A Case Study on Volatility in Financial Time Series

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Outline

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Goal - **Convince you that WGAN is the "best" GAN**

What does it mean to learn a probability distribution?

When learning generative models, we assume the data we have comes from some unknown distribution $\mathbb{P}_r$.

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1. Directly learn the probability density function $\mathbb{P}_\theta$ and then optimize through maximum likelihood estimation

2. Learn a function that transforms an existing distribution Z into $\mathbb{P}_\theta$. Here, g_θ is some differentiable function, Z is a common distribution (usually uniform or Gaussian), and $\mathbb{P}_\theta = g_\theta(Z)$

Maximum Likelihood approach is problematic

Recall that for continuous distributions $\mathbb{P}$ and $\mathbb{Q}$ the KL divergence is:

$$KL(\mathbb{P}||\mathbb{Q}) = \int_x \mathbb{P}(x) \log \frac{\mathbb{P}(x)}{\mathbb{Q}(x)} dx$$

and given function $\mathbb{P}_\theta$, the MLE objective is

$$\max_{\theta \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^{m} \log \mathbb{P}_\theta(x^{(i)})$$

In the limit (as $m \to \infty$), samples will appear based on the data distribution $\mathbb{P}_r$, so

$$\lim_{m \to \infty} \max_{\theta \in \mathbb{R}^d} \frac{1}{m} \sum_{i=1}^{m} \log \mathbb{P}_\theta(x^{(i)}) = \max_{\theta \in \mathbb{R}^d} \int_x \mathbb{P}_r(x) \log \mathbb{P}_\theta(x) dx$$

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- This unfortunately introduces some error, and empirically people have needed to add a lot of random noise to make models train

Transforming an existing distribution

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VAEs focus on the approximate likelihood of the examples and so share the limitation that you need to fiddle with additional noise terms.

GANs offer much more flexibility but their training is unstable.

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How do we define d?

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χ - compact metric set (such as the space of images $[0,1]^d$)
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Kullback-Leibler (KL) divergence

$$KL(\mathbb{P}_r || \mathbb{P}_\theta) = \int_x \mathbb{P}_r(x) \log \frac{\mathbb{P}_r(x)}{\mathbb{P}_\theta(x)} d\mu(x)$$

where both $\mathbb{P}_r$ and $\mathbb{P}_\theta$ are assumed to be absolutely continuous with respect to a same measure μ defined on χ.

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Jensen-Shannon (JS) Divergence

$$JS(\mathbb{P}_r, \mathbb{P}_\theta) = KL(\mathbb{P}_r || \mathbb{P}_m) + KL(\mathbb{P}_\theta || \mathbb{P}_m)$$

where $\mathbb{P}_m$ is the mixture $(\mathbb{P}_r + \mathbb{P}_\theta)/2$

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Earth-Mover (EM) distance or Wasserstein-1

$$W(\mathbb{P}_r, \mathbb{P}_\theta) = \inf_{\gamma \in \Pi((\mathbb{P}_r, \mathbb{P}_\theta)} \mathbb{E}_{(x,y)\sim\gamma}[||x - y||]$$

where $\Pi(\mathbb{P}_r, \mathbb{P}_\theta)$ denotes the set of all join distributions $\gamma(x, y)$ whose marginals are respectively $\mathbb{P}_r$ and $\mathbb{P}_\theta$

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Transport Plan

Each $\gamma \in \Pi$ is a transport plan and to execute the plan, for all x, y move $\gamma(x, y)$ mass from x to y.

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This shows why the marginals of $\gamma \in \Pi$ must be $\mathbb{P}_r$ and $\mathbb{P}_\theta$. For scoring, the effort spent is

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Computing the infimum of this over all valid γ gives the earth mover distance

Learning Parallel Lines Example

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Let $Z \sim U[0,1]$ and let $\mathbb{P}_0$ be the distribution of $(0, Z) \in \mathbb{R}^2$, uniform on a straight vertical line passing through the origin. Now let $g_\theta(z) = (\theta, z)$ with θ a single real parameter.

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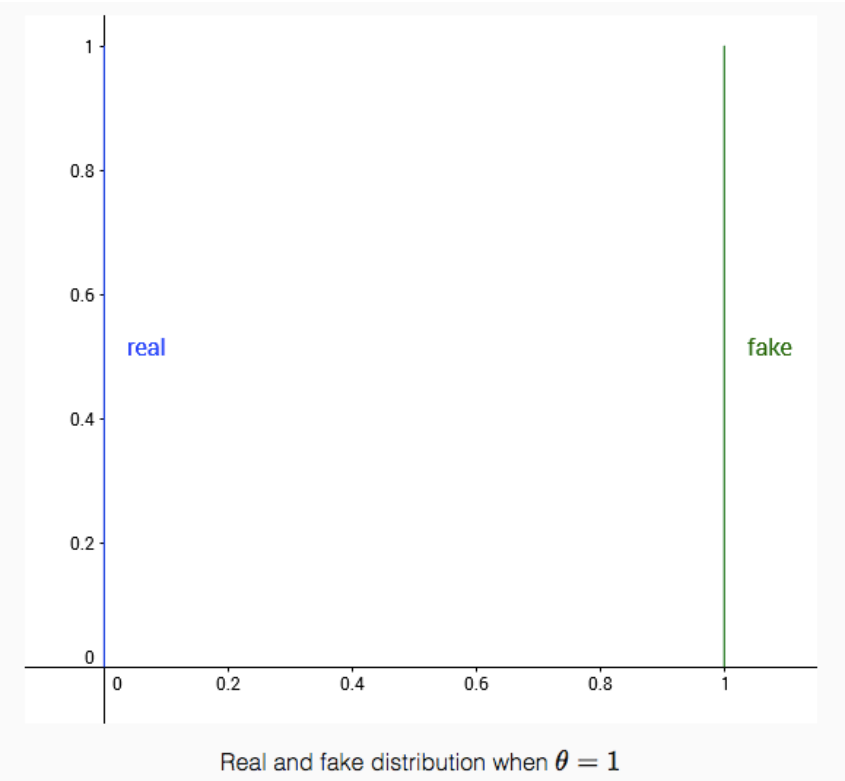

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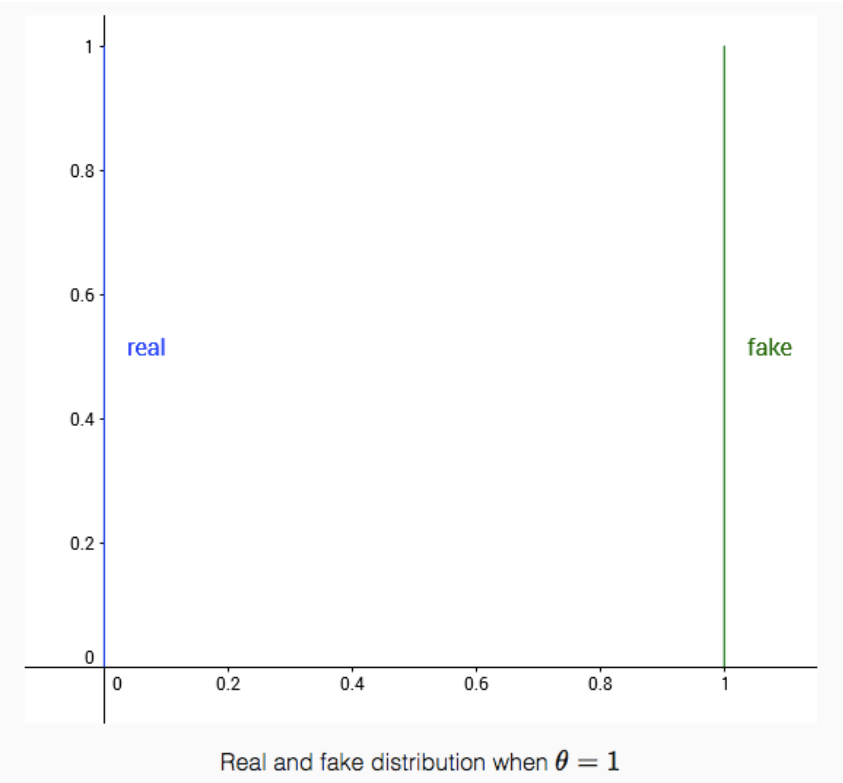

Real and fake distribution when $\theta = 1$

We'd like our optimization algorithm to learn to move θ to 0. As $\theta \to 0$, the distance $d(\mathbb{P}_0, \mathbb{P}_\theta)$ should decrease.

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For many common distance functions, this doesn't happen.

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$$\delta(\mathbb{P}_0, \mathbb{P}_\theta) = \begin{cases} 1 & \text{if } \theta \neq 0 \\ 0 & \text{if } \theta = 0 \end{cases}$$

$$JS(\mathbb{P}_0, \mathbb{P}_\theta) = \begin{cases} \log 2 & \text{if } \theta \neq 0 \\ 0 & \text{if } \theta = 0 \end{cases}$$

$$KL(\mathbb{P}_\theta, \mathbb{P}_0) = KL(\mathbb{P}_0, \mathbb{P}_\theta) = \begin{cases} +\infty & \text{if } \theta \neq 0 \\ 0 & \text{if } \theta = 0 \end{cases}$$

$$W(\mathbb{P}_0, \mathbb{P}_\theta) = |\theta|$$

Theoretical Justification

Theorem (1)

Let $\mathbb{P}_r$ be a fixed distribution over χ. Let Z be a random variable over another space $\mathcal{Z}$. Let $g : \mathcal{Z} \times \mathbb{R}^d \to \chi$ be a function, that will be denote $g_\theta(z)$ with z the first coordinate and θ the second. Let $\mathbb{P}_\theta$ denote the distribution of $g_\theta()$. Then,

1. *If g is continuous in θ, so is $W(\mathbb{P}_r, \mathbb{P}_\theta)$.*
2. *If g is locally Lipschitz and satisfies regularity assumption 1, then $W(\mathbb{P}_r, \mathbb{P}_\theta)$ is continuous everywhere, and differentiable almost everywhere*
3. *Statements 1-2 are false for the Jensen-Shannon divergence $JS(\mathbb{P}_r, \mathbb{P}_\theta)$ and all the KLs.*

Theoretical Justification

Theorem (2)

Let $\mathbb{P}$ be a distribution on a compact space χ and $(\mathbb{P}_n)_{n\in\mathbb{N}}$ be a sequence of distributions on χ. Then, considering all limits as $n \to \infty$,

1. *The following statements are equivalent*
   - $\delta(\mathbb{P}_n, \mathbb{P}) \to 0$
   - $JS(\mathbb{P}_n, \mathbb{P}) \to 0$
2. *The following statements are equivalent*
   - $W(\mathbb{P}_n, \mathbb{P}) \to 0$
   - $\mathbb{P}_n \xrightarrow{D} \mathbb{P}$ *where* $\xrightarrow{D}$ *represents convergence in distribution for random variables*
3. $KL(\mathbb{P}_n||\mathbb{P}) \to 0$ *or* $KL(\mathbb{P}||\mathbb{P}_n) \to 0$ *imply the statements in (1).*
4. *The statements in (1) imply the statements in (2).*

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The *generator* network G maps a source of noise to the input space.

The *discriminator* network D receives either a generated sample or a true data sample and must distinguish between the two.

The generator is trained to fool the discriminator.

Generative Adversarial Networks

Formally we can express the game between the generator G and the discriminator D with the minimax objective:

$$\min_G \max_D \mathbb{E}_{x \sim \mathbb{P}_r}[\log(D(x))] + \mathbb{E}_{\widetilde{x} \sim \mathbb{P}_g}[\log(1 - D(\widetilde{x})]$$

where $\mathbb{P}_r$ is the data distribution and $\mathbb{P}_g$ is the model distribution implicitly defined by $\widetilde{x} = G(z)$, $z \sim p(z)$

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- If the discriminator is trained to optimality before each generator parameter update, minimizing the value function amounts to minimizing the Jensen-Shannon divergence between the data and model distributions on x
- This is expensive and often leads to vanishing gradients as the discriminator saturates
- In practice, this requirement is relaxed, and the generator and discriminator are update simultaneously

Kantorivich-Rubinstein Duality

Unfortunately, computing the Wasserstein distance exactly is intractable.

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However, a result from the Kantorivich-Rubinstein Duality (Villani 2008) shows W is equivalent to

$$W(\mathbb{P}_r, \mathbb{P}_\theta) = \sup_{||f||_L \leq 1} \mathbb{E}_{x\sim\mathbb{P}_r}[f(x)] - \mathbb{E}_{x\sim\mathbb{P}_\theta}[f(x)]$$

where the supremum is taken over all 1-Lipschitz functions

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Calculating this is still intractable, but now it's easier to approximate.

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Suppose we have a parametrized function family $\{f_w\}_{w \in W}$, where w are the weights and W is the set of all possible weights

Furthermore suppose these functions are all K-Lipschitz for some K.

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Furthermore suppose these functions are all K-Lipschitz for some K. Then we have

$$\max_{w \in W} \mathbb{E}_{x \sim \mathbb{P}_r}[f_w(x)] - \mathbb{E}_{x \sim \mathbb{P}_\theta}[f_w(x)] \leq \sup_{||f||_L \leq K} \mathbb{E}_{x \sim \mathbb{P}_r}[f(x)] - \mathbb{E}_{x \sim \mathbb{P}_\theta}[f(x)]$$

$$= K \cdot W(\mathbb{P}_r, \mathbb{P}_\theta)$$

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Suppose we have a parametrized function family $\{f_w\}_{w \in W}$, where w are the weights and W is the set of all possible weights

Furthermore suppose these functions are all K-Lipschitz for some K. Then we have

$$\max_{w \in W} \mathbb{E}_{x \sim \mathbb{P}_r}[f_w(x)] - \mathbb{E}_{x \sim \mathbb{P}_\theta}[f_w(x)] \leq \sup_{||f||_L \leq K} \mathbb{E}_{x \sim \mathbb{P}_r}[f(x)] - \mathbb{E}_{x \sim \mathbb{P}_\theta}[f(x)]$$

$$= K \cdot W(\mathbb{P}_r, \mathbb{P}_\theta)$$

If $\{f_w\}_{w \in W}$ contains the true supremum among K-Lipschitz functions, this gives the distance exactly.

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In practice this won't be true!

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We can then backpropagate through $W(\mathbb{P}_r, g_\theta(Z))$ to get the gradient for θ.

$$\begin{aligned}\nabla_\theta W(\mathbb{P}_r, \mathbb{P}_\theta) &= \nabla_\theta(\mathbb{E}_{x\sim\mathbb{P}_r}[f_w(x)] - \mathbb{E}_{z\sim Z}[f_w(g_\theta(z))]) \\ &= -\mathbb{E}_{z\sim Z}[\nabla_\theta f_w(g_\theta(z))]\end{aligned}$$

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Important Detail

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To guarantee this is true, the authors use weight clamping. The weights w are constrained to lie within $[-c, c]$, by clipping w after every update to w.

Wasserstein GAN 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

Comparison with Standard GANs

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- In GANs, the discriminator maximizes

$$\frac{1}{m}\sum_{i=1}^{m}\log D(x^{(i)}) + \frac{1}{m}\sum_{i=1}^{m}\log(1 - D(g_\theta(z^{(i)})))$$

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- Consequently, we're updating G against an objective that kind of aims towards the JS divergence, but doesn't go all the way
- In constrast, because the Wasserstein distance is differentiable nearly everywhere, we can (and should) train f_w to convergence before each generator update, to get as accurate an estimate of $W(\mathbb{P}_r, \mathbb{P}_\theta)$ as possible

Properties of optimal WGAN critic

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To understand why weight clipping is problematic in WGAN critic we need to understand what are the properties of the optimal WGAN critic?

Properties of optimal WGAN critic

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If the optimal critic under the Kantorovich-Rubinstein dual D^* is differentiable, and x is a point from our generator distribution $\mathbb{P}_\theta$, then there is a point y sampled from the true distribution $\mathbb{P}_r$ such that the gradient of D^* at all points $x_t = (1-t)x + ty$ lie on a straight line between x and y.

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In other words, $\nabla D^*(x_t) = \frac{y - x_t}{||y - x_t||}$.

This implies that the optimal WGAN critic has gradients with norm 1 almost everywhere under $\mathbb{P}_r$ and $\mathbb{P}_\theta$

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This implies we should directly constrain the gradient norm of our critic function with respect to its input.

Enforcing a soft version of this we get:

$$L = \underbrace{\mathop{\mathbb{E}}_{\tilde{\boldsymbol{x}} \sim \mathbb{P}_g} [D(\tilde{\boldsymbol{x}})] - \mathop{\mathbb{E}}_{\boldsymbol{x} \sim \mathbb{P}_r} [D(\boldsymbol{x})]}_{\text{Original critic loss}} + \underbrace{\lambda \mathop{\mathbb{E}}_{\hat{\boldsymbol{x}} \sim \mathbb{P}_{\hat{\boldsymbol{x}}}} \left[(\|\nabla_{\hat{\boldsymbol{x}}} D(\hat{\boldsymbol{x}})\|_2 - 1)^2 \right]}_{\text{Our gradient penalty}}$$

WGAN with gradient penalty

Algorithm 1 WGAN with gradient penalty. We use default values of $\lambda = 10$, $n_{\text{critic}} = 5$, $\alpha = 0.0001$, $\beta_1 = 0.5$, $\beta_2 = 0.9$.

Require: The gradient penalty coefficient λ, the number of critic iterations per generator iteration n_{critic}, the batch size m, Adam hyperparameters α, β_1, β_2.
Require: initial critic parameters w_0, initial generator parameters θ_0.

while θ has not converged **do**
  for $t = 1, ..., n_{\text{critic}}$ **do**
    for $i = 1, ..., m$ **do**
      Sample real data $\boldsymbol{x} \sim \mathbb{P}_r$, latent variable $\boldsymbol{z} \sim p(\boldsymbol{z})$, a random number $\epsilon \sim U[0, 1]$.
      $\tilde{\boldsymbol{x}} \leftarrow G_\theta(\boldsymbol{z})$
      $\hat{\boldsymbol{x}} \leftarrow \epsilon \boldsymbol{x} + (1 - \epsilon)\tilde{\boldsymbol{x}}$
      $L^{(i)} \leftarrow D_w(\tilde{\boldsymbol{x}}) - D_w(\boldsymbol{x}) + \lambda(\|\nabla_{\hat{\boldsymbol{x}}} D_w(\hat{\boldsymbol{x}})\|_2 - 1)^2$
    end for
    $w \leftarrow \text{Adam}(\nabla_w \frac{1}{m} \sum_{i=1}^{m} L^{(i)}, w, \alpha, \beta_1, \beta_2)$
  end for
  Sample a batch of latent variables $\{\boldsymbol{z}^{(i)}\}_{i=1}^{m} \sim p(\boldsymbol{z})$.
  $\theta \leftarrow \text{Adam}(\nabla_\theta \frac{1}{m} \sum_{i=1}^{m} -D_w(G_\theta(\boldsymbol{z})), \theta, \alpha, \beta_1, \beta_2)$
end while