A model-independent likelihood function for the Belle II $B^+ \to K^+\nu\bar{\nu}$ analysis

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in collaboration with

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Reusability in HEP

Publishing statistical models: Getting the most out of particle physics experiments

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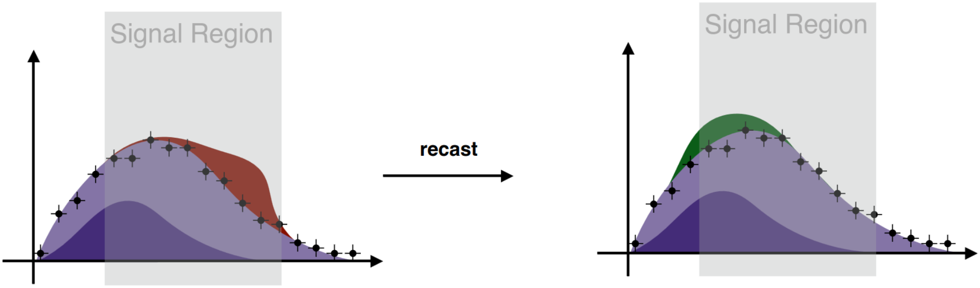
Forum [8], with the current status and updated recommendations presented in Ref. [6]. This paper takes these decade-long efforts to what we argue is the logical conclusion: if we wish to maximize the scientific impact of particle physics experiments, decades into the future, we should make the publication of full statistical models, together with the data to convert them into likelihood functions, standard practice. A statistical model provides the complete mathematical description of an experimental analysis and is, therefore, the appropriate starting

[arXiv:2109.04981 [hep-ph]]

Shortcomings of model-dependencies in analyses

- **Limited interpretability** in terms of any BSM or future SM physics with different kinematic predictions.

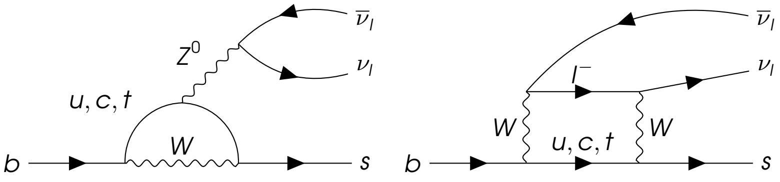
Idea behind reinterpretation



original analysis (w.r.t **model A**) original analysis (recast to **model B**)

[source]

Why reinterpret $B^+ \to K^+ \nu\bar{\nu}$?



- Suppression of FCNCs in the SM.

➜ Tree level BSM effects could substantially affect observables.

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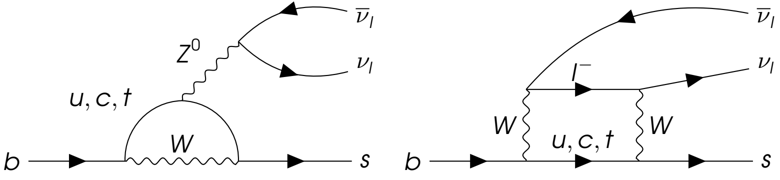

- Suppression of FCNCs in the SM.

➜ Tree level BSM effects could substantially affect observables.

- **Benefits of reinterpretation**
  - **Sensitivity** to any current or future (B)SM prediction.
  - **Exclusion** limits in BSM parameter space inferable.
  - **Combinations** with other measurements possible.

Analysis

Where is the model dependence?

The Belle II $B^+ \to K^+ \nu\bar{\nu}$ analysis

1. Two consecutive BDTs separate signal from background.
2. Signal MC weighted according to SM kinematic prediction.
   $\to$ **model dependence**
3. Max. likelihood fit in bins of $p_T(K^+) \times BDT_2$.

[hepdata.130199]
[Phys.Rev.Lett.127.181802]

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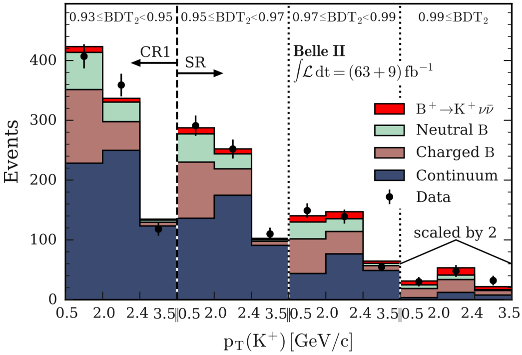

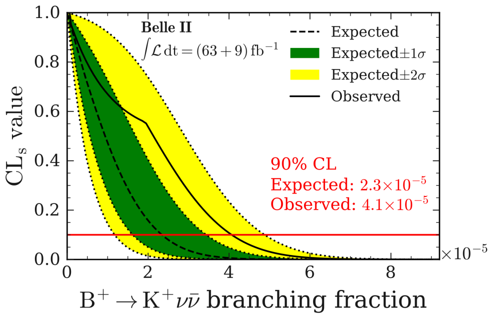

$\mathcal{B}(B^+ \to K^+ \nu\bar{\nu}) < 4.1 \times 10^{-5}$@90%CL

Reweighting approach

How do we obtain new signal templates?

Reweighting recipe

Recipe

1. Find kinematic dependence of measured observable: $\Gamma(q^2)$, $q^2 = (p_\nu + p_{\bar{\nu}})^2$

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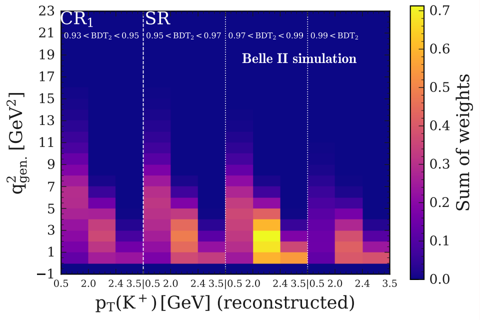
2. Get distributions of kinematic d.o.f (q^2)

$$N_{klm} = \underbrace{p_T \times BDT_2}_{\text{analysis binning}} \times \underbrace{q^2_{gen.}}_{\text{kinematic d.o.f}}$$



Reweighting approach

Recipe

1. Find kinematic dependence of theoretical prediction: $\Gamma(q^2)$, $q^2 = (p_\nu + p_{\bar{\nu}})^2$
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$$N_{k\,l\,m} = \underbrace{p_T \times BDT_2}_{\text{analysis binning}} \times \underbrace{q^2_{gen.}}_{\text{kinematic d.o.f}}$$

3. Apply weights in bins of kinematic d.o.f. (phase space (PHSP): $\mathcal{M} = 1$)

$$N_{k\,l} = \sum_{m \in q^2} N^{\text{PHSP}}_{k\,l\,m} \, w_m = \sum_{m \in q^2} N^{\text{PHSP}}_{k\,l\,m} \int_{\text{bin } m} dq^2 \frac{d\Gamma^{(B)SM}}{dq^2} \left(\frac{d\Gamma^{\text{PHSP}}}{dq^2} \right)^{-1}$$

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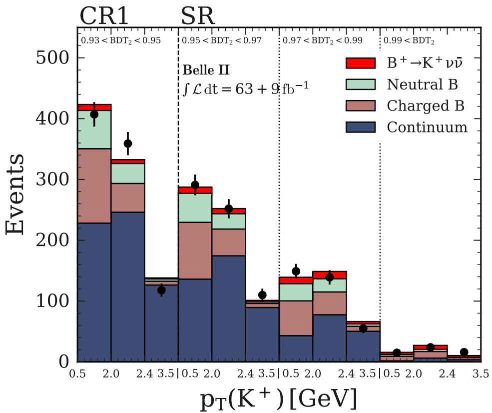
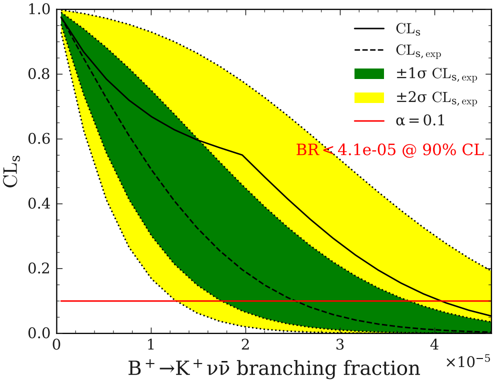
Benefits

+ Fast
+ Versatile
+ Easily publishable

Validation: Reproducing the upper limit





$\mathcal{B}(B^+ \to K^+ \nu\bar{\nu}) < 4.1 \times 10^{-5}$@90%CL

pyhf.readthedocs.io

Theory

How can we parametrize our model dependence?

(B)SM theory predictions

- Parametrize decay rate within the weak effective theory

$$\mathcal{L}_{SM} \to \mathcal{L}_{WET} = \sum C_i \, \mathcal{O}_i$$

- Capture BSM physics above electroweak symmetry breaking scale with

$$C_{SL} + C_{SR} \qquad C_{VL} + C_{VR} = C_{VL}^{SM} + C_{VL}^{NP} + C_{VR} \qquad C_{TL}$$

eos.github.io

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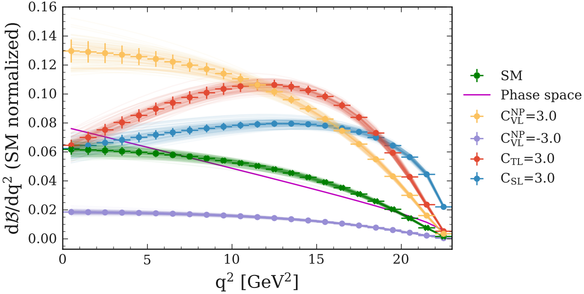
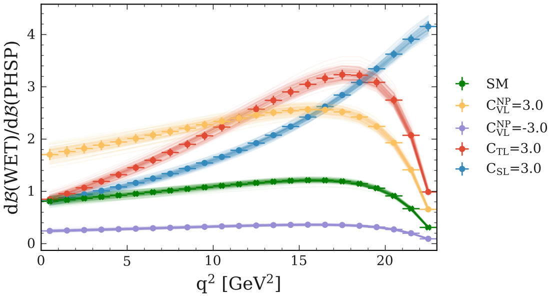




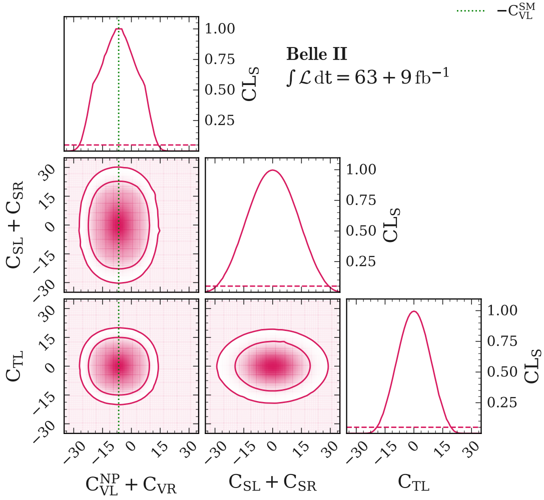
Fruits of reinterpretation

What do we get from all this?

Wilson coefficient exclusion limits

- pyhf + EOS → fast & reliable
- Exclusion limits @95%CL

$$|C_{VL}^{SM} + C_{VL}^{NP} + C_{VR}| < 20.6$$
$$|C_{SL} + C_{SR}| < 29.3$$
$$|C_{TL}| < 19.4$$



∂ifferentiable ℒikelihoods

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Analysis update: $B^+ \to K^+\nu\bar{\nu}$ @ 362 fb^{-1}

Inclusive $\mathcal{B} = \left(2.8^{+0.5}_{-0.5}{}^{+0.5}_{-0.5}\right) \times 10^{-5}$

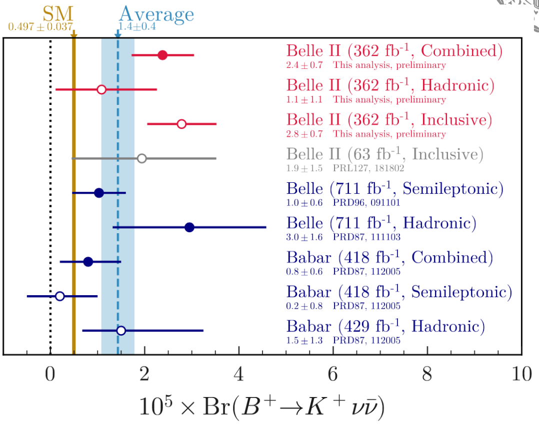
Hadronic $\mathcal{B} = \left(1.1^{+0.9}_{-0.8}{}^{+0.8}_{-0.5}\right) \times 10^{-5}$

Combined $\mathcal{B} = \left(2.4^{+0.5}_{-0.5}{}^{+0.5}_{-0.4}\right) \times 10^{-5}$

Significance of the **combined** result:

- 3.6σ wrt. null hypothesis
- 2.8σ wrt. SM

First evidence of $B^+ \to K^+\nu\bar{\nu}$



Model-independent likelihood method will be applied and published.

Presented at EPS 2023

Summary

- **Challenge**
  - Neutrino-induced experimental complexities

  ➜ **model-dependent results**
- **Solution**
  - **Model-independent likelihood function**
    Maximum likelihood fits for any given (B)SM signal prediction.
- **Benefits**
  - **Exclusions in BSM parameter space.**
  - **Combinations** with other channels and/or experiments.
  - Individual model studies with provided decay rate predictions.
- **Significance**
  - Publishing such likelihoods is crucial for a full exploitation of experimental results.

Belle II EOS pyhf ∂ifferentiable ℒikelihoods

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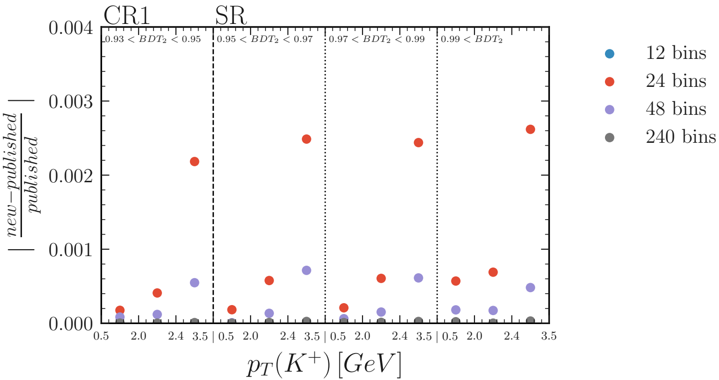
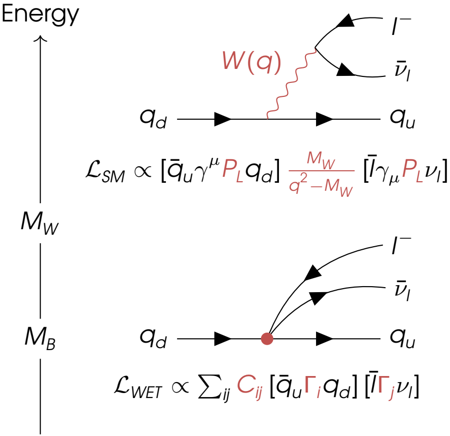
Binning choice

We compared the relative accuracy of the binned weighting (new) with the event-by-event weighting (published).



Effective field theory

- **High energy collisions**
  Enough energy to radiate off an on-shell (massive) W boson.
- **Lower energy quark decays**
  W boson is always off-shell.



$$\mathcal{L}_{SM} \propto [\bar{q}_u \gamma^\mu P_L q_d] \frac{M_W}{q^2 - M_W} [\bar{l} \gamma_\mu P_L \nu_l]$$

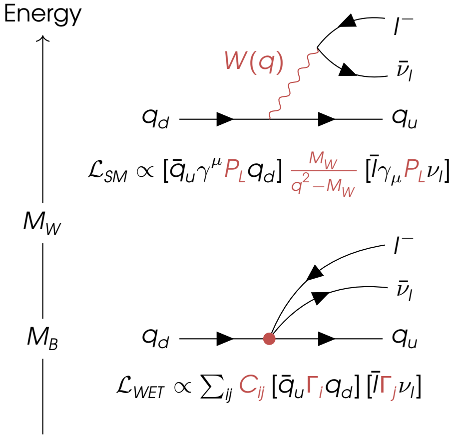
$$\mathcal{L}_{WET} \propto \sum_{ij} C_{ij} [\bar{q}_u \Gamma_i q_d] [\bar{l} \Gamma_j \nu_l]$$

Effective field theory

- **High energy collisions**
  Enough energy to radiate off an on-shell (massive) W boson.
- **Lower energy quark decays**
  W boson is always off-shell.
- **Weak effective theory**
  W is integrated out – effects are encoded in new couplings

$$\mathcal{L}_{SM} \to \mathcal{L}_{WET} = \sum C_i \, \mathcal{O}_i$$

➜ Model independent **parametrization**, constrained only by Wilson coefficients C_i.



Weak Effective Theory for $B \to K\nu\bar{\nu}$

Contribution operators

The effective Lagrangian is

$$\mathcal{L}^{WET} = \sum_{X=L,R} C_{\mathrm{VX}}\, \mathcal{O}_{\mathrm{VX}} + \sum_{X=L,R} C_{\mathrm{SX}}\, \mathcal{O}_{\mathrm{SX}} + C_{\mathrm{TL}}\, \mathcal{O}_{\mathrm{TL}} + \text{h.c.}$$

The $d = 6$ contributing operators in and beyond the SM are given by

$$\mathcal{O}_{\mathrm{VL}} = \left(\overline{\nu_L}\gamma_\mu \nu_L\right)\left(\overline{s_L}\gamma^\mu b_L\right) \qquad \mathcal{O}_{\mathrm{VR}} = \left(\overline{\nu_L}\gamma_\mu \nu_L\right)\left(\overline{s_R}\gamma^\mu b_R\right)$$

$$\mathcal{O}_{\mathrm{SL}} = \left(\overline{\nu_L^c}\nu_L\right)\left(\overline{s_R} b_L\right) \qquad \mathcal{O}_{\mathrm{SR}} = \left(\overline{\nu_L^c}\nu_L\right)\left(\overline{s_L} b_R\right)$$

$$\mathcal{O}_{\mathrm{TL}} = \left(\overline{\nu_L^c}\sigma_{\mu\nu} \nu_L\right)\left(\overline{s_R}\sigma^{\mu\nu} b_L\right)$$

[arXiv:2111.04327 [hep-ph]]

Weak Effective Theory for $B \to K\nu\bar{\nu}$

Decay width

Decay width dependence on the Wilson coefficients is given by

$$\frac{d\Gamma\left(B \to K\nu\bar{\nu}\right)}{dq^2} = \frac{\sqrt{\lambda_{BK}}q^2}{(4\pi)^3 m_B^3}\left[\frac{\lambda_{BK}}{24q^2}\left|f_+(q^2)\right|^2 \left|C_{\mathrm{VL}} + C_{\mathrm{VR}}\right|^2 + \frac{\left(m_B^2 - m_K^2\right)^2}{8\left(m_b - m_s\right)^2}\left|f_0(q^2)\right|^2 \left|C_{\mathrm{SL}} + C_{\mathrm{SR}}\right|^2 + \frac{2\lambda_{BK}}{3\left(m_B + m_K\right)^2}\left|f_T(q^2)\right|^2 \left|C_{\mathrm{TL}}\right|^2\right]$$

valid for $J^P = 0^-$ kaon states.

[arXiv:2111.04327 [hep-ph]]

Implementation

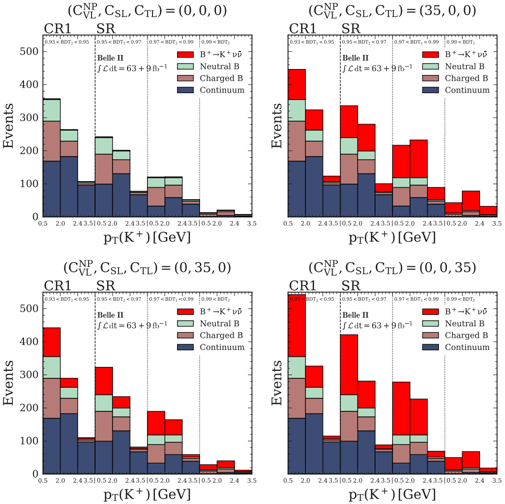
eos.github.io

- Calculate theoretical predictions
- Theory parameters: Wilson coefficients & hadronic parameters

pyhf.readthedocs.io

- Built a "custom modifier" that generates new signal template from theory parameters.
- Theory parameters become fitting parameters.

Expected yields



Parameter space selection

The definition of Wilson coefficients in `arXiv:2111.04327 [hep-ph]` compared to the values used in EOS are

$$C_{paper} = -\frac{4G_F}{\sqrt{2}}\frac{\alpha}{2\pi}V_{ts}^*V_{tb}\left(\frac{X}{\sin^2\theta_W}\right) = -\frac{4G_F}{\sqrt{2}}\frac{\alpha}{2\pi}V_{ts}^*V_{tb}C_{EOS} \approx \frac{1}{615TeV^2}C_{EOS}.$$

We get a rough estimate of the parameter space from `arXiv:2111.04327 [hep-ph]`:

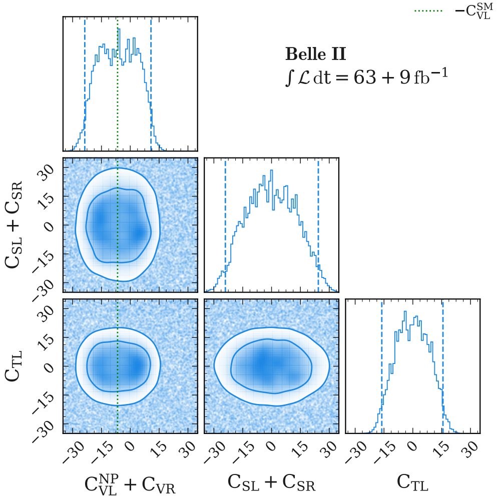
Operator	Value (paper) $[\mathrm{TeV}^{-2}]$	Value (EOS)	NP scale $[\mathrm{TeV}]$	Observable
$\mathcal{O}^{\mathrm{VL,NP}}_{\nu d,\alpha\alpha sb}$	0.028	17.2	6	$B \to K^*\nu\nu$
$\mathcal{O}^{\mathrm{VR}}_{\nu d,\alpha\alpha sb}$	0.021	12.9	7	$B \to K\nu\nu$
$\mathcal{O}^{\mathrm{VL}}_{\nu d,\gamma\delta sb}$	0.014	8.61	9	$B \to K^*\nu\nu$
$\mathcal{O}^{\mathrm{SL}}_{\nu d,\gamma\gamma sb}$	0.012	7.38	10	$B \to K^{(*)}\nu\nu$
$\mathcal{O}^{\mathrm{SL}}_{\nu d,\gamma\delta sb}$	0.009	5.54	10	$B \to K^{(*)}\nu\nu$
$\mathcal{O}^{\mathrm{TL}}_{\nu d,\gamma\delta sb}$	0.002	1.23	25	$B \to K^*\nu\nu$

Hence, choosing an upper bound of $C_{EOS} \leq 35$ completely covers branching ratio values of up to $Br \leq 1.1 \times 10^{-3}$.

Cross check: Bayesian sampling

As an alternative approach, we found exclusion limits in the space of Wilson coefficients by sampling random points in theory space.

- We performed a ML fit for each sample, with fixed signal strength.
- The likelihood is used as a weight for each sample.
- The dashed lines include the 95% central region for each distribution.
- The contours correspond to 68% (inner) and 95% (outer) intervals.

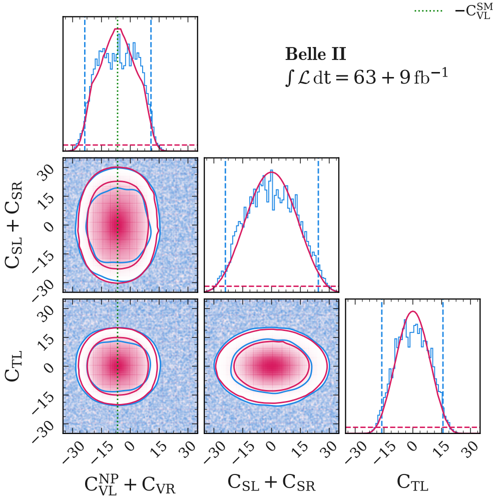


Contour overlay

We compare the two different methods by overlaying their contours.

- The 2d contours overlay very well.
- The 1d contours have a slightly different peak structure.
- The frequentist approach has slightly more conservative limits (1d distributions).

Since the exclusion criterium is different for the two cases, we should only compare the exclusion contours.



Hadronic parameters

Form factors are parameterized using the BCL parametrization

$$f_0\left(q^2\right) = \frac{\mathcal{L}}{1 - \frac{q^2}{M^2_{B^*_{s0}}}} \sum_{n=0}^{N-1} a_n^0 z^n$$

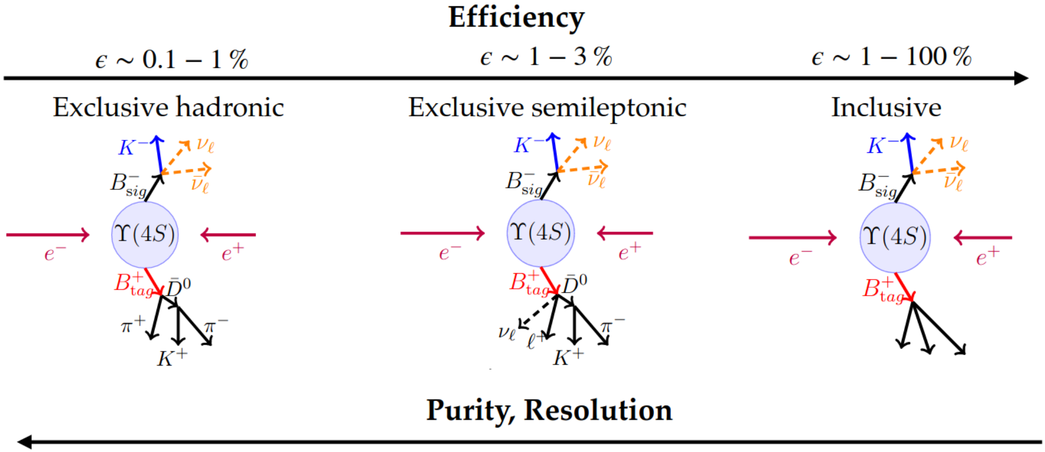
$$f_+\left(q^2\right) = \frac{\mathcal{L}}{1 - \frac{q^2}{M^2_{B^*_s}}} \sum_{n=0}^{N-1} a_n^+ \left(z^n - \frac{n}{N}(-1)^{n-N} z^N\right)$$

$$f_T\left(q^2\right) = \frac{\mathcal{L}}{1 - \frac{q^2}{M^2_{B^*_s}}} \sum_{n=0}^{N-1} a_n^T \left(z^n - \frac{n}{N}(-1)^{n-N} z^N\right),$$

The correlation matrix between the hadronic parameters.

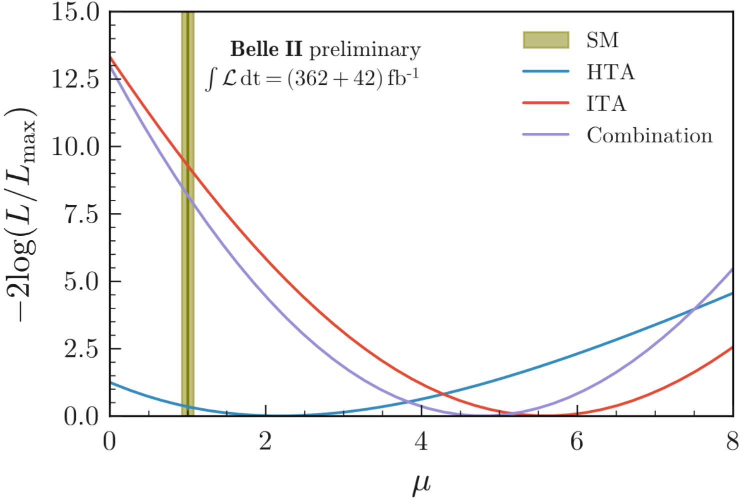
	a_0^+	a_1^+	a_2^+	a_1^0	a_2^0	a_0^T	a_1^T
a_0^+	1.00	0.67	0.33	0.94	0.83	0.43	0.34
a_1^+	0.67	1.00	0.86	0.73	0.70	0.22	0.39
a_2^+	0.33	0.86	1.00	0.39	0.41	0.04	0.26
a_1^0	0.94	0.73	0.39	1.00	0.96	0.40	0.37
a_2^0	0.83	0.70	0.41	0.96	1.00	0.34	0.33
a_0^T	0.43	0.22	0.04	0.40	0.34	1.00	0.89
a_1^T	0.34	0.39	0.26	0.37	0.33	0.89	1.00
a_2^T	0.21	0.42	0.44	0.23	0.23	0.71	0.91

Reconstruction techniques



Different reconstruction techniques lead to nearly orthogonal data samples

Analysis update: $B^+ \to K^+ \nu\bar{\nu}$ @ 362 fb^{-1}



pyhf

For observed event counts $\boldsymbol{n}$ the likelihood function is composed of

$$L(\boldsymbol{n}, \boldsymbol{a} \mid \boldsymbol{\eta}, \boldsymbol{\chi}) = \underbrace{\prod_{c \in \text{ channels}} \prod_{b \in \text{ bins}} \text{Pois}\left(n_{cb} \mid \nu_{cb}(\boldsymbol{\eta}, \boldsymbol{\chi})\right)}_{\substack{\text{Simultaneous measurement} \\ \text{of multiple channels}}} \quad \underbrace{\prod_{\chi \in \boldsymbol{\chi}} c_{\chi}\left(a_{\chi} \mid \chi\right)}_{\substack{\text{constraint terms} \\ \text{for "auxiliary measurements"}}}$$

with free and constrained parameters $\boldsymbol{\eta}, \boldsymbol{\chi}$, respectively,

$$L(\boldsymbol{x} \mid \phi) = L(\boldsymbol{x} \mid \overbrace{\boldsymbol{\eta}}^{\text{free}}, \underbrace{\boldsymbol{\chi}}_{\text{constrained}}) = f(\boldsymbol{x} \mid \overbrace{\boldsymbol{\psi}}^{\text{parameters of interest}}, \underbrace{\boldsymbol{\theta}}_{\text{nuisance parameters}})$$

The auxiliary measurements $\boldsymbol{a}$ are a frequentist approach to count modification.
The expected number of events for each channel and in each bin is

$$\nu_{cb}(\phi) = \sum_{s \in \text{ samples}} \nu_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi}) = \sum_{s \in \text{ samples}} \underbrace{\prod_{\kappa \in \boldsymbol{\kappa}} \kappa_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi})}_{\text{multiplicative modifiers}} \left(\nu_{scb}^{0}(\boldsymbol{\eta}, \boldsymbol{\chi}) + \underbrace{\sum_{\Delta \in \boldsymbol{\Delta}} \Delta_{scb}(\boldsymbol{\eta}, \boldsymbol{\chi})}_{\text{additive modifiers}}\right).$$

Modifiers and constraints

Description	Modification	Constraint Term c_χ	Input
Uncorrelated Shape	$\kappa_{scb}(\gamma_b) = \gamma_b$	$\prod_b \text{Pois}\left(r_b = \sigma_b^{-2} \middle| \rho_b = \sigma_b^{-2}\gamma_b\right)$	σ_b
Correlated Shape	$\Delta_{scb}(\alpha) = f_p\left(\alpha \middle| \Delta_{scb,\alpha=-1}, \Delta_{scb,\alpha=1}\right)$	$\text{Gaus}\left(a = 0 \middle| \alpha, \sigma = 1\right)$	$\Delta_{scb,\alpha=\pm1}$
Normalisation Unc.	$\kappa_{scb}(\alpha) = g_p\left(\alpha \middle| \kappa_{scb,\alpha=-1}, \kappa_{scb,\alpha=1}\right)$	$\text{Gaus}\left(a = 0 \middle| \alpha, \sigma = 1\right)$	$\kappa_{scb,\alpha=\pm1}$
MC Stat. Uncertainty	$\kappa_{scb}(\gamma_b) = \gamma_b$	$\prod_b \text{Gaus}\left(a_{\gamma_b} = 1 \middle| \gamma_b, \delta_b\right)$	$\delta_b^2 = \sum_s \delta_{sb}^2$
Luminosity	$\kappa_{scb}(\lambda) = \lambda$	$\text{Gaus}\left(l = \lambda_0 \middle| \lambda, \sigma_\lambda\right)$	$\lambda_0, \sigma_\lambda$
Normalisation	$\kappa_{scb}(\mu_b) = \mu_b$		
Data-driven Shape	$\kappa_{scb}(\gamma_b) = \gamma_b$		