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Unifying GANs and Score-Based Diffusion as Generative Particle Models

J.-Y. Franceschi,[1] M. Gartrell,[1] L. Dos Santos,[1,*] T. Issenhuth,[1,2,*] E. de Bézenac,[3,*] M. Chen,[4,*] A. Rakotomamonjy[1,*]

[1]Criteo AI Lab [2]LIGM, Ecole des Ponts, Univ Gustave Eiffel, CNRS [3]SAM, D-MATH, ETH Zürich [4]Valeo.ai

Our Contributions

- We unify gradient flows, score-based diffusion models, and GANs in a single framework.
- We represent generated data as moving particles. A model is defined by:
  - a gradient vector field that the particles follow either at inference or training time;
  - the possibility of incorporating a generator that smooths this movement.
- This suggests the existence of hybrid models:
  - a generator trained with diffusion guidance (Score GANs);
  - a GAN trained without a generator (Discriminator Flows).
- We experimentally verify our findings.

GANs vs Diffusion

Traditional opposition in the literature.

GANs → Generator trained by discriminating true vs fake data.
- Generator (manifold learning).
- Close to SOTA performance.
- Harder to optimize.
- Fast inference.

Diffusion → Learns to progressively reverse a data degradation process.
- No generator (on the data space).
- SOTA performance.
- Easier to optimize.
- Slow inference.

From PMs to Int-PMs

- We assign to each generated particle $x = g_\theta(z)$ the same loss as in PMs: $\mathcal{L}_{\text{gen}}(\theta) = -\mathbb{E}_{z\sim p_z}\Big[h_{\rho_t}\big(g_\theta(z)\big)\Big]$.
- We do not take into account the dependency of ρ_t w.r.t. θ_t, to mimic PMs: $\rho = \mathrm{StopGradient}(g_\theta \sharp p_z)$.
- Continuous-time gradient descent:
$$\frac{\mathrm{d}\theta_t}{\mathrm{d}t} = -\nabla_{\theta_t}\mathcal{L}_{\text{gen}}(\theta_t) = \eta\nabla_{\theta_t}\mathbb{E}_{z\sim p_z}\Big[h_{\rho_t}\big(g_{\theta_t}(z)\big)\Big] = \eta\mathbb{E}_{z\sim p_z}\Big[\nabla_{\theta_t}g_{\theta_t}(z)\nabla h_{\rho_t}\big(g_{\theta_t}(z)\big)\Big].$$
- Evolution of particles:
$$\frac{\mathrm{d}g_{\theta_t}(z)}{\mathrm{d}t} = \nabla_{\theta_t}g_{\theta_t}(z)^\top\frac{\mathrm{d}\theta_t}{\mathrm{d}t} = \eta\mathbb{E}_{z'\sim p_z}\Big[\nabla_{\theta_t}g_{\theta_t}(z)^\top\nabla_{\theta_t}g_{\theta_t}(z')\nabla h_{\rho_t}\big(g_{\theta_t}(z')\big)\Big].$$

Particle-Based Framework

Generated particles $x_t \sim \rho_t$ follow a gradient vector field ∇h_{ρ_t}, i.e. optimize an objective h_{ρ_t}.

Wasserstein Gradient

$$-\nabla_W\mathcal{F}(\rho_t) = -\nabla\frac{\partial\mathcal{F}(\rho_t)}{\partial\rho_t}$$

Log Ratio Gradient

$$\alpha_t\nabla\log\Big[p_{\text{data}} \star k^{\sigma(t)}_{\text{RBF}}\Big] - \beta_t\nabla\log\rho_t$$

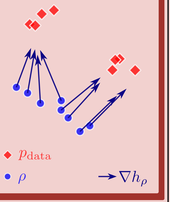
Discriminator Gradient

$$-\nabla\big(c\circ f_{\rho_t}\big)$$

where f_{ρ_t} discriminates ρ_t from p_{data}

Particle Models (No Generator)

- At generation / inference time t:
$$x_0 \sim \pi = \rho_0,\ \mathrm{d}x_t = \nabla h_{\rho_t}(x_t)\,\mathrm{d}t.$$
- Independently moving particles.
- Each x_t individually follows a **gradient ascent** path on $h_{\rho_t}(x_t)$.
- h_ρ is usually a predefined functional approximated with neural networks.

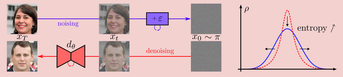


Wasserstein Gradient Flows

- Gradient descent for functionals over distributions $\mathcal{F}$ (Santambrogio, 2017).

Objective $\mathcal{F}(\rho)$		h_ρ
Forward KL	$\mathbb{E}_\rho \log \rho/p_{\text{data}}$	$-\log \rho/p_{\text{data}}$
f-divergence	$\mathbb{E}_{p_{\text{data}}} f\big(\rho/p_{\text{data}}\big)$	$-f'\big(\rho/p_{\text{data}}\big)$
Squared MMD w.r.t. kernel k	$\mathbb{E}_{\substack{x,x'\sim\rho\\ y,y'\sim p_{\text{data}}}}\begin{bmatrix}k(x,x')\\+k(y,y')\\-2k(x,y)\end{bmatrix}$	$\mathbb{E}_{y\sim p_{\text{data}}}\big[k(y,\cdot)\big] - \mathbb{E}_{x\sim\rho}\big[k(x,\cdot)\big]$
Entropy	$\mathbb{E}_\rho \log\rho$	$-\log\rho$

Score-Based Diffusion



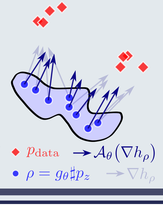
- Using Jordan et al. (1998) in Song et al. (2019) and Karras et al. (2022):
$$\mathrm{d}x_t = \alpha_t\nabla\log\Big[p_{\text{data}} \star k^{\sigma(t)}_{\text{RBF}}\Big](x_t)\,\mathrm{d}t + \sqrt{2\beta_t}\,\mathrm{d}W_t \quad\Leftrightarrow\quad -\beta_t\nabla\log\rho_t\,\mathrm{d}t.$$

Discriminator Flows

- Particles directly follow the discriminator gradient.
- The discriminator is simultaneously trained and used to generate data.

Interacting Particle Models (Generator)

- Training with **the same loss**:
$$\mathcal{L}_{\text{gen}}(\theta) = -\mathbb{E}_{z\sim p_z}\Big[h_{\rho_t}\big(g_\theta(z)\big)\Big].$$
- At training time t:
$$\mathrm{d}g_{\theta_t}(z) = \eta\big[\mathcal{A}_{\theta_t}(z)\big]\big(\nabla h_{\rho_t}\big)\,\mathrm{d}t.$$
- Generalization of PMs where particles interact with each other.



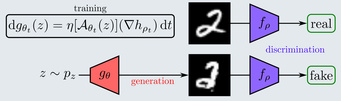
Stein Gradient Flows

- Stein gradient flows (Liu, 2017) are kernelized Wasserstein gradient flows:
$$\mathrm{d}x_t = \mathbb{E}_{x'_t\sim\rho_t}\Big[k\big(x_t,x'_t\big)\nabla h_{\rho_t}\big(x'_t\big)\Big]\,\mathrm{d}t.$$
- Int-PMs under mild hypotheses (generalization of Durr et al. (2022)).
- Hint towards the same h_ρ being used in a PM and an Int-PM.

Score GANs

- Estimate ∇h_ρ with two score matching networks and use it in parameter update equation of generator training.
- Data score (pretrained like diffusion): $s^{p_{\text{data}}}_\psi(\cdot,\sigma) \equiv \nabla\log\big[p_{\text{data}} \star k^\sigma_{\text{RBF}}\big]$.
- Gen. score (continuously updated like a discriminator): $s^\rho_\phi \equiv \nabla\log\rho$.

GANs



- Gradient descent-ascent on the min-max objective yields the generator loss:
$$\mathcal{L}_{\text{GAN}}(g_\theta) = \mathbb{E}_{z\sim p_z}\Big[\big(c\circ f_\rho\big)\big(g_\theta(z)\big)\Big].$$

Smoothing Operator

- $\mathcal{A}_{\theta_t}(z)$ is a linear operator on vector fields (kernel integral operator):
$$\big[\mathcal{A}_{\theta_t}(z)\big](V) \triangleq \mathbb{E}_{z'\sim p_z}\Big[k_{g_{\theta_t}}(z,z')V\big(g_{\theta_t}(z')\big)\Big],\ k_{g_{\theta_t}}(z,z') \triangleq \nabla_{\theta_t}g_{\theta_t}(z')^\top\nabla_{\theta_t}g_{\theta_t}(z).$$
- $k_{g_{\theta_t}}$ is the generator's matrix Neural Tangent Kernel (NTK, Jacot et al., 2018).
- Special case: $k_{g_{\theta_t}}(z,z') = \delta_{z=z'}I_d$ (generator with infinite capacity).
  - No interaction between particles: $\big[\mathcal{A}_{\theta_t}(z)\big](V) = V\big(g_\theta(z)\big)$.
  - $\mathrm{d}g_{\theta_t}(z) = \nabla h_{\rho_t}\big(g_{\theta_t}(z)\big)\,\mathrm{d}t$: we retrieve PMs.
- General case: $\mathcal{A}_{\theta_t}$ represents the parameterization of ρ as a manifold.
  - $\mathcal{A}_{\theta_t}$ smooths the original vector field ∇h_{ρ_t} by convolving it with k.
  - Particles interact with each other through generator parameterization.

Other Models & Flows

- Int-PMs and Stein (generalization of Durr et al. (2022)): $k\Big(g_{\theta_t}(z), g_{\theta_t}(z')\Big) = k_{g_{\theta_t}}(z,z')$ in the NTK regime.
- Langevin diffusion (Song et al., 2019) is a KL flow.
- Under some hypotheses, GANs are Stein flows (Franceschi et al., 2022; Yi et al., 2023): KL flow for f-divergence GANs, squared MMD for IPM GANs.
- As a consequence, under similar hypotheses, Discriminator Flows with the same losses are Wasserstein flows.
- Many methods use neural networks to approximate the flow (Alvarez-Melis et al., 2022; Heng et al., 2023).

Score GANs in Practice

- Two practical issues:
  - sliced score matching to train s^ρ_ϕ;
  - scheduling σs w.r.t. training time t.
- We randomly sample σ and also noise the particles:
$$\nabla h_\rho = \nabla\log[p_{\text{data}} \star k^\sigma_{\text{RBF}}] - \nabla\log[\rho_t \star k^\sigma_{\text{RBF}}],$$
$$\equiv \widetilde{\nabla h}_\rho(\cdot,\sigma) = s^{p_{\text{data}}}_\psi(\cdot,\sigma) - s^\rho_\phi(\cdot,\sigma).$$
- Generator update:
  - few-step training of s^ρ_ϕ with denoising score matching;
  - gradient descent step:
$$\theta \leftarrow \theta + \eta\mathop{\mathbb{E}}_{\sigma\sim p_\sigma,\varepsilon\sim\mathcal{N}(0,\sigma I_D),z\sim p_z}\Big[\nabla_\theta g_\theta(z)\widetilde{\nabla h}_\rho\big(g_\theta(z)+\varepsilon,\sigma\big)\Big].$$

Discr. Flows in Practice

- Discriminator loss:
$$\mathcal{L}_{\text{d}}(f;\rho,p_{\text{data}}) = \mathbb{E}_\rho[a\circ f] - \mathbb{E}_{p_{\text{data}}}[b\circ f] + \mathcal{R}(f;\rho,p_{\text{data}}).$$
- Naive training: successive f_{ρ_t} trainings and ρ_t updates.
- For efficiency purposes, we simultaneously learn all time-parameterized discriminators: $f_{\rho_t} = f_\phi(\cdot,t)$.
- Training step:
  - sample $t \sim \mathcal{U}\big([0,1]\big)$, $x_0 \sim \pi$;
  - compute $x_t = -\eta\int_0^t\nabla\big(c\circ f_\phi(\cdot,s)\big)(x_s)\,\mathrm{d}s$;
  - train $f_\phi(\cdot,t)$ to discriminate between x_t and p_{data}.
- Generalization of some gradient flows.

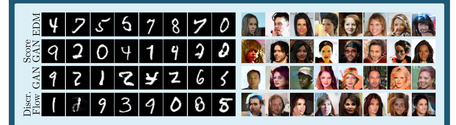
Links

Article

Code and samples

- Code for all models and baselines.
- Animated samples.

Experimental Results



Dataset	PMs (no generator)		Int-PMs (generator)	
	EDM	Discr. Flow	GAN	Score GAN
MNIST	3	4	3	15
CelebA	10	41	19	35

- Hybrid models are viable, support theory.
- EDM: diffusion (Karras et al., 2022).

Properties

- **Discr. flows** learn a path to the data distribution, unlike **diffusion**.
- **PMs vs Int-PMs**: Int-PMs are prone to mode collapse but are faster than PMs at inference and have better latent space properties.

Perspectives

- Our work paves the way for new hybrid models.
- Model improvements: Score GANs for score distillation, Discr. Flows for generation efficiency.
- Framework improvements: convergence, second-order and discrete-time optimization, more accurate GAN modeling.

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