Probabilistic Inverse Optimal Transport

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Abstract

Optimal transport (OT) formalizes the problem of finding an optimal coupling between probability measures given a cost matrix. The inverse problem of inferring the cost given a coupling is Inverse Optimal Transport (IOT). IOT is less well understood than OT. We formalize and systematically analyze the properties of IOT using tools from the study of entropy-regularized OT. Theoretical contributions include characterization of the manifold of cross-ratio equivalent costs, the implications of model priors, and derivation of an MCMC sampler. Empirical contributions include visualizations of cross-ratio equivalent effect on basic examples and simulations validating theoretical results.

1 Introduction

Inverse Optimal Transport (Stuart and Wolfram, 2020; Li et al., 2019; Paty and Cuturi, 2020) has received less systematic attention than (entropy-regularized) Optimal Transport (OT) (Villani, 2008; Cuturi, 2013). Formulation and investigation of the general problem of probabilistic inference of latent costs from stochastic couplings given priors has not been systematically undertaken. Like EOT, IOT inherits interesting geometric structure from Sinkhorn scaling (Sinkhorn, 1964), which gives rise to natural questions about the nature of posterior distributions, the existence of samplers, and questions about the feasibility and effectiveness of inferences from observed couplings to underlying costs.

In recent years IOT problems have been studied and applied in many areas. Practical examples include: (1) inferring the cost criterion of international migration (Stuart and Wolfram, 2020); (2) estimating the marriage matching affinity (Dupuy et al., 2019); (3) learning interaction cost function from noisy and incomplete matching matrix and make prediction on new matching (Li et al., 2019). These works provide methodologies to solve certain IOT problems, while in our article we provide a framework for analyzing the general problem to understand the geometric properties of probabilistic inverse optimal transport (PIOT).

Our contributions include: (1) formulating the PIOT problem and provide basic results; (2) characterizing the geometry of the support manifold of PIOT solutions along with the implications of prior distributions on posterior inference; (3) presenting MCMC algorithms for posterior inference which derives directly from properties of Sinkhorn scaling; (4) demonstrating the ability of PIOT through simulating general examples.

Notation: \( \mathbb{R}^+ \) denotes the extended non-negative reals \( \mathbb{R}^* \cup \{+\infty\} \). \( \Delta_k \) is the \( k \)-dimensional simplex. For a space \( X \), \( P(X) \) denotes the set of distributions over \( X \). Matrices are in uppercase and their elements are in the corresponding lowercase. For a matrix \( A_{m \times n} \), \( a_1, \ldots, a_n \) denotes columns of \( A \). Column normalizing a matrix \( A_{m \times n} \) with respect to a \( n \)-dim row vector \( \nu \) is defined as \( \text{Col}(A, \nu) = \text{Adiag}(\nu) A \), where \( 1_m \) is a \( m \)-dim row vector with each element equals to 1. \( \nu \) with respect to \( \nu \) is omitted when \( \nu = 1_n \). Row normalization is defined in the same fashion.

2 Background and Related Work

Given two spaces \( X = \{x_1, \ldots, x_m\} \) and \( Y = \{y_1, \ldots, y_n\} \), let \( T = (t_{ij})_{m \times n} \in (\mathbb{R}^*)^{m \times n} \) be a coupling that records the co-occurrence distribution between \( X \) and \( Y \). Note that \( t_{ij} \) is allowed to be zero here. Each element \( t_{ij} \) represents the probability of observing \( x_i \) and \( y_j \) simultaneously. The interaction between \( X \) and \( Y \) can be captured by a cost matrix \( C = (c_{ij})_{m \times n} \in (\mathbb{R}^*)^{m \times n} \), where \( c_{ij} \) measures the underlying cost of coupling \( x_i \) and \( y_j \). Hence, the prob-

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Probabilistic inference on the underlying structure over X and Y is then to obtain \( P(C|T) \), the distribution over all possible \( C \) given an observed coupling \( T \).

**Entropy regularized optimal transport** is a fundamental building block in modelling \( P(C|T) \). Given a cost matrix \( C \) and distributions \( \mu, \nu \) over \( X \) and \( Y \) respectively, the entropy regularized optimal transport (EOT) (Cuturi, 2013; Peyré et al., 2019) solves the optimal coupling \( T^\lambda \) that minimizes the entropy regularized cost of transfer \( X \) with distribution \( \mu \) into \( Y \) with distribution \( \nu \). Thus for a parameter \( \lambda > 0 \):

\[
T^\lambda = \text{argmin}_{T \in U(\mu, \nu)} \left\{ \langle C, T \rangle - \frac{1}{\lambda} H(T) \right\} \quad (1)
\]

where \( U(\mu, \nu) \) is the set of all couplings between \( \mu \) and \( \nu \) (i.e. joint distributions with marginals \( \mu \) and \( \nu \)), \( \langle C, T \rangle = \sum_{i \in X, j \in Y} c_{ij} t_{ij} \) is the Frobenius inner product between \( C \) and \( T \), and \( H(T) := -\sum_{i=1}^{m} \sum_{j=1}^{n} t_{ij} \log t_{ij} \) is the entropy of \( T \). \( T^\lambda \) is called an optimal coupling with parameter \( \lambda \).

**Sinkhorn scaling** is used to efficiently compute optimal couplings. \((\mu, \nu)\)-Sinkhorn Scaling (SK) (Sinkhorn, 1964) of a matrix \( M \) is the iterated alternation between row normalization of \( M \) with respect to \( \mu \) and column normalization of \( M \) with respect to \( \nu \). (Cuturi, 2013) proved that: given a cost matrix \( C \), the optimal coupling \( T^\lambda \) between \( \mu \) and \( \nu \) can be solved by applying \((\mu, \nu)\)-Sinkhorn scaling on the negative exponential cost matrix \( K^\lambda \), where \( K^\lambda = e^{-\lambda C} = (e^{-\lambda c_{ij}})_{m \times n} \).

**Example 2.1.** Let \( \mu = \nu = (\frac{3}{8}, \frac{5}{8}) \), \( C = (\frac{\ln 1}{\ln 4}, \frac{\ln 2}{\ln 4}, \frac{\ln 1}{\ln 4}) \).

For \( \lambda = 1 \), we may obtain \( T \) by applying SK scaling on \( K^1 = e^{-C} = (\frac{1}{1/4}, \frac{1/2}{1/4}) \). First, row normalize \( K^1 \) with respect to \( \mu \) results: \( K^1_1 = (\frac{1/4}{1/8}, \frac{1/2}{1/2}) \). Then column normalization of \( K^1_1 \) with respect to \( \nu \) outputs \( K^1_2 = (\frac{1/4}{1/8}, \frac{1/2}{1/2}) \). As \( K^1_1 = K^1_2 \), the SK scaling has converged with \( T = K^1 \) in general, multiple iterations may be required to reach the limit.

Given a coupling \( T \), the inference on the cost matrix \( C \) can be formulated as an inverse entropy regularized optimal transport problem. Given \( \lambda \), EOT is the map \( \Phi: (\mathbb{R}^n)^{m \times n} \times \mathcal{P}(\mathbb{R}^m) \times \mathcal{P}(\mathbb{R}^n) \to \mathcal{P}((\mathbb{R}^n)^{m \times n}) \) with \( \Phi(C, \mu, \nu) = T^\lambda \). Therefore inverse entropy regularized optimal transport (IOT) can be defined as \( \Phi^{-1} : T^\lambda \to \{(C, \mu, \nu)\} \), where \( \{(C, \mu, \nu)\} \) represents the preimage set of \( T^\lambda \) under \( \Phi \).

**Remark 2.2.** In IOT, when \( T^\lambda \) is observed without any noise, \( T^\lambda \) completely determines \( \mu \) and \( \nu \). Indeed \( (C, \mu, \nu) \in \Phi^{-1}(T^\lambda) \) implies that \( T^\lambda \in U(\mu, \nu) \). Thus \( \mu \) and \( \nu \) must equal the row and column marginals of \( T^\lambda \). Hence we may reduce IOT into \( \Phi^{-1} : T^\lambda \to \{C\} \).

Further, note that \( \Phi^{-1} : T^\lambda \to \{C\} \) is not well-defined as a function, since \( T^\lambda \) does not uniquely determine cost \( C \). For instance, any matrix \( C' \) in form of \( C' = \begin{pmatrix} \ln \alpha - \frac{1}{\ln \beta - 1} & \ln \alpha - \frac{2}{\ln \beta - 1} \\ \ln \beta - 4 & \ln \beta - 1 \end{pmatrix} \), for \( \alpha, \beta > 0 \) outputs the same optimal coupling \( T \) as \( C \) in Example 2.1.

**Related Work.** The forward OT problem has a long history and is an active field of research (Kantorovich, 1942; Villani, 2008; Peyré et al., 2019; Genevay et al., 2016). Applications in machine learning include: supervised learning (Frogner et al., 2015), Bayesian inference (El Moselhy and Marzouk, 2012), generative models (Salimans et al., 2018), Transfer learning (Courty et al., 2016), and NLP (Alaux et al., 2018).

However, the inverse OT problem is much less studied. The few existing inverse OT papers (Dupuy et al., 2019; Li et al., 2019; Li et al., 2019; Stuart and Wolfram, 2020), to our best knowledge, all focused on obtaining a unique approximation of the ‘ground truth’ \( C^* \), even though \( \Phi^{-1}(T) \) contains a set of cost matrices. To output an estimate of \( C^* \), existing approaches place constraints on the cost matrix. For example in Stuart and Wolfram (2020), \( C \) has to be either a Toeplitz matrix or determined by a given graph structure. In Li et al. (2019), \( C \) must be constructed from a metric over a space where both \( X \) and \( Y \) are able to be embedded in, plus \( X \) and \( Y \) need to have the same dimensionality. In Dupuy et al. (2019), the affinity matrix has a low-rank constraint. These assumptions do not hold in general.

We aim to analyze the intrinsic properties and the underlying geometric structure of the set \( \{C\} = \Phi^{-1}(T^\lambda) \) for the general case in the following sections. To simplify the notation, we will omit the superscript \( \lambda \), and fix \( \lambda = 1 \) unless otherwise stated.

### 3 Probabilistic inverse optimal transport

**Definition 3.1.** Let \( T \) be a noisy observation of the optimal coupling \( T^* \). **Probabilistic inverse optimal transport** is defined as:

\[
P(C|T) = \int_{T^* \in (\mathbb{R}^n)^{m \times n}} P(C|T^*)P(T^*|T)dT^*, \quad (2)
\]

where \( P(C|T^*) \) is obtained through Bayes’ Rule:

\[
P(C|T^*) = \frac{P(T^*|C)P_0(C)}{P(T^*)}, \quad (3)
\]

\( P_0(C) \) is a prior of cost matrix \( C \) over \((\mathbb{R}^n)^{m \times n}; \)
\( P(T^*) = \int P(T^*|C)P_0(C)dC \) is the normalizing constant; Likelihood \( P(T|C) = 1 \) if \( C \in \Phi^{-1}(T) \), oth-
3.1 No observation noise

As a direct application of Definition 3.1, we have:

**Proposition 3.2.** $P(C|T)$ is supported on the intersection between $\Phi^{-1}(T)$ and the domain of $P_0(C)$.

Moreover, we have that $P(C|T) = \frac{P_0(C)}{\int_{\Phi^{-1}(T)} P_0(C) dC}$.

Therefore, characterization of $\Phi^{-1}(T)$ is essential to understand the manifold where the posterior distribution $P(C|T)$ is supported on.

Notice that for any $C \in \Phi^{-1}(T)$, a Sinkhorn scaling of $K = e^{-C}$ results in $T$, and each step of Sinkhorn Scaling is a normalization which equivalent to multiplication of a diagonal matrix. We show that:

**Proposition 3.3.** Let $T$ be a non-negative optimal coupling of dimension $m \times n$. $C \in \Phi^{-1}(T)$ if and only if for every $\epsilon > 0$, there exist two positive diagonal matrices $D^r = \text{diag}(d^r_1, \ldots, d^r_m)$ and $D^c = \text{diag}(d^c_1, \ldots, d^c_n)$ such that: $|D^r K D^c - T| < \epsilon$, where $K = e^{-C}$ and $|\cdot|$ is the $L^1$ norm. In particular, if $T$ is a positive matrix, then $C \in \Phi^{-1}(T)$ if and only if there exist positive diagonal matrices $D^r, D^c$ such that $D^r K D^c = T$, i.e.

$$\Phi^{-1}(T) = \{ C | \exists D^r, D^c \text{ s.t. } K = D^r T D^c \} \quad (4)$$

Proposition 3.3 identifies a key feature of matrices in $\Phi^{-1}(T)$. However, it is not easy to verify whether an arbitrary matrix belongs to $\Phi^{-1}(T)$ nor reveal any underlying geometric structure of $\Phi^{-1}(T)$.

Towards these goals, we now introduce an equivalent condition: cross ratio equivalence between positive matrices, and show that the IOT set $\Phi^{-1}(T)$ can be completely characterized by $T$’s cross ratios.

**Definition 3.4.** Let $A, B$ be positive $m \times n$ matrices. $A$ is cross ratio equivalent to $B$, denoted by $A \underset{c.r.}{\sim} B$, if all cross ratios of $A$ and $B$ are the same, i.e.

$$r_{ijk}^{kl}(A) := \frac{a_{ik} a_{jl}}{a_{il} a_{jk}} = \frac{b_{ij} b_{kl}}{b_{il} b_{jk}} := r_{ijk}^{kl}(B)$$

holds for any $i, j \in \{1, \ldots, m\}$ and $k, l \in \{1, \ldots, n\}$.

**Lemma 3.5.** For two positive matrices $A, B$, $A \underset{c.r.}{\sim} B$ if and only if there exist positive diagonal matrices $D^r$ and $D^c$ such that $A = D^r T D^c$.

**Theorem 3.6.** Let $T$ be an observed positive optimal coupling of dimension $m \times n$. Then $\Phi^{-1}(T)$ is a hyperplane of dimension $m + n - 1$ embedded in $(\mathbb{R}^*)^{m \times n}$, which consists all the cost matrices that of the form:

$$\Phi^{-1}(T) = \{ C \in (\mathbb{R}^*)^{m \times n} | K = e^{-C} \underset{c.r.}{\sim} T \}. \quad (5)$$

Cross ratio equivalence provides a strong connection between IOT and algebraic geometry. Algebraically, cross ratios generate the set of algebraic invariants of matrix scaling. Thus the set of all scale reachable matrices from a coupling $T$, i.e. $\Phi_K^{-1}(T) = \{ K | D^r K D^c \} = \{ K = e^{-C} | C \in \Phi^{-1}(T) \}$ forms an algebraic variety defined by the cross-ratios of $T$. Geometrically, the set $\Phi_K^{-1}(T)$ forms a special manifold (Fienberg, 1968). $T$ is the unique intersection between $\Phi_K^{-1}(T)$ and the hyperplane determined by the linear marginal conditions.

**Remark 3.7.** Since a matrix $T$ and its normalization $T / \sum_{ij} t_{ij}$ have the same cross ratios (hence have the same image under IOT), we may relax the distribution constraint on the observed coupling $T$. In this case, instead of probability, $t_{ij}$ represents the frequency of observing $x_i$ and $y_j$ simultaneously.

**Example 3.8.** Let $T = \left( \begin{array}{ccc} 1 & 2 & 3 \\ 2 & 3 & 1 \end{array} \right)$. $T$ has three cross ratios $r_{1212}(T) = \frac{1}{3}, r_{1213}(T) = \frac{1}{2}, r_{1223} = \frac{2}{3}$. Only two are independent as $r_{1213}(T) = r_{1212}(T) * r_{1223}(T)$. Hence $\Phi_K^{-1}(T)$ is the solution set of the algebraic equation:

$$\left\{ \begin{array}{c} k_{11} k_{22} + k_{12} k_{21} = 3/4 \\ k_{12} k_{23} + k_{13} k_{22} = 2/9 \end{array} \right. \iff \left\{ \begin{array}{c} 4k_{11} k_{22} - 3k_{12} k_{21} = 0 \\ 9k_{12} k_{23} - 2k_{13} k_{22} = 0 \end{array} \right.$$

Further as $k_{ij} = e^{-c_{ij}}$, we obtain that $\Phi^{-1}(T)$ is the 4-dim hyperplane defined by the linear equations:

$$\left\{ \begin{array}{c} c_{12} + c_{21} - c_{11} - c_{22} = \ln(3/4) \\ c_{13} + c_{22} - c_{12} - c_{23} = \ln(2/9) \end{array} \right. \quad (6a) \quad (6b)$$

**Remark 3.9.** For a $m \times n$ matrix $A$, although there are $\binom{n}{2}$ ways to choose $i, j, k, l$ to form cross ratios of $A$, not all are independent as seen in Example 3.8. A set of independent cross ratios that generates the entire collection of cross ratios is called a basis. For example, it is easy to check that $B = \{ r_{ijkl}(A) | j = 2, \ldots, m, k = 2, \ldots, n \}$ forms a basis for $A$.

Observed $T$ is assumed to be a positive matrix for the rest of the paper, the case when $T$ is non-negative can be derived using machinery of maximal partial pattern developed in (Wang et al., 2019).

**Support manifold.** Since $\text{Supp}[P(C|T)] = \Phi^{-1}(T) \cap \text{Domain}[P_0(C)]$, different priors would add different constraints on $C$, which will result different submanifolds embed in the hyperplane formed by $\Phi^{-1}(T)$.

For instance, suppose $P_0(C)$ follows a Dirichlet distribution over the entire matrix $(P_1)$. Then

$$\text{Supp}[P(C|T)] = \{ C \in (\mathbb{R}^*)^{m \times n} | e^{-C} \underset{c.r.}{\sim} T, \sum_{ij} c_{ij} = 1 \}. \quad (5)$$

Proofs for all results are included in the supplemental materials.
Notice that $K$ encodes the cross ratios of $T$, and to avoid the estimation of $\lambda$, it is handy to directly put prior over $K = e^{-C}$. For example, assume that $P_0(K)$ is the distribution where each column follows an independent Dirichlet distribution $(\mathcal{P}_2)$ with hyper-parameter $\alpha$. Then the domain of $P_0(K)$ is $\mathcal{P}(\mathbb{R}^n)^m$.

Therefore, based on Eq. (4), we have the intersection of the form:

$$\text{supp}[P(C|T)] = \{C|\exists D^r \text{ s.t. } K = \text{Col}(D^r T)\} \quad (7)$$

**Remark 3.10.** Eq. (7) indicates that (i) a known column of $K$ uniquely determines all the other columns. Indeed, denote the $j$-th column of $K, T$ by $k_j, t_j$. For a known column $k_j$, let $d_i = k_{ij}/t_{ij}$ and $D^r = \text{diag}(d_1, \ldots, d_m)$. Then the $l$-th column $k_l$ equals to the column normalization of $D^r t_l$. (ii) for any $v \in \mathcal{P}(\mathbb{R}^n)^m$, there exists a $K \in \text{supp}(P(K|T))$ such that $k_j = v$. Therefore, we have:

**Corollary 3.11.** Under prior $P_2$, the projection of $\text{supp}[P(K|T)]$ onto each column is a $(m-1)$-dimensional manifold that is homeomorphic to the simplex $\Delta_m-1$.

**Subspace of Supp**[$P(C|T)$]. Let $C_s$ be the submatrix of the cost $C$ that corresponds to $X_s \times Y_s$, where $X_s = \{x_1, \ldots, x_s\} \subset X, Y_s = \{y_1, \ldots, y_s\} \subset Y$. In this section, we characterize the support of $P(C_s|T)$ as a subspace of $\text{supp}(P(C|T))$.

Denote the sub-coupling of $T$ corresponding to $C_s$ by $T_s$. According to Eq. (4) and Eq. (5), the projection of $\Phi^{-1}(T)$ onto the cost over $X_s \times Y_s$ is in form of:

$$\Phi^{-1}_s(T) := \{C_s|C_s \text{ is submatrix of } C \in \Phi^{-1}(T)\}$$

$$= \{C_s|\exists D^s_s, D^c_s \text{ s.t. } K_s = D^s_s T_s D^c_s\}$$

$$= \{C_s|K_s = e^{-C_s}, K_s \sim T_s\}$$

$$\text{Supp}[P(C_s|T)]$$

is determined by $\Phi^{-1}_s(T)$ and the prior $P_0(C)$. Intuitively, $\text{supp}[P(C_s|T)]$ contains all the matrices $C_s \in \Phi^{-1}_s(T)$ such that there exists a proper extension of $D^s_s, D^c_s$ to $D^r, D^c$ such that $D^r T D^c$ is in the domain of $P_0(C)$.

Take prior $P_2$ as an example. Since the domain for a column of $K$ is a copy of $\Delta_m-1$ as shown in Corollary 3.11, the domain for a column of $K_s = e^{-C_s}$ is then a copy of $\Sigma_s = \{k = (k_1, \ldots, k_s) \in (\mathbb{R}^+)^s|k_1 + \cdots + k_s < 1\}$. Hence, $\text{supp}[P(C_s|T)]$ should be contained in the set:

$$W_s = \{C_s|\exists \text{ diagonal matrices } D^s_s, D^c_s \text{ s.t. } K_s = D^s_s T_s D^c_s \text{ and } 1_{s_1} K_s = (a_1, \ldots, a_{s_2}), a_i < 1\}$$

It is important to note that $\text{supp}[P(C_s|T)]$ is a proper subset of $W$. As $K_s$ is a submatrix of $K$, the choice of $D^s_s$ must form a proper column normalizing constant of a $D^r T$. Thus, the choice of $D^s_s = \text{diag}(d_1^s, \ldots, d_m^s)$ must guarantee that there exist an extension of $D^s_s$, denoted by $D^r = \text{diag}(d_1^r, \ldots, d_m^r)$, with $d_{s_1+1}^r, \ldots, d_m^r > 0$, such that the $j$-th column sum of $D^r T$ is $1/d_j^r$. Let $T_{m-s}$ be the submatrix of $T$ corresponding to $\{x_{s+1}, \ldots, x_m\} \times Y$. We show that:

**Proposition 3.12.** $C_s \in \text{supp}[P(C_s|T)]$ if and only if there exists positive diagonal matrices $D^r_s, D^c_s$ such that $K_s = D^r_s T_s D^c_s$ and the system of equations $(x_1, \ldots, x_{m-s})T_{m-s} = (1/d_1^s, \ldots, 1/d_m^s) - 1_s D^c_s T_s$ have a set positive solution for $(x_1, \ldots, x_m)$. We say $P(C_s|T)$ is compatible.

**Incomplete Observation.** Say $T$ is observed with $t_{m_1}$ missing. Then generically, we have:

$$\text{supp}[P(C_s|T)] = \cup_{\tilde{T} \in U(T)} \text{supp}[P(C_s|\tilde{T})]$$

where $U(T)$ is the set of matrices with $T$ completed by a choice of $t_{m_1} > 0$. Given a prior, say $P_1$, we have:

$$\text{supp}[P(C_s|T)] = \{C|\exists c_{m_1} > 0 \text{ s.t. } K_s \sim \tilde{T}, \sum_{ij} c_{ij} = 1\}$$

where $\tilde{T}$ is $T$ with $t_{m_1}$ as its $m_1$-th element. With prior $P_2$, according to (7) we have:

$$\text{supp}[P(C_s|T)] = \{C|\exists D^r, t_{m_1} > 0, \text{ s.t. } K = \text{Col}(D^r \tilde{T})\}$$

Moreover, according to Remark 3.10, a known column $k_l$ of $K$ completely determines another fully observed column. Hence with a missing element in the first column, $k_l$ determines an one dimensional set $\mathcal{K}_l$ for $k_l$. In particular, let $D^r = \text{diag}(d_1, \ldots, d_m)$, where $d_i = k_{il}/t_{il}$. We show that:

**Corollary 3.13.** Under prior $P_2$, $K_l$ is a line segment in $\Delta_{m-1}$ that can be parameterized as: $K_l = \{d_{il} t_{l1}, \ldots, d_{m} t_{l1}\}/\sum_{i=1}^m d_{il} t_{i1}, t_{i1} \in (0, \infty)\}$. Note that for different choice of priors, $K_l$ could be a curve instead of a line segment. Denote the prior imposed constraint on $k_l$ by $f_l(k_l) = 0$, the ratio imposed linear constraint on $k_l$ by $f_l(k_l) = 0$, where $f_l(k_l) = k_{i1} - d_{i1} t_{il} / (d_{i1} t_{il})$, for $i = 2, \ldots, m-1$. Then $\mathcal{K}_l$ is the solution set for system of equations $\{f_1, f_2, \ldots, f_{m-1}\}$. With Dirichlet prior, $f_1$ is also linear, so $\mathcal{K}_l$ is a line segment.

### 3.2 With observation noise

First, for any two observed couplings with the same dimension, we introduce a natural distance between their images under IOT.

**Corollary 3.14.** Let $T_1, T_2$ be two positive matrices of dimension $m \times n$. The hyperplanes $\Phi^{-1}(T_1)$ and $\Phi^{-1}(T_2)$, have the same normal direction. In particular, if $T_1 \sim T_2$ then $\Phi^{-1}(T_1) = \Phi^{-1}(T_2)$. Otherwise $\Phi^{-1}(T_1)$ is parallel to $\Phi^{-1}(T_2)$. 

Therefore, $\Phi^{-1}(T_1), \Phi^{-1}(T_2)$ are either the same or parallel hyperplanes embedded in $(\mathbb{R}^+)^{m \times n}$. The distance between IOT of $T_1$ and $T_2$, denoted by $d(\Phi^{-1}(T_1), \Phi^{-1}(T_2))$ is then well-defined to be the Euclidean distance between $\Phi^{-1}(T_1)$ and $\Phi^{-1}(T_2)$.

Moreover, $\Phi^{-1}(T)$ is completely determined by $T$’s cross ratios. So $d(\Phi^{-1}(T_1), \Phi^{-1}(T_2))$ can be expressed in terms of cross ratios of $T_1$ and $T_2$. We now illustrate how to obtain $d(\Phi^{-1}(T_1), \Phi^{-1}(T_2))$.

**Example 3.15.** Let $T_1 = T$ in Example 3.8, $T_2 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}$. Then $\Phi^{-1}(T_1)$ is the hyperplane shown in Eq. (9). Taking $r_{1212}, r_{1213}$ as $T$’s cross ratio basis, then we have $\Phi^{-1}(T_2)$ is:

\[
\begin{align*}
  c_{12} + c_{21} - c_{11} - c_{22} &= \ln(1/3) \quad (8a) \\
  c_{13} + c_{22} - c_{12} - c_{23} &= \ln(1/3) \quad (8b)
\end{align*}
\]

Both $\Phi^{-1}(T_1)$ and $\Phi^{-1}(T_2)$ are intersections of two 5-dim hyperplanes (i.e. (6a) \(\cap\) (6b) and (8a) \(\cap\) (8b)) with the same coefficient, so they are parallel. Let the Dihedral angle between (6a) and (6b) be $\theta$. It is easy to check $\cos \theta = 1/2$. So we have

\[
d(\Phi^{-1}(T_1), \Phi^{-1}(T_2)) = \sqrt{\ln^2 \frac{2}{3} + \ln^2 \frac{2}{3} - \ln \frac{2}{3} \ln \frac{2}{3}}.
\]

**Remark 3.16.** The hyperparameter $\lambda$ in Eq.(1) can be viewed as a greedy data selection. For a forward EOT problem, $\lambda$ raises the cross ratios of $K = e^{-\lambda}$ to a power of $\lambda$. Hence, $\lambda$ either exaggerates or suppresses the cross ratios of $T$, depending on whether $\lambda$ is greater or less than 1 (Wang et al., 2020). Conversely, given a backward IOT problem, for a fixed coupling $T$, the larger the $\lambda$ is assumed, the smaller the cross ratios of $K$ are. Moreover, for a pair of observed couplings $T_1$ and $T_2$, the equations for hyperplanes corresponding $\Phi^{-1}(T_1), \Phi^{-1}(T_2)$ with different choices of $\lambda$, only differ on the constants by a scalar, i.e. $d_\lambda(\Phi^{-1}(T_1), \Phi^{-1}(T_2)) = d(\Phi^{-1}(T_1), \Phi^{-1}(T_2))/\lambda$. Therefore, the larger $\lambda$ is assumed, the smaller the distance between $\Phi^{-1}(T_1)$ and $\Phi^{-1}(T_2)$ are.

Assuming uniform prior $P_0(C)$ over $(\mathbb{R}^+)^{m \times n}$, we now investigate $P(C|T)$ under two common noise types. Results for other specific priors can be obtained by restricting the generic results to the prior’s domain. Without loss, we will assume noise only occurs on one element of $T$, say $t_{11}$, as the general case may be treated as compositions of such.

**Bounded noise.** Suppose that $t_{11}$ is perturbed by a uniform noise from $t_{11}$, i.e. $t_{11}' = t_{11} + \epsilon$, where $\epsilon$ is a random variable with uniform distribution over $[-a, a]$, for $a > 0$.

Theorem 3.6 and Corollary 3.14 imply that $P(C|T)$ is supported on a collection of parallel hyperplanes within bounded distance away from $\Phi^{-1}(T)$. More precisely, we show:

**Proposition 3.17.** For a coupling $T$, assume uniform observation noise on $t_{11}$ with bounded size $a$,

\[
supp[P(C|T)] = \cup_{T' \in \mathcal{B}_a(T)} \Phi^{-1}(T'),
\]

where $\mathcal{B}_a(T)$ is the set of matrices $T'$ of the same dimension as $T$ with the property that: $t_{11}' > 0$, $|t_{11}' - t_{11}| \leq a$ and $t_{ij}' = t_{ij}$ for other $i, j$. Moreover, $\Phi^{-1}(T')$ can be expressed as intersection of two hyperplanes (may be in different dimensions): one with equation: $c_{11} + c_{22} - c_{12} - c_{21} = -\ln \frac{t_{11}' t_{22}'}{t_{12}' t_{21}'}$, and the other equation does not depend on the value of $t_{11}'$. Assume the angle between these two hyperplanes is $\theta$. Then $d(\Phi^{-1}(T'_1), \Phi^{-1}(T'_2)) \leq \ln \frac{1+a}{1-a}/\sin \theta$, for $T'_1, T'_2 \in \mathcal{B}_a(T)$.

**Example 3.18.** Let $T$ be the same as Example 3.8. Suppose there is a bounded noise $\epsilon$ on $t_{11}$ of size $a > 0$. Hence, $\supp[P(C|T)]$ is the union of a collection of hyperplanes $\mathcal{B}_a(T)$ of the form for $\epsilon \in [-a, a]$:

\[
\begin{align*}
  c_{12} + c_{21} - c_{11} - c_{22} &= \ln(3 + 3\epsilon)/4 \quad (9a) \\
  c_{13} + c_{22} - c_{12} - c_{23} &= \ln(2/9) \quad (9b)
\end{align*}
\]

Let the angle between (9a) and (9b) be $\theta$. Computation shows that $\sin \theta = \sqrt{3}/2$. Hence for $T'_1, T'_2 \in \mathcal{B}_a(T)$, $d(\Phi^{-1}(T'_1), \Phi^{-1}(T'_2)) \leq \sqrt{3}\ln(1+a)$.

**Gaussian noise.** Suppose that $t_{11}$ is perturbed by a Gaussian distribution from $t_{11}$ centered at zero, i.e. $t_{11}' = t_{11} + \epsilon$, where $\epsilon \sim \mathcal{N}(0, \sigma^2)$ with standard deviation $\sigma > 0$.

Gaussian distribution is defined over the entire real line, so $\supp[P(C|T)] = \cup_{T' \in \mathcal{L}(T)} \Phi^{-1}(T')$, where $\mathcal{L}(T)$ is the set of matrices $T'$ of the same dimension as $T$ with the property that: $t_{11} > 0$ and $t_{ij}' = t_{ij}$ for $(i, j) \neq (1, 1)$. In particular, cross ratios of $T'$ that depend on $t_{11}$ can be an arbitrary number. Hence, similar to the case of missing elements in $T$, $P(C|T)$ is supported on a hyperplane that is one dimensional higher than $P(C|T')$. In particular, we show:

**Proposition 3.19.** Let $T$ be an observed coupling of dimension $m \times n$ with Gaussian noise on $t_{11}$. Further, let $\mathcal{B}$ be a basis for cross ratios of $m \times n$ matrices, that contains only one cross ratio depending on $t_{11}$. Eliminate the cross ratio depending on $t_{11}$ in $\mathcal{B}$, denote the new set by $\mathcal{B}^*$. Then:

\[
supp[P(C|T)] = \{ c | r(K) = r(T) \text{ for } r \in \mathcal{B}^* \}
\]

In particular, $P(C|T)$ is supported on a hyperplane that is one dimensional higher than $P(C|T')$ for any $T' \in \mathcal{L}(T)$.

**Example 3.20.** Let $T$ be the same as Example 3.8. Suppose there is a Gaussian noise $\epsilon \sim \mathcal{N}(0, \sigma^2)$ on
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t_{11}$. Hence, $\text{supp}[P(C|T)]$ is the union of a collection of hyperplanes $L(T)$ of the form:

\begin{align}
 c_{12} + c_{21} - c_{11} - c_{22} &= \ln[(3 + 3\epsilon)/4] \\
 c_{13} + c_{22} - c_{12} - c_{23} &= \ln(2/9) 
\end{align}

Here $3 + 3\epsilon > 0$ and $\epsilon \sim N(0, \sigma^2)$ imply that $\epsilon \in (-1, \infty)$, which further suggests that Eq. (10a) does not put any restriction on $c_{12} + c_{21} - c_{11} - c_{22}$. Hence:

$$\text{supp}[P(C|T)] = \{C|c_{13} + c_{22} - c_{12} - c_{23} = \ln(2/9)\}.$$

**Remark 3.21.** In this case, $P(C|T)$ is not uniform over its support. According to Eq \((2)\), $P(C|T) \propto P(T_C|T)$ where $T_C \in L(T)$ and $K = e^{-C} \overset{\infty}{\preceq} T_C$. In particular, $P(C|T)$ has the highest probability on the hyperplane $\Phi^{-1}(T)$. If further constraints are added to the cost matrix $C$ such that there is a unique $C \in \Phi^{-1}(T)$ that meets such constraints, then one may obtain a maximum a posteriori estimation of $C$. This explains why the simulation for the general case \(^2\) in Section 4.4 of (Stuart and Wolfram, 2020) failed to identify a unique cost matrix: $P(C|T)$ is supported on an entire hyperplane. Maximum a posteriori estimations of $C$ were successfully obtained in both the graph and Toeplitz cases (Stuart and Wolfram, 2020).

4 Algorithm

Approximate inference via MCMC. Given a perfectly observed $T$ and $P_0(C)$, we propose a Markov Chain Monte Carlo (MCMC) method for sampling $P(C|T)$ (see Algorithm 1). At iteration $i$, denote the current cost $C$ by $C^{(i)}$, $K^{(i)} = e^{-C^{(i)}}$. We generate two vectors $D^r$ and $D^c$ with each element sampled from an exponential of a Gaussian distribution $N(0, \sigma^2)$. $K^{(i+1)}$ is then obtained by $K^{(i+1)} = \text{diag}(D^r) K^{(i)} \text{diag}(D^c)$. The acceptance ratio, $r = \frac{P(-\ln(K^{(i+1)}|T)}{P(-\ln(K^{(i)}|T)} \frac{p_0(C^{(i)}, \beta)}{p_0(C^{(i+1)}, \beta)}$, where $\beta$ is the hyperparameter of prior $P_0(C)$. Equality $(*),$ holds because our proposal preserves the cross-ratios, so we are guaranteed to stay on the manifold of support. Therefore, $P(T|C)$ is always 1 and is omitted (see Proposition 3.2). We accept or reject the move by comparing the acceptance ratio to an uniform random variable, $u$, which concludes a single step of the MCMC algorithm. We refer this method as MetroMC.

Metropolis-Hastings Monte Carlo method. We can avoid dealing with the parameter $\lambda$ by putting a prior on $K$. However, the MetroMC has long autocorrelation time for such priors. In each iteration,

**Algorithm 1: MetroMC**

Inputs: coupling $T$, variance $\sigma$, Prior parameters $\beta$, uniform random variable $u \in [0, 1]$;  
Initialization: $C^{(0)} = -\ln(K^{(0)})$; 
$K^{(0)} = T_{m \times n}$; 

for $i = 1$ to ITERMAX do 

$D^r = \text{exp}(N(0, \sigma \star I_m))$; 
$D^c = \text{exp}(N(0, \sigma \star I_n))$; 
$K^{(i+1)} \leftarrow \text{diag}(D^r) K^{(i)} \text{diag}(D^c)$; 
$C^{(i+1)} = -\ln(K^{(i+1)})$; 
$a \leftarrow P(C^{(i+1)}|T)/P(C^{(i)}|T)$; 
if $a > u$ then 

Accept $C^{(i+1)}$; 
else 

Reject $C^{(i+1)}$; 
$C^{(i+1)} \leftarrow C^{(i)}$

Output: $C$.

$K^{(i+1)}$ is obtained by multiplying random factors on $K^{(i)}$, whereas $C^{(i+1)}$ is obtained by adding random factors on $C^{(i)}$. In more detail, rows of $K^{(i)}$ are scaled by exponential of Gaussian variables a lot of time only a few of rows are at the same scale. After the columns are normalized, the rows that have large scale will have most of the weight in a column, which means we will sample a lot on the boundaries of the support. In order to improve the efficiency, we utilize the Metropolis-Hastings (Hastings, 1970) sampling method.

Now we propose an algorithm to sample from $P(K|T)$ with a prior on $K$. The sufficient condition for the ergodicity of the MCMC method is detailed balance, which is defined as $\pi(K)Q(K|K')A(K', K) = \pi(K')Q(K'|K)A(K, K')$, where $\pi(K)$ is the stationary distribution, $Q(K'|K)$ is the proposal transition probability from a state $K$ to $K’$ and $A(K’, K)$ is the acceptance probability which we choose

$$A(K’, K) = \min\left(1, \frac{P(K') Q(K|K')}{P(K) Q(K'|K)}\right).$$

We replace the acceptance probability $a$ in Alg. 1 with Eq. (11). We refer this algorithm as the MHMC.

The proposal transition probability $Q(K'|K)$ is defined as follows. In each iteration of MHMC, we draw a random number $\epsilon_i$ from a Gaussian distribution $N(0, \sigma^2)$, where $\sigma$ depends on the row sums of $K$. More precisely, $\sigma = \sigma_0 * s_i^\gamma + \delta$, where $\sigma_0$, $\gamma$, and $\delta$ are hyper-parameters for the model and $s_i = \sum_j K_{ij}$. $K' = \text{diag}(D^r) K$, where $D^r_i = \epsilon^{[0, \ldots, 0, \epsilon_i, 0, \ldots, 0]}$.

We scale a row at once, so in each step the acceptance ratio is reduced to $A(s_i'|s_i)$. To compute

\(^2\)Stuart and Wolfram (2020) requires the diagonal elements of $C$ be zeros in the general case.
it we need \( Q(s' | s_i) = F_N(x = \ln(s' / s_i), \mu, \sigma) \) and \( Q(s_i | s' ) = F_N(x = \ln(s_i / s'), \mu', \sigma') \), where \( F_N(x, \mu, \sigma) \) is the Gaussian probability density function.

5 Simulations on synthetic data

Visualizing subspaces of \( \text{supp}(P(K|T)) \). Fig 1(a-c) illustrates support of \( 2 \times 2 \) subspaces \( \text{supp}(P(K^*|T)) \), for a \( 4 \times 4 \) coupling \( T \) under prior \( P_2 \). In each plot, a \( T \) is sampled from a Dirichlet distribution \(^3\). Consider submatrix \( K_s = [k_{11}, k_{12}, k_{21}, k_{22}] \) of \( K \). According to section 3.1, both columns \( k_1, k_2 \) of \( K_s \) lie in a copy of \( \Sigma_2 \). Each colored triangle mark represents a uniformly sampled \( k_1 \), from \( \Sigma_2 \). A sampled \( k_1 \) determines a \( D_s = \text{diag}\{k_{11}, k_{12}, k_{21}, k_{22}\} \), which further determines a set \( \mathcal{K}_2 \) for \( k_2 \) shown by solid segment with the same color. Projection of \( W \) into the simplex corresponding to \( k_2 \), denoted by \( W_2 \), is shown by the dashed ray. Here, \( \mathcal{K}_2 \) is obtained by: \( \text{fix } k_1 = (k_{11}, k_{21})^T, \text{further sample } k_{31} \text{ and } k_{41} \text{ to form the first column of } \mathcal{K}_2 \). Then compute and plot the uniquely determined \( k_2 \). As predicted in section 3.1, \( \mathcal{K}_2 \) is only a subset of \( W_2 \). The sizes and locations of \( \mathcal{K}_2 \) in \( W_2 \) vary according to cross ratios of \( T \).

![Figure 1](image1.png)

**Figure 1:** Visualization of \( 2 \times 2 \) subspaces of \( \text{supp}(P(K|T)) \). In each plot, a \( T \) is sampled from a Dirichlet distribution. Each colored mark represents a uniformly sampled \( k_1 = (k_{11}, k_{21})^T \). Solid segment with the same color plots the corresponding set \( \mathcal{K}_2 \) for the second column, and the dashed ray plots \( W_2 \).

Visualizing \( \text{supp}(P(K|T)) \) with incomplete observations. Fig 2 illustrates the \( \text{supp}(P(K|T)) \) for a \( 3 \times 3 \) observation \( T \) with \( t_{31} \) missing under prior \( P_2 \). Columns of three sampled \( K \in \text{supp}(P(K|T)) \) are plotted in three colored copies \( \Delta_2 \) as shown. Here, three \( k_2 \) are sampled uniformly from the middle \( \Delta_2 \). The uniquely determined \( k_3 \) are shown in the right \( \Delta_2 \). The corresponding set for \( k_1 \) \( (K_1) \) is plotted in the left \( \Delta_2 \). \( K_1 \) is obtained by uniformly sample a thousand \( t_{31} \) from \([0, 10]\). Each \( t_{31} \) uniquely determines a \( k_1 \). As explained in Corollary 3.13, each \( K_1 \) forms a line segments. The slope of each line is determined by \( T \)'s cross ratios.

\(^3\)All observed coupling \( T \) in this section are presented in the supplement material.

![Figure 2](image2.png)

**Figure 2:** Visualization of \( \text{supp}(P(K|T)) \) for a \( 3 \times 3 \) observed \( T \) with \( t_{31} \) missing. Three sampled \( K \in \text{supp}(P(K|T)) \) are shown here with each column is plotted in a copy of \( \Delta_2 \) as shown. Colored dots in the middle \( \Delta_2 \) represents uniformly sampled \( k_2 \)'s. The uniquely determined \( k_3 \)'s are shown on the right, the set \( K_1 \) for the corresponding \( k_1 \)'s is shown on the left.

Visualizing \( \text{supp}(P(K|T)) \) through MHMC. Now we utilize MHMC to visualize \( \text{supp}(P(K|T)) \) and see the effect of cross-ratios. Under prior \( P_2 \) with \( \alpha = 1 \), Fig. 3 illustrates the posterior distributions \( P(K|T) \) of \( 3 \times 3 \) coupling \( T \).

We choose \( \alpha = 1 \) for the Dirichlet prior \( P_0(K) \), \( \sigma_0 = 0.5 \), \( \gamma = 3 \), and \( \delta = 1.0 \). We run for 10,000 burn-in steps and take 10,000 samples with lags of 100. The choices of these numbers are validated in Supplemental Material. Three columns \( \text{red, green, and blue colors, respectively} \) of each \( T \) are plotted on a one simplex in the left of Fig. 3. Locations of these points illustrate the relations between each column encoded by the cross ratios of \( T \). The right of Fig. 3 plots columns of sampled \( K \) from \( P(K|T) \) with corresponding \( T \) to the left. We clearly see how the cross-ratio of \( T \) affects \( P(K|T) \). If one column of \( T \) is close to one edge, then the posterior distribution of that column will be denser on that edge; on the other hand, if a column of \( T \) is located near the center, then the posterior is more evenly distributed on a simplex. E.g. in the top case, the effects on red and blue are exaggerated because the effect depends on relative position (and similarly for the red in the middle panel).

Bounded noise on observed plan. Given an observed noisy \( T \), we assume \( t_{11} \) was perturbed by a bounded noise \( \epsilon \) sampled uniformly from distribution \([-a, a]\) with \( a = 0.01 \). Assuming prior \( P_1 \) for \( P_0(C) \) with symmetric Dirichlet parameter equals to 1, we use MetroMC to sample \( P(C|T) \).

Notice that initializing \( K^{(0)} = T \) may cause the corresponding \( C^{(0)} \) lies outside the domain of \( P_0(C) \) as \( \sum_{ij} c_{ij}^{(0)} = \sum_{ij} -\ln(t_{ij}) \) is not guaranteed be 1. This will cause an extremely long burning time. In order fix this issue, we scale \( K^{(0)} \) by a constant when necessary. Scaling does not change the cross-ratios, hence it equivalent to a move within \( \Phi^{-1}(T) \).

For each iteration in the MCMC method we generate
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Figure 3: (Left.) The columns of three $T$ matrices plotted on the same simplex: $t_1, t_2, t_3$ are shown in Red, green for , blue. (Right.) Samples from posterior distribution $P(K|T)$. Each column of inferred matrices $K$ are plotted in a separate simplex, indicated by corresponding color.

$m + n - 1$ (rather than $m + n$) independent Gaussian random numbers with $\sigma = 0.02$ to construct vectors $D^T$ and $D^C$ satisfying $\sum_{i,j} \ln(d^T_i) + \ln(d^C_j) = 0$. The purpose of the above condition is to ensure that the newly generated sample lies on the support of the posterior. Otherwise, the acceptance rate will be extremely low. Because $C$ is a positive matrix, the MetroMC method rejects any sample of $K$ if $\max_{(i,j)} k_{i,j} \geq 1$.

Fig. 4 shows the MetroMC results on the inferred cost matrices $C$ for a given $3 \times 3$ coupling $T$. For each simulation we burn in 10,000 steps and take 100,000 samples with lags of 100. The acceptance rates range from 0.51 to 0.58. Noise level $\epsilon$ is indicated by colors. The Left panel plots components for a cross-ratio depend on $t_{11}$: $(c_{11} + c_{22})$ by solid curves and plots $(c_{21} + c_{12})$ by dashed curves. The Right panel plots components for a cross-ratio dose not depend on $t_{11}$: $(c_{12} + c_{23})$ by solid curves and plots $(c_{13} + c_{22})$ by dashed curves. All the curves are broadened using the Gaussian kernel density estimation (KDE) method with a bandwidth of 0.05. Fig. 4 illustrates that curves for $(c_{11} + c_{22})$ and $(c_{21} + c_{12})$ with a fixed $\epsilon$, i.e. curves in the same color, are in the same shape. The off-set of curves varies as the noisy level changes. Whereas off-set between curves for $c_{12} + c_{23}$ and $(c_{13} + c_{22})$ on the right panel remains a constant for any choice of $\epsilon$. This is consistent with our theoretical result in Prop. 3.17 that: $(c_{11} + c_{22}) - (c_{21} + c_{12}) = -\ln t_{11}^2 t_{22}^2$ depends on $\epsilon$ where as $(c_{12} + c_{23}) - (c_{13} + c_{22}) = -\ln t_{13}^2 t_{23}^2$ is a constant.

Gaussian noise on observed plan. We start with a Toeplitz ground truth cost function $C^g$ and obtain a OT plan, $T^g$, with $C^g$ and uniform $\mu, \nu$. A random Gaussian noise $\epsilon \sim \mathcal{N}(0, 0.004^2)$, about 4% of the average value of $T$, is added to $t_{12}^g$, and the corrupted plan $T = T^g + \epsilon$. We then infer the posterior distribution $P(C|T)$. We put a $P_1$ prior on $C$ with the hyperparameters follows toeplitz matrix format. Inference is done by first generating 10 random numbers $\epsilon^*_i \sim \mathcal{N}(0, 0.004^2)$ and apply the noise on $t_{12}$ to get $T^* = T + \epsilon^*_i$. Then, we utilize MHMC on every $T^*_i$ to obtain $P(C|T^*_i)$, and finally $P(C|T) \approx \sum_i P(C|T^*_i)$.

For the MHMC method, we burn in 10,000 steps and then take 10,000 samples with lags of 200 steps for each $P(C|T^*_i)$. For each step, we use the same sampling procedure as described in the bounded noise case but use a Gaussian standard deviation of 0.003. The acceptance rates are around 0.52-0.70.

The posterior distributions of each element of the inferred $C$ are shown in Fig. 5. The inferred distributions are close to the ground truth costs which are indicated by blue dashed lines. We demonstrate that our method successfully make accurate inferences using soft constraints, $P_0(C)$, with the results comparable to hard constraints imposed by (Stuart and Wolfram, 2020).

6 Conclusion

We have generalized prior treatments of IOT by defining and studying the underlying support manifold and associated inference problems. We provide general MCMC methods for inference over general priors on discrete costs and induced kernels. Simulations illustrate underlying geometric structure and show the feasibility and effectiveness of the inference.

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Supplementary for Probabilistic Inverse Optimal Transport

1 Proofs and Definitions for Section 3

Proposition 3.2. When \( T = T^* \), \( P(C|T) \) is supported on the intersection between \( \Phi^{-1}(T) \) and the domain of \( P_0(C) \), moreover, we have that \( P(C|T) = \frac{P_0(C)}{\int_{\Phi^{-1}(T)} P_0(C) dC} \).

Proof. When \( T = T^* \), Eq (2) and Eq (3) imply that: \( P(C|T) = \frac{P(T|C)P_0(C)}{P(T)} \), \( P(T) > 0 \) is the normalizing constant, so \( \text{Supp}[P(C|T)] = \text{Supp}[P(T|C)|\text{Domain}[P_0(C)] \). Note that \( P(T|C)P_0(C) = P_0(C) \) for \( C \in \Phi^{-1}(T) \), otherwise \( P(T|C)P_0(C) = 0 \). Hence the proposition holds.

Proposition 3.3. Let \( T \) be a non-negative optimal coupling of dimension \( m \times n \). \( C \in \Phi^{-1}(T) \) if and only if for every \( \epsilon > 0 \), there exist two positive diagonal matrices \( D^r = \text{diag}(d^r_1, \ldots, d^r_m) \) and \( D^c = \text{diag}(d^c_1, \ldots, d^c_n) \) such that: \( |D^r K D^c - T| < \epsilon \), where \( K = e^{-C} \) and \( |\cdot| \) is the \( L^1 \) norm. In particular, if \( T \) is a positive matrix, then \( C \in \Phi^{-1}(T) \) if and only if there exist positive diagonal matrices \( D^r, D^c \) such that \( D^r K D^c = T \), i.e.

\[
\Phi^{-1}(T) = \{ C | D^r \text{ and } D^c \text{ s.t. } K = D^r T D^c \}
\]

Proof. Let the row and column of marginals of \( T \) be \( \mu \) and \( \nu \). Then \( C \in \Phi^{-1}(T) \) if and only if \((\mu, \nu)\)-Sinkhorn scaling of \( K \) converges to \( T \) in \( L^1 \) norm (for finite matrices, convergence in all \( L^k \) norms are equivalent). Notice that a row (column) normalization step in the Sinkhorn scaling is equivalent to a left(right) matrix multiplication of a positive diagonal matrix. Indeed, let \( K_0 = K, r_0 = K_0 \mathbf{1}_m \) (vector for row sums of \( K_0 \)), \( D^r_0 = \text{diag}(\mu/\nu) \). Here \( r_0 \) represents element-wise division. Let \( K'_0 \) be the matrix obtained by row normalization of \( K_0 \) with respect to \( \mu \). Then \( K'_0 = D^r_0 K_0 \). Similarly, let \( K_1 = K'_{100} K_0 \) be the matrix obtained by column normalization of \( K'_0 \) with respect to \( \nu \). Then \( K_1 = K'_0 D^c_0 \), where \( D^c_0 = \text{diag}(\nu/\nu) \). Iteratively, we have \( K_s = \Pi^s_1 D^r_s K_0 \Pi^s_1 D^c_s \).

The only if direction \([C \in \Phi^{-1}(T) \implies \text{existence of } D^r \text{ and } D^c \text{ for any } \epsilon] \): \( C \in \Phi^{-1}(T) \implies (\mu, \nu)\)-Sinkhorn scaling of \( K \) converges to \( T \), for any \( \epsilon > 0 \), there exists \( N > 0 \) such that for any \( s > N \), \( |K_s - T| < \epsilon \), where \( K_s = \Pi^s_1 D^r_s K \Pi^s_1 D^c_s \). Let \( D^r = \Pi^s_1 D^r_s \), \( D^c = \Pi^s_1 D^c_s \), the only if direction is complete.

The if direction \([\text{existence of } D^r \text{ and } D^c \text{ for any } \epsilon \implies C \in \Phi^{-1}(T)] \): Let the limit of \((\mu, \nu)\)-Sinkhorn scaling on \( K \) be \( K^* \). Hence \( K^* \) and \( T \) have the same marginals and pattern. According to Lemma A.3 of (Wang et al., 2019), \( K^* \) and \( T \) are diagonally equivalent. Further by Proposition 1 of (Pretzel, 1980) \( K^* = T \).

In particular, when \( T \) is a positive matrix, \( K \) must also be a positive matrix. Then \( K^* \) and \( T \) have the same pattern. \( T = \lim_{s \to \infty} \Pi^s_1 D^r_s K \Pi^s_1 D^c_s \) implies that \( \lim_{s \to \infty} \Pi^s_1 D^r_s \) and \( \lim_{s \to \infty} \Pi^s_1 D^c_s \) exist. Hence the claim. (Rothblum and Schneider, 1989; Idel, 2016)

Lemma 3.5. For two positive matrices \( A, B \), \( A \preceq \preceq B \) if and only if there exist positive diagonal matrices \( D^r \) and \( D^c \) such that \( A = D^r B D^c \).

Proof. The if direction: \( A = D^r B D^c \implies \frac{a_{ik} a_{jl}}{a_{il} a_{jk}} = \frac{d^r_i b_{ik} d^c_k \cdot d^r_j b_{jl} d^c_l}{d^r_i b_{il} d^c_l \cdot d^r_j b_{jk} d^c_k} = \frac{b_{ik} b_{jl}}{b_{il} b_{jk}} \implies A \preceq \preceq B \).

The only if direction: Let the dimension of \( A, B \) be \( m \times n \), we will prove by induction on \( m + n \).

Step 1. Assume the dimension of \( A, B \) is \( 2 \times 2 \). Let the marginal of \( A \) be \( \mu_A \) and \( \nu_A \), and \( B^* = \Phi(B, \mu_A, \nu_A) \). Then \( A \) and \( B^* \) have the same marginals and cross ratios, which put four same independent constraints on elements of \( A \) and \( B \), hence \( A = B^* = D^r B D^c \) for some \( D^r, D^c \). step 2. Assume the statement holds for \( m + n < N \).
Now assume that $m + n = N$. Denote the submatrices of $A$ and $B$ consisted by their first $n - 1$ by $A_1$ and $B_1$. $A \sim B \iff A_1 \sim B_1$. By the inductive assumption, there exist diagonal matrices $D^t_1$ and $D^c_1$ such that $A_1 = D^t_1 B_1 D^c_1$. Further $\alpha^t_{i,j}\alpha^c_{i,n} = \lambda^t_{i,j}\lambda^c_{i,n}b_{in}$ holds for any $i \in \{1, \ldots, m\}$ imply that there exists an $d > 0$ such that $a_n = d \cdot b_n$. Let $D^t = D^t_1$, $D^c = \text{diag} D^c_1, d$, we have $A = D^t BD^c$ holds. Hence the only if direction is completed.

**Theorem 3.6.** Let $T$ be an observed positive optimal coupling of dimension $m \times n$. Then $\Phi^{-1}(T)$ is a hyperplane of dimension $m + n - 1$ embedded in $(\mathbb{R}^*)^{m \times n}$, which consists all the cost matrices that of the form:

$$
\Phi^{-1}(T) = \{ C \in (\mathbb{R}^*)^{m \times n} | K = e^{-C} \sim T \}.
$$

**Proof.** Combining Proposition 3.3 and Lemma 3.5, we have Eq. (1) holds. Hence $\Phi^{-1}(T)$ contains all the matrices $C$ satisfying the following set of equations: $k_{ik}k_{jl} = t_{ik}t_{jl}$ for any $i, j \in \{1, \ldots, m\}$ and $k, l \in \{1, \ldots, n\}$, where $K = e^{-C}$, i.e. $k_{ik} = e^{-c_{ik}}$. Thus $\Phi^{-1}(T)$ is the solution set of the system of linear equations:

$$
c_{il} + c_{jk} - c_{ik} - c_{jl} = \ln(t_{ik}t_{jl}) - \ln(t_{il}t_{jk})
$$

Further Remark 3.9 shows that there are only $(m - 1)(n - 1)$ independent equations in the system (2). Hence $\Phi^{-1}(T)$ is a hyperplane of dimension $mn - (m - 1)(n - 1) = m + n - 1$.

**Corollary 3.11.** Under prior $P_2$, the projection of $\text{supp}[P(K|T)]$ onto each column is a $(m - 1)$-dimensional manifold that is homeomorphic to the simplex $\Delta_{m-1}$.

**Proof.** According to prior $P_2$, for any $K \in \text{supp}[P(K|T)]$, each column of $K$ sums to 1. Hence the projection of $\text{supp}[P(K|T)]$ onto any $j$-th column is embedded in the simplex $\Delta_{m-1}$. To show ‘homeomorphic’, we only need to show that for each $v \in \Delta_{m-1}$, there exists a $K \in \text{supp}[P(K|T)]$ such that $k_j = v$. As discussed in Remark 3.10, let $D'' = \text{diag}(v, t_j)$, $K' = \text{Col}(D''T)$. It’s easy to check that $K' \in \text{supp}[P(K|T)]$, and $k'_j = v$. Hence the corollary holds.

**Proposition 3.12.** $C_{s} \in \text{supp}[P(C_{s}|T)]$ if and only if there exists positive diagonal matrices $D^r_{1}, D^r_{2}$ such that $K_s = D^r_{1}T_s D^r_{2}$ and the system of equations shown below have a set positive solution for $\{x_1, \ldots, x_{m-s}\}$.

$$
(x_1, \ldots, x_{m-s}) \text{\text{Tr}}_{m-s} = (1/d^r_1, \ldots, 1/d^r_{s}) - 1_s D^r_s T_s
$$

**Proof.** The if direction: Let $(x_1, \ldots, x_{m-s})$ be a positive solution of Eq. (3), let $D'' = \text{diag}(D''_s, x_1, \ldots, x_{m-s})$ be an extension of $D''$. Denote the column sum of $D''T$ by $v'$. Then Eq. (3) implies that $v'_i = d^r_i$ for $i \in \{1, \ldots, s\}$. Let $D^c = \text{diag}(D^c_1, t_{s+1}, \ldots, t_n)$. It is clear that $K' = D''TD''^c \in \text{supp}[P(K|T)]$, and $K_s$ is $K'$’s submatrix corresponding to $X_s \times Y_s$.

The only if direction: for $C_s \in \text{supp}[P(C_{s}|T)]$, let $K_s = e^{-C_s}$ be the submatrix of $K' \in \text{textsupp}[P(K|T)]$.

Then there exist $D'\nu$, $D'\nu^c$ such that $K', D''TD''^c \in \text{supp}[P(K|T)]$. Let the corresponding submatrices of $D'$, $D'\nu^c$ be $D'_s, D''_s$. We have $K_s = D'_s T_s D''_s$. It is easy to verify that $(d'_{s+1}, \ldots, d_n)$ is a positive solution for Eq. (3). Hence the proof is completed.

**Corollary 3.13.** Under prior $P_2$, $K_1$ is a line segment in $\Delta_{m-1}$ that can be parameterized as: $K_1 = \{(d_{1t_1}, \ldots, d_{m_t} t_{m}) \sum_{t=1}^{m} d_{1t1} t_{m} \in (0, \infty)\}$.

**Proof.** Corollary 3.11 implies that $K_1 \subset \Delta_{m-1}$. Further Remark 3.10 implies that for each choice of $t_{m} > 1$, a known $k_t$ uniquely determines a point in form of $(d_{1t1}, \ldots, d_{m_t} t_{m}) \sum_{t=1}^{m} d_{1t1}$ in $K_1$. Hence the corollary holds.

**Corollary 3.14.** Let $T_1, T_2$ be two positive matrices of dimension $m \times n$. The hyperplanes $\Phi^{-1}(T_1)$ and $\Phi^{-1}(T_2)$, have the same normal direction. In particular, if $T_1 \sim T_2$ then $\Phi^{-1}(T_1) = \Phi^{-1}(T_2)$. Otherwise $\Phi^{-1}(T_1)$ is parallel to $\Phi^{-1}(T_2)$.

**Proof.** According to the proof of Theorem 3.6 above, both $\Phi^{-1}(T_1)$ and $\Phi^{-1}(T_2)$ are defined by system of equations in form of Eq. (2). In particular, they have the same coefficients, only the constants on the right side of the equations are different. Hence, $\Phi^{-1}(T_1)$ and $\Phi^{-1}(T_2)$, have the same normal direction.
Proposition 3.17. For a coupling $T$, assume uniform observation noise on $t_{11}$ with bounded size $a$,

$$\text{supp}[P(C|T)] = \cup_{T' \in \mathbb{B}_a(T)} \Phi^{-1}(T'),$$

where $\mathbb{B}_a(T)$ is the set of matrices $T'$ of the same dimension as $T$ with the property that: $t_{11}' > 0$, $|t_{11}' - t_{11}| \leq a$ and $t_{ij}' = t_{ij}$ for other $i, j$. Moreover, $\Phi^{-1}(T')$ can be expressed as intersection of two hyperplanes (may be in different dimensions): one with equation: $c_{11} + c_{22} - c_{21} - c_{12} = -\ln t_{11}'t_{22}/t_{12}'t_{21}'$, and the other equation does not depend on the value of $t_{11}'$. Assume the angle between these two hyperplanes is $\theta$. Then $d(\Phi^{-1}(T_1), \Phi^{-1}(T_2)) \leq \ln t_{11}'t_{22}/t_{12}'t_{21}' / \sin \theta$

Proof. With bounded noise on $t_{11}$, the domain for $t_{11}'$ is $[t_{11} - a, t_{11} + a] \cap \{t_{11}' > 0\}$. Hence Eq. (4) holds. $\Phi^{-1}(T')$ is defined by the cross ratios of $T$ as shown in Eq. (2). Using cross-ratio basis say $B = \{r_{m,j,k}(T')|j = 1, \ldots, m-1, k = 1, \ldots, n-1\}$, Eq. 2 can be simplified into a system with only independent $(m-1)(n-1)$, where only the equation defined by $r_{m11}(T')$ involves $t_{11}'$, the other equations can be combined into one equation by substitutions. Each of these two equations determines a hyperplane, hence $\Phi^{-1}(T')$ can be expressed as the intersection of two hyperplanes. Moreover, let the defining hyperplanes for $T^1, T^2 \in \mathbb{B}_a(T)$ be $\{H_1^1, H_1^2\}$ and $\{H_2^1, H_2^2\}$ respectively, where $H_1^i$ is the one defined by $c_{11} + c_{mn} - c_{1m} - c_{m1} = \ln(t_{11}'t_{mn}) - \ln(t_{11}'t_{mn})$, where $i = 1, 2$. Then the Euclidean distance between $H_1^1, H_1^2$ is $d(H_1^1, H_1^2) = |\ln t_{11}' - \ln t_{11}'| \leq |\ln(t_{11} + a) - \ln(t_{11} - a)|$. Notice that $H_2^1 = H_2^2$. So the distance between $\Phi^{-1}(T^1), \Phi^{-1}(T^2)$ is bounded by $(\ln(t_{11} + a) - \ln(t_{11} - a))/\sin \theta$.

Proposition 3.19. Let $T$ be an observed coupling of dimension $m \times n$ with Gaussian noise on $t_{11}$. Further, let $B$ be a basis for cross ratios of $m \times n$ matrices, that contains only one cross ratio depending on $t_{11}$. Eliminate the cross ratio depending on $t_{11}$ in $B$, denote the new set by $B^-$. Then:

$$\text{supp}[P(C|T)] = \{C|r(K) = r(T) \text{ for } r \in B^-\}$$

In particular, $P(C|T)$ is supported on a hyperplane that is one dimensional higher than $P(C|T')$ for any $T' \in L(T)$.

Proof. Since the domain for $\epsilon \sim \mathcal{N}(0, \sigma^2)$ is $(-\infty, \infty)$, hence the domain for possible $t_{11}^*$ is $(0, \infty)$. Thus the observation $T$ essentially put no constraint on the cross ratio of $T^*$ depends on $t_{11}$. Hence $\text{supp}[P(C|T)] = \{C|r(K) = r(T) \text{ for } r \in B^-\}$. As only one equation was eliminated, so $P(C|T)$ is supported on a hyperplane that is one dimensional higher than $P(C|T')$ for any $T' \in L(T)$.

2 Additional details of experiments

2.1 Auto-correlation function.

To monitor the efficiency of our MC methods, we compute the auto-correlation function during the burn-in phase and choose the lags accordingly.

The auto-correlation function is defined as

$$R(t) = \frac{1}{(N-t)\sigma^2} \sum_{i=1}^{N-t} \sum_{i,j}(K_{i,j}^{(t)} - \bar{K}_{i,j}) \cdot (K_{i,j}^{(t+t)} - \bar{K}_{i,j}),$$

where $N$ is the total number of samples generated, $(i,j)$ runs over all indices of the matrices $K$, $\bar{K}$ is the mean averaging over all the samples, and $\sigma^2 = \sum_{i,j} \sigma_{K,i,j}$ is the variance.

2.2 Re-normalization of $T$ for MetroMC over prior $P_1$.

For using this method, not every random $T$ satisfies the condition such that $C^{(0)} = -\ln(K^{(0)}) = -\ln(T)$ lies on the support of the posterior, therefore, we need to re-normalize $T$ so that $C^{(0)} - \ln[T/F(T)]$ is on the support. $F(T)$ is defined as

$$F(T) = \exp \left(1 + \sum_{i=1}^{m} \sum_{j=1}^{n} \log(T_{i,j}) \right).$$

(6)
2.3 MHMC on uniform matrix.

In this section, we validate our MHMC algorithm by apply it to an uniform $T$, i.e $T_{m,n} = 1/m$ under prior $P_2$. The cross-ratios of $T$ are all 1 and stay the same for all inferred sample $K^{(i)}$. Thus, each $K^{(i)}$ has same copies of $n$ columns. We compare posterior sampled by MHMC to a $m$-dimensional uniform symmetric Dirichlet distribution generated by the SciPy package (Virtanen et al., 2020).

We perform our MHMC algorithm on a $3 \times 3$ uniform matrix with prior $P_2$ and the Dirichlet concentration parameter $\alpha$ are the same for every element. We choose $\alpha = 1$ for the Dirichlet parameter, $\sigma_0 = 0.5$, $\gamma = 3$, and $\delta = 1.0$. We run for 10,000 burn-in steps and take 10,000 samples with lags of 100. The result is shown in Fig. S1. We choose the lag by observing the auto-correlation function in the burn in, where the chain becomes uncorrelated after $\sim 100$ steps. Also, the running averages of the row sums are stable at taking 10,000 samples, which means 10,000 samples can effectively represent the posterior distribution.

The posterior distribution (Shown in top right of Fig. S1.) is compared to the distribution $P(K|T)$ of three-dimensional vectors generated by Dirichlet vector sampler (Virtanen et al., 2020) with symmetric $\alpha = 1$ in top left of Fig. S1. The results are comparable, which suggests that our MHMC method is able to generate distributions which well represent the support of the posterior distributions.

Figure S1: (Top left.) The distributions of each component of three-dimensional Dirichlet vectors with symmetric $\alpha = 1$ generated using SciPy package. (Top right.) The distributions of each component of the first column of $P(K|T)$ sampled by the MHMC method. (Lower left.) The auto-correlation function of the MHMC simulation. The black dashed lines indicate the range $[-1/e, 1/e]$. (Lower right.) The running average of the row sums of the MHMC simulation.

2.4 MetroMC on uniform matrix.

We test MetroMC on 3x3 uniform $T$, where $T_{i,j} = 1/(m \times n)$, and assume the prior $P_1$ is put on $C$. We take $K^{(0)} = T/F(T)$. For each MC iteration we sample $m+n-1$ Gaussian random numbers with standard deviations
of 0.02 for the diagonal matrices $D^r$ and $D^c$ satisfying the condition

$$\sum_{i,j} \ln(d^r_i) + \ln(d^c_j) = 0.$$  \hspace{1cm} (7)

We burn in 10,000 steps and take 100,000 samples with 100 lags in between. The Gaussian Kernel density estimation (KDE) of each component of $P(C|T)$ is demonstrated in Fig. S2. We use bandwidths of 0.05 for all the Gaussian KDE in this article. There are a few notable features. First, we assume a Dirichlet prior on the whole $C$ matrix, the distributions will be smaller at large values because each large value will suppress the value of the other elements. Second, since we have cross-ratio $= 1$ everywhere in $T$ and prior $P_1$ on $C$, there will not be a single element with value close to one. Otherwise, the cross-ratio involving that element could never be 1 anymore. Also, for the same reason all distributions should be similar.

Figure S2: (Top.) The distribution of each matrix element of $P(C|T)$ with a uniform $T$ and a prior $P_1$ over $C$ matrix. (Bottom left.) The autocorrelation function of the simulation. (Bottom right.) The running averages of the row sums.
2.5 Supporting plots for the MetroMC method on noisy T.

In this section, we provide data for diagnostics of the MetroMC simulations on the noise models in section 5 of the main text.

**Bounded noise on observed plan.** The autocorrelation function and the running averages of row sums of the samples for each noise are plotted in Fig. S3. In the simulation we set 100 for the lags by observing that the chains become uncorrelated after \( \sim 100 \) steps for all cases. We take 100,000 samples in total for all cases since the running averages are stable at (or before) 100,000 MC steps, which means the samples reaches a stationary distribution.

![Plots](image.png)

**Figure S3:** MC diagnostics for the Bounded noise example. (a.) The autocorrelation funciton for all noises. (b.)-(f.) The running averages of row sums of the samples for noises -0.01, -0.005, 0.0, 0.005, and 0.01 added to \( t_{11} \), respectively.

**Gaussian noise on observed plan.** The autocorrelation function and the running averages of row sums of the samples for the 10 Gaussian noises are plotted in Fig. S4. We set 200 for the lags since the chains become uncorrelated after \( \sim 180 \) steps for all cases. 10,000 samples are taken for all cases since the running averages of the row sums are stable at 10,000 MC steps.
Figure S4: MC diagnostics for the Bounded noise example. (a.) The autocorrelation function for all noises. (b.)-(k.) The running averages of row sums of the samples for the 10 random Gaussian noises added to $t_{12}$.

### 2.6 Matrices.

We list the matrices used in section 5: **Simulations on synthetic data** below.

The three $T$ matrices in Fig. 1 are

$$T_a = \begin{bmatrix} 0.3096 & 0.3785 & 0.0544 & 0.2575 \\ 0.2522 & 0.3203 & 0.1860 & 0.2415 \\ 0.4318 & 0.1433 & 0.4196 & 0.0053 \\ 0.0064 & 0.1579 & 0.3400 & 0.4957 \end{bmatrix},$$

$$T_b = \begin{bmatrix} 0.2532 & 0.4143 & 0.2894 & 0.0431 \\ 0.1925 & 0.0548 & 0.0958 & 0.6569 \\ 0.4459 & 0.0905 & 0.3480 & 0.1156 \\ 0.1083 & 0.4404 & 0.2669 & 0.1844 \end{bmatrix},$$
The matrix $T_c$ in Fig. 2 is

$$T_c = \begin{bmatrix}
0.4790 & 0.0994 & 0.0838 & 0.3378 \\
0.1343 & 0.1514 & 0.1920 & 0.5224 \\
0.1678 & 0.6182 & 0.1963 & 0.0177 \\
0.2189 & 0.1310 & 0.5279 & 0.1222 \\
\end{bmatrix}.$$  

The matrix $T$ in Fig. 2 is

$$T = \begin{bmatrix}
0.4583 & 0.2297 & 0.2633 \\
0.4631 & 0.4785 & 0.2755 \\
0.0785 & 0.2919 & 0.4611 \\
\end{bmatrix}.$$  

The matrices $T$ in Fig. 3 are

$$T_1 = \begin{bmatrix}
0.1104 & 0.0684 & 0.1545 \\
0.0505 & 0.2401 & 0.0428 \\
0.1725 & 0.0249 & 0.1360 \\
\end{bmatrix},$$

$$T_2 = \begin{bmatrix}
0.0950 & 0.1100 & 0.1283 \\
0.1155 & 0.0343 & 0.1835 \\
0.1228 & 0.1890 & 0.0215 \\
\end{bmatrix},$$

$$T_3 = \begin{bmatrix}
0.1053 & 0.1193 & 0.1088 \\
0.2148 & 0.0090 & 0.1096 \\
0.0133 & 0.2051 & 0.1150 \\
\end{bmatrix}.$$  

The matrix $T$ for the bounded noise case is

$$T = \begin{bmatrix}
0.1067 & 0.1141 & 0.1125 \\
0.1175 & 0.1052 & 0.1106 \\
0.1092 & 0.1139 & 0.1102 \\
\end{bmatrix}.$$  

The ground truth $C^g$ in the Gaussian noise example is

$$C^g = \begin{bmatrix}
0.2604 & 0.0521 & 0.0104 \\
0.0208 & 0.2604 & 0.0521 \\
0.0625 & 0.0208 & 0.2604 \\
\end{bmatrix},$$  

and the hyperparameter matrix for the prior is

$$\alpha = \begin{bmatrix}
25.0 & 5.0 & 1.9 \\
3.0 & 25.0 & 5.0 \\
6.0 & 3.0 & 25.0 \\
\end{bmatrix}.$$  

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