

19 Generative Adversarial Networks

Goal

Push-forward, Generative Adversarial Networks, min-max optimization, duality.

Alert 19.1: Convention

Gray boxes are not required hence can be omitted for unenthusiastic readers.

This note is likely to be updated again soon.

Example 19.2: Simulating distributions

Suppose we want to sample from a Gaussian distribution with mean \mathbf{u} and covariance S . The typical approach is to first sample from the standard Gaussian distribution (with zero mean and identity covariance) and then perform the transformation:

$$\text{If } \mathbf{Z} \sim \mathcal{N}(\mathbf{0}, \mathbb{I}), \quad \text{then } X = \mathsf{T}(\mathbf{Z}) := \mathbf{u} + S^{1/2}\mathbf{Z} \sim \mathcal{N}(\mathbf{u}, S).$$

Similarly, we can sample from a χ^2 distribution with zero mean and degree d by the transformation:

$$\text{If } \mathbf{Z} \sim \mathcal{N}(\mathbf{0}, \mathbb{I}_d), \quad \text{then } X = \mathsf{T}(\mathbf{Z}) := \sum_{j=1}^d Z_j^2 \sim \chi^2(d).$$

In fact, we can sample from any distribution F on \mathbb{R} by the following transformation:

$$\text{If } Z \sim \mathcal{N}(0, 1), \quad \text{then } X = \mathsf{T}(Z) := F^{-1}(\Phi(Z)) \sim F, \quad \text{where } F^{-1}(z) = \min\{x : F(x) \geq z\},$$

and Φ is the cumulative distribution function of standard normal.

Theorem 19.3: Transforming to any probability measure

Let μ be a diffuse (Borel) probability measure on a polish space Z and similarly ν be any (Borel) probability measure on another polish space X . Then, there exist (measurable) maps $\mathsf{T} : Z \rightarrow X$ such that

$$\text{If } Z \sim \mu, \quad \text{then } X := \mathsf{T}(Z) \sim \nu.$$

□

Recall that a (Borel) probability measure is diffuse iff any single point has measure 0. For less mathematical readers, think of $Z = \mathbb{R}^p$, $X = \mathbb{R}^d$, μ and ν as probability densities on the respective Euclidean spaces.

Alert 19.4: A whole new world

Recall that in sigmoid belief network (Section 18) we **specify** the conditional densities $p(x_j | x_{<j})$. The problem of this approach is that we have to *commit to* a particular parametric form for each conditional (e.g. Bernoulli or Gaussian), and the only thing we can tune is the parameters of the chosen conditional (e.g. mean or variance). However, Theorem 19.3 suggests a more powerful way: we can simply learn a parameterized map T_θ , where $\mathsf{T}_\theta(\mathbf{Z})$ models the target density (with say $\mathbf{Z} \sim \mathcal{N}(\mathbf{0}, \mathbb{I}_p)$).

Definition 19.5: Push-forward generative modeling

Given an i.i.d. sample $\mathbf{X}_1, \dots, \mathbf{X}_n \sim \chi$, we can now estimate the target density χ by the following push-forward approach:

$$\inf_{\theta} D(\mathbf{X}, \mathsf{T}_\theta(\mathbf{Z})),$$

where say $\mathbf{Z} \sim \mathcal{N}(\mathbf{0}, \mathbb{I}_p)$, $\mathsf{T}_\theta : \mathbb{R}^p \rightarrow \mathbb{R}^d$, and $\mathbf{X} \sim \chi$ (the true underlying data generating distribution). The function D is a “distance” that measures the closeness of our (true) data distribution (represented by \mathbf{X}) and model distribution (represented by $\mathsf{T}_\theta(\mathbf{Z})$). By minimizing D we bring our model $\mathsf{T}_\theta(\mathbf{Z})$ close to our data \mathbf{X} .

Remark 19.6: The good, the bad, and the beautiful

One big advantage of the push-forward approach in Definition 19.5 is that after training (e.g. finding a reasonable θ) we can *effortlessly generate new data*: we sample $\mathbf{Z} \in \mathcal{N}(\mathbf{0}, \mathbb{I}_d)$ and then set $\mathbf{X} = \mathsf{T}_\theta(\mathbf{Z})$. This is in sharp contrast with RBM and DBN where we still need to run the (slow) Gibbs sampling to generate new samples.

On the flip side, we **no longer have any explicit form for the model density** (namely, that of $\mathsf{T}_\theta(\mathbf{Z})$ when $p < d$). In contrast, we know the exact form of the density of RBM (up to a normalization constant) and DBN. This **renders direct maximum likelihood estimation of θ impossible**.

This is where we need the beautiful idea called **duality**. Basically, we need to distinguish two distributions: the data distribution represented by a sample \mathbf{X} and the model distribution represented by a sample $\mathsf{T}_\theta(\mathbf{Z})$. We distinguish them by running many tests, represented by functions f :

$$\sup_{f \in \mathcal{F}} |E f(\mathbf{X}) - E \mathsf{T}_\theta(\mathbf{Z})|.$$

If the class of tests \mathcal{F} we run is dense enough, then we would be able to tell the difference between the two distributions and provide feedback for the model θ to improve, until we no longer can tell the difference.

Definition 19.7: f -divergence (Csiszár 1963; Morimoto 1963; Ali and Silvey 1966)

Let $f : \mathbb{R}_+ \rightarrow \mathbb{R}$ be a strictly convex function (see Definition 3.9) with $f(1) = 0$. We define the following **f -divergence** to measure the closeness of two pdfs p and q :

$$D_f(p||q) := \int f(p(\mathbf{x})/q(\mathbf{x})) \cdot q(\mathbf{x}) \, d\mathbf{x}, \quad (19.1)$$

where we assume $q(\mathbf{x}) = 0 \implies p(\mathbf{x}) = 0$ (otherwise we put the divergence to ∞).

For two random variables $Z \sim q$ and $X \sim p$, we sometimes abuse the notation to mean

$$D_f(X||Z) := D_f(p||q).$$

Csiszár, Imre (1963). “Eine informationstheoretische Ungleichung und ihre Anwendung auf den Beweis der Ergodizität von Markoffschen Ketten”. *Magyar. Tud. Akad. Mat. Kutató Int. Közl.*, vol. 8, pp. 85–108.

Morimoto, Tetsuzo (1963). “Markov Processes and the H -Theorem”. *Journal of the Physical Society of Japan*, vol. 18, no. 3, pp. 328–331.

Ali, S. M. and S. D. Silvey (1966). “A General Class of Coefficients of Divergence of One Distribution from Another”. *Journal of the Royal Statistical Society. Series B (Methodological)*, vol. 28, no. 1, pp. 131–142.

Exercise 19.8: Properties of f -divergence

Prove the following:

- $D_f(p||q) \geq 0$, with 0 attained iff $p = q$;
- $D_{f+g} = D_f + D_g$ and $D_{sf} = sD_f$ for $s > 0$;
- Let $g(t) = f(t) + s(t - 1)$ for any s . Then, $D_g = D_f$;
- If $p(\mathbf{x} = 0) \iff q(\mathbf{x} = 0)$, then $D_f(p||q) = D_{f^\circ}(q||p)$, where $f^\circ(t) := t \cdot f(1/t)$;
- f° is (strictly) convex, $f^\circ(1) = 0$ and $(f^\circ)^\circ = f$;

The second last result indicates that f -divergences are not usually symmetric. However, we can always symmetrize them by the transformation: $f \leftarrow f + f^\circ$.

Example 19.9: KL and LK

Let $f(t) = t \log t$, then we obtain the **Kullback-Leibler** (KL) divergence:

$$\text{KL}(p\|q) = \int p(\mathbf{x}) \log(p(\mathbf{x})/q(\mathbf{x})) \, d\mathbf{x}.$$

Reverse the inputs we obtain the reverse KL divergence:

$$\text{LK}(p\|q) := \text{KL}(q\|p).$$

Verify by yourself that the underlying function $f = -\log$ for reverse KL.

Example 19.10: More divergences, more fun

Derive the formula for the following f -divergences:

- χ^2 -divergence: $f(t) = (t - 1)^2$;
- **Hellinger** divergence: $f(t) = (\sqrt{t} - 1)^2$;
- total variation: $f(t) = |t - 1|$;
- Jensen-**Shannon** divergence: $f(t) = t \log t - (t + 1) \log(t + 1) + \log 4$;
- Rényi divergence (Rényi 1961): $f(t) = \frac{t^\alpha - 1}{\alpha - 1}$ for some $\alpha > 0$ (for $\alpha = 1$ we take limit and obtain ?).

Which of the above are symmetric?

Rényi, Alfréd (1961). “On Measures of Entropy and Information”. In: *Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability*, pp. 547–561.

Definition 19.11: Fenchel conjugate function

For any extended real-valued function $f : \mathcal{V} \rightarrow (-\infty, \infty]$ we define its Fenchel conjugate function as:

$$f^*(\mathbf{x}^*) := \sup_{\mathbf{x}} \langle \mathbf{x}, \mathbf{x}^* \rangle - f(\mathbf{x}).$$

According to one of the rules in Exercise 3.13, f^* is always a convex function (of \mathbf{x}^*).

If $\text{dom } f$ is nonempty and **closed**, and f is continuous, then

$$f^{**} := (f^*)^* = f.$$

This remarkable property of convex functions will now be used!

Example 19.12: Fenchel conjugate of JS

Consider the convex function that defines the Jensen-Shannon divergence:

$$f(t) = t \log t - (t + 1) \log(t + 1) + \log 4. \quad (19.2)$$

We derive its Fenchel conjugate:

$$f^*(s) = \sup_t st - f(t) = \sup_t st - t \log t + (t + 1) \log(t + 1) - \log 4.$$

Taking derivative w.r.t. t we obtain

$$s - \log t - 1 + \log(t + 1) + 1 = 0 \iff t = \frac{1}{\exp(-s) - 1},$$

and plugging it back we get

$$\begin{aligned} f^*(s) &= \frac{s}{\exp(-s) - 1} - \frac{1}{\exp(-s) - 1} \log \frac{1}{\exp(-s) - 1} + \frac{\exp(-s)}{\exp(-s) - 1} \log \frac{\exp(-s)}{\exp(-s) - 1} - \log 4 \\ &= \frac{s}{\exp(-s) - 1} - \frac{1}{\exp(-s) - 1} \log \frac{1}{\exp(-s) - 1} + \frac{\exp(-s)}{\exp(-s) - 1} \log \frac{1}{\exp(-s) - 1} - \frac{s \exp(-s)}{\exp(-s) - 1} - \log 4 \\ &= -s - \log(\exp(-s) - 1) - \log 4 \\ &= -\log(1 - \exp(s)) - \log 4. \end{aligned} \tag{19.3}$$

Using conjugation again, we obtain the important formula:

$$f(t) = \sup_s st - f^*(s) = \sup_s st + \log(1 - \exp(s)) + \log 4.$$

Exercise 19.13: More conjugates

Derive the Fenchel conjugate of the other convex functions in Example 19.9 and Example 19.10.

Definition 19.14: Generative adversarial networks (GAN) (Goodfellow et al. 2014)

We are now ready to define the original GAN, which amounts to using the Jensen-Shannon divergence in Definition 19.5:

$$\inf_{\theta} \text{JS}(\mathbf{X} \parallel \mathbb{T}_{\theta}(\mathbf{Z})), \quad \text{where} \quad \text{JS}(\mathbf{p} \parallel \mathbf{q}) = D_f(\mathbf{p} \parallel \mathbf{q}) = \text{KL}(\mathbf{p} \parallel \frac{\mathbf{p} + \mathbf{q}}{2}) + \text{KL}(\mathbf{p} \parallel \frac{\mathbf{p} + \mathbf{q}}{2}),$$

and the convex function f is defined in (19.2), along with its Fenchel conjugate f^* given in (19.3).

To see how we can circumvent the lack of an explicit form of the density $\mathbf{q}(\mathbf{x})$ of $\mathbb{T}_{\theta}(\mathbf{Z})$, we expand using duality:

$$\begin{aligned} \text{JS}(\mathbf{X} \parallel \mathbb{T}_{\theta}(\mathbf{Z})) &= \int_{\mathbf{x}} f(\mathbf{p}(\mathbf{x})/\mathbf{q}(\mathbf{x}))\mathbf{q}(\mathbf{x}) \, d\mathbf{x} \\ &= \int_{\mathbf{x}} [\sup_s s\mathbf{p}(\mathbf{x})/\mathbf{q}(\mathbf{x}) - f^*(s)]\mathbf{q}(\mathbf{x}) \, d\mathbf{x} \\ &= \int_{\mathbf{x}} [\sup_s s\mathbf{p}(\mathbf{x}) - f^*(s)\mathbf{q}(\mathbf{x})] \, d\mathbf{x} \\ &= \sup_{S: \mathbb{R}^d \rightarrow \mathbb{R}} \int_{\mathbf{x}} S(\mathbf{x})\mathbf{p}(\mathbf{x}) \, d\mathbf{x} - \int_{\mathbf{x}} f^*(S(\mathbf{x}))\mathbf{q}(\mathbf{x}) \, d\mathbf{x} \\ &= \sup_{S: \mathbb{R}^d \rightarrow \mathbb{R}} \text{ES}(\mathbf{X}) - \text{E}f^*(S(\mathbb{T}_{\theta}(\mathbf{Z}))). \end{aligned}$$

Therefore, if we parameterize the test function S by ϕ (say a deep net), then we obtain a lower bound of the Jensen-Shannon divergence for minimizing:

$$\inf_{\theta} \sup_{\phi} \text{ES}_{\phi}(\mathbf{X}) - \text{E}f^*(S_{\phi}(\mathbb{T}_{\theta}(\mathbf{Z}))).$$

Of course, we cannot compute either of the two expectations, so we use sample average to approximate them:

$$\inf_{\theta} \sup_{\phi} \hat{\text{E}}S_{\phi}(\mathbf{X}) - \hat{\text{E}}f^*(S_{\phi}(\mathbb{T}_{\theta}(\mathbf{Z}))), \tag{19.4}$$

where the first sample expectation \hat{E} is simply the average of the given training data while the second sample expectation is the average over samples generated by the model $T_{\theta}(\mathbf{Z})$ (recall Remark 19.6).

In practice, both T_{θ} and S_{ϕ} are represented by deep nets, and the former is called the generator while the latter is called the discriminator. Our final objective (19.4) represents a two-player game between the generator and the discriminator. At equilibrium (if any) the generator is forced to mimic the (true) data distribution (otherwise the discriminator would be able to tell the difference and incur a loss for the generator).

See Algorithm 3.46 for a simple algorithm for solving (19.4).

Goodfellow, Ian, Jean Pouget-Abadie, Mehdi Mirza, Bing Xu, David Warde-Farley, Sherjil Ozair, Aaron Courville, and Yoshua Bengio (2014). “Generative Adversarial Nets”. In: *NIPS*.

Remark 19.15: Approximation

We made a number of approximations in Definition 19.14. Thus, technically speaking, the final GAN objective (19.4) no longer minimizes the Jensen-Shannon divergence. Nock et al. (2017) and Liu et al. (2017) formally studied this approximation trade-off.

Nock, Richard, Zac Cranko, Aditya K. Menon, Lizhen Qu, and Robert C. Williamson (2017). “ f -GANs in an Information Geometric Nutshell”. In: *NIPS*.

Liu, Shuang, Léon Bottou, and Kamalika Chaudhuri (2017). “Approximation and convergence properties of generative adversarial learning”. In: *NIPS*.

Exercise 19.16: Catch me if you can

Let us consider the game between the generator $q(\mathbf{x})$ (the implicit density of $T_{\theta}(\mathbf{Z})$) and the discriminator $S(\mathbf{x})$:

$$\inf_q \sup_S \int_{\mathbf{x}} S(\mathbf{x})p(\mathbf{x}) \, d\mathbf{x} + \int_{\mathbf{x}} \log(1 - \exp(S(\mathbf{x})))q(\mathbf{x}) \, d\mathbf{x} + \log 4.$$

- Fixing the generator q , what is the optimal discriminator S ?
- Plugging the optimal discriminator S back in, what is the optimal generator?
- Fixing the discriminator S , what is the optimal generator q ?
- Plugging the optimal generator q back in, what is the optimal discriminator?

Exercise 19.17: KL vs. LK

Recall that the f -divergence $D_f(p||q)$ is infinite iff for some \mathbf{x} , $p(\mathbf{x}) \neq 0$ while $q(\mathbf{x}) = 0$. Consider the following twin problems:

$$q_{\text{KL}} := \operatorname{argmin}_{q \in \mathcal{Q}} \text{KL}(p||q)$$

$$q_{\text{LK}} := \operatorname{argmin}_{q \in \mathcal{Q}} \text{LK}(p||q).$$

Recall that $\operatorname{supp}(p) := \operatorname{cl}\{\mathbf{x} : p(\mathbf{x}) \neq 0\}$. What can we say about $\operatorname{supp}(p)$, $\operatorname{supp}(q_{\text{KL}})$ and $\operatorname{supp}(q_{\text{LK}})$? What about JS?

Definition 19.18: f -GAN (Nowozin et al. 2016)

Following Nowozin et al. (2016), we summarize the main idea of f -GAN as follows:

- **Generator:** Let μ be a **fixed reference** probability measure on space Z (usually the standard normal distribution) and $Z \sim \mu$. Let ν be any target probability measure on space X and $X \sim \nu$. Let $\mathcal{T} \subseteq \{\mathbf{T} : Z \rightarrow X\}$ be a class of transformations. According to Theorem 19.3 we know there exist

transformations T (which *may or may not* be in our class \mathcal{T}) so that $T(Z) \sim X \sim \nu$. Our goal is to **approximate such transformations T using our class \mathcal{T}** .

- **Loss:** We use the f -divergence to measure the closeness between the target X and the transformed reference $T(Z)$:

$$\inf_{T \in \mathcal{T}} D_f(X \| T(Z)).$$

In fact, any loss function that allows us to distinguish two probability measures can be used. However, we face an additional difficulty here: the densities of X and $T(Z)$ (w.r.t. a third probability measure λ) are not known to us (especially the former) so we cannot naively evaluate the f -divergence in (19.1).

- **Discriminator:** A simple variational reformulation will resolve the above difficulty! Indeed,

$$\begin{aligned} D_f(X \| T(Z)) &= \int f\left(\frac{d\nu}{d\tau}(\mathbf{x})\right) d\tau(\mathbf{x}) && (T(Z) \sim \tau) \\ &= \int \sup_{s \in \text{dom}(f^*)} \left[s \frac{d\nu}{d\tau}(\mathbf{x}) - f^*(s) \right] d\tau(\mathbf{x}) && (f^{**} = f) \\ &\geq \sup_{S \in \mathcal{S}} \int \left[S(\mathbf{x}) \frac{d\nu}{d\tau}(\mathbf{x}) - f^*(S(\mathbf{x})) \right] d\tau(\mathbf{x}) && (\mathcal{S} \subseteq \{S : X \rightarrow \text{dom}(f^*)\}) \\ &= \sup_{S \in \mathcal{S}} \mathbf{E}[S(X)] - \mathbf{E}[f^*(S(T(Z)))] && (\text{equality if } f' \left(\frac{d\nu}{d\tau} \right) \in \mathcal{S}), \end{aligned}$$

so our estimation problem reduces to the following minimax zero-sum game:

$$\inf_{T \in \mathcal{T}} \sup_{S \in \mathcal{S}} \mathbf{E}[S(X)] - \mathbf{E}[f^*(S(T(Z)))].$$

By replacing the expectations with empirical averages we can (approximately) solve the above problem with classic stochastic algorithms.

- **Reparameterization:** The class of functions \mathcal{S} we use to test the difference between two probability measures in the f -divergence must have their range contained in the domain of f^* . One convenient way to enforce this constraint is to set

$$\mathcal{S} = \sigma \circ \mathcal{U} := \{\sigma \circ U : U \in \mathcal{U}\}, \quad \sigma : \mathbb{R} \rightarrow \text{dom}(f^*), \quad \mathcal{U} \subseteq \{U : X \rightarrow \mathbb{R}\},$$

where the functions U are unconstrained and the domain constraint is enforced through a *fixed* “activation function” σ . With this choice, the **final f -GAN problem we need to solve is:**

$$\inf_{T \in \mathcal{T}} \sup_{U \in \mathcal{U}} \mathbf{E}[\sigma \circ U(X)] - \mathbf{E}[(f^* \circ \sigma)(U(T(Z)))].$$

Typically we choose an **increasing σ** so that the composition $f^* \circ \sigma$ is “nice.” Note that the **monotonicity of σ implies the same monotonicity of the composition $f^* \circ \sigma$** (since f^* is always increasing as f is defined only on \mathbb{R}_+). In this case, we prefer to pick a test function U so that $U(X)$ is large while $U(T(Z))$ is small. This choice aligns with the goal to “maximize target and minimize transformed reference,” although the opposite choice would work equally well (merely a sign change).

Nowozin, Sebastian, Botond Cseke, and Ryota Tomioka (2016). “ f -GAN: Training Generative Neural Samplers using Variational Divergence Minimization”. In: *NIPS*.

Remark 19.19: f -GAN recap

To specify an f -GAN, we need:

- A reference probability measure μ : should be easy to sample and typically we use standard normal;

- A class of transformations (generators): $\mathcal{T} \subseteq \{T : Z \rightarrow X\}$;
- An **increasing** convex function $f^* : \text{dom}(f^*) \rightarrow \mathbb{R}$ with $f^*(0) = 0$ and $f^*(s) \geq s$ (or equivalently an f -divergence);
- An **increasing** activation function $\sigma : \mathbb{R} \rightarrow \text{dom}(f^*)$ so that $f^* \circ \sigma$ is “nice”;
- A class of *unconstrained* test functions (discriminators): $\mathcal{U} \subseteq \{U : X \rightarrow \mathbb{R}\}$ so that $\mathcal{S} = \sigma \circ \mathcal{U}$.

Definition 19.20: Wasserstein GAN (WGAN) (Arjovsky et al. 2017)

If we let the test functions range over the set of all 1-Lipschitz continuous functions \mathcal{L} , we then obtain WGAN:

$$\inf_{\theta} \sup_{S \in \mathcal{L}} \text{ES}(\mathbf{X}) - \text{ES}(T_{\theta}(\mathbf{Z})),$$

which corresponds to the dual of the 1-Wasserstein distance.

Arjovsky, Martin, Soumith Chintala, and Léon Bottou (2017). “Wasserstein Generative Adversarial Networks”. In: *ICML*.

Definition 19.21: Maximum Mean Discrepancy GAN (MMD-GAN)

If, instead, we choose the test functions from a reproducing kernel Hilbert space (RKHS), then we obtain the so-called MMD-GAN (Dziugaite et al. 2015; Li et al. 2015; Li et al. 2017):

$$\inf_{\theta} \sup_{S \in \mathcal{H}_{\kappa}} \text{ES}(\mathbf{X}) - \text{ES}(T_{\theta}(\mathbf{Z})),$$

where \mathcal{H}_{κ} is the unit ball of the RKHS induced by the kernel κ .

Dziugaite, Gintare Karolina, Daniel M. Roy, and Zoubin Ghahramani (2015). “Training generative neural networks via maximum mean discrepancy optimization”. In: *UAI*.

Li, Yujia, Kevin Swersky, and Rich Zemel (2015). “Generative Moment Matching Networks”. In: *ICML*.

Li, Chun-Liang, Wei-Cheng Chang, Yu Cheng, Yiming Yang, and Barnabas Poczos (2017). “MMD GAN: Towards Deeper Understanding of Moment Matching Network”. In: *NIPS*.