Generative Adversarial Networks

Machine Learning and Data Mining

Maxim Borisyak

National Research University Higher School of Economics (HSE)

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Generative models

Generative models

- Informally, given samples we wish to learn underlying distribution in form of sampling procedure.
- Formally, given samples of a random variable X, we wish to find X', so that:

$$P(X) \approx P(X')$$

Types of generative models

Fitting density function $P(X)$ (or a function $f(x)$ proportional to the density):

- partition function Z for $f(x)$ might be an issue:
  - for energy models Contrastive Devergence keeps Z finite (ideally constant);
- sampling might be an issue:
  - Gibbs sampling works ok if $P(x^i \mid x^{-i})$ is analytically known and simple enough.

Going deep:

- RBM is intrinsically one-layer model;
- Deep Boltzmann machines:
  - Gibbs sampling becomes less efficient than for RBM.

Types of generative procedures

Options for defining a random variables:

- specify $P(X)$ and use general sampling algorithm (e.g. Gibbs sampling);
- **learn sampling procedure directly**, e.g.:

$$\begin{aligned} X &= f(Z); \\ Z &\sim \mathrm{SimpleDistribution}; \end{aligned}$$

Fitting Distributions

Notation: Q - ground truth distribution, P - model.

Maximum Likelihood:

$$\begin{aligned}\mathcal{L} &= \sum_i \log P(x_i) \approx \mathop{\mathbb{E}}_{x \sim Q} \log P(x) \to_P \min; \\ \mathrm{KL}(Q \,\|\, P) &= \mathop{\mathbb{E}}_{x \sim Q} \log Q(x) - \mathop{\mathbb{E}}_{x \sim Q} \log P(x) \to_P \min .\end{aligned}$$

Jensen-Shannon distance:

$$\begin{aligned}\mathrm{JS}(P, Q) &= \frac{1}{2}\left[\mathrm{KL}(P \,\|\, M) + \mathrm{KL}(Q \,\|\, M)\right] \to_P \min; \\ M &= \frac{1}{2}(P + Q).\end{aligned}$$

Generative Adversarial Networks

Approximating JS distance

$$\mathrm{JS}(P,Q) = \frac{1}{2}\left[\mathop{\mathbb{E}}_{x\sim P} \log\frac{P(x)}{M(x)} + \mathop{\mathbb{E}}_{x\sim Q} \log\frac{Q(x)}{M(x)}\right] =$$

$$\frac{1}{2}\left[\mathop{\mathbb{E}}_{x\sim P} \log\frac{P(x)}{P(x)+Q(x)} + \mathop{\mathbb{E}}_{x\sim Q} \log\frac{Q(x)}{P(x)+Q(x)}\right] + \log 2 =$$

$$\mathop{\mathbb{E}}_{x\sim M} \frac{P(x)}{P(x)+Q(x)} \log\frac{P(x)}{P(x)+Q(x)} +$$

$$\mathop{\mathbb{E}}_{x\sim M} \frac{Q(x)}{P(x)+Q(x)} \log\frac{Q(x)}{P(x)+Q(x)} + \log 2$$

Approximating JS distance

$$\mathrm{JS}(P,Q) = \mathop{\mathbb{E}}_{x\sim M} \frac{P(x)}{P(x)+Q(x)} \log \frac{P(x)}{P(x)+Q(x)} +$$

$$\mathop{\mathbb{E}}_{x\sim M} \frac{Q(x)}{P(x)+Q(x)} \log \frac{Q(x)}{P(x)+Q(x)} + \log 2$$

Let's introduce y: $y = 1$ if x is sampled from P and $y = 0$ for Q:

$$\mathrm{JS}(P,Q) - \log 2 =$$

$$\mathop{\mathbb{E}}_{x\sim M} \left[P(y=1 \mid x) \log P(y=1 \mid x) + P(y=0 \mid x) \log P(y=0 \mid x)\right] =$$

$$\mathop{\mathbb{E}}_{x\sim M} \left[\mathop{\mathbb{E}}_{y} [y \mid x] \log P(y=1 \mid x) + (1 - \mathop{\mathbb{E}}_{y} [y \mid x]) \log P(y=0 \mid x)\right]$$

Approximating JS distance

$$\mathrm{JS}(P, Q) - \log 2 =$$

$$\mathop{\mathbb{E}}_{x \sim M} \left[\mathop{\mathbb{E}}_{y} [y \mid x] \log P(y = 1 \mid x) + (1 - \mathop{\mathbb{E}}_{y} [y \mid x]) \log P(y = 0 \mid x) \right] =$$

$$\mathop{\mathbb{E}}_{x \sim M, y} y \, \log P(y = 1 \mid x) + (1 - y) \log P(y = 0 \mid x)$$

$$\boxed{\mathrm{JS}(P, Q) = \log 2 - \min_{f} \left[\mathcal{L}_{\text{crossentropy}}(f \mid P, Q) \right]}$$

Approximating JS distance

$$\arg\min_{P} \mathrm{JS}(P, Q) = \arg\max_{P} \left[\min_{f} \mathcal{L}_{\mathrm{crossentropy}}(f \mid P, Q)\right]$$

- JS-distance between distributions P and Q can be measured by training a discriminative model with cross-entropy loss;
- distribution P can trained by ascending loss of a trained discriminative model.

Game interpretation

$$\mathcal{L}(\theta, \psi) = -\frac{1}{2}\left[\mathop{\mathbb{E}}_{x \sim Q} \log f_\theta(x) + \mathop{\mathbb{E}}_{z \sim Z} \log\left(1 - f_\theta(g_\psi(z))\right)\right]$$

- discriminative model: **discriminator** $f(x)$;
- generative model: **generator** $x' = g(z)$;

Min-max game:

- goal of discriminator: distinguish between real and generated samples:

$$\mathcal{L}(\theta, \psi) \to_\theta \min$$

- goal of generator: 'fool' discriminator:

$$\mathcal{L}(\theta, \psi) \to_\psi \max$$

Adversarial Training

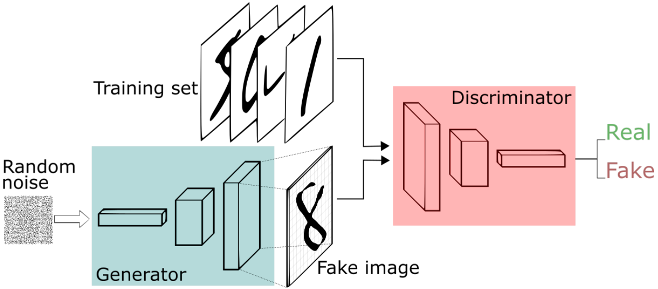
Algorithm 1 Generative Adversarial Training

Require: generative model g parametrized by ψ,
discriminative model f parametrized by θ,
sample of real data X

while not enough **do**
  for $i := 1, \ldots, n$ **do**
    sample real data $\{x_j\}_{j=1}^{k}$
    sample latent variables $\{z_j\}_{j=1}^{l}$
    $\theta \leftarrow \theta + \frac{\lambda}{2} \nabla_\theta \left[\sum_j \log f_\theta(x_j) + \sum_j \log\left(1 - f_\theta(g_\psi(z_j))\right) \right]$
  end for
  sample latent variables $\{z_j\}_{j=1}^{l}$
  $\psi \leftarrow \psi - \frac{\alpha}{2} \nabla_\psi \left[\sum_j \log\left(1 - f_\theta(g_\psi(z_j))\right) \right]$
end while

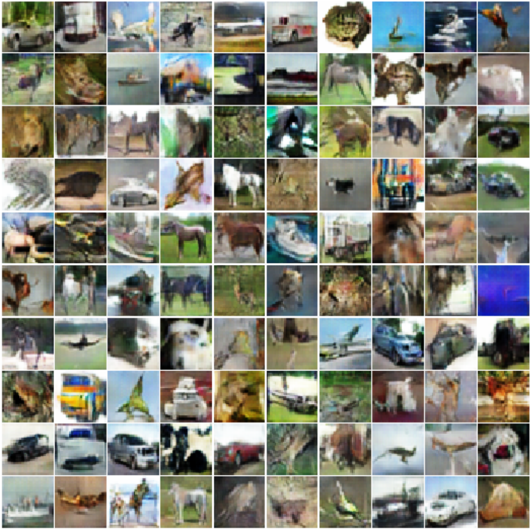
Generative Adversarial Networks

- generator and discriminator are usually deep neural networks;
- latent variables z are usually chosen to be easy to sample, e.g. $\mathcal{N}^n(0,1)$.



Source: https://sthalles.github.io/assets/dcgan/GANs.png

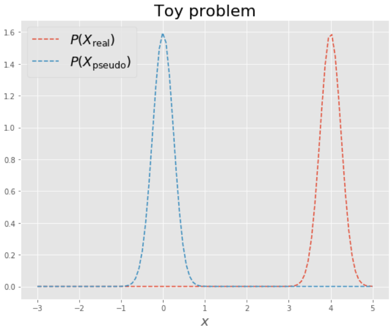
CIFAR examples



Discussion

Consider toy problem:

- powerfull discriminator;
- (almost) disjoint supports:
  - unlucky initial guess;
  - target data is on low-dimensional manifold;



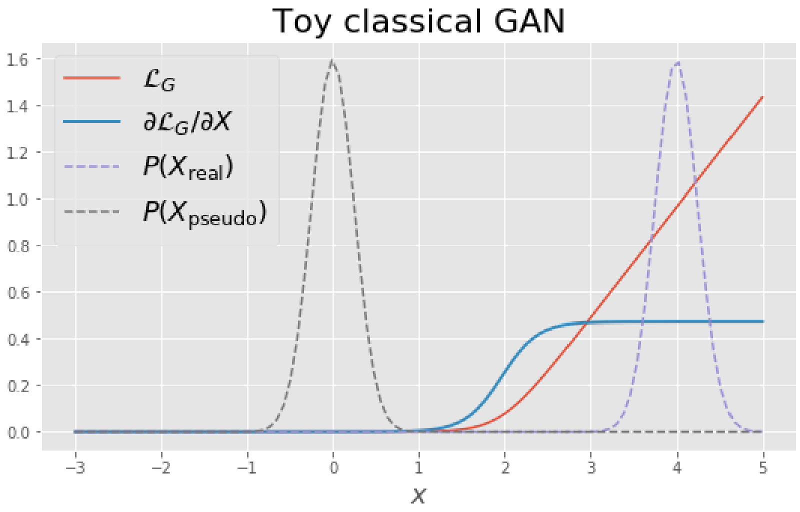
Discussion

After training discriminator:

$$\begin{aligned}\frac{\partial \mathcal{L}(\theta, \psi)}{\partial \psi} &= -\frac{1}{1 - f(g(z))} \cdot \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial \psi}; \\ f(g(z)) &\approx 0; \\ \frac{f}{\partial g} &\approx 0.\end{aligned}$$

$\Rightarrow$ gradients tend to vanish on early stages.

Discussion



Toy classical GAN
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
$\mathcal{L}_G$
$\partial\mathcal{L}_G/\partial X$
$P(X_{\text{real}})$
$P(X_{\text{pseudo}})$
−3
−2
−1
0
1
2
3
4
5
X

GAN training tricks

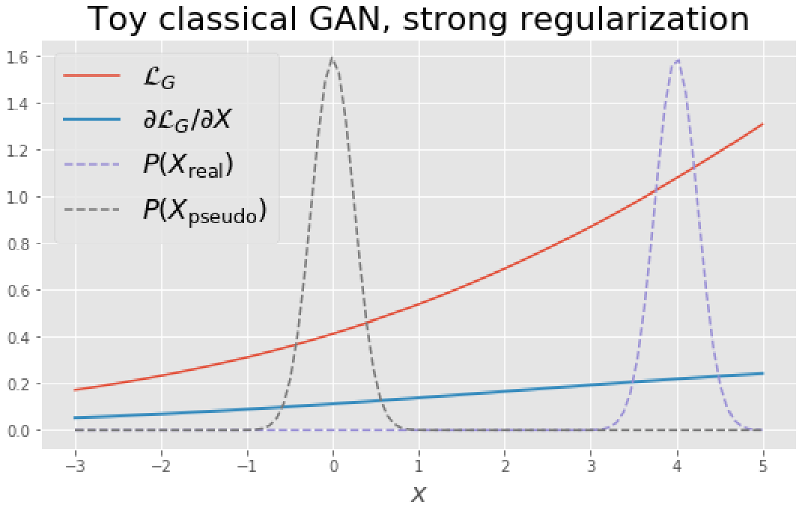
Fight for the gradients

Start with heavily restricted discriminator:

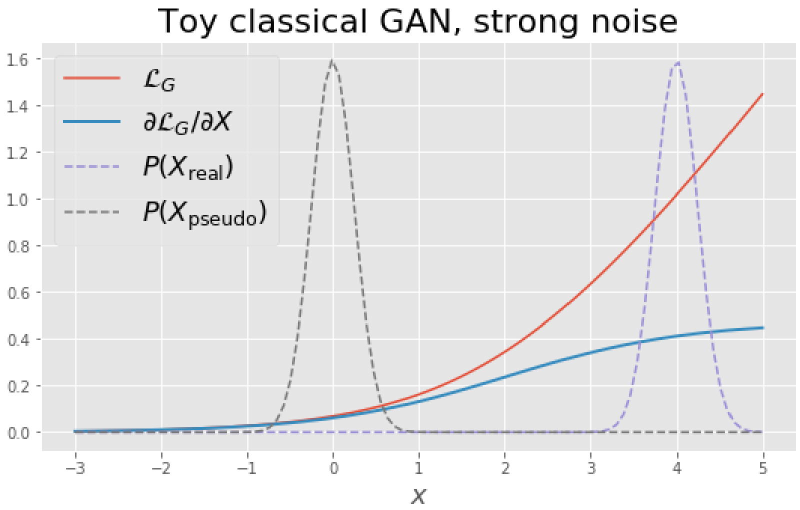
- don’t train discriminator fully:
    - poor-man solution;
- add noise to the samples:
    - especially nicely works for target on low-dimensional manifolds;
    - easy to control.
- heavy regularization.

As learning progresses gradually relax restrictions.

Fight for the gradients



Fight for the gradients



Fight for the gradients

Discriminator stop criteria:

```
for epoch in ...:
  while loss > C1:
    loss = train_discriminator()

  while loss < C2:
    loss = train_generator()
```

Ensemble of discriminators

- if discriminator $f_1 \in \mathcal{F}_1$ covers all possible $f_2 \in \mathcal{F}_2$, i.e. $\mathcal{F}_2 \subset \mathcal{F}_1 \subseteq \mathcal{F}$, then:

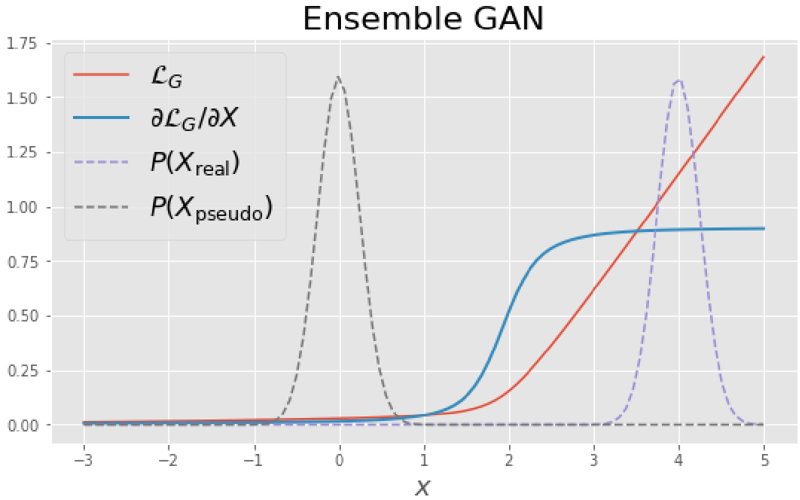
$$\log 2 - \mathrm{JS}(X, g(Z)) = \min_{f \in \mathcal{F}} \mathcal{L}(f, g) \leq \min_{f \in \mathcal{F}_1} \mathcal{L}(f, g) \leq \min_{f \in \mathcal{F}_2} \mathcal{L}(f, g)$$

- simple discriminator tend to provide gradients for a larger set of g, but don't lead to exact solution;
- powerful discriminator provide precise solution, but suffer from vanishing gradients.

Ensemble of discriminators with capacities from low to sufficient:

- provide gradient on early stages;
- lead to the precise solution.

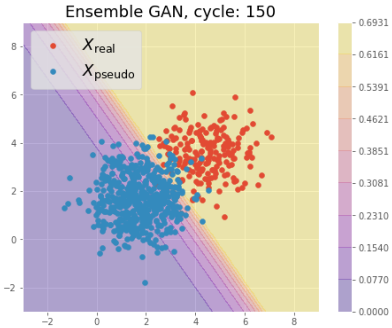
Ensemble of discriminators

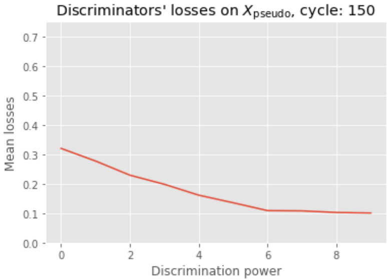


Bonus

Using ensemble of discriminators progress of training can be estimated by sum of individual losses:

$$\mathcal{L} = \sum_i \mathcal{L}^i$$





Mode collapse

Often generator learns to output constant:

- syndrome of poorly trained discriminator;
- might occur while using early stopping of discriminator training:
  - that is why it is a poor solution.
- ensure, discriminator is trained sufficiently long;
- prevent gradient vanishing by another methods.

Feature matching

Let h be some **feature**, then feature matching is an auxiliary objective:

$$\mathcal{L}_{\text{fm}} = \| \mathop{\mathbb{E}}_{x \sim \text{data}} h(x) - \mathop{\mathbb{E}}_{z \sim Z} h(g(z)) \|^2$$

Mini-batch discrimination

Instead of predicting label for a single sample, predict a single label for the whole mini-batch:

- prevents mode collapse by producing equivalent gradients to a multiple points.

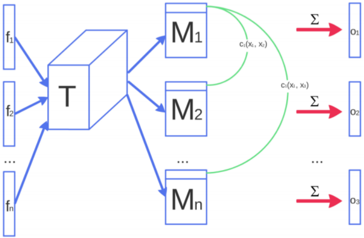


Figure 1: Figure sketches how mini-batch discrimination works. Features $\mathbf{f}(\boldsymbol{x}_i)$ from sample $\boldsymbol{x}_i$ are multiplied through a tensor T, and cross-sample distance is computed.

EBGAN and WGAN

Fight for the gradients

A lot of problems with training GANs can be traced to problem of maintaining balance between:

- vanishing gradients;
- sufficiently trained discriminator.

Fully trained discriminator $\Rightarrow$ vanishing gradients.

Poorly trained discriminator $\Rightarrow$ mode collapse.

These properties are fundamental for Jensen-Shannon metric.

Energy-Based GAN

Energy-Based GAN utilizes different loss function:

$$\mathcal{L} = \mathop{\mathbb{E}}_{x \sim \mathrm{data}} E(x) + \mathop{\mathbb{E}}_{z \sim Z} [m - E(g(z))]_+$$

$$\begin{aligned}
\mathcal{L}_f &= \mathop{\mathbb{E}}_{x \sim \mathrm{data}} E(x) + \mathop{\mathbb{E}}_{z \sim Z} [m - E(g(z))]_+ \to \min; \\
\mathcal{L}_g &= \mathop{\mathbb{E}}_{z \sim Z} E(g(z)) \to \min;
\end{aligned}$$

where:

- $E(x) > 0$ - an energy function;
- m - margin, a hyperparameter;
- $[a]_+ = \max(0, a)$.

Energy-Based GAN

- corresponds to minimization of Total-Variation distance:

$$\mathrm{TV}(P, Q) = \sum_x |P(x) - Q(x)|$$

- the most popular choice of energy function is MSE of an AutoEncoder:

$$E(x) = \|x - \mathrm{AE}(x)\|^2$$

- discriminator tend to have gradients almost everywhere;
- discriminator should be trained until convergence, i.e. as long as possible.

Wasserstein GAN

Wasserstein or Earth-Mover distance:

$$W(P,Q) = \inf_{\Gamma \in \Pi(P,Q)} \mathop{\mathbb{E}}_{(x,y)\sim\Gamma} \|x - y\|$$

where:

- $\Pi(P,Q)$ - set of all possible joint distributions Γ with marginals P and Q.

$$W(P,Q) = \sup_{\|f\|_L \le 1} \mathop{\mathbb{E}}_{x\sim\mathrm{data}} f(x) - \mathop{\mathbb{E}}_{z\sim Z} f(g(z))$$

where:

- $\|f\|_L = \sup \|\nabla f\|$ - Lipschitz constant for f.

Wasserstein GAN

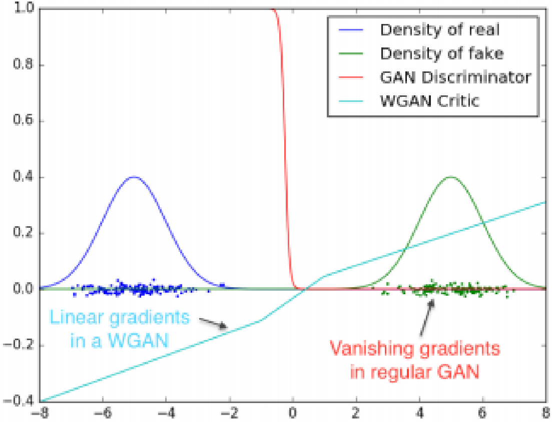


Figure 2: Optimal discriminator and critic when learning to differentiate two Gaussians. As we can see, the traditional GAN discriminator saturates and results in vanishing gradients. Our WGAN critic provides very clean gradients on all parts of the space.

Wasserstein GAN training

Algorithm 2 Wasserstein GAN trainin

while not enough **do**
  for $i := 1, \ldots, n$ **do**
    sample real data $\{x_j\}_{j=1}^k$
    sample latent variables $\{z_j\}_{j=1}^l$
    $g_\theta \leftarrow \nabla_\theta \left[\frac{1}{k}\sum_j f_\theta(x_j) - \frac{1}{l}\sum_j f_\theta(g_\psi(z_j))\right]$
    $\theta \leftarrow \theta + \alpha \mathrm{RMSProp}(\theta, g_\theta)$
    $\theta \leftarrow \mathrm{clip}(\theta, -1, 1)$
  end for
  sample latent variables $\{z_j\}_{j=1}^l$
  $g_\psi = -\nabla_\psi \left[\frac{1}{l}\sum_j f_\theta(g_\psi(z_j))\right]$
  $\psi \leftarrow \psi - \alpha \mathrm{RMSProp}(\psi, g_\psi)$
end while

Beyond generative

Conditional GAN

Allows to train a conditional generator $g(z, y)$:

- both discriminator and generator receive condition.

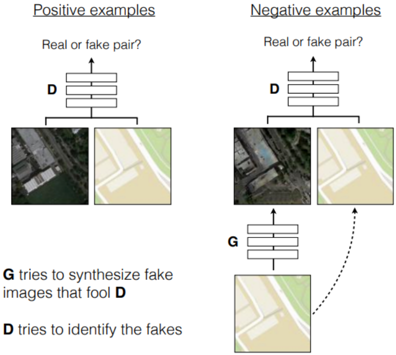


Figure 2: Training a conditional GAN to predict aerial photos from maps. The discriminator, D, learns to classify between real and synthesized pairs. The generator learns to fool the discriminator. Unlike an unconditional GAN, both the generator and discriminator observe an input image.

For image to image translation, loss:

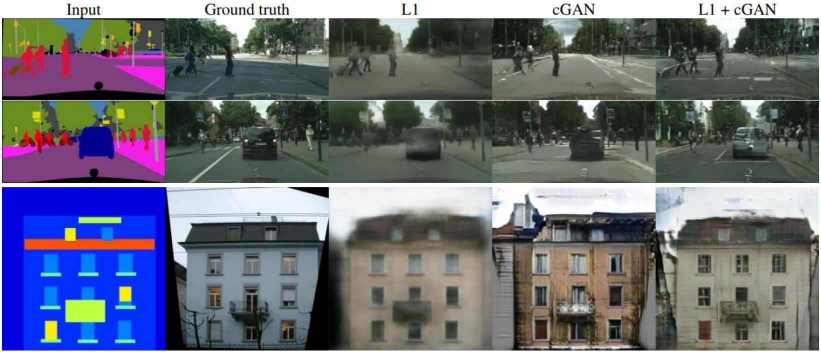
$$\mathcal{L} = \frac{1}{n}|f(x) - y| + \lambda\mathcal{L}_{\mathrm{GAN}}$$

where:

- $\mathcal{L}_{\mathrm{GAN}}$ - GAN loss on small image patches;

produces highly realistic images.

GAN as auxiliary loss



Summary

Summary

Generative Adversarial Networks:

- utilize adversary to measure statistical distance:
    - classical GAN estimates Jensen-Shannon distance;
    - EB-GAN estimates total-variation distance;
    - W-GAN estimates Wasserstein distance.
- can be modified to learn conditional distributions;
- can be used as auxiliary loss.

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