Regression using Energy-Based Models and Noise Contrastive Estimation

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Energy-Based Models for Deep Probabilistic Regression
Fredrik K. Gustafsson, Martin Danelljan, Goutam Bhat, Thomas B. Schön
The European Conference on Computer Vision (ECCV), 2020

How to Train Your Energy-Based Model for Regression
Fredrik K. Gustafsson, Martin Danelljan, Radu Timofte, Thomas B. Schön
The British Machine Vision Conference (BMVC), 2020

Accurate 3D Object Detection using Energy-Based Models
Fredrik K. Gustafsson, Martin Danelljan, Thomas B. Schön
Preprint

Deep Energy-Based NARX Models
Johannes Hendriks, Fredrik K. Gustafsson, Antônio Ribeiro, Adrian Wills, Thomas B. Schön
Preprint

An **energy-based model (EBM)** specifies a probability distribution $p(x;\theta)$ over $x \in \mathcal{X}$ directly via a parameterized scalar function $f_\theta : \mathcal{X} \to \mathbb{R}$:

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By defining $f_\theta(x)$ using a deep neural network (DNN), $p(x;\theta)$ becomes expressive enough to learn practically any distribution from observed data.

Energy-Based Models

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where $f_\theta(x)$ commonly is defined using a DNN.

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The EBM $p(x;\theta) = e^{f_\theta(x)} / \int e^{f_\theta(\tilde{x})} d\tilde{x}$ is thus a highly expressive model that puts minimal restricting assumptions on the true distribution $p(x)$.

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(Compare with normalizing flows which are specifically designed to be easy to both evaluate and sample. EBMs instead prioritize maximum expressivity)

The definition of an EBM $p(x;\theta)$,

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In particular, EBMs are challenging to train. A variety of different approaches have therefore been explored in literature.

A very recent tutorial on the subject:

How to Train Your Energy-Based Models
Yang Song, Diederik P. Kingma
arXiv:2101.03288

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Regression: learn to predict a continuous target $y^\star \in \mathcal{Y} = \mathbb{R}^K$ from a corresponding input $x^\star \in \mathcal{X}$, given a training set $\mathcal{D}$ of i.i.d. input-target pairs, $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^N$, $(x_i, y_i) \sim p(x, y)$.

Energy-Based Models for Regression

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We address this task by modelling the distribution $p(y|x)$ with a *conditional* EBM:

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Here, $f_\theta : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ is a DNN that maps any input-target pair $(x, y) \in \mathcal{X} \times \mathcal{Y}$ directly to a scalar $f_\theta(x, y) \in \mathbb{R}$, and $Z(x, \theta)$ is the input-dependent partition function.

Energy-Based Models for Regression

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EBMs for Regression: train a DNN $f_\theta : \mathcal{X} \times \mathcal{Y} \to \mathbb{R}$ to predict a scalar value $f_\theta(x, y)$, then model $p(y|x)$ with the conditional EBM $p(y|x;\theta)$:

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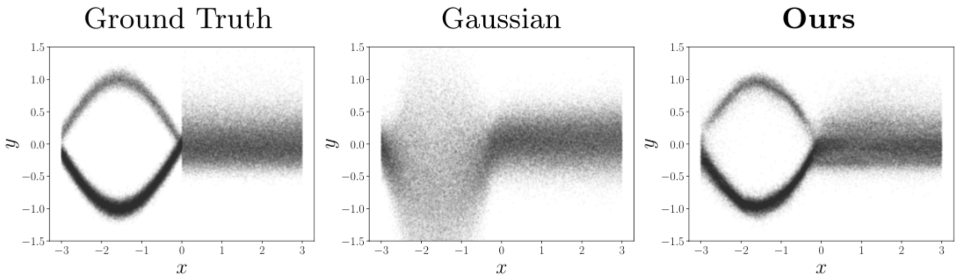
The EBM $p(y|x;\theta)$ can learn complex target distributions directly from data:



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We have applied the approach to various regression problems:

- Age estimation, $\mathcal{Y} = \mathbb{R}$.
- Head-pose estimation, $\mathcal{Y} = \mathbb{R}^3$.
- 2D bounding box regression (object detection, visual tracking), $\mathcal{Y} = \mathbb{R}^4$.
- 3D bounding box regression (3D object detection in LiDAR point clouds), $\mathcal{Y} = \mathbb{R}^7$.
- System identification, $\mathcal{Y} = \mathbb{R}$.

Energy-Based Models for Regression - Prediction

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Given an input $x^\star$ at test time, we usually predict $y^\star$ by maximizing $p(y|x^\star;\theta)$:

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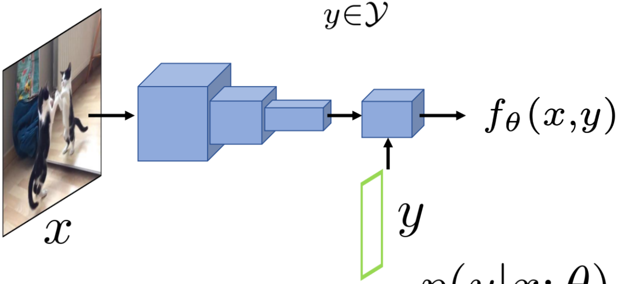
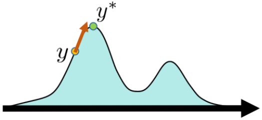
In practice, $y^\star = \operatorname{argmax}_y f_\theta(x^\star, y)$ is approximated by refining an initial estimate $\hat{y}$ via T steps of gradient ascent,

$$y \leftarrow y + \lambda \nabla_y f_\theta(x^\star, y),$$

thus finding a local maximum of $f_\theta(x^\star, y)$. Evaluation of the partition function $Z(x^\star, \theta)$ is therefore *not* required.

$$y^* = \underset{y\in\mathcal{Y}}{\arg\max}\, p(y|x;\theta) = \underset{y\in\mathcal{Y}}{\arg\max}\, f_\theta(x,y)$$





$$p(y|x;\theta) = \frac{e^{f_\theta(x,y)}}{\int e^{f_\theta(x,\tilde{y})}\mathrm{d}\tilde{y}}$$

Energy-Based Models for Regression - Training

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The DNN $f_\theta(x, y)$ can be trained using various methods for fitting a density $p(y|x;\theta)$ to observed data $\{(x_i, y_i)\}_{i=1}^N$.

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Generally, the most straightforward such method is probably to minimize the negative log-likelihood $\mathcal{L}(\theta) = -\sum_{i=1}^N \log p(y_i|x_i;\theta)$, which for the EBM $p(y|x;\theta)$ is given by,

$$\mathcal{L}(\theta) = \sum_{i=1}^N \log\left(\int e^{f_\theta(x_i,y)} dy\right) - f_\theta(x_i, y_i).$$

Energy-Based Models for Regression - Training

$$p(y|x;\theta) = \frac{e^{f_\theta(x,y)}}{Z(x,\theta)}, \quad Z(x,\theta) = \int e^{f_\theta(x,\tilde{y})} d\tilde{y}.$$

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In **Energy-Based Models for Deep Probabilistic Regression**, we simply approximated this intractable integral using importance sampling.

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Importance sampling:

$$\begin{aligned}
-\log p(y_i|x_i;\theta) &= \log\left(\int e^{f_\theta(x_i,y)} dy\right) - f_\theta(x_i,y_i) \\
&= \log\left(\int \frac{e^{f_\theta(x_i,y)}}{q(y)} q(y) dy\right) - f_\theta(x_i,y_i) \\
&\approx \log\left(\frac{1}{M}\sum_{k=1}^{M} \frac{e^{f_\theta(x_i,y^{(k)})}}{q(y^{(k)})}\right) - f_\theta(x_i,y_i), \quad y^{(k)} \sim q(y).
\end{aligned}$$

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Various alternative techniques could however also be employed to train the DNN $f_\theta(x, y)$, including noise contrastive estimation (NCE) and score matching.

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In **How to Train Your Energy-Based Model for Regression**, we therefore studied in detail how EBMs should be trained specifically for regression problems.

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In **How to Train Your Energy-Based Model for Regression**, we therefore studied in detail how EBMs should be trained specifically for regression problems.

We compared six methods on the task of 2D bounding box regression, and concluded that a simple extension of NCE should be considered the go-to training method.

Energy-Based Models for Regression - Training using NCE

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Noise contrastive estimation (NCE) entails learning to discriminate between observed data examples and samples drawn from a noise distribution.

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Noise contrastive estimation (NCE) entails learning to discriminate between observed data examples and samples drawn from a noise distribution.

Specifically, the DNN $f_\theta(x,y)$ is trained by minimizing the loss $J(\theta) = -\frac{1}{N}\sum_{i=1}^{N} J_i(\theta)$,

$$J_i(\theta) = \log \frac{\exp\{f_\theta(x_i, y_i^{(0)}) - \log q(y_i^{(0)}|y_i)\}}{\sum_{m=0}^{M} \exp\{f_\theta(x_i, y_i^{(m)}) - \log q(y_i^{(m)}|y_i)\}},$$

where $y_i^{(0)} \triangleq y_i$, and $\{y_i^{(m)}\}_{m=1}^{M}$ are M samples drawn from a noise distribution $q(y|y_i)$ that depends on the true target y_i.

Energy-Based Models for Regression - Training using NCE

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Effectively, $J(\theta)$ is the softmax cross-entropy loss for a classification problem with $M+1$ classes (which of the $M+1$ values $\{y_i^{(m)}\}_{m=0}^{M}$ is the true target y_i?).

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A simple yet effective choice for the noise distribution $q(y|y_i)$ is a mixture of K Gaussians centered at y_i,

$$q(y|y_i) = \frac{1}{K}\sum_{k=1}^{K} \mathcal{N}(y; y_i, \sigma_k^2 I).$$

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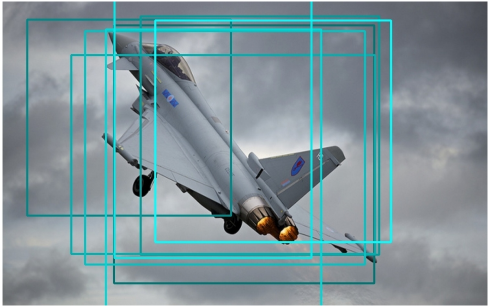

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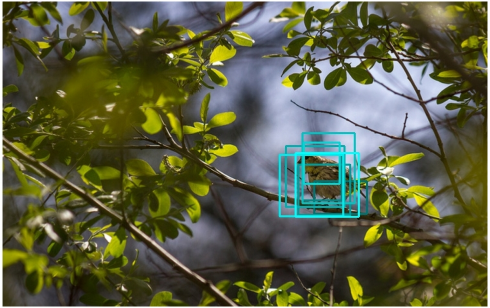

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