Study Material - Youtube

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Video Overview

This lecture, "Mathematical Foundations of Generative AI: Wasserstein GANs," provides a detailed explanation of Wasserstein Generative Adversarial Networks (WGANs). It addresses the critical training instability issues found in standard GANs, such as vanishing gradients, and introduces the Wasserstein distance as a superior alternative to the f-divergences (like Jensen-Shannon) used in traditional GANs. The instructor explains that the Wasserstein distance, rooted in the theory of optimal transport, offers a "softer" and more meaningful measure of the difference between two probability distributions, providing useful gradients even when their supports do not overlap. The lecture culminates in deriving the WGAN objective function through the Kantorovich-Rubinstein duality and outlining the practical algorithm for training these more stable models.

Learning Objectives

Upon completing this lecture, students will be able to: - **Identify the primary causes of training instability** in standard GANs, particularly the issue of saturating divergence metrics when distribution supports are disjoint. - **Understand the intuitive concept of the Wasserstein distance** as the "Earth Mover's Distance" and its connection to optimal transport. - **Formulate the primal definition of the Wasserstein distance**, including the concepts of a transport plan and the set of all valid joint distributions. - **Appreciate the intractability of the primal form** and the necessity of a dual formulation. - **Comprehend the Kantorovich-Rubinstein duality** and its role in making the Wasserstein distance computationally feasible. - **Define the 1-Lipschitz constraint** and understand its critical importance in the WGAN framework. - **Formulate the WGAN objective function** as a min-max game between a generator and a "critic." - **Describe the WGAN training algorithm**, including the practical method of weight clipping or normalization to enforce the Lipschitz constraint.

Prerequisites

To fully grasp the concepts in this lecture, students should have a solid understanding of: - **Generative Adversarial Networks (GANs):** The basic architecture and adversarial training process. - **Probability Theory:** Concepts of probability distributions, probability density functions (PDFs), probability mass functions (PMFs), and expectation. - **Calculus and Optimization:** Gradient descent, minimization, and maximization. - **Linear Algebra:** Norms of vectors and matrices. - **f-Divergences:** A conceptual understanding of measures like Jensen-Shannon (JS) divergence and why they might fail.

Key Concepts Covered in This Video

- **Training Instability in GANs:** Vanishing gradients due to non-overlapping supports of real and generated data distributions.
- **Wasserstein-1 Distance (Earth Mover's Distance):** A metric measuring the minimum cost to transform one distribution into another.
- **Optimal Transport:** The mathematical theory behind the Wasserstein distance.
- **Transport Plan (γ):** A joint distribution describing how to move mass from one distribution to another.
- **Kantorovich-Rubinstein Duality:** A dual formulation of the Wasserstein distance that is more computationally tractable.
- **1-Lipschitz Functions:** Functions whose gradient norm is bounded by 1, crucial for the dual formulation.
- **Critic:** The discriminator-like network in a WGAN, which estimates the Wasserstein distance.
- **WGAN Objective Function:** The min-max objective derived from the Kantorovich-Rubinstein duality.
- **Weight Clipping/Normalization:** A practical technique to enforce the 1-Lipschitz constraint on the critic's weights.

Understanding Wasserstein GANs (WGANs)

This section delves into the core concepts of Wasserstein GANs, starting with the problem they solve, introducing the Wasserstein distance, and finally detailing the WGAN algorithm.

The Problem with Standard GANs: Saturating Divergence

At the heart of a standard GAN is the minimization of a divergence metric between the real data distribution (P_x) and the generated data distribution (P_θ). Often, this is the Jensen-Shannon (JS) divergence.

A significant problem arises from the **Manifold Hypothesis**, which posits that high-dimensional data (like images) lies on low-dimensional manifolds. In the initial stages of training, the manifolds of the real data and the randomly generated data are almost certain to be disjoint (i.e., they do not overlap).

> **Key Insight (00:11):** When the supports of two distributions, P_x and P_θ, do not align or overlap, the JS divergence between them is a constant ($\log 2$). This means the gradient of the divergence with respect to the generator's parameters (θ) is zero. This phenomenon is known as **gradient saturation** or **vanishing gradients**, which makes it impossible for the generator to learn and improve.

The solution proposed is to use a "softer" divergence metric that provides a meaningful, non-zero gradient even when the distribution supports are disjoint.

A New Metric: The Wasserstein Distance

The Wasserstein distance, also known as the **Earth Mover's Distance (EMD)**, is a metric from the field of **Optimal Transport** (00:31). It offers a more robust way to measure the distance between two probability distributions.

Intuitive Foundation: The Earth Mover's Distance

Imagine two distributions as two different piles of dirt. The EMD is the minimum "cost" or "work" required to move the dirt from the first pile and arrange it to form the second pile. The cost is calculated as:

Cost = (Amount of Dirt Moved) × (Distance Moved)

The "optimal" plan is the one that minimizes this total cost. This concept is powerful because even if the two piles of dirt are far apart (disjoint supports), there is still a well-defined, non-zero cost to move one to the other. The further apart they are, the higher the cost. This property ensures that we always have a meaningful measure of distance and, consequently, a useful gradient for optimization.

Mathematical Analysis: The Primal Form of Wasserstein Distance

(02:05) The formal definition of the Wasserstein-1 distance is based on finding the optimal "transport plan."

Let P_x and $P_{\hat{x}}$ be two probability distributions. The Wasserstein-1 distance between them is defined as:

$$W(P_x, P_{\hat{x}}) = \inf_{\gamma \in \Pi(P_x, P_{\hat{x}})} \mathbb{E}_{(x,\hat{x})\sim\gamma}[\|x - \hat{x}\|]$$

Let's break down this formula: - $\Pi(P_x, P_{\hat{x}})$: This represents the set of **all possible joint distributions** $\gamma(x, \hat{x})$ whose marginal distributions are P_x and $P_{\hat{x}}$. This means: - $\int p(x, \hat{x})d\hat{x} = p_x(x)$ - $\int p(x, \hat{x})dx = p_{\hat{x}}(\hat{x})$ - $\gamma(x, \hat{x})$: Each joint distribution γ is a **transport plan**. It specifies how much mass should be moved from a point x (from distribution P_x) to a point $\hat{x}$ (to form distribution $P_{\hat{x}}$). - $\|x - \hat{x}\|$: This is the cost of moving one unit of mass from location x to location $\hat{x}$. It's the distance between the two points. - $\mathbb{E}_{(x,\hat{x})\sim\gamma}[\|x - \hat{x}\|]$: This is the expected cost, or total work, for a specific transport plan γ. It is calculated as $\iint \gamma(x, \hat{x})\|x - \hat{x}\|dxd\hat{x}$. - inf **(Infimum)**: This indicates that we are searching for the minimum cost over all possible valid transport plans. The transport plan that achieves this minimum is the "optimal transport plan."

> **Problem:** This primal form is computationally intractable because the space of all possible joint distributions $\Pi(P_x, P_{\hat{x}})$ is immense and cannot be easily searched.

Making Wasserstein Distance Practical: Kantorovich-Rubinstein Duality

To overcome the intractability of the primal form, WGANs leverage a powerful mathematical result known as the **Kantorovich-Rubinstein Duality** (39:07). This theorem provides an alternative, dual formulation for the Wasserstein-1 distance.

The Dual Formulation

The duality states that the Wasserstein-1 distance is equivalent to:

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

Here's the breakdown of the dual form: - sup **(Supremum)**: We are now maximizing over a set of functions instead of minimizing over a set of distributions. - f: This is a function, which in the context of WGANs is called the **critic**. It is a real-valued function that we will approximate with a neural network, denoted as $f_w(x)$ with parameters w. - $\|f\|_L \leq 1$: This is the critical **1-Lipschitz constraint**. A function is 1-Lipschitz if the absolute value of its slope is at most 1 everywhere. Formally:

$$|f(x_1) - f(x_2)| \leq |x_1 - x_2| \quad \forall x_1, x_2$$

This is equivalent to stating that the norm of its gradient is at most 1:

$$\|\nabla_x f(x)\| \leq 1$$

This dual formulation is much more practical. We can use a neural network for the critic f_w and find the best parameters w through gradient ascent to approximate the supremum.

The WGAN Algorithm

The WGAN framework uses the dual form of the Wasserstein distance to define its objective function.

The WGAN Objective

The goal of the generator (G_θ) is to minimize the Wasserstein distance between the real distribution P_x and the generated distribution P_θ. The critic (f_w) aims to maximize this same distance. This leads to the following min-max objective:

$$\min_\theta \max_w \left(\mathbb{E}_{x \sim P_x}[f_w(x)] - \mathbb{E}_{z \sim p(z)}[f_w(G_\theta(z))] \right)$$

subject to the constraint that f_w is a 1-Lipschitz function.

The following diagram illustrates the WGAN training process, which is an adversarial game based on this objective.

```
flowchart TD
    subgraph Generator Training
        Z["Noise `z`"] --> G["Generator `G_theta`"]
        G --> X_hat["Fake Data `x_hat`"]
        X_hat --> C["Critic `f_w`"]
        C --> L_G["Generator Loss<br/>`-f_w(x_hat)`"]
        L_G --> U_G["Update `theta` via<br/>Gradient Descent"]
    end

    subgraph Critic Training
        X["Real Data `x`"] --> C
        X_hat --> C
        C --> L_C["Critic Loss<br/>`f_w(x_hat) - f_w(x)`"]
        L_C --> U_C["Update `w` via<br/>Gradient Ascent"]
        U_C --> WC["Weight Clipping/Normalization<br/>Enforce Lipschitz Constraint"]
    end

    U_G --> G
    WC --> C
```

Figure 1: A flowchart illustrating the adversarial training process in a Wasserstein GAN. The generator tries to minimize the Wasserstein distance, while the critic tries to maximize it.

Enforcing the 1-Lipschitz Constraint

The most challenging part of implementing a WGAN is enforcing the 1-Lipschitz constraint on the critic network f_w. The original paper proposed a simple solution:

- **Weight Clipping:** After each gradient update on the critic's weights w, clip them to a small, fixed range (e.g., $[-0.01, 0.01]$).

The instructor also mentions a more modern approach (45:24):

- **Weight Normalization:** After each gradient step, normalize the weights of the critic network such that their L2 norm is 1: $\|w\|_2 = 1$.

This constraint is crucial because it prevents the critic from becoming too powerful too quickly, allowing for more stable training and providing meaningful gradients to the generator.

Key Takeaways from This Video

- **WGANs solve GAN instability:** They replace the saturating JS divergence with the non-saturating Wasserstein distance, which provides useful gradients even when distribution supports are disjoint.

- **Wasserstein Distance is Optimal Transport Cost:** It represents the minimum "work" needed to transform one distribution into another.
- **Kantorovich-Rubinstein Duality is Key:** It transforms an intractable minimization problem over distributions into a tractable maximization problem over 1-Lipschitz functions.
- **The Discriminator becomes a Critic:** In WGANs, the discriminator is replaced by a "critic" that learns a 1-Lipschitz function to help estimate the Wasserstein distance.
- **Training is More Stable:** The WGAN objective leads to more stable training and avoids issues like mode collapse, although it requires careful handling of the Lipschitz constraint.

Self-Assessment for This Video

1. **Conceptual Question:** In your own words, explain the "Earth Mover's Distance" analogy for the Wasserstein distance. Why is this metric better suited for comparing distributions with disjoint supports than the JS divergence?
2. **Mathematical Formulation:**
   - Write down the primal form of the Wasserstein-1 distance. What does the term $\Pi(P_x, P_{\hat{x}})$ represent?
   - Write down the dual form of the Wasserstein-1 distance using the Kantorovich-Rubinstein duality. What is the key constraint placed on the function f?
3. **WGAN Algorithm:**
   - What is the role of the "critic" in a WGAN, and how does it differ from a standard GAN's "discriminator"?
   - Describe the objective function for the WGAN. What is the generator trying to minimize, and what is the critic trying to maximize?
4. **Practical Implementation:** The Kantorovich-Rubinstein duality requires the critic to be a 1-Lipschitz function. What practical method was mentioned in the lecture to enforce this constraint on a neural network critic? Why is this step necessary for stable training?
5. **Problem Solving:** Suppose the real data distribution P_x is a single point mass at $x = 0$, and the generated distribution P_θ is a single point mass at $x = \theta$. What is the JS divergence between them? What is the Wasserstein distance? How does this simple example illustrate the advantage of WGANs?