Flexible conditional normalizing-flow distributions over manifolds: the jammy-flows toolkit

Thorsten Glüsenkamp, May 1st 2024, EuCAIFCon flash talk

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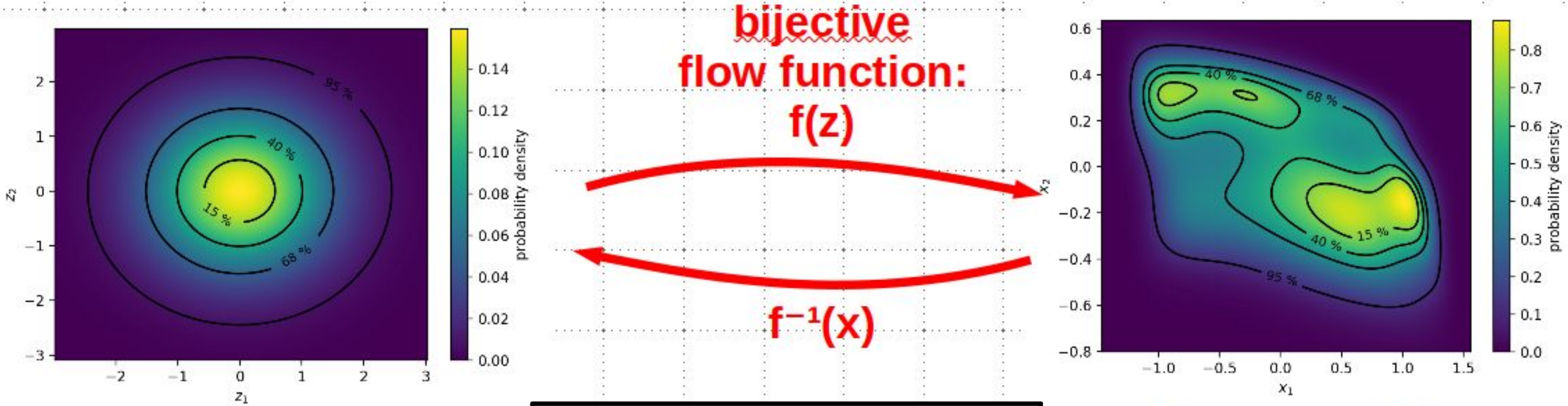
Normalizing flows are great, but….



Auxiliary base space "z":

$p_0(z) = \mathcal{N}(z; \mathbf{0}, \mathbb{1})$

Target space "x":

$p_\theta(x|y) = p_0(f^{-1}_{g_\theta(y)}(x)) \cdot |\det J^{-1}_{g_\theta(y)}(x)|$

… implementations are

- often scattered around in their own repositories
- often not really suited for physics ("image-focused flows")
- often complicated to set up, especially the conditioning

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Jammy Flows

([1] https://github.com/thoglu/jammy_flows)

Joint **A**utoregressive **M(MY)**anifold normalizing **flows**

setup complex normalizing flows in 1 line of code [1]

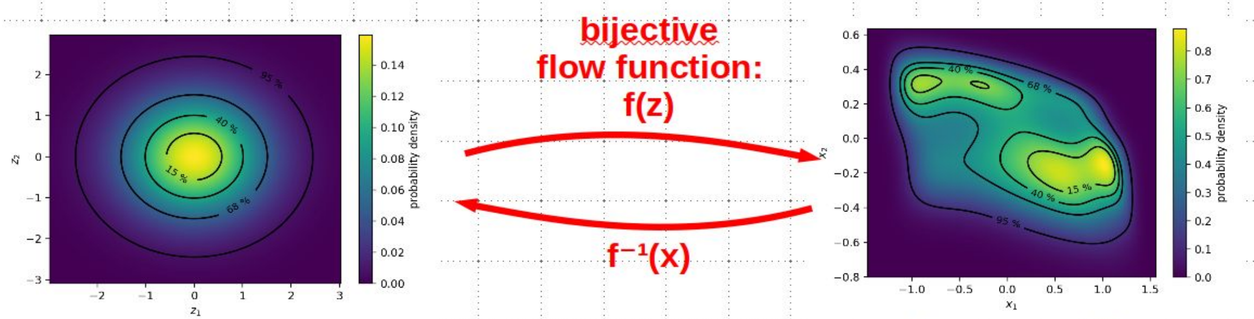
Euclidean ($\mathbb{R}^4$)

$$f(\vec{z}) = \Phi_t(\Phi_g(\Phi_g(\vec{z})))$$

Arg 1: Manifold

Arg 2: Flow function f(z)

```
pdf=jammy_flows.pdf("e4", "ggt")
```



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Supports various manifolds + autoregressive linking

Joint Autoregressive M(MY)anifold normalizing flows
setup complex normalizing flows in 1 line of code [1]

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```
pdf=jammy_flows.pdf("e4", "ggt")
```

Autoregressive ($S^2 \times \Delta^2 \times \mathbb{R}^3$)

$$f(\vec{z}) = \begin{bmatrix} \Phi_n(\Phi_n(\vec{z_1})) \\ \Phi_{w,x1}(\vec{z_2}) \\ \Phi_{g,x1,x2}(\Phi_{g,x1,x2}(\Phi_{g,x1,x2}(\Phi_{g,x1,x2}(\vec{z_3})))) \end{bmatrix}$$

```
pdf=jammy_flows.pdf("s2+c2+e4", "nn+w+gggg")
```

2-sphere (S^2)

$$f(\vec{z}) = \Phi_v(\Phi_v(\Phi_v(\vec{z})))$$

```
pdf=jammy_flows.pdf("s2", "vvv")
```

Interval (-3 to 3)

$$f(\vec{z}) = \Phi_r(\Phi_r(\Phi_r(\Phi_r(\Phi_r(\vec{z})))))$$

```
pdf=jammy_flows.pdf("i1_-3_3", "rrrrr")
```

Probability simplex (Δ^3)

$$f(\vec{z}) = \Phi_w(\Phi_w(\vec{z}))$$

```
pdf=jammy_flows.pdf("c3", "ww")
```

Syntax reflects normalizing flow-defining function f(z)

Flow abbreviations:

- "t" – affine flow
- "g" – Gaussianzation flows [2]
- "v" – Exponential map flows [3]
- "n" – Recursive flows on the 2-sphere [5]
- "w" – Simplex flow [6]
- "r" – neural spline flows [4]

+ a few more in the package

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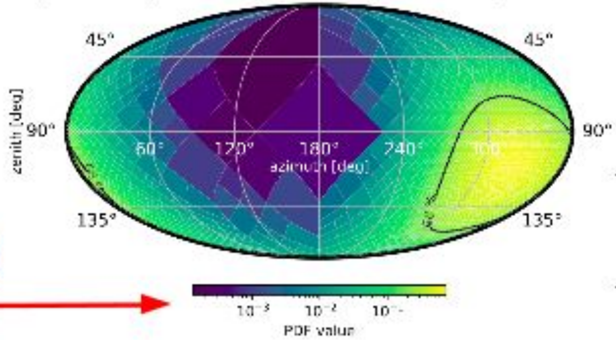
Features

Many state-of-the-art normalizing flows that can be autoregressively linked, customized, and made conditional. Autoregressive routing generalizes structure from inverse autoregressive flows [7].

Convenience functions for ...

- $1^{st} + 2^{nd}$ moments
- asymmetry measure (higher order moments) (see [9])
- entropy
- coverage (Gaussian base used for all manifolds – see [8])
- plotting (adaptive healpix for spherical PDFs)
- easy to add new layers



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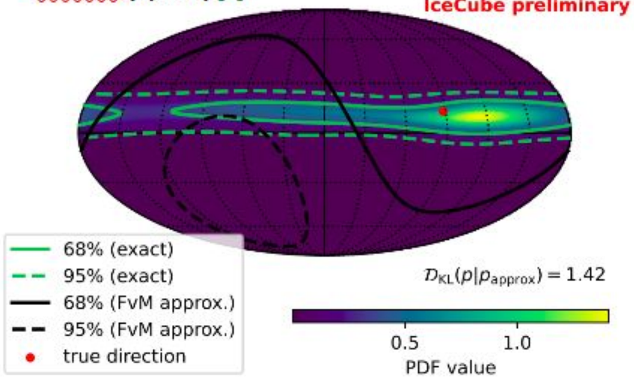
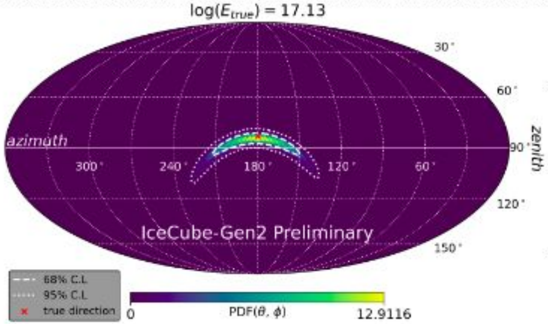
Applied in IceCube and IceCube-Gen2 for per-event posterior inference

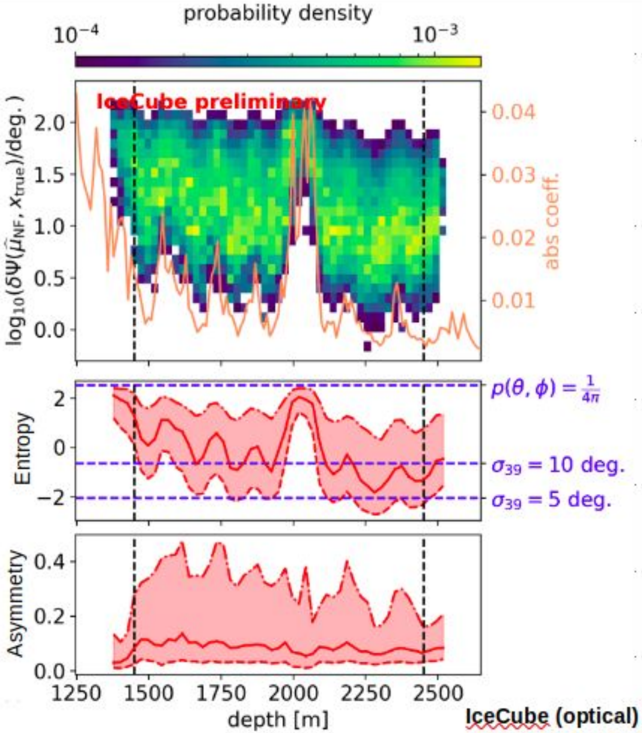
IceCube (optical) [9]





IceCube-Gen2 (radio) [10]

Directional posterior resolution vs depth (~50k electron neutrinos)



IceCube (optical) [9]

Posterior properties reflect detector properties (South Pole ice properties vary with depth)

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