
Machine Learning tools in the search for leptoquarks in final states with taus, b-jets and MET at the LHC

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Outline

Signal and background

- Scalar-leptoquarks

- Selection cuts and comparison with an ATLAS collaboration analysis

From Machine Learning to significances

- How to link ML classifiers with standard statistical tests

Results: expected significance

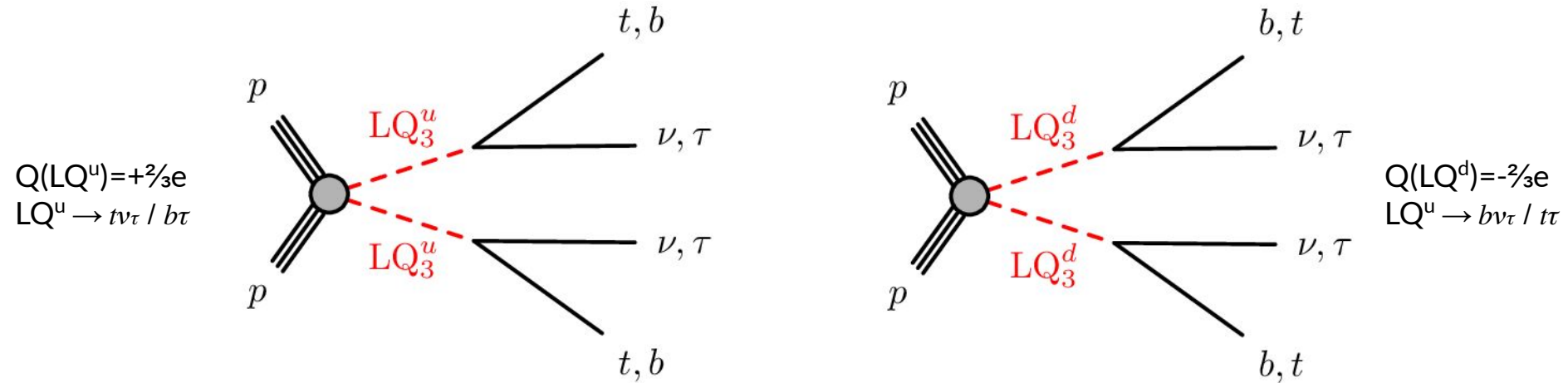
- 95% C.L. expected exclusion contours for $m(\text{LQ})$ vs $\text{BR}(\text{LQ} \rightarrow q\ell)$

Signal and Backgrounds

Signal: pair production of scalar-leptoquarks

Leptoquarks are motivated by GUT (also used to explain B-anomalies)

Only decays into third-generation leptons and quarks (minimal Buchmüller–Rückl–Wyler model)

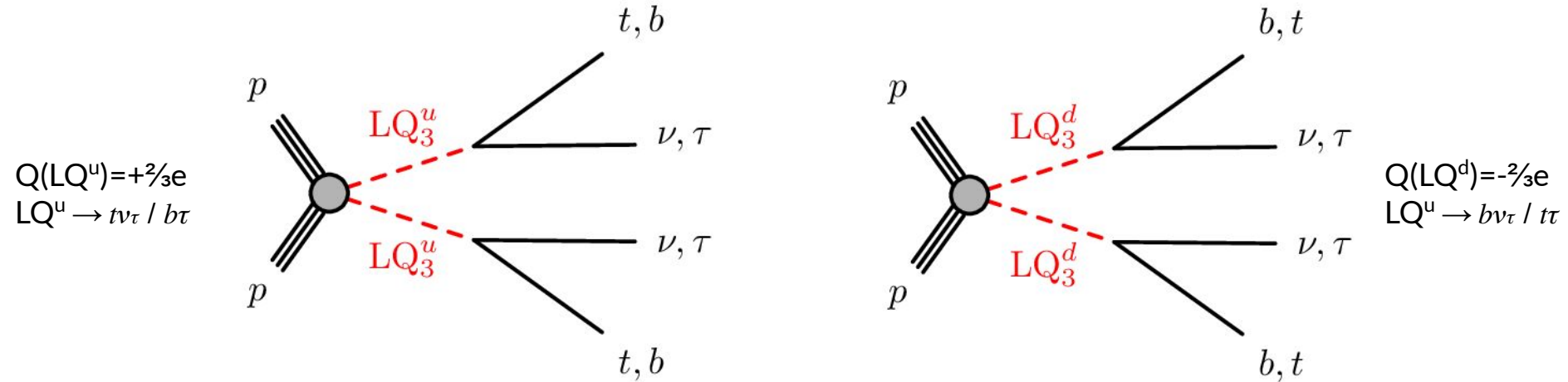


2 parameters: $m(LQ^{u/d})$, leptoquark mass and
 $BR(LQ^{u/d} \rightarrow q\ell)$, the branching fraction into a quark and a charged lepton.

$$BR(LQ^{u/d} \rightarrow q\nu) = 1 - BR(LQ^{u/d} \rightarrow q\ell)$$

Signal: pair production of scalar-leptoquarks

For a $BR(LQ^{u/d} \rightarrow q\ell) \sim 0.5$ most of the decays of the pair of third-generation leptoquarks yield a final state with one tau lepton, two b -jets and large MET from the tau neutrino.



Events with final states with:

- 1 hadronically decaying tau leptons ($p_T > 20 \text{ GeV}$, $|\eta| < 2.5$),
- at least 2 b -tagged jets ($p_T > 20 \text{ GeV}$, $|\eta| < 2.5$),
- large missing transverse momentum ($\text{MET} > 280 \text{ GeV}$)
- no light leptons (e/μ)

Background: SM

ATLAS analysis, Phys. Rev. D 104, (2021) 112005, arXiv:2108.07665

	Single-tau SR (binned in $p_T(\tau)$)					
	[50, 100] GeV		[100, 200] GeV		> 200 GeV	
Observed	8		6		2	
Total bkg.	10.1	± 1.8	5.1	± 1.1	2.05	± 0.64
$t\bar{t}$ (2 real τ)	—		—		—	
$t\bar{t}$ (1 real τ)	4.8	± 1.2	2.69	± 0.88	0.64	± 0.29
$t\bar{t}$ -fake	2.83	± 0.87	0.66	± 0.17	0.185	± 0.072
Single top	0.85	$^{+0.86}_{-0.85}$	0.54	± 0.54	0.57	± 0.56
W + jets	0.34	± 0.12	0.64	± 0.24	0.37	± 0.12
Z + jets	0.275 ± 0.081		0.043 ± 0.022		0.123 ± 0.048	
Multiboson	0.163 ± 0.037		0.111 ± 0.030		$0.030^{+0.032}_{-0.030}$	
$t\bar{t} + V$	0.65	± 0.16	0.31	± 0.12	0.092	± 0.035
$t\bar{t} + H$	0.10	± 0.10	$0.060^{+0.061}_{-0.060}$		$0.028^{+0.029}_{-0.028}$	
Other top	0.096 ± 0.074		0.091 ± 0.049		0.0120 ± 0.0084	

Different selection cuts

ATLAS analysis, Phys. Rev. D 104, (2021) 112005, arXiv:2108.07665

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at least 2 b -tagged jets ($p_T > 20 \text{ GeV}$, $|\eta| < 2.5$),
large missing transverse momentum ($E_T^{\text{miss}} > 280 \text{ GeV}$)
no light leptons (e/μ)

ATLAS signal enriched region: $\sum m_T(b_{1,2}) = m_T(b_1) + m_T(b_2) > 700 \text{ GeV}$

$$m_T(\tau) > 150 \text{ GeV}$$

$$s_T = p_T(\tau) + p_T(\text{jet}_1) + p_T(\text{jet}_2) > 600 \text{ GeV}$$

where $m_T^2(\mathbf{p}_T, \mathbf{E}_T^{\text{miss}}) = 2 p_T E_T^{\text{miss}} (1 - \cos \Delta\phi(\mathbf{p}_T, \mathbf{E}_T^{\text{miss}}))$ is the stransverse mass

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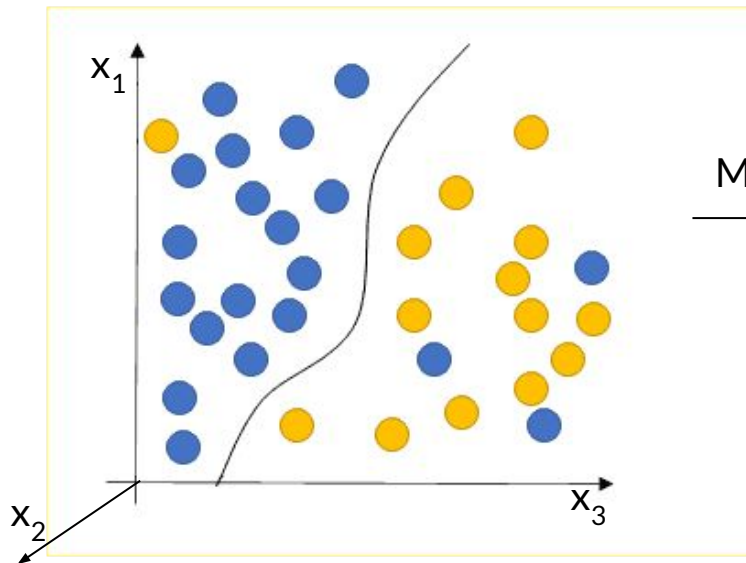
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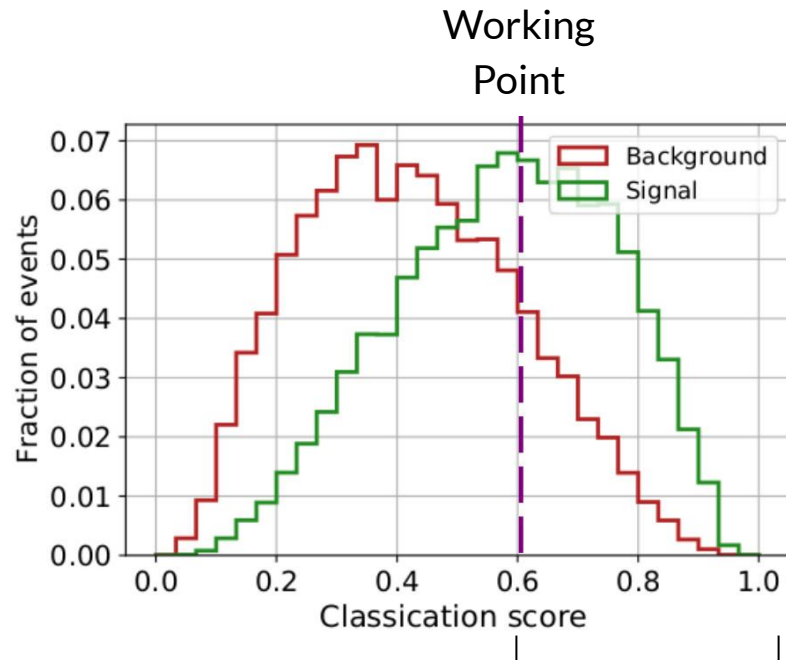
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From ML to significances

Expected significance



ML
→

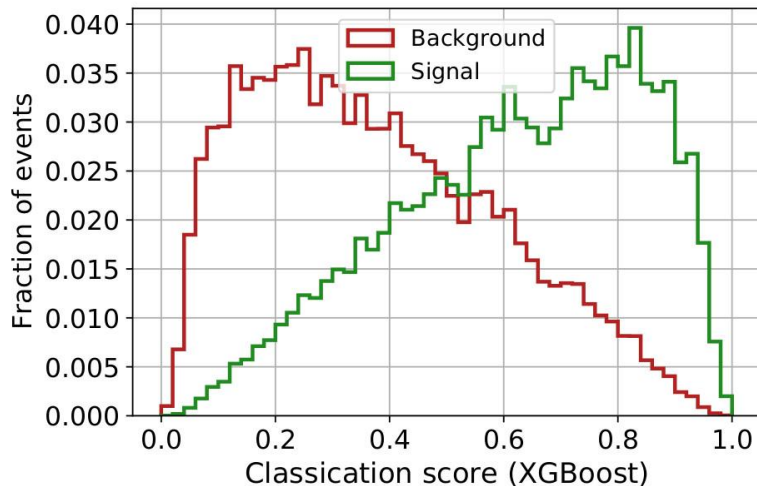


Defining a Working Point ~ design observable, define a working region

In that signal enriched region
(we discard events outside of it) → significance ~ $\frac{S}{\sqrt{B}}$

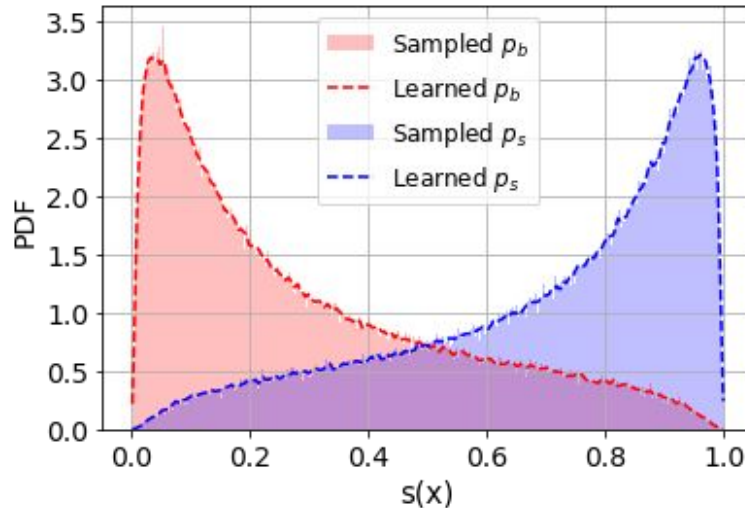
Expected significance

We used the *full 1D* ML classifier output $o(x)$ with the standard statistical tests (without defining a working point) to compute the significance



$o(\bar{x})$ Binned Likelihood method

$$\text{med} [Z_0^{\text{binned}}|1] = \left[2 \sum_{d=1}^D \left((S_d + B_d) \text{Ln} \left(1 + \frac{S_d}{B_d} \right) - S_d \right) \right]^{1/2}$$



$o(\bar{x})$ Unbinned method

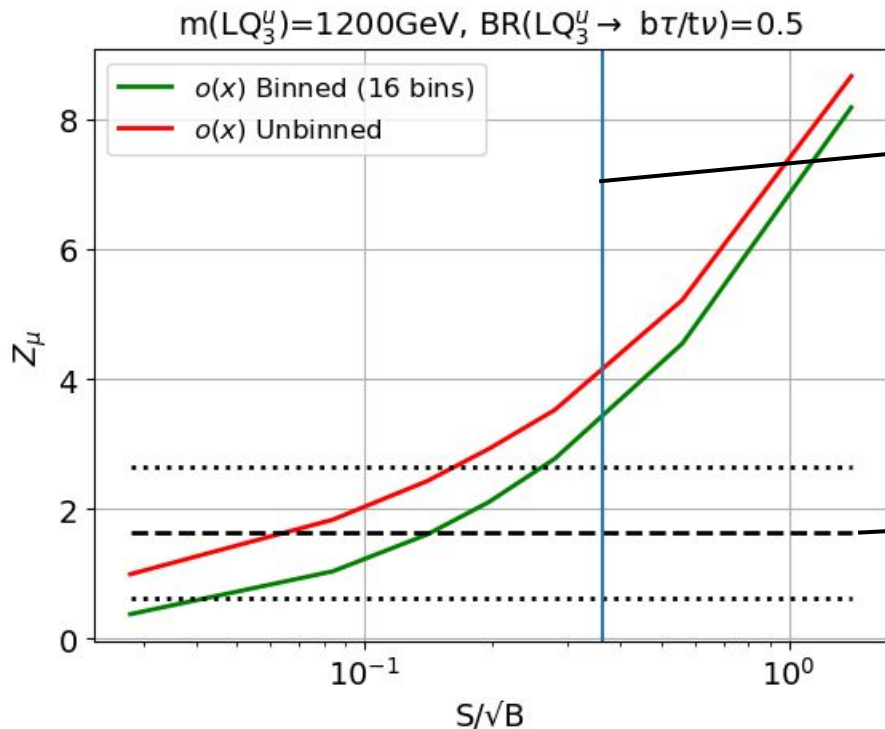
Use KDE to estimate the B and S PDFs.

↳ Calculate Z building pseudo-experiments

Results

Results

Example $m(\text{LQ}^u) = 1200 \text{ GeV}$, and $\text{BR}(\text{LQ}^u \rightarrow q\ell) = 0.5$



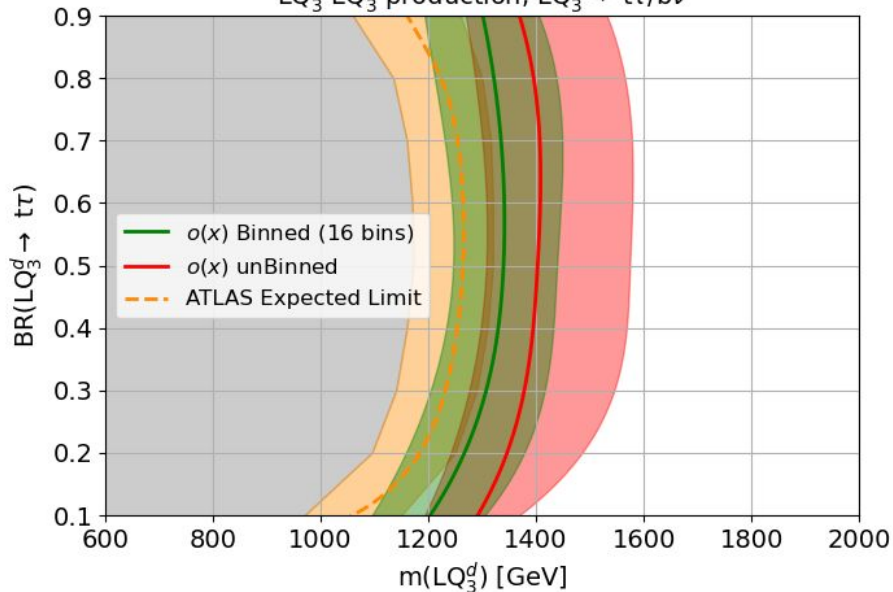
Expected
signal-to-background ratio
for this parameter point.

$Z > 1.64 \rightarrow \text{excluded at}$
95% C.L.

Results

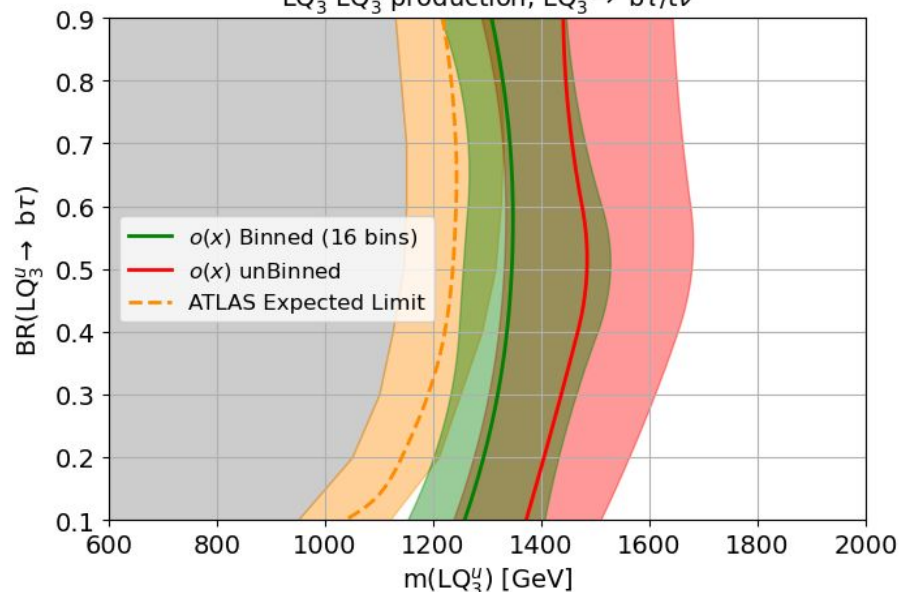
Down-type Leptoquarks

$LQ_3^d LQ_3^d$ production, $LQ_3^d \rightarrow t\tau/b\nu$



Up-type Leptoquarks

$LQ_3^u LQ_3^u$ production, $LQ_3^u \rightarrow b\tau/t\nu$



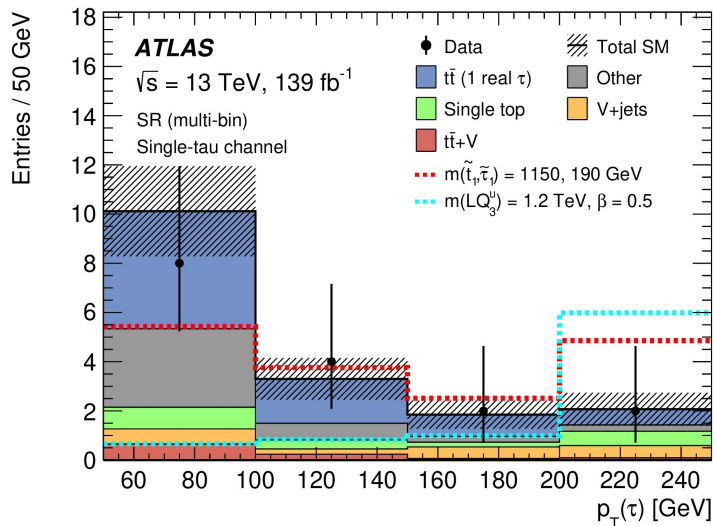
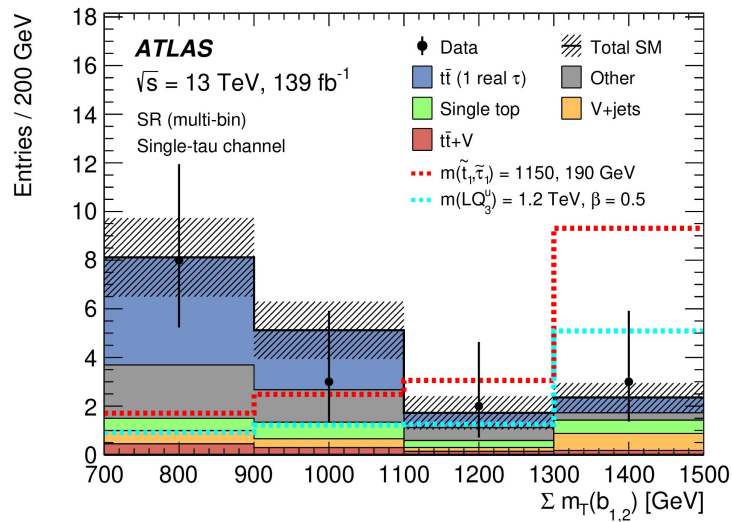
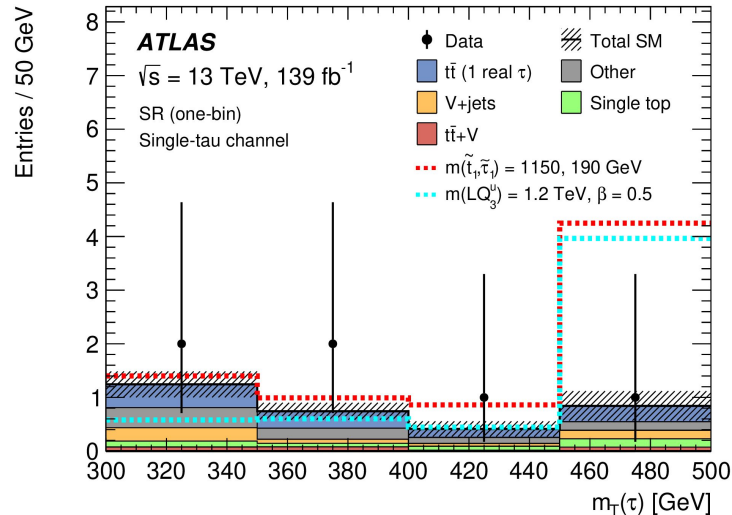
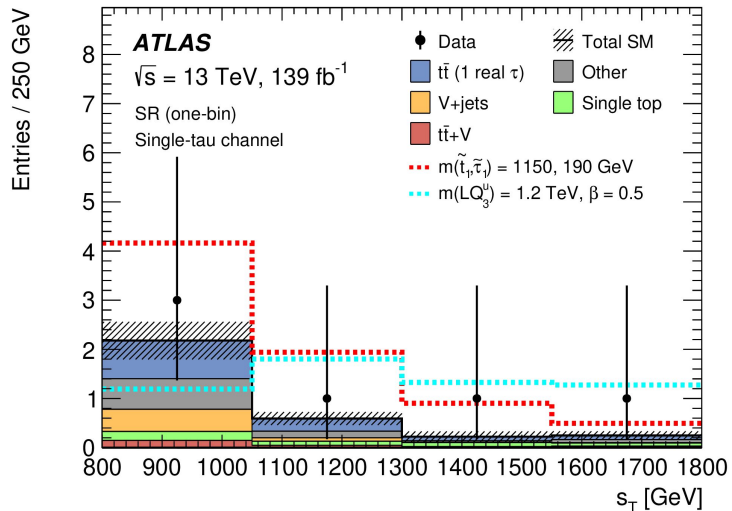
For both types of scalar leptoquarks, the expected exclusion contours extend to masses around 1.25 TeV (ATLAS), 1.35 TeV (Binned), 1.45 TeV (Unbinned) at the 95% confidence level for intermediate values of the branching fraction $BR(LQ^{u/d} \rightarrow q\ell)$

Conclusions

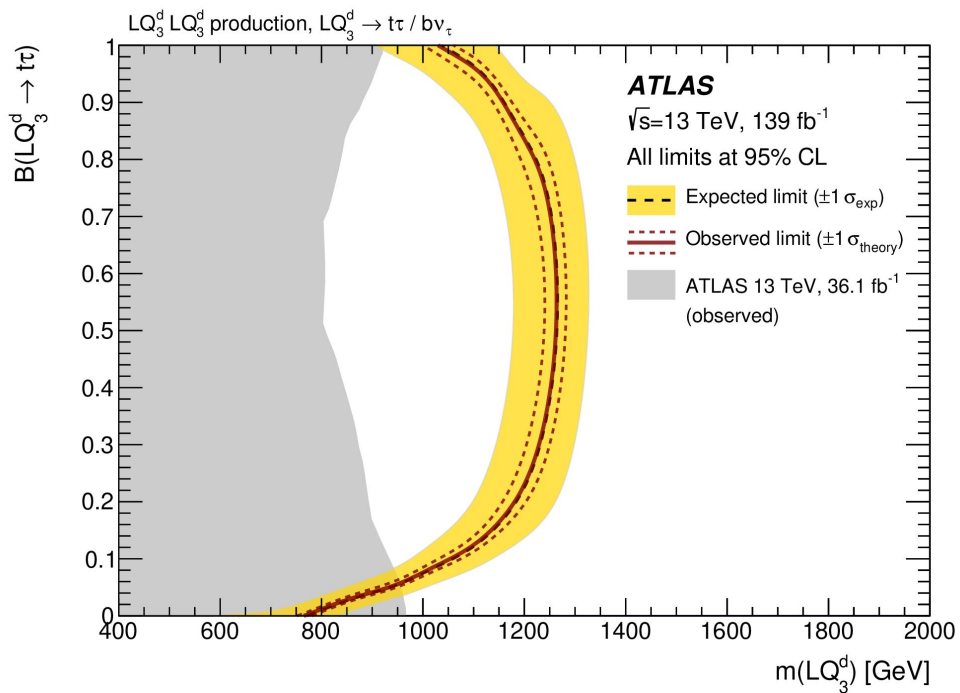
- Search for new phenomena in final states with hadronically decaying tau leptons, b -jets and large missing transverse momentum
→ third-generation scalar leptoquarks (motivated by GUT).
- As a ***proof of concept*** we used ML algorithms with simple selection cuts and compared them to an ATLAS analysis.
- We use the full classifier output (no working points) to estimate the significances.
- For both types of scalar leptoquarks, expected exclusion contours up to masses
1.25 TeV (ATLAS)
1.35 TeV (Binned)
1.45 TeV (Unbinned)
at the 95% confidence level for intermediate values of the branching fraction
 $BR(LQ^{u/d} \rightarrow q\ell)$

Thank you!

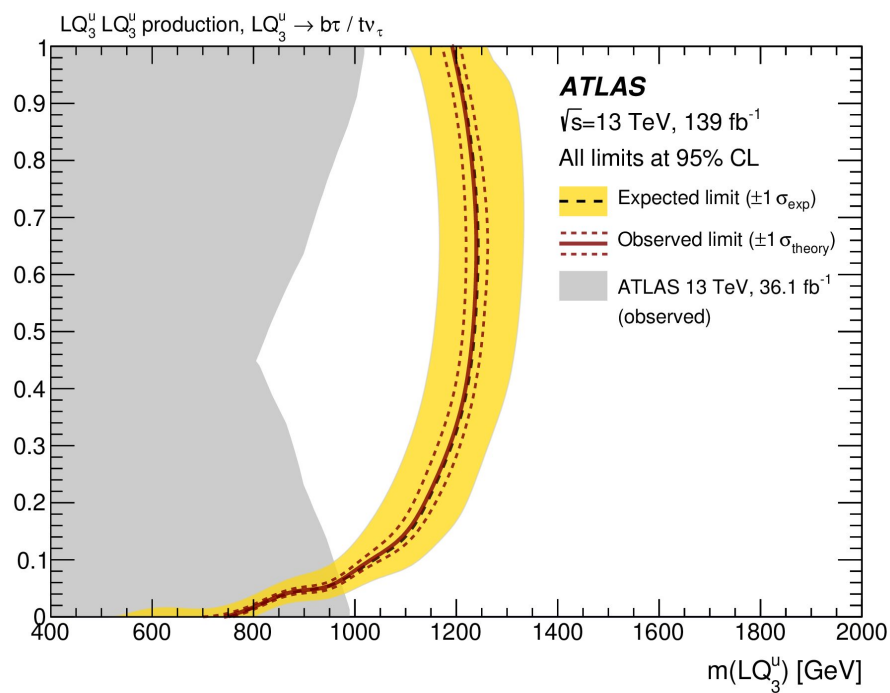
Back up



Down-type Leptoquarks



Up-type Leptoquarks



Leptoquark model

Buchmüller–Rückl–Wyler model, Phys. Lett. B 191 (1987) 442

We start from an effective lagrangian with the most general dimensionless, $SU(3) \times SU(2) \times U(1)$ invariant couplings of scalar and vector leptoquarks satisfying baryon and lepton number conservation:

$$\mathcal{L} = \mathcal{L}_{F=2} + \mathcal{L}_{F=0}, \quad (1a)$$

$$\begin{aligned} \mathcal{L}_{F=2} = & (g_{1L} \bar{q}_L^c i\tau_2 \ell_L + g_{1R} \bar{u}_R^c e_R) S_1 \\ & + \tilde{g}_{1R} \bar{d}_R^c e_R \tilde{S}_1 + g_{3L} \bar{q}_L^c i\tau_2 \boldsymbol{\tau} \ell_L S_3 \\ & + (g_{2L} \bar{d}_R^c \gamma^\mu \ell_L + g_{2R} \bar{q}_L^c \gamma^\mu e_R) V_{2\mu} \\ & + \tilde{g}_{2L} \bar{u}_R^c \gamma^\mu \ell_L \tilde{V}_{2\mu} + \text{c.c.}, \end{aligned} \quad (1b)$$

$$\begin{aligned} \mathcal{L}_{F=0} = & (h_{2L} \bar{u}_R \ell_L + h_{2R} \bar{q}_L i\tau_2 e_R) R_2 + \tilde{h}_{2L} \bar{d}_R \ell_L \tilde{R}_2 \\ & + (h_{1L} \bar{q}_L \gamma^\mu \ell_L + h_{1R} \bar{d}_R \gamma^\mu e_R) U_{1\mu} \\ & + \tilde{h}_{1R} \bar{u}_R \gamma^\mu e_R \tilde{U}_{1\mu} + h_{3L} \bar{q}_L \boldsymbol{\tau} \gamma^\mu \ell_L U_{3\mu} + \text{c.c.} \end{aligned} \quad (1c)$$

The Yukawa-type interaction of the leptoquarks with the quark-lepton pair are determined by two parameters:

- a common coupling strength λ ($=g, h$) and,
- an additional parameter β , with the coupling to a quark and a charged lepton given by $(\sqrt{\beta})\lambda$, and the coupling to a quark and a neutrino by $[\sqrt{(1-\beta)}]\lambda$.

The branching fraction $BR(LQ^{u/d} \rightarrow q\ell) \approx \beta$, except for kinematic effects arising from the mass differences of the decay products.

λ set to 0.3 close to the electromagnetic coupling $e=\sqrt{4\pi\alpha}$, resulting in a $LQ^{u/d}$ width equal to $\sim 0.2\%$ of its mass

Leptoquark model

Buchmüller–Rückl–Wyler model, Phys. Lett. B 191 (1987) 442

Table 1

Quantum numbers of scalar and vector leptoquarks with $SU(3) \times SU(2) \times U(1)$ invariant couplings to quark–lepton pairs ($Y = Q_{\text{em}} - T_3$).

	Spin	$F = 3B + L$	$SU(3)_c$	$SU(2)_w$	$U(1)_Y$
S_1	0	−2	3^*	1	$\frac{1}{3}$
\tilde{S}_1	0	−2	3^*	1	$\frac{4}{3}$
S_3	0	−2	3^*	3	$\frac{1}{3}$
V_2	1	−2	3^*	2	$\frac{5}{6}$
\tilde{V}_2	1	−2	3^*	2	$-\frac{1}{6}$
R_2	0	0	3	2	$\frac{7}{6}$
\tilde{R}_2	0	0	3	2	$\frac{1}{6}$
U_1	1	0	3	1	$\frac{2}{3}$
\tilde{U}_1	1	0	3	1	$\frac{5}{3}$
U_3	1	0	3	3	$\frac{2}{3}$

Leptoquark model

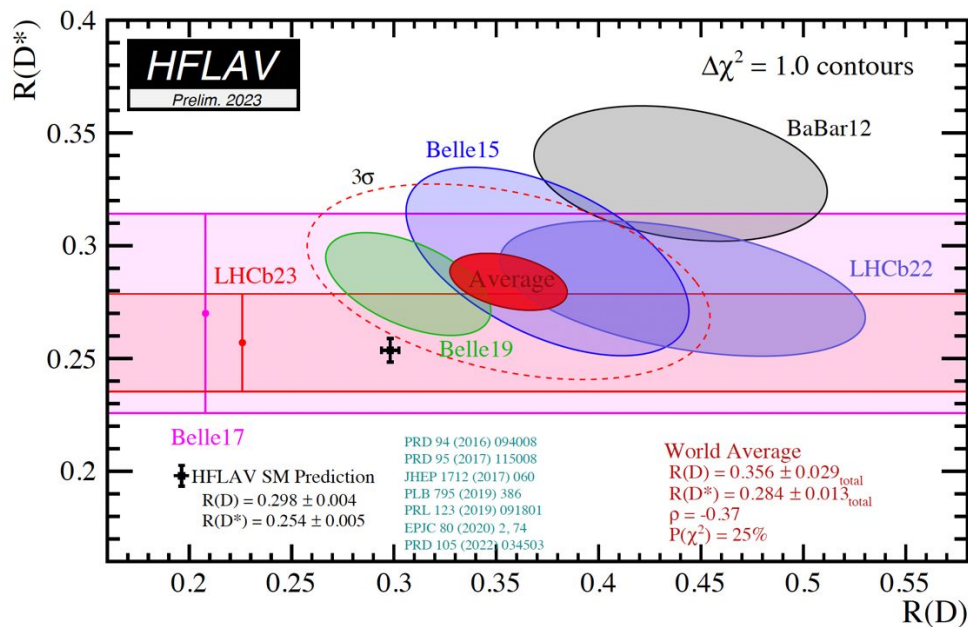
Buchmüller–Rückl–Wyler model, Phys. Lett. B 191 (1987) 442

Table 2

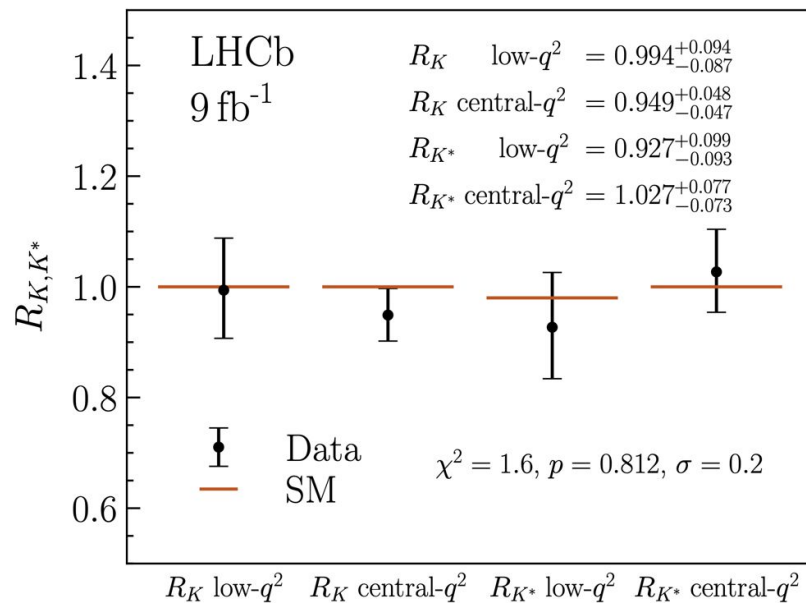
Couplings of scalar and vector leptoquarks to quark–lepton pairs. The subscripts L,R of the couplings refer to the lepton chirality.

Channel	$F = -2$, scalars			$F = -2$, vectors	
	S_1	\tilde{S}_1	S_3	V_2	\tilde{V}_2
$e_{L,R}^- u$	$g_{1L,R}$	–	$-g_{3L}$	g_{2R}	\tilde{g}_{2L}
$\nu_L d$	$-g_{1L}$	–	$-g_{3L}$	g_{2L}	–
$e_{L,R}^- d$	–	\tilde{g}_{1R}	$-\sqrt{2} g_{3L}$	$g_{2L,R}$	–
$\nu_L u$	–	–	$\sqrt{2} g_{3L}$	–	\tilde{g}_{2L}
Channel	$F = 0$, vectors			$F = 0$, scalars	
	U_1	\tilde{U}_1	U_3	R_2	\tilde{R}_2
$e_{L,R}^- \bar{d}$	$h_{1L,R}$	–	$-h_{3L}$	$-h_{2R}$	\tilde{h}_{2L}
$\nu_L \bar{u}$	h_{1L}	–	h_{3L}	h_{2L}	–
$e_{L,R}^- \bar{u}$	–	\tilde{h}_{1R}	$\sqrt{2} h_{3L}$	$h_{2L,R}$	–
$\nu_L \bar{d}$	–	–	$\sqrt{2} h_{3L}$	–	\tilde{h}_{2L}

B-anomalies



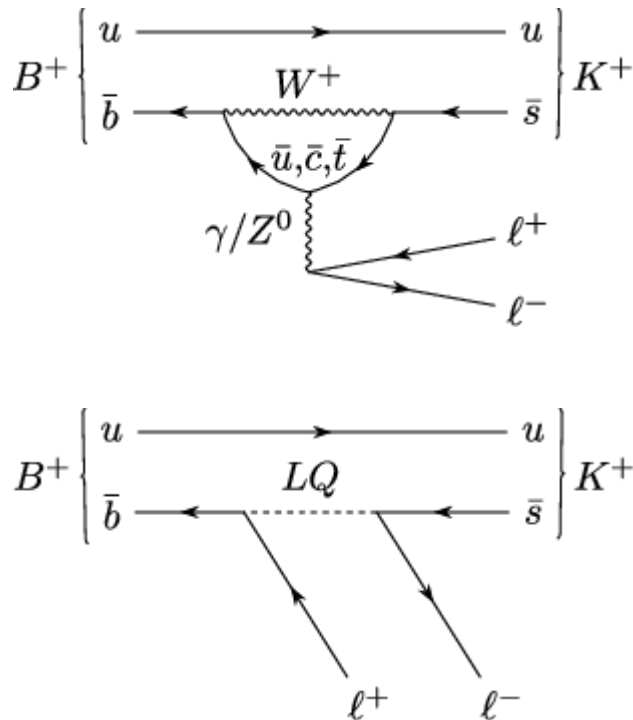
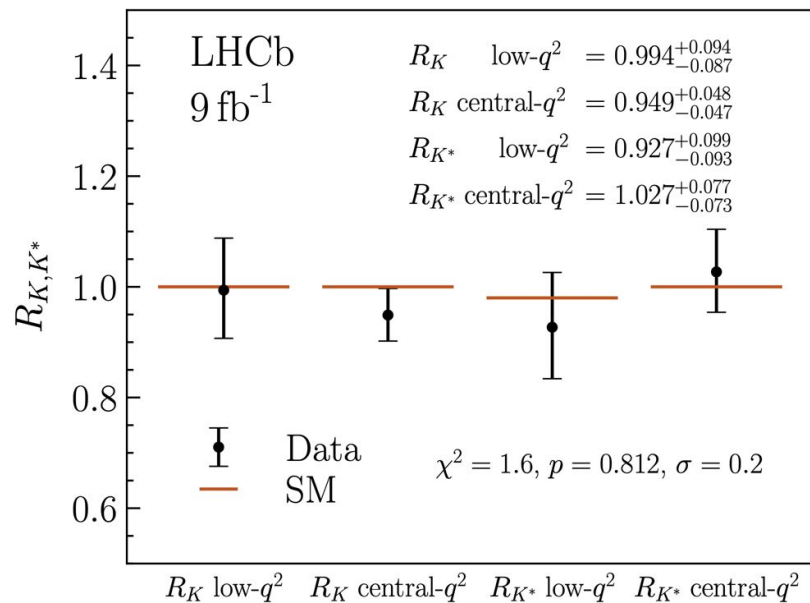
Status of the charged-current LFU ratios $R(D)$ and $R(D^*)$.



Measurements of the e/μ LFU ratios reported by LHCb in December 2022.

Fully compatible with the SM

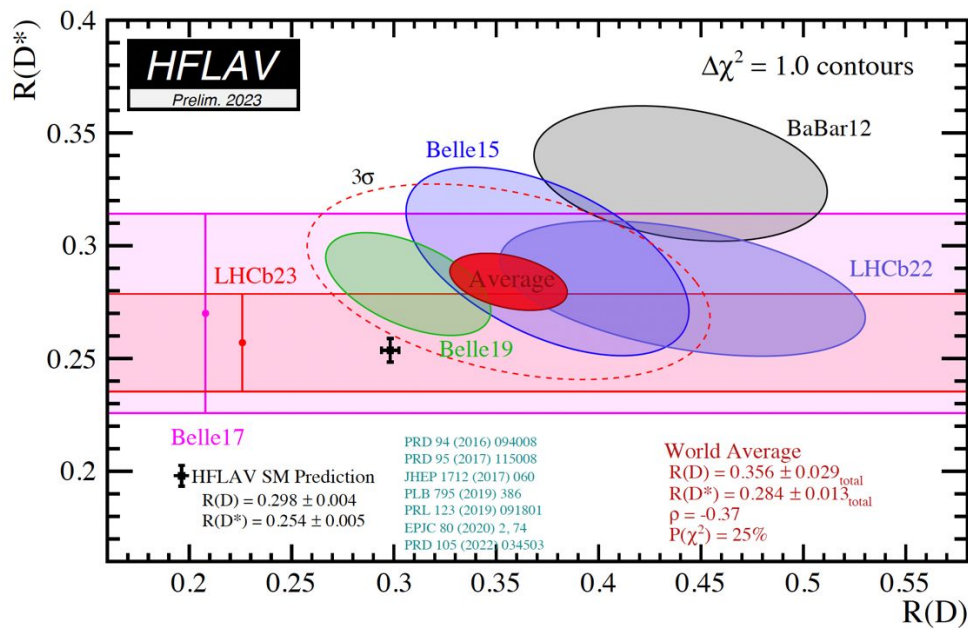
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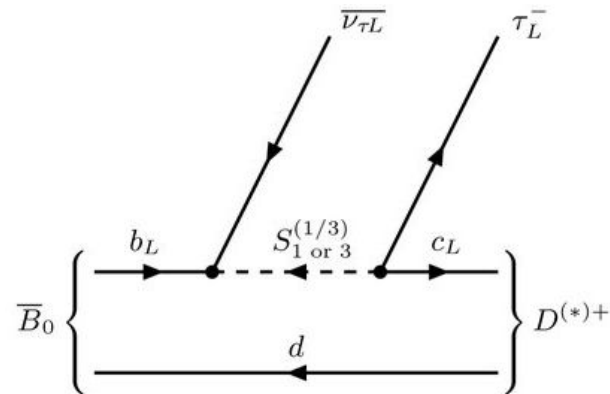
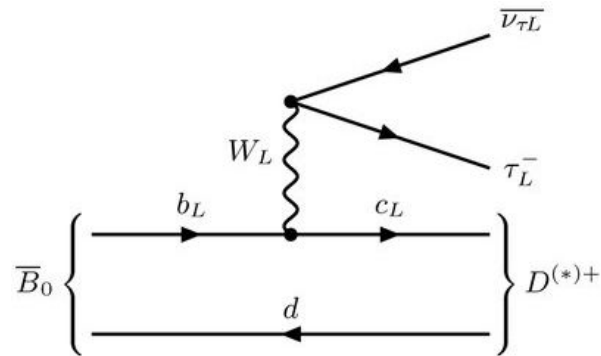
$$R_{K^{(*)}}^{[q_1^2, q_2^2]} = \frac{\text{Br}'(B \rightarrow K^{(*)} \mu \mu)}{\text{Br}'(B \rightarrow K^{(*)} e e)}$$

B-anomalies



Status of the charged-current LFU ratios $R(D)$ and $R(D^*)$.

$$R_{D^{(*)}} = \left. \frac{\text{Br}(B \rightarrow D^{(*)} \tau \bar{\nu})}{\text{Br}(B \rightarrow D^{(*)} \ell \bar{\nu})} \right|_{\ell \in \{e, \mu\}}$$



Supervised Learning

Input

Labeled data $D = \{(\bar{x}_1, t_1), \dots, (\bar{x}_n, t_n)\}$

$\{\bar{x}_i\}$: features, e.g. $p_T, \Delta\phi_{12}, E_t^{\text{miss}}$

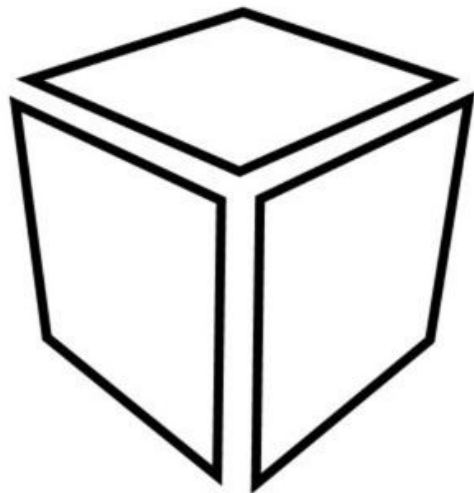
$\{t_i\}$: target, e.g. for classification:

1 for *signal*

0 for *background*

Train
dataset \bar{x}

dataset \bar{x}
Train



ML classifier

Output

The algorithm finds a mapping:

ideally $o(\bar{x}_i) = t_i$

for classification: $o(\bar{x}_i) \in [0, 1]$

ML output
 $o(\bar{x})$

$o(\bar{x})$
ML output

Always 1D

Supervised Learning

New data

Data sample that we do not know if it is Signal or Background

S or B
label ??

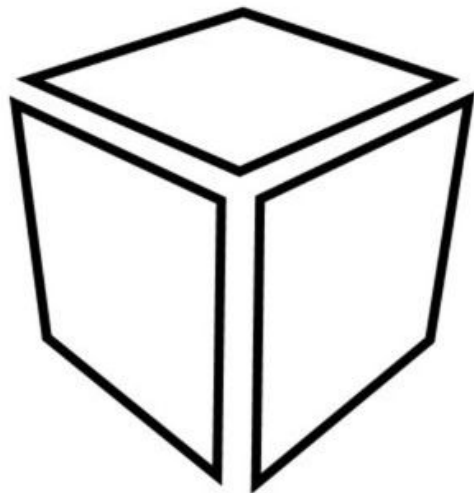
Prediction

To assign a label a threshold or working point (WP) is needed

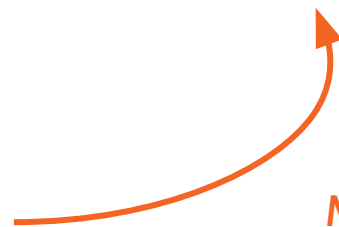
if $o(x) < WP$ label \rightarrow '0' \rightarrow **B**
if $o(x) > WP$ label \rightarrow '1' \rightarrow **S**

Test
dataset \bar{x}

dataset \bar{x}
test



ML classifier



ML output
 $o(\bar{x})$

$o(\bar{x})$
ML output

Always 1D

Machine Learned-Likelihood (MLL)

Likelihood to define the statistical model for N independent measurements, with a set of observables x_i

$$\mathcal{L}(\mu, s, b) = p(N, \{x_i, i = 1, \dots, N\} | \mu, s, b) = \underbrace{\text{Pois}(N | \mu S + B)}_{\substack{\sim \text{global info} \\ \text{ensemble factor}}} \underbrace{\prod_{i=1}^N p(x_i | \mu, s, b)}_{\substack{\sim \text{local info} \\ \text{event-by-event}}}$$

with:

- S the expected total signal yield
- B the expected total background yield

$$\bullet \quad p(x | \mu, s, b) = \frac{B}{\mu S + B} p_b(x) + \frac{\mu S}{\mu S + B} p_s(x)$$

$$p_s(x) = p(x | s)$$

$$p_b(x) = p(x | b)$$

- μ the signal strength defines the hypothesis we are testing for:

background-only hypothesis $\rightarrow \mu = 0$

background-plus-signal hypothesis $\rightarrow \mu = 1$

Machine Learned-Likelihood (MLL)

The relevant test statistic for **discovery** limits (very similar for exclusion):

discovery corresponds to studying background-only hypothesis $\mu = 0$

using the Likelihood

$$q_0 = \begin{cases} -2 \text{Ln} \frac{\mathcal{L}(0, s, b)}{\mathcal{L}(\hat{\mu}, s, b)} & \text{if } \hat{\mu} \geq 0, \\ 0 & \text{if } \hat{\mu} < 0, \end{cases}$$

$$q_0 = \begin{cases} -2\hat{\mu}S + 2 \sum_{i=1}^N \text{Ln} \left(1 + \frac{\hat{\mu}S}{B} \frac{p_s(x_i)}{p_b(x_i)} \right) & \text{if } \hat{\mu} \geq 0, \\ 0 & \text{if } \hat{\mu} < 0. \end{cases}$$

where $\hat{\mu}$ is the parameter that maximizes the likelihood

$$\sum_{i=1}^N \frac{p_s(x_i)}{\hat{\mu}S p_s(x_i) + B p_b(x_i)} = 1.$$

Machine Learned-Likelihood (MLL)

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discovery corresponds to studying background-only hypothesis $\mu = 0$

We need

$$p_s(x) = p(x|s)$$

$$p_b(x) = p(x|b)$$

Machine Learned-Likelihood (MLL)

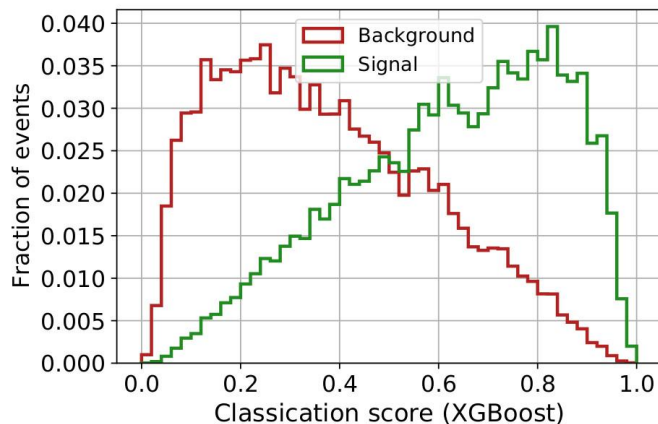
Replace the densities for the one-dimensional manifolds obtained with a machine-learning classifier.

The classification score that maximizes the binary cross-entropy approaches:

$$o(x) = \frac{p_s(x)}{p_s(x) + p_b(x)}$$

Dimensional reduction by dealing with $o(x)$ instead of x

$$p_b(x) \rightarrow \tilde{p}_b(o(x)), \quad \text{and} \quad p_s(x) \rightarrow \tilde{p}_s(o(x))$$



where $\tilde{p}_{s,b}(o(x))$ are the distributions of $o(x)$ for signal and background, obtained by evaluating the classifier on a set of pure signal or background events, respectively.

Machine Learned-Likelihood (MLL)

Then, the relevant test statistic for **discovery** limits

$$q_0 = \begin{cases} -2\hat{\mu}S + 2 \sum_{i=1}^N \text{Ln} \left(1 + \frac{\hat{\mu}S}{B} \frac{\tilde{p}_s(o(x_i))}{\tilde{p}_b(o(x_i))} \right) & \text{if } \hat{\mu} \geq 0, \\ 0 & \text{if } \hat{\mu} < 0, \end{cases}$$

with $\hat{\mu}$ the parameter that maximizes the likelihood

$$\sum_{i=1}^N \frac{\tilde{p}_s(o(x_i))}{\hat{\mu}S \tilde{p}_s(o(x_i)) + B \tilde{p}_b(o(x_i))} = 1$$

We can estimate numerically the q_0 distribution.

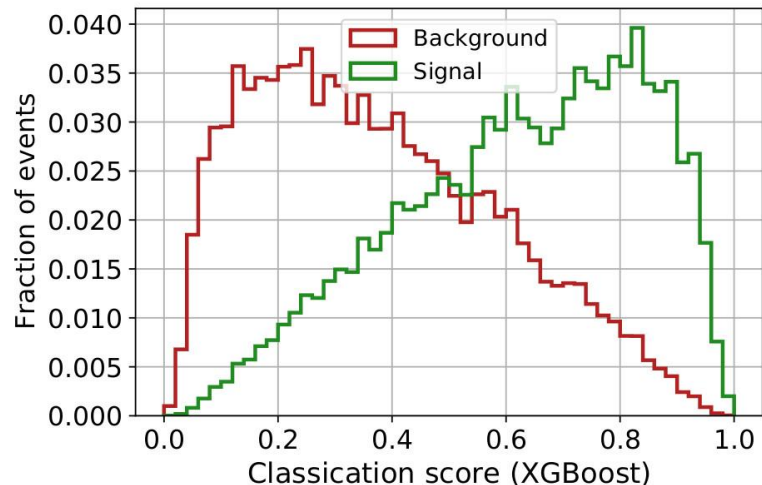
The median expected significance assuming signal-plus-background hypothesis ($\mu'=1$) is

$$Z_0 \rightarrow \text{med} [Z_0|1] = \sqrt{\text{med} [q_0|1]}$$

Density estimation

We want to retrieve the density function from which the samples were generated

$$p_b(x) \rightarrow \tilde{p}_b(o(x)), \quad \text{and} \quad p_s(x) \rightarrow \tilde{p}_s(o(x))$$



The original space, x , can be high-dimensional
but the classifier output $\mathbf{o}(x)$ is **always one-dimensional**

- To avoid binning, we use a non-parametric method:

Kernel Density Estimation (KDE)

Kernel Density Estimation (KDE)

$$p_{s,b}(o(x)) = \frac{1}{N} \sum_i^N \kappa_\epsilon [o(x) - o(x_i)]$$

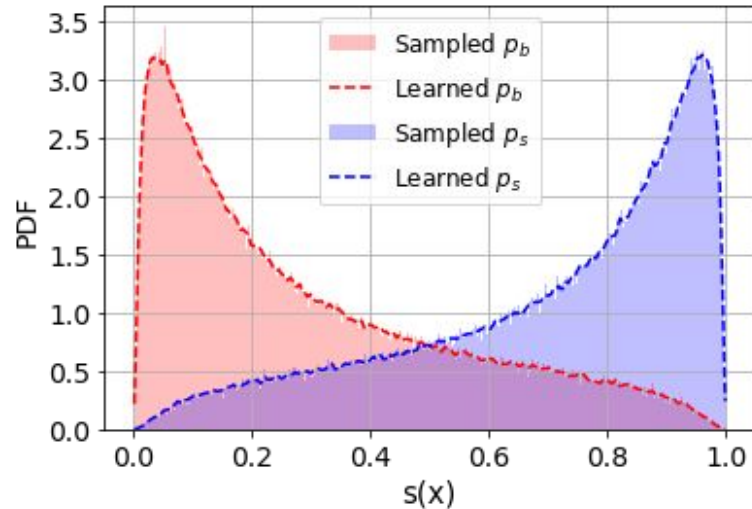
where κ_ϵ is a kernel function that depends on the "smoothing" scale, or bandwidth parameter ϵ .

We use the Epanechnikov kernel

$$\kappa_\epsilon(u) = \begin{cases} \frac{1}{\epsilon} \frac{3}{4} (1 - (u/\epsilon)^2), & \text{if } |u| \leq \epsilon \\ 0, & \text{otherwise} \end{cases}$$

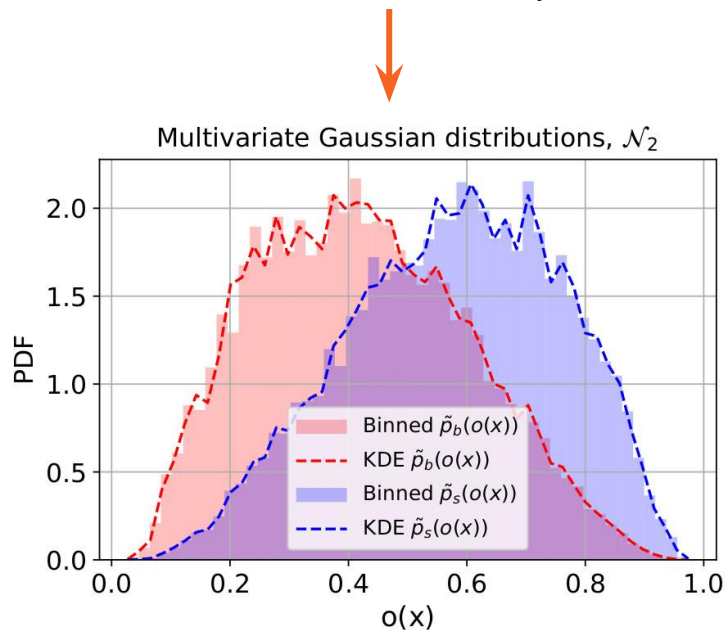
The bandwidth parameter ϵ is key

- if ϵ is too low the model may overfit
- if ϵ is too high the model may underfit



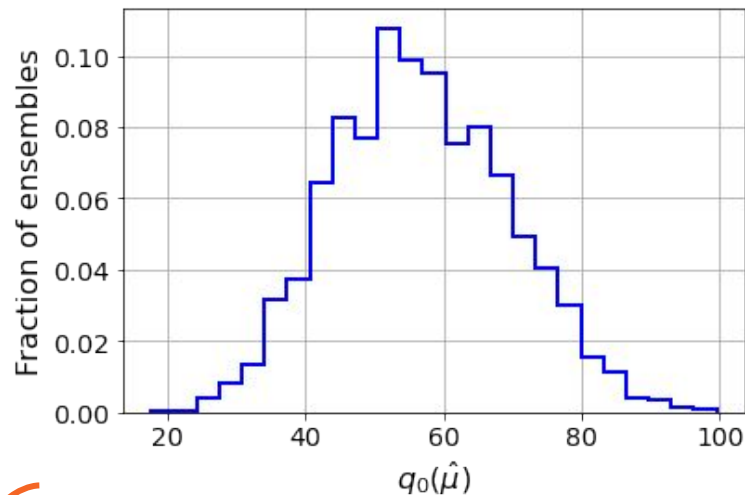
Machine Learned-Likelihood (MLL)

Train supervised per-even classifier:
XGBoost with 1M events per class



Evaluate $o(x)$ with the test data-set
Find the distributions with KDE

Build toy ensembles of fixed B and S (each one represent a possible experimental result)
and evaluate the test statistic q_0



Calculate the significance

$$Z = \sqrt{\text{med}[q_0]}$$

Machine Learned-Likelihood (MLL)

First find $\hat{\mu}$ (for each ensemble)

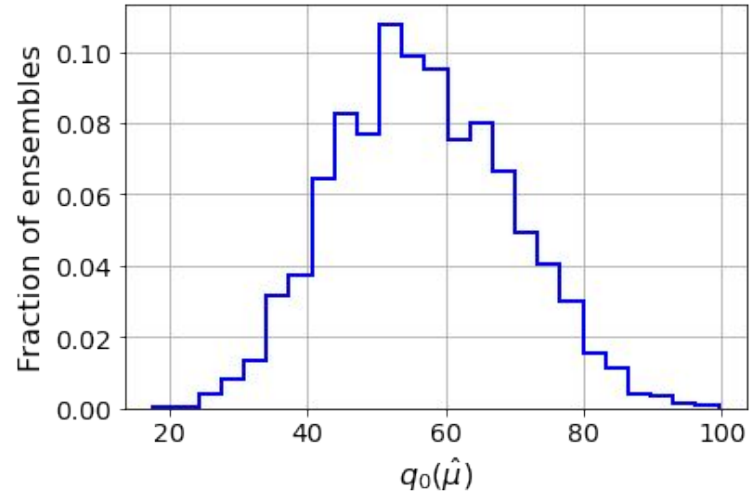
$$\sum_{i=1}^N \frac{\tilde{p}_s(o(x_i))}{\hat{\mu} S \tilde{p}_s(o(x_i)) + B \tilde{p}_b(o(x_i))} = 1$$

↓
summation over the events of
each ensemble (build a lot)

Estimate numerically the test
statistic (for each ensemble)

$$q_0 = \begin{cases} -2\hat{\mu}S + 2 \sum_{i=1}^N \text{Ln} \left(1 + \frac{\hat{\mu}S}{B} \frac{\tilde{p}_s(o(x_i))}{\tilde{p}_b(o(x_i))} \right) & \text{if } \hat{\mu} \geq 0, \\ 0 & \text{if } \hat{\mu} < 0, \end{cases}$$

Build toy ensembles of fixed B and S (each one
represent a possible experimental result)
and evaluate the test statistic q_0



Calculate the significance

$$Z = \sqrt{\text{med}[q_0]}$$

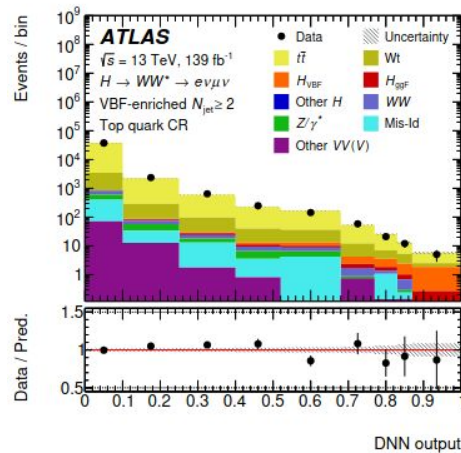
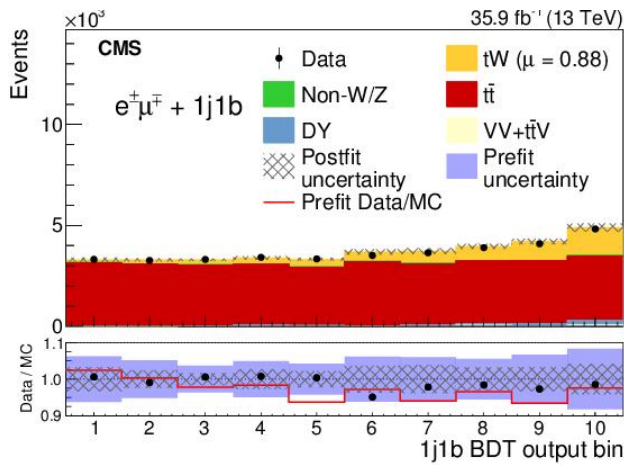
Traditional Binned-Likelihood (BL) method

The Likelihood for D bins, where in each bin d , B_d : the expected number of background events, S_d : the expected number of signal events, and N_d : the measured number of events,

$$\mathcal{L}(\mu, s, b) = \prod_{d=1}^D \text{Pois}(N_d | \mu S_d + B_d)$$

The median discovery significance

$$\text{med} [Z_0^{\text{binned}} | 1] = \left[2 \sum_{d=1}^D \left((S_d + B_d) \text{Ln} \left(1 + \frac{S_d}{B_d} \right) - S_d \right) \right]^{1/2} \xrightarrow[\sqrt{B} \gg 1]{S \ll B} \frac{S}{\sqrt{B}}$$



Machine Learned-Likelihood (MLL)

The relevant test statistic for **exclusion** limits (very similar for exclusion):

exclusion corresponds to
studying signal+background
hypothesis $\mu = 1$

using the Likelihood

$$\tilde{q}_\mu = \begin{cases} 0 & \text{if } \hat{\mu} > \mu, \\ -2 \text{Ln} \frac{\mathcal{L}(\mu, s, b)}{\mathcal{L}(\hat{\mu}, s, b)} & \text{if } 0 \leq \hat{\mu} \leq \mu, \\ -2 \text{Ln} \frac{\mathcal{L}(\mu, s, b)}{\mathcal{L}(0, s, b)} & \text{if } \hat{\mu} < 0, \end{cases}$$

$$\tilde{q}_\mu = \begin{cases} 0 & \text{if } \hat{\mu} > \mu \\ 2(\mu - \hat{\mu})S - 2 \sum_{i=1}^N \text{Ln} \left(\frac{B p_b(x_i) + \mu S p_s(x_i)}{B p_b(x_i) + \hat{\mu} S p_s(x_i)} \right) & \text{if } 0 \leq \hat{\mu} \leq \mu \\ 2\mu S - 2 \sum_{i=1}^N \text{Ln} \left(1 + \frac{\mu S p_s(x_i)}{B p_b(x_i)} \right) & \text{if } \hat{\mu} < 0; \end{cases}$$

where $\hat{\mu}$ is the parameter that maximizes the likelihood

$$\sum_{i=1}^N \frac{p_s(x_i)}{\hat{\mu} S p_s(x_i) + B p_b(x_i)} = 1.$$

The median expected significance
assuming background-only
hypothesis ($\mu'=0$) is

$$Z_\mu \rightarrow \text{med} [Z_\mu | 0] = \sqrt{\text{med} [\tilde{q}_\mu | 0]}$$