High Dimensional Predictive Inference

Ed George University of Pennsylvania (joint work with Larry Brown, Feng Liang, and Xinyi Xu)

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I. The Hunt for Shrinkage Estimators Begins

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 - Canonical Problem: Observe X | µ ~ N_p(µ, I) and estimate µ by µ̂ under

$$R_Q(\mu, \hat{\mu}) = E_{\mu} \|\hat{\mu}(X) - \mu\|^2$$

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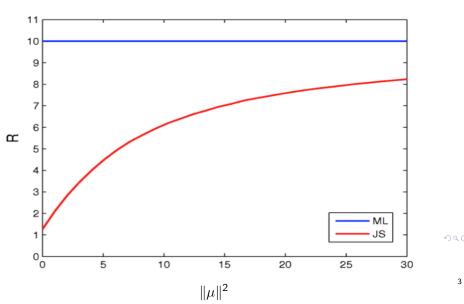
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- ► A Shocking Discovery: µ̂_{MLE} is inadmissible when p ≥ 3. (Stein 1956)
- An Explicit Better Estimator Appears: The James-Stein estimator

$$\hat{\mu}_{JS} = \left(1 - rac{p-2}{\|X\|^2}
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(James and Stein 1961)

• The risk of $\hat{\mu}_{MLE}$ and the risk of $\hat{\mu}_{JS}$ various values of μ



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- For a prior $\pi(\mu)$, the Bayes rule under $R_Q(\mu, \hat{\mu})$ is

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- Stein (1962) suggests an empirical Bayes motivation for µ_{JS}. The focus of the hunt turns to Bayes.
- For a prior $\pi(\mu)$, the Bayes rule under $R_Q(\mu, \hat{\mu})$ is

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• Remark: The (formal) Bayes rule under $\pi_U(\mu) \equiv 1$ is

$$\hat{\mu}_U(X) \equiv \hat{\mu}_{MLE}(X) = X$$

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• $\hat{\mu}_H(X)$, the Bayes rule under the Harmonic prior

$$\pi_H(\mu) = \|\mu\|^{-(p-2)}$$

dominates $\hat{\mu}_U$ when $p \ge 3$. (Stein 1974)

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• $\hat{\mu}_a(X)$, the Bayes rule under $\pi_a(\mu)$ where

$$\mu \mid s \sim N_p\left(0, s \, I\right), \quad s \sim (1+s)^{a-2}$$

dominates $\hat{\mu}_U$ and is proper Bayes when p = 5 and $a \in [.5, 1)$ or when $p \ge 6$ and $a \in [0, 1)$. (Strawderman 1971)

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A Unifying Phenomenon: These domination results can be attributed to properties of the marginal distribution of X = under π_H → ∞ and π_a. • The Bayes rule under $\pi(\mu)$ can be expressed as

$$\hat{\mu}_{\pi}(X) = E_{\pi}(\mu \mid X) = X + \nabla \log m_{\pi}(X)$$

where

$$m_{\pi}(X) \propto \int e^{-(X-\mu)^2/2} \pi(\mu) \, d\mu$$

is the marginal of X under $\pi(\mu)$. $(\nabla = (\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_p})')$ (Brown 1971)

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• The risk improvement of $\hat{\mu}_{\pi}(X)$ over $\hat{\mu}_{U}(X)$ can be expressed as

$$\begin{aligned} R_Q(\mu, \hat{\mu}_U) - R_Q(\mu, \hat{\mu}_\pi) &= E_\mu \left[\|\nabla \log m_\pi(X)\|^2 - 2\frac{\nabla^2 m_\pi(X)}{m_\pi(X)} \right] \\ &= E_\mu \left[-4\nabla^2 \sqrt{m_\pi(X)} / \sqrt{m_\pi(X)} \right] \implies \implies \infty \propto n \\ \nabla^2 &= \sum_i \frac{\partial^2}{\partial x_i^2} \end{aligned}$$

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(Stein 1974, 1981)

That µ̂_H(X) dominates µ̂_U when p ≥ 3, follows from the fact that the marginal m_π(X) under π_H is superharmonic, i.e.

$$abla^2 m_\pi(X) \leq 0$$

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That µ̂_a(X) dominates µ̂_U when p ≥ 5 (and conditions on a), follows from the fact that the sqrt of the marginal under π_a is superharmonic, i.e.

$$abla^2 \sqrt{m_\pi(X)} \leq 0$$

(Fourdrinier, Strawderman and Wells 1998)

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$$L(\mu, q(y \mid x)) = \int p(y \mid \mu) \log \frac{p(y \mid \mu)}{q(y \mid x)} dy$$

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Risk function

$$R_{\mathcal{K}\mathcal{L}}(\mu,q) = \int \mathcal{L}(\mu,q(y \mid x)) \ p(x \mid \mu) \ dx = \mathcal{E}_{\mu}[\mathcal{L}(\mu,q(y \mid X))]^{-1}$$

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• For a prior $\pi(\mu)$, the Bayes rule under $R_{KL}(\mu, q)$ is

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- ▶ p_U(y | x) is best invariant and minimax with constant risk. (Murray 1977, Ng 1980, Barron and Liang 2003)
- Shocking Fact: $p_U(y \mid x)$ is inadmissible when $p \ge 3$.

• $p_H(y \mid x)$, the Bayes rule under the Harmonic prior

$$\pi_H(\mu) = \|\mu\|^{-(p-2)},$$

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A Key Question: Are these domination results attributable to the properties of m_π?

• Let $m_{\pi}(x; v_x)$ denote the marginal of $X \mid \mu \sim N_p(\mu, v_x I)$ under $\pi(\mu)$.

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- **Lemma**: The Bayes rule $p_{\pi}(y \mid x)$ can be expressed as

$$p_{\pi}(y \mid x) = \frac{m_{\pi}(w; v_w)}{m_{\pi}(x; v_x)} p_U(y \mid x)$$

where

$$W = \frac{v_y X + v_x Y}{v_x + v_y} \sim N_p(\mu, v_w I)$$

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Using this, the risk improvement can be expressed as

$$R_{KL}(\mu, p_U) - R_{KL}(\mu, p_\pi) = \int \int p_{v_x}(x|\mu) p_{v_y}(y|\mu) \log \frac{p_\pi(y, |x)}{p_U(y|x)} dx dy$$

= $E_{\mu, v_w} \log m_\pi(W; v_w) - E_{\mu, v_w} \log m_\pi(X; v_x)$ ¹¹

An Analogue of Stein's Unbiased Estimate of Risk

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An Analogue of Stein's Unbiased Estimate of Risk

Theorem:

$$\frac{\partial}{\partial v} E_{\mu,v} \log m_{\pi}(Z;v) = E_{\mu,v} \left[\frac{\nabla^2 m_{\pi}(Z;v)}{m_{\pi}(Z;v)} - \frac{1}{2} \|\nabla \log m_{\pi}(Z;v)\|^2 \right]$$
$$= E_{\mu,v} \left[2\nabla^2 \sqrt{m_{\pi}(Z;v)} / \sqrt{m_{\pi}(Z;v)} \right]$$

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$$= E_{\mu,v} \left[2\nabla^2 \sqrt{m_{\pi}(Z;v)} / \sqrt{m_{\pi}(Z;v)} \right]$$

Proof relies on using the heat equation

$$rac{\partial}{\partial v}m_{\pi}(z;v)=rac{1}{2}
abla^2m_{\pi}(z;v),$$

Brown's representation and Stein's Lemma.

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Let m_π(z; v) be the marginal distribution of Z | μ ~ N_p(μ, vI) under π(μ).

- Let m_π(z; v) be the marginal distribution of Z | μ ∼ N_p(μ, vI) under π(μ).
- ► Theorem: If m_π(z; v) is finite for all z, then p_π(y | x) will be minimax if either of the following hold:
 - 1. $m_{\pi}(z; v)$ is superharmonic
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- Corollary: If m_π(z; v) is finite for all z, then p_π(y | x) will be minimax if π(μ) is superharmonic.

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- Corollary: If m_π(z; v) is finite for all z, then p_π(y | x) will be minimax if π(μ) is superharmonic.
- p_π(y | x) will dominate p_U(y | x) in the above results if the set ≥ ∞∞ superharmonicity is strict on some interval.

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▶ Because π_H is superharmonic, it is immediate that p_H(y | x) dominates p_U(y | x) and is minimax.

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- ▶ Because √m_a is superharmonic (under suitable conditions on a), it is immediate that p_a(y | x) dominates p_U(y | x) and is minimax.
- It also follows that any of the improper superharmonic t-priors of Faith (1978) or any of the proper generalized t-priors of Fourdrinier, Strawderman and Wells (1998) yield Bayes rules that dominate p_U(y | x) and are minimax.

III. Predictive "Shrinkage"

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III. Predictive "Shrinkage"

Our Lemma representation

$$p_H(y \mid x) = \frac{m_H(w; v_w)}{m_H(x; v_x)} p_U(y \mid x)$$

shows how $p_H(y | x)$ "shrinks $p_U(y | x)$ towards 0" by an adaptive multiplicative factor.

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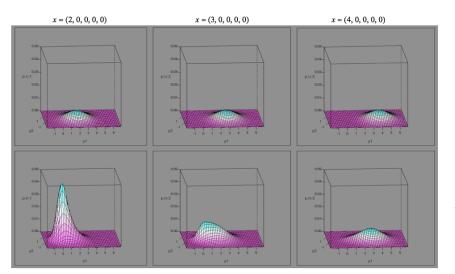
shows how $p_H(y | x)$ "shrinks $p_U(y | x)$ towards 0" by an adaptive multiplicative factor.

► Note the analogies with the Bayes rule $\hat{\mu}_{\pi}(X) = E_{\pi}(\mu \mid X)$ whose coordinates are

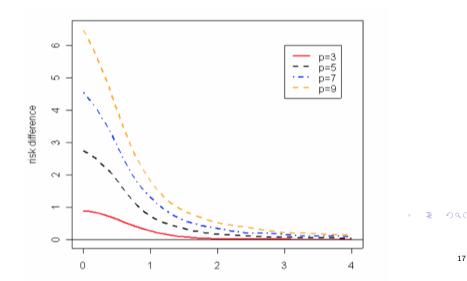
$$\left(1+\frac{(\nabla\log m_{\pi}(X))_{i}}{X_{i}}\right) X_{i}$$

Predictive Shrinkage in Action

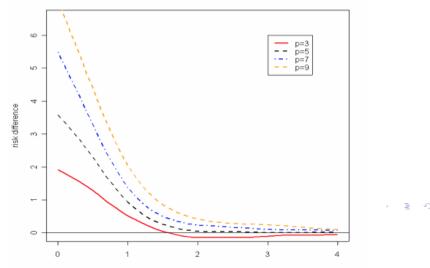
• The contrast between $p_U(y | x)$ and $p_H(y | x)$ for various values of x



▶ The risk function difference $[R_{KL}(\mu, p_U) - R_{KL}(\mu, p_H)]$ is largest at $\mu = 0$, and then asymptotes to 0 as $||\mu|| \rightarrow \infty$.



The risk function difference [R_{KL}(µ, p_U) − R_{KL}(µ, p_a)] is largest at µ = 0, and then asymptotes to 0 as ||µ|| → ∞.



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and corresponding recentered marginal

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This yields a predictive distribution

$$p_{\pi}^{b}(y \mid x) = \frac{m_{\pi}^{b}(w; v_{w})}{m_{\pi}^{b}(x; v_{x})} p_{U}(y \mid x)$$

that now shrinks $p_U(y | x)$ towards b rather than 0.

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- Letting P_Bz be the projection of z onto B, shrinkage towards B is obtained by using the recentered prior

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which yields the reecentered marginal

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If m^B_π(z; v) satisfies any of our superharmonic conditions for minimaxity, then p^B_π(y | x) will dominate p_U(y | x) and be minimax.

Minimax Multiple Predictive Shrinkage

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► For any spherically symmetric prior, a set of subspaces B₁,..., B_N, and corresponding probabilities w₁,..., w_N, consider the recentered mixture prior

$$\pi_*(\mu) = \sum_{i=1}^N w_i \, \pi^{B_i}(\mu),$$

and corresponding recentered mixture marginal

$$m_*(z;v)=\sum_1^N w_i m_\pi^{B_i}(z;v).$$

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and corresponding recentered mixture marginal

$$m_*(z; v) = \sum_1^N w_i m_{\pi}^{B_i}(z; v).$$

Applying the µ
_π(X) = X + ∇ log m_π(X) construction with m_∗(X; v
) ∽ ∽ ∽ yields minimax multiple shrinkage estimators of µ. (George 1986)

• Applying the predictive construction with $m_*(z; v)$ yields

$$p_*(y \mid x) = \sum_{i=1}^N p(B_i \mid x) p_{\pi}^{B_i}(y \mid x)$$

where $p_{\pi}^{B_i}(y \mid x)$ is a single target predictive distribution and

$$p(B_i \mid x) = \frac{w_i m_{\pi}^{B_i}(x; v_x)}{\sum_{i=1}^{N} w_i m_{\pi}^{B_i}(x; v_x)}$$

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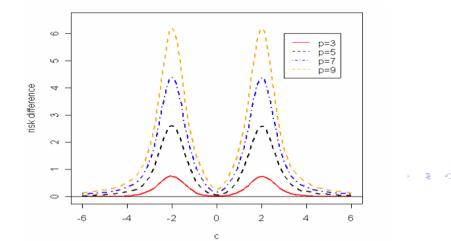
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► Theorem: If each m^{B_i}_π(z; v) is superharmonic, then p_{*}(y | x) will dominate p_U(y | x) and will be minimax.

▶ The risk reduction obtained by the multiple shrinkage predictor p_{H^*} which adaptively shrinks $p_U(y | x)$ towards the closer of the two points $b_1 = (2, ..., 2)$ and $b_2 = (-2, ..., -2)$ using equal weights $w_1 = w_2 = 0.5$



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 Comparing Stein's unbiased quadratic risk expression with our unbiased KL risk expression reveals

$$R_Q(\mu, \hat{\mu}_U) - R_Q(\mu, \hat{\mu}_\pi) = -2 \left[\frac{\partial}{\partial v} E_{\mu, v} \log m_\pi(Z; v) \right]_{v=1}$$

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 Combined with our previous KL risk difference expression reveals a fascinating connection

$$R_{KL}(\mu, p_U) - R_{KL}(\mu, p_\pi) = \frac{1}{2} \int_{v_w}^{v_x} \frac{1}{v^2} \left[R_Q(\mu, \hat{\mu}_U) - R_Q(\mu, \hat{\mu}_\pi) \right]_v dv$$

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Ultimately it is this connection that yields the similar conditions for minimaxity and domination in both problems. Can we go further?

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• Let $B_{KL}(\pi, q) \equiv E_{\pi}[R_{KL}(\mu, q)]$ be the average KL risk of $q(y \mid x)$ under π .

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- ► Theorem (Blyth's Method): If there is a sequence of finite nonnegative measures satisfying π_n({µ : ||µ|| ≤ 1}) ≥ 1 such that

$$B_{KL}(\pi_n,q) - B_{KL}(\pi_n,p_{\pi_n}) \rightarrow 0$$

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• **Theorem**: For any two Bayes rules p_{π} and p_{π_n}

$$B_{\mathcal{KL}}(\pi_n, p_{\pi}) - B_{\mathcal{KL}}(\pi_n, p_{\pi_n}) = \frac{1}{2} \int_{v_w}^{v_x} \frac{1}{v^2} \left[B_Q(\pi_n, \hat{\mu}_{\pi}) - B_Q(\pi_n, \hat{\mu}_{\pi_n}) \right]_v dv$$

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- Let B_{KL}(π, q) ≡ E_π[R_{KL}(μ, q)] be the average KL risk of q(y | x) under π.
- ► Theorem (Blyth's Method): If there is a sequence of finite nonnegative measures satisfying π_n({µ : ||µ|| ≤ 1}) ≥ 1 such that

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Using the explicit construction of π_n(µ) from Brown and Hwang (1984), we obtain tail behavior conditions that prove admissibility of p_U(y | x) when p ≤ 2, and admissibility of p_H(y | x) when p ≥ 3.

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- Theorem: In the KL risk problem, all the admissible procedures are Bayes or formal Bayes procedures.
- ➤ Our proof uses the weak* topology from L[∞] to L¹ to define convergence on the action space which is the set of all proper densities on R^p.
- A Sketch of the Proof:
 - 1. All the admissible procedures are non-randomized.
 - For any admissible procedure p(· | x), there exists a sequence of priors π_i(μ) such that p_{πi}(· | x) → p(· | x) weak* for a.e. x.
 - 3. We can find a subsequence $\{\pi_{i''}\}$ and a limit prior π such that $p_{\pi_{i''}}(\cdot | x) \to p_{\pi}(\cdot | x)$ weak* for almost every x. Therefore, $p(\cdot | x) = p_{\pi}(\cdot | x)$ for a.e. x, i.e. $p(\cdot | x)$ is a Bayes or a formal Bayes rule.

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- ► Observe $X_{m \times 1} = A_{m \times p} \beta_{p \times 1} + \varepsilon_{m \times 1}$ and predict $Y_{n \times 1} = B_{n \times p} \beta_{p \times 1} + \tau_{n \times 1}$
 - $\varepsilon \sim N_m(0, I_m)$ is independent of $\tau \sim N_n(0, I_n)$

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• Given a prior π on β , the Bayes procedure $p_{\pi}^{L}(y \mid x)$ is

$$p_{\pi}^{L}(y \mid x) = \frac{\int p(x \mid A\beta)p(y \mid B\beta)\pi(\beta)d\beta}{\int p(x \mid A\beta)\pi(\beta)d\beta}$$

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► The Bayes procedure p^L_U(y | x) under the uniform prior π_U ≡ 1 is minimax with constant risk

The Key Marginal Representation

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The Key Marginal Representation

For any prior π ,

$$p_{\pi}^{L}(y \mid x) = \frac{m_{\pi}(\hat{\beta}_{x,y}, (C'C)^{-1})}{m_{\pi}(\hat{\beta}_{x}, (A'A)^{-1})} p_{U}^{L}(y \mid x)$$

where $C_{(m+n) \times p} = (A', B')'$ and

$$\hat{\beta}_{x} = (A'A)^{-1}A'x \sim N_{p}(\beta, (A'A)^{-1})$$
$$\hat{\beta}_{x,y} = (C'C)^{-1}C'(x', y')' \sim N_{p}(\beta, (C'C)^{-1})$$

► Here the difference between the KL risks of p^L_U(y | x) and p^L_π(y | x) can be expressed as

$$R_{KL}(\beta, p_U^L) - R_{KL}(\beta, p_{\pi}^L) = E_{\beta, (C'C)^{-1}} \log m_{\pi}(\hat{\beta}_{x,y}; (C'C)^{-1}) - E_{\beta, (A'A)^{-1}} \log m_{\pi}(\hat{\beta}_x; (A'A)^{-1})$$

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• Minimaxity of $p_{\pi}^{L}(y \mid x)$ is here obtained when

$$rac{\partial}{\partial \omega} E_{\mu,V_\omega} \log m_\pi(Z;V_\omega) < 0$$

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This leads to weighted superharmonic conditions on m_π and π for minimaxity.

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Thank you!