Entropic-Regularized Gromov-Wasserstein Discrepancy

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1 Problem Formulation

Given two metric measure spaces (X_1, d_1, μ_1) and (X_2, d_2, μ_2), the **Gromov-Wasserstein discrepancy** measures their distance. It is defined as:

$$2\mathrm{d}_1(x_1, x_1')d_2(x_2, x_2'), \mathrm{d}\gamma(x_1, x_2)$$

where $\Pi(X_1, X_2)$ is the set of joint measures on $X_1 \times X_2$ with marginals μ_1 and μ_2. We relax this to the **entropic-regularized** Gromov-Wasserstein discrepancy, maximizing the joint entropy subject to approximating the original discrepancy:

$$^2_e((X_1, d_1, \mu_1), (X_2, d_2, \mu_2)) = \max_{\gamma \in \Pi(X_1, X_2)} H(\gamma) \qquad \text{s.t.} \qquad GW_2^2(\gamma) \leq \epsilon$$

2 Example: Comparing Graphs

We have two graphs $G1$ and $G2$ that we want to compare. To measure the distance between them, we use the entropic-regularized Gromov-Wasserstein discrepancy:

We start with measures μ_1 on the nodes of $G1$ and μ_2 on the nodes of $G2$. These are the "input" measures we want to match.

We initialize a joint measure μ on $G1 \times G2$, where μ defines correspondences between nodes in the two graphs. The marginals of μ likely do not match μ_1 and μ_2.

We project μ onto the marginal constraints by solving:

$$\mu_{k+1} =_{\mu \in \Pi(G1, G2)} D(\mu, \mu_k) \qquad \text{s.t.} \qquad \text{marginals}(\mu) = (\mu_1, \mu_2)$$

This finds the measure μ_{k+1} closest to μ_k (in Bregman divergence) whose marginals match (μ_1, μ_2). We update $\mu = \mu_{k+1}$, projecting onto the constraints.

We project μ onto the entropy constraints by solving:

$$\mu_{k+1} =_{\mu:D(\mu,\mu_k)\leq\epsilon} H(\mu)$$

This increases the entropy of μ as much as possible, within an epsilon ball of the current solution. We update $\mu = \mu_{k+1}$, projecting onto the entropy objective.

We repeat these projections, tuning μ to find the right balance. The final joint measure μ defines a correspondence between nodes in $G1$ and $G2$ with marginals nearly matching (μ_1, μ_2), and maximum entropy.

The distance between $G1$ and $G2$ is defined in terms of the joint measure μ and its projections. Maximizing the entropy of μ results in a more robust distance metric.

3 Algorithm Overview

The optimization problem is solved via an iterative Bregman projection algorithm. The main steps are:

- Initialize a joint measure $\mu_0 \in \Pi(G1, G2)$ satisfying the marginal constraints.
- Project onto marginal constraints. Update to the projected measure.
- Project onto entropy constraints. Update to the projected measure.
- Repeat the projections, tuning μ to balance the marginals and entropy.

The final μ encodes a correspondence between $G1$ and $G2$ with marginals μ_1 and μ_2 and maximum entropy, representing their discrepancy.

4 Discussion

- Strict convexity from the entropy term, avoiding local optima.
- Robustness by spreading mass, reducing outlier influence.
- Relaxed constraints allowing some error to gain entropy.
- Automated tuning of the entropy weight via projections.
- Encodes complex relationships, not just one-to-one matchings.

The Bregman projections are key to handling the constraints and optimizing the entropy. They keep the solution feasible while driving progress, converging to the balance between competing objectives.