

# Supporting Information for Fast Burst-Sparsity Learning Based Baseline Correction (FBSL-BC) Algorithm for Signals of Analytical Instruments

Haoran Li,<sup>†</sup> Suyi Chen,<sup>†</sup> Jisheng Dai,<sup>\*,†</sup> Xiaobo Zou,<sup>\*,‡</sup> Tao Chen,<sup>¶</sup> Tianhong  
Pan,<sup>§</sup> and Melvin Holmes<sup>||</sup>

<sup>†</sup>*School of Electrical and Information Engineering, Jiangsu University, Zhenjiang 212013,  
China*

<sup>‡</sup>*School of Food and Biological Engineering, Jiangsu University, Zhenjiang 212013, China*

<sup>¶</sup>*Department of Chemical and Process Engineering, University of Surrey, Guildford GU2  
7XH, United Kingdom*

<sup>§</sup>*School of Electrical Engineering and Automation, Anhui University, Hefei, 230061, China*

<sup>||</sup>*School of Food Science and Nutrition, University of Leeds, Leeds LS2 9JT, United  
Kingdom*

E-mail: jsdai@ujs.edu.cn; xiaobo@ujs.edu.cn

## Supporting Information Contents

The update solutions with Lemma 1;

Pseudo Code of FBSL-BC;

### Figures

Figure S-1: Comparison among FBSL-BC, SBL-BC and SSFBCSP for simulated spectrum with exponential baseline. a) simulated spectrum, b) FBSL-BC, c) SBL-BC, d) SSFBCSP with  $\lambda_1 = \{10^4, 10^6, 10^5\}$  and  $\lambda_2 = \{10^{-3}, 10^{-1}, 10^{-1}\}$ .

Figure S-2: NMSE results under different SNR for simulated data with exponential baseline, where  $\lambda_1 = 10^5$ ,  $\lambda_2 = 10^{-2}$ ,  $\lambda^{\text{ALS}} = 10^5$ ,  $p^{\text{ALS}} = 0.005$  and  $\lambda^{\text{air}} = 10^4$ .

Figure S-3: The baseline correction results of corn spectrum (with added noise,  $\text{SNR} = 50\text{dB}$ ) and estimated baseline. a) FBSL-BC, b) SBL-BC, c) SSFBCSP, d) airPLS.

Figure S-4: The baseline correction results of Huangshan Maofeng Tea spectrum. a) FBSL-BC, b) SBL-BC, c) SSFBCSP and d) airPLS.

Figure S-5: Comparison of baseline correction results for GmeliniteNa Raman spectral with  $\text{SNR} = 50\text{dB}$ . a) FBSL-BC, b) airPLS ( $\lambda^{\text{air}} = 10^9$ ), c) SBL-BC, d) SSFBCSP ( $\lambda_1 = 10^6$  and  $\lambda_2 = 10^{-2}$ ).

Figure S-6: Comparison of baseline correction results for Cassiterite Raman spectral with  $\text{SNR} = 40\text{dB}$ . a) FBSL-BC, b) airPLS ( $\lambda^{\text{air}} = 10^9$ ), c) SBL-BC, d) SSFBCSP ( $\lambda_1 = 10^6$  and  $\lambda_2 = 10^{-2}$ ).

Figure S-7: Comparison of baseline correction results for Marialite Raman spectra with  $\text{SNR} = 30\text{dB}$ . a) FBSL-BC, b) airPLS ( $\lambda^{\text{air}} = 10^9$ ), c) SBL-BC, d) SSFBCSP ( $\lambda_1 = 10^6$  and  $\lambda_2 = 10^{-2}$ ).

Figure S-8: The sparse coefficients for three mineral Raman datasets, a) SBL-BC, b) FBSL-BC.

## Tables

Table S-1: Comparison of averaged RMSECV among airPLS ( $\lambda^{\text{air}} = 10^8$ ), arPLS ( $\lambda^{\text{ar}} = 10^5$ ), SSFBCSP ( $\lambda_1 = 10^4$  and  $\lambda_2 = 10^{-2}$ ), SBL-BC ( $\rho = 10^5$ ) and FBSL-BC.

Table S-2: Comparison of averaged RMSEP results among airPLS ( $\lambda^{\text{air}} = 10^8$ ), arPLS ( $\lambda^{\text{ar}} = 10^5$ ), SSFBCSP ( $\lambda_1 = 2 \times 10^5$  and  $\lambda_2 = 10^{-2}$ ), SBL-BC ( $\rho = 10^5$ ) and FBSL-BC.

## The proof of Lemma 1

**Lemma. 1:** The optimal solutions to (20)–(25) are given as follows:

$$q^{(r+1)}(\mathbf{W}) = \prod_{g=1}^G \mathcal{N}(\mathbf{w}_g | \hat{\mathbf{w}}_g^{(r+1)}, \boldsymbol{\Sigma}^{(r+1)}), \quad (1)$$

$$q^{(r+1)}(\alpha) = \Gamma\left(\alpha \middle| e + \frac{1}{2}LG, f_\alpha^{(r+1)}\right), \quad (2)$$

$$q^{(r+1)}(\boldsymbol{\gamma}) = \prod_{l=1}^L \Gamma\left(\gamma_l \middle| e_l^{(r+1)}, f_l^{(r+1)}\right), \quad (3)$$

$$q^{(r+1)}(\mathbf{h}) = \prod_{l=1}^L \prod_{k \in \{-1, 0, 1\}} \hat{h}_{l,k}^{(r+1)} \delta(h_l - k), \quad (4)$$

$$q^{(r+1)}(\beta) = \Gamma\left(\beta \middle| e + \frac{1}{2}LG, f_\beta^{(r+1)}\right), \quad (5)$$

$$q^{(r+1)}(\mathbf{B}) = \prod_{g=1}^G \mathcal{N}(\mathbf{b}_g | \hat{\mathbf{b}}_g^{(r+1)}, \boldsymbol{\Sigma}_b^{(r+1)}), \quad (6)$$

where

$$\boldsymbol{\Sigma}^{(r+1)} = \left( \hat{\alpha}^{(r)} \mathbf{A}_L^T \mathbf{A}_L + \sum_{k \in \{-1, 0, 1\}} \boldsymbol{\Psi}_k^{(r)} \boldsymbol{\Lambda}_k^{(r)} \right)^{-1}, \quad (7)$$

$$\hat{\mathbf{w}}_g^{(r+1)} = \hat{\alpha}^{(r)} \boldsymbol{\Sigma}^{(r+1)} \mathbf{A}_L^T (\mathbf{x}_g - \hat{\mathbf{b}}_g^{(r)}), \quad (8)$$

$$f_\alpha^{(r+1)} = f + \frac{1}{2} \sum_{g=1}^G \left( \|\mathbf{x}_g - \mathbf{A}_L \hat{\mathbf{w}}_g^{(r+1)} - \hat{\mathbf{b}}_g^{(r)}\|_2^2 + \text{tr}\{\mathbf{A}_L \boldsymbol{\Sigma}^{(r+1)} \mathbf{A}_L^T + \boldsymbol{\Sigma}_b^{(r)}\} \right), \quad (9)$$

$$\hat{\alpha}^{(r+1)} = \langle \alpha \rangle_{q^{(r+1)}(\alpha)} = (e + \frac{1}{2}LG) / f_\alpha^{(r+1)}, \quad (10)$$

$$e_l^{(r+1)} = e + \frac{G}{2} (\hat{h}_{l+1,-1}^{(r)} + \hat{h}_{l,0}^{(r)} + \hat{h}_{l-1,1}^{(r)}), \quad (11)$$

$$f_l^{(r+1)} = f + \frac{1}{2} \sum_{g=1}^G (\hat{h}_{l+1,-1}^{(r)} \varpi_{l+1,g}^{(r+1)} + \hat{h}_{l,0}^{(r)} \varpi_{l,g}^{(r+1)} + \hat{h}_{l-1,1}^{(r)} \varpi_{l-1,g}^{(r+1)}), \quad (12)$$

$$\hat{\gamma}_l^{(r+1)} = \langle \gamma_l \rangle_{q^{(r+1)}(\gamma_l)} = e_l^{(r+1)} / f_l^{(r+1)}, \quad (13)$$

$$\hat{h}_{l,k}^{(r+1)} = \frac{\exp(\nu_{l,k}^{(r+1)})}{\sum_{k \in \{-1,0,1\}} \exp(\nu_{l,k}^{(r+1)})}, \quad (14)$$

$$f_{\beta}^{(r+1)} = f + \frac{1}{2} \sum_{g=1}^G \left( \|\mathbf{D}_L \hat{\mathbf{b}}_g^{(r)}\|^2 + \text{tr}\{\mathbf{D}_L \boldsymbol{\Sigma}_b^{(r)} \mathbf{D}_L^T\} \right), \quad (15)$$

$$\hat{\beta}^{(r+1)} = \langle \beta \rangle_{q^{(r+1)}(\beta)} = (e + \frac{1}{2}LG)/(f_{\beta}^{(r+1)}), \quad (16)$$

$$\boldsymbol{\Sigma}_b^{(r+1)} = \left( \hat{\alpha}^{(r+1)} \mathbf{I} + \hat{\beta}^{(r+1)} \mathbf{D}_L^T \mathbf{D}_L \right)^{-1}, \quad (17)$$

$$\hat{\mathbf{b}}_g^{(r+1)} = \hat{\alpha}^{(r+1)} \boldsymbol{\Sigma}_b^{(r+1)} \left( \mathbf{x}_g - \mathbf{A}_L \hat{\mathbf{w}}_g^{(r+1)} \right). \quad (18)$$

with  $\boldsymbol{\Psi}_k^{(r)} = \text{diag}\{\hat{h}_{1,k}^{(r)}, \hat{h}_{2,k}^{(r)}, \dots, \hat{h}_{L,k}^{(r)}\}$ ,  $\boldsymbol{\Lambda}_k^{(r)} = \text{diag}\{\hat{\gamma}_{1+k}^{(r)}, \hat{\gamma}_{2+k}^{(r)}, \dots, \hat{\gamma}_{L+k}^{(r)}\}$ ,  $\varpi_{l,g}^{(r+1)} = \langle w_{l,j}^2 \rangle_{q^{(r+1)}(w_j)} = [\hat{w}_{l,g}^{(r+1)}]_j^2 + [\boldsymbol{\Sigma}^{(r+1)}]_{l,l}$ ,  $\nu_{l,k}^{(r+1)} = \frac{G}{2} (\widehat{\ln \gamma_{l+k}})^{(r+1)} - \frac{1}{2} \sum_{g=1}^G \hat{\gamma}_{l+k}^{(r+1)} \varpi_{l,g}^{(r+1)}$ , and  $(\widehat{\ln \gamma_l})^{(r+1)} = \langle \ln \gamma_l \rangle_{q^{(r+1)}(\gamma_l)} = \Psi(e_l^{(r+1)}) - \ln(f_l^{(r+1)})$ .

*Proof.* The joint distribution  $p(\mathbf{X}, \mathbf{W}, \mathbf{h}, \boldsymbol{\gamma}, \mathbf{B}, \alpha, \beta)$  can be factorized by

$$p(\mathbf{X}, \mathbf{W}, \mathbf{h}, \boldsymbol{\gamma}, \mathbf{B}, \alpha, \beta) = p(\mathbf{X}|\mathbf{W}, \mathbf{B}, \alpha) p(\mathbf{W}|\boldsymbol{\gamma}, \mathbf{h}) p(\boldsymbol{\gamma}) p(\mathbf{h}) p(\mathbf{B}|\beta) p(\beta) p(\alpha) \quad (19)$$

The stationary solution can be obtained by following iteratively update strategy:

$$\ln q^{(r+1)}(\Omega_1) \propto \langle \ln p(\mathbf{X}, \Omega) \rangle_{q^{(r)}(\Omega_2) q^{(r)}(\Omega_3) q^{(r)}(\Omega_4) q^{(r)}(\Omega_5) q^{(r)}(\Omega_6)}, \quad (20)$$

$$\ln q^{(r+1)}(\Omega_2) \propto \langle \ln p(\mathbf{X}, \Omega) \rangle_{q^{(r+1)}(\Omega_1) q^{(r)}(\Omega_3) q^{(r)}(\Omega_4) q^{(r)}(\Omega_5) q^{(r)}(\Omega_6)}, \quad (21)$$

$$\ln q^{(r+1)}(\Omega_3) \propto \langle \ln p(\mathbf{X}, \Omega) \rangle_{q^{(r+1)}(\Omega_1) q^{(r+1)}(\Omega_2) q^{(r)}(\Omega_4) q^{(r)}(\Omega_5) q^{(r)}(\Omega_6)}, \quad (22)$$

$$\ln q^{(r+1)}(\Omega_4) \propto \langle \ln p(\mathbf{X}, \Omega) \rangle_{q^{(r+1)}(\Omega_1) q^{(r+1)}(\Omega_2) q^{(r+1)}(\Omega_3) q^{(r)}(\Omega_5) q^{(r)}(\Omega_6)}, \quad (23)$$

$$\ln q^{(r+1)}(\Omega_5) \propto \langle \ln p(\mathbf{X}, \Omega) \rangle_{q^{(r+1)}(\Omega_1) q^{(r+1)}(\Omega_2) q^{(r+1)}(\Omega_3) q^{(r+1)}(\Omega_4) q^{(r)}(\Omega_6)}, \quad (24)$$

$$\ln q^{(r+1)}(\Omega_6) \propto \langle \ln p(\mathbf{X}, \Omega) \rangle_{q^{(r+1)}(\Omega_1) q^{(r+1)}(\Omega_2) q^{(r+1)}(\Omega_3) q^{(r+1)}(\Omega_4) q^{(r+1)}(\Omega_5)}, \quad (25)$$

Substituting (19) into (20), we obtain

$$\begin{aligned} & \ln q^{(r+1)}(\mathbf{W}) \\ & \propto \langle \ln p(\mathbf{X}|\mathbf{W}, \mathbf{B}, \alpha) p(\mathbf{W}|\boldsymbol{\gamma}, \mathbf{h}) \rangle_{q^{(r)}(\alpha)q^{(r)}(\boldsymbol{\gamma})q^{(r)}(\mathbf{h})q^{(r)}(\mathbf{B})} \end{aligned} \quad (26)$$

$$\propto -\frac{1}{2}\hat{\alpha}^{(r)} \sum_{g=1}^G \|\mathbf{x}_g - \mathbf{A}_L \mathbf{w}_g - \hat{\mathbf{b}}_g^{(r)}\|_2^2 - \frac{1}{2} \sum_{g=1}^G \mathbf{w}_g^T (\boldsymbol{\Psi}_{-1}^{(r)} \boldsymbol{\Lambda}_{-1}^{(r)} + \boldsymbol{\Psi}_0^{(r)} \boldsymbol{\Lambda}_0^{(r)} + \boldsymbol{\Psi}_1^{(r)} \boldsymbol{\Lambda}_1^{(r)}) \mathbf{w}_g, \quad (27)$$

where  $\boldsymbol{\Psi}_k^{(r)} = \text{diag}\{\hat{h}_{1,k}^{(r)}, \hat{h}_{2,k}^{(r)}, \dots, \hat{h}_{L,k}^{(r)}\}$  with  $\hat{h}_{l,k}^{(r)} = q^{(r)}(h_l = k)$ ,  $\boldsymbol{\Lambda}_k^{(r)} = \text{diag}\{\hat{\gamma}_{1+k}^{(r)}, \hat{\gamma}_{2+k}^{(r)}, \dots, \hat{\gamma}_{L+k}^{(r)}\}$ , and  $\hat{\mathbf{b}}_g^{(r)} = \langle \mathbf{b} \rangle_{q^{(r)}(\mathbf{b}_g)}$ . It shows that  $q^{(r+1)}(\mathbf{w}_g)$ s are separable and follow Gaussian distributions:

$$q^{(r+1)}(\mathbf{w}_g) = \mathcal{N}(\mathbf{w}_g | \hat{\mathbf{w}}_g^{(r+1)}, \boldsymbol{\Sigma}^{(r+1)}), \quad g = 1, 2, \dots, G, \quad (28)$$

where

$$\boldsymbol{\Sigma}^{(r+1)} = \left( \hat{\alpha}^{(r)} \mathbf{A}_L^T \mathbf{A}_L + \sum_{k \in \{-1, 0, 1\}} \boldsymbol{\Psi}_k^{(r)} \boldsymbol{\Lambda}_k^{(r)} \right)^{-1}, \quad (29)$$

$$\hat{\mathbf{w}}_g^{(r+1)} = \hat{\alpha}^{(r)} \boldsymbol{\Sigma}^{(r+1)} \mathbf{A}_L^T (\mathbf{x}_g - \hat{\mathbf{b}}_g^{(r)}). \quad (30)$$

Substituting (19) into (21), we obtain

$$\begin{aligned} & \ln q^{(r+1)}(\alpha) \\ & \propto \langle \ln p(\mathbf{X}|\mathbf{W}, \mathbf{B}, \alpha) p(\alpha) \rangle_{q^{(r+1)}(\mathbf{W})q^{(r)}(\mathbf{B})} \end{aligned} \quad (31)$$

$$\propto -\frac{1}{2}\alpha \sum_{g=1}^G \left( \|\mathbf{x}_g - \mathbf{A}_L \hat{\mathbf{w}}_g^{(r+1)} - \hat{\mathbf{b}}_g^{(r)}\|_2^2 + \text{tr}\{\mathbf{A}_L \boldsymbol{\Sigma}^{(r+1)} \mathbf{A}_L^T + \boldsymbol{\Sigma}_b^{(r)}\} \right) - \alpha f + (e + LG/2 - 1) \ln \alpha. \quad (32)$$

Hence,  $q^{(r+1)}(\alpha)$  obeys a Gamma distribution:

$$q^{(r+1)}(\alpha) = \Gamma\left(\alpha \middle| e + \frac{1}{2}LG, f_\alpha^{(r+1)}\right), \quad (33)$$

where  $f_\alpha^{(r+1)} = f + \frac{1}{2} \sum_{g=1}^G \left( \|\mathbf{x}_g - \mathbf{A}_L \hat{\mathbf{w}}_g^{(r+1)} - \hat{\mathbf{b}}_g^{(r)}\|_2^2 + \text{tr}\{\mathbf{A}_L \boldsymbol{\Sigma}^{(r+1)} \mathbf{A}_L^T + \boldsymbol{\Sigma}_b^{(r)}\} \right)$ .

Substituting (19) into (22), we obtain

$$\begin{aligned} & \ln q^{(r+1)}(\boldsymbol{\gamma}) \\ & \propto \langle \ln p(\mathbf{W} | \boldsymbol{\gamma}, \mathbf{h}) p(\boldsymbol{\gamma}) \rangle_{q^{(r+1)}(\mathbf{W}) q^{(r)}(\mathbf{h})} \end{aligned} \quad (34)$$

$$\begin{aligned} & \propto \sum_{l=1}^L -\gamma_l \left( f + \frac{1}{2} \sum_{g=1}^G \left( \hat{h}_{l+1,-1}^{(r)} \varpi_{l+1,g}^{(r+1)} + \hat{h}_{l,0}^{(r)} \varpi_{l,g}^{(r+1)} + \hat{h}_{l-1,1}^{(r)} \varpi_{l-1,g}^{(r+1)} \right) \right) \\ & + \sum_{l=1}^L \left( e + \frac{G}{2} (\hat{h}_{l+1,-1}^{(r)} + \hat{h}_{l,0}^{(r)} + \hat{h}_{l-1,1}^{(r)}) - 1 \right) \ln \gamma_l. \end{aligned} \quad (35)$$

It shows that  $q^{(r+1)}(\gamma_l)$ s are also separable and follow Gamma distributions:

$$q^{(r+1)}(\gamma_l) = \Gamma\left(\alpha \middle| e_l^{(r+1)}, f_l^{(r+1)}\right), \quad l = 1, 2, \dots, L, \quad (36)$$

where  $e_l^{(r+1)} = e + \frac{G}{2} (\hat{h}_{l+1,-1}^{(r)} + \hat{h}_{l,0}^{(r)} + \hat{h}_{l-1,1}^{(r)})$  and  $f_l^{(r+1)} = f + \frac{1}{2} \sum_{g=1}^G (\hat{h}_{l+1,-1}^{(r)} \varpi_{l+1,g}^{(r+1)} + \hat{h}_{l,0}^{(r)} \varpi_{l,g}^{(r+1)} + \hat{h}_{l-1,1}^{(r)} \varpi_{l-1,g}^{(r+1)})$ .

Substituting (19) into (23), we obtain

$$\ln q^{(r+1)}(\mathbf{h}) \propto \langle \ln p(\mathbf{W} | \boldsymbol{\gamma}, \mathbf{h}) p(\mathbf{h}) \rangle_{q^{(r+1)}(\mathbf{W}) q^{(r+1)}(\boldsymbol{\gamma})}. \quad (37)$$

Because  $h_l$  takes values from  $\{-1, 0, 1\}$  only, we can directly calculate  $q^{(r+1)}(h_l = k)$ ,  $k \in \{1, 0, 1\}$ :

$$\ln q^{(r+1)}(h_l = k) \propto \underbrace{\frac{G}{2} (\widehat{\ln \gamma_{l+k}})^{(r+1)} - \frac{1}{2} \sum_{g=1}^G \hat{\gamma}_{l+k}^{(r+1)} \varpi_{l,g}^{(r+1)}}_{\triangleq \nu_{l,k}^{(r+1)}}, \quad (38)$$

where  $(\widehat{\ln \gamma_l})^{(r+1)} = \langle \ln \gamma_l \rangle_{q^{(r+1)}(\gamma_l)} = \Psi(e_l^{(r+1)}) - \ln(f_l^{(r+1)})$ . Since  $\sum_{k \in \{-1, 0, 1\}} q^{(r+1)}(h_l = k)$ , we have

$$\hat{h}_{l,k}^{(r+1)} = q^{(r+1)}(h_l = k) = \frac{\exp(\nu_{l,k}^{(r+1)})}{\sum_{k \in \{-1, 0, 1\}} \exp(\nu_{l,k}^{(r+1)})}, \quad k \in \{-1, 0, 1\}. \quad (39)$$

Finally, the update rules for  $q^{(r+1)}(\beta)$  and  $q^{(r+1)}(\mathbf{B})$  coincide with the ones in , whose proofs are omitted for brevity.  $\square$

For the computational efficiency, we can similarly set  $\hat{\beta} = \rho \hat{\alpha}^{(r+1)}$  and  $\hat{\alpha}^{(r+1)} \boldsymbol{\Sigma}_b^{(r+1)} = (\mathbf{I} + \rho \cdot \mathbf{D}_L^T \mathbf{D}_L)^{-1}$ , and then (18) can be simplified as:

$$\hat{\mathbf{b}}_g^{(r+1)} = (\mathbf{I} + \rho \cdot \mathbf{D}_L^T \mathbf{D}_L)^{-1} \left( \mathbf{x}_g - \mathbf{A}_L \hat{\mathbf{w}}_g^{(r+1)} \right), \quad (40)$$

where  $\rho$  can be simply choose from  $\{10^4, 10^5, 10^7, 10^8\}$



## Pseudo Code of FBSL-BC

---

**Algorithm 1** FBSL-BC
 

---

1. Input:  $\mathbf{x}$  and  $G$ .
  2. Down-sample  $\mathbf{x}$  into  $\mathbf{x}_g$ s,
  3. Initialize  $\hat{\alpha}^{(0)}$ ,  $\hat{\gamma}^{(0)}$ ,  $\hat{h}_{l,k}^{(0)}$ s,  $\Sigma_b^{(0)}$  and  $\hat{\mathbf{b}}_g^{(0)}$ s, and set  $r = 0$ ,  $e = 10^{-10}$  and  $f = 10^{-10}$ .
  4. Repeat the following steps:
    - a) Update  $\Sigma^{(r+1)}$  and  $\hat{\mathbf{w}}_g^{(r+1)}$ s using (7) and (8), and then project  $\hat{\mathbf{w}}_g^{(r+1)}$ s to their non-negative parts.
    - b) Update  $\hat{\alpha}^{(r+1)}$  using (10) and let  $\hat{\alpha}^{(r+1)} = \min\{\hat{\alpha}^{(r+1)}, 10^5\}$ .
    - c) Update  $\hat{\gamma}_l^{(r+1)}$ s using (13).
    - d) Update  $\hat{h}_{l,k}^{(r+1)}$ s using (14).
    - e) Update  $\hat{\mathbf{b}}_g^{(r+1)}$ s using (40).
    - f) Update  $\sigma_l^2$ s using the variance refinement.
    - g) Let  $r = r + 1$  and go back to Step-4a until a given threshold is reached.
  5. Output:  $\hat{\mathbf{w}}_g^{(r)}$ s and  $\hat{\mathbf{b}}_g^{(r)}$ s.
-

# Figures

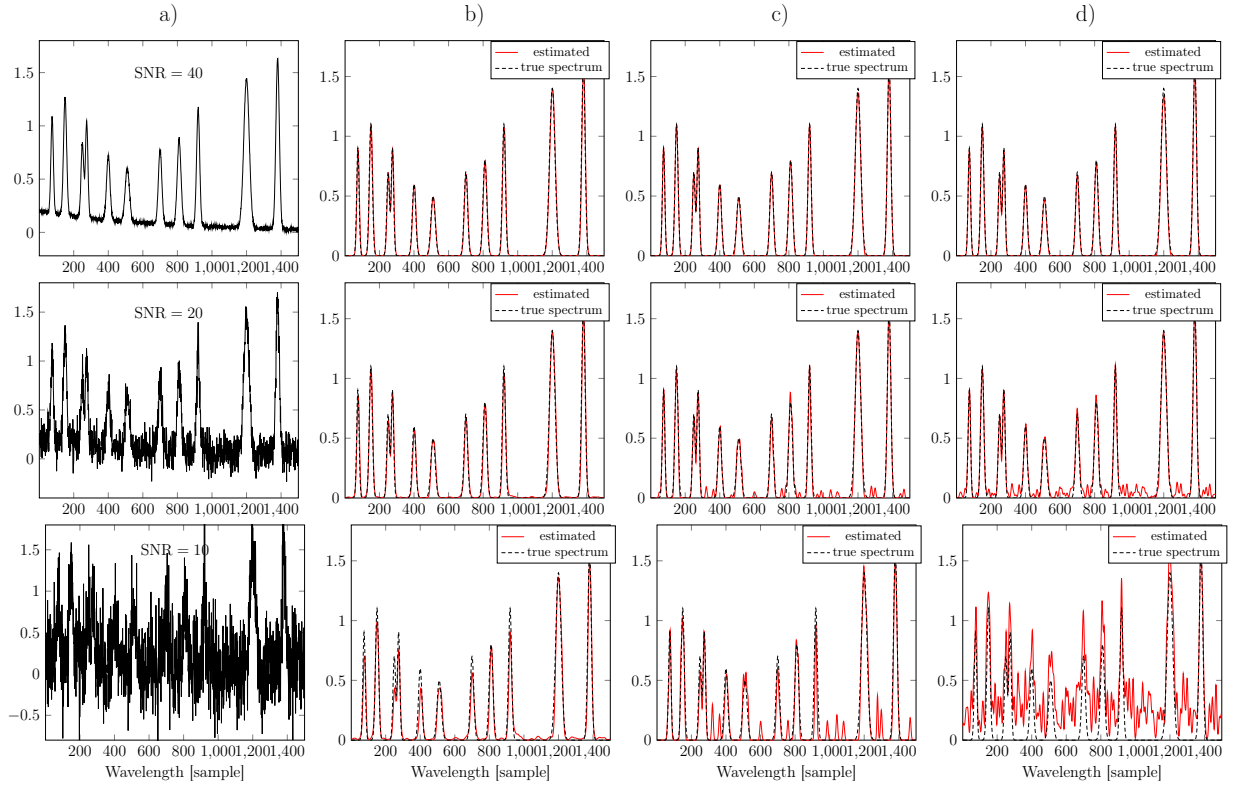


Figure S-1: Comparison among FBSL-BC, SBL-BC and SSFBCSP for simulated spectrum with exponential baseline. a) simulated spectrum, b) FBSL-BC, c) SBL-BC, d) SSFBCSP with  $\lambda_1 = \{10^4, 10^6, 10^5\}$  and  $\lambda_2 = \{10^{-3}, 10^{-1}, 10^{-1}\}$ .

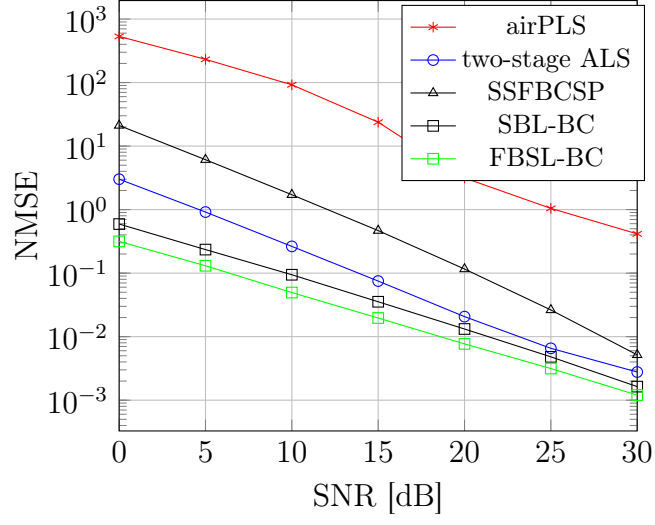


Figure S-2: NMSE results under different SNR for simulated data with exponential baseline, where  $\lambda_1 = 10^5$ ,  $\lambda_2 = 10^{-2}$ ,  $\lambda^{\text{ALS}} = 10^5$ ,  $p^{\text{ALS}} = 0.005$  and  $\lambda^{\text{air}} = 10^4$ .

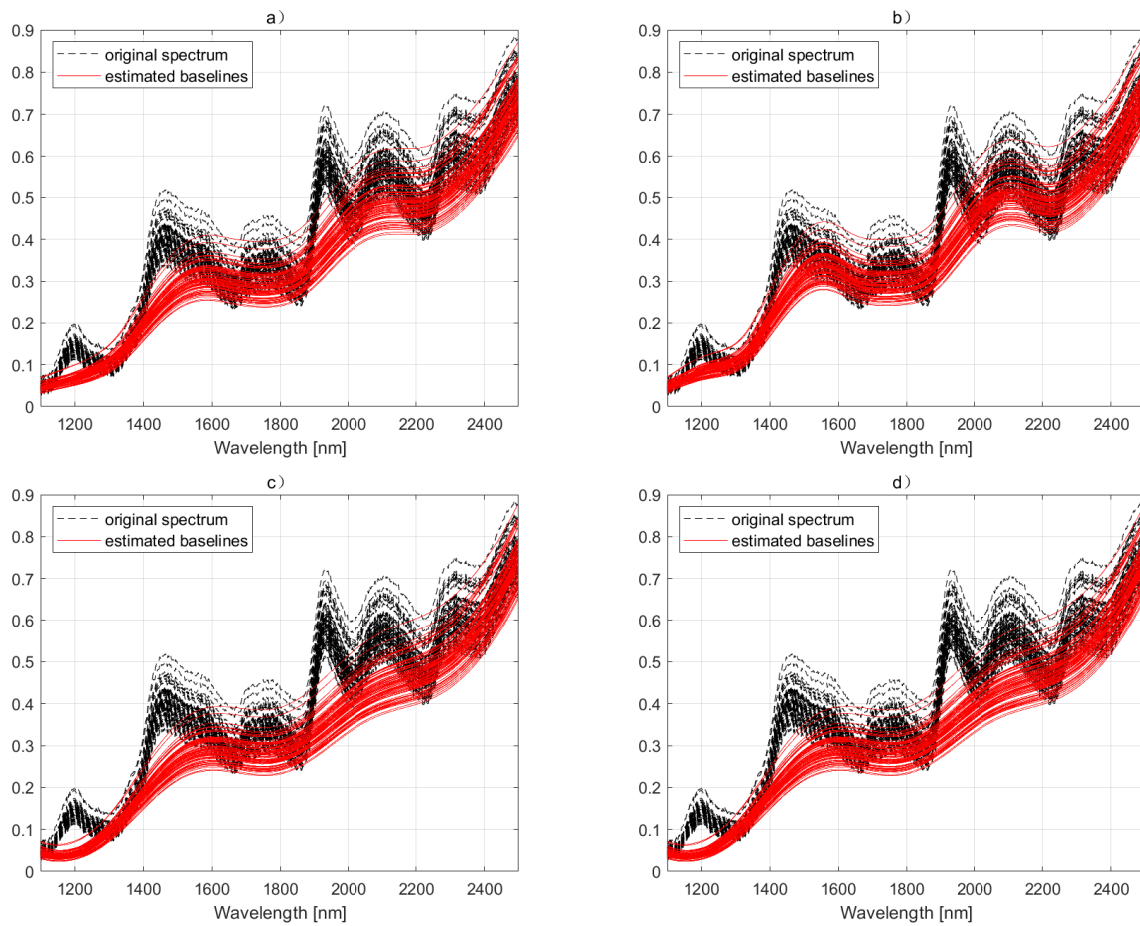


Figure S-3: The corn spectrum (with added noise, SNR = 50dB) and estimated baseline.  
a) FBSL-BC, b) SBL-BC, c) SSFBCSP, d) airPLS.

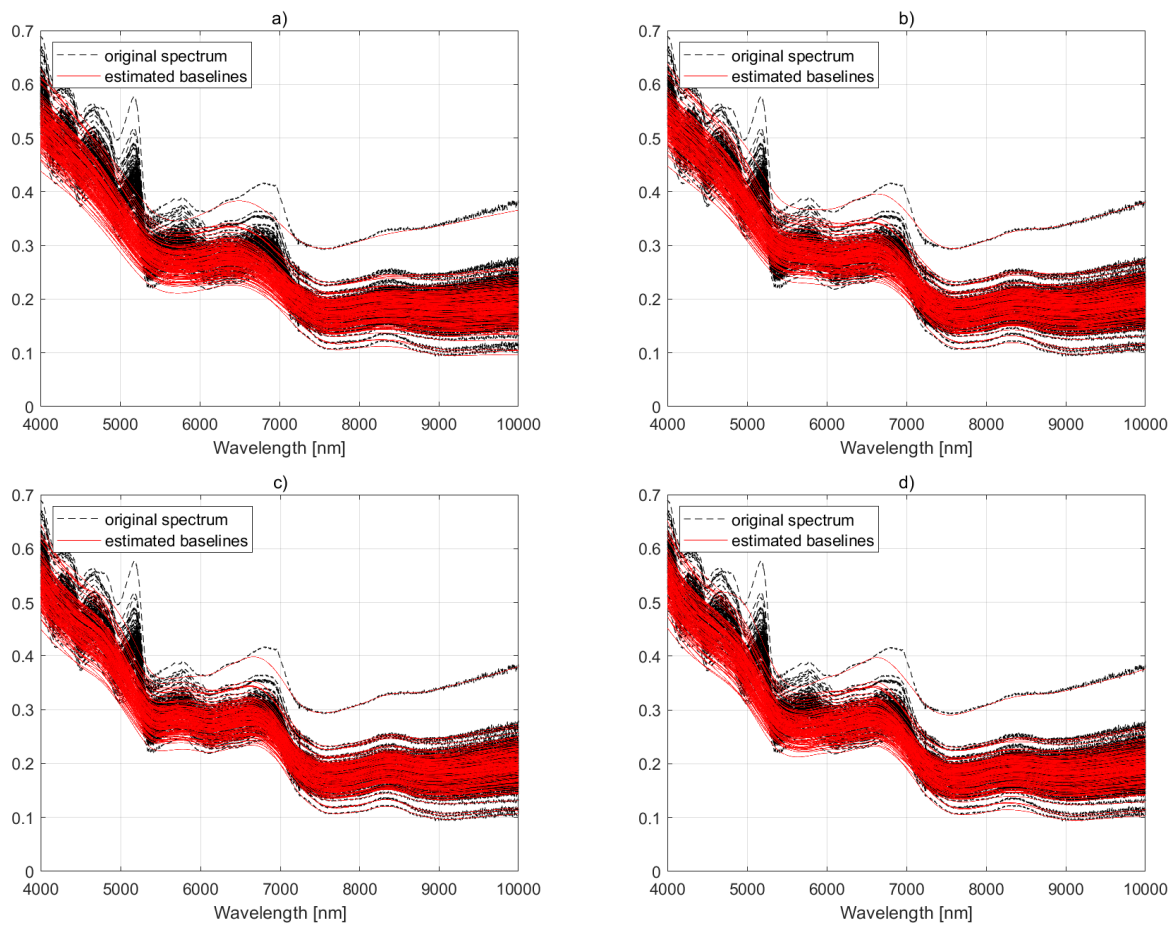


Figure S-4: The original tea spectrum and estimated baseline. a) FBSL-BC, b) SBL-BC, c) SSFBCSP and d) airPLS.

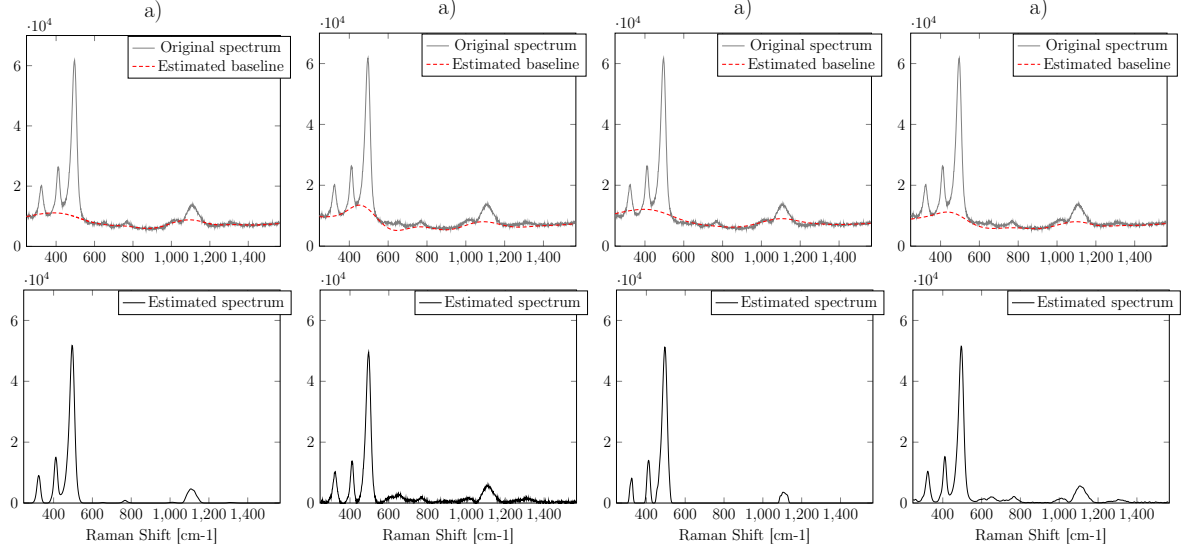


Figure S-5: Comparison of baseline correction results for GmeliniteNa Raman spectral with  $\text{SNR} = 50\text{dB}$ . a) FBSL-BC, b) airPLS ( $\lambda^{\text{air}} = 10^9$ ), c) SBL-BC, d) SSFBCSP ( $\lambda_1 = 10^6$  and  $\lambda_2 = 10^{-2}$ ).

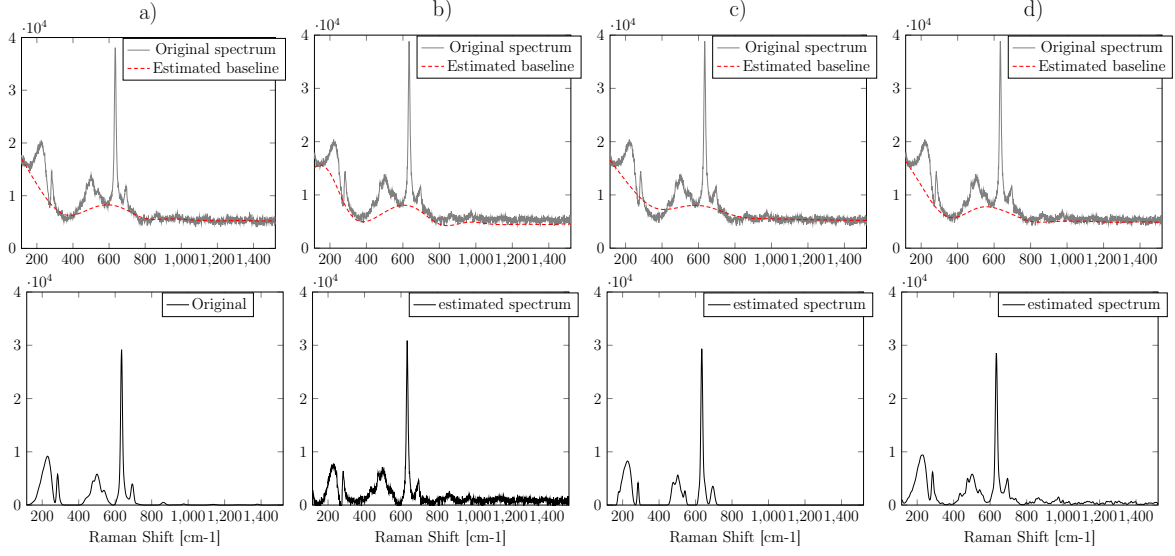


Figure S-6: Comparison of baseline correction results for Cassiterite Raman spectral with  $\text{SNR} = 40\text{dB}$ . a) FBSL-BC, b) airPLS ( $\lambda^{\text{air}} = 10^9$ ), c) SBL-BC, d) SSFBCSP ( $\lambda_1 = 10^6$  and  $\lambda_2 = 10^{-2}$ ).

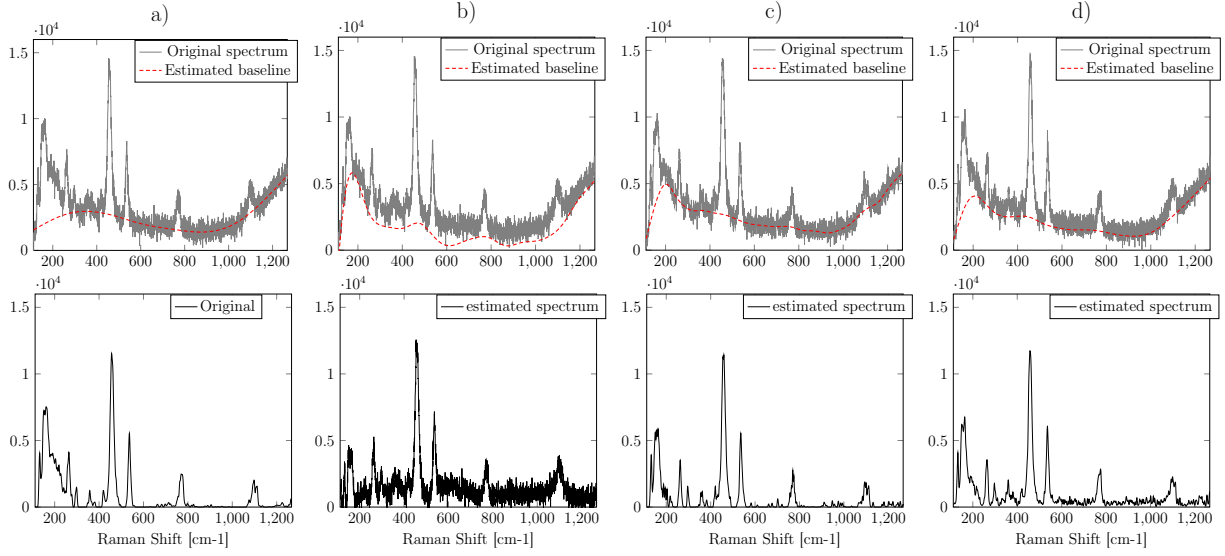


figure S-7: Comparison of baseline correction results for Marialite Raman spectra with  $\text{SNR} = 30\text{dB}$ . a) FBSL-BC, b) airPLS ( $\lambda^{\text{air}} = 10^9$ ), c) SBL-BC, d) SSFBCSP ( $\lambda_1 = 10^6$  and  $\lambda_2 = 10^{-2}$ ).



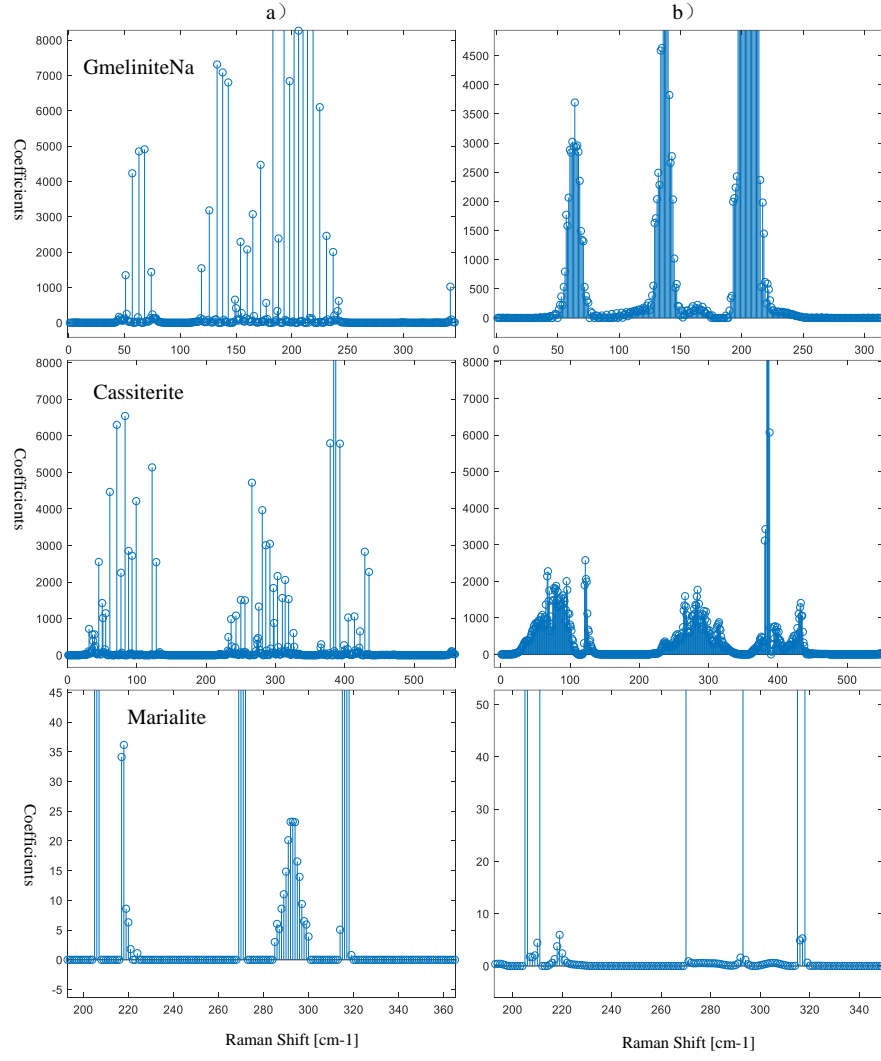


Figure S-8: The sparse coefficients for three mineral Raman datasets, a) SBL-BC, b) FBSL-BC.

## Tables

Table S-1: Comparison of averaged RMSECV among airPLS ( $\lambda^{\text{air}} = 10^8$ ), arPLS ( $\lambda^{\text{ar}} = 10^5$ ), SSFBCSP ( $\lambda_1 = 10^4$  and  $\lambda_2 = 10^{-2}$ ), SBL-BC ( $\rho = 10^5$ ) and FBSL-BC.

	Moisture	Oil	Protein	Starch
airPLS	0.0418	0.0421	0.0641	0.1633
arPLS	0.0485	0.0404	0.0721	0.1590
SSFBCSP	0.0462	0.0396	0.0640	0.1549
SBL-BC	0.0451	0.0386	0.0643	<b>0.1442</b>
FBSL-BC	<b>0.0403</b>	<b>0.0374</b>	<b>0.0611</b>	0.1579

Table S-2: Comparison of averaged RMSEP results among airPLS ( $\lambda^{\text{air}} = 10^8$ ), arPLS ( $\lambda^{\text{ar}} = 10^5$ ), SSFBCSP ( $\lambda_1 = 2 \times 10^5$  and  $\lambda_2 = 10^{-2}$ ), SBL-BC ( $\rho = 10^5$ ) and FBSL-BC.

	Moisture	Oil	Protein	Starch
airPLS	0.0676	0.0684	0.1113	0.2741
arPLS	0.0741	0.0664	0.1214	0.2620
SSFBCSP	0.0712	0.0662	0.1091	0.2635
SBL-BC	0.0700	<b>0.0609</b>	0.1019	<b>0.2545</b>
FBSL-BC	<b>0.0684</b>	0.0627	<b>0.0981</b>	0.2729