Inspiration from Calc

$$\int_{x=0}^{\infty} 2x e^{-x^2} \, dx =$$

$$x = \sqrt{u}$$

$$\int_{x=0}^{\infty} 2x e^{-x^2} \, dx = \int_{u=0}^{\infty} e^{-u} \, du = -e^{-u} \Big|_0^{\infty} = 1$$

$$\begin{cases} \text{Set } u = x^2 \\ du = 2x\,dx \end{cases}$$

Observe: ① e^{-u} is a prob. density on $[0, \infty)$.

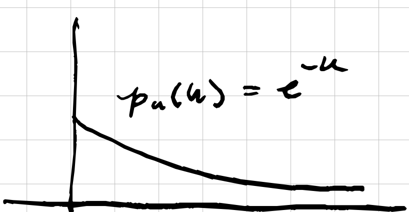
② $2x e^{-x^2}$ " " " " " "

③ $\begin{cases} u = x^2 : [0,\infty) \xrightarrow{\text{bij, diff.}} [0,\infty) \\ x = \sqrt{u} \quad " \quad " \quad " \end{cases}$

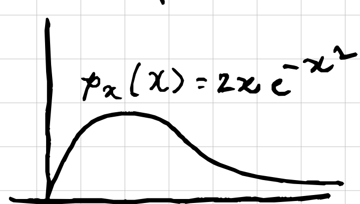
$$u(x) = x^2 \qquad \frac{du}{dx} = 2x$$

$$x(u) = \sqrt{u} \qquad \frac{dx}{du} = \frac{1}{2\sqrt{u}}$$

$$p_u(u) \longmapsto p_u(u(x)) \left| \frac{du}{dx}(x) \right|$$



$\longleftrightarrow$

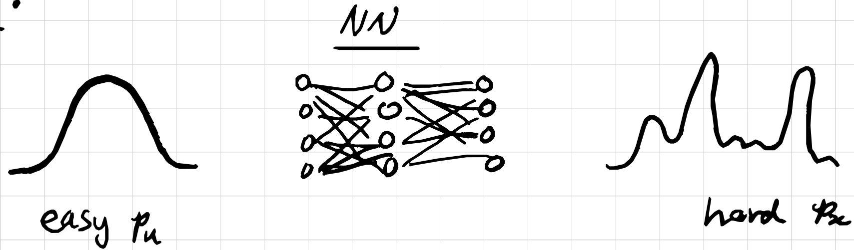


In general, i.e. $u, x \in \mathbb{R}^n$

n×n Jacobian matrix

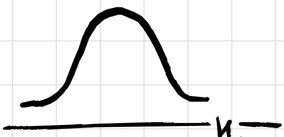
$$p_x(x) = p_u(u(x)) \left| \det \underbrace{u'(x)}_{J_u(x)} \right|$$

Idea:



Idea:

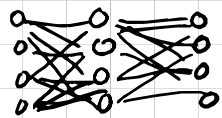
$u \in \mathbb{R}^n$



u

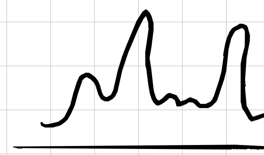
easy p_u (Normal)

NN



$T_\theta(u) = x$

$x \in \mathbb{R}^n$



x

hard p_x^*

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① Set p_u = standard Normal

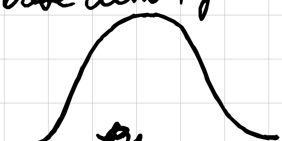
② Create NN so that it is a diffeomorphism

- every layer is bijective (all have n-nodes!)
- " " " diff'ble.

③ Create a loss fn: $KL(p_x, p_x^*)$ OR $KL(p_u^*, p_u)$

Observe: OR

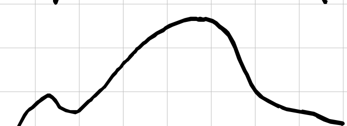
base density



p_u

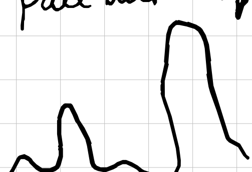
$\xrightarrow{T_\theta \#}$

push thru of p_u



$p_x(x) = p_u(T^{-1}(x))\,|\det J_{T^{-1}}(x)|$

pull back of p_x^*



$p_u^*(u) = p_x^*(T(u))\,|\det J_T(u)|$

$\xleftarrow{T_\theta^{-1} \#}$

Target density

$p_x^*(x)$

Recall

$$KL(p,q) = \int \log\left(\frac{p}{q}\right) dp$$

$$= \int_x \log\left(\frac{p(x)}{q(x)}\right) p(x)\, dx$$

$$= \sum_i \log\left(\frac{p(x_i)}{q(x_i)}\right) p(x_i) \cdot 1$$

Properties: $KL(p,q) \geq 0$

$\quad\quad\quad\quad$ " $\quad = 0 \iff p = q$ a.e. dp

In general $\quad KL(p,q) \neq KL(q,p)$

& Δ-ineq. doesn't hold.

Theorem: $KL(p_u, p_u^*) = KL(p_x, p_x^*)$

& $KL(p_u^*, p_u) = KL(p_x^*, p_x)$.

Proof: FTONF

We have 2 options!

Forward KL $\quad KL(p^*, p)$

Reverse KL $\quad KL(p, p^*)$

Cheat Sheet

$$KL(p, q) = \int \log\left(\frac{p}{q}\right) dp$$

If $x_i \overset{IID}{\sim} p$

$$\approx \frac{1}{N} \sum_{i=1}^{N} \log\left(\frac{p(x_i)}{q(x_i)}\right)$$

We have 2 options:

target — pushthru, θ lives here

① **Foward KL** $KL(p_x^*, p_x)$

$$= \int \log\left(\frac{p_x^*}{p_x}\right) dp_x^*.$$

If you have a data set $\{x_i\}_{i=1}^{N} \overset{IID}{\sim} \underbrace{p_x^*}_{\text{unknown data dist.}}$

& you want to generate more

$$\approx \frac{1}{N} \sum_{i=1}^{N} \left[\underbrace{\log p_x^*(x_i)}_{\text{constant in } \theta} - \log p_x(x_i, \theta)\right]$$

$$= \text{const} - \frac{1}{N} \sum_{i=1}^{N} \log p_x(x_i, \theta)$$

$$\min_\theta KL(p_x^*, p_x) \iff \max_\theta \frac{1}{N} \sum_{i=1}^{N} \log p_x(x_i, \theta)$$

This is an MLE!

$$= \boxed{\max_\theta \frac{1}{N} \sum_i \log\left(p_u\left(T_\theta^{-1}(x_i)\right)\right) + \log\left(\left|\det J_{T_\theta^{-1}}(x_i)\right|\right)}$$

(*) Normal

Requirements!

① Must be able to computationally invert T

② Compute det J

Use Case 1   I have $\{x_i\}_{i=1}^{N} \overset{\text{IID}}{\sim} \underbrace{p_x^*}_{\text{unknown data density}}$

I want to generate more data.

How?

① Create NF T_θ - NN s.t.
- every layer is invertible & diff
- Can compute $\underbrace{T_\theta^{-1}}_{??}$ & $\underbrace{|\det J_{T^{-1}_\theta}|}_{\text{OK w/ cleverness}}$ (yikes!)

② Training $\overset{\text{Forward KL}}{\text{Minimize}}$ $KL(P_*, P)$
$\Updownarrow$
Maximize (*)   (MLE)

③ Sample $\{u_j\} \sim N(0, I) = p_u$

Compute $x_j = T(u_j) \sim p_x \approx p_x^*$

Main hurdle is that you need to invert the NN to sample / train

② Reverse KL $\underline{KL(p, p^*)}$

$$KL(p_x, p_x^*) = \int \log\left(\frac{p_x}{p_x^*}\right) dp_x$$

$u = T^{-1}(x)$

$$= \int \log\left(\frac{p_u}{p_u^*}\right) dp_u$$

Sample $u_i \overset{iid}{\sim} p_u$

$$\approx \frac{1}{N} \sum_{i=1}^{N} \underbrace{\log(p_u(u_i))}_{\text{constant in } \theta} - \underbrace{\log(p_u^*(u_i))}_{\theta \text{ here!}}$$

(**) minimize $-\frac{1}{N} \sum \log\left[\underbrace{p_x^*(\underbrace{T_\theta(u_i)}_{x_i})} \underbrace{\left|\det J_{T_\theta}(u_i)\right|} \right]$

Need to compute

- $p_x^*(\cdot)$ up to a (positive) constant

- Need to compute $|\det T_\theta(\cdot)|$ ← ok w/ Clever NF

$$P(\phi \mid \text{data}) = \frac{p(\text{data} \mid \phi) \underbrace{p(\phi)}_{\text{prior}}}{\int_\phi p(\text{data} \mid \phi) p(\phi) d\phi}$$

constant

2^{nd} use case

Some unknown constant.

I can compute $p^*(x) \cdot Z$

I want to sample $x \sim p^*$

How?

1. Create NF T
   - feed fwd N.N.
   - bijective diff.
   - so that I can compute J_T

2. Training: Minimize Reverse KL = (**)

3. Sampling: Sample $u_i \sim p_u$ $(N(0,I))$
   $x_i = T_\theta(u_i) \sim p_x \approx p_x^*$

	Continuous Data	Discrete Data
Discrete Flows	OG NFs	Categorical NFs Discrete NFs
Continuous Flows	Neural ODEs	?

- p_u
- $u = T(x) \iff x = T^{-1}(u)$

$$p_u \longmapsto T\# p_u = p_x(x) := p_u(\underbrace{T^{-1}(x)}_{u(x)}) \mid \det \underbrace{(T^{-1})'(x)}_{u'(x)} \mid$$

Note

$$P_x(x \in [3,4]) = \int_{x \in [3,4]} 2x e^{-x^2} dx$$

$u = x^2$

$\frac{du}{dx} = 2x$

$$= \int_{u \in [9,16]} e^{-u} du = P_u(u([3,4]))$$

Recall some facts:

① $(f_1 \circ f_2)'(x) = \underbrace{f_1'(f_2(x))}\, f_2'(x)$

$= J_{f_1}(f_2(x)) \cdot J_{f_2}(x)$

② $\det(AB) = \det(A)\det(B)$.

③ $\det(A^{-1}) = \det(A)^{-1}$

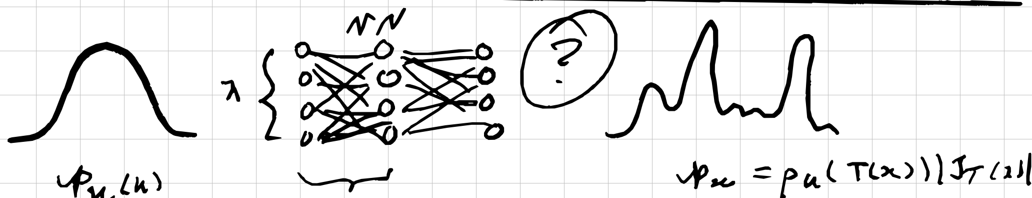
④ $(AB)^{-1} = B^{-1}A$

⑤ $\left.\begin{matrix} u = f(x) \\ x = f^{-1}(u) \end{matrix}\right\}$ $[f'(x)]^{-1} = [f^{-1}(u)]'$

Goal is to sample from <u>target</u> density

$p_x^*(x)$, $x \in \mathbb{R}^n$

① Pick easy base density $p_u(u)$ (Standard Normal)



② NN → every layer is a bijection $\mathbb{R}^n \to \mathbb{R}^n$, & differentiable

$x = f(u)$
$\quad\ d\ \theta$

② Create a NN so that it is a diffeomorphism

(each layer is same dim., 1-1, , differentiable)

<u>Observe</u>: 4 distributions