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

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For the ith component:

1. 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 $k \leq \alpha$, then
   \[ \delta_a = 0 \]
   else
   \[ r = c_i - c_i\text{-hat} \]
5. \[ \delta_a = \sum \sum (r \times r^T) \]
   where, \( c_i\text{-hat} = [(u_i(:,2:nf) s_i (2:nf,2:nf) v_i(:,2:nf))]
6. end if

%%%% 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
   \[ \delta_a = 0 \]
else
   \[ \delta_a = \text{sum} \text{sum}(r*r') \]
end