

# Tsallis Regularized Optimal Transport and Ecological Inference — Supplementary Material —

## Abstract

This is the supplementary material to the AAAI'17 paper "Tsallis Regularized Optimal Transport and Ecological Inference", by B. Muzellec, R. Nock, G. Patrini and F. Nielsen.

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## Supplementary Material: proofs

### 2 Proof of Theorem 3

The proof encompasses a more general statement than that of Theorem 3 since we show that  $M$  may actually not even be a distance matrix for the Theorem to hold.

( $\star$ ) Let  $M \in \mathbb{R}_+^{n \times n}$  be a distance matrix, and  $q, q' \in \mathbb{R} - \{1\}, q \neq q'$  (the case when  $q = 1$  xor  $q' = 1$  can be treated in a similar fashion). We suppose wlog that the support does not reduce to a singleton (otherwise the solution to optimal transport is trivial). Rescaling  $M$  and a constant row vector and a constant column vector, the solution of  $\text{TROT}(q, \lambda, M)$  can be written wlog as

$$p_{ij} = \exp_q(-1) \exp_q^{-1}(m_{ij}) . \quad (1)$$

Assume there exists a  $\lambda' \in \mathbb{R}$  such that the solution of  $\text{TROT}(q', \lambda', M)$  is equal to that of  $\text{TROT}(q, \lambda, M)$ . This is equivalent to saying that there exists  $\alpha, \beta \in \mathbb{R}^n$  such that

$$\exp_q(m_{ij}) = \exp_{q'}(\alpha_i + \lambda' m_{ij} + \beta_j) , \forall i, j . \quad (2)$$

Composing with  $\log_{q'}$  and rearranging, this implies that

$$f_{q',q}^{\lambda'}(m_{ij}) = \alpha_i + \beta_j , \forall i, j , \quad (3)$$

where

$$f_{q',q}^{\lambda'}(x) \doteq \log_{q'} \circ \exp_q - \lambda' \text{Id} . \quad (4)$$

Now, remark that, since  $M$  is a distance,  $m_{ii} = 0, \forall i$  because of the identity of the indiscernibles, and so  $\alpha_i + \beta_i = f_{q',q}^{\lambda'}(0) = 0$ , implying  $\alpha = -\beta$ .  $f_{q',q}^{\lambda'}$  is differentiable. Let:

$$\begin{aligned} g_{q',q}^{\lambda'}(x) &\doteq \frac{d}{dx} f_{q',q}^{\lambda'}(x) \\ &= \exp_q^{q-q'}(x) - \lambda' ; \\ h_{q',q}^{\lambda'}(x) &\doteq \frac{d}{dx} g_{q',q}^{\lambda'}(x) \\ &= (q - q') \cdot \exp_q^{2q-q'-1}(x) . \end{aligned} \quad (5)$$

If we assume wlog that  $q > q'$ , then  $g_{q',q}^{\lambda'}$  is increasing and zeroes at most once over  $\mathbb{R}$ , eventually on some  $m^*$  that we define as:

$$m^* \doteq \begin{cases} \log_q \left( \lambda'^{\frac{1}{q-q'}} \right) & \text{if } (\lambda' > 1) \wedge (0 \in \text{Im} g_{q',q}^{\lambda'}) \\ +\infty & \text{otherwise} \end{cases} . \quad (7)$$

Notice that  $m^* > 0$  and  $f_{q',q}^{\lambda'}$  is bijective over  $(0, m^*)$ . Suppose wlog that  $m_{ij} \leq m^*, \forall i, j$ . Otherwise, all distances are scaled by the same real so that  $m_{ij} \leq m^*, \forall i, j$ :

this does not alter the property of  $M$  being a distance. A distance being symmetric, we also have  $m_{ij} = m_{ji}$  and since  $f_{q',q}^{\lambda'}$  is strictly increasing in the range of distances, then we get from eq. (3) that  $\alpha_i + \beta_j = \alpha_j + \beta_i, \forall i, j$  and so  $\alpha_i - \alpha_j = \beta_i - \beta_j = -(\alpha_i - \alpha_j)$  (since  $\alpha = -\beta$ ). Hence, there exists a real  $\alpha$  such that  $\alpha = \alpha \cdot \mathbf{1}$ . We get, in matrix form

$$f_{q',q}^{\lambda'}(M) = \alpha \mathbf{1}^\top + \mathbf{1} \beta^\top \quad (8)$$

$$= \alpha \cdot \mathbf{1} \mathbf{1}^\top - \alpha \cdot \mathbf{1} \mathbf{1}^\top = 0 . \quad (9)$$

Hence,  $m_{ij} = m_{ii}, \forall i, j$  and the support reduces to a singleton (because of the identity of the indiscernibles), which is impossible.

( $\star$ ) Remark that the proof also works when  $M$  is not a distance anymore, but for example contains all arbitrary non negative matrices. To see this, we remark that the right hand side of eq. (8) is a matrix of rank no larger than 2. Since  $f_{q',q}^{\lambda'}$  is continuous, we have

$$\text{Im}(f_{q',q}^{\lambda'}) \doteq \mathcal{J} \subseteq \mathbb{R}$$

where  $\mathcal{J}$  is not reduced to a singleton and so the left hand side of eq. (8) spans matrices of arbitrary rank. Hence, eq. (8) cannot always hold.

### 3 Proof of Theorem 4

Denote

$$f_{ij} : p_{ij} \rightarrow p_{ij} m_{ij} - \frac{1}{\lambda(1-q)} (p_{ij}^q - p_{ij}) .$$

$f_{ij}$  is twice differentiable on  $\mathbb{R}_{+*}$ , and

$$\frac{d^2}{dx^2} f_{ij}(x) = \frac{q}{\lambda} x^{q-2} > 0$$

for any fixed  $q > 0$ , and so  $f_{ij}$  is strictly convex on  $\mathbb{R}_{+*}$ . We also remark that  $U(\mathbf{r}, \mathbf{c})$  is a non-empty compact subset of  $\mathbb{R}^{n \times n}$ . Indeed,  $\mathbf{r} \mathbf{c}^\top \in U(\mathbf{r}, \mathbf{c}), \forall P \in U(\mathbf{r}, \mathbf{c}), \|P\|_1 = 1$  (which proves boundedness) and  $U(\mathbf{r}, \mathbf{c})$  is a closed subset of  $U(\mathbf{r}, \mathbf{c})$  (being the intersection of the pre-images of singletons by continuous functions). Hence, since  $\langle P, M \rangle - \frac{1}{\lambda} H_q(P) = \sum_{i,j} f_{ij}(p_{ij})$ , there exists a unique minimum of this function in  $U(\mathbf{r}, \mathbf{c})$ .

To prove the analytic shape of the solution, we remark that  $\text{TROT}(q, \lambda, M)$  consists in minimizing a convex function given a set of affine constraints, and so the KKT conditions are necessary and sufficient. The KKT conditions give

$$p_{ij} = \exp_q(-1) \exp_q^{-1}(\alpha_i + \lambda m_{ij} + \beta_j) ,$$

where  $\alpha, \beta \in \mathbb{R}^n$  are Lagrange multipliers.

Finally, let us show that Lagrange multipliers  $\alpha, \beta \in \mathbb{R}^n$  are unique up to an additive constant. Assume that  $\alpha, \alpha', \beta, \beta' \in \mathbb{R}^n$  are such that

$$\begin{aligned} \forall i, j, p_{ij} &= \exp_q(-1) \exp_q^{-1}(\lambda m_{ij} + \alpha_i + \beta_j) \\ &= \exp_q(-1) \exp_q^{-1}(\lambda m_{ij} + \alpha'_i + \beta'_j) , \end{aligned}$$

where  $P$  is the unique solution of  $\text{TROT}(q, \lambda, M)$ . This implies

$$\alpha_i + \beta_j = \alpha'_i + \beta'_j, \forall i, j ,$$

*i.e.*

$$\alpha_i - \alpha'_i = \beta'_j - \beta_j, \forall i, j .$$

In particular, if there exists  $i_0$  and  $C \neq 0$  such that  $\alpha_{i_0} - \alpha'_{i_0} = C$ , then  $\forall j, \beta'_j = \beta_j + C$  and in turn  $\forall i, \alpha_i = \alpha'_i + C$ , which proves our claim.

## 4 Proof of Theorems 5 and 6

For reasons that we explain now, we will in fact prove Theorem 6 before we prove Theorem 5.

Had we chosen to follow [4], we would have replaced  $\text{TROT}(q, \lambda, M)$  by:

$$d_{M, \alpha, q}(\mathbf{r}, \mathbf{c}) \doteq \min_{\substack{P \in U(\mathbf{r}, \mathbf{c}) \\ H_q(P) - H_q(\mathbf{r}) - H_q(\mathbf{c}) \geq \alpha}} \langle P, M \rangle , \quad (10)$$

for some  $\alpha > 0$ . Both problems are equivalent since  $\lambda$  in  $\text{TROT}(q, \lambda, M)$  plays the role of the Lagrange multiplier for the entropy constraint in eq. (10) [4, Section 3], and so *there exists* an equivalent value of  $\alpha^*$  for which both problems coincide:

$$d_{M, \alpha^*, q}(\mathbf{r}, \mathbf{c}) = d_M^{\lambda^*, q}(\mathbf{r}, \mathbf{c}) , \quad (11)$$

so eq. (10) indeed matches  $\text{TROT}(q, \lambda, M)$ . It is clear from eq. (11) that  $\alpha$  does not depend solely on  $\lambda$ , *but also* (eventually) on all other parameters, including  $\mathbf{r}, \mathbf{c}$ .

This would not be a problem to state the triangle inequality *for*  $d_{M, \alpha, q}$ , as in [4] ( $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \Delta_n$ ):

$$d_{M, \alpha, q}(\mathbf{x}, \mathbf{z}) \leq d_{M, \alpha, q}(\mathbf{x}, \mathbf{y}) + d_{M, \alpha, q}(\mathbf{y}, \mathbf{z}) . \quad (12)$$

However,  $\alpha$  is *fixed* and in particular different from the  $\alpha^*$  that guarantee eq. (11) — and there might be three different sets of parameters for  $d_M^{\lambda, q}$  as it would equivalently appear from eq. (12). Under the simplifying assumption that only  $\lambda$  changes, we might just get from eq. (12):

$$d_M^{\lambda^*, q}(\mathbf{x}, \mathbf{z}) \leq d_M^{\lambda^*, q}(\mathbf{x}, \mathbf{y}) + d_M^{\lambda''^*, q}(\mathbf{y}, \mathbf{z}) , \quad (13)$$

with  $\lambda^* \neq \lambda'^* \neq \lambda''^*$ . Worse, the transportation plans may change with  $\lambda$ : for example, we may have

$$\arg \min_{P \in U(\mathbf{x}, \mathbf{z})} d_M^{\lambda_1, q}(\mathbf{x}, \mathbf{z}) \neq \arg \min_{P \in U(\mathbf{x}, \mathbf{z})} d_M^{\lambda_2, q}(\mathbf{x}, \mathbf{z}) ,$$

with  $\lambda_1 \neq \lambda_2$  and  $\lambda_1, \lambda_2 \in \{\lambda^*, \lambda'^*, \lambda''^*\}$ . So, the triangle inequality for  $d_M^{\lambda, q}$  that follows from ineq. (12) does not allow to control the parameters of  $\text{TROT}(q, \lambda, M)$  nor the optimal transportation plans that follows. It does not show a problem in regularizing the optimal transport distance, but rather that the distance  $d_{M, \alpha, q}$  chosen from eq. (11) does not completely fulfill its objective in showing that regularization in  $d_M^{\lambda, q}$  still keeps some of the attractive properties that unregularized optimal transport meets.

To bypass this problem and establish a statement involving a distance in which all parameters are in the clear and optimal transportation plans still coincide with  $d_M^{\lambda, q}$ , we chose to rely on measure:

$$d_M^{\lambda, q, \beta}(\mathbf{r}, \mathbf{c}) \doteq \min_{P \in U(\mathbf{r}, \mathbf{c})} \langle P, M \rangle - \frac{1}{\lambda} \cdot (H_q(P) - \beta \cdot (H_q(\mathbf{r}) + H_q(\mathbf{c}))) ,$$

where  $\beta$  is some *constant*. There is one trivial but crucial fact about  $d_M^{\lambda, q, \beta}(\mathbf{r}, \mathbf{c})$ : regardless of the choice of  $\beta$ , its optimal transportation plan is the *same* as for  $\text{TROT}(q, \lambda, M)$ .

**Lemma 1** *For any  $\mathbf{r}, \mathbf{c} \in \Delta_n$  and constant  $\beta \in \mathbb{R}$ , let*

$$P_1 \doteq \arg \min_{P \in U(\mathbf{r}, \mathbf{c})} \langle P, M \rangle - \frac{1}{\lambda} \cdot (H_q(P) - \beta \cdot (H_q(\mathbf{r}) + H_q(\mathbf{c}))) . \quad (14)$$

$$P_2 \doteq \arg \min_{P \in U(\mathbf{r}, \mathbf{c})} \langle P, M \rangle - \frac{1}{\lambda} \cdot (H_q(P)) . \quad (15)$$

Then  $P_1 = P_2$ .

**Theorem 2** *The following holds for any fixed  $q \geq 1$  (unless otherwise stated):*

- for **any**  $\beta \geq 1$ ,  $d_M^{\lambda, 1, \beta}$  satisfies the triangle inequality;
- for the choice  $\beta = 1/2$ ,  $d_M^{\lambda, q, 1/2}$  satisfies the following weak version of the identity of the indiscernibles: if  $\mathbf{r} = \mathbf{c}$ , then  $d_M^{\lambda, q, 1/2}(\mathbf{r}, \mathbf{c}) \leq 0$ .
- for the choice  $\beta = 1/2$ ,  $\forall \mathbf{r} \in \Delta_n$ , choosing the (no) transportation plan  $P = \text{Diag}(\mathbf{r})$  brings

$$\langle P, M \rangle - \frac{1}{\lambda} \cdot \left( H_q(P) - \frac{1}{2} \cdot (H_q(\mathbf{r}) + H_q(\mathbf{r})) \right) = 0 .$$

**Remark:** the last property is trivial but worth stating since the (no) transportation plan  $P = \text{Diag}(\mathbf{r})$  also satisfies  $P = \arg \min_{Q \in U(\mathbf{r}, \mathbf{r})} \langle Q, M \rangle$ , which zeroes the (no) transportation distance  $d_M(\mathbf{r}, \mathbf{r})$ . Remark that in this case,  $P = \text{Diag}(\mathbf{r})$  amounts to making no transportation in the support of the marginal, hence the "(no) transportation" name.

**Proof** To prove the Theorem, we need another version of the Gluing Lemma with entropic constraints [4, Lemma 1], generalized to handle Tsallis entropy.

**Lemma 3 (Refined gluing Lemma)** Let  $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \Delta_n$ . Let  $P \in U(\mathbf{x}, \mathbf{y})$  and  $Q \in U(\mathbf{y}, \mathbf{z})$ . Let  $S \in \mathbb{R}^{n \times n}$  defined by general term

$$s_{ik} \doteq \sum_j \frac{p_{ij} q_{jk}}{y_j} . \quad (16)$$

The following holds about  $S$ :

1.  $S \in U(\mathbf{x}, \mathbf{z})$ ;
2. if  $q \geq 1$ , then:

$$\begin{aligned} H_q(S) - H_q(\mathbf{x}) - H_q(\mathbf{z}) \\ \geq H_q(P) - H_q(\mathbf{x}) - H_q(\mathbf{y}) . \end{aligned} \quad (17)$$

**Proof** The proof essentially builds upon [4, Lemma 1]. We remark that  $S$  can be built by

$$s_{ik} = \sum_j t_{ijk} , \quad (18)$$

where  $\forall i, j, k \in \{1, 2, \dots, n\}$ , we have

$$t_{ijk} \doteq \begin{cases} \frac{p_{ij} q_{jk}}{y_j} & \text{if } y_j \neq 0 \\ 0 & \text{otherwise} \end{cases} . \quad (19)$$

$S$  is a transportation matrix between  $\mathbf{x}$  and  $\mathbf{z}$ . Indeed,

$$\begin{aligned} \sum_i \sum_j s_{ijk} &= \sum_j \sum_i \frac{p_{ij} q_{jk}}{y_j} \\ &= \sum_j \frac{q_{jk}}{y_j} \sum_i p_{ij} \\ &= \sum_j \frac{q_{jk}}{y_j} y_j = \sum_j q_{jk} = z_k ; \\ \sum_k \sum_j s_{ijk} &= \sum_j \sum_k \frac{p_{ij} q_{jk}}{y_j} \\ &= \sum_j \frac{p_{ij}}{y_j} \sum_k q_{jk} \\ &= \sum_j \frac{p_{ij}}{y_j} y_j = \sum_j p_{ij} = x_i . \end{aligned}$$

So,  $S \in U(\mathbf{x}, \mathbf{z})$ . To prove ineq. (17), we need the following definition from [6].

**Definition 4** [6] *Let  $X$  and  $Y$  denote random variables. The Tsallis conditional entropy of  $X$  given  $Y$ , and Tsallis joint entropy of  $X$  and  $Y$ , are respectively given by:*

$$\begin{aligned} H_q(X|Y) &\doteq - \sum_{x,y} p(x,y)^q \log_q p(x|y) , \\ H_q(X, Y) &\doteq - \sum_{x,y} p(x,y)^q \log_q p(x,y) . \end{aligned}$$

The Tsallis mutual entropy of  $X$  and  $Y$  is defined by

$$\begin{aligned} I_q(X; Y) &\doteq H_q(X) - H_q(X|Y) \\ &= H_q(X) + H_q(Y) - H_q(X, Y) . \end{aligned}$$

We have made use of the simplifying notation that removes variables names when unambiguous, like  $p(x) \doteq p(X = x)$ . Let  $X, Y, Z$  be random variables jointly distributed as  $T$ , that is, for any  $x, y, z$ ,

$$p(x, y, z) = \frac{p(x, y)p(y, z)}{p(y)} \quad (20)$$

It follows from that and Bayes rule that:

$$\begin{aligned} p(x|y) &= \frac{p(x, y)}{p(y)} \\ &= \frac{p(x, y, z)}{p(y, z)} , \forall z \\ &= p(x|y, z) , \forall z , \end{aligned} \quad (21)$$

and so

$$\begin{aligned} I_q(X; Z|Y) &\doteq H_q(X|Y) - H_q(X|Y, Z) \\ &= 0 . \end{aligned} \quad (22)$$

It comes from [6, Theorem 4.3],

$$I_q(X; Y, Z) = I_q(X; Z) + I_q(X; Y|Z) \quad (23)$$

$$= I_q(X; Y) + I_q(X; Z|Y) , \quad (24)$$

but since  $I_q(X; Z|Y) = 0$ , we obtain

$$I_q(X; Y) = I_q(X; Z) + I_q(X; Y|Z) . \quad (25)$$

It also follows from [6, Theorem 3.4] that  $I_q(X; Y|Z) \geq 0$  whenever  $q \geq 1$ , and so

$$I_q(X; Y) \geq I_q(X; Z) , \forall q \geq 1 . \quad (26)$$

Now, it comes from Definition 4 and the definition of  $X, Y$  and  $Z$  from eq. (20),

$$\begin{aligned} -I_q(X; Y) &= H_q(X, Y) - H_q(X) - H_q(Y) \\ &= H_q(P) - H_q(\mathbf{x}) - H_q(\mathbf{y}) , \end{aligned} \quad (27)$$

$$\begin{aligned} -I_q(X; Z) &= H_q(X, Z) - H_q(X) - H_q(Z) \\ &= H_q(S) - H_q(\mathbf{x}) - H_q(\mathbf{z}) . \end{aligned} \quad (28)$$

Since  $P \in U_\lambda(\mathbf{x}, \mathbf{y})$ , by assumption, we obtain from ineq. (26) that whenever  $q \geq 1$ ,

$$H_q(S) - H_q(\mathbf{x}) - H_q(\mathbf{z}) \geq H_q(P) - H_q(\mathbf{x}) - H_q(\mathbf{y}) ,$$

as claimed. ■

We can now prove Theorem 2. Shannon's entropy is denoted  $H_1$  for short.

Define for short

$$\Delta \doteq H_1(P) + H_1(Q) - H_1(S) - 2\beta \cdot H_1(\mathbf{y}) , \quad (29)$$

where  $P, Q, S$  are defined in Lemma 3. It follows from the definition of  $S$  and [4, Proof of Theorem 1] that

$$\begin{aligned} d_M^{\lambda, q, \beta}(\mathbf{x}, \mathbf{z}) &\doteq \min_{R \in U(\mathbf{x}, \mathbf{z})} \langle R, M \rangle - \frac{1}{\lambda} \cdot (H_1(R) - \beta \cdot (H_1(\mathbf{x}) + H_1(\mathbf{z}))) \\ &\leq \langle S, M \rangle - \frac{1}{\lambda} \cdot (H_1(S) - \beta \cdot (H_1(\mathbf{x}) + H_1(\mathbf{z}))) \\ &\leq \langle P, M \rangle + \langle Q, M \rangle - \frac{1}{\lambda} \cdot (H_1(S) - \beta \cdot (H_1(\mathbf{x}) + H_1(\mathbf{z}))) \\ &= \langle P, M \rangle - \frac{1}{\lambda} \cdot (H_1(P) - \beta \cdot (H_1(\mathbf{x}) + H_1(\mathbf{y}))) \\ &\quad + \langle Q, M \rangle - \frac{1}{\lambda} \cdot (H_1(Q) - \beta \cdot (H_1(\mathbf{y}) + H_1(\mathbf{z}))) \\ &\quad + \frac{1}{\lambda} \cdot (H_1(P) + H_1(Q) - H_1(S) - 2\beta \cdot H_1(\mathbf{y})) \\ &\doteq d_M^{\lambda, q, \beta}(\mathbf{x}, \mathbf{y}) + d_M^{\lambda, q, \beta}(\mathbf{y}, \mathbf{z}) + \frac{1}{\lambda} \cdot \Delta . \end{aligned} \quad (30)$$

We now show that  $\Delta \leq 0$ . For this, observe that ineq. (17) yields:

$$\begin{aligned} \Delta &\leq (H_1(S) + H_1(\mathbf{y}) - H_1(\mathbf{z})) \\ &\quad + H_1(Q) - H_1(S) - 2\beta \cdot H_1(\mathbf{y}) \\ &= H_1(Q) - H_1(\mathbf{y}) - H_1(\mathbf{z}) + 2(1 - \beta)H_1(\mathbf{y}) , \end{aligned} \quad (31)$$

and, by definition of  $Q, \mathbf{y}, \mathbf{z}$ ,

$$\begin{aligned} H_1(Q) - H_1(\mathbf{y}) - H_1(\mathbf{z}) &\doteq H_1(Y, Z) - H_1(Y) - H_1(Z) . \end{aligned} \quad (32)$$



Shannon's entropy of a joint distribution is maximal with independence:  $H_1(Y, Z) \leq H_1(Y \times Z) = H_1(Y) + H_1(Z)$ , so we get from eq. (31) after simplifying

$$\Delta \leq 2(1 - \beta)H_1(\mathbf{y}) . \quad (33)$$

Hence if  $\beta \geq 1$ , then  $\Delta \leq 0$ . We get that for any  $\beta \geq 1$ ,

$$d_M^{\lambda,1,\beta}(\mathbf{x}, \mathbf{z}) \leq d_M^{\lambda,1,\beta}(\mathbf{x}, \mathbf{y}) + d_M^{\lambda,1,\beta}(\mathbf{y}, \mathbf{z}) , \quad (34)$$

and  $d_M^{\lambda,1,\beta}$  satisfies the triangle inequality. For  $\beta = 1/2$ , it is trivial to check that for any  $\mathbf{x} \in \Delta_n$ , the (no) transportation plan  $P = \text{Diag}(\mathbf{x})$  is in  $U(\mathbf{x}, \mathbf{x})$  and satisfies

$$\begin{aligned} \langle P, M \rangle - \frac{1}{\lambda} \cdot \left( H_q(P) - \frac{1}{2} \cdot (H_q(\mathbf{x}) + H_q(\mathbf{x})) \right) \\ = 0 - \frac{1}{\lambda} \cdot (H_q(\mathbf{x}) - H_q(\mathbf{x})) = 0 . \end{aligned} \quad (35)$$

This ends the proof of Theorem 2. ■

Notice that Theorem 6 is in fact a direct consequence of Theorem 2. To finish up, we now prove Theorem 5. To simplify notations, let

$$U_\alpha(\mathbf{r}, \mathbf{c}) \doteq \left\{ \begin{array}{l} P \in U(\mathbf{r}, \mathbf{c}) : \\ H_q(P) - H_q(\mathbf{r}) - H_q(\mathbf{c}) \geq \alpha(\lambda) \end{array} \right\} . \quad (36)$$

Suppose  $P, Q$  in Lemma 3 are such that  $P, Q \in U_\lambda(\mathbf{x}, \mathbf{y})$ . In this case,

$$H_q(P) - H_q(\mathbf{x}) - H_q(\mathbf{y}) \geq \alpha \quad (37)$$

and so point 2. in Lemma 3 brings

$$H_q(S) - H_q(\mathbf{x}) - H_q(\mathbf{z}) \geq \alpha , \quad (38)$$

so  $S \in U_\lambda(\mathbf{x}, \mathbf{z})$ . The proof of [4, Theorem 1] can then be used to show that  $\forall \mathbf{x}, \mathbf{y}, \mathbf{z} \in \Delta_n$ ,

$$d_{M,\alpha,q}(\mathbf{x}, \mathbf{z}) \leq d_{M,\alpha,q}(\mathbf{x}, \mathbf{y}) + d_{M,\alpha,q}(\mathbf{y}, \mathbf{z}) . \quad (39)$$

It is easy to check that  $d_{M,\alpha,q}$  is non negative and that  $\mathbb{1}_{\{\mathbf{r}=\mathbf{c}\}}d_{M,\alpha,q}(\mathbf{r}, \mathbf{c})$  meets, in addition, the identity of the indiscernibles. This achieves the proof of Theorem 5.

## 5 Proof of Theorem 7

**Basic facts and definitions** — In this proof, we make two simplifying assumptions: (i) we consider matrices either as matrices or as vectorized matrices without ambiguity, and (ii) we let  $\phi(P) \doteq -H_q(P)$ , noting that the domain of  $\phi$  is  $\Delta_{n^2}$  (nonnegative matrices with row- and column-sums in the simplex) when  $P \in U(\mathbf{r}, \mathbf{c})$ . Since  $\phi$  is convex, we can define a *Bregman divergence* with generator  $D_\phi$  [2] as:

$$D_\phi(P||R) \doteq \phi(P) - \phi(R) - \langle \nabla \phi(R), P - R \rangle .$$

We define

$$a_{ij} \doteq \alpha_i + \lambda m_{ij} + \beta_j , \quad (40)$$

so that

$$p_{ij} = \exp_q(-1) \exp_q^{-1}(a_{ij}) \quad (41)$$

in eq. (7) (main file). Finally, let us denote for short

$$D_q(P\|R) \doteq K_{1/q}(P^q, R^q) , \quad (42)$$

so that we can, reformulate eq. (6) (main file) as:

$$d_M^{\lambda, q}(\mathbf{r}, \mathbf{c}) = \frac{1}{\lambda} \cdot \min_{P \in U(\mathbf{r}, \mathbf{c})} D_q(P\|\tilde{U}) + g(M) , \quad (43)$$

and our objective "reduces" to the minimization of  $D_q(P\|\tilde{U})$  over  $U(\mathbf{r}, \mathbf{c})$ . In so-TROT (Algorithm 1), we just care for a single constraint out of the two possible in  $U(\mathbf{r}, \mathbf{c})$ , so we will focus without loss of generality on the row constraint and therefore to the solution of:

$$P^* \doteq \arg \min_{P \in \mathbb{R}_+^{n \times n} : P\mathbf{1} = \mathbf{r}} D_q(P\|\tilde{U}) . \quad (44)$$

The same result would apply to the column constraint.

**Convergence proof** — We reuse the theory of *auxiliary functions* developed for the iterative constrained minimization of Bregman divergences [2, 5]. We reuse notation "◊" following [3, 7] and define for any  $\mathbf{y} \in \mathbb{R}^n$ ,  $P \in \mathbb{R}^{n \times n}$  matrix  $\mathbf{y} \diamond_q P \in \mathbb{R}^{n \times n}$  such that

$$\begin{aligned} (\mathbf{y} \diamond_q P)_{ij} & \\ & \doteq \frac{\exp_q^{-1}(y_i) p_{ij}}{\exp_q \left[ (1-q) y_i \exp_q^{1-q}(y_i) \log_q(p_{ij}) \right]} . \end{aligned} \quad (45)$$

We also define key matrix  $\tilde{P} \in \mathbb{R}^{n \times n}$  with:

$$\tilde{P} \doteq \mathbf{r} \mathbf{c}^\top . \quad (46)$$

Let us denote

$$\begin{aligned} \mathcal{Q} & \doteq \left\{ \begin{array}{l} Q \in \mathbb{R}^{n \times n} : \\ Q = \exp_q(-1) \exp_q^{-1}(\boldsymbol{\alpha}^\top \mathbf{1} + \lambda M + \mathbf{1}^\top \boldsymbol{\beta}) , \text{ with } \boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{R}^n \end{array} \right\} . \\ \mathcal{P} & \doteq \{ P \in \Delta_{n^2} : P\mathbf{1} = \tilde{P}\mathbf{1} = \mathbf{r} \} . \end{aligned}$$

One function will be key.

**Definition 5** We define  $A(P, \mathbf{y}) \doteq \sum_i A_i(P, \mathbf{y})$ , with:

$$\begin{aligned} A_i(P, \mathbf{y}) & \doteq y_i r_i + \sum_j (p_{ij}^q - \exp_q^q(-1) \exp_q^{-q}(a_{ij} - y_i)) . \end{aligned} \quad (47)$$

Here  $a_{ij}$  is defined in eq. (40),  $r_i$  is the  $i$ -th coordinate in  $\mathbf{r}$  (the row marginal constraint), and  $\mathbf{y} \in \mathbb{R}^n$ .

**Lemma 6** For any  $\mathbf{y}$ ,

$$A(P, \mathbf{y}) = D_\phi(\tilde{P} \| P) - D_\phi(\tilde{P} \| \mathbf{y} \diamond_q P) . \quad (48)$$

Furthermore,  $A(P, \mathbf{0}) = 0$ .

**Proof** We have

$$\begin{aligned} & D_\phi(\tilde{P} \| P) - D_\phi(\tilde{P} \| \mathbf{y} \diamond_q P) \\ & = -D_\phi(P \| \mathbf{y} \diamond_q P) \\ & \quad + \langle \tilde{P} - P, \nabla \phi(\mathbf{y} \diamond_q P) - \nabla \phi(P) \rangle . \end{aligned}$$

■

Because a Bregman divergence is non-negative and  $A(P, \mathbf{0}) = 0$ , if, as long as there exists some  $\mathbf{y}$  for which  $A(P, \mathbf{y}) > 0$  we keep on updating  $P$  by replacing it by  $\mathbf{y}^* \diamond_q P$  such that  $A(P, \mathbf{y}^*) > 0$ , then the sequence

$$P_0 = \tilde{U} \rightarrow P_1 \doteq \mathbf{y}_0^* \diamond_q P_0 \rightarrow P_2 \doteq \mathbf{y}_1^* \diamond_q P_1 \cdots \quad (49)$$

will converge to a limit matrix in the sequence,

$$\lim_j P_j \doteq \mathbf{y}_{j-1}^* \diamond_q P_{j-1} . \quad (50)$$

This matrix turns out to be the one we seek.

**Theorem 7** Let  $P_{j+1} \doteq \mathbf{y}_j \diamond_q P_j$  (with  $P_0 \doteq \tilde{U}$ ) be such that  $A(P_j, \mathbf{y}_j) > 0, \forall j \geq 0$ , and the sequence ends when no such  $\mathbf{y}_j$  exists. Then  $\mathcal{S} \doteq \{P_j\}_{j \geq 0} \subset \mathcal{Q}$ . If furthermore  $\mathcal{S}$  lies in a compact of  $\bar{\mathcal{Q}}$ , then it satisfies

$$P^* \doteq \lim_j P_j = \arg \min_{P \in \mathcal{P}} D_q(P \| \tilde{U}) . \quad (51)$$

**Proof sketch:** The proof relies on two steps, first that

$$P^* \doteq \lim_j P_j = \arg \min_{P \in \mathcal{P}} D_\phi(P \| \tilde{U}) , \quad (52)$$

and then the fact that (51) holds as well, which "amounts" to replacing  $D_\phi$ , which is Bregman, by  $D_q$ , which is *not*. Because it is standard in Bregman divergences, we sketch the first step. The fundamental result we use is adapted from [5] (see also [3, Theorem 1]).

**Theorem 8** Suppose that  $D_\phi(\tilde{P}, \tilde{U}) < \infty$ . Then there exists a unique  $P^*$  satisfying the following four properties:

1.  $P^* \in \mathcal{P} \cap \bar{\mathcal{Q}}$
2.  $\forall P \in \mathcal{P}, \forall R \in \bar{\mathcal{Q}}, D_\phi(P\|R) = D_\phi(P\|P^*) + D_\phi(P^*\|R)$
3.  $P^* = \arg \min_{P \in \mathcal{P}} D_\phi(P\|\tilde{U})$
4.  $P^* = \arg \min_{R \in \bar{\mathcal{Q}}} D_\phi(\tilde{P}\|R)$

Moreover, any of these four properties determines  $P^*$  uniquely.

It is not hard to check that  $\tilde{U} \in \bar{\mathcal{Q}}$  and whenever  $P_j \in \bar{\mathcal{Q}}$ , then  $\mathbf{y} \diamond_q P_j \in \bar{\mathcal{Q}}, \forall \mathbf{y}$ , so we indeed have  $\mathcal{S} \subset \bar{\mathcal{Q}}$ . With the constraint that  $A(P_j, \mathbf{y}_j) > 0, \forall j \geq 0$ , it follows from Lemma 6 that  $A(P, \mathbf{y})$  is an auxiliary function for  $\mathcal{S}$  [3] if we can show in addition that if  $\mathbf{y} = \mathbf{0}$  is a maximum of  $A(P, \mathbf{y})$ , then  $P \in \mathcal{P}$ . To remark that this is true, we have

$$\nabla A(P, \mathbf{y})_{\mathbf{y}} = \mathbf{r} - P\mathbf{1} , \quad (53)$$

so whenever  $A(P, \mathbf{y})$  reaches a maximum in  $\mathbf{y}$ , we indeed have  $P\mathbf{1} = \mathbf{r}$  and so  $P \in \mathcal{P}$ , and if  $\mathbf{y} = \mathbf{0}$  then because a Bregman divergence satisfies the identity of the indiscernibles, if  $\mathbf{y} = \mathbf{0}$  is the maximum, then  $\mathcal{S}$  has converged to some  $P^*$ . From 4. above, we get

$$P^* = \arg \min_{R \in \bar{\mathcal{Q}}} D_\phi(\tilde{P}\|R) , \quad (54)$$

and so from 3. above, we also get

$$P^* = \arg \min_{P \in \mathcal{P}} D_\phi(P\|\tilde{U}) . \quad (55)$$

To "transfer" this result to  $D_q$ , we just need to remark that there is one remarkable trivial equality:

$$D_\phi(P\|R) = D_q(P\|R) - \sum_{i,j} (p_{ij}^q - r_{ij}^q) , \quad (56)$$

so that even when  $K_{1/q}$  is not a Bregman divergence for a general  $q$ , it still meets the Bregman triangle equality [1].

**Lemma 9** We have;

$$\begin{aligned} & D_q(P\|R) + D_q(R\|S) - D_q(P\|S) \\ &= D_\phi(P\|R) + D_\phi(R\|S) - D_\phi(P\|S) \\ &= \langle P - R, \nabla \phi(S) - \nabla \phi(R) \rangle . \end{aligned} \quad (57)$$

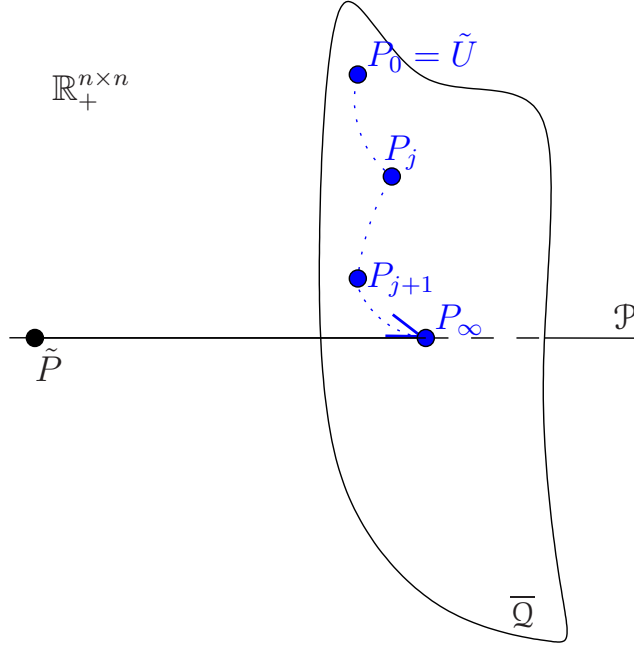


Figure 1: High level overview of the proof of Theorem 7 (see text for details).

Hence, point 2. implies as well

$$D_q(P\|R) = D_q(P\|P^*) + D_q(P^*\|R) , \quad (58)$$

$\forall P \in \mathcal{P}, \forall R \in \bar{Q}$ , and so  $D_q(P\|\tilde{U}) = D_q(P\|P^*) + D_q(P^*\|\tilde{U}), \forall P \in \mathcal{P}$ , so that we also have (since  $D_q$  is non negative and satisfies  $D_q(P\|P) = 0$ )

$$P^* = \arg \min_{P \in \mathcal{P}} D_q(P\|\tilde{U}) ,$$

as claimed (end of the proof of Theorem 7).  $\square$

Figure 1 summarizes Theorem 7. We are left with the problem of finding an auxiliary function for the sequence  $\mathcal{S}$ , which we recall boils down to finding, whenever it exists, some  $\mathbf{y}$  such that  $A(P, \mathbf{y}) > 0$ .

**Theorem 10**  $A(P, \mathbf{y})$  is an auxiliary function for  $\mathcal{S}$  for the sequence of updates  $\mathbf{y}$  given as in steps 6-11 of SO-TROT (Algorithm 1).

**Proof** We shall need the complete Taylor expansion of  $A(P, \mathbf{y})$ .

**Lemma 11** Let us denote for short  $\gamma \doteq 1 - q$ . The Taylor series expansion of  $A_i(P, \mathbf{y})$

(as defined in Definition 5) is:

$$\begin{aligned}
A_i(P, \mathbf{y}) &= y_i(r_i - \sum_j p_{ij}) \\
&\quad - \sum_j p_{ij} \sum_{k=2}^{\infty} \left[ \frac{1}{k} \prod_{l=1}^{k-1} (\gamma + q/l) \right] y_i^k \left( \frac{p_{ij}}{q} \right)^{k-1}. \tag{59}
\end{aligned}$$

**Proof** Let us denote  $f(x) = \exp_q^{-q}(x)$ . We have:

$$\begin{aligned}
\frac{d}{dx} f(x) &= q \exp_q^{1-q}(x) \frac{d}{dx} \exp_q^{-1}(x) \\
&= -q \exp_q^{-1}(x). \tag{60}
\end{aligned}$$

A simple recursion also shows ( $\forall k \geq 2$ ):

$$\begin{aligned}
\frac{d^k}{dx^k} \exp_q^{-1}(x) &= (-1)^k \left[ \prod_{i=1}^k (i - (i-1)q) \right] \exp_q^{kq - (k+1)}(x),
\end{aligned}$$

which yields  $\forall k \geq 1$ ,

$$\begin{aligned}
\frac{d^k}{dx^k} f(x) &= -q \frac{d^{k-1}}{dx^{k-1}} \exp_q^{-1}(x) \\
&= (-1)^k q \left[ \prod_{i=1}^{k-1} (i\gamma + q) \right] \exp_q^{-(k-1)\gamma - 1}(x).
\end{aligned}$$

Since  $\exp_q^q(-1) = \exp_q(-1)/q$  and  $\forall i, j, p_{ij} = \exp_q(-1) \exp_q^{-1}(a_{ij})$ , writing the Taylor development of  $f$  at point  $a_{ij}$  evaluated at  $y_i$ , and adding the  $y_i r_i + \sum_j p_{ij}^q$  term, we obtain the desired result. ■

We have two special reals to define,  $t_i$  and  $z_i$ . If  $r_i \leq \sum_j p_{ij}$ , we let  $t_i$  denote the maximum of the second order approximation of  $A_i(P, \mathbf{y})$ ,

$$T_i^{(2)}(y_i) \doteq y_i(r_i - \sum_j p_{ij}) - \frac{y_i^2}{2} \sum_j \frac{p_{ij}^{1+\gamma}}{q}, \tag{61}$$

i.e. the root of

$$\frac{d}{dy} T_i^{(2)}(y_i) = (r_i - \sum_j p_{ij}) - y_i \sum_j \frac{p_{ij}^{1+\gamma}}{q}.$$

If  $\sum_j p_{ij} \leq r_i$ , we let  $z_i$  be the the largest root of

$$\begin{aligned} R_i &\doteq (r_i - \sum_j p_{ij}) \\ &\quad - y_i \sum_j \frac{p_{ij}^{1+\gamma}}{q} - y_i^2 (2-q) \sum_j \frac{p_{ij}^{1+2\gamma}}{q^2} . \end{aligned} \quad (62)$$

We shall see that  $z_i$  is positive. Let  $y_i^* \doteq t_i$  if  $r_i \leq \sum_j p_{ij}$ , and  $y_i^* \doteq z_i$  otherwise. We first make the assumption that

$$\left| \frac{y_i^* p_{ij}^\gamma}{q} \cdot \left( \gamma + \frac{q}{3} \right) \right| \leq \frac{1}{2}, \forall i, j . \quad (63)$$

Under this assumption, we have two cases.

( $\star$ ) Case  $r_i \leq \sum_j p_{ij}$ . By definition, we have in this case that  $y_i = t_i \leq 0$  in SO-TROT (Step 10). We also have

$$\begin{aligned} A_i(P, \mathbf{y}) &= T^{(2)}(y_i) \\ &\quad - \underbrace{\sum_j p_{ij} \sum_{k=3}^{\infty} \left[ \frac{1}{k} \prod_{l=1}^{k-1} (\gamma + q/l) \right] y_i^k \left( \frac{p_{ij}^\gamma}{q} \right)^{k-1}}_{\doteq S_3} . \end{aligned} \quad (64)$$

Since  $y_i = t_i \leq 0$ ,  $S_3$  is an alternating series, that is a series whose general term is alternatively positive and negative. Under assumption (63), the module of its general term is decreasing. A classic result on series allows us to deduce from this fact that (a)  $S_3 \ll \infty$  and (b) the sign of  $S_3$  is that of its first term, *i.e.*, it is negative. Since  $A_i(P, \mathbf{y}) = T^{(2)}(y_i) - S_3$ , we have that

$$A_i(P, \mathbf{y}) \geq T^{(2)}(y_i) = 0 . \quad (65)$$

Note also that  $A_i(P, \mathbf{y}) = 0$  iff  $\sum_j p_{ij} = r_i$  as  $T^{(2)}(y_i)$  is decreasing on  $[t_i, 0]$  and  $T^{(2)}(0) = 0$ . Hence, for the choice in Step 10,  $A_i(P, \mathbf{y})$  is an auxiliary function for variable  $i$ .

( $\star$ ) Case  $\sum_j p_{ij} \leq r_i$ : we still have  $A_i(P, \mathbf{y}) = T^{(2)}(y_i) - S_3$ , but this time  $y_i$  will be positive, ensuring  $y_i(r_i - \sum_j p_{ij}) \geq 0$ . We first show that  $S_3$  is upperbounded by a

geometric series under assumption (63):

$$\begin{aligned}
S_3 &= \sum_j p_{ij} y_i^3 \left( \frac{p_{ij}^\gamma}{q} \right)^2 \sum_{k=0}^{\infty} \frac{y_i^k}{k+3} \left[ \prod_{l=1}^{k+2} (\gamma + q/l) \right] \left( \frac{p_{ij}^\gamma}{q} \right)^k \\
&\leq \sum_j p_{ij} (1 - q/2) \frac{y_i^3}{3} \left( \frac{p_{ij}^\gamma}{q} \right)^2 \sum_{k=0}^{\infty} \left( \frac{y_i p_{ij}^\gamma}{q} (\gamma + q/3) \right)^k \\
&= \sum_j p_{ij} (1 - q/2) \frac{y_i^3}{3} \left( \frac{p_{ij}^\gamma}{q} \right)^2 \times \frac{1}{1 - \frac{y_i p_{ij}^\gamma}{q} (\gamma + q/3)} \\
&\leq (2 - q) \sum_j p_{ij} \frac{y_i^3}{3} \left( \frac{p_{ij}^\gamma}{q} \right)^2,
\end{aligned}$$

which conveniently yields

$$A_i(P, \mathbf{y}) \geq T^{(2)}(y_i) - (2 - q) \sum_j p_{ij} \frac{y_i^3}{3} \left( \frac{p_{ij}^\gamma}{q} \right)^2. \quad (66)$$

The derivative of the right-hand term of (66) is  $R_i$  defined in eq. (62) above. Let us define:

$$a \doteq (2 - q) \sum_j \frac{p_{ij}^{1+2\gamma}}{q^2}, \quad (67)$$

$$b \doteq \sum_j \frac{p_{ij}^{1+\gamma}}{q}, \quad (68)$$

$$c \doteq -(r_i - \sum_j p_{ij}). \quad (69)$$

We have  $ac < 0$  and consequently the discriminant  $\Delta \doteq b^2 - 4ac > b^2$ , implying  $R_i$  has a positive root  $z_i \doteq (-b + \sqrt{\Delta})/(2a)$  which maximises the right-hand term of 66, and is such that this right-hand term is positive. Further, we again have that  $z_i = 0$  iff  $\sum_j p_{ij} = r_i$ . It is easy to check that  $z_i = y_i$  in Step 8 of SO-TROT, for which we check that  $A_i(P, \mathbf{y}) \geq 0$ , with equality iff  $\sum_j p_{ij} = r_i$ . Hence, for the choice in Step 8,  $A_i(P, \mathbf{y})$  is an auxiliary function for variable  $i$ .

We can now conclude that under assumption (63),  $A(P, \mathbf{y})$  is an auxiliary function.

If assumption (63) does not hold, then notice that this cannot hold at convergence for coordinate  $i$ . For this reason,  $r_i \neq \sum_j p_{ij}$  and the sign  $\text{sign}(r_i - \sum_j p_{ij})$  is also well defined. Therefore, we just need to pick a value for  $y_i \neq 0$  which guarantees



$A_i(P, \mathbf{y}) > 0$ . To do so, we pick

$$y_i = \frac{q \cdot \text{sign}(r_i - \sum_j p_{ij})}{(6 - 4q) \cdot \max_j p_{ij}^{1-q}}, \quad (70)$$

remarking that this  $y_i$  indeed violates (63) (recalling  $\gamma \doteq 1 - q$ ). We also have  $|y_i| \in (0, n^{2(1-q)}/2]$ . Notice that this choice guarantees  $A_i(P, \mathbf{y}) > 0$ . (end of the proof of Theorem 10) ■

Theorems 7 and 10 altogether prove Theorem 7.

## Supplementary Material: experiments

### 6 Per county error distribution, TROT survey vs Florida average

Figure 2 displays the empirical distribution of the errors for TROT vs Florida average. While not being a true distribution of the solution error of TROT — in a Bayesian sense —, the graph should convey the intuition that algorithms with a distribution that shrinks around zero provide better inference.

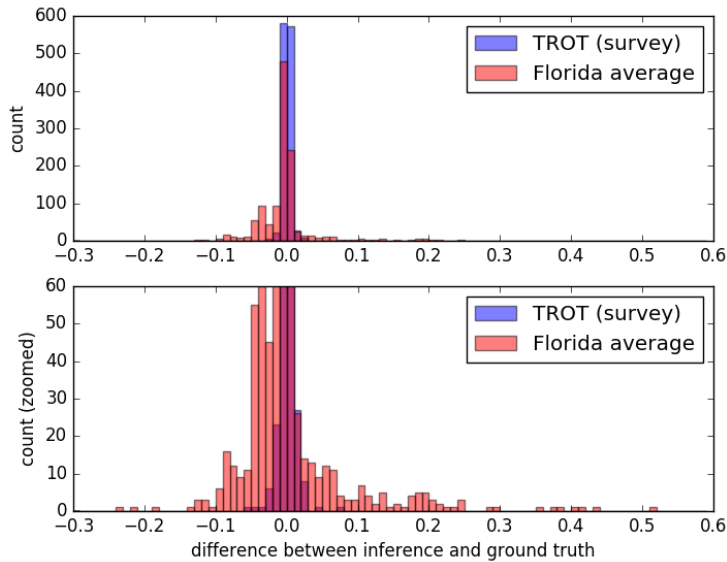


Figure 2: (Signed) error distribution of TROT compared to Florida-average.

## 7 Per county errors, TROT survey vs TROT $11^\top$

Figure 3 confronts the prediction errors by county of TROT when we use  $M = M^{\text{sur}}$  (survey) and  $M = M^{\text{no}} (= 11^\top)$  as cost matrix: while the overall performance of the two algorithms is very close, the graph demonstrates that TROT optimized with  $M^{\text{sur}}$  achieves very often smaller error, although the average error is worsen by few particularly bad counties.

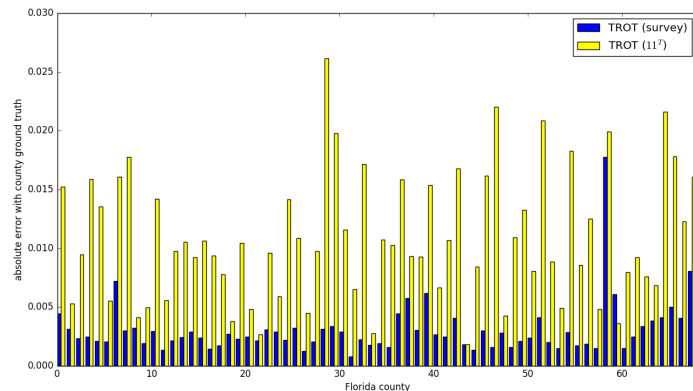


Figure 3: Absolute error of TROT optimized with  $M$  compared to with no prior.

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