Envelopes: Methods for Efficient Estimation in Multivariate Statistics

Dennis Cook

School of Statistics
University of Minnesota

Collaborating with
Bing Li, Francesca Chiaromonte, Zhihua Su, Inge Helland & Xin Zhang
How do envelopes work?

Multivariate regression with two responses, $Y_1$ and $Y_2$, and a single predictor, $X = 0$ or 1, to indicate two populations.

$$
Y = \left( \begin{array}{c} Y_1 \\ Y_2 \end{array} \right) = \left( \begin{array}{c} \alpha_1 \\ \alpha_2 \end{array} \right) + \left( \begin{array}{c} \beta_1 \\ \beta_2 \end{array} \right) X + \left( \begin{array}{c} \epsilon_1 \\ \epsilon_2 \end{array} \right)
$$

$\alpha_1 = E(Y_1|X = 0)$, $\beta_1 = E(Y_1|X = 1) - E(Y_1|X = 0)$,
$\alpha_2 = E(Y_2|X = 0)$, $\beta_2 = E(Y_2|X = 1) - E(Y_2|X = 0)$.

Standard estimators are obtained by substituting sample moments.
Schematic representation of an envelope analysis
Schematic representation of an envelope analysis
Schematic representation of an envelope analysis
Schematic representation of an envelope analysis
Schematic representation of an envelope analysis
Schematic representation of an envelope analysis
Wheat protein data

\((Y_1, Y_2)\) are spectral intensities at two wave lengths for high (red) and low protein wheat. \(n = 50\).

SE’s for 2 elements in \(\hat{\beta}\):

- Standard estimator: 8.6, 9.5
- Envelope estimator: 0.4, 0.6
- \(n \sim 20,000\)
Wheat protein data

Standard analysis

Envelope analysis

Dennis Cook | Envelopes: Methods for Efficient Estimation in Multivariate Statistics
Heights of Boys and Girls Ages 13 and 14

Figure 7: Graphical representation of the envelope estimator.
Multivariate linear regression

\[ Y_i = \alpha + \beta X_i + \varepsilon_i, \quad i = 1, \ldots, n \]

- \( Y \in \mathbb{R}^r \): multivariate response
- \( X \in \mathbb{R}^p \): non-stochastic predictors centered at 0
- \( \varepsilon \in \mathbb{R}^r \): normal errors, mean 0 and covariance \( \Sigma > 0 \)
- \( \alpha \in \mathbb{R}^r \): unknown intercept
- \( \beta \in \mathbb{R}^{r \times p} \): unknown coefficients
- Goal: estimate \( \beta \), prediction.

MLE \( \hat{\beta}_{\text{Std}} \) of \( \beta \) is obtained by doing \( r \) univariate linear regressions, one for each response.
Rationale for envelopes

Envelopes arise by parameterizing the MLM in terms of the smallest subspace \( \mathcal{E} \subseteq \mathbb{R}^r \) so that \( (P_{\mathcal{E}} = \text{projection onto } \mathcal{E}, \ Q_{\mathcal{E}} = I - P_{\mathcal{E}}) \)

\[
Q_{\mathcal{E}} Y \mid X \sim Q_{\mathcal{E}} Y \\
P_{\mathcal{E}} Y \perp Q_{\mathcal{E}} Y \mid X
\]

This implies that the impact of \( X \) on \( Y \) is concentrated in \( P_{\mathcal{E}} Y \). We refer to \( P_{\mathcal{E}} Y \) and \( Q_{\mathcal{E}} Y \) informality as the material and immaterial parts of \( Y \).
The conditions $Q_\varepsilon Y \mid X \sim Q_\varepsilon Y$ and $P_\varepsilon Y \perp Q_\varepsilon Y \mid X$ hold if and only if

$$\text{span}(\beta) \subseteq \mathcal{E}$$

$$\Sigma = P_\varepsilon \Sigma P_\varepsilon + Q_\varepsilon \Sigma Q_\varepsilon.$$ 

- $\mathcal{E}$ envelops $\mathcal{B} := \text{span}(\beta)$.
- $\mathcal{E}$ is a **reducing subspace** of $\Sigma$.
- Formally, the intersection of all subspaces $\mathcal{E}$ with these properties is called the $\Sigma$-envelope of $\mathcal{B}$ and represented as $\mathcal{E}_\Sigma(\mathcal{B})$ with $u = \dim(\mathcal{E}_\Sigma(\mathcal{B}))$. 
Dennis Cook | Envelopes: Methods for Efficient Estimation in Multivariate Statistics
Let the columns of the semi-orthogonal matrices $\Gamma \in \mathbb{R}^{r \times u}$ and $\Gamma_0 \in \mathbb{R}^{r \times (r-u)}$ be bases for $\mathcal{E}_\Sigma(\mathcal{B})$ and $\mathcal{E}_{\Sigma}^{\perp}(\mathcal{B})$.

Then $\beta = \Gamma \eta$. $\Sigma = \Gamma \Omega \Gamma + \Gamma_0 \Omega_0 \Gamma_0^T$, where $\Omega > 0$ and $\Omega_0 > 0$.

Envelope Model:

$$Y = \alpha + \Gamma \eta X + \epsilon, \quad \Sigma = \Gamma \Omega \Gamma + \Gamma_0 \Omega_0 \Gamma_0^T.$$

Estimation via maximum likelihood with $u$ determined by AIC, BIC, likelihood ratio testing, cross validation or a holdout sample.

We are still interested in $\beta$ and $\Sigma$, which depend on the envelope $\mathcal{E}_\Sigma(\mathcal{B})$, but not on the particular basis $\Gamma$ selected to represent it.
Maximum likelihood estimators

The estimated envelope \( \hat{\mathcal{E}}_\Sigma(\mathcal{B}) \) can be represented as

\[
\hat{\mathcal{E}}_\Sigma(\mathcal{B}) = \arg \min_{\mathcal{S}} \left( \log |P_{\mathcal{S}S_Y|X}P_{\mathcal{S}|0} + \log |Q_{\mathcal{S}S_Y}Q_{\mathcal{S}|0}| \right),
\]

where \( | \cdot |_0 \) means the product of the non-zero eigenvalues, \( \mathcal{S} \) is a \( u \)-dim subspace of \( \mathbb{R}^r \) and \( S(\cdot) = \) sample covariance matrix.

Let \( \hat{\Gamma} \) be a basis for \( \hat{\mathcal{E}}_\Sigma(\mathcal{B}) \). Estimators of other parameters:

- \( \hat{\beta} = P_{\hat{\Gamma}} \hat{\beta}_{\text{Std}}, \)
- \( \hat{\eta} = \hat{\Gamma}^T \hat{\beta}_{\text{Std}}. \)
- \( \hat{\Omega} = \hat{\Gamma}^T S_{Y|X} \hat{\Gamma}, \quad \hat{\Omega}_0 = \hat{\Gamma}_0^T S_Y \hat{\Gamma}_0. \)
Asymptotic variance of the MLE

\[ \sqrt{n}[\text{vec}(\hat{\beta}) - \text{vec}(\beta)] \xrightarrow{\mathcal{D}} N_{rp}(0, V) \]

\[ V = \text{avar}\{ \sqrt{n}\text{vec}[\hat{\beta}] \} \]
\[ = \text{avar}\{ \sqrt{n}\text{vec}[\hat{\beta}_\Gamma] \} + \text{avar}\{ \sqrt{n}\text{vec}[Q\Gamma\hat{\beta}_\eta] \} \]
\[ \leq \text{avar}(\text{vec}[\hat{\beta}_{\text{Std}}]) \]

The efficiency gains can be massive, particularly when \( \| \Omega \| \ll \| \Omega_0 \| \). \( \| \cdot \| = \text{spectral norm} \)

\[ \Sigma = \Gamma\Omega\Gamma^T + \Gamma_0\Omega_0\Gamma_0^T = \text{material var.} + \text{immaterial var.} \]
Cattle data

The life cycle of the stomach and gut worm

Experiment: Two treatments, each assigned randomly to 30 cows. Weight measured at weeks 2, 4, 6, …, 16, 18, 19. Do the treatment have a differential effect; if so, about when it is first apparent?
Profile plot of cattle data

\[ Y_i = \alpha + \beta X_i + \varepsilon_i, \quad X = 0, 1 \]

\[ \hat{\beta}_{\text{Std}} = \bar{Y}_{\text{trt1}} - \bar{Y}_{\text{trt2}} \]
Mean profile plot of cattle data

\[ \max_i \left| \frac{1}{SE(\beta_{Std,i})} \right| \approx 1.3. \]  

LRT stat. for \( \beta = 0 \) is about 27 on 10 df.
Fitted profile plots, after inferring that $u = 5$. From envelope fit, $|\hat{\beta}_i|/SE(\hat{\beta}_i) > 4.1$ for $i \geq 10$. 
Cattle weight, week 12 vs week 14
Air pollution data in Los Angeles

- 42 measurements at noon
- $Y$: measurements for CO, NO, NO2, O3 and HC.
- $X$: wind speed and solar radiation
- $\hat{u} = 1$, $\|\hat{\Omega}\| = 0.21$ and $\|\hat{\Omega}_0\| = 36.3$.
- SE ratios for sm/em: 1.7 $\sim$ 163.
### Individual SE ratios

<table>
<thead>
<tr>
<th>4.3</th>
<th>5.7</th>
<th>CO</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6</td>
<td>4.7</td>
<td>NO</td>
</tr>
<tr>
<td>51</td>
<td>68</td>
<td>NO2</td>
</tr>
<tr>
<td>123</td>
<td>163</td>
<td>O3</td>
</tr>
<tr>
<td>1.7</td>
<td>2.0</td>
<td>HC</td>
</tr>
</tbody>
</table>
Egyptian Skulls

- 4 measurements \( Y \) in cm on 30 male skulls in each of 5 epochs, 4000, 3300, 1850, 200 BC & 150 AD, included as indicators \( X \).

- \( Y = \alpha + \beta_{3300}X_1 + \beta_{1850}X_2 + \beta_{200}X_3 + \beta_{150}X_4 + \epsilon \)

- We inferred that \( u = 1 \) so the envelope model becomes

\[
Y = \alpha + \Gamma\{\eta_{3300}X_1 + \eta_{1850}X_2 + \eta_{200}X_3 + \eta_{150}X_4\} + \epsilon,
\]

- Since \( \hat{u} = 1 \), we can easily plot \( \hat{\Gamma^T}Y \) vs epoch.
Skull Boxplots vs Epoch
Reducing $X$ and Partial least squares
PLS formulation

With \( X \) random we consider the same model

\[
Y_i = \alpha + \beta X_i + \varepsilon_i, \quad i = 1, \ldots, n,
\]

but now the goal is to reduce \( X \). PLS operates by

1. Reducing \( X \rightarrow \hat{\Phi}^T X \) by using an iterative algorithm
2. Fitting \( Y = \alpha + \eta^T \{\hat{\Phi}^T X\} + \varepsilon \) using OLS
3. Estimating \( \hat{\beta}_{\text{pls}} = \hat{\Phi} \hat{\eta} = P_{\hat{\Phi}}(S_X) B^T \)
SIMPLS algorithm for $\hat{\Phi}$ (de Jong, 1993)

Set $w_0 = 0$ and let $\hat{\Phi}_k = (w_0, \ldots, w_k) \in \mathbb{R}^{p \times k}$. Then given $\hat{\Phi}_k$, the next vector $w_{k+1}$ is constructed as

$$S_k = \text{span}(S_X \hat{\Phi}_k)$$

$$w_{k+1} = \ell_{\text{max}}(Q_{S_k} S_{XY} S_{XY}^T Q_{S_k})$$

$$\hat{\Phi}_{k+1} = (w_0, \ldots, w_k, w_{k+1})$$

for $k = 1, \ldots, m - 1$. $m$, the number of components, is chosen by cross-validation or a hold-out sample. Then $\hat{\Phi} = \hat{\Phi}_m$.

Envelope connection: With known $m$, $\text{span}(\hat{\Phi}_m)$ is a $\sqrt{n}$-consistent estimator of the $\Sigma_X$-envelope of $\text{span}(\beta^T)$, $E_{\Sigma_X}(B')$, where $B' = \text{span}(\beta^T)$ and $m = \text{dim}(E_{\Sigma_X}(B'))$. 
Alternatively, we can use an envelope estimator for the same tasks:

\[
Y = \alpha + \eta^T \{ \phi^T X \} + \varepsilon
\]

\[
\Sigma_X = \phi \Delta \phi^T + \phi_0 \Delta_0 \phi_0^T
\]

\[
\Sigma = \Sigma
\]

\[
\hat{\beta} = B P^{T} \phi(S_X)
\]

where

\[
\hat{\phi} = \arg \min_{S} \{ \log |P_S S_X Y P_S|_0 + \log |Q_S S_X Q_S|_0 \}
\]

and \( S \) is an \( m \)-dim subspace of \( \mathbb{R}^p \).
Predict protein content \((Y, r = 1)\) of beef based on spectral measurements at \(p = 50\) wave lengths, \(n = 103\).
NIR analysis of biscuit dough

Predict fat, sucrose, flower and water content ($Y$, $r = 4$) of biscuit dough based on spectral measurements at $p = 20$ wavelengths, 39 training samples & 31 testing samples, created on different occasions. Comparison criterion is the SS prediction error on the testing samples.
Figure 8.1: Prediction sum of square errors on the testing set. X-axis denote the numbers of components for PLS and simultaneous envelope $X$-dimension, $d_X$, where the $Y$-dimension of simultaneous envelope is fixed at $d_Y = 2$. To help visualization, the CCA performance is not included and the SSE for CCA are all greater than OLS no matter how many components to use.
Simulations

Top: \( r = 1, p = 10, u = 8. \) \( \Sigma_X = 200 \phi \phi^T + 50 \phi_0 \phi_0^T \)

Bottom: \( r = 1, p = 7, u = 2. \) \( \Sigma_X = \phi \Delta \phi^T + \phi_0 \Delta_0 \phi_0^T \)

eigenvalues: 0.07 and 1.6 for \( \Delta \); between 3 and 584 for \( \Delta_0 \).
Beyond linear models

Suppose we have an an asymptotically normal estimator $\hat{\theta}$ of $\theta \in \mathbb{R}^p$, $\sqrt{n}(\hat{\theta} - \theta) \rightarrow N(0, V(\theta))$.

The estimator can often be improved by projecting it onto a root-$n$ consistent estimator of the $V(\theta)$-envelope of span($\theta$).

1. Reproduces all of the known envelope methods, and applicable to GLMs.
2. Links envelopes to a pre-specified estimator, MLE, robust estimator, OLS, .... Likelihood not required.
3. $V(\theta)$ can now depend on the parameter being estimated, plus perhaps nuisance parameters.
4. Extends to matrix and array-valued parameters via “tensor envelopes.”
Let \((B, B_0)\) denote an orthogonal basis of \(\mathbb{R}^p\), where \(B \in \mathbb{R}^{p \times q}\), \(B_0 \in \mathbb{R}^{p \times (p-q)}\) and \(\text{span}(B) \subseteq \mathcal{E}_M(B)\). Then \(v \in \mathcal{E}_{B_0^TMB_0}(B_0^T B)\) implies that \(B_0v \in \mathcal{E}_M(B)\).
1 Set initial value $g_0 = G_0 = 0$.
2 For $k = 0, \ldots, u - 1$, $g_{k+1} \in \mathbb{R}^q$ is obtained direction in the envelope $\mathcal{E}_{\mathbf{V}(\theta)}(\text{span}(\theta))$ as follows,
   1 Let $G_k = (g_1, \ldots, g_k)$ if $k \geq 1$ and let $(G_k, G_0k)$ be an orthogonal basis for $\mathbb{R}^q$.
   2 Define the stepwise objective function
     
     $$L_k(w) = \log(w^T A_k w) + \log(w^T B_{k}^{-1} w),$$  
     \hfill (1)

     where $A_k = G_{0k}^T \hat{\mathbf{V}}(\theta) G_{0k}$, $B_k = G_{0k}^T \hat{\mathbf{V}}(\theta) G_{0k} + G_{0k}^T \hat{\theta} \hat{\theta}^T G_{0k}$ and $w \in \mathbb{R}^{q-k}$.
3 Solve $w_{k+1} = \arg \min_w L_k(w)$ subject to a length constraint $w^T w = 1$.
4 Define $g_{k+1} = G_{0k} w_{k+1}$ to be the unit length $(k + 1)$-th stepwise direction.
Computing for linear model applications:

MatLab toolbox:
http://code.google.com/p/envlp/.

Thank you!
Envelopes and MSE
Dennis Cook | Envelopes: Methods for Efficient Estimation in Multivariate Statistics
Other envelope application in MLMs

- **Partial response envelopes** for part of $\beta = (\beta_1, \beta_2)$. (Su and Cook, *Biometrika*, 2011)

\[
Y = \alpha + \beta_1 X_1 + \beta_2 X_2 + \varepsilon \\
= \alpha + \Gamma \eta X_1 + \beta_2 X_2 + \varepsilon \\
\Sigma = \Gamma \Omega \Gamma^T + \Gamma_0 \Omega_0 \Gamma_0^T
\]

- **Simultaneous envelopes** for reducing $X$ and $Y$ (Cook and Zhang, *Technometrics*, to appear)

\[
Y = \alpha + \beta X + \varepsilon \\
= \alpha + \Gamma \eta \Phi^T X + \varepsilon \\
\Sigma = \Gamma \Omega \Gamma^T + \Gamma_0 \Omega_0 \Gamma_0^T \\
\Sigma_X = \Phi \Delta \Phi^T + \Phi_0 \Delta_0 \Phi_0^T
\]
- Scaled predictor envelopes, when predictors are in different scales. (Su and Cook, submitted)
  \[ Y = \alpha + \eta^T \Phi^T \Lambda^{-1} X + \varepsilon, \]
  \[ \Sigma_X = \Lambda \Phi \Delta \Phi^T \Lambda + \Lambda \Phi_0 \Delta_0 \Phi_0^T \Lambda, \]
  \[ \Lambda = \text{diag}(1, \lambda_2, \ldots, \lambda_p) \]

- Scaled response envelopes, when responses are in different scales. (Su and Cook, *Biometrika*, 2013)

- Inner envelopes, when envelopes don’t offer improvement. (Su and Cook, *Biometrika*, 2012) – based on the largest reducing subspace of \( \Sigma \) that is contained within span(\( \beta \)).

<table>
<thead>
<tr>
<th>Week</th>
<th>B</th>
<th>B/se(B)</th>
<th>$\hat{\beta}$</th>
<th>$\hat{\beta}/se(\hat{\beta})$</th>
<th>se(B)/se($\hat{\beta}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2.43</td>
<td>0.83</td>
<td>-2.17</td>
<td>-1.67</td>
<td>2.25</td>
</tr>
<tr>
<td>4</td>
<td>3.33</td>
<td>1.05</td>
<td>-0.48</td>
<td>-0.65</td>
<td>4.27</td>
</tr>
<tr>
<td>6</td>
<td>3.13</td>
<td>0.89</td>
<td>0.88</td>
<td>1.23</td>
<td>4.89</td>
</tr>
<tr>
<td>8</td>
<td>4.73</td>
<td>1.22</td>
<td>2.38</td>
<td>2.82</td>
<td>4.56</td>
</tr>
<tr>
<td>10</td>
<td>4.73</td>
<td>1.14</td>
<td>2.89</td>
<td>4.14</td>
<td>5.94</td>
</tr>
<tr>
<td>12</td>
<td>5.50</td>
<td>1.30</td>
<td>5.40</td>
<td>5.30</td>
<td>4.15</td>
</tr>
<tr>
<td>14</td>
<td>-4.80</td>
<td>-1.11</td>
<td>-5.09</td>
<td>-5.55</td>
<td>4.69</td>
</tr>
<tr>
<td>16</td>
<td>-4.53</td>
<td>-0.97</td>
<td>-4.62</td>
<td>-5.36</td>
<td>5.40</td>
</tr>
<tr>
<td>18</td>
<td>-2.87</td>
<td>-0.54</td>
<td>-3.67</td>
<td>-4.06</td>
<td>5.86</td>
</tr>
<tr>
<td>19</td>
<td>5.00</td>
<td>0.86</td>
<td>4.21</td>
<td>4.92</td>
<td>6.78</td>
</tr>
</tbody>
</table>

We would need $n \sim 1500$ for OLS to match the envelope results.
The standard MLE is $\hat{\beta}_{\text{Std}} = (5.5, -4.8)^T$ with bootstrap standard errors $(4.2, 4.4)^T$, while the envelope estimate is $\hat{\beta} = (5.4, -5.1)^T$ with bootstrap standard errors $(1.12, 1.07)^T$.

About 1500 observations would be needed for a likelihood analysis to yield the standard errors from an envelope analysis with 60 observations.
Heights of Boys and Girls
Heights of Boys and Girls Ages 13 and 14

- \( \| \hat{\Omega} \| = 1.57 \) and \( \| \hat{\Omega}_0 \| = 79.5 \).
Heights of Boys and Girls Ages 17 and 18

\[ \| \hat{\Omega} \| = 118.7 \text{ and } \| \hat{\Omega}_0 \| = 0.16. \]

SE ratios for sm/em: 1.01 and 0.99
# Heights of Boys and Girls: Bootstrap SEs

**Table:** Bootstrap and estimated asymptotic standard errors of the two elements in $\hat{\beta}$ under the standard model (SM) and envelope model (EM).

<table>
<thead>
<tr>
<th>Response</th>
<th>SM</th>
<th>BSM</th>
<th>EM</th>
<th>BEM</th>
<th>SM/EM</th>
<th>BSM/BEM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Age 13</td>
<td>1.60</td>
<td>1.80</td>
<td>0.188</td>
<td>0.191</td>
<td>8.49</td>
<td>9.44</td>
</tr>
<tr>
<td>Age 14</td>
<td>1.61</td>
<td>1.81</td>
<td>0.187</td>
<td>0.190</td>
<td>8.61</td>
<td>9.64</td>
</tr>
<tr>
<td>Age 17</td>
<td>1.32</td>
<td>1.36</td>
<td>1.31</td>
<td>1.30</td>
<td>1.01</td>
<td>1.04</td>
</tr>
<tr>
<td>Age 18</td>
<td>1.33</td>
<td>1.37</td>
<td>1.34</td>
<td>1.37</td>
<td>0.99</td>
<td>1.01</td>
</tr>
</tbody>
</table>