MML lecture extra notes, Nov 19, 2021

Further discussions on finding stationary points for PCA's Lagrangian

The constrained optimisation problem for PCA (from the maximum variance perspective) is:

$$\begin{aligned} \min_{\{\mathbf{b}_1,...,\mathbf{b}_M\}} \quad & -\sum_{m=1}^{M} \mathbf{b}_m^\top \mathbf{S} \mathbf{b}_m, \\ \text{subject to} \quad & ||\mathbf{b}_m||_2^2 = 1, \; m = 1, ..., M \\ & \mathbf{b}_i \perp \mathbf{b}_j, \quad \forall i \neq j. \end{aligned} \tag{1}$$

The corresponding Lagrangian is:

$$L(\{\mathbf{b}_m\}, \{\lambda_m\}, \{\gamma_{ij}\}) = -\sum_{m=1}^{M} \mathbf{b}_m^\top \mathbf{S} \mathbf{b}_m + \sum_{m=1}^{M} \lambda_m (||\mathbf{b}_m||_2^2 - 1) + \sum_{i<j} \gamma_{ij} \mathbf{b}_i^\top \mathbf{b}_j. \tag{2}$$

To find the minimum of the constrained optimisation problem we need to find the stationary points for L first, i.e. we need to find $\{\mathbf{b}_m\}, \{\lambda_m\}, \{\gamma_{ij}\}$ to satisfy both the stationarity and primal feasibility conditions:

- stationarity: $\nabla_{\mathbf{b}_m} L(\{\mathbf{b}_m\}, \{\lambda_m\}, \{\gamma_{ij}\}) = \mathbf{0}, m = 1, ..., M$;
- primal feasibility: $||\mathbf{b}_m||_2^2 = 1, m = 1, ..., M$, $\mathbf{b}_i \perp \mathbf{b}_j, \forall i \neq j$.

In the lecture, when we find the solutions for $\{\mathbf{b}_m\}$ to satisfy the stationarity condition

$$\nabla_{\mathbf{b}_m} L(\{\mathbf{b}_m\}, \{\lambda_m\}, \{\gamma_{ij}\}) = -2\mathbf{S}\mathbf{b}_m + 2\lambda_m \mathbf{b}_m + \sum_{i<m} \gamma_{im} \mathbf{b}_i + \sum_{j>m} \gamma_{mj} \mathbf{b}_j = \mathbf{0}, \tag{3}$$

we make use of the primal feasibility condition and left-multiply the gradient with $\mathbf{b}_j$ (for some $j \neq m$) to obtain a new condition for $\mathbf{b}_m$:

$$-\mathbf{b}_m^\top (\mathbf{S}\mathbf{b}_m - \lambda_m \mathbf{b}_m) = 0. \tag{4}$$

As primal feasibility also requires $||\mathbf{b}_m||_2^2 = 1$, we concluded that a solution of this stationarity condition would be to set $(\mathbf{b}_m, \lambda_m) = (\boldsymbol{q}_d, \Lambda_{dd})$ for one of the eigenvector-eigenvalue pair of $\mathbf{S} = \mathbf{Q}\Lambda\mathbf{Q}^\top$. In such case we can also set $\gamma_{ij} = 0$ and this will ensure $\nabla_{\mathbf{b}_m} L(\{\mathbf{b}_m\}, \{\lambda_m\}, \{\gamma_{ij}\}) = 0$.

Here we justify why eigenvectors are the only possible solutions for $\mathbf{b}_m$ when concerning the stationarity and primal feasibility conditions. The reduced condition (4) only requires the two vectors $\mathbf{b}_m$ and $\mathbf{S}\mathbf{b}_m - \lambda_m \mathbf{b}_m$ to have inner product zero, which does not necessarily require $\mathbf{S}\mathbf{b}_m - \lambda_m \mathbf{b}_m = \mathbf{0}$. Indeed, by representing $\mathbf{b}_m$ using the orthonormal basis $\mathbf{Q}$ (i.e. $\mathbf{b}_m = \sum_{d=1}^{D} \beta_{md} \boldsymbol{q}_d$ for some coordinates $\{\beta_{md}\}$), one can show that (recall that $||\mathbf{b}_m||_2^2 = 1$ means $\sum_{d=1}^{D} \beta_{md}^2 = 1$)

$$-\mathbf{b}_m^\top (\mathbf{S}\mathbf{b}_m - \lambda_m \mathbf{b}_m) = \sum_{d=1}^{D} \beta_{md}^2 (\Lambda_{dd} - \lambda_m) = 0 \quad \Rightarrow \quad \lambda_m = \sum_{d=1}^{D} \beta_{md}^2 \Lambda_{dd}. \tag{5}$$

In other words, if we have $M << D$, e.g. $M = 2, D = 50$, one can still design $\mathbf{b}_1 = \sum_{d=1}^{2} \beta_{1d} \boldsymbol{q}_d$ and $\mathbf{b}_2 = \sum_{d=3}^{4} \beta_{2d} \boldsymbol{q}_d$ and the corresponding λ_1, λ_2 to satisfy condition (4) and primal feasibility. However, notice that $\mathbf{S}\mathbf{b}_m - \lambda_m \mathbf{b}_m = \sum_{d=1}^{D} \beta_{md} (\Lambda_{dd} - \lambda_m) \boldsymbol{q}_d$ which means the designed $\mathbf{b}_1 \in span\{\boldsymbol{q}_1, \boldsymbol{q}_2\}$ and $\mathbf{b}_2 \in span\{\boldsymbol{q}_3, \boldsymbol{q}_4\}$. This also means for any value of γ_{ij}, we can show that $\nabla_{\mathbf{b}_1} L \neq 0$ and $\nabla_{\mathbf{b}_2} L \neq 0$ (see eq. (3)), as $\mathbf{b}_2$ is perpendicular to $\mathbf{S}\mathbf{b}_1 - \lambda_1 \mathbf{b}_1$ when $\mathbf{S}\mathbf{b}_1 - \lambda_1 \mathbf{b}_1 \neq \mathbf{0}$, and vice versa. Therefore the only way to satisfy both the stationarity and primal feasibility conditions is to make $\mathbf{S}\mathbf{b}_m - \lambda_m \mathbf{b}_m = \mathbf{0}$ which returns eigenvectors as solutions.