# Learning Dynamic Generative Models via Causal Optimal Transport

Beatrice Acciaio
London School of Economics

with Michael Munn (Google NY), and Tianlin Xu (LSE)

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# Idea in a nutshell

Let me tell you where we are heading to...

- We observe an **i.i.d. sample**, where every element is a path/evolution of some process of interest (asset price process, LOB, volatility surface, audio data,...)
- We want to understand the **distribution** underlying the sample
- We want to train a generator to:
  - **generate** new real-looking samples (e.g. to extend the available data set for training and evaluation of trading strategies)
  - **predict** the evolution of the path given that we observe part of it
- For this we use some **dynamic modification of GANs**

# Outline

- Introduction to Generative Adversarial Networks (GANs)
- Our toolkit: Causal Optimal Transport (COT)
- Dynamic GANs via COT
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Adversarial: set a **Discriminator D** against G, to stimulate G to do a better job

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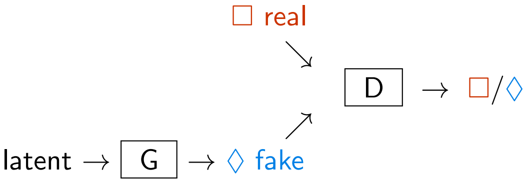
- In a loop, we train: **G** to generate real-looking samples, and
  **D** to recognize whether an element comes from real data or is fake (generated by G).
- G and D compete with each other, which drives both of them to improve, until the generated samples are indistinguishable from the genuine data (zero-sum game).



# Generative Adversarial Networks

- training data $\{x^i\}_{i=1}^N$ on $\mathcal{X}$, empirical distribution $\mu = \frac{1}{N}\sum_{i=1}^N \delta_{x^i}$
- latent space $\mathcal{Z}$, $\dim(\mathcal{Z}) \ll \dim(\mathcal{X})$, noise distribution $\zeta \in \mathcal{P}(\mathcal{Z})$
- $g_\theta : \mathcal{Z} \to \mathcal{X}$ generates samples, $\nu_\theta = g_{\theta\#}\zeta \in \mathcal{P}(\mathcal{X})$ (cf. $\mu$)
- $f_\varphi : \mathcal{X} \to [0,1]$ outputs high value if D believes input likely to be real

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**Problem formulation** in original GANs (Goodfellows et al. 2014):

$$\inf_\theta \sup_\varphi \left\{ \mathbb{E}^{x\sim\mu}[\ln f_\varphi(x)] + \mathbb{E}^{z\sim\zeta}[\ln(1 - f_\varphi(g_\theta(z)))] \right\}$$

**D:** learn $f_\varphi$ (via NN) s.t. $f_\varphi(\text{real}) \sim 1$, $f_\varphi(\text{fake}) \sim 0$

**G:** learn decoding map $g_\theta$ (via NN) to maximally confuse D

# Generative Adversarial Networks

**Why not Maximum Likelihood Estimation?**

- Density fitting: $d\nu_\theta(x) = p_\theta(x)dx$
- MLE: $\sup_\theta \frac{1}{N}\sum_{i=1}^N \ln p_\theta(x^i) \;\longleftrightarrow\; \inf_\theta H(\mu|\nu_\theta)$, where $H(.|.)$ relative entropy
- But $\nu_\theta$ has no density in $\mathcal{X}$, supports of $\nu_\theta$ and $\mu$ may even be non-overlapping (MLE not well defined)

$\Rightarrow$ look for a more flexible discrepancy to compare $\mu$ and $\nu_\theta$. Use a metric that can handle measures with non-overlapping supports.

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**Problems** (with original GANs):

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Example: Wasserstein distance $\mathcal{W}_1(\mu, \nu_\theta) = \inf\{\mathbb{E}^\pi[\|x - y\|] : \pi_1 = \mu, \pi_2 = \nu_\theta\}$

$$\Longrightarrow \qquad \underbrace{\inf_\theta}_{G} \; \underbrace{\mathcal{W}_1(\mu, \nu_\theta)}_{D}$$

# Wasserstein GANs (Arjovsky et al., Gulrajani et al. 2017)

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$\rightarrow$ enforce Lip constraint via gradient penalization (easier and regularized)

$$\inf_{\theta} \sup_{\varphi} \left\{\mathbb{E}^{\mu}[f_\varphi(x)] - \mathbb{E}^{\nu_\theta}[f_\varphi(y)] \ + \text{Lip. penalization}\right\}$$

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- Continuity: if $\theta \mapsto g_\theta$ cont. $\Rightarrow$ $\theta \mapsto \mathcal{W}_1(\mu, \nu_\theta)$ cont.
- Convergence: WGANs converge if D always trained till optimality
- WGANs outperform MLE and MLE-NN unless exact parametric form of data is known

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$\hookrightarrow$ dual OT (Arjovsky et al. 2017, Gulrajani et al. 2017)
continuity $\checkmark$, convergence $\checkmark$, stability $\times$

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$\rightarrow$ We consider a **dynamic framework**: to **generate paths** (data = time series)

- we mimic primal OT approach by Genevay et al.
- we need a **good distance for sequential data**

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# Classical Monge-Kantorovich Optimal Transport

Given Polish probability spaces $(\mathcal{X}, \mu), (\mathcal{Y}, \nu)$, move the mass from $\mu$ to $\nu$ minimizing the cost of transportation $c : \mathcal{X} \times \mathcal{Y} \to [0, \infty]$:

$$\mathrm{OT}(\mu, \nu, c) := \inf \left\{ \mathbb{E}^{\pi}[c(x, y)] : \pi \in \Pi(\mu, \nu) \right\},$$

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$\to$ **Dynamic framework** (e.g. $\mathcal{X} = \mathcal{Y} = \mathbb{R}^{d \times T}$) something that evolves in time:
"move distribution of a process $X$ into distribution of a process $Y$"

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**Causal Optimal Transport problem:**

$$\mathrm{COT}(\mu, \nu, c) := \inf \left\{ \mathbb{E}^{\pi}[c(X, Y)] : \pi \in \Pi^{\text{causal}}(\mu, \nu) \right\},$$

where $\Pi^{\text{causal}}(\mu, \nu) = \{\pi \in \Pi(\mu, \nu) : \pi \text{ causal}\}$

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# Dynamic Generative Adversarial Networks via COT

**Our approach:**

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- We build some modification of GAN where D computes distance between the real distribution $\mu$ and the generated distribution $\nu_\theta$ via causal optimal transport
- Inspired by Genevay, Peyré and Cuturi, we consider the primal COT problem and add an entropic regularization $\rightarrow$ Sinkhorn algorithm
- Causality provides a family of cost functions $\rightarrow$ D computes the worst case OT distance w.r.t. these cost functions (D is learning the cost function)

# Dynamic Generative Adversarial Networks via COT

1. We regularize the causal transport:

$$\mathrm{COT}^{\varepsilon}(\mu, \nu, c) := \inf_{\pi \in \Pi^{\text{causal}}(\mu,\nu)} \left\{ \mathbb{E}^{\pi}[c(x, y)] + \varepsilon H(\pi | \mu \otimes \nu) \right\},$$

$$\mathrm{COT}^{\varepsilon}(\mu, \nu, c) \xrightarrow[\varepsilon \to 0]{} \mathrm{COT}(\mu, \nu, c) \quad \text{(A., Backhoff, Jia 2020)}$$

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3. We remove the bias $\rightarrow$ Sinkhorn divergence:

$$\mathcal{W}_{c+s,\varepsilon}(\mu,\nu) := \mathrm{OT}^{\varepsilon}(\mu,\nu,c+s) - \tfrac{1}{2}\mathrm{OT}^{\varepsilon}(\mu,\mu,c+s) - \tfrac{1}{2}\mathrm{OT}^{\varepsilon}(\nu,\nu,c+s)$$

# Dynamic Generative Adversarial Networks via COT

**Causal Wasserstein GAN**:

$$\boxed{\inf_{\theta} \sup_{\varphi} \mathcal{W}_{c_\varphi,\varepsilon}(\mu, \nu_\theta)}$$

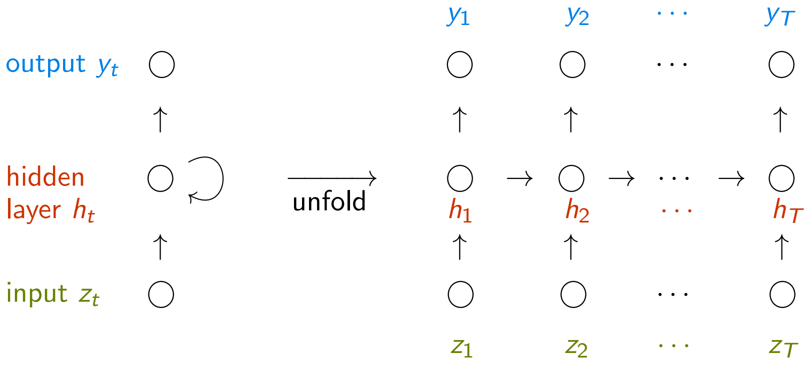
$\rightarrow$ D learns $c_\varphi$, that is, the cost function (worst-case distance)

$\rightarrow$ G learns $\nu_\theta$, that is, the best generating function $g_\theta$ ($\nu_\theta = g_{\theta\#}\zeta$)

- the cost functions $c_\varphi$ are of the form appearing in the dualization of causality
- $\varphi$ ad $\theta$ learned through "dynamic architectures", such as Recurrent Neural Networks and Convolutionals Neural Networks

# Training architecture: example

## Basic Recurrent Neural Network




$h_t = \sigma(Az_t + Bh_{t-1} + a)$ network memory, $\sigma$ activation functions

$y_t = Cs_t$, $\theta = \{A, B, C, a\}$ parameters: weight matrices and bias vectors

# The algorithm

To solve the min-max problem, we approximate $\mathcal{W}_{c_\varphi,\epsilon}(\mu,\nu_\theta)$:

- sample mini-batches from real data and from latent space $\hookrightarrow$ emp.distr. $\hat{\mu},\hat{\nu}_\theta$
- penalize cost functions $c_\varphi = c + s$ for which $s \notin \mathbb{S}$
- compute $\inf_{\pi\in\Pi(\hat{\mu},\hat{\nu}_\theta)} \left\{\mathbb{E}^\pi[c_\varphi] + \epsilon H(\pi|\hat{\mu}\otimes\hat{\nu}_\theta)\right\}$ by Sinkhorn algorithm (Cuturi 2013), by considering a pre-determined # iterations

$$\Rightarrow \quad \widehat{\mathcal{W}}_{c_\varphi,\epsilon}(\hat{\mu},\hat{\nu}_\theta)$$

Use stochastic Gradient Ascent/Descent to update parameters:

$$\varphi_{n+1} = \varphi_n + \alpha\,\nabla_\varphi \widehat{\mathcal{W}}_{c_\varphi,\epsilon}(\hat{\mu},\hat{\nu}_\theta)$$

$$\theta_{n+1} = \theta_n - \alpha\,\nabla_\theta \widehat{\mathcal{W}}_{c_\varphi,\epsilon}(\hat{\mu},\hat{\nu}_\theta)$$

# Pseudo-code

**Data:** $\theta_0$, $\varphi_0$, $\{x^i\}_{i=1}^N$, $\zeta$, $\epsilon$, batch size $m$, Sinkhorn iter., learning rate $\alpha$, critic iter. $n_c$
**Result:** $\theta$, $\varphi$
$\theta \leftarrow \theta_0$, $\varphi \leftarrow \varphi_0$
**for** $k = 1, 2, \dots$ **do**
  **for** $l = 1, 2, \dots, n_c$ **do**
    Sample: $\{x^i\}_{i=1}^m$ from real data, and $\{z^i\}_{i=1}^m$ from $\zeta$
    $y^i \leftarrow g_\theta(z^i)$
    $\varphi \leftarrow \varphi + \alpha \nabla_\varphi \left( \widehat{\mathcal{W}}_{c_\varphi, \epsilon}(\hat{\mu}, \hat{\nu}_\theta) \right)$
  **end**
  Sample: $\{x^i\}_{i=1}^m$ from real data, and $\{z^i\}_{i=1}^m$ from $\zeta$
  $y^i \leftarrow g_\theta(z^i)$
  $\theta \leftarrow \theta - \alpha \nabla_\theta \left( \widehat{\mathcal{W}}_{c_\varphi, \epsilon}(\hat{\mu}, \hat{\nu}_\theta) \right)$
**end**

# Prediction rather than generation

→ Causal Wasserstein GANs: learn how to **generate real-looking evolutions** given an observed dataset.

→ WIP: develop a conditional modification of the algorithm, for **time-series trend prediction**, so that we feed the beginning of a sequence and the generator produces some reasonable continuation.

- Mathematically: easy modification
- But may require different choice of architectures

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**Initial testing:**

- We have been testing some easy-to check features on simulated data, e.g. reproducing periodic curves.
- Now we are testing on standard datasets, such as audio datasets (NSynth); and MNIST (yes, I know, not truly sequential..)

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**Financial applications: data-driven model-independent analysis**

- Robust pricing of financial derivatives
- Volatility prediction
- Prediction of evolution of LOB

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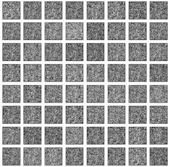
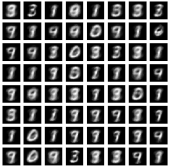
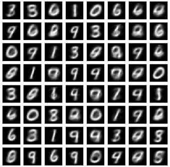


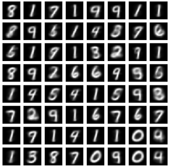
1 iteration (1.1 sec)



300 iterations (4.5 min)



15k iterations (5h)



40k iterations (14h)

MNIST: batch size 32, critic 1, $\epsilon = 0.8$, Sinkhorn iter. 30, learning rate 0.0001

# Literature


- Acciaio, Backhoff, Jia: Cournot-Nash equilibrium and optimal transport in a dynamic setting, 2020
- Arjovsky, Chintala, Bottou: Wasserstein GAN, 2017
- Cuturi: Sinkhorn distances: Lightspeed computation of OT, 2013
- Genevay, Peyré, Cuturi: Learning Generative Models with Sinkhorn Divergences, 2017
- Goodfellows et al.: Generative Adversarial Networks, 2014
- Gulrajani et al.: Improved Training of Wasserstein GANs, 2017

**Thank you for your attention!**