Diffusion Models

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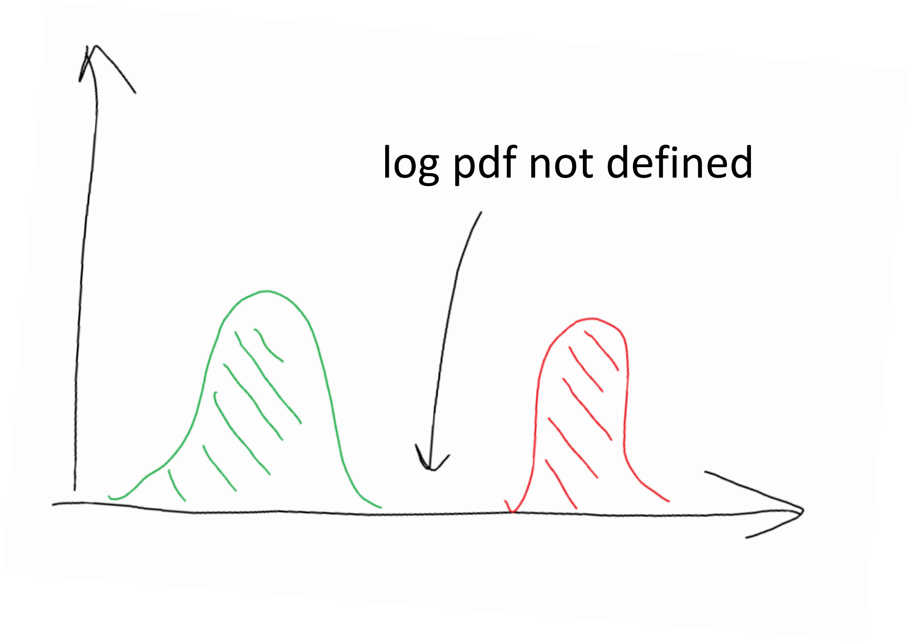
As score matching models

- Score matching estimates the gradient of log prob in data space and generates samples by some variation of gradient ascent.
- It is good but has some downsides.
- Extra backpropagations to estimate trace of score gradient.
- Manifold hypothesis.
- Low data density regions have bad score estimates.
- It’s hard to transition between disconnected supports.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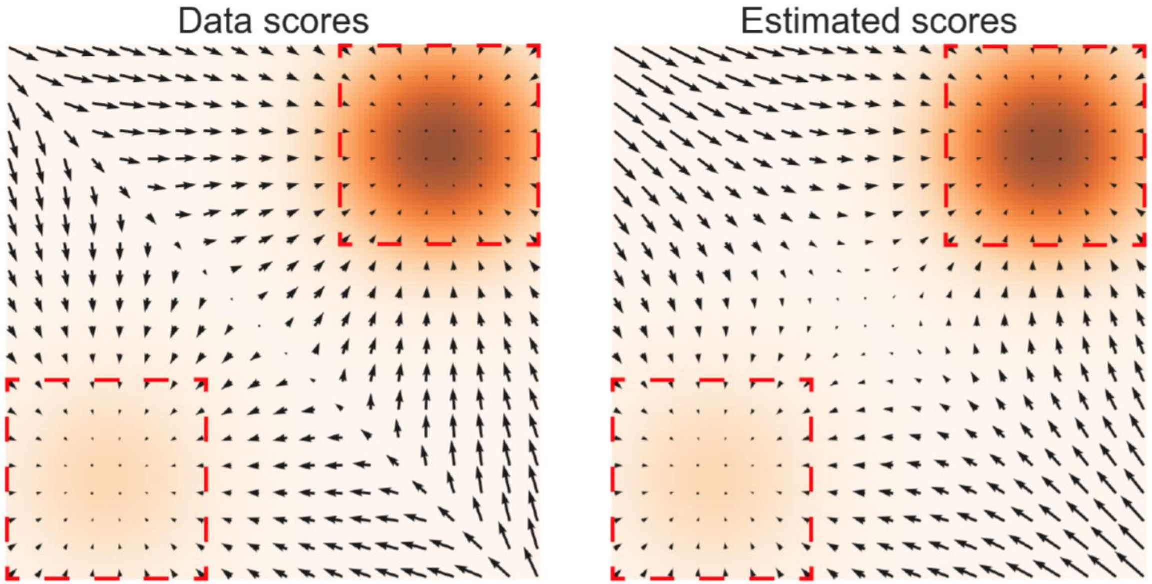

Data scores
Estimated scores

As score matching models

- Let’s perturb data with various levels of Gaussian noise and train a noise conditional network to estimate score.
- High noise fills low density regions and gives a common support.
- Low noise is almost indistinguishable from true data.
- Sample using annealed Langevin dynamics (ALS).
- Our loss becomes:

$$\ell(\boldsymbol{\theta};\sigma) \triangleq \frac{1}{2}\mathbb{E}_{p_{\text{data}}(\mathbf{x})}\mathbb{E}_{\tilde{\mathbf{x}}\sim\mathcal{N}(\mathbf{x},\sigma^2 I)}\left[\left\|\mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}},\sigma)+\frac{\tilde{\mathbf{x}}-\mathbf{x}}{\sigma^2}\right\|_2^2\right] \qquad \mathcal{L}(\boldsymbol{\theta};\{\sigma_i\}_{i=1}^L) \triangleq \frac{1}{L}\sum_{i=1}^{L}\lambda(\sigma_i)\ell(\boldsymbol{\theta};\sigma_i)$$

Algorithm 1 Annealed Langevin dynamics.

Require: $\{\sigma_i\}_{i=1}^{L}, \epsilon, T.$

1: Initialize $\tilde{\mathbf{x}}_0$

2: **for** $i \leftarrow 1$ to L **do**

3: $\quad \alpha_i \leftarrow \epsilon \cdot \sigma_i^2/\sigma_L^2$ $\quad \triangleright$ α_i is the step size.

4: $\quad$ **for** $t \leftarrow 1$ to T **do**

5: $\quad\quad$ Draw $\mathbf{z}_t \sim \mathcal{N}(0, I)$

6: $\quad\quad$ $\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \dfrac{\alpha_i}{2}\mathbf{s}_{\boldsymbol{\theta}}(\tilde{\mathbf{x}}_{t-1}, \sigma_i) + \sqrt{\alpha_i}\,\mathbf{z}_t$

7: $\quad$ **end for**

8: $\quad \tilde{\mathbf{x}}_0 \leftarrow \tilde{\mathbf{x}}_T$

9: **end for**

return $\tilde{\mathbf{x}}_T$

Too many hyperparameters

- How can we come up with good noise levels?
- What about sampling step size?
- And the number of steps?

Noise levels

- Smallest noise level has to be indistinguishable.
- Transition probabilities decay exponentially.
- Choose largest noise level at least as large as the maximum Euclidean distance between all pairs of training data.
- Samples have to cover high density regions of previous noise level.
- Choose a geometric progression with common ratio dependent on data dimensionality.

ALS parameters

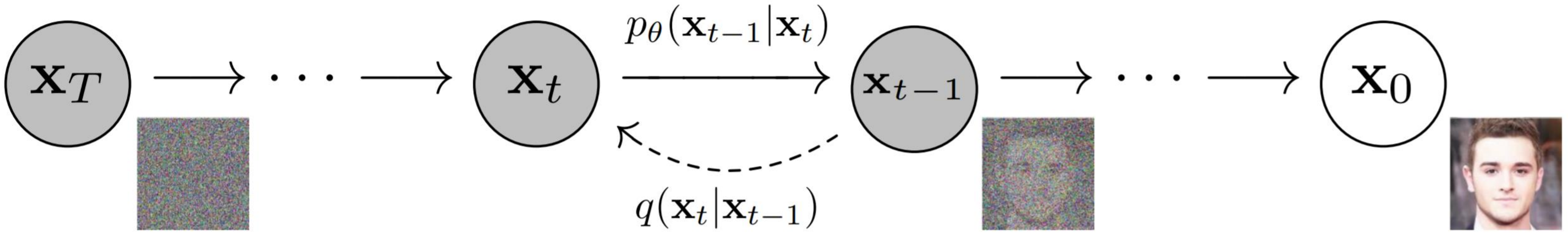
- We want sampling variance to be as close to noise level as possible.
- Can be computed analytically for one data point.
- Choose T as large as possible and optimize the step size making variance ratio as close to 1 as possible.

Other tricks

- Hard to condition on noise level (is it really?).
- Make an unconditional score estimation network and divide its output by noise std.
- Samples are empirically very unstable and exhibit artifacts such as common color shift.
- Apply EMA over model weights.

As nonequilibrium thermodynamics

- Let’s gradually perturb our data with small noise.
- Reverse diffusion process has the same functional form.
- We have to predict mean and variance.
- Train by maximizing variational lower bound.
- Generate by gradually denoising samples from stationary distribution.



$\mathbf{x}_T$
$\mathbf{x}_t$
$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$
$\mathbf{x}_{t-1}$
$q(\mathbf{x}_t|\mathbf{x}_{t-1})$
$\mathbf{x}_0$

$$L \geq \int d\mathbf{x}^{(0\cdots T)} q\left(\mathbf{x}^{(0\cdots T)}\right) \cdot$$
$$\log\left[p\left(\mathbf{x}^{(T)}\right) \prod_{t=1}^{T} \frac{p\left(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}\right)}{q\left(\mathbf{x}^{(t)}|\mathbf{x}^{(t-1)}\right)}\right]$$

$$K = -\sum_{t=2}^{T} \int d\mathbf{x}^{(0)} d\mathbf{x}^{(t)} q\left(\mathbf{x}^{(0)}, \mathbf{x}^{(t)}\right) \cdot$$
$$D_{KL}\left(q\left(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}, \mathbf{x}^{(0)}\right) \middle|\middle| p\left(\mathbf{x}^{(t-1)}|\mathbf{x}^{(t)}\right)\right)$$
$$+ H_q\left(\mathbf{X}^{(T)}|\mathbf{X}^{(0)}\right) - H_q\left(\mathbf{X}^{(1)}|\mathbf{X}^{(0)}\right) - H_p\left(\mathbf{X}^{(T)}\right).$$

As nonequilibrium thermodynamics

- We’re now working with Gaussian noise only.
- Let’s set variance to a time dependent constant.

Loss reparameterization

- Let's rewrite our loss.
- We can remove the factor between estimated noise difference norm to obtain a simplified objective.
- Score matching objective and variance lower bound maximization are very similar.

$$\mathbb{E}_{\mathbf{x}_0,\boldsymbol{\epsilon}}\left[\frac{\beta_t^2}{2\sigma_t^2\alpha_t(1-\bar{\alpha}_t)}\left\|\boldsymbol{\epsilon}-\boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0+\sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon},t)\right\|^2\right]$$

Algorithm 1 Training

repeat
  $\mathbf{x}_0 \sim q(\mathbf{x}_0)$
  $t \sim \mathrm{Uniform}(\{1, \dots, T\})$
  $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  Take gradient descent step on
  $$\nabla_\theta \left\| \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_\theta(\sqrt{\bar{\alpha}_t}\mathbf{x}_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}, t) \right\|^2$$
until converged

Algorithm 2 Sampling

$\mathbf{x}_T \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $t = T, \dots, 1$ **do**
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$ if $t > 1$, else $\mathbf{z} = \mathbf{0}$
  $\mathbf{x}_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(\mathbf{x}_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\boldsymbol{\epsilon}_\theta(\mathbf{x}_t, t)\right) + \sigma_t \mathbf{z}$
end for
return $\mathbf{x}_0$

How to obtain exact log likelihoods?

- Let's set the last term of reversed process to a discrete decoder.
- We can now estimate the conditional probability by calculating an integral.

$$p_\theta(\mathbf{x}_0|\mathbf{x}_1) = \prod_{i=1}^{D} \int_{\delta_-(x_0^i)}^{\delta_+(x_0^i)} \mathcal{N}(x; \mu_\theta^i(\mathbf{x}_1, 1), \sigma_1^2)\, dx$$

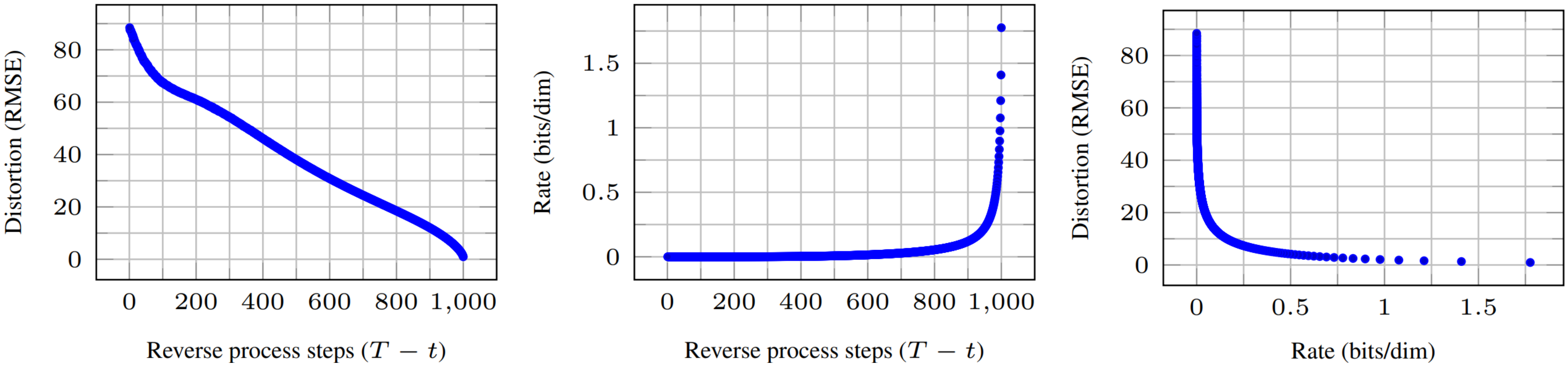
$$\delta_+(x) = \begin{cases} \infty & \text{if } x = 1 \\ x + \frac{1}{255} & \text{if } x < 1 \end{cases} \qquad \delta_-(x) = \begin{cases} -\infty & \text{if } x = -1 \\ x - \frac{1}{255} & \text{if } x > -1 \end{cases}$$

Different objectives

- Simplified objective makes low noise level loss relatively more important and improves sample quality.
- Predicting noise gives similar results to estimating mean of Gaussian.

Lossy compression

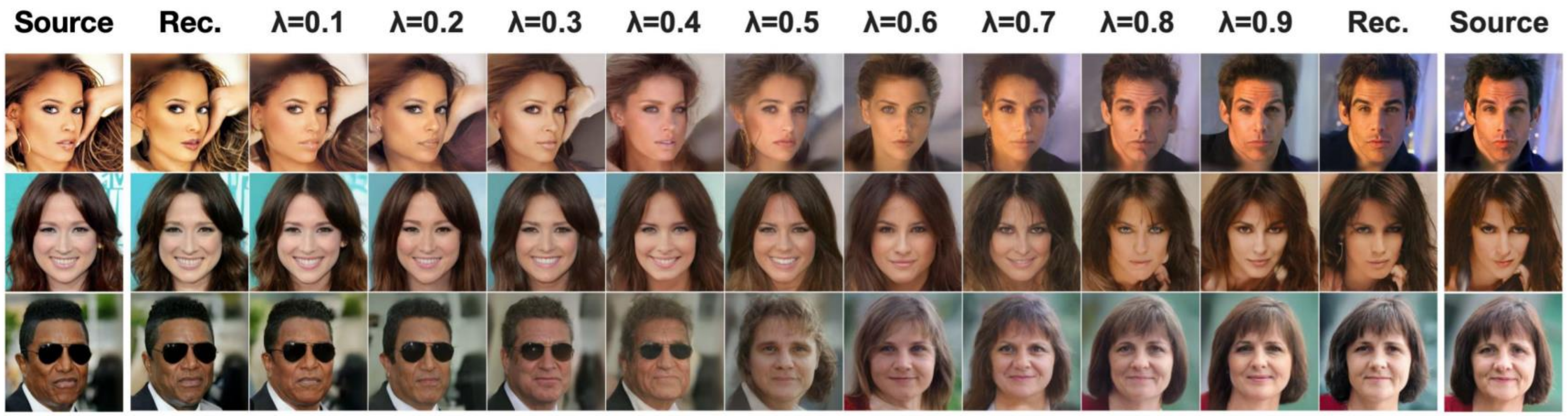
- KL divergence corresponds to rate (?).
- RMSE corresponds to distortion.
- Let’s plot them.
- Turns out that the majority of our codelength encodes impeccable details, which is not optimal.
- I’m not sure if I got this right.



Distortion (RMSE)
80
60
40
20
0
0
200
400
600
800
1,000
Reverse process steps $(T - t)$
Rate (bits/dim)
1.5
1
0.5
0
0
200
400
600
800
1,000
Reverse process steps $(T - t)$
Distortion (RMSE)
80
60
40
20
0
0
0.5
1
1.5
Rate (bits/dim)

Extra details

- Diffusion process that masks first T pixels corresponds to an autoregressive model.
- Interpolating in latent space works particularly well.

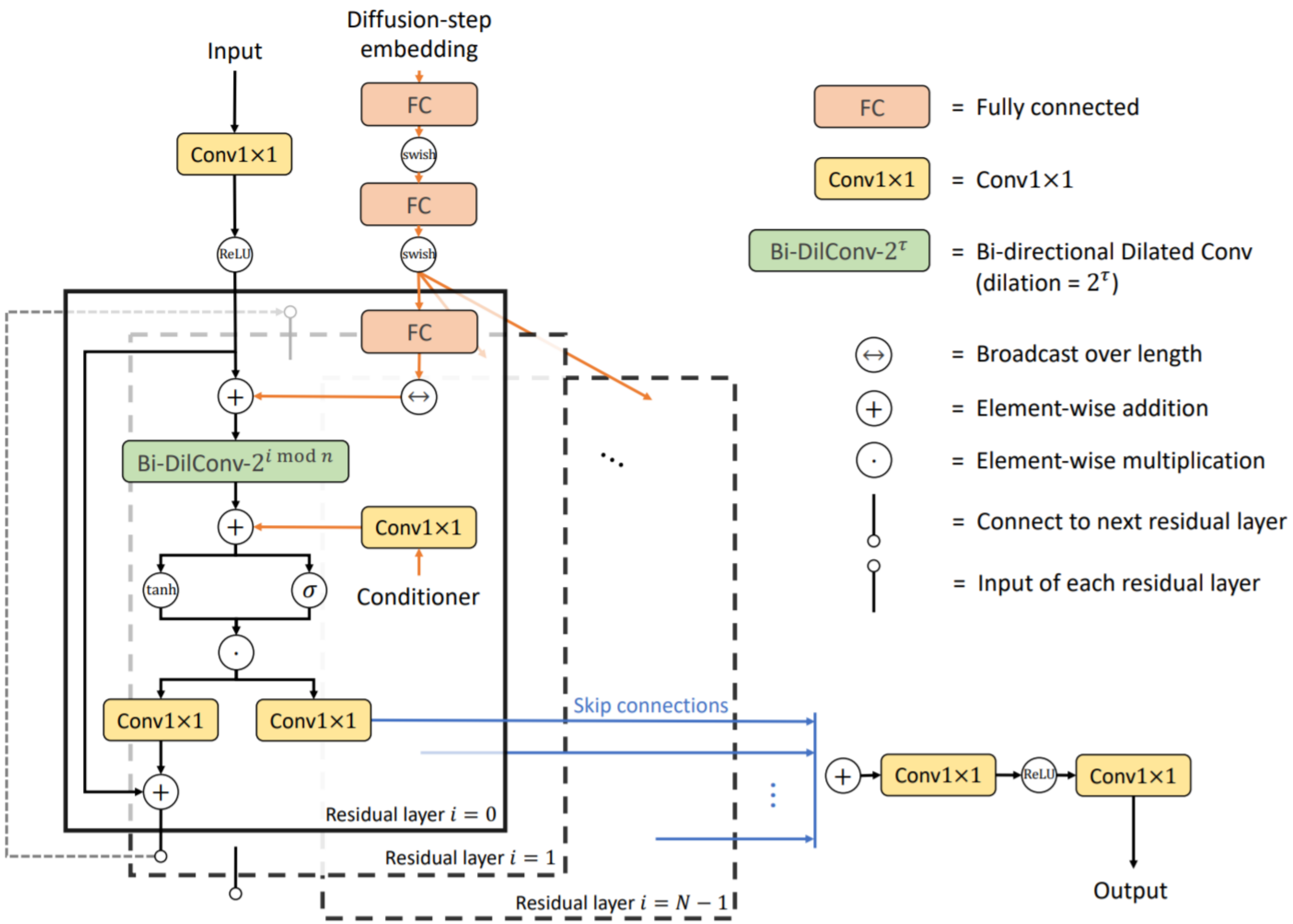


Advantages in audio generation

- Diffusion models avoid mode/posterior collapse.
- Non-autoregressive which means faster parallel synthesis.
- Very flexible architecture.
- Does not require auxiliary losses (e.g. Mel spectrogram loss).
- Provides intuitive speed/quality tradeoff by varying number of denoising steps.

DiffWave

- Bidirectional dilated convolutions.
- N residual layers divided into m blocks.
- Dilation is doubled at each layer within each block.
- Big receptive fields because of multiple denoising steps.
- Positional embeddings of timesteps from transformers.
- Let’s upsample local conditioning to the same length.
- We can then add both local and global conditioning as bias terms after dilated convolutions by using 1x1 conv.
- We can use faster noise schedules at inference to increase speed.



Input
Diffusion-step embedding
Conv1×1
FC
swish
FC
swish
ReLU
FC
Bi-DilConv-$2^{i \bmod n}$
Conv1×1
Conditioner
tanh
σ
Conv1×1
Conv1×1
Skip connections
Residual layer $i = 0$
Residual layer $i = 1$
Residual layer $i = N-1$
Conv1×1
ReLU
Conv1×1
Output
FC = Fully connected
Conv1×1 = Conv1×1
Bi-DilConv-2^{τ} = Bi-directional Dilated Conv (dilation = 2^{τ})
= Broadcast over length
= Element-wise addition
= Element-wise multiplication
= Connect to next residual layer
= Input of each residual layer

DiffWave results

- Performs well at neural vocoding.
- Better MOS than WaveNet at 6.91M vs 4.57M parameters.
- Real-time generation but still much slower than flow based models (1.1-5.6x vs 40+x).
- Completely destroys everybody at unconditional and class-conditional generation.
- Zero-shot speech denoising and latent space interpolation is also available.

Table 1: The model hyperparameters, model footprint, and 5-scale Mean Opinion Score (MOS) with 95% confidence intervals for WaveNet, ClariNet, WaveFlow, WaveGlow and the proposed DiffWave on the **neural vocoding** task. ↑ means the number is the higher the better, and ↓ means the number is the lower the better.

Model	T	T_{infer}	**layers**	**res. channels**	**#param(↓)**	**MOS(↑)**
WaveNet	—	—	30	128	4.57M	**4.43** $\pm$ 0.10
ClariNet	—	—	60	64	2.17M	4.27 $\pm$ 0.09
WaveGlow	—	—	96	256	87.88M	4.33 $\pm$ 0.12
WaveFlow	—	—	64	64	5.91M	4.30 $\pm$ 0.11
WaveFlow	—	—	64	128	22.25M	4.40 $\pm$ 0.07
DiffWave $_{\text{BASE}}$	20	20	30	64	2.64M	4.31 $\pm$ 0.09
DiffWave $_{\text{BASE}}$	40	40	30	64	2.64M	4.35 $\pm$ 0.10
DiffWave $_{\text{BASE}}$	50	50	30	64	2.64M	**4.38** $\pm$ 0.08
DiffWave $_{\text{LARGE}}$	200	200	30	128	6.91M	**4.44** $\pm$ 0.07
DiffWave $_{\text{BASE}}$ (Fast)	50	6	30	64	2.64M	*4.37* $\pm$ 0.07
DiffWave $_{\text{LARGE}}$ (Fast)	200	6	30	128	6.91M	*4.42* $\pm$ 0.09
Ground-truth	—	—	—	—	—	4.52 $\pm$ 0.06

Table 2: The automatic evaluation metrics (FID, IS, mIS, AM, and NDB$/K$), and 5-scale MOS with 95% confidence intervals for WaveNet, WaveGAN, and DiffWave on the **unconditional** generation task. $\uparrow$ means the number is the higher the better, and $\downarrow$ means the number is the lower the better.

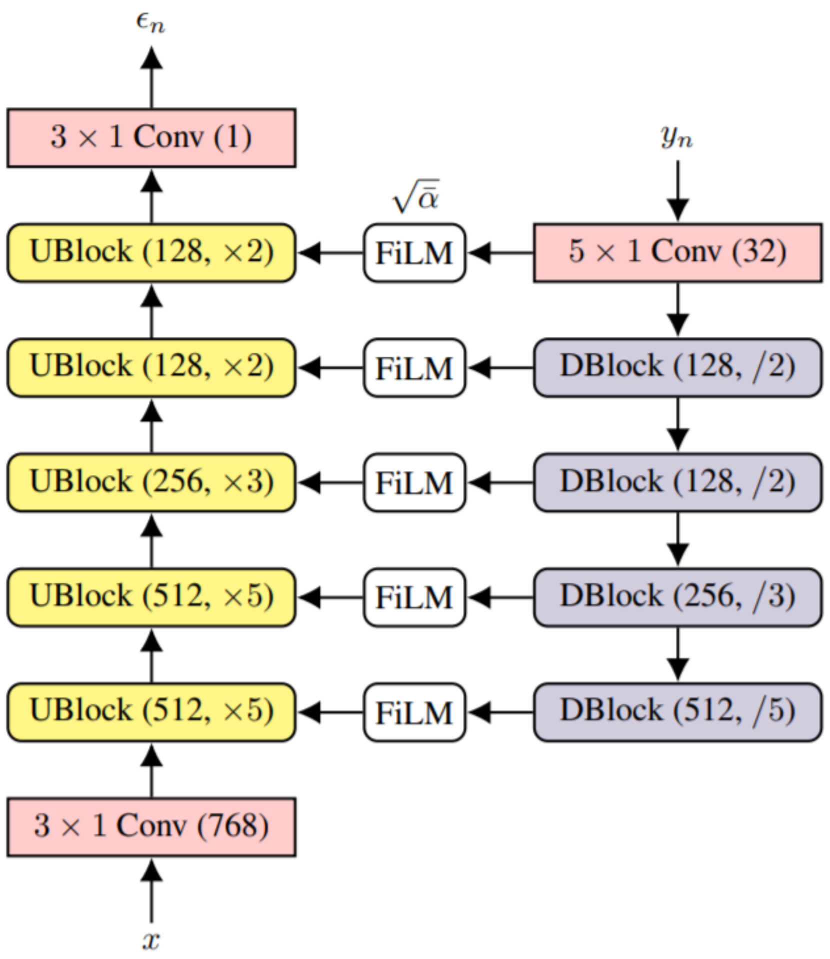
Model	**FID**($\downarrow$)	**IS**($\uparrow$)	**mIS**($\uparrow$)	**AM**($\downarrow$)	**NDB**$/K$($\downarrow$)	**MOS**($\uparrow$)
WaveNet-128	3.279	2.54	7.6	1.368	0.86	1.34 ± 0.29
WaveNet-256	2.947	2.84	10.0	1.260	0.86	1.43 ± 0.30
WaveGAN	1.349	4.53	36.6	0.796	0.78	2.03 ± 0.33
DiffWave	**1.287**	**5.30**	**59.4**	**0.636**	**0.74**	$\mathbf{3.39} \pm 0.32$
Trainset	0.000	8.48	281.4	0.164	0.00	—
Testset	0.011	8.47	275.2	0.166	0.10	3.72 ± 0.28

Table 3: The automatic evaluation metrics (Accuracy, FID-class, IS, mIS), and 5-scale MOS with 95% confidence intervals for WaveNet and DiffWave on the **class-conditional** generation task.

Model	**Accuracy**($\uparrow$)	**FID-class**($\downarrow$)	**IS**($\uparrow$)	**mIS**($\uparrow$)	**MOS**($\uparrow$)
WaveNet-128	56.20%	7.876±2.469	3.29	15.8	1.46 ± 0.30
WaveNet-256	60.70%	6.954±2.114	3.46	18.9	1.58 ± 0.36
DiffWave	91.20%	1.113±0.569	6.63	117.4	$\mathbf{3.50} \pm 0.31$
DiffWave (deep & thin)	**94.00%**	**0.932**±0.450	**6.92**	**133.8**	3.44 ± 0.36
Trainset	99.06%	0.000±0.000	8.48	281.4	—
Testset	98.76%	0.044±0.016	8.47	275.2	3.72 ± 0.28

WaveGrad

- Let’s use diffusion models in TTS.
- Network similar to a feature pyramid.
- Uses spatial feature-wise linear modulation for conditioning.
- Proposes conditioning on the fraction of true signal instead of on the timestamp which provides better generalization between noise schedules.
- Authors also suggest Fibonacci and manual noise schedules.


ϵ_n
3×1 Conv (1)
y_n
$\sqrt{\bar{\alpha}}$
UBlock (128, $\times 2$)
FiLM
5×1 Conv (32)
UBlock (128, $\times 2$)
FiLM
DBlock (128, /2)
UBlock (256, $\times 3$)
FiLM
DBlock (128, /2)
UBlock (512, $\times 5$)
FiLM
DBlock (256, /3)
UBlock (512, $\times 5$)
FiLM
DBlock (512, /5)
3×1 Conv (768)
x

WaveGrad results

- Large model with 1000 iterations achieves a MOS of 4.51 (4.58 GT).
- Base model with 6 iterations achieves a MOS of 4.41 with good real-time factors (0.2 on NVIDIA V100 and 1.5 on CPU).

Model	**MOS (↑)**
WaveRNN	4.49 ± 0.04
Parallel WaveGAN	3.92 ± 0.05
MelGAN	3.95 ± 0.06
Multi-band MelGAN	4.10 ± 0.05
GAN-TTS	4.34 ± 0.04
WaveGrad	
Base (6 iterations, continuous noise levels)	4.41 ± 0.03
Base (1,000 iterations, discrete indices)	4.47 ± 0.04
Large (1,000 iterations, discrete indices)	4.51 ± 0.04
Ground Truth	4.58 ± 0.05

Iterations (schedule)	**LS-MSE (↓)**	**MCD (↓)**	**FFE (↓)**	**MOS (↑)**
WaveGrad conditioned on discrete index				
25 (Fibonacci)	283	3.93	3.3%	3.86 ± 0.05
50 (Linear $(1 \times 10^{-4}, 0.05)$)	181	3.13	3.1%	4.42 ± 0.04
1,000 (Linear $(1 \times 10^{-4}, 0.005)$)	116	2.85	3.2%	4.47 ± 0.04
WaveGrad conditioned on continuous noise level				
6 (Manual)	217	3.38	2.8%	4.41 ± 0.04
25 (Fibonacci)	185	3.33	2.8%	4.44 ± 0.04
50 (Linear $(1 \times 10^{-4}, 0.05)$)	177	3.23	2.7%	4.43 ± 0.04
1,000 (Linear $(1 \times 10^{-4}, 0.005)$)	106	2.85	3.0%	4.46 ± 0.03

Questions?