Generative Ratio Matching Networks

Akash Srivastava[*,1,2], Kai Xu[*,3], Michael U. Gutmann[3], Charles Sutton[3,4,5]

∗ denotes equal contributions
[1]MIT-IBM Watson AI Lab [2]IBM Research [3]University of Edinburgh [4]Google AI [5]Alan Turing Institute

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Introduction and motivations

Implicit deep generative models: $x = \mathrm{NN}(z; \theta)$ where $z \sim$ noise

Maximum mean discrepancy networks (MMD-nets)

- ❌ can only work well with **low-dimensional** data
- ✅ are very **stable** to train by avoiding the saddle-point optimization problem

Adversarial generative models (e.g. GANs, MMD-GANs)

- ✅ can generate **high-dimensional** data such as natural images
- ❌ are very **difficult** to train due to the saddle-point optimization problem

Q: Can we have two ✅✅?
A: Yes. Generative ratio matching (GRAM) is a *stable* learning algorithm for *implicit* deep generative models that does **not** involve a saddle-point optimization problem and therefore is easy to train 🎉.

Background: maximum mean discrepancy

The maximum mean discrepancy (MMD) between two distributions p and q is defined as

$$\mathrm{MMD}_{\mathcal{F}}(p, q) = \sup_{f \in \mathcal{F}} \left(\mathbb{E}_p[f(x)] - \mathbb{E}_q[f(x)] \right)$$

Gretton et al. (2012) shows that it is sufficient to choose $\mathcal{F}$ to be a unit ball in an reproducing kernel Hilbert space (RKHS) $\mathcal{R}$ with a characteristic kernel k s.t.

$$\mathrm{MMD}_{\mathcal{F}}(p, q) = 0 \iff p = q$$

The empirical estimate of the (squared) MMD with $x_i \sim p$ and $y_j \sim q$ by Monte Carlo is

$$\hat{\mathrm{MMD}}^2_{\mathcal{R}}(p, q) = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i'=1}^{N} k(x_i, x_{i'}) - \frac{2}{NM} \sum_{i=1}^{N} \sum_{j=1}^{M} k(x_i, y_j) + \frac{1}{M^2} \sum_{j=1}^{M} \sum_{j'=1}^{M} k(y_j, y_{j'})$$

MMD-nets trains neural generators by minimizing this empirical estimate.

Background: density ratio estimation via moment matching

Density ratio estimation: find $\hat{r}(x) \approx r(x) = \frac{p(x)}{q(x)}$ with samples from p and q

Finite moments under the fixed design setup gives $\hat{\mathbf{r}}_q = [\hat{r}(x_1^q), ..., \hat{r}(x_M^q)]$ for $x^q \sim q$

$$\min_r \left(\int \phi(x) p(x) dx - \int \phi(x) r(x) q(x) dx \right)^2$$

Huang et al. (2007) shows that by changing $\phi(x)$ to $k(x;.)$, where k is a characteristic kernel in RKHS, we can match infinite moments and the optimization below agrees with the true $r(x)$

$$\min_{r \in \mathcal{R}} \left\| \int k(x;.) p(x) dx - \int k(x;.) r(x) q(x) dx \right\|_{\mathcal{R}}^2$$

Analytical solution: $\hat{\mathbf{r}} = \mathbf{K}_{q,q}^{-1} \mathbf{K}_{q,p} \mathbf{1}$, where $[\mathbf{K}_{p,q}]_{i,j} = k(x_i^p, x_j^q)$ given samples $\{x_i^p\}$ and $\{x_j^q\}$.

GRAM: an overview

Two targets in the training loop

1. Learning a projection function f_θ that maps the data space into a low-dimensional manifold which preserves the density ratio between data and model.
   - "Preserves": $\frac{p_x(x)}{q_x(x)} = \frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))}$, measured by $D(\theta) = \int q_x(x) \left(\frac{p_x(x)}{q_x(x)} - \frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} \right)^2 dx$
   - ❓ $\frac{p_x(x)}{q_x(x)}$ is hard to estimate in the high-dimensional space ...
2. Matching the model G_γ to data in the low-dimensional manifold by minimizing MMD
   - 👍 MMD works well in low dimensional space
   - $\mathrm{MMD} = 0$ ➡️ $\frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} = 1$ ➡️ $\frac{p_x(x)}{q_x(x)} = 1$

Both with empirical estimates based on samples from the data $\{x_i^p\}$ and the model $\{x_j^q\}$.

f_θ and G_γ are simultaneously updated.

GRAM: tractable ratio matching

1️⃣ Learning the projection function $f_\theta(x)$ by minimizing the squared difference

$$
\begin{aligned}
D(\theta) &= \int q_x(x) \left(\frac{p_x(x)}{q_x(x)} - \frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} \right)^2 dx \\
&= C - 2 \int p_x(x) \frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} dx + \int q_x(x) \left(\frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} \right)^2 dx \\
&= C - 2 \int \bar{p}(f_\theta(x)) \frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} df_\theta(x) + \int \bar{q}(f_\theta(x)) \left(\frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} \right)^2 df_\theta(x) \\
&= C' - \left(\int \bar{q}(f_\theta(x)) \left(\frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} \right)^2 df_\theta(x) - 1 \right) = C' - \mathrm{PD}(\bar{q}, \bar{p})
\end{aligned}
$$

... or by equivalently maximizing the Pearson divergence 😄.

A reminder on LOTUS: $\int p(x) g(f(x)) dx = \int p(f(x)) g(f(x)) df(x)$

[1]: A derivation of the reverse order for a special case of projection functions was also shown in (Sugiyama et al., 2011).

GRAM: Pearson divergence maximization

Monte Carlo approximation of PD

$$\mathrm{PD}(\bar{q}, \bar{p}) = \int \bar{q}(f_\theta(x)) \left(\frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))} \right)^2 df_\theta(x) - 1 \approx \frac{1}{N} \sum_{i=1}^{N} \left(\frac{\bar{p}(f_\theta(x_i^q))}{\bar{q}(f_\theta(x_i^q))} \right)^2 - 1$$

where $x_i^q \sim q_x$ or equivalently $f_\theta(x_i^q) \sim \bar{q}$.

Given samples $\{x_i^p\}$ and $\{x_j^q\}$, we use the density ratio estimator based on infinite moments matching (Huang et al., 2007, Sugiyama et al., 2012) under the fixed-design setup

$$\hat{\mathbf{r}}_{q,\theta} = \mathbf{K}_{q,q}^{-1} \mathbf{K}_{q,p} \mathbf{1} = [\hat{r}_\theta(x_1^q), \ldots, \hat{r}_\theta(x_M^q)]^\top$$

where $[\mathbf{K}_{p,q}]_{i,j} = k(f_\theta(x_i^p), f_\theta(x_j^q))$ and $r_\theta(x) = \frac{\bar{p}(f_\theta(x))}{\bar{q}(f_\theta(x))}$.

GRAM: matching projected model to projected data

2️⃣ Minimizing the empirical estimator of MMD in the low-dimensional manifold

$$\min_{\gamma}\Bigg[\frac{1}{N^2}\sum_{i=1}^{N}\sum_{i'=1}^{N}k(f_\theta(x_i), f_\theta(x_{i'})) - \frac{2}{NM}\sum_{i=1}^{N}\sum_{j=1}^{M}k(f_\theta(x_i), f_\theta(G_\gamma(z_j))) + \frac{1}{M^2}\sum_{j=1}^{M}\sum_{j'=1}^{M}k(f_\theta(G_\gamma(z_j)), f_\theta(G_\gamma(z_{j'})))\Bigg]$$

with respect to its parameters γ.

GRAM: the complete algorithm

Loop until convergence

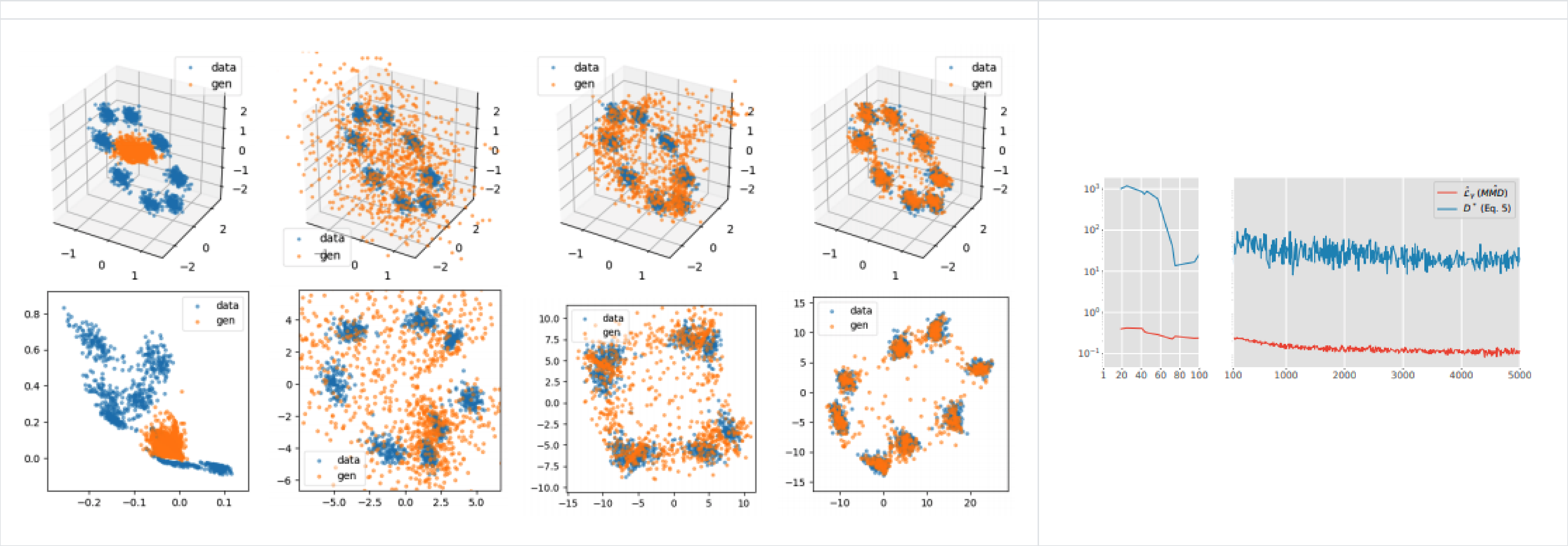
1. Sample a minibatch of data and generate samples from G_γ
2. Project data and generated samples using f_θ
3. Compute the kernel Gram matrices using Gaussian kernels in the projected space
4. Compute the objectives for f_θ and G_γ using the same kernel Gram matrices
5. Backprop two objectives to get the gradients for θ and γ
6. Perform gradient update for θ and γ

😎 Fun fact: the objectives in our GRAM algorithm both heavily relies on the use of kernel Gram matrices.

How do GRAM-nets compare to other deep generative models

GAN	MMD-net	MMD-GAN	GRAM-net
$\begin{tikzcd} z \sim p_z \arrow[d, "\gamma"] & \\ x^q \arrow[d, "\theta"] \arrow[dr, "\theta"] & x^p \sim p_x \arrow[d, dashed, "\theta"] \\ \mathcal{L}_\gamma \arrow[r, dotted, no head] & \mathcal{L}_\theta \end{tikzcd}$	$\begin{tikzcd} z \sim p_z \arrow[d, "\gamma"] & x^p \sim p_x \arrow[d] \\ x^q \arrow[r] & \mathbf{K} \arrow[dl] \\ \mathcal{L}_\gamma & \end{tikzcd}$	$\begin{tikzcd} z \sim p_z \arrow[d, "\gamma"] & x^p \sim p_x \arrow[d, "\theta"] \\ x^q \arrow[d, "\theta"] & f_\theta(x^p) \arrow[d] \\ f_\theta(x^q) \arrow[r] & \mathbf{K} \arrow[dl] \arrow[d] \\ \mathcal{L}_\gamma \arrow[r, dotted, no head] & \mathcal{L}_\theta \end{tikzcd}$	$\begin{tikzcd} z \sim p_z \arrow[d, "\gamma"] & x^p \sim p_x \arrow[d, "\theta"] \\ x^q \arrow[d, "\theta"] & f_\theta(x^p) \arrow[d] \\ f_\theta(x^q) \arrow[r] & \mathbf{K} \arrow[dl] \arrow[d] \\ \mathcal{L}_\gamma & \mathcal{L}_\theta \end{tikzcd}$

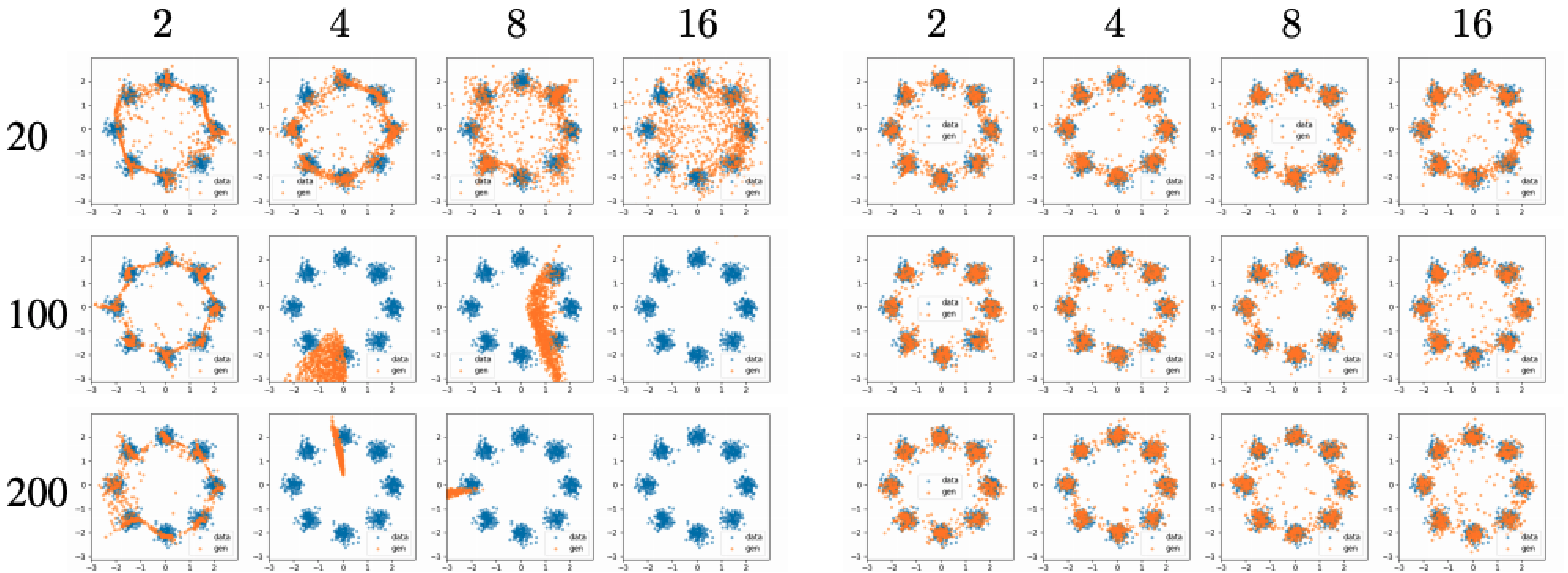
Illustration of GRAM training



Blue: data, Orange: samples

Top: original, Bottom: projected

Evaluations: the stability of models

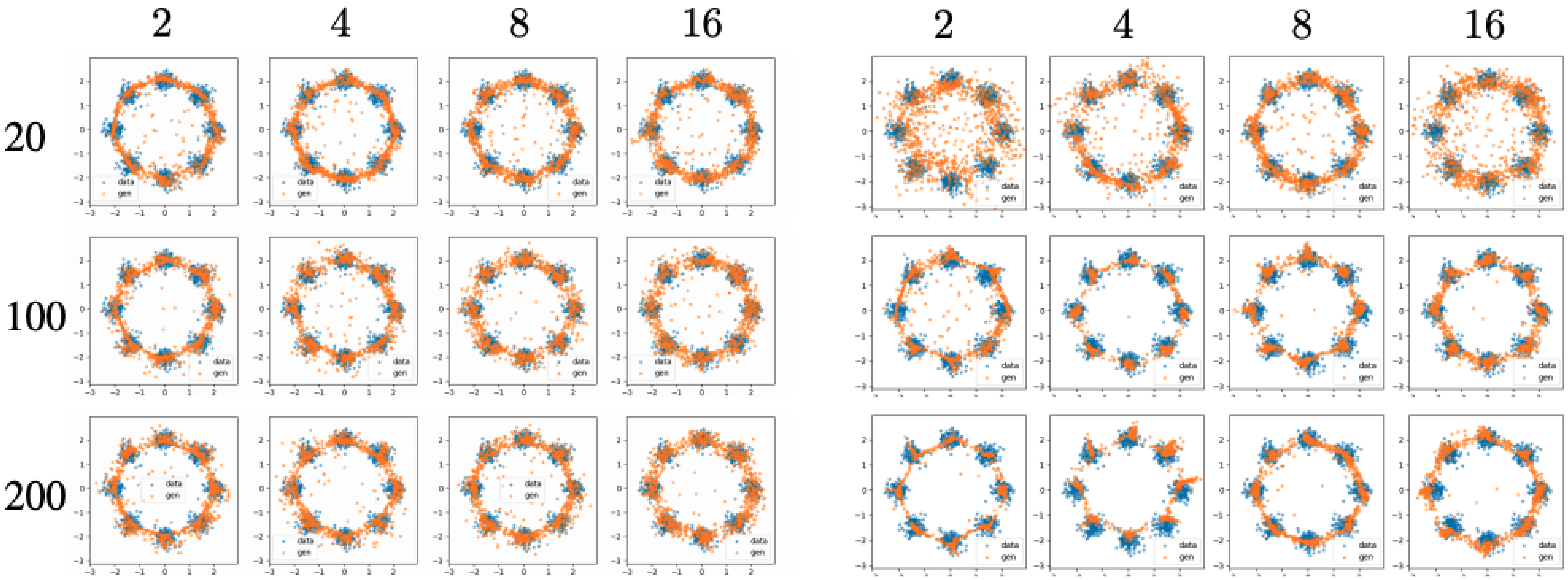


(a) GAN

(b) GRAM-net

x-axis = noise dimension and y-axis = generator layer size

Evaluations: the stability of models (continued)



(a) MMD-nets (b) MMD-GANs

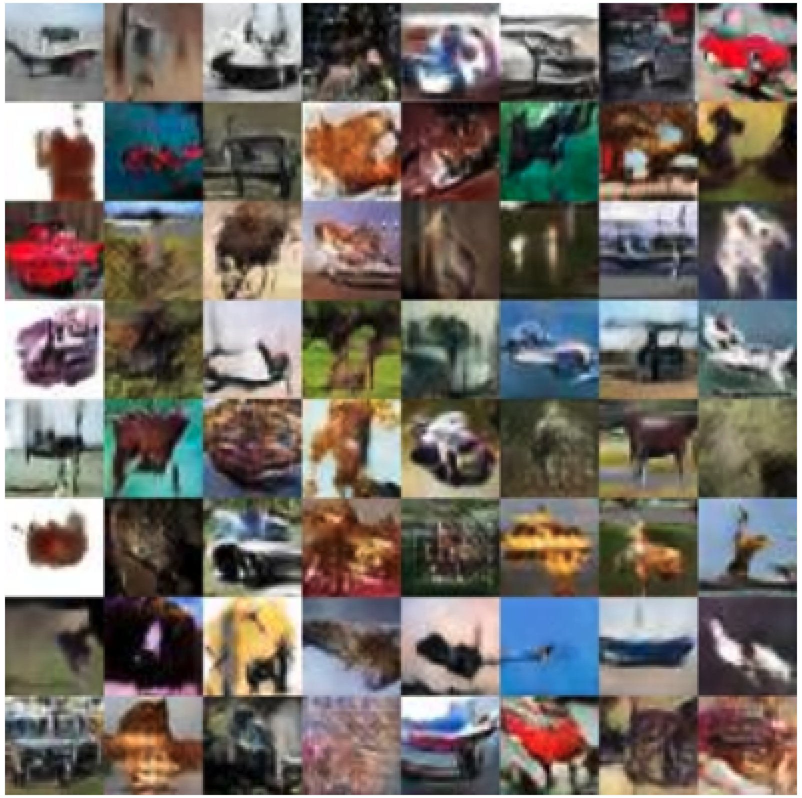
x-axis = noise dimension and y-axis = generator layer size

Quantitative results: sample quality

Table 1: Sample quality (measured by FID; lower is better) of GRAM-nets compared to GANs.

Arch.	**Dataset**	**MMD-GAN**	**GAN**	**GRAM-net**
DCGAN	Cifar10	40.00 ± 0.56	26.82 ± 0.49	$\mathbf{24.85 \pm 0.94}$
Weaker	Cifar10	210.85 ± 8.92	31.64 ± 2.10	$\mathbf{24.82 \pm 0.62}$
DCGAN	CelebA	41.105 ± 1.42	30.97 ± 5.32	$\mathbf{27.04 \pm 4.24}$

Qualitative results: random samples



(a) CIFAR10

(b) CelebA

The end