Generalized Energy-Based Models

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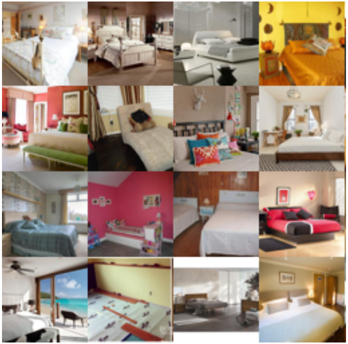
Deepmind

Columbia Statistics, 2023

Training generative models

- Have: One collection of samples X from unknown distribution P.
- Goal: generate samples Q that look like P

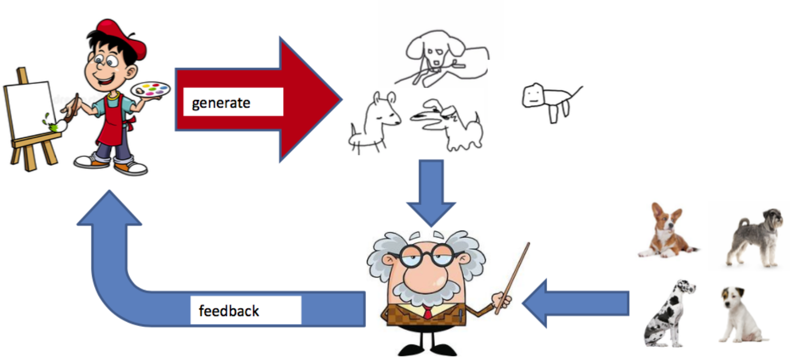


LSUN bedroom samples P

Generated Q, MMD GAN

Role of divergence $D(P, Q)$?

Visual notation: GAN setting



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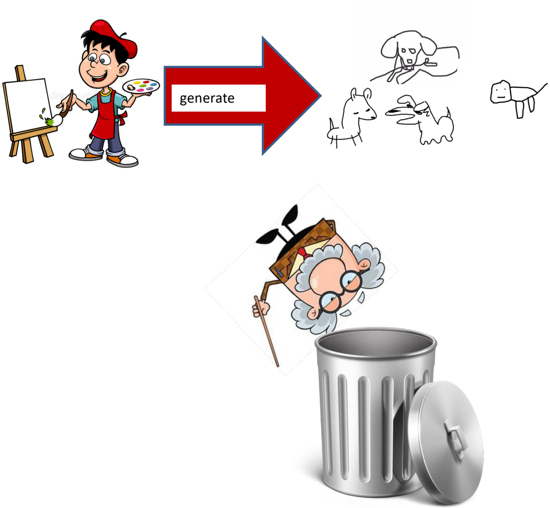


Outline

Divergences $D(P, Q)$

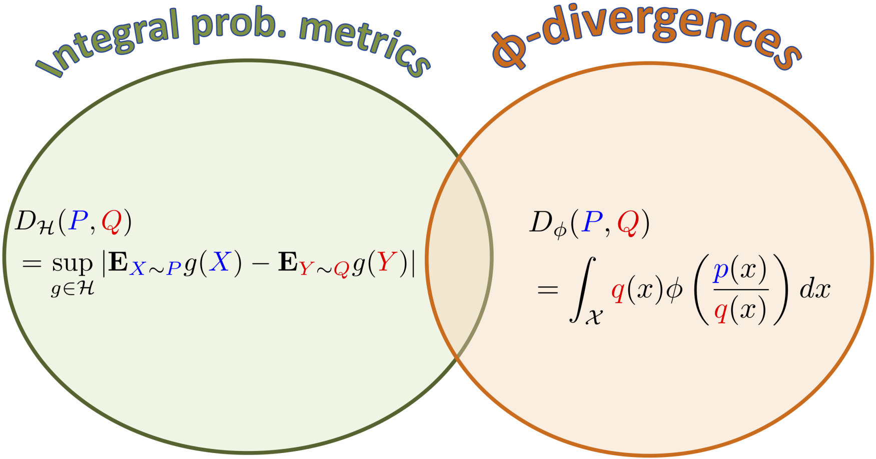
- ϕ-divergences (f-divergences) and a variational lower bound (KL)

Generalized energy-based models

- "Like a GAN" but incorporate critic into sample generation
- Perform better than using generator alone

Arbel, Zhou, G., Generalized Energy Based Models (ICLR 2021)

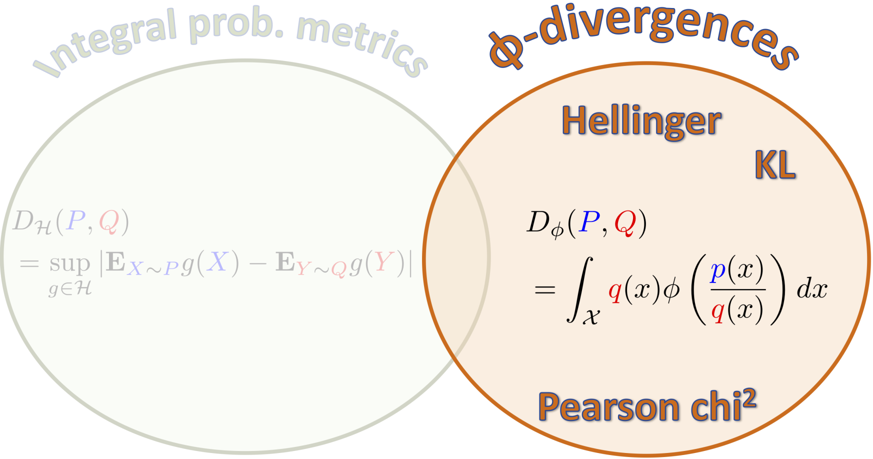
Divergences



$$D_{\mathcal{H}}(P, Q) = \sup_{g \in \mathcal{H}} \left| \mathbf{E}_{X \sim P} g(X) - \mathbf{E}_{Y \sim Q} g(Y) \right|$$

$$D_{\phi}(P, Q) = \int_{\mathcal{X}} q(x) \phi\left(\frac{p(x)}{q(x)}\right) dx$$

The ϕ-divergences



The ϕ-divergences

Define the ϕ-divergence(f-divergence):

$$D_\phi(P, Q) = \int \phi\left(\frac{p(z)}{q(z)}\right) q(z)dz$$

where ϕ is convex, lower-semicontinuous, $\phi(1) = 0$.

- Example: $\phi(u) = u\log(u)$ gives KL divergence,

$$D_{KL}(P, Q) = \int \log\left(\frac{p(z)}{q(z)}\right) p(z)dz$$
$$= \int \left(\frac{p(z)}{q(z)}\right) \log\left(\frac{p(z)}{q(z)}\right) q(z)dz$$

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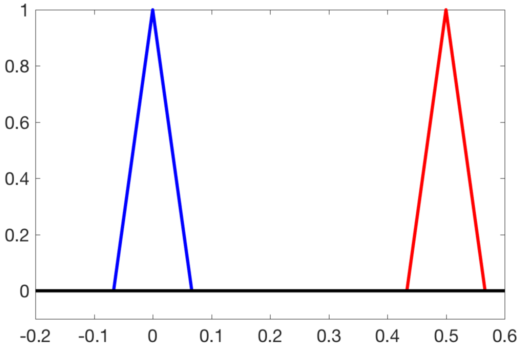
Are ϕ-divergences good critics?

Simple example: disjoint support.

Goodfellow et al. (NeurIPS 2014), Arjovsky and Bottou [ICLR 2017]

$$D_{KL}(P, Q) = \infty \qquad D_{JS}(P, Q) = \log 2$$



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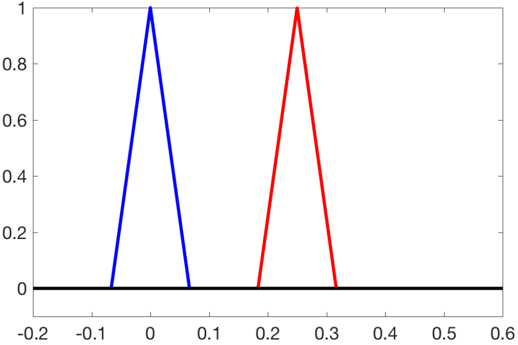
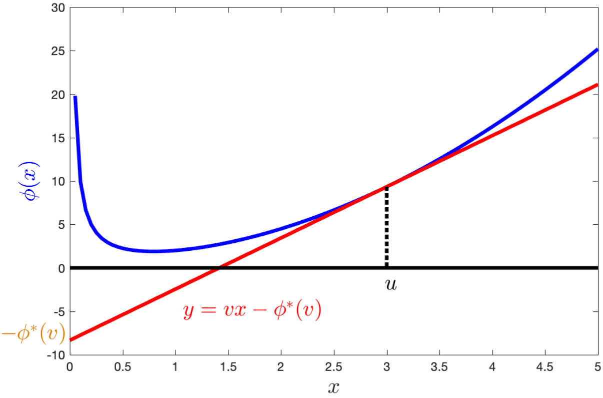


ϕ-divergences in practice

Notation: the conjugate (Fenchel) dual

$$\phi^*(v) = \sup_{u \in \mathbb{R}} \{uv - \phi(u)\}.$$



- $\phi^*(v)$ is negative intercept of tangent to ϕ with slope v

ϕ-divergences in practice

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- For a convex l.s.c. ϕ we have

$$\phi^{**}(x) = \phi(x) = \sup_{v \in \mathbb{R}} \{xv - \phi^*(v)\}$$

ϕ-divergences in practice

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- KL divergence:

$$\phi(x) = x \log(x) \qquad \phi^*(v) = \exp(v - 1)$$

A variational lower bound

A lower-bound ϕ-divergence approximation:

$$D_\phi(P, Q) = \int q(z)\phi\left(\frac{p(z)}{q(z)}\right) dz$$

Nguyen, Wainwright, Jordan, IEEE Transactions on Information Theory (2010);
Nowozin, Cseke, Tomioka, NeurIPS (2016)

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$\phi^*(v)$ is dual of $\phi(x)$.

A variational lower bound

A lower-bound ϕ-divergence approximation:

$$
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&\geq \sup_{f \in \mathcal{H}} \mathrm{E}_P f(X) - \mathrm{E}_Q \phi^*(f(Y))
\end{aligned}
$$

(restrict the function class)

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(restrict the function class)

Bound tight when:

$$f^\diamond(z) = \partial\phi\left(\frac{p(z)}{q(z)}\right)$$

if ratio defined.

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Case of the KL

$$D_{KL}(P, Q) = \int \log\left(\frac{p(z)}{q(z)}\right) p(z)\, dz$$

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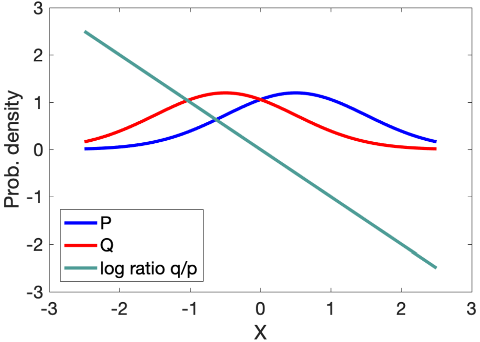

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$$\approx \sup_{f \in \mathcal{H}} \left[-\frac{1}{n}\sum_{j=1}^{n} f(x_i) - \frac{1}{n}\sum_{i=1}^{n} \exp(-f(y_i))\right] + 1$$

$$x_i \overset{\text{i.i.d.}}{\sim} P$$

$$y_i \overset{\text{i.i.d.}}{\sim} Q$$

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This is a

KL

Approximate

Lower-bound

Estimator.

Nguyen, Wainwright, Jordan, IEEE Transactions on Information Theory (2010);
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The KALE divergence

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Empirical properties of KALE

$$KALE(P, Q; \mathcal{H}) = \sup_{f \in \mathcal{H}} -E_P f(X) - E_Q \exp(-f(Y)) + 1$$

$$f = \langle w, \phi(x) \rangle_{\mathcal{H}} \qquad \mathcal{H} \text{ an RKHS}$$

$$\|w\|^2_{\mathcal{H}} \quad \text{penalized :}$$

Glaser, Arbel, G. "KALE Flow: A Relaxed KL Gradient Flow for Probabilities with Disjoint Support," (NeurIPS 2021, Section 2)

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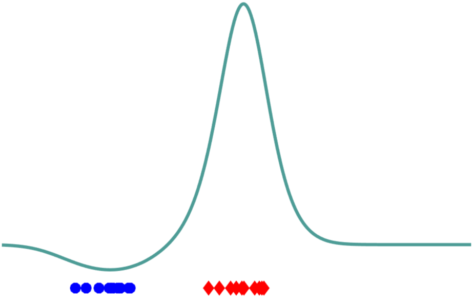
$$\|w\|_{\mathcal{H}}^2 \quad \text{penalized : KALE smoothie}$$

$$KALE(Q, P; \mathcal{H}) = 0.18$$



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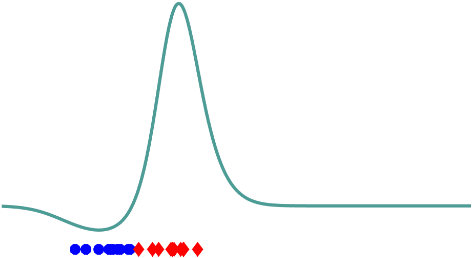
$$KALE(Q, P; \mathcal{H}) = 0.12$$



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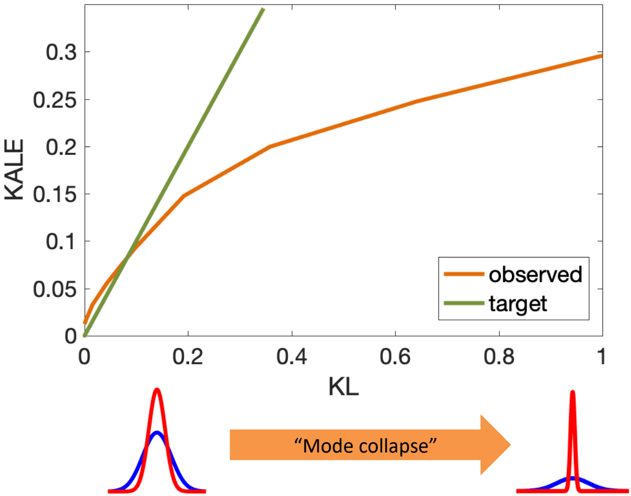
The KALE smoothie and "mode collapse"

- Two Gaussians with same means, different variance



Example thanks to M. Arbel and M. Rosca

Topological properties of KALE (1)

Key requirements on $\mathcal{H}$ and $\mathcal{X}$:

- Compact domain $\mathcal{X}$,
- $\mathcal{H}$ dense in the space $C(\mathcal{X})$ of continuous functions on $\mathcal{X}$ wrt $\|\cdot\|_\infty$.
- If $f \in \mathcal{H}$ then $-f \in \mathcal{H}$ and $cf \in \mathcal{H}$ for $0 \leq c \leq C_{\mathtt{max}}$.

Theorem: $KALE(P, Q; \mathcal{H}) \geq 0$ and $KALE(P, Q; \mathcal{H}) = 0$ iff $P = Q$.

Zhang, Liu, Zhou, Xu, and He. "On the Discrimination-Generalization Tradeoff in GANs"

(ICLR 2018, Corollary 2.4; Theorem B.1)
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$\mathcal{H}$ dense in $C(\mathcal{X})$ for $\mathcal{X} \subset \mathbb{R}^d$ when:

$$\mathcal{H} = \text{span}\{\sigma(w\top x + b) : [w, b] \in \Theta\}$$

$\sigma(u) = \max\{u, 0\}^\alpha$, $\alpha \in \mathbb{N}$, and $\{\lambda\theta : \lambda \ge 0, \theta \in \Theta\} = \mathbb{R}^{d+1}$.

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Topological properties of KALE (2)

Additional requirement: all functions in $\mathcal{H}$ Lipschitz in their inputs with constant L

Theorem: $KALE(P, Q^n; \mathcal{H}) \to 0$ iff $Q^n \to P$ under the weak topology.

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Partial proof idea:

$$\begin{aligned}
KALE(P, Q; \mathcal{H}) &= -\int f \, dP - \int \exp(-f) \, dQ + 1 \\
&= \int f(x) \, dQ(x) - f(x') \, dP(x') \\
&\quad - \int \underbrace{(\exp(-f) + f - 1)}_{\geq 0} \, dQ \\
&\leq \int f(x) \, dQ(x) - f(x') \, dP(x') \leq L W_1(P, Q)
\end{aligned}$$

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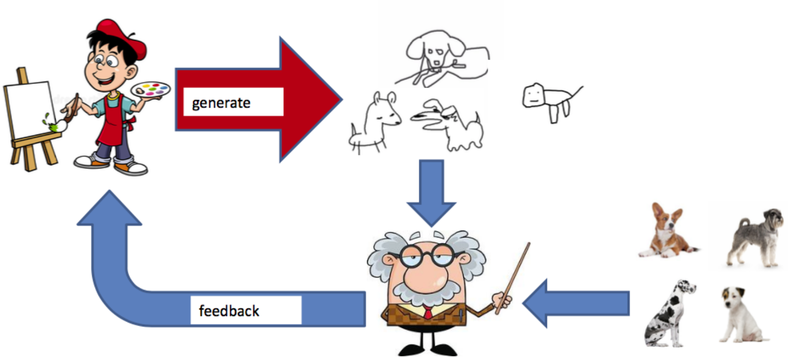
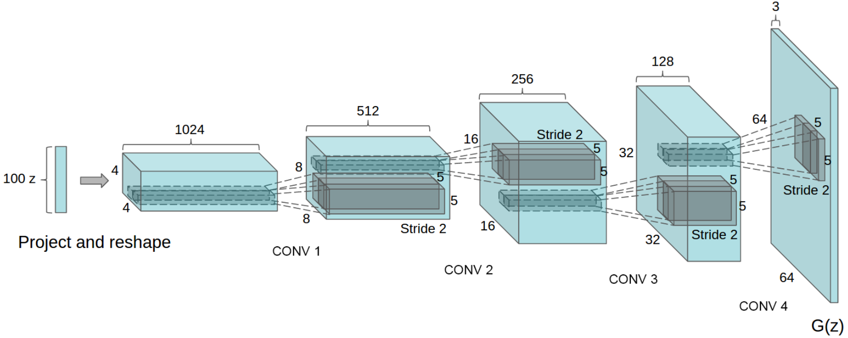


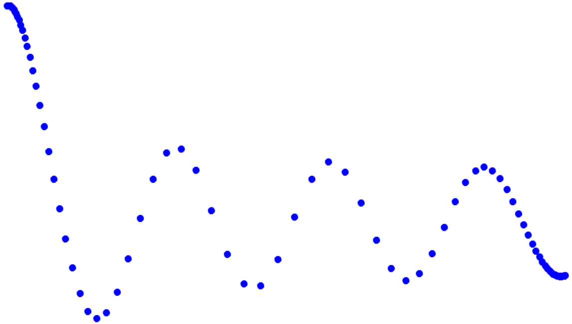
Reminder: the generator



Radford, Metz, Chintala, ICLR 2016

Generalized Energy-Based Models - the idea

Target distribution P



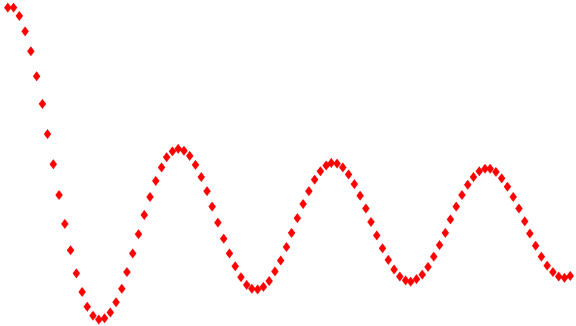
Arbel, Zhou, G. (ICLR 2021)

Generalized Energy-Based Models - the idea

GAN (generator)

$$X \sim Q_\theta \quad \Longleftrightarrow \quad X = B_\theta(Z), \quad Z \sim \eta,$$

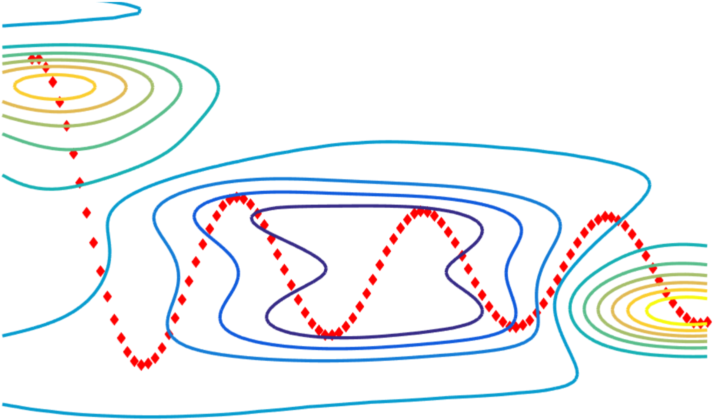
correct support but wrong mass



Arbel, Zhou, G. (ICLR 2021)

Generalized Energy-Based Models - the idea

Log energy function and Q_θ



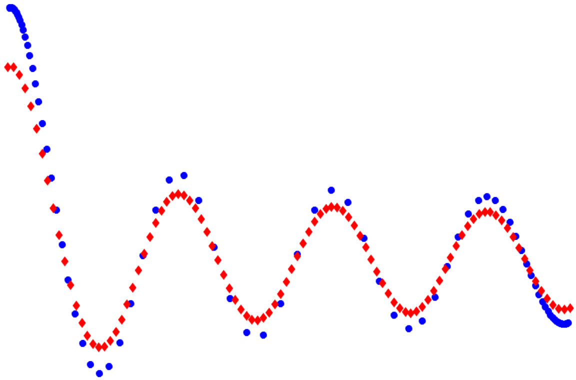
Key:

- Orange: increase mass
- Blue: reduce mass

Arbel, Zhou, G. (ICLR 2021)

Generalized Energy-Based Models - the idea

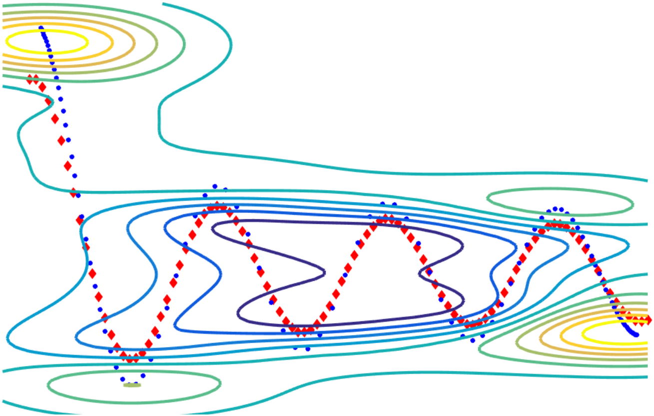
Target distribution P and GAN (generator) Q_θ, wrong support and wrong mass



Arbel, Zhou, G. (ICLR 2021)

Generalized Energy-Based Models - the idea

Log energy function, P, and Q_θ



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Generalized energy-based models

Define a model $Q_{B_\theta, E}$ as follows:

- Sample from generator with parameters θ

$$X \sim Q_\theta \quad \iff \quad X = B_\theta(Z), \quad Z \sim \eta$$

- Reweight the samples according to importance weights:

$$f_{Q,E}(x) = \frac{\exp(-E(x))}{Z_{Q_\theta,E}}, \qquad Z_{Q,E} = \int \exp(-E(x))\, d\, Q_\theta(x),$$

  where $E \in \mathcal{E}$, the energy function class.

  $f_{Q,E}(x)$ is Radon-Nikodym derivative of $Q_{B_\theta, E}$ wrt Q_θ.

- When Q_θ has density wrt Lebesgue on $\mathcal{X}$, standard energy-based model (special case)
- Sample from model via HMC on posterior of Z.

Arbel, Zhou, G. (ICLR 2021)

How do we learn the energy E?

How do we learn the energy E?

Fit the model using Generalized Log-Likelihood:

$$\mathcal{L}_{P,Q}(E) := \int \log(f_{Q,E})\, dP = -\int E\, dP - \log Z_{Q,E}$$

- When $KL(P, Q_\theta)$ well defined, above is Donsker-Varadhan lower bound on KL
  - tight when $E(z) = -\log(p(z)/q(z))$.
- However, Generalized Log-Likelihood still defined when P and Q_θ mutually singular (as long as E smooth)!

KALE and the energy function

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One last trick...(convexity of exponential)

$$-\log \int \exp(-E)\, dQ_\theta \geq -c - e^{-c} \int \exp(-E)\, dQ_\theta + 1$$

tight whenever $c = \log \int \exp(-E)\, dQ_\theta$.

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Generalized Log-Likelihood has the lower bound:

$$\mathcal{L}_{P,Q}(E) \geq -\int (E + c)\, dP - \int \exp(-E - c)\, dQ_\theta + 1$$

$$:= \mathcal{F}(P, Q_\theta; \mathcal{E} + \mathbb{R})$$

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This is the KALE! with function class $\mathcal{E} + \mathbb{R}$.

KALE and the energy function

Fit the model using Generalized Log-Likelihood:

$$\mathcal{L}_{P,Q}(E) := \int \log(f_{Q,E})\, dP = -\int E\, dP - \log \int \exp(-E)\, dQ_\theta$$

One last trick...(convexity of exponential)

$$-\log \int \exp(-E)\, dQ_\theta \geq -c - e^{-c} \int \exp(-E)\, dQ_\theta + 1$$

tight whenever $c = \log \int \exp(-E)\, dQ_\theta$.

Generalized Log-Likelihood has the lower bound:

$$\mathcal{L}_{P,Q}(E) \geq -\int (E + c)\, dP - \int \exp(-E - c)\, dQ_\theta + 1$$
$$:= \mathcal{F}(P, Q_\theta; \mathcal{E} + \mathbb{R})$$

Jointly maximizing yields the maximum likelihood energy E^* and corresponding $c^* = \log \int \exp(-E)\, dQ_\theta$.

Training the base measure (generator)

Recall the generator:

$$X = B_\theta(Z), \quad Z \sim \eta$$

Define: $\mathcal{K}(\theta) := \mathcal{F}(P, Q_\theta; \mathcal{E} + \mathbb{R})$

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Theorem: $\mathcal{K}$ is lipschitz and differentiable for almost all $\theta \in \Theta$ with:

$$\nabla \mathcal{K}(\theta) = Z_{Q,E^*}^{-1} \int \nabla_x E^*(B_\theta(z)) \nabla_\theta B_\theta(z) \exp(-E^*(B_\theta(z)))\eta(z)\, dz.$$

where E^* achieves supremum in $\mathcal{F}(P, Q; \mathcal{E} + \mathbb{R})$.

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Assumptions:

- Functions in $\mathcal{E}$ parametrized by $\psi \in \Psi$, where Ψ compact,
  - jointly continous w.r.t. (ψ, x), L-lipschitz and L-smooth w.r.t. x.
- $(\theta, z) \mapsto B_\theta(z)$ jointly continuous wrt (θ, z), $z \mapsto B_\theta(z)$ uniformly Lipschitz w.r.t. z, lipschitz and smooth wrt θ (see paper: constants depend on z)

Sampling from the model

Consider end-to-end model $Q_{B_\theta, E}$, where recall that
$X = B_\theta(Z), \quad Z \sim \eta,$

$$f_{B,E}(x) := \frac{\exp(-E(x))}{Z_{Q,E}}$$

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$$f_{B,E}(x) := \frac{\exp(-E(x))}{Z_{Q,E}}$$

For a test function g,

$$\int g(x)dQ_{B,E}(x) = \int g(B(z))f_{B,E}(B(z))\eta(z)dz$$

Posterior latent distribution therefore

$$\nu_{B,E}(z) = \eta(z)f_{B,E}(B(z))$$

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Posterior latent distribution therefore

$$\nu_{B,E}(z) = \eta(z) f_{B,E}(B(z))$$

Sample $z \sim \nu_{B,E}$ via Langevin diffusion-derived algorithms (MALA, ULA, HMC,...) to exploit gradient information.

Generate new samples in $\mathcal{X}$ via

$$X \sim Q_{B,E} \quad \Longleftrightarrow \quad Z \sim \nu_{B,E}, \quad X = B_\theta(Z).$$

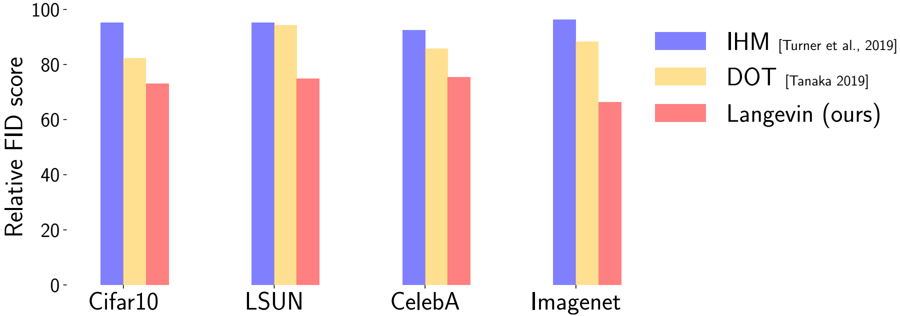
Experiments

Examples: sampling at modes

Tempered GEBM Cifar10 samples at different stages of sampling using a Kinetic Langevin Algorithm (KLA). Early samples → late samples. Model run at *low temperature* ($\beta = 100$) for better quality samples.

Sampling at modes: results

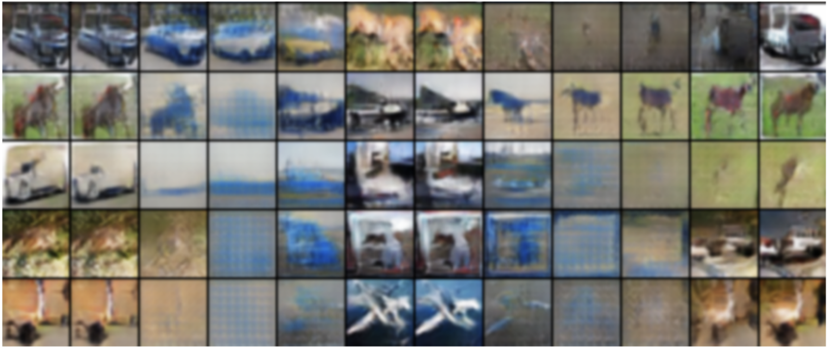
The relative FID score: $\frac{\mathrm{FID}(Q_{B_\theta,E})}{\mathrm{FID}(B_\theta)}$



For a given generator B_θ and energy E, samples always better (FID score) than generator alone.

Examples: moving between modes

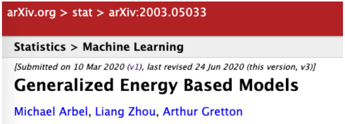
Tempered GEBM Cifar10 samples at different stages of sampling using KLA. Early samples → late samples.
Model run at *lower friction* (but still low temperature, $\beta = 100$) for mode exploration.



Summary

- Generalized energy based model:
  - End-to-end model incorporating generator and critic
  - Always better samples than generator alone.
- ICLR 2021

https://github.com/MichaelArbel/GeneralizedEBM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Generalized Energy Based Models

Michael Arbel, Liang Zhou, Arthur Gretton

Summary

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Research support

Work supported by:

The Gatsby Charitable Foundation

Deepmind

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Post-credit scene: MMD flow

From NeurIPS 2019:

Maximum Mean Discrepancy Gradient Flow

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Sanity check: reduction to EBM case

Base measure B_θ is real NVP with closed-form density.