



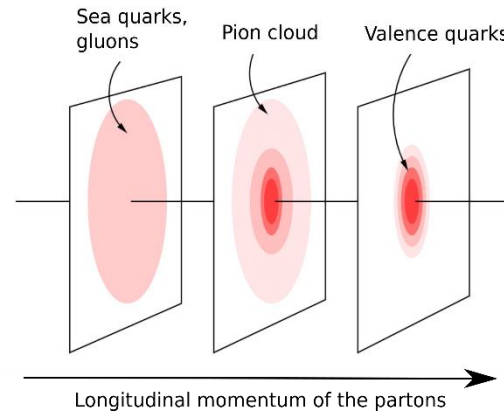
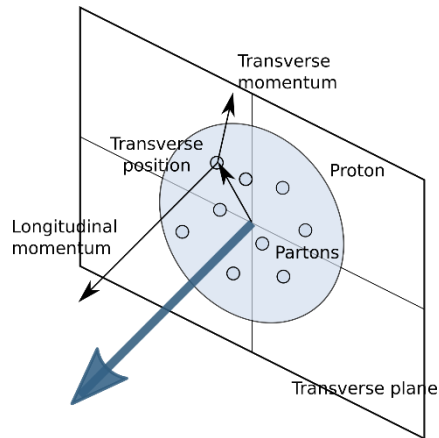
MACHINE LEARNING FOR CLAS12 DATA ANALYSIS WITH GENERALIZED ADDITIVE MODELS

IN2P3/IRFU workshop | Noëlie Cherrier

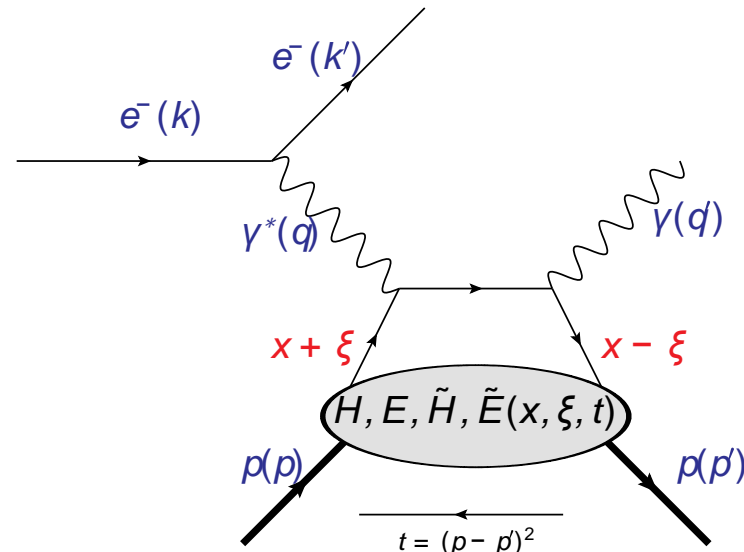


INTRODUCTION

- 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)

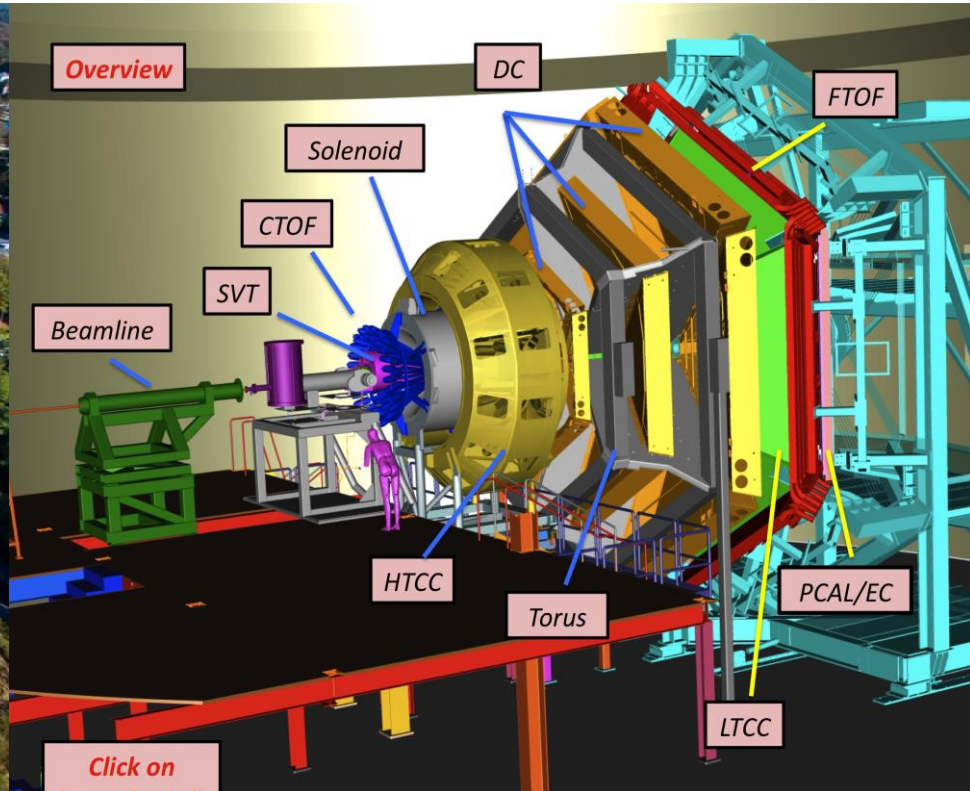


INTRODUCTION

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

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

Machine learning approach to be compared to classical approach



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

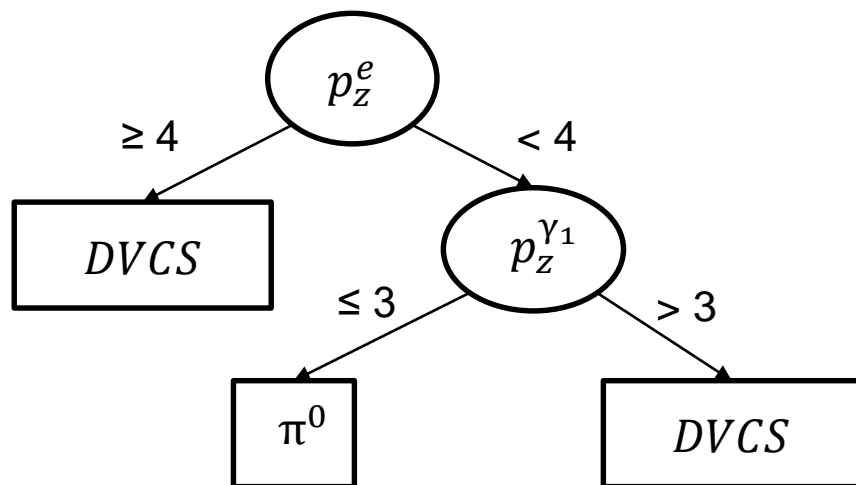


The lack of interpretability is controversial

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

Models for which post-hoc analysis
is not needed



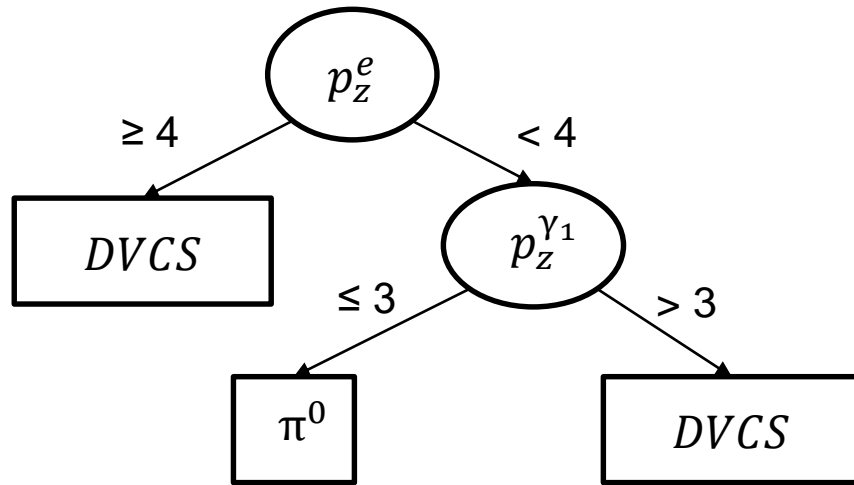
Decision trees

Rule bases

```
(inv_masss_g1g2 in [-inf, -inf, 0.665977, 0.666042]) and (inv_masss_g1g2 in [0.007705, 0.007706, inf, inf]) => Class=DVMP (CF = 0.8)
(energy_g1 in [-inf, -inf, 2.209962, 2.21012]) and (cone_angle_g1 in [-inf, -inf, 16.272992, 16.275288]) => Class=DVMP (CF = 0.76)
(energy_g1 in [-inf, -inf, 3.100969, 3.101338]) and (MM_eg1 in [0.525376, 0.525439, inf, inf]) => Class=DVMP (CF = 0.65)
(energy_g1 in [-inf, -inf, 1.735166, 2.66702]) and (MM_eg1 in [-1.85998, -1.857006, inf, inf]) => Class=DVMP (CF = 0.61)
(MM_eg1 in [1.298545, 1.304201, inf, inf]) and (energy_g1 in [-inf, -inf, 4.182, 4.182101]) => Class=DVMP (CF = 0.66)
(energy_g1 in [3.333313, 3.333823, inf, inf]) and (MM_eg1 in [-inf, -inf, 0.96117, 0.961204]) => Class=DVCS (CF = 0.82)
(energy_g1 in [3.100909, 3.101237, inf, inf]) and (MM_eg1 in [-inf, -inf, 1.084021, 1.084045]) => Class=DVCS (CF = 0.8)
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(cone_angle_g1 in [16.137178, 21.604087, inf, inf]) and (MM_egg1 in [-inf, -inf, -0.538689, -0.537701]) => Class=DVCS (CF = 0.56)
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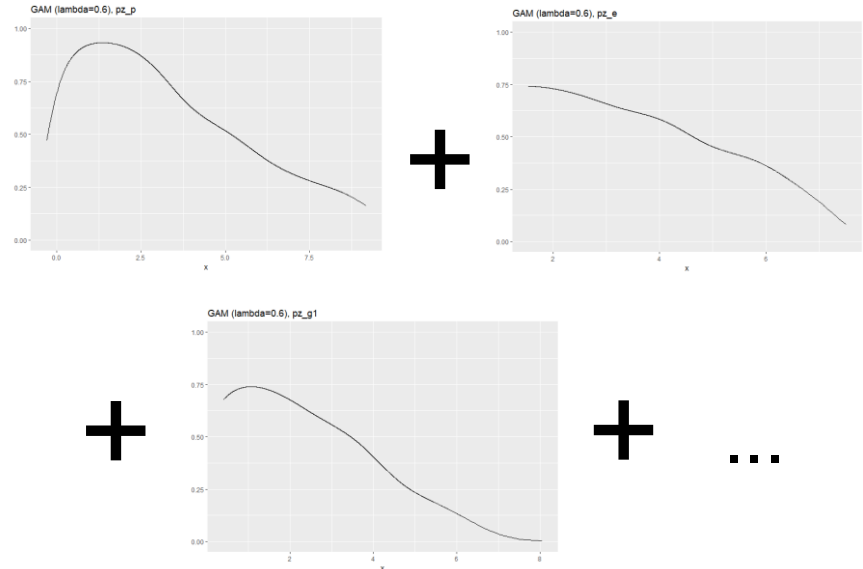


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$$g(E(Y)) = \beta_0 + f_1(x_1) + f_2(x_2) + f_3(x_3) + \dots + f_m(x_m)$$

Generalized Additive Models (GAM)

GENERALIZED ADDITIVE MODELS (GAM)

Generalized Linear Models (GLM) :

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

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

Hastie, T. J. (1986). Generalized additive models. In *Statistical models in S* (pp. 249-307). Routledge.

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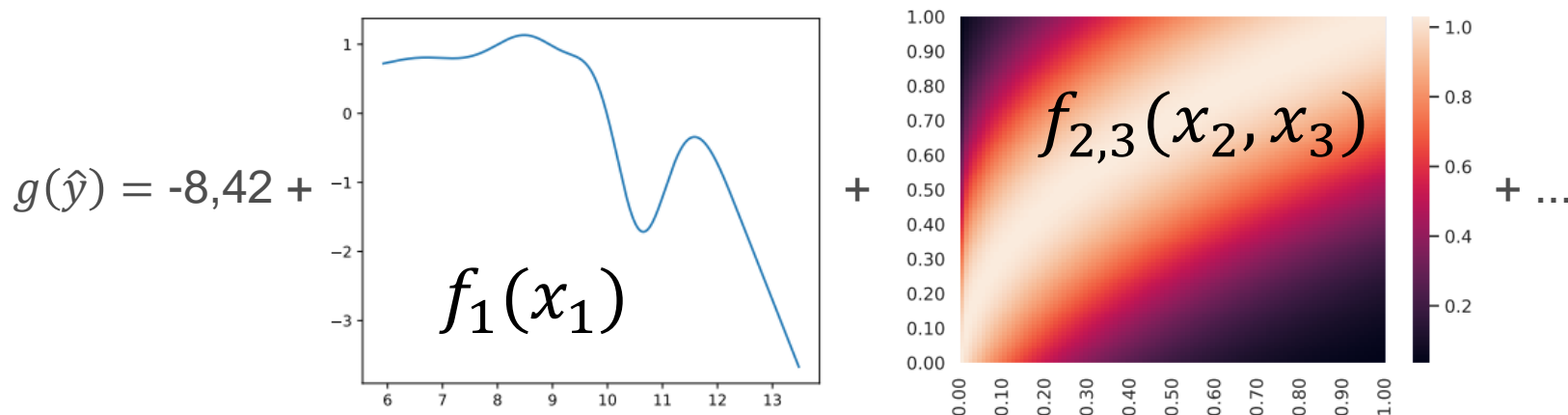
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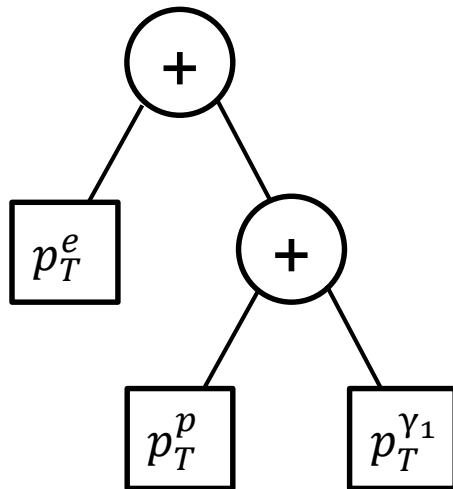
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HOW TO USE PHYSICS KNOWLEDGE?

1. 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

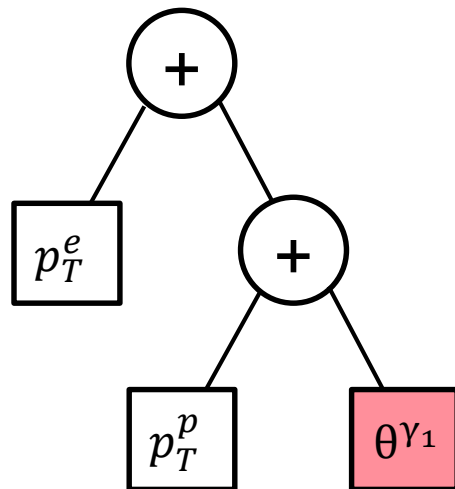
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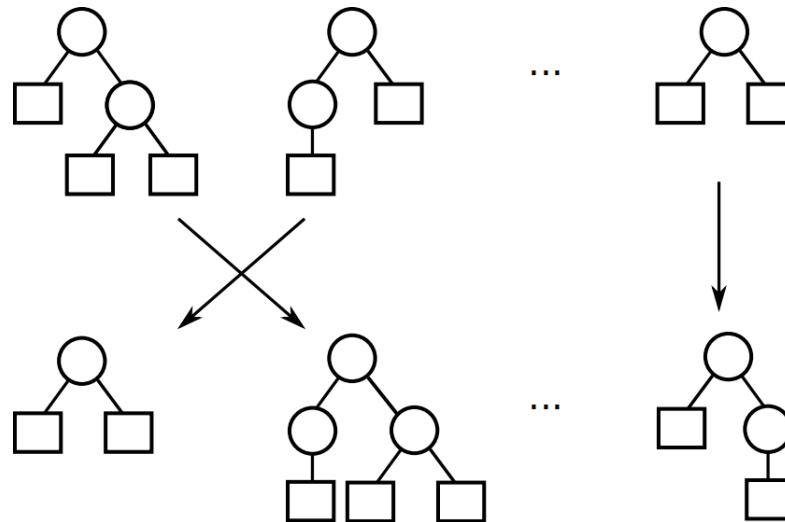
Cherrier, N., Poli, J. P., Defurne, M., & Sabatié, F. (2019, June). Consistent Feature Construction with Constrained Genetic Programming for Experimental Physics. In *2019 IEEE Congress on Evolutionary Computation (CEC)* (pp. 1650-1658). IEEE.

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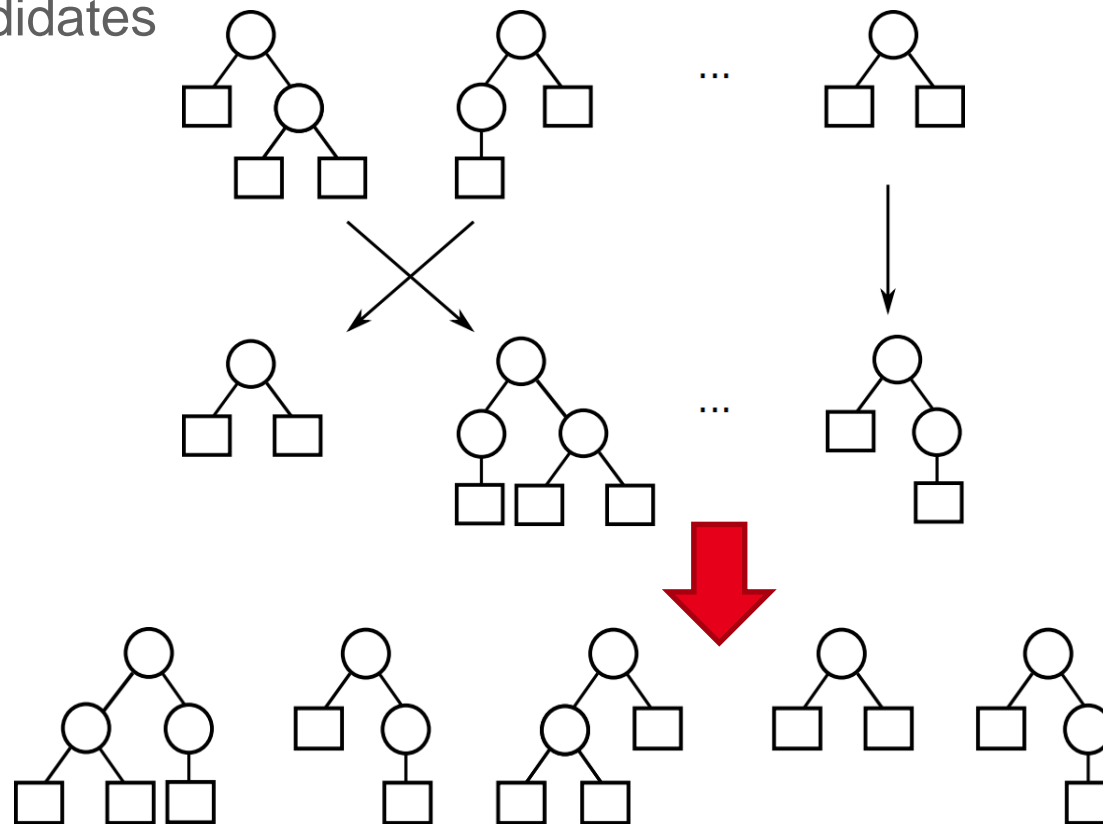


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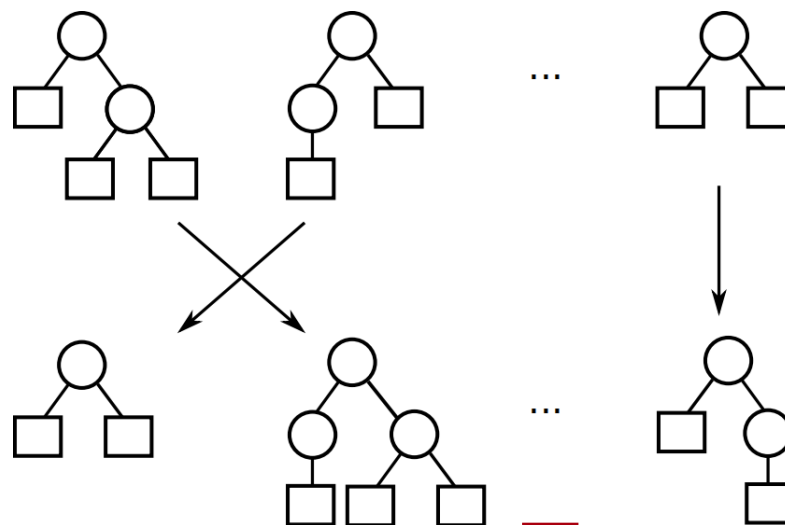


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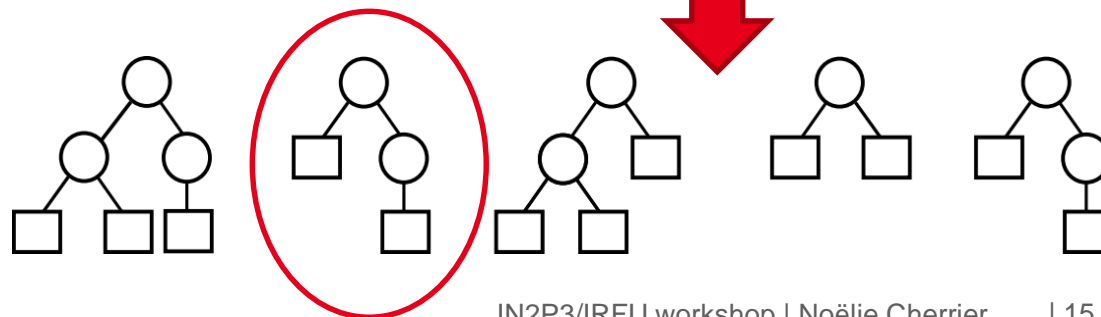
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Evaluation function?



FEATURE CONSTRUCTION IN GA2M

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

→ **gradient boosting**

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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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4) Compute the new model: $g(\hat{y}) = g(\hat{y}) + f_1(x_1)$ (or $g(\hat{y}) + f_{1,2}(x_1, x_2)$) and the new residual $r = y - \hat{y}$, and go back to step 2

FEATURE CONSTRUCTION IN GA2M

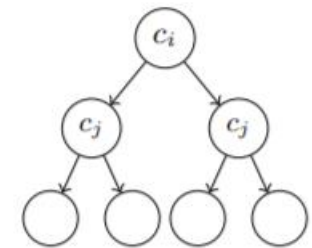
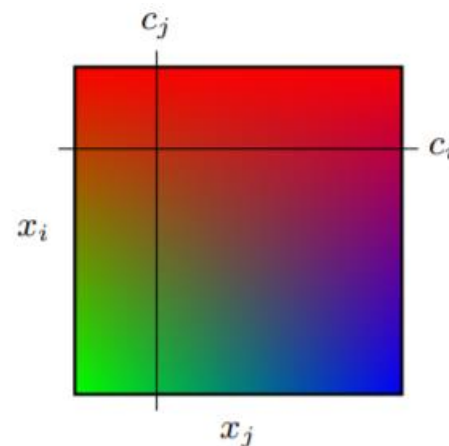
Fitness function for the Genetic Programming algorithm:

Single feature case

Shallow tree (maximum 4 leaves)
Feature fitness: RMS error of the
inducted tree with the residual $y - \hat{y}$

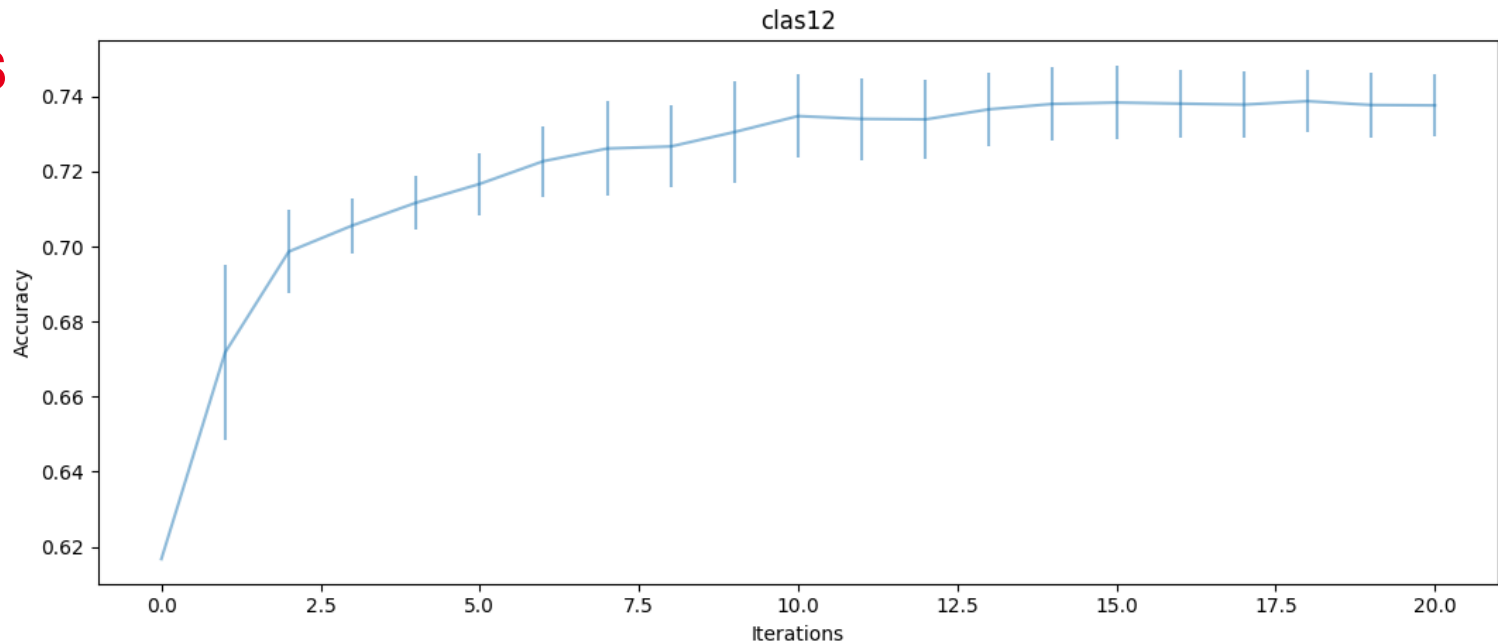
Feature pair case

FAST algorithm, the target being the
residual $y - \hat{y}$



Lou, Y., Caruana, R., Gehrke, J., & Hooker, G. (2013, August). Accurate intelligible models with pairwise interactions. *ACM SIGKDD 2013*.

RESULTS



Neural network	$0.7012 \pm 0,0062$
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Linear SVM	0.6911
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C4.5 with feature construction	$0.7266 \pm 0,0086$ (15 nodes using feature construction)
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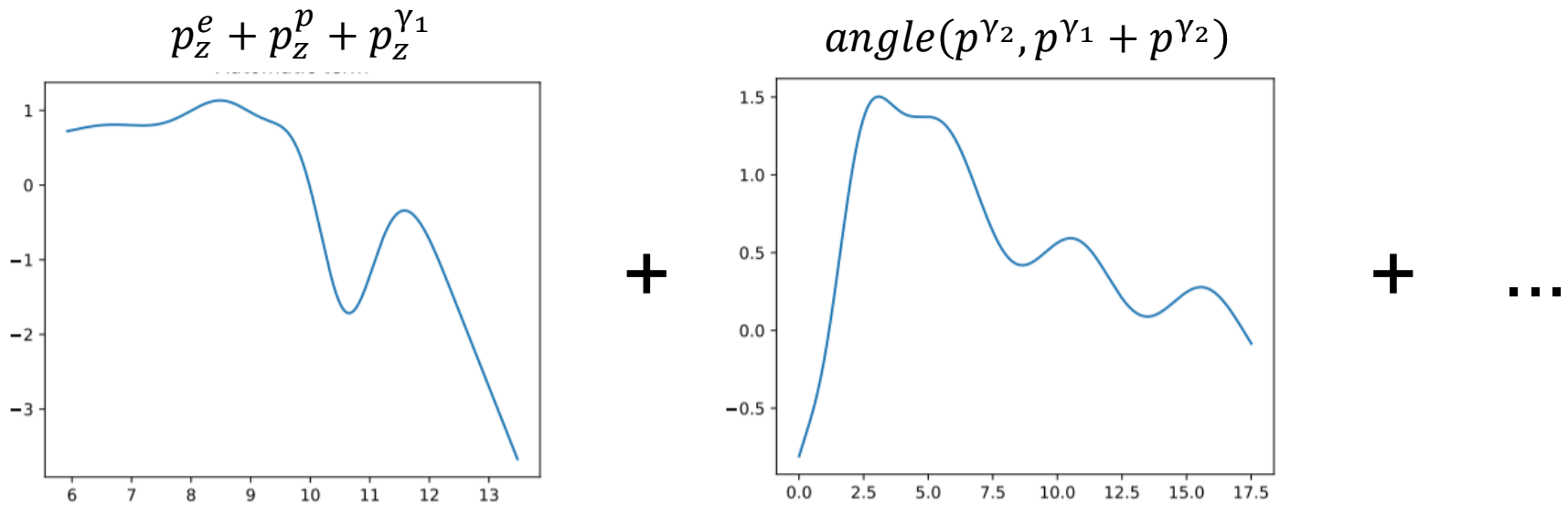
AdaBoost with feature construction	0.7280 ± 0.0063 (50 trees of 1 node each with feature construction)
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Gradient Boosting with feature construction	0.7446 ± 0.0071 (100 trees of 7 nodes each with feature construction)
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Baselines:

RESULTS

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



HOW TO USE PHYSICS KNOWLEDGE?

1. Feature construction
2. Using assumption on variable distributions to guide GAM/GA2M fitting

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Some works use the a priori monotonicity of the input variables w.r.t. the target

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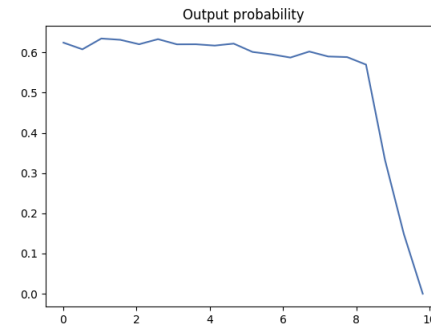
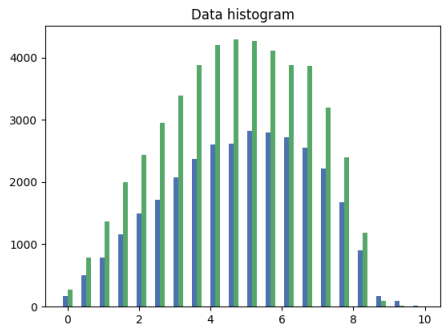
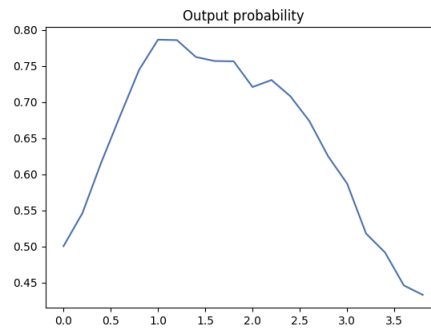
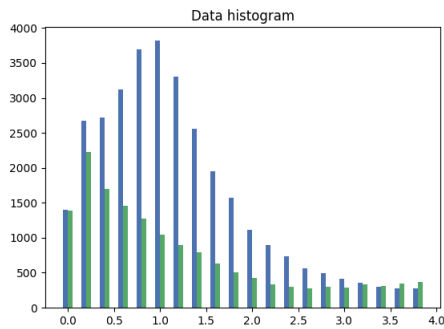
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Monotonicity in physics?



Angle between hypothetical π^0 and photon

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

Missing mass $ep \rightarrow e\gamma$

$$\sqrt{(\|p^e\| + \|p^{\gamma_1}\| - 10,6 - M_p)^2 - \|p^e + p^{\gamma_1}\|^2}$$

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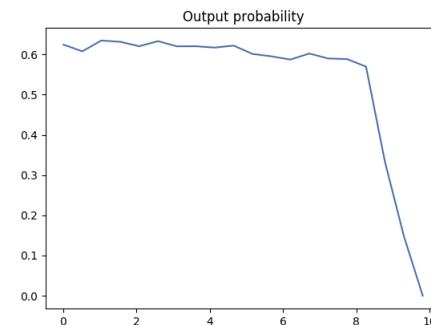
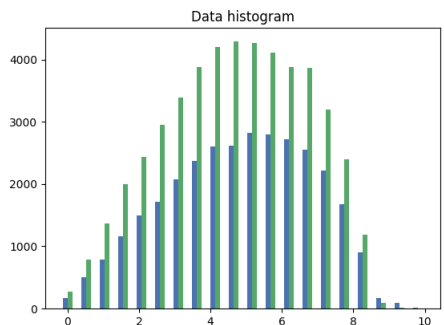
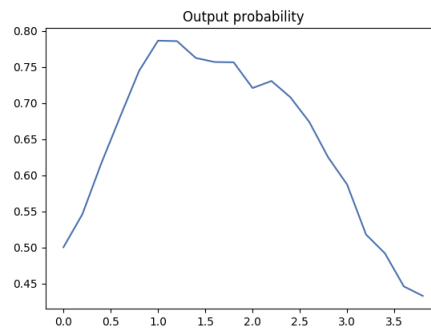
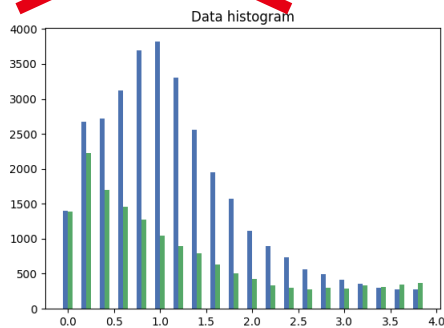
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~~Monotonicity in physics?~~

Bitonicity



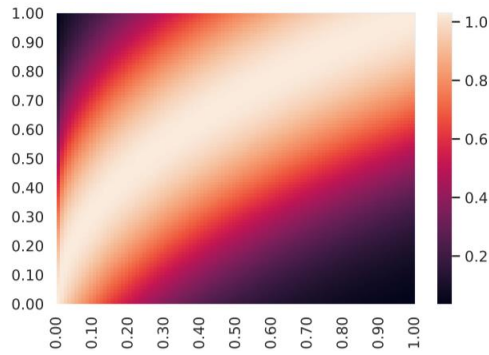
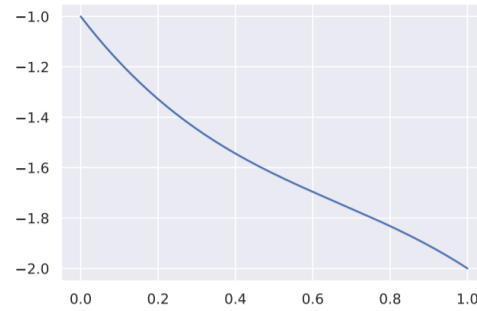
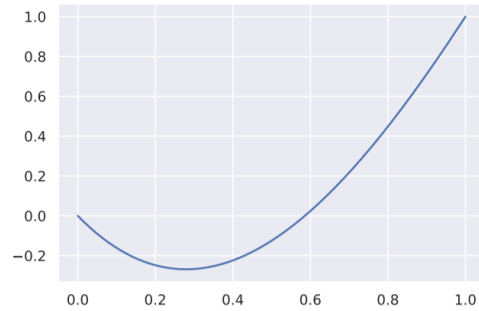
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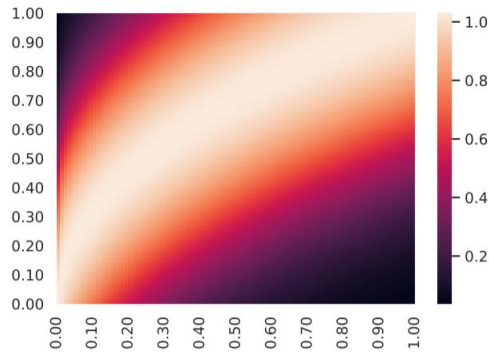
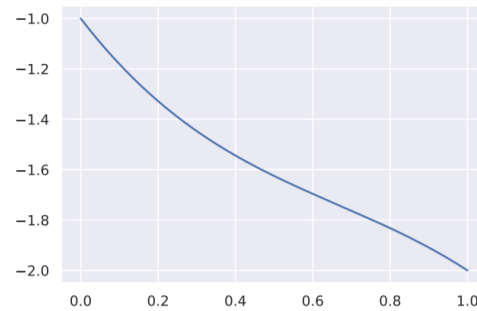
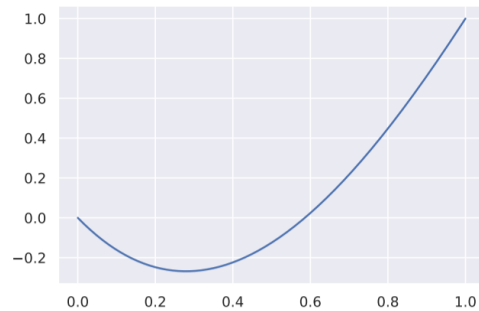
BITONICITY



Bitonicity: either monotonic, or increasing then decreasing, or decreasing then increasing (i.e. unimodal)

Bitonicity criteria:
difference between the function and its cumulative maximum/minimum

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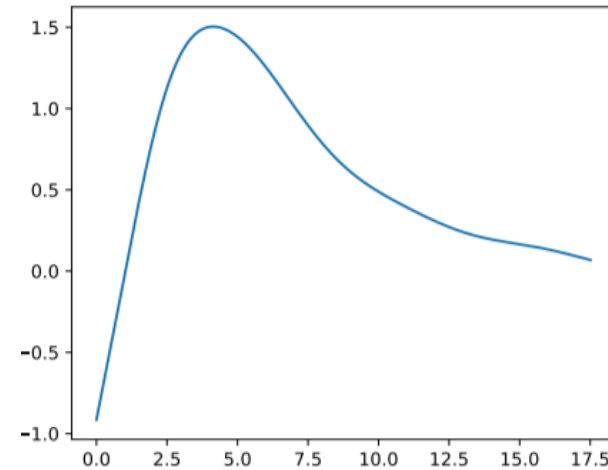
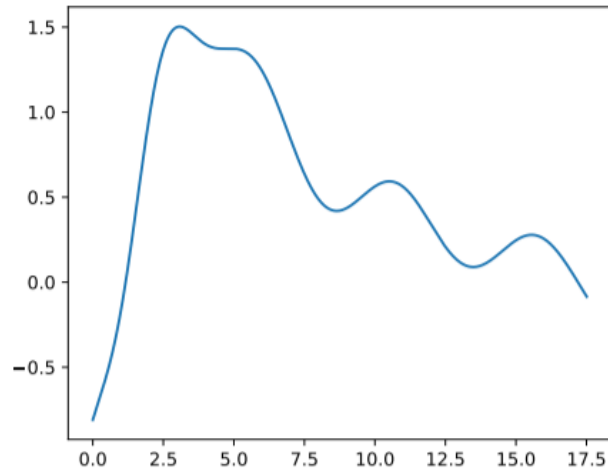
Bitonicity criteria:
difference between the function and its cumulative maximum/minimum

Penalization:

- in feature construction: $\text{fitness} = s - \lambda b$
- in shape functions with regularization in spline fitting

RESULTS

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

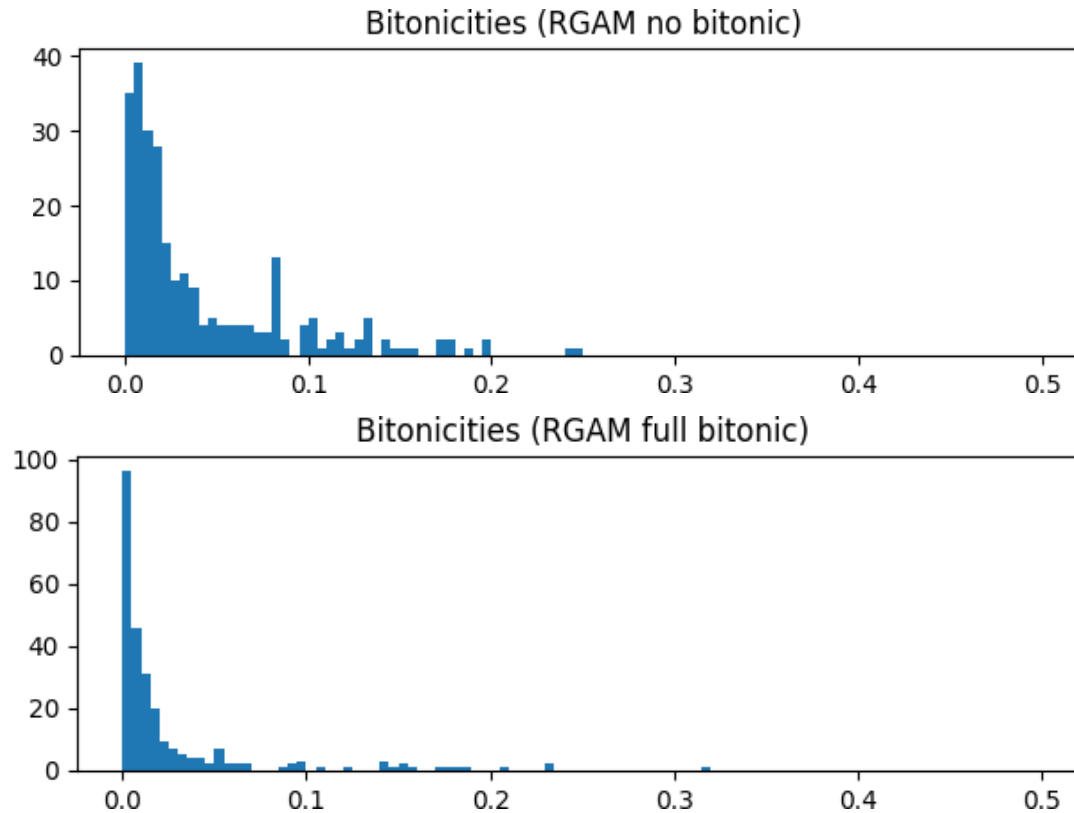


	Accuracy	Bitonicity score (penalty)
Without bitonicity constraint	0.738 ± 0.008	0.041 ± 0.048
With bitonicity constraint	0.735 ± 0.006	0.025 ± 0.046

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	Accuracy	Bitonicity score (penalty)
Without bitonicity constraint	0.738 ± 0.008	0.041 ± 0.048
With bitonicity constraint	0.735 ± 0.006	0.025 ± 0.046

Bitonicity penalties distributions:



CONCLUSION

- GAM and GA2M: intelligible models, not perfectly transparent but more flexible than a rule base
- Gives good results on CLAS12 data particularly when exploiting feature construction
- Prior knowledge to include: bitonicity of the most discriminative variables
- Using this prior knowledge leads to simpler models that remain efficient
 - Enforcing bitonicity is equivalent to increasing the regularization parameter
 - The model is more understandable when it matches prior knowledge on the input variables

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Thank you for listening!

