Deep learning

11.2. Wasserstein GAN

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Arjovsky et al. (2017) pointed out that $D_{JS}$ does not account [much] for the metric structure of the space.

\[
D_{JS}(\mu, \mu') = \min(\delta, |x|) \left( \frac{1}{\delta} \log \left( 1 + \frac{1}{2\delta} \right) - \left( 1 + \frac{1}{\delta} \right) \log \left( 1 + \frac{1}{\delta} \right) \right)
\]

Hence all $|x|$ greater than $\delta$ are seen the same.
An alternative choice is the “earth moving distance”, or Wasserstein distance, which intuitively is the minimum mass displacement to transform one distribution into the other.

\[
\mu = \frac{1}{4} \mathbf{1}_{[1,2]} + \frac{1}{4} \mathbf{1}_{[3,4]} + \frac{1}{2} \mathbf{1}_{[9,10]} \quad \mu' = \frac{1}{2} \mathbf{1}_{[5,7]}
\]

\[
W(\mu, \mu') = 4 \times \frac{1}{4} + 2 \times \frac{1}{4} + 3 \times \frac{1}{2} = 3
\]
Intuitively, it increases monotonically with the distance between modes

\[ W(\mu, \mu') = \frac{1}{2} |x| \]
The Wasserstein distance can be defined as

\[ W(\mu, \mu') = \min_{q \in \Pi(\mu, \mu')} \mathbb{E}_{(X, X') \sim q} \left[ \|X - X'\| \right], \]

where \( \Pi(\mu, \mu') \) is the set of distributions over \( \mathcal{X}^2 \) whose marginals are \( \mu \) and \( \mu' \).

So while it would make a lot of sense to look for a generator matching the density for this metric, that is

\[ G^* = \arg\min_G W(\mu, \mu_G). \]

the definition of \( W \) is not an operational way of estimating it.
A duality theorem from Kantorovich and Rubinstein implies

$$W(\mu, \mu') = \max_{\|f\|_L \leq 1} \mathbb{E}_{X \sim \mu} [f(X)] - \mathbb{E}_{X \sim \mu'} [f(X)]$$

where

$$\|f\|_L = \max_{x, x'} \frac{\|f(x) - f(x')\|}{\|x - x'\|}$$

is the Lipschitz seminorm.
\[\mu = \frac{1}{4}1_{[1,2]} + \frac{1}{4}1_{[3,4]} + \frac{1}{2}1_{[9,10]} \quad \mu' = \frac{1}{2}1_{[5,7]}\]

\[W(\mu, \mu') = \left(3 \times \frac{1}{4} + 1 \times \frac{1}{4} + 2 \times \frac{1}{2}\right) - \left(-1 \times \frac{1}{2} - 1 \times \frac{1}{2}\right) = 3\]
Using this result, we are looking for a generator

$$G^* = \arg\min_G W(\mu, \mu_G)$$

$$= \arg\min_G \max_{\|D\|_1 \leq 1} \left( E_{X \sim \mu} [D(X)] - E_{X \sim \mu_G} [D(X)] \right),$$

where the max is now an optimized predictor.

This is very similar to the original GAN formulation, except that the value of $D$ is not interpreted through a log-loss, and there is a strong regularization on $D$. 
The main issue in this formulation is to optimize the network $D$ under a constraint on its Lipschitz seminorm

$$\|D\|_L \leq 1.$$ 

Arjovsky et al. achieve this by clipping $D$'s weights.
The two main benefits observed by Arjovsky et al. are

- A greater stability of the learning process, both in principle and in their experiments: they do not witness “mode collapse”.

- A greater interpretability of the loss, which is a better indicator of the quality of the samples.
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.

(Arjovsky et al., 2017)
Figure 4: JS estimates for an MLP generator (upper left) and a DCGAN generator (upper right) trained with the standard GAN procedure. Both had a DCGAN discriminator. Both curves have increasing error. Samples get better for the DCGAN but the JS estimate increases or stays constant, pointing towards no significant correlation between sample quality and loss. Bottom: MLP with both generator and discriminator. The curve goes up and down regardless of sample quality. All training curves were passed through the same median filter as in Figure 3.

(Arjovsky et al., 2017)
Figure 3: Training curves and samples at different stages of training. We can see a clear correlation between lower error and better sample quality. Upper left: the generator is an MLP with 4 hidden layers and 512 units at each layer. The loss decreases consistently as training progresses and sample quality increases. Upper right: the generator is a standard DCGAN. The loss decreases quickly and sample quality increases as well. In both upper plots the critic is a DCGAN without the sigmoid so losses can be subjected to comparison. Lower half: both the generator and the discriminator are MLPs with substantially high learning rates (so training failed). Loss is constant and samples are constant as well. The training curves were passed through a median filter for visualization purposes.

(Arjovsky et al., 2017)
However, as Arjovsky et al. wrote:

“Weight clipping is a clearly terrible way to enforce a Lipschitz constraint. If the clipping parameter is large, then it can take a long time for any weights to reach their limit, thereby making it harder to train the critic till optimality. If the clipping is small, this can easily lead to vanishing gradients when the number of layers is big, or batch normalization is not used (such as in RNNs).”

(Arjovsky et al., 2017)

In some way, the resulting Wasserstein GAN (WGAN) trades the difficulty to train $G$ for the difficulty to train $D$.

In practice, this weakness results in extremely long convergence time.
Spectral Normalization
Miyato et al. (2018) proposed to control the Lipschitz constant of $\mathbf{D}$ by rescaling its weights, so that all the linear layers have their singular values lesser than 1, and consequently Lipschitz constant, lesser than 1.

If the non-linear layers are also Lipschitz of constant lesser than 1 (e.g. ReLU), this is a sufficient condition.

**Spectral Normalization** is a layer normalization that estimates the largest singular value of a weight matrix, and rescale it accordingly.

While computing the SVD of a matrix is expensive, computing [a good approximation of] the largest SV can be done iteratively for a reasonable cost.
The largest singular value of a matrix $W$ is also its spectral norm

$$\sigma(W) = \max_{h: \|h\|_2 \leq 1} \|Wh\|_2.$$ 

To calculate it, the power iteration method starts with two random vectors $u_0$ and $v_0$, and with

$$v_{n+1} = \frac{W^T u_n}{\|W^T u_n\|_2}$$

$$u_{n+1} = \frac{Wv_{n+1}}{\|Wv_{n+1}\|_2}$$

we have

$$\sigma(W) = \lim_{n \to \infty} u_n^T W v_n$$
W = torch.empty(15, 15).normal_()
print(W.svd().S.max())

u = torch.empty(W.size(0)).normal_()

for k in range(10):
    v = W.t() @ u
    v = v / v.norm()
    u = W @ v
    u = u / u.norm()

print(u.t() @ W @ v)

prints

tensor(7.9129)
tensor(7.9129)
Miyato et al. update $u_n$ and $v_n$ before every gradient step, and rescale the weight matrix accordingly.

The same can be done in PyTorch with torch.nn.utils.spectral_norm, that wraps any linear layer into a module that performs the normalization.
m = nn.Linear(5, 5)
print(m.weight.svd().S.max())

x = torch.randn(100, 5)
optimizer = torch.optim.SGD(m.parameters(), lr = 1e-1)

for k in range(100):
    loss = -m(x).norm()
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

print(m.weight.svd().S.max())

prints

tensor(0.9277, grad_fn=<MaxBackward1>)
tensor(114.1429, grad_fn=<MaxBackward1>)}
m = nn.Linear(5, 5)
print(m.weight.svd().S.max())

m = nn.utils.spectral_norm(m)

x = torch.rand(100, 5)
optimizer = torch.optim.SGD(m.parameters(), lr = 1e-1)

for k in range(100):
    loss = -m(x).norm()
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

print(m.weight.svd().S.max())

prints

tensor(0.8716, grad_fn=<MaxBackward1>)
tensor(1.0000, grad_fn=<MaxBackward1>)
References