Improved Autoregressive Modeling with Distribution Smoothing

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Let $\{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$ — D-dimensional i.i.d samples from a continuous data distribution $p_{\text{data}}(\boldsymbol{x})$

Property

An autoregressive model decomposes a joint distribution into univariate conditionals [2]:

$$p(\boldsymbol{x}) = \prod_{i=1}^{D} p\left(x_i \mid \boldsymbol{x}_{<i}\right)$$

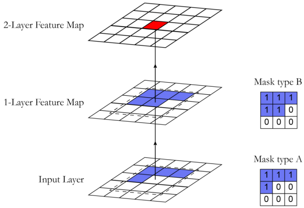
Goal

Find θ — parameters of the model such that $p_\theta(\boldsymbol{x}) \approx p_{\text{data}}(\boldsymbol{x})$

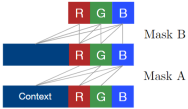
A commonly used approach for density estimation is maximum likelihood estimation (MLE), i.e., by maximizing

$$L(\theta) \triangleq \frac{1}{N} \sum_{i=1}^{N} \log p_\theta\left(\boldsymbol{x}_i\right)$$

PixelCNN [3]



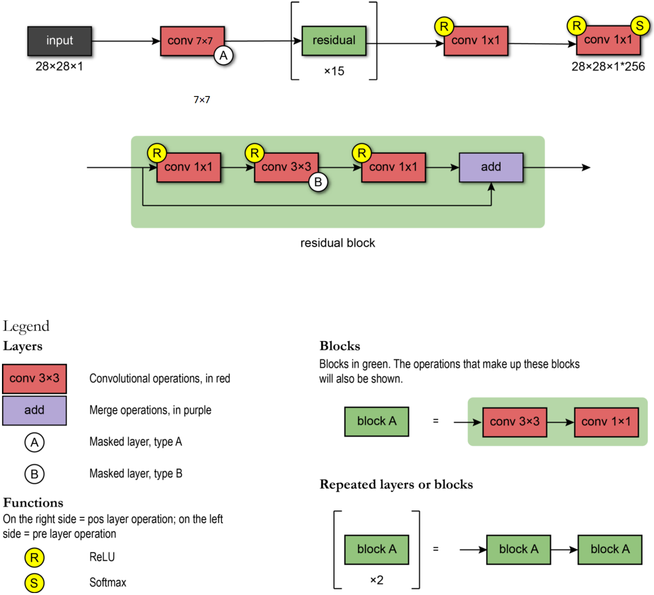
Masking 1



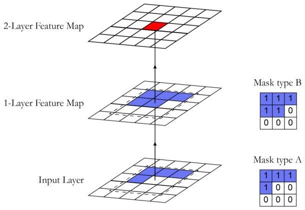
Masking 2

Image source

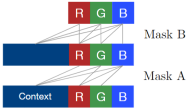
PixelCNN [3]



Architecture of the PixelCNN

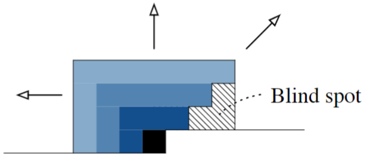


Masking 1

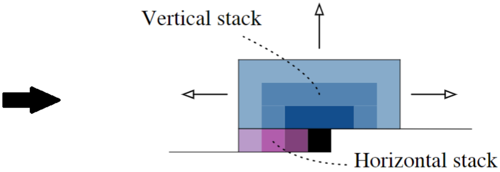


Masking 2

Gated PixelCNN [4]

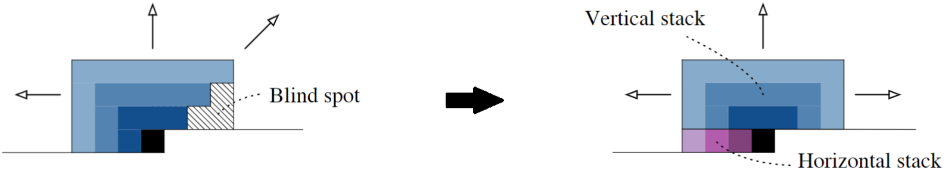


Problem

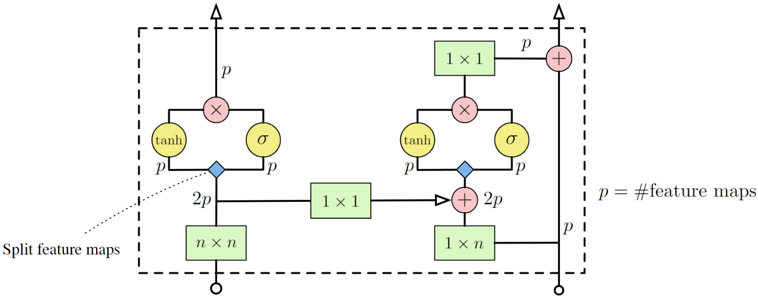


Solution

Gated PixelCNN [4]



Problem Solution



A single layer in the Gated PixelCNN architecture

PixelCNN++ [5]

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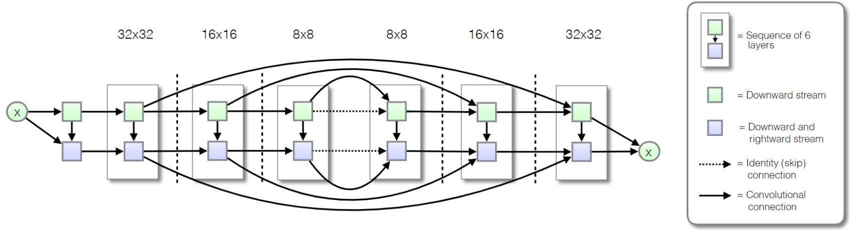

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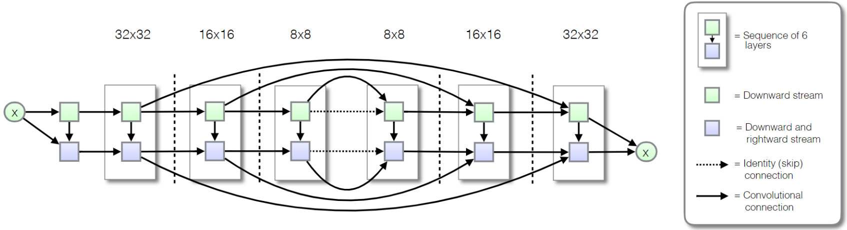

- adding short-cut connections

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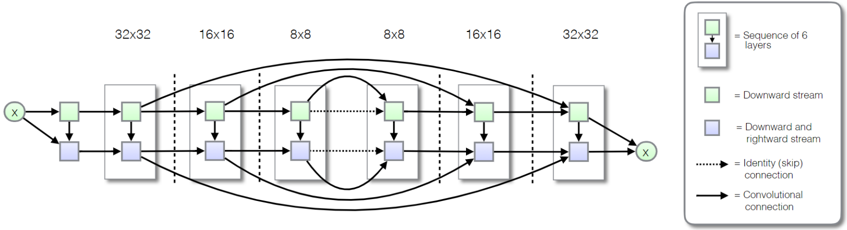
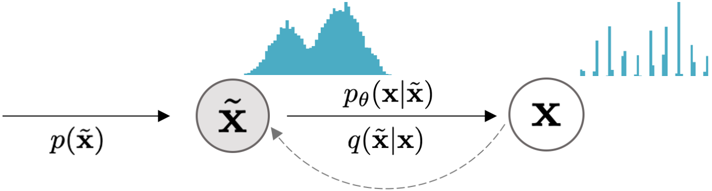


- adding short-cut connections
- regularization using dropout

For complete details see here

General idea



Overview of the method
($\tilde{x}$ — the smoothed data, $q(\tilde{x} \mid x)$ — the smoothing distribution) [1]

Problem 1: Manifold hypothesis

Many real world data distributions (e.g.natural images) **may lie in the vicinity of a low-dimensional manifold** and can often **have complicated densities with sharp transitions** (i.e. high Lipschitz constants) that are difficult to model.

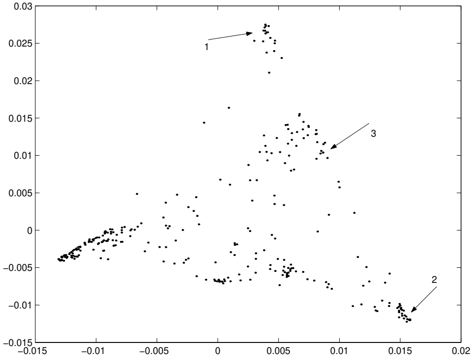


Figure (a): The 300 most frequent words of the Brown corpus represented in the spectral domain.

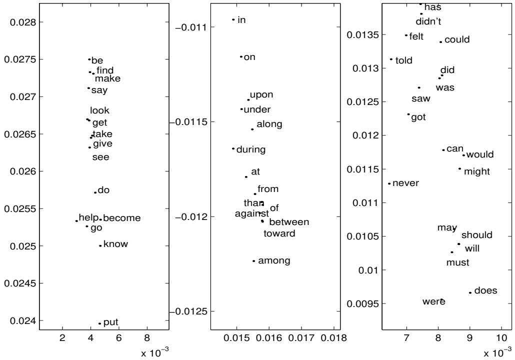
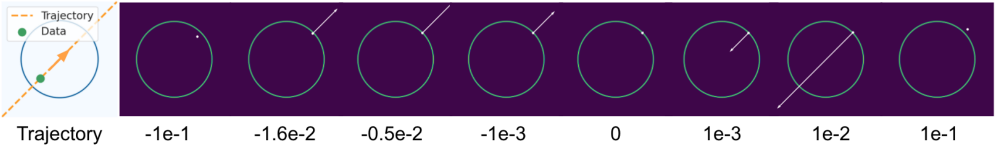


Figure (b): Fragments labeled by arrows: (left) infinitives of verbs, (middle) prepositions, and (right) mostly modal and auxiliary verbs.

Image source: (Belkin M., Niyogi P., 2003)

Problem 1: Manifold hypothesis



Ring distribution (almost a unit circle) formed by rotating the 1-d Gaussian distribution $\mathcal{N}\left(1, 0.01^2\right)$ around the origin. The data location for each figure is $(\sqrt{0.5}+c, \sqrt{0.5}+c)$, where c is the number below each figure and $(\sqrt{0.5}, \sqrt{0.5})$ is the upper right intersection of the trajectory with the unit circle. [1]

Problem 2: Compounding errors

$$p(\boldsymbol{x}) = \prod_{i=1}^{D} p\left(x_i \mid \boldsymbol{x}_{<i}\right)$$

Compounding errors **comes from the inaccurate approximation of the conditional distributions.**

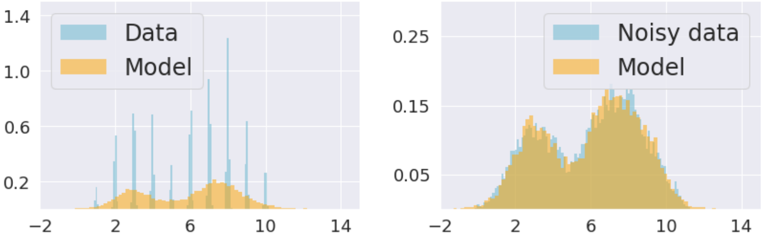
The reasons for this may be:

- Curse of dimensionality + very limited amount of training data (in some cases)
- The current state is based on the values of the previous states
- Adversarial attacks

Theorem 1 Let:

1. $p(x)$ — a continuous 1-d distribution that is supported on $\boldsymbol{R}$
2. $q(\tilde{x} \mid x)$ — 1-d distribution that is:
   - symmetric (i.e. $q(\tilde{x} \mid x) = q(x \mid \tilde{x})$)
   - stationary (i.e. translation invariant)
   - $\lim_{x \to \infty} p(x) q(x \mid \tilde{x}) = 0$ for any given $\tilde{x}$

Then: $\mathrm{Lip}(q(\tilde{x})) \leq \mathrm{Lip}\left(p_{\text{data}}\ (x)\right)$,
where $q(\tilde{x}) \triangleq \int q(\tilde{x} \mid x) p(x) dx$ and $\mathrm{Lip}(\cdot)$ denotes the Lipschitz constant of the given $1 - d$ function.



(a) Data (b) Smoothed data

Illustration of Theorem 1 [1]

Proposition 1 (Informal) Let:

1. $q(\tilde{\boldsymbol{x}} \mid \boldsymbol{x})$ is such that:
   - symmetric
   - stationary
   - has small variance
   - has negligible higher order moments (i.e. very small)

Then:

$$\boldsymbol{E}_{p_{\text{data}}(\boldsymbol{x})} \boldsymbol{E}_{q(\tilde{\boldsymbol{x}}|\boldsymbol{x})} [\log p_\theta(\tilde{\boldsymbol{x}})] \approx \boldsymbol{E}_{p_{\text{data}}(\boldsymbol{x})} \left[\log p_\theta(\boldsymbol{x}) + \frac{\eta}{2} \sum_i \frac{\partial^2 \log p_\theta}{\partial x_i^2} \right]$$

for some constant η.

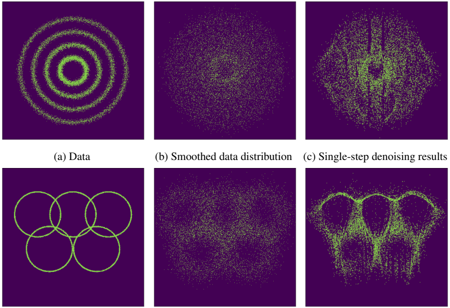
Since the samples from p_{data} should be close to a local maximum of the model, this encourages the second order gradients computed at a data point $\boldsymbol{x}$ to become closer to zero (if it were positive then $\boldsymbol{x}$ will not be a local maximum), creating a smoothing effect.

Introducing 2^{nd} distribution: $p_\theta(x \mid \tilde{x})$

Case 1 $q(\tilde{\boldsymbol{x}} \mid \boldsymbol{x}) = \mathcal{N}\left(\tilde{\boldsymbol{x}} \mid \boldsymbol{x}, \sigma^2 I\right)$ and σ is small

Single-step denoising [6]

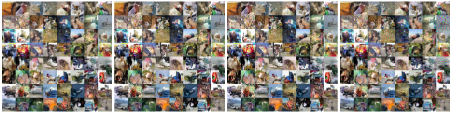
$$\overline{\boldsymbol{x}} = \tilde{\boldsymbol{x}} + \sigma^2 \nabla_{\tilde{x}} \log p_\theta(\tilde{\boldsymbol{x}})$$



(a) Data (b) Smoothed data distribution (c) Single-step denoising results

(d) Data (e) Smoothed data distribution (f) Single-step denoising results

Example of "single-step denoising"



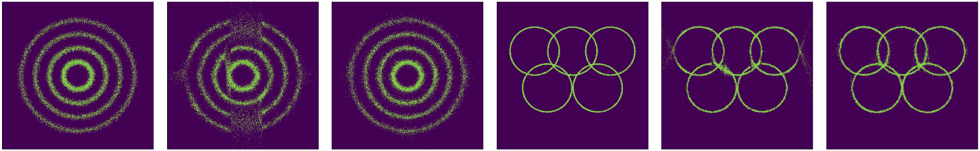
(a) $\sigma = 0$ (Original) (b) $\sigma = 0.01$ (c) $\sigma = 0.05$ (d) $\sigma = 0.1$

"Single-step denoising" on PixelCNN++ trained on unsmoothed data

Case 2 General case

Maximizing an evidence lower bound (ELBO)[1]

$$\log p_\theta(x) \geq \mathbb{E}_{p_{\mathbf{data}}(x)}\left[\mathbb{E}_{q(\tilde{x}|x)}[\log p_\theta(\tilde{x})] - \mathbb{E}_{q(\tilde{x}|x)}[\log q(\tilde{x} \mid x)] + \mathbb{E}_{q(\tilde{x}|x)}[\log p_\theta(x \mid \tilde{x})]\right]$$



(a) Rings (b) MADE (6) (c) Ours (3) (d) Olympics (e) MADE (6) (f) Ours (3)

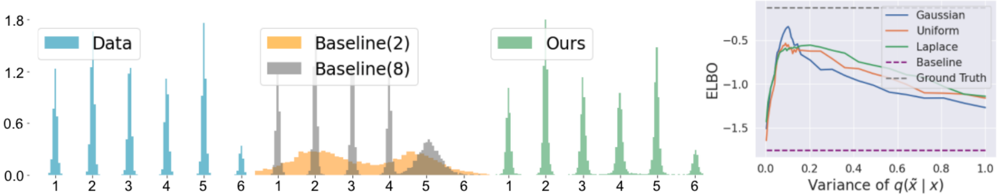
We use a MADE model with comparable number of parameters for both our method and the baseline

Dataset	RealNVP	CIF-RealNVP	MADE (3 mixtures)	MADE (6 mixtures)	Ours (3 mixtures)
Rings	2.81	2.81	3.26	2.81	**2.71**
Olympics	1.80	1.74	1.27	**0.80**	**0.80**

Negative log-likelihoods on 2-d synthetic datasets (lower is better))

[1] Formula derivation

Choosing the smoothing distribution



Density estimation on 1-d synthetic dataset. In the second figure, the digit in the paren-thesis denotes the number of mixture components used in the baseline mixture of logistics model.

For each type of distribution, we perform a grid search to find the optimal variance. Since our approach requires the modeling of both $p_\theta(\tilde{\boldsymbol{x}})$ and $p_\theta(\boldsymbol{x} \mid \tilde{\boldsymbol{x}})$, we stack $\tilde{\boldsymbol{x}}$ and $\boldsymbol{x}$ together, and
use a MADE model [7] with a mixture of two logistic components to parameterize $p_\theta(\tilde{\boldsymbol{x}})$ and $p_\theta(\boldsymbol{x} \mid \tilde{\boldsymbol{x}})$ at the same time. For the baseline model, we train a mixture of logistics model directly on $p_{\text{data}}(\boldsymbol{x})$.

Column 1 Column 2 Column 3 Column 4

From left to right: **Column 1**: samples from $p_\theta(\tilde{x})$. **Column 2**: "single-step denoising" samples from $p_\theta(\tilde{x})$. **Column 3** 3 : samples from $p_\theta(x \mid \tilde{x})$. **Column 4**: samples from the baseline PixelCNN++ model with parameters comparable to the sum of total parameters of $p_\theta(\tilde{x})$ and $p_\theta(x \mid \tilde{x})$.

Model	Inception ↑	FID ↓	BPD ↓
PixelCNN (Oord et al., 2016b)	4.60	65.93	**3.14**
PixelIQN (Ostrovski et al., 2018)	5.29	49.46	-
EBM (Du & Mordatch, 2019)	6.02	40.58	-
i-ResNet (Behrmann et al., 2019)	-	65.01	3.45
MADE (Germain et al., 2015)	-	-	5.67
Glow (Kingma & Dhariwal, 2018)	-	46.90	3.35
Single-step (Ours)	$7.50 \pm .08$	57.53	-
Two-step (Ours)	$\mathbf{7.84} \pm .07$	**29.83**	≤ 3.53

Trained on unconditional CIFAR-10. Inception (higher is better) and FID scores (lower is better). "Single-step" samples are generated solely by $p_\theta(\tilde{\boldsymbol{x}})$. "Two-step" samples are generated by drawing samples from $p_\theta(\tilde{\boldsymbol{x}})$ and then "denoised" by $p_\theta(\boldsymbol{x} \mid \tilde{\boldsymbol{x}})$.

We use PixelCNN++ (Salimans et al., 2017) as the model architecture for both $p_\theta(\tilde{\boldsymbol{x}})$ and $p_\theta(\boldsymbol{x} \mid \tilde{\boldsymbol{x}})$.

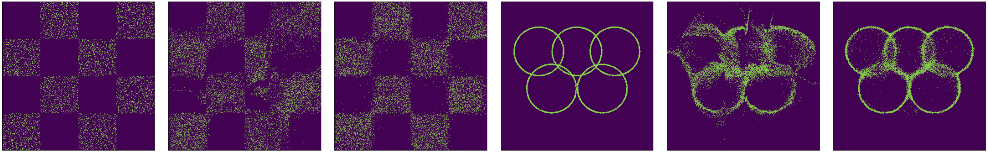
(a) CIFAR10 inpainting (b) CelebA inpainting

Inpainting results from our two-step method

(a) Noisy MNIST (b) MNIST denoising (c) Noisy CIFAR10 (d) CIFAR10 denoising

Denoising with $p_\theta(x \mid \tilde{x})$

Normalizing flows [8]



(a) Data (b) RealNVP (c) Ours (d) Data (e) RealNVP (f) Ours

We compare the RealNVP model trained with randomize smoothing, where we use $p_\theta(\boldsymbol{x} \mid \tilde{\boldsymbol{x}})$ (also a RealNVP) to revert the smoothing process, with a RealNVP trained with the original method but with comparable number of parameters.

Model/Dataset	checkerboard	Olympics
Original	3.72	1.80
Ours	**3.64**	**1.32**

NLL on the datasets. Distribution are modeled as RealNVP

[1] Improved autoregressive modeling with distribution smoothing.
https://openreview.net/pdf?id=rJA5Pz7lHKb, 2021.

[2] Tim Salimans, Andrej Karpathy, Xi Chen, and Diederik P Kingma.
Pixelcnn++: Improving the pixelcnn with discretized logistic mixture likelihood and other modifications.
arXiv:1701.05517, 2017.

[3] A aron van den Oord, Nal Kalchbrennern, and Koray Kavukcuoglu.
Pixel recurrent neural networks.
https://arxiv.org/pdf/1601.06759.pdf, 2016.

[4] A aron van den Oord, Nal Kalchbrennern, Koray Kavukcuoglu et al.
Conditional image generation with pixelcnn decoders.
https://arxiv.org/pdf/1606.05328.pdf, 2016.

[5] Tim Salimansn, Andrej Karpathyn, Xi Chenn, Diederik P. Kingmas.
Pixelcnn++: Improving the pixelcnn with discretized logistic mixture likelihood and other modifications.
https://arxiv.org/pdf/1701.05517.pdf, 2017.

[6] Saeed Saremi, Arash Mehrjou, Bernhard Sch olkop, and Aapo Hyv arinen.

Deep energy estimatornetworks.
arXiv:1805.08306, 2018.

[7] Mathieu Germain, Karol Gregor, Iain Murray, and Hugo Larochelleen.
Made: Masked autoencoder fordistribution estimation.
InInternational Conference on Machine Learning, pp. 881–889, 2015.

[8] Laurent Dinh, Jascha Sohl-Dickstein, and Samy Bengio.
Density estimation using real nvp.
arXiv:1605.08803, 2016.