Shape Constraints, Compound Decisions and Empirical Bayes Rules

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Joint work with Ivan Mizera (U. of Alberta)
An Empirical Bayes Homework Problem

Suppose you observe a sample \( \{Y_1, \ldots, Y_n\} \) and \( Y_i \sim \mathcal{N}(\mu_i, 1) \) for \( i = 1, \ldots, n \), and would like to estimate all of the \( \mu_i \)'s under squared error loss. We might call this “incidental parameters with a vengeance.”
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Fact 1. If the \( \mu_i \) are drawn iid-ly from a known distribution \( F \) so the \( Y_i \) have density,

\[
g(y) = \int \phi(y - \mu) dF(\mu),
\]

then the Bayes rule is:

\[
\delta(y) = y + \frac{g'(y)}{g(y)}
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**Fact 2.** If \( F \) is unknown, one can try to estimate \( g \) and plug it into the Bayes rule, but exponential family considerations dictate that \( \hat{\delta}(\cdot) \) should be monotone increasing.
We’d like to estimate the $\mu_i$’s with something other than the naïve decision rule, $\mu_i = Y_i$. For example, if we thought that $F$ were $\mathcal{N}(\mu_0, \sigma_0^2)$ we would have,

$$\delta(y) = y + \frac{g'(y)}{g(y)} = \mu_0 + \frac{\sigma_0^2}{1 + \sigma_0^2} (y - \mu_0).$$

Note that in this case, $Y \sim \mathcal{N}(\mu_0, 1 + \sigma_0^2)$, so we can estimate $(\mu_0, \sigma_0^2)$ at $\sqrt{n}$ rate, and we obtain a variant of the celebrated James-Stein (1960) estimator. When the prior mean, $\mu_0 = 0$, and the prior variance, $\sigma_0^2 = 1$, then the optimal rule is “shrink by half.”

$$\delta(y) = y/2$$
Unobserved Heterogeneity

More generally we can consider models of the form:

\[ g(y) = \int \varphi(y, \theta) \, dF(\theta), \]

where \( \varphi \) is a known parametric likelihood, and \( F \) is again a mixing distribution over the parameter \( \theta \).
Unobserved Heterogeneity

More generally we can consider models of the form:

\[ g(y) = \int \varphi(y, \theta) dF(\theta), \]

where \( \varphi \) is a known parametric likelihood, and \( F \) is again a mixing distribution over the parameter \( \theta \).

In survival analysis these are called "fraility" models, or in the terminology of Heckman and Singer (1984) models of "unobserved heterogeneity."
A natural question would be: When can we identify $\varphi$ and $F$ based on knowledge of the mixture distribution $G$. Not surprisingly, the answer is only with further assumptions. Two favorable special cases:

- Gaussian Location Family When $g(y) = \int \varphi(y-\theta) dF(\theta)$, $\psi_G(t) \equiv \int e^{iyt} g(y) dy = \int \int e^{iyt} \varphi(y-\theta) dF(\theta) = e^{-t^2/2} \int e^{i\theta t} dF(\theta)$, so uniqueness of the characteristic function for $G$ assures identifiability of $F$.

- General Location Families When $g(y) = \int \varphi(y-\theta) dF(\theta)$, we have, $\psi_G(t) = \psi_{\varphi}(t) \psi_F(t)$, so unless $\psi_{\varphi}(t) = 0$ over an open interval, $F$ is again uniquely defined.
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Most of the applications of our homework problem choose $\phi$ as a one parameter exponential family with a "natural" parameter, $\theta$, so we may write,

$$\phi(y, \theta) = m(y) e^{y\theta} h(\theta)$$

Quadratic loss implies that the Bayes rule is a conditional mean:

$$\delta_G(y) = \mathbb{E}[\Theta|Y = y]$$

$$= \int \theta \phi(y, \theta) dF / \int \phi(y, \theta) dF$$

$$= \int \theta e^{y\theta} h(\theta) dF / \int e^{y\theta} h(\theta) dF$$

$$= \frac{d}{dy} \log \left( \int e^{y\theta} h(\theta) dF \right)$$

$$= \frac{d}{dy} \log \left( g(y)/m(y) \right)$$
Standard Gaussian Case

In the homework problem,

$$\varphi(y, \theta) = \phi(y - \theta) = K \exp\{- (y - \theta)^2 / 2\} = Ke^{-y^2/2} \cdot e^{y\theta} \cdot e^{-\theta^2/2}$$

So $$m(y) = e^{-y^2/2}$$ and the logarithmic derivative yields our Bayes rule:

(Fact 1) $$\delta(y) = \frac{d}{dy} \left[ \frac{1}{2} y^2 + \log g(y) \right] = y + \frac{g'(y)}{g(y)}.$$
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For Fact 2, note that,

\[ \delta'_G(y) = \frac{d}{dy} \left[ \frac{\int \theta \varphi dF}{\int \varphi dF} \right] = \frac{\int \theta^2 \varphi dF}{\int \varphi dF} - \left( \frac{\int \theta \varphi dF}{\int \varphi dF} \right)^2 \]
\[ = \mathbb{E}[\Theta^2 | Y = y] - (\mathbb{E}[\Theta | Y = y])^2 \]
\[ = \mathbb{V}[\Theta | Y = y] \geq 0, \]

implying that \( \delta_G \) must be monotone. This is the monotone likelihood ratio property of the exponential family coming into play.
Estimating $\delta(y)$

So far we have emphasized knowing the form of the mixing distribution $F$ as well as $\varphi$, what if $F$ is unknown? If $F$ is known up to a finite dimensional parameter, then there is quite a lot of literature on special cases.

For example, in Johnstone and Silverman’s (2004) paper “Needles and Straw in Haystacks,” they consider prior densities of the form:

$$f(u) = (1 - w)\delta_0(u) + w\gamma(u)$$

so $F$ has mass $1 - w$ at zero, and its remaining mass spread according to a density $\gamma$ which is taken either to be Laplace (double exponential) or as a beta mixture of normals with Cauchy tails. They construct empirical Bayes estimators that estimate the mass $w$ and the scale of the $\gamma$ density. Estimators are then selected as the median of the posterior, or the mean, and a quite extensive simulation experiment conducted.
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Data is generated from 12 distinct models, all of the form:

\[ Y_i = \mu_i + u_i, \quad u_i \sim \mathcal{N}(0, 1), \quad i = 1, \ldots, 1000. \]

Of the \( n = 1000 \) observations \( n - k \) of the \( \mu_i = 0 \), and the remaining \( k \) take one of the four values \( \{3, 4, 5, 7\} \). There are three choices of \( k \): \( \{5, 50, 500\} \). There are 50 replications for each of the 12 experimental settings and 18 different competing estimators.
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Performance is measured by the mean (over replications) of the sum (over the \( n = 1000 \) observations) of squared errors, so a score of 500 means that the mean squared prediction error is 0.5, or half of what the naïve prediction \( \hat{\mu}_i = Y_i \) would yield if the \( \mu_i \) were all zero.
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Non-parametric Empirical Bayes

What about nonparametric estimation of the mixture density $g$? Brown and Greenshtein (Annals, 2009) propose estimating $g$ by standard fixed bandwidth kernel methods and they compare performance of the resulting estimated Bayes rule with various other methods including the 18 methods investigated by Johnstone and Silverman, employing their simulation design. For these simulations they employ bandwidth $h = 1.15$. 

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But our homework asked for a monotone Bayes rule.

Find a density estimate \( \hat{g} \) for the mixture density such that

\[
\hat{\delta}(y) = y + \frac{\hat{g}'(y)}{\hat{g}(y)}
\]

is monotone increasing, or equivalently, such that,

\[
K(y) = \frac{1}{2} y^2 + \log \hat{g}(y)
\]

is convex. This problem is closely related to recent work on estimating log-concave densities, e.g. Cule, Samworth and Stewart (JRSSB, 2010), K and Mizera (Annals, 2010), Seregin and Wellner (2010).
Monotone Empirical Bayes Rules

We could, as van Houwelingen and Stijnen (Stat. Ned., 1983), try to make a preliminary (kernel) density estimate and then monotonize its logarithmic derivative, but why not maximum likelihood?

\[
\hat{g} = \text{argmax}\{ \sum_{i=1}^{n} \log g(Y_i) | \int g \, dy = 1, \ K(y) \in \mathcal{K} \},
\]

where \( \mathcal{K} \) is the convex cone of convex functions. This can be solved by standard interior point methods, or equivalently we can solve the dual problem of minimizing Shannon entropy or the Kullback-Leibler distance between the estimated density and a uniform density on the support of the empirical df.

Solutions have piecewise linear \( K \) functions, and rather funny looking \( \hat{g} \)’s.
Discrete Formulation

Let $h(y) = -\log g(y)$, and write the primal problem as,

$$(P) \quad \max_{\alpha} \{ w^\top \alpha - \sum c_i e^{\alpha_i} \mid D\alpha + 1 \geq 0 \}.$$ 

and dual problem as,

$$(D) \quad \min_{\nu} \{ \sum c_i g_i \log g_i + 1^\top \nu \mid g = C^{-1}(\nu + D^\top \nu), \nu \geq 0 \}.$$
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\]

For example with \( F \sim U[5, 15] \) we obtain estimates like this:
Revenge of the MLE

How well do these monotone Bayes rules perform in the Johnstone and Silverman sweepstakes?
Revenge of the MLE

How well do these monotone Bayes rules perform in the Johnstone and Silverman sweepstakes?

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</table>

Shockingly well, actually. But as ever so, there is disappointment just around the corner.

Roger Koenker (UIUC)
Revenge of the MLE

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<tr>
<td></td>
<td>$\hat{\delta}$</td>
<td>3 4 5 7</td>
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<tr>
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<td></td>
<td></td>
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<td></td>
<td>488 310 145 22</td>
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<td></td>
</tr>
<tr>
<td>$\tilde{\delta}_{1.15}$</td>
<td>53 49 42 27</td>
<td></td>
<td></td>
<td></td>
<td>179 136 81 40</td>
<td></td>
<td></td>
<td></td>
<td>484 302 158 48</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>J-S Min</td>
<td>34 32 17 7</td>
<td></td>
<td></td>
<td></td>
<td>201 156 95 52</td>
<td></td>
<td></td>
<td></td>
<td>829 730 609 505</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Shockingly well, actually. But as ever so, there is disappointment just around the corner.
Revenge$^2$ of the MLE

Kiefer and Wolfowitz (1956) reconsidering the Neyman and Scott (1948) problem showed that non-parametric maximum likelihood could be used to establish consistent estimators even when the number of incidental parameters tended to infinity. Laird (1978) and Heckman and Singer (1984) suggested that the EM algorithm could be used to compute the MLE in such cases.

Jiang and Zhang (Annals, 2009) adapt this approach for the empirical Bayes problem: Let $u_i: i = 1, \ldots, m$ denote a grid on the support of the sample $Y_i$'s, then the prior (mixing) density $f$ is estimated by the fixed point iteration:

$$\hat{f}(k+1)_j = \frac{1}{n} \sum_{i=1}^n \hat{f}(k)_j \phi(Y_i - u_j)\sum_{j=1}^m \hat{f}(k)_{\ell} \phi(Y_i - u_{\ell}),$$

and the implied Bayes rule becomes at convergence:

$$\hat{\delta}(Y_i) = \sum_{j=1}^m u_j \phi(Y_i - u_j)\hat{f}_j \sum_{j=1}^m \phi(Y_i - u_j)\hat{f}_j.$$
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$$
\hat{f}_j^{(k+1)} = n^{-1} \sum_{i=1}^{n} \frac{\hat{f}_j^{(k)} \phi(Y_i - u_j)}{\sum_{\ell=1}^{m} \hat{f}_\ell^{(k)} \phi(Y_i - u_\ell)},
$$

and the implied Bayes rule becomes at convergence:

$$
\hat{\delta}(Y_i) = \frac{\sum_{j=1}^{m} u_j \phi(Y_i - u_j) \hat{f}_j}{\sum_{j=1}^{m} \phi(Y_i - u_j) \hat{f}_j}.
$$
The Incredible Lethargy of EM-ing

Unfortunately, EM fixed point iterations are notoriously slow and this is especially apparent in the Kiefer and Wolfowitz setting. Solutions approximate discrete (point mass) distributions, but EM goes ever so slowly. (Approximation is controlled by the grid spacing of the $u_i$'s.)
Accelerating EM

There is a large literature on accelerating EM iterations, but none of the recent developments (that I tried) seemed to help very much. Eventually it occurred to me that the problem could be reformulated as a maximum likelihood problem to exploit interior point methods for solving convex programs. Consider,

\[
\max_{f \in F} \sum_{i=1}^{n} \log \left( \sum_{j=1}^{m} \phi(y_i - u_j) f_j \right),
\]

or reformulating slightly,

\[
\min \left\{ -\sum_{i=1}^{n} \log(y_i) \mid A z = y, \ z \in S \right\},
\]

where \(A = (\phi(y_i - u_j))\) and \(S = \{ s \in \mathbb{R}^m \mid 1^\top s = 1, \ s \geq 0 \}\). So \(z_j\) denotes the estimated mixing density estimate \(\hat{f}\) at the grid point \(u_j\), and \(y_i\) denotes the estimated mixture density estimate, \(\hat{g}\), at \(Y_i\).
Interior Point vs. EM

![Graph showing the comparison between Interior Point and EM methods, with various lines representing different models and parameters.](image)

- **GMLEBIP**
- **GMLEBEM: m=10^2**
- **GMLEBEM: m=10^4**
- **GMLEBEM: m=10^5**
Interior Point vs. EM

In the foregoing test problem we have $n = 200$ observations and $m = 300$ grid points. Timing and accuracy is summarized in this table.

<table>
<thead>
<tr>
<th>Estimator</th>
<th>EM1</th>
<th>EM2</th>
<th>EM3</th>
<th>IP</th>
</tr>
</thead>
<tbody>
<tr>
<td>Iterations</td>
<td>100</td>
<td>10,000</td>
<td>100,000</td>
<td>15</td>
</tr>
<tr>
<td>Time</td>
<td>1</td>
<td>37</td>
<td>559</td>
<td>1</td>
</tr>
<tr>
<td>$L(g) - 422$</td>
<td>0.9332</td>
<td>1.1120</td>
<td>1.1204</td>
<td>1.1213</td>
</tr>
</tbody>
</table>

Comparison of EM and Interior Point Solutions: Iteration counts, log likelihoods and CPU times (in seconds) for three EM variants and the interior point solver.

Scaling problem sizes up, the deficiency of the EM approach is even more serious.
In the (now familiar) Johnstone and Silverman sweepstakes we have the following comparison of performance.

<table>
<thead>
<tr>
<th>Estimator</th>
<th>k = 5</th>
<th>k = 50</th>
<th>k = 500</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>$\hat{\delta}_{\text{MLE-IP}}$</td>
<td>33</td>
<td>30</td>
<td>16</td>
</tr>
<tr>
<td>$\hat{\delta}_{\text{MLE-EM}}$</td>
<td>37</td>
<td>33</td>
<td>21</td>
</tr>
<tr>
<td>$\delta$</td>
<td>37</td>
<td>34</td>
<td>21</td>
</tr>
<tr>
<td>$\tilde{\delta}_{1.15}$</td>
<td>53</td>
<td>49</td>
<td>42</td>
</tr>
<tr>
<td>J-S Min</td>
<td>34</td>
<td>32</td>
<td>17</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>$\hat{\delta}_{\text{MLE-IP}}$</td>
<td>153</td>
<td>107</td>
<td>51</td>
</tr>
<tr>
<td>$\hat{\delta}_{\text{MLE-EM}}$</td>
<td>162</td>
<td>111</td>
<td>56</td>
</tr>
<tr>
<td>$\delta$</td>
<td>173</td>
<td>121</td>
<td>63</td>
</tr>
<tr>
<td>$\tilde{\delta}_{1.15}$</td>
<td>179</td>
<td>136</td>
<td>81</td>
</tr>
<tr>
<td>J-S Min</td>
<td>201</td>
<td>156</td>
<td>95</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>$\hat{\delta}_{\text{MLE-IP}}$</td>
<td>454</td>
<td>276</td>
<td>127</td>
</tr>
<tr>
<td>$\hat{\delta}_{\text{MLE-EM}}$</td>
<td>458</td>
<td>285</td>
<td>130</td>
</tr>
<tr>
<td>$\delta$</td>
<td>488</td>
<td>310</td>
<td>145</td>
</tr>
<tr>
<td>$\tilde{\delta}_{1.15}$</td>
<td>484</td>
<td>302</td>
<td>158</td>
</tr>
<tr>
<td>J-S Min</td>
<td>829</td>
<td>730</td>
<td>609</td>
</tr>
</tbody>
</table>

Here MLE-EM is Jaing and Zhang’s (2009) Bayes rule with their suggested 100 EM iterations. It does somewhat better than the shape constrained estimator, but the interior point version MLE-IP does even better.
... , but how does it work in theory?

The fundamental theorem of compound decisions (Robbins (1951)) asserts that the multivariate problem of estimating all the \(\theta\)'s can be reduced to

\[
R^*(G_n) = \min_{t \in T} R(t, G_n) = \min_{t \in T} \mathbb{E}_{G_n}(t(Y_i) - \xi)^2
\]

that is, to finding a Bayes Rule for the univariate problem:

\[
Y|\xi \sim \mathcal{N}(\xi, 1), \quad \xi \sim G,
\]

with \(G = G_n\), the empirical df of the \(\theta\)'s, over the class of Borel functions.
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$$Y|\xi \sim N(\xi, 1), \quad \xi \sim G,$$

with $G = G_n$, the empirical df of the $\theta$’s, over the class of Borel functions. We can constrain the class, $T$ in various ways:

- Linear $t(\cdot)$ – James-Stein estimator,
- soft thresholding $t(\cdot)$ – Stein unbiased risk estimator (SURE),
- hard thresholding $t(\cdot)$ – FDR/generalized $C_p$ estimator,
- posterior medians – Johnstone and Silverman’s EBThresh
Adaptive Minimaxity and the Oracle

Comparing performance with that of the Oracle estimator using $F = F_n$:

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<th>$k = 50$</th>
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<td>3 4 5 7</td>
<td></td>
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<td></td>
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<td></td>
</tr>
<tr>
<td>Oracle</td>
<td>27 22 12 1</td>
<td>144 93 46 3</td>
<td>443 273 128 8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\hat{\delta}_{\text{MLE-IP}}$</td>
<td>33 30 16 8</td>
<td>153 107 51 11</td>
<td>454 276 127 18</td>
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Question: How can such poor estimates of the mixing distribution produce such good performance for their associated Bayes rules?
Discrete Approximations and Entropy

The mixing density may be poor, but the mixture density is still quite good:

**Lemma**: (Zhang) Let \( g_F(y) = \int \phi(y - u) \, dF(u) \), then for any \( F \) there exists a discrete \( F_m \), with support \([-M - a, M + a]\) and at most
\[ m = (2 \lfloor 6a^2 \rfloor + 1)(2M/a + 2) + 1 \]
atoms such that
\[ \| g_F - g_{F_m} \|_{\infty, M} \leq \phi(a)(1 + \phi(0)). \]
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\[
\| g_F - g_{F_m} \|_{\infty, M} \leq \phi(a)(1 + \phi(0)).
\]

The existence of such parsimonious discrete approximations yield a good entropy bound (covering number) for the class of distributions and thus a large deviation inequality for the Hellinger error of the (generalized) MLE. This in turn yields strong bounds on the "regret" for the associated Bayes rules relative to the Oracle bound.
Adaptive Minimaxity

For their approximate MLE-EM Bayes rules Jiang and Zhang prove:

**Theorem:** For the normal mixture problem, with a (complicated) weak \( p \)th moment restriction on \( \Theta \), the approximate non-parametric MLE, \( \hat{\theta} = \hat{\delta}_{\hat{F}_n}(Y) \) is adaptively minimax, i.e.

\[
\sup_{\theta} \mathbb{E}_{n,\theta} L_n(\hat{\theta}, \theta) \rightarrow 1,
\]

\[
\inf_{\tilde{\theta}} \sup_{\theta \in \Theta} \mathbb{E}_{n,\theta} L_n(\tilde{\theta}, \theta)
\]

The weak \( p \)th moment condition encompasses a much broader class of both deterministic and stochastic classes \( \Theta \).
Conclusions and Extensions

- Empirical Bayes methods, employing maximum likelihood, offer some advantages over other thresholding and kernel methods,
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- Kiefer-Wolfowitz type non-parametric MLEs, while computationally somewhat more demanding, perform even better, especially after replacing EM by interior point computational methods. For large sample sizes, further binning is needed to make the interior point methods practical.
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- Kiefer-Wolfowitz type non-parametric MLEs, while computationally somewhat more demanding, perform even better, especially after replacing EM by interior point computational methods. For large sample sizes, further binning is needed to make the interior point methods practical.
- There are many opportunities for linking such methods to various semi-parametric estimation problems a la Heckman and Singer (1983) and van der Vaart (1996).