# Two Generator Game: Learning to Sample via Linear Goodness-of-Fit Test

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## Background

- Learning the probability distribution of high-dimensional data.
- GANs are a type of implicit generative models (IGMs).
- Existing GAN models are fundamentally two-sample test problems.
- We summarize existing GAN models into two categories:
  - ▷ Integral Probability Metric (IPM).

$$\delta(\mathbf{p},\mathbf{q}) = \sup_{\mathbf{f}\in\mathcal{F}} \left| \int_{\mathcal{X}} \mathbf{f}(\mathbf{x})\mathbf{p}(\mathbf{x})\mathbf{d}\mathbf{x} - \int_{\mathcal{X}} \mathbf{f}(\mathbf{x}')\mathbf{q}(\mathbf{x}')\mathbf{d}\mathbf{x}' \right|.$$

    Wasserstein GANs (WGANs), MMD-GAN
  - ▷ $\zeta$-divergence

$$\delta_\zeta(\mathbf{p},\mathbf{q}) = \int_{\mathcal{X}} \mathbf{q}(\mathbf{x})\zeta\left(\frac{\mathbf{p}(\mathbf{x})}{\mathbf{q}(\mathbf{x})}\right)\mathbf{d}\mathbf{x},$$

    where $\zeta$ is a convex, lower-semicontinuous, satisfying $\zeta(\mathbf{1}) = \mathbf{0}$.
    GAN, least squares GAN
- Analyzing and comparing distributions without imposing any parametric assumptions
  - ▷ Two-sample test:
    Whether two distributions $\mathbf{p}$ and $\mathbf{q}$ are different based on

$$\mathcal{D}_\mathbf{x} = \{\mathbf{x}_\mathbf{i}\}_{\mathbf{i}=\mathbf{1}}^{\mathbf{n}} \subset \mathcal{X} \subseteq \mathbb{R}^\mathbf{d} \sim \mathbf{p}$$
$$\mathcal{D}_\mathbf{y} = \{\mathbf{y}_\mathbf{j}\}_{\mathbf{j}=\mathbf{1}}^{\mathbf{m}} \subset \mathcal{Y} \subseteq \mathbb{R}^\mathbf{d} \sim \mathbf{q}$$

  - ▷ Goodness-of-fit test:
    How well a given model density $\mathbf{p}$ fits a set of given samples

$$\mathcal{D}_\mathbf{x} = \{\mathbf{x}_\mathbf{i}\}_{\mathbf{i}=\mathbf{1}}^{\mathbf{n}} \subset \mathcal{X} \subseteq \mathbb{R}^\mathbf{d} \sim \mathbf{q}$$

## Contributions

- Deep energy adversarial network (DEAN):
  A new paradigm that casts the generative adversarial learning as a goodness-of-fit (GOF) test problem.
- A novel two generator game via GOF tests:
  - ▷ One explicit generator is designed to learn an energy-based distribution (EBD), which maps the real data to a scalar energy-based probability.
  - ▷ The other implicit generator is trained by minimizing the vFSSD between the EBD and the generated data.
- A two-level alternative optimization procedure to train the explicit and implicit generative networks, such that the hyper-parameters can also be automatically learned.

## Energy Estimator Network

Energy-based models $\mathcal{E}_\theta(\mathbf{x}) : \mathcal{X} \to \mathbb{R}$ associate an energy value with a sample $\mathbf{x}$, where $\theta$ are the parameters. We can obtain a distribution based on $\mathcal{E}_\theta(\mathbf{x})$,

$$\mathbf{p}(\mathbf{x};\theta) = \frac{\mathbf{1}}{\mathbf{Z}_\theta}\exp(-\mathcal{E}_\theta(\mathbf{x})).$$

Now we define the loss function of the explicit generative network (EGN) of DEAN as follows:

$$\min_{\theta_\mathbf{e}} \mathcal{E}(\mathbf{x};\theta_\mathbf{e}) + \left[\gamma - \mathcal{E}\left(\mathbf{G}(\mathbf{z};\theta_\mathbf{g}^*);\theta_\mathbf{e}\right)\right]^+, \tag{1}$$

where $\mathcal{E}(\mathbf{x};\theta_\mathbf{e})$ is an *energy model* parameterized by $\theta_\mathbf{e}$, $[\cdot]^+ = \max(\cdot,\mathbf{0})$ and $\gamma$ is a given positive margin. When the network parameters $\theta_\mathbf{e}^*$ are optimized, we can define a probability distribution

$$\mathbf{p}(\mathbf{x};\theta_\mathbf{e}^*) = \frac{\mathbf{1}}{\mathbf{Z}_{\theta_\mathbf{e}^*}}\exp(-\mathcal{E}(\mathbf{x};\theta_\mathbf{e}^*)).$$

## Energy Estimator Network

We consider a deep auto-encoder as a more complex energy model

$$\mathcal{E}(\mathbf{x};\theta) = \|\mathbf{x} - \mathbf{AE}(\mathbf{x};\theta_\mathbf{e})\|,$$

where $\mathbf{AE}(\mathbf{x};\theta_\mathbf{e})$ denotes a deep auto-encoder parameterized by $\theta_\mathbf{e}$. For the optimized parameters $\theta_\mathbf{e}^*$, we can define

$$\mathbf{p}(\mathbf{x};\theta_\mathbf{e}^*) = \frac{\mathbf{1}}{\mathbf{Z}_{\theta_\mathbf{e}^*}}\exp(-\mathcal{E}(\mathbf{x};\theta_\mathbf{e}^*)).$$

## GOF-driven Generator Network

Kernel Stein operator can be written as

$$(\mathbf{T}_\mathbf{p}\mathbf{f})(\mathbf{x}) = \sum_{\mathbf{i}=\mathbf{1}}^{\mathbf{d}} \left(\frac{\partial \log \mathbf{p}(\mathbf{x})}{\partial \mathbf{x}_\mathbf{i}}\mathbf{f}_\mathbf{i}(\mathbf{x}) + \frac{\partial \mathbf{f}_\mathbf{i}(\mathbf{x})}{\partial \mathbf{x}_\mathbf{i}}\right) = \langle \mathbf{f}, \omega_\mathbf{p}(\mathbf{x},\cdot)\rangle_{\mathcal{F}^\mathbf{d}}.$$

Now we introduce the kernel Stein discrepancy (KSD), which is formulated as

$$\mathrm{KSD}[\mathcal{F}^\mathbf{d},\mathbf{p},\mathcal{D}_\mathbf{x}] = \sup_{\|\mathbf{f}\|_{\mathcal{F}^\mathbf{d}}\le\mathbf{1}} \langle \mathbf{f}, \mathbf{E}_{\mathbf{x}\sim\mathbf{q}}\omega_\mathbf{p}(\mathbf{x},\cdot)\rangle := \|\mathbf{g}(\cdot)\|_{\mathcal{F}^\mathbf{d}}, \tag{2}$$

where $\mathbf{g}(\cdot) = \mathbf{E}_{\mathbf{x}\sim\mathbf{q}}\omega_\mathbf{p}(\mathbf{x},\cdot)$. The statistic of the finite set Stein discrepancy (FSSD) is defined as

$$\mathrm{FSSD}[\mathcal{F}^\mathbf{d},\mathbf{p},\mathcal{D}_\mathbf{x}] = \frac{\mathbf{1}}{\mathbf{dJ}}\sum_{\mathbf{i}=\mathbf{1}}^{\mathbf{d}}\sum_{\mathbf{j}=\mathbf{1}}^{\mathbf{J}} \mathbf{g}_\mathbf{i}^2(\mathbf{v}_\mathbf{j}).$$

The unbiased estimator of FSSD is defined as

$$\widehat{\mathrm{FSSD}}^2[\mathcal{F}^\mathbf{d},\mathbf{p},\mathcal{D}_\mathbf{x}] = \frac{\mathbf{2}}{\mathbf{n(n-1)}}\sum_{\mathbf{i}<\mathbf{j}} \mathbf{\Delta}(\mathbf{x}_\mathbf{i},\mathbf{x}_\mathbf{j}),$$

where $\mathbf{\Delta}(\mathbf{x},\mathbf{y}) = \tau(\mathbf{x})^\mathrm{T}\tau(\mathbf{y})$. To alleviate the impact of dimension and stabilize the statistic, we introduce

$$\mathbf{vFSSD}[\mathbf{p},\mathcal{D}_\mathbf{x}] = \frac{\mathbf{1}}{\hat{\sigma}_{\mathbf{H}_1}}\widehat{\mathrm{FSSD}}^2[\mathbf{p},\mathcal{D}_\mathbf{x}].$$

## GOF-driven Generator Network

Now we define the loss function of the IGN as follows:

$$\min_{\theta_\mathbf{g}} \max_{\xi} \mathbf{vFSSD}_\xi\left[\mathbf{p}(\mathbf{x};\theta_\mathbf{e}^*),\mathcal{D}_{\mathbf{x}'}\right], \tag{3}$$

where $\xi = \left\{\{\mathbf{v}_\mathbf{i}\}_{\mathbf{i}=\mathbf{1}}^{\mathbf{J}}, \sigma_\mathbf{k}\right\}$ denotes the hyper-parameters of vFSSD, including the kernel parameter $\sigma_\mathbf{k}$ and $\mathbf{J}$ test locations $\{\mathbf{v}_\mathbf{i}\}_{\mathbf{i}=\mathbf{1}}^{\mathbf{J}}$. We present the following two objectives, (4) and (5), to optimize Equation (3) and improve the test power of DEAN.

$$\max_{\xi} \mathbf{vFSSD}_\xi\left[\mathbf{p}(\mathbf{y};\theta_\mathbf{e}^*),\mathcal{D}_{\mathbf{x}'^*}\right], \tag{4}$$

where $\mathcal{D}_{\mathbf{x}'^*} = \left\{\mathbf{x}_\mathbf{i}'^* := \mathbf{G}(\mathbf{z}_\mathbf{i};\theta_\mathbf{g}^*)\right\}_{\mathbf{i}=\mathbf{1}}^{\mathbf{n}}$ and $\mathbf{G}(\mathbf{z}_\mathbf{i};\theta_\mathbf{g}^*)$ is a deep network with the optimized parameter $\theta_\mathbf{g}^*$. The hyper-parameters $\xi = \left\{\{\mathbf{v}_\mathbf{i}\}_{\mathbf{i}=\mathbf{1}}^{\mathbf{J}}, \sigma_\mathbf{k}\right\}$ will be optimized in Equation (4).

$$\min_{\theta_\mathbf{g}} \mathbf{vFSSD}_{\xi^*}\left[\mathbf{p}(\mathbf{y};\theta_\mathbf{e}^*),\mathcal{D}_{\mathbf{x}'}\right], \tag{5}$$

where $\xi^* = \left\{\{\mathbf{v}_\mathbf{i}^*\}_{\mathbf{i}=\mathbf{1}}^{\mathbf{J}}, \sigma_\mathbf{k}^*\right\}$ denotes the optimized hyper-parameters, and the parameters $\theta_\mathbf{g}$ for $\mathcal{D}_{\mathbf{x}'} = \left\{\mathbf{x}_\mathbf{i}' := \mathbf{G}(\mathbf{z}_\mathbf{i};\theta_\mathbf{g})\right\}_{\mathbf{i}=\mathbf{1}}^{\mathbf{n}}$ will be optimized.

## Theorem

*We assume that $\mathcal{D}_{\mathbf{x}'}$ is drawn from $\mathbf{p}_{\mathbf{x}'}$. If $\kappa$ is a universal and analytic kernel;*
$\mathbf{E}_{\mathbf{a}\sim\mathbf{p}_{\mathbf{x}'}}\mathbf{E}_{\mathbf{b}\sim\mathbf{p}_\mathbf{e}}\left[\mathbf{s}^\mathrm{T}(\mathbf{a})\mathbf{s}(\mathbf{b})\kappa(\mathbf{a},\mathbf{b}) + \mathbf{s}^\mathrm{T}(\mathbf{b})\nabla_\mathbf{a}\kappa(\mathbf{a},\mathbf{b}) + \mathbf{s}^\mathrm{T}(\mathbf{a})\nabla_\mathbf{b}\kappa(\mathbf{a},\mathbf{b}) + \sum_{\mathbf{i}=\mathbf{1}}^{\mathbf{d}}\frac{\partial^2\kappa(\mathbf{a},\mathbf{b})}{\partial \mathbf{a}_\mathbf{i}\partial \mathbf{b}_\mathbf{i}}\right] < \infty$
*with* $\mathbf{s}(\mathbf{a}) = \nabla_\mathbf{a}\log \mathbf{p}_\mathbf{e}(\mathbf{a})$; $\mathbf{E}_{\mathbf{a}\sim\mathbf{p}_{\mathbf{x}'}}\|\nabla_\mathbf{a}\log \mathbf{p}_\mathbf{e}(\mathbf{a}) - \nabla_\mathbf{a}\log \mathbf{p}_{\mathbf{x}'}(\mathbf{a})\|^2 < \infty$;
$\lim_{\|\mathbf{a}\|\to\infty} \mathbf{p}_\mathbf{e}(\mathbf{a})\mathbf{g}(\mathbf{a}) = \mathbf{0}$, *where* $\mathbf{g}(\cdot)$ *is given in Eq. (2) in Section 4.2; for any* $\mathbf{J} \ge \mathbf{1}$, *almost surely* $\mathrm{FSSD}[\mathbf{p}_\mathbf{e},\mathcal{D}_{\mathbf{x}'}] = \mathbf{0}$ *if and only if* $\mathbf{p}_{\mathbf{x}'} = \mathbf{p}_\mathbf{e}$.

## Theorem

*Let* $\mathbf{\Lambda}(\theta_\mathbf{e}) = \mathcal{E}(\mathbf{x};\theta_\mathbf{e}) + \left[\gamma - \mathcal{E}\left(\mathbf{G}(\mathbf{z};\theta_\mathbf{g}^*);\theta_\mathbf{e}\right)\right]^+$. *The minimum of* $\mathbf{\Lambda}(\theta_\mathbf{e})$ *is achieved if and only if* $\mathbf{p}_\mathbf{e} = \mathbf{p}_\mathbf{x}$. *With the optimized* $\theta_\mathbf{e}^*$, $\int_{\mathbf{x},\mathbf{z}} \mathbf{\Lambda}(\theta_\mathbf{e}^*)\mathbf{p}_\mathbf{x}(\mathbf{x})\mathbf{p}_\mathbf{z}(\mathbf{z})\mathbf{d}\mathbf{x}\mathbf{d}\mathbf{z} = \gamma$.