Subspace Detours Meet Gromov-Wasserstein

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OTML 2021
13/12/2021
Gromov-Wasserstein Distance

Let \((X, d_X, \mu), (Y, d_Y, \nu)\) be metric-measures spaces (mm-spaces).

**Gromov-Wasserstein**

\[
GW(X, Y) = \inf_{\gamma \in \Pi(\mu, \nu)} \iint (c_X(x, x') - c_Y(y, y'))^2 \, d\gamma(x, y) d\gamma(x', y')
\]

with \(\Pi(\mu, \nu) = \{\gamma \in \mathcal{P}(X \times Y), \pi_1^#\gamma = \mu, \pi_2^#\gamma = \nu\}\).

**Examples**

For \(X = \mathbb{R}^p, Y = \mathbb{R}^q\),

- \(c_X(x, x') = d_X(x, x'), c_Y(y, y') = d_Y(y, y)\)
- \(c_X(x, x') = \|x - x'\|^2_2, c_Y(y, y') = \|y - y'\|^2_2\)
- \(c_X(x, x') = \langle x, x' \rangle_p, c_Y(y, y') = \langle y, y' \rangle_q\)

**Properties:**

- Distance between mm-spaces up to isometries
- Invariances
Let \((X, d_X, \mu), (Y, d_Y, \nu)\) be metric-measure spaces (mm-spaces).

\[
GW(X, Y) = \inf_{\gamma \in \Pi(\mu, \nu)} \iint (c_X(x, x') - c_Y(y, y'))^2 \, d\gamma(x, y) \, d\gamma(x', y')
\]

with \(\Pi(\mu, \nu) = \{\gamma \in \mathcal{P}(X \times Y), \pi_1^\# \gamma = \mu, \pi_2^\# \gamma = \nu\}\).

**Practical Issues:**

- Computational Complexity: \(O(n^4)\)

**Proposed Solution:**

- Entropic Regularization [Peyrée et al., 2016]
- Low rank constraints [Scetbon et al., 2021]
- Sliced Gromov-Wasserstein [Vayer et al., 2019]
- Minibatch estimators [Fatras et al., 2021]
Subspace Detour approach [Muzellec and Cuturi, 2019]:

- Choose a subspace $E$
- Project the measures: $\mu_E = \pi^E_\# \mu$ and $\nu_E = \pi^E_\# \nu$
- Take the optimal coupling $\gamma^*_E \in \Pi(\mu_E, \nu_E)$
- Find a coupling $\gamma \in \Pi_E(\mu, \nu) = \{ \gamma \in \Pi(\mu, \nu) | (\pi^E, \pi^E)_\# \gamma = \gamma^*_E \}$

Coupling on the whole set:

- Monge-Independent plan:
  $$\pi_{MI} = \gamma^*_E \otimes (\mu_{E\perp|E} \otimes \nu_{E\perp|E})$$

- Monge-Knothe plan:
  $$\pi_{MK} = \gamma^*_E \otimes \gamma^*_{E\perp|E}$$
Motivation

Figure: From left to right: Data (moons), OT plan obtained with GW for $c(x, x') = \|x - x'\|_2^2$, Data projected on the 1st axis, OT plan obtained between the projected measures, Data projected on their 1st PCA component, OT plan obtained between the projected measures.

Subspace Detour approach for GW: Let $\mu \in \mathcal{P}(\mathbb{R}^p)$, $\nu \in \mathcal{P}(\mathbb{R}^q)$,

- Choose subspace $E \subset \mathbb{R}^p$ and $F \subset \mathbb{R}^q$
- Project the measures: $\mu_E = \pi_E \# \mu$ and $\nu_F = \pi_F \# \nu$
- Take the optimal coupling $\gamma^*_{E,F} \in \Pi(\mu_E, \nu_F)$
- Find a coupling $\gamma \in \Pi_{E,F}(\mu, \nu) = \{\gamma \in \Pi(\mu, \nu) | (\pi^E, \pi^F) \# \gamma = \gamma^*_{E \times F}\}$
\[ GW_{E,F}(\mu, \nu) = \inf_{\gamma \in \Pi_{E,F}(\mu, \nu)} \iint (c_X(x, x') - c_Y(y, y'))^2 \, d\gamma(x, y) d\gamma(x', y') \]

Properties:

- Let \( \pi_{MK} = \gamma^*_{E \times F} \otimes \gamma^*_{E^\perp \times F^\perp} |_{E \times F} \), then
  \[
  \pi_{MK} \in \arg\min_{\gamma \in \Pi_{E,F}(\mu, \nu)} \iint (c_X(x, x') - c_Y(y, y'))^2 \, d\gamma(x, y) d\gamma(x', y').
  \]

- \( GW_{E,F} \) invariant w.r.t isometries of the form \( f = (Id_E, f_{E^\perp}) \) for
  \[
  c_X(x, x') = \|x - x'\|_2^2, \quad c_Y(y, y') = \|y - y'\|_2^2 \quad \text{or} \quad c_X(x, x') = \langle x, x' \rangle_p, \quad c_Y(y, y') = \langle y, y' \rangle_q.
  \]
Choice of subspace

- Better sample complexity on lower dimensional spaces [Vayer et al., 2018]
- Better computational cost with 1D subspaces: $O(n \log n)$ [Vayer et al., 2019]

Choice of subspace?

- Euclidean spaces: PCA
- Graphs: Fiedler vector
- Gradient descent over Stiefel manifold
Application

Ground Truth | GW (Adjacency) | GW (Weighted Adjacency) | GW (Heat Kernel) | GW (Geodesic distance)
Conclusion

Thank you!


