1 Introduction

Unweighted principal components analysis is performed by applying appropriate row and/or column centering and/or scaling to obtain suitable transformed matrix X and then solving for the singular value decomposition (SVD)

$$X = UDV^T \tag{1}$$

with the solution satisfying various relationships with the eigenvalue decompositions of the symmetric matrices X^TX and XX^T; for example,

$$XX^TU = UD^2 \tag{2a}$$

$$X^TXV = VD^2 \tag{2b}$$

One approach to weighted principal components analysis results from replacing the matrices X^TX (proportional to the column-wise covariance matrix) with X^TW^2X and XX^T (proportional to row-wise covariance) with WXX^TW, where W is a diagonal matrix with w_{ii}^2 representing the weight assigned to row i.

Weighted problem then replaces (2) with

$$WXX^TWU = UD^2 \tag{3a}$$

$$X^TW^2XV = VD^2 \tag{3b}$$

These weighted eigenproblems may be solved via the SVD of WX:

$$WX = UDV^T \tag{4}$$

(with U, V orthogonal and D diagonal), or

$$w_{ii}x_{ig} = \sum_q u_{iq}d_{qq}v_{gq} \tag{5}$$

2 Differentiate Eigenproblems

We are interested here in the changes ΔU, ΔD, and ΔV to U, D, and V which result from an infinitesimal change ΔW to the weight matrix W.

First note that

$$0 = (U + \Delta U)^T(U + \Delta U) - I = (\Delta U)^TU + U^T\Delta U \tag{6}$$

or

$$(\Delta U)^TU = -U^T\Delta U \tag{7}$$

shows that $(\Delta U)^TU$ is antisymmetric. Similarly, for V:

$$(\Delta V)^TV = -V^T\Delta V \tag{8}$$

Now,

$$(\Delta W)XX^TW + WXX^T(\Delta W) = (\Delta U)D^2U^T + 2UD(\Delta D)U^T + UD^2(\Delta U)^T \tag{9}$$

Writing $M = (\Delta W)XX^TW + WXX^T(\Delta W)$, let's try

$$U^TMU = U^T\Delta UD^2 + 2D\Delta D + D^2(\Delta U)^TU \tag{10a}$$

$$= U^T\Delta UD^2 + 2D\Delta D - D^2U^T\Delta U \tag{10b}$$

or

$$\sum_{i,j} u_{iq} m_{ij} u_{jr} = \sum_i u_{iq} \Delta u_{ir} d_{rr}^2 - \sum_i u_{iq} \Delta u_{ir} d_{qq}^2 + 2\delta_{qr} d_{qq} \Delta d_{qq} \tag{11}$$

For $q = r$,

$$\sum_{i,j} u_{iq} m_{ij} u_{jq} = 2 d_{qq} \Delta d_{qq} \tag{12}$$

implying

$$\Delta d_{qq} = \frac{\sum_{i,j} u_{iq} m_{ij} u_{jq}}{2 d_{qq}} \tag{13}$$

For $q \neq r$,

$$\sum_{i,j} u_{iq} m_{ij} u_{jr} = \sum_i u_{iq} \Delta u_{ir} (d_{rr}^2 - d_{qq}^2) \tag{14}$$

or

$$\sum_i u_{iq} \Delta u_{ir} = \frac{1}{d_{rr}^2 - d_{qq}^2} \sum_{i,j} u_{iq} m_{ij} u_{jr} \tag{15}$$

Premultiplying by u_{kq} and summing over q,

$$\Delta u_{kr} = u_{kr} \sum_i u_{ir} \Delta u_{ir} + \sum_{q \neq r} \frac{u_{kq}}{d_{rr}^2 - d_{qq}^2} \sum_{i,j} u_{iq} m_{ij} u_{jr} \tag{16}$$

but $\sum_i u_{iq} \Delta u_{ir} = -\sum_i \Delta u_{iq} u_{ir}$ implies that $\sum_i u_{ir} \Delta u_{ir} = 0$, so

$$\Delta u_{kr} = \sum_{q \neq r} \frac{u_{kq}}{d_{rr}^2 - d_{qq}^2} \sum_{i,j} u_{iq} m_{ij} u_{jr} \tag{17}$$

Similarly, defining $N = 2X^T W \Delta W X$

$$\Delta d_{qq} = \frac{\sum_{g,h} v_{gq} n_{gh} v_{hq}}{2 d_{qq}} \tag{18}$$

and

$$\Delta v_{fr} = \sum_{q \neq r} \frac{v_{fq}}{d_{rr}^2 - d_{qq}^2} \sum_{g,h} v_{gq} n_{gh} v_{hr} \tag{19}$$

3 Differentiate SVD Directly

Analysis above complicated by non-square X. In this case, can use equations above for ΔD and whichever of ΔU or ΔV is square; the remaining derivative can be calulated directly from the definition of SVD:

$$(W + \Delta W)\, X = (U + \Delta U)(D + \Delta D)(V + \Delta V)^T \tag{20a}$$

$$\Delta W\, X = \Delta U\, D V^T + U \Delta D\, V^T + U D (\Delta V)^T \tag{20b}$$

$$\Delta U = \Delta W\, X V D^{-1} - U \Delta D\, D^{-1} - U D (\Delta V)^T V D^{-1} \tag{20c}$$

$$(\Delta V)^T = D^{-1} U^T \Delta W\, X - D^{-1} U^T \Delta U\, D V^T - D^{-1} \Delta D\, V^T \tag{20d}$$

4 Arbitrary Changes to X

In order to approximate the changes to the SVD under a perturbation $X \mapsto X + \Delta X$, replace equation (9) with

$$\Delta X X^T + X(\Delta X)^T = (\Delta U)D^2U^T + 2UD(\Delta D)U^T + UD^2(\Delta U)^T \tag{21}$$

Defining $A = \Delta X X^T + X(\Delta X)^T$, we can follow the same logic as above to obtain

$$\Delta d_{qq} = \frac{\sum_{i,j} v_{iq} a_{ij} v_{jq}}{2d_{qq}} \tag{22a}$$

$$\Delta u_{kr} = \sum_{q \neq r} \frac{u_{kq}}{d_{rr}^2 - d_{qq}^2} \sum_{i,j} u_{iq} a_{ij} u_{jr} \tag{22b}$$

and, with $B = (\Delta X)^T X + X^T \Delta X$

$$\Delta d_{qq} = \frac{\sum_{g,h} v_{gq} b_{gh} v_{hq}}{2d_{qq}} \tag{23a}$$

$$\Delta v_{fr} = \sum_{q \neq r} \frac{v_{fq}}{d_{rr}^2 - d_{qq}^2} \sum_{g,h} v_{gq} b_{gh} v_{hr} \tag{23b}$$

Again, if X is not square, can use whichever of (22) or (23) deals with smaller matrix U or V and then obtain the remaining matrix directly from

$$X + \Delta X = (U + \Delta U)(D + \Delta D)(V + \Delta V)^T \tag{24a}$$

$$\Delta X = \Delta U\, DV^T + U \Delta D\, V^T + UD(\Delta V)^T \tag{24b}$$

$$\Delta U = \Delta X\, V D^{-1} - U \Delta D\, D^{-1} - UD(\Delta V)^T V D^{-1} \tag{24c}$$

$$(\Delta V)^T = D^{-1}U^T \Delta X - D^{-1} U^T \Delta U\, DV^T - D^{-1} \Delta D\, V^T \tag{24d}$$