Generative Adversarial Networks

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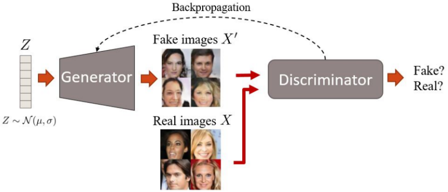
Density estimation

- Consider i.i.d. sample $x_1, ...x_N$, $x_i \sim p(x)$.
- We want to sample $\widehat{x}_{N+1}, \widehat{x}_{N+2}, ...$ from similar distribution.
- Statistical approach:
  - May take $q_\theta(x) \approx p(x)$ and sample from $q_\theta(x)$.
  - hard to estimate in high dimensional space
- Generative adversarial network (GAN):
  - replace hard problem (densitiy estimation in high dim. space) with easy problem-binary classification
  - train discriminator, discriminating x from $\widehat{x}$
  - fixed discriminator acts as trained loss function for improving generator $\widehat{x} = g(z)$,$z \sim p(z)$.

Intuition of adversarial learning

Generative adversarial learning for images:



GAN training overview.

Analogy for bank and a money counterfeiter (having a spy in the bank).

- they compete, until money counterfeiter learns to make perfect money replicas!

Seminal paper on GAN[1]

- Two networks:
  - generator $G(z) : Z \to X$
    - outputs generated object x
  - discriminator $D(x) : X \to [0, 1]$
    - probability that x **is real** rather than generated by G.

[1] Link to paper.

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        - probability that x **is real** rather than generated by G.
- Define
    - $p(x)$ - true data distribution (from training set)
    - $q(x)$ - generated data distribution $x \sim q(x) = G(z)$, $z \sim p(z)$.
        - $p(z)$ - standard distribution (Gaussian or other-spherical recommended).

[1] Link to paper.

Game

- Probability that x is correctly classified by discriminator:

$$\begin{cases} D(x), & x \text{ is real} \\ 1 - D(x), & x \text{ is fake} \end{cases}$$

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- Log-probability of correct classification by discriminator:
    - given that $p(real) = p(fake) = \frac{1}{2}$

$$V(D, G) = \mathbb{E}_{x \sim p(x)} [\log D(x)] + \mathbb{E}_{z \sim p(z)} [\log(1 - D(G(z)))]$$

Game

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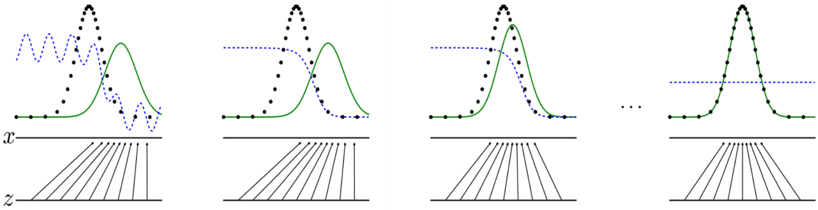
- D and G play two-player game with minimax function $V(G, D)$:

$$\min_G \max_D V(D, G)$$

Illustration of incremetal learning

Incremental learning of D and G:



black dotted: $p(x)$ - density of true samples
green: $q(x)$ - density of fake samples
blue dashed: $D(x) = p(x \text{ is true}|x)$

Losses

D task (for fixed G):

$$\mathbb{E}_{x\sim p(x)}\left[\log D(x)\right] + \mathbb{E}_{z\sim p(z)}\left[\log(1 - D(G(z)))\right] \to \max_{D}$$

G task (for fixed D):

$$\mathbb{E}_{z\sim p(z)}\left[\log(1 - D(G(z)))\right] \to \min_{G}$$

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- **Thus $G(z)$ learns to sample realistic samples from $p(x)$.**
- D and G should be trained syncronously.
    - if too much training of D, G will get zero-gradient, no feedback!
    - if too much training of G, it may converge to $\arg\max_x D(x)$.

Algorithm

for number of training iterations **do**

for k steps **do**

- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Sample minibatch of m examples $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
- Update the discriminator by ascending its stochastic gradient:

$$\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[\log D\left(\boldsymbol{x}^{(i)}\right) + \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right)\right].$$

end for

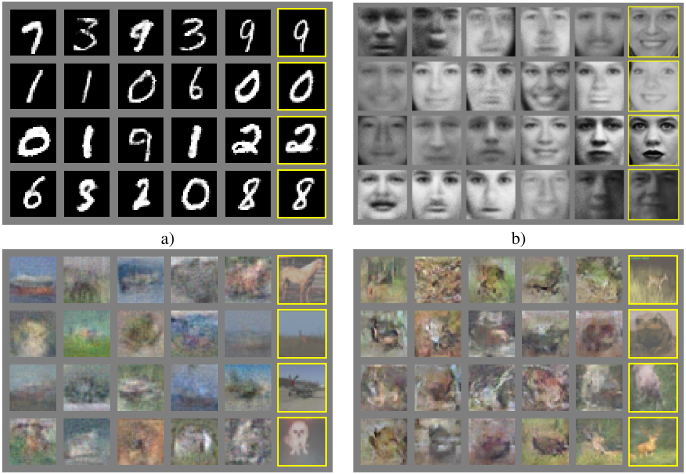
- Sample minibatch of m noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
- Update the generator by descending its stochastic gradient:

$$\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log\left(1 - D\left(G\left(\boldsymbol{z}^{(i)}\right)\right)\right).$$

end for

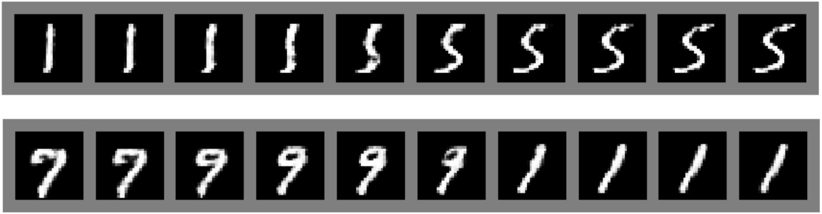
The gradient-based updates can use any standard gradient-based learning rule. We used momentum in our experiments.

Generated images



Interpolation in latent space

Linear interpolation of objects in latent space:



Optimal D^* given fixed G

Suppose D is flexible enough to take arbitrary values.

Theorem: For fixed G optimal discriminator is:

$$D^*(x|G) = \frac{p(x)}{p(x)+q(x)}$$

Optimal D^* given fixed G

Suppose D is flexible enough to take arbitrary values.

Theorem: For fixed G optimal discriminator is:

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Proof:

$$V(G, D) = \int_x p(x) \log(D(x))dx + \int_z p(g(z)) \log(1 - D(g(z)))dz =$$
$$= \int_x p(x) \log(D(x))dx + q(x) \log(1 - D(x))dx$$

Applying for $\forall x \in X$ $\arg\max_{d\in\mathbb{R}} \{p \log(d) + q \log(1 - d)\} = \frac{p}{p+q}$ for any $p, q \in \mathbb{R}$ obtain

$$\arg\max_D V(G, D) = \frac{p(x)}{p(x) + q(x)}$$

Optimal G^*

Theorem: given optimal D^*, optimal G^* should yield $q(x) = p(x)$.

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Proof:
Let G^* correspond to $q^*(x)=p(x)$. Then

$$
\begin{aligned}
& V(G^*,D^*(G))= \\
& =\int_x p(x)\log\frac{p(x)}{p(x)+q^*(x)}dx+\int_x q(x)\log\frac{q(x)}{p(x)+q^*(x)}dx \\
& =\int_x p(x)\log\frac{1}{2}dx+\int_x q(x)\log\frac{1}{2}dx=2\log\frac{1}{2}=-2\log 2
\end{aligned}
$$

Optimal G^* given D^*

$V(G^*, D^*(G)) = \min_G V(G, D^*(G))$, because

$$
\begin{aligned}
& V(G, D^*) - V(G^*, D^*) \\
= & \int_x p(x) \log \frac{p(x)}{p(x)+q(x)} dx + \int_x q(x) \log \frac{q(x)}{p(x)+q(x)} dx \\
& + \int_x p(x) \log 2 dx + \int_x q(x) \log 2 dx \\
= & \int_x p(x) \log \frac{p(x)}{\frac{p(x)+q(x)}{2}} dx + \int_x q(x) \log \frac{q(x)}{\frac{p(x)+q(x)}{2}} dx \\
= & KL\left(p(x) || \frac{p(x)+q(x)}{2}\right) + KL\left(q(x) || \frac{p(x)+q(x)}{2}\right) \geq 0
\end{aligned}
$$

1. Simple GAN
    - Model
    - Practical recommendations

Finding unstable saddle-point

D task (for fixed G):

$$\mathbb{E}_{x\sim p(x)}\left[\log D(x)\right]+\mathbb{E}_{z\sim p(z)}\left[\log(1-D(G(z)))\right]\to\max_{D}$$

G task (for fixed D):

$$\mathbb{E}_{z\sim p(z)}\left[\log(1-D(G(z)))\right]\to\min_{G}$$

Finding saddle-point $\min_G \max_D V(D,G)$ is very unstable.

- requires a lot of fine-tuning, see link to recommendations.

Problem of smart discriminator

Problem:

- On early iterations G generates poor fakes.
- It becomes very easy for D to discriminate.
- So $D(G(z)) \approx 0 => \nabla_{\theta_G} \log(1 - D(G(z)) \approx 0$ => no training in G.

Problem of smart discriminator: solutions

Improve G from another criterion:

$$\mathbb{E}_{z\sim p(z)}\left[\log(D(G(z)))\right] \to \max_{G}$$

- G is still tuned to fool the discriminator: $\uparrow D(G(z))$
- $\log(\cdot)$ exponentially amplifies small changes in $D(G(z))$ near zero.
- G gets non-degenerate feedback.
- D, G game stops being game with zero-sum.

Problem of smart discriminator: solutions

- occasionally flip labels when training D
- or use soft labels (1->uniform[0.7, 1.2], 0->uniform[0, 0.3])
- or add noise to input of $D(\cdot)$

Intuition:

- discriminator solves classification in more noisy setting and its predictions become smoother, so $\not\approx 0$

More recommendations

- Track failures early:
  - D loss goes to 0: failure mode
  - check norms of gradients: they should not be high
- If you have object labels, use them by training combined discriminator-classifier
  - weight sharing helps!

Mode collapse

- We proved that $\arg\max_G V(G, D^*(G)) = G^*$, yielding $q^*(x) = p(x)$
- Finding $D^*(G)$ for every change in G is impractical
- Practical task: improve G for fixed D: $\arg\max_G V(G, D)$
    - Can give mode collapse: $G(z) \equiv const \equiv \arg\max_x D(x)$
- Solutions to mode collapse
    - add stochasticity to G:
        - add Gaussian noise to inner layers (Zhao et. al. EBGAN).
        - add dropout in both train and test phase
    - add penalty for too close $G(z_1), G(z_2), ...G(z_K)$ where $z_1, ...z_K$ are mini-batch initializations.

Possible initializations

- May initialize G with right half of VAE.
- May initialize first layers of D with classification net (e.g. VGG).

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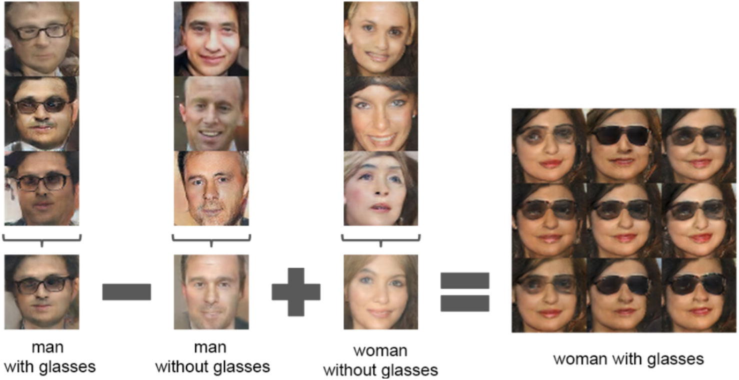
Deep convolutional GAN (DCGAN)[2]

Generates photorealistic 64x64 images (bedrooms in this case).

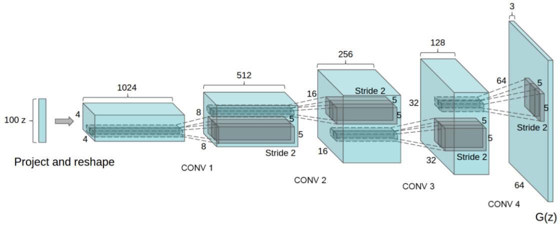
[2] https://arxiv.org/pdf/1511.06434.pdf

Latent space arithmetics



Generator

Uses fully-convolutional generator:



Architecture guidelines for stable DCGANs

1. Replace any pooling layers with fractional-strided convolutions in G and strided convolutions in D.
2. Use LeakyReLU activation in the discriminator for all layers.
3. Use batchnorm in both the generator and the discriminator.
4. Remove fully connected hidden layers for deeper architectures.
5. Use ReLU activation in generator for all layers except for the output, which uses Tanh.

Intuition: 1 and 2 allow better propagation of gradients.

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Proposed approachArticle about Wasserstein GAN

Proposed approach for generator:

1. $z \sim p(z)$ (e.g. $\sim \mathcal{N}(0, I)$)
2. $x = g_\theta(z)$, so $x \sim q_\theta(x)$ [distribution of generator]

We want $p(x) \approx q_\theta(x)$, so we require $\rho(p(x), q_\theta(x)) \to \min_\theta$.

- $\rho(\cdot, \cdot)$ is distance between probability distributions

By using Earth mover distance we get non-trivial distances even when domains of $p(x)$ and $q(x)$ don't intersect!

Popular distances

Let $x \in \mathcal{X}$ and define Σ-all measurable subsets of $\mathcal{X}$.

- Total Variation (TV):

$$\delta(p,q) = \sup_{A \in \Sigma} |p(A) - q(A)|$$

- Kullback-Leibler (KL) divergence:

$$KL(p||q) = \int p(x) \ln\left(\frac{p(x)}{q(x)}\right) dx$$

  - asymmetric
  - infinite if exist regions where $q(x) = 0$ and $p(x) \neq 0$.

Popular distances

- Jensen-Shannon (JS) divergence:

$$JS(p,q) = KL(p||a) + KL(q||a)$$

  where $a(x) := (p(x) + q(x))/2$.

- Earth-Mover (EM) distance or Wasserstein-1:

$$W(p,q) = \inf_{\gamma \in \Pi(p,q)} \mathbb{E}_{(x,y)\sim\gamma}\left[\|x-y\|\right]$$

  where $\Pi(p,q)$ is a set of all densities$\in \mathbb{R}^{2D}$, having
  - p - marginal distribution along $1:D$ dimensions
  - q - marginal distribution along $D+1:2D$ dimensions.

Example

Setup-consider 2D r.v. belonging to 1D manifold:

- $z \sim U[0,1]$
- p:=distribution of $(0,z) \in \mathbb{R}^2$.
- q_θ:=distribution of $(\theta,z) \in \mathbb{R}^2$ for some $\theta \in \mathbb{R}$.

Distance values $\rho(p, q_\theta)$:

$$W(p, q_\theta) = |\theta|$$

$$\delta(p, q_\theta) = \begin{cases} 1, & \theta \neq 0 \\ 0, & \theta = 0 \end{cases}$$

$$KL(p||q_\theta) = KL(q_\theta||p) = \begin{cases} +\infty, & \theta \neq 0 \\ 0, & \theta = 0 \end{cases}$$

$$JS(p, q_\theta) = \begin{cases} \ln 2, & \theta \neq 0 \\ 0, & \theta = 0 \end{cases}$$

If sequence $\theta_t \to 0$ then $\rho(p_r, p_{\theta_t}) \to 0$ only according to

Theory

- W is the weakest distance among δ, KL, JS.
    - i.e. convergence $p_t(\cdot) \to p(\cdot)$ for δ, KL, JS implies $p_t(\cdot) \to p(\cdot)$ for W
- $W(p_t, p) \to 0 \iff p_t(\cdot) \xrightarrow{\mathcal{D}} p(\cdot)$ (convergence by distribution).
- if $g_\theta(z)$ - continuous in $\theta \implies W(p_r, p_\theta)$ - continuous in θ.
- if $g_\theta(z)$ - multi-layer perceptron with smooth Lipshitz activations oe ReLU, then
    - $W(p, q_\theta)$ - continuous w.r.t. θ everywhere.
    - $W(p, q_\theta)$ - differentiable w.r.t. θ almost everywhere.

Kantorovich-Rubinstein duality

- $f(x)$ is K-Lipshitz if $\forall x, x' \in dom(f)$:
$$f(x) - f(x') \le K \left\|x - x'\right\|$$
- Intuitively K-Lipshitz means at any point x variation of $f(x + \Delta x)$ stays withing conus.

Wasserstein distance can be estimated with **Kantorovich-Rubinstein duality**:

$$W(p, q_\theta) = \sup_{\|f\|_L \le 1} \mathbb{E}_{x\sim p}\left[f(x)\right] - \mathbb{E}_{x\sim q_\theta}\left[f(x)\right]$$

where supremum is taken w.r.t all 1-Lipshitz functions.

- if $f(x)$ is taken among K-Lipshitz functions, duality will estimate $K \cdot W(p, q_\theta)$.
- since we want $W(p, q_\theta) \to \min$, multiplier K is not important.

Practical estimation of Wasserstein distance

- We may estimate Wassterstein distance with parametrized family of K-Lipshitz functions $\{f_w\}_{w \in W}$.
- f_w is taken as multi-layer perceptron with typical activations and constrained weights $W \in [-0.01, 0.01]^{\#weights}$ (to ensure K-Lipshitz property)
- For such function family:

1. $\max_{w \in W} \mathbb{E}_{x \sim p}[f_w(x)] - \mathbb{E}_{z \sim p(z)}[f_w(g_\theta(x))]$ - maximum **is achieved**.
2. $\nabla_\theta W(p, q_\theta) \propto -\mathbb{E}_{z \sim p(z)}[\nabla f(g_\theta(z)]$

Algorithm

Algorithm 1 WGAN, our proposed algorithm. All experiments in the paper used the default values $\alpha = 0.00005$, $c = 0.01$, $m = 64$, $n_{\text{critic}} = 5$.

Require: : α, the learning rate. c, the clipping parameter. m, the batch size. n_{critic}, the number of iterations of the critic per generator iteration.

Require: : w_0, initial critic parameters. θ_0, initial generator's parameters.

while θ has not converged **do**

  for $t = 0, ..., n_{\text{critic}}$ **do**

    Sample $\{x^{(i)}\}_{i=1}^m \sim \mathbb{P}_r$ a batch from the real data.

    Sample $\{z^{(i)}\}_{i=1}^m \sim p(z)$ a batch of prior samples.

    $g_w \leftarrow \nabla_w \left[\frac{1}{m}\sum_{i=1}^m f_w(x^{(i)}) - \frac{1}{m}\sum_{i=1}^m f_w(g_\theta(z^{(i)}))\right]$

    $w \leftarrow w + \alpha \cdot \text{RMSProp}(w, g_w)$

    $w \leftarrow \text{clip}(w, -c, c)$

  end for

  Sample $\{z^{(i)}\}_{i=1}^m \sim p(z)$ a batch of prior samples.

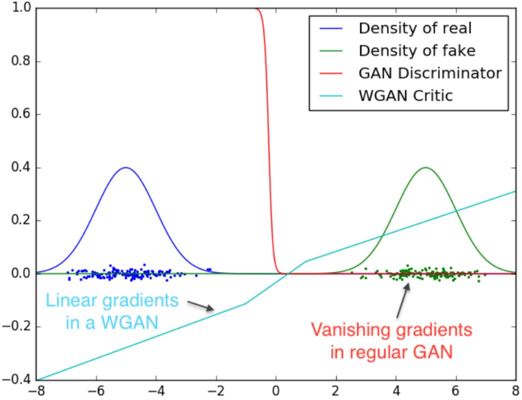
  $g_\theta \leftarrow -\nabla_\theta \frac{1}{m}\sum_{i=1}^m f_w(g_\theta(z^{(i)}))$

  $\theta \leftarrow \theta - \alpha \cdot \text{RMSProp}(\theta, g_\theta)$

end while

Wasserstein GAN

For distinct $p(x)$ and $q(x)$ and tunded D usual GAN can't train ($\nabla D(G(z)) \approx 0$), but WGAN can.



Benefits

Benefits of WGAN:

- Objective convergence criterion $W(p, q_\theta)$
  - in usual GAN generator and discriminator optimize different functions
- For distinct $p(x)$ and $q(x)$ and tunded D usual GAN can't train ($\nabla D(G(z)) \approx 0$), but WGAN can.
- No mode collapse because $W(p, \delta(x - \arg\max_u p(u)) > W(p, p)$
- More stable convergence&results for different architectures of generator/discriminator.

Wasserstein GAN with gradient penalty[3]

Another way to enforce Lipshitz property:

- remove weights clipping
- add regularizer $\lambda\left(\|\nabla_x f(x)\|_2 - 1\right)^2$ in optimization.
    - because Lipshitz property of order 1: $\|\nabla_x f(x)\|_2 \leq 1$

[3] Gulrajani et al. 2017

DCGAN vs. WGAN vs. WGAN-GP

Gives better quality for variable model design:

Conclusion

- GAN - method to generate new realistic samples based on $x_1, ...x_N$.
- Original approach suffers from:
  - smart discriminator => ≈ 0 gradients for G
    - flip labels, use soft labels, WassersteinGAN
  - mode collapse in G
    - use Gaussian noise, dropout in G
    - use WassersteinGAN (brings closer whole distributions)
- DCGAN - GAN designed for images generation.
  - fully convolutional G
  - in D to propagate $\neq 0$ gradients:
    - max-pooling -> strided conv
    - ReLU->LeakyReLU.