Supplementary Materials for "Fast envelope algorithms"

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1 Proof for Proposition 3

We first prove the following:

$$\begin{aligned} \mathrm{F}(\mathbf{A}_0) &= \log|\mathbf{A}_0^T\mathbf{M}\mathbf{A}_0| + \log|\mathbf{A}_0^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{A}_0| && \text{(A1)} \\ &\leq \log|\mathbf{A}_0^T\mathbf{M}\mathbf{A}_0| + \log|\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{A}_0| && \text{(A2)} \\ &= 0, && \text{(A3)} \end{aligned}$$

where the inequality (A2) is because $\mathbf{M} > 0$ and $\mathbf{U} \geq 0$, and hence $(\mathbf{M}+\mathbf{U})^{-1} \leq \mathbf{M}^{-1}$ and $\mathbf{A}_0^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{A}_0 \leq \mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{A}_0$. To show the equality (A3), we need to apply Lemma 2 in the Appendix of (Cook et al., 2013): $|\mathbf{A}^T\mathbf{M}\mathbf{A}| = |\mathbf{M}| \times |\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{A}_0|$ for any $\mathbf{M} > 0$ and any orthogonal basis $(\mathbf{A}, \mathbf{A}_0) \in \mathbb{R}^{p\times p}$. Therefore, in (A2), $\log|\mathbf{A}_0^T\mathbf{M}\mathbf{A}_0| + \log|\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{A}_0| = \log|\mathbf{A}_0^T\mathbf{M}\mathbf{A}_0| + \log|\mathbf{A}^T\mathbf{M}\mathbf{A}| - \log|\mathbf{M}|$, which equals to zero because $\mathrm{span}(\mathbf{A})$ is a reducing subspace of $\mathbf{M}$.

Turning to the second part of the proposition, we decompose $\mathbf{U} = \mathbf{u}\mathbf{u}^T$, where $\mathbf{u}$ has full column rank, and decompose $(\mathbf{I} + \mathbf{u}^T\mathbf{M}^{-1}\mathbf{u})^{-1} = \mathbf{b}\mathbf{b}^T$. Let $\mathbf{C} = (\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{A}_0)^{-1}$. Then using the Woodbury identity for matrix inverses (i.e. $(\mathbf{D}+\mathbf{X}\mathbf{E}\mathbf{X}^T)^{-1} = \mathbf{D}^{-1} + \mathbf{D}^{-1}\mathbf{X}(\mathbf{E}^{-1} +$

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$\mathbf{X}^T\mathbf{D}^{-1}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{D}^{-1}$ for square and invertible matrices $\mathbf{D}$ and $\mathbf{E}$) and a common determinant identity (i.e. $|\mathbf{D}+\mathbf{X}\mathbf{E}\mathbf{X}^T| = |\mathbf{D}|\cdot|\mathbf{E}|\cdot|\mathbf{E}^{-1}+\mathbf{X}^T\mathbf{D}^{-1}\mathbf{X}|$) we have

$$\begin{aligned}
\log|\mathbf{A}_0^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{A}_0| &= \log|\mathbf{A}_0^T(\mathbf{M}+\mathbf{u}\mathbf{u}^T)^{-1}\mathbf{A}_0| \\
&= \log|\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{A}_0 - \mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{u}\mathbf{b}\mathbf{b}^T\mathbf{u}^T\mathbf{M}^{-1}\mathbf{A}_0| \\
&= \log|\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{A}_0| + \log|\mathbf{I} - \mathbf{b}^T\mathbf{u}^T\mathbf{M}^{-1}\mathbf{A}_0\mathbf{C}\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{u}\mathbf{b}|.
\end{aligned}$$

Since $\mathrm{span}(\mathbf{A}_0)$ is a reducing subspace of $\mathbf{M}$, $\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{A}_0 = (\mathbf{A}_0^T\mathbf{M}\mathbf{A}_0)^{-1}$ and thus

$$\log|\mathbf{A}_0^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{A}_0| = -\log|\mathbf{A}_0^T\mathbf{M}\mathbf{A}_0| + \log|\mathbf{I} - \mathbf{b}^T\mathbf{u}^T\mathbf{M}^{-1}\mathbf{A}_0\mathbf{C}\mathbf{A}_0^T\mathbf{M}^{-1}\mathbf{u}\mathbf{b}|.$$

It follows that $F(\mathbf{A}_0) = 0$ if and only if $\mathbf{b}^T\mathbf{u}^T\mathbf{M}^{-1}\mathbf{A}_0 = 0$. Since $\mathbf{b}$ has full column rank, this holds if and only if $\mathrm{span}(\mathbf{M}^{-1}\mathbf{u}) \subseteq \mathrm{span}(\mathbf{A})$. Since $\mathrm{span}(\mathbf{A})$ reduces $\mathbf{M}$, this holds if and only if $\mathrm{span}(\mathbf{u}) \subseteq \mathrm{span}(\mathbf{A})$.

To prove $\mathcal{E}_{\mathbf{M}}(\mathbf{U}) = \mathbf{A}\mathcal{E}_{\mathbf{A}^T\mathbf{M}\mathbf{A}}(\mathbf{A}^T\mathbf{U}\mathbf{A})$, we first need to establish $\mathrm{span}(\mathbf{A}^T\mathbf{U}\mathbf{A}) \subseteq \mathrm{span}(\mathbf{A}^T\mathbf{M}\mathbf{A})$ (cf. Definition 2). Since $\mathrm{span}(\mathbf{U}) \subseteq \mathrm{span}(\mathbf{M})$, there is a matrix $\mathbf{B}$ so that $\mathbf{U} = \mathbf{M}\mathbf{B}$. Thus

$$\mathrm{span}(\mathbf{A}^T\mathbf{U}\mathbf{A}) = \mathrm{span}(\mathbf{A}^T\mathbf{U}) = \mathrm{span}(\mathbf{A}^T\mathbf{M}\mathbf{B}) \subseteq \mathrm{span}(\mathbf{A}^T\mathbf{M}) = \mathrm{span}(\mathbf{A}^T\mathbf{M}\mathbf{A}).$$

We next let $\mathcal{E}_1 = \mathcal{E}_{\mathbf{A}^T\mathbf{M}\mathbf{A}}(\mathbf{A}^T\mathbf{U}\mathbf{A})$ when used as a subscript. The conclusion can be deducted from the following quantities:

$$\begin{aligned}
\mathbf{M} &= \mathbf{P}_{\mathbf{A}}\mathbf{M}\mathbf{P}_{\mathbf{A}} + \mathbf{Q}_{\mathbf{A}}\mathbf{M}\mathbf{Q}_{\mathbf{A}} \\
&= \mathbf{A}(\mathbf{A}^T\mathbf{M}\mathbf{A})\mathbf{A}^T + \mathbf{Q}_{\mathbf{A}}\mathbf{M}\mathbf{Q}_{\mathbf{A}} \\
&= \mathbf{A}(\mathbf{P}_{\mathcal{E}_1}\mathbf{A}^T\mathbf{M}\mathbf{A}\mathbf{P}_{\mathcal{E}_1} + \mathbf{Q}_{\mathcal{E}_1}\mathbf{A}^T\mathbf{M}\mathbf{A}\mathbf{Q}_{\mathcal{E}_1})\mathbf{A}^T + \mathbf{Q}_{\mathbf{A}}\mathbf{M}\mathbf{Q}_{\mathbf{A}} \\
&= \mathbf{A}\mathbf{P}_{\mathcal{E}_1}\mathbf{A}^T\mathbf{M}\mathbf{A}\mathbf{P}_{\mathcal{E}_1}\mathbf{A}^T + (\mathbf{A}\mathbf{Q}_{\mathcal{E}_1}\mathbf{A}^T + \mathbf{Q}_{\mathbf{A}})\mathbf{M}(\mathbf{A}\mathbf{Q}_{\mathcal{E}_1}\mathbf{A}^T + \mathbf{Q}_{\mathbf{A}}),
\end{aligned}$$

where the final equation holds because $\mathbf{A}\mathbf{Q}_{\mathcal{E}_1}\mathbf{A}^T\mathbf{M}\mathbf{Q}_{\mathbf{A}} = \mathbf{A}\mathbf{Q}_{\mathcal{E}_1}(\mathbf{A}^T\mathbf{M}\mathbf{A}_0)\mathbf{A}_0 = 0$ and because $\mathbf{A}\mathbf{P}_{\mathcal{E}_1}\mathbf{A}^T$ and $(\mathbf{A}\mathbf{Q}_{\mathcal{E}_1}\mathbf{A}^T + \mathbf{Q}_{\mathbf{A}})$ are orthogonal projections. It follows that $\mathrm{span}(\mathbf{A}\mathbf{P}_{\mathcal{E}_1}\mathbf{A}^T) = \mathbf{A}\mathcal{E}_{\mathbf{A}^T\mathbf{M}\mathbf{A}}(\mathbf{A}^T\mathbf{U}\mathbf{A})$ is a reducing subspace of $\mathbf{M}$ that contains $\mathrm{span}(\mathbf{U})$. The envelope equality $\mathcal{E}_{\mathbf{M}}(\mathbf{U}) = \mathbf{A}\mathcal{E}_{\mathbf{A}^T\mathbf{M}\mathbf{A}}(\mathbf{A}^T\mathbf{U}\mathbf{A})$ follows from the minimality of $\mathcal{E}_{\mathbf{A}^T\mathbf{M}\mathbf{A}}(\mathbf{A}^T\mathbf{U}\mathbf{A})$.

2 Proof for Proposition 4 and Proposition 5

We first establish the results in Proposition 5 about $\widetilde{u}$. Recall that $\widetilde{u}$ is the number of eigenvectors from the decomposition $\mathbf{M} = \sum_{i=1}^{p} \lambda_i \mathbf{v}_i \mathbf{v}_i^T$ used in Step 1 of Algorithm 2 that are not orthogonal to $\mathrm{span}(\mathbf{U})$ and that, from Proposition 1, $\mathcal{E}_{\mathbf{M}}(\mathbf{U}) = \sum_{j=1}^{q} \mathbf{P}_j \mathcal{U}$ for q projections $\mathbf{P}_j$, $j = 1, \ldots, q$, onto the distinct (and unique) eigenspaces of $\mathbf{M}$. For these eigenspaces, if $\mathrm{span}(\mathbf{P}_j) \subseteq \mathcal{E}_{\mathbf{M}}(\mathbf{U})$ for some $j = 1, \ldots, q$, then the associated eigenvectors will be guaranteed to intersect with $\mathrm{span}(\mathbf{U})$ because of the minimality of the envelope. If $\mathrm{span}(\mathbf{P}_j) \subseteq \mathcal{E}_{\mathbf{M}}^{\perp}(\mathbf{U})$ for some $j = 1, \ldots, q$, then the associated eigenvectors will be orthogonal to $\mathrm{span}(\mathbf{U})$. Thus for the first part of Proposition 5, if all eigenspaces are contained in either $\mathcal{E}_{\mathbf{M}}(\mathbf{U})$ or $\mathcal{E}_{\mathbf{M}}^{\perp}(\mathbf{U})$, then $u = \widetilde{u}$ and equals to the sum of the dimensions of eigenspaces that are contained in $\mathcal{E}_{\mathbf{M}}(\mathbf{U})$. However, if some eigenspace $\mathrm{span}(\mathbf{P}_j)$ intersect with both $\mathcal{E}_{\mathbf{M}}(\mathbf{U})$ and $\mathcal{E}_{\mathbf{M}}^{\perp}(\mathbf{U})$, then by $\mathcal{E}_{\mathbf{M}}(\mathbf{U}) = \sum_{j=1}^{q} \mathbf{P}_j \mathcal{U}$ we have $\mathbf{P}_j \mathcal{U} \subseteq \mathcal{E}_{\mathbf{M}}(\mathbf{U})$ and $\mathbf{P}_j \mathcal{U}^{\perp} \subseteq \mathcal{E}_{\mathbf{M}}^{\perp}(\mathbf{U})$. Since any vector in the eigenspace $\mathrm{span}(\mathbf{P}_j)$ is a eigenvector for $\mathbf{M}$, therefore different eigen-decomposition leads to different number $\widetilde{u}$. Depending on the particular eigen-decomposition, $\widetilde{u}$ can be any integer from u to $u + K$, where K is the sum of the dimensions of all such eigenspaces that intersect with both the envelope and the orthogonal completion of the envelope.

To prove Proposition 4, we let $\mathcal{I}$ denote the index set of the $\widetilde{u}$ eigenvectors that are not orthogonal to $\mathrm{span}(\mathbf{U})$, and let $\mathcal{I}_0$ denote the remaining indices in $\{1, \ldots, p\}$. Then we have $\mathbf{v}_i \cap \mathcal{E}_{\mathbf{M}}(\mathbf{U}) \neq 0$ and $\mathbf{v}_i^T \mathbf{U} \mathbf{v}_i > 0$ for $i \in \mathcal{I}$ and $\mathbf{v}_i \in \mathcal{E}_{\mathbf{M}}^{\perp}(\mathbf{U})$ for $i \in \mathcal{I}_0$. Now we finally turn to the function $\mathrm{F}(\mathbf{v}_i)$. From Proposition 3, we know that $\mathrm{F}(\mathbf{v}_i) = 0$ for $i \in \mathcal{I}_0$. For $i \in \mathcal{I}$, let $\mathbf{P}_{\mathcal{E}}$ and $\mathbf{Q}_{\mathcal{E}}$ denote the projection onto $\mathcal{E}_{\mathbf{M}}(\mathbf{U})$ and $\mathcal{E}_{\mathbf{M}}^{\perp}(\mathbf{U})$, respectively. Then it is straightforward to see that,

$$(\mathbf{M} + \mathbf{U})^{-1} = \{\mathbf{P}_{\mathcal{E}}(\mathbf{M} + \mathbf{U})\mathbf{P}_{\mathcal{E}} + \mathbf{Q}_{\mathcal{E}} \mathbf{M} \mathbf{Q}_{\mathcal{E}}\}^{-1} = \mathbf{P}_{\mathcal{E}}(\mathbf{M} + \mathbf{U})^{-1}\mathbf{P}_{\mathcal{E}} + \mathbf{Q}_{\mathcal{E}} \mathbf{M}^{-1} \mathbf{Q}_{\mathcal{E}}. \quad \text{(A1)}$$

Because $\mathbf{v}_i^T \mathbf{U} \mathbf{v}_i > 0$ for $i \in \mathcal{I}$ we have $\mathbf{v}_i^T (\mathbf{M} + \mathbf{U})^{-1} \mathbf{v}_i < \mathbf{v}_i^T \mathbf{M}^{-1} \mathbf{v}_i$, and thus $f_i < 0$ for $i \in \mathcal{I}$. Ordering $f_1, \ldots, f_p$ monotonically, we have $f_{(p)} \leq \ldots \leq f_{(p-\widetilde{u}+1)} < f_{(p-\widetilde{u})} = \ldots = f_{(1)} = 0$. For $d \geq \widetilde{u}$, $\mathrm{span}(\mathbf{A}_0)$ is a subset of $\mathcal{E}_{\mathbf{M}}^{\perp}(\mathbf{U})$ and thus $\mathrm{F}(\mathbf{A}_0) = 0$ from equation

(A1). By construction, both $\mathrm{span}(\mathbf{A})$ and $\mathrm{span}(\mathbf{A}_0)$ are always reducing subspaces of $\mathbf{M}$. Thus applying Proposition 3, we have $\mathbf{A}\mathcal{E}_{\mathbf{A}^T\mathbf{M}\mathbf{A}}(\mathbf{A}^T\mathbf{U}\mathbf{A}) = \mathcal{E}_{\mathbf{M}}(\mathbf{U})$ for $d \geq u$.

3 Proof for Proposition 6

Because the objective function $\mathrm{F}(\mathbf{A}_0)$ is a smooth and differentiable function in $\mathbf{M}$ and $\mathbf{U}$, it follows that $\mathrm{F}_n(\widehat{\mathbf{A}}_0) = \mathrm{F}(\widehat{\mathbf{A}}_0) + O_p(n^{-1/2})$. To see this treat $\mathrm{F}_n(\widehat{\mathbf{A}}_0) = \log|\widehat{\mathbf{A}}_0^T\widehat{\mathbf{M}}\widehat{\mathbf{A}}_0| + \log|\widehat{\mathbf{A}}_0^T(\widehat{\mathbf{M}}+\widehat{\mathbf{U}})^{-1}\widehat{\mathbf{A}}_0| = f(\widehat{\mathbf{M}}, \widehat{\mathbf{U}}, \widehat{\mathbf{A}}_0)$ as a function of $\widehat{\mathbf{M}}$, $\widehat{\mathbf{U}}$ and $\widehat{\mathbf{A}}_0$. Then we have $\mathrm{F}(\widehat{\mathbf{A}}_0) = f(\mathbf{M}, \mathbf{U}, \widehat{\mathbf{A}}_0)$. The partial derivatives of $f(\mathbf{M}, \mathbf{U}, \widehat{\mathbf{A}}_0)$ with respect to $\mathbf{M}$ and $\mathbf{U}$ can be computed (not shown here) and are bounded because $\partial \log|\mathbf{X}|/\partial\mathbf{X} = \mathbf{X}^{-1}$ for symmetric positive definite matrix $\mathbf{X}$ and the components $(\widehat{\mathbf{A}}_0^T\mathbf{M}\widehat{\mathbf{A}}_0)^{-1}$, $(\widehat{\mathbf{A}}_0^T\widehat{\mathbf{M}}\widehat{\mathbf{A}}_0)^{-1}$, $(\widehat{\mathbf{A}}_0^T(\widehat{\mathbf{M}} + \widehat{\mathbf{U}})^{-1}\widehat{\mathbf{A}}_0)^{-1}$ and $(\widehat{\mathbf{A}}_0^T(\mathbf{M} + \mathbf{U})^{-1}\widehat{\mathbf{A}}_0)^{-1}$ are bounded with probability 1. Since $f(\mathbf{M}, \mathbf{U}, \widehat{\mathbf{A}}_0)$ is smooth and differentiable with respect to its first two arguments, $\widehat{\mathbf{M}} - \mathbf{M} = O_p(n^{-1/2})$ and $\widehat{\mathbf{U}} - \mathbf{U} = O_p(n^{-1/2})$, it follows by a Taylor expansion that $f(\widehat{\mathbf{M}}, \widehat{\mathbf{U}}, \widehat{\mathbf{A}}_0) - f(\mathbf{M}, \mathbf{U}, \widehat{\mathbf{A}}_0) = O_p(n^{-1/2})$. From the $\sqrt{n}$-consistency of eigenvectors, we have $\widehat{\mathbf{A}}_0^T\mathbf{M}\widehat{\mathbf{A}}_0 = \mathbf{A}_0^T\mathbf{M}\mathbf{A}_0 + O_p(n^{-1/2})$ and $\widehat{\mathbf{A}}_0^T(\mathbf{M}+\mathbf{U})^{-1}\widehat{\mathbf{A}}_0 = \mathbf{A}_0^T(\mathbf{M}+\mathbf{U})^{-1}\mathbf{A}_0 + O_p(n^{-1/2})$. Therefore, $\mathrm{F}(\widehat{\mathbf{A}}_0) = \mathrm{F}(\mathbf{A}_0) + O_p(n^{-1/2})$.

4 Additional numerical results for Section 4.2

In Section 4.2, we analyzed the meat protein data set following the previous studies in Cook et al. (2013) and Cook and Zhang (2016). Recall that in Section 4.2, we used the protein percentage of $n = 103$ meat samples as the univariate response variable $Y_i \in \mathbb{R}^1$, $i = 1, \ldots, n$, and use corresponding $p = 50$ spectral measurements from near-infrared transmittance at every fourth wavelength between 850nm and 1050nm as the predictor $\mathbf{X}_i \in \mathbb{R}^p$. We then randomly split the data into a testing sample and a training sample in a 1:4 ratio and recorded the prediction mean squared errors (PMSE) and repeated this procedure 100 times. Figure 4.1 summarized the averaged prediction mean squared errors (PMSE) for the four estimators (ECD, 1D, ECS-ECD, and ECS-1D). The ECD algorithm was proven again to be the most reliable

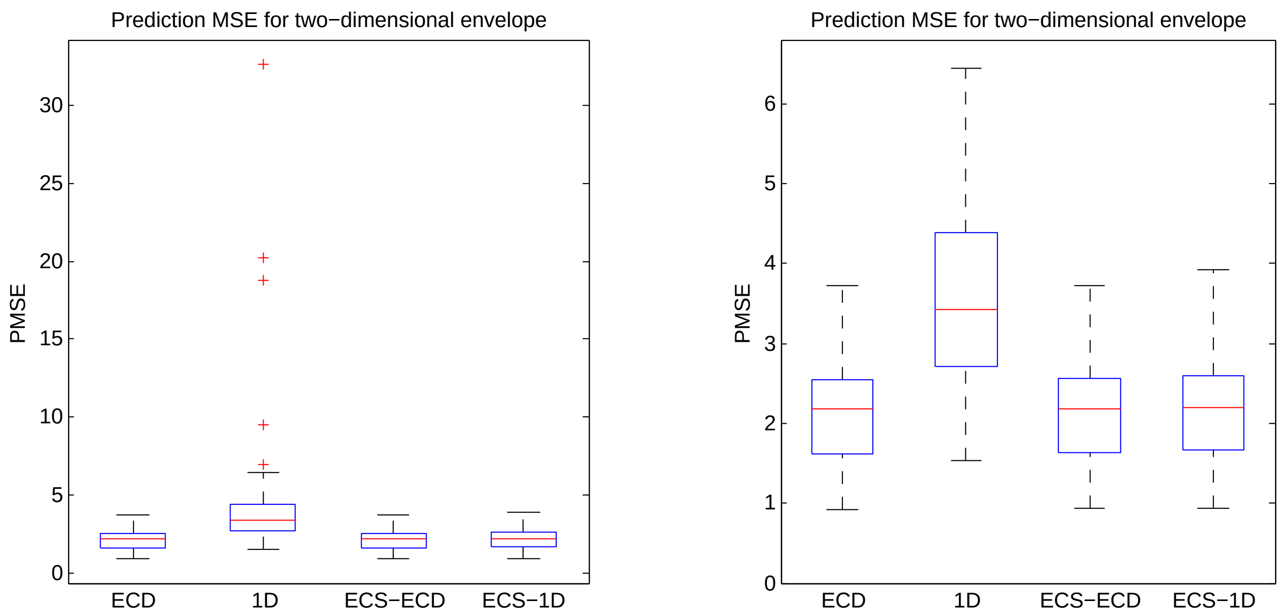

Figure A1: Meat Protein Data: prediction mean squares error comparison of ECD and 1D algorithms when $u = 2$. The left panel summarized all the 100 PMSE for each of the four estimators; the right panel is the zoomed-in view of the left panel, that is after deleting the 5 outliers of the 1D algorithm's PMSE.

one, while the performances of both the ECS-1D and the ECS-ECD estimators are very similar to that of the ECD algorithm. For $u = 2$, we have observed a big difference between the 1D and the ECD algorithm. Since both algorithms are under the same sequential 1D framework of (Cook and Zhang, 2016) and are trying to optimize the same objective function, we further examined their differences more carefully. In Figure A1, we have the side-by-side boxplot of the 100 PMSE for all the four estimators. The means of the PMSE over the 100 data sets for each estimators are: 2.15 (ECD); 4.79 (1D); 2.16 (ECS-ECD); 2.19 (ECS-1D), while the medians are: 2.13 (ECD), 3.53 (1D), 2.13 (ECS-ECD), 2.17 (ECS-ECD).

References

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