Normalising Flows for Particle Cloud Generation

IML Machine Learning Working Group, 11.10.2022 Benno Käch, Dirk Krücker, Isabell Melzer-Pellmann, Moritz Scham, Simon Schnake benno.kaech@desy.de

HELMHOLTZAI



CLUSTER OF EXCELLENCE QUANTUM UNIVERSE



Artwork by $\text{DALL} - \text{E} \cdot 2$

Normalising Flows

- Find invertible functions to transform data distribution to Normal distribution
- Invertible functions due to smart construction: Coupling Layers
- Stack multiple Coupling Layers for expressivity
- Contrast to $\text{GAN} \rightarrow \text{Stable Maximum-Likelihood training}$



Coupling Layers

Invertibility by Construction

• Neural Networks for parameters θ of transformation f

Application: Particle Cloud Generation

JetNet [1] Datasets

- Gluon, light and top-quark Pythia jets, clustered by anti- k_T
- Jets of about $p_T^{\rm jet} \sim 1~TeV$
- Particles: tuples of $(\eta^{\rm rel},\phi^{\rm rel},p_T^{\rm rel})$ relative to jet axis, massless
- p_T^{rel} normalised to total p_T of jet
- Constrained to max 30 particles/jet \rightarrow 90 dimensions
- Invariant jet mass $m^2 = \sum_{i=0}^{\infty} \overrightarrow{p}_i^2$
- Size $\sim 150'000$ Samples
- (70/30) Train/Test split

Normalising Flow Architecture & Training

- Top-Quark \rightarrow Complex jet substructure
- Flat Dense Normalising Flow: 90 dimensional latent space
- No permutation invariant encoding, particles ordered by p_T^{rel}
- Jets with less < 30 particles zero-padded & noise added $O(10^{-7})$
- No inductive bias \rightarrow contrast to other generative models
- Adam Optimiser
- Batch Normalisation
- Dropout during training/evaluation

First Results

Implementation by nflows [2]

- Affine coupling layers
- 4 layer ResNets for coupling layer parameters
- Significant disagreement in inclusive marginals

All Particles

Rational Quadratic Spline Coupling

Proposed by Durkan and Bekasov et al. [3], also in nflows [2]

- Affine coupling lacks flexibility
- Element-wise monotonic ratio of quadratic splines
- Monotonic \rightarrow analytically invertible
- K bins $\rightarrow (3K 1)$ NN outputs per dimension

7

Rational Quadratic Splines - Results

Distributions for Individual Particles

• Same architecture as before, RQS instead of Affine Coupling

Generated individual particle distributions compatible with ground truth

Assessing Performance

Same Metrics as in [2]

- Logprob well-motivated from theory \rightarrow But devil is in the details
- Track multiple metrics for performance:
 - Wasserstein-1 distance W_1 on different distributions (see below)
 - Fréchet ParticleNet Distance (FPND) [2]
 - Coverage (COV)
 - Minimum Matching Distance (MMD)

In-sample distances								
Parton	$W_1^M(\times 10^{-3})$	$W_1^P(\times 10^{-3})$	$W_1^{EFP}(\times 10^{-5})$	FPND	$\mathrm{COV}\uparrow$	MMD		
Gluon	0.5 ± 0.1	0.4 ± 0.2	0.4 ± 0.4	0.01	0.56	0.036		
Light Quark	0.42 ± 0.09	0.6 ± 0.4	0.5 ± 0.5	0.01	0.55	0.024		
Top Quark	0.5 ± 0.1	0.6 ± 0.4	1.1 ± 0.4	0.03	0.56	0.072		

Wasserstein Distance

- Formally: $W_1(\mathbb{P}_r, \mathbb{P}_g) := \inf_{\gamma \in \Gamma(\mathbb{P}_r, \mathbb{P}_g)} \mathbb{E}_{(x, y) \sim \gamma}[|x y|]$
- Not tractable for $\dim(X \sim \mathbb{P}_g) > 1$
 - W_1^P : average of W_1 over (η, ϕ, p_T)
 - W_1^M : invariant jet mass
 - W_1^{EFP} : 5 Energy Flow Polynomials [4] (n=4,d=4)

In-sample distances

Parton	$W_1^M(\times 10^{-3})$	$W_1^P(\times 10^{-3})$	$W_1^{EFP}(\times 10^{-5})$	FPND	$\mathrm{COV}\uparrow$	MMD
Gluon	0.5 ± 0.1	0.4 ± 0.2	0.4 ± 0.4	0.01	0.56	0.036
Light Quark	0.42 ± 0.09	0.6 ± 0.4	0.5 ± 0.5	0.01	0.55	0.024
Top Quark	0.5 ± 0.1	0.6 ± 0.4	1.1 ± 0.4	0.03	0.56	0.072

DESY. | Benno Kaech | benno.kaech@desy.de

[4] Komiske et al., Energy flow polynomials: <u>A complete linear basis for jet sbstructure</u>, arxiv.org/abs/1712.07124 **10**

Fréchet ParticleNet Distance (FPND) [2]

• Inspired from Fréchet Inception Distance (FID) for image generation [5]

 $W_1^P(\times 10^{-3})$

 0.4 ± 0.2

 0.6 ± 0.4

 0.6 ± 0.4

Wasserstein-2 distance between Gaussians fitted to activations in first FC layer
 of ParticleNet [6] of MC & ML generated jets

In-sample distances

 0.4 ± 0.4

 0.5 ± 0.5

 1.1 ± 0.4

 $W_1^{EFP}(\times 10^{-5})$

Sensitive to output quality & mode collapse

 $W_1^M(\times 10^{-3})$

 0.5 ± 0.1

 0.5 ± 0.1

 0.42 ± 0.09

11

Parton

Gluon

Light Quark

Top Quark

[2] Kansal et al., <u>Particle Cloud Generation with Message Passing Generative Adversarial Networks</u>, arxiv.org/abs/2106.11535
 [5] Heusel et al., <u>GANs Trained by a Two Time-Scale Update Rule Converge to a Local Nash Equilibrium</u>, arxiv.org/abs/1706.08500
 [6] Qu et al., <u>ParticleNet: Jet Tagging via Particle Clouds</u>, arxiv.org/abs/1902.08570

 $\text{COV} \uparrow$

0.56

0.55

0.56

FPND

0.01

0.01

0.03

Pitfall of Vanilla Normalising Flows

Due to Coupling Layer construction?

Dimensionality Scaling of Normalising Flows

DESY. | Benno Kaech | benno.kaech@desy.de

Conditioned Normalising Flows

- Add additional variables to parameter NN
- Increase expressivity of parameter NN
- Needed during sampling

Sampling Conditioned Normalising Flows

- Mass is 1D variable → Universality of the uniform:
 one-dimensional random variable transformed with its cumulative density function is uniformly distributed
- Interpolate CDF with Monotone Piecewise Cubic Polynomials $[7] \rightarrow$ invertible
- Jet Generation:
 - 1. Sample 1D uniform
 - 2. Apply inverted monotonic cubic interpolation $\rightarrow m_{\rm cond}$
 - 3. Sample D = 90 Normal $\rightarrow z$
 - 4. Generate jets $x = f(z \mid m_{cond})$

Conditioned Normalising Flows

- Fixes mass modelling
- Improves nearly every other metric

Mass Constraint

- Constrain Normalising Flow to produce jet with mass same as condition
 - Generate jet $x_{gen} = f(z \mid m_{cond})$
 - Calculate jet mass $m_{\text{gen}} = m(\mathbf{x}_{\text{gen}})$
 - Add loss $L = \|m_{\rm gen} m_{\rm cond}\|^2$ to nLL loss
- During training Normalising Flow trained using both directions

Constrained & Conditioned Normalising Flows

-0.1

-0.1

CNF (m)

- Perfect mass modelling ٠
- Tradeoff with other metrics → Hyperparameter?

DESY. | Benno Kaech | benno.kaech@desy.de

But Point Clouds Have Variable Sizes?

- Introduce number particles in jet as 2^{nd} condition
- Switch datasets: 99 % of Top-quark jets have 30 particles \rightarrow Light Quarks
- Particles [k + 1,...,n] set to zero for jet with $n_{cond} = k$
- Sampling Condition: Number particles discrete \rightarrow Decompose $p(m, n) = p(n)p(m \mid n)$

Number Particles per Jet

Results on Light Quark Initiated Jets - No Condition

Model $W_1^M(\times 10^{-3})$ $W_1^P(\times 10^{-3})$ $W_1^{EFP}(\times 10^{-5})$ FPNDCOV \uparrow MMDVNF 3.5 ± 0.3 2.3 ± 0.4 3 ± 1 2.100.540.025

DESY. | Benno Kaech | benno.kaech@desy.de

Results on Light Quark Initiated Jets - Two Conditions

 \rightarrow Conditioning with number particles \rightarrow No significant improvement

Results

Jet Class	Model	$W_1^M(\times 10^{-3})$	$W_1^P(\times 10^{-3})$	$W_1^{EFP}(\times 10^{-5})$	FPND	$\mathrm{COV}\uparrow$	MMD
	MP-MP	0.7 ± 0.2	0.9 ± 0.3	0.7 ± 0.7	0.12	0.56	0.037
	MP_LFC-MP	0.69 ± 0.07	1.8 ± 0.3	0.9 ± 0.2	0.20	0.54	0.037
	VNF	5.5 ± 0.7	2.9 ± 0.7	4.4 ± 0.8	2.32	0.54	0.035
Gluon	CNF (m)	0.9 ± 0.1	0.6 ± 0.3	0.9 ± 0.5	0.68	0.54	0.036
	CNF (m,n)	0.9 ± 0.3	0.7 ± 0.2	0.9 ± 0.5	0.70	0.55	0.034
	CCNF (m)	0.9 ± 0.2	0.5 ± 0.2	1.1 ± 0.5	1.10	0.55	0.036
	CCNF (m,n)	0.6 ± 0.5	0.8 ± 0.1	0.9 ± 0.8	0.72	0.56	0.035
	MP-MP	0.6 ± 0.2	4.9 ± 0.5	0.7 ± 0.4	0.35	0.50	0.026
	MP_LFC-MP	0.7 ± 0.2	2.6 ± 0.4	0.9 ± 0.9	0.08	0.52	0.037
	VNF	3.5 ± 0.3	2.3 ± 0.4	3 ± 1	2.10	0.54	0.025
Light Quark	CNF (m)	1.1 ± 0.2	1.3 ± 0.3	$\boldsymbol{0.7\pm0.3}$	0.78	0.55	0.024
	CNF (m,n)	1.8 ± 0.2	0.9 ± 0.5	0.9 ± 0.4	0.64	0.54	0.025
	CCNF (m)	0.9 ± 0.3	0.6 ± 0.2	0.7 ± 0.3	0.71	0.54	0.024
	CCNF (m,n)	1.0 ± 0.3	1.2 ± 0.4	0.8 ± 0.5	1.99	0.51	0.026
	MP-MP	0.6 ± 0.2	2.3 ± 0.3	2 ± 1	0.37	0.57	0.071
	MP_LFC-MP	0.9 ± 0.3	2.2 ± 0.7	2 ± 1	0.93	0.56	0.073
Top Quark	VNF	6.4 ± 0.2	2.2 ± 0.2	14 ± 1	7.91	0.56	0.071
	CNF (m)	1.7 ± 0.3	1.1 ± 0.3	5 ± 1	4.53	0.55	0.073
	CNF (m,n)	0.9 ± 0.5	1.5 ± 0.1	7 ± 2	3.46	0.56	0.071
	CCNF (m)	0.7 ± 0.3	12.2 ± 0.1	9 ± 1	9.16	0.38	0.083
	CCNF (m,n)	1.1 ± 0.5	3.7 ± 0.3	13 ± 3	6.34	0.55	0.073

DESY. | Benno Kaech | benno.kaech@desy.de

Results - Strength

Jet Class	Model	$W_1^M(\times 10^{-3})$	$W_1^P(\times 10^{-3})$	$W_1^{EFP}(\times 10^{-5})$	FPND	$\mathrm{COV}\uparrow$	MMD
	MP-MP	0.7 ± 0.2	0.9 ± 0.3	0.7 ± 0.7	0.12	0.56	0.037
	MP_LFC-MP	0.69 ± 0.07	1.8 ± 0.3	0.9 ± 0.2	0.20	0.54	0.037
	VNF	5.5 ± 0.7	2.9 ± 0.7	4.4 ± 0.8	2.32	0.54	0.035
Gluon	CNF (m)	0.9 ± 0.1	0.6 ± 0.3	0.9 ± 0.5	0.68	0.54	0.036
	CNF (m,n)	0.9 ± 0.3	0.7 ± 0.2	0.9 ± 0.5	0.70	0.55	0.034
	CCNF (m)	0.9 ± 0.2	$oldsymbol{0.5}\pm0.2$	1.1 ± 0.5	1.10	0.55	0.036
	CCNF (m,n)	0.6 ± 0.5	0.8 ± 0.1	0.9 ± 0.8	0.72	0.56	0.035
	MP-MP	0.6 ± 0.2	4.9 ± 0.5	0.7 ± 0.4	0.35	0.50	0.026
	MP_LFC-MP	0.7 ± 0.2	2.6 ± 0.4	0.9 ± 0.9	0.08	0.52	0.037
	VNF	3.5 ± 0.3	2.3 ± 0.4	3 ± 1	2.10	0.54	0.025
Light Quark	CNF (m)	1.1 ± 0.2	1.3 ± 0.3	0.7 ± 0.3	0.78	0.55	0.024
	CNF (m,n)	1.8 ± 0.2	0.9 ± 0.5	0.9 ± 0.4	0.64	0.54	0.025
	CCNF (m)	0.9 ± 0.3	$\boldsymbol{0.6\pm0.2}$	$\boldsymbol{0.7\pm0.3}$	0.71	0.54	0.024
	CCNF (m,n)	1.0 ± 0.3	1.2 ± 0.4	0.8 ± 0.5	1.99	0.51	0.026
	MP-MP	0.6 ± 0.2	2.3 ± 0.3	2 ± 1	0.37	0.57	0.071
	MP_LFC-MP	0.9 ± 0.3	2.2 ± 0.7	2 ± 1	0.93	0.56	0.073
	VNF	6.4 ± 0.2	2.2 ± 0.2	14 ± 1	7.91	0.56	0.071
Top Quark	CNF (m)	1.7 ± 0.3	1.1 ± 0.3	5 ± 1	4.53	0.55	0.073
	CNF (m,n)	0.9 ± 0.5	1.5 ± 0.1	7 ± 2	3.46	0.56	0.071
	CCNF (m)	0.7 ± 0.3	12.2 ± 0.1	9 ± 1	9.16	0.38	0.083
	CCNF (m,n)	1.1 ± 0.5	3.7 ± 0.3	13 ± 3	6.34	0.55	0.073

Normalising Flows handle marginal distributions well

Results - Weaknesses

Jet Class	Model	$W_1^M(\times 10^{-3})$	$W_1^P(\times 10^{-3})$	$W_1^{EFP}(\times 10^{-5})$	FPND	$\mathrm{COV}\uparrow$	MMD
	MP-MP	0.7 ± 0.2	0.9 ± 0.3	0.7 ± 0.7	0.12	0.56	0.037
	MP_LFC-MP	0.69 ± 0.07	1.8 ± 0.3	0.9 ± 0.2	0.20	0.54	0.037
	VNF	5.5 ± 0.7	2.9 ± 0.7	4.4 ± 0.8	2.32	0.54	0.035
Gluon	CNF (m)	0.9 ± 0.1	0.6 ± 0.3	0.9 ± 0.5	0.68	0.54	0.036
	CNF (m,n)	0.9 ± 0.3	0.7 ± 0.2	0.9 ± 0.5	0.70	0.55	0.034
	CCNF (m)	0.9 ± 0.2	0.5 ± 0.2	1.1 ± 0.5	1.10	0.55	0.036
	CCNF (m,n)	$oldsymbol{0.6}\pm0.5$	0.8 ± 0.1	0.9 ± 0.8	0.72	0.56	0.035
	MP-MP	0.6 ± 0.2	4.9 ± 0.5	0.7 ± 0.4	0.35	0.50	0.026
	MP_LFC-MP	0.7 ± 0.2	2.6 ± 0.4	0.9 ± 0.9	0.08	0.52	0.037
	VNF	3.5 ± 0.3	2.3 ± 0.4	3 ± 1	2.10	0.54	0.025
Light Quark	CNF (m)	1.1 ± 0.2	1.3 ± 0.3	0.7 ± 0.3	0.78	0.55	0.024
	CNF (m,n)	1.8 ± 0.2	0.9 ± 0.5	0.9 ± 0.4	0.64	0.54	0.025
	CCNF (m)	0.9 ± 0.3	0.6 ± 0.2	0.7 ± 0.3	0.71	0.54	0.024
	CCNF (m,n)	1.0 ± 0.3	1.2 ± 0.4	0.8 ± 0.5	1.99	0.51	0.026
	MP-MP	0.6 ± 0.2	2.3 ± 0.3	2 ± 1	0.37	0.57	0.071
	MP_LFC-MP	0.9 ± 0.3	2.2 ± 0.7	$\mathfrak{I} \perp \mathfrak{I}$	0.93	0.56	0.073
	VNF	6.4 ± 0.2	2.2 ± 0.2	14 ± 1	7.91	0.56	0.071
Top Quark	CNF (m)	1.7 ± 0.3	1.1 ± 0.3	5 ± 1	4.53	0.55	0.073
	CNF (m,n)	0.9 ± 0.5	1.5 ± 0.1	7 ± 2	3.46	0.56	0.071
	CCNF (m)	0.7 ± 0.3	12.2 ± 0.1	9 ± 1	9.16	0.38	0.083
	CCNF (m,n)	1.1 ± 0.5	3.7 ± 0.3	13 ± 3	6.34	0.55	0.073

But still significantly worse on some metrics

Summary

- Normalising Flows light, quick & stable alternative to GANs
- Training duration $\sim 1-2 \ h$ on NVIDIA P100
- Significant differences on FPND
- Difficulties in modelling global features
- Conditioning enhances expressivity
- Normalising Flows handle variable number particles well
- Mass Constraint \rightarrow mass modelling $\overline{\mathbf{V}}$ overall performance \mathbf{i}

Any Questions?

Backup

Coupling Layers

How to Construct Invertible Functions with a Tractable Determinant

• Partition input into $(\mathbf{x}^A, \mathbf{x}^B) \in \mathbb{R}^d \times \mathbb{R}^{D-d}, D = 90, d = 45$

• Construct map element-wise:
$$f_{\theta}(x) = \begin{cases} z_i^A = x_i^A \\ z_i^B = s_{\theta(x^A)}(x_i^B) \end{cases} \Leftrightarrow f_{\theta}^{-1}(z) = \begin{cases} x_i^A = z_i^A \\ x_i^B = s_{\theta(z^A)}^{-1}(z_i^B) \end{cases}$$
$$\Rightarrow \frac{df}{dx} = \begin{bmatrix} \mathbb{I} & 0 \\ \frac{dz_B}{dx_A} & \frac{ds_{\theta(x^A)}}{dx^B} \end{bmatrix} \Rightarrow \det \frac{df}{dx} = \prod_{i=d+1}^D \frac{ds_i^{\theta(x_A)}}{dx_i^B}$$

- $s_{\theta}(x)$ simple parametrised function but θ arbitrarily complex \rightarrow NN for parameters θ
- Affine: $s_{\theta = (\theta_1, \theta_2)}(x) = x_B \odot \theta_1(x_A) + \theta_2(x_A)$

Affine vs Spline

Training vs Validation Logprobs, and Metrics

Possible Explanation why Max-Likelihood is not Enough

- Maximum likelihood consistent → can learn any distribution given **infinite** data & perfect model class
- Under model misspecification and finite data \rightarrow produces models that overgeneralise
- Minimising Forward KL-Divergence: equivalent to Maximum Likelihood

Normalising Flows

In more formal language

• Main foundation: Change of Variables formula, $z = f_{\theta}(x)$

$$p_{X}(\boldsymbol{x}) = p_{Z}(f_{\theta}(\boldsymbol{x})) \left| \det \frac{df_{\theta}}{d\boldsymbol{x}} \right| = p_{Z}(z) \left| \det \frac{df_{\theta}^{-1}}{dz} \right|^{-1}$$

• 2 Constraints: Invertible functions, Jacobi-Matrix tractable

• Stack transformations:
$$z = z_K = f^{(K)} \circ \cdots \circ f^{(0)}(z_0 = x)$$

 \rightarrow Invertible with determinant $\prod_{i=0}^K \det \left| \frac{df_{\theta}^{(i)}}{d\mathbf{x}_i} \right|$

• Optimise with negative Log-Likelihood:

$$\boldsymbol{\theta} = -\arg\min_{\boldsymbol{\theta}} \sum_{\boldsymbol{x} \in X} \log p_{\boldsymbol{x}}(\boldsymbol{x}) = \arg\min_{\boldsymbol{\theta}} \sum_{\boldsymbol{x} \in X} \left(\frac{f(\boldsymbol{x})^2}{2} - \sum_{i=0}^{K} \left| \det \frac{df_{\boldsymbol{\theta}}^{(i)}}{d\boldsymbol{x}_i} \right| \right)$$

DESY. | Benno Kaech | benno.kaech@desy.de

Affine Marginals

Hardest Particle

Inclusive Distributions for Fewer Particles

DESY. | Benno Kaech | benno.kaech@desy.de

34

Inclusive Distributions for Fewer Particles

n=10 and n=15

All Particles

Limited Condition

Precision of Mass Conditioning

Accuracy of Mass Conditioning

Correlation Plots

 η_{rel}

Correlation Plots

 ϕ_{rel}

Correlation Plots

 p_T

2D Histograms $\eta^{rel}\phi^{rel}$

DESY. | Benno Kaech | benno.kaech@desy.de

2D Histograms

 $\phi^{rel} p_T^{rel}$

2D Histograms $\eta^{rel} p_T^{rel}$

Oversampling

Using 1 Condition

Normalising Flows are BIG

Layer (type:depth-idx)	Param #	
TransGan		
CompositeTransform: 1-2		
ModuleList: 2-1		
PiecewiseRationalQuadraticC	ouplingTransform: 3-1	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-2	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-3	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-4	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-5	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-6	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-7	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-8	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-9	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-10	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-11	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-12	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-13	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-14	437,366
PiecewiseRationalQuadraticC	ouplingTransform: 3-15	437,366
Flow: 1-3	6,560,490	
CompositeTransform: 2-2	(recursive))
ModuleList: 3-16	(recursive)	
StandardNormal: 2-3	_	
Identity: 2-4		

Flow: 1	1-3		6,	560,490			
L-Co	ompos	eTransform: 2-2		(recursive)			
L	—Mo	uleList: 3-16		(recursive)			
		PiecewiseRationa	alQuadraticCoupl	ingTransform: 4-16	(recursive)		
		ResidualNet	:: 5-46	(recursive)			
		Linear:	6-31	(recursive)			
		Module	eList: 6-32	(recursive))		
		Re-Re-	esidualBlock: 7-9	1 (recursi	ve)		
		Re-Re-	esidualBlock: 7-9	2 (recursi	ve)		
		Linear:	6-33	(recursive)			
		Dropout: 5-9	99				
		Dropout: 5-	100				