Normalizing flows for discrete data

Emiel Hoogeboom, Jorn Peters, Rianne van den Berg* & Max Welling.







Integer discrete flows and lossless compression Emiel Hoogeboom, Jorn Peters, Rianne van den Berg, Max Welling

Normalizing flows

Quantized RV's

Images

Compression

Discrete Flows: Invertible Generative Models of Discrete Data

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Probable inputs map to shorter codes and improbable inputs are mapped to longer codes.

Minimum code length for a symbol x is close to

$$-\log D(x)$$

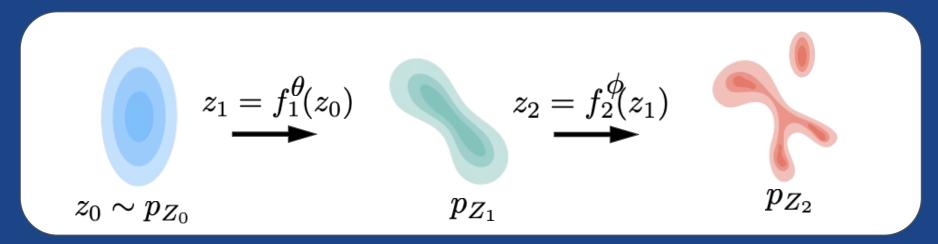
a_i	$c(a_i)$	p_i	$h(p_i)$	l_i
a	0	$1/_{2}$	1.0	1
b	10	$1/_{4}$	2.0	2
С	110	$1/_{8}$	3.0	3
d	111	$1/_{8}$	3.0	3

Minimum expected code length:

$$\mathbb{E}_{x \sim D}[|c(x)|] \ge \mathbb{E}_{x \sim \mathcal{D}}[-\log p_{\theta}(x)] \ge \mathcal{H}(\mathcal{D}) = \mathbb{E}_{x \sim \mathcal{D}}[-\log \mathcal{D}(x)]$$

NORMALIZING FLOWS: CONTINUOUS RANDOM VARIABLES

Idea: Apply a sequence of invertible transformations to a random variable.



$$p(z_1|z_0) = \delta(z_1 - f_1(z_0))$$

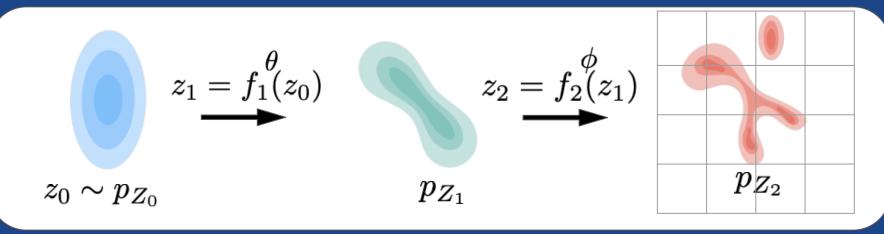
$$p(z_1) = \int p(z_1|z_0) p(z_0) \; \mathrm{d}z_0 = p(f_1^{-1}(z_1)) \left| rac{\partial z_1}{\partial z_0}
ight|^{-1}$$

NAIVE LOSSLESS COMPRESSION FOR NORMALIZING FLOWS

Entropy encoders require as input:

- Input in the form of symbols
- The distribution of the symbols

Quantize latent distribution



Leads to reconstruction error \rightarrow needs to be encoded too for lossless compression.

NORMALIZING FLOWS FOR INTEGER VALUED DATA

Problem formulation: Define invertible

$$f_{ heta}: \mathbb{Z}^d \mapsto \mathbb{Z}^d$$

Simplest solution: Take RealNVP and make suitable for integers.



$$z = egin{bmatrix} z_1 \ z_2 \end{bmatrix} \leftarrow egin{bmatrix} x_1 \ s^{ heta}(x_1) \odot x_2 + t^{ heta}(x_1) \end{bmatrix}$$



$$x = egin{bmatrix} x_1 \ x_2 \end{bmatrix} \leftarrow egin{bmatrix} z_1 \ (z_2 - t^{ heta}(z_1)) igorims s^{ heta}(z_1) \end{bmatrix}$$



NORMALIZING FLOWS FOR INTEGER VALUED DATA

Problem formulation: Define invertible

$$f_{ heta}: \mathbb{Z}^d \mapsto \mathbb{Z}^d$$

Simplest solution: Take RealNVP and make suitable for integers.



$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ x_2 + t^{\theta}(x_1) \end{bmatrix}$$



$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leftarrow \begin{bmatrix} z_1 \\ z_2 - t^{\theta}(z_1) \end{bmatrix}$$



NORMALIZING FLOWS FOR INTEGER VALUED DATA

Problem formulation: Define invertible

$$f_{ heta}: \mathbb{Z}^d \mapsto \mathbb{Z}^d$$

Simplest solution: Take RealNVP and make suitable for integers.



$$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ x_2 + [t^{\theta}(x_1)] \end{bmatrix}$$



Use straight-through estimator to backprop gradients



$$x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \leftarrow \begin{bmatrix} z_1 \\ z_2 - \lfloor t^{\theta}(z_1) \rfloor \end{bmatrix}$$



OBTAINING THE DENSITY

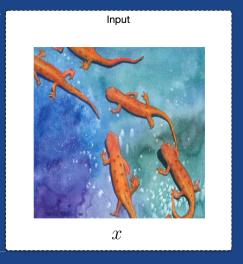
Continuous random variables:

$$p(x) = \int p(x|z)p(z) dz = \int \delta(x - f(z))p(z) dz = p(f^{-1}(x)) \left| \frac{\partial x}{\partial z} \right|^{-1}$$

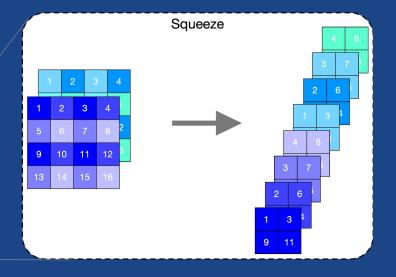
Discrete random variables:

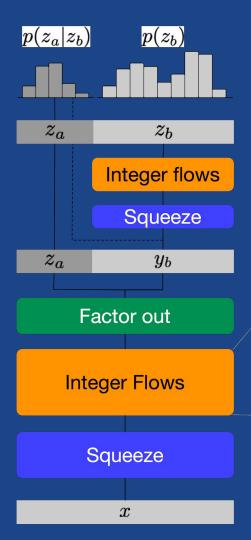
$$p(x) = \sum_{z} p(x|z)p(z) = \sum_{z} \delta_{z,f^{-1}(x)}p(z) = p(f^{-1}(x))$$

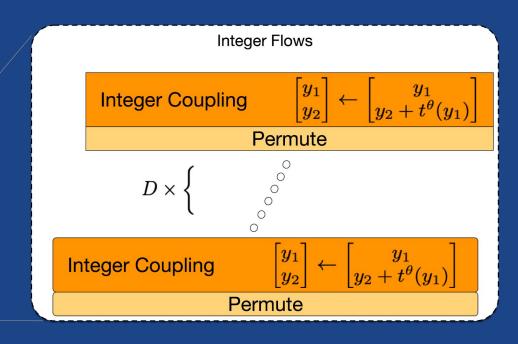
$p(z_a|z_b)$ $p(z_b)$ z_a z_b Integer flows Squeeze z_a y_b Factor out **Integer Flows** Squeeze



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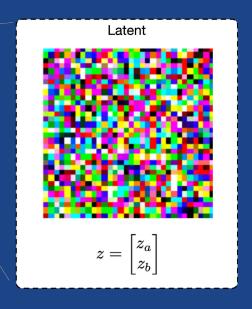




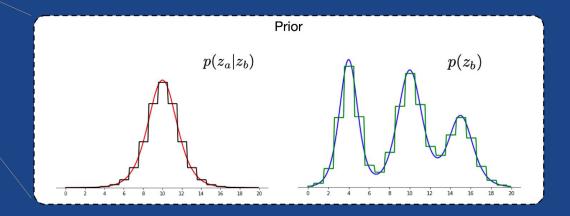


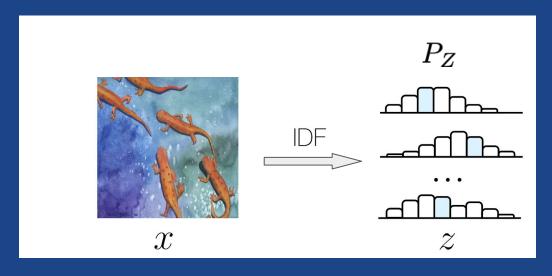
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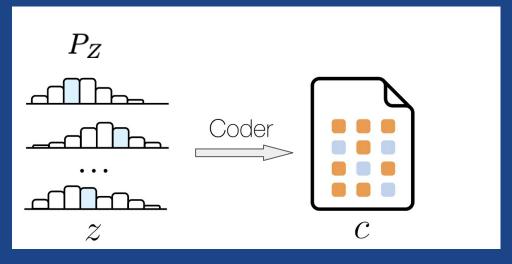


$p(z_a|z_b)$ $p(z_b)$ z_a z_b Integer flows Squeeze z_a y_b Factor out **Integer Flows** Squeeze \boldsymbol{x}





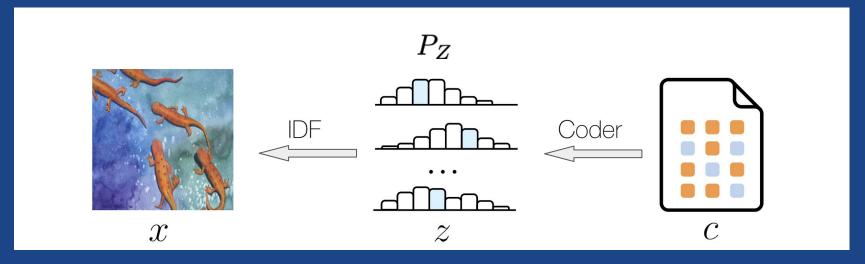






High-probability $z \rightarrow Short code$

Low-probability $z \rightarrow Long code$





High-probability $z \rightarrow Short code$

Low-probability $z \rightarrow Long code$

RESULTS

Table 1: Compression performance of IDFs on CIFAR10, ImageNet32 and ImageNet64 in bits per dimension, and compression rate (shown in parentheses). The Bit-Swap results are retrieved from [23]. The column marked IDF[†] denotes an IDF trained on ImageNet32 and evaluated on the other datasets.

Dataset	IDF	${ m IDF}^{\dagger}$	Bit-Swap	FLIF [34]	PNG	JPEG2000
CIFAR10	3.34 (2.40×)	3.60 (2.22×)	$3.82(2.09\times)$	4.37 (1.83×)	5.89 (1.36×)	5.20 (1.54×)
ImageNet32	$4.18 (1.91 \times)$	$4.18 (1.91 \times)$	$4.50 (1.78 \times)$	$5.09(1.57\times)$	$6.42 (1.25 \times)$	$6.48 (1.23 \times)$
ImageNet64	$3.90 (2.05 \times)$	$3.94 (2.03 \times)$	_	$4.55 (1.76 \times)$	$5.74 (1.39 \times)$	$5.10 (1.56 \times)$

Table 3: Generative modeling performance of IDFs and comparable flow-based methods in bits per dimension (negative log₂-likelihood).

Dataset	IDF	Continuous	RealNVP	Glow	Flow++
CIFAR10	3.32	3.31	3.49	3.35	3.08
ImageNet32	4.16	4.13	4.28	4.09	3.86
ImageNet64	3.90	3.85	3.98	3.81	3.69

MEDICAL DATA: HISTOLOGY DATA

Resolution: 2000 x 2000 pixels

IDF trained on 80 x 80 px patches

patch-wise compression (each patch is considered independent)

Sampled patches: 80 x 80 pixels

Dataset	IDF	JP2-WSI	FLIF [34]	JPEG2000
Histology	2.42 (3.19×)	3.04 (2.63×)	4.00 (2.00×)	4.26 (1.88×)

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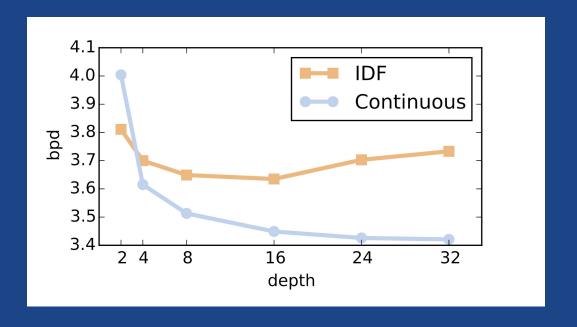
$p(z_b)$ $p(z_a|z_b)$ z_b Integer flows Squeeze z_a y_b Factor out **Integer Flows** Squeeze \boldsymbol{x}



DIRECTIONS FOR IMPROVEMENT

Problem: discrete flows don't always benefit from more flow layers.

Hypothesis: gradient bias in straight through estimator is the cause.



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DISCRETE FLOWS

Discrete but not ordinal data with finite number of classes

Focus: generative modeling for text (character level)

Architecture variants:

- Autoregressive layers
- Coupling layer/bi-partite layers

INTEGER DISCRETE FLOWS

Ordinal discrete data with possibly infinite number of classes

Focus: lossless source compression for images

Architecture variants:

Coupling layer/bi-partite layers

DISCRETE FLOWS

Bipartite bijector

$$\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \leftarrow \begin{bmatrix} x_1 \\ [s(x_1) \odot x_2 + t(x_1)] \bmod K \end{bmatrix}$$

Autoregressive bijector

$$z_d = [s_d(x_{1:d-1}) \odot x_d + t_d(x_{1:d-1})] \mod K$$

$$t: \{0, 1, ..., K-1\} \mapsto \{0, 1, ..., K-1\}$$

 $s: \{0, 1, ..., K-1\} \mapsto \{1, ..., K-1\}$

Only invertible if s and K are coprime

$$t_d = \text{one_hot}(\arg\max(\theta_d))$$

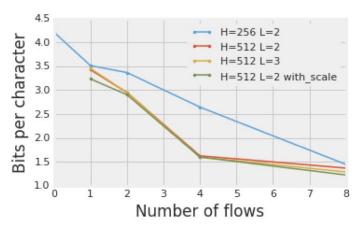
$$\frac{\partial t_d}{\partial \theta_d} \approx \frac{\partial}{\partial \theta_d} \operatorname{softmax} \left(\frac{\theta_d}{\tau} \right)$$

RESULTS

	Test NLL (bpc)	Generation
3-layer LSTM (Merity et al., 2018)	1.18 ³	3.8 min
Ziegler and Rush (2019) (AF/SCF)	1.46	-
Ziegler and Rush (2019) (IAF/SCF)	1.63	=
Bipartite flow	1.38	0.17 sec

Table 3: Character-level language modeling results on Penn Tree Bank.

RESULTS



	bpc	Gen.
LSTM (Coojimans+2016)	1.43	19.8s
64-layer Transformer (Al-Rfou+2018)	1.13	35.5s
Bipartite flow (4 flows, w/ σ)	1.60	0.15s
Bipartite flow (8 flows, w/o σ)	1.29	0.16s
Bipartite flow (8 flows, w/ σ)	1.23	0.16s

Figure 3: Character-level language modeling results on text8. The test bits per character decreases as the number of flows increases. More hidden units H and layers L in the Transformer per flow, and applying a scale transformation instead of only location, also improves performance.

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