Accelerating the search for mass bumps using the Data-Directed Paradigm

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Introduction

Motivation

What? → Train a neural network to **identify mass bumps in real data** without the need of simulation or analytical fit to estimate the background

- Rapidly scan many different regions of the observable-space
- Complementary to the standard analysis approach

Why? → Exploit the **discovery potential of the data**

- Impossible to cover all possible searches with the traditional analysis
- Many possible resonances in unexplored final states

Existing searches for two-body resonances[1]

	e	μ	τ	q/g	b	t	γ	Z/W	H	BSM → $SM_1 \times SM_1$				BSM → $SM_1 \times SM_2$				BSM → complex			
										q/g	γ/π^0's	b	$\cdots$	tZ/H	bH		$\cdots$	$\tau qq'$	eqq'	$\mu qq'$	$\cdots$
e	[37, 38]	[39, 40]	[39]	∅	∅	∅	[41]	[42]	∅	∅	∅	∅		∅	∅	∅		∅	[43, 44]	∅	
μ		[37, 38]	[39]	∅	∅	∅	[41]	[42]	∅	∅	∅	∅		∅	∅	∅		∅	∅	[43, 44]	
τ			[45, 46]	∅	[47]	∅	∅	∅	∅	∅	∅	∅		∅	∅	∅		[48, 49]	∅	∅	
q/g				[29, 30, 50, 51]	[52]	∅	[53, 54]	[55]	∅	∅	∅	∅		∅	∅	∅		∅	∅	∅	
b					[29, 52, 56]	[57]	[54]	[58]	[59]	∅	∅	∅		[60]	∅	∅		∅	∅	∅	
t						[61]	∅	[62]	[63]	∅	∅	∅		[64]	[60]	∅		∅	∅	∅	
γ							[65, 66]	[67–69]	[68, 70]	∅	∅	∅		∅	∅	∅		∅	∅	∅	
Z/W								[71]	[71]	∅	∅	∅		∅	∅	∅		∅	∅	∅	
H									[72, 73]	[74]	∅	∅		∅	∅	∅		∅	∅	∅	
BSM → $SM_1 \times SM_1$: q/g										∅	∅	∅		∅	∅	∅		∅	∅	∅	
γ/π^0's											[75]	∅		∅	∅	∅		∅	∅	∅	
b												[76, 77]		∅	∅	∅		∅	∅	∅	
$\vdots$																					
$\vdots$																					

[1] J. H. Kim et al., J. High Energ. Phys. **2020**, 30 (2020), arXiv:1907.06659 [hep-ph]

Data-Directed Paradigm

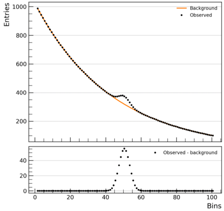
- The **Data Directed Paradigm (DDP)** is a search strategy to efficiently identify regions of interest in the data. It requires two ingredients:

Property of the SM
on which deviations can be searched for

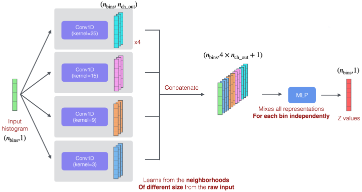
+

Tool to scan the observable-space
in search for deviations

e.g. smoothly falling invariant mass



e.g. NN getting statistical significance for bumps

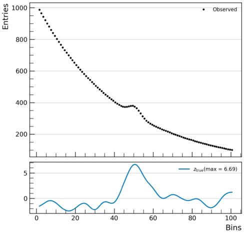


- Proof of concept performed for **symmetries**[2] and **bump searches**[3]

[2] S. Volkovich et al., Eur. Phys. J. C **82**, 265 (2022), arXiv:2107.11573 [hep-ex]
[3] M. Birman et al., Eur. Phys. J. C **82**, 508 (2022), arXiv:2203.07529 [hep-ph]

Bump search with DDP

- Bump search performed with a **network mapping invariant mass distribution to statistical significance**
  - **Input**: vector of bin entries from invariant mass histogram
  - **Target**: vector of statistical significance Z from likelihood-ratio test
  - Representative of an ideal analysis without modelling uncertainties



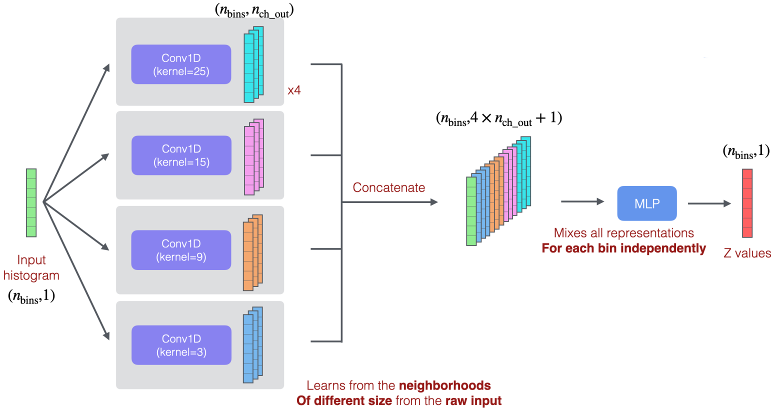
- Exploit its full potential with as **many final states** as possible
  - Multiple combinations of **objects** at the LHC
  - **Selections** on variables such as H_T, E_{Tmiss}, leading object p_T, etc

Electron	Leptonic Z
Muon	Boosted hadronic W/Z
Photon	Boosted top
Jet	High mass jet (m > 200 GeV)

Neural network and synthetic data generation

Implementation

- **Architecture:**
  - Use of 1D convolution layers followed by a dense layer
  - Intuitive and agnostic to the number of bins in the histogram

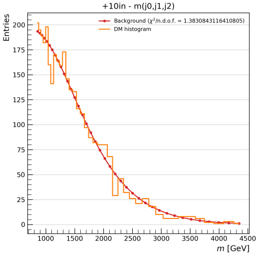


Synthetic data generation

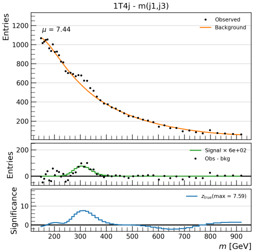
- **Data generation workflow**:
  1. Obtain background shapes
     - Analytical functions

$$be^{-ax},\quad ax+b,\quad \frac{1}{ax}+b,\quad \frac{1}{ax^2}+b,\quad \frac{1}{ax^3}+b,$$
$$\frac{1}{ax^4}+b,\quad a\left(x-x_2\right)^2+y_2,\quad -a\cdot\ln\left(x\right)+b,$$
$$\left(y_1-y_2\right)\cos\left(a\left(x-b\right)\right)+y_2,\quad \cosh\left(a\left(x-x_2\right)\right)+b.$$

     - Fits to simulation data



  2. Inject signal
     - Select background
     - Generate Gaussian signal
     - Combine both into **observed histogram**
     - Poisson fluctuate the histogram
     - Calculate **true significance** with likelihood-ratio test



- **Training data**:
  - Histograms with 30 to 100 bins
  - Broad dynamic range, from 10 to 100k entries per bin
  - Signals injected from broad significance range, from 1 to 20σ

Dark Machines sample description

- Using the **Dark Machines** dataset[4]
  - Designed to test anomaly detection techniques
  - Contains all of the **highest cross-section processes** at the LHC
  - Generation with Madgraph and Pythia, including fast detector simulation using Delphes
  - Events divided into signal regions/channels
    e.g. channel 3, which is more inclusive with cuts on $E_{Tmiss} > 100$ GeV and $H_T \geq 600$ GeV
  - Dataset equivalent to 10 fb^{-1}

SM processes			
Physics process	Process ID	σ (pb)	N_{tot} ($N_{10\,\text{fb}^{-1}}$)
$pp \to jj(+2j)$	njets	$19718_{H_T>600\text{GeV}}$	415331302 (197179140)
$pp \to l^{\pm}\nu_l(+2j)$	w_jets	$10537_{H_T>100\text{GeV}}$	135692164 (105366237)
$pp \to \gamma j(+2j)$	gam_jets	$7927_{H_T>100\text{GeV}}$	123709226 (79268824)
$pp \to l^+l^-(+2j)$	z_jets	$3753_{H_T>100\text{GeV}}$	60076409 (37529592)
$pp \to t\bar{t}(+2j)$	ttbar	541	13590811 (5412187)
$pp \to t + \text{jets}(+2j)$	single_top	130	7223883 (1297142)
$pp \to \bar{t} + \text{jets}(+2j)$	single_topbar	112	7179922 (1116396)
$pp \to W^+W^-(+2j)$	ww	82.1	17740278 (821354)
$pp \to W^{\pm}t(+2j)$	wtop	57.8	5252172 (577541)
$pp \to W^{\pm}\bar{t}(+2j)$	wtopbar	57.8	4723206 (577541)
$pp \to \gamma\gamma(+2j)$	2gam	47.1	17464818 (470656)
$pp \to W^{\pm}\gamma(+2j)$	Wgam	45.1	18633683 (450672)
$pp \to ZW^{\pm}(+2j)$	zw	31.6	13847321 (315781)
$pp \to Z\gamma(+2j)$	Zgam	29.9	15909980 (299439)
$pp \to ZZ(+2j)$	zz	9.91	7118820 (99092)
$pp \to h(+2j)$	single_higgs	1.94	2596158 (19383)
$pp \to t\bar{t}\gamma(+2j)$	ttbarGam	1.55	95217 (15471)
$pp \to t\bar{t}Z$	ttbarZ	0.59	300000 (5874)
$pp \to t\bar{t}h(+1j)$	ttbarHiggs	0.46	200476 (4568)
$pp \to \gamma t(+2j)$	atop	0.39	2776166 (3947)
$pp \to t\bar{t}W^{\pm}$	ttbarW	0.35	279365 (3495)
$pp \to \gamma\bar{t}(+2j)$	atopbar	0.27	4770857 (2707)
$pp \to Zt(+2j)$	ztop	0.26	3213475 (2554)
$pp \to Z\bar{t}(+2j)$	ztopbar	0.15	2741276 (1524)
$pp \to t\bar{t}t\bar{t}$	4top	0.0097	399999 (96)
$pp \to t\bar{t}W^+W^-$	ttbarWW	0.0085	150000 (85)

[4] T. Aarrestad et al., SciPost Phys. **12**, 043 (2022), arXiv:2105.14027 [hep-ph]

Histogram production

- Consider all possible **combinations of objects and selections**
  - With 0 to 4 objects per type
  - Additional kinematic cuts:
    $E_{Tmiss} > 200, 500$ GeV; leading object $p_T > 100, 200, 400$ GeV, ...
- Split the sub-dataset according to **jet multiplicity**
  - 0 jet, 1 jet, 2 jets, ... , ≥ 6 jets (depends on the available stat)
  - Should allow to improve S/B
  - Help reducing look-elsewhere effect (since bump should appear at the same place in neighboring jet multiplicities)
- **Build variables** from available objects
  - Mass distributions of the objects and their combinations
  - Transverse mass distributions including E_{Tmiss}
  - For jets, use only the 4 leading jets using b-tagging information
- Find the **maximum of the histogram** and start from there

- $1\mu + 3j$ + $E_{Tmiss} > 200$ GeV
  + $0e, 0\gamma, 0T, 0Z, 0Wh, 0HM$
- $1W + 1Z + 3j$ + $p_T(Z) > 100$ GeV
  + $0e, 0\gamma, 0T, 0HM$
- $\ldots$

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$1\mu + 3j + E_{Tmiss} > 200$ GeV
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- $1\mu + 3j$ + $E_{Tmiss} > 200$ GeV
  + $0e, 0\gamma, 0T, 0Z, 0Wh, 0HM$
  - $m(\mu j_1)$, $m(\mu j_1 E_{Tmiss})$, ...
  - $m(\mu j_1 j_2)$, $m(\mu j_1 j_2 E_{Tmiss})$, ...
  - ...
- $1W + 1Z + 3j$ + $p_T(Z) > 100$ GeV
  + $0e, 0\gamma, 0T, 0HM$
  - $m(Wh, j_1)$, $m(Wh, j_1, E_{Tmiss})$...
  - $m(j_1 j_2)$, $m(j_1 j_2, E_{Tmiss})$...
  - ...
- ...

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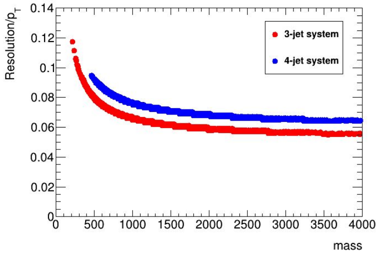
+ $0e, 0\gamma, 0T, 0HM$
- $m(Wh, j_1)$, $m(Wh, j_1, E_{Tmiss})$...
- $m(j_1 j_2)$, $m(j_1 j_2, E_{Tmiss})$...
- ...

...

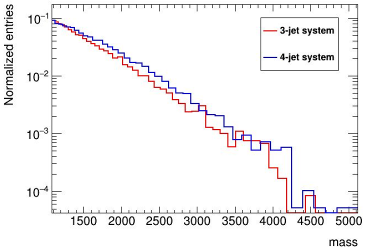
Total of **30 000 mass histograms**

Processing and calibration

- In real data, signal width determined by **detector resolution**
  - Different for different final states and/or mass
  - Narrow signal should produce a bump in few bins
- **Rebin histogram** to reflect the detector resolution we would see in actual experimental data
  - e, μ, γ: Delphes Card formulas, depends on p_T and η
  - jets: ATLAS report on jet resolution, depends on p_T
  - *HM*/*T*/*Wh* accounts for 3/3/2 jets
  - Using $p_T \approx m/2$ approximation



Resolution is higher for $m(4j)$ than $m(3j)$, also larger for small masses



Binning reflects this with larger bin width when resolution is smaller

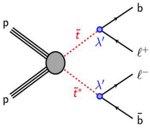
Dark Machines datasets

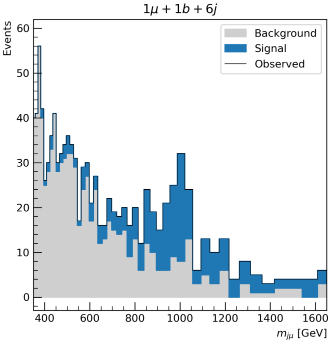
- **Background-only datasets**:
  - Obtain shapes to be included in the training sample
  - Assess false positive rate

- **BSM signal datasets**:
  - Simulated signal data added on top of the backgrounds
  - Test the network in a more realistic scenario
  - Different levels of difficulty (e.g. cross-section, mass values, etc)

Some of the new physics models we have available include:

- RPV stop $\longrightarrow b\ell$
- $W' \longrightarrow WZ \longrightarrow \ell\nu qq, qq\nu\nu$
- $LQ \longrightarrow beb\mu, bebe, t\nu t\nu$
- $Z' \longrightarrow 3l$

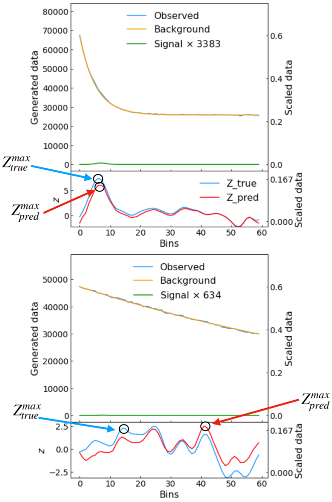




Performance and finding BSM signals

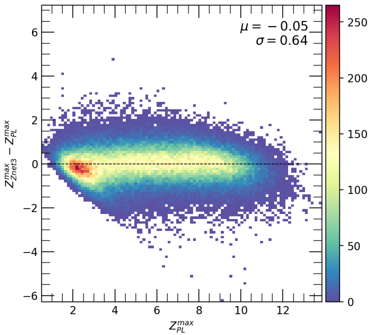
Performance over synthetic data

- Performance quantified in terms of the **difference between predicted and true maximum significance**
  - Z^{max}_{true}: maximal significance calculated via the likelihood ratio test
  - Z^{max}_{pred}: maximal predicted significance
- Majority of entries should have $Z^{max}_{pred} - Z^{max}_{true}$ close to 0 with the smallest variance possible
- **Non-zero significance** for background-only histograms
  - Due to look-elsewhere-effect
  - Could artificially bias the performance at low significance

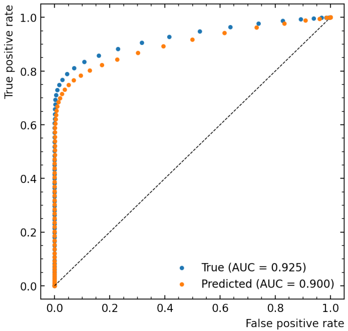


Performance on the testing sample

- Trained model **accurately predicts maximum significance** with no bias and a variance of ± 0.64

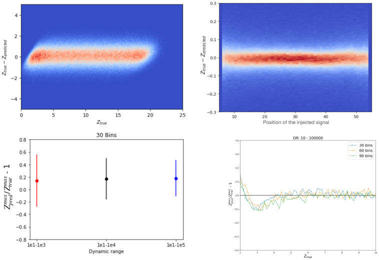


- **Excellent discriminating performance** of signal and background with an AUC of 0.900

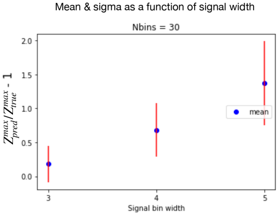


Performance stability

- Good agreement between Z_{pred}^{max} and Z_{true}^{max} is **stable**
  - For all Z_{true}^{max}
  - Over all mass range
  - For all dynamic ranges
  - For linear combinations of the functions

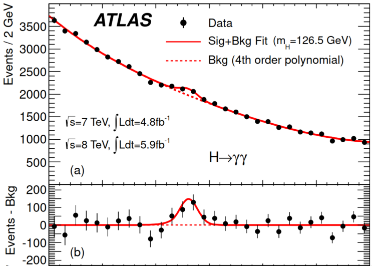


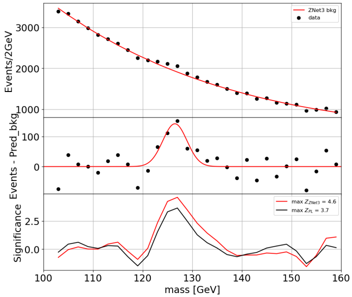
- Training with fixed signal width has **increased bias as signal width increases**
  - Same behaviour regardless of number of bins and dynamic range
  - Accurate calibration takes time (and the DDP should work fast)
  - Room for improvement, yet well defined behaviour



Finding BSM signals

- Promising results when **finding the Higgs bump**
  - Data sampled from the ATLAS plot[5] using a digitizer





- ✓ Predicted resonance at the correct mass
- ! Predicted significance of 4.6σ whereas the ATLAS significance is 3.7σ

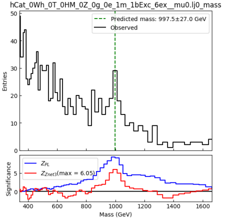
[5] ATLAS Collaboration, Physics Letters B **716**, 1–29 (2012), arXiv:1207.7214 [hep-ex]

Finding BSM signals

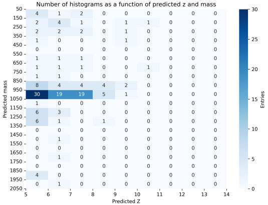
- Tested over **simulated BSM signals** added to the Dark Machines background

RPV stop $\rightarrow b\ell$

$m(j\mu)$ at 1μ+1b+6j



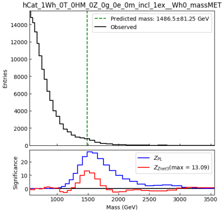
Histograms with $Z_{pred}^{max} \geq 5$



- Successfully finds an excess at the expected mass of the stop at 1 TeV

$W' \rightarrow WZ$

$m(Wh, E_{Tmiss})$ at 1Wh+1j



- Successfully finds bump for W' (with a boosted Z in the final state)

- Other signals tested and successfully found include $LQ \rightarrow beb\mu$, $bebe$ and $Z' \rightarrow 3\ell$
- **False-positive rate of 0.1%** when tested over background-only sample

Conclusion

Final remarks

- **Data directed paradigm bump search** to scan unexplored final states in search for resonances
  - Target smoothly falling invariant mass spectra across a variety of final states
  - Exploit full potential of data without the need of simulation or analytical fit
- **Network implementation and performance**
  - Using Dark Machines datasets with highest cross-section processes at the LHC
  - Produce mass histograms with binning that reflects detector resolution
  - Successfully finds Higgs bump and BSM signals on top of the Dark Machines background, such as RPV stop and W'
- **Future developements**
  - Application to real experimental data, focusing on Run 2
  - Use full MC simulation data with basic selections
  - First iteration using single-lepton trigger and same objects
  - Eventually adding more objects, such as large-R jets

Appendix

Calculation of target significance

For each bin i, we perform a **hypothesis test** and obtain a significance value z_i (see arXiv:1007.1727)

- **Step 1:** Define the shape of the signal S for which we are looking, e.g. a Gaussian centered on bin i
  - We are currently using the mass values on the x-axis

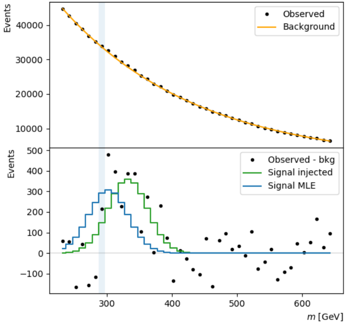
$$s_i = \int_{\mathrm{bin}\,i} f(x; x_0, \sigma)\,\mathrm{d}x \approx f(x; x_0, \sigma)\Delta x$$

$$\begin{cases} x_0 = \text{center of bin } i \\ \sigma = \text{width of bin } i \times \text{given number of bins} \end{cases}$$

- **Step 2:** Obtain the **maximum likelihood estimator** $\hat{\mu}$ for this signal S
  - Expected value is $N_{\mathrm{exp}} = b_i + \mu s_i$

$$\hat{\mu} = \arg\min - \ln[L(\mu)]$$

$$-\ln[L(\mu)] = -\sum_i N_{\mathrm{obs}} \ln(N_{\mathrm{exp}}) - N_{\mathrm{exp}} + \ln\left(\frac{1}{N_{\mathrm{obs}}!}\right)$$



- **Observed data (N_{obs})** is the synthetic data
- **Unfluctuated background (b)** is our null hypothesis
- **Injected signal** is the one added into the observed data
- **Test signal** is the signal that maximizes the likelihood for each bin

Calculation of target significance

For each bin i, we perform a **hypothesis test** and obtain a significance value z_i (see arXiv:1007.1727)

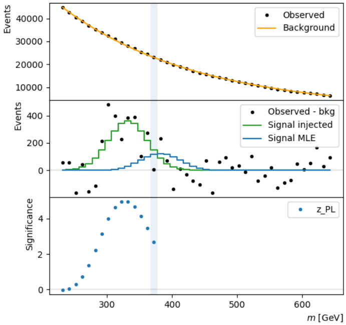
- **Step 3:** Obtain the **likelihood** for both the background-only hypothesis and the maximum-likelihood estimator (MLE) signal hypothesis
  - $-\ln[L(\mu = 0)] \rightarrow$ Background-only ($N_{\mathrm{exp}} = b_i$)
  - $-\ln[L(\mu = \hat{\mu})] \rightarrow$ Signal MLE ($N_{\mathrm{exp}} = b_i + \hat{\mu} s_i$)
- **Step 4:** Obtain the significance using the **profile likelihood ratio** test

If $\hat{\mu} \geq 0$:

$$z_i = \sqrt{q_0} \quad \text{with} \quad q_0 = -2 \ln \left[\frac{L(0)}{L(\hat{\mu})} \right]$$

If $\hat{\mu} < 0$:

$$z_i = -\sqrt{-q_0} \quad \text{with} \quad q_0 = \begin{cases} -2 \ln \left[\frac{L(\hat{\mu})}{L(0)} \right], \text{if two-sided} \\ 0, \text{otherwise} \end{cases}$$



- **Observed data (N_{obs})** is the synthetic data
- **Unfluctuated background (b)** is our null hypothesis
- **Injected signal** is the one added into the observed data
- **Test signal** is the signal that maximizes the likelihood for each bin

Background functions in the framework

$ax + b$

```
def linear(x, p0, p1):
    return p0 * x + p1
```

ae^{-bx}

```
def exponential(x, p0, p1):
    return p0 * np.exp(-p1 * x)
```

$\frac{1}{ax} + b$

```
def one_over_x(x, p0, p1):
    return 1/(p0*x) + p1
```

$a(x - x_{max})^2 + y_{min}$

```
def parabola_half(x, p0, p1, x2, y2):
    return p0*(x - x2)**2 + y2
```

$\frac{1}{ax^2} + b$

```
def one_over_x_squared(x, p0, p1):
    return 1/(p0*x**2) + p1
```

$\Delta y \cos[a(x - b)] + y_{max}$

```
def cos_quarter(x, p0, p1, y1, y2):
    return (y1 - y2)*np.cos(p0*(x - p1)) + y1
```

$\frac{1}{ax^3} + b$

```
def one_over_x_cubed(x, p0, p1):
    return 1/(p0*x**3) + p1
```

$-a \ln(x) + b$

```
def ln_negative(x, p0, p1):
    return -p0*np.log(x) + p1
```

$\frac{1}{ax^4} + b$

```
def one_over_x_to_4th(x, p0, p1):
    return 1/(p0*x**4) + p1
```

$\cosh[a(x - x_{max})] + b$

```
def cosh_half(x, p0, p1, x2):
    return np.cosh(p0*(x - x2)) + p1
```

$\frac{1}{ax^n} + b$

```
def one_over_x_to_nth(x,p0,p1,n):
    return 1/(p0*x**n) + p1
```

$\rightarrow$ where n is taken randomly from the range [0.01, 10]