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A Neural Tangent Kernel Perspective of GANs

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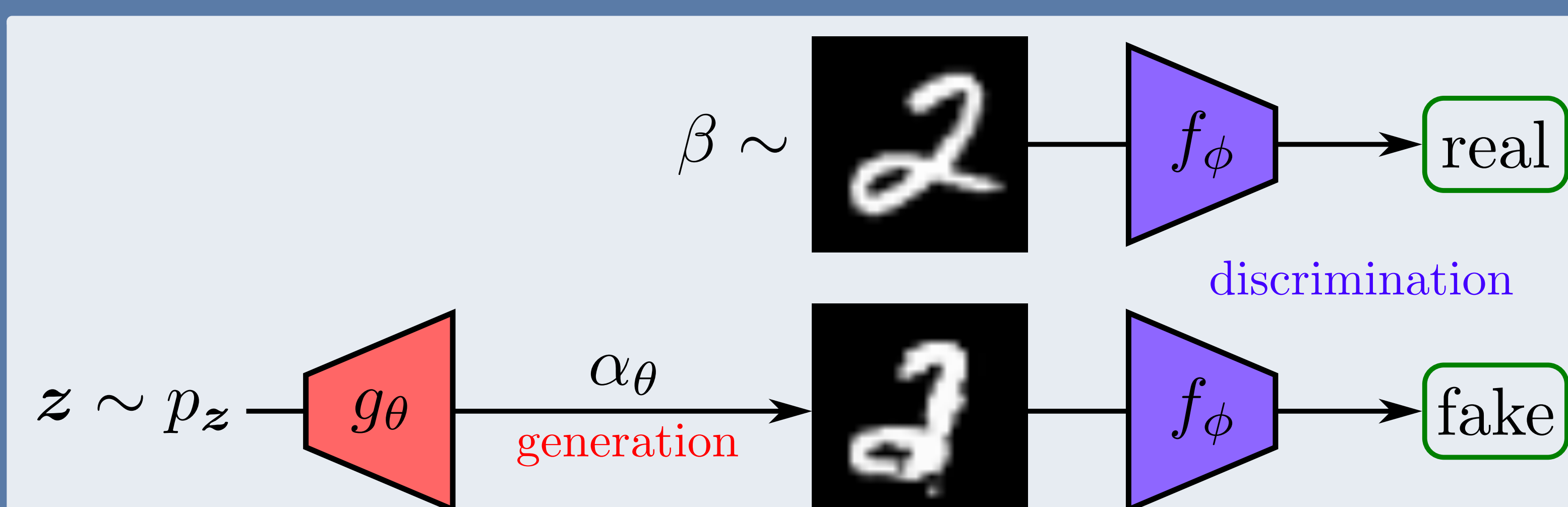
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Motivation & Outline

- Many analyses cannot explain GAN training as they fail to take into account alternating optimization and model the architecture and implicit biases of the discriminator.
- We propose a theoretical framework solving these issues using the theory of Neural Tangent Kernels.
- We deduce new insights about the flow and convergence of the generated distribution during training.

Generative Adversarial Networks



$$\inf_{\theta} \sup_{\phi} \mathcal{L}(g_{\theta}, f_{\phi}) = \inf_{\theta} \mathcal{L}(g_{\theta}, f_{\phi}^*) \approx \inf_{\theta} \mathcal{C}(\alpha_{\theta}, \beta),$$

$$\mathcal{L}(g_{\theta}, f_{\phi}) = \mathbb{E}_{x \sim \alpha_{\theta}} [(a \circ f_{\phi})(x)] - \mathbb{E}_{y \sim \beta} [(b \circ f_{\phi})(y)].$$

E.g. for vanilla GAN \mathcal{C} is a Jensen-Shannon, for WGAN it is the 1-Wasserstein, for LSGAN it is a χ^2 -divergence.

Issue 1: Alternating Optimization

- In practice, GANs are optimized alternatingly, f_{ϕ} and g_{θ} being considered to be independent of each other.

$$\theta \leftarrow \theta - \eta \nabla_{\theta} \mathcal{L}(g_{\theta}, f_{\phi});$$

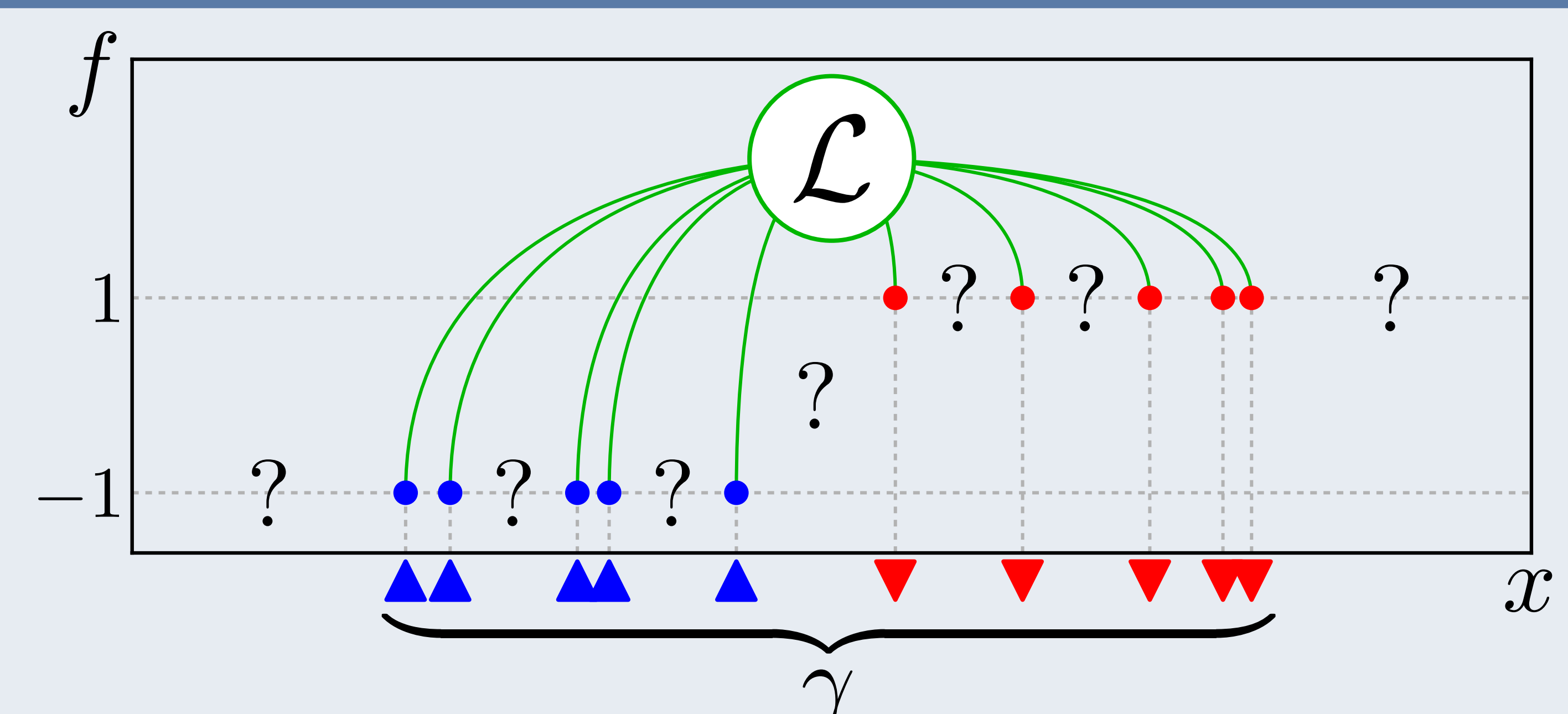
$$\phi \leftarrow \phi + \lambda \nabla_{\phi} \mathcal{L}(g_{\theta}, f_{\phi}).$$

- Gradient received by g_{θ} :

$$\nabla_{\theta} \mathcal{L}(g_{\theta}, f_{\phi}^*) \Rightarrow \nabla_{\theta} \mathcal{L}(g_{\theta}, f_{\phi}).$$

- This changes the true generator loss \mathcal{C} . Hence, sound studies should model alternating optimization.

Issue 2: Ill-Defined Discr. Gradients



In an alternating optimization setting:

$$\nabla_{\theta} \mathcal{L}(g_{\theta}, f) = \mathbb{E}_{z \sim p_z} [\nabla_{\theta} g_{\theta}(z)^{\top} \nabla_x (a \circ f)(x)|_{x=g_{\theta}(z)}].$$

- The gradient of the generator requires ∇f (chain rule).
- Without any assumption on the structure of f , as \mathcal{L} is only defined on training points γ , ∇f is not defined.
- The parameter gradient of the generator is thus also ill-defined.
- Analyses need to take into account the structure of f .

Our solution: Modeling discriminator training as a neural network via its NTK.

A Background on NTKs

The Neural Tangent Kernel: For a neural network f_{ϕ} with parameters ϕ , its NTK $k_{f_{\phi}}$ is defined as:

$$k_{f_{\phi}}(x, y) \triangleq \langle \partial_{\phi} f_{\phi}(x), \partial_{\phi} f_{\phi}(y) \rangle.$$

In the infinite-width limit of f , during training:

$$k_{f_{\phi}}(x, y) = k(x, y).$$

Kernel Integral Operator and RKHS:

$$\mathcal{T}_{k, \gamma}: L^2(\gamma) \rightarrow \mathcal{H}_k^{\gamma}, h \mapsto \int_x k(\cdot, x) h(x) d\gamma(x),$$

where $\mathcal{H}_k^{\gamma} \subseteq L^2(\Omega)$ is the RKHS of k generated by γ .

Discriminator Inner Loop

We consider the NNs in the NTK regime. This enables a theoretical study of their evolution w.r.t. training time t :

$$\partial_t f_t = \mathcal{T}_{k, \gamma}(\nabla^{\gamma} \mathcal{L}_{\alpha}(f_t)).$$

Discriminator Structure:

Under mild assumptions, f_t is uniquely defined and:

$$\forall t \in \mathbb{R}_+, f_t = f_0 + \mathcal{T}_{k, \gamma} \left(\int_0^t \nabla^{\gamma} \mathcal{L}_{\alpha}(f_s) ds \right) \in f_0 + \mathcal{H}_k^{\gamma}.$$

- $\mathcal{T}_{k, \gamma}$ smooths out gradients over the whole input space by sending them into \mathcal{H}_k^{γ} .
- \mathcal{H}_k^{γ} depends on discriminator architecture.

Differentiability of the Discriminator:

The discriminator trained with gradient descent is infinitely differentiable (almost) everywhere.

- The spatial gradient of the discriminator ∇f_t is well-defined.
- The parameter gradient of the generator $\nabla_{\theta} \mathcal{L}(g_{\theta}, f_t)$ is well-defined.

Underlying NTK Regularity Results

To prove the above results, we establish novel regularity results on NTKs. Given, for the network f :

- a standard architecture (fully connected, convolutional, residual, etc.),
- a standard activation function (tanh, softplus, ReLU-like, sigmoid, Gaussian, etc.),

we prove that the NTK k of f is:

- smooth almost everywhere if the network has non-null bias terms.
- smooth everywhere if the activation is smooth.

These results, obtained from similar regularity results on the conjugate kernel of f , then transfer to f .

Resulting Convergence Results

Our finer-grained framework allows us to derive novel convergence insights, with highlighted results below.

Gradient Flow of Generated Distribution:

$$\partial_t \alpha_t^z = -\nabla_{\mathcal{G}_{k_g}} \mathcal{C}(\alpha_t)$$

$$= \nabla_x \cdot \left(\alpha_t^z \mathcal{T}_{k_g, p_z} \left(z \mapsto \nabla_x (a \circ f_{\alpha_t})(x)|_{x=g_{\ell}(z)} \right) \right),$$

where α_t^z is the distribution of $(z, g_{\ell}(z))$ under $z \sim p_z$.

- In the non-interacting case, i.e. $\mathcal{T}_{k_g, p_z} = \text{id}$, this corresponds to a Wasserstein gradient flow:

$$\partial_t \alpha_t = -\nabla_{\mathcal{G}_{k_g}} \mathcal{C}(\alpha_t) = -\nabla_{\mathcal{W}} \mathcal{C}(\alpha_t).$$

- In the general case, this is a gradient flow in a Stein geometry defined by the generator's NTK k_g .
- $\mathcal{C}(\alpha_t)$ is automatically decreasing via this gradient flow, as fast as possible (locally).

IPM GANs ($a = b = \text{id}$) and NTK MMD:

We find $f_t = f_0 + t \left(\mathbb{E}_{x \sim \alpha} [k(x, \cdot)] - \mathbb{E}_{y \sim \beta} [k(y, \cdot)] \right)$, hence, if $f_0 = 0$:

$$\mathcal{C}(\alpha) = \mathcal{L}_{\alpha}(f_t) \propto \text{MMD}_k^2(\alpha, \beta).$$

Empirical Study

- We assess the adequacy of our framework by observing how close finite and infinite-width regimes are.
- We study the convergence of GANs on empirical distributions in the non-interacting case ($\mathcal{T}_{k_g, p_z} = \text{id}$).
- We discover the singular performance of ReLU architectures for generative modeling and explain it by studying generator gradients with our framework.

Toolkit GAN(TK)²

- GAN analysis toolkit based on our framework.
- Written in JAX with the Neural Tangents library.
- Link to paper and code \rightarrow

