MOMENTUM-IMBUED LANGEVIN DYNAMICS (MILD) FOR FASTER SAMPLING

N. Shetty[1], M. Bandla[2], N. Neema[2], S. Asokan[3], C. S. Seelamantula[1]
[1]Department of Electrical Engineering, [2]Department of Computer Science and Automation, Indian Institute of Science, Bengaluru; [3]Microsoft Research Lab India, Bengaluru

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SAMPLING AND OPTIMIZATION

- We propose a novel sampling algorithm Momentum-Imbued Langevin Dynamics (MILD).
- MILD is inspired by momentum-based accelerated gradient descent used in convex optimization techniques.
- MILD can be combined with pre-trained score-based diffusion models.
- It speeds up sampling by a factor of two to five in terms of the number of function evaluations (NFEs).

Gradient Descent Optimization

$$\min_{\boldsymbol{x}} f(\boldsymbol{x})$$

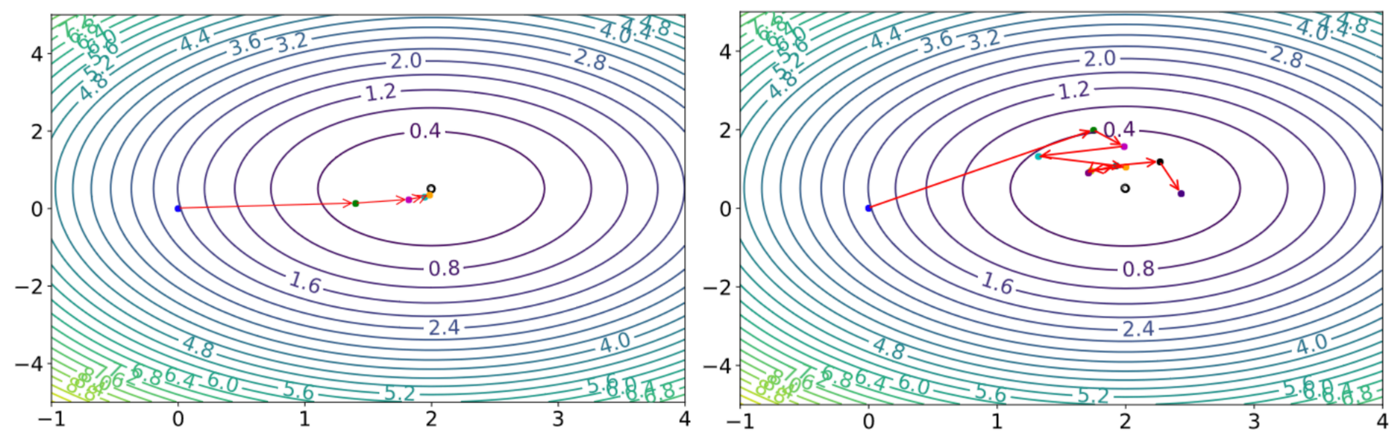
$$\boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \alpha_t \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_t)$$

Langevin Monte Carlo Sampling

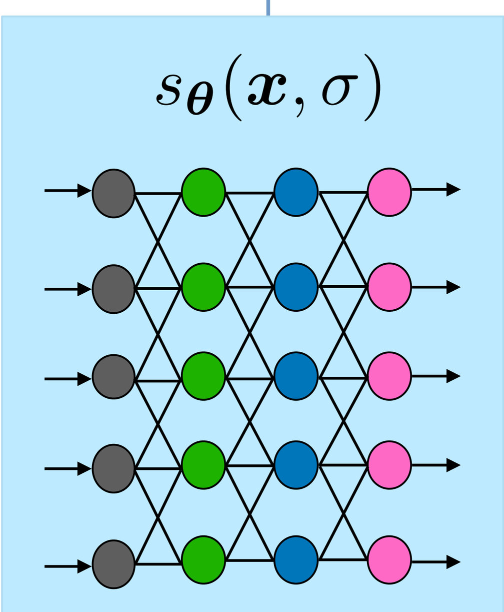
Sample from $p(\boldsymbol{x}) = \frac{\exp(-f(\boldsymbol{x}))}{Z}$

$$\boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \alpha_t \nabla_{\boldsymbol{x}} \log p(\boldsymbol{x}_t) + \sqrt{2\alpha_t}\boldsymbol{z}_t$$

$$\boldsymbol{x}_{t+1} = \boldsymbol{x}_t - \alpha_t \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_t) + \sqrt{2\alpha_t}\boldsymbol{z}_t$$

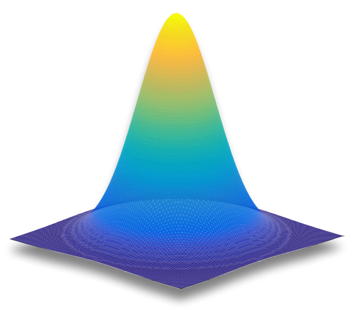


MOMENTUM-IMBUED LANGEVIN DYNAMICS (MILD) SAMPLER



PRE-TRAINED SCORE NETWORK

MILD



$$\boldsymbol{x}_0 \sim \mathcal{N}(\mathbf{0}, \mathbb{I})$$
$$\boldsymbol{v}_0 = \mathbf{0}$$

MOMENTUM-IMBUED LANGEVIN DYNAMICS

$$\boldsymbol{v}_{t+1} = \gamma \boldsymbol{v}_t + \alpha_i s_{\boldsymbol{\theta}}(\boldsymbol{x}_t + \gamma \boldsymbol{v}_t, \sigma_i)$$
$$\boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \boldsymbol{v}_{t+1} + \sqrt{2\alpha_i}\boldsymbol{z}_t$$

$t = 1, \ldots, T$ $\quad i = 1, \cdots, L$

$\mathbf{x}_{LT}$

PROPOSED SAMPLER

EXPERIMENTAL RESULTS

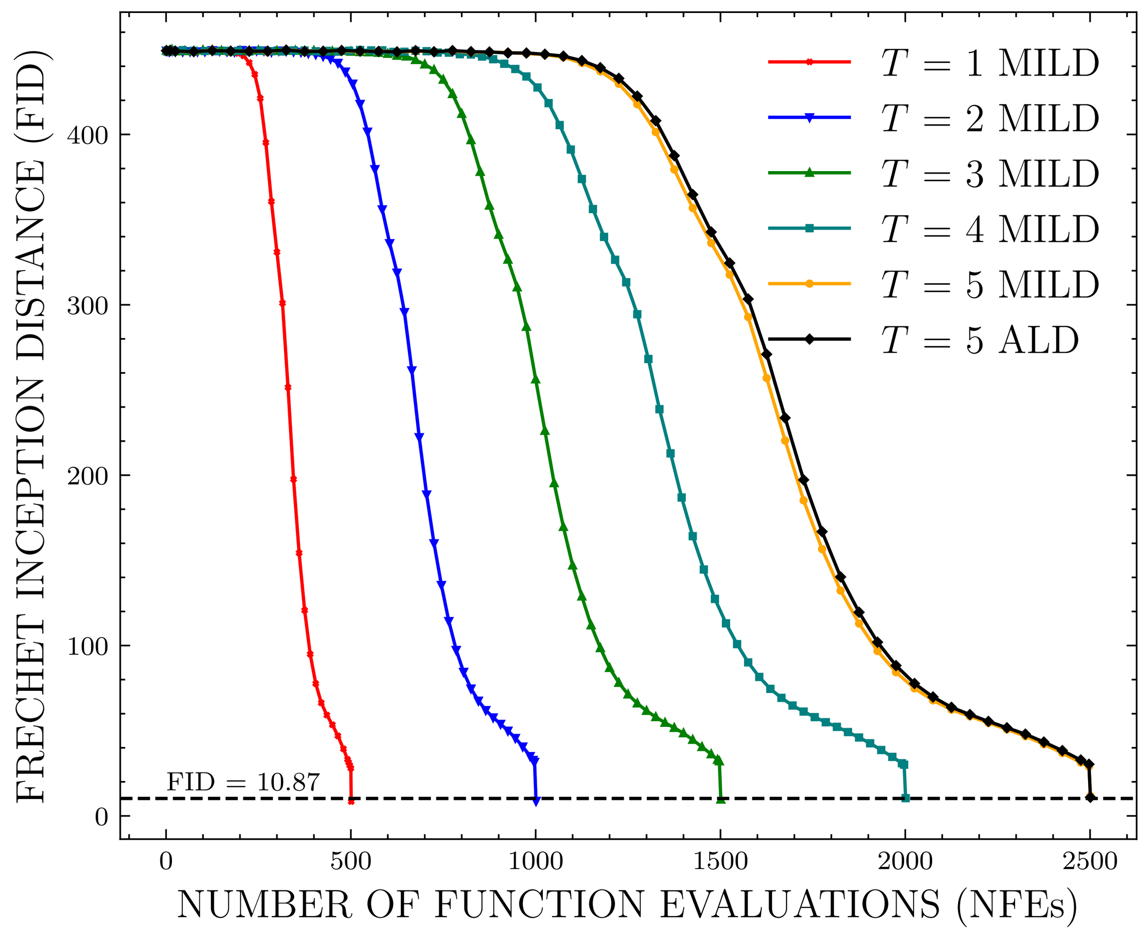
Table 1: FID values for samples generated using annealed Langevin dynamics (ALD) and momentum-imbued Langevin dynamics (MILD) for the pre-trained NCSN [1] and NCSN++ [2] models. L denotes the number of noise levels, and T denotes the sampling steps at each noise-scale. $L \times T$ is the total number of sampling steps.

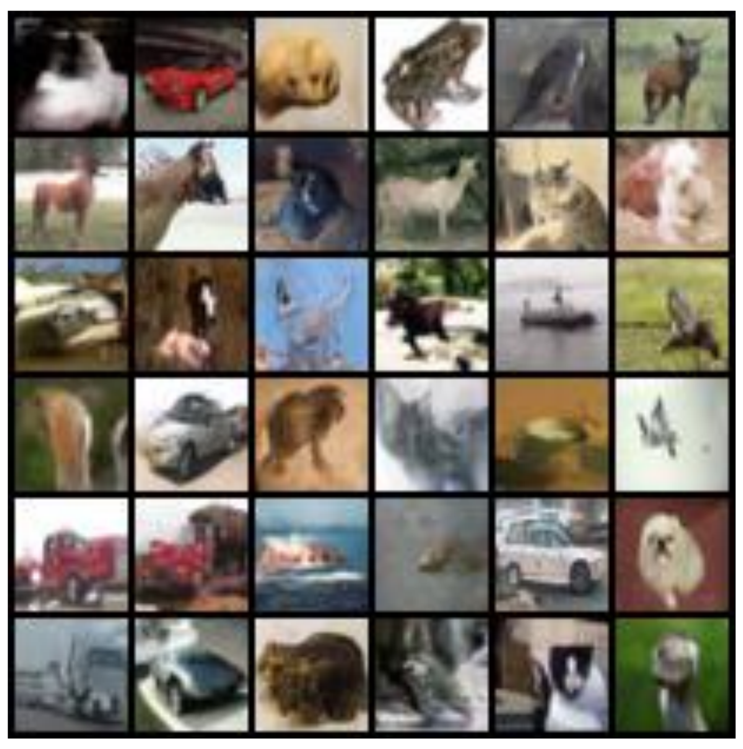
NCSN	Dataset	L	T	FID
ALD	CIFAR-10 (32×32)	10	100	**25.32**
MILD **(Ours)**	CIFAR-10 (32×32)	10	100	46.98
		10	50	28.23
		10	40	29.78
		10	30	40.35
		10	20	41.18
ALD	CelebA (32×32)	10	100	75.78
MILD **(Ours)**	CelebA (32×32)	10	100	81.85
		10	50	70.97
		10	40	**70.48**
		10	30	71.14
		10	20	73.25

NCSN++	Dataset	L	T	FID
ALD	CIFAR-10 (32×32)	232	5	12.9
MILD **(Ours)**	CIFAR-10 (32×32)	232	5	12.97
		232	4	**12.43**
		232	3	12.55
		232	2	13.58
		232	1	15.5
ALD	CelebA (64×64)	500	5	11.1
MILD **(Ours)**	CelebA (64×64)	500	5	10.93
		500	4	9.91
		500	3	9.37
		500	2	**8.59**
		500	1	8.98

Algorithm 1: Faster generative sampling with momentum-imbued Langevin dynamics (MILD).

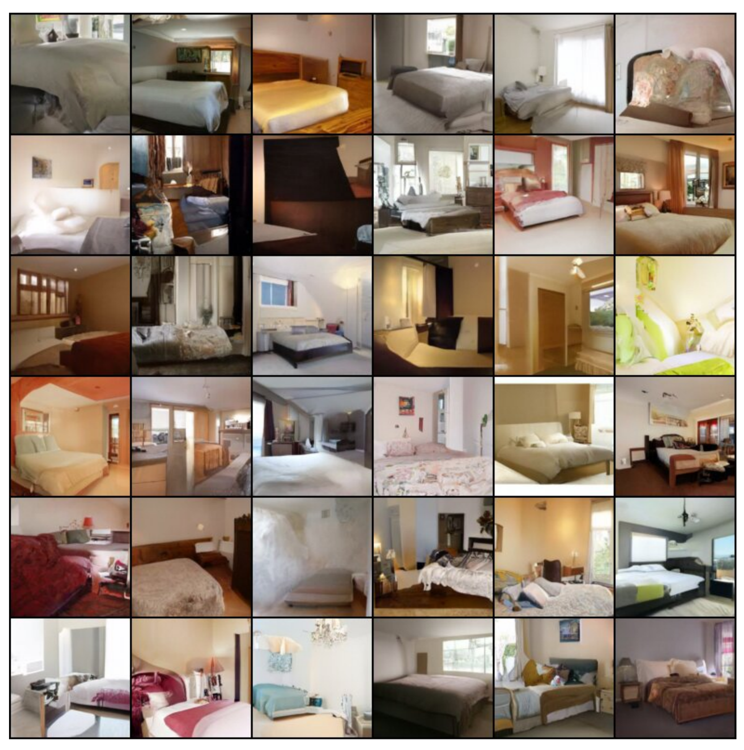
Input: $\{\sigma_i\}_{i=1}^{L}, \varepsilon, T, \gamma$, score-network $s_{\boldsymbol{\theta}}$
Initialize: $\boldsymbol{x}_0 \sim \mathcal{N}(\mathbf{0}, \mathbb{I})$, $\boldsymbol{v}_0 = \mathbf{0}$
for $i = 1$ *to* L **do**
  $\alpha_i = \frac{\varepsilon \cdot \sigma_i^2}{\sigma_L^2}$
  for $t = 0$ *to* $T - 1$ **do**
    Draw $\boldsymbol{z}_t \sim \mathcal{N}(\mathbf{0}, \mathbb{I})$
    $\boldsymbol{v}_{t+1} = \gamma \boldsymbol{v}_t + \alpha_i s_{\boldsymbol{\theta}}(\boldsymbol{x}_t + \gamma \boldsymbol{v}_t, \sigma_i)$
    $\boldsymbol{x}_{t+1} = \boldsymbol{x}_t + \boldsymbol{v}_{t+1} + \sqrt{2\alpha_i}\boldsymbol{z}_t$
  $\boldsymbol{x}_0 \leftarrow \boldsymbol{x}_T$
  $\boldsymbol{v}_0 \leftarrow \boldsymbol{v}_T$
if denoise $\boldsymbol{x}_T$ **then**
  return $\boldsymbol{x}_T + \sigma_T^2 s_\theta(\boldsymbol{x}_T, \sigma_T)$
else
  return $\boldsymbol{x}_T$





CIFAR10

CELEBA



LSUN BEDROOMS

TAKE-HOME MESSAGE

Incorporating momentum clearly accelerates the sampling speed as well as improves the quality of the generated samples (as measured by FID). Obtaining theoretical guarantees on the rate of convergence for faster sampling is a potential direction for future research.

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