Introduction to Score-matching

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Goals

1. What is an energy-based model and why are they hard to train?
2. What is score-matching, and how can it be used to train an EBM?
3. How does score-matching relate to diffusion models?

Energy-Based Models (EBM)

Problem setup: Density estimation

- Observations from true model $x \sim p^*(x)$

- Ideally: Learn a model $p(x)$ that's close to $p^*(x)$
  - Capture uncertainty / variability over x

- Participation: Give examples of an x we model, and how $p(x)$ is parameterized
  - Ex: Language modeling uses Transformers for $p(x) = \prod_t p(x_t | x_{<t})$

Running example: Image generation

- "Solved": Finite-class density estimation
    - Softmax assigns a score to each $E(x)$ then normalizes

Energy fn

$$softmax(x) = \frac{\exp(E(x))}{\sum_x \exp(E(x))}$$

normalizing constant

partition function

- Image generation
    - Every change in a single pixel is a new class
    - Size: 1024 x 1024, each pixel has 256 * 3 values

Image generation models

- Autoregressive: Break down generation from left-to-right

$$p(x) = \prod_t p(x_{ij} | x_{<i,j}, x_{\bullet,<j})$$

- Latent variable model: Specify break down more flexibly

$$p(x) = \sum_z p(x|z)p(z)$$

- Energy-based model: Don't force breakdown of decision process

$$p(x) = \frac{E(x)}{\int_x E(x)}$$

EBM drawing

- Example:

x = cat or cow

$$\overbrace{E(x)} = \underbrace{\sum_i E_i(x)}$$

$E_0 \Rightarrow$ cat head

$E_1 \Rightarrow$ cow head

$E_2 \Rightarrow$ tail

$E_0(x)$

100

$E_1(x)$

200

$E_2(x)$

100

$p($  $)$

$$\frac{\underbrace{\overset{100}{E_0} + \overset{100}{E_2}}}{(\underset{100}{E_0} + \underset{100}{E_2}) + (\underset{100}{E_1} + \underset{200}{E_2})} = \frac{2}{5}$$

What is an EBM?

- Globally normalized over images x

$$p(x) = \frac{\exp(E(x))}{Z}$$

$$Z = \int_x \exp(E(x))$$

- Computation of the partition function Z is hard
  - Integrate $E(x)$ over all possible images
- Goal of training: maximize likelihood (minimize KL div)
  - Need to compute $p(x)$ and therefore Z
  - Next: How to avoid computing partition function Z

Score-matching: Training an EBM

KL divergence to Fisher divergence

- Standard: Minimize KL divergence

$$E_{p^*(x)} \log \frac{\overbrace{p^*(x)}^{\text{data}}}{\underbrace{p(x)}_{\text{model}}} = \cancel{E_{p^*(x)} \log p^*(x)} \overbrace{- E_{p^*(x)} \log p(x)}^{\text{cross-entropy}}$$

$p^*(x) = p(x)$

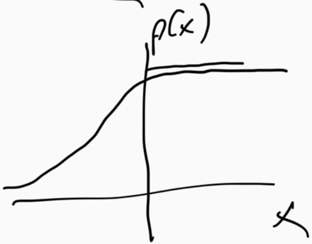
pointwise

- Issue: Can't compute $p(x)$ because of Z

- Instead: Give up on equality := KL div

Approximation lemma (made up)

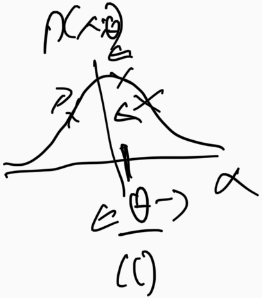
- Two continuous functions are equal iff they are pointwise equal $p^*(x) = p(x)$
- ALSO: Two continuous functions are equal iff their derivatives are equal $\nabla_x p^*(x) = \nabla_x p(x)$ up to a constant



Fisher divergence intuition

$\rightarrow \nabla_\theta \log p(x;\theta) \neq$

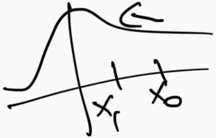
- If two density fns are equal, have the same Stein score $s(x) = \nabla_x \underbrace{\log p(x)}$
- Can use the Stein score to get good samples / find likely x
  - Langevin dynamics: follow score + noise
- Lose ability to compute likelihoods, can only use score model for sampling



(1) $\nabla_\theta \log p(x;\theta)$

(2) $\nabla_x \log p(x;\theta)$

$x^{(0)} \rightarrow$ following $\nabla_x \log p(x)$



Minimize Fisher divergence = Score matching

- Minimize Fisher divergence to avoid computing Z

$$E_{p^*(x)} \left\| \nabla_x \log \frac{p^*(x)}{p(x)} \right\|_2^2 = E_{p^*(x)} \left\| \nabla_x \log p^*(x) - \nabla_x \log p(x) \right\|_2^2$$

- Notation: Introduce Stein score $s(x) = \nabla_x \log p(x)$

$$E_{p^*(x)} \left\| \nabla_x \log p^*(x) - \nabla_x \log p(x) \right\|_2^2 = E_{p^*(x)} \left\| \nabla_x \log p^*(x) - s(x) \right\|_2^2$$

- Parameterize $s(x)$ directly instead of $p(x)$, avoid computing Z

Issues in training an EBM

Fisher Div

$$\underbrace{E_{p^*(x)}}\,\|\nabla_x \log \overbrace{\underbrace{p^*(x)}}\, - s(x)\|_2^2$$

1) Solved: Cant compute $p(x)$ b/c of Z => model Stein score $\underbrace{s(x) = \nabla_x \log p(x)}$

2) Unknown p^*: Dont know $p^*(x)$ or its score

3) Covariate shift: $E_{p^*(x)}$ is problematic because of covariate shift

Avoiding p^*: Implicit score matching

Hyvarinen 2005

- Can rewrite the explicit score matching objective to avoid p^*

$$\min \quad E_{p^*(x)}\left[\|\nabla_x \cancel{\log p^*(x)} - s(x)\|_2^2\right] \approx E_{p^*(x)}\left[\frac{1}{2}\|s(x)\|_2^2 + tr(\nabla_x s(x))\right] \qquad (1)$$

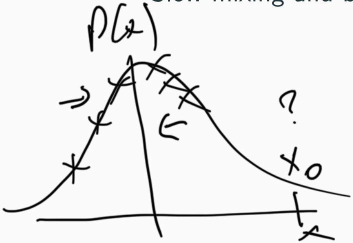
- Second term is nasty: $s(x) \in R^d$, $\nabla_x s(x) \in R^{d\times d}$ $\quad s(x) = \nabla_x \log p(x)$
- Solution: Use Hutchinson's trace estimator

$$E_{p^*(x)}\left[\frac{1}{2}\|s(x)\|_2^2 + tr(\nabla_x s(x))\right] = E_{v\sim N(0,I_d)}E_{p^*(x)}\left[\frac{1}{2}\|s(x)\|_2^2 + v^T\nabla_x s(x))v\right]$$

- Easy to implement with pytorch

Covariate shift

- Sample via Langevin dynamics := Start with random point and follow score + noise
  - Score is trained on examples drawn from $p^*(x)$
  - Score is bad on regions of low $p^*(x)$, eg random points
  - Slow mixing and bad samples



Solution to cov shift

- Solution: sample perturbed $x \sim p^*(x)$ with multiple noise scales $\{\sigma_i\}$
  - Interpretation: Data augmention + smooth out samples
  - Need to have score model condition on noise $s(x; \sigma_i)$

$\sigma_1 = 0.1$

$N(x, 0.1)$

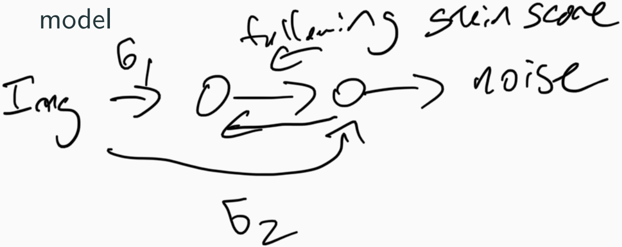
Summary

- Intractable partition function => Model (Stein) score
  - Pointwise equality => derivative equality
  - Lose ability to compute likelihoods, can only use score model for sampling
  - Sample via Langevin dynamics (follow grad+noise)
- Don't know data score: Rewrite objective to avoid $\nabla_x p^*(x)$
  - Results in some nasty expressions => Estimate with Hutchinson trace estimator
- Add multiple noise scales to help learning score at random points

Connection to diffusion models

Diffusion models

- Hierarchical VAE perspective: forward / reverse process vs noised marginals + score model



- SDE: continuous-time extension of score matching (time = the noise scale)

Credits

- Ayan Das' blog post
- Lyu 2009
- Vincent 2011
- Song 2019