Machine learning for analytic calculations in theoretical physics

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SDU

HAMLET Physics 2025
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[2502.05121] with M. von Hippel

see also [2502.09544] by Song, Yang, Cao, Luo, Zhu

see also [2504.16045] by M. Zeng

work in progress with J. Berman, F. Charton and M. Zeng

DANMARKS FRIE FORSKNINGSFOND   QM Centre for Quantum Mathematics   ℏQTC   VILLUM FONDEN

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ML for analytic calculations in theoretical physics

Typical machine learning applications: Noisy numeric real-world data

Theoretical physics: Exact analytic calculations

ML for analytic calculations in theoretical physics

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Solutions hard to calculate but easy to check
$\Rightarrow$ Case for **Machine Learning**

ML for analytic calculations in theoretical physics

Typical machine learning applications: Noisy numeric real-world data

Theoretical physics: Exact analytic calculations

Solutions hard to calculate but easy to check
$\Rightarrow$ Case for **Machine Learning**

Examples

- Symbol bootstrap
  [Cai, Charton, Cranmer, Dixon, Merz, Nolte, **MW** (2024)]
  $\rightarrow$ My talk at HAMLET Physics 2024

- Spinor-helicity simplifications [Cheung, Dersy, Schwartz (2024)]
- Integration-by-parts reduction
  [Hippel, **MW** (2025)], [Song, Yang, Cao, Luo, Zhu (2025)], [Zeng (2025)] $\rightarrow$ this talk

The problem in a nutshell

Alternative title: ML for Linear Algebra

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Why? Isn't ML harder than Linear Algebra?

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Why? Isn't ML harder than Linear Algebra?

Problem: Given a large set S of redundant linear equations, pick a small subset $s \subset S$ that still allows to uniquely solve for a given set of unknowns

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Why? Isn't ML harder than Linear Algebra?

Problem: Given a large set S of redundant linear equations, pick a small subset $s \subset S$ that still allows to uniquely solve for a given set of unknowns

Challenge: $|\{s \subset S\}| = 2^{|S|}$ $\rightarrow$ Heuristics $\rightarrow$ ML

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Fundamental Physics

Aim: Understand fundamental constituents of **matter** & **interactions**!

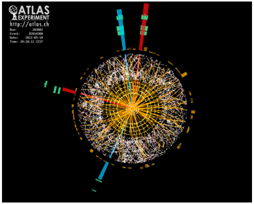

Image: ATLAS

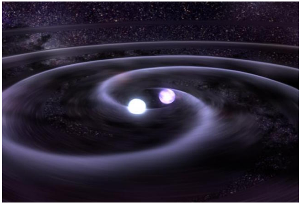
Image: NASA/Goddard Space Flight Center

New experiments $\Rightarrow$ Need for high-precision theory predictions!

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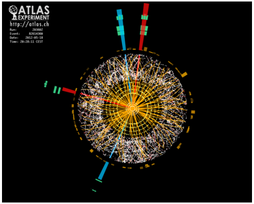

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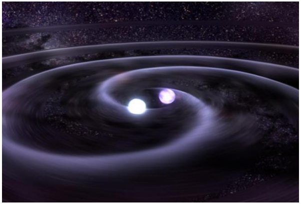
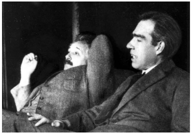


Image: NASA/Goddard Space Flight Center

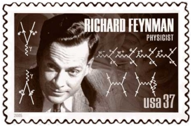
New experiments $\Rightarrow$ Need for high-precision theory predictions!

Theoretical framework:
Quantum Field Theory $=$ Special relativity $+$ Quantum Mechanics



Pipeline for calculating precision predictions

Feynman diagrams → Feynman integrals → Master integrals → Predictions

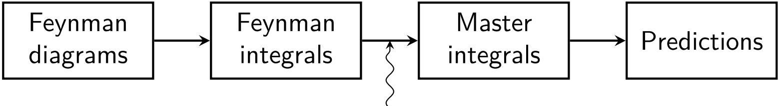


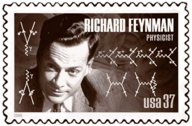
Feynman integrals: $\sim 10^5$

IBP reduction

Master integrals: $\sim 10^2$

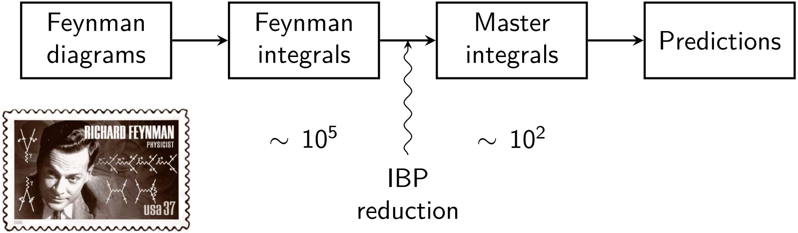
Pipeline for calculating precision predictions





What is integration-by-parts (IBP) reduction?

Pipeline for calculating precision predictions



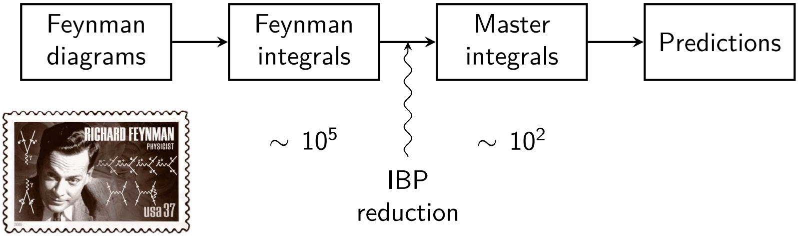
What is integration-by-parts (IBP) reduction?

$\langle$Feynman integrals$\rangle$ = vector space of finite dimension

[Smirnov, Petukhov (2010)]

$\Rightarrow \exists$ finite basis $\{I_1, \ldots, I_N\}$ a.k.a. master integrals

Pipeline for calculating precision predictions



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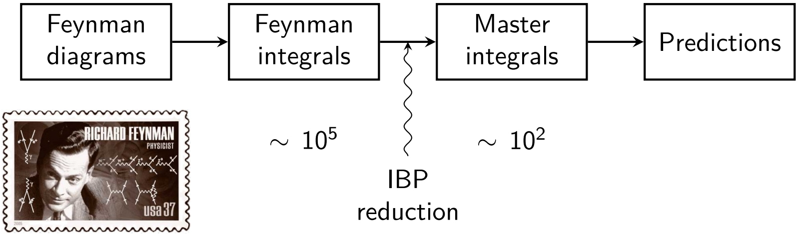

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Bottle neck of many calculations!

e.g. 300k CPU hours [Driesse, Jakobsen, Mogull, Plefka, Sauer, Usovitsch (2024)]

Feynman integrals and IBP identities

General family of Feynman integrals

$$I_{a_1,\ldots,a_n} = \int \frac{\prod_{l=1}^{L} d^D k_l}{\prod_{i=1}^{n} [D_i(k_1^\mu, \ldots, k_L^\mu)]^{a_i}}$$

where $a_i \in \mathbb{Z}$, $L \in \mathbb{N}$, $k_l \in \mathbb{R}^D$, $\mu = 1, \ldots, D$ and D_i polynomials

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Integration-by-part identities [Chetyrkin, Tkachov (1981)]

$$0 = \int \prod_{i=1}^{L} d^D k_i \sum_{\mu=1}^{D} \frac{d}{d k_l^\mu} \frac{q^\mu}{\prod_{i=1}^{n} D_i{}^{a_i}} = \text{linear combination of } I_{a'_1,\dots a'_n}$$

for any $q \in \mathbb{R}^D$ with $a'_i = a_i, a_i \pm 1$

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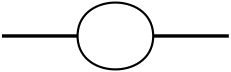
Integration-by-part identities can't be solved for generic a_i
$\rightarrow$ specify to particular values $S \subset \mathbb{Z}^n$ and solve via Laporta's algorithm

[Laporta (2000)]

A simple example

Integral family example: Bubble integral



$$I_{a_1,a_2} = \int \frac{d^D k}{(k^2 - m^2)^{a_1} \left[(p-k)^2\right]^{a_2}}$$

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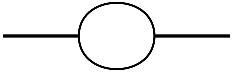

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Integration-by-part identities for $q = p, k$:

$$0 = (D-2a_1-a_2) I_{a_1,a_2} - 2a_1 m^2 I_{a_1+1,a_2} - a_2(m^2-p^2) I_{a_1,a_2+1} - a_2 I_{a_1-1,a_2+1}$$

$$0 = (a_2-a_1) I_{a_1,a_2} - a_1(m^2+p^2) I_{a_1+1,a_2} - a_2(m^2-p^2) I_{a_1,a_2+1} - a_2 I_{a_1-1,a_2+1} + a_1 I_{a_1+1,a_2-1}$$

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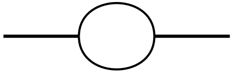

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Possible master integrals $I_{1,1}$, $I_{2,0}$

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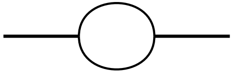

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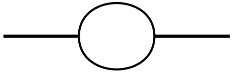

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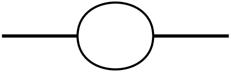
Task: IBP reduce $I_{2,1}$

Solution: Picking $a_1 = a_2 = 1$ above $\Rightarrow I_{2,1} = \frac{D-3}{m^2-p^2} I_{1,1} - \frac{1}{m^2-p^2} I_{2,0}$

Integral family example: Bubble integral



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Homework: IBP reduce $I_{5,5}$

Seeding strategies

How to choose seeds? Heuristics!

Define for $(a_1, \ldots, a_n) \in \mathbb{Z}^n$:

$$t \equiv \sum_{a_i>0} 1\,, \qquad r \equiv \sum_{a_i>0} a_i\,, \qquad d \equiv r - t\,, \qquad s \equiv -\sum_{a_i<0} a_i$$

Rectangular Seeding: $S_1 = \{(a_1, \ldots, a_n) \in \mathbb{Z}^n | r \leq r_{\max} \wedge s \leq s_{\max}\}$
w/ parameters $r_{\max}, s_{\max}$

Golden Rule: $S_2 = \{(a_1, \ldots, a_n) \in S_1 | d \leq d_{\max}\}$ w/ parameter $d_{\max}$

[Laporta (2000)]

Homework: IBP reduce $I_{5,5} \to S_1 = S_2 = \{(a_1, a_2) \in \mathbb{Z}^2 | r \leq 9 \wedge s \leq 0\}$

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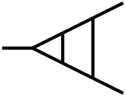
Improved Seeding: $S_3 = \{(a_1, \ldots, a_n) \in S_2 | s \leq t - l + 1\}$ w/ parameter l

$\Rightarrow$ **Order of magnitude improvements** in number of seeds and time!

[Usovitsch (talk in 2023)]

Idea: **Use ML to discover better heuristics**
for picking seeds $s \subset S$

*Always test using  with $a_1, \ldots, a_7$

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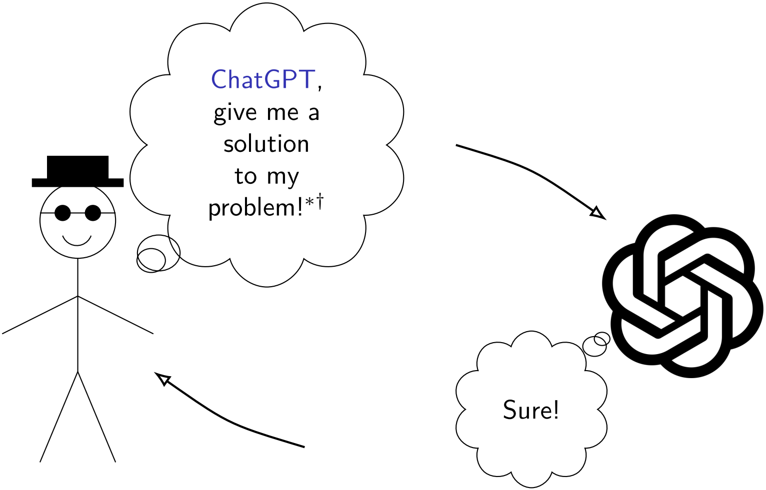
What is funsearch?

funsearch [Romera-Paredes, Barekatain, Novikov, Balog, Kumar, Dupont, Ruiz, Ellenberg, Wang, Fawzi, Kohli, Fawzi (2023)]

Solving problems by automated brainstorming

Funsearch in a nutshell



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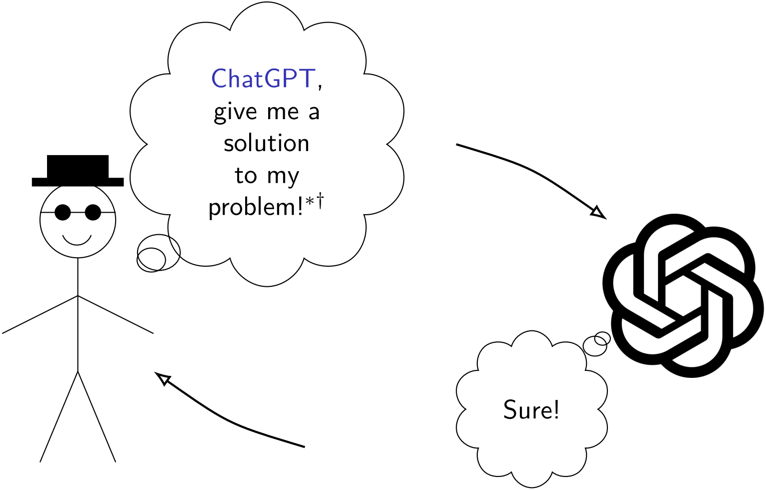

* As python code, so I can check how good it is

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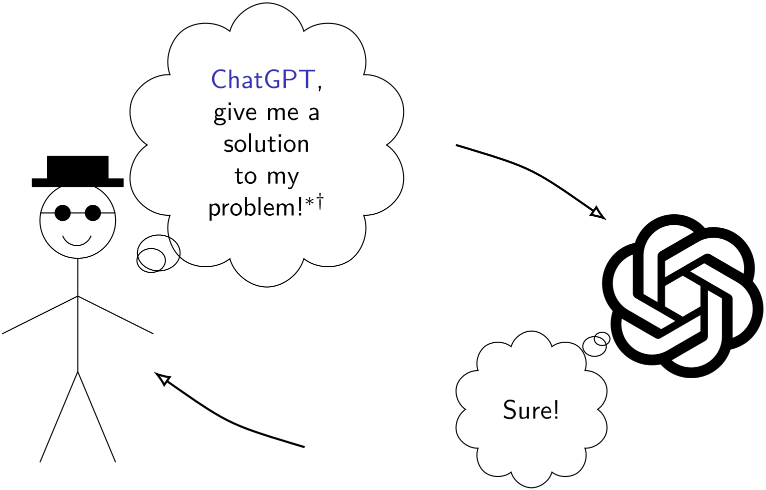
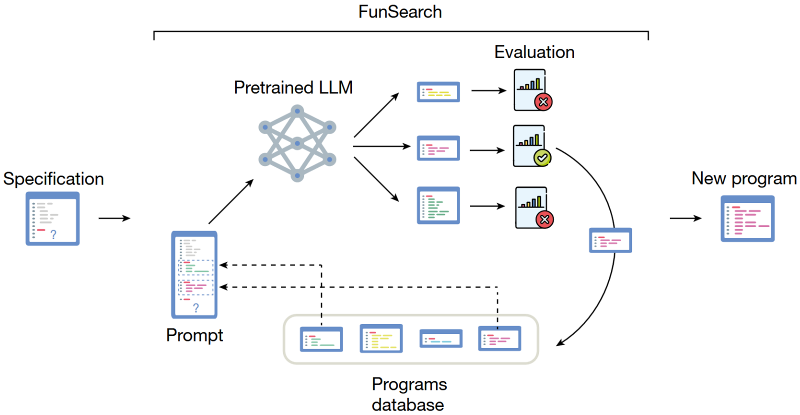


* As python code, so I can check how good it is

† Given those two solutions from earlier already that worked pretty well

Funsearch in slightly longer



[Romera-Paredes, Barekatain, Novikov, Balog, Kumar, Dupont, Ruiz, Ellenberg, Wang, Fawzi, Kohli, Fawzi (2023)]

Properties of funsearch

Some properties:

- Variant of genetic programming, but unconstrained
- Output is python code

$\Rightarrow$ interpretable

$\Rightarrow$ generalizable

[Romera-Paredes, Barekatain, Novikov, Balog, Kumar, Dupont, Ruiz, Ellenberg, Wang, Fawzi, Kohli, Fawzi (2023)]

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Fitness

- Gauß elimination $\mathcal{O}(|s|^3) \to$ less seeds is better
- Fitness $= \begin{cases} -|s| & \text{if } \exists \text{ solution} \\ -|s| - |S| & \text{if } \nexists \text{ solution} \end{cases}$

[von Hippel, **MW** (2025)]

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- Fitness $= \begin{cases} -|s| & \text{if } \exists \text{ solution} \\ -|s| - |S| & \text{if } \nexists \text{ solution} \end{cases}$ [von Hippel, **MW** (2025)]
- Sparse $\to$ Refined fitness $= \#$ element-wise operations [Zeng (2025)]

Experiment with funsearch

Starting point corresponding to a golden rule system with $d_{\max} = 1$:

```python
def priority(a_list: list[int]) -> bool:
    """Decides whether to include the seed a_list in the ibp system.
      Returns True or False."""

    len_alist=len(a_list)

    #Number of propagators, which are entries in a_list greater than zero
    num_props=sum(map(lambda x: 1 if x>0 else 0,a_list))

    #Numbers of numerators, which are entries in a_list less than zero
    numerators=sum(map(lambda x: 1 if x<0 else 0,a_list))

    #Dots, the sum of all entries in a_list greater than one
    dots=sum(map(lambda x: x-1 if x>1 else 0,a_list))

    #The simplest choice: if there is more than one dot, exclude the seed
    #else include it
    if dots>1:
      return False
    else:
      return True
```

$\Rightarrow$ 2,148 seeds

[von Hippel, **MW** (2025)]

Experimental results

After 2,400 generation: 2,148 seeds $\rightarrow$ 92 seeds
$\widehat{=}$ improved seeding strategy with $d_{\max} = 0$ and $l = 4$
$\Rightarrow$ **Rediscovered state of the art!**

[von Hippel, **MW** (2025)]

Experimental results

After 2,400 generation: 2,148 seeds $\rightarrow$ 92 seeds
$\hat{=}$ improved seeding strategy with $d_{\max} = 0$ and $l = 4$
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After 3,800 generation: 2,148 seeds $\rightarrow$ 88 seeds
$\hat{=}$ improved seeding strategy $+$ $t \geq 4$
$\Rightarrow$ **Improvement on state of the art!**

[von Hippel, **MW** (2025)]

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Classic genetic programming

Funsearch: unconstrained + slow → Exploration

Classic genetic programming

Funsearch: unconstrained $+$ slow $\rightarrow$ Exploration

Classic genetic programming: constrained $+$ fast $\rightarrow$ Exploitation
e.g. [Distributed Evolutionary Algorithms in Python (DEAP)]

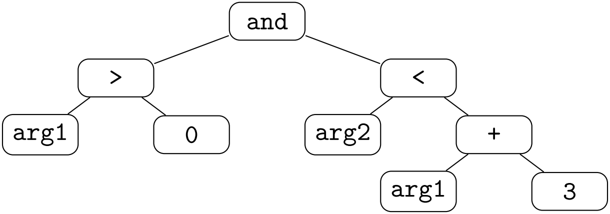
Classic genetic programming

Funsearch: unconstrained + slow → Exploration

Classic genetic programming: constrained + fast → Exploitation
e.g. [Distributed Evolutionary Algorithms in Python (DEAP)]

Syntax trees

```
def func(arg1,arg2):
    return arg1>0 and arg2<arg1+3
```



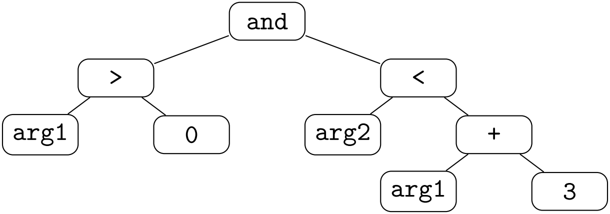
Classic genetic programming

Funsearch: unconstrained + slow → Exploration

Classic genetic programming: constrained + fast → Exploitation
e.g. [Distributed Evolutionary Algorithms in Python (DEAP)]

Syntax trees

```
def func(arg1, arg2):
    return arg1>0 and arg2<arg1+3
```



3+True Nonsense ⇒ **Strongly typed genetic programming**

Strongly typed genetic programming

Evolving trees $=$ grafting


Image: nwtree.com

Strongly typed genetic programming

Evolving trees = grafting

Image: nwtree.com

Cross-over Replace random sub-tree by random sub-tree of another tree
Mutation Replace random sub-tree by random new sub-tree

Strongly typed genetic programming

Evolving trees = grafting


Image: nwtree.com

Cross-over Replace random sub-tree by random sub-tree of another tree
Mutation Replace random sub-tree by random new sub-tree

Building blocks

- Arguments built from $(a_1, \ldots, a_n) \in \mathbb{Z}$: $\sum_{a_i>0} a_i$, $\sum_{a_i>1} a_i$, $-\sum_{a_i<0} a_i$, $\sum_{a_i} a_i$, $\sum_{a_i>0} 1$, $\sum_{a_i>1} 1$, $\sum_{a_i<0} 1$, $\sum_{a_i=0} 1$, $\sum_{a_i=1} 1$, n
- Primitives: `and`, $>$, $<$, $=$, $+$, $-$
- Terminal elements: `True`, $r_{\max}$, $s_{\max}$, $-10, \ldots, +10$

Experimental results

After 18 generation: 2,148 seeds $\rightarrow$ 88 seeds
$\hat{=}$ improved seeding strategy $+$ $t \geq 4$
$\Rightarrow$ **Same result as funsearch but faster!**

[von Hippel, **MW** (2025)]

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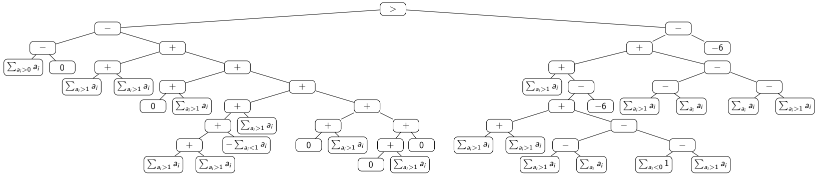
Final tree



[von Hippel, **MW** (2025)]

Table of contents

Conclusion

- **Bottle neck** for analytic calculations in theoretical physics:
  IBP reductions

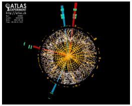


Image: ATLAS

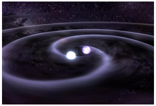
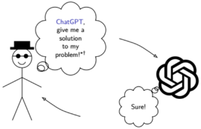
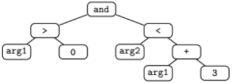


Image: NASA/Goddard Space Flight Center

- **Challenge:** Pick set $s \subset S$ of linear equations
- **ML approach:**
  - funsearch



  - strongly typed genetic programming

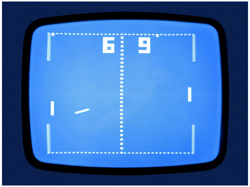


⇒ Improvement over state of the art ⇒ **Proof of principle!**

[von Hippel, **MW** (2025)]

Outlook

- funsearch $\rightarrow$ AlphaEvolve
  [Novikov,Vũ,Eisenberger,Dupont,Huang,Wagner,Shirobokov,Kozlovskii et al. (2025)]
- Gamification $\rightarrow$ RL
  [Zeng (2025)], [Berman, Charton, **MW**, Zeng (in progress)]



- Generalization & Deployment
  - Interpret $\Rightarrow$ Deploy analytic seeding strategy
  - Finite field techniques $\rightarrow$ Training budget of $10^5 - 10^6$ runs
    $\Rightarrow$ Deploy ML
- ...

Image: Road Travel America

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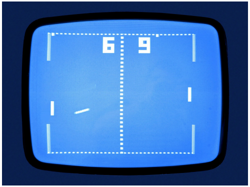

- Generalization & Deployment
  - Interpret ⇒ Deploy analytic seeding strategy
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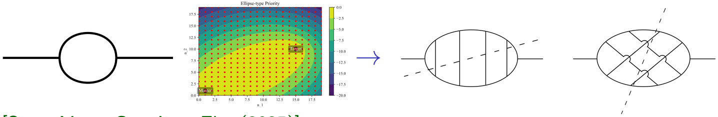
- ...

Thank you!


Image: Road Travel America

Option A

Interpretable $\Rightarrow$ **Deploy analytic seeding strategy**

- $t \geq 4$ [von Hippel, **MW** (2025)]
- 

[Song, Yang, Cao, Luo, Zhu (2025)]

Option A

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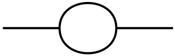
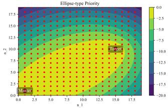
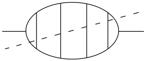
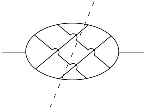
-  

$\rightarrow$  

  [Song, Yang, Cao, Luo, Zhu (2025)]

Option B

Finite field techniques [von Manteuffel, Schabinger (2014)], [Peraro (2016)]

- Run for $D, m_i, s_{ij} \in \mathbb{F}_p$
- Reconstructs rational dependence on D, m_i, s_{ij}

$\rightarrow$ Training budget of $10^5 - 10^6$ runs $\Rightarrow$ **Deploy ML**