On Out-of-distribution Detection with Energy-based Models

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Project page: https://www.daml.in.tum.de/ood-ebm/

TL;DR

- EBMs do **not** strictly outperform Normalizing Flows across multiple training methods.
- Semantic features induced by **supervision improves OOD detection** in recent discriminative EBMs [2].
- **Architectural modifications** can also be used to improve OOD detection with EBMs.

What is an energy-based model?

EBM defines a probability distribution over the data $\mathbf{x} \in \mathbb{R}^D$ through the energy function E_θ as

$$p_\theta(\mathbf{x}) = \frac{\exp(-E_\theta(\mathbf{x}))}{Z(\theta)} \quad (1)$$

where $Z(\theta) = \int \exp(-E_\theta(\mathbf{x}))d\mathbf{x}$ is the normalizing constant.

Properties:

✓ Flexible transformations	✗ Exact density evaluation
✓ Dimensionality reduction	✗ No direct maximum likelihood training

Why study EBMs for OOD detection?

- Recent research on density estimation focuses on exact likelihood methods.
- Findings of superior OOD detection performance of EBMs without analysis in JEMs [2].

→ Hypotheses for better OOD detection vs. Normalizing Flows:

	Normalizing Flows	EBM
Dimensionality reduction	Operate in $\mathbb{R}^D$	$E_\theta : \mathbb{R}^D \mapsto \mathbb{R}$
Supervision	Not considered	Used in JEM [2]

How to train an EBM?

Since maximum likelihood training is not possible, we consider three different approaches:

Sliced score matching (SSM) [4]. Efficient update formula based on random projection

$$\mathbb{E}_{p_v}\mathbb{E}_{p(x)}\left[v^T \nabla_x s_\theta(x) v + \frac{1}{2}\|s_\theta(x)\|_2^2\right]$$

where $s_\theta(x) = \nabla_x p_\theta(x)$ and $v \sim p_v$ is a simple distribution of random vectors.

Contrastive divergence (CD) [3]. Approximation of the gradient of the maximum likelihood objective by

$$\nabla_\theta p_\theta(x) = \mathbb{E}_{p_\theta(x')}\left[\nabla_\theta E_\theta(x')\right] - \nabla_\theta E_\theta(x)$$

VERA [1]. Learn the parameters ϕ of a auxiliary distribution q_ϕ as the optimum of

$$\log Z(\theta) = \max_{q_\phi} \mathbb{E}_{q_\phi(x)}\left[f_\theta(x)\right] + H(q_\phi)$$

which can be plugged into 1 to obtain an alternative method for training EBMs with a variational approximation to estimate the entropy term $H(q_\phi)$.

Experiments & Results

Differentiation of natural and non-natural dataset.

Natural OOD: Requires learning semantic features to differentiate, e.g., images of classes not in training set.
Non-natural OOD: Requires detection farther from the training data manifold, e.g., noise, OODomain

Are EBMs better than Normalizing Flows?

EBMs do not consistently outperform Normalizing Flows across different training methods (Improvements: CD 11.9%, VERA 4.3%, SSM -4.3%)
→ Dimensionality reduction is not significant

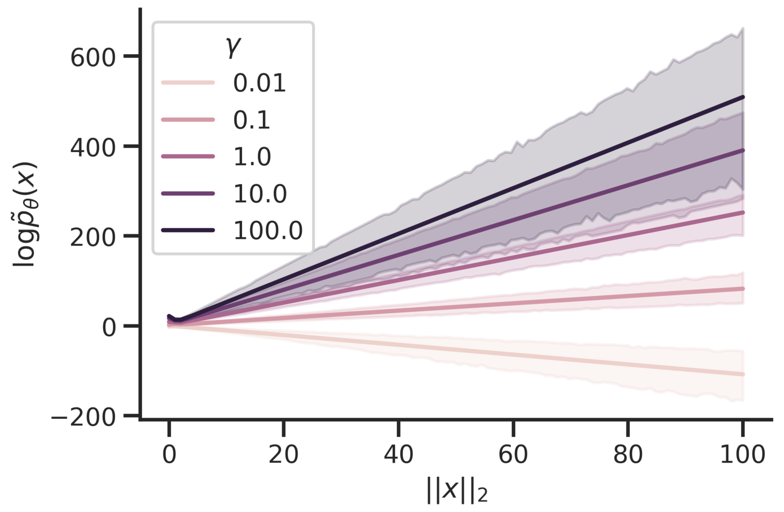
Does supervision improve OOD detection?

Use Joint Energy model (JEM) which incorporates supervision through cross-entropy objective.

Model	ID dataset	Natural	Non-natural
CD	CIFAR-10	-10.82	-9.11
	FMNIST	47.17	3.24
	Segment	1.85	0.89
	Sensorless	29.72	-0.02
SSM	CIFAR-10	7.33	-27.94
	FMNIST	50.61	-20.26
	Segment	25.89	-21.94
	Sensorless	22.13	-40.73
VERA	CIFAR-10	-1.16	-3.00
	FMNIST	33.66	-15.53
	Segment	4.98	-0.57
	Sensorless	97.93	0.07

% improvement in AUC-PR

- Supervision improves some results significantly on *natural* OOD datasets, but degrade on *non-natural* datasets.
- Investigation shows: Weighting parameter of cross-entropy loss γ affects the density estimates far from training data
  → *Non-natural* data becomes harder to detect



Sidestepping tuning of γ

Intoduce supervision indirectly by training on embeddings obtained from classification model.

Model	ID dataset	Natural	Non-natural
CD	CIFAR-10	48.60	3.37
	FMNIST	95.79	-13.52
SSM	CIFAR-10	53.84	-2.31
	FMNIST	58.40	59.59
VERA	CIFAR-10	50.16	16.97
	FMNIST	15.12	1.80

% improvement in AUC-PR

- OOD detection significantly improves on *natural* and in cases on *non-natural* datasets
- Shows that vanilla EBMs struggle to extract high-level, semantic features

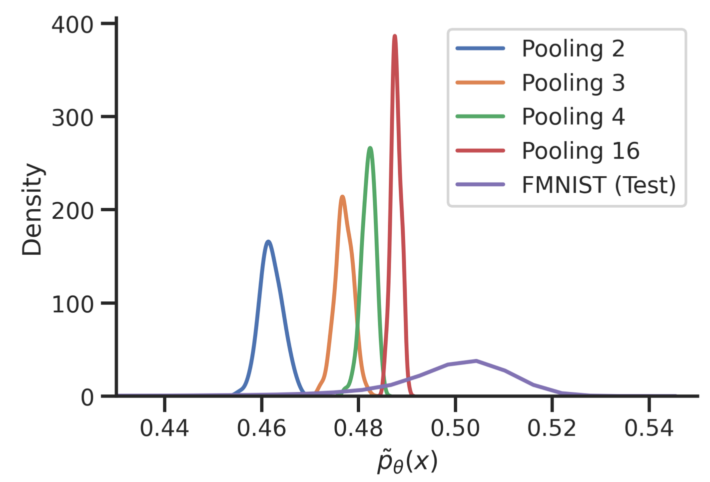
Can we encourage semantic features?

Introduce bottlenecks through 1×1 convolutions into the architecture.

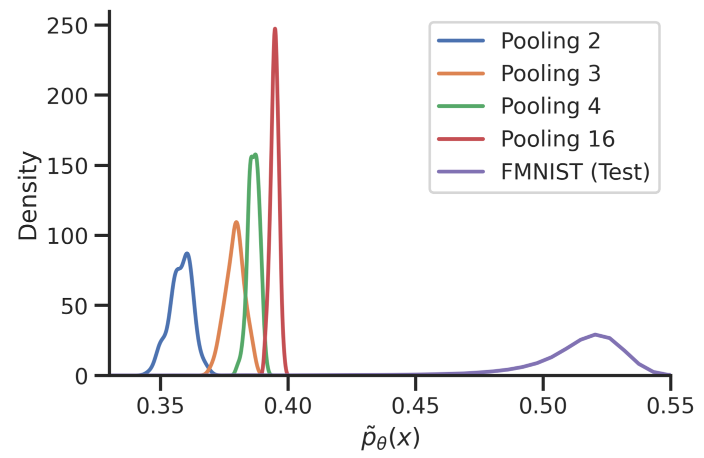
Model	ID dataset	Natural	Non-natural
CD	CIFAR-10	20.18	20.38
	FMNIST	67.95	10.88
SSM	CIFAR-10	14.76	33.34
	FMNIST	1.75	-5.92
VERA	CIFAR-10	19.66	33.22
	FMNIST	26.84	32.94

% improvement in AUC-PR

- OOD detection improves consistently upon the baseline EBMs by learning higher-level features
- The difference in density assigned for low-level features to images increases significantly



No Bottleneck.



With Bottleneck.

References

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[2] W. Grathwohl, K.-C. Wang, J.-H. Jacobsen, D. Duvenaud, M. Norouzi, and K. Swersky. Your Classifier is Secretly an Energy Based Model and You Should Treat it Like One. *arXiv:1912.03263 [cs, stat]*, Sept. 2020.

[3] G. E. Hinton. Training Products of Experts by Minimizing Contrastive Divergence. *Neural Computation*, 14(8):1771–1800, Aug. 2002.

[4] Y. Song, S. Garg, J. Shi, and S. Ermon. Sliced Score Matching: A Scalable Approach to Density and Score Estimation. *arXiv:1905.07088 [cs, stat]*, June 2019.