Study Material - Youtube

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Video Overview

This lecture, "W2L5: Generative modelling via variational divergence minimization," delves into the theoretical foundations of how generative models learn to approximate complex data distributions through variational methods. Prof. Prathosh A P presents the mathematical framework that underpins many successful generative models, including Variational Autoencoders (VAEs) and certain GAN formulations. The lecture establishes the connection between information theory, variational inference, and practical generative modeling, showing how divergence minimization provides a principled approach to learning probability distributions from data.

Learning Objectives

Upon completing this lecture, a student will be able to: * **Understand Variational Principles:** Grasp how variational methods provide tractable approximations to intractable problems. * **Master Divergence Measures:** Distinguish between different divergence measures and their properties in generative modeling. * **Apply KL Divergence:** Use Kullback-Leibler divergence for distribution approximation and its role in VAEs. * **Derive ELBO:** Understand the Evidence Lower Bound and its central role in variational inference. * **Connect Theory to Practice:** Link mathematical derivations to implementation in modern generative models.

Prerequisites

To fully understand the concepts in this video, students should have: * **Probability Theory:** Joint, marginal, and conditional probability distributions * **Information Theory:** Entropy, mutual information, and basic information-theoretic measures * **Calculus:** Multivariable calculus, particularly integration and expectation calculations * **Optimization:** Understanding of constrained optimization and Lagrange multipliers * **Variational Calculus:** Basic concepts of functional derivatives (helpful but not essential)

Key Concepts Covered

- Variational Inference Principles
- KL Divergence and Its Properties
- Evidence Lower Bound (ELBO)
- Jensen's Inequality Applications
- Reparameterization Tricks

- Forward vs Reverse KL Divergence

Variational Divergence Minimization Framework

The Central Problem

Generative modeling fundamentally involves learning a complex, unknown probability distribution $p_{data}(x)$ from observed samples. However, directly modeling this distribution is often intractable due to:

1. **High Dimensionality:** Real data (images, text, audio) exists in extremely high-dimensional spaces
2. **Complex Dependencies:** The true data distribution may have intricate correlations
3. **Normalization Constants:** Computing partition functions becomes computationally prohibitive

The Variational Solution: Instead of directly modeling $p_{data}(x)$, we approximate it with a simpler, parameterized distribution $q_\theta(x)$ and minimize the divergence between them.

Mathematical Framework

The General Variational Principle

Given an intractable target distribution $p(x)$ and a family of tractable approximating distributions $\{q_\theta(x) : \theta \in \Theta\}$, we seek:

$$\theta^* = \arg\min_{\theta \in \Theta} D(p \| q_\theta)$$

where $D(p \| q_\theta)$ is a divergence measure quantifying the "distance" between distributions.

Properties of Divergence Measures

A proper divergence measure $D(p \| q)$ must satisfy: 1. **Non-negativity:** $D(p \| q) \geq 0$ for all p, q 2. **Identity:** $D(p \| q) = 0$ if and only if $p = q$ (almost everywhere) 3. **Asymmetry:** Generally $D(p \| q) \neq D(q \| p)$

Note: Unlike distances, divergences are typically asymmetric, leading to different optimization behaviors.

KL Divergence: The Foundation

Definition and Properties

The **Kullback-Leibler (KL) divergence** from distribution q to distribution p is:

$$D_{KL}(p \| q) = \int p(x) \log \frac{p(x)}{q(x)} dx = \mathbb{E}_{x \sim p} \left[\log \frac{p(x)}{q(x)} \right]$$

Key Properties: 1. **Information-Theoretic Interpretation:** Measures the information lost when using q to approximate p 2. **Asymmetry:** $D_{KL}(p \| q) \neq D_{KL}(q \| p)$ in general 3. **Convexity:** $D_{KL}(p \| q)$ is convex in both arguments 4. **Connection to Entropy:** $D_{KL}(p \| q) = H(p, q) - H(p)$ where $H(p, q)$ is cross-entropy

Forward vs Reverse KL Divergence

The choice of direction has significant implications:

Forward KL: $D_{KL}(p_{data} \| q_\theta)$ - **Mode-Seeking:** q_θ tends to cover all modes of p_{data} - **Over-Dispersed:** May spread probability mass too broadly - **Inclusive:** Penalizes q_θ for assigning low probability where p_{data} has high probability

Reverse KL: $D_{KL}(q_\theta \| p_{data})$ - **Mode-Covering:** q_θ focuses on dominant modes of p_{data} - **Under-Dispersed:** May miss minor modes - **Exclusive:** Penalizes q_θ for assigning high probability where p_{data} has low probability

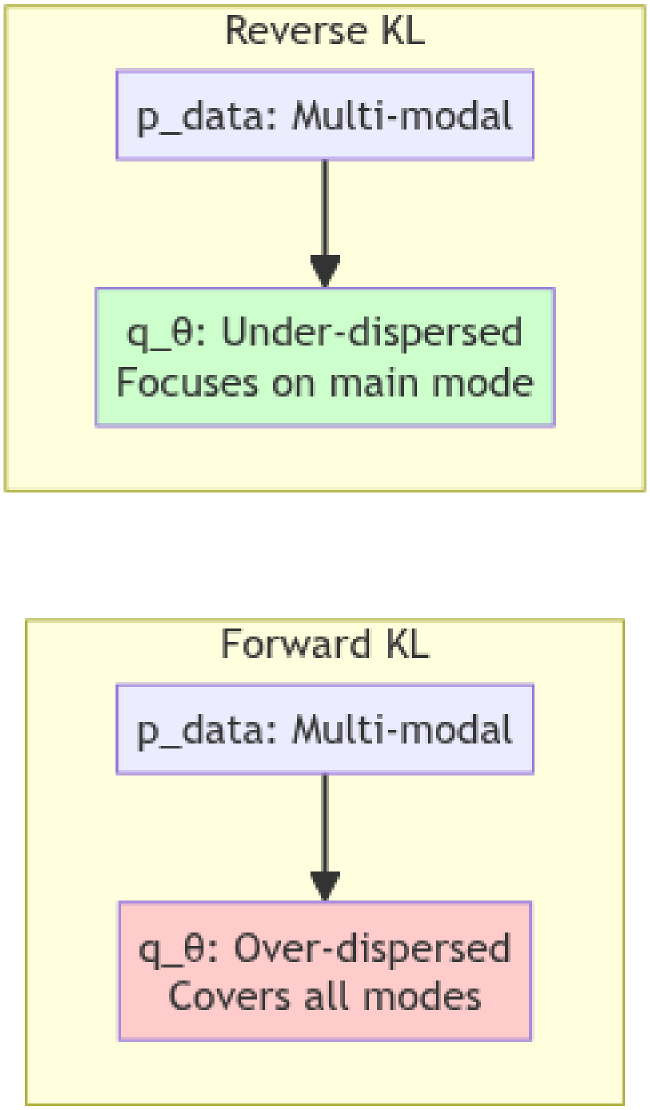

Figure 1: Behavioral differences between forward and reverse KL divergence optimization.

The Evidence Lower Bound (ELBO)

Derivation from Intractable Evidence

Consider a latent variable model where we want to maximize the log-evidence:

$$\log p(x) = \log \int p(x|z)p(z)dz$$

This integral is typically intractable. Using variational inference with an approximate posterior $q(z|x)$:

$$\log p(x) = \mathbb{E}_{q(z|x)}[\log p(x)] = \mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{p(z|x)}\right]$$

Applying the identity $\frac{p(x,z)}{p(z|x)} = \frac{p(x,z)\cdot q(z|x)}{p(z|x)\cdot q(z|x)}$:

$$\log p(x) = \mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right] + \mathbb{E}_{q(z|x)}\left[\log \frac{q(z|x)}{p(z|x)}\right]$$

$$= \mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right] + D_{KL}(q(z|x)\|p(z|x))$$

Since $D_{KL}(q(z|x)\|p(z|x)) \geq 0$, we have:

$$\log p(x) \geq \mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right] = \mathcal{L}(x,q)$$

ELBO Components

The **Evidence Lower Bound (ELBO)** can be decomposed as:

$$\mathcal{L}(x,q) = \mathbb{E}_{q(z|x)}[\log p(x|z)] - D_{KL}(q(z|x)\|p(z))$$

Interpretation: 1. **Reconstruction Term:** $\mathbb{E}_{q(z|x)}[\log p(x|z)]$ - How well can we reconstruct x from latent z 2. **Regularization Term:** $D_{KL}(q(z|x)\|p(z))$ - How close is the approximate posterior to the prior

Jensen's Inequality Application

An alternative derivation uses Jensen's inequality for the concave logarithm function:

$$\log p(x) = \log \mathbb{E}_{q(z|x)}\left[\frac{p(x,z)}{q(z|x)}\right] \geq \mathbb{E}_{q(z|x)}\left[\log \frac{p(x,z)}{q(z|x)}\right]$$

This provides a direct path to the ELBO without explicitly introducing the KL divergence term.

Mathematical Foundations of Divergence Measures

f-Divergences: A General Framework

The KL divergence belongs to a broader family of **f-divergences** defined by:

$$D_f(p\|q) = \int q(x) f\left(\frac{p(x)}{q(x)}\right) dx$$

where f is a convex function with $f(1) = 0$.

Important f-Divergences

1. KL Divergence: $f(t) = t \log t$

$$D_{KL}(p\|q) = \int p(x) \log \frac{p(x)}{q(x)} dx$$

2. Reverse KL: $f(t) = -\log t$

$$D_{KL}(q\|p) = \int q(x) \log \frac{q(x)}{p(x)} dx$$

3. Jensen-Shannon Divergence: Symmetric divergence

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

where $m = \frac{1}{2}(p+q)$

4. Wasserstein Distance: Based on optimal transport

$$W_1(p,q) = \inf_{\gamma \in \Pi(p,q)} \mathbb{E}_{(x,y)\sim\gamma}[\|x-y\|]$$

Variational Representation of Divergences

Many divergences admit **dual representations** that are useful for optimization:

KL Divergence Dual Form

$$D_{KL}(p\|q) = \sup_f \left\{ \mathbb{E}_p[f(x)] - \log \mathbb{E}_q[e^{f(x)}] \right\}$$

This representation is particularly useful when p is known through samples but q is parameterized.

Jensen-Shannon Dual Form

$$JS(p\|q) = \log 2 + \frac{1}{2} \sup_D \left\{ \mathbb{E}_p[\log D(x)] + \mathbb{E}_q[\log(1 - D(x))] \right\}$$

This is the mathematical foundation underlying the original GAN objective.

Reparameterization Trick

The Challenge

Direct optimization of $\mathbb{E}_{q_\theta(z)}[f(z)]$ with respect to θ is difficult because the expectation is over a distribution that depends on θ.

The Solution

For certain distributions, we can reparameterize $z \sim q_\theta(z)$ as:

$$z = g_\theta(\epsilon) \text{ where } \epsilon \sim p(\epsilon)$$

and $p(\epsilon)$ is independent of θ.

Example: Gaussian Distribution If $q_\theta(z) = \mathcal{N}(\mu_\theta, \sigma_\theta^2)$, then:

$$z = \mu_\theta + \sigma_\theta \cdot \epsilon \text{ where } \epsilon \sim \mathcal{N}(0,1)$$

Gradient Computation

$$\nabla_\theta \mathbb{E}_{q_\theta(z)}[f(z)] = \nabla_\theta \mathbb{E}_{p(\epsilon)}[f(g_\theta(\epsilon))] = \mathbb{E}_{p(\epsilon)}[\nabla_\theta f(g_\theta(\epsilon))]$$

This allows Monte Carlo estimation of gradients:

$$\nabla_\theta \mathbb{E}_{q_\theta(z)}[f(z)] \approx \frac{1}{L} \sum_{l=1}^{L} \nabla_\theta f(g_\theta(\epsilon^{(l)}))$$

Practical Optimization Considerations

Numerical Stability

1. **Log-Sum-Exp Trick:** For computing $\log \sum_i e^{x_i}$ numerically
2. **Gradient Clipping:** Preventing exploding gradients in deep networks
3. **Annealing Schedules:** Gradually adjusting the regularization weight

Convergence Properties

1. **Local vs Global Optima:** Variational objectives may have multiple local minima
2. **Initialization Sensitivity:** Starting points can significantly affect final solutions
3. **Learning Rate Schedules:** Adaptive optimization for better convergence

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Key Takeaways from This Video

- **Variational Principle:** Approximating intractable distributions through tractable parameterized families provides a principled approach to generative modeling.
- **Divergence Choice Matters:** Different divergences (forward KL, reverse KL, JS) lead to different optimization behaviors and model characteristics.
- **ELBO Foundation:** The Evidence Lower Bound decomposes into reconstruction and regularization terms, providing interpretable training objectives.
- **Reparameterization Trick:** Enables efficient gradient-based optimization of variational objectives through Monte Carlo estimation.
- **Mathematical Rigor:** Understanding the theoretical foundations allows for principled design choices and debugging of generative models.
- **Practical Implementation:** Theoretical insights directly translate to implementation considerations in modern deep learning frameworks.

Self-Assessment for This Video

1. **Divergence Properties:** What are the key mathematical properties that make KL divergence suitable for variational inference?

2. **Forward vs Reverse KL:** Explain the behavioral differences between optimizing $D_{KL}(p_{data} \| q_\theta)$ vs $D_{KL}(q_\theta \| p_{data})$ and when you might prefer each.

3. **ELBO Derivation:** Derive the Evidence Lower Bound starting from $\log p(x)$ and explain each step of the mathematical transformation.

4. **Reparameterization:** Why is the reparameterization trick necessary for gradient-based optimization? Provide a concrete example with Gaussian distributions.

5. **f-Divergences:** How does the KL divergence fit into the broader framework of f-divergences? What other divergences might be useful for generative modeling?

6. **Practical Implementation:** How would you implement ELBO optimization in PyTorch, including proper handling of the reparameterization trick?
7. **Convergence Analysis:** What factors might cause variational optimization to converge to poor local optima, and how can these issues be mitigated?
8. **Information Theory Connection:** Explain the information-theoretic interpretation of the KL divergence and how it relates to the concept of "information lost" in approximation.