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# Generalized Belief Transport: Supplementary Material

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## 1 Additional Materials

**Cooperative Communication.** *Cooperative communication* formalizes a single problem comprised of interactions between two processes: teaching and learning. The teacher and learner have beliefs about hypotheses, which are represented as probability distributions. The process of teaching is to select data that move the learner’s beliefs from some initial state, to a final desired state. The process of learning is then, given the data selected by the teacher, infer the beliefs of the teacher. The teacher’s selection and learner’s inference incur costs. The agents minimize the cost to achieve their goals. Communication is successful when the learner’s belief, given the teacher’s data, is moved to the target distribution.

Formally, denote the common ground between agents: the shared priors on  $\mathcal{H}$  and  $\mathcal{D}$  by  $\mathbb{P}(h)$  and  $\mathbb{P}(d)$ , the shared initial matrix over  $\mathcal{D}$  and  $\mathcal{H}$  by  $M$  of size  $|\mathcal{D}| \times |\mathcal{H}|$ . In general, up to normalization,  $M$  is simply a non-negative matrix which also specifies the consistency between data and hypotheses<sup>1</sup>

In cooperative communication, a learner’s goal is to minimize the cost of transforming the observed data distribution  $\mathbb{P}(\mathcal{D})$  to the shared prior over hypotheses  $\mathbb{P}(\mathcal{H})$ . A learner’s cost matrix  $C^L = (C_{ij}^L)_{|\mathcal{M}| \times |\mathcal{H}|}$  is defined as  $C_{ij}^L = -\log M$ . A *learning plan* is a joint distribution  $L = (L_{ij})$ , where  $L_{ij} = P_L(d_i, h_j)$  represents the probability of the learner inferring  $h_j$  given  $d_i$ . It is proved in [Wang et al., 2019] that:

**Proposition S.1.** *Optimal cooperative communication plans,  $L$ , is the EOT plan with cost  $C^L$  and marginals being  $\eta = \mathbb{P}(d)$  and  $\theta = \mathbb{P}(h)$ .*

## 2 Proofs

**Proposition 1.** *The UOT problem with cost matrix  $C$ , marginals  $\theta, \eta$  and parameters  $\epsilon = (\epsilon_P, \epsilon_\eta, \epsilon_\theta)$  generates the same UOT plan as the UOT problem with  $tC$ ,  $\theta, \eta$ ,  $t\epsilon = (t\epsilon_P, t\epsilon_\eta, t\epsilon_\theta)$  for any  $t \in (0, \infty)$ .*

*Proof.* Consider that the UOT problem solution is

$$P^\epsilon(C, \eta, \theta) = \arg \min_{P \in (\mathbb{R}_{\geq 0})^{n \times m}} \{ \langle C, P \rangle - \epsilon_P H(P) + \epsilon_\eta \text{KL}(P\mathbf{1}|\eta) + \epsilon_\theta \text{KL}(P^T\mathbf{1}|\theta) \}. \quad (1)$$

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<sup>1</sup>Data,  $d_i$ , are consistent with a hypothesis,  $h_j$ , when  $M_{ij} > 0$ .

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**Algorithm 1** Unbalanced Sinkhorn Scaling
 

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**input:**  $C, \theta, \eta, \epsilon = (\epsilon_P, \epsilon_\eta, \epsilon_\theta)$ ,  $N$  stopping condition  $\omega$   
**initialize:**  $\mathbf{K} = \exp(-\epsilon_P C)$ ,  $\mathbf{v}^{(0)} = \mathbf{1}_m$   
**while**  $k < N$  **and not**  $\omega$  **do**  
    $\mathbf{u}^{(k)} \leftarrow \left(\frac{\eta}{K\mathbf{v}^{(k-1)}}\right)^{\frac{\epsilon_\eta}{\epsilon_\eta + \epsilon_P}}$ ,  $\mathbf{v}^{(k)} \leftarrow \left(\frac{\theta}{K^T\mathbf{u}^{(k)}}\right)^{\frac{\epsilon_\theta}{\epsilon_\theta + \epsilon_P}}$   
**end while**  
**output:**  $M = \text{diag}(u)K\text{diag}(v)$

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where the objective function is linear on  $C$  and  $\epsilon$ .

$$\begin{aligned}
 P^{t\epsilon}(tC, \eta, \theta) &= \arg \min_{P \in (\mathbb{R}_{\geq 0})^{n \times m}} \{ \langle tC, P \rangle - t\epsilon_P H(P) + t\epsilon_\eta \text{KL}(P\mathbf{1}|\eta) + t\epsilon_\theta \text{KL}(P^T\mathbf{1}|\theta) \} \\
 &= \arg \min_{P \in (\mathbb{R}_{\geq 0})^{n \times m}} t \cdot \{ \langle C, P \rangle - \epsilon_P H(P) + \epsilon_\eta \text{KL}(P\mathbf{1}|\eta) + \epsilon_\theta \text{KL}(P^T\mathbf{1}|\theta) \} \\
 &= P^\epsilon(C, \eta, \theta).
 \end{aligned} \tag{2}$$

□

**Proposition 2.** *The UOT plan  $P$  in Equation 1, as a function of  $\epsilon$ , is continuous in  $(0, \infty) \times [0, \infty)^2$ . Furthermore,  $P$  is differentiable with respect to  $\epsilon$  in the interior.*

*Proof.* For simplicity, in this proof, for a vector  $v$ , we use both  $v_i$  and  $v(i)$  to represent a component of  $v$ .

By definition, the UOT plan  $P$  minimizes the objective function  $\Omega(P; \epsilon) = \langle C, P \rangle - \epsilon_P H(P) + \epsilon_\eta \text{KL}(P\mathbf{1}|\eta) + \epsilon_\theta \text{KL}(P^T\mathbf{1}|\theta)$ . Since  $\Omega$  is a strict convex function on  $P$ , there is only one minimal  $P$ . So the UOT plan  $P$  is the solution to  $\nabla_P \Omega = 0$ . From a direct calculation,

$$(\nabla_P \Omega)_{ij} = C_{ij} + \epsilon_P \ln P_{ij} + \epsilon_\eta (\ln(\sum_{k=1}^m P_{ik}) - \ln \eta(i)) + \epsilon_\theta (\ln(\sum_{k=1}^n P_{kj}) - \ln \theta(j))$$

and

$$(\nabla_P^2 \Omega)_{ijkl} = \frac{\epsilon_P \delta_{ik} \delta_{jl}}{P_{ij}} + \frac{\epsilon_\eta \delta_{ik}}{\sum_{t=1}^m P_{it}} + \frac{\epsilon_\theta \delta_{jl}}{\sum_{t=1}^n P_{tj}}.$$

As we assume that  $P_{ij} > 0$  for all  $i, j$ , all the terms above are well-defined. Besides,  $\nabla_P \Omega$  is  $C^1$  on  $\eta, \theta$  and  $\epsilon$ . Therefore, we can show  $P^\epsilon(C, \eta, \theta)$  is continuous not only on  $\epsilon$  but also on  $\eta$  and  $\theta$  after checking Hessian. From implicit function theorem, if we show the above Hessian is invertible for  $\epsilon_P > 0$ , then the results of the proposition are true. Equivalently, it suffices to show that  $\det H \neq 0$  where matrix  $H$  is the flattened  $\nabla_P^2 \Omega$  by mapping  $(i, j, k, l) \mapsto (im + j, km + l)$ .

**Invertibility of  $H$ .** Let  $\mathbf{r}$  be the vector of reciprocals of row sums of  $P$ , i.e.,  $r_i = 1 / (\sum_j P_{ij})$ , and similarly, let  $\mathbf{c}$  be the vector of reciprocals of column sums of  $P$ , i.e.,  $c_j = 1 / (\sum_i P_{ij})$ . Then

$$(\nabla_P^2 \Omega)_{ijkl} = \frac{\epsilon_P \delta_{ik} \delta_{jl}}{P_{ij}} + \epsilon_\eta \delta_{ik} r_i + \epsilon_\theta \delta_{jl} c_j.$$

Let  $\phi$  be the map  $(i, j) \mapsto (im + j)$ , then  $\phi$  induces a reshaping of  $P$  to a vector of size  $mn$ , denoted by  $P^\phi$ . When there is no ambiguity, we may omit the  $\phi$  superscript.

Further define  $p^\phi$  as a vector of dimension  $mn$  where  $p_k^\phi = \epsilon_P / P_k^\phi$ . By definition,  $H^\phi = \epsilon_P (\text{diag}(p^\phi)) + \epsilon_\eta \mathbb{1}_m \otimes (\text{diag}(\mathbf{r})) + \epsilon_\theta (\text{diag}(\mathbf{c})) \otimes \mathbb{1}_n$  where  $\mathbb{1}_k$  is the  $k \times k$  matrix of ones, and  $A \otimes B$  is Kronecker product (tensor product of matrices). Decompose  $H = D + G$  where  $D = \epsilon_P (\text{diag}(p^\phi))$  and  $G = \epsilon_\eta \mathbb{1}_m \otimes (\text{diag}(\mathbf{r})) + \epsilon_\theta (\text{diag}(\mathbf{c})) \otimes \mathbb{1}_n$ .

From now on, we may use  $P$ -row,  $P$ -column to represent  $i, j$  style indices, and  $G$ -row,  $G$ -column or simply row/column to represent those of  $G$ , or the ones in range  $[1, mn]$ .  $D$  is diagonal, and  $\det G = 0$ . Furthermore,

(\*) any row or column of  $G$  with index  $k$  can be represented by an entry position  $(i, j)$  of  $P$  by inverse of  $\phi$ , and any rows of indices  $k_1, k_2, k_3, k_4$  corresponding to  $(i_1, j_1), (i_1, j_2), (i_2, j_1), (i_2, j_2)$  (i.e., determined as intersections of two  $P$ -rows and two  $P$ -columns) is linearly dependent:  $G_{(k_1, \cdot)} + G_{(k_4, \cdot)} - G_{(k_2, \cdot)} - G_{(k_3, \cdot)} = \mathbf{0}$ , we denote this property as (\*).

Structure of  $\det H$ : Let  $D = \text{diag}(p_1, p_2, \dots, p_{mn})$ , then  $\det H$  is a polynomial on  $p_k$ 's with constant term 0. Each term in  $\det H$  is of form  $f(\mathcal{I}) \left( \prod_{k \notin \mathcal{I}} p_k \right)$  for each subset  $\mathcal{I} \subseteq \{1, 2, \dots, mn\}$ , and the coefficient  $f(\mathcal{I}) = \det G_{(\mathcal{I}, \mathcal{I})}$  where  $G_{(\mathcal{I}, \mathcal{I})}$  is the submatrix with lines of indices not in  $\mathcal{I}$ , i.e., the entries of  $G_{(\mathcal{I}, \mathcal{I})}$  are of the form  $G_{ij}$  with  $i \in \mathcal{I}$  and  $j \in \mathcal{I}$ .

Next we show that  $f(\mathcal{I})$  is nonnegative for all  $\mathcal{I}$ , then with  $p_k > 0$  for all  $k$ , we can conclude that  $\det H > 0$ . Since  $\mathcal{I} \subseteq \{1, 2, \dots, mn\}$ ,  $\phi^{-1}(\mathcal{I}) \subseteq \{1, 2, \dots, n\} \times \{1, 2, \dots, m\}$ , and  $\phi$  is a bijection, we may not distinguish  $\mathcal{I}$  from  $\phi^{-1}(\mathcal{I})$ , in order to make the statement neater.

**1. [Operation-(\*) on  $\mathcal{I}$ ]:** We want to investigate the operations on  $\mathcal{I}$  producing a subset  $\mathcal{J}$  such that  $f(\mathcal{I}) = f(\mathcal{J})$ . By the properties of determinant, (\*) induces one operation: when  $\mathcal{I}$  containing 4 integer pairs which can form the vertices of a rectangle,  $f(\mathcal{I}) = 0$ . Moreover, for any  $k_1, k_2, k_3, k_4$  such indices in (\*), we can generate row  $G_{(k_4, \cdot)}$  by  $G_{(k_4, \cdot)} = G_{(k_2, \cdot)} + G_{(k_3, \cdot)} - G_{(k_1, \cdot)}$ , then if  $\{k_1, k_2, k_3\} \subseteq \mathcal{I}$ , we can build  $G_{(k_4, \cdot)}$  on any  $G_{(k_i, \cdot)}$ , thus the determinant  $\det G_{(\mathcal{I}, \mathcal{I})}^{row} = \pm \det G_{(\mathcal{I}, \mathcal{I})}$  (positive for  $k_2$  and  $k_3$ , negative for  $k_1$ ). Similarly, if we follow the same operation on columns, we have  $\det G_{(\mathcal{I}, \mathcal{I})}^{col} = \pm \det G_{(\mathcal{I}, \mathcal{I})}$ . And when doing both,  $\det G_{(\mathcal{I}, \mathcal{I})}^{col-row} = \det G_{(\mathcal{I}, \mathcal{I})}$ . Therefore, we know that if  $k_1, k_2, k_3 \in \mathcal{I}$ , and  $\mathcal{J} = \{k_4\} \cup \mathcal{I} \setminus \{k_i\}$  for any  $i = 1, 2, 3$ , then  $f(\mathcal{I}) = f(\mathcal{J})$ . Such operations changing  $\mathcal{I}$  to  $\mathcal{J}$  is denoted by operation-\*. In short, an operation-\* moves an end of a small ‘‘L-shaped’’ set of 3 pairs along a  $P$ -row or a  $P$ -column, producing another L-shaped set of 3 pairs.

**2. [Regularized form of  $\mathcal{I}$ , and decomposition of nondegenerate regularized form  $\mathcal{I}^\sharp$  into L-shaped subsets]:** Once  $\mathcal{I}$  or any  $\mathcal{J}$  equivalent to  $\mathcal{I}$  via operations-\* contains 4 pairs satisfying condition (\*),  $f(\mathcal{I}) = 0$ , then we call  $\mathcal{I}$  degenerate. In decomposing  $\mathcal{I}$ , when we find it degenerate, we stop since  $f(\mathcal{I})$  is known.

We decompose  $\mathcal{I}$  as set of pairs inductively in the following way before stopping. Start with any  $(i, j) \in \mathcal{I}$ , we look for pairs of form  $(i, l)$  and  $(k, j)$  in  $\mathcal{I}$ , adding them into the subset  $A_{(i, j)}$  containing  $(i, j)$ . Then check the degeneracy, by looking for whether  $\mathcal{I}$  contains a point  $(k, l)$  with  $(i, l), (j, k) \in A_{(i, j)}$ , whenever  $\mathcal{I}$  is degenerate, we stop since  $f(\mathcal{I}) = 0$ . Next we enlarge  $A_{(i, j)}$  by changing the set  $\mathcal{I}$  to a regularized form using operation-\*'s. For each  $(k, l)$  with  $(i, l) \in A_{(i, j)}$ , then  $(k, j)$  can be constructed on  $(k, l)$  via an operation-\* with  $(i, j)$  and  $(i, l)$ . Thus we modify  $\mathcal{I}$  into  $\mathcal{J} = (i, l) \cup \mathcal{I} \setminus (k, l)$  that  $f(\mathcal{I}) = f(\mathcal{J})$ , and adding  $(i, l)$  into set  $A_{(i, j)}$ . Similar process can be done for those  $(k, l) \in \mathcal{I}$  with  $(k, j) \in A_{(i, j)}$ .

After regularizing  $\mathcal{I}$  and enlarging  $A_{(i, j)}$  to maximum about  $(i, j)$ , we get a regularized form  $\mathcal{J}$  of  $\mathcal{I}$ , with  $f(\mathcal{I}) = f(\mathcal{J})$ , and a component  $A_{(i, j)}$  of L-shape. The set of  $\mathcal{J} \setminus A_{(i, j)}$  has no elements of form  $(k, l)$  with  $(i, l) \in A_{(i, j)}$  or  $(k, j) \in A_{(i, j)}$ , as they are already moved to  $A_{(i, j)}$  by operation-\*. Therefore,  $\mathcal{J} \setminus A_{(i, j)}$  is supported on a rectangular region by deleting all  $P$ -rows  $(k, \cdot)$ 's and  $P$ -columns  $(\cdot, l)$ 's where  $k, l$ 's occur in  $A_{(i, j)}$ .

Repeating the L-shaped component construction above for  $\mathcal{J} \setminus A_{(i, j)}$ , we can transform  $\mathcal{I}$  into a regularized form (not unique or standard)  $\mathcal{I}^\sharp$  and we have a decomposition  $\mathcal{I}^\sharp = \bigcup A_{(i_t, j_t)}$  into L-shaped components, which do not intersect with each other. The name ‘‘regularized form’’ is given to the transformed set with a L-shaped decomposition, and since only operation-\* is applied,  $f(\mathcal{I}) = f(\mathcal{I}^\sharp)$ .

**3. [Properties between the L-shaped subsets:]** For each  $\mathcal{I}$  which we did not conclude  $f(\mathcal{I}) = 0$  in the last step, we get  $\mathcal{I}^\sharp$  and a decomposition  $\mathcal{I}^\sharp = \bigcup_{t \in T} A_t$  into L-shaped subsets.

The construction of components  $A_t$  induces such a property: for two distinct components  $A_t$  there is no elements  $(i, j) \in A_t$  and  $(k, l) \in A_s$ , in normal words, the  $A_t$  occupies certain  $P$ -rows and  $P$ -columns which is distinct from those of  $A_s$ .

For  $(i, j)$  and  $(k, l)$  with  $i \neq k$  and  $j \neq l$ ,  $G_{im+j, km+l} = 0$  from the formula that  $G_{im+j, km+l} = \epsilon_\eta r_i \delta_{ik} + \epsilon_\theta c_j \delta_{jl}$ . Therefore, the decomposition  $\mathcal{I}^\sharp = \bigcup_{t \in T} A_t$  induces a decomposition of matrix

$G_{(\mathcal{I}^\#, \mathcal{I}^\#)}$  into blockwise diagonal matrix

$$\begin{bmatrix} G_{A_1, A_1} & 0 & \dots & 0 \\ 0 & G_{A_2, A_2} & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & G_{A_t, A_t} \end{bmatrix} \quad (3)$$

So for a decomposition  $\mathcal{I}^\# = \bigcup_{t \in T} A_t$ , we have  $f(\mathcal{I}^\#) = \prod_{t \in T} f(A_t)$ .

**4.** [ $f(A)$  for an L-shaped component]: The last part is to show  $f(A) > 0$  for all L-shaped components. Recall that  $G_{im+j, km+l} = \epsilon_\eta r_i \delta_{ik} + \epsilon_\theta c_j \delta_{jl}$ , so for  $A$  an L-shaped component with  $s$   $P$ -rows and  $t$   $P$ -columns,  $G_{(A, A)}$  in general is of form

$$G_{(A, A)} = \begin{bmatrix} r_1 + c_1 & \dots & r_1 & r_1 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ r_1 & \dots & r_1 + c_{t-1} & r_1 & 0 & \dots & 0 \\ r_1 & \dots & r_1 & r_1 + c_t & c_t & \dots & c_t \\ 0 & \dots & 0 & c_t & c_t + r_2 & \dots & c_t \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & c_t & c_t & \dots & c_t + r_s \end{bmatrix} \quad (4)$$

Recall the formula  $\det \begin{bmatrix} E & B \\ C & D \end{bmatrix} = \det(E) \det(D - CE^{-1}B)$  and the matrix determinant lemma

$$\det(\text{diag}(c) + r\mathbf{1}\mathbf{1}^T) = (1 + r\mathbf{1}^T \text{diag}(c)^{-1} \mathbf{1}) \det(\text{diag}(c)) = \prod c_i (1 + \sum (r/c_i)).$$

If  $s = 1$  or  $t = 1$ , the determinant of  $G_{(A, A)}$  can be calculated directly by the matrix determinant lemma above.

If  $s > 1$  and  $t > 1$ , we cut Eq. (4) into 4 blocks  $\begin{bmatrix} E & B \\ C & D \end{bmatrix}$  where  $E$  contains the upper left  $t \times t$  part,  $B$  is zero but the last row,  $C$  is zero but the last column,  $D$  is a matrix in a similar form as  $E$ .

According to the characters of  $B, C$  stated above, it can be found that  $CE^{-1}B = c_t^2 \mathbf{1} E_{t,t}^{-1} \mathbf{1}^T$  which is an  $s \times s$ -matrix. The entry  $E_{t,t}^{-1} = \det E_{(1:t-1, 1:t-1)} / \det E$  where  $E_{(1:t-1, 1:t-1)}$  is the matrix  $E$  without the last row and last column, moreover,  $E_{t,t}^{-1} = \left( \prod_1^{t-1} c_i (1 + \sum_1^{t-1} (r_1/c_i)) \right) / \left( \prod_1^t c_i (1 + \sum_1^t (r_1/c_i)) \right) = \frac{1 + \sum_1^{t-1} (r_1/c_i)}{c_t (1 + \sum_1^t (r_1/c_i))} < 1/c_t$ . Therefore,  $CE^{-1}B = \lambda \mathbf{1}\mathbf{1}^T$  with  $\lambda < c_t$  and  $D - CE^{-1}B = \text{diag}(r_{2:s}) + (c_t - \lambda) \mathbf{1}\mathbf{1}^T$ , whose determinant is positive according to the matrix determinant lemma.

As a consequence,  $\det G_{(A, A)} > 0$  for each L-shaped components  $A$ . So combining the discussions in [1-4], we have  $\det H = \det(D + G) > 0$ .

Then the implicit function theorem implies the differentiability of  $P^\epsilon$  on  $\epsilon$ .  $\square$

**Proposition 3.** For any finite  $s_P, s_\eta, s_\theta \geq 0$ , the limit of  $P^\epsilon$  exists as  $\epsilon$  approaches to  $(\infty, s_\eta, s_\theta)$ . In fact,  $\lim_{\epsilon \rightarrow (\infty, s_\eta, s_\theta)} P_{ij}^\epsilon = 1$  for all  $i, j$  (Limit 1). Moreover,  $P^\epsilon$  converges to the solution to

$$\min \langle C, P \rangle - s_P H(P) + s_\theta KL(P^T \mathbf{1} | \theta), \text{ with constraint } P\mathbf{1} = \eta, \quad (5)$$

as  $\epsilon \rightarrow (s_P, \infty, s_\theta)$  (Limit 2). Similarly,  $P^\epsilon$  converges to the solution to

$$\min \langle C, P \rangle - s_P H(P) + s_\eta KL(P\mathbf{1} | \eta), \text{ with constraint } P^T \mathbf{1} = \theta, \quad (6)$$

as  $\epsilon \rightarrow (s_P, s_\eta, \infty)$  (Limit 3). And in the case when  $\epsilon \rightarrow (s_P, \infty, \infty)$ , the matrix  $P^\epsilon$  converges to the EOT solution (Limit 4):

$$\min \langle C, P \rangle - s_P H(P), \text{ with constraints } P^T \mathbf{1} = \theta \text{ and } P\mathbf{1} = \eta. \quad (7)$$

When  $\epsilon \rightarrow (\infty, \infty, s_\theta)$ ,  $(\infty, s_\eta, \infty)$  or  $(\infty, \infty, \infty)$ , the limit does not exist, but the directional limits can be calculated..

*Proof.* Recall that  $H(P) = -\sum_{ij}(P_{ij} \ln P_{ij} - P_{ij})$ ,  $(\nabla_P H)_{ij} = -\ln P_{ij}$ , and  $H(P)$  is strictly concave, therefore  $H$  has a unique maximum  $mn$  at  $P_{ij} = 1$ , denoted by  $\mathbb{1}$ . Similarly,  $KL(a|b) = \sum_i(a_i(\ln a_i - \ln b_i) - a_i + b_i)$ ,  $\nabla_a KL(a|b)_i = \ln a_i - \ln b_i$ ,  $KL$  is strictly convex, therefore  $KL$  has a minimum 0 at  $a_i = b_i$  for all  $i$ .

**Limit 1.** Shown by contradiction: When  $\epsilon \rightarrow (\infty, s_\eta, s_\theta)$ , suppose the limit  $\lim_{\epsilon \rightarrow (\infty, s_\eta, s_\theta)} P_{ij}^\epsilon$  for some  $(i, j)$  does not exist, or is not 1. Thus there is  $e > 0$  that, for any  $\delta > 0$  and  $N > 0$ , there exists a parameter  $\epsilon_1 = (\epsilon_P, \epsilon_\eta, \epsilon_\theta)$  such that  $\epsilon_P > N$ ,  $|\epsilon_\eta - s_\eta| < \delta$  and  $|\epsilon_\theta - s_\theta| < \delta$ , satisfying  $|P_{ij}^\epsilon - 1| > e$ .

However, for any  $0 < e < 1/2$ , let  $\delta = 1$ , let  $E = (1+e) \ln(1+e) - (1+e) + 1 > 0$ ,  $\min \Omega(P; \epsilon) \leq \Omega(\mathbb{1}; \epsilon) < C$  for some  $G > 0$  where  $(\mathbb{1})_{ij} = 1$  for all  $(i, j)$ , and any  $\epsilon \in \{(\epsilon_P, \epsilon_\eta, \epsilon_\theta) : s_\eta/2 < \epsilon_\eta < 3s_\eta/2, s_\theta/2 < \epsilon_\theta < 3s_\theta/2, \}$ . So there is a  $N > 0$  such that  $NE > G + \max_{ij} C_{ij} + mn + L$  where  $L = -\inf\{\epsilon_\eta KL(P\mathbb{1}|\eta) + \epsilon_\theta KL(P^T\mathbb{1}|\theta)\}$ , meaning those  $P$  with  $|P_{ij} - 1| > e$  for some  $(i, j)$  is not minimizing  $\Omega$ .

The contradiction indicates that  $\lim_{\epsilon \rightarrow (\infty, s_\eta, s_\theta)} P_{ij}^\epsilon = 1$  for all  $i, j$ .

**Limit 2 & 3:** The situation of  $\epsilon_\theta \rightarrow \infty$  and  $\epsilon_\eta \rightarrow \infty$  are similar, so we only prove for  $\epsilon_\theta \rightarrow \infty$  case. Let  $\hat{P}$  denote the solution to Eq. (6).

Let  $\hat{P}$  be the solution to the optimization with constraints. We first show that  $\lim_{\epsilon \rightarrow (s_P, s_\eta, \infty)} \sum_{k=1}^n P_{kj}^\epsilon = \theta_j$ .

This is similar to limit 1. Suppose the limit either does not exist or is not  $\theta_j$ , then there exists an  $e > 0$  such that for any  $N > 0$ ,  $\delta > 0$ , there exists  $\epsilon_\theta > N$ ,  $|\epsilon_\eta - s_\eta| < \delta$  and  $|\epsilon_P - s_P| < \delta$ , such that

$$\left| \sum_{k=1}^n P_{kj}^\epsilon - \theta_j \right| > e \quad (8)$$

for some  $j$ . Thus  $KL((P^\epsilon)^T \mathbb{1} | \theta) > E$  for some  $E > 0$ . Consider that  $\langle C, P \rangle \geq 0$ ,  $H(P) \geq -mn$  and  $KL(P\mathbb{1}|\eta) \geq 0$  are lower bounded, we can take sufficiently large  $N$  such that the  $P^\epsilon$  satisfying Eq. (8) satisfy  $\Omega(P^\epsilon; \epsilon) > \Omega(\hat{P}; \epsilon)$ , making  $P^\epsilon$  fail to optimize  $\Omega(\cdot; \epsilon)$ , which is a contradiction. Thus we have  $\lim_{\epsilon \rightarrow (s_P, s_\eta, \infty)} \sum_{k=1}^n P_{kj}^\epsilon = \theta_j$ .

For each  $\epsilon = (\epsilon_P, \epsilon_\eta, \epsilon_\theta)$ , let  $\theta^\epsilon$  denote the  $(P^\epsilon)^T \mathbb{1}$ , then for any  $\epsilon$ , the solution  $P^\epsilon$  is also the solution to

$$\min_P \langle C, P \rangle + \epsilon_P H(P) + \epsilon_\eta KL(P\mathbb{1}|\eta), \text{ with constraint } P^T \mathbb{1} = \theta^\epsilon. \quad (9)$$

Denote  $\Phi(P, \epsilon_P, \epsilon_\eta) := \langle C, P \rangle + \epsilon_P H(P) + \epsilon_\eta KL(P\mathbb{1}|\eta)$  When  $\epsilon_P \in (0, \infty)$ , the new objective function  $\Phi(P, \epsilon_P, \epsilon_\eta)$  is continuous on  $P$  and  $\epsilon_P, \epsilon_\eta$ , and each minimization problem gets a unique solution since the objective function is strictly convex. Therefore, the limit  $\lim_{\epsilon \rightarrow (s_P, s_\eta, \infty)} P^\epsilon = \hat{P}$ . We show this via contradiction:

Suppose the opposite, there exists some  $\xi > 0$  such that  $\|P^\epsilon - \hat{P}\|_2 > \xi$  for  $\epsilon$  arbitrarily close to  $(s_P, s_\eta, \infty)$ . Let

$$\alpha := \inf_{P^T e = \theta, \|P - \hat{P}\|_2 > \xi} \Phi(P, s_P, s_\eta) - \Phi(\hat{P}, s_P, s_\eta),$$

$\alpha > 0$  since the minimum  $\hat{P}$  is unique and the objective is strictly convex. The sets  $P^T e = \theta^\epsilon$  is compact since it is closed and bounded, so there exists bounds  $b = (b_1, b_2, b_3)$  for  $\epsilon = (\epsilon_P, \epsilon_\eta, \epsilon_\theta)$  such that in the bound where  $|\epsilon_P - s_P| < b_1$ ,  $|\epsilon_\eta - s_\eta| < b_2$  and  $\epsilon_\theta > b_3$ ,  $\max \Phi(P, s_P, s_\eta) - \Phi(P^\sharp, \epsilon_P, \epsilon_\eta) < \alpha/3$  for  $P$  with  $P^T e = \theta$  and  $P^\sharp$  its Euclidean projection to  $\{P^T e = \theta^\epsilon\}$ , and  $\max \Phi(P, \epsilon_P, \epsilon_\eta) - \Phi(P^b, s_P, s_\eta) < \alpha/3$  for  $P$  with  $P^T e = \theta^\epsilon$  and  $P^b$  its Euclidean projection to  $\{P^T e = \theta\}$ .

Let  $\epsilon$  be a parameter in the above bound  $b$  to  $(s_P, s_\eta, \infty)$ , where  $P = \operatorname{argmin}_{P^T e = \theta^\epsilon} \Phi(P, \epsilon_P, \epsilon_\eta)$  is  $\xi$  far from  $\hat{P}$ . Then  $\Phi(P, \epsilon_P, \epsilon_\eta) > \Phi(P^b, s_P, s_\eta) - \alpha/3 > \Phi(\hat{P}, s_P, s_\eta) + 2/3\alpha > \Phi(\hat{P}^\sharp, \epsilon_P, \epsilon_\eta) + \alpha/3 > \Phi(\hat{P}^\sharp, \epsilon_P, \epsilon_\eta)$ , which is a contradiction to the assumption that  $P$  is the argmin.

**Limit 4:** Similar to the previous two limits, we can say that  $\lim_{\epsilon \rightarrow (s_P, \infty, \infty)} \sum_{k=1}^n P_{kj}^\epsilon = \theta_j$  and  $\lim_{\epsilon \rightarrow (s_P, \infty, \infty)} \sum_{k=1}^m P_{ik}^\epsilon = \eta_i$ . Then the problem becomes the EOT problem, which has a unique solution.

**Boundaries at  $\epsilon_\eta = 0$  or  $\epsilon_\theta = 0$ :** It is simple to check the continuity when  $\epsilon_\eta \rightarrow 0$  or  $\epsilon_\theta \rightarrow 0$ . From Prop. 2, the continuity and differentiability hold for  $\epsilon_\eta \rightarrow 0$  or  $\epsilon_\theta \rightarrow 0$  when  $\epsilon_P > 0$ .

**Nonexistence of the limits when  $\epsilon_P, \epsilon_\eta \rightarrow \infty$ , and directional limits:** Let a sequence  $\epsilon_1, \epsilon_2, \dots$  where  $\epsilon_i = (\epsilon_P^i, \epsilon_\eta^i, \epsilon_\theta^i)$  satisfy  $\lim \epsilon_P^i = \lim \epsilon_\eta^i = \infty$  and  $\lim(\epsilon_\eta^i/\epsilon_P^i) = t$ , then the limit  $P$  of  $P^{\epsilon_i}$  satisfy  $P_{ij} = t(\ln c_j - \ln n)/(t+1)$ , since the limit minimizes the following objective function

$$H(P) + tKL(P\mathbf{1}|\eta).$$

The reason is, as  $\sum \eta_i = 1$ ,  $H(P)$  and  $KL(P\mathbf{1}|\eta)$  cannot vanish for the same  $P$ , thus the minima of objective function approaches to infinity, therefore the finite terms  $\langle C, P \rangle$  and  $\epsilon_\theta KL(P^T \mathbf{1}|\theta)$  tend to have no effect on the minimal point  $P$  as  $\epsilon_P, \epsilon_\eta$  increases to infinity.

A direct consequence of the above discussion is, when  $t$  changes, the limits  $P$  of those sequences changes, which indicates that the limit of  $P^\epsilon$  as  $\epsilon \rightarrow (\infty, \infty, s_\theta)$  fails to exist. And similar situation happens when  $\epsilon \rightarrow (\infty, s_\eta, \infty)$

**Nonexistence of the limits when  $\epsilon_P, \epsilon_\eta, \epsilon_\theta \rightarrow \infty$ , and directional limits :** Similar to the discussions above, let the sequence  $\epsilon_1, \epsilon_2, \dots$  where  $\epsilon_i = (\epsilon_P^i, \epsilon_\eta^i, \epsilon_\theta^i)$  satisfy  $\lim_{i \rightarrow \infty} \epsilon_i = (\infty, \infty, \infty)$ . Further let  $\lim(\epsilon_\eta^i/\epsilon_P^i) = u$ ,  $\lim(\epsilon_\theta^i/\epsilon_P^i) = w$ , then  $P^{\epsilon_i}$  converges to the solution to the problem

$$H(P) + uKL(P\mathbf{1}|\eta) + wKL(P^T \mathbf{1}|\theta),$$

which could be considered as another UOT problem with cost function constantly 0. □

**Corollary 4.** Consider a UOT problem with cost  $C = -\log \mathbb{P}(d|h)$ , marginals  $\theta = \mathbb{P}(h)$ ,  $\eta \in \mathcal{P}(\mathcal{D})$ . The optimal UOT plan  $P^{(1, \epsilon_\eta, \epsilon_\theta)}$  converges to the posterior  $\mathbb{P}(h|d)$  as  $\epsilon_\eta \rightarrow 0$  and  $\epsilon_\theta \rightarrow \infty$ . Bayesian inference is a special case of GBT with  $\epsilon = (1, 0, \infty)$ .

*Proof.* As direct application of Limit 3 of Proposition 3, we only need to show that the optimal plan  $P^{(1, 0, \infty)}$  is proportional to the posterior  $\mathbb{P}(h|d)$ .

$$P^{(1, 0, \infty)} = \arg \min_{P \in U(\theta)} K(P) := \arg \min_{P \in U(\theta)} \{\langle C, P \rangle - H(P)\}. \quad (10)$$

where  $U(\theta) = \{P \in \mathcal{M}(D \times H) | P^T \mathbf{1} = \theta\}$ .

Let  $\lambda \in \mathbb{R}^{+m}$ , consider the corresponding Lagrangian problem:

$$L(P, \lambda) := \langle C, P \rangle - H(P) + \langle \lambda, (P^T \mathbf{1} - \theta) \rangle$$

Partial derivatives  $\partial_{P_{ij}} = 0$  and  $\partial_{\lambda_j} L = 0$  result the following system of equations:

$$\log P_{ij} - \log \mathbb{P}(d_i|h_j) + \lambda_j = 0 \quad \sum_i P_{ij} - \mathbb{P}(h_j) = 0 \quad (11)$$

Calculation shows that the solution to Equation 11 is  $P_{ij} = \frac{\mathbb{P}(d_i|h_j)\mathbb{P}(h_j)}{\sum_i \mathbb{P}(d_i|h_j)} = \mathbb{P}(d_i|h_j)\mathbb{P}(h_j) \propto \mathbb{P}(h_j|d_i)$ . Hence the proof is completed. □

**Corollary 5.** Consider a UOT problem with  $\theta \in \mathcal{P}(\mathcal{H})$ ,  $\eta = \mathbb{P}(d)$ . The optimal UOT plan  $P^{(\epsilon_P, \infty, 0)}$  converges to  $\eta \otimes \mathbf{1}$  as  $\epsilon_P \rightarrow \infty$ . Frequentist Inference is a special case of GBT with  $\epsilon = (\infty, \infty, 0)$ .

*Proof.* As direct application of Proposition 3, we only need to show that  $P^{(\infty, \infty, 0)} = \eta \otimes \mathbf{1}$ . Notice that the limit problem

$$P^\epsilon(C, \eta, \theta) = \arg \min_{P \in (\mathbb{R}_{\geq 0})^{n \times m}} \{\langle C, P \rangle - \epsilon_P H(P) + \epsilon_\eta KL(P\mathbf{1}|\eta) + \epsilon_\theta KL(P^T \mathbf{1}|\theta)\}. \quad (12)$$

as  $\epsilon \rightarrow (\infty, \infty, 0)$  along  $\epsilon_P$ -up direction is equivalent to

$$P^{(\infty, \infty, 0)} = \arg \min_{P \in (\mathbb{R}_{\geq 0})^{n \times m}} H(P), \text{ with constraint } P\mathbf{1} = \eta \quad (13)$$

Hence  $P^{(\infty, \infty, 0)} = \eta \otimes \mathbf{1}$ .  $\square$

**Corollary 6.** *Let cost  $C = -\log M$ , marginals  $\theta = \mathbb{P}(h)$  and  $\eta = \mathbb{P}(d)$ . The optimal UOT plan  $P^{(1, \epsilon_\eta, \epsilon_\theta)}$  converges to the optimal plan  $L$  as  $\epsilon_\eta \rightarrow \infty$  and  $\epsilon_\theta \rightarrow \infty$ . Cooperative Inference is a special case of GBT with  $\epsilon = (1, \infty, \infty)$ , which is exactly entropic Optimal Transport [Cuturi, 2013].*

*Proof.* According to proposition 1,  $L = P^{(1, \infty, \infty)}$ , and the convergence result is a direct application of Limit 4 of Proposition 3  $\square$

**Corollary 7.** *Consider a UOT problem with cost  $C = -\log \mathbb{P}(d, h)$ ,  $m = n$ , and marginals  $\theta = \eta$  are uniform. The optimal UOT plan  $P^{(\epsilon_P, \epsilon_\eta, \epsilon_\theta)}$  approaches to a diagonal matrix as  $\epsilon_\eta, \epsilon_\theta \rightarrow \infty$  and  $\epsilon_P \rightarrow 0$ . In particular, discriminative learner is a special case of GBT with  $\epsilon = (0, \infty, \infty)$ , which is exactly classical Optimal Transport [Villani, 2008].*

*Proof.* Limit 4 of Proposition 3 implies the convergence of  $P^{(\epsilon_P, \epsilon_\eta, \epsilon_\theta)} \rightarrow P^{(0, \infty, \infty)}$  as  $\epsilon_\eta, \epsilon_\theta \rightarrow \infty$  and  $\epsilon_P \rightarrow 0$ . When  $m = n$ ,  $P^{(0, \infty, \infty)}$  is a permutation matrix is the result of Wang et al. [2020b][Proposition 8].  $\square$

**Proposition 8.** *In GBT with  $\epsilon_\theta = \infty$ , cost  $C$  and current belief  $\theta$ . The learner updates  $\theta$  with UOT plan in the same way as applying Bayes rule with likelihood from  $P^\epsilon(C, \eta, \theta)$ , and prior  $\theta$ .*

*Proof.* From the GBT algorithm (Algorithm 1 in the main text), for a general data point  $d^i$  chosen, the GBT takes the vector normalization of some row  $P^\epsilon$ , i.e.,  $\theta^i = P^\epsilon_{(i, \cdot)} / (\sum_j P^\epsilon_{ij})$ .

On the other hand, when we apply Bayes rule to  $P^\epsilon$ , prior is  $\theta = \mathbb{P}(h)$ , likelihood  $\mathbb{P}(d|h)$  is the column normalization of  $P^\epsilon$ , satisfying  $\mathbb{P}(d^i|h^j) = P^\epsilon_{ij} / (\sum_i P^\epsilon_{ij}) = P^\epsilon_{ij} / \theta_j$ . The last equality is because  $\theta(i) = \sum_j P^\epsilon_{ij}$  when  $\epsilon_\theta = \infty$ . So the posterior  $\mathbb{P}(h|d^i)$  is the vector normalization of  $\mathbb{P}(d^i|h)\mathbb{P}(h)$ , by  $\mathbb{P}(d^i|h^j)\mathbb{P}(h^j) = P^\epsilon_{ij} / \theta_j * \theta_j = P^\epsilon_{ij}$ . Therefore,  $\mathbb{P}(h^j|d^i) = \theta^j(h^j)$ .  $\square$

Now, we introduce some notations will be used in the following proofs.

**Notations.** Denote the set of all possible belief by  $\Delta = \mathcal{P}(\mathcal{H})$ . Distribution of  $\Theta_k$  is denoted by  $\mu_k$ . We only consider the case where no two hypotheses are the same in  $\mathcal{H}$ . Hence we make the following assumption that columns of  $\exp(-\epsilon_P C)$  are not differ by a multiplicative scalar, i.e. columns of  $C$  are not differ by an additive scalar.

**Lemma S.2.** *For  $\epsilon = (\epsilon_P, \infty, \infty)$ ,  $\epsilon_P \in (0, \infty)$ , given cost  $C$  with initial belief  $\theta_0 \in \mathcal{P}(\mathcal{H})$  and fixed teaching and learning distribution  $\eta_k = \eta \in \mathcal{P}(\mathcal{D})$  for all  $k$ , then the belief random variables  $(\Theta_k)_{k \in \mathbb{N}}$  have the same expectation on  $h$ :  $\mathbb{E}_{\Theta_k}[\theta(h)] = \theta_0(h)$ .*

*Proof.* We start the proof by showing  $\mathbb{E}_{\Theta_k}[\theta(h)] = \mathbb{E}_{\Theta_{k-1}}[\theta(h)]$  for  $k \geq 1$ . Notice that given cost  $C$  and data marginal  $\eta$ , an observed data  $d \in \mathcal{D}$  and UOT planning uniquely determines a map from a learner's initial belief  $\theta_{k-1}$  to one's posterior belief  $\theta_k$ . Denote this map by  $T_d : \theta_{k-1} \mapsto \theta_k$ . Let the distribution of  $\Theta_{k-1}$  over  $\mathcal{P}(\mathcal{H})$  be  $\mu_{k-1}$ , denote its support by  $S_{k-1}$ . Then the following holds:

$$\begin{aligned} \mathbb{E}_{\Theta_k}[\theta(h^j)] &= \sum_{\theta \in S_{k-1}} \mu_{k-1}(\theta) \sum_{d^i \in \mathcal{D}} \eta^i T_{d^i}(\theta)(h^j) = \sum_{\theta \in S_{k-1}} \mu_{k-1}(\theta) \sum_{d^i \in \mathcal{D}} \eta^i \frac{M_k(i, j)}{\eta^i} \\ &= \sum_{\theta \in S_{k-1}} \mu_{k-1}(\theta) \sum_{d^i \in \mathcal{D}} M_k(i, j) = \sum_{\theta \in S_{k-1}} \mu_{k-1}(\theta) \theta(h^j) = \mathbb{E}_{\Theta_{k-1}}[\theta(h)] \end{aligned}$$

Hence  $\mathbb{E}_{\Theta_k}[\theta(h)] = \mathbb{E}_{\Theta_{k-1}}[\theta(h)] = \dots = \mathbb{E}_{\Theta_0}[\theta(h)] = \theta_0(h)$ .

□

**Theorem 10 (PS).** Consider a learning problem with initial belief  $\theta_0 \in \mathcal{P}(\mathcal{H})$ , and the true hypothesis  $h^*$  defined by  $\eta \in \mathcal{P}(\mathcal{D})$ . If the learner's data distribution  $\eta_k = \eta$ , then belief random variables  $(\Theta_k)_{k \in \mathbb{N}}$  converge to the random variable  $Y$  in probability, where  $Y = \sum_{h \in \mathcal{H}} \theta_0(h) \delta_h$  and  $Y$  is supported on  $\{\delta_h\}_{h \in \mathcal{H}}$  with  $\mathbb{P}(Y = \delta_h) = \theta_0(h)$  for  $\epsilon_\eta = \epsilon_\theta = \infty$  and  $\epsilon_P \in (0, \infty)$ .

*Proof.* Step 1: First, we show the following claim inspired the proof proposition 5.1 in Wang et al. [2020a]

**Claim:**  $\lim_{k \rightarrow \infty} \mu_k(\Delta_\epsilon) = 0$ , for any  $\epsilon > 0$ , where  $\Delta_\epsilon := \{\theta \in \Delta : \theta(h) \leq 1 - \epsilon, \forall h \in \mathcal{H}\}$ .

Assume the claim does not hold, then there exists  $\alpha > 0$  and a subsequence  $(\mu_{k_i})_{i \in \mathbb{N}}$  such that  $\mu_{k_i}(\Delta_\epsilon) > \alpha$  for all  $i$ .

Let the center of  $\Delta$  be  $u$ , we define  $L(\mu) := \mathbb{E}_\mu f(\theta)$ , where  $f(\theta) = \|\theta - u\|_2^2$ , ( $f$  may also be chosen as entropy  $H(\theta)$ ). Then  $L(\mu_{k+1}) = \mathbb{E}_{\mu_k}(\mathbb{E}_{d \sim \eta} f(T_d(\theta)))$ .

Notice that  $f$  is strictly convex, by Jensen's inequality,

$$\mathbb{E}_{d \sim \eta} f(T_d(\theta)) \stackrel{(a)}{\geq} f(\mathbb{E}_{d \sim \eta} T_d(\theta)) \stackrel{(b)}{=} f(\theta) \quad (14)$$

Here (b) holds because:

$$\mathbb{E}_{d \sim \eta} T_d(\theta) \stackrel{(c)}{=} \sum_{d^i \in \mathcal{D}} \eta^i \cdot (M_k(i, \_)/\eta^i) = \sum_{d^i \in \mathcal{D}} M_k(i, \_) \stackrel{(d)}{=} \theta \quad (15)$$

(c), (d) hold since  $M_k$  has marginals  $\eta, \theta$ .

Moreover, equality holds in (a) if and only if  $T_d(\theta) = \theta$  for all  $d \in \mathcal{D}$ . Thus rows of  $M_k$  are the same up to a scalar. This implies either (1) only one column of  $M_k$  is none zero, thus  $\Theta_k \equiv \delta_h$  for some  $h$  or (2)  $M_k$  has at least two columns are differed by a scalar.

In the case of (1), if  $\theta_0 \neq \delta_h$ ,  $\Theta_k \equiv \delta_h$  is contradict to Lemma 8. Otherwise,  $Y = \delta_h$ , the result holds. In the case of (2), according to Wang et al. [2019],  $M_k$  is cross-ratio equivalent to  $\exp(-\epsilon_P C)$ , hence  $\exp(-\epsilon_P C)$  has two columns differ by a multiplicative scalar, contradict to the assumption.

Thus for any  $\theta \in \Delta_\epsilon$ ,  $\mathbb{E}_{d \sim \eta} f(T_d(\theta)) > f(\theta)$ . Therefore  $L(\mu_{k+1}) > L(\mu_k)$  for any  $k$ .

Moreover, notice that  $\Delta_\epsilon$  is compact, there is a lower bound  $\beta > 0$ , such that  $\mathbb{E}_{d \sim \eta} f(T_d(\theta)) - f(\theta) > \beta$  for all  $\theta \in \Delta_\epsilon$ . Therefore:

$$\begin{aligned} L(\mu_{k_i+1}) &= \mathbb{E}_{\theta_{k_i+1} \in \Delta_\epsilon}(\mathbb{E}_{d \sim \eta} f(T_d(\theta))) + \mathbb{E}_{\theta_{k_i+1} \in \Delta \setminus \Delta_\epsilon}(\mathbb{E}_{d \sim \eta} f(T_d(\theta))) \\ &> \mathbb{E}_{\theta_{k_i} \in \Delta_\epsilon}(f(\theta)) + \mathbb{E}_{\theta_{k_i} \in \Delta \setminus \Delta_\epsilon}(f(\theta)) + \alpha * \beta \\ &= L(\mu_{k_i}) + \alpha * \beta. \end{aligned} \quad (16)$$

Thus  $L(\mu_{k_i+s}) > L(\mu_{k_i}) + s * \alpha * \beta \rightarrow \infty$  as  $s \rightarrow \infty$ . On the other hand, by definition,  $f(\theta)$  is bounded above by the diameter of  $\Delta$  under  $l^2$  norm, so  $L(\mu)$  is also bounded above. Contradiction! Therefore, the Claim holds.

Step 2. We show  $\lim_{k \rightarrow \infty} \mathbb{P}(\Theta_k \in \Delta_{1-\epsilon}^h) = \lim_{k \rightarrow \infty} \mu_k(\Delta_{1-\epsilon}^h) = \theta_0(h)$ , for all  $h \in \mathcal{H}$  where  $\Delta_{1-\epsilon}^h := \{\theta \in \Delta : \theta(h) > 1 - \epsilon\}$ .

For a fixed  $h \in \mathcal{H}$ , we have:

$$\begin{aligned} \theta_0(h) &\stackrel{(a)}{=} \mathbb{E}_{\Theta_k}(\theta(h)) \stackrel{(b)}{=} \mathbb{E}_{\theta_k \in \Delta_{1-\epsilon}^h}(\theta(h^j)) + \mathbb{E}_{\theta_k \in \Delta_{1-\epsilon}^u}(\theta(h)) + \mathbb{E}_{\theta_k \in \Delta_\epsilon}(\theta(h)) \\ &\stackrel{(c)}{\leq} \mu_k(\Delta_{1-\epsilon}^h) \cdot 1 + \mu_k(\Delta_{1-\epsilon}^u) \cdot \epsilon + \mu_k(\Delta_\epsilon) \cdot 1 \\ &= \mu_k(\Delta_{1-\epsilon}^h) + \epsilon + \mu_k(\Delta_\epsilon) \end{aligned}$$

where  $\Delta_{1-\epsilon}^u$  denotes the union of all the other corners of  $\Delta$ , i.e.  $\Delta_{1-\epsilon}^u := \cup_{h' \in \mathcal{H} \setminus h} \Delta_{1-\epsilon}^{h'}$ . Here (a) is direct application of Lemma 8; (b) holds since  $\Delta = \Delta_{1-\epsilon}^h \cup \Delta_{1-\epsilon}^u \cup \Delta_\epsilon$ . (c) holds because in general

$\theta(h^j) < 1$ , and  $\theta(h^j) < \epsilon$  for any  $\theta \in \Delta_{1-\epsilon}^u$ . Therefore,  $0 \leq \theta_0(h) - \mu_k(\Delta_{1-\epsilon}^h) \leq \epsilon + \mu_k(\Delta_\epsilon) \rightarrow \epsilon$  as  $k \rightarrow \infty$  hold for any choice of  $\epsilon$ . Pick a sequence of  $\epsilon \rightarrow 0$ , we have that  $\lim_{k \rightarrow \infty} \mu_k(\Delta_{1-\epsilon}^h) = \theta_0(h)$ .

Hence combining results from Step 1 and Step 2, we have shown  $\Theta_k$  converges to  $Y$  in probability:  $\mathbb{P}(|\Theta_k - Y| > \epsilon) \leq \mu_k(\Delta_\epsilon) + \sum_{h \in \mathcal{H}} (\theta_0(h) - \mu_k(\Delta_{1-\epsilon}^h)) \rightarrow 0$  as  $k \rightarrow \infty$ . Hence the proof is completed.  $\square$

**Corollary 11.** *Given a fixed data sequence  $d_i$  sampled from  $\eta$ , if  $\theta_k$  converges to  $\delta_{h^j}$ , then the  $j$ -th column of  $M_k$  converges to  $\eta$ .*

*Proof.* For  $\epsilon > 0$ , there exists  $N > 0$  such that  $\theta_k(h^j) > 1 - \epsilon$  for any  $k > N$ . So  $\sum_{j' \neq j} M_k(i, j') < \epsilon$  for any  $d_i \in \mathcal{D}$ , on the other hand  $\sum_{j'} M_k(i, j') = \eta_i$ . This implies that  $\eta_i - \epsilon < M_k(i, j) < \eta_i$ , so  $M_k(i, j) \rightarrow \eta_i$  as  $\epsilon \rightarrow 0$ . Therefore the  $j$ -th column of  $M_k$  converges to  $\eta$ .  $\square$

**Proposition 12.** *Consider a learning problem with cost  $C$ , initial belief  $\theta_0 \in \mathcal{P}(\mathcal{H})$ , the true hypothesis  $h^*$  defined by  $\eta \in \mathcal{P}(\mathcal{D})$ . If the learner updates the estimation  $\eta_k$  with observed data (sampled from  $\eta$ ) as stated above, then belief random variables  $(\Theta_k)_{k \in \mathbb{N}}$  satisfies that for any  $s > 0$ ,  $\lim_{k \rightarrow \infty} \sum_{h \in \mathcal{H}} \mathbb{P}(\Theta(h) > 1 - s) = 1$ . As a consequence,  $M_k$  as the transport plan has a dominant column ( $h^j$ ) with total weights  $> 1 - s$ , and  $|(M_k)_{ij} - \eta_k(i)| < s$ . In fact, as long as the sequence of  $\eta_k$  as random variables converges to  $\eta$  in probability, the above proposition holds.*

*Proof.* The proof is similar to Step 1 of Theorem 10. The major difference is that data are sampled from  $\eta$  in each step, whereas the learner only has an estimation  $\eta_k$  at round  $k$ . Therefore, under current condition, equality (b) of Eq 14 need to be modified as following:

$$\mathbb{E}_{d \sim \eta} T_d(\theta_k) = \sum_{d^i \in \mathcal{D}} \eta^i \cdot (M_k(i, -) / \eta_k^i) = \sum_{d^i \in \mathcal{D}} M_k(i, -) \cdot \frac{\eta^i}{\eta_k^i} = \theta_k \odot \mathbf{v}_k. \quad (17)$$

where  $\mathbf{v}_k = (\frac{\eta^i}{\eta_k^i})$  is a vector of the size of the data set  $\mathcal{D}$ , and  $\odot$  represents element-wise product. Hence  $\mathbb{E}_{d \sim \eta} f(T_d(\theta_k)) = f(\theta_k \odot \mathbf{v}_k)$  holds for all  $\theta_k \in \Delta$ . Since  $\eta_k \rightarrow \eta$  as  $k \rightarrow \infty$ . For any  $\alpha * \beta > 0$ , there exists  $N > 0$  such that for  $k > N$ ,  $|1 - \frac{\eta^i}{\eta_k^i}| < \sqrt{\frac{\alpha * \beta}{2n}}$ . Hence:  $|f(\theta_k \odot \mathbf{v}_k) - f(\theta_k)| \leq \frac{\alpha * \beta}{2}$ . Then corresponding to Eq 16, for  $k_i > N$ , we have:

$$\begin{aligned} L(\mu_{k_i+1}) &= \mathbb{E}_{\theta_{k_i+1} \in \Delta_\epsilon} (\mathbb{E}_{d \sim \eta} f(T_d(\theta))) + \mathbb{E}_{\theta_{k_i+1} \in \Delta \setminus \Delta_\epsilon} (\mathbb{E}_{d \sim \eta} f(T_d(\theta))) \\ &> \mathbb{E}_{\theta_{k_i} \in \Delta_\epsilon} (f(\theta_k \odot \mathbf{v}_k)) + \mathbb{E}_{\theta_{k_i} \in \Delta \setminus \Delta_\epsilon} (f(\theta_k \odot \mathbf{v}_k)) + \alpha * \beta \\ &> \mathbb{E}_{\theta_{k_i} \in \Delta_\epsilon} (f(\theta_k)) + \mathbb{E}_{\theta_{k_i} \in \Delta \setminus \Delta_\epsilon} (f(\theta_k)) - \frac{\alpha * \beta}{2} + \alpha * \beta \\ &= L(\mu_{k_i}) + \frac{\alpha * \beta}{2}. \end{aligned}$$

Hence the contradiction on the upper bound of  $L(\mu_{k_i+1})$  still holds, which shows the claim that:  $\lim_{k \rightarrow \infty} \mu_k(\Delta_\epsilon) = 0$ . So  $\lim_{k \rightarrow \infty} \sum_{h \in \mathcal{H}} \mathbb{P}(\Theta(h) > 1 - s) = 1$ . The proof for the second part of the proposition follows exactly as Corollary 11.  $\square$

**Proposition 14.** *For  $\epsilon = (\epsilon_P, \epsilon_\eta, 0)$  with  $\epsilon_P \in (0, \infty)$ , as  $\eta_k \rightarrow \eta$  almost surely, the sequence  $\Theta_k$  of posteriors as a sequence of random variables converges in probability to variable  $\Theta$ , where  $\mathbb{P}(\Theta = \mathbf{v}^i) = \eta(i)$  and  $\mathbf{v}^i = P_{(i, -)} / (\sum_{j=1}^m P_{ij})$  and  $P = P^\epsilon(C, \eta, \theta)$ . Therefore, for any  $s > 0$ ,  $\lim_{k \rightarrow \infty} \sum_{h \in \mathcal{H}} \mathbb{P}(|\Theta_k(h) - 1| < s) = 0$  for generic (for all but in a closed subset) cost  $C$  and  $\eta, \theta$ .*

*Proof.* First,  $\epsilon_\theta = 0$  means that  $P^\epsilon(C, \eta, \theta)$  is independent of  $\theta$ . Therefore,  $M_k = P^\epsilon(C, \eta_k, \theta)$  and has a limit  $P^\epsilon(C, \eta, \theta)$ , regardless of the concrete posterior  $\theta_k$ . From construction of GBT, the posterior  $\Theta_k$  is determined by  $\mathbb{P}(\Theta_k = \mathbf{w}_k^i) = \eta(i)$  where  $\mathbf{w}_k^i = (M_k)_{(i, -)} / \sum_{j=1}^m (M_k)_{ij}$ . Given the coupling  $(\Theta_k, \Theta)$  by setting only  $\mathbb{P}(\Theta_k = \mathbf{w}_k^i, \Theta = \mathbf{v}^i) = \eta(i)$  for each  $i$ , we may calculate  $\mathbb{P}(|\Theta_k - \Theta| < s)$  converge to 1 as  $M_k$  converge to  $P^\epsilon(C, \eta, \theta)$ .

For generic  $C, \eta, \theta$ , the probability of  $P^\epsilon(C, \eta, \theta)$  having a row with only one nonzero entry is 0.  $\square$

**Remark:** As  $\eta_k \rightarrow \eta$  almost surely, for any  $e > 0$ , there exists  $N > 0$ , such that, when  $k > N$ , the probability of having  $\eta_k$   $e$ -close to  $\eta$  is 1. Thus in almost all episodes, with generic  $C, \eta, \theta$ , when  $e$  is small enough, for any  $\|\eta' - \eta\| < e$  (using  $p - \infty$  norm, same for below), the row-normalized (to  $\mathbb{1}_n$ ) UOT plans

$$\max_i \|P_r^\epsilon(C, \eta', \theta)_{(i, \cdot)} - P_r^\epsilon(C, \eta, \theta)_{(i, \cdot)}\| < \frac{1}{4} \min_{i, j} \|P_r^\epsilon(C, \eta, \theta)_{(i, \cdot)} - P_r^\epsilon(C, \eta, \theta)_{(j, \cdot)}\|$$

where  $P_r^\epsilon$  is the row normalization of  $P^\epsilon$ .

Therefore, for such  $e$ , we may find an  $N > 0$  such that for any  $k, k' > N$ ,  $P_r^\epsilon(C, \eta_k, \theta) \neq P_r^\epsilon(C, \eta_{k'}, \theta)$ . However, for generic  $\eta$ , say, no entry of  $\eta$  is 0,  $\|\theta_k - \theta_{k'}\| < e$  when  $k, k' > N$  and  $d_k \neq d_{k'}$ . Thus the posterior sequence of almost every episode fails to converge.

The original statement of the following Proposition is problematic, we changed the statement accordingly.

**Proposition 16.** *For a Bayesian learner, the posterior sequence  $\{\Theta_k\}$  converges almost surely to  $\delta_h$  where  $h = \arg \min_{h' \in \mathcal{H}} KL(\bar{\eta} | M_{(\cdot, h')})$  and  $M = e^{-C/\epsilon_P}$ ,  $\bar{\eta} = \frac{1}{p} \sum_{k=0}^{p-1} \eta_k$ .*

*Proof.* Based on the proof of Prop. 9, the behavior of the posterior sequence is determined by teaching data governed by the Central Limit Theorem.

We calculate  $\log(\Theta_k(h')/\Theta_k(h))$  for any  $h' \neq h$ . With a tuple  $(d_0, d_1, \dots, d_k)$  of data points sampled from  $\bar{\eta}$  periodically,

$$\begin{aligned} \log(\theta_k(h')/\theta_k(h)) &= \sum_{s=0}^k (\log(M_{(d_s, h')}) - \log(M_{(d_s, h)})) \\ &= \sum_{d \in \mathcal{D}} \lambda_d (\log(M_{(d, h')}) - \log(M_{(d, h)})) \\ &= t (KL(\lambda | M_{(\cdot, h')}) - KL(\lambda | M_{(\cdot, h)})) . \end{aligned} \quad (18)$$

where  $\lambda$  is the empirical distribution of the data points  $(d_0, d_1, \dots, d_k)$ .

According to the central limit theorem, the teacher following  $\bar{\eta}$  produces a sequence with associated empirical distribution  $\bar{\eta}$  almost surely. Thus the posterior sequence converges to  $\delta_h$  with  $h$  of the greatest KL-divergence.  $\square$

**Proposition 17.** *For  $\epsilon$  in the interior of the cube, for (PS) problem, the sequence  $\{\vec{\Theta}_t\}$  (random variables over  $\mathcal{P}(\mathcal{H})^p$ ) form a time-homogeneous Markov chain. For (RS) problem,  $\{(\vec{\Theta}_t, \frac{1}{pt} \sum_{k=0}^{p-1} t\eta_k)\}$ , the random variable sequence producing samples  $\{(\vec{\theta}_t, \frac{1}{pt} \sum_{k=0}^{p-1} \delta_{d_k})\}$ , forms a Markov chain.*

*Proof.* Define  $\Phi_t = (\vec{\Theta}_t, \frac{1}{pt} \sum_{k=0}^{p-1} t\eta_k)$ , whose sample is  $\phi_t = (\vec{\theta}_t, \lambda_t)$  where  $\vec{\theta}_t = (\theta_{(t-1)p}, \theta_{(t-1)p+1}, \dots, \theta_{tp-1})$  and  $\lambda_t$  is the empirical (statistical) distribution of the set of taught data points  $\{d_0, d_1, \dots, d_{tp-1}\}$ .

Since in (PS) problem,  $\theta_k$  is determined by  $\theta_{k-1}$ , a fixed  $\eta$  and  $d_{k-1}$ , via the UOT solution. Thus,  $\Theta_k$  depends on  $\Theta_{k-1}$  only. So,  $\vec{\Theta}_t$  depends only on  $\vec{\Theta}_{t-1}$ , showing that  $\vec{\Theta}_t$  is time-homogeneous Markovian.

For (RS) problem,  $\lambda_t$  is determined by  $\lambda_{t-1}$  and the sample  $(d_{(t-1)p}, d_{(t-1)p+1}, \dots, d_{tp-1})$  from  $\bar{\eta}$ , and  $\vec{\theta}_t$  is determined by  $\vec{\theta}_{t-1}$  (in fact, just the last element  $\theta_{(t-1)p-1}$ ) and  $\lambda_{t-1}$ . Therefore, we get the Markovianess.  $\square$

### 3 Additional Simulations

Interpolation between learning models can be investigated properly under GBT. Human learners appear to be capable of moving between different learning models gradually. Consider an individual at a carnival who is playing a game. At each of 10 trials, a bit of information is provided, but the available reward decreases. The individual has a pool of tickets with which they can bet on the outcome at each trial. The question is how the individual should update their beliefs in order to maximize their rewards. On the first trial, their belief update, in order to accurately reflect the evidence, should follow Bayes rule. However, for the last trial, one should focus bets on the most probable outcome in order to maximize chances for rewards, that is, their beliefs should be optimized for discriminating among the possible outcomes. GBT offers a coherent way of interpolating between these two approaches to provide candidate strategies on the intermediate steps. Such situations are common where there is an explicit constraint on the time horizon after which point no further evidence can be obtained, and there are incentives to act early, rather than to wait until evidence has fully accumulated; for example, identifying dangerous situations (tiger or not? poisonous or not?).

We now demonstrate how continuity of GBT (section 3.1) allows one to gradually interpolate between Bayesian and discriminative learning over steps (rather than a sharp switch).

#### 3.1 Simulation Setup

Suppose a learner who observes data sampled from a true hypothesis  $\mathbb{P}(d|h^*)$ , and needs to make a conclusion on whether  $h^*$  is one of the hypotheses in  $\mathcal{H}$  within a fixed number  $N$  of observations.

Here we compare a baseline learner who utilizes Bayesian inference ( $\epsilon = (1, 0, \infty)$ ) on the first  $N - 1$  observations, and switch to discriminative learning ( $\epsilon = (0, \infty, \infty)$ ) on the last observation, against learners who interpolate from Bayesian to discriminative learning gradually along a sequence of models on curves in GBT. Two curves along with intermediate models are shown red and orange in Figure 1.

We take a random sampled  $M$  of shape  $4 \times 4$  as an example,

$$M = \begin{bmatrix} 0.225779 & 0.014886 & 0.433787 & 0.050735 \\ 0.613779 & 0.322347 & 0.172658 & 0.109262 \\ 0.069799 & 0.620178 & 0.29083 & 0.243635 \\ 0.090643 & 0.042588 & 0.102725 & 0.596368 \end{bmatrix}.$$

Thus  $|\mathcal{H}| = |\mathcal{D}| = 4$ . Set  $N = 10$  and start from uniform  $\theta = (0.25, 0.25, 0.25, 0.25)$ .

Simulation details: We perform 40000 trials in total. For each trial  $s$  (or say each episode), we uniformly sample  $X_s \in \mathcal{P}(\mathcal{H})$ , and let the true hypothesis  $h^*$  be a normalized (thus a distribution) column of  $M$ , uniformly sampled from the 4 columns. While teaching the episode, in each round, we sample a hypothesis  $h \in \mathcal{H}$  following  $X_s$ , then sample a data  $d$  following the column of  $M$  corresponding to  $d$ . During inference, we set  $\eta_k$  by counting the frequency of each  $d \in \mathcal{D}$  (starting from 1 to avoid 0 in  $\eta_k$ ) and then normalize, as stated in **(RS)** model in Sec. 3.

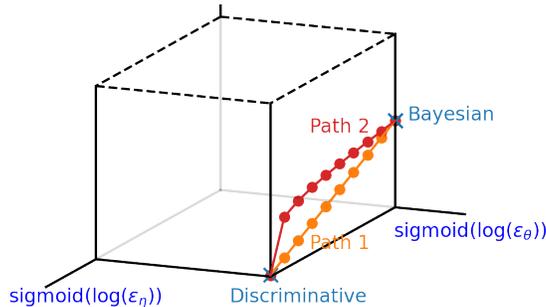


Figure 1: Baseline (sharp change) and two paths we follow on the parameter space of GBT.

### 3.2 Results

Following paths shown in Fig. 1, for baseline (blue, left), path 1 (orange, middle), and path 2 (red, right), the distribution of maximal component of each posterior at round 10 are shown in histograms of 30, and the entropy of these posteriors are plotted in the lower three figures.

Conclusiveness (minimal  $l^1$  distance between posterior and a 1-hot vector) and posterior entropy are plotted as histograms. The results show that the smoother path may lead to a more conclusive posterior. Numerical results: Conclusiveness of **Blue**: mean 0.9406, standard deviation 0.1300. Conclusiveness of **Orange**: mean 0.9964, standard deviation 0.0327. Conclusiveness of **Red**: mean 0.9834, standard deviation 0.0676. Furthermore, compared with a sudden jump, gradual interpolations have lower entropy. Numerical results: entropy of **Blue**: mean 0.1261, standard deviation 0.2435, entropy of **Orange**: mean 0.0079, standard deviation 0.0629; entropy of **Red**: mean 0.0388, standard deviation 0.1336.

Thus learning tends to be more conclusive along these paths. Here conclusiveness means that the ability of getting a conclusion (one component of the posterior eventually becoming dominant). Furthermore, the entropy distributions shown in the lower figures also illustrate this point, as compare to baseline, gradual interpolations have lower entropy.

It is necessary to consider that, the two paths and interpolations are chosen for demonstration purpose, by no means they are optimal. However, we believe GBT is capable of facilitating exploration of such optimization.

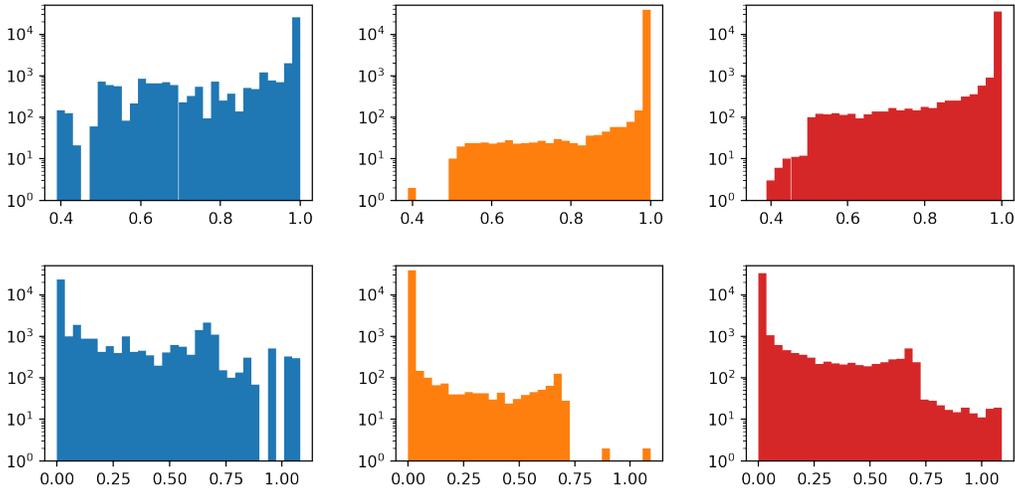


Figure 2: Results. Upper: distribution of maximal component of posterior. Lower: Entropy distribution of posteriors. Left: baseline. Middle: along path 1. Right, along path 2.

### 3.3 Sequential GBT: Dynamic

There are some more data from simulation, all with  $M$  of size  $3 \times 3$ , exploring the effects of varying  $\epsilon$  and choosing different  $M$ .

We first investigate the behavior when  $\epsilon = (1, \epsilon_\eta, \epsilon_\theta)$  where  $\epsilon_\eta, \epsilon_\theta \in [0, \infty)$ . We choose a grid  $(10^{-2}, 10^{-1}, \dots, 10^9)^2$  and measure asymptotic diverging distance  $\frac{1}{p} \sum_{k=(t-1)p}^{tp-1} \|\mathbb{E}[\Theta_k] - \mathbb{E}[\Theta_t]\|_2$  at each point in the grid, where  $M$  and the circular teaching path is shown in Fig. 3 (a), and the result is shown in (b). The ‘‘asymptotic’’ value is the average of last 5 periods in the 15 period simulations where  $t = 15$ , period  $p = 20$  and total steps  $k = 300$  in each episode (empirically, the last 5 periods are usually stable enough to represent the asymptotic situation). The mean of 10240 episodes are taken to estimate the expectation of  $\Theta_k$  and  $\Theta_t$ . We see a higher contribution of  $\epsilon_\theta$  than  $\epsilon_\eta$  in controlling the posteriors’ converging either to a point or to an attractive curve.

Next, we choose a set of  $M$  randomly, and set the teacher teaching along a circle of period 20. We are interested in the relation between the matrix and the area ratio (posterior loop divided by the teaching

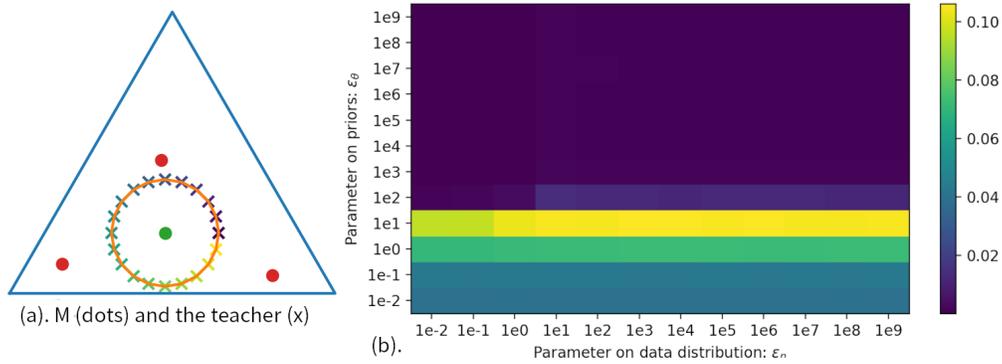


Figure 3: Influence of  $\epsilon$  on the average distance between stable posterior and the Euclidean barycenter of each posterior period. (a) The setup,  $M$  and the teaching path. (b). the result. With the asymptotic average diverging distance of each period represented by colors of each cell, and the parameter  $\epsilon$  represented by positions, it can be seen from the figure that when  $\epsilon_\theta$  is large, the average posterior tends to converge and fail to detect the periodicity of teacher. The most sensitive  $\epsilon$  occurs when  $\epsilon_\theta \approx 10$ .

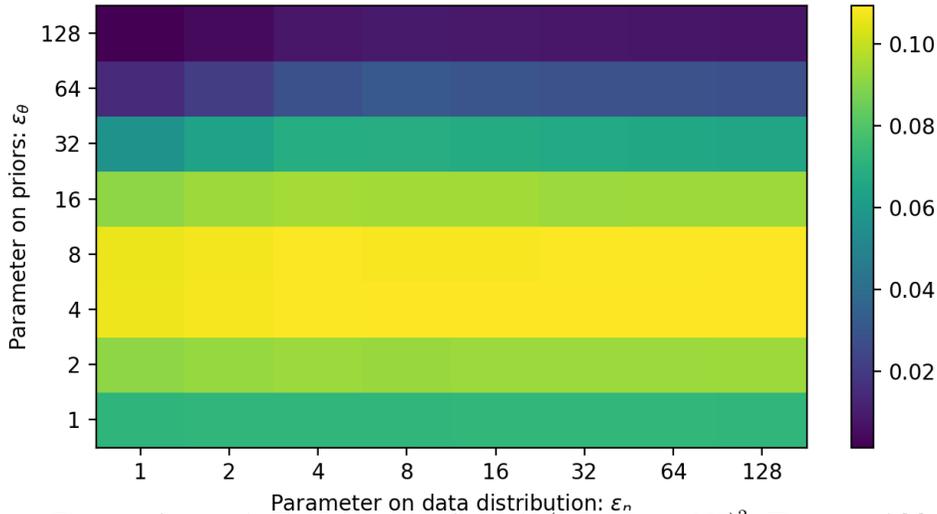


Figure 4: The same figure as in Fig. 3 (b), with a finer grid  $(1, 2, 4, 8, \dots, 128)^2$ . The setup of  $M$  and the teacher stays the same as in Fig. 3 (a)

loop). In Fig. 5, the area ratio roughly follows a linear relation to the area of the 3 columns of  $M$  (equivalently, a constant times  $\det(M)$ ). A linear regression with the  $R$  value 0.997 shows that the slope is 0.318 and the intercept is 0.005.

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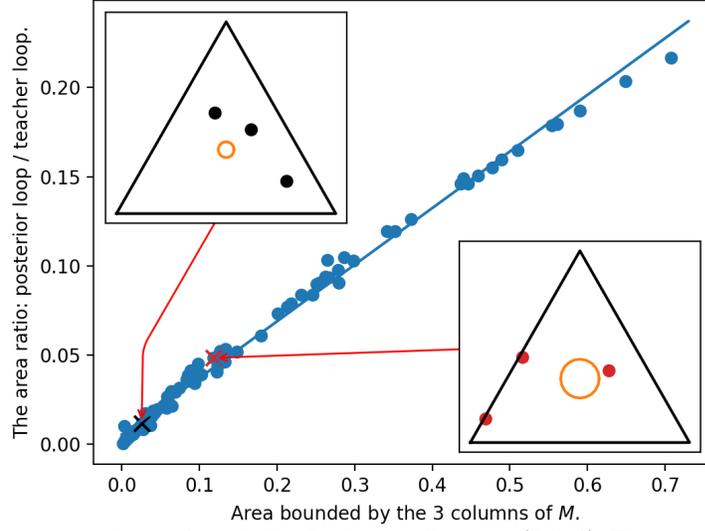


Figure 5: Area ratio v.s. the area bounded by 3 columns of  $M$ .  $\epsilon = (1, 1, 1)$ . There are 69 points plotted. The small figures show the setup — matrix  $M$  and the teaching path — for two of the points in the plot.

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