Event Generation with Normalizing Flows: i-flow

— Particle Physics in Computing Frontier, IBS Daejeon —

Claudius Krause

Fermi National Accelerator Laboratory

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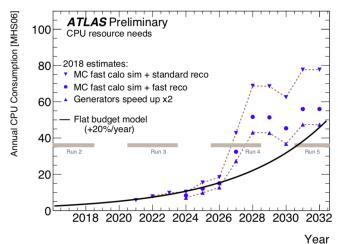




Alexander von Humboldt Stiftung/Foundation

In collaboration with: Christina Gao, Stefan Höche, Joshua Isaacson, Holger Schulz arXiv: 1912.abcde and arXiv: 1912.fghii

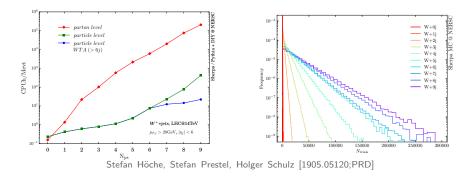
Monte Carlo Simulations are increasingly important.



https://twiki.cern.ch/twiki/bin/view/AtlasPublic/ComputingandSoftwarePublicResults

- ⇒ MC event generation is needed for signal and background predictions.
- ⇒ The required CPU time will increase in the next years.

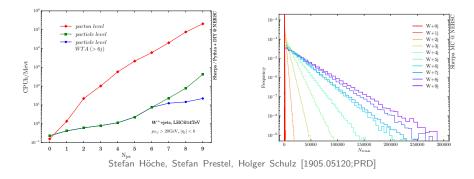
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The bottlenecks for evaluating large final state multiplicities are

- a slow evaluation of the matrix element
- a low unweighting efficiency

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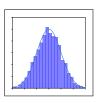


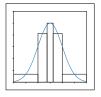
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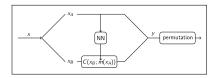
Part I: Monte Carlo Integration and Importance Sampling





Part II: Existing Algorithms

Part III: Normalizing Flows

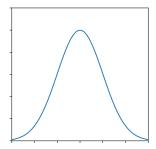




I: There are two problems to be solved...

 $f(\vec{x})$

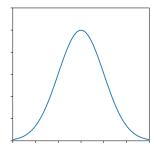
 $d\sigma(p_i, \vartheta_i, \varphi_i)$



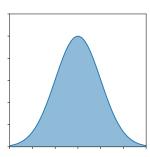


I: There are two problems to be solved...

$$f(\vec{x}) \Rightarrow F = \int f(\vec{x}) d^D x$$
 $d\sigma(p_i, \vartheta_i, \varphi_i) \Rightarrow \sigma = \int d\sigma(p_i, \vartheta_i, \varphi_i), \quad D = 3n_{\text{final}} - 4$





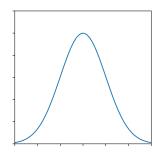




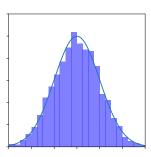
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Given a distribution $f(\vec{x})$, how can we sample according to it?



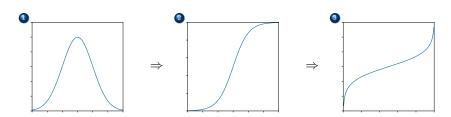






I: ... but they are closely related.

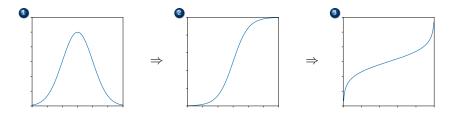
- Starting from a pdf, ...
- 2 ... we can integrate it and find its cdf, ...
- ... to finally use its inverse to transform a uniform distribution.





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- Starting from a pdf, ...
- 2 ... we can integrate it and find its cdf, ...
- ... to finally use its inverse to transform a uniform distribution.



⇒ We need a fast and effective numerical integration!



I: Importance Sampling is very efficient for high-dimensional integration.

$$\int_0^1 f(x) \ dx \qquad \xrightarrow{\text{MC}} \qquad \frac{1}{N} \sum_i f(x_i) \qquad x_i \dots \text{uniform}$$

$$= \int_0^1 \frac{f(x)}{q(x)} \ q(x) dx \qquad \xrightarrow{\text{IMC} \atop \text{importance sampling}} \qquad \frac{1}{N} \sum_i \frac{f(x_i)}{q(x_i)} \qquad x_i \dots q(x)$$



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We therefore have to find a q(x) that

- approximates the shape of f(x).
- is "easy" enough such that we can sample from its inverse cdf.



I: The unweighting efficiency measures the quality of the approximation q(x).

- If q(x) = const., each event x_i would require a weight of $f(x_i)$ to reproduce the distribution of f(x). \Rightarrow "Weighted Events"
- If $q(x) \propto f(x)$, all events would have the same weight as the distribution reproduces f(x) directly. \Rightarrow "Unweighted Events"



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- To unweight, we need to accept/reject each event with probability $\frac{f(x_i)}{\max f(x)}$. The resulting set of kept events is unweighted and reproduces the shape of f(x).
- The unweighting efficiency η gives the fraction of events that "survives" this procedure.

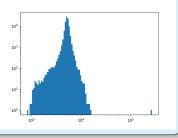
$$\eta = \frac{\# \text{ accepted events}}{\# \text{ all events}} = \frac{\text{mean } w}{\text{max } w}$$
, with $w_i = \frac{p(x_i)}{q(x_i)} = \frac{f(x_i)}{Fq(x_i)}$.



I: The usual definition of unweighting efficiency is unstable if many events are generated.

Problems of the old definition:

- The maximum grows with the number of events drawn.
- If more points are drawn than used in training, the chance for outliers increases a lot.
- Generating smaller subsets doesn't work, because we want a globally unweighted set of events.

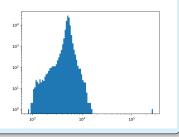




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Our new definition:

- ullet Assuming we used N_{opt} events during optimization, draw nN_{opt} events.
- ullet Now, select m replicas of N_{opt} events each and find their maximum weight.
- Compute the total maximum as the median of the individual maxima.
- We expect a few overweight events that can either be discarded or included with their weights set to w_{max} (Requiring further control plots!).



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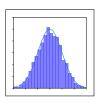
for example: $N_{\text{opt}} = 20000$ $nN_{\text{opt}} = 10^6$ m = 1000

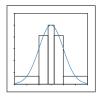
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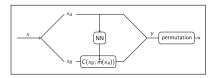
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II: The VEGAS algorithm is very efficient.

The VEGAS algorithm

Peter Lepage 1980

- assumes the integrand factorizes and bins the 1-dim projection.
- then adapts the bin edges such that area of each bin is the same.







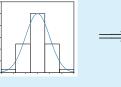


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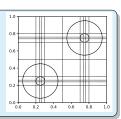
Peter Lepage 1980

- assumes the integrand factorizes and bins the 1-dim projection.
- then adapts the bin edges such that area of each bin is the same.





- It does have problems if the features are not aligned with the coordinate axes.
- The current python implementation also uses stratified sampling.

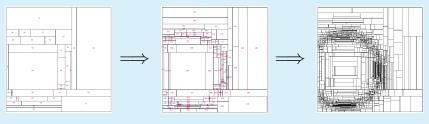




II: The Foam algorithm resolves correlations.

The Foam algorithm S. Jadach [physics/0203033]

- In the exploration phase, the integration domain is consecutively split into cells.
- In the generation phase, a cell is chosen at random and a point is drawn uniformly from within that cell.

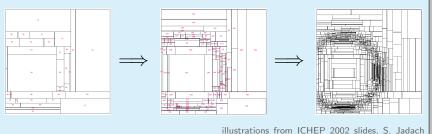




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- It captures correlations.
- However, within each cell q(x) = const.



II: There are two different approaches to generate events with Machine Learning Techniques.

Generate events directly using GANs.

Suyong Choi et al. [next talk]; Bendavid [1707.00028]; Otten et al. [1901.0875]; Hashemi et al. [1901.05282]; Di Sipio et al. [1903.02433]; Butter et al. [1907.03764]; Carrazza et al. [1909.01359]

- √ Several orders of magnitude faster.
- ✓ Generates unweighted events directly.
- Need existing event sample to train.
- × Results can be biased if not trained right.

Learn q(x) to improve importance sampling.

Bendavid [1707.00028]; Klimek/Perelstein [1810.11509]; i-flow [this talk]

- ✓ Insufficient training just yields high uncertainties, no bias.
- ✓ Events are generated from scratch, no pre-existing set is needed.
- × Resulting set of events still needs to be unweighted.



II: The Loss function quantifies our goal.

We have different choices:

Kullback-Leibler (KL) divergence:

$$D_{KL} = \int p(x) \log \frac{p(x)}{q(x)} dx$$
 $\approx \frac{1}{N} \sum \frac{p(x_i)}{q(x_i)} \log \frac{p(x_i)}{q(x_i)}, \quad x_i \dots q(x)$

• Pearson χ^2 divergence:

$$D_{\chi^2} = \int \frac{(\rho(x) - q(x))^2}{q(x)} dx \qquad \approx \qquad \frac{1}{N} \sum \frac{\rho(x_i)^2}{q(x_i)^2} - 1, \qquad x_i \dots q(x)$$

Exponential divergence:

$$D_{exp} = \int p(x) \log \left(\frac{p(x)}{q(x)}\right)^2 dx \quad \approx \quad \frac{1}{N} \sum \frac{p(x_i)}{q(x_i)} \log \left(\frac{p(x_i)}{q(x_i)}\right)^2, \quad x_i \dots q(x)$$

We use the ADAM optimizer for stochastic gradient descent:

- The learning rate for each parameter is adapted separately, but based on previous iterations.
- This is effective for sparse and noisy functions. Kingma/Ba [arXiv:1412.6980]



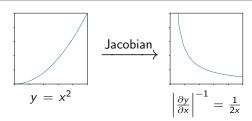
II: Using the NN as coordinate transform is too costly.

We could use the NN as nonlinear coordinate transform:

- We use a deep NN with n_{dim} nodes in the first and last layer to map a uniformly distributed x to a target q(x).
- The distribution induced by the map y(x) (=NN) is given by the Jacobian of the map:

$$q(y) = q(y(x)) = \left| \frac{\partial y}{\partial x} \right|^{-1}$$

Klimek/Perelstein [arXiv:1810.11509]





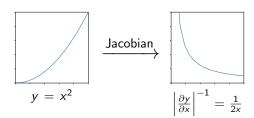
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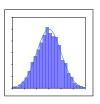
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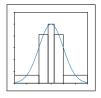


 \Rightarrow The Jacobian is needed to evaluate the loss and to sample. However, it scales as $\mathcal{O}(n^3)$ and is too costly for high-dimensional integrands!

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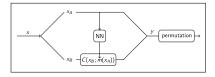
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III: Normalizing Flows are numerically cheaper.

A Normalizing Flow:

- is a bijective, smooth mapping between two statistical distributions.
- is composed of a series of easy transformations, the "Coupling Layers".
- is still flexible enough to learn complicated distributions.
- \Rightarrow The NN does not learn the transformation, but the parameters of a series of easy transformations.



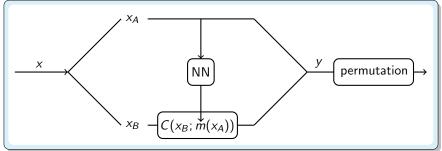
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- \Rightarrow The NN does not learn the transformation, but the parameters of a series of easy transformations.
 - The idea was introduced as "Nonlinear Independent Component Estimation" (NICE) in Dinh et al. [arXiv:1410.8516].
 - In Rezende/Mohamed [arXiv:1505.05770], Normalizing Flows were first discussed with planar and radial flows.
 - Our approach follows the ideas of Müller et al. [arXiv:1808.03856], but with the modifications of Durkan et al. [arXiv:1906.04032].
 - Our code uses TensorFlow 2.0, www.tensorflow.org.



III: The Coupling Layer is the fundamental Building Block



$$y_A = x_A$$

$$y_{B,i} = C(x_{B,i}; m(x_A))$$

inverse:

$$x_A = y_A$$

$$x_{B,i} = C^{-1}(y_{B,i}; m(x_A))$$

separable in $x_{B,i}$.

Jacobian:

$$\left|\frac{\partial y}{\partial x}\right| = \begin{vmatrix} 1 & \frac{\partial C}{\partial x_B} \\ 0 & \frac{\partial C}{\partial x_B} \end{vmatrix} = \Pi_i \frac{\partial C(x_{B,i}; m(x_A))}{\partial x_{B,i}}$$

The C are numerically cheap, invertible, and

$$\Rightarrow \mathcal{O}(n)$$



III: The Coupling Function is a piecewise approximation to the cdf.







 $\label{eq:mulliprob} \text{M\"{u}ller et al. } \left[\text{arXiv:}1808.03856\right]$

The NN predicts the pdf bin heights Q_i .



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piecewise linear coupling function:





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Müller et al. [arXiv:1808.03856]

$$C = \sum_{k=1}^{b-1} Q_k + \alpha Q_b$$

$$\alpha = \frac{x - (b-1)w}{w}$$

$$\left| \frac{\partial C}{\partial x_B} \right| = \prod_i \frac{Q_{b_i}}{w}$$



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rational quadratic spline coupling function:

Durkan et al. [arXiv:1906.04032]

Gregory/Delbourgo [IMA Journal of Numerical Analysis, '82]



$$C = \frac{a_2\alpha^2 + a_1\alpha + a_0}{b_2\alpha^2 + b_1\alpha + b_0}$$

- still rather easy
- more flexible

The NN predicts the cdf bin widths, heights, and derivatives that go in $a_i \& b_i$.



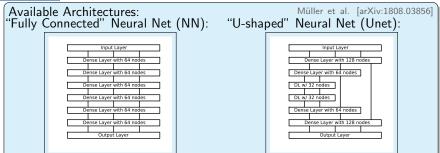
III: We need $\mathcal{O}(\log n)$ Coupling Layers.

How many Coupling Layers do we need?

- Enough to learn all correlations between the variables.
- As few as possible to have a fast code.
- This depends on the applied permutations and the $x_A x_B$ -splitting: (pppttt) \leftrightarrow (tttppp) vs. (pppptt) \leftrightarrow (ttpppp)
- More pass-through dimensions (p) means more points required for accurate loss.
- Fewer pass-through dimensions means more CLs needed.
- For $\#p \approx \#t$, we can prove: $4 \le \#CLs \le 2 \log_2 n_{dim}$

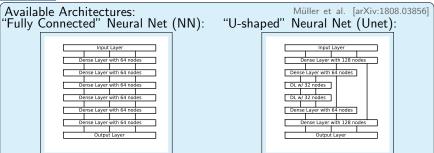


III: We utilize different NN architectures.





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There are different ways to encode the input dimensions x_A . For example $x_A = (0.2, 0.7)$:

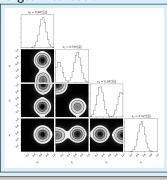
- direct: $x_i = (0.2, 0.7)$
- one-hot (8 bins): $x_i = ((0, 1, 0, 0, 0, 0, 0, 0), (0, 0, 0, 0, 0, 1, 0, 0))$
- one-blob (8 bins): $x_i = ((0.55, 0.99, 0.67, 0.16, 0.01, 0, 0, 0), (0, 0, 0.01, 0.11, 0.55, 0.99, 0.67, 0.16))$

Müller et al. [arXiv:1808.03856]

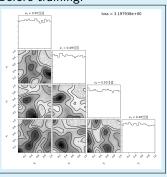


Our test function: 2 Gaussian peaks, randomly placed in a 4d space.

Target Distribution:



Before training:



• Final Integral: 0.0063339(41)

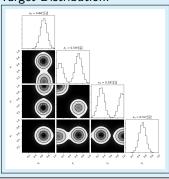
• VEGAS plain: 0.0063349(92)

• VEGAS full: 0.0063326(21)

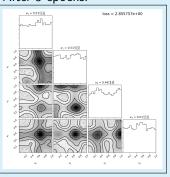


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Target Distribution:



After 5 epochs:



• Final Integral: 0.0063339(41)

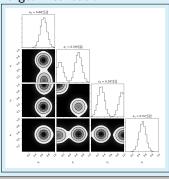
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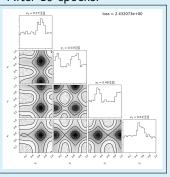


Our test function: 2 Gaussian peaks, randomly placed in a 4d space.

Target Distribution:



After 10 epochs:



• Final Integral: 0.0063339(41)

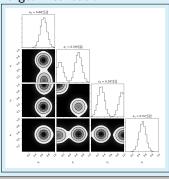
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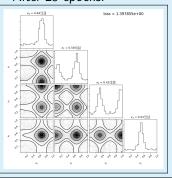


Our test function: 2 Gaussian peaks, randomly placed in a 4d space.

Target Distribution:



After 25 epochs:



• Final Integral: 0.0063339(41)

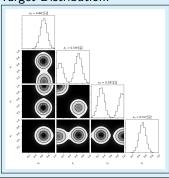
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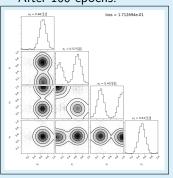


Our test function: 2 Gaussian peaks, randomly placed in a 4d space.

Target Distribution:



After 100 epochs:



• Final Integral: 0.0063339(41)

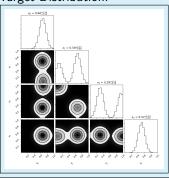
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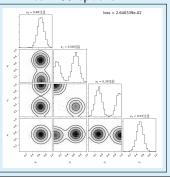


Our test function: 2 Gaussian peaks, randomly placed in a 4d space.

Target Distribution:



After 200 epochs:



• Final Integral: 0.0063339(41)

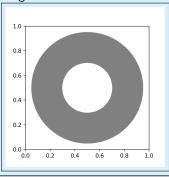
• VEGAS plain: 0.0063349(92)

• VEGAS full: 0.0063326(21)

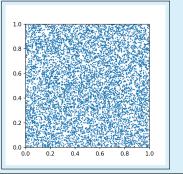


Our test function: a 2d ring function.

Target Distribution:



Before training:

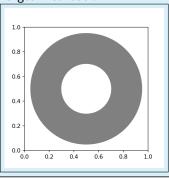


• Final cut efficiency: 89 % Untrained efficiency: 51 %

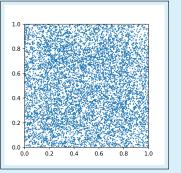


Our test function: a 2d ring function.

Target Distribution:



After 10 epochs:

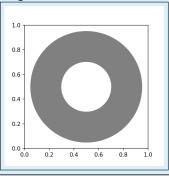


• Final cut efficiency: 89 % Untrained efficiency: 51 %

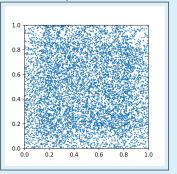


Our test function: a 2d ring function.

Target Distribution:



After 20 epochs:

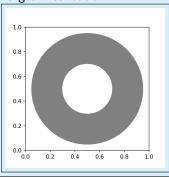


• Final cut efficiency: 89 % Untrained efficiency: 51 %

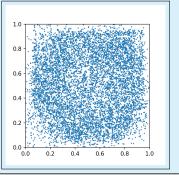


Our test function: a 2d ring function.

Target Distribution:



After 50 epochs:

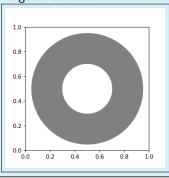


• Final cut efficiency: 89 % Untrained efficiency: 51 %

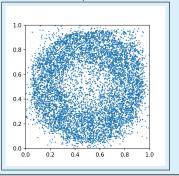


Our test function: a 2d ring function.

Target Distribution:



After 100 epochs:

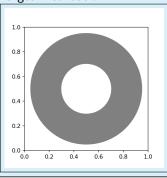


• Final cut efficiency: 89 % Untrained efficiency: 51 %

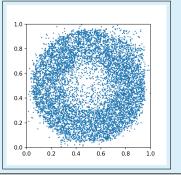


Our test function: a 2d ring function.

Target Distribution:



After 200 epochs:

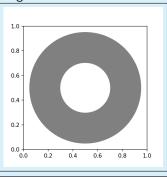


• Final cut efficiency: 89 % Untrained efficiency: 51 %

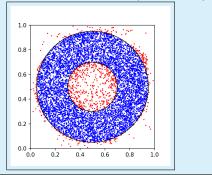


Our test function: a 2d ring function.

Target Distribution:



Final Distribution (500 epochs):



• Final cut efficiency: 89 % Untrained efficiency: 51 %



III: Sherpa needs a high-dimensional integrator.

Sherpa is a Monte Carlo event generator for the Simulation of High-Energy Reactions of PArticles. We use Sherpa to

- compute the matrix element of the process.
- map the unit-hypercube of our integration domain to momenta and angles. To improve efficiency, Sherpa uses a recursive multichannel algorithm.

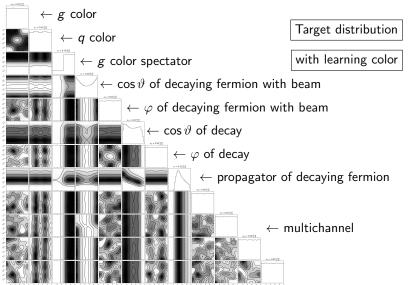
$$\Rightarrow n_{dim} = \underbrace{3n_{final} - 4}_{\text{kinematics}} + \underbrace{n_{final} - 1}_{\text{multichannel}}$$

• However, the COMIX++ ME-generator uses color-sampling, so we should also integrate over final state color configurations. While this improves the efficiency, it is not possible to handle group processes like W+nj with a single flow.

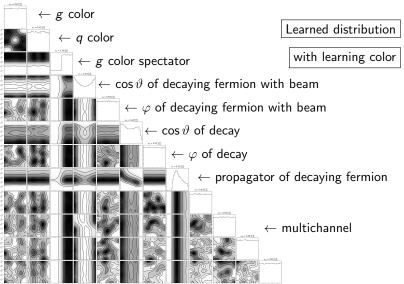
$$\Rightarrow n_{dim} = 4n_{final} - 4 + 2n_{color}$$

https://sherpa.hepforge.org/

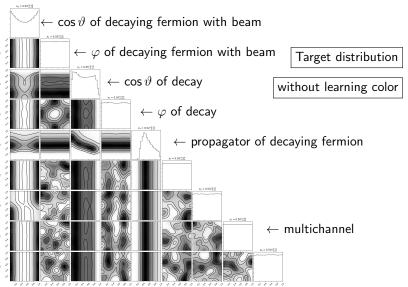




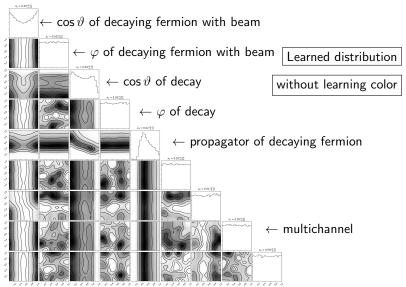






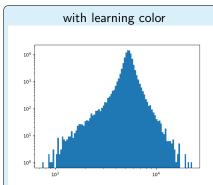




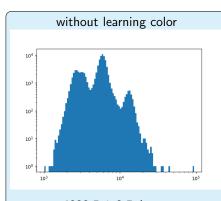




III: Comparing $e^+e^- \rightarrow 3j$ with and without learning color.



- $\sigma = 4879.8 \pm 5.3$ pb
- $\eta_{\sf new} = 45\%$
- Cut efficiency: 92 %
- 20 overweight events in 100k



- $\sigma = 4883.5 \pm 8.5 \mathrm{pb}$
- $\eta_{\sf new} = 25\%$
- Cut efficiency: 92 %
- 20 overweight events in 100k



III: Hyperparameter Optimization is difficult.

There are many hyperparameters that we have to optimize:

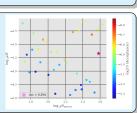
- network architecture:DNN vs. U-Net, # layers, # nodes
- learning schedule:
 schedule function (const., exponential, ...), initial learning rate, decay
 rate and step size, ...
- training: which loss function, # epochs, # samples per epoch
- normalizing flow specific:
 # (input/output) bins, input encoding (one blob, direct), how to split dims inside CL, # CLs, which function in the CLs



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There are many hyperparameters that we have to optimize:

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- training:which loss function, # epochs, # samples per epoch
- normalizing flow specific:
 # (input/output) bins, input encoding (one blob, direct), how to split dims inside CL, # CLs, which function in the CLs
- We scan a subset of the hyperparameters with a Sobol sequence on NERSC.
- We focus on the process $pp \rightarrow W + 1i$.
- We apply the best point to $pp \rightarrow W + nj$.





III: High Multiplicities are still difficult to learn.

unweighting efficiency		LO QCD			
$\langle w \rangle / w_{\rm max}$		n = 0	n = 1	n =2	n = 3
$W^+ + n$ jets	Sherpa 2.2.7	$2.4 \cdot 10^{-1}$	$3.2 \cdot 10^{-2}$	$7.6 \cdot 10^{-3}$	$1.8 \cdot 10^{-3}$
	Sherpa 3.x.y	$2.5\cdot 10^{-1}$	$2.9\cdot 10^{-2}$	$7.3 \cdot 10^{-3}$	$2.0\cdot 10^{-3}$
	NN+NF	$5.8\cdot10^{-1}$	$1.3\cdot 10^{-1}$	$1.2\cdot 10^{-2}$	$2.1\cdot 10^{-3}$
	Gain	2.3	4.3	1.7	1.1
$W^- + n$ jets	Sherpa 2.2.7	$3.1\cdot 10^{-1}$	$2.8\cdot 10^{-2}$	$7.9\cdot 10^{-3}$	$2.5\cdot 10^{-3}$
	Sherpa 3.x.y	$2.4\cdot 10^{-1}$	$4.4\cdot10^{-2}$	$9.4\cdot10^{-3}$	$2.1\cdot 10^{-3}$
	NN+NF	$6.0\cdot10^{-1}$	$1.2\cdot 10^{-1}$	$1.7\cdot 10^{-2}$	$2.4\cdot 10^{-3}$
	Gain	2.5	2.6	1.8	1.1
Z + n jets	Sherpa 2.2.7	$2.9\cdot 10^{-1}$	$3.6\cdot10^{-2}$	$1.4\cdot10^{-2}$	$3.1\cdot 10^{-3}$
	Sherpa 3.x.y	$4.3\cdot 10^{-1}$	$3.9\cdot 10^{-2}$	$1.4\cdot10^{-2}$	$3.3\cdot 10^{-3}$
	NN+NF	$5.1\cdot 10^{-1}$	$1.3\cdot 10^{-1}$	$1.9\cdot 10^{-2}$	$3.1\cdot 10^{-3}$
	Gain	1.2	3.5	1.4	0.95



III: There are numerous ways to improve i-flow in the near future.

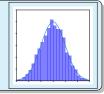
- adjust hyperparameters
- use a CNN in the CL
- introduce Conditional Normalizing Flows or Discrete Flows to improve the multichannel or color sampling

```
Winkler et al. [1912.00042]; Tran et al. [1905.10347]
```

- "learn" the permutations: using 1×1 convolutions Kingma/Dhariwal [1807.03039]
- improve memory consumption with checkpointing Chen et al. [1604.06174]
- . . .

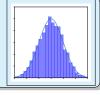
Event Generation with Normalizing Flows: i-flow

• I introduced the concepts of numerical integration and importance sampling.



Event Generation with Normalizing Flows: i-flow

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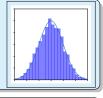


- I discussed "traditional" algorithms like, VEGAS or Foam.
- I compared ML approaches: learning q(x) vs. GANs



Event Generation with Normalizing Flows: i-flow

• I introduced the concepts of numerical integration and importance sampling.



- I discussed "traditional" algorithms like, VEGAS or Foam.
- I compared ML approaches: learning q(x) vs. GANs



- I presented the idea of Normalizing Flows and showed their performance in test functions.
- I showed preliminary results for $pp \rightarrow W + nj$ with Sherpa.

