$\frac{[\mathbf{X}^\top \mathbf{u}]_+}{\|\mathbf{u}\|_2^2}$ solves $\min_{\mathbf{v}\geq 0} \|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2$

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A non-negative constrained minimization problem

Given $\mathbf{X} \in \mathbb{R}^{m \times n}$, $\mathbf{u} \in \mathbb{R}^m$ and $\mathbf{u} \neq 0$, find the vector $\mathbf{v} \in \mathbb{R}^n_+$ by solving

$$\min_{\mathbf{v} \geq 0} \|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2,$$

where

- $\mathbf{v} \geq 0$ means all elements in the vector $\mathbf{v}$ are non-negative
- $\mathbf{u}\mathbf{v}^\top$ is vector outer product

Theorem. For the problem mentioned above, the unique and optimal solution has close form expression

$$\frac{[\mathbf{X}^\top \mathbf{u}]_+}{\|\mathbf{u}\|_2^2},$$

where $[\mathbf{X}^\top \mathbf{u}]_+ = \max(0, \mathbf{X}^\top \mathbf{u})$ and 0 is the zero vector with length n.

Next few pages : prove this small theorem.

Proving $\frac{[\mathbf{X}^\top \mathbf{u}]_+}{\|\mathbf{u}\|_2^2}$ solves $\min_{\mathbf{v}\geq 0} \|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2$ uniquely. (1/3)

Proof. Let $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_n]$ and $\mathbf{v} = [v_1, v_2, ..., v_n]$. Then we express $\|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2$ as

$$\|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2 = \sum_{i=1}^{n} \|\mathbf{u}v_i - \mathbf{x}_i\|_2^2 = \sum_{i=1}^{n} \|\mathbf{u}\|_2^2 v_i^2 - 2\mathbf{u}^\top \mathbf{x}_i v_i + \|\mathbf{x}_i\|_2^2$$

Let $f(v_i) = \|\mathbf{u}v_i - \mathbf{x}_i\|_2^2$. Then we have

$$\min_{\mathbf{v}\geq 0} \|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2 = \sum_{i=1}^{n} \min_{v_i \geq 0} f(v_i)$$

So we only need to analyze how to minimize $f(v_i)$ for each v_i.

What we do : set the gradient $\dfrac{\partial f(v_i)}{\partial v_i} = 2\|\mathbf{u}\|_2^2 v_i - 2\mathbf{u}^\top \mathbf{x}_i$ to zero.

Proving $\frac{[\mathbf{X}^\top \mathbf{u}]_+}{\|\mathbf{u}\|_2^2}$ solves $\min\limits_{\mathbf{v}\geq 0} \|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2$ uniquely. (2/3)

Note that we do not specify the signs of the elements on $\mathbf{u}$ and $\mathbf{X}$: we are given $\mathbf{X} \in \mathbb{R}^{m\times n}$ and $\mathbf{u} \in \mathbb{R}^{m\times 1}$ not $\mathbf{X} \in \mathbb{R}_+^{m\times n}$ nor $\mathbf{u} \in \mathbb{R}_+^{m\times 1}$.
Hence we have to consider two cases : $\mathbf{u}^\top \mathbf{x}_i < 0$ or $\mathbf{u}^\top \mathbf{x}_i \geq 0$.

Case 1. $\mathbf{u}^\top \mathbf{x}_i \geq 0$, we can solve v_i by setting $\dfrac{\partial f(v_i)}{\partial v_i} = 0$ as

$$\frac{\partial f(v_i)}{\partial v_i} = 2\|\mathbf{u}\|_2^2 v_i - 2\mathbf{u}^\top \mathbf{x}_i = 0 \implies v_i = \frac{\mathbf{u}^T \mathbf{x}_i}{\|\mathbf{u}\|_2^2}.$$

i.e. when $\mathbf{u}^\top \mathbf{x}_i \geq 0$, the solution to $\min\limits_{\mathbf{v}\geq 0} \|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2$ is $v_i = \dfrac{\mathbf{u}^T \mathbf{x}_i}{\|\mathbf{u}\|_2^2}$.

Note

- $\mathbf{u} \neq 0$ and the equal sign in $\mathbf{u}^\top \mathbf{x}_i \geq 0$ means $\mathbf{x}_i$ can be zero
- such solution is unique

Proving $\frac{[\mathbf{X}^\top \mathbf{u}]_+}{\|\mathbf{u}\|_2^2}$ solves $\min\limits_{\mathbf{v}\geq 0} \|\mathbf{u}\mathbf{v}^\top - \mathbf{X}\|_F^2$ uniquely. (3/3)

Case 2. $\mathbf{u}^\top \mathbf{x}_i < 0$, the term $-2\mathbf{u}^\top \mathbf{x}_i = +2|\mathbf{u}^T \mathbf{x}_i| > 0$, then

$$f(v_i) \quad = \quad \|\mathbf{u}\|_2^2 v_i^2 + 2|\mathbf{u}^\top \mathbf{x}_i| v_i + \|\mathbf{x}_i\|_2^2,$$

i.e. $f(v_i)$ is a quadratic function with positive coefficients (note that $\mathbf{u} \neq 0$). By high school algebra we know that

- $f(v_i)$ opens upward (V-shape)
- the valley of $f(v_i)$ is at $-\dfrac{|\mathbf{u}^\top \mathbf{x}_i|}{\|\mathbf{u}\|_2^2} < 0$

So the best non-negative solution v_i^* that is closest to the optimal solution (the valley) is at $v_i = 0$. (Draw the valley diagram to convince yourself)

Conclusion :

- When $\mathbf{u}^T \mathbf{x}_i \geq 0$, the solution to $\min\limits_{\mathbf{v}\geq 0} \|\mathbf{u}\mathbf{v}^T - \mathbf{X}\|_F^2$ is $\mathbf{v} = \dfrac{\mathbf{X}^T \mathbf{u}}{\|\mathbf{u}\|_2^2}$
- When $\mathbf{u}^T \mathbf{x}_i < 0$, the solution to $\min\limits_{\mathbf{v}\geq 0} \|\mathbf{u}\mathbf{v}^T - \mathbf{X}\|_F^2$ is $\mathbf{v} = 0$
- Combine both cases, the statement is proved.

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