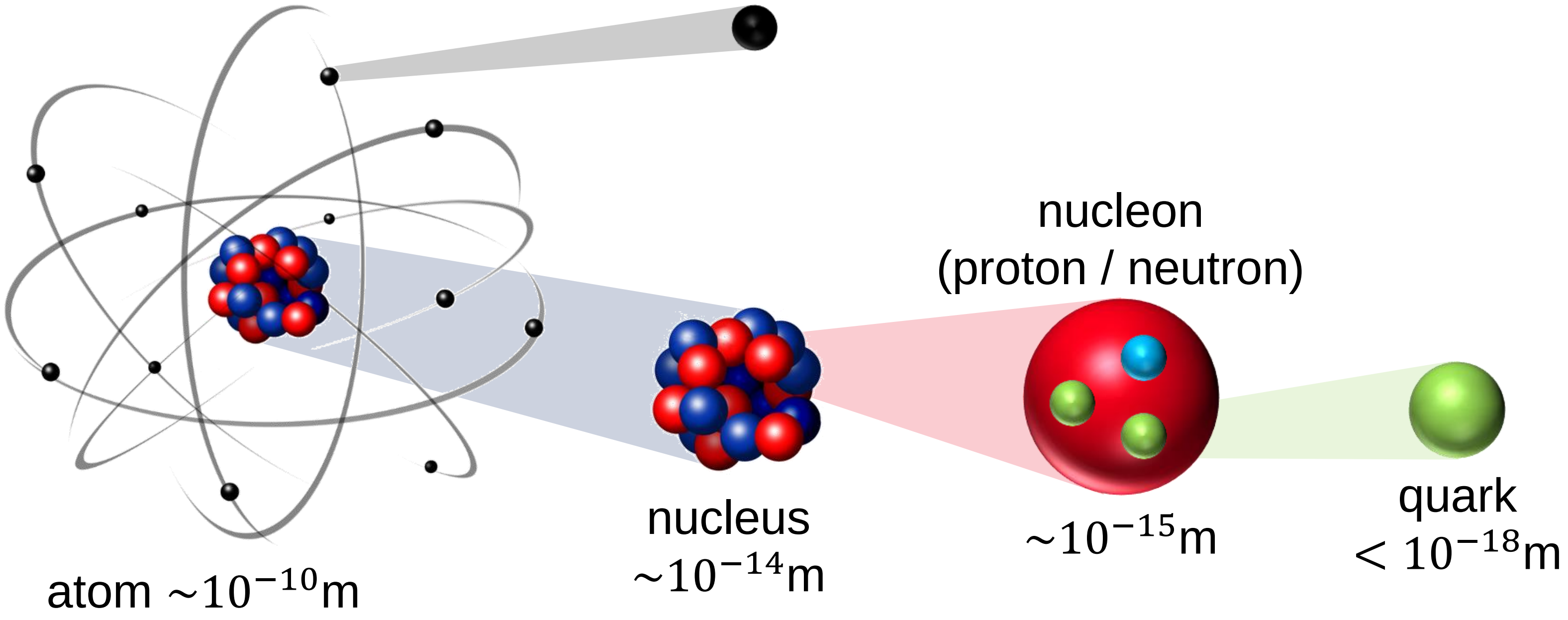
INTERPRETABLE MACHINE LEARNING FOR CLAS12 DATA ANALYSIS

InTheArt | Noëlie Cherrier

OUTLINE

- Introduction
- Feature construction: principle
- Feature construction: practical use in algorithms
  - → Trees and ensemble models
  - → Generalized Additive Models (GAM)
- CLAS12 data analysis
  - → Comparison with classical and neural network approach
  - → Transfer learning

INTRODUCTION



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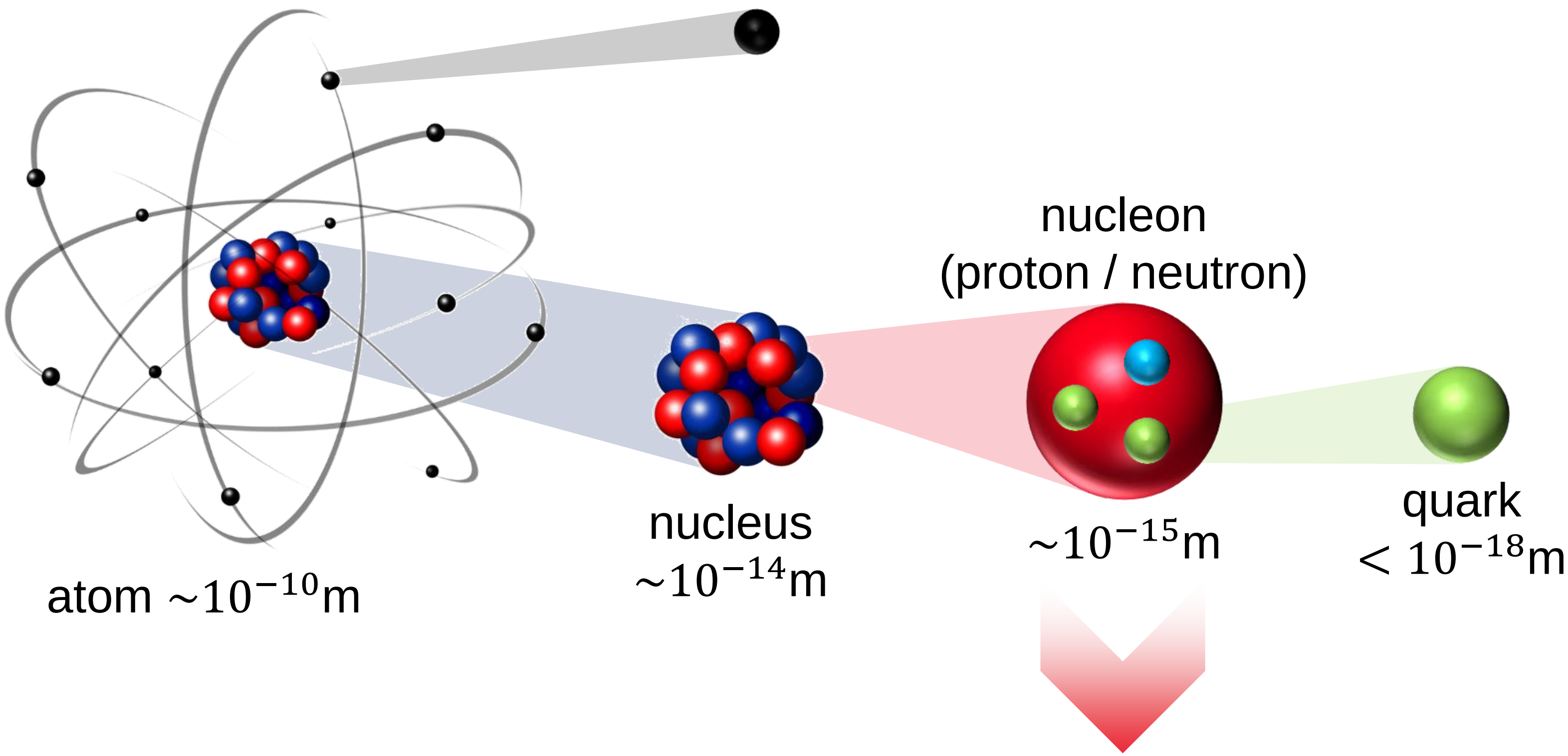
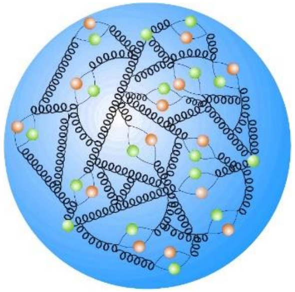


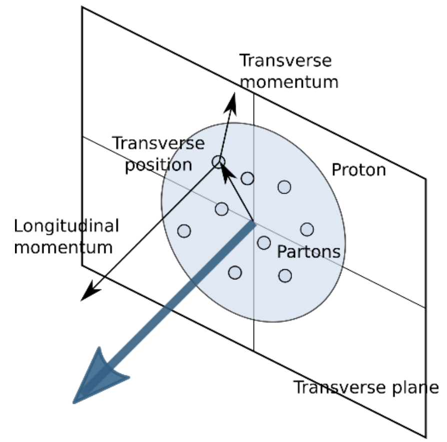
Objective: study the proton structure

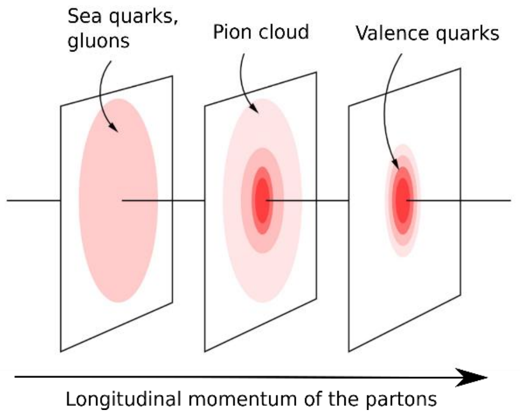


INTRODUCTION

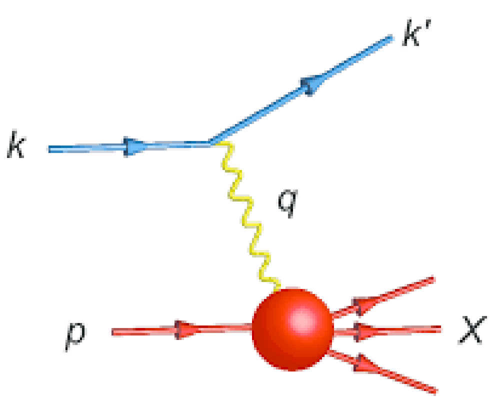
- Physics objective: tomography of the nucleon through **Generalized Parton Distributions** (GPDs)

  ⟶ Correlation between longitudinal momentum and transverse position of the partons in the nucleon





- Accessed through exclusive inelastic processes including **Deeply Virtual Compton Scattering** (DVCS)



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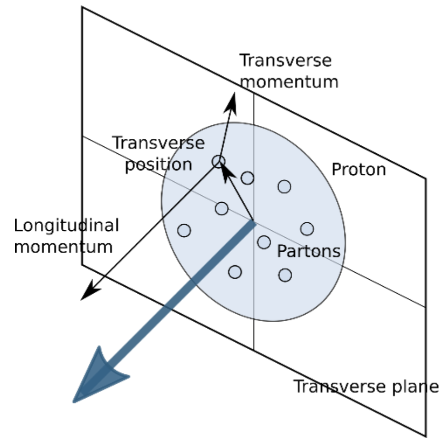

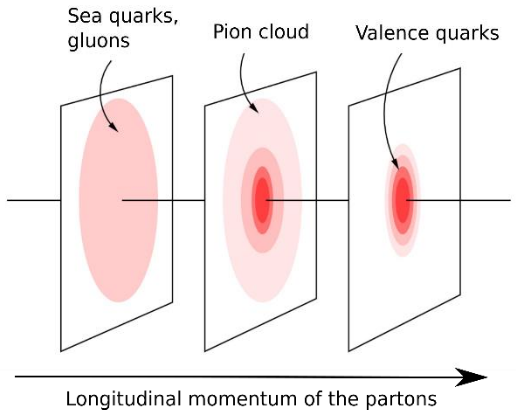

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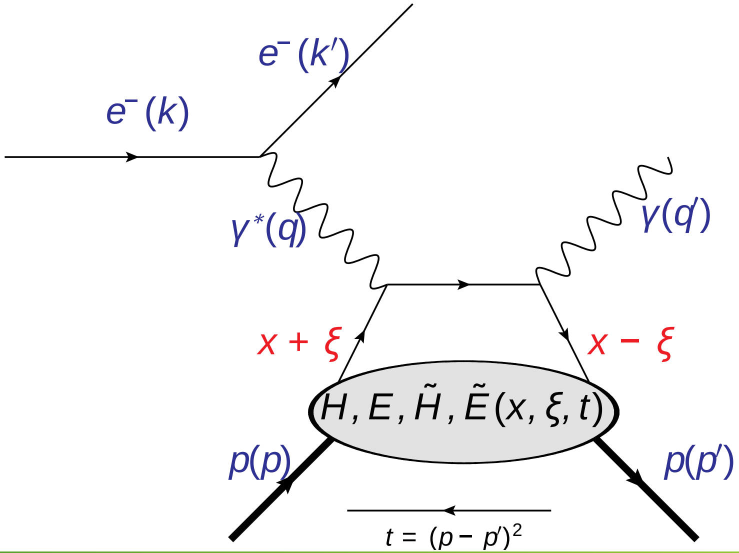
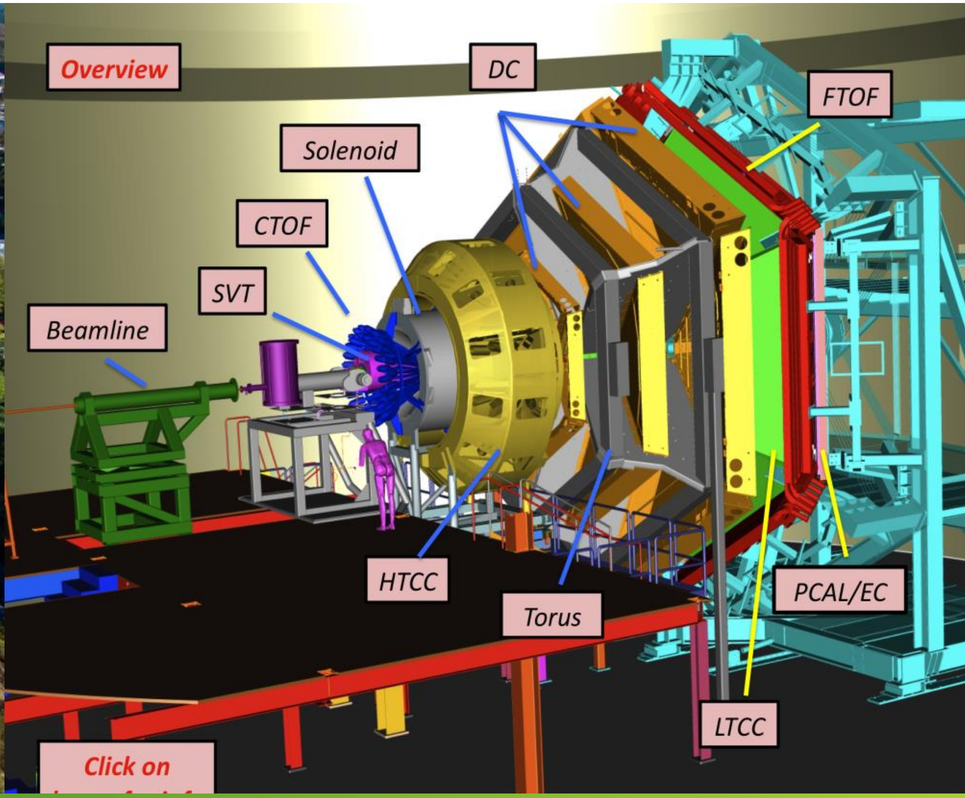


INTRODUCTION

- Jefferson Lab: 10.6 GeV electron beam
- CLAS12 data taking since 2018: hydrogen target

Event classification task: isolate DVCS events ($ep \to ep\gamma$)



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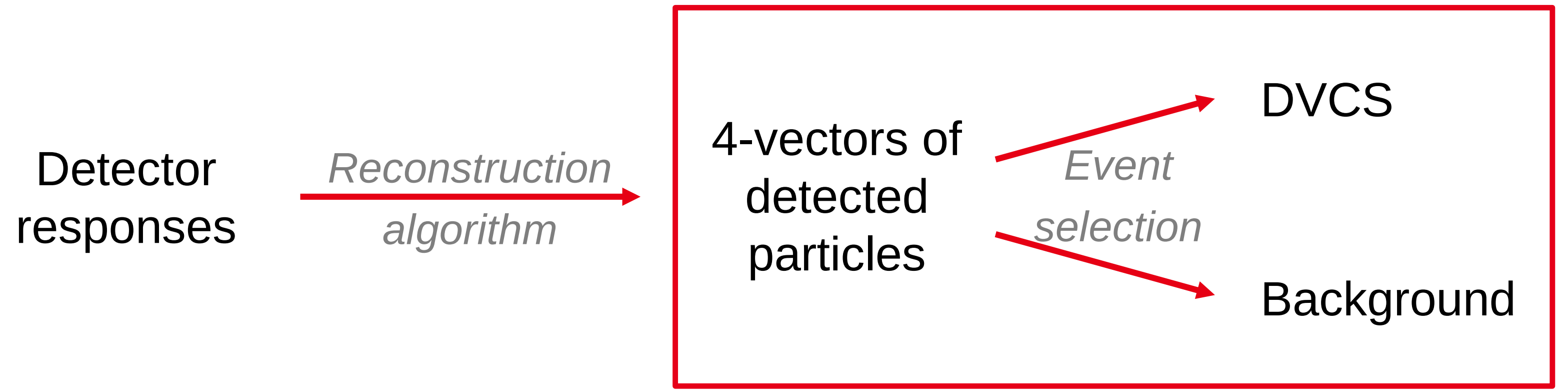
Event classification task: isolate DVCS events ($ep \rightarrow ep\gamma$)

Machine learning approach to be compared to classical approach



Main background: π^0-production events $ep \rightarrow ep\pi^0 \rightarrow ep\gamma\gamma$

INTERPRETABLE / TRANSPARENT / INTELLIGIBLE MACHINE LEARNING

- **Interpretability**: it is defined as the ability to explain or to provide the meaning in understandable terms to a human

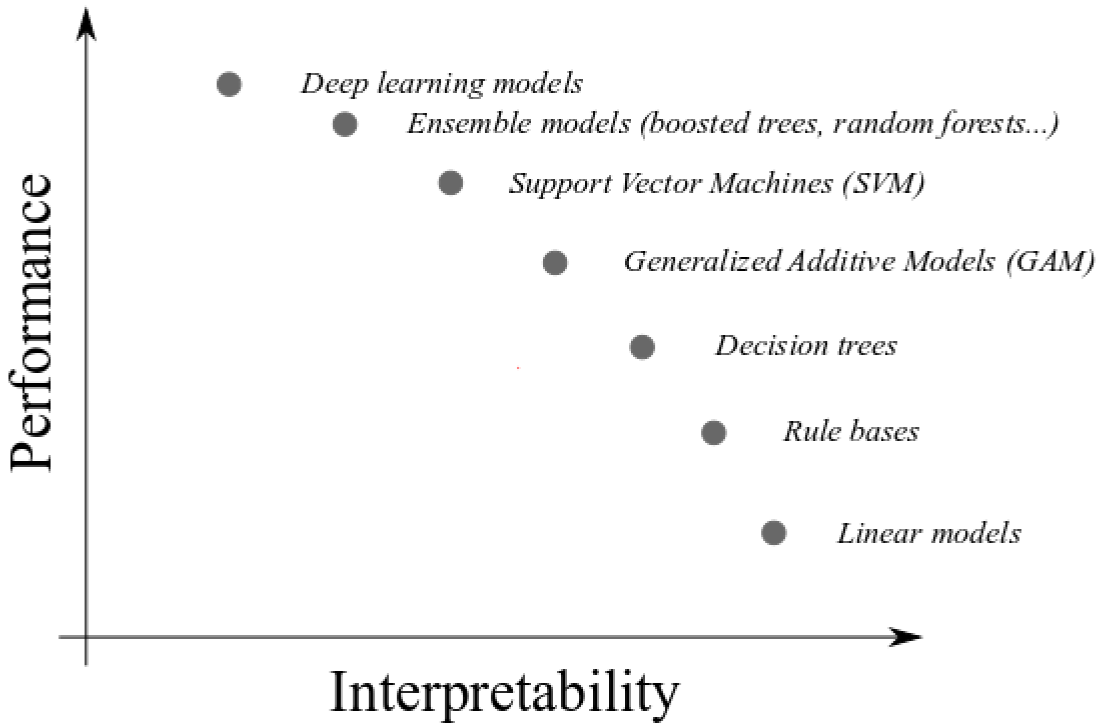
- **Transparency**: a model is considered to be transparent if by itself it is understandable. A model can feature different degrees of understandability

- **Intelligibility** (or understandability) denotes the characteristic of a model to make a human understand its function – how the model works – without any need for explaining its internal structure or the algorithmic means by which the model processes data internally

⚠ The lack of interpretability is controversial

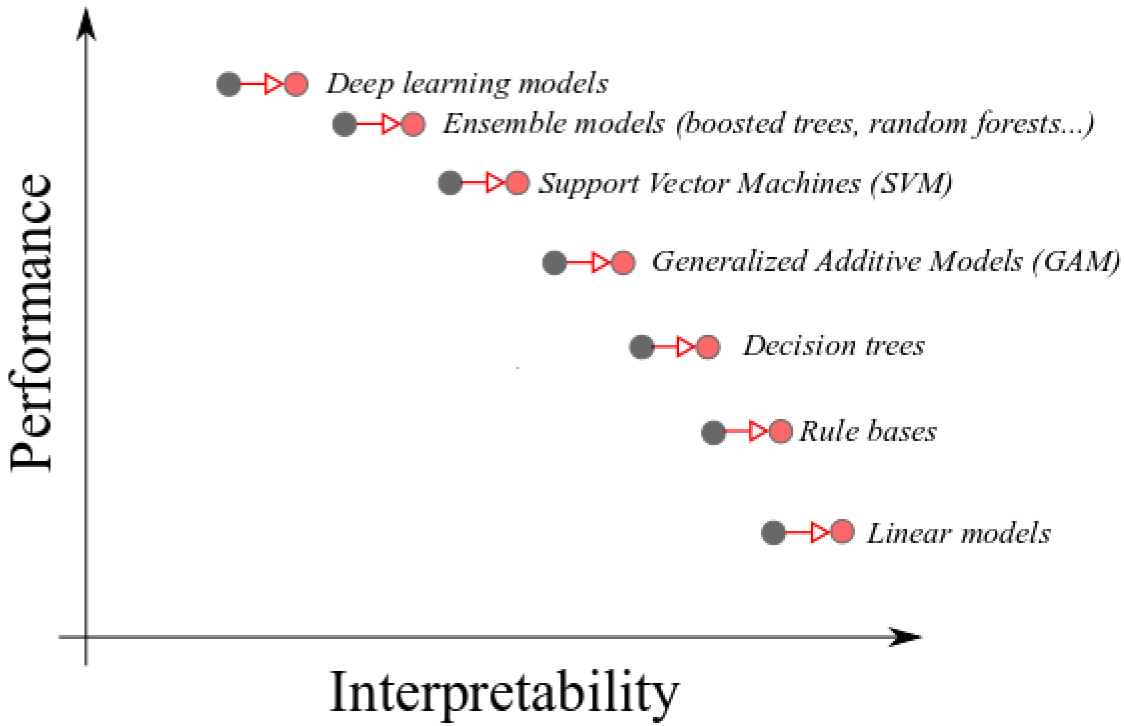
Arrieta, Alejandro Barredo, et al. "Explainable Artificial Intelligence (XAI): Concepts, Taxonomies, Opportunities and Challenges toward Responsible AI." *Information Fusion* (2019).

INTERPRETABLE / TRANSPARENT / INTELLIGIBLE MACHINE LEARNING



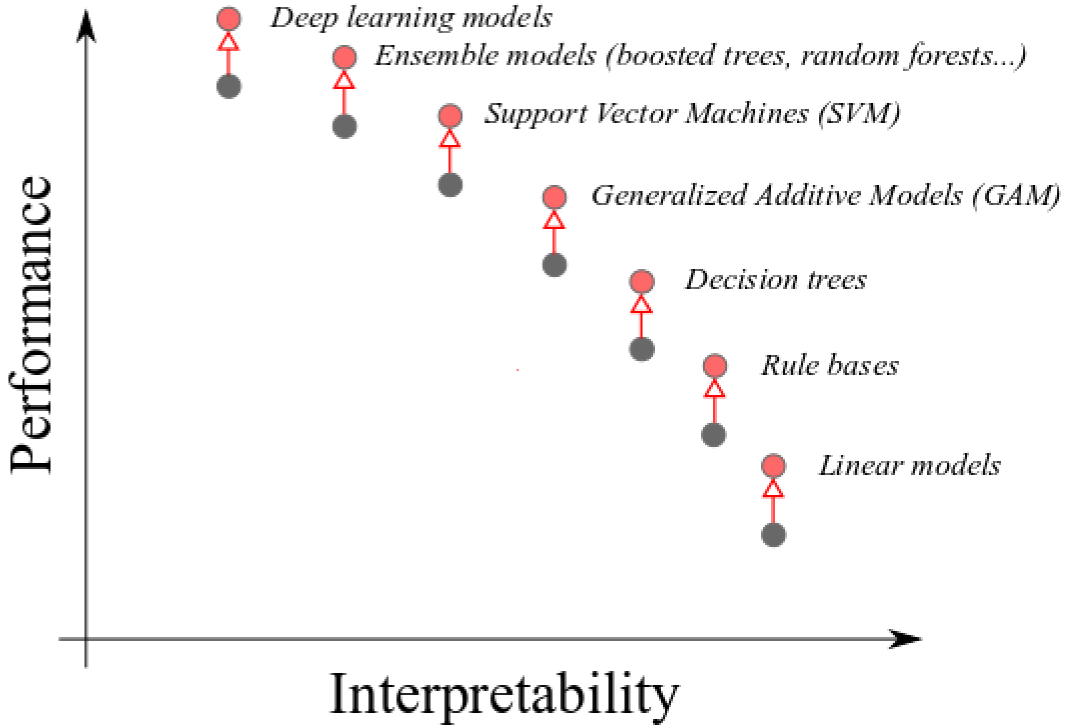
INTERPRETABLE / TRANSPARENT / INTELLIGIBLE MACHINE LEARNING

Post-hoc explainability methods (feature importance, simplification...)



INTERPRETABLE / TRANSPARENT / INTELLIGIBLE MACHINE LEARNING

Make up for the model drawbacks (notably internal representation)



FEATURE CONSTRUCTION: PRINCIPLE

FEATURE CONSTRUCTION

Motivation: these models do not build a sufficiently complex internal representation of the data

$p_x^e \quad \varphi^\tau$

θ^γ

p_T^{lep}

$\longrightarrow$

$p_z^e + p_z^p + p_z^{\gamma_1}$

$\cos(\theta^{lep} - \theta^\tau)$

$angle(p^{\gamma_1}, p^{\gamma_1} + p^{\gamma_2})$

$\cos(\varphi^{lep} - \varphi^\tau)$

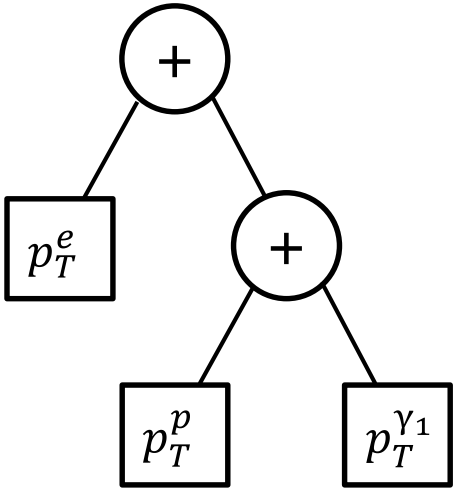
Base variables — Discriminative and intelligible features

In machine learning: feature engineering, feature construction

FEATURE CONSTRUCTION

Motivation: these models do not build a sufficiently complex internal representation of the data

Constrained Genetic Programming: evolve a population of high-level feature candidates



Feature candidate example
→ Nodes are mathematical operators
→ Leaves are base variables

Cherrier, N., Poli, J. P., Defurne, M., & Sabatié, F. (2019, June). Consistent Feature Construction with Constrained Genetic Programming for Experimental Physics. In *2019 IEEE Congress on Evolutionary Computation (CEC)* (pp. 1650-1658). IEEE.

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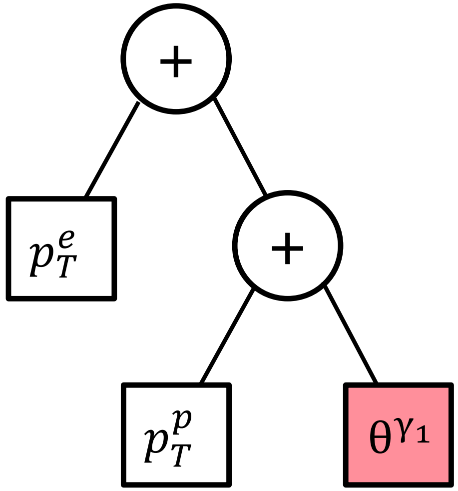

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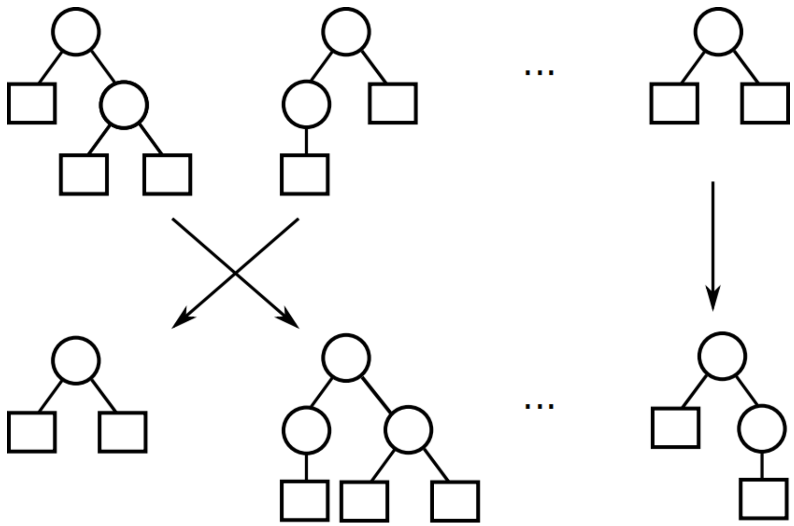
FEATURE CONSTRUCTION

Grammar-guided Genetic Programming

```
<start> ::= <E> | <A> | <F>
<E> ::= <E> + <E> | <E> - <E> | <E> * <F>
       | <E> / <F> | sqrt(<E2>) | <termE>
<A> ::= <A> + <A> | <A> - <A> | acos(<F>)
       | asin(<F>) | atan(<F>) | <termA>
<F> ::= <F> + <F> | <F> - <F> | <F> * <F>
       | <F> / <F> | <E> / <E> | <A> / <A>
       | cos(<A>) | sin(<A>) | tan(<A>)
       | <termF>
<E2> ::= <E2> + <E2> | <E2> - <E2>
       | <E> * <E> | <E2> * <F> | <E2> / <F>
       | square(<E>) | <termE2>
```

Ratle, A., & Sebag, M. (2001). Grammar-guided genetic programming and dimensional consistency: application to non-parametric identification in mechanics. Applied Soft Computing, 1(1), 105-118.

FEATURE CONSTRUCTION

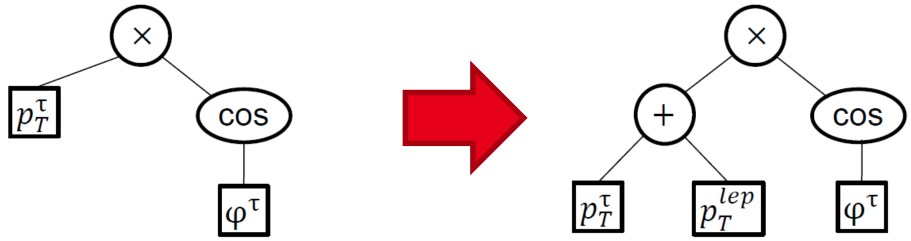


Generation n

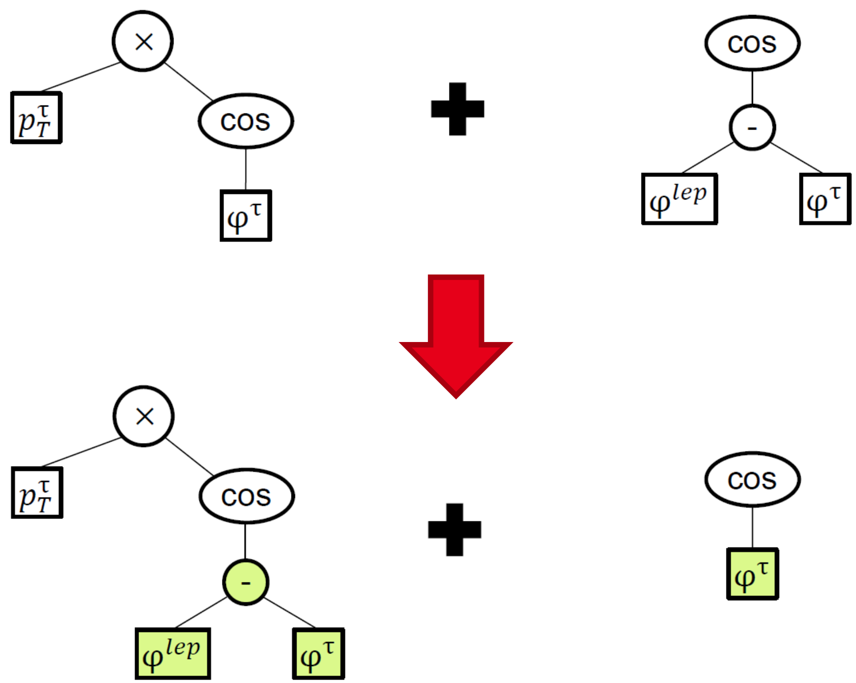
Offspring

FEATURE CONSTRUCTION

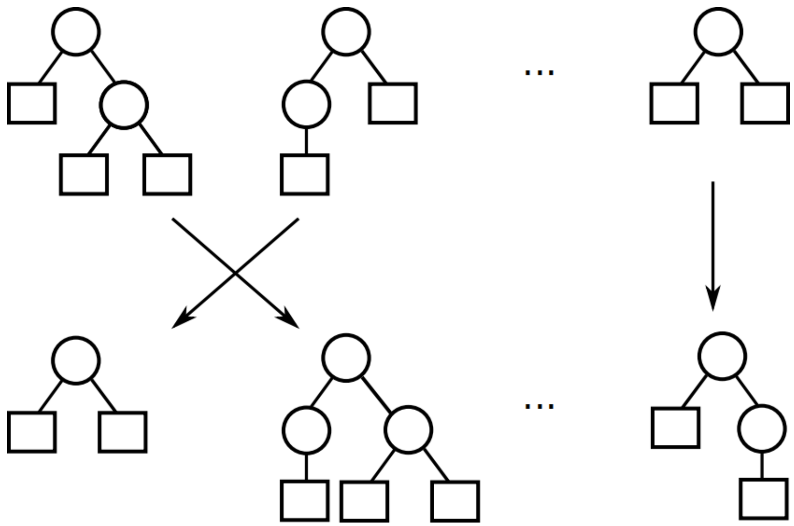
Mutation



Crossover



FEATURE CONSTRUCTION



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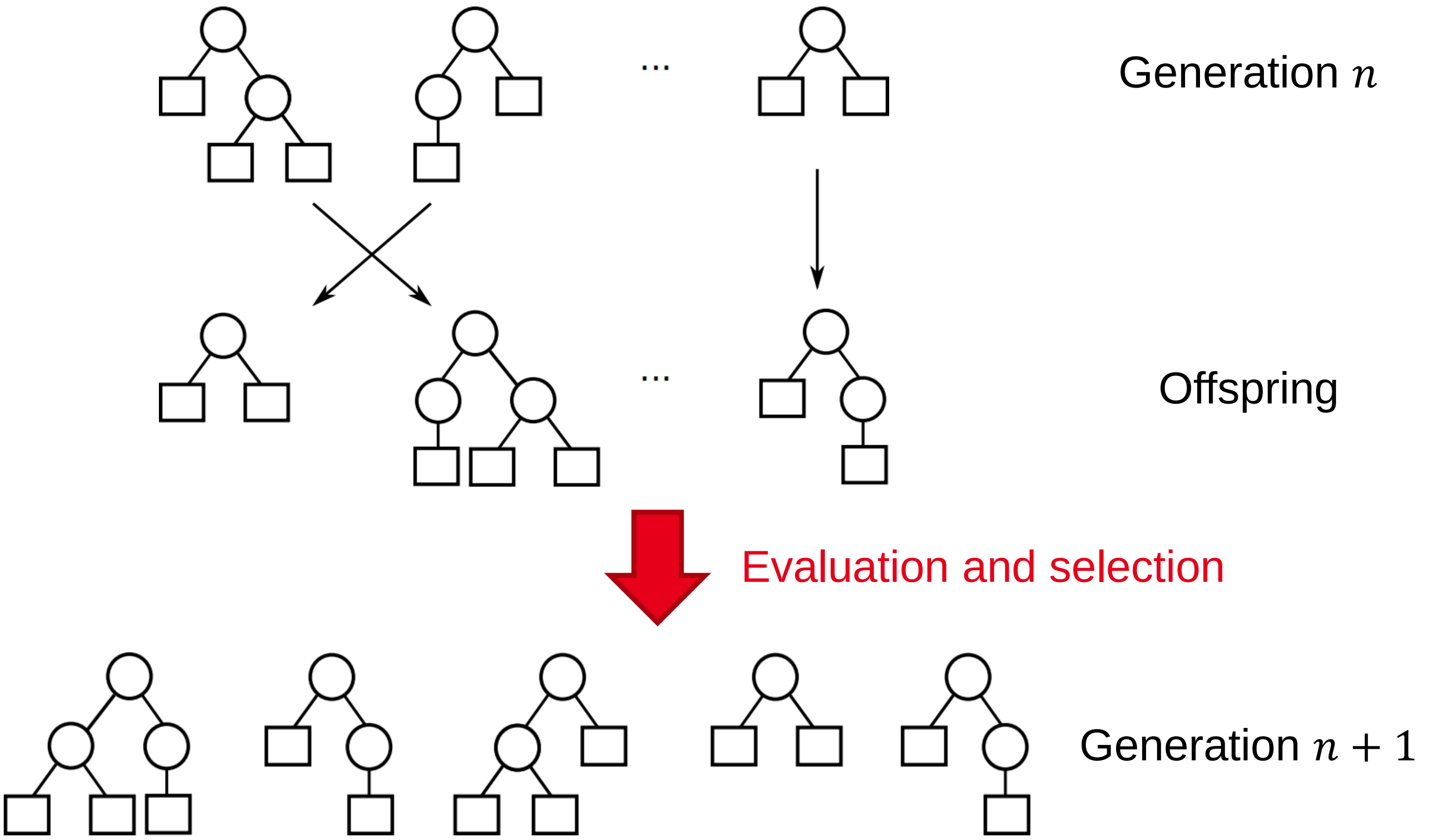
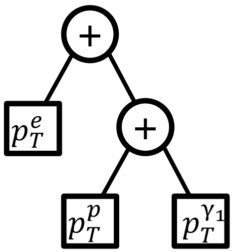


FEATURE CONSTRUCTION

Different FC methods, main difference = how to evaluate the feature candidates

Filter, wrapper, or embedded methods

prior FC
(before learning the ML model)



$\longrightarrow \quad p_T^e + p_T^p + p_T^{\gamma_1}$

Filter

Information gain, Gini index, ... of the candidate feature

Wrapper

Inclusion into the initial list:

$p_T^e, \Theta^e, \varphi^e, p_T^p, \Theta^p, \varphi^p$, etc., $p_T^e + p_T^p + p_T^{\gamma_1}$

and training of a ML algorithm
(the fitness of the candidate is the test score of the ML algorithm)

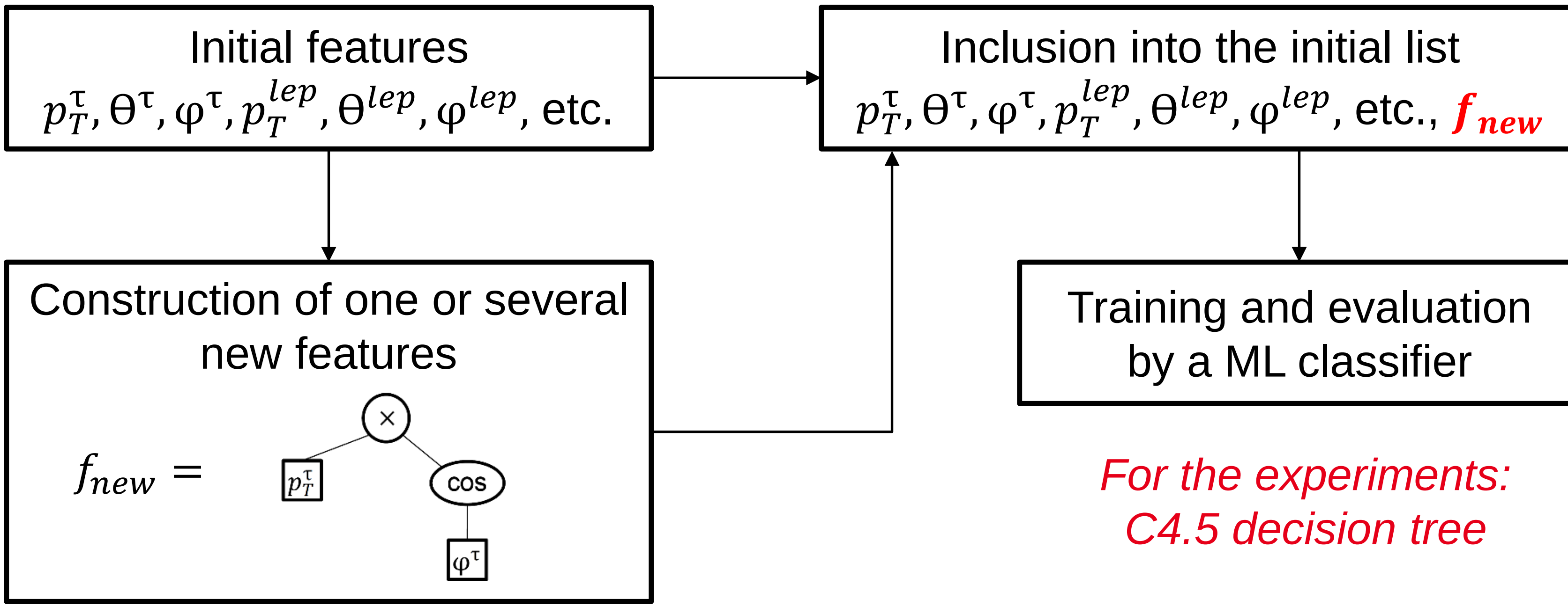
Embedded

Build features during the induction process, usually with filter fitness functions

- *Decision trees and ensemble methods*
- *Generalized Additive Models*

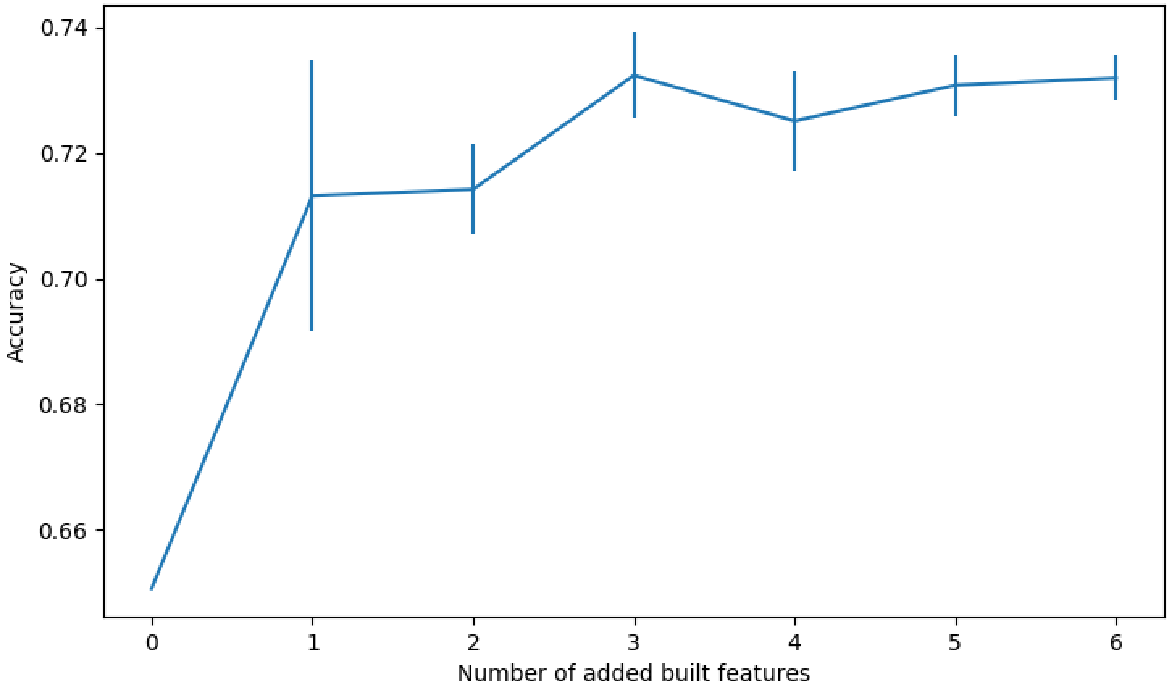
FEATURE CONSTRUCTION: PRACTICAL USE IN ML ALGORITHMS

PRIOR FEATURE CONSTRUCTION



For the experiments:
C4.5 decision tree

PRIOR FEATURE CONSTRUCTION



$$p_z^e + p_z^{\gamma_1} + p_z^p$$

$$(\cos(\phi^{\gamma_1} - \phi^{\gamma_2}) + 9)\cos(\theta^{\gamma_1} - \theta^{\gamma_2})$$

$$\phi^{\gamma_1} - \phi^{\gamma_2}$$

EMBEDDED FEATURE CONSTRUCTION: IN TREES

Cherrier, N., Defurne, M., Poli, J. P., & Sabatié, F. (2019). Embedded Constrained Feature Construction for High-Energy Physics Data Classification. In *Workshop on Machine Learning for the Physical Sciences, NeurIPS* 2019.

p_x^e φ^τ

θ^γ

p_T^{lep}

Features in the dataset

Constrained Genetic Programming →

$p_z^e + p_z^p + p_z^{\gamma_1}$

$\cos(\theta^{lep} - \theta^\tau)$

$angle(p^{\gamma_1}, p^{\gamma_1} + p^{\gamma_2})$

$\cos(\varphi^{lep} - \varphi^\tau)$

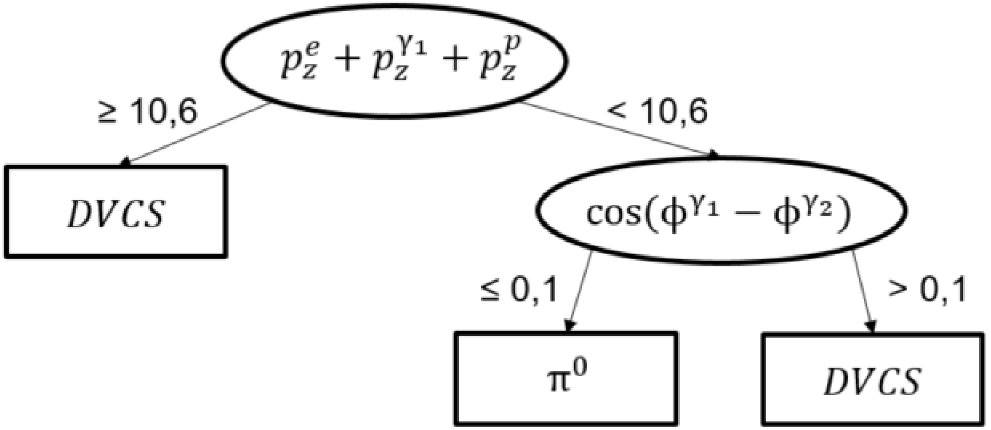
Discriminative and intelligible features

embedded into tree node induction

Fitness: tree splitting criterion (information gain, Gini index, ...)

✓ Faster construction

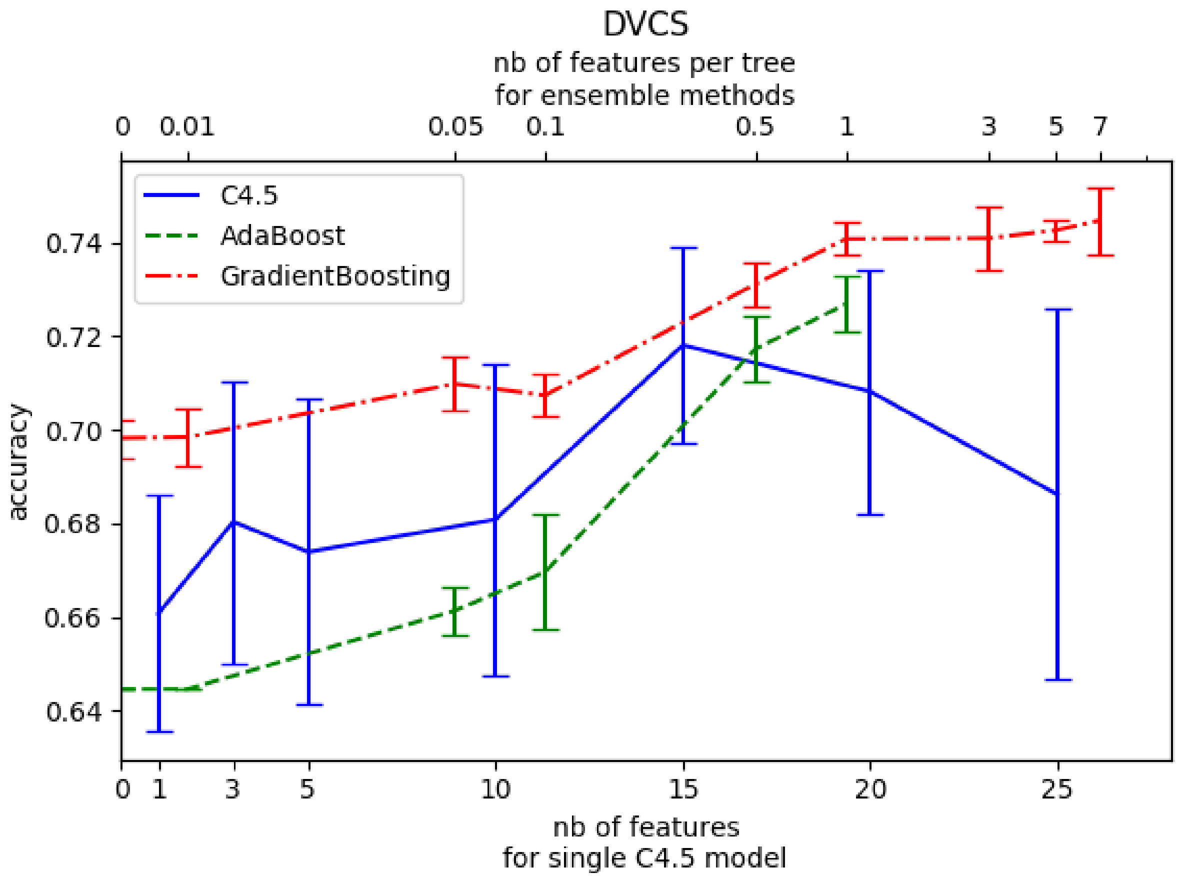
("filter" methods are faster to evaluate than training a whole ML model)



EMBEDDED FEATURE CONSTRUCTION: IN TREES

“Weak” learner in ensemble methods: decision tree with embedded feature construction

<u>ex:</u> AdaBoost, gradient boosting, XGBoost, etc.



GENERALIZED ADDITIVE MODELS (GAM)

$\hat{y}$ predicted output
y true output
x_1, ..., x_d input variables

Generalized Linear Models (GLM) :

$$g(\hat{y}) = \beta_0 + \beta_1 x_1 + \ldots + \beta_d x_d$$

$g(\hat{y}) = \hat{y}$ for regression, $g(\hat{y}) = \ln(\frac{\hat{y}}{1-\hat{y}})$ for classification

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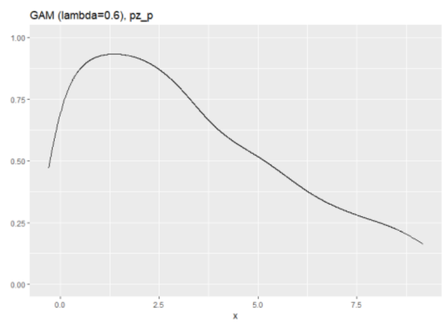
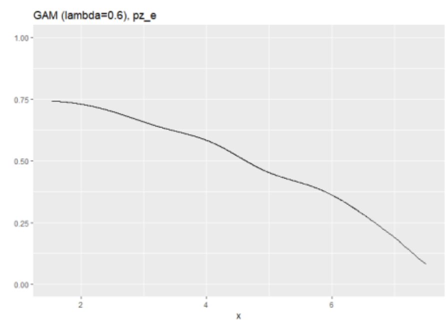
Generalized Additive Models (GAM) :

$$g(\hat{y}) = \beta_0 + f_1(x_1) + \ldots + f_d(x_d)$$



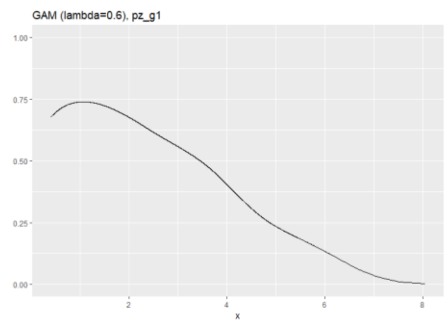
$f_1(x_1)$

+



$f_2(x_2)$

+



$f_3(x_3)$

+ ...

Hastie, T. J. (1986). Generalized additive models. In *Statistical models in S* (pp. 249-307). Routledge.
Lou, Y., Caruana, R., Gehrke, J., & Hooker, G. (2013, August). Accurate intelligible models with pairwise interactions. *ACM SIGKDD 2013.*

EMBEDDED FEATURE CONSTRUCTION: IN GAM

Idea: build one feature at a time, associated with one term of the GAM

$\longrightarrow$ **gradient boosting**

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Objective function: minimize the cross entropy $-y\ln(\hat{y}) - (1-y)\ln(1-\hat{y})$

1) Compute $\beta_0 = \ln\left(\frac{p_0}{1-p_0}\right)$ to form the 1st model $g(\hat{y}) = \beta_0$.
The residual is $r = y - \hat{y} = y - p_0$ (p_0 proportion of the majority class)

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Fitness function for the Genetic Programming algorithm:

- Shallow tree (maximum 4 leaves)
- Feature fitness: RMS error of the inducted tree with the residual

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Fitness function for the Genetic Programming algorithm:

- Shallow tree (maximum 4 leaves)
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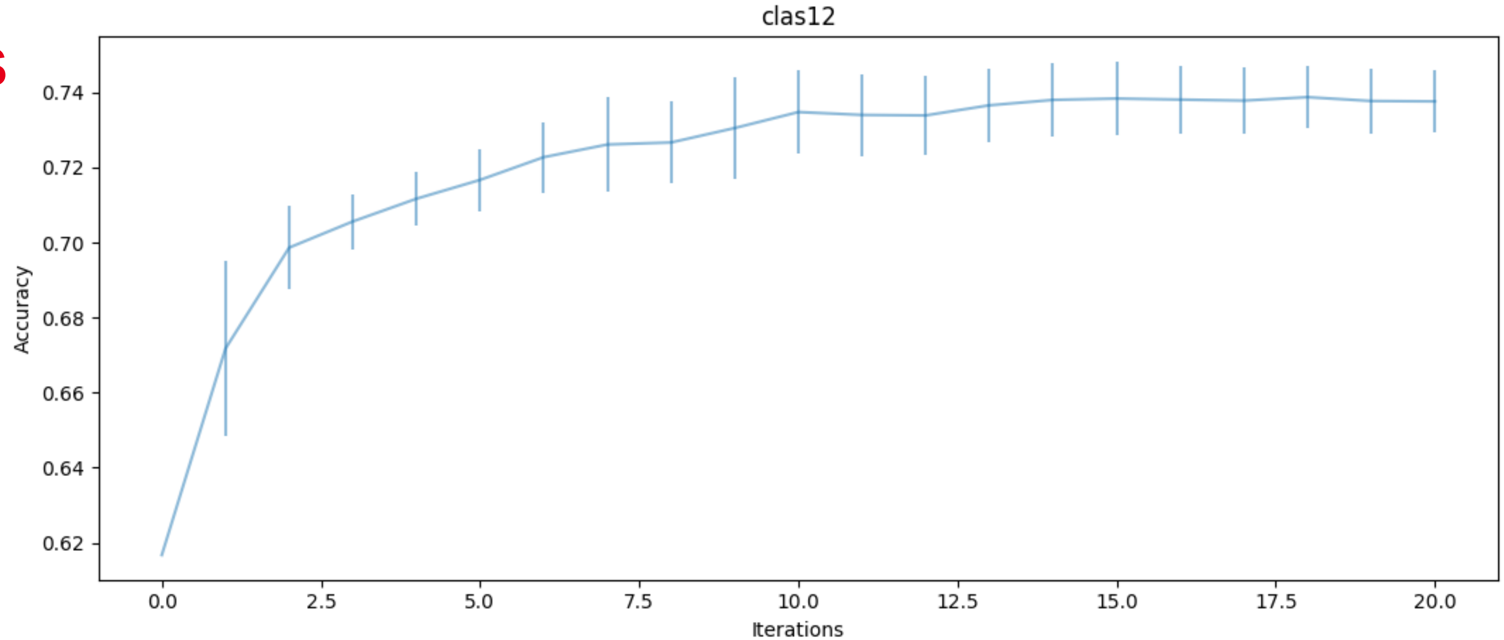
3) Fit a shape function $f_1(x_1)$ to the residual

4) Compute the new model: $g(\hat{y}) = g(\hat{y}) + f_1(x_1)$ and the new residual $r = y - \hat{y}$, and go back to step 2

RESULTS



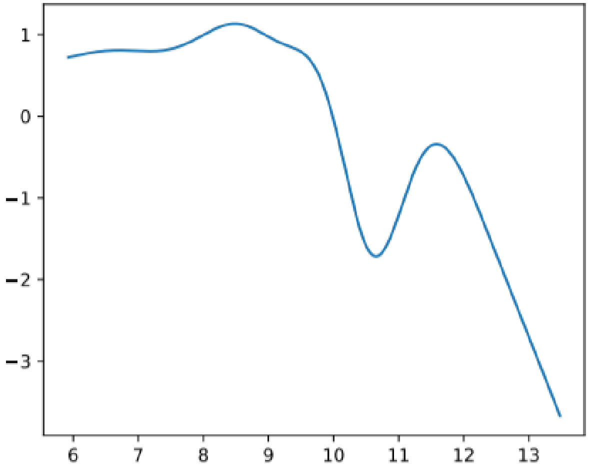
Baselines:

Neural network (2 hidden layers of size 100)	0.7012 ± 0,0062
Linear SVM	0.6911
C4.5 with feature construction	0.718 ± 0,020 (15 nodes using feature construction)
AdaBoost with feature construction	0.7280 ± 0.0063 (50 trees of 1 node each with feature construction)
Gradient Boosting with feature construction	0.7446 ± 0.0071 (100 trees of 7 nodes each with feature construction)

RESULTS

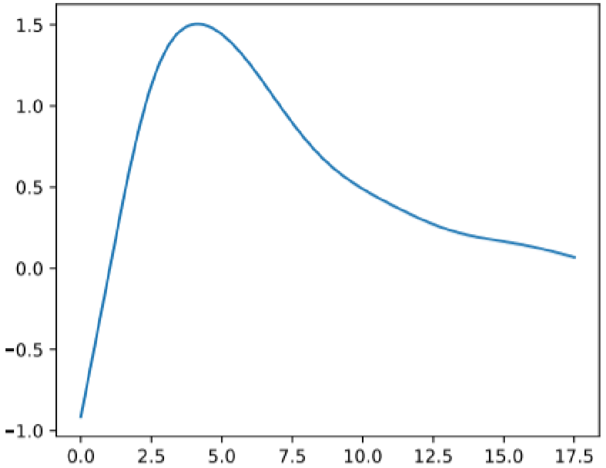
Example of a model (the lower the y value, the higher the probability to have a DVCS event):

$$p_z^e + p_z^p + p_z^{\gamma_1}$$



$+$

$$angle(p^{\gamma_2}, p^{\gamma_1} + p^{\gamma_2})$$



$+ \quad \ldots$

CLAS12 DATA ANALYSIS

COMPARISON WITH OTHER ANALYSIS APPROACHES

Classical DVCS event selection

$$-0{,}05\ GeV^2 \leq {MM^2}_{ep\to ep\gamma X} \leq 0{,}05\ GeV^2$$

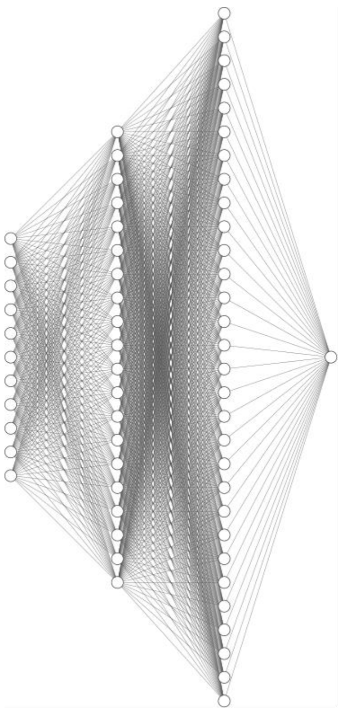
$$0{,}1\ GeV \leq MM_{ep\to e\gamma X} \leq 1{,}7\ GeV$$

$$-1\ GeV \leq missing\ energy \leq 2\ GeV$$

$$missing\ p_T\ (ep \to epX) \leq 0{,}4\ GeV$$

$$cone\ angle \leq 4°$$

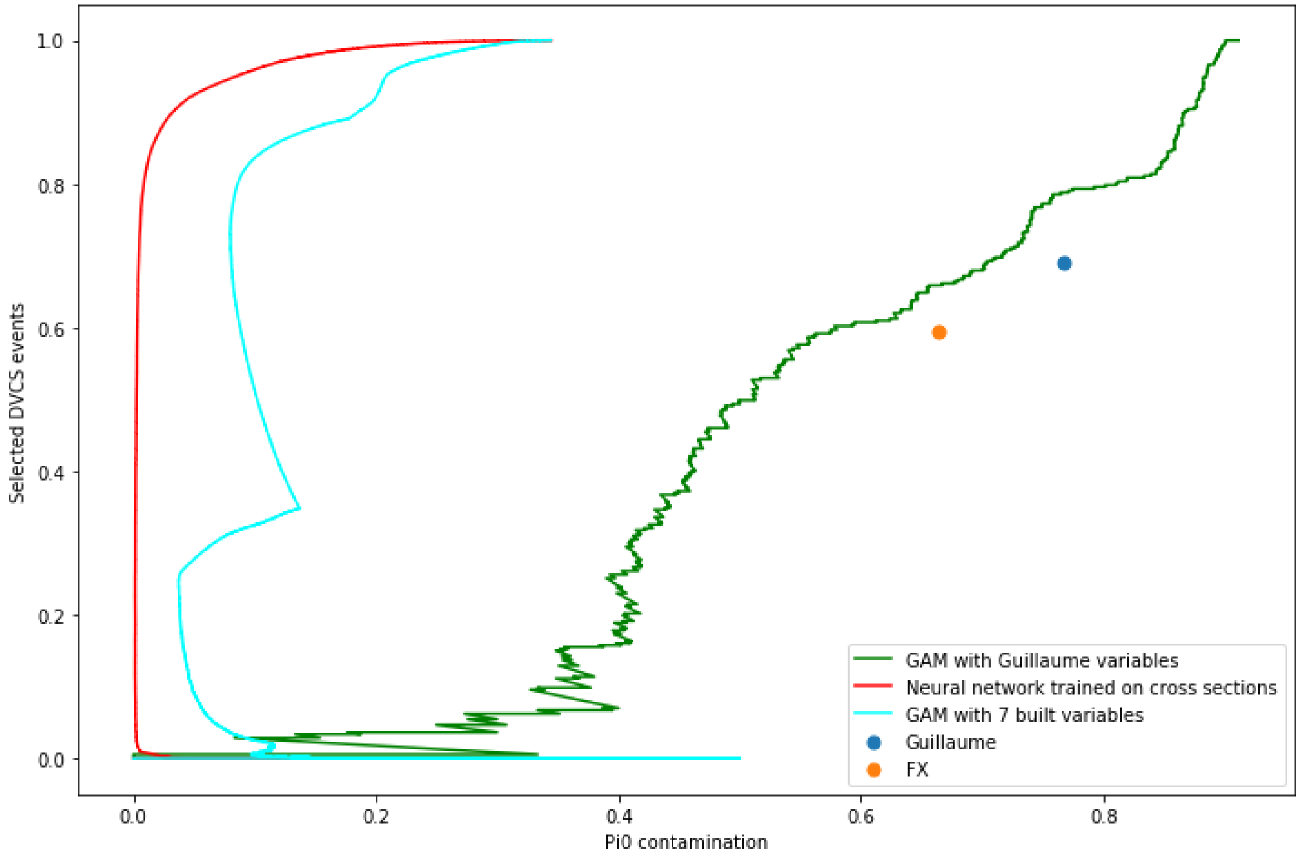
Neural network approach



2 hidden layers of size (20, 30)
11 high-level input features

COMPARISON WITH OTHER ANALYSIS APPROACHES

Y axis: percentage of selected DVCS events among all existing DVCS in simulated data
X axis: percentage of Pi0 events still present in the selected subset



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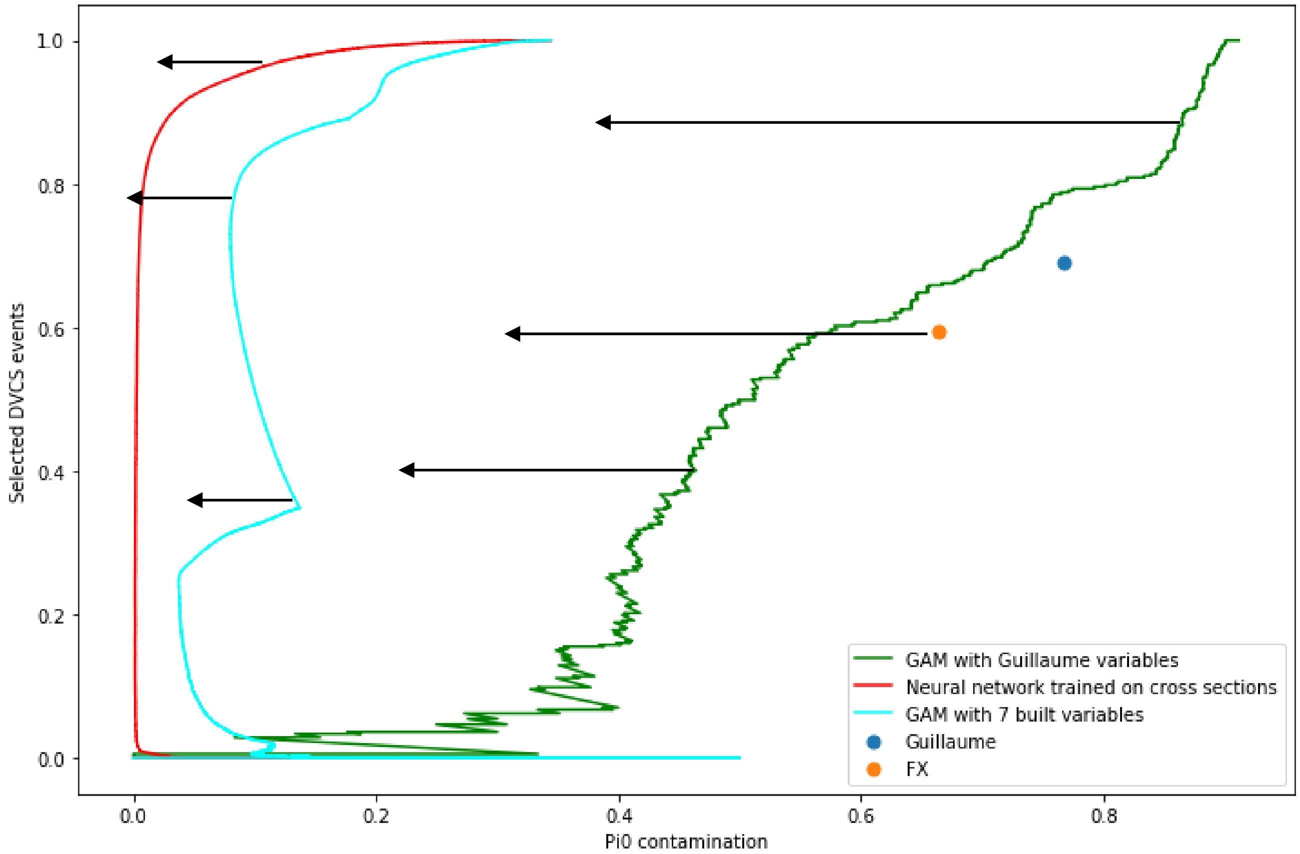
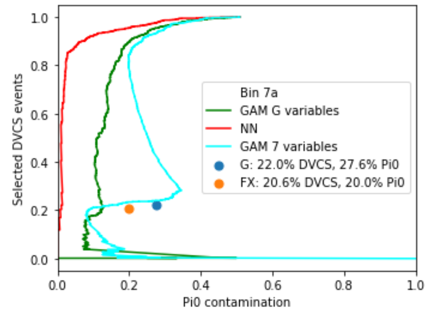
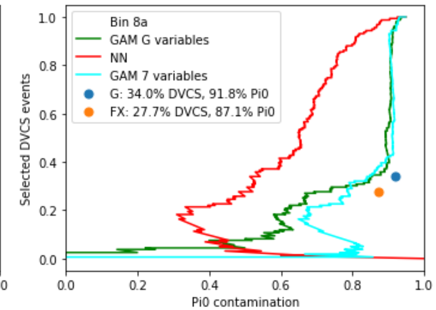
! Pi0 subtraction method

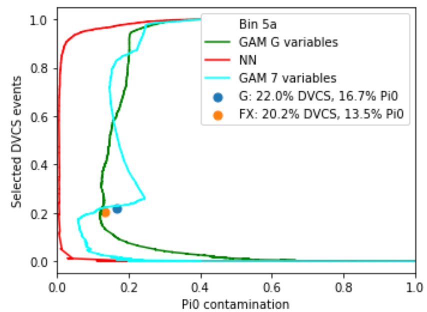


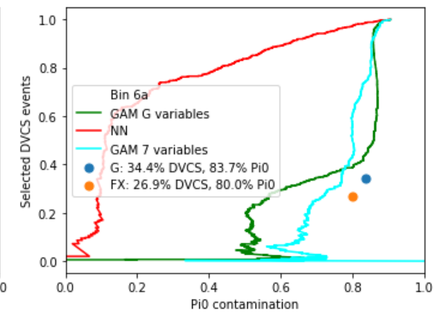
COMPARISON WITH OTHER ANALYSIS APPROACHES

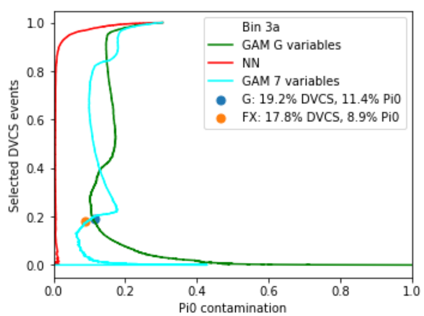
$$-\frac{t}{Q^2} \geq 0{,}25$$

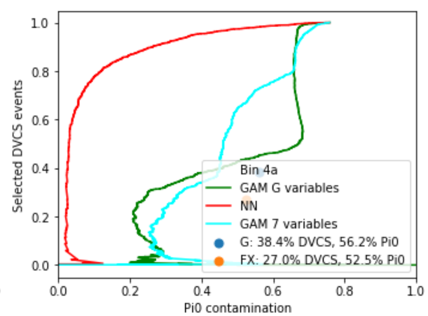


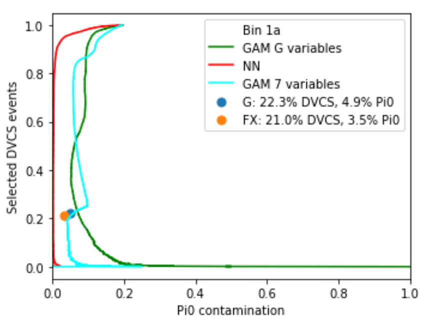


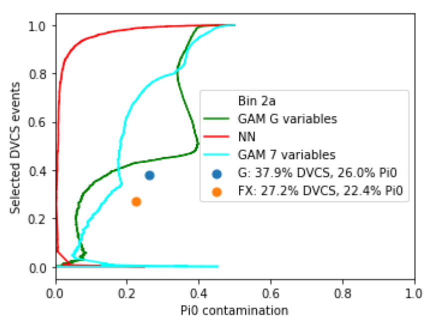






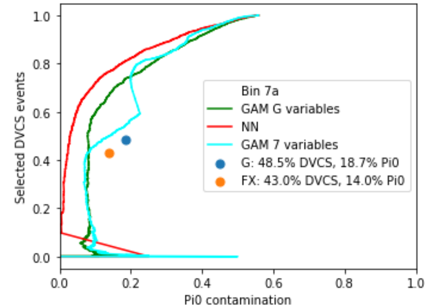


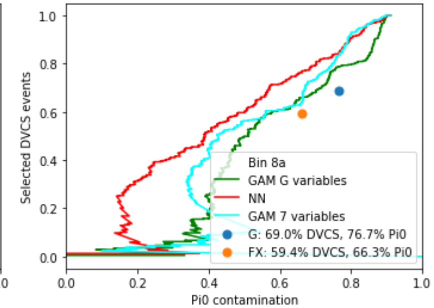


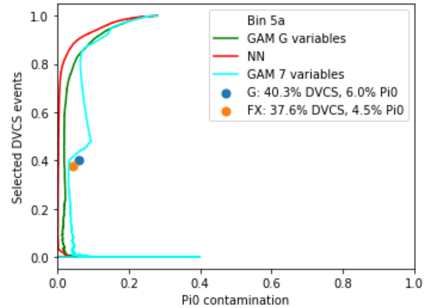


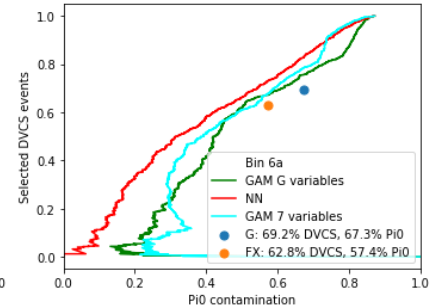
COMPARISON WITH OTHER ANALYSIS APPROACHES

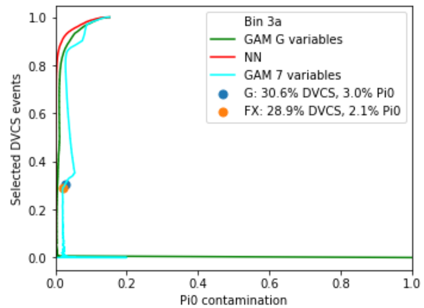
$$-\frac{t}{Q^2} < 0{,}25$$

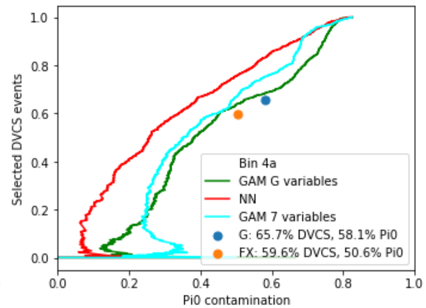


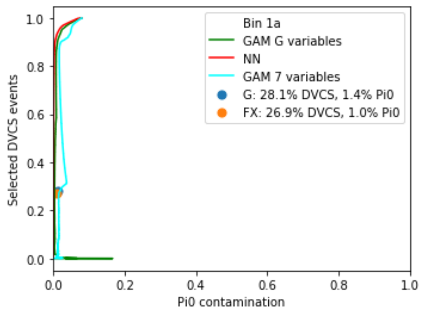


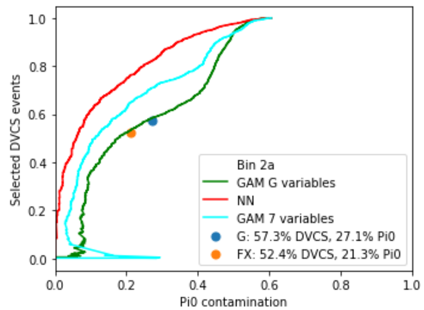










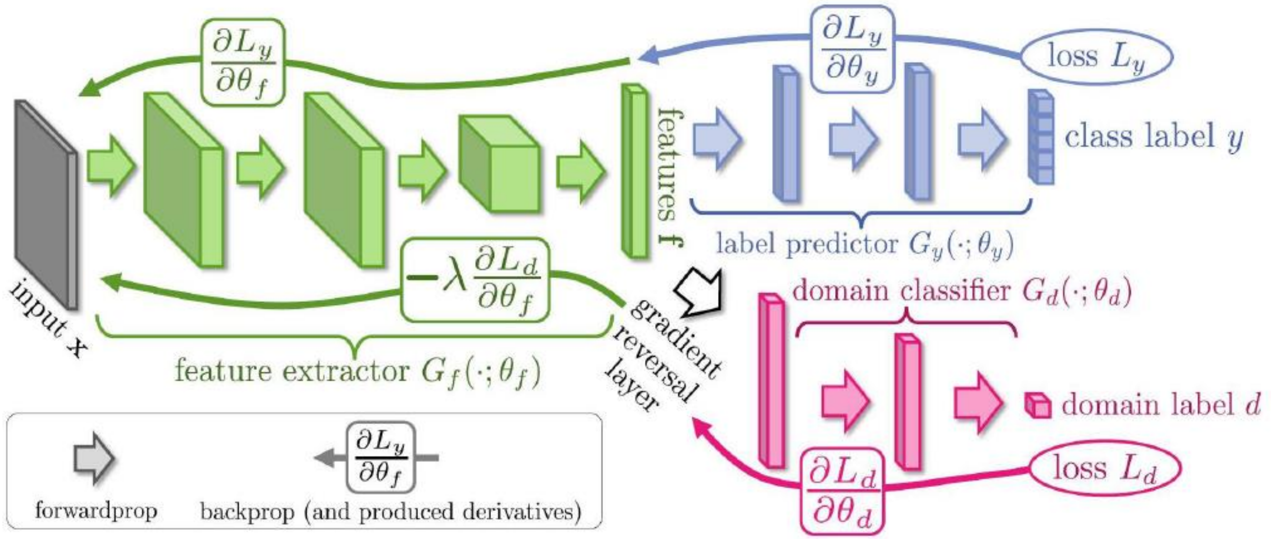


TRANSFER LEARNING

Issues:

- Shifts due to detector resolutions and calibrations
- Different data distributions (due to cross sections)
- New classes present in real data but not in simulations (other physics processes, accidental background, ...)

First approach from the neural network track:



$$\mathcal{L} = \mathcal{L}_y - \lambda\, \mathcal{L}_d$$

Ganin, Y., & Lempitsky, V. (2014). Unsupervised domain adaptation by backpropagation. *arXiv preprint arXiv:1409.7495*

Baalouch, M., Defurne, M., Poli, J. P., & Cherrier, N. (2019). Sim-to-Real Domain Adaptation For High Energy Physics. In *Workshop on Machine Learning for the Physical Sciences, NeurIPS* 2019.

TRANSFER LEARNING

Two approaches to transfer learning or domain adaptation for interpretable ML models:

- Modify thresholds and leaf weights by learning a transformation from source to target data
- Find a domain-invariant feature representation

Ideas:

- Select a subset of data containing only π_0-production events and learn the transformation on this subset
- Weight real events to “remove” the influence of cross-sections and get distributions comparable to those of simulated data

Still work in progress!

CONCLUSION

- Analysis of CLAS12 data to select DVCS events
- Feature construction principle: get new discriminative high-level variables
- Implementation in several “interpretable” algorithms
- Comparison with other analysis methods
- Still work to do with transfer learning to be able to apply all of this on real data

Thank you!