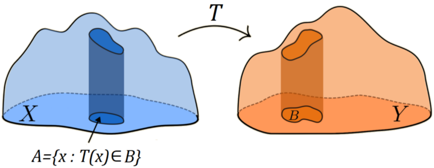
Introduction to Optimal Transport[1][2][3]

"Moving Sandcastles in the Air"

J. Setpal

March 26, 2025



[1]Peyré, Cuturi. [Arxiv 2020]
[2]Arjovsky, et. al. [Arxiv 2017]
[3]Heitz, et. al. [CVPR 2021]

Outline

1. Motivation
2. Monge Problem, Kantorovich Relaxation
3. Kantorovich Problem's Dual Formulation
4. Optimal Transport Induces a Distance
5. Wasserstein GANs

Outline

Why Should We Care? (1/3)

Monge likes playing with sandcastles.

He wonders, “What is the most efficient way to move this marvellous sandcastle from the beach to my house?”

And **Optimal Transport** was born.

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Why should you care:

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Why should you care:

1. You like playing with sandcastles.
2. You're interested in any of the following research foci:
    a. **Neural Style Transfer:**

Why Should We Care? (2/3)

2. b. **Sentence Similarity** (Word Mover's Distance):

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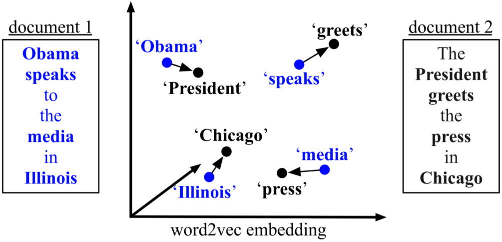
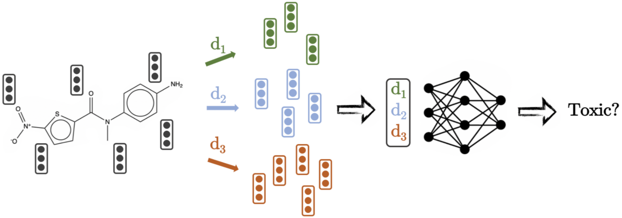
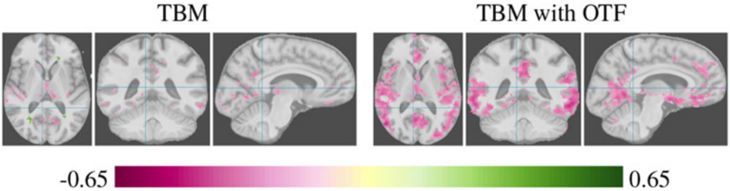


c. **Graph Neural Networks** (Better Representation Learning):



Why Should We Care? (3/3)

2. d. **Medical Imaging** (Gray Matter Tissue loss for Dementia):



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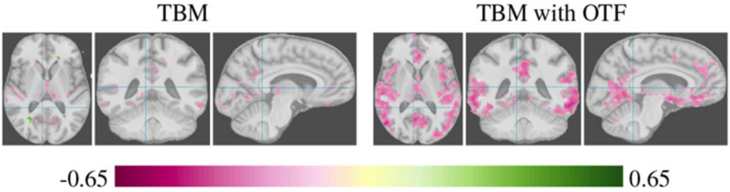
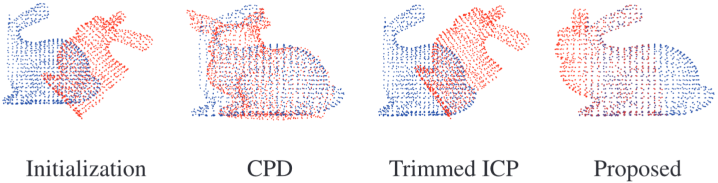


e. **Robust Point-Cloud Matching:**



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Geometry Induced by OT on the Probability Simplex

We start with the probability simplex:

$$\Sigma_n := \left\{ \boldsymbol{a} \in \mathbb{R}_+^n : \sum_{i=1}^{n} \boldsymbol{a}_i = 1 \right\} \tag{1}$$

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Aside

OT literature deals with both discrete and continuous measures using the same framework. We'll focus mostly on the discrete setting.

Monge's Assignment Problem (1/2)

Monge asks us to transfer measure α to a new measure β while also minimizing the total cost of transportation.

$$\alpha(x) = \sum_{i=1}^{n} \boldsymbol{a}_i \chi_{x_i}(x), \quad \beta(y) = \sum_{i=1}^{m} \boldsymbol{b}_i \chi_{y_i}(y) \tag{3}$$

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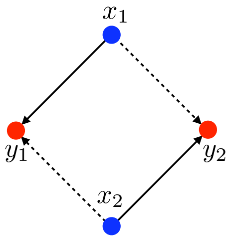
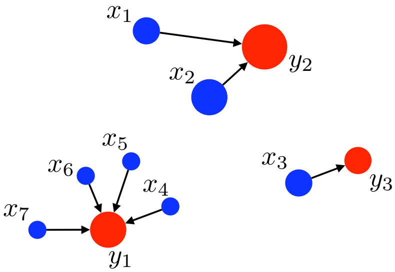
If $n = m$, $T \in \text{Perm}(n)$.

Monge's Assignment Problem (2/2)

Two visual examples of optimal transport:





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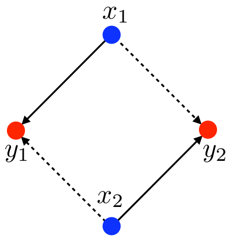

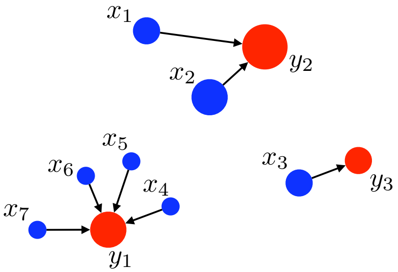

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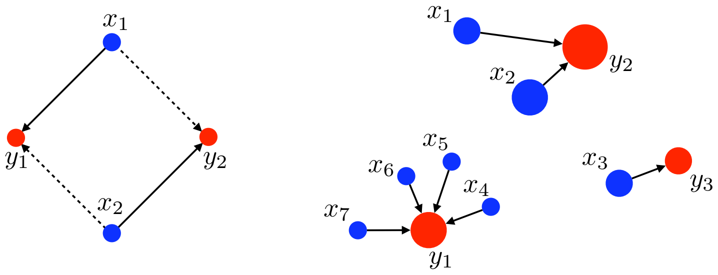

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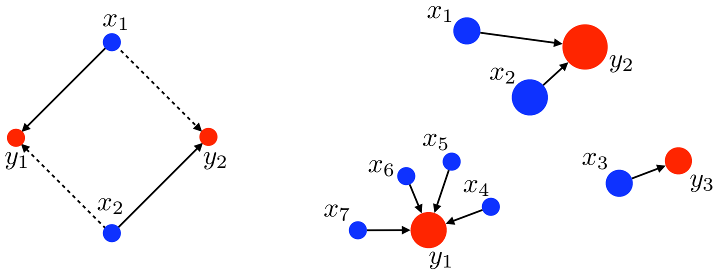

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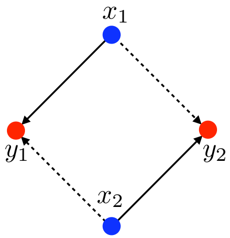

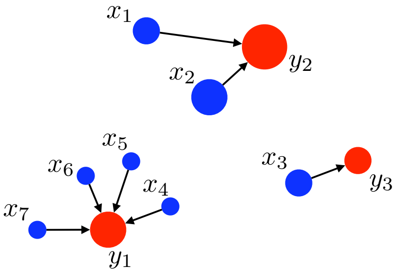

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1. The optimal transport map is not necessarily unique.
2. The current formulation does not allow mass-splitting.
3. If $m > n$ there is no feasible transport plan.
4. Complexity scales sharply and optimization landscape is non-convex.

Push-Forward & Pull-Back Operators

For every valid transport map, we know that the following is satisfied:

$$\forall j \in \{1, \ldots, m\}, \quad \boldsymbol{b}_j = \sum_{i : T(i) = y_j} \boldsymbol{a}_i \tag{5}$$

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We define the **Push-Forward operator** $T_\sharp$ to map a transport plan over an entire measure space.

$$T_\sharp : \mathcal{M}(X) \to \mathcal{M}(Y), \quad \beta = T_\sharp \alpha := \sum_{i}^{n} \boldsymbol{a}_i \chi_{T(x_i)} \tag{6}$$

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Push-Forward and Pull-Back operators are related as follows:

$$\forall (\alpha, g) \in \mathcal{M}(\mathcal{X}) \times \mathcal{C}(\mathcal{Y}), \quad \int_{\mathcal{Y}} g d(T_\sharp \alpha) = \int_{\mathcal{X}} T^\sharp g d\alpha \tag{8}$$

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Basically, we allow mass splitting. Instead of a transport map, we define a family of coupling matrices where each $\boldsymbol{P} \in \mathbb{R}_+^{n \times m}$ is a valid coupling:

$$\mathcal{U}(\boldsymbol{a}, \boldsymbol{b}) := \left\{ \boldsymbol{P} \in \mathbb{R}_+^{n \times m} : \underbrace{\boldsymbol{P}\mathbb{1}_m = \boldsymbol{a}, \boldsymbol{P}^T \mathbb{1}_n = \boldsymbol{b}}_{\text{mass conservation}} \right\} \tag{9}$$

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Finally, our new optimization objective is as follows:

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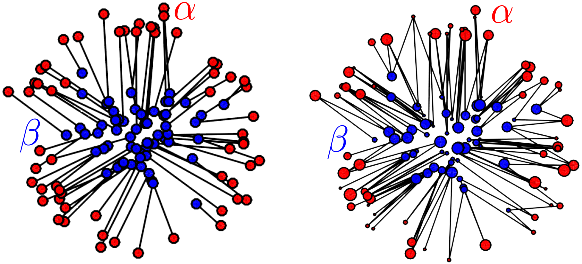
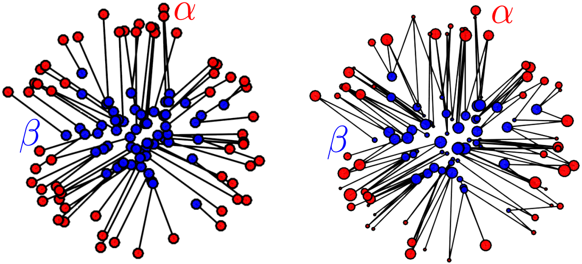
BIG Observation: This is a linear program.

Kantorovich Relaxation (2/2)





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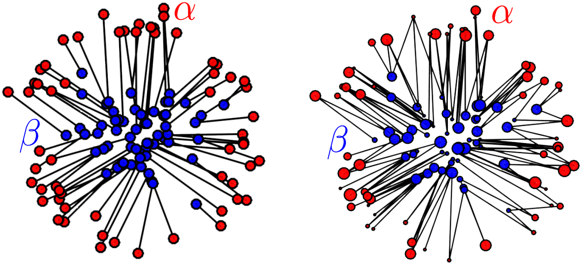

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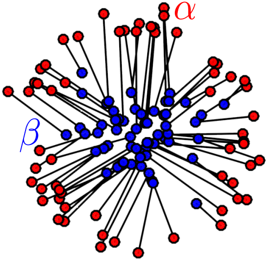

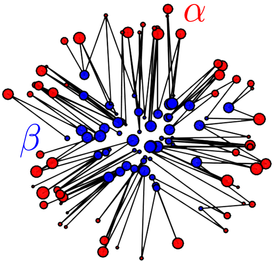

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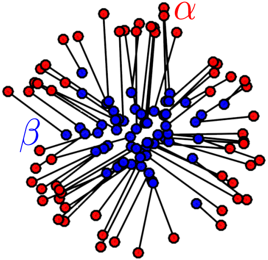

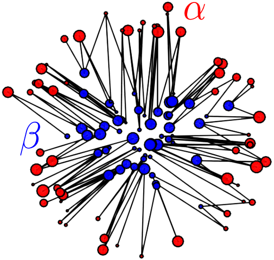

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2. Each coupling $\boldsymbol{P}$ is symmetric: $\boldsymbol{P} \in \mathcal{U}(\boldsymbol{a}, \boldsymbol{b}) \iff \boldsymbol{P}^T \in \mathcal{U}(\boldsymbol{a}, \boldsymbol{b})$.

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4. The optimal value for the primal problem *equals* the dual $\iff$ the program has an optimal solution – by **Strong Duality Theorem**.
5. If we know an optimal solution exists, we can choose to solve the easier problem and get the same answer.

Kantorovich Dual

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From there, we have the following dual problem:

$$L_{\boldsymbol{C}}(\boldsymbol{a}, \boldsymbol{b}) = \max_{\boldsymbol{f}, \boldsymbol{g} \in \mathcal{R}(\boldsymbol{C})} \langle \boldsymbol{f}, \boldsymbol{a} \rangle + \langle \boldsymbol{g}, \boldsymbol{b} \rangle \tag{13}$$

The dual variables, here $\boldsymbol{f}, \boldsymbol{g}$ are called Kantorovich Potentials.

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To check the optimality of the vendor's prices, the operator can use $\boldsymbol{C}_{i,j}$:

$$\forall(i,j), \quad \boldsymbol{f}_i + \boldsymbol{g}_j \overset{?}{\leq} \boldsymbol{C}_{i,j} \tag{16}$$

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p-Wasserstein Distance (1/2)

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Using this, we define the **Wasserstein Distance**:

$$W_p(\boldsymbol{a}, \boldsymbol{b}) := L_{\boldsymbol{D}^p}(\boldsymbol{a}, \boldsymbol{b})^{1/p} \tag{17}$$

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$$W_2(T_{\tau\sharp}\alpha, T_{\tau'\sharp}\beta)^2 = W_2(\tilde{\alpha}, \tilde{\beta})^2 - \|\boldsymbol{m}_\alpha - \boldsymbol{m}_\beta\|^2 \tag{18}$$

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   This distinction implies a two-fold comparison: the shapes of measures α and β, and the distance between their means.

Sliced Wasserstein Distance (1/4)

One special case of Optimal Transport is the 1-D case; $\mathcal{X} = \mathbb{R}$. Assuming uniform weights[4] and $c(x, y) = \|x - y\|_p^p$, we have:

$$\alpha = \frac{1}{n} \sum_{i=1}^{n} \chi_{x_i}, \quad \beta = \frac{1}{n} \sum_{i=1}^{n} \chi_{y_i} \tag{19}$$

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This **reduces OT to a sorting problem**, and can be solved in $\mathcal{O}(n \log n)$.

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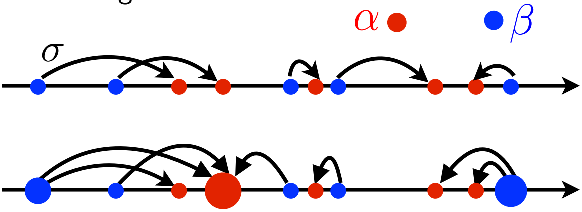
Visual for discrete and generic cases:



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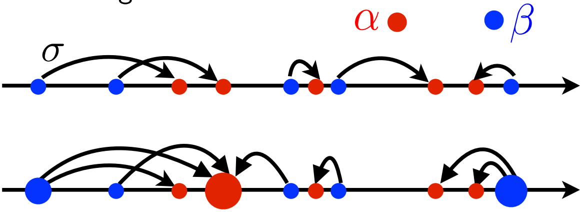

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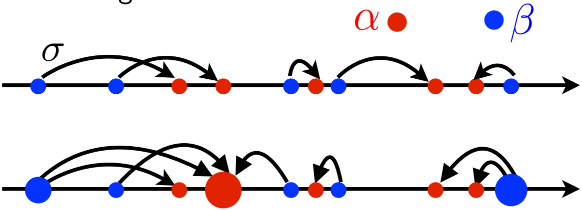

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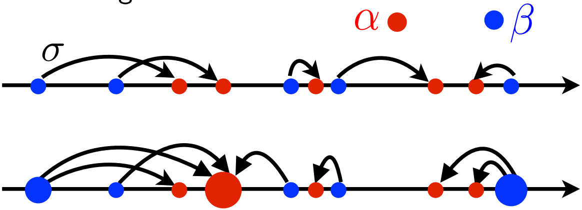

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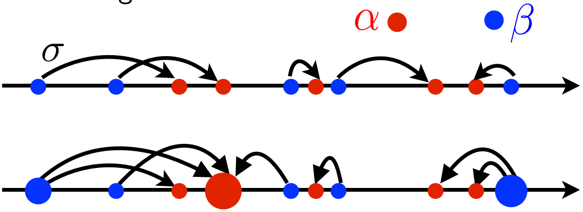

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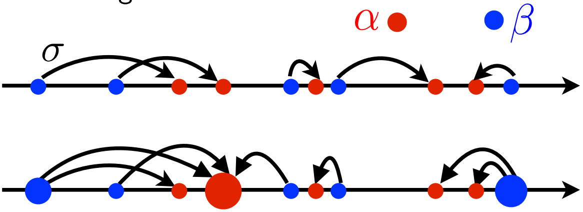

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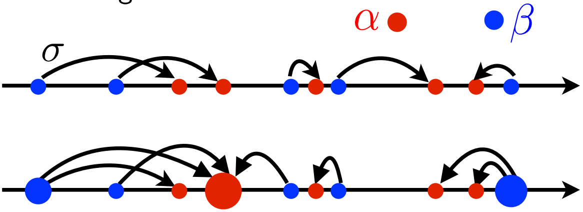

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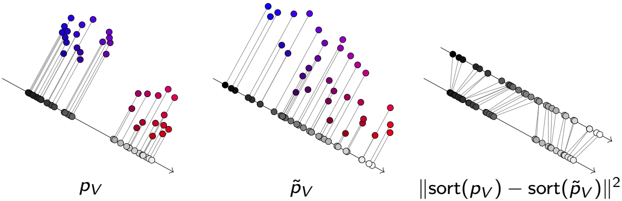
Caveat: This is is no longer the p-Wasserstein Distance.

Sliced Wasserstein Distance (3/4)

Here's what that looks like visually, for a single direction:



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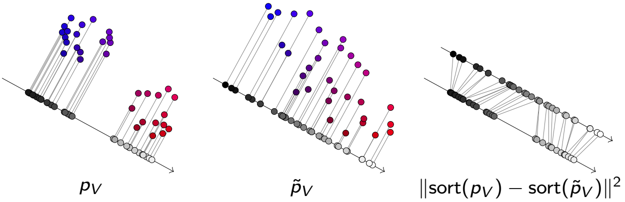
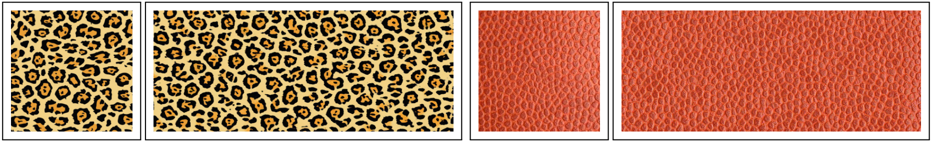


Crucially, Sliced Wasserstein Distance is **differentiable**, which enables us to use optimize transport cost using neural nets. E.g. texture matching:

input **generated** **input** **generated**



Sliced Wasserstein Distance (4/4)

Spatial Priors: Projections act on point clouds, which rids spatial information in learning the input distribution.

Sliced Wasserstein Distance ($^4/_4$)

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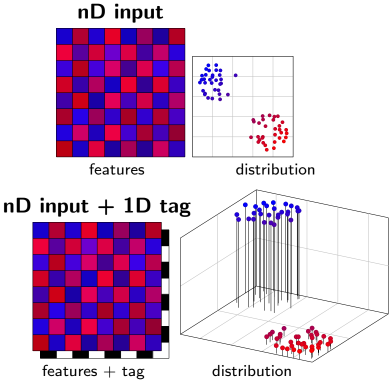
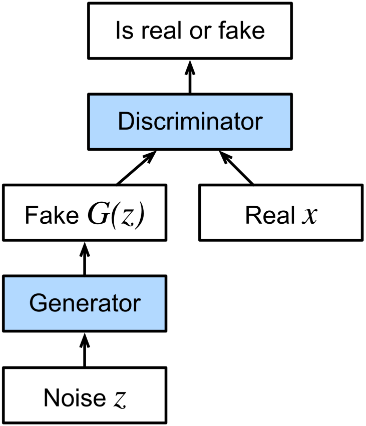
A trick to recover spatial structure is to cluster-sort by spatial dimension:



Outline

Wasserstein GAN Setup



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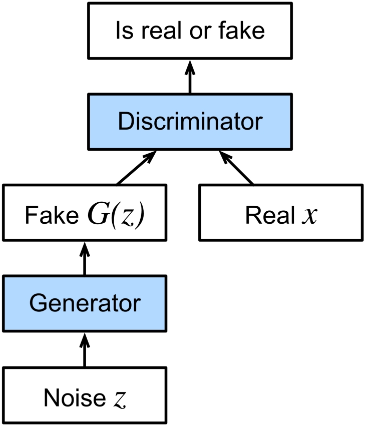

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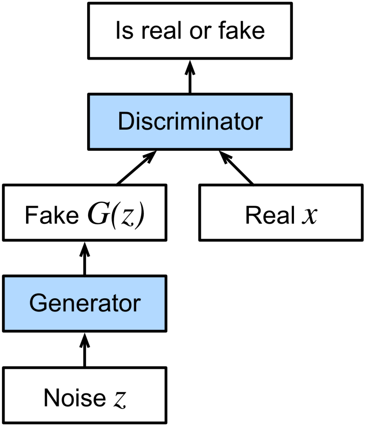

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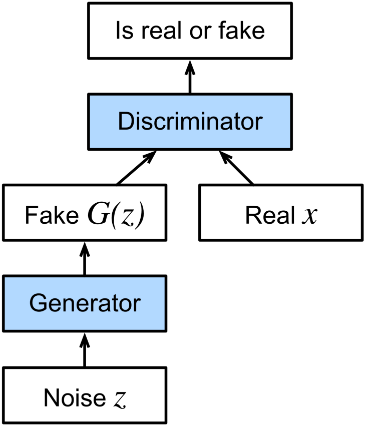

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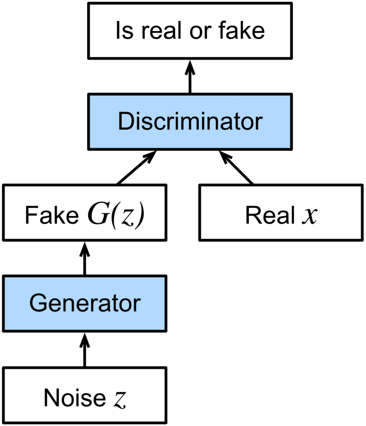

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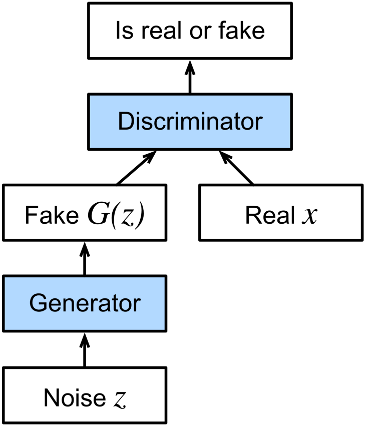

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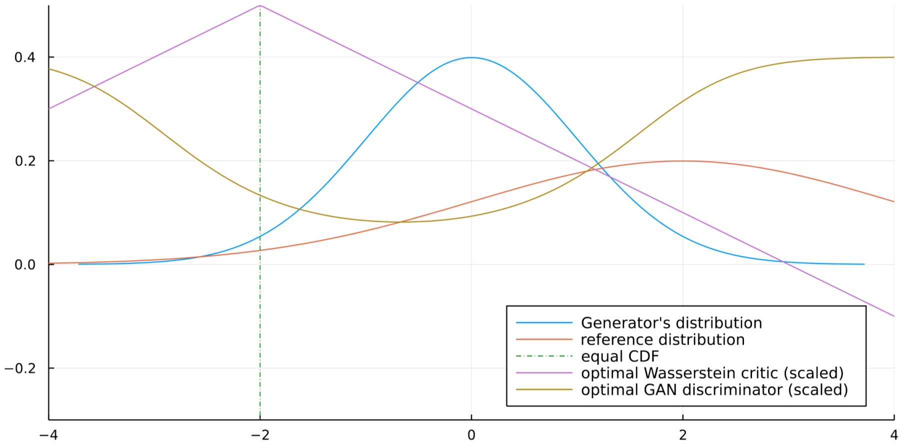
New **Discriminator** $f_\xi : \mathbb{R}^{C \times D_1 \times D_2} \to \mathbb{R}$ which models Wasserstein Distance.

Training WGANs

Algorithm 1 WGAN training algorithm. $\eta = 10^{-5},\ c = 0.01,\ n_{\text{critic}} = 5,\ n_{\text{iter}} = 500.$

for $t = 0, \ldots, n_{\text{iter}}$ **do**
  for $t = 0, \ldots, n_{\text{critic}}$ **do**
    Sample $\{x_i\}_{i=1}^{B} \sim \mathcal{D}^B$ a batch from the real data.
    Sample $\{z_i\}_{i=1}^{B} \sim \mathcal{P}^B$ a batch of prior samples.
    $g_\xi \leftarrow \nabla_\xi \left[\frac{1}{B}\sum_{i=1}^{B} f_\xi(x_i) - \frac{1}{B}\sum_{i=1}^{B} f_\xi(G_\theta(z_i))\right]$
    $\xi \leftarrow \xi + \eta \cdot \text{Adam}(g_\xi)$
    $\xi \leftarrow \text{clip}(\xi, -c, c)$
  end for
  Sample $\{z_i\}_{i=1}^{B} \sim \mathcal{P}(z)$ a batch of prior samples.
  $g_\theta \leftarrow -\nabla_\theta \frac{1}{B}\sum_{i=1}^{B} f_\xi(G_\theta(z_i))$
  $\theta \leftarrow \theta - \eta \cdot \text{Adam}(g_\theta)$
end for

Critic Improvements from Wasserstein GANs



Code Example – Training WGANs

If you can view this screen, I am making a mistake.

Thank you!

Have an awesome rest of your day!

Slides: `https://jinen.setpal.net/slides/ot.pdf`