Residual Flows

for Invertible Generative Modeling

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Invertible Residual Networks (i-ResNet)

It can be shown that residual blocks

$$y = f(x) = x + g(x)$$

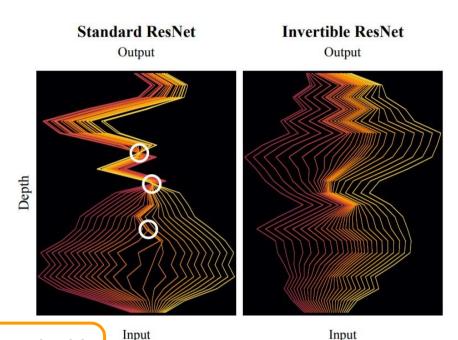
can be inverted by fixed-point iteration

$$x^{(i)} = y - g(x^{(i-1)})$$

and has a unique inverse (ie. invertible)

if

$$|g(x) - g(y)| < |x - y|$$



i.e. Lipschitz. Enforced with spectral normalization.

(Behrmann et al. 2019)

Applying Change of Variables to i-ResNets

lf

$$y = f(x) = x + g(x)$$

Then

$$\log p(x) = \log p(f(x)) + \log \left| \det \frac{df(x)}{dx} \right|$$
$$\log p(x) = \log p(f(x)) + \sum_{i=1}^{\infty} \frac{(-1)^{k+1}}{k} \operatorname{tr}([J_g(x)]^k)$$

Enter the "Russian roulette" estimator (Kahn, 1955). Suppose we want to estimate

$$\sum_{k=1}^{\infty} \Delta_k \qquad \qquad \text{(Require } \sum_{k=1}^{\infty} |\Delta_k| < \infty \text{)}$$

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(Require $\sum_{k=1}^{\infty} |\Delta_k| < \infty$)

Flip a coin b with probability q.

$$\mathbb{E}\left[\Delta_1 + \right]$$

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Flip a coin b with probability **q**.

$$\mathbb{E}\left[\Delta_1 + \left[\begin{array}{cc} & & \\ & & \end{array}\right] \mathbb{1}_{b=0} + \left[\begin{array}{cc} \\ \end{bmatrix} \mathbb{1}_{b=1}\right]$$

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Flip a coin b with probability q.

$$\mathbb{E}\left[\Delta_{1} + \left[\frac{1}{1-q} \sum_{k=2}^{\infty} \Delta_{k}\right] \mathbb{1}_{b=0} + [0] \mathbb{1}_{b=1}\right]$$

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Flip a coin b with probability q.

$$\mathbb{E}\left[\Delta_{1} + \left[\frac{1}{1-q}\sum_{k=2}^{\infty}\Delta_{k}\right]\mathbb{1}_{b=0} + [0]\mathbb{1}_{b=1}\right]$$

$$= \Delta_{1} + \left[\frac{1}{1-q}\sum_{k=2}^{\infty}\Delta_{k}\right](1-q)$$

$$= \sum_{k=1}^{\infty}\Delta_{k}$$
Has probability evaluated in features.

Has probability q of being evaluated in **finite** time.

If we repeatedly apply the same procedure *infinitely many times*, we obtain an unbiased estimator of the infinite series.

$$\sum_{k=1}^{\infty} \Delta_k = \mathbb{E}_{n \sim p(N)} \left[\sum_{k=1}^n \frac{\Delta_k}{\mathbb{P}(N \geq k)} \right]$$
 Computed in finite time

Directly sample the first successful coin toss.

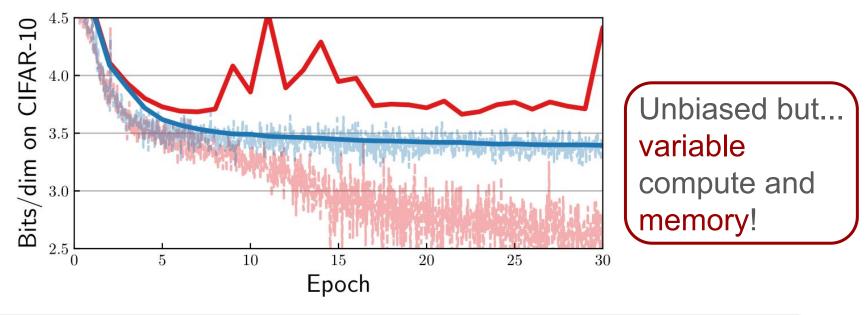
k-th term is weighted by prob. of seeing >= k tosses.

Computed in **finite** time with **prob. 1**!!

Residual Flow:

$$\log p(x) = \log p(f(x)) + \mathbb{E}_{n,v} \left[\sum_{k=1}^{n} \frac{(-1)^{k+1}}{k} \frac{v^{T} [J_g(x)]^{k} v}{\mathbb{P}(N \ge k)} \right]$$

Decoupled Training Objective & Estimation Bias



--- i-ResNet (**Biased** Train Estimate) --- Residual Flow (**Unbiased** Train Estimate) --- Residual Flow (Actual Test Value)

Constant-Memory Backpropagation

Naive gradient computation:

$$\mathbb{E}_{n,v} \left[\sum_{k=1}^{n} \alpha_k \frac{\partial v^T [J_g(x)]^k v}{\partial \theta} \right] \qquad \text{1. Estimate}$$
 2. Differentiate

Alternative (Neumann series) gradient formulation:

$$\mathbb{E}_{n,v}\left[\left(\sum_{k=1}^{n}\alpha_k v^T [J_g(x)]^k\right) \frac{\partial J_g(x)v}{\partial \theta}\right] \qquad \text{ Differentiate 2. Estimate}$$

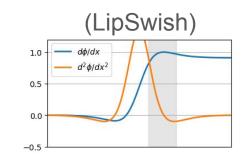
1. Analytically

Don't need to store random number of terms in memory!!

Density Estimation Experiments

Contribution Summary:

- Unbiased estimator of log-likelihood.
- Memory-efficient computation of log-likelihood.
- LipSwish activation function [not discussed in talk].

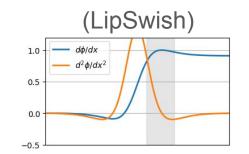


| Model | MNIST | CIFAR-10 | ImageNet 32 | ImageNet 64 | CelebA-HQ 256 |
|----------------------------------|-------|-------------|-------------|-------------|---------------|
| Real NVP (Dinh et al., 2017) | 1.06 | 3.49 | 4.28 | 3.98 | _ |
| Glow (Kingma and Dhariwal, 2018) | 1.05 | 3.35 | 4.09 | 3.81 | 1.03 |
| FFJORD (Grathwohl et al., 2019) | 0.99 | 3.40 | | | |
| Flow++ (Ho et al., 2019) | _ | 3.29 (3.09) | — (3.86) | — (3.69) | |
| i-ResNet (Behrmann et al., 2019) | 1.05 | 3.45 | _ | _ | _ |
| Residual Flow (Ours) | 0.970 | 3.280 | 4.010 | 3.757 | 0.992 |

Density Estimation Experiments

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| Training Setting | MNIST | CIFAR-10 | CIFAR-10 [†] |
|---|-------|----------|-----------------------|
| $\overline{i-ResNet} + ELU$ | 1.05 | 3.45 | 3.66~4.78 |
| ${\sf Residual\ Flow\ +\ ELU}$ | 1.00 | 3.40 | 3.32 |
| ${\sf Residual\ Flow} + {\sf LipSwish}$ | 0.97 | 3.39 | 3.28 |

Table: Ablation results. †Larger network.

Qualitative Samples

CelebA: Data Residual Flow

| CelebA: | Data | CelebA: |

CIFAR10:





| Model | CIFAR10 FID |
|---------------|-------------|
| PixelCNN* | 65.93 |
| PixelIQN* | 49.46 |
| i-ResNet | 65.01 |
| Residual Flow | 46.37 |
| DCGAN* | 37.11 |
| WGAN-GP* | 36.40 |
| | |

Qualitative Samples

<u>CelebA:</u> Data Residual Flow





CelebA-HQ 256x256:



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Thanks for Listening!

Code and pretrained models: https://github.com/rtqichen/residual-flows





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