Unifying MadNIS and Amplitude Surrogates for NLO

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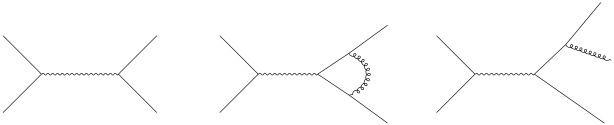
Cross section at Next to Leading Order

Cross section at Next-to-Leading-Order (NLO) combines three contributions



(a) Born (b) Virtual (c) Real emission

Virtual and real diagrams IR divergent; sum is finite (KLN theorem)

$$d\sigma^{\mathsf{NLO}} = \underbrace{\int_{\mathsf{d}\Phi_n} \left[d\sigma^{\mathsf{B}} + d\sigma^{\mathsf{V}} \right]}_{n\text{-body}} + \underbrace{\int_{\mathsf{d}\Phi_{n+1}} d\sigma^{\mathsf{R}}}_{(n+1)\text{-body}} \tag{1}$$

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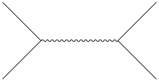
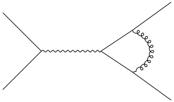
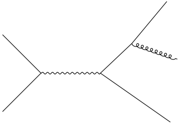


(a) Born



(b) Virtual



(c) Real emission

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$$d\sigma^{\mathsf{NLO}} = \underbrace{\int_{\mathsf{d}\Phi_n} \left[d\sigma^{\mathsf{B}} + d\sigma^{\mathsf{V,reg}} + d\sigma^{\mathsf{I}}\right]}_{n\text{-body}} + \underbrace{\int_{\mathsf{d}\Phi_{n+1}} \left(d\sigma^{\mathsf{R}} - d\sigma^{\mathsf{S}}\right)}_{(n+1)\text{-body}} \tag{1}$$

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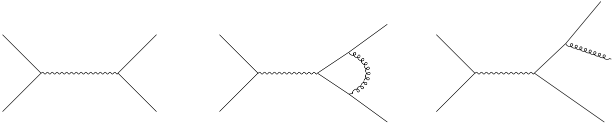

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Key point

Sum is finite but separate integrals are not; possible to implement analytical cancellation in numerical methods

FKS subtraction scheme

Store the cancellation in real part of dσ.

$$\mathrm{d}\sigma^{\mathsf{R}} \to \sum_{ij\in\text{sectors}} \mathrm{d}\sigma^{\mathsf{R}}_{ij} \propto |\mathcal{M}|^2 \mathcal{S}_{ij}\xi_i^2(1-y_{ij}) = \Sigma_{ij} \tag{2}$$

$\mathcal{S}_{ij}$: sector partition function
ξ_i: energy of emitted gluon
y_{ij}: collinearity of sector pair

Implicitly we translate the integration into the following numerical integral (well behaved):

$$d\sigma^{\mathsf{R}} \to \sum_{ij} \int_{\mathrm{d}\Phi_n} \mathrm{d}\xi_i \mathrm{d}y_{ij} \, \frac{\Sigma_{ij} - \overbrace{\boxed{\Sigma_{ij}(\text{sing.})}}^{\text{pole subtraction}}}{\underbrace{\boxed{\xi_i(1-y_{ij})}}_{\text{regularization terms}}}$$

numerically hard:
0/0 if not careful!

Takeaway

FKS method: phase space partitioning, singular region regularization

Full subtracted term

$$
\begin{aligned}
\mathrm{d}\sigma_{ij}^{\mathsf{R}} - \mathrm{d}\sigma_{ij}^{\mathsf{S}} \propto \frac{1}{\xi_i^2(1-y_{ij})} \Big[& \Sigma_{ij}(\Phi_n, \xi_i, y_{ij}, \varphi_i) \\
& -\Sigma_{ij}(\Phi_n, \xi_i, 1, \varphi_i)\, \Theta(y_{ij} - 1 + \delta) \\
& -\Sigma_{ij}(\Phi_n, 0, y_{ij}, \varphi_i)\, \Theta(\xi_{\mathsf{cut}} - \xi_i) \\
& +\Sigma_{ij}(\Phi_n, 0, 1, \varphi_i)\, \Theta(y_{ij} - 1 + \delta)\, \Theta(\xi_{\mathsf{cut}} - \xi_i) \Big]\,.
\end{aligned} \tag{3}
$$

- Subtraction of the *regularized* object Σ_{ij}
- Construction of different kinematics for subtraction terms

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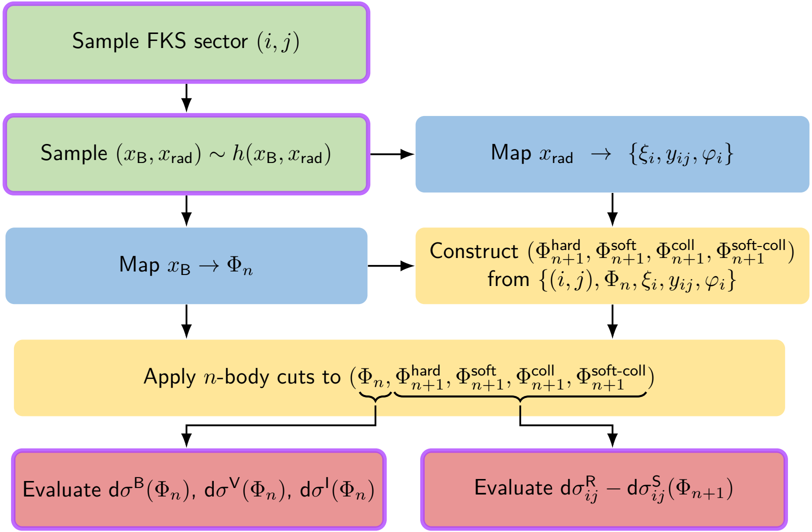
Cut hyperparameters

Cross section independent of δ, ξ_{cut}: hyperparameters to be optimized

Sampling algorithm for MC integration



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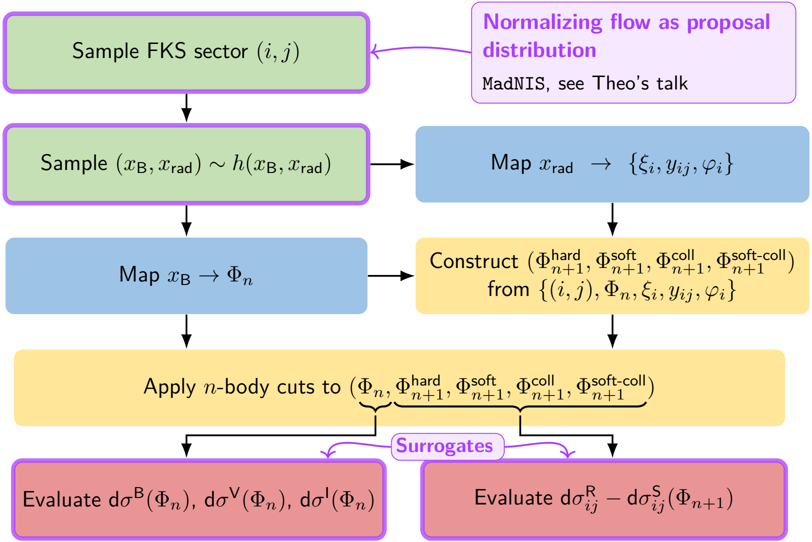
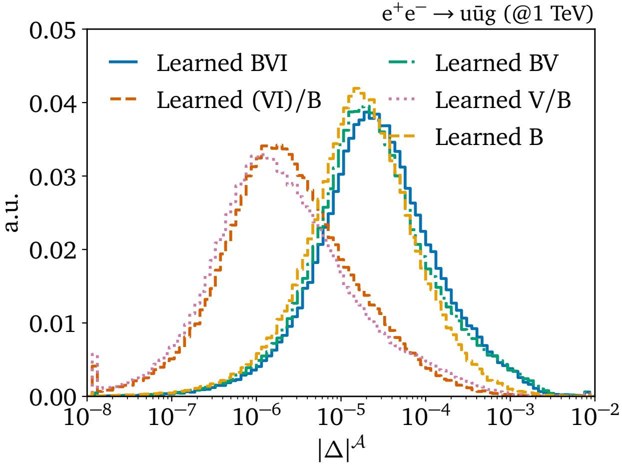


MLP results: virtual surrogate



- Simple MLP; input are Φ_n and $\log s_{ij}$
- $|\Delta| = \left|\frac{\text{true} - \text{pred}}{\text{true}}\right|$
- Different target parameterization: $\frac{\text{V}}{\text{B}}$ easiest to learn

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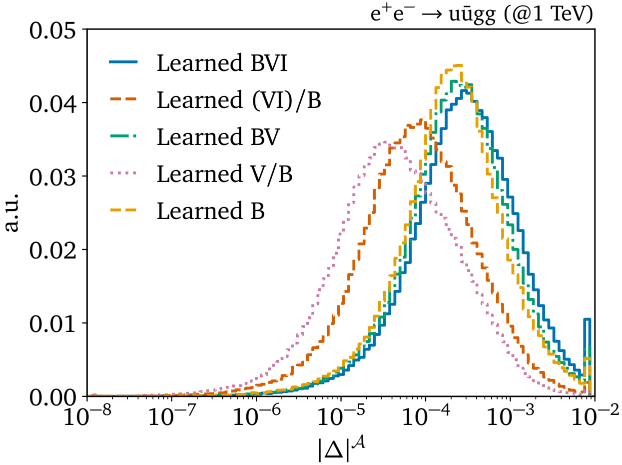

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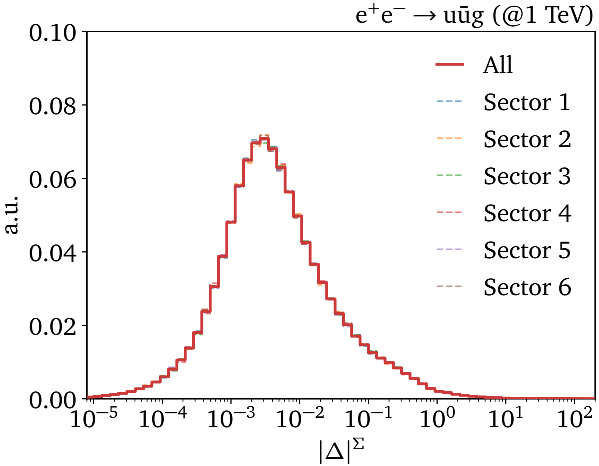
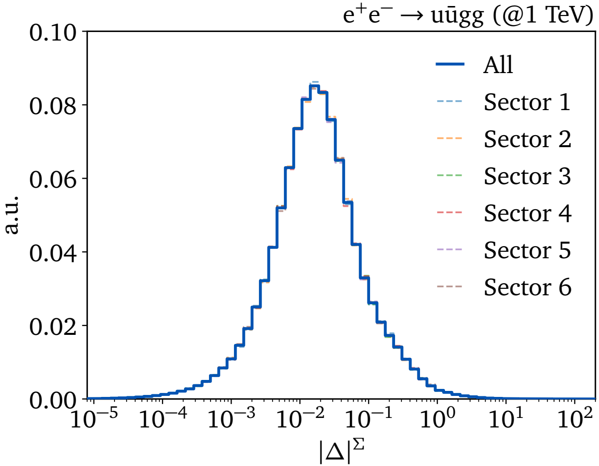
MLP results: real surrogate



- Simple MLP; input are Φ_n, lin-$\log s_{ij}$ and radiation var.s
- Same metrics as before
- Worse performance overall $\to$ real test comes in integration

MLP results: real surrogate



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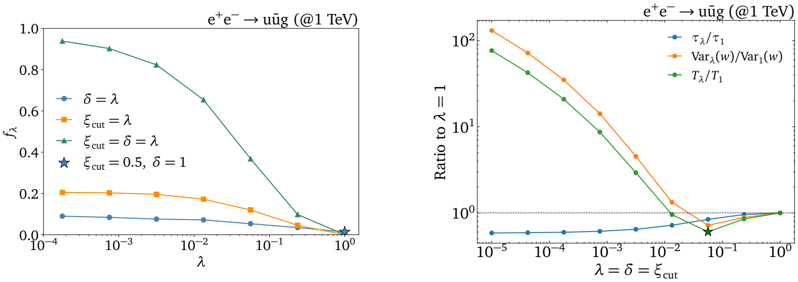
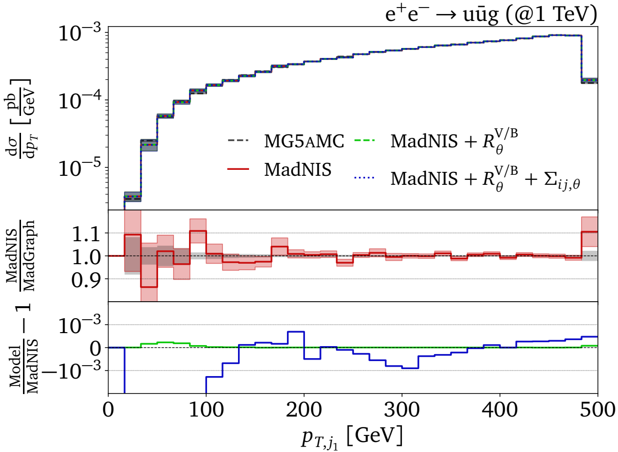
Optimizing the subtraction threshold



Fraction of surrogate calls f_λ (left) and evaluation-time/variance figure of merit (right) vs subtraction threshold λ.

- Smaller λ: less subtraction support $\to$ more surrogate calls, but larger integrand variance
- Minimize total evaluation time $T_\lambda(\varepsilon)$ at fixed precision ε
- Optimum: $\lambda \approx 0.05$ ($f_\lambda \approx 40\%$) for 3-jet, $\lambda \approx 0.01$ ($f_\lambda \approx 65\%$) for 4-jet

MLP in integration: observable plots



- Errors with virtual surrogate within relative 10^{-3}
- Real surrogate (only inactive subtraction) mantain precision
- Consistent with VEGAS (MadGraph line for reference)

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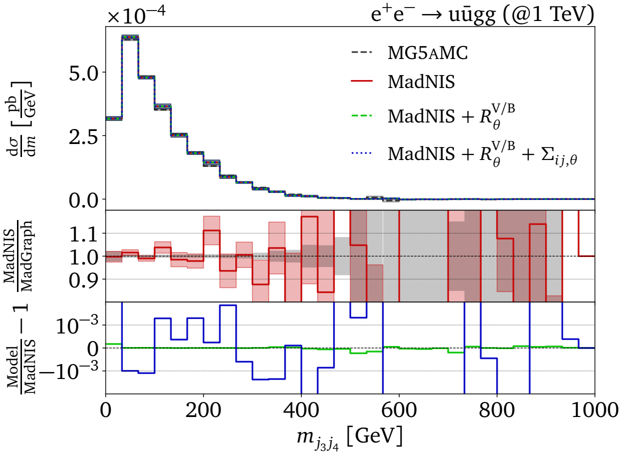

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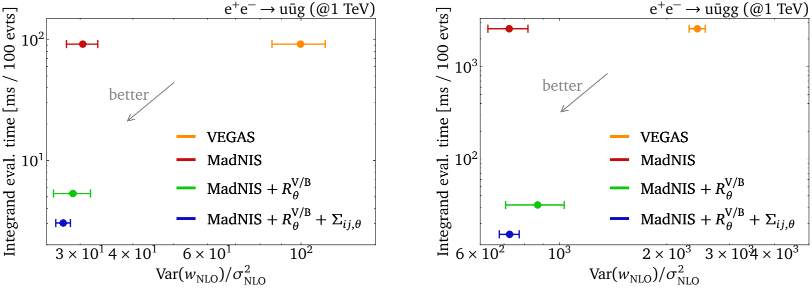
Cross sections: VEGAS vs MadNIS (+ surrogates)

Sampling mode	Surrogates $R_\theta^{\mathsf{V/B}}$	Surrogates $\Sigma_{ij,\theta}$	$e^+e^- \to u\bar{u}g$ σ_{NLO} [pb]	$e^+e^- \to u\bar{u}g$ $\mathsf{Var}(w_{\mathsf{NLO}})/\sigma^2_{\mathsf{NLO}}$	$e^+e^- \to u\bar{u}gg$ σ_{NLO} [pb]	$e^+e^- \to u\bar{u}gg$ $\mathsf{Var}(w_{\mathsf{NLO}})/\sigma^2_{\mathsf{NLO}}$
VEGAS	✗	✗	0.107 50(34)	100(14)	0.087 69(27)	2400(130)
MadNIS	✗	✗	0.107 60(19)	30.4(26)	0.087 29(15)	720(90)
MadNIS	✓	✗	0.107 59(18)	28.8(29)	0.087 11(18)	870(160)
MadNIS	✓	✓	0.107 65(18)	27.4(11)	0.087 38(15)	730(50)

Cross section and relative variance for each sampling/surrogate setup (mean $\pm$ std. dev. over 5 runs).

- Excellent agreement in σ_{NLO} across all setups
- Need 3–$4\times$ more phase-space points with VEGAS to reach MadNIS precision

Acceleration: timing vs relative variance



Evaluation time vs relative variance: $e^+e^- \to u\bar{u}g$ (left), $e^+e^- \to u\bar{u}gg$ (right).

- `MadNIS` and `VEGAS` with actual amplitudes: same evaluation time, but $3\times$ smaller RV
- Combined speed-up at fixed precision: $\sim110\times$ (3-jet), $\sim570\times$ (4-jet)

Outlook

- MadNIS works for NLO runs too
- Surrogates are precise enough to guarantee compatibility with true matrix element integration
- Possible next steps:
  - Higher final state multiplicites
  - Move to pp collisions
  - Extend real surrogates usage

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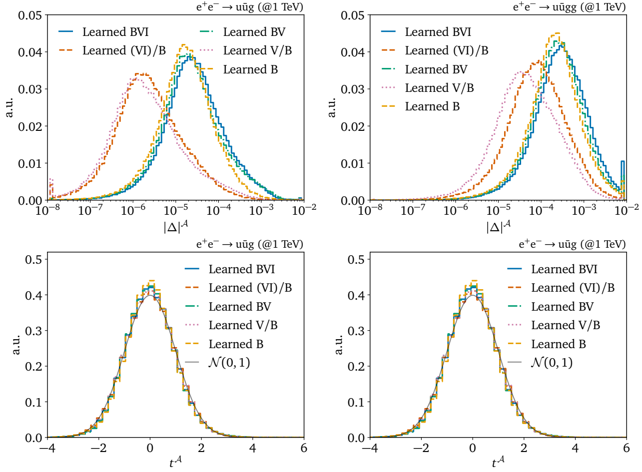
Thank you for your attention!

Backup

MLP results: virtual surrogate (with pull plots)



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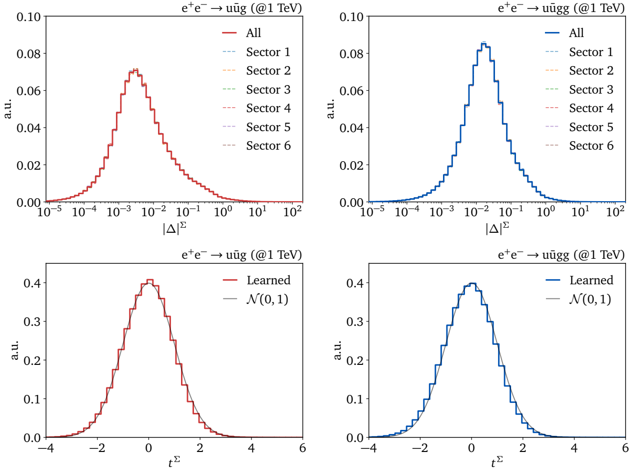

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Further histograms

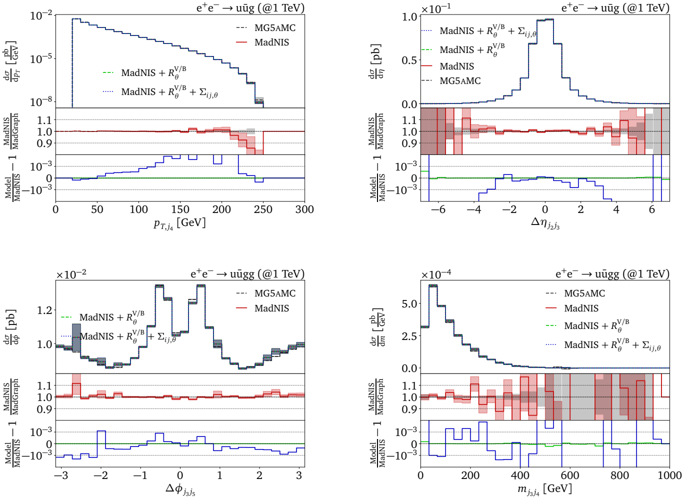

Figure: Additional observables: $e^+e^- \to u\bar{u}g$ (top), $e^+e^- \to u\bar{u}gg$ (bottom).