

# Learning Energy-Based Models by Cooperative Diffusion Recovery Likelihood

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# Introduction: Energy Based Model

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- Energy-based models (EBMs) provide a powerful formulation for estimating the distribution of random variable  $\mathbf{x}$

$$p_{\theta}(\mathbf{x}) = \frac{1}{Z_{\theta}} \exp(f_{\theta}(\mathbf{x})),$$

- EBMs have exhibited their flexibility and practicality in a variety of application scenarios.

GRAPHEBM: MOLECULAR GRAPH GENERATION WITH ENERGY-BASED MODELS

Reduce, Reuse, Recycle: Compositional Generation with Energy-Based Diffusion Models and MCMC

Patchwise Generative ConvNet: Training Energy-Based Models from a Single Natural Image for Internal Learning

Likelihood-Based Generative Radiance Field with Latent Space Energy-Based Model for 3D-Aware Disentangled Image Representation

Generative PointNet: Deep Energy-Based Learning on Unordered Point Sets for 3D Generation, Reconstruction and Classification

Energy-based Out-of-distribution Detection

Versatile Energy-Based Probabilistic Models for High Energy Physics

Learning Neural Set Functions Under the Optimal Subset Oracle

End-to-End Stochastic Optimization with Energy-Based Model

Molecule Design by Latent Space Energy-Based Modeling and Gradual Distribution Shifting

BEEF: BI-COMPATIBLE CLASS-INCREMENTAL LEARNING VIA ENERGY-BASED EXPANSION AND FUSION

Learning Energy-Based Prior Model with Diffusion-Amortized MCMC

Energy-Based Continuous Inverse Optimal Control

Maximum Likelihood Learning of Unnormalized Models for Simulation-Based Inference

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And many other interesting works

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# Introduction: Energy Based Model

Training energy-based models (EBMs) on high-dimensional data can be both challenging and time-consuming. There exists a noticeable gap in sample quality between EBMs and other generative frameworks like GANs and diffusion models.

Models	FID ↓
EBM based method	
NT-EBM (Nijkamp et al., 2022)	78.12
LP-EBM (Pang et al., 2020)	70.15
Adaptive CE (Xiao & Hari, 2022)	65.01
EBM-SR (Nijkamp et al., 2019)	44.50
JEM (Grathwohl et al., 2020)	38.40
EBM-IG (Du & Mordatch, 2019)	38.20
EBM-FCE (Gao et al., 2020)	37.30
CoopVAEBM (Xie et al., 2021b)	36.20
CoopNets (Xie et al., 2018a)	33.61
Divergence Triangle (Han et al., 2020)	30.10
VARA (Grathwohl et al., 2021b)	27.50
EBM-CD (Du et al., 2021)	25.10
GEBM (Arbel et al., 2021)	19.31
HAT-EBM (Hill et al., 2022)	19.30
CF-EBM (Zhao et al., 2021)	16.71
CoopFlow (Xie et al., 2022)	15.80
CLEL-base (Lee et al., 2023)	15.27
VAEBM (Xiao et al., 2021)	12.16
DRL (Gao et al., 2021)	9.58
CLEL-large (Lee et al., 2023)	8.61
EGC (Unsupervised) (Guo et al., 2023)	5.36

Models	FID ↓
GAN based method	
WGAN-GP (Gulrajani et al., 2017)	36.40
SN-GAN (Mivato et al., 2018)	21.70
BigGAN (Brock et al., 2019)	14.80
StyleGAN2-DiffAugment (Zhao et al., 2020)	5.79
Diffusion-GAN (Xiao et al., 2022)	3.75
StyleGAN2-ADA (Karras et al., 2020)	2.92
Score based and Diffusion method	
NCSN (Song & Ermon, 2019)	25.32
NCSN-v2 (Song & Ermon, 2020)	10.87
NCSN++ (Song et al., 2021)	2.20
DDPM Distillation (Luhman & Luhman, 2021)	9.36
DDPM++(VP, NLL) (Kim et al., 2021)	3.45
DDPM (Ho et al., 2020)	3.17
DDPM++(VP, FID) (Kim et al., 2021)	2.47

FID Score for CIFAR-10 unconditional Generation

# Challenges of Training EBM

- The training of EBM requires sampling from the current estimated distribution

$$\mathcal{L}'(\theta) = \mathbb{E}_{p_{\text{data}}} \left[ \frac{\partial}{\partial \theta} f_{\theta}(\mathbf{x}) \right] - \mathbb{E}_{p_{\theta}} \left[ \frac{\partial}{\partial \theta} f_{\theta}(\mathbf{x}) \right],$$

- Sampling is often achieved through MCMC, which can be challenging with high-dimensional data;
- Previous work [7] proposed to estimate a sequence of EBMs defined on increasingly noisy versions of the data and jointly estimate them by maximizing recovery likelihood.

# Diffusion Recovery Likelihood (DRL)

- Assume a sequence of noisy training example perturbed by a Gaussian diffusion process:  $\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_T$ .
- $\mathbf{x}_{t+1} = \alpha_{t+1}\mathbf{x}_t + \sigma_{t+1}\boldsymbol{\epsilon}$ ,  $\mathbf{x}_0 \sim p_{\text{data}}$ ,  $\boldsymbol{\epsilon} \sim \mathcal{N}(0, \mathbf{I})$ .
- Denote  $\mathbf{y}_t = \alpha_{t+1}\mathbf{x}_t$  and fit  $p_{\theta}(\mathbf{y}_t) = \frac{1}{Z_{\theta,t}} \exp(f_{\theta}(\mathbf{y}_t; t))$  for marginal distribution;

- The conditional distribution is given by

$$p_{\theta}(\mathbf{y}_t | \mathbf{x}_{t+1}) = \frac{1}{\tilde{Z}_{\theta,t}(\mathbf{x}_{t+1})} \exp\left(f_{\theta}(\mathbf{y}_t; t) - \frac{1}{2\sigma_{t+1}^2} \|\mathbf{y}_t - \mathbf{x}_{t+1}\|^2\right)$$

- Sample iteratively with Langevin dynamics:

$$\tilde{\mathbf{y}}_t^{\tau+1} = \tilde{\mathbf{y}}_t^{\tau} + \frac{s_t^2}{2} \left( \nabla_{\mathbf{y}} f_{\theta}(\tilde{\mathbf{y}}_t^{\tau}; t) - \frac{1}{\sigma_{t+1}^2} (\tilde{\mathbf{y}}_t^{\tau} - \mathbf{x}_{t+1}) \right) + s_t \boldsymbol{\epsilon}^{\tau}$$

# Cooperative Diffusion Recovery Likelihood (CDRL)

- Although DRL makes sampling easier by sampling from  $p_{\theta}(\mathbf{y}_t|\mathbf{x}_{t+1})$ , the initialization of MCMC sampling  $\mathbf{x}_{t+1}$ , may still be far from the data manifold of  $\mathbf{y}_t$ .
- We propose to learn an extra initializer model to further close this gap  $q_{\phi}(\mathbf{y}_t|\mathbf{x}_{t+1}) \sim \mathcal{N}(\mathbf{g}_{\phi}(\mathbf{x}_{t+1}; t), \tilde{\sigma}_t^2 \mathbf{I})$ .
- Cooperative Training:
  - Given observation  $\mathbf{x}_{t+1}$ , initializer  $q_{\phi}$  makes the initial guess  $\hat{\mathbf{y}}_y$ .
  - $\hat{\mathbf{y}}_t$  is then modified by learned recovery-likelihood through Langevin sampling to get  $\tilde{\mathbf{y}}_t$ .
  - Update initialized using modified samples as target:

$$\mathcal{L}_t(\phi) = \frac{1}{n} \sum_{i=1}^n \left[ -\frac{1}{2\tilde{\sigma}_t^2} \|\tilde{\mathbf{y}}_{t,i} - \mathbf{g}_{\phi}(\mathbf{x}_{t+1}, i; t)\|^2 \right]$$

- Update energy models using modified samples:

$$\nabla_{\theta} \mathcal{J}_t(\theta) = \nabla_{\theta} \left[ \frac{1}{n} \sum_{i=1}^n f_{\theta}(\mathbf{y}_{t,i}; t) - \frac{1}{n} \sum_{i=1}^n f_{\theta}(\tilde{\mathbf{y}}_{t,i}; t) \right]$$



# Sampling of CDRL

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## Algorithm 2 CDRL Sampling

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**Input:** (1) Number of noise levels  $T$ ; (2) Number of Langevin sampling steps  $K$  at each noise level; (3) Langevin step size at each noise level  $\delta_t$ ; (4) Trained EBM  $f_\theta$ ; (5) Trained initializer  $g_\phi$ ;

**Output:** Samples  $\tilde{\mathbf{x}}_0$

Randomly initialize  $\mathbf{x}_T \sim \mathcal{N}(0, I)$ .

**for**  $t = T - 1$  **to** 0 **do**

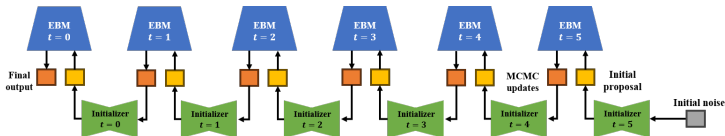
    Generate initial proposal  $\hat{\mathbf{y}}_t$ .

    Update  $\hat{\mathbf{y}}_t$  to  $\tilde{\mathbf{y}}_t$  by  $K$  iterations of Langevin Sampling.

    Let  $\tilde{\mathbf{x}}_t = \tilde{\mathbf{y}}_t / \alpha_{t+1}$ .

**end for**

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# Unconditional Generation

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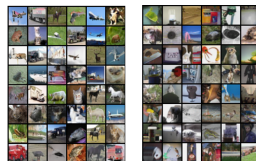
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Models	FID ↓	Models	FID ↓
EBM based method		Other likelihood based method	
NT-EBM (Nijkamp et al., 2022)	78.12	VAE (Kingma & Welling, 2014)	78.41
LP-EBM (Pang et al., 2020)	70.15	PixelCNN (Salimans et al., 2017)	65.93
Adaptive CE (Xiao & Han, 2022)	65.01	PixelIQN (Ostrovski et al., 2018)	49.46
EBM-SR (Nijkamp et al., 2019)	44.50	Residual Flow (Chen et al., 2019)	47.37
JEM (Grathwohl et al., 2020)	38.40	Glow (Kingma & Dhariwal, 2018)	45.99
EBM-IG (Du & Mordatch, 2019)	38.20	DC-VAE (Parmar et al., 2021)	17.90
EBM-FCE (Gao et al., 2020)	37.30		
CoopVAEBM (Xie et al., 2021b)	36.20	GAN based method	
CoopNets (Xie et al., 2018a)	33.61	WGAN-GP (Gulrajani et al., 2017)	36.40
Divergence Triangle (Han et al., 2020)	30.10	SN-GAN (Miyato et al., 2018)	21.70
VARA (Grathwohl et al., 2021b)	27.50	BigGAN (Brock et al., 2019)	14.80
EBM-CD (Du et al., 2021)	25.10	StyleGAN2-DiffAugment (Zhao et al., 2020)	5.79
GEBM (Arbel et al., 2021)	19.31	Diffusion-GAN (Xiao et al., 2022)	3.75
HAT-EBM (Hill et al., 2022)	19.30	StyleGAN2-ADA (Karras et al., 2020)	2.92
CF-EBM (Zhao et al., 2021)	16.71		
CoopFlow (Xie et al., 2022)	15.80	Score based and Diffusion method	
CLEL-base (Lee et al., 2023)	15.27	NCSN (Song & Ermon, 2019)	25.32
VAEBM (Xiao et al., 2021)	12.16	NCSN-v2 (Song & Ermon, 2020)	10.87
DRL (Gao et al., 2021)	9.58	NCSN++ (Song et al., 2021)	2.20
CLEL-large (Lee et al., 2023)	8.61	DDPM Distillation (Luhman & Luhman, 2021)	9.36
EGC (Unsupervised) (Guo et al., 2023)	5.36	DDPM++(VP, NLL) (Kim et al., 2021)	3.45
CDRL (Ours)	4.31	DDPM (Ho et al., 2020)	3.17
CDRL-large (Ours)	3.68	DDPM++(VP, FID) (Kim et al., 2021)	2.47

FID scores for CIFAR-10 Unconditional Generation



CIFAR-10 Samples ImageNet (32 × 32) Samples

Models	FID ↓
EBM-IG (Du & Mordatch, 2019)	60.23
PixelCNN (Salimans et al., 2017)	40.51
EBM-CD (Du et al., 2021)	32.48
CF-EBM (Zhao et al., 2021)	26.31
CLEL-base (Lee et al., 2023)	22.16
DRL (Gao et al., 2021)	- (not converge)
DDPM++(VP, NLL) (Kim et al., 2021)	8.42
<b>CDRL (Ours)</b>	<b>9.35</b>

FID scores for ImageNet (32 × 32) Unconditional Generation

# Sampling Acceleration

We applied post-training techniques to accelerate sampling.

- Langevin sampling step:

$$\tilde{\mathbf{y}}_t^{\tau+1} = \tilde{\mathbf{y}}_t^{\tau} + \frac{s_t^2}{2} \left( \nabla_{\mathbf{y}} f_{\theta}(\tilde{\mathbf{y}}_t^{\tau}; t) - \frac{1}{\sigma_{t+1}^2} (\tilde{\mathbf{y}}_t^{\tau} - \mathbf{x}_{t+1}) \right) + s_t \epsilon^{\tau},$$

- We decrease the number of sampling steps, and meanwhile adjust the MCMC sampling step size to be inversely proportional to the square root of the number of sampling steps.

Models	Number of noise level $\times$ Number of MCMC steps	FID $\downarrow$
DRL (Gao et al., 2021)	$6 \times 30 = 180$	9.58
CDRL	$6 \times 15 = 90$	4.31
CDRL (step 8)	$6 \times 8 = 48$	4.58
CDRL (step 5)	$6 \times 5 = 30$	5.37
CDRL (step 3)	$6 \times 3 = 18$	9.67

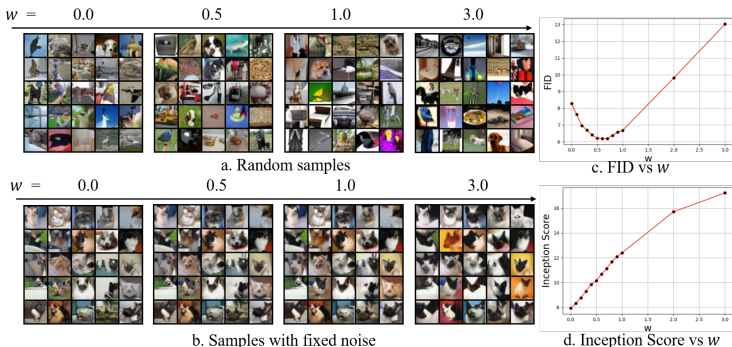
FID scores for CIFAR-10 with Sampling Adjustment

# Conditional Generation

Following [15], we can apply classifier-free guidance to CDRL by estimating both conditional and unconditional distributions.

$$\log \tilde{p}_\theta(\mathbf{y}_t | c) = (w + 1)f_\theta(\mathbf{y}_t; c, t) - wf_\theta(\mathbf{y}_t; t) + \text{const.}$$


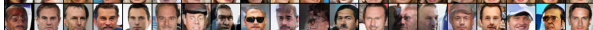






$$\tilde{q}_\phi(\mathbf{y}_t | c, \mathbf{x}_{t+1}) \sim \mathcal{N}((w + 1)\mathbf{g}_\phi(\mathbf{x}_{t+1}; c, t) - w\mathbf{g}_\phi(\mathbf{x}_{t+1}; t), \tilde{\sigma}_t^2 \mathbf{I}).$$



# Attribution-Compositional Generation

Similar to [5][20], given two energy functions trained on two conditionally independent concepts  $c_1$  and  $c_2$ , we can estimate the energy conditioning on both concepts using:

$$\log p_{\theta}(\mathbf{x}|c_1, c_2) = \log p_{\theta}(\mathbf{x}|c_1) + \log p_{\theta}(\mathbf{x}|c_2) - \log p_{\theta}(\mathbf{x}) + \text{const.}$$

	Male	Smile	Young
	×	-	-
	√	-	-
	×	×	-
	×	√	-
	×	-	×
	×	-	√
	×	√	×
	×	√	√

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# Out-Of-Distribution Detection

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- The fitted energy function in CDRL naturally forms a score reflecting the log-likelihood of the data.
- We employ the model trained on CIFAR-10 as a detector and use the energy at the lowest noise level to serve as the OOD prediction score.

	Cifar-10 interpolation	Cifar-100	CelebA
PixelCNN (Salimans et al., 2017)	0.71	0.63	-
GLOW (Kingma & Dhariwal, 2018)	0.51	0.55	0.57
NVAE (Vahdat & Kautz, 2020)	0.64	0.56	0.68
EBM-IG (Du & Mordatch, 2019)	0.70	0.50	0.70
VAEBM (Xiao et al., 2021)	0.70	0.62	0.77
EBM-CD (Du et al., 2021)	0.65	0.83	-
CLEL-Base (Lee et al., 2023)	0.72	0.72	0.77
<b>CDRL (ours)</b>	0.75	0.78	0.84

AUROC scores in OOD detection using CDRL and other explicit density models on CIFAR-10

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# Conclusion and our contributions

This paper tries to push forward the progress of development of Energy Based Models.

- We propose cooperative diffusion recovery likelihood (CDRL) that tractably and efficiently learns and samples from a sequence of EBMs and MCMC initializers;
- Empirically we demonstrate that CDRL achieves significant improvements on sample quality compared to existing EBM approaches;
- We show that CDRL has great potential to enable more efficient sampling with sampling adjustment techniques;
- We demonstrate CDRL's ability in various tasks like unconditional generation, conditional generation, compositional generation, out-of-distribution (OOD) detection, etc.

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# Thank you for listening!

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