Discrete Probabilistic Inverse Optimal Transport ICML 2022 @ Baltimore

Wei-Ting Chiu^{1,*}, Pei Wang^{1,*}, Patrick Shafto^{1,2}

iamwtchiu@gmail.com, peiwang425@gmail.com, patrick.shafto@gmail.com

Department of Mathematics and Computer Science, Rutgers University Newark, NJ ² School of Mathematics, Institute for Advanced Study (IAS), Princeton NJ * Equal contribution

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- Inverse OT is the problem of inferring the latent costs C from observed T.
 - It arises naturally in many domains, such as: cost of international migrations.



$$C = ?$$
 – Existing works.

Is
$$C$$
 unique? - No!!

Space of all possible C? – Our work.

- Entropy regularized OT (EOT): a map $\Phi:(C,\mu,\nu)\to T$.
- Inverse OT is defined as $\Phi^{-1}: T \to \{(C, \mu, \nu)\}$ not unique!!!.
- Goal: We aim to analyze the intrinsic properties of the entire cost space.

Probability Inverse Optimal Transport (PIOT)



Given a noisy observation T of T^* , PIOT is defined as:

$$P(C|T) = \int_{T^* \in (\mathbb{R}^*)^{m \times n}} P(C|T^*) P(T^*|T) dT^*, \tag{1}$$

where $P(C|T^*)$ is obtained through Bayes' Rule:

$$P(C|T^*) = \frac{P(T^*|C)P_0(C)}{P(T^*)},\tag{2}$$

Likelihood $P(T^*|C)=1$ if $C\in\Phi^{-1}(T^*)$, otherwise $P(T^*|C)=0$;

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Support manifold $\Phi^{-1}(T)$ – No noise



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Definition. Positive matrices A, B are cross ratio equivalent, $A \stackrel{c.r.}{\sim} B$, if:

$$r_{ijkl}(A) := \frac{a_{ik}a_{jl}}{a_{il}a_{jk}} = \frac{b_{ik}b_{jl}}{b_{il}b_{jk}} := r_{ijkl}(B).$$
(3)

Theorem. Given positive T of dimension $m \times n$, $\Phi^{-1}(T)$ is a hyperplane of dimension m+n-1, consists cost matrices C satisfying $e^{-C} \stackrel{c.r.}{\sim} T$.

 $lackbox{ Supp}[P(C|T)]$ for different priors, incomplete observations, submanifolds.

Support manifold - With noise

Lemma. Given T_1, T_2 , hyperplanes $\Phi^{-1}(T_1)$, $\Phi^{-1}(T_2)$ are the same or parallel.

The distance between IOT of T_1 and T_2 is then well-defined to be the Euclidean distance between $\Phi^{-1}(T_1)$ and $\Phi^{-1}(T_2)$.

Proposition. Given T, assume uniform noise on t_{11} with bounded size a, then

$$supp[P(C|T)] = \bigcup_{T' \in \mathbb{B}_a(T)} \Phi^{-1}(T')$$
 a collection of hyperplanes.



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Approximate inference via MCMC



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- Use MCMC method for inferring cost function *C*
- Advantages:
 - Flexibility on choice of prior $P_0(C)$ or $P_0(K)$
 - Generally inferring a set of possible C instead of a single one
- Procedure: given $K^{(0)} = T$; $K^{(i+1)} = \operatorname{diag} D^r K^{(i)} \operatorname{diag} D^c$
- Acceptance ratio *a* depending on the prior:
 - Prior on C: Metropolis (MetroMC): $a = \frac{P(-\ln(K^{(i+1)})|T)}{P(-\ln(K^{(i)}|T)} \stackrel{(*)}{=} \frac{P_0(C^{i+1},\beta)}{P_0(C^i,\beta)}$
 - Prior on K: Metropolis-Hasting (MHMC): $a = \min\left(1, \frac{P(K')}{P(K)} \frac{Q(K|K'))}{Q(K'|K)}\right)$
- Accept move if $a > u \in [0, 1)$.

Visualizing support of P(K|T)

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- Demonstrate effect of cross-ratio equivalence on P(K|T)
- Prior over K is possible and suitable for visualization
- Column-wise Dirichlet prior for $P_0(K)$
 - lacktriangle Visualizing supp[P(K|T)]: plotting columns of T & columns of P(K|T)





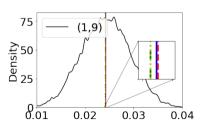




Synthetic data: symmetric cost with noise

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- Accurate cost inference with relative error $< 10^{-3}$;
- $C_{ij}^g = \left| \frac{(i-j)}{n} \right|^p + 10^{-4} * U_{[0,1)} \text{ (blue)}^1$
- Median of the posterior distribution (red)
- Compare with Ma et al. (arXiv:2002.09650) (yellow & green)



¹The inset in the figure has a range of $C^g \pm 10^{-4}$.

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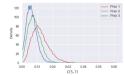
Real-world data: European migration flow (1)

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- Ground truth cost not available.
- Inferred cost inversely proportional to log of migration flow
- Consider 3 priors, stronger prior gives sharper posterior
- PIOT with soft constrain is less biased





Ground truth T^g Inferred cost C

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Real-world data: European migration flow (2)



- Evaluate predictability of PIOT on 2 cases: T with (1) noise (2) missing value
 - Procedure: T –[PIOT] $\rightarrow P(C|T)$ –[EOT] $\rightarrow P(T')$; $T^p = \overline{P(T')}$
 - NOISE: $T_{ij} = T_{ij}^g + \epsilon_{ij}$; MISSING VALUE: $T_{ij} \in [100, 25000)$
- $\bullet \ \ \textit{Accurate predictions on noisy/missing elements} \rightarrow \textit{PIOT infers cost well} \\$

				Missing value		
	(3,6)	(4,5)	(5,7)	(3,6)	(4,5)	(5,7)
T^g	452	6635	16560	452	6635	16560
T^p	454	6593	$16560 \\ 16515$	3699	7462	12349
$-\Delta$.45%	.87%	.25%	26%	6.6%	34%

Table: Comparison between the predicted coupling, T^p , with the ground truth coupling, T^g . $\Delta = (T^p - T^g)/\overline{T}^g$. Corresponding element is corrupted by a 4% Gaussian noise on the left column, and missing on the right column.

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In this work we

- formulate PIOT and identify the support manifold for latent costs
- characterize the geometry of the support manifold
- analyze the support manifold for noisy and incomplete observations
- develop MCMC algorithms for posterior inference
- demonstrate PIOT through simulations on general examples

Thank you!







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