Learning Energy-based Model via Dual-MCMC Teaching

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NEURAL INFORMATION PROCESSING SYSTEMS

Preliminary I: Energy-based Model

Energy-based Model (EBM). The EBM can be defined with probability density as

$$\pi_\alpha(\mathbf{x}) = \frac{1}{\mathrm{Z}(\alpha)} \exp\left[f_\alpha(\mathbf{x})\right]$$

Maximum Likelihood Estimation (MLE). With observed examples $\{\mathbf{x}^{(i)}, i = 1, 2, ..., n\}$, learning of EBM can be done via MLE with the gradient computed as

$$\frac{\partial}{\partial \alpha} L_\pi(\alpha) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})}[\frac{\partial}{\partial \alpha} f_\alpha(\mathbf{x})] - \mathbb{E}_{\pi_\alpha(\mathbf{x})}[\frac{\partial}{\partial \alpha} f_\alpha(\mathbf{x})]$$

Limitation. The MLE learning requires sampling from the EBM, which can be achieved by Markov Chain Monte Carlo (MCMC) sampling, such as the Langevin dynamics,

$$\mathbf{x}_{\tau+1} = \mathbf{x}_\tau + s\frac{\partial}{\partial \mathbf{x}_\tau} \log \pi_\alpha(\mathbf{x}_\tau) + \sqrt{2s}U_\tau$$

However, such Langevin dynamics typically start from noise points, which may take a long time to converge and mix between different modes.

Preliminary II: Generator Model

Generator Model. The generator model seeks to explain the observation signal $\mathbf{x}$ by a latent vector $\mathbf{z}$ and can be specified as

$$p_\theta(\mathbf{x}, \mathbf{z}) = p(\mathbf{z})p_\theta(\mathbf{x}|\mathbf{z})$$

where $p(\mathbf{z})$ is the known prior distribution such as unit Gaussian, and $p_\theta(\mathbf{x}|\mathbf{z})$ is the generation model.

Maximum Likelihood Estimation (MLE). The MLE learning of the generator model computes log-likelihood over the observed examples. The gradient is computed as

$$\frac{\partial}{\partial \theta} L_p(\theta) = \mathbb{E}_{p_{\text{data}}(\mathbf{x})p_\theta(\mathbf{z}|\mathbf{x})}[\frac{\partial}{\partial \theta} \log p_\theta(\mathbf{x}, \mathbf{z})]$$

Limitation. The MLE learning requires sampling from the generator posterior, which can be done by MCMC sampling as,

$$\mathbf{z}_{\tau+1} = \mathbf{z}_\tau + s\frac{\partial}{\partial \mathbf{z}_\tau} \log p_\theta(\mathbf{z}_\tau|\mathbf{x}) + \sqrt{2s}U_\tau$$

However, noise-initialized Langevin dynamics can be ineffective in traversing the latent space and hard to mix.

Proposed Method

Inference Model. The generator model can be utilized as the **initializer** model for the MCMC sampling of EBM, while for the MCMC sampling of the generator posterior, an inference model is thus introduced,

$$q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mu_\phi(\mathbf{x}), V_\phi(\mathbf{x}))$$

which aims to initialize the MCMC generator posterior sampling.

Joint Density. With the EBM, generator and inference model, joint densities can be formulated as

$$P_\theta(\mathbf{x}, \mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z})$$
$$\Pi_{\alpha,\phi}(\mathbf{x}, \mathbf{z}) = \pi_\alpha(\mathbf{x})q_\phi(\mathbf{z}|\mathbf{x})$$
$$Q_\phi(\mathbf{x}, \mathbf{z}) = p_{\text{data}}(\mathbf{x})q_\phi(\mathbf{z}|\mathbf{x})$$

Dual-MCMC Teaching. In addition, we introduce two joint densities that incorporate the MCMC sampling as revision processes,

$$P_{\theta,\alpha}(\mathbf{x}, \mathbf{z}) = \mathcal{T}_\alpha^{\mathbf{x}} p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z}) \quad Q_{\phi,\theta}(\mathbf{x}, \mathbf{z}) = p_{\text{data}}(\mathbf{x})\mathcal{T}_\theta^{\mathbf{z}} q_\phi(\mathbf{z}|\mathbf{x})$$

Learning energy-based model. Therefore, learning the EBM is based on the minimization of KL divergences as

$$\mathrm{KL}(\tilde{Q}_{\phi_t,\theta_t}(\mathbf{x}, \mathbf{z})\|\Pi_{\alpha,\phi}(\mathbf{x}, \mathbf{z})) - \mathrm{KL}(\tilde{P}_{\theta_t,\alpha_t}(\mathbf{x}, \mathbf{z})\|\Pi_{\alpha,\phi}(\mathbf{x}, \mathbf{z}))$$

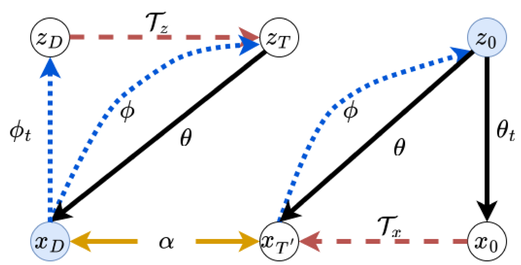
Learning generator model. The generator model is learned through the minimization of KL divergences as

$$\mathrm{KL}(\tilde{Q}_{\phi_t,\theta_t}(\mathbf{x}, \mathbf{z})\|P_\theta(\mathbf{x}, \mathbf{z})) + \mathrm{KL}(\tilde{P}_{\theta_t,\alpha_t}(\mathbf{x}, \mathbf{z})\|P_\theta(\mathbf{x}, \mathbf{z}))$$

Learning inference model. The generator model is learned through the minimization of KL divergences as

$$\mathrm{KL}(\tilde{Q}_{\phi_t,\theta_t}(\mathbf{x}, \mathbf{z})\|Q_\phi(\mathbf{x}, \mathbf{z})) + \mathrm{KL}(\tilde{P}_{\theta_t,\alpha_t}(\mathbf{x}, \mathbf{z})\|\Pi_{\alpha,\phi}(\mathbf{x}, \mathbf{z}))$$

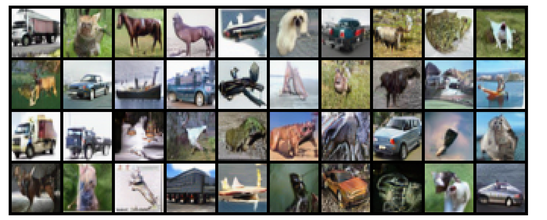
Illustration for Dual-MCMC Teaching.



Experiment: Image Modelling

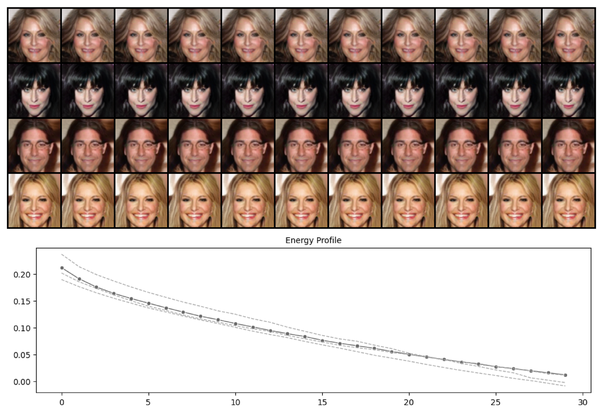
Methods	CIFAR-10 IS (↑)	CIFAR-10 FID (↓)	CelebA-64 FID (↓)
Ours	**8.55**	**9.26**	**5.15**
Cooperative EBM	6.55	33.61	16.65
Amortized EBM	6.65	-	-
Divergence Triangle	7.23	30.10	18.21
No MCMC EBM	-	27.5	-
Short-run EBM	6.21	-	23.02
IGEBM	6.78	38.2	-
ImprovedCD EBM	7.85	25.1	-
Diffusion EBM	8.30	9.58	5.98
VAEBM	8.43	12.19	5.31

Methods	CelebA-HQ-256	LSUN-Church-64
Ours	**15.89**	**4.56**
Diffusion EBM	-	7.02
VAEBM	20.38	13.51
NCP-VAE	27.79	-
GLOW	68.93	59.35
PGGAN	21.7	6.1



Experiment: MCMC Revision

Visualize of Langevin Transition on $\mathbf{x}$.



MCMC revision on $\mathbf{x}$. The leftmost images are sampled from the generator model, and the rightmost images are at the final step of the EBM-guided MCMC sampling. **Bottom:** Energy profile over steps. Only minor changes can be observed during the transition, suggesting that the generator has matched the EBM-guided MCMC revision.

Experiment: Inference and Generator Model

Image Reconstruction.

Methods	CIFAR-10	CelebA-64
VAE	0.0341	0.0438
ABP	0.0183	0.0277
Cooperative EBM	0.0271	0.0387
Divergence Triangle	0.0237	0.0281
Ours (Inf)	0.0214	0.0227
Ours (Inf+L=10)	**0.0072**	**0.0164**

Interpolation on Latent Space.

The *top* and *bottom* three rows indicate image generation and reconstruction, respectively.