Efficient Machine Learning for new physics discoveries

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Master Thesis in Computer Science

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Artificial intelligence (AI)

Machine Learning + Data

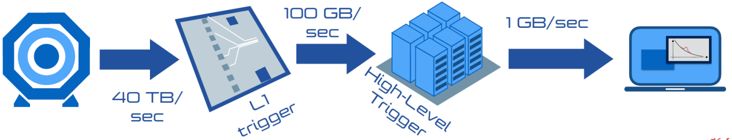
The costs of AI

GPT-3 (175B parameters)†:

- 355 years of GPU training
- $ 4.6 M

† https://lambdalabs.com/blog/demystifying-gpt-3/

Machine Learning for High Energy Physics



This thesis

Efficient Machine Learning for High Energy Physics

Model	Training time	Resources
Our approach	$\mathcal{O}(\mathrm{s})$	**Single GPU machine**
Neural networks	$\mathcal{O}(h)$	Farm of CPUs

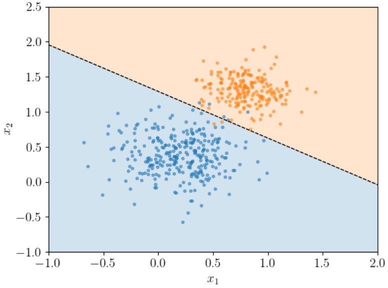
Supervised learning

Given a *training set*

$$(x_i, y_i)_{i=1}^{n} \in (\mathbb{R}^d \times \{0,1\})^n$$

find a *map*

$$f_n(x_{\text{new}}) \sim y_{\text{new}}$$



Loss & target functions

Empirical Risk Minimization: $$f_n = \arg\min \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(x_i))$$

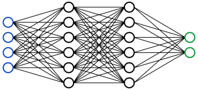
Logistic loss: $$\ell(y, f(x)) = \log(1 + e^{yf(x)}) \longrightarrow \lim_{n\to\infty} f_n = \log \frac{p(1|x)}{p(0|x)}$$

Models

$$f_w(x) = w^T x$$

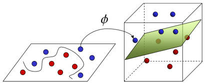
Neural networks

$$w^T \sigma(B^T x)$$

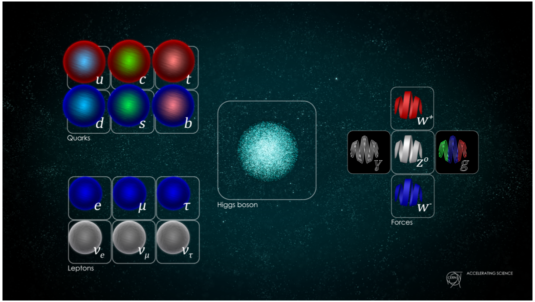


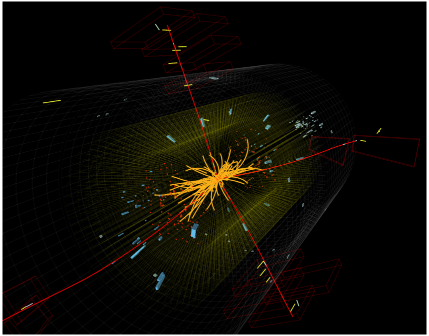
Kernel methods

$$w^T \Phi(x)$$



Theory vs Data





Theory vs Data

$$\{x_i\}_{i=1}^{\mathcal{N}_0} \sim p(x|0), N(0) \longleftarrow \text{ Standard Model (\textit{known})}$$

$$\{x_j\}_{j=1}^{\mathcal{N}_1} \sim p(x|1), N(1) \longleftarrow \text{ Data (\textit{true, unknown})}$$

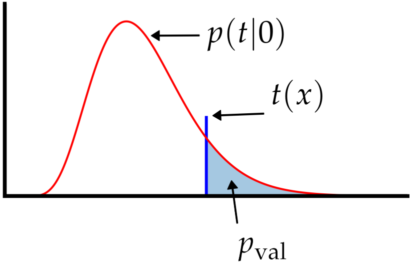
$$p(x \mid 0) = p(x \mid 1)\ ?$$

Idea hypothesis testing

1. $f_n(x) \approx \log \frac{p(x|1)}{p(x|0)} \longrightarrow t(x)$

2. toy experiments: $p(t|0)$

3. p-value: p_{val}



Remarks

- inspired by D'Agnolo et. al.[†]
- unbalanced problem with $\mathcal{N}_0 \gg \mathcal{N}_1$
- multiple training with $N_{\text{toy}} = \mathcal{O}(100)$

[†] D'Agnolo, R. T., & Wulzer, A. (2019). *Learning new physics from a machine.* Physical Review D, 99(1), 015014.

Weighted logistic loss

$$\ell(y, f(x)) = y\, \beta_1 \, \log\left(1 + e^{-f(x)}\right) + \, (1-y)\, \beta_0 \, \log\left(1 + e^{f(x)}\right)$$

$$\lim_{n \to \infty} f_n = \frac{\beta_1}{\beta_0} \frac{p(1|x)}{p(0|x)}$$

Physics-informed weights

$$\begin{cases} \beta_1 = \dfrac{\mathcal{N}_0}{N(0)} \\ \beta_0 = 1 \end{cases}$$

$$f_n \approx \log\left[\frac{n(x|1)}{n(x|0)}\right], \text{ with } n(x) = Np(x) \longrightarrow t(x)$$

Kernel logistic regression

$$\min_{w} L(f_w) + \lambda R(f_w)$$

$$f_w(x) = \sum_{i=1}^{n} w_i \, k(x, x_i), \quad \text{with} \quad k(x, x_i) = \exp\left(-\frac{\|x - x_i\|^2}{2\sigma^2}\right)$$

LogFalkon†

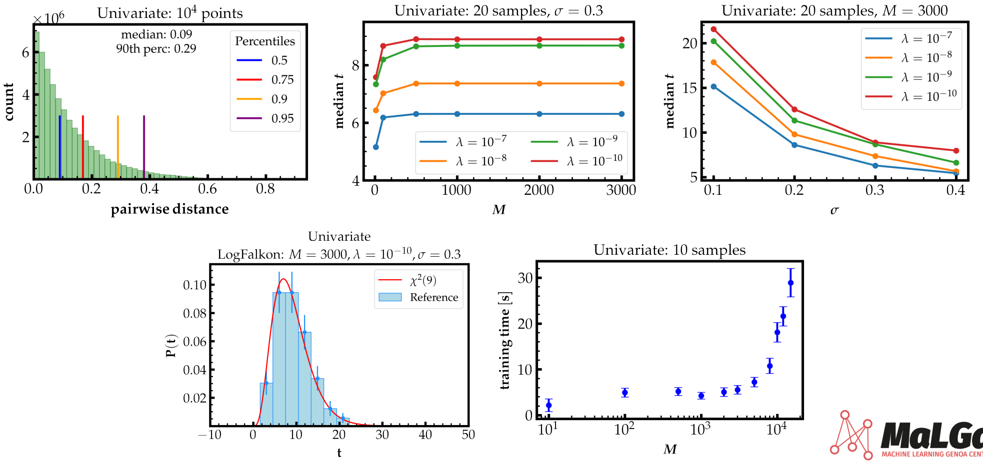
$$f_w(x) = \sum_{i=1}^{\mathbf{M}} w_i k(x, x_i)$$

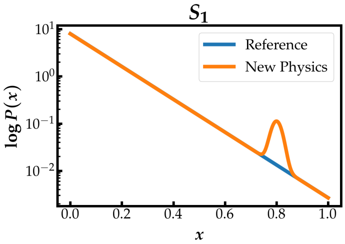
with $\{x_1, x_2, \ldots, x_{\mathbf{M}}\} \subseteq \{x_1, x_2, \ldots, x_n\}$ called Nystrom centers.

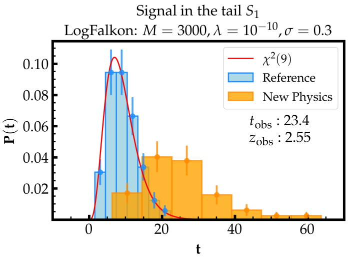
Tune: $\boxed{M, \lambda, \sigma}$

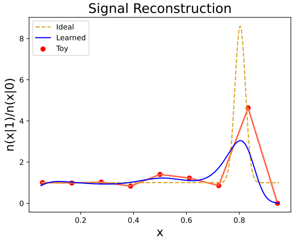
† Meanti, G., et. al. (2020). *Kernel methods through the roof: handling billions of points efficiently.* Advances in Neural Information Processing Systems, 33, 14410-14422.

Hyperparameter tuning









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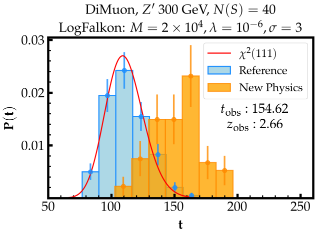
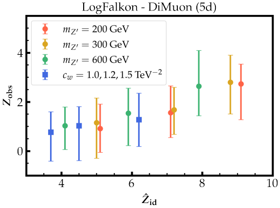
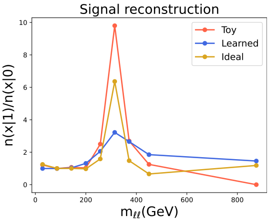
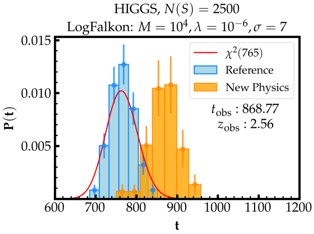
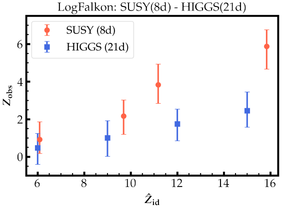
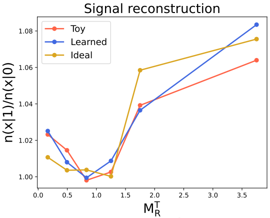






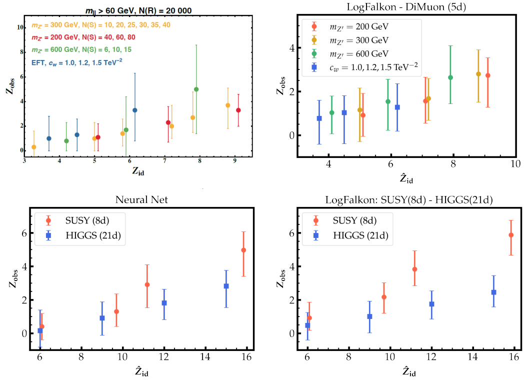






D'Agnolo, et. al. (2021). *Learning multivariate new physics.* The European Physical Journal C, 81(1), 1-21.
Baldi, P., et. al. (2014). *Searching for exotic particles in high-energy physics with deep learning.* Nature communications, 5(1), 1-9.

Comparison with neural networks



Model	DiMuon	SUSY	HIGGS
LogFalkon	**88.7 $\pm$ 1.9 s**	**44.8 $\pm$ 1.5 s**	**89.7 $\pm$ 2.2 s**
Neural networks	4.23 $\pm$ 0.73 h	73.1 $\pm$ 10 h	112 $\pm$ 9 h

MaLGa MACHINE LEARNING GENOA CENTER

Contributions

- An efficient ML framework for High Energy Physics
- A software library (Python)
- Extensive experiments

Future work

- Other datasets and domains
- Anomaly detection / Semi-supervised learning

Thank you!

Test statistic

$$\mathcal{L}(\mathcal{D}, y) = e^{-N(y)} N(y)^{\mathcal{N}_y} \prod_{x \in \mathcal{D}} p(x|y)$$

$$t = -2 \log \frac{\mathcal{L}(\mathcal{D}, 0)}{\mathcal{L}(\mathcal{D}, 1)} = - -2 \sum_{x,y} \left[(1-y) \frac{N(0)}{\mathcal{N}_0} \left(e^{f(x)} - 1 \right) - y f(x) \right]$$