Electronic Supplementary Material (ESI) for Analyst.

Supplemental Material Soft-trilinear constraints for improved quantitation in Multivariate Curve Resolution

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For the *i*th component:

a. Fold the current estimate of the concentration profile of component *i* into a matrix

2. Apply PCA to the matrix
3. Calculate the value of *k* according to equation 4.
4. if $k<=\alpha$, then

   $\delta_{\alpha}=0$

   else

   $\mathbf{r} = \mathbf{c}_{i}-\mathbf{c}_{i\text{-hat}}$

5. $\delta_{\alpha} = \sum\sum(r \times r^{T})$

   where, $\mathbf{c}_{i\text{-hat}}=|(\mathbf{u}_{c}(:,2{:}nf)\ \mathbf{s}_{c}(2{:}nf,2{:}nf)\ \mathbf{v}^{T}_{c}(:,2{:}nf))|$

6. end if

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%%%% c is the folded concentration matrix
%%%% nf is number of augmented data matrices
% nf=3 as an example
[u,s,v]=svds(c,nf);  %%%%%%%%c is the concentration matrix of component i.
var=sum(diag(s).^2);
k=((s(2,2)^2+s(3,3)^2)/var)*100;
t=s(2:nf,2:nf)*v(:,2:nf)';
c_hat=abs(u(:,2:nf)*t);
r=cp-c_hat; %%%%% residual
%%%%%%%% define alpha
if k<=alpha
 δα==0;
else
 δα=sum(sum(r*r'));
end
```