career horizons.**

Mastering the game of Go with deep neural networks and tree search, <https://doi.org/10.1038/nature16961>

Learning to Control

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Learning to Walk via Deep Reinforcement Learning <https://arxiv.org/abs/1812.11103>

Modern machine learning **boosts control technologies**. AI, gaming, robotic, self-driving vehicle, etc.

Learning from Complexity

Conv 1: Edge+Blob

Conv 3: Texture

Conv 5: Object Parts

Fc8: Object Classes

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Machine learning model can **extract information from complex dataset.** More classical algorithm counter part may take **years of development.**

The Black-box Dilemma

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Deep learning may yield great improvements. Having the "best classification performance" is not always sufficient. Forming an understand of the processes at play is often crucial.

Physics Knowledge

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Machine Learning can **help understand Physics**.

1.75

 1.50

1.25

 $\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{bmatrix}$

0.75

0.50

0.25

0.00

 0.4

0.3

 $\begin{array}{c}\n\text{Density} \\
0.2\n\end{array}$

 0.1

 0.8

0.7 0.6

 $\frac{5}{2}$ 0.5
0.4

 0.3 0.2 0.1

Learning Observables

Search in the space of functions using decision ordering. Simplified to the energy flow polynomial subspace. Extract set of EFP that matches DNN performance.

Use Physics

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Let the model **include Physics principles** to master convergence

Inductive Bias

Embed the symmetry and invariance in the model. Economy of model parameters.

$$
\mathcal{F}_{i} \mapsto W \cdot \left(\mathcal{F}_{i} \oplus \mathcal{F}_{i}^{\otimes 2} \oplus \sum_{j} f\left(p_{ij}^{2}\right) \cdot p_{ij} \otimes \mathcal{F}_{j}\right) \qquad \text{Lorentz group quiva}
$$

 (c)

Jet Tagging

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Graph-based models have recently achieved state-of-the-art jet tagging performance on benchmarks, and in analysis. Still a very rich field, in particular in developing inductive bias in the model (symmetry, invariance, …). Kinematic regression, substructure assignment, … also possible thanks to model flexibility.

Operation Vectorization

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ANN ≡ matrix operations ≡ parallelizable

$$
\begin{bmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \\ w_{13} & w_{23} \end{bmatrix} \cdot \begin{bmatrix} i_1 \\ i_2 \end{bmatrix} = \begin{bmatrix} (w_{11} \times i_1) + (w_{21} \times i_2) \\ (w_{12} \times i_1) + (w_{22} \times i_2) \\ (w_{13} \times i_1) + (w_{23} \times i_2) \end{bmatrix}
$$

Computation of prediction from artificial neural network model can be **vectorized to a large extend.**

Hyper-Fast Prediction

Synthesizing FPGA firmware from trained ANN

<https://fastmachinelearning.org/hls4ml/>

J. Duarte et al[.\[1804.06913\]](https://arxiv.org/abs/1804.06913)

Artificial neural network model can be **executed efficiently on FPGA**, GPU, TPU, ...

Inference Engines

Growing list of deep learning accelerators. Location of the device is driven by the environment (Trigger, Grid, HPC, …).

"Remote accelerator"

[\[1811.04492\],](https://arxiv.org/abs/1811.04492) [\[2007.10359\],](https://arxiv.org/abs/2007.10359) [\[2007.14781\]](https://arxiv.org/abs/2007.14781)

Model Compression

Model inference can be accelerated by reducing the number and size of operations.

The Standard Model

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Well demonstrated effective model. Good amount of detailed, **"labelled" simulation available**.

Slide: A. Wulzner [\[H&N\]](http://www.weizmann.ac.il/conferences/SRitp/Aug2019/)

The Sea Beyond Standard Model

"Almost" Simple H₁

Focus on few sharply-defined alternative models (e.g., the Higgs)

Case-by-case design of **optimal test**

"Very" Composite H_1

Huge set of alternatives Case-by-case optimisation unfeasible The right H₁ likely not yet formulated

Event Triggering

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Select what is important to keep for analysis. Ultra fast decision in hardware and software.

Reconstruction of the event under limited latency / bandwidth. **Better resolution** help lowering background trigger rates, **Faster algorithms** helps making more refined decisions.

Reconstructing Collisions

63 From detector signal to high-level features using **mostly pattern recognition**. Complex and **computing intensive** series of tasks.

Event Processing

Dimensionality reduction

Globalization of information

Simulating Collisions

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Non-differentiable, **computing intensive** sequence of **complex simulators** of the signal expected from the detectors.

Reconstruction ◦ Simulation ∼ Identity

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Simulation aims at predicting the outcome of collisions. Reconstruction aims at inverting it. Multiple ways to connect intermediate steps with deep learning.

The Computing Cost of Science

Ever growing needs for computing resource. Slowdown of classical architecture, over growth of GPU architecture.

Annual CPU Consumption [MHS06]

Possible Utilizations

Accuracy Speed

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Interpretable

➔ **Fast surrogate** models (trigger, simulation, etc) ; even better if more accurate. ➔ **More accurate** than existing algorithms (tagging, regression, etc) ; even better if faster. ➔ Model performing **otherwise impossible tasks** (operations, etc)

