Notes WB project

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1 Notes on RD spliting method

Suppose we want to solve the following problem:

$$\min f(x) + g(x) \tag{1}$$

With f and g closed, convex, proper functions such that $\mathbf{Dom}(f) \cap \mathbf{Dom}(g) \neq \emptyset$ and $\mathbf{Im}(f) = \mathbf{Im}(g) = \mathbb{R} \cup \{\infty\}$, if the following operator is simple to compute for f and g:

$$\mathbf{prox}_f(\hat{x}) = \mathbf{argmin}_x f(x) + \tfrac{1}{2}||x - \hat{x}||^2$$

We can solve problem (1) with the Douglas–Rachford iterations, we start with a y^0 and a proximal parameter $\rho > 0$, we do:

$$\begin{cases} x^{k+1} = \mathbf{Prox}_{f\rho}(y^k) \\ \hat{x}^{k+1} = \mathbf{Prox}_{g\rho}(2x^{k+1} - y^k) \\ y^{k+1} = y^k + \hat{x}^{k+1} - x^{k+1} \end{cases} \tag{2}$$

So lets now look at our problem:

$$\begin{cases} \min_{\pi \geq 0} \langle c, \pi \rangle \\ \mathbf{s.t}\ \pi \in \mathcal{K} \end{cases}$$

This problem is equivalent to the following:

$$\min \langle c, \pi \rangle + \mathcal{I}_{\pi \geq 0}(\pi) + \mathcal{I}_{\mathcal{K}}(\pi)$$

If we let $f(\pi) = \mathcal{I}_{\mathcal{K}}(\pi)$ and $g(\pi) = \langle c, \pi \rangle + \mathcal{I}_{\pi \geq 0}(\pi)$ we get exactly the proposed iteration:

- Begin with $\theta^0 = (\theta^{1,0}, \ldots, \theta^{M,0})$
- For $k = 1, 2, 3, \ldots$ do:

$$\begin{cases} \pi^{k+1} = \mathbf{Proj}_{\mathcal{K}}(\theta^k), \\ \hat{\pi}^{k+1} = \mathrm{argmin}_{\pi \geq 0} \langle c, \pi \rangle + \dfrac{\rho}{2} \|\pi - (2\pi^{k+1} - \theta^k)\|^2, \\ \theta^{k+1} = \theta^k + \hat{\pi}^{k+1} - \pi^{k+1}. \end{cases}$$

Lets prove the convergence of the DR algo. First we reformulate the algorithm as fixed point iteration:

$$y_{k+1} = F(y_k)$$

With (here we set the proximal parameter $\rho = 1$ for simplicity)

$$F(y) = y + \mathbf{Prox}_g(2\mathbf{Prox}_f(y) - y) - \mathbf{Prox}_f(y)$$

To this end we prove the following:

Theorem 1.1. *y is a fixed point of F iff $x = \boldsymbol{Prox}_f(y)$ satisfies $0 \in \partial f(x) + \partial g(x)$, that is:*

$$y = F(y) \iff 0 \in \partial f(\boldsymbol{Prox}_f(y)) + \partial g(\boldsymbol{Prox}_f(y))$$

Proof. Supose $F(y) = y$ and $x = \mathbf{Prox}_f(y)$, this is equivalent to:

$$\begin{aligned} F(y) = y &= y + \mathbf{Prox}_g(2x - y) - x \\ x &= \mathbf{Prox}_g(2x - y) \end{aligned}$$

So, for x we have: $x = \mathbf{Prox}_f(y) = \mathbf{Prox}_g(2x - y)$ we have this if and only if $y - x \in \partial f$ and $x - y \in \partial g$. We get that if $F(y) = y$ then $0 = (y - x) + (x - y) \in \partial f(x) + \partial g(x)$.

Using this we can set $-z = y - x \in \partial f(x)$ and like thtis $z \in \partial g(x)$ then using the equivalences above:

$$x = \mathbf{Prox}_f(y) \text{ and } x = \mathbf{Prox}_g(2x - y)$$

If we substitute onto the definition of F we get $F(y) = y + x - x = y$ □

The operator F is know as the Douglas-Rashford operator, we will prove that F is a *firmly non expansive* map:

Definition 1. *A map $T : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ is firmly nonexpansive if:*

$$||T(w) - T(w')||_2^2 \leq \langle w - w', T(w) - T(w') \rangle$$

For all $w, w' \in \mathbb{R}^n$

Frist we prove:

Theorem 1.2. *The proximal operator of a convex closed function $f : \mathbb{R}^n \longrightarrow \mathbb{R}$ such that $\boldsymbol{Im}(f) = \mathbb{R} \cup \{\infty\}$ is firmly nonexpansive.*

Proof. Let $u_1 = \mathbf{Prox}_f(x_1)$ and $u_2 = \mathbf{Prox}_f(x_2)$ that is:

$$x_1 - u_1 \in \partial f(u_1), x_2 - u_2 \in \partial f(u_2)$$

Since ∂f is monotone:

$$\langle x_1 - u_1 - (x_2 - u_2), u_1 - u_2 \rangle \geq 0$$
$$\langle x_1 - x_2, u_1 - u_2 \rangle \geq ||u_1 - u_2||_2^2$$

□

Now we prove:

Theorem 1.3. *The Douglas-Rashford is a simply nonexpansive map*

Proof. Let $w, w' \in \mathbb{R}^n$, $y = \mathbf{Prox}_f(w)$ and $x = \mathbf{Prox}_g(2y - w)$ so that: $T(w) = x + w - y$. as we know, the proximal maps satisfy:

$$||y - y'||_2^2 \leq \langle y - y', w - w' \rangle$$
$$||x - x'||_2^2 \leq \langle x - x', 2(y - y') - (w - w') \rangle$$

We can then write:

$$\begin{aligned}
\|T(w) - T(w')\|_2^2 &= \|x - x' + w - w' - (y - y')\|_2^2 \\
&= \|x - x'\|_2^2 + \|w - w'\|_2^2 + \|y - y'\|_2^2 \\
&\quad + 2\langle x - x', w - w' \rangle - 2\langle x - x', y - y' \rangle - 2\langle y - y', w - w' \rangle \\
&\leq \langle x - x', w - w' \rangle + \|w - w'\|_2^2 - \langle y - y', w - w' \rangle \\
&= \langle (x + w - y) - (x' + w' - y'),\, w - w' \rangle \\
&= \langle T(w) - T(w'),\, w - w' \rangle.
\end{aligned}$$

□

To get to our finst result we prove the folllowing lema:
If T is firmly non expansive, then $G = I - T$ is also firmly non expansive

Proof. We have that:

$$\begin{aligned}
||Gw - Gw'||_2^2 &= ||w - w'||_2^2 + ||Tw - Tw'||_2^2 - 2\langle w - w', Tw - Tw' \rangle \\
&\leq ||w - w'||_2^2 - \langle w - w', Tw - Tw' \rangle \\
&= \langle w - w', Gw - Gw' \rangle
\end{aligned}$$

□

We now get to our main result:

Theorem 1.4. *Assume $T : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ a firmly non expansive map that has at least one fixed point w^*. Then the iterations $w_{k+1} = T(w_k)$ converges to some fixed point of T, and:*

$$\min_{0 \leq j \leq k-1} ||w_j - T(w_j)||_2^2 \leq \frac{||w_0 - w^*||_2^2}{k}$$

Proof. Let w^* be a fixed point of T, then for any w we have:

$$||T(w) - w^*||_2^2 - ||w - w^*||_2^2 \leq \langle w - w^*, T(w) - w^* \rangle - ||w - w^*||_2^2 \tag{3}$$

$$= \langle w - w^*, -G(w) \rangle \leq -||G(w)||_2^2 \tag{4}$$

(We used that G is simply nonexpansive, and $G(0) = 0$). Summing the inequalities arising from the iterations we get:

$$\sum_{i=0}^{k-1} ||G(w_i)||_2^2 \leq ||w_0 - w^*||_2^2$$

Let $r = \min_{0 \leq i \leq k-1} ||G(w_i)||_2^2$, we get that:

$$r \leq \frac{1}{k} \sum_{i=0}^{k-1} ||G(w_i)||_2^2 \leq \frac{||w_0 - w^*||_2^2}{k}$$

We now show that the sequence generated by the iterations converges to w^*. The equations (3) and (4) shows that the sequence $||w_i - w^*||_2$ is non increasing for any ficed point w^*, in particular (w_i) is bounded and therefore it has a limit point $\bar{w}$. First, since G is continuos and $||G(w_i)|| \longrightarrow 0$ we mus have that $G(\bar{w}) = 0$, therefore $\bar{w}$ is a fixed point of T. So the sequence $||w_i - \bar{w}||_2$ converges to 0 so: $w_i \longrightarrow \bar{w}$ □

2 Notes on possible restrictions

2.1 Restriction on the Frobenius norm

As we impose a restriction on the transport plans such that:

$$||\pi^m||_F = \sqrt{\sum_{r=1}^{R} \sum_{s=1}^{S^m} |\pi^m_{r,s}|^2} \leq \tau$$

We are saying that the total energy of our transport plans is bounded, meaning that we cannot transport a high amount of mass, this can lead to a more robust barycenter facing outliers. How to choose τ so that the WB problem is feasible? If we choose τ too small the problem becomes infeasible, if too large the constraint becomes useless.

One possible application would be in medical images: Given images that represent certain patients with certain pathology and we want to find the "mean" patient, we would like the barycenter to be robust when a patient is an outlier.

Now lets look at our version of the problem with this constrain:

$$\begin{cases} \min_{\pi \geq 0} \langle c, \pi \rangle \\ \textbf{s.t } \pi \in \mathcal{K} \\ \pi^m \in \mathcal{B}_\tau^{||\cdot||_F^m}(0) \text{ for all } m = 1, ..., M \end{cases} \tag{5}$$

With $\mathcal{B}_\tau^{||\cdot||_F^m}(0) = \{A \in \mathbb{R}^{R\times S^m} : ||A||_F \leq \tau\}$

We now will take a look at the feasibility of this problem, as it depends on the value of τ. First we take a look at the inequality:

$$||\pi^m||_F^2 = \sum_{r=1}^{R}\sum_{s=1}^{S^m} |\pi_{r,s}^m|^2 < \sum_{r=1}^{R}\sum_{s=1}^{S^m} |\pi_{r,s}^m| = 1$$

So if $\tau \geq 1$ the constrain is useless. We may use Cauchy Schwarz and see that: if $x = (\pi_{r,s}^m) \in \mathbb{R}^{RS^m}$ (the vector corresponding to the entries of π^m) and y is the vector of ones on $\mathbb{R}^{RS^m}$, we see that:

$$\langle x, y\rangle^2 = (\sum_{r=1}^{R}\sum_{s=1}^{S^m} |\pi_{r,s}^m|) = 1 \leq RS^m \sum_{r=1}^{R}\sum_{s=1}^{S^m} |\pi_{r,s}^m|^2 = RS^m ||\pi^m||_F^2$$

(Note that we have equality iff the plans are uniformly distributed) So, we have that, for π^m:

$$||\pi^m||_F \geq \frac{1}{\sqrt{RS^m}}$$

So $\tau > \max_m \frac{1}{\sqrt{RS^m}}$

We could also say that, as the set $\mathcal{K}$ is amused to be non empty we could take a $\bar{\pi} = (\bar{\pi}^1, ...\bar{\pi}^M) \in \mathcal{K}$ and define: $\tau_\pi = \max_{m=1,\dots,M} ||\pi^m||_F$ we get that, for all $m = 1, ..., M$, $||\pi^m|| \leq \tau_\pi$. If we make: $\tau^* = \inf_{\pi\in\mathcal{K}} \tau_\pi$ we could say that $\max_m \frac{1}{\sqrt{RS^m}} \leq \tau^* \leq \tau_\pi \forall \pi \in \mathcal{K}$.

Finally, our problem is feasible if: $\max_m \frac{1}{\sqrt{RS^m}} < \tau < 1 \forall m = 1, ..., M$

We can write it as, understanding the indicator functions being evaluated on each plan π^m:

$$\min_\pi \langle c, \pi\rangle + \mathcal{I}_{\pi\geq 0}(\pi) + \mathcal{I}_{\mathcal{K}}(\pi) + \mathcal{I}_{\mathcal{B}_\tau^{||\cdot||_F^m}(0)}(\pi)$$

If we let $f(\pi) = \mathcal{I}_{\mathcal{K}}(\pi)$ and $g(\pi) = \langle c, \pi\rangle + \mathcal{I}_{\pi\geq 0}(\pi) + \mathcal{I}_{\mathcal{B}_\tau^{||\cdot||_F}(0)}(\pi)$ we get that both of this functions are convex and closed, so we can apply the RD algo:

- Begin with $\theta^0 = (\theta^{1,0}, \dots, \theta^{M,0})$
- For $k = 1, 2, 3, \dots$ do:

$$\begin{cases} \pi^{k+1} = \mathbf{Proj}_{\mathcal{K}}(\theta^k), \\ \hat{\pi}^{k+1} = \text{argmin}_\pi \langle c, \pi\rangle + \mathcal{I}_{\pi\geq 0}(\pi) + \mathcal{I}_{\mathcal{B}_\tau^{||\cdot||_F{}^m}(0)}(\pi) + \frac{\rho}{2}||\pi - (2\pi^{k+1} - \theta^k)||^2, \\ \theta^{k+1} = \theta^k + \hat{\pi}^{k+1} - \pi^{k+1}. \end{cases}$$

Lets take a closer look at the second steep:

$$\begin{aligned} &\operatorname*{argmin}_\pi \langle c, \pi\rangle + \mathcal{I}_{\pi\geq 0}(\pi) + \mathcal{I}_{\mathcal{B}_\tau^{||\cdot||_F{}^m}(0)}(\pi) + \frac{\rho}{2}||\pi - (2\pi^{k+1} - \theta^k)||^2 \\ &= \operatorname*{argmin}_{\pi\geq 0, ||\pi^m||_F \leq \tau, m=1,\dots,M} \langle c, \pi\rangle + \frac{\rho}{2}||\pi - (2\pi^{k+1} - \theta^k)||^2 \end{aligned}$$

Now:

$$\begin{aligned}
\langle c, \pi \rangle + \frac{\rho}{2}||\pi - (2\pi^{k+1} - \theta^k)||^2 &= \langle c, \pi \rangle + \frac{\rho}{2}||\pi||^2 + \langle \pi, -\rho(2\pi^{k+1} - \theta^k) \rangle + \frac{\rho}{2}||2\pi^{k+1} - \theta^k||^2 \\
&= \frac{\rho}{2}\left[||\pi||^2 + 2\langle \pi, \frac{c}{\rho} - (2\pi^{k+1} - \theta^k) \rangle\right] \\
&= \frac{\rho}{2}||\pi - (2\pi^{k+1} - \theta^k - \frac{c}{\rho})||^2
\end{aligned}$$

Were the terms that don't depend on π were not taken into account due to the **argmin** operator. We conclude that the second steep is reduced to computing:

$$\underset{\pi \geq 0, ||\pi^m||_F \leq \tau, m=1,\ldots,M}{\text{argmin}} ||\pi - (2\pi^{k+1} - \theta^k - \frac{c}{\rho})||^2$$

That is, is the projection of $2\pi^{k+1} - \theta^k - \frac{c}{\rho}$ on the set: $\{\pi | \pi \geq 0, ||\pi^m||_F \leq \tau, m = 1, ..., M\}$. Next we will look at how to compute this projection, which, as the inequality of the Frobenius norm applies on each of the M matrices, can be decomposed into M smaller problems:

Given a matrix A we want to solve:

$$\min_{X \geq 0, ||X||_F \leq \tau} \frac{1}{2}||X - A||_F^2$$

We proceed then to use the KKT conditions. Frist we write the lagrangian:

$$\mathcal{L}(X, \lambda, M) = \frac{1}{2}||X - A||_F^2 + \frac{\lambda}{2}(||X||_F^2 - \tau^2) - \langle M, X \rangle$$

With $M \geq 0$ Note that we have replaced the constraint $||\pi^m||_F \leq \tau$ with the equivalent constraint: $\frac{1}{2}||\pi^m||_F^2 \leq \frac{1}{2}\tau^2$What happens when $X = 0$? The overcome this issue, the simplest trick is to replace the constraint $||X||_F \leq \tau$ with the equivalent one: $\frac{1}{2}||X||_F^2 \leq \frac{1}{2}\tau^2$. This new constraint is differentiable and had gradient X. Now the KKT conditions are:

- $\nabla_X \mathcal{L} = X - A + \lambda X - M = 0$ this gradient is incorrect that is:

$$(1 + \lambda)X = A + M$$

- $\lambda(||X||_F - \tau) = 0$, $M_{ij}X_{ij} = 0, \forall i, j$
- $||X||_F \leq \tau, X_{ij} \geq 0$
- $\lambda, M_{ij} \geq 0, \forall i, j$

From the stationary condition:

$$(1 + \lambda)X_{ij} = A_{ij} + M_{ij}$$

This leads to two cases, if $X_{ij} > 0$, then we have: $M_{ij} = 0$, therefore: $X_{ij} = \frac{A_{ij}}{1+\lambda}$ and $A_{ij} > 0$. If $A_{ij} \leq 0$ then we must have $X_{ij} = 0$, we get then:

$$X = \frac{A_+}{1 + \lambda}$$

Now, if $\lambda = 0$, $X = A_+$ and $||A_+||_F \leq \tau$. And if $\lambda > 0$ we must have $||X||_F = \tau$ and:

$$|||A_+||_F = \tau(1 + \lambda) > \tau$$

We can conclude that:

$$\min_{X \geq 0, ||X||_F \leq \tau} \frac{1}{2}||X - A||_F^2 = \begin{cases} A_+, \text{ if } ||A_+||_F \leq \tau \\ \frac{\tau A_+}{||A_+||} \text{ if } ||A_+||_F > \tau \end{cases} = \frac{\tau}{\max\{\tau, ||A_+||_F\}} A_+$$

Then our algo is then:

Algorithm 1 Method of Averaged Marginals - Bounds Frobenius norm

Input: Let initial point $p^0 \in H$, scalar $\rho > 0$, probability vectors $q^m \in \Delta_{S^m}$, cost matrices $c^m \in \mathbb{R}^{R \times S^m}$, $m = 1, \ldots, M$, be given, coefficient τ such that $\max_m \frac{1}{\sqrt{RS^m}} < \tau < 1$

Initialization: Define $a_m := \left(\frac{1}{S^m}\right) / \left(\sum_{j=1}^{M} \frac{1}{S^j}\right)$ and set $\mathfrak{p}^m \leftarrow p^0$ for all $m = 1, \ldots, M$. Initialize $\theta_{rs}^m \leftarrow \frac{r_r^0}{S^m} + \frac{q_s^m}{R} - \frac{1}{RS^m}$ for all m, r, s

while not converged **do**

  $p \leftarrow \mathrm{Proj}_{X \cap H}\left(\sum_{m=1}^{M} a_m \mathfrak{p}^m\right)$

  for $m = 1, \ldots, M$ **do**

    $\mathfrak{q}^m \leftarrow (\theta^m)^\top \mathbf{1}_R$

    $\gamma^m \leftarrow (\mathfrak{q}^m)^\top \mathbf{1}_{S^m} - 1$

    $\beta \leftarrow \frac{p - \mathfrak{p}^m}{S^m} + \frac{q^m - \mathfrak{q}^m}{R} + \frac{\gamma^m}{RS^m}$

    $\alpha \leftarrow \frac{\tau}{\max\{\tau, ||(\theta^m + 2\beta - c^m/\rho)_+||_F\}}$

    for $r = 1, \ldots, R$ **do**

      for $s = 1, \ldots, S^m$ **do**

        $\theta_{rs}^m \leftarrow \alpha(\theta_{rs}^m + 2\beta_{rs} - c_{rs}^m/\rho)_+ - \beta_{rs}$

      end for

    end for

    $\mathfrak{p}^m \leftarrow \theta^m \mathbf{1}_{S^m}$

  end for

end while

return p

2.2 Bounds on the elements of the plans

We could also investigate how we can implement constrains of the form: $0 \leq \pi_{r,s} \leq u$, for a given u, this, as the Frobenius norm, cloud make the barycenter more smooth and protect it against outliers (As if we have one, the mass of this outlier has to be distributed, in a function of u among the points on the barycenter's support).

We can then set $\mathcal{A}$? $\mathcal{A} = \{\pi | 0 \leq \pi^m_{r,s} \leq u\}$ and our problem would be:

$$\begin{cases} \min_{\pi \geq 0} \langle c, \pi \rangle \\ \textbf{s.t } \pi \in \mathcal{K} \\ \quad \pi^m \in \mathcal{A} \end{cases} \tag{6}$$

Wich can be restated as:

$$\min_{\pi} \langle c, \pi \rangle + \mathcal{I}_{\pi \geq 0}(\pi) + \mathcal{I}_{\mathcal{K}}(\pi) + \mathcal{I}_{\mathcal{A}}(\pi)$$

If we let $f(\pi) = \mathcal{I}_{\mathcal{K}}(\pi)$ and $g(\pi) = \langle c, \pi \rangle + \mathcal{I}_{\pi \geq 0}(\pi) + \mathcal{I}_{\mathcal{A}}(\pi)$, As both of this functions are convex and closed we can apply the RD algo:

- Begin with $\theta^0 = (\theta^{1,0}, \ldots, \theta^{M,0})$
- For $k = 1, 2, 3, \ldots$ do:

$$\begin{cases} \pi^{k+1} = \textbf{Proj}_{\mathcal{K}}(\theta^k), \\ \hat{\pi}^{k+1} = \text{argmin}_{\pi} \langle c, \pi \rangle + \mathcal{I}_{\pi \geq 0}(\pi) + \mathcal{I}_{\mathcal{A}}(\pi) + \frac{\rho}{2} ||\pi - (2\pi^{k+1} - \theta^k)||^2, \\ \theta^{k+1} = \theta^k + \hat{\pi}^{k+1} - \pi^{k+1}. \end{cases}$$

Again the second steep is just:

$$\underset{\pi \geq 0, \pi \in \mathcal{A}}{\text{argmin}} \langle c, \pi \rangle + \frac{\rho}{2} ||\pi - (2\pi^{k+1} - \theta^k)||^2$$

Following the same argument as before, we conclute that we just hace to compute:

$$\underset{\pi \geq 0, \pi \in \mathcal{A}}{\text{argmin}} ||\pi - (2\pi^{k+1} - \theta^k - \frac{c}{\rho})||^2$$

So we proceed to computing this projection. we note that if $0 \leq \pi_{i,j} \leq u$ we automatically get $0 \leq \pi$, like this we can ignore the first constrain.

Let C be a matrix, we want:

$$\underset{0 \leq \pi_{i,j} \leq u \forall i,j}{\text{argmin}} ||\pi - C||^2$$

Recall that: $||\pi - C||^2 = \sum_{i,j}(\pi_{ij} - C_{ij})^2$ so our problem is separable on the entries of the matrices, therefore, we focus now on solving:

$$\min_{0 \leq x \leq u} (x - C_{ij})$$

The lagrangian of this problem is:

$$\mathcal{L}(x, \lambda_1, \lambda_2) = (x - C_{ij})^2 - \lambda_1 x + \lambda_2 (x - u)$$

And the KKT conditions are:

- $\frac{\partial \mathcal{L}}{\partial x} = 2(x - c) - \lambda_1 + \lambda_2 = 0$
- $0 \leq x \leq u$
- $\lambda_1 \geq 0, \lambda_2 \geq 0$
- $\lambda_1 x = 0, \lambda_2 (x - u) = 0$

We have then tree cases, we leet $c = C_{i,j}$:

- $0 < c < u$, here we can take $x = c$, therefore $\lambda_1 = \lambda_2$ and as $x > 0$, $\lambda_1 = \lambda_2 = 0$ and therefore we conclude that c is our solution
- $c \leq 0$, we take $x = 0$, so:$\lambda_2 = 0$ and $\lambda_1 = -2c \geq 0$, so our optimal is $x = c$
- $c \geq u$, we propose $x = u$, we then hace $\lambda_1 = 0$ and $\lambda_2 = 2(c - u) \geq 0$.

We conclute that:

$$\min_{0 \leq x \leq u} (x - C_{ij}) = \min\{\max\{C_{i,j}, 0\}, u\}$$

Coming back to our original matrix problem:

$$\underset{0 \leq \pi_{i,j} \leq u \forall i,j}{\text{argmin}} ||\pi - C||^2 = \min\{\max\{C, 0\}, u\}$$

With the operations taken component wise.

Our new algo is then:

Algorithm 2 Method of Averaged Marginals - Bounds on capacity

Input: Let initial point $p^0 \in H$, scalar $\rho > 0$, probability vectors $q^m \in \Delta_{S^m}$, and cost matrices $c^m \in \mathbb{R}^{R \times S^m}$, $m = 1, \ldots, M$, be given

Initialization: Define $a_m := \left(\frac{1}{S^m}\right) / \left(\sum_{j=1}^{M} \frac{1}{S^j}\right)$ and set $\mathfrak{p}^m \leftarrow p^0$ for all $m = 1, \ldots, M$. Initialize $\theta^m_{rs} \leftarrow \frac{r_r^0}{S^m} + \frac{q_s^m}{R} - \frac{1}{RS^m}$ for all m, r, s

while not converged **do**

  $p \leftarrow \mathrm{Proj}_{X \cap H}\left(\sum_{m=1}^{M} a_m \mathfrak{p}^m\right)$

  for $m = 1, \ldots, M$ **do**

    $\mathfrak{q}^m \leftarrow (\theta^m)^\top \mathbf{1}_R$

    $\gamma^m \leftarrow (\mathfrak{q}^m)^\top \mathbf{1}_{S^m - 1}$

    for $r = 1, \ldots, R$ **do**

      for $s = 1, \ldots, S^m$ **do**

        $\beta \leftarrow \frac{p_r - \mathfrak{p}_r^m}{S^m} + \frac{q_s^m - \mathfrak{q}_s^m}{R} + \frac{\gamma^m}{RS^m}$

        $\theta^m_{rs} \leftarrow \min\{\max\{\theta^m_{rs} + \beta - c^m_{rs}/\rho, -\beta\}, u - \beta\}$

      end for

    end for

    $\mathfrak{p}^m \leftarrow \theta^m \mathbf{1}_{S^m}$

  end for

end while

return p

2.3 Restrictions on the resulting baricenter

One way to impose restrictions on the barycenter trough restrictions on the plans is to note the following: On the set $\mathcal{K}$ we know that the plans should satisfy:

$$p = \pi^1 \mathbf{1}_{S^1} = \pi^2 \mathbf{1}_{S^2} = \cdots = \pi^M \mathbf{1}_{S^M} \in H$$

With p being the probability distribution of the Barycenter. We note that if we want to impose some constrains on the barycenter (say for instance that it should be on a closed non empty set X I am not sure it we need X to be convex) we could add another constrain:

$$\forall m, \pi^m \mathbf{1}_{S^m} \in X$$

We could therefore define a set $\mathcal{C} = \{\pi = (\pi^1, \ldots, \pi^M) | \quad \pi^m \mathbf{1}_{S^m} \in X \, \forall \, m\}$, so our probolem:

$$\begin{cases} \min_{\pi \geq 0} \langle c, \pi \rangle \\ \quad \textbf{s.t } \pi \in \mathcal{K} \\ \qquad \pi \in \mathcal{C} \end{cases} = \min_{\pi} \langle c, \pi \rangle + \mathcal{I}_{\pi \geq 0}(\pi) + \mathcal{I}_{\mathcal{K}}(\pi) + \mathcal{I}_{\mathcal{C}}(\pi)$$

If we let $f(\pi) = \mathcal{I}_{\pi \geq 0}(\pi)$ and $g(\pi) = \min_{\pi} \langle c, \pi \rangle + \mathcal{I}_{\pi \geq 0}(\pi) + \mathcal{I}_{\mathcal{C}}(\pi)$ we see that f is convex and for g to be convex we just need to show that the set $\mathcal{C}$ is convex, for that it suffices to show that, for a given m, the set $\{\pi^m \mathbf{1}_{S^m} \in X\}$ is convex (Its non empty because X is non empty and we could take an element $x \in X$ and put it in the principal diagonal of π^m).

Let then be $\pi_1^m, \pi_2^m \in \mathcal{C}$ and $\theta_1, \theta_2 \geq 0, \theta_1 + \theta_2 = 1$, we then have:

$$(\theta_1 \pi_1^m + \theta_2 \pi_2^m) \mathbf{1}_{S^m} = \theta_1 \pi_1^m \mathbf{1}_{S^m} + \theta_2 \pi_2^m \mathbf{1}_{S^m} = \theta_1 x_1 + \theta_2 x_2$$

With $x_1 = \pi_1^m \mathbf{1}_{S^m}, x_2 = \pi_1^m \mathbf{2}_{S^m}$. As $\pi_2^m \mathbf{1}_{S^m}, \pi_2^m \mathbf{1}_{S^m} \in X$ and this set is convex we get that: $\theta_1 x_1 + \theta_2 x_2 \in X$.

So if the set X is convex then g is convex. Therefore we could apply our algo:

$$\begin{cases} \pi^{k+1} = \mathbf{Proj}_{\mathcal{K}}(\theta^k) \\ \hat{\pi}^{k+1} = \text{argmin}_{\pi} \langle c, \pi \rangle + \mathcal{I}_{\pi \geq 0}(\pi) + \mathcal{I}_{\mathcal{C}}(\pi) + \frac{\rho}{2} ||\pi - (2\pi^{k+1} - \theta^k)||^2 \\ \theta^{k+1} = \theta^k + \hat{\pi}^{k+1} - \pi^{k+1} \end{cases}$$

the second steep is:

$$\text{argmin}_{\pi \geq 0, \pi \in \mathcal{C}} \langle c, \pi \rangle + \frac{\rho}{2} ||\pi - (2\pi^{k+1} - \theta^k)||^2$$

Which is just:

$$\text{argmin}_{\pi \geq 0, \pi \in \mathcal{C}} ||\pi - (2\pi^{k+1} - \theta^k - \frac{c}{p})||^2$$

As the restrictions on π are component wise we could just divide this problem on M subproblems:

$$\hat{\pi}_m^{k+1} = \text{argmin}_{\pi_m \geq 0, \pi_m \mathbf{1}_{S^m} \in X} ||\pi_m - (2\pi_m^{k+1} - \theta_m^k - \frac{c_m}{p})||^2$$

We will know focus on computing this projection for a suitable matrix A:

$$\text{argmin}_{Y \geq 0, Y\mathbf{1} \in X} ||Y - A||^2$$

For some sets X. For instance, lets set $X = \{p : p_r \leq u_r\}$ for given $u_r > 0\, \forall\, r$ and $\sum_{r=1}^R u_r > 1$, The Lagrangian of this problem is:

$$\mathcal{L}(Y, \lambda, \mu) = \frac{1}{2}||Y - A||^2 + \sum_r \lambda_r (\sum_j Y_{rj} - u_r) - \sum_{r,j} \mu_{rj} Y_{rj}$$

If we do component by component the KKT conditions are:

- $\frac{\partial \mathcal{L}}{\partial Y_{rj}} = Y_{rj} - A_{rj} + \lambda_r - \mu_{rj} = 0$
- $Y_{r,j} \geq 0, \sum_j Y_{rj} \leq u_r$
- $\lambda_r \geq 0, \mu_{r,j} \geq 0$
- $\lambda_r(\sum_j Y_{r,j} - u_r) = 0, \mu_{r,j} Y_{r,j} = 0$

If $Y_{r,j} > 0$: we get that $\mu_{r,j} = 0$ and plugging in the stationary condition: $Y_{rj} = A_{rj} - \lambda_r$ and $A_{r,j} > \lambda_r$. If $Y_{r,j} = 0$, we get that $\mu_{rj} = \lambda_r - A_{rj} \geq 0$ so $\lambda_r \geq A_{rj}$, we get that:

$$Y_{r,j} = \max\{A_{r,j} - \lambda_r, 0\}$$

To determine λ_r we see that:

$$\sum_{j=1}^n \max\{A_{r,j} - \lambda_r, 0\} \leq u_r \ , \lambda_r(\sum_j \max\{A_{r,j} - \lambda_r, 0\} - u_r) = 0$$

Let's define then:

$$\phi_r(\lambda) = \sum_{j=1}^n \max\{A_{r,j} - \lambda_r, 0\}, \ \lambda \geq 0$$

As this function is a sum of continuous functions, it is continuous, we also see that:

$$\phi_r(0) = \sum_{j=1}^n \max\{A_{r,j}, 0\}, \ \lim_{\lambda \longrightarrow 0} \phi_r(\lambda) = 0$$

For a fixed j take $\lambda_1 < \lambda_2$, so we get: $A_{r,j} - \lambda_1 > A_{r,j} - \lambda_2$ so we get: $\max\{A_{r,j} - \lambda_1, 0\} \geq \max\{A_{r,j} - \lambda_2, 0\}$. Summing over j we get:

$$\phi_r(\lambda_1) \geq \phi_r(\lambda_2)$$

We will know see that $\phi_r(\lambda)$ is strictly monotone.

Let's suppose that $\phi_r(\lambda_1) = \phi_r(\lambda_1)$ (with $\lambda_1 < \lambda_2$) and that there exists j' such that $\max\{A_{r,j'} - \lambda_1, 0\} > \max\{A_{r,j'} - \lambda_2, 0\}$, so:

$$\begin{aligned}\phi_r(\lambda_1) = \sum_j \max\{A_{r,j} - \lambda_1, 0\} &= \max\{A_{r,j'} - \lambda_1, 0\} + \sum_{j \neq j'} \max\{A_{r,j} - \lambda_1, 0\} \\ &> \max\{A_{r,j'} - \lambda_2, 0\} + \sum_{j \neq j'} \max\{A_{r,j} - \lambda_2, 0\} = \phi_r(\lambda_2)\end{aligned}$$

Which contradicts $\phi_r(\lambda_1) = \phi_r(\lambda_1)$, we conclude that $\max\{A_{r,j} - \lambda_1, 0\} = \max\{A_{r,j} - \lambda_2, 0\}$ for all j if $\phi_{r,j}(\lambda_1) = \phi_{r,j}(\lambda_2)$.

We now have, for a fixed j, three possibilities:

- $A_{rj} \leq \lambda_1$: We get: $A_{rj} - \lambda_1,\ A_{rj} - \lambda_2 \leq 0$ so $\max\{A_{rj} - \lambda_1, 0\} = \max\{\ A_{rj} - \lambda_2, 0\} = 0$
- $\lambda_1 < A_{r,j} \leq \lambda_2$: In this case: $A_{rj} - \lambda_1 > 0,\ A_{rj} - \lambda_2 \leq 0$, so: $\max\{A_{rj} - \lambda_1, 0\} > \max\{\ A_{rj} - \lambda_2, 0\}$
- $\lambda_2 < A_{rj}$: It follows that, $A_{rj} - \lambda_1 >\ A_{rj} - \lambda_2 > 0$ and: $\max\{A_{rj} - \lambda_1, 0\} > \max\{\ A_{rj} - \lambda_2, 0\}$

So all of the elements of the sum are equal (for their sums to be equal) if, for all $j, A_{rj} \leq \lambda_1$ which means that: $\phi_r(\lambda_1) = 0$.

We just show that: $\phi_r(\lambda_1) = \phi_r(\lambda_2) \implies \phi_r(\lambda_1) = 0$ so by contrapositive: $\phi_r(\lambda_1) > 0 \implies \phi_r(\lambda_1) > \phi_r(\lambda_2)$, so we just shown that if $\lambda_1 < \lambda_2 \implies \phi_r(\lambda_1) > \phi_r(\lambda_2)$, so ϕ_r is strictly decreasing.

Coming back to the computation of λ_r we are looking to solve the following equation:

$$\phi_r(\lambda) \leq u_r, \lambda(\phi_r(\lambda) - u_r) = 0$$

We have two cases:

- $\phi_r(0) \leq u_r$: As the function is strictly deceasing we cannot get back to the value u_r so the second equation is valid if and only if $\lambda = 0$
- $\phi_r(0) > u_r$: We cannot, as before, let $\lambda = 0$ but the intermediate value theorem states that there exist a (unique in our case) λ such that $\phi_r(\lambda) = u_r$

So we conclude that λ_r is uniquely determinate for each r.

The only problem is how to determine λ_r, lets fix a row r on A, as before we can define: $\phi_r(\lambda) = \sum_{j=1}^n \max\{A_{r,j} - \lambda_r, 0\}$ if $\phi_r(0) \leq u_r$ we set $\lambda = 0$. If this is not the case (that is, when $\phi_r(0) = \sum_{j=1}^n \max\{A_{r,j}, 0\} > u_r$) we seek to solve:

$$\phi_r(\lambda) = u_r$$

If λ is a solution, then there exists a set $I_\lambda = \{j : \ A_{r,j} - \lambda > 0\}$ such that: if $j \in I_\lambda, Y_{i,j} = A_{ij} - \lambda$ and if $j \notin I_\lambda, Y_{ij} = 0$, suppose that $k = |I_\lambda|$. If we knew K:

$$u_r = \sum_{j \in I_\lambda} A_{r,j} - \lambda, \ \lambda = \frac{\sum_{j \in I_\lambda} A_{r,j} - u_r}{k}$$

Our problem is to find now k, if we order the entries of the row r in decreasing order we then know that there exist a k such that:

$$A_{r,1} \geq A_{r,2} \geq \cdots \geq A_{r,k} > \lambda \geq A_{r,k+1} \geq \cdots \geq A_{r,n}$$

We see that the $j \leq k, j \leftrightarrow I_\lambda$ so we take: $\lambda = \frac{\sum_{j=1}^{k} A_{r,j}^{k} - u_r}{k}$

We are then ready to state the algo corresponding to the projection $\operatorname{argmin}_{Y \geq 0, Y\mathbf{1} \in X} ||Y - A||^2$:

Algorithm 3 Projection onto $\mathcal{C} = \{Y : Y \geq 0, \ Y\mathbf{1} \leq u\}$

Input: A matrix $A \in \mathbb{R}^{R \times n}$, a vector $u \in \mathbb{R}^R$ with $u_r > 0, \ \sum_{r=1}^{R} u_r > 1$
for $r = 1, \ldots, R$ **do**
    if $\sum_{j=1}^{n} \max\{A_{r,j}, 0\} \leq u_r$ **then**
        $\lambda_r = 0$
    else
        Order the entries of the r-th row: $A_{1,r} \geq A_{2,r} \geq \cdots \geq A_{n,r}$
        Compute cumulative sums: $S_k = \sum_{j=1}^{k} A_{r,j}, \quad k = 1, \ldots, n$
        Find $k_r = \max_k \{A_{r,k} > \frac{S_k - u_r}{k}\}$
        Set $\lambda_r = \frac{S_{k_r} - u_r}{k_r}$
    end if
    for $j = 1, \ldots, n$ **do**
        $Y_{r,j} = \max\{A_{r,j} - \lambda_r, 0\}$
    end for
end for
Return Y

With this we now state our main algorithm for this part:

Algorithm 4 Method of Averaged Marginals - Bounds on resulting barycenter

Input: Let initial point $p^0 \in H$, scalar $\rho > 0$, probability vectors $q^m \in \Delta_{S^m}$, cost matrices $c^m \in \mathbb{R}^{R \times S^m}$, $m = 1, \dots, M$ and a vector $u \in \mathbb{R}^R$ with $u_r > 0$, $\sum_{r=1}^R u_r > 1$, be given

Initialization: Define $a_m := \left(\frac{1}{S^m}\right) / \left(\sum_{j=1}^M \frac{1}{S^j}\right)$ and set $\mathfrak{p}^m \leftarrow p^0$ for all $m = 1, \dots, M$. Initialize $\theta^m_{rs} \leftarrow \frac{r^0_r}{S^m} + \frac{q^m_s}{R} - \frac{1}{RS^m}$ for all m, r, s

while not converged **do**

  $p \leftarrow \mathrm{Proj}_{X \cap H}\left(\sum_{m=1}^M a_m \mathfrak{p}^m\right)$

  for $m = 1, \dots, M$ **do**

    $\mathfrak{q}^m \leftarrow (\theta^m)^\top \mathbf{1}_R$

    $\gamma^m \leftarrow (\mathfrak{q}^m)^\top \mathbf{1}_{S^m - 1}$

    $\beta \leftarrow \frac{p - \mathfrak{p}^m}{S^m} + \frac{q^m - \mathfrak{q}^m}{R} + \frac{\gamma^m}{RS^m}$

    for $r = 1, \dots, R$ **do**

      for $s = 1, \dots, S^m$ **do**

        $\theta^m_{rs} \leftarrow \mathbf{Algo}_3(\theta^m + 2\beta - c^m/\rho)_{r,s} - \beta_{r,s}$

      end for

    end for

    $\mathfrak{p}^m \leftarrow \theta^m \mathbf{1}_{S^m}$

  end for

end while

return p

2.4 Restriction on transporting mass far away

Imagine we have a set of medical images, for instance fMRI, of patients with certain pathologies, and we want to obtain a "mean" of the fMRI with the objective to get a unified way to identify a patient and to develop a treatment.

If we find the usual barycenter we could get a fMIR that shows unusual activities or even non-anatomically accurate behaviors, for instance connecting two regions of the brain that rarely connect, to counter this we could impose that the cost of moving mass bettewn distant regios (or in our case, pixels) is more expensive. There are many ways of doing this, for instance we could transform the cost matrix:

$$C_{ij} = d_{ij}^p \text{ with } p > 1$$

Or if we want a more geometrical cost (imposing a linear cost for the pixels in a radius r):

$$c_{ij} = d_{ij} + \beta \max\{0, d_{ij} - r\}^q \text{ with } q \geq 2$$

3 Notes on section 10.3 of Computational Optimal Transport from Peyré and Cuturi

On the section mentioned they take a look to the following problem:

$$\min_{\pi \in \mathcal{U}(\alpha,\beta)} \{ \int_{\mathcal{X}\times\dagger} c(x,y) d\pi(x,y) : \pi \in \mathcal{C} \}$$

That is, the OT problem with restrictions on the couplings. They give two examples:

- A capacity constrain, that is, the density of the transport plan is bounded: $\{\pi : \rho_\pi \leq k\}$, which we have already seen.
- Also, another constrain that finds applications on finance is the constraint on the conditional mean of the couplings:

  $$\{\pi : \forall x \in \mathbb{R}^d, \int_{\mathbb{R}^d} y \frac{d\pi(x,y)}{d\alpha(x) d\beta(y)} d\beta(y) = x\}$$

  This imposes that the barycentric map (A map that, given a transport plan π, for each x gives us the barycenter of the points that get mass from it) is the identity. They mention that this set is usually empty. Nevertheless if the two measures are in "convex order" this set is not empty.

Just to clarify:

Definition 2. *Let α, β two probability measures on $\mathbb{R}^d$ with finite first moment, we say that $\alpha \leq_{cx} \beta$, α is convex dominated by β if and only if:*

$$\int \phi d\alpha \leq \int \phi d\beta$$

For all convex functions ϕ for wich the integrals are well defined

They also state that the second constrain is more difficult to implement numerically, and can lead to "multivariate" Monge maps.

One of the most interesting insights that they present is that using an entropic penalization on this problem, we can solve it in an proximately using Dijkstra's algorithm. This requires computing the projection onto $\mathcal{C}$ for the **KL** divergence: They mention that this is easy with the first constrain but harder (requires sub iterations) on the second constrain. I believe this could be another interesting algorithm.

4 References

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