NOTES ON ENTROPIC REGULARIZATION

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1. Statement

The original problem is

$$\begin{aligned} &\min \sum_{i,j} P_{ij} C_{ij} \\ &\text{s.t. } \mathbf{P}\mathbb{1} = \mathbf{a} \\ &\qquad \mathbf{P}^T \mathbb{1} = \mathbf{b} \end{aligned}$$

Denote the feasible region by $\mathbf{U}(\mathbf{a}, \mathbf{b})$. *Entropic regularization* considers the following modified problem:

$$L_{\mathbf{C}}^{\epsilon}(\mathbf{a}, \mathbf{b}) = \min_{\mathbf{P} \in \mathbf{U}(\mathbf{a}, \mathbf{b})} \sum_{i,j} P_{ij} C_{ij} + \epsilon \underbrace{\sum_{i,j} P_{ij} (\log P_{ij} - 1)}_{-H(\mathbf{P})}.$$

We can show that the negative entropy $-H(\mathbf{P})$ is 1-strongly convex (i.e. Hessian minus I is positive semi-definite). Thus the objective is ϵ-strongly convex. The strong convexity means that the optimum $\mathbf{P}_\epsilon$ is unique. Unsurprisingly, $\mathbf{P}_\epsilon \to \mathbf{P}^\star$ as $\epsilon \to 0$ where $\mathbf{P}^\star$ is the maximal-entropy solution to the original problem $L_{\mathbf{C}}^0$. Moreover, note that if $\epsilon \to \infty$, we are essentially maximizing the entropy, and unsurprisingly, the maximal entropy solution is $\mathbf{a}\mathbf{b}^T$: In terms of probability, maximal entropy joint distribution is assuming independence.

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We can reformulate the problem via *KL projection*. Note that minimizing the regularized objective is akin to minimizing

$$\begin{aligned}
&\sum_{i,j} \frac{1}{\epsilon} P_{ij} C_{ij} + P_{ij}(\log P_{ij} - 1) + e^{-C_{ij}/\epsilon} \\
&= \sum_{i,j} P_{ij} \left(\log P_{ij} - \log \left(e^{-C_{ij}/\epsilon} \right) \right) - P_{ij} + + e^{-C_{ij}/\epsilon} \\
&= \sum_{i,j} P_{ij} \log \frac{P_{ij}}{K_{ij}} - P_{ij} + K_{ij} =: \mathrm{KL} \binom{\mathbf{P}}{\mathbf{K}},
\end{aligned}$$

where $\mathbf{K}_{ij} = \exp(-C_{ij}/\epsilon)$ is called a *Gibbs kernel*. Thus the problem is akin to projecting $\mathbf{K}$ onto $\mathbf{U}(\mathbf{a}, \mathbf{b})$ via the KL-divergence as a distance metric.

The Lagrangian of the regularized problem is

$$\begin{aligned}
\mathrm{Lagrange}(\mathbf{P}, \mathbf{f}, \mathbf{g}) = &\sum_{i,j} P_{ij} C_{ij} + \epsilon \sum_{i,j} P_{ij}(\log P_{ij} - 1) \\
&+ \sum_i f_i \left(a_i - \sum_j P_{ij} \right) + \sum_j g_j \left(b_j - \sum_i P_{ij} \right),
\end{aligned}$$

for which the first-order conditions yield

$$C_{ij} + \epsilon \log P_{ij} - f_i - g_j = 0.$$

Rewriting yields

$$P_{ij} = e^{f_i/\epsilon} e^{-C_{ij}/\epsilon} e^{g_j/\epsilon} = u_i K_{ij} v_j$$

for some $\mathbf{u}, \mathbf{v}$. The condition prescribed by $\mathbf{U}(\mathbf{a}, \mathbf{b})$, written via $\mathbf{u}, \mathbf{v}$, yield

$$\mathbf{u} \odot (\mathbf{K}\mathbf{v}) = \mathbf{a} \quad \mathbf{v} \odot (\mathbf{K}^T \mathbf{u}) = \mathbf{b}.$$

Since the optimum is unique, we need only find $\mathbf{u}, \mathbf{v}$ such that these conditions hold.

Given $\mathbf{v}$, we can compute $\mathbf{u}$ via $\mathbf{u} = \frac{\mathbf{a}}{\mathbf{K}\mathbf{v}}$ and vice versa. This motivates Sinkhorn's algorithm by initializing $\mathbf{v}^{(0)} = \mathbb{1}$ and computing

$$\mathbf{u}^{(\ell+1)} = \frac{\mathbf{a}}{\mathbf{K}\mathbf{v}^{(\ell)}} \quad \mathbf{v}^{(\ell+1)} = \frac{\mathbf{b}}{\mathbf{K}^T u^{(\ell+1)}}$$

It has been shown (2017!) that Sinkhorn updates achieves a τ-approximate solution of the unregularized problem in $O(n^2 \log(n) \tau^{-3})$ update iterations.