Hunting new physics with Deep Learning: Physics-case of vector-like fermions and exotic scalars

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Work done in collaboration with: António P. Morais, Felipe F. Freitas, Roman Pasechnik, Cesar Bonilla, A. E. Cárcamo Hernández, Rui Santos, António Onofre, P.M. Ferreira and Vasileios Vatellis

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Science Coffee seminars - Lund University, Sweden

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The Standard Model (**SM**) is the basis by which all subatomic interactions are described. **However**, some unanswered questions remain . . .

- Inability to explain the observed particle spectra (family replication, masses and couplings hierarchies, neutrino masses);
- Lack of a Dark matter (**DM**) candidate;
- Hiearchy problem;
- $(g-2)_\mu$ anomaly, R_{D,D^*} tension, matter/anti-matter asymmetry;
- Naive quantization of gravity leads to a non-renormalizable theory, etc;

A simple observation $\Longrightarrow$ **SM is not the ultimate theory**

Potential solution! $\rightarrow$ **Grand Unification ?**

At a high energy scale, all interactions are unified in a **single group**,

$$\mathcal{G}_U \subset \underbrace{\mathrm{SU}(3)_\mathrm{C} \times \mathrm{SU}(2)_\mathrm{L} \times \mathrm{U}(1)_\mathrm{Y}}_{\mathrm{SM}}.$$

New physics emerges at low scales, at order of TeV:

- **Vector-like fermions:** Both quark and lepton types. $\mathrm{SU}(2)_\mathrm{L}$ does not distinguish chiralities;
- **Leptoquarks:** Direct consequence of quark-lepton unification;
- **Extended scalar sector:** New Higgs doublets and scalar singlets;
- **Right-handed neutrinos:** Majorana or Dirac type;

The story of SM is incomplete, **but we have not found anything new!** That means

- New physics is **heavy**, i.e., of the TeV-PeV order (or beyond);
- New physics is **weakly coupled to the SM**, i.e., low couplings;

As constraints on new physics become increasingly tighter, computational resources become more and more important.

We need

- **Powerful, reliable and proven** methods to deal with weak signals in the ocean of the SM background;
- The methods **must be comfortable** in dealing with **large** datasets.

Machine learning to the rescue !

JHEP
PUBLISHED FOR SISSA BY SPRINGER
RECEIVED: *October 12, 2020*
REVISED: *November 22, 2020*
ACCEPTED: *November 23, 2020*
PUBLISHED: *January 14, 2021*

Phenomenology of vector-like leptons with Deep Learning at the Large Hadron Collider

Felipe F. Freitas,[a] João Gonçalves,[a] António P. Morais[a] and Roman Pasechnik[b]

(a) Published on JHEP

Eur. Phys. J. C (2022) 82:826
https://doi.org/10.1140/epjc/s10052-022-10799-8
THE EUROPEAN PHYSICAL JOURNAL C
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Regular Article - Theoretical Physics

Phenomenology at the large hadron collider with deep learning: the case of vector-like quarks decaying to light jets

Felipe F. Freitas[1,a], João Gonçalves[1,b], António P. Morais[1,c], Roman Pasechnik[2,d]
[1] Departamento de Física da Universidade de Aveiro and Centre for Research and Development in Mathematics and Applications (CIDMA), Campus de Santiago, 3810-183 Aveiro, Portugal
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(b) Published on EPJC

JHEP
PUBLISHED FOR SISSA BY SPRINGER
RECEIVED: *August 17, 2021*
REVISED: *December 22, 2021*
ACCEPTED: *January 3, 2022*
PUBLISHED: *January 26, 2022*

Collider signatures of vector-like fermions from a flavor symmetric model

Cesar Bonilla,[a] A.E. Cárcamo Hernández,[b,c,d] João Gonçalves,[e,f] Felipe F. Freitas,[e,f] António P. Morais[e,f] and R. Pasechnik[g]

(c) Published on JHEP

Collider phenomenology of new neutral scalars in a flavoured multi-Higgs model

P.M. Ferreira[1,2,*] João Gonçalves[3,†] Antonio P. Morais[3,4,‡] António Onofre[5,§] Roman Pasechnik[6,¶] and Vasileios Vatellis[3**]

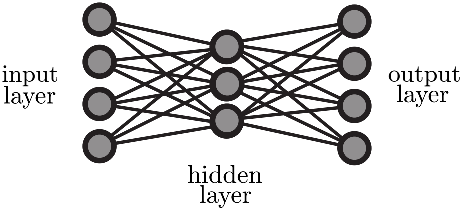
(d) Submitted to PRD

Deep Learning (DL) $\rightarrow$ Extracting high-level features from input data

Universal approximation theorem [Kurt Hornik, Neural Networks. **4** (2): 251–257]

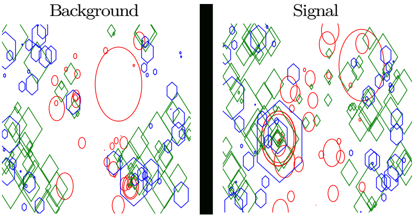
$\Downarrow$

Approximate any function, for an arbitrary number of layers!



Detects small deviations in classes $\Rightarrow$ Perfect for **classfication tasks**!

(a) For cats and dogs



(b) For detector images

```
neurons = 512
activ = 'sigmoid'
initl = 'RandomNormal'
loss  = 'binary_crossentropy'
metric = 'accuracy'
a1     = 1.e-7
a2     = 1.e-7
alp    = 0.1
nb_classes = 5

def NN_model():
    model = Sequential()
    #Input layer
    nn = model.add(Dense(neurons, input_dim=X_train.shape[1], kernel_initializer=initl,
                   kernel_regularizer=regularizers.l1_l2(l1=a1, l2=a2)))
    model.add(Activation(activ))

    #2nd layer
    model.add(Dense(neurons, kernel_initializer=initl,
              kernel_regularizer=regularizers.l1_l2(l1=a1, l2=a2)))
    model.add(Activation(activ))

    #3rd layer
    model.add(Dense(neurons, kernel_initializer=initl,
              kernel_regularizer=regularizers.l1_l2(l1=a1, l2=a2)))
    model.add(Activation(activ))

    #4th layer
    model.add(Dense(neurons, kernel_initializer=initl,
              kernel_regularizer=regularizers.l1_l2(l1=a1, l2=a2)))
    model.add(Activation(activ))

    #Output layer
    model.add(Dense(nb_classes, init=initl , activation=activ ))

    model.compile(loss=loss, optimizer=Adam(), metrics=[metric])
    return model
```

```
neurons = 512
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alp    = 0.1
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```

- Number of neurons: **Arbitrary**;
- Activation functions: **10 +** in Keras (with tunable parameters);
- Initializers: **10 +** in Keras (with tunable parameters);
- ...

```
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a2    = 1.e-7
alp   = 0.1
nb_classes = 5
```

A lot of free parameters to tune in architectural building

⇓

Calls for some optimization procedure → **Genetic algorithms!**

```
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    model.add(Activation(activ))

    #Output layer
    model.add(Dense(nb_classes, init=initl , activation=activ ))

    model.compile(loss=loss, optimizer=Adam(), metrics=[metric])
    return model
```
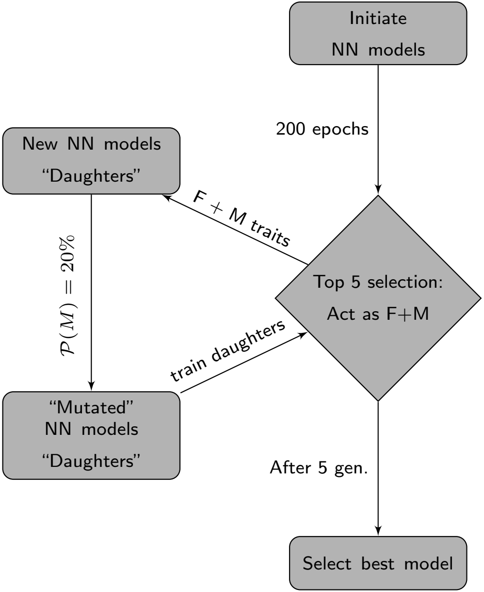

Algorithm Felipe F. Freitas et. al JHEP 01 (2021) 076:

- Randomly generate N models, by pooling a list of hyper-parameters;
- Train: Top 5 models are used to breed daughter networks;
- Add mutation probability. Train daughters and iterate the cycle.

Nice **advantages**:

- Simplifies network construction. Simple way to find the best hyperparameters;
- Straightforward way to maximize distinct metrics.



The best neural model is chosen based on two distinct metrics

- Asimov significance defined as

$$\mathcal{Z}_A = \left[2\left((s+b)\ln\left(\frac{(s+b)(b+\sigma_b^2)}{b^2+(s+b)\sigma_b^2}\right) - \frac{b^2}{\sigma_b^2}\ln\left(1+\frac{\sigma_b^2 s}{b(b+\sigma_b^2)}\right)\right)\right]^{1/2}$$

  Loss function is defined as $L = 1/(\mathcal{Z}_A + \epsilon)$. ϵ regularizes the loss function.
  Adam Elwood and Dirk Krücker arXiv:1806.00322

- Accuracy with binary cross-entropy loss function

$$L = -\frac{1}{N}\sum_{i=1}^{N} y_i \log(p_{\hat{y}_i}) + (1-y_i)\log(1-p_{\hat{y}_i}),$$

  with N being the number of points, y the ground truth label (0 if background and 1 if signal) and p_{y_i} the probability of being signal.

Contrary to what you may think, building neural networks is the easy part $\rightarrow$ **Data representation** is the part where the most careful considerations are taken

- Represent data as **numerical tabular sets** Felipe F. Freitas et. al JHEP 01 (2021) 076. Most straightforward;
- **Jet Images:** Associate energy deposited in the calorimeter with a pixel in the (η, ϕ) plane Luke de Oliveira et. al JHEP 07 (2016) 069;
- **Graph representation:** Map path of charged particles into a graph Xiangyang Ju et.al NeurIPS 2019. Particle cloud representation Huilin Qu and Loukas Gouskos Phys.Rev.D 101 (2020) 5, 056019.

In this presentation I will only focus on models whose data is represented by numerical and image data.

JHEP

Published for SISSA by Springer

Received: *October 12, 2020*
Revised: *November 22, 2020*
Accepted: *November 23, 2020*
Published: *January 14, 2021*

Phenomenology of vector-like leptons with Deep Learning at the Large Hadron Collider

Felipe F. Freitas,[a] João Gonçalves,[a] António P. Morais[a] and Roman Pasechnik[b]

At the low energy limit, this framework results in 2 new **VLQs** at TeV scale.

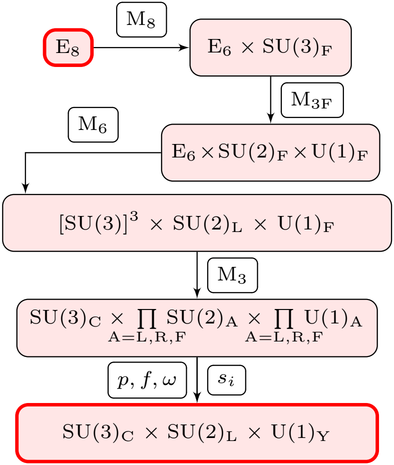
3 generations of **VLLs** with two distinct scenarios

- Two light states ($m < 1$ TeV) and one heavy state ($m > 1$ TeV);
- One light state and two heavy states.

A total of 15 **neutrino states**

- 9 $\mathrm{SU(2)_L}$ doublets (6 BSM and 3 SM-like);
- 6 $\mathrm{SU(2)_L}$ singlets (all BSM).

The framework allows for the existence of sterile neutrinos (in the keV-MeV range).



Prospects for New Physics from gauge Left-Right-Colour-Family Grand Unification. António P. Morais, Roman Pasechnik, Werner Porod, Eur.Phys.J.C 80 (2020) 12, 1162;

Phenomenology of vector-like leptons with Deep Learning at the Large Hadron Collider. **J. Gonçalves***, Felipe F. Freitas, António P. Morais, Roman Pasechnik. doi: 10.1007/JHEP01(2021)076*

Vector-like leptons (VLLs) $\rightarrow$ Both left and right-handed components transform identically under $\mathrm{SU}(2)_\mathrm{L}$.

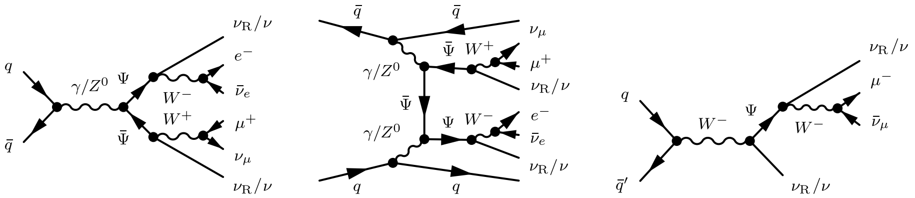
It is a common prediction from E_8 GUT models

- Either at a low-scale ($\Lambda_\mathrm{GUT} \sim 10^9$ GeV) [Alfredo Aranda et. al arXiv:2107.05495];
- Or at a high-scale one ($\Lambda_\mathrm{GUT} \sim 10^{16}$ GeV) [António P. Morais et. al Eur.Phys.J.C 80 (2020) 12, 1162].

Mass generated at loop-level after SUSY breaking. Masses go from hundreds of GeV to the low TeV scale.

Limited constraints [CMS Collaboration Phys. Rev. D 100, 052003 (2019)], [L3 Collaboration Phys.Lett.B517:75-85,2001]. Masses greater than 100.8 GeV. If it couples exclusively to the tau, exclusion goes to 790 GeV.

Single and pair-production topologies at the LHC. ν_{R} in the keV range and acts as missing energy.



(a) ZA topology (b) VBF topology (c) VLBSM topology

For simplicity, we consider flavour opposite final states. Event selection via simple cuts:

1. Charged leptons with $p_T > 25$ GeV and $|\eta| \leq 5$;
2. Missing transverse energy $\not{E}_T > 15$ GeV;
3. Jets: $\Delta R = 1.0$, $p_T > 35$ GeV and $|\eta| \leq 5$.

Event generation flow: `SARAH` $\rightarrow$ `MadGraph` $\rightarrow$ `Pythia8` $\rightarrow$ `Delphes` $\rightarrow$ `ROOT`.

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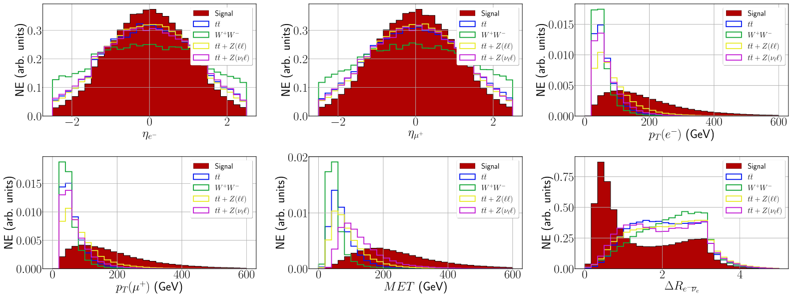
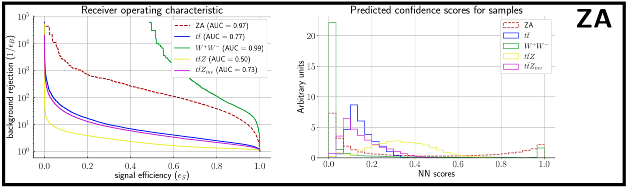
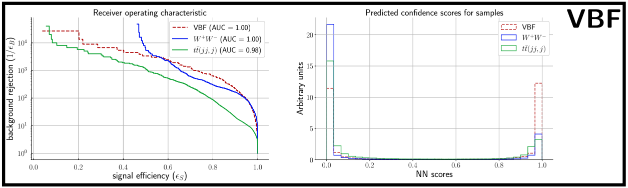


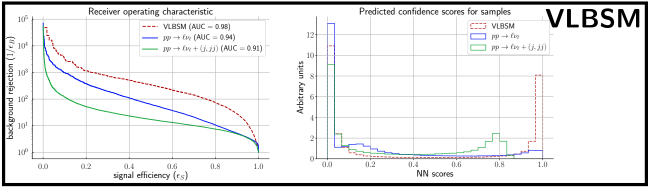
Feed the neural net high-level kinematics (mass distributions, pseudorapidity, transverse momentum, etc) for signal/background topologies.

Some cuts may be imposed to reduce backgrounds → **Unbalanced datasets!**

- Generate more Monte-Carlo: **Computational inefficient**;
- Oversample minority classes (e.g. `SMOTE` algorithm N. V. Chawla et. al JAIR: Vol 16, Issue 1, Jan. 2002);
- Associate weights with events [J, Byrd and Z. C. Lipton arXiv: 1812.03372].







Luminosity: $3000\ \mathrm{fb}^{-1}$; Mass: 677 GeV

The selected architectures are capable of separating signal events from background with efficiencies **greater than 90%**.

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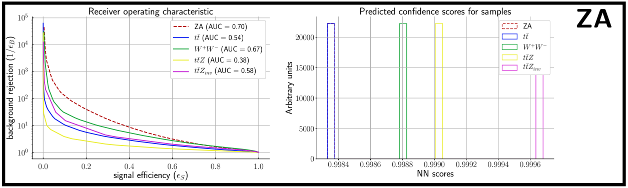

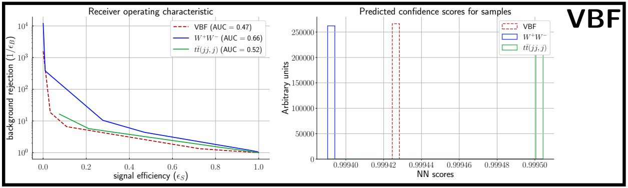

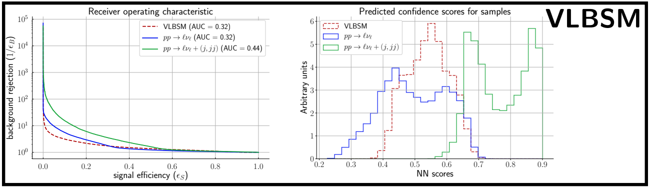

Luminosity: 3000 fb^{-1}; Mass: 677 GeV

Models with the Asimov significance as a loss function result in networks with lower accuracy.

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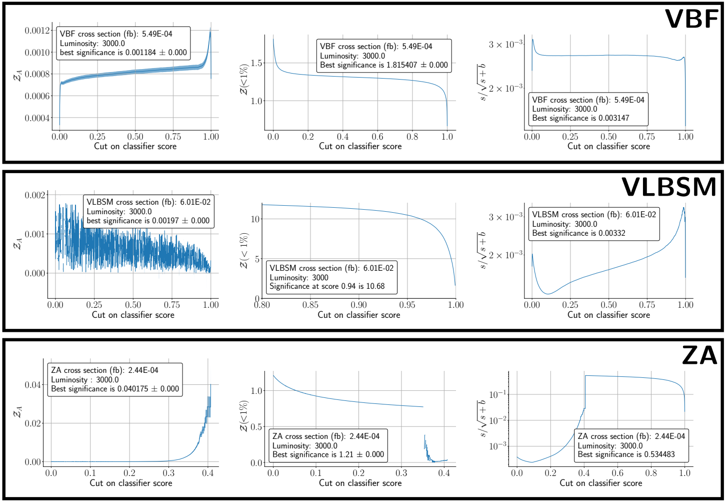

$$\boxed{\mathcal{Z}_A} : \sigma_C = 0.04\sigma, \ \boxed{\mathcal{Z}(<1\%)} : 13.71\sigma, \ \boxed{s/\sqrt{s+b}} : \sigma_C = 0.55\sigma.$$

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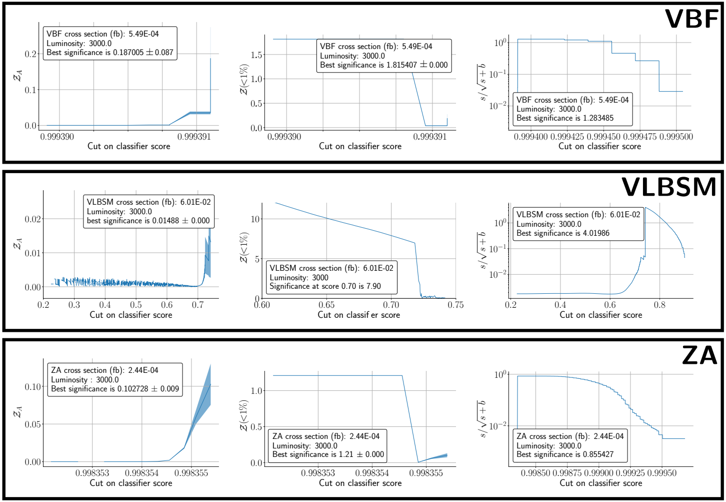

$$\boxed{\mathcal{Z}_A} : \sigma_C = 0.33\sigma, \quad \boxed{\mathcal{Z}(<1\%)} : 10.93\sigma, \quad \boxed{s/\sqrt{s+b}} : \sigma_C = 6.16\sigma.$$

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Mass of e_4	$s/\sqrt{s+b}$			$\mathcal{Z}(<1\%)$			$\mathcal{Z}_A$		
	ZA	VBF	VLBSM	ZA	VBF	VLBSM	ZA	VBF	VLBSM
200 GeV	4.01	9.4×10^{-3}	0.31	12.18	2.83	12.95	2.05	2.47×10^{-3}	1.41
486 GeV	0.95	1.51	6.66×10^{-3}	2.59	2.13	7.83	0.12	4.6×10^{-4}	2.15×10^{-4}
677 GeV	0.53	3.15×10^{-3}	3.32×10^{-3}	1.21	1.82	10.68	0.040	1.18×10^{-3}	1.97×10^{-3}
868 GeV	0.26	0.93	6.18×10^{-4}	0.52	1.32	6.60	0.01	0.30	2.47×10^{-4}
1250 GeV	0.05	4.37×10^{-4}	1.20×10^{-4}	0.17	0.59	4.90	4.28×10^{-4}	2.05×10^{-4}	2.65×10^{-3}

Table: Accuracy metric for $\mathcal{L}=3000$ fb^{-1}.

Mass of e_4	$s/\sqrt{s+b}$			$\mathcal{Z}(<1\%)$			$\mathcal{Z}_A$		
	ZA	VBF	VLBSM	ZA	VBF	VLBSM	ZA	VBF	VLBSM
200 GeV	6.10	2.00	12.65	12.18	2.83	12.70	4.44	0.145	4.28
486 GeV	1.77	1.50	11.26	2.60	2.13	8.62	0.30	0.53	0.20
677 GeV	0.86	1.28	4.02	1.21	1.82	7.90	0.11	0.187	0.015

Table: Asimov metric for $\mathcal{L}=3000$ fb^{-1}.

- Heavy states ($m > 1$ TeV) have reduced significance. Still above 5σ;
- Light states should have a strong presence at HL-LHC ($\mathcal{Z}(<1\%) = 27.86\sigma$ @ 200 GeV);
- We have higher significance for Asimov metric genetic algorithm.

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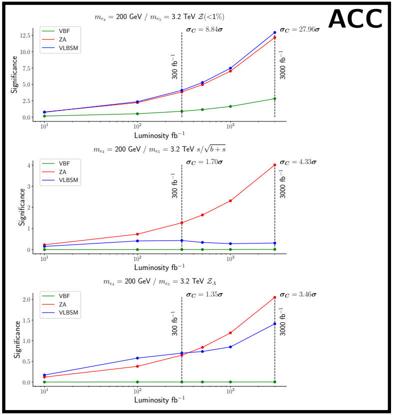

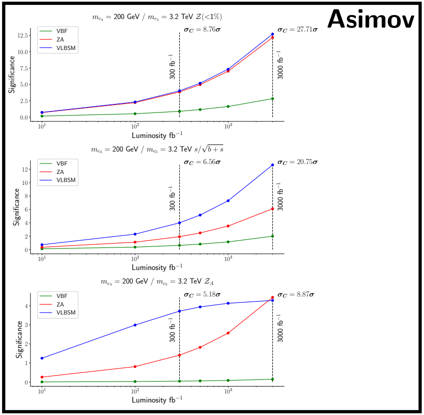

- Significance as a function of luminosity. $300\ \mathrm{fb}^{-1} \rightarrow$ Run-III;
- Utilizing the Asimov metric in the genetic algorithm, we can already obtain results above 5σ **for all** three metrics. We can **already probe them** at run-III of the LHC.

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Eur. Phys. J. C (2022) 82:826
https://doi.org/10.1140/epjc/s10052-022-10799-8

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Regular Article - Theoretical Physics

Phenomenology at the large hadron collider with deep learning: the case of vector-like quarks decaying to light jets

Felipe F. Freitas[1,a], **João Gonçalves**[1,b], **António P. Morais**[1,c], **Roman Pasechnik**[2,d]

[1] Departamento de Física da Universidade de Aveiro and Centre for Research and Development in Mathematics and Applications (CIDMA), Campus de Santiago, 3810-183 Aveiro, Portugal
[2] Department of Astronomy and Theoretical Physics, Lund University, Sölvegatan 14A, 223-62 Lund, Sweden

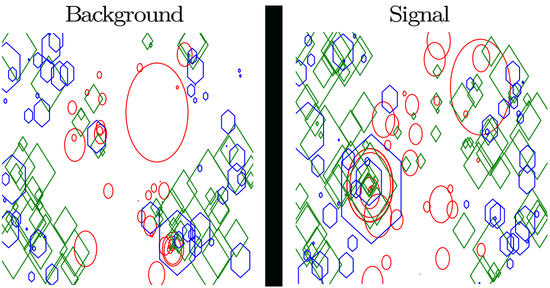
- Inspired by the GUT model António P. Morais et.al Eur.Phys.J.C 80 (2020) 12, 1162; Felipe F. Freitas et. al JHEP 01 (2021) 076:

$$\mathcal{L}_{\mathsf{y}} =(Y^a)_{iJ}\left(\bar{Q}_{\mathrm{L}}\right)^i(D_{\mathrm{R}})^J\phi_a + (\Gamma^a)_{ij}\left(\bar{Q}_{\mathrm{L}}\right)^i(d_{\mathrm{R}})^j\phi_a + (\Delta^a)_{ij}\left(\bar{Q}_{\mathrm{L}}\right)^i(u_{\mathrm{R}})^j\tilde{\phi}_a + \\ + (\Pi^a)_{ij}\left(\bar{L}\right)^i(e_{\mathrm{R}})^j\phi_a + \text{h.c.}\,.$$

- **2 generations** of down-type VLQs. Masses are predicted to be around the TeV scale António P. Morais et.al Eur.Phys.J.C 80 (2020) 12, 1162;
- Extended CKM mixing

$$V_{\mathsf{CKM}} = U_L^u \cdot P \cdot (U_L^d)^\dagger = \begin{pmatrix} V_{\mathrm{CKM}}^{\mathrm{SM}} & V_{\mathrm{CKM}}^{\mathrm{VLQs}} \end{pmatrix}\,,$$

Focus on benchmarks where VLQ couples with **1st/2nd** generation quarks.

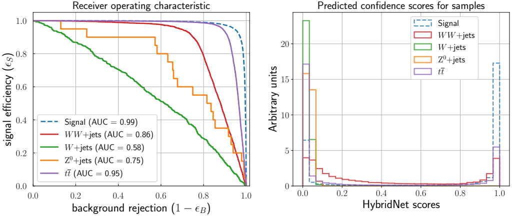


New physics at TeV order → Highly boosted decay products that needs to separated from multijet background at hadron colliders;

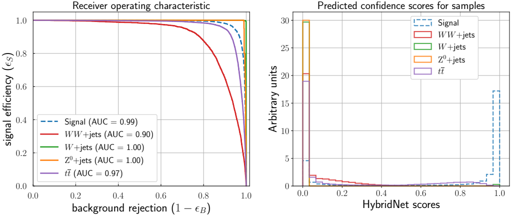
Jet Images: Associate energy deposited in the calorimeter with a pixel in the (η, ϕ) plane [Luke de Oliveira et. al JHEP 07 (2016) 069].

- Enhance classification with **jet kinematics** (multiplicity, mass, ΔR, ...);
- **Abstract Images**: Richer substructure;
- We have obtained efficiencies **greater** than only using kinematic data [Felipe F. Freitas et. al EPJC **82**, 826 (2022)].

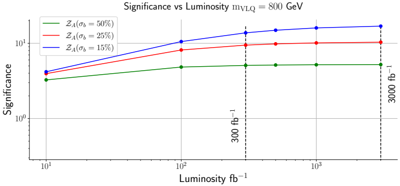
From paper: Phenomenology at the large hadron collider with deep learning: the case of vector-like quarks decaying to light jets. **J. Gonçalves**, Felipe F. Freitas, António P. Morais, Roman Pasechnik. doi: 10.1140/epjc/s10052-022-10799-8



(d) Kinematic



(e) Kinematic + Abstract Images



1. Focusing on VLQ signatures for **decays into light jets**.
2. Use of **Abstract Images** heavily improves the **accuracy** of the neural network
3. Can exclude VLQs at the high-luminosity/run-III phase of the LHC, even for systematics of **50% !**

From paper: Phenomenology at the large hadron collider with deep learning: the case of vector-like quarks decaying to light jets. **J. Gonçalves**, Felipe F. Freitas, António P. Morais, Roman Pasechnik. doi: 10.1140/epjc/s10052-022-10799-8

Collider phenomenology of new neutral scalars in a flavoured multi-Higgs model

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António Onofre[5],§ Roman Pasechnik[6],¶ and Vasileios Vatellis[3]**

Model used in this work first introduced in [Pedro M. Ferreira et al. arXiv:2202.13153]. 2HDM + singlet with a non-trivial $\mathrm{U}(1)'$ flavour symmetry. Yukawa Lagrangian

$$-\mathcal{L}_{\text{Yukawa}} = \overline{q_L^0}\Gamma_a\Phi^a d_R^0 + \overline{q_L^0}\Delta_a\tilde{\Phi}^a u_R^0 + \text{H.c.} + \overline{\ell_L^0}\Pi_a\Phi^a e_R^0 + \overline{\ell_L^0}\Sigma_a\tilde{\Phi}^a\nu_R + \frac{1}{2}\overline{\nu_R^c}\left(\mathrm{A} + \mathrm{B}S + \mathrm{C}S^*\right)\nu_R + \text{H.c.}\,,$$

Scalar potential:

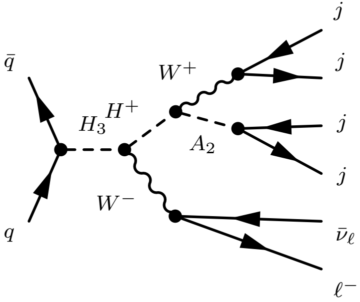
$$\begin{aligned} V_0 = \;& \mu_a^2|\Phi^a|^2 + \lambda_a|\Phi^a|^4 + \lambda_3|\Phi_1|^2|\Phi_2|^2 + \lambda_4|\Phi_1^\dagger\Phi_2|^2 + {\mu_S}^2|S|^2 + \lambda_1'|S|^4 \\ & + \lambda_2'|\Phi_1|^2|S|^2 + \lambda_3'|\Phi_2|^2|S|^2 \quad (a=1,2), \\ V_1 = \;& \mu_3^2\Phi_2^\dagger\Phi_1 + \frac{1}{2}\mu_b^2 S^2 + a_1\Phi_1^\dagger\Phi_2 S + a_2\Phi_1^\dagger\Phi_2 S^\dagger + a_3\Phi_1^\dagger\Phi_2 S^2 + \text{H.c.}\,, \end{aligned}$$

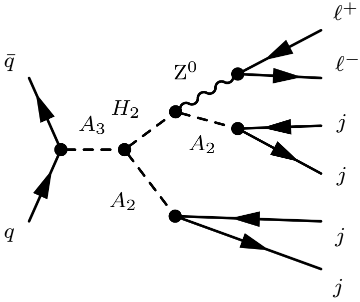
Once the fields develop VEVs, we have **3 CP-even states** (h, H_2, H_3), **2 CP-odd states** (A_2, A_3) and a **singly charged scalar** ($H^\pm$).

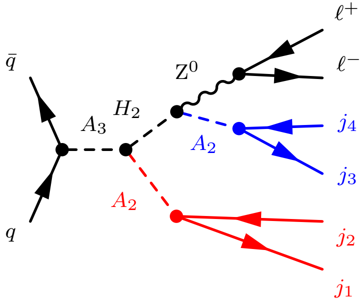
In general (**with some exceptions!**), most searches focus on BSM Higgs decays to heavy SM states

- Limited searches for decays into **1st/2nd gen.** chiral quarks
- Charged Higgs primarily probed in the $tbH^{\pm}$ vertex
- Limited searches for decays involving **multiple BSM Higgs**.

Additional parameter space can be probed in more complex final states, involving **various BSM scalars**







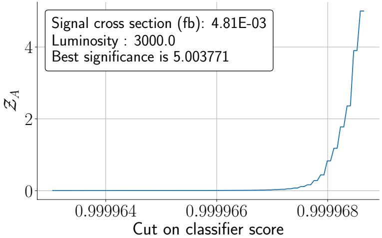
- Mass information can be use to match pairs of jets to original scalars fields;
- $\Delta M = M(j_1, j_2) - M(j_3, j_4) < \varepsilon$:
  - **Signal**: small ε;
  - **Background**: Arbitrary ε;
- Loop over all possible combinations of jets and select the pairs with smallest ε.

Match jets to H_2 scalar: $\min\left(\left|M(j_n, j_m) - M(\mathrm{Z}^0) - M(H_2)\right|\right)$

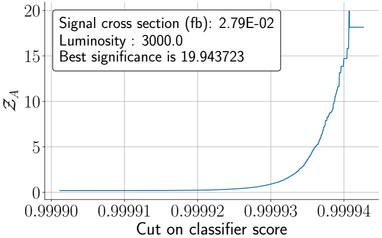
If the minimum is for pair (j_3, j_4), then this is matched to the blue leg and the pair (j_1, j_2) is matched to the red leg.

Since ε is expected to be arbitrary, the matching procedure can help reduce backgrounds for small values of ε.

$M(j) > 10$ GeV and $\Delta M < 35$ GeV



(a) $M_{A_2} = 215$ GeV$/M_{H_2} = 400$ GeV



(b) $M_{A_2} = 300$ GeV$/M_{H_2} = 600$ GeV

Relaxed constraints on jet mass distributions increases the significance. Particularly helpful for lower mass scalar fields. Still, **high cuts** on data for optimal results.

To summarize . . .

- I discuss have discussed how **Deep learning** algorithms can be used in collider phenomenology of generic BSM models;
- I shown these tools in action for various BSM models, including models with **vector-like fermions** and **neutral scalars**;
- For optimization of neural networks, I have presented a **genetic algorithm** that best maximize the statistical significance;
- In principle, the process itself is **model-independent**, in the sense that the neural models are agnostic to the BSM details. They only need the data.

Hunting new physics with Deep Learning: Physics-case of vector-like fermions and exotic scalars

Thank you for your attention

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Centro 2020
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