"Hyper-K physics workshop at DIPC"

(June 2023)

"MACHINE LEARNING IN PARTICLE PHYSICS"

Bryan Zaldivar (Valencia)

Outline

- What does machine learning bring to physics?
- Some examples of different uses of ML for Dark Matter [DISCLAIMER]
- Good practices when applying ML to physics

MOTIVATION

* Physical knowledge of background is limited
  (common problem in astrophysics)

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e.g. • γ-rays
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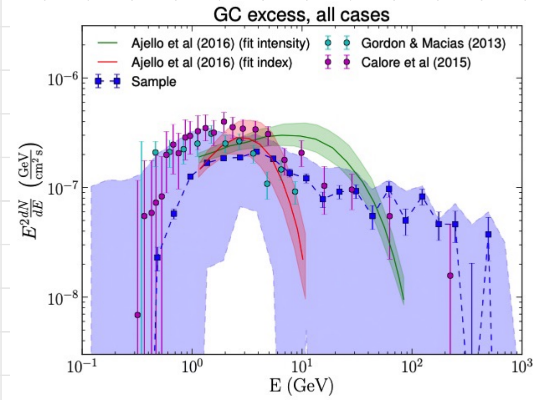
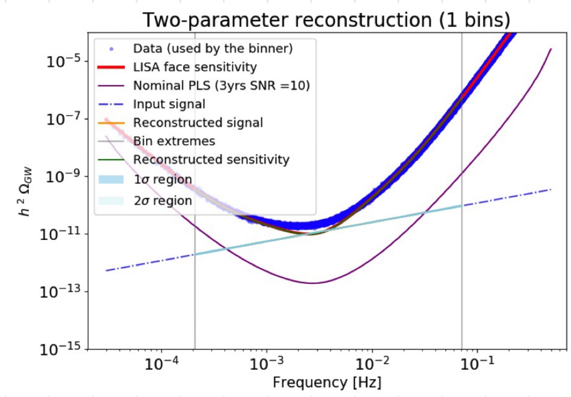
Fermi-LAT, 1704.03910



Caprini et al, 1906.09244



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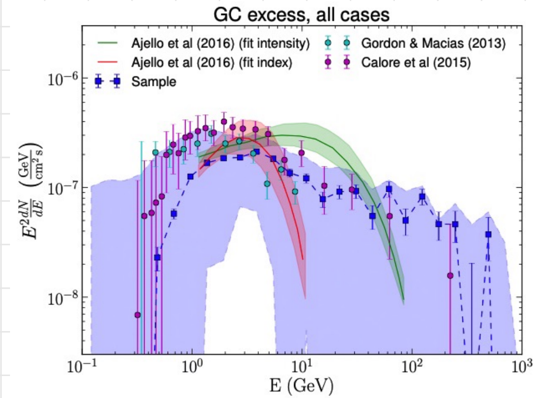

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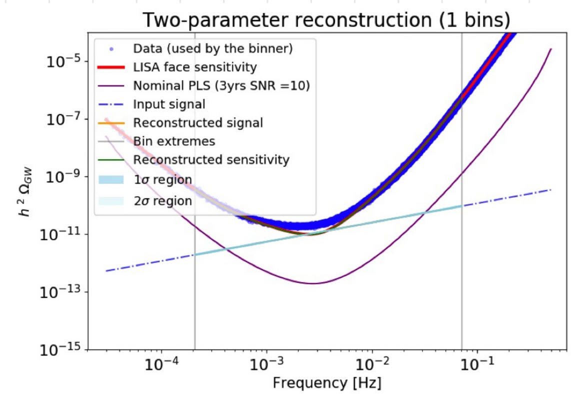

Signal + Background $\Longleftrightarrow$ Data

interest
(Physical model)

nuisance
(data-driven model)

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* Physics well known, but observables very complicated to compute

(complex topology, particle misidentification, etc)

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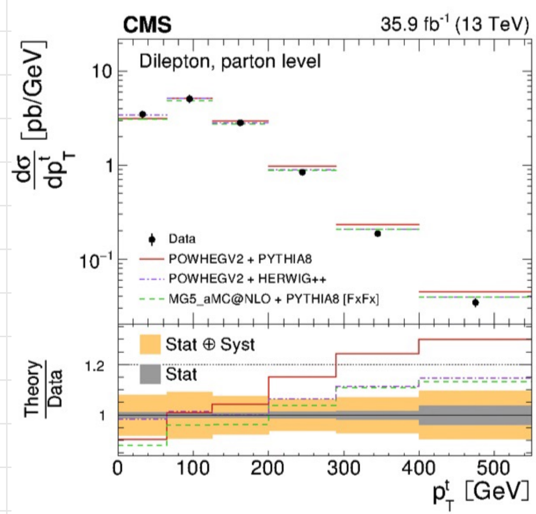
TOP-17-014-PAS



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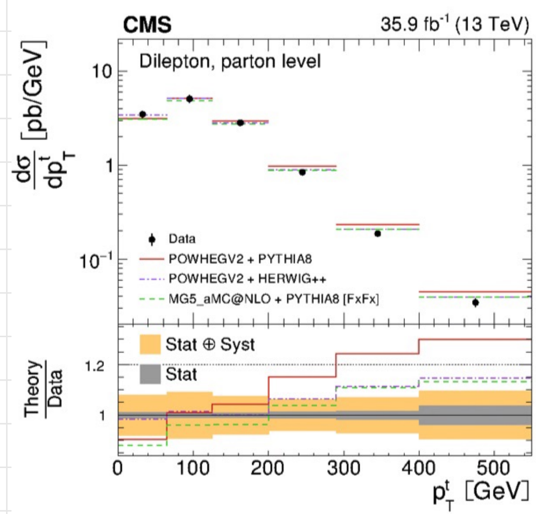
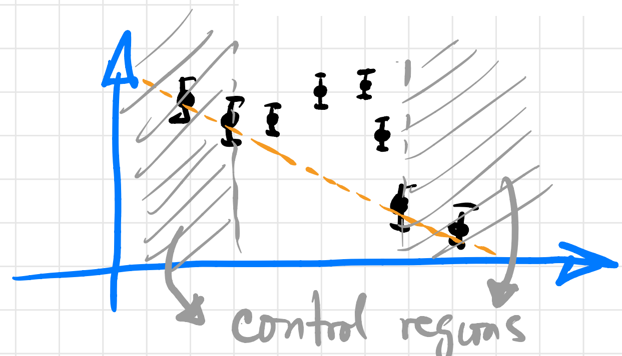


Data-driven methods to infer the background from inter/extrapolations



MOTIVATION

Snowmass, 2209.07426

Name	Technology	Target	Active Mass	Experiment Location	Start Ops	End Ops
Currently Running or Under Construction						
LZ	TPC	LXe	7,000 kg	SURF	2021	2026
PandaX-4T	TPC	LXe	4,000 kg	CJPL	2021	2025
XENONnT	TPC	LXe	7,000 kg	LGNS	2021	2025
DEAP-3600	Scintillator	LAr	3,300 kg	SNOLAB	2016	2025
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DAMA/LIBRA	Scintillator	NaI	250 kg	LNGS	2003	
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SABRE PoP	Scintillator	NaI	5 kg	LNGS	2021	2022
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CDEX-10	Ionization (77K)	Ge	10 kg	CJPL	2016	
EDELWEISS III (High Field)	Cryo Ionization / HV	Ge	33 g	LSM	2019	
SuperCDMS CUTE	Cryo Ionization / HV	Ge/Si	5 kg/1 kg	SNOLAB	2020	2022
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CRESST-III (HW Tests)	Bolometer Scintillation	CaWO4		LNGS	2020	
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NEWS-G	Gas Drift	CH4		SNOLAB	2020	2025
DAMIC-M prototype	CCD Skipper	Si	18 g	LSM	2022	2023
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SENSEI	CCD Skipper	Si	2 g	Fermilab	2019	2020
SENSEI	CCD Skipper	Si	100 g	SNOLAB	2021	2023

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ALETHEIA	TPC	He		China Inst. At. Energy		
TESSERACT	Cryo TES	LHe, SiO_2, Al_2O_3, GaAs		undetermined	2026	
CYGNO	Gas Directional	He + CF_4	0.5 - 1 kg	LNGS	2024	
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Windchime	Accelerometer array			Multiple sites		
MAGNETO-χ	Cryogenic MMC	Diamond, Sapphire, etc.				

Experiment	Final state	Threshold/sensitivity	Field of view	Location
Current experiments				
Fermi	Photons	10 MeV – 10^3 GeV	Wide	Space
HESS	Photons	30 GeV - 100 TeV	Targeted	Namibia
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Future experiments				
CTA	Photons	20 GeV - 300 TeV	Targeted	Chile & Spain
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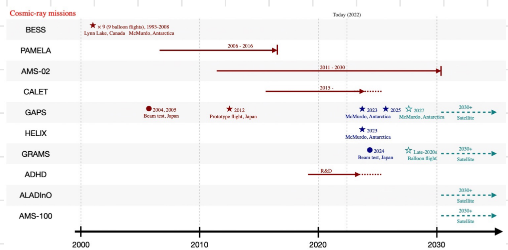

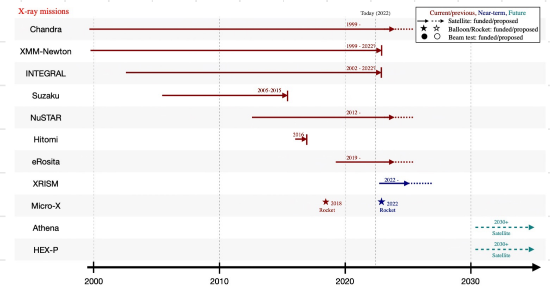

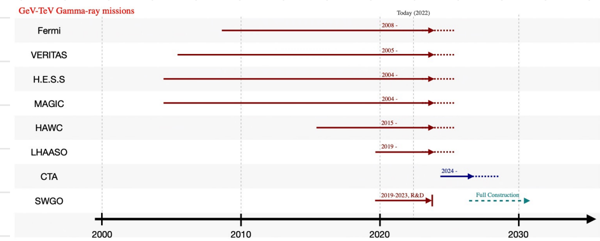

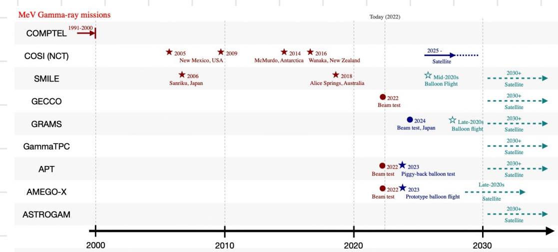

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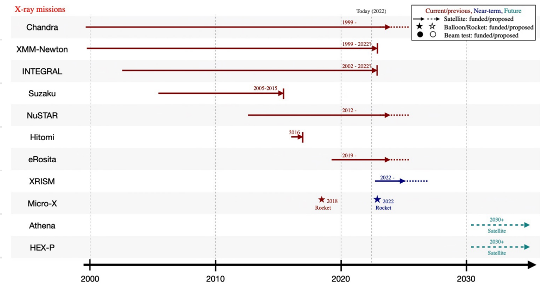
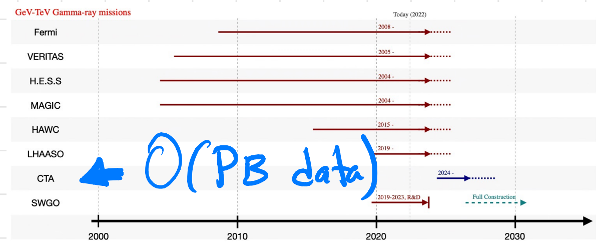
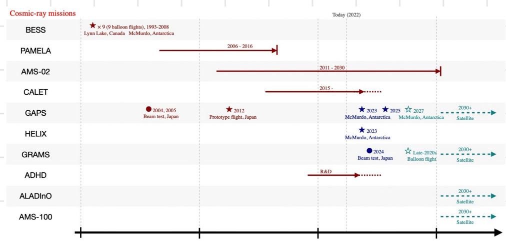
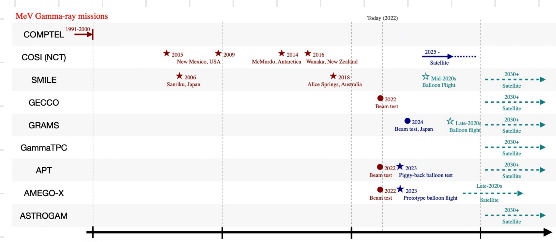




O(PB data)





O(40) experiments operative in near future!

MOTIVATION

* Statistical bottleneck

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* Statistical bottleneck

- More complex datasets

$\Downarrow$

More complex physical modeling

$\Downarrow$

More complex simulator

MOTIVATION

* Statistical bottleneck

- More complex datasets

↓

More complex physical modeling

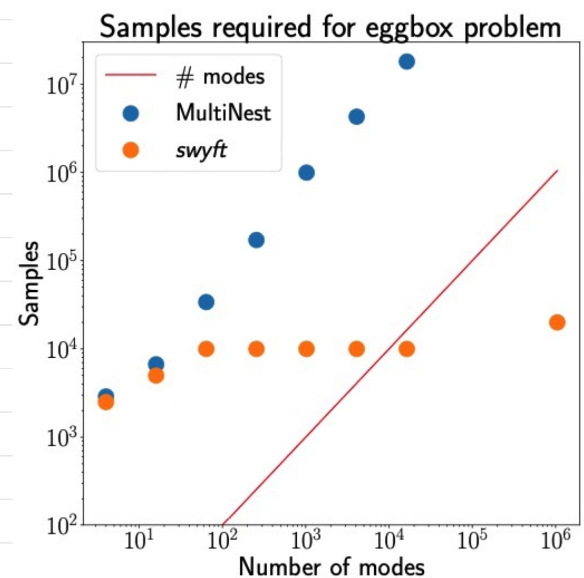
↓

More complex simulators

↓

Better statistical treatment!

Miller et al, 2011.13951



- better scaling
- more descriptive
- Higher statistical power

MOTIVATION

* Hints about the underlying physics

MOTIVATION

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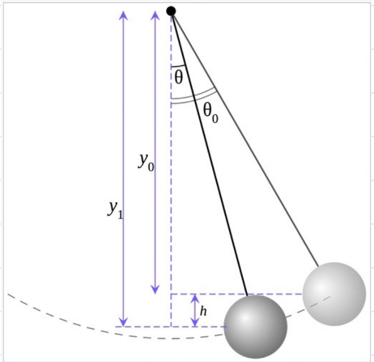
- The intrinsic dimension of → # physical variables
  - Single pendulum : 2
  - Lava lamp : ?



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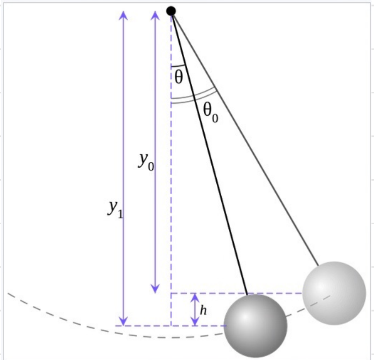


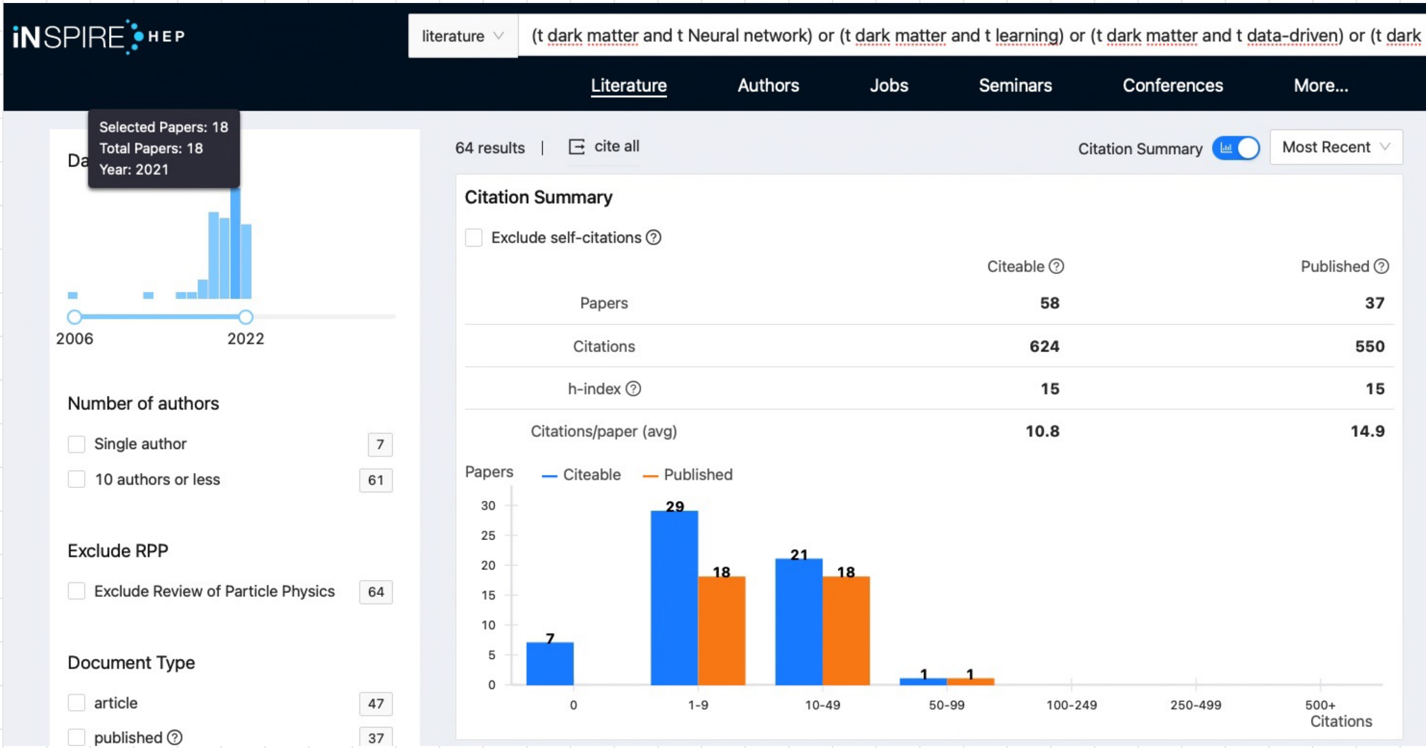
Statistical model (ML)

ID = 7 − 8

(see 2112.10755)

DARK MATTER WITH MACHINE LEARNING

[likely same trend in other areas]



Two main ML paradigms
used in physics

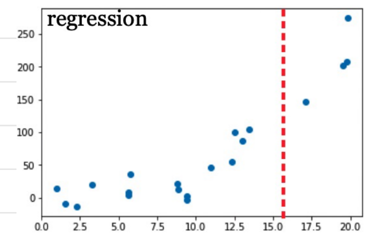
SUPERVISED LEARNING

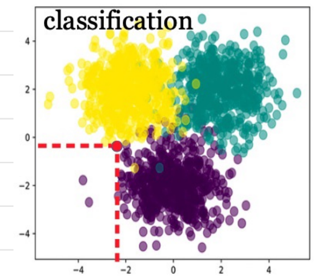
Tasks

1) Estimate underlying distribution

$$y(\vec{x}) \sim p\left(f(\vec{x};\vec{\theta}), \sigma\right)$$

$$\text{data} = \{\vec{x}_i, y_i\}$$





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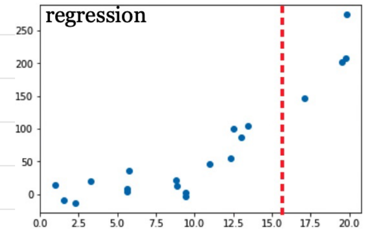
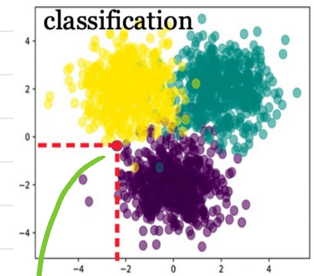
- Assume shape of p,
  estimate $f(\vec{x},\vec{\theta})$ with a ML model

[useful for estimating nuisance contributions,
(c.f. Motivation #1)]





2) Prediction for new $\vec{x}$

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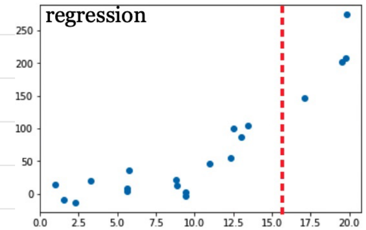

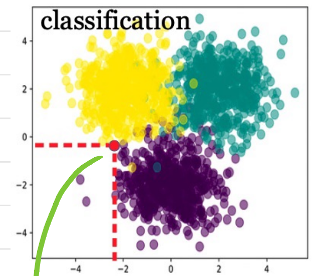

- Assume shape of p,
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  [useful for estimating nuisance contributions,
  (c.f. Motivation #1)]

2) Prediction for new $\vec{x}$

- $f(\vec{x},\vec{\theta})$ given by a physics model (infer physical parameters $\vec{\theta}$)
  Estimate shape of p with a ML procedure

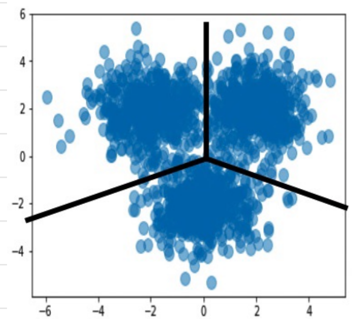
UNSUPERVISED LEARNING

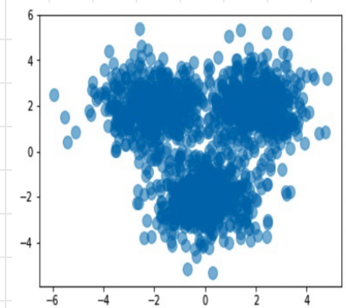
data $= \{ \vec{x}_i \}$

Tasks

1) Clusterize the data

(very useful e.g. in collider physics)





UNSUPERVISED LEARNING

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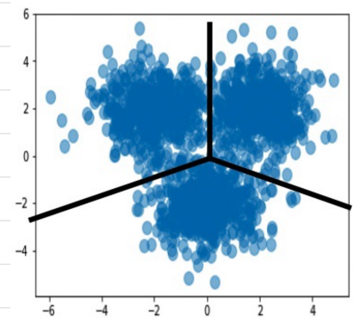
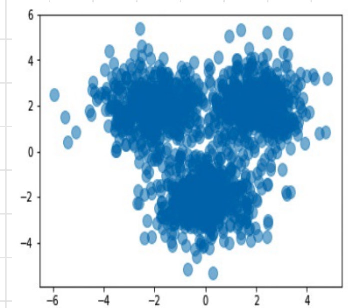
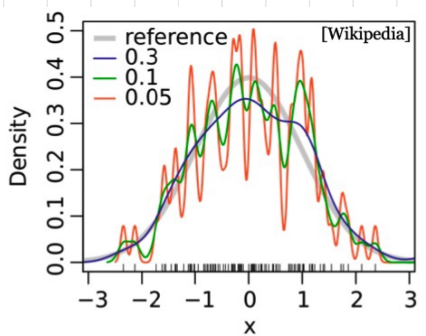




Tasks

1) Clusterize the data
(very useful e.g. in collider physics)

2) Probability density estimation
(astrophysics, cosmology, everywhere...)



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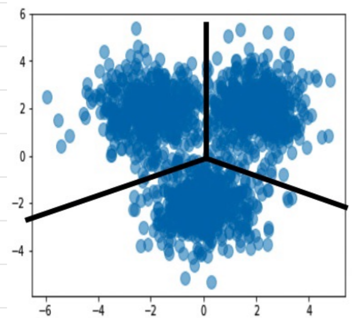

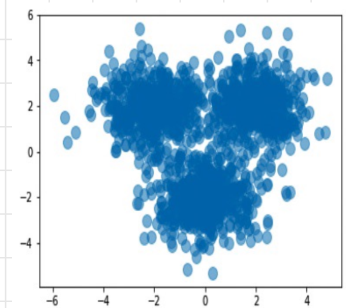

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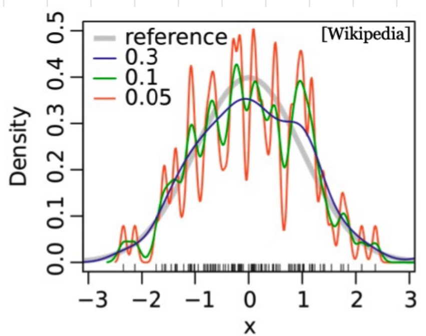
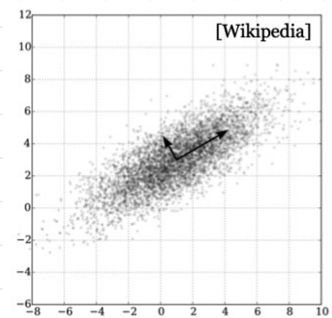


3) Dimensionality reduction
(everywhere)



Some examples of applications

[by no means exhaustive!!]

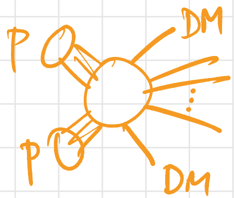
I DM searches at the LHC (Banerjee et al, 1705.02327)

(I) DM searches at the LHC (Banerjee et al, 1705.02327)

- What is the motivating issue?

Final state topology may be quite complex

$\Rightarrow$ potentially large phase space!



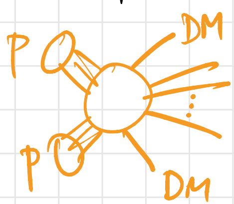
traditional analyses (e.g. cut-based) may give poor performance

(I) DM searches at the LHC (Banerjee et al, 1705.02327)

• What is the motivating issue?

Final state topology may be quite complex

$\Rightarrow$ potentially large phase space!



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Frame it into a ML classification problem

(optimize signal-to-bckg ratio)

ML classifier is (formally) an approx to the

$$TS = \frac{p(x\,|\,H_0)}{p(x\,|\,H_1)}$$

highest statistical power

$\hookrightarrow$ Neural network, Boosted Decision Trees, ...

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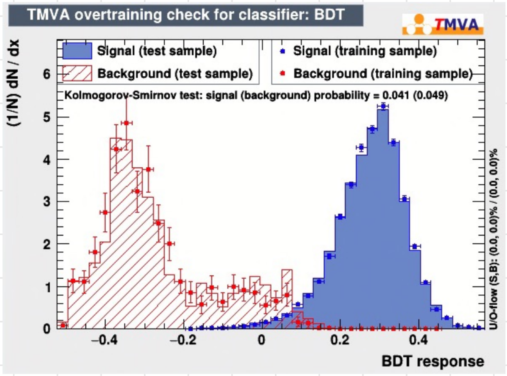
↳ simple case study with a monojet signal



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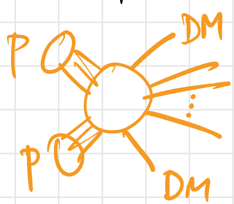

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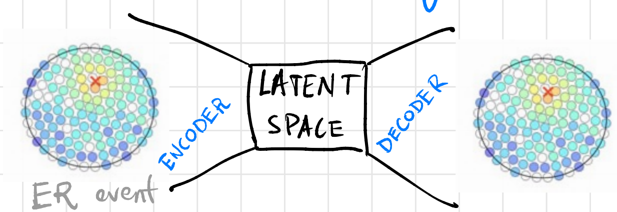

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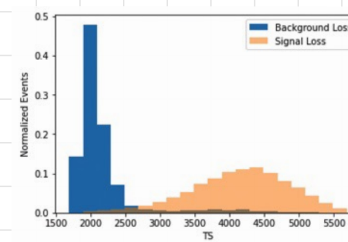
The resulting distribution should be distinguishable from the bckg one



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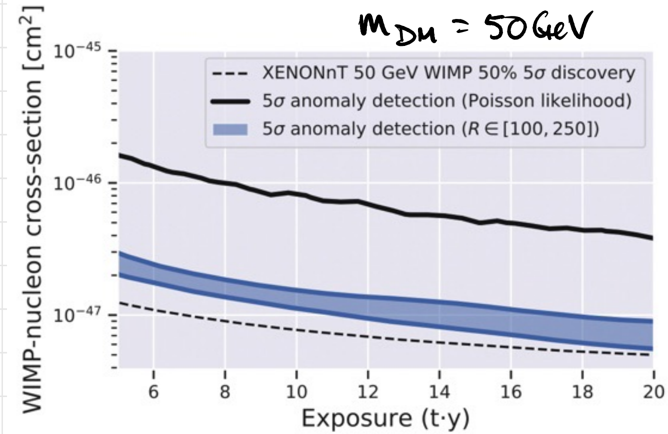
$m_{DM} = 50\,\mathrm{GeV}$



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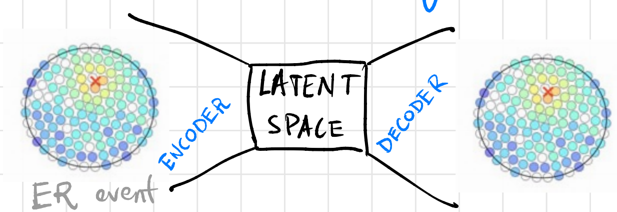

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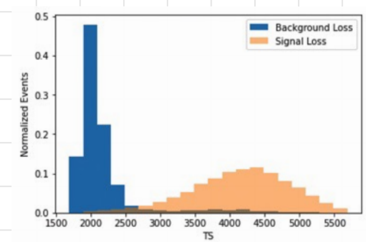

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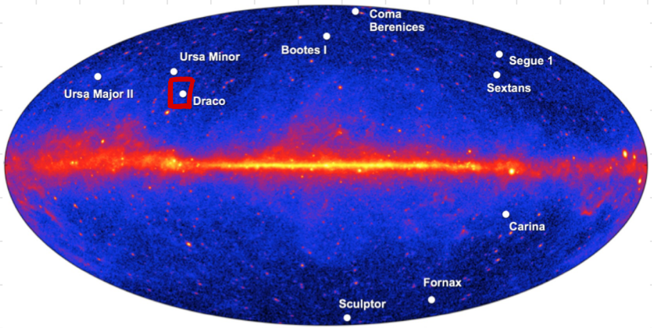
Fermi γ-rays at dSphs



Motivation

1) Typical bckg estimation has limitations
   * Templates are biased (limited knowledge of physics)
   * Local fitting of templates (no global consistency)
   * No clear way of accounting for prediction uncertainties

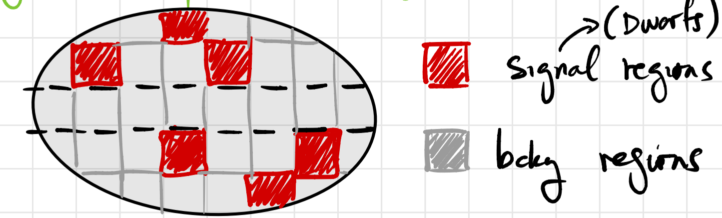
(Calore, Serpico, Zaldivar, 1803.05508) cont...

Aiming for a global, unbiased estimation of the background probability distribution

(Calore, Serpico, Zaldivar, 1803.05508) cont...

Aiming for a global, unbiased estimation of the background probability distribution

Idea:



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Aiming for a global, unbiased estimation of the background probability distribution

$$\text{Data} = \{\vec{x}_i, y_i\}_{i=1}^{N}$$

$N \to$ all pixels of the sky

$\vec{x}_i$: spatial coordinates

y_i: counts

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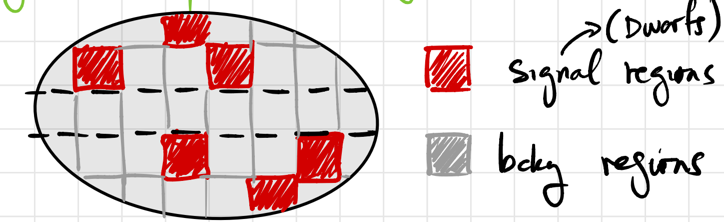

$$p(\vec{x}, y) = \frac{1}{N} \sum_i k_\alpha(\vec{x}-\vec{x}_i) \cdot g_\beta(y-y_i)$$

↳ unbiased estimator of the true PDF

$k_\alpha(\cdot)$, $g_\beta(\cdot)$: kernel functions

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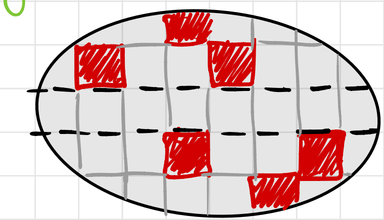

signal regions $\to$ (Dwarfs)

bckg regions

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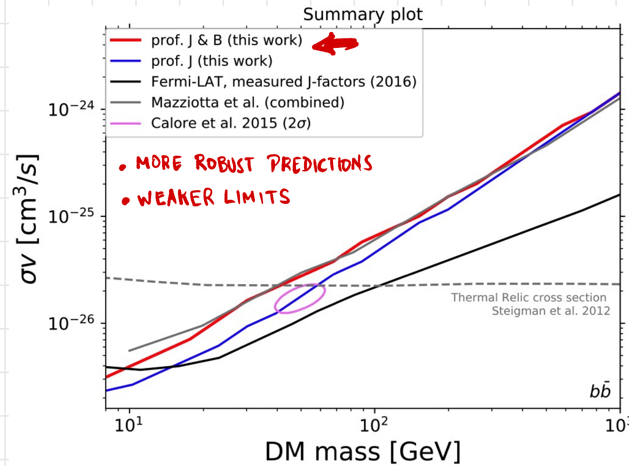

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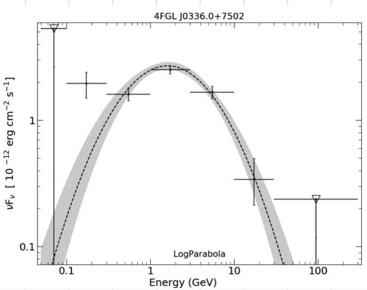
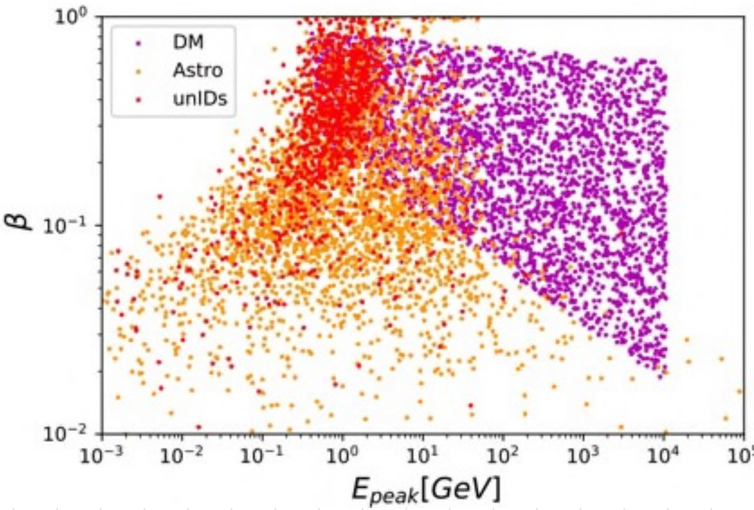
Astrophysical sources vs. Dark Matter sources



✓ ✓ Energy spectrum

✓ X Exp. uncertainties

✓ X Detection significance



Idea: DM inherits statistical properties of the unID's

(Gammaldi et al, 2207.09307) cont...

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Not so: input data have uncertainties

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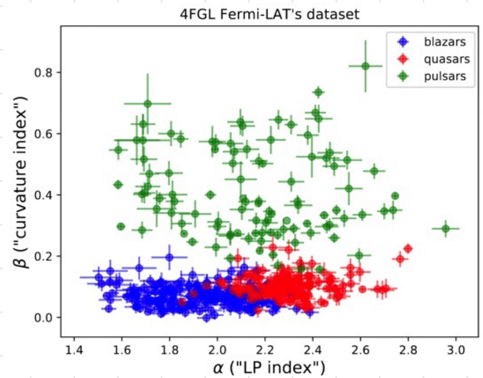
[Villacampa et al, 2001.10523]



Gaussian Process model

$\vec{x} \sim N(\vec{\mu}, \vec{\sigma})$

latent variables to be inferred

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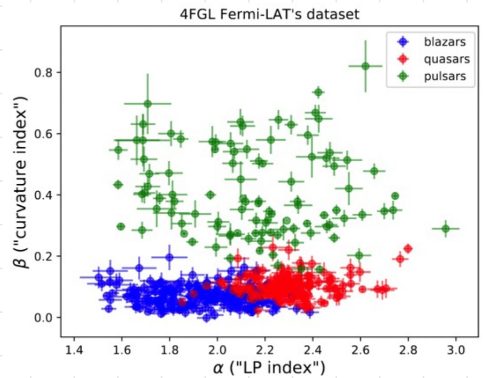

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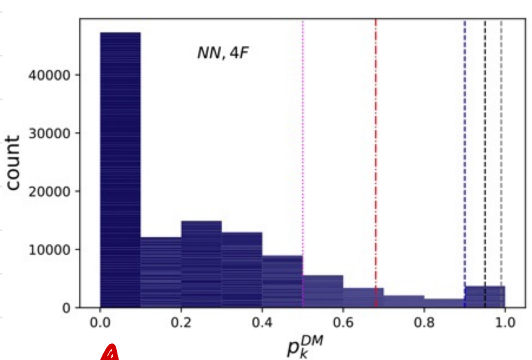
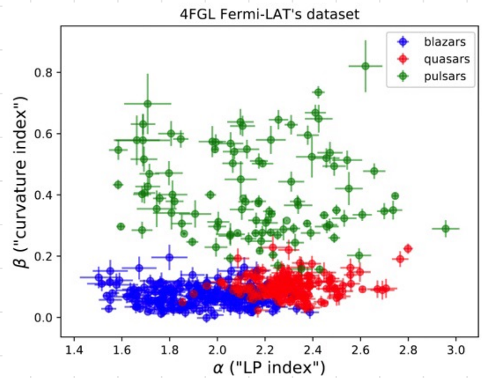


No statistically significant evidence for DM



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V Warm dark matter mass from strong lensing

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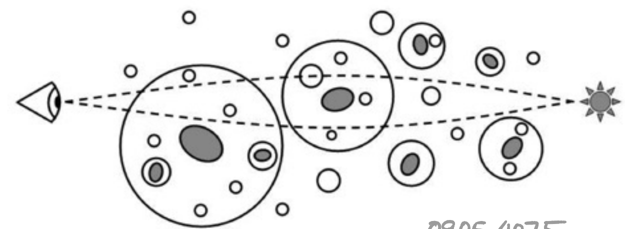

0905.4075

nuisance
- Size and position of the main lens
- Brightness distribution and position of the source
- Position, mass, distance, etc of all the subhalos

→ Warm dark matter mass ← parameter of interest

Typical MCMC algorithms don't scale well with dimensionality of the param. space

(Anau Montel et al, 2205.09126) cont...

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Solution

Estimate $p(\vec{\theta} \mid \text{data})$ directly with a neural network

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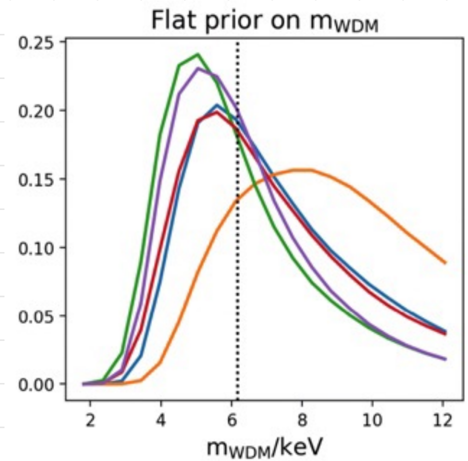
$\Bigg\}$ Inferring the warm DM mass $\Rightarrow$



Important warnings to beware of

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Facts:

- Very large models (DNNs) have built-in overfitting control
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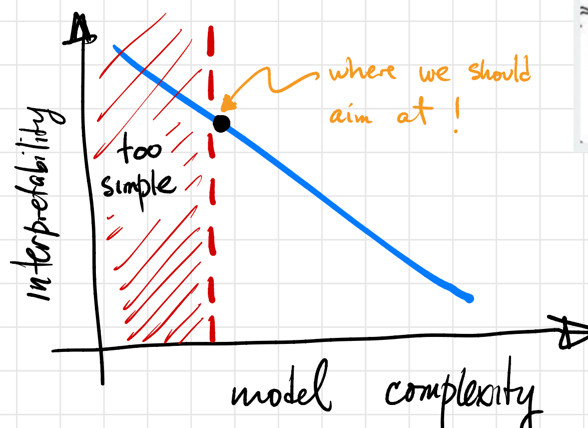

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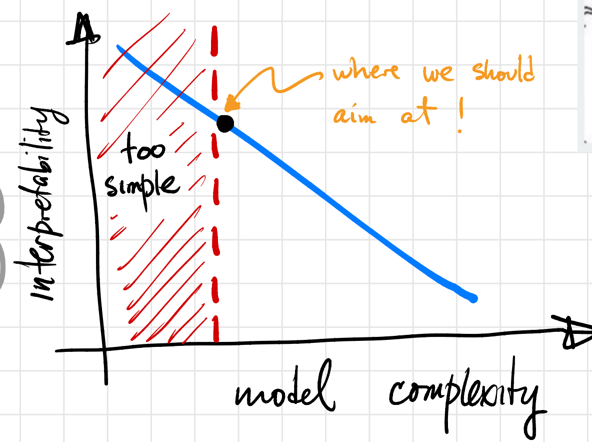
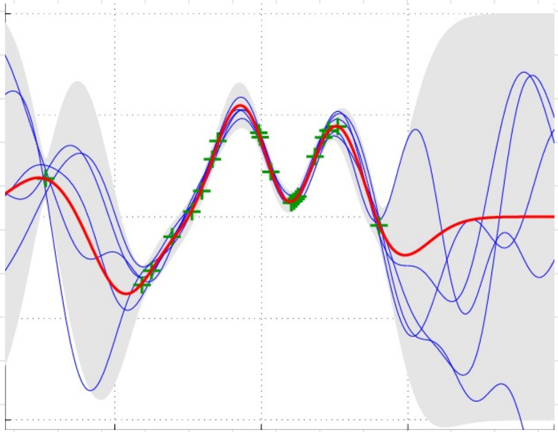


Remember that polymials are also -as neural nets- Universal approximators !!

ii) Uncertainties related to the modeling itself

(a.k.a. "epistemic" uncertainties)



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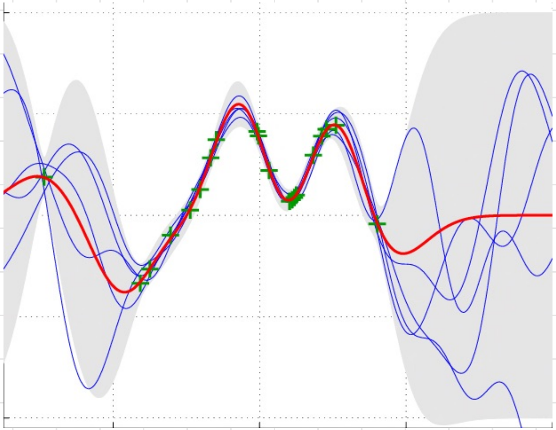

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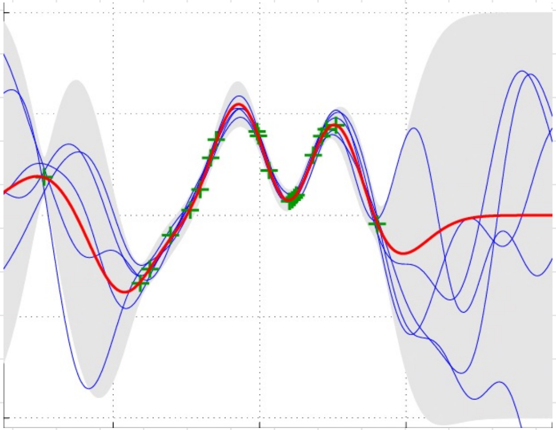

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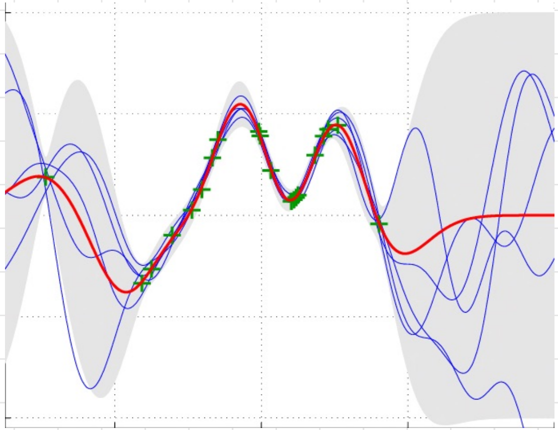

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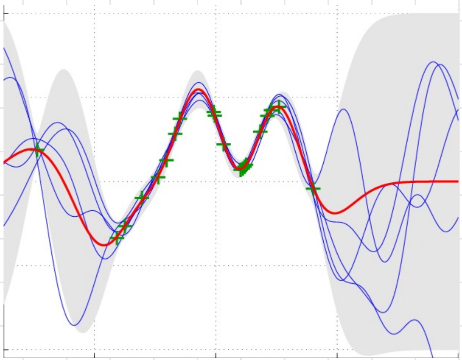
- Cats don't have error bars (maybe) but in science, uncertainty estimation is mandatory!

iii) ML predictions vs. physical plausibility

How many of these possible solutions are physically meaningful ?

[a priori no physics knowledge]



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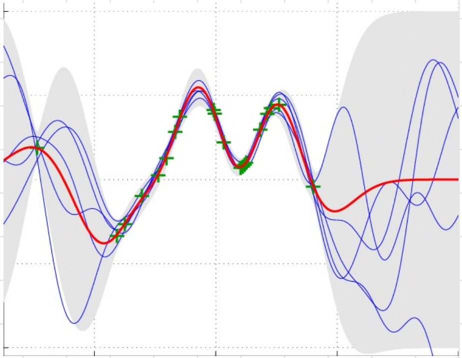

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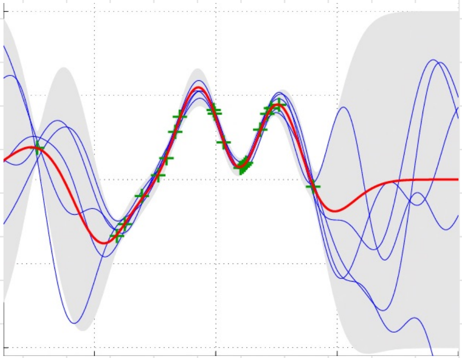

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Data

$\{\vec{x}_i, y_i\}$

Statistical (ML) model

$P(y \mid f_{ML}(\vec{x}, \vec{\theta}))$

Loss function   Partial diff. eq.

$$-\ln p(y \mid f_{ML}) + \mathcal{F}(f_{ML}, \partial_{\vec{x}} f_{ML})$$

Take-home messages

* ML is proving to be an essential tool in modern physics (unfortunately embedded in a gigantic hype)

* As physicists, we have the responsability to make use of such tools in a scientific meaningful way

* ML for science still in its infancy
  ⇒ A lot to do in Physics–ML symbiosis