Study Material - Youtube

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Video Overview

This technical lecture, "W2L7: Generative adversarial networks Formulation," provides a rigorous mathematical treatment of the GAN framework introduced in the previous lecture. Prof. Prathosh A P delves deep into the theoretical foundations, presenting detailed mathematical proofs, convergence analysis, and the connection between the GAN objective and information-theoretic measures. This lecture transforms the intuitive understanding of adversarial learning into precise mathematical statements, enabling students to understand not just how GANs work, but why they work from a theoretical perspective.

Learning Objectives

Upon completing this lecture, a student will be able to: * **Master GAN Mathematics:** Derive and understand the complete mathematical formulation of the GAN objective function. * **Analyze Optimal Solutions:** Prove the existence and properties of optimal discriminator and generator networks. * **Connect to Information Theory:** Understand the relationship between GAN training and Jensen-Shannon divergence minimization. * **Evaluate Convergence Properties:** Analyze when and why GAN training converges to the global optimum. * **Apply Theoretical Insights:** Use mathematical understanding to guide practical implementation and debugging.

Prerequisites

To fully understand the concepts in this video, students should have: * **Advanced Calculus:** Multivariable calculus, optimization theory, and Lagrange multipliers * **Probability Theory:** Probability density functions, expectations, and measure theory basics * **Information Theory:** Entropy, mutual information, KL divergence, and Jensen-Shannon divergence * **Functional Analysis:** Basic understanding of function spaces and optimization over function classes * **Game Theory:** Nash equilibria and minimax theorems

Key Concepts Covered

- Rigorous GAN Objective Derivation
- Optimal Discriminator Analysis
- Jensen-Shannon Divergence Connection
- Global Optimum Characterization
- Convergence Guarantees and Limitations

- Practical Training Algorithm Analysis

Mathematical Formulation of GANs

The Complete GAN Framework

Problem Setup

Given a dataset $\{x_1, x_2, ..., x_n\}$ drawn from an unknown data distribution $p_{data}(x)$, we want to learn a generator function $G : \mathcal{Z} \to \mathcal{X}$ that maps from a simple noise distribution $p_z(z)$ to the complex data distribution.

Key Components: - **Data Space:** $\mathcal{X} \subseteq \mathbb{R}^d$ (e.g., images as vectors) - **Latent Space:** $\mathcal{Z} \subseteq \mathbb{R}^k$ (typically $k \ll d$) - **Generator:** $G_\theta : \mathcal{Z} \to \mathcal{X}$ parameterized by θ - **Discriminator:** $D_\phi : \mathcal{X} \to [0, 1]$ parameterized by ϕ

The Minimax Objective

The GAN training objective is formulated as a **minimax game**:

$$\min_G \max_D V(D, G) = \mathbb{E}_{x \sim p_{data}(x)}[\log D(x)] + \mathbb{E}_{z \sim p_z(z)}[\log(1 - D(G(z)))]$$

Alternative Formulation with Generated Distribution: Let $p_g(x)$ denote the distribution of samples $G(z)$ when $z \sim p_z(z)$. Then:

$$V(D, G) = \int_{\mathcal{X}} p_{data}(x) \log D(x) dx + \int_{\mathcal{X}} p_g(x) \log(1 - D(x)) dx$$

Discriminator's Perspective

For a fixed generator G, the discriminator solves:

$$\max_D V(D, G) = \max_D \int_{\mathcal{X}} [p_{data}(x) \log D(x) + p_g(x) \log(1 - D(x))] dx$$

Pointwise Optimization: Since the integral can be maximized pointwise, for each $x \in \mathcal{X}$:

$$\frac{\partial}{\partial D(x)} [p_{data}(x) \log D(x) + p_g(x) \log(1 - D(x))] = 0$$

$$\frac{p_{data}(x)}{D(x)} - \frac{p_g(x)}{1 - D(x)} = 0$$

Optimal Discriminator: Solving for $D(x)$:

$$D^*(x) = \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}$$

Generator's Perspective

Substituting the optimal discriminator D^* back into the objective:

$$C(G) = \max_D V(D, G) = V(D^*, G)$$

$$= \mathbb{E}_{x\sim p_{data}}\left[\log \frac{p_{data}(x)}{p_{data}(x) + p_g(x)}\right] + \mathbb{E}_{x\sim p_g}\left[\log \frac{p_g(x)}{p_{data}(x) + p_g(x)}\right]$$

Connection to Information Theory

Jensen-Shannon Divergence

The generator's objective can be rewritten in terms of the **Jensen-Shannon (JS) divergence**:

Definition of JS Divergence:

$$JS(p\|q) = \frac{1}{2}KL(p\|m) + \frac{1}{2}KL(q\|m)$$

where $m = \frac{1}{2}(p + q)$ is the mixture distribution.

Theorem: The generator's objective is:

$$C(G) = -\log(4) + 2 \cdot JS(p_{data}\|p_g)$$

Proof of JS Connection

Starting from the generator objective:

$$C(G) = \int_{\mathcal{X}} p_{data}(x) \log \frac{p_{data}(x)}{p_{data}(x) + p_g(x)} dx + \int_{\mathcal{X}} p_g(x) \log \frac{p_g(x)}{p_{data}(x) + p_g(x)} dx$$

Step 1: Add and subtract $\log 2$ terms:

$$C(G) = \int_{\mathcal{X}} p_{data}(x) \log \frac{2p_{data}(x)}{p_{data}(x) + p_g(x)} dx + \int_{\mathcal{X}} p_g(x) \log \frac{2p_g(x)}{p_{data}(x) + p_g(x)} dx - 2\log 2$$

Step 2: Recognize the mixture distribution $m(x) = \frac{p_{data}(x)+p_g(x)}{2}$:

$$C(G) = KL(p_{data}\|m) + KL(p_g\|m) - \log 4$$

Step 3: Apply JS divergence definition:

$$C(G) = 2 \cdot JS(p_{data}\|p_g) - \log 4$$

Properties of the JS Formulation

1. **Non-negativity:** $JS(p_{data}\|p_g) \geq 0$ with equality iff $p_{data} = p_g$
2. **Symmetry:** $JS(p\|q) = JS(q\|p)$
3. **Bounded:** $0 \leq JS(p\|q) \leq \log 2$
4. **Global Minimum:** $C(G)$ achieves its global minimum of $-\log 4$ when $p_g = p_{data}$

Detailed Convergence Analysis

Existence of Global Optimum

Theorem (Global Optimum): If both G and D have sufficient capacity (can represent any function), then the global optimum of the minimax game exists and satisfies: - $p_g^* = p_{data}$ - $D^*(x) = \frac{1}{2}$ for all x

Proof Sketch: 1. **Minimum Value:** Since $JS(p_{data} \| p_g) \geq 0$, we have $C(G) \geq -\log 4$ 2. **Achievability:** The minimum $C(G) = -\log 4$ is achieved when $p_g = p_{data}$ 3. **Uniqueness:** The JS divergence equals zero only when distributions are identical

Practical Convergence Challenges

Despite theoretical guarantees, practical GAN training faces several challenges:

1. Limited Capacity: Real neural networks have finite capacity, violating the theoretical assumptions

2. Non-Convex Optimization: The minimax objective is non-convex in the parameters, leading to local optima

3. Training Dynamics: Alternating optimization may not converge to the Nash equilibrium

4. Gradient Quality: Discrete training steps and finite sample sizes introduce noise

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Theoretical Analysis and Convergence

Training Algorithm Analysis

Practical Training Procedure

The theoretical minimax formulation translates to the following algorithm:

```
for epoch in range(num_epochs):
    for batch in dataloader:
        # Step 1: Update Discriminator
        for d_step in range(k_discriminator):
            real_batch = sample_real_data()
            fake_batch = G(sample_noise())

            d_loss_real = -log(D(real_batch))
            d_loss_fake = -log(1 - D(fake_batch))
            d_loss = d_loss_real + d_loss_fake

            optimize_discriminator(d_loss)

        # Step 2: Update Generator
        for g_step in range(k_generator):
            fake_batch = G(sample_noise())
            g_loss = -log(D(fake_batch))  # Original formulation
            # g_loss = log(1 - D(fake_batch))  # Alternative formulation

            optimize_generator(g_loss)
```

Alternative Generator Objectives

The original generator objective $\min_G \mathbb{E}_{z\sim p_z}[\log(1 - D(G(z)))]$ can suffer from **vanishing gradients** when the discriminator is highly confident.

Alternative Objective:

$$\max_G \mathbb{E}_{z\sim p_z}[\log D(G(z))]$$

Comparison: - **Original:** Minimizes $\log(1-D(G(z)))$ - **Alternative:** Maximizes $\log D(G(z))$

The alternative provides stronger gradients when $D(G(z))$ is small but changes the equilibrium properties.

Convergence in Function Space

Theorem (Convergence in Function Space): Consider the continuous-time gradient dynamics in function space:

$$\frac{\partial D}{\partial t} = \nabla_D V(D, G)$$
$$\frac{\partial G}{\partial t} = -\nabla_G V(D, G)$$

Under certain regularity conditions, this system converges to the Nash equilibrium.

Discrete-Time Analysis

For discrete updates with learning rates α_D and α_G:

$$D_{t+1} = D_t + \alpha_D \nabla_D V(D_t, G_t)$$
$$G_{t+1} = G_t - \alpha_G \nabla_G V(D_t, G_t)$$

Stability Conditions: - Learning rates must satisfy certain bounds - The ratio α_G/α_D affects convergence properties - Too large learning rates can cause oscillatory behavior

Mode Collapse Analysis

Mathematical Characterization

Mode Collapse occurs when the generator G maps multiple distinct noise vectors to the same or very similar outputs, reducing sample diversity.

Formal Definition: Mode collapse occurs when:

$$\exists x^* \text{ such that } \int_{\mathcal{Z}} \|G(z) - x^*\|^2 p_z(z) dz \text{ is small}$$

Theoretical Causes

1. Discriminator Overfitting: If D becomes too good at distinguishing real from fake samples, G receives poor gradient information.

2. Generator Optimization Landscape: The loss surface for G may have many local minima corresponding to collapsed modes.

3. Training Dynamics: Sequential optimization can lead to cyclical behavior where the generator jumps between modes.

Prevention Strategies

1. Regularization Terms: Add penalty terms to encourage diversity:

$$L_G = -\mathbb{E}[\log D(G(z))] + \lambda \mathbb{E}[\|G(z_1) - G(z_2)\|^2]$$

2. Modified Objectives: Use Wasserstein GAN or other divergences that provide better gradient properties.

3. Training Balance: Carefully balance discriminator and generator update frequencies.

Practical Implementation Considerations

Gradient Flow Analysis

The gradient of the generator loss with respect to generated samples:

$$\frac{\partial}{\partial G(z)}[-\log D(G(z))] = -\frac{1}{D(G(z))}\frac{\partial D(G(z))}{\partial G(z)}$$

Issues: - When $D(G(z)) \approx 0$, gradients explode - When $D(G(z)) \approx 1$, gradients vanish - Requires careful balance for stable training

Architectural Considerations

Generator Architecture: - **Deconvolutional layers** for upsampling - **Batch normalization** for training stability - **Activation functions:** ReLU for hidden layers, Tanh for output

Discriminator Architecture: - **Convolutional layers** for feature extraction - **Leaky ReLU** to avoid sparse gradients - **No batch normalization** in discriminator (can harm training)

Hyperparameter Sensitivity

Critical Hyperparameters: 1. **Learning Rates:** α_G and α_D ratio affects convergence 2. **Batch Size:** Larger batches provide more stable gradients 3. **Network Capacity:** Balance between generator and discriminator capacity 4. **Update Frequency:** Ratio of discriminator to generator updates

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Key Takeaways from This Video

- **Mathematical Rigor:** The GAN framework has solid theoretical foundations grounded in game theory and information theory.
- **Optimal Solutions:** Under ideal conditions, GANs provably recover the true data distribution with the discriminator outputting 1/2 everywhere.
- **JS Divergence Connection:** GAN training is equivalent to minimizing the Jensen-Shannon divergence between data and generated distributions.
- **Convergence Challenges:** Despite theoretical guarantees, practical training faces issues due to non-convexity and limited network capacity.
- **Training Dynamics:** The alternating optimization procedure requires careful balancing to avoid instabilities and mode collapse.
- **Implementation Insights:** Theoretical understanding provides guidance for practical design choices in architecture and hyperparameters.

Self-Assessment for This Video

1. **Optimal Discriminator Derivation:** Derive the optimal discriminator $D^*(x)$ for a fixed generator. Show all mathematical steps.

2. **JS Divergence Connection:** Prove that the generator objective $C(G) = -\log(4) + 2 \cdot JS(p_{data} \| p_g)$. Explain each step of the derivation.

3. **Global Optimum Properties:** What are the properties of the global optimum in the GAN minimax game? Why does $D^*(x) = 1/2$ at equilibrium?

4. **Convergence Analysis:** Under what conditions do GANs theoretically converge? What practical factors prevent this convergence?

5. **Alternative Generator Objectives:** Compare the original generator objective $\min_G \mathbb{E}[\log(1 - D(G(z)))]$ with the alternative $\max_G \mathbb{E}[\log D(G(z))]$. What are the trade-offs?
6. **Mode Collapse:** Provide a mathematical characterization of mode collapse. What causes it from a theoretical perspective?
7. **Gradient Analysis:** Analyze the gradient flow for the generator. When do gradients vanish or explode, and how does this affect training?
8. **Practical Implementation:** How do the theoretical insights guide practical implementation choices for GAN architectures and training procedures?