

Projection onto simplex

- ▶ The simplex and the projection onto simplex by POCS.
- ▶ Driving the solution of projection by partial Lagrangian.
- ▶ The solution of projection onto simplex is a thresholding operator.
- ▶ The threshold is the root of a piecewise linear equation.
- ▶ The threshold can be solved by sorting with complexity $\mathcal{O}(n \log n)$.

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Simplex

- ▶ The r -dimensional (regular) simplex is the set of nonnegative vector with elements sum up to a . Mathematically, it is

$$\Delta = \left\{ \mathbf{x} \in \mathbb{R}^r \mid \langle \mathbf{x}, \mathbf{1}_r \rangle = a, \mathbf{x} \geq 0 \right\}.$$

- ▶ The r -dimensional unit simplex is a simplex with $a = 1$:

$$\Delta = \left\{ \mathbf{x} \in \mathbb{R}^r \mid \langle \mathbf{x}, \mathbf{1}_r \rangle = 1, \mathbf{x} \geq 0 \right\}.$$

- ▶ Δ is a closed and convex set: for $\mathbf{x}, \mathbf{y} \in \Delta$,

$$\langle \lambda \mathbf{x} + (1 - \lambda) \mathbf{y}, \mathbf{1}_r \rangle = \lambda \langle \mathbf{x}, \mathbf{1}_r \rangle + (1 - \lambda) \langle \mathbf{y}, \mathbf{1}_r \rangle = \lambda a + (1 - \lambda) a = a.$$

- ▶ We now consider how to solve the problem: projection onto simplex

$$\mathbf{x} = P_{\Delta}(\mathbf{y}) = \operatorname{argmin}_{\mathbf{x} \in \Delta^r} \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2^2.$$

Projections onto convex sets (POCS)

- ▶ The simplex set is the intersection of two sets:

$$\Delta = \underbrace{\{\mathbf{x} \in \mathbb{R}^n \mid \langle \mathbf{x}, \mathbf{1}_r \rangle = 1\}}_{C_1} \cap \underbrace{\{\mathbf{x} \in \mathbb{R}^r \mid x_i \geq 0\}}_{C_2}$$

where C_1 is a hyperplane and C_2 is the nonnegative orthant.

- ▶ As projection onto C_1 and projection onto C_2 have simple closed-form sol., thus $P_\Delta(\mathbf{y})$ solved by POCS

$$P_\Delta(\mathbf{y}) = P_{C_1 \cap C_2}(\mathbf{y}) = P_{C_2}(P_{C_1} \dots (P_{C_2}(P_{C_1}(\mathbf{y}))) \dots),$$

where POCS works if $C_1 \cap C_2 \neq \emptyset$.

- ▶ Another POCS using averaged projection: starting at \mathbf{x}_0 , iterate the following

$$\mathbf{x}_{k+1} = \frac{1}{2} \left(P_{C_1}(\mathbf{x}_k) + P_{C_2}(\mathbf{x}_k) \right),$$

until converges.

The Lagrangian

- ▶ The two projections

$$P_{C_1} = \max\{\mathbf{x}, 0\}, \quad P_{C_2} = \mathbf{x} - \frac{\sum_i x_i - 1}{n} \mathbf{1}.$$

POCS approach seem expensive and indirect. Can we do better?

- ▶ We now consider the Lagrangian of the problem

$$\operatorname{argmin}_{\mathbf{x} \geq 0, \langle \mathbf{x}, \mathbf{1}_r \rangle = 1} \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2^2.$$

- ▶ A trick: ignore the nonnegativity constraint now, **focus on the equality constraint**. The “partial” Lagrangian is

$$L(\mathbf{x}, \mu) = \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2^2 + \mu(\langle \mathbf{x}, \mathbf{1}_r \rangle - 1),$$

where μ is the Lagrangian multiplier.

The dual gives a hint

- ▶ Recall Lagrangian is a min-max problem: to get the optimal point, we need to minimize L w.r.t. \mathbf{x} and maximize L w.r.t. μ .

Now, consider minimization of L w.r.t. \mathbf{x} , **with $\mathbf{x} \geq 0$ in mind**:

$$\min_{\mathbf{x} \geq 0} L(\mathbf{x}, \mu) = \min_{\mathbf{x} \geq 0} \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2^2 + \mu(\langle \mathbf{x}, \mathbf{1}_r \rangle - 1).$$

- ▶ The problem is on \mathbf{x} , remove unrelated terms gives

$$\begin{aligned} \min_{\mathbf{x} \geq 0} L(\mathbf{x}, \mu) &= \min_{\mathbf{x} \geq 0} \frac{1}{2} \|\mathbf{x} - \mathbf{y}\|_2^2 + \langle \mathbf{x}, \mu \mathbf{1}_r \rangle \\ &= \min_{\mathbf{x} \geq 0} \sum_{i=1}^r \underbrace{\frac{1}{2} (x_i - y_i)^2 + \mu x_i}_{=l_i(x_i)} \end{aligned}$$

L is minimized if all l_i are minimized.

- ▶ The minimization of l_i are scalar problems in the form

$$\min_{x \geq 0} \underbrace{\frac{1}{2} (x - y)^2 + \mu x}_{=l(x)}.$$

The solution is a thresholding operator

- ▶ By 1st-order optimality condition / Fermat's rule, the minimizer of $l(x)$ is $y - \mu$.
 - ▶ If $y - \mu \geq 0$, then $x = y - \mu$ is the feasible optimal sol..
 - ▶ If $y - \mu < 0$, then $x = 0$ is the feasible optimal sol..

Hence, the solution of the minimization of l_i is

$$x_i = [y_i - \mu]_+ := \max\{0, y_i - \mu\}.$$

- ▶ The (feasible) minimizer of L is thus

$$[y - \mu \mathbf{1}_r]_+.$$

- ▶ Therefore, the solution of the projection $P_{\Delta}(\mathbf{y})$ is just a thresholding operator: for the vector \mathbf{y} , subtract each elements by μ . If the result is negative, replace it by zero.
- ▶ The question is : how to find μ ?

How to find μ

- ▶ Recall primal feasibility

$$\langle x, \mathbf{1}_r \rangle = 1, \mathbf{x} \geq 0.$$

Using summation sign

$$\sum_i x_i = a, \mathbf{x} \geq 0.$$

- ▶ Put the solution $\mathbf{x} = [y - \mu \mathbf{1}_r]_+$ into the primal feasibility, and note that

$$\sum_i [y_i - \mu]_+ = a, \quad \underbrace{[y - \mu \mathbf{1}_r]_+ \geq 0}_{\text{always true}}.$$

- ▶ Therefore, to find μ , the key is to solve the nonlinear equation

$$\sum_i \max\{0, y_i - \mu\} = a,$$

or more precisely, a piecewise linear equation.

Solving the piecewise linear equation

$$\sum_i \max\{0, y_i - \mu\} = a.$$

- ▶ Recall a property of max: if $y_i \leq \mu$, the max term becomes zero. Then the nonlinear equation can be expressed as

$$\sum_{j: y_j > \mu} (y_j - \mu) = a.$$

That is, only the components of \mathbf{y} that is large enough will contribute to the formation of μ . In other words, small components in \mathbf{y} can be ignored.

- ▶ As the size of components in \mathbf{y} matters, we can solve μ by a sorting method with general complexity $\mathcal{O}(n \log n)$. See [here](#) for details.

Solving the piecewise linear equation by sorting

- ▶ Assume elements in \mathbf{y} are sorted: $y_1 \geq y_2 \geq \dots \geq y_n$. Define the set

$$\mathcal{J} = \{j \mid y_j > \mu\}, \quad |\mathcal{J}| = K.$$

Then the piecewise linear equation becomes

$$\sum_{j \in \mathcal{J}} y_j - K\mu = a, \quad \implies \quad \mu = \frac{\sum_{j \in \mathcal{J}} y_j - a}{K}.$$

- ▶ The key now is how to find K . It is the largest j such that

$$y_K - \mu > 0.$$

As $y_K - \mu > 0$ is equivalent to $\max\{0, y_K - \mu\} \neq 0$, meaning y_K (the K -th largest component in \mathbf{y}), contributes to the formation of μ .

Summary of solving the piecewise linear equation by sorting

$$\sum_i \max\{0, y_i - \mu\} = a.$$

- ▶ Step-1. Sort \mathbf{y} .
- ▶ Step-2. Find K , which is the largest integer within $\{1, 2, \dots, n\}$ such that $y_K - \frac{\sum_{j \in \mathcal{J}} y_j - a}{K} > 0$.
- ▶ Step-3. Output $\mu = \frac{\sum_{j \in \mathcal{J}} y_j - a}{K}$.
- ▶ The most expensive part in this approach is step-1, using quick sort, the worst computational complexity is $\mathcal{O}(n \log n)$.
- ▶ This method is first proposed in: Held, M., Wolfe, P., Crowder, H.: Validation of subgradient optimization. Math. Program. (1974)

Last page – summary

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