Inference through optimal transport

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Dynamics and Data Assimilation, Physiology and Bioinformatics: Mathematics at the Interface of Theory and Clinical Application

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The problem

Data:

xⁱ: state

z^i : factors

- a^i : action
- g^i : reference group

Goal:

Estimate $\rho(x|z_*, a_*, g_*)$ or simulate $x_*^j \sim \rho(: |z_*, a_*, g_*)$.

Examples:

Diagnosis, forecast, treatment effect estimation

Conditional density simulation through the optimal transport barycenter problem

Include the action a among the factors z, forget temporarily the reference group g.

Remove from x the variability attributable to z through a map y = T(x; z) such that $\mu(y) = T \# \rho(x|z)$ is independent of z. Among such maps T, select the minimizer of a cost function C(T) associated with data distortion.



$$x^{i} \sim \rho\left(:|z^{i}\right) \rightarrow y^{i} = T\left(x^{i}; z^{i}\right) \rightarrow x^{i}_{*} = T^{-1}\left(y^{i}; z_{*}\right) \sim \rho\left(:|z_{*}\right)$$

An example: hourly temperature in Ithaca, NY

- Set 1: Static covariates: time of day, day of year, year.
- Set 2: Static + local temperature 24 hours before.
- Set 3: Static + temperature at 3 locations 36 hours before.



Figure: Observations, estimated median and 95% confidence interval.

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Capturing idiosyncratic factors through sub-sampling



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Trajectories

$$y_* = T(x_*; z_*, a_*)).$$

In time, under a prescribed action a(t):

$$\mathbf{x}_*(t) = \mathcal{T}^{-1}(\mathbf{y}_*; \mathbf{z}(t), \mathbf{a}(t)) \sim
ho\left(: | \mathbf{z}(t), \mathbf{a}(t), \mathbf{g}_*
ight)$$

In action:

$$x_*(t) = \mathcal{T}^{-1}(y_*; z_*, a) \sim
ho\left(: | z_*, a, g_*
ight)$$

Sensitivity, attribution:

$$x_*(t) = T^{-1}(y_*; z, a_*) \sim \rho(: | z, a_*, g_*)$$

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Factor discovery

Find additional latent factors z_l explaining, jointly with the known factors z_k , as much variability in x as possible:



 $z_l = rgmin var \left[\mu(y) = T \# \rho(x|z)\right], \quad z = \{z_k, z_l\}$

but
$$var[\rho] = \min C(T) + var[\mu]$$
, so

$$\max_{z_l} \min_{T(x,z)} C(T)$$

To conclude

The barycenter problem provides a natural framework for inference and control, suitable for analysis at various levels of granularity/individualization.

Left out of this talk: how to formulate and solve the data-driven barycenter problem. That's where much of the math fun is! Some ingredients: weak formulation of the push-forward condition, maps built from continuous flows, minimax problems.

Also left our of this talk: biomedical applications. Work in progress!

Much more to do.

Thanks!