Generative Modeling

Normalizing flows

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LAMBDA • HSE

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In this Lecture

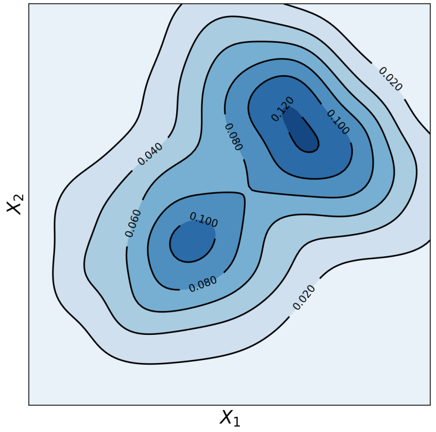
- Normalizing flows problem statement.
- Block schemes for Normalizing flows.
- MAF/IAF duality

Motivation

Motivation

$x_i \sim p_x(x)$

$p_x(x)$ - ?

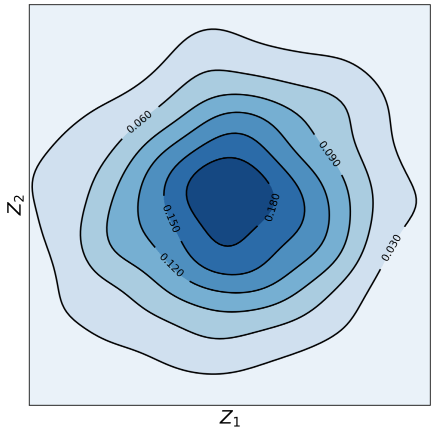


$\boldsymbol{z = f(x)}$

$\boldsymbol{x = T(z)}$

$z_i \sim p_z(z)$

$p_z(z)$ - known



- Generative model:
  - Likelihood evaluation;
  - Sampling procedure.
- Use **deterministic map** to known distribution.

Change of variables

For $\boldsymbol{p_z}(z)$ some pdf and $\mathrm{z} = \boldsymbol{f}(x)$ known then $p_x(x)$:

Ratio of volume ∂z to new volume ∂x

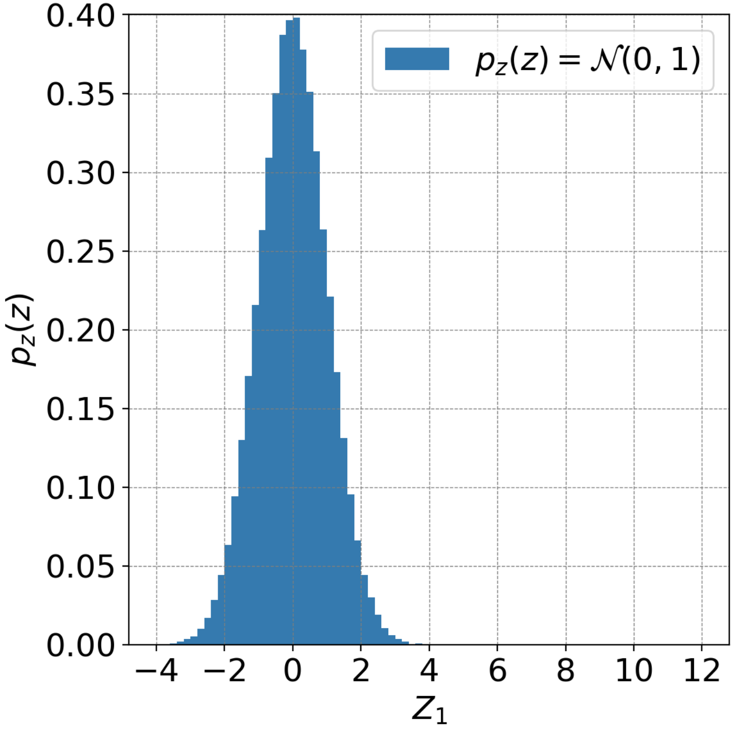
$$p_x(x_i) = \boldsymbol{p_z}\left(\boldsymbol{f}(x_i)\right)\left|\det \frac{\partial \boldsymbol{f}(x_i)}{\partial x_i}\right|,$$

1st derivative matrix:

$$\frac{\partial \boldsymbol{f}(x_i)}{\partial x_i} = \begin{pmatrix} \frac{\partial \boldsymbol{f}(x_i)_1}{\partial x_{i1}} & \cdots & \frac{\partial \boldsymbol{f}(x_i)_1}{\partial x_{in}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \boldsymbol{f}(x_i)_m}{\partial x_{i1}} & \cdots & \frac{\partial \boldsymbol{f}(x_i)_m}{\partial x_{in}} \end{pmatrix}.$$

1D example

$$z = f(x) = 0.5x - 2.5$$



$x_i \sim p_x(x)$

$p_x(x)$ - ?

$z_i \sim p_z(z)$

$p_z(z) = \mathcal{N}(0,1)$

1D example

For function $\boldsymbol{f}(x)$:

$$z = \boldsymbol{f}(x) = 0.5x - 2.5$$

Jacobi matrix:

$$\frac{\partial \boldsymbol{f}(x_i)}{\partial x_i} = (0.5)$$

Jacobian:

$$\left| \det \frac{\partial \boldsymbol{f}(x_i)}{\partial x_i} \right| = 0.5$$

1D example

Change of variables formulas:

$$p_x(x_i) = \boldsymbol{p_z}(\boldsymbol{f}(x_i)) \left|\det \frac{\partial \boldsymbol{f}(x_i)}{\partial x_i}\right|,$$

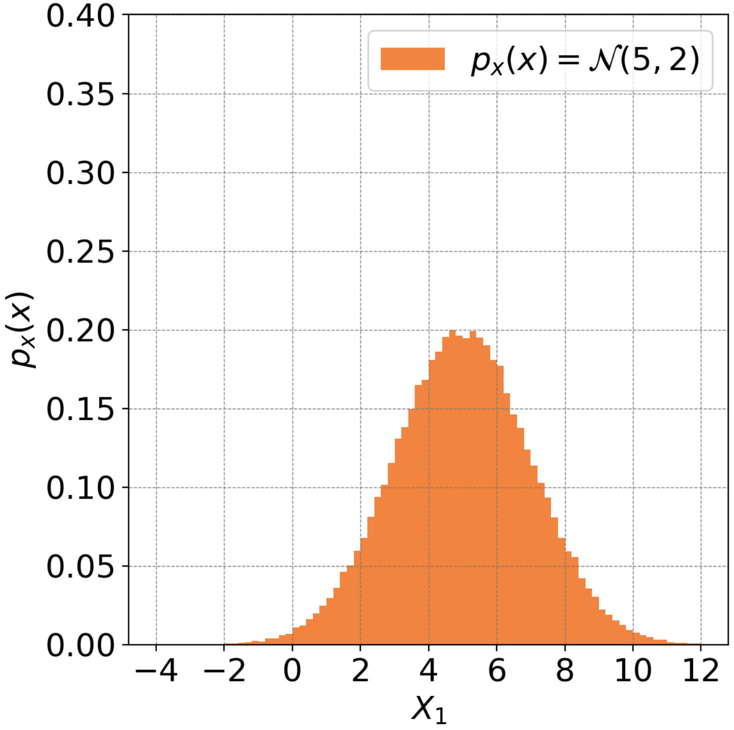
Using normal distribution definition:

$$\boldsymbol{p_z}(z_i) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(z_i)^2}{2}}$$

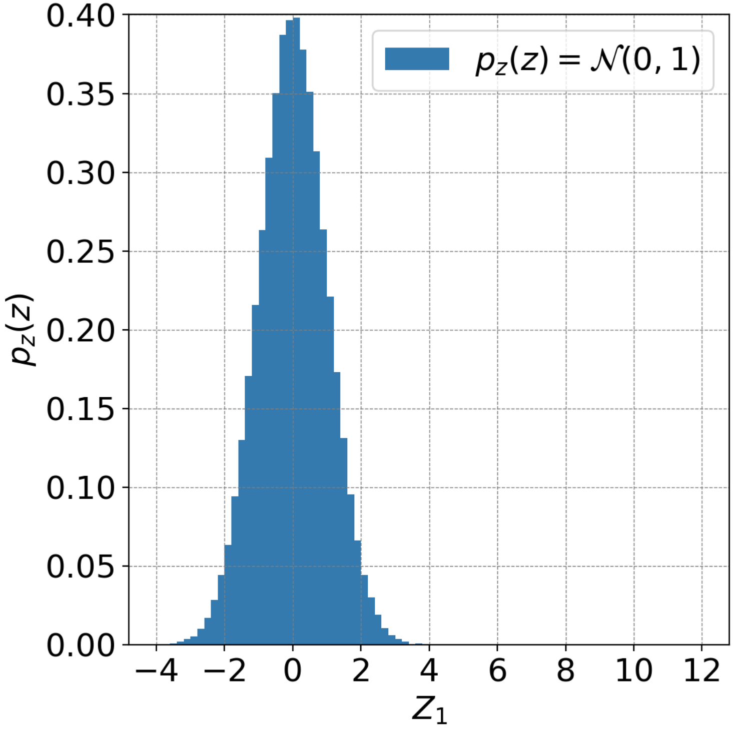
$$p_x(x_i) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(0.5x_i - 2.5)^2}{2}} * 0.5$$

$$= \frac{1}{2\sqrt{2\pi}} e^{-\frac{(x_i - 5)^2}{2*2^2}} = \mathcal{N}(5, 2)$$

1D example



$$z = f(x) = 0.5x - 2.5$$



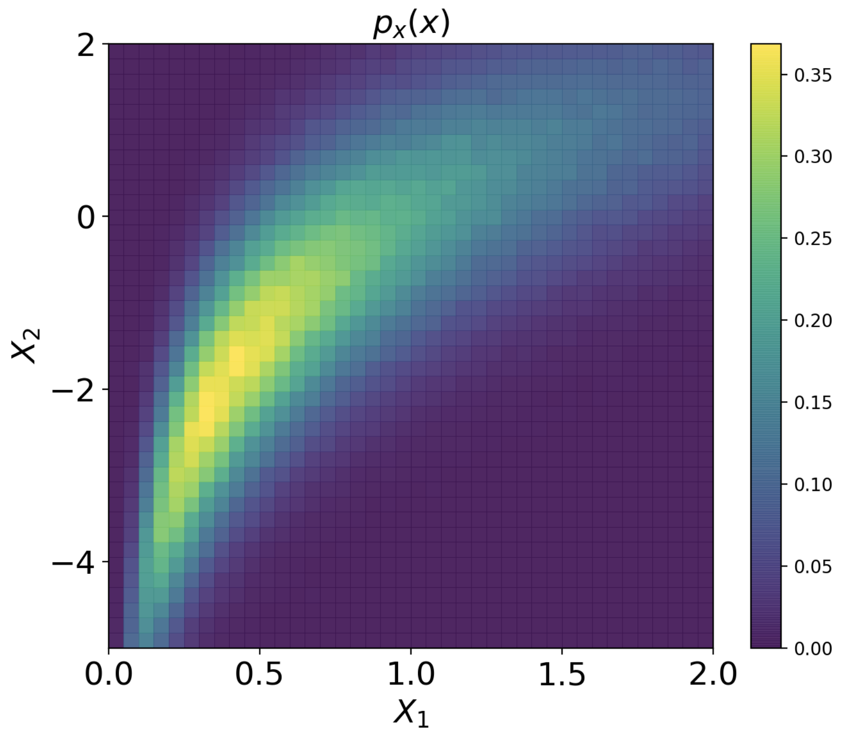
$$x_i \sim p_x(x)$$

$$p_x(x) = \mathcal{N}(5, 2)$$

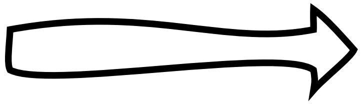
$$z_i \sim p_z(z)$$

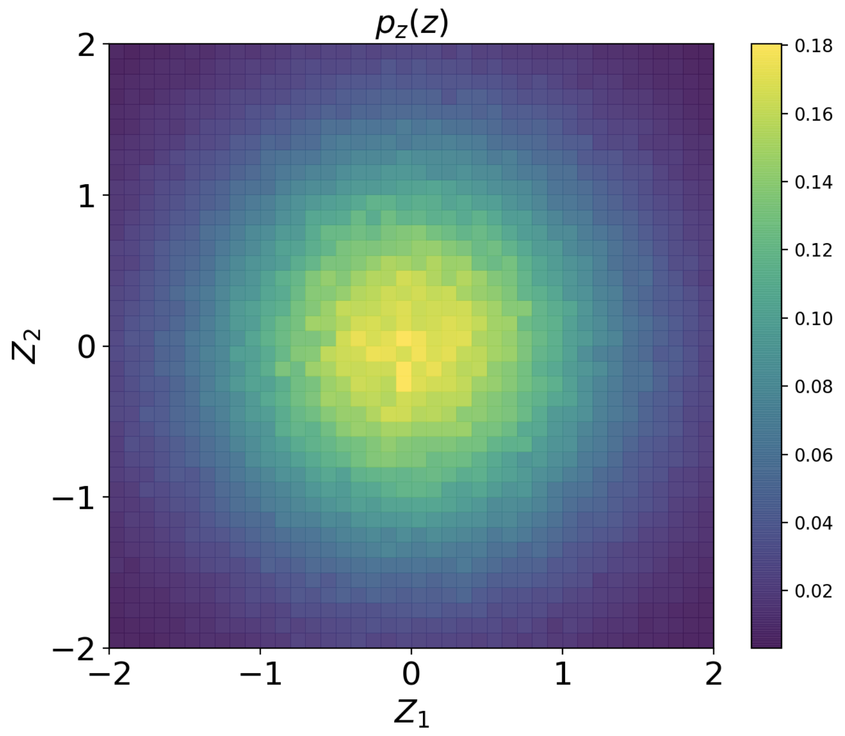
$$p_z(z) = \mathcal{N}(0, 1)$$

2D example



$$f(x) = \begin{cases} z_1 = \ln x_1 \\ z_2 = x_2 - 2\ln x_1 \end{cases}$$





$$x_i \sim p_x(x)$$

$$z_i \sim p_z(z)$$

$p_x(x)$ - ?

$$p_z(z) = \frac{1}{2\pi} e^{-\frac{z_1^2 + z_2^2}{2}}$$

2D example

For function:

$$z = \boldsymbol{f}(x) = \begin{cases} z_1 = \ln x_1 \\ z_2 = x_2 - 2\ln x_1 \end{cases}$$

Linear derivatives are:

$$\frac{\partial \boldsymbol{f}(x)}{\partial x} = \begin{pmatrix} {}^{1}\!/_{x_1} & 0 \\ {}^{-2}\!/_{x_{x1}} & 1 \end{pmatrix}$$

Jacobian:

$$\left|\det \frac{\partial \boldsymbol{f}(x)}{\partial x}\right| = \frac{1}{x_1}$$

2D example

Change of variables:

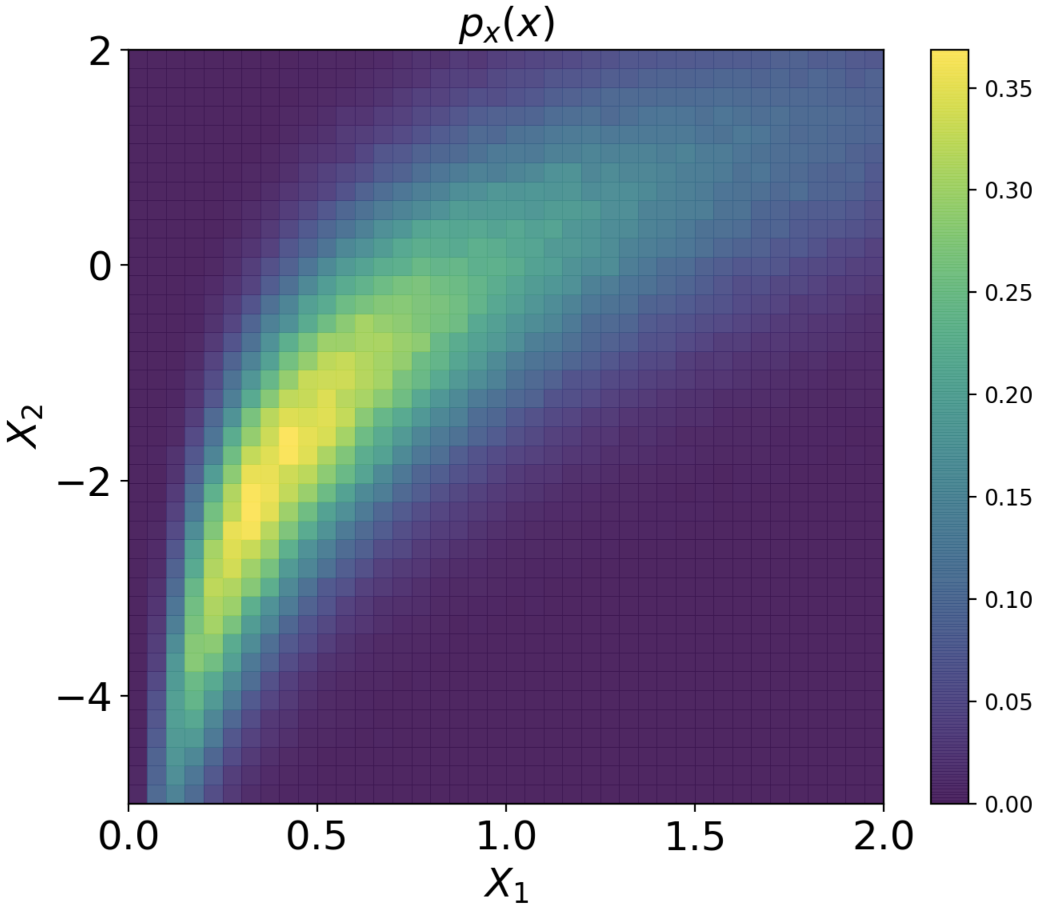
$$p_x(x_i) = \boldsymbol{p_z}\left(\boldsymbol{f}(x_i)\right)\left|\det\frac{\partial \boldsymbol{f}(x_i)}{\partial x_i}\right|,$$

Insert known shapes:

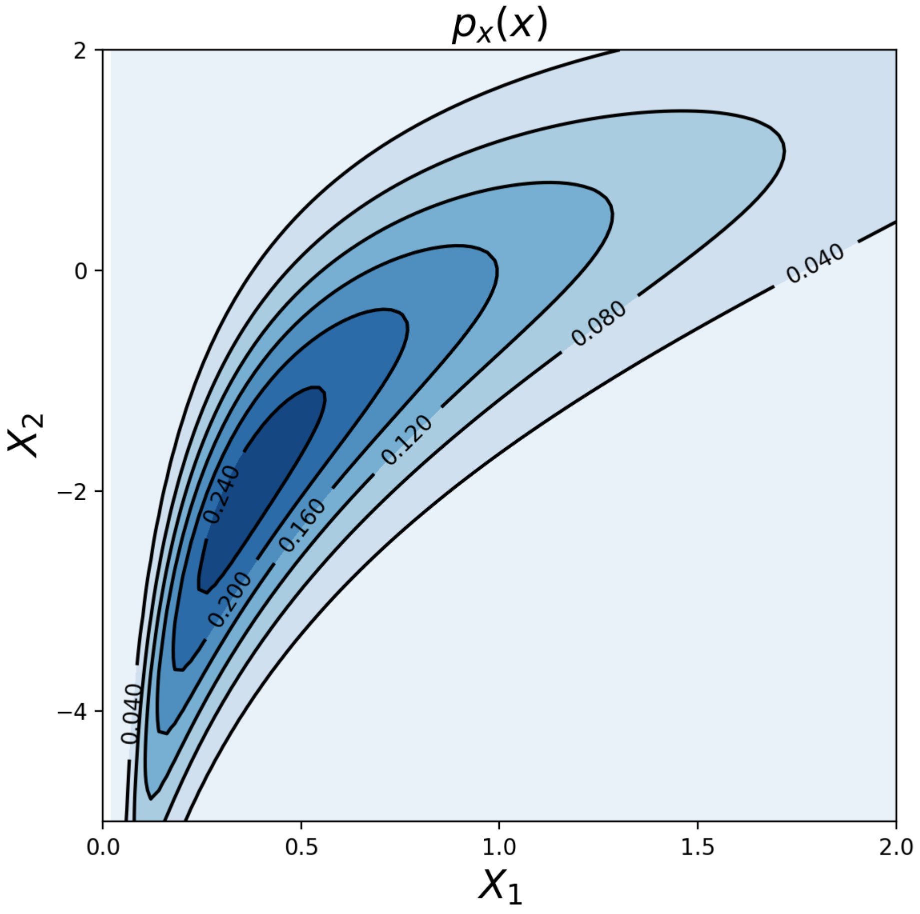
$$\boldsymbol{p_z}(z_i) = \frac{1}{2\pi}e^{-\frac{z_1^2+z_2^2}{2}}$$

$$p_x(x_i) = \frac{1}{2\pi}e^{-\frac{(\ln x_1)^2+(x_2-2\ln x_1)^2}{2}} * \frac{1}{x_1}$$

2D example



Experiment



Theory

Motivation recap

- Use **deterministic map** to known distribution:

$$\boldsymbol{z} = \boldsymbol{f}(\boldsymbol{x}).$$

- In this case, change of variables formula:

$$p_x(\boldsymbol{x}) = \boldsymbol{p_z}\big(\boldsymbol{f}(\boldsymbol{x})\big)\left|\det\frac{\partial\boldsymbol{f}(\boldsymbol{x})}{\partial\boldsymbol{x}}\right|.$$

- Inverse map:

$$\boldsymbol{x} = \boldsymbol{T}(\boldsymbol{z}).$$

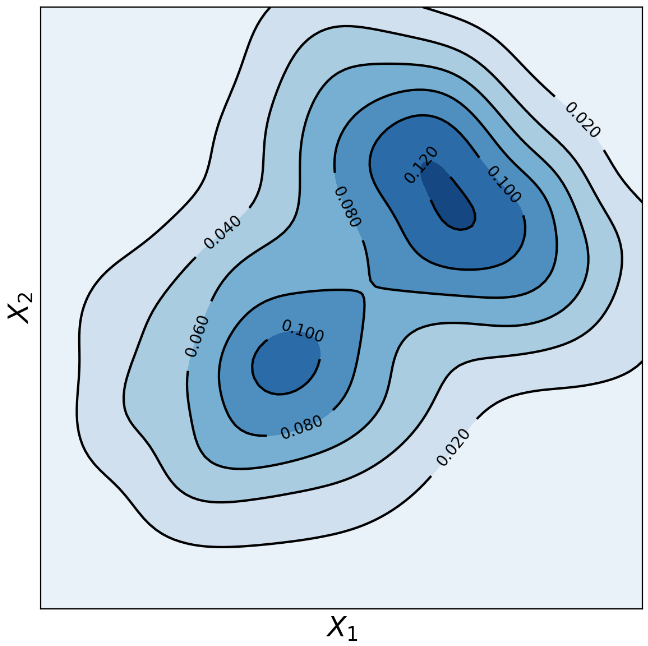
- In this case, change of variables formula:

$$\boldsymbol{p_z}(\boldsymbol{z}) = p_x\big(\boldsymbol{T}(\boldsymbol{z})\big)\left|\det\frac{\partial\boldsymbol{T}(\boldsymbol{z})}{\partial\boldsymbol{z}}\right|.$$

Motivation

$x_i \sim p_x(x)$

$p_x(x)$ - ?



Sampling

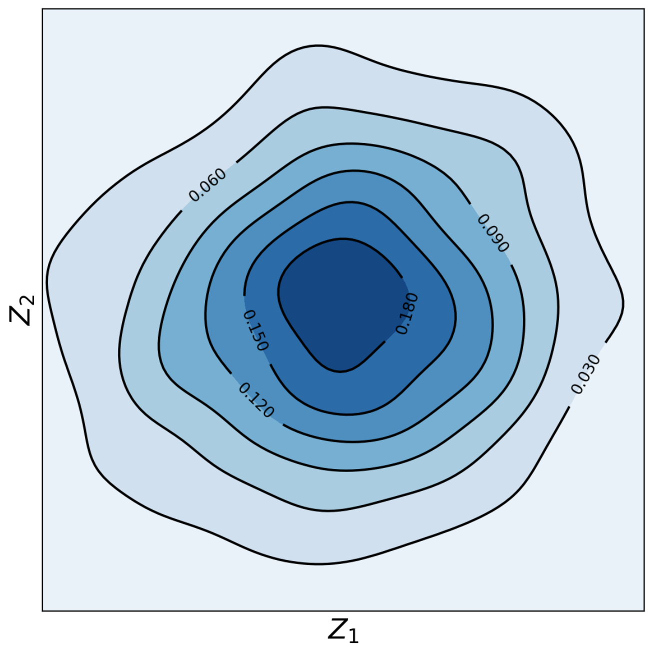
$\boldsymbol{x = T(z)}$

Likelihood evaluation

$\boldsymbol{z = f(x)}$

$z_i \sim p_z(z)$

$p_z(z)$ - known



Can we have invertible function?

Motivation recap

f:

- Invertible.
- Differentiable.

- Use **deterministic map** to known distribution:

$$\boldsymbol{z} = \boldsymbol{f}(\boldsymbol{x}).$$

- In this case, change of variables formula:

$$p_x(\boldsymbol{x}) = \boldsymbol{p_z}\big(\boldsymbol{f}(\boldsymbol{x})\big)\left|\det\frac{\partial \boldsymbol{f}(\boldsymbol{x})}{\partial \boldsymbol{x}}\right|.$$

- Inverse map:

$$\boldsymbol{x} = \boldsymbol{T}(\boldsymbol{z}) = \boldsymbol{f}^{-1}(\boldsymbol{z}).$$

- In this case, change of variables formula:

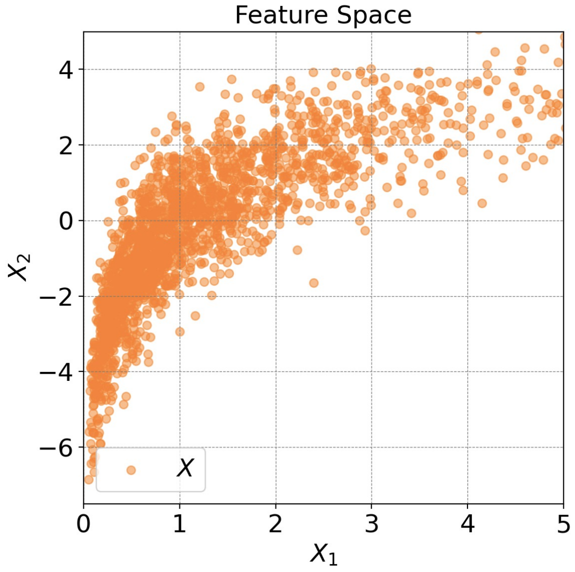
$$\boldsymbol{p_z}(\boldsymbol{z}) = p_x\big(f^{-1}(\boldsymbol{z})\big)\left|\det\frac{\partial \boldsymbol{f}^{-1}(z)}{\partial z}\right| = p_x\big(f^{-1}(z)\big)\left|\det\frac{\partial \boldsymbol{f}(z)}{\partial z}\right|^{-1}.$$

Normalizing flows

Problem Statement

$x_i \sim p_x(x)$ – data

$p_x(x)$ – ?

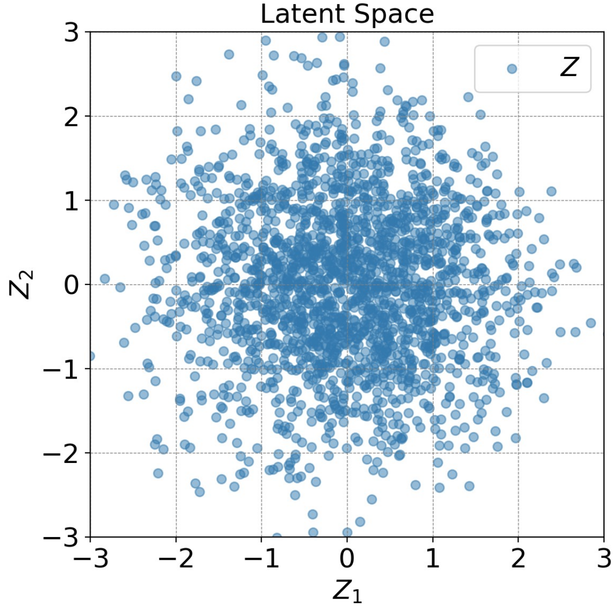


$z = \boldsymbol{f}(x)$ – ?

$\boldsymbol{x = f^{-1}(z)}$ - ?

$z_i \sim p_z(z)$

$p_z(z)$ known



- **We have:** real objects $\{x_i\}$
- **Task:** find invertible and differentiable f: $z_i = \boldsymbol{f}(x_i)$, such that $z_i \sim \boldsymbol{p_z}(z)$. For some known: $\boldsymbol{p_z}(z)$.

Loss function

Use log-likelihood:

$$\log \mathcal{L} = -\frac{1}{n}\sum_{i=1}^{n} \log p_x(x_i)$$

Change of variables:

$$p_x(x_i) = \boldsymbol{p_z}\left(\boldsymbol{f}(x_i)\right)\left|\det \frac{\partial \boldsymbol{f}(x_i)}{\partial x_i}\right|$$

Thus:

$$\log \mathcal{L} = -\frac{1}{n}\sum_{i=1}^{n}\left(\log \boldsymbol{p_z}\left(\boldsymbol{f}(x_i)\right) + \log\left|\det \frac{\partial \boldsymbol{f}(x_i)}{\partial x_i}\right|\right)$$

Training Algorithm

for number of training iterations **do:**

- Sample m of real objects $\{x_1, x_2, \dots, x_m\}$.
- Calculate loss function:

$$L = -\frac{1}{m}\sum_{i=1}^{m}\left(\log \boldsymbol{p_z}(\boldsymbol{f}(x_i)) + \log\left|\det\frac{\partial \boldsymbol{f}(x_i)}{\partial x_i}\right|\right)$$

- Update parameters of the function $z_i = \boldsymbol{f}(x_i)$:

$$\theta_f = \theta_f - \nabla_{\theta_f} L$$

Generation Algorithm

- Sample m objects $\{z_1, z_2, \dots, z_m\}$.
- Generate new objects using the learned function:

$$x_i = \boldsymbol{f}^{-1}(z_i)$$

Planar flows

- Transformation:

$$x = f_\theta^{-1}(z) = z + uh(w^T z + b),$$

$\theta = (w \in \mathbb{R}^D, u \in \mathbb{R}^D, b \in \mathbb{R})$ – parameters, $h(.)$ – elementwise nonlinearity.

- Linear derivative matrix:

$$\frac{\partial f_\theta^{-1}}{\partial z} = I + uh'(w^T z + b)w^T.$$

- Jacobian:

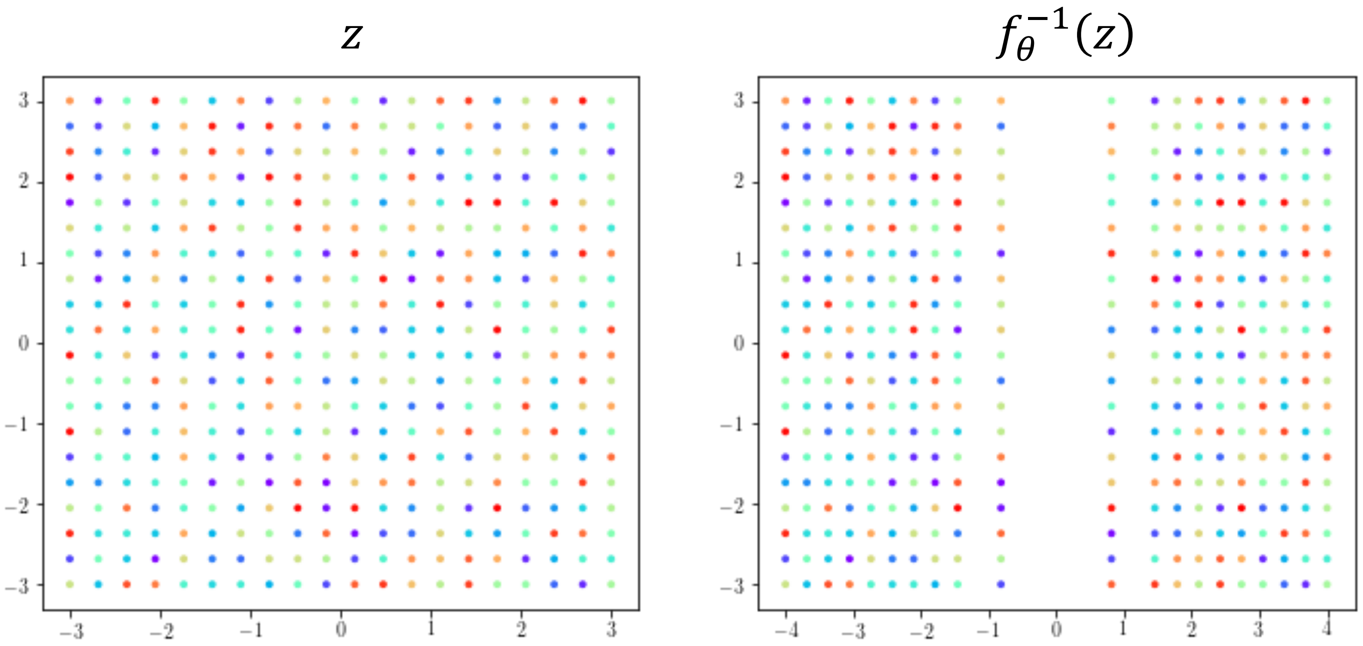
$$\det \frac{\partial f_\theta^{-1}}{\partial z} = 1 + h'(w^T z + b)w^T u.$$

Is it invertible? For $\boldsymbol{h}(.) = \tanh(.)$ need $\boldsymbol{w}^T\boldsymbol{u} > -1$.

Planar flows: grid behavior

$$x = f_\theta^{-1}(z) = z + uh(w^T z + b)$$

$$w = [5;\ 0]^T$$
$$u = [1;0]^T$$
$$b = 0$$
$$h(x) = \tanh(x)$$

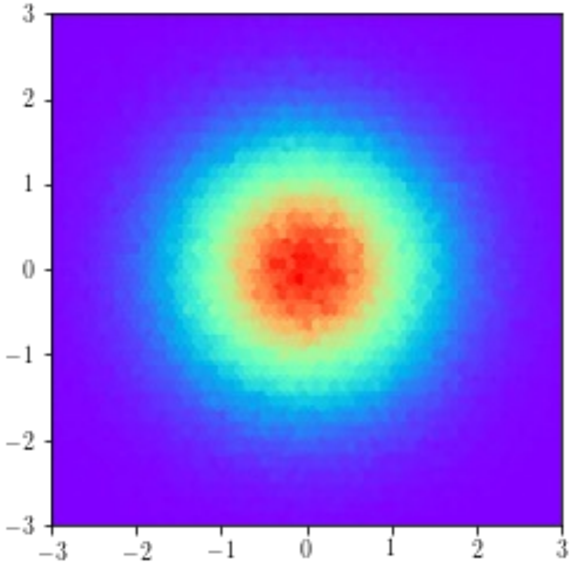


$$x = f_\theta^{-1}(z) = \begin{cases} z_1 + \tanh(5z_1) \\ z_2 \end{cases}$$

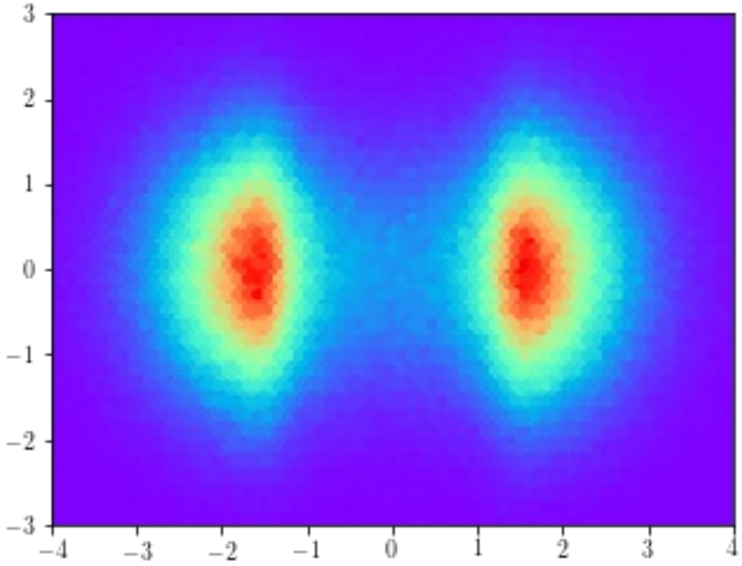
Grid will be pushed away from zero.

Planar flows: one step

$$x = f_\theta^{-1}(z) = \begin{cases} z_1 + \tanh(5z_1) \\ z_2 \end{cases}$$



$$x = f^{-1}(z)$$

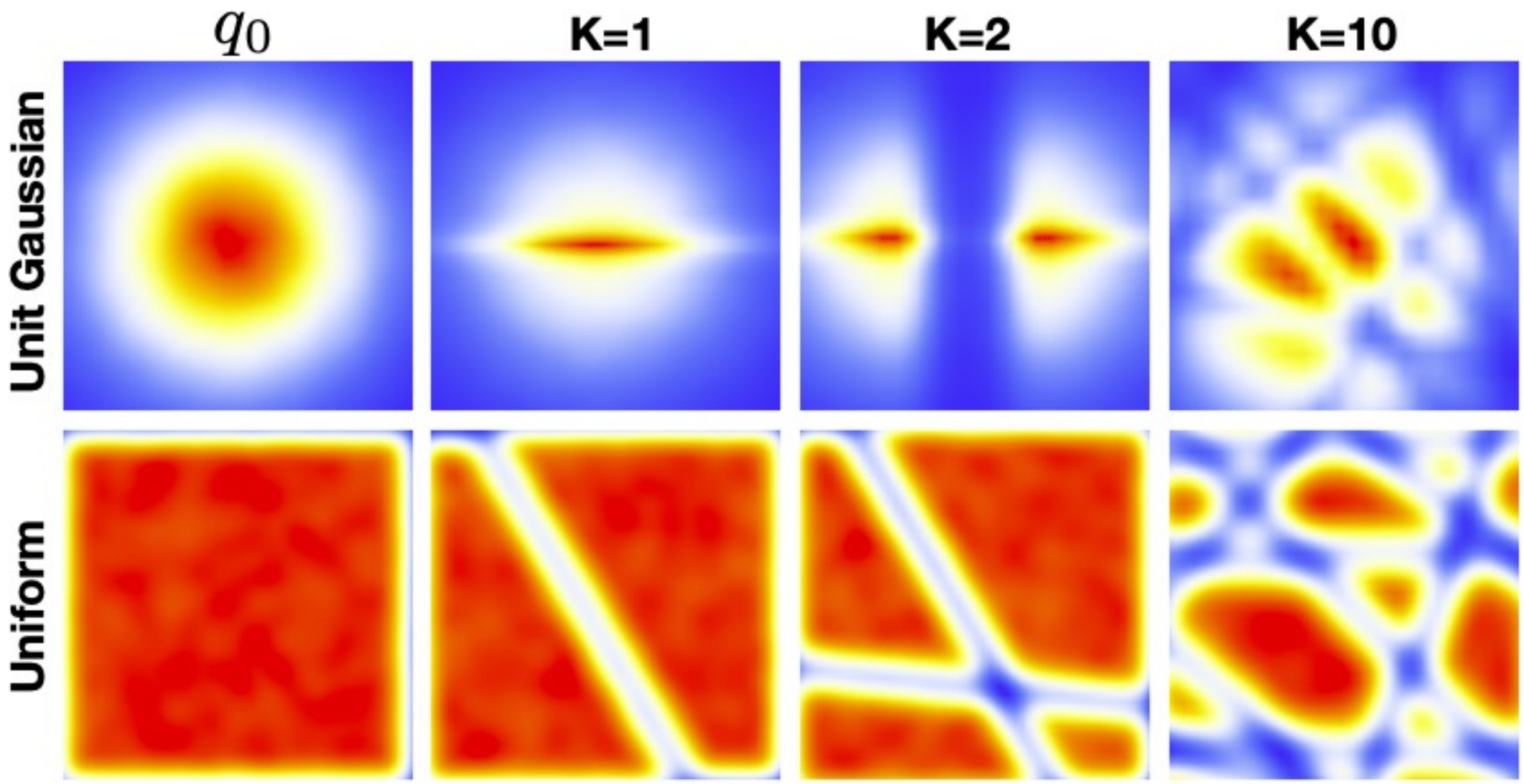


We can obtain a more complicated figure.

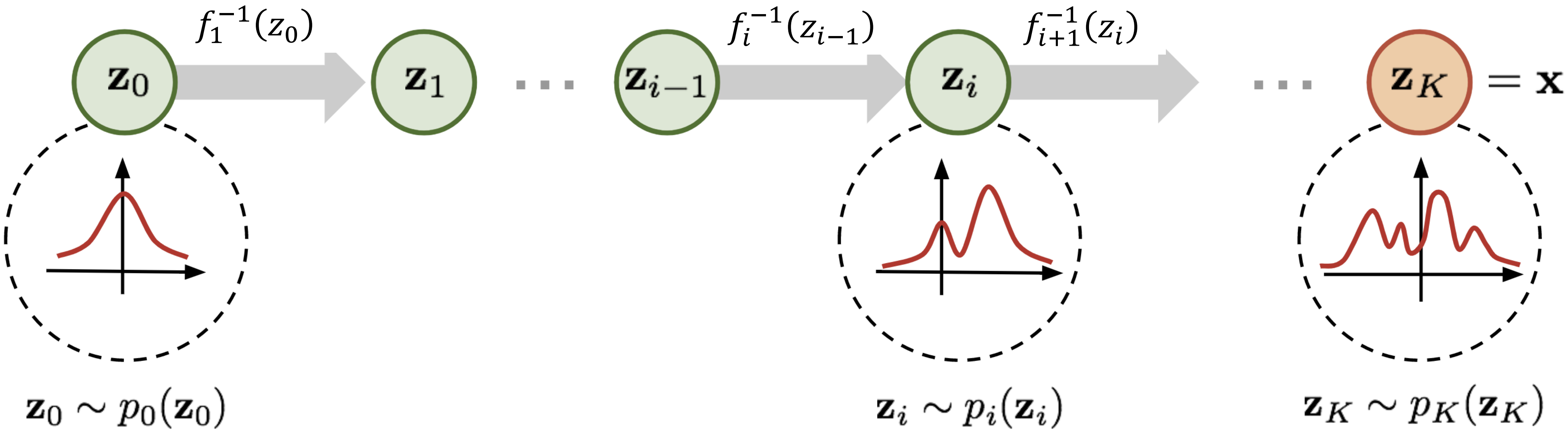
Planar flows: more steps

$$x = f_\theta^{-1}(z) = z + uh(w^T z + b)$$

Change transformation parameters at each step K for any prior distribution.

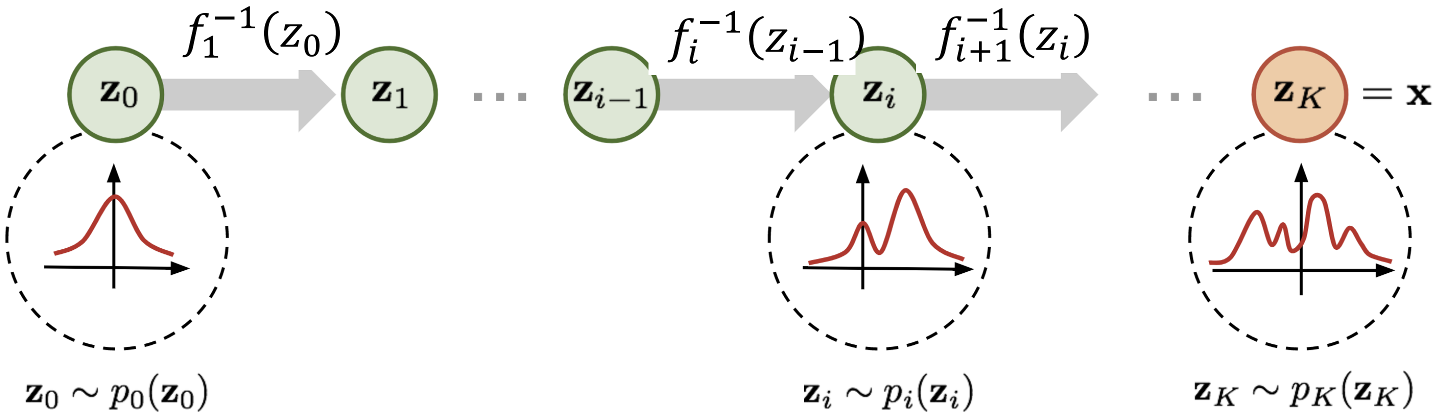


Stack more layers



- We take several transformations consecutively.
- At each layer we have new function.

Layers in Flows



Let $z_0 = \boldsymbol{f}_1(z_1), z_1 = \boldsymbol{f}_2(x)$.

Then:

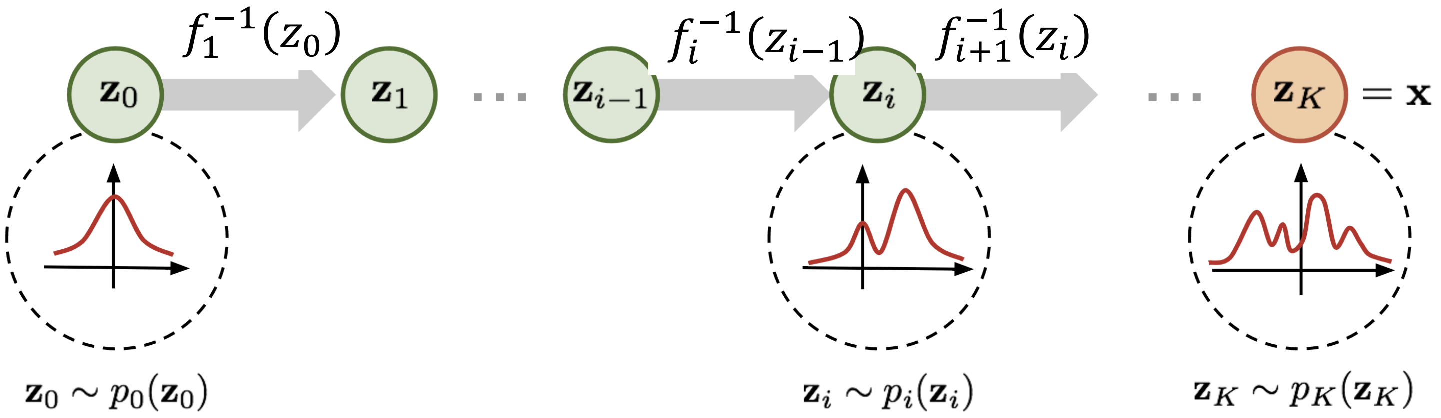
$$p_x(x) = \boldsymbol{p}_y(\boldsymbol{f}_2(x)) \left|\det \frac{\partial \boldsymbol{f}_2(x)}{\partial x}\right|$$

$$p_{z_1}(z_1) = \boldsymbol{p}_{z_0}(\boldsymbol{f}_1(z_1)) \left|\det \frac{\partial \boldsymbol{f}_1(z_1)}{\partial z_1}\right|$$

Which means:

$$p_x(x) = \boldsymbol{p}_{z_0}\left(\boldsymbol{f}_2(\boldsymbol{f}_1(x))\right) \left|\det \frac{\partial \boldsymbol{f}_1(z_1)}{\partial z_1}\right| \left|\det \frac{\partial \boldsymbol{f}_2(x)}{\partial x}\right|$$

Layers in Flows



Let $z_0 = \boldsymbol{f}_1(z_1), z_1 = \boldsymbol{f}_2(x)$.

Then:

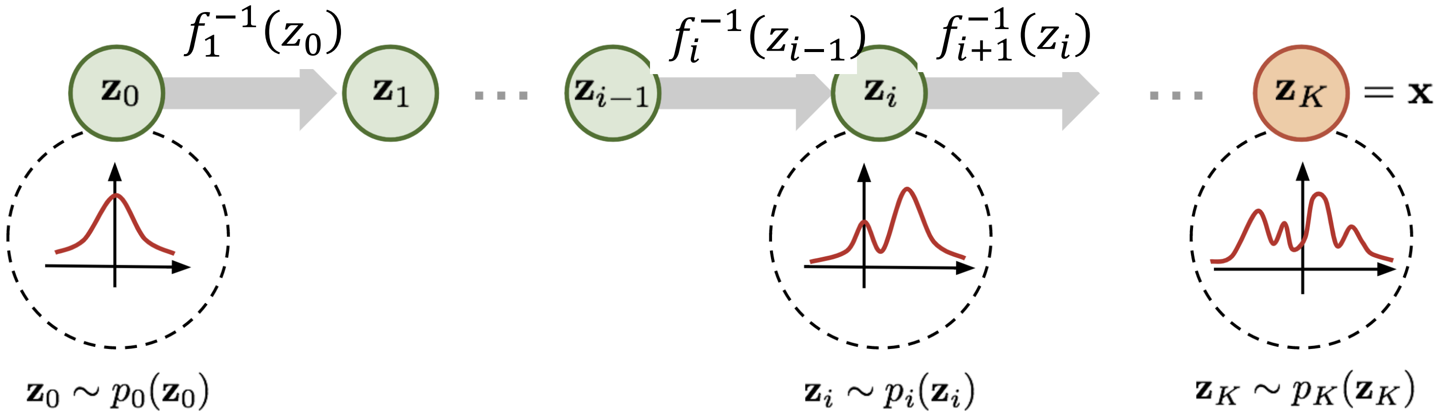
$$p_x(x) = \boldsymbol{p_y}(\boldsymbol{f}_2(x)) \left|\det \frac{\partial \boldsymbol{f}_2(x)}{\partial x}\right|$$

$$p_{z_1}(z_1) = \boldsymbol{p}_{\boldsymbol{z_0}}(\boldsymbol{f}_1(z_1)) \left|\det \frac{\partial \boldsymbol{f}_1(z_1)}{\partial z_1}\right|$$

Which means:

$$p_x(x) = \boldsymbol{p}_{\boldsymbol{z}_0}\left(\boldsymbol{f}_2(\boldsymbol{f}_1(x))\right) \left|\det \frac{\partial \boldsymbol{f}_1(z_1)}{\partial z_1}\right| \left|\det \frac{\partial \boldsymbol{f}_2(x)}{\partial x}\right|$$

Flow discussion



$$p_x(x) = \boldsymbol{p}_{\boldsymbol{z}_0}(\boldsymbol{f}_{\boldsymbol{K}}(\ldots(\boldsymbol{f}_{\boldsymbol{1}}(x)))) \left|\det \frac{\partial \boldsymbol{f}_{\boldsymbol{1}}(z_1)}{\partial z_1}\right| \ldots \left|\det \frac{\partial \boldsymbol{f}_{\boldsymbol{K}}(z_k)}{\partial z_k}\right|.$$

- It is possible to obtain $p_x(x)$ consecutively changing observables.
- The overall transformation is invertible if individual layers are invertible.
- Dimensions of each observable is the same.
- Fit is performed using ML estimate.
- Need to calculate determinant.

Jacobian Problems

$$\frac{\partial \boldsymbol{f}(x_i)}{\partial x_i} = \begin{pmatrix} \frac{\partial \boldsymbol{f}(x_i)_1}{\partial x_{i1}} & \cdots & \frac{\partial \boldsymbol{f}(x_i)_1}{\partial x_{in}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \boldsymbol{f}(x_i)_m}{\partial x_{i1}} & \cdots & \frac{\partial \boldsymbol{f}(x_i)_m}{\partial x_{in}} \end{pmatrix}$$

- dxd determinant is **too expensive** to compute with $\mathcal{O}(d^3)$ computations.
- **Idea: take only transformations with triangular matrix, in this case $\mathcal{O}(d)$ computations.**
- **Bogachev theorem**: There always exists a unique (up to ordering) increasing triangular map that transforms a source density to a target density.

We came to autoregressive models.

Block models

Block matrix for Jacobian

$$\frac{\partial \boldsymbol{f}(x)}{\partial x} = \begin{pmatrix} \mathbb{I}_d & 0 \\ \frac{\partial z_{d+1:D}}{\partial x_{d+1:D}} & S \end{pmatrix}$$

- Randomly choose d such that we have two disjoint subsets of observables: $z_{1:d}$ and $z_{d+1:D}$.
- Insert a block transform.
- Repeat for several layers.
- If needed insert scaling layers.
- Fit simultaneously.

Non-linear Independent Components Estimation

$$z = \boldsymbol{f}(x) = \begin{cases} z_{1:d} = x_{1:d} \\ z_{d+1:D} = x_{d+1:D} - m(x_{1:d}) \end{cases}$$

- $\boldsymbol{m}(x_{1:d})$ – **neural networks** with d inputs and $D - d$ outputs;
- easy to invert;
- scaling layer $x_i = s_i z_i$ can be added.
- $\det J = \prod_{i=1}^{n} s_i$.
- Based on NADE autoregressive model.

Non-linear Independent Components Estimation

(a) Model trained on MNIST

(b) Model trained on TFD

https://arxiv.org/abs/1410.8516

Real-NVP

$$z = \boldsymbol{f}(x) = \begin{cases} z_{1:d} = x_{1:d} \\ z_{d+1:D} = x_{d+1:D} \odot \exp\big(\boldsymbol{s}(x_{1:d})\big) + \boldsymbol{t}(x_{1:d}) \end{cases}$$

- $\boldsymbol{s}(x_{1:d})$ и $\boldsymbol{t}(x_{1:d})$ – **neural networks** with d inputs and $D-d$ outputs.
- Invertible.
- $\det J_k = \exp \sum_{i=d+1}^{D} \big(\alpha_\theta(z_{1:d})\big)_i$ for k-th layer.
- Inspired by RNADE.

https://arxiv.org/abs/1605.08803

R-NVP: results

Рис.: https://github.com/laurent-dinh/laurent-dinh.github.io/blob/master/img/real_nvp_fig/celeba_samples.png

Discussion

- Normalizing flows based on block scheme have nice results.
- Block scheme allows for autoregressive model insertion.
- Fairly fast: need only one pass to get the sampling and likelihood evaluation, can run in parallel.
- Autoregressive quality is not conserved in multiple layers.

Masked Autoregressive Flow (MAF)

Masked Autoregressive Flow (MAF)

$$z = \boldsymbol{f}(x) = \begin{cases} z_1 = (x_1 - \mu_1)\exp(-s_1) \\ \dots \\ z_k = (x_k - \boldsymbol{\mu_k}(x_{1:k-1})) \odot \exp(-\boldsymbol{s_k}(x_{1:k-1})) \\ \dots \end{cases}$$

- $\boldsymbol{\mu_d}(x_{1:d-1})$ и $\boldsymbol{s_d}(x_{1:d-1})$ – **neural networks.**
- MADE architecture inspired.
  - Fast in likelihood evaluation.
  - Slow ancestral sampling.

https://arxiv.org/abs/1705.07057

Masked Autoregressive Flow (MAF): Jacobian

- Low-triangular matrix

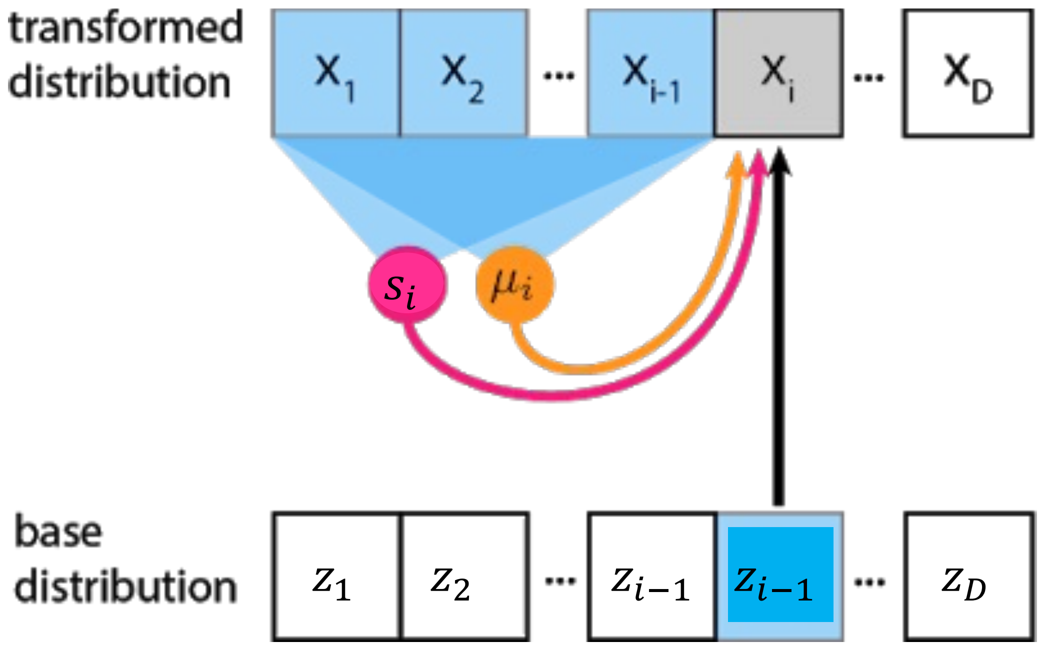
$$\frac{\partial \boldsymbol{f}(x)}{\partial x} = \begin{pmatrix} \exp(-\boldsymbol{s_1}) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ \frac{\partial z_D}{\partial x_1} & \cdots & \exp(-\boldsymbol{s_D}(x_{1:D-1})) \end{pmatrix}$$

- Jacobian:

$$\left|\det \frac{\partial \boldsymbol{f}(x)}{\partial x}\right| = \exp(-\sum_{j=1}^{D} \boldsymbol{s_d}(x_{1:d-1}))$$

MAF sampling

$$x = f^{-1}(z) = \begin{cases} x_1 = z_1 \exp(s_1) + \mu_1 \\ x_d = z_d \exp(\boldsymbol{s_d}(x_{1:d-1})) + \boldsymbol{\mu_d}(x_{1:d-1}) \end{cases}$$



- Forward pass:

  $z \sim N(0;1)$

  $x_1 = \exp(s_1)\, z_1 + \mu_1$

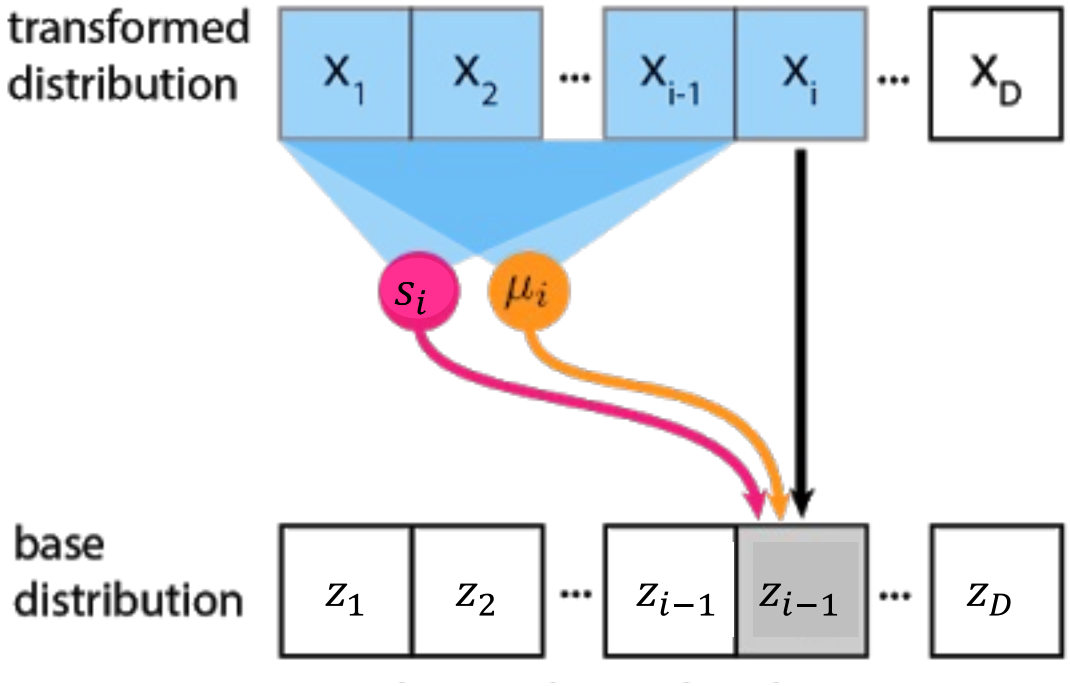
  $x_2 = \exp\big(s_2(x_1)\big)\, z_2 + \mu_2(x_1)$

  And so on.

  Consecutive and slow.

MAF Likelihood evaluation

$$z = \boldsymbol{f}(x) = \begin{cases} z_1 = (x_1 - \mu_1)\exp(-s_1) \\ z_k = (x_k - \boldsymbol{\mu_k}(x_{1:k-1})) \odot \exp(-\boldsymbol{s_k}(x_{1:k-1})) \end{cases}$$



- Inverse pass:

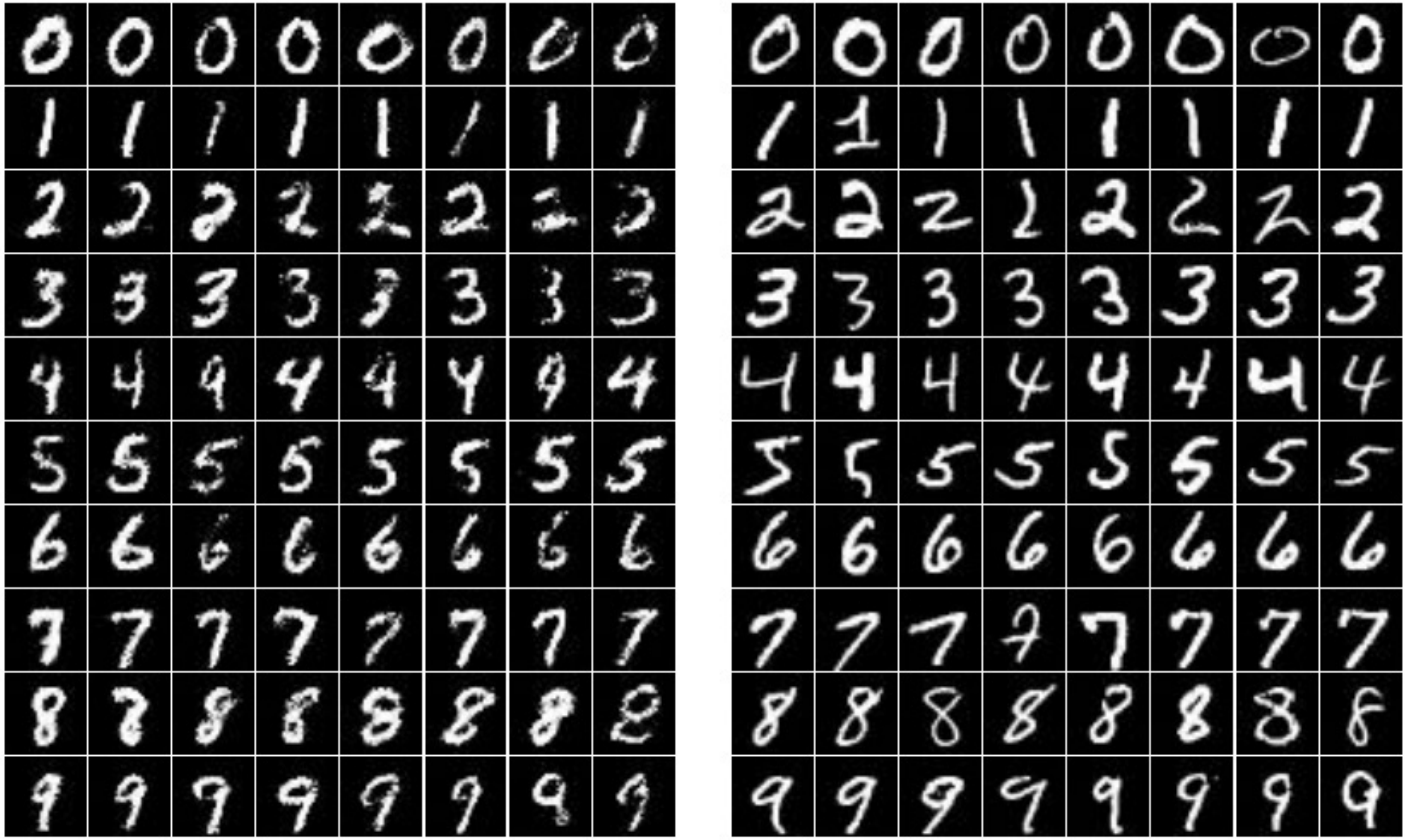
  compute all μ and s;

  evaluate z.

Likelihood evaluation is fast and parallelizable.

Training is fast.

MAF: results



(a) Generated images (b) Real images

Figure 3: Class-conditional generated and real images from MNIST. Rows are different classes. Generated images are sorted by decreasing log likelihood from left to right.

Inverse Autoregressive Flow (IAF)

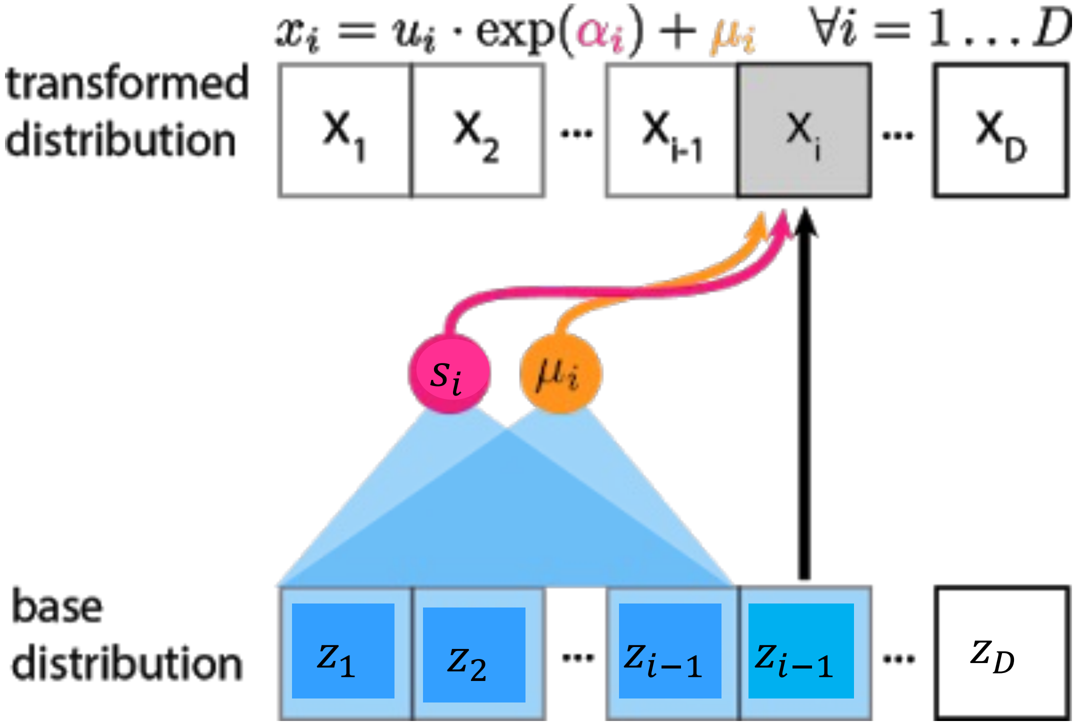
$$z = \boldsymbol{f}(x) = \begin{cases} z_1 = (x_1 - \mu_1)\exp(-s_1) \\ z_d = (x_d - \boldsymbol{\mu_d}(z_{1:d-1}))\exp(-\boldsymbol{s_d}(z_{1:d-1})) \end{cases}$$

- $\boldsymbol{\mu_d}(z_{1:d-1})$ и $\boldsymbol{s_d}(z_{1:d-1})$ – **neural networks.**
- Similar to MAF but with inverse problems by construction:
  - Fast to sample.
  - Slow to evaluate likelihood.

https://arxiv.org/abs/1606.04934

Inverse Autoregressive Flow (IAF)

$$x = f^{-1}(z) = \begin{cases} x_1 = z_1 \exp(s_1) + \mu_1 \\ x_d = z_d \exp(\boldsymbol{s_d}(z_{1:d-1})) + \boldsymbol{\mu_d}(z_{1:d-1}) \end{cases}$$



- Forward pass:

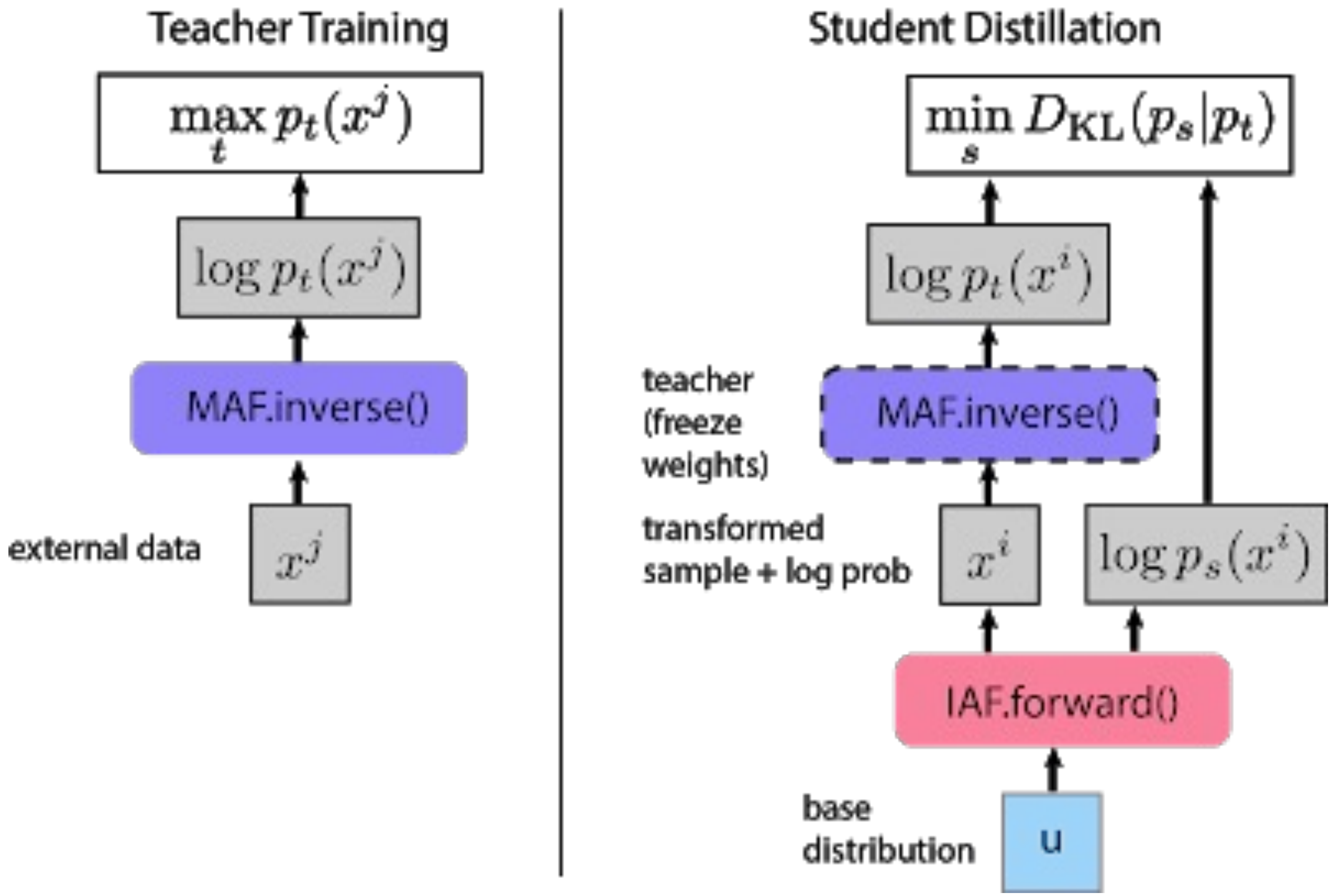
  compute all μ and s;

  evaluate x.

Sampling is fast and parallelizable.

Training is slow.

Probability Density Distillation



- Two-part training with a teacher and student model.
- Teacher (MAF) trained first, then student (IAF) initialized.
- Student, s, is trained to match the teachers' distribution t using KL divergence:

$$KL(p_s||p_t) = H(p_s, p_t) - H(p_s).$$

Which is evaluated using MAF.

https://arxiv.org/pdf/1711.10433.pdf

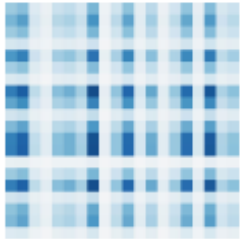
Conclusions

Conclusions

1. Det Identities

Planar NF
Sylvester NF
...

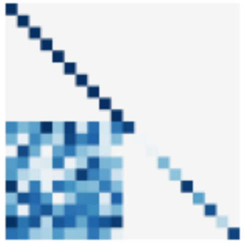
Jacobian



(Low rank)

2. Coupling Blocks

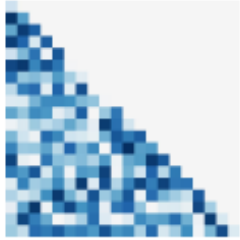
NICE
Real NVP
Glow
...



(Lower triangular + structured)

3. Autoregressive

Inverse AF
Neural AF
Masked AF
...



(Lower triangular)

4. Unbiased Estimation

FFJORD
Residual Flows

(Arbitrary)