







The Threshold Selection Problem

Given

• data
$$X_i \sim N(\mu_i, 1), \quad i = 1, ..., n$$

• some threshold rule, e.g.

$$\hat{\theta}_i = \begin{cases} X_i & |X_i| \ge t\\ 0 & |X_i| < t \end{cases}$$

How to "reliably" choose $\hat{t} = \hat{t}(X_1, \ldots, X_n)$?

- case study using Growing Gaussian Models
- well studied, but complicated by **phase changes** (v. sparse \rightarrow sparse \rightarrow dense signals μ)
- no 'best' solution;
- An apparently *ad hoc* Empirical Bayes compromise

Agenda

- Transform shrinkage & block structure
 - why data-dependent thresholds matter
- Reduction to Single Sequence (Growing Gaussian) model
- An *ad hoc* mixture model
 - posterior median thresholding
 - Empirical Bayes threshold choice
 - comparison with other methods (SURE, FDR)
- Adapting to phase changes in the GG model
- Adapting to phase changes in wavelet shrinkage

An "Easy" Example



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Transform Shrinkage Approach



Processing step:

• Operations on groups (blocks) $d_j = (d_{jk} : k = 1, ..., n_j)$

•
$$\eta: d_j \to \hat{d}_j$$

Features of block processing:

- creates more homogeneous subgroups
- ignores cross block dependence

Block structure in many transform problems

Direct data: y = f + z

- 1-d signals:
 - might choose subblocks within levels
 - blocking of Fourier coefficients
- Images:
 - wavelet bases: resolution level \times channel
 - ridgelet bases (or frames), brushlets, curvelets ...

Indirect data: y = Kf + z

- *K* (linear) operator: integration, Radon transform, convolution/blurring....
- If ∃ near diagonalization in some transform domain

$$y_{Jk} = \alpha_J \theta_{Jk} + z_{Jk}, \qquad k \in B_J, J \in \mathcal{J}$$

Indirect data Examples

- Fourier transform (deconvolution)
- Singular value decomposition (SVD)
- Wavelet-vaguelette decomposition (WVD): $\{v_{Jk}\}, \{w_{Jk}\}$ such that

$$Kv_{Jk} = \alpha_J w_{Jk}$$

- Certain wavelet packet bases: e.g. mirror wavelets for deconvolution
 - Mallat CNES example

'Truth' and Blurred Data



Wiener filter vs. Mirror Wavelets



SNR = 32.7db

SNR = 34.1db

Choice of basis/transform

- Try to choose transform domain so that
 - a) signal coefficients are sparse,
 - b) noise is relatively white *within blocks*
- "sparse": energy is concentrated in a few components

Examples:

Smooth signals: Oscillatory signals: Point singularities: Line singularities: Fourier basis, energy in low frequencies wavelet or cosine packet bases wavelet bases ridgelet, curvelet bases

Henceforth, we assume this has been done ...

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Why threshold choice matters, I

Portion of Ion Channel Signal



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$\sqrt{2\log n}$ thresholds: 8.9 % errors



FDR, q = 0.05 thresholds: 6.7% errors



E-Bayes thresholds: 2.9% errors



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Single sequence problem

Single block (e.g. level in wavelet transform)

$$X_i = \mu_i + z_i, \qquad z_i \stackrel{ind}{\sim} N(0, 1) \quad i = 1, 2, \dots, n$$

 μ is **fixed** & unknown, z is random. ("many normal means problem")

- e.g. for wavelet blocks, $n = 2^j$, but not necessarily
- Want to adapt well to sparsity in the sequence μ , while also dealing well with 'dense' cases.
- a "growing Gaussian" model, since n = # variables \nearrow

Why threshold choice matters, II

 $\mu_i \sim U(-5,5)$ with probability .0005, .002, .01, .05, .2, 1









Optimal thresholds vary with sparsity:



Coordinatewise Non-linearity

$$\hat{\mu}_i(x) = \eta(x_i, \hat{t})$$

Extreme Examples:

Hard: Soft: $\eta(x_i, t) = x_i I\{|x_i| > t\}$ $\eta(x_i, t) = \operatorname{sign}(x)(|x_i| - t)_+$



For example: • $\eta(x,t) = (1 - \frac{t^2}{x^2})_+ x$ (Breiman's n.n. garrote) • posterior *median* (later)

Two (somewhat) uncoupled issues

- choice of *non-linearity*: problem dependent, e.g.
 - hard thresh: preserves peak heights, good L_2 error
 - soft thresh: smoother visual appearance
 - intermediate choices
- choice of *threshold value* Dichotomy:
 - subjective/previous experience (e.g. 3σ 5σ)
 - vs. *automatic*

Focus here on threshold choice

Goals for a Thresholding Method

- data adaptive (to sparse **and** dense sequences)
- stable
- computable, with software
- good performance
 - on simulations
 - on data
 - in theory

E-Bayes on sparse mixtures is one solution: near minimax across several goals: {theory, simulation, data, software }

This talk: how and why E-Bayes works theoretical basis for adaptivity and robustness claims

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Ad Hoc Mixture Model

Prior:
$$\mu_i \overset{i.i.d.}{\sim} f(\mu) = (1 - \mathbf{w})\delta_0(\mu) + \mathbf{w}\gamma(\mu)$$

i.e.

$$X_i \sim \begin{cases} \phi(x) & \text{w. prob} \quad 1 - \mathbf{w} \\ g(x) = \int \phi(x - \mu) \gamma(\mu) d\mu & \text{w. prob} \quad \mathbf{w} \end{cases}$$

Given w, posteriors for μ_i are **independent**

 \Rightarrow Bayes estimates for ℓ_q loss:

$$\hat{\mu}_i(x) = \hat{\mu}(x_i; w) = \operatorname{argmin}_a E[|\mu_i - a|^q | x_i]$$

Posterior mean/median/mode for $q = 2/\mathbf{q} = \mathbf{1}/q = 0$

Posterior median does thresholding



Posterior median does thresholding



 \Rightarrow posterior median has:

- threshold zone: $\hat{\mu}(x; w) = 0 \Leftrightarrow |x| \le t(w)$
- shrinkage: $|\hat{\mu}(x;w)| \leq x$

Two Specific Examples



Key properties

Typical priors:
$$\gamma(\mu) = \frac{1}{2}ae^{-a|\mu|}$$
 [Laplace]
 $\sim \begin{cases} N(0, \theta^{-1} - 1) \\ \theta \sim Beta(\frac{1}{2}, 1) \end{cases}$ [Quasi-Cauchy]

Consequences:

- Small $w \Leftrightarrow \text{Large threshold } t(w)$
- Bounded shrinkage property: $\exists b \text{ s.t. for all } x, w$ $|x - \hat{\mu}(x; w)| \leq t(w) + b$



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Estimation of *w***: Marginal Max. Likelihood**

Log-likelihood: $\ell(w) = \sum_{i=1}^{n} \log\{(1-w)\phi(X_i) + wg(X_i)\}$

Score function:

$$S(w) = \ell'(w) = \sum_{i} \frac{g(X_i) - \phi(X_i)}{\phi(X_i) + w[g(X_i) - \phi(X_i)]}$$
$$= \sum_{i} \frac{\beta(X_i)}{1 + w\beta(X_i)},$$

where the mixture ratio

$$\beta(x) = \frac{g(x)}{\phi(x)} - 1. \qquad (g = \gamma \star \phi)$$

S(w) is monotone \searrow , so estimate w from $S(\hat{w}) = 0$. \rightarrow "E-Bayes" estimate: $\hat{t} = t(\hat{w})$.

Why MML might fail: Heavy tails of $\beta(\boldsymbol{x})$



Infinite Variance! Var $S(0) = \infty$, since Var $\beta(X) = \infty$

Why MML might fail: Heavy tails of $\beta(\boldsymbol{x})$



Why MML works: Heavy tails of $\beta(\boldsymbol{x})$

$$S(\hat{w}) = \sum_{i} \beta(x_i, \hat{w}) = 0$$

Note: at \hat{w} , bimodality of $\beta(x_i, \hat{w})$:

$$\beta(x, \hat{w}) = \frac{\beta(x)}{1 + w\beta(x)}$$
$$\approx \begin{cases} 1/w & \beta(x) \text{ large} \\ \beta(x) & \beta(x) \text{ small} \end{cases}$$

For simulation examples:





Why MML works: Heavy tails of $\beta(\boldsymbol{x})$

Hence

- Unique MMLE $S(\hat{w}) = 0$,
- easy to compute,

• extreme bimodality of
$$\beta(x_i, \hat{w}) = \frac{\beta(x_i)}{1 + \hat{w}\beta(x_i)}$$

So heavy tails of β (and monotonicity)

$$\Rightarrow$$
 stability & low variance of \hat{w} .
Likelihood vs Risk Minima

- Compare locations of likelihood and loss minima
- *q*-minima are often close; E-Bayes quite close
- Percent increase from minimum at E-Bayes solution often small



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Stein's Unbiased Risk Estimate (SURE)

• Choose t to minimize – for **soft** thresholding –

$$\hat{U}(t) = n + \sum_{1}^{n} x_k^2 \wedge t^2 - 2\sum_{1}^{n} I\{x_k^2 \le t^2\}$$
$$\hat{t}_{SURE} = \underset{0 \le t \le \sqrt{2\log n}}{\operatorname{argmin}} \hat{U}(t)$$

- some good theory, but unstable and
- doesn't handle sparse cases well
- instability is inherent to SURE on thresholds
 - similar plots for SURE for *posterior medians*

Unbiased risk vs Score criteria



False Discovery Rate (FDR)

- decreasing magnitudes $|x|_{(1)} \ge |x|_{(2)} \ge \ldots \ge |x|_{(n)}$
- quantile boundary $t_k = \sigma z(\frac{q}{2} \cdot \frac{k}{n})$
- FDR parameter $q \in (0, 1/2]$
- crossing index $\hat{k}_F = \max\{k : |x|_k \ge t_k\}$



N.B.: doesn't handle **dense** signals well (for q small):

E-Bayes thresholds: 2.9% errors



FDR chooses large t in dense cases



- $\sqrt{2\log n}$ too big at coarse j
- SURE too low at fine j
- FDR(.05) still too big at coarse *j*
- EBayes: good transition across scales

Where we're headed (i)

Claim: Sparse-mixture E-Bayes thresholding is near-optimal over several goals

{ **theory**, simulation, data, software }

Last three: see IMJ & B.W. Silverman, AOS, 2004 in press,

- "Needles and Straw in Haystacks: Empirical Bayes Estimates of Possibly Sparse Sequences",
- "Empirical Bayes selection of wavelet thresholds",
- and **numerous references to other work** therein!

and available software, at

• www.stats.ox.ac.uk/~silverma/

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Where we're headed (ii)

• Presence of **phase changes**

v.sparse \rightarrow *sparse* \rightarrow *dense*

challenges good threshold selection in sequence model.

- not all a priori reasonable methods are in fact satisfactory in adapting over the range of phases
- Some methods (E-Bayes, penalized least squares ...) can be shown to do so
- (adaptation to) phase changes in function estimation

Regular \rightarrow Critical \rightarrow Logarithmic

flows from phase changes in (growing) Gaussian sequence models

Theory for adaptive thresholds

Goals:

- flexible adaptation small risk for small $\|\mu\|_p$
- robustness

bounded risk for all μ

• variety of losses $\ell_q, 0 < q < 2$

A priori – not clear for MML:

- **know** that prior is wrong: μ is arbitary
- how does $\mathcal{L}(t(\hat{w}))$ depend on μ ?



Region

Non-zero signal

Typical near-mmx estimator

Minimax risk for ℓ_p balls

- a family of benchmarks, using
 - $\ell_p(C) = \{\mu : \sum_{i=1}^n |\mu_i|^p \le C^p\}$
 - p enforces sparsity (when < 2)
 - C measures size (and, indirectly, sparsity)

• using
$$\ell_q \text{ loss } (0 < q \le 2)$$

 $R_{p,q}^{SS}(C,n) := \inf_{\hat{\mu}} \sup_{\mu \in \ell_p(C)} E \sum_{1}^{n} |\hat{\mu}_i - \mu_i|^q$

- increases from 0 to $nE|Z|^q$ with C from 0 to ∞
- want $\hat{\mu}$ to adapt to unknown p, C (for all q)
- an essential feature: **'phase changes'**:

v.sparse
$$\rightarrow$$
 sparse \rightarrow *dense*



estimator





Bounds for estimated threshold \hat{t} :

Response to sparsity: $\|\mu\|_p$ **small** $\Rightarrow \hat{t}$ 'large' With high probability, uniformly over $n^{-1} \sum |\mu_i|^p \leq \eta^p$,

$$\hat{t}^2 > \begin{cases} 2\log\eta^{-p} + (p-1)\log\log\eta^{-p} & \text{if } \eta^p \ge \frac{\log^2 n}{n} \\ 2\log n & -(5-p)\log\log n & \text{if } \eta^p < \frac{\log^2 n}{n} \end{cases}$$

Response to 'density': $\|\mu\|_0$ **large** $\Rightarrow \hat{t}$ 'small'

Density exceeds π on $D_{\tau}(\pi) = \{\mu : n^{-1} \#\{i : |\mu_i| \ge \tau\} \ge \pi\}$ With high probability, uniformly over $\mu \in D_{\tau}(\pi)$

 $\hat{t} \le t(\tau, \pi)$

where $t(\tau, \pi) \searrow$ as $\pi \nearrow$.

[Actually true for "pseudo-threshold" $\xi = \beta^{-1}(1/w)$]

Main Adaptivity result for E-Bayes(A)

For $n \ge n_0$ and all $0 < p, q \le 2$ and all C > 0,

$$\sup_{\mu \in \ell_p(C)} E \|\hat{\mu}_{EB} - \mu\|_q^q \le c \left[R_{p,q}^{SS}(C,n) + n^{-A} (\log n)^{(q-1)/2} \right]$$

[if A = 0, same result with error $(\log n)^{2+(q-p)/2}$]

Applies to **any** estimator $\hat{\mu}_i(x, \hat{w}) = \eta(x_i, t(\hat{w}))$ if

- $\eta(x,t)$ is bounded threshold shrinkage rule
- \hat{w} is chosen by Empirical Bayes

E-Bayes(A) To ensure v. small mean ℓ_q error when μ small, need thresholds $> \sqrt{2 \log n}$. Theory suggests an **ad hoc** fix: let A > 0, and

$$\hat{t}_A = \begin{cases} \hat{t} & \text{if } \hat{t}^2 \leq 2\log n - 5\log\log n \\ \sqrt{2(1+A)\log n} & o/w \end{cases}$$



Contrast with some existing results



[Birgé - Massart (2001): adaptivity for ℓ_2 loss; non-asymptotic bounds; *via* complexity penalized least squares; C-H Zhang: nonparametric E-Bayes]

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Function Estimation

Back to $y_i = f(i/n) + \sigma \epsilon_i$ (non-parametric reg'n) $Y_t = \int_0^t f(s) ds + N^{-1/2} W_t$ (Gaussian White Noise) $y_{jk} = \theta_{jk} + N^{-1/2} z_{jk}$ (wavelet coefficients)

Goal: apply results for single sequence model to each (wavelet) level

Issue: consequences of phase changes?

or

or

Phase Change in Rates: (q > p)



 σ , loss derivatives

Assumptions

Smoothness: $\alpha \leftrightarrow \#$ derivatives for f $(\alpha > 1/2 - 1/p)$ $p \leftrightarrow \text{ index of average smoothness}, p \leq \infty$

$$\theta \in B^{\alpha}_{p,\infty}(C):$$
 $\sum_{k=1}^{2^{j}} |\theta_{jk}|^{p} \le C^{p} 2^{-ap}, \quad \forall j, \quad a = \alpha + 1/2 - 1/p$

Error Measures: $\sigma \leftrightarrow \#$ derivatives estimated, $0 \le \sigma < \alpha - (1/p - 1/q)$ $q \leftrightarrow$ index of average error, $q \le 2$

$$E\|\hat{\theta} - \theta\|_{B^{\sigma}_{q,q}}^{q} = \sum_{j} 2^{sqj} E\|\hat{\theta}_{j} - \theta_{j}\|_{q}^{q}, \qquad s = \sigma + 1/2 - 1/q$$

 \sim estimation of θ^{th} derivative in L_q :

$$a_0 \|\theta\|_{B^{\sigma}_{q,2}}^q \le \int |f^{(\sigma)}|^q \le a_1 \|\theta\|_{B^{\sigma}_{q,q}}^q$$

Phase Change in Rates

Assume
$$a > 0, \sigma \ge 0, \alpha > \sigma + (1/p - 1/q)_{+}$$

Rates:

$$\mathbf{r} = \frac{\alpha - \sigma}{2\alpha + 1}, \qquad \mathbf{r'} = \frac{a - s}{2a}$$

Minimax risk (DJKP, 95):

Phase Change in Rates: (q > p)



 σ , loss derivatives

. – p.62

$$[a = \alpha + 1/2 - 1/p; \qquad s = \sigma + 1/2 - 1/q]$$

Levelwise (Empirical Bayes) Thresholding

or

For $y_i =$

empirical wavelet coefficients of data (at j^{th} level)

data in dyadic form of Gaussian white noise model $y_{jk} = \theta_{jk} + N^{-1/2} z_{jk}$ $j \ge 0, k = 1, \dots, 2^j$.

use

variance-1 single sequence E-Bayes(A); with w estimated separately at each level j:

$$\hat{\theta}_j^{EB} = N^{-1/2} \hat{\mu}_{EB} (N^{1/2} y_j; \hat{w}_j)$$

 $[\text{If } j \ge \log_2 N \text{, set } \hat{\theta}_j^{EB} = 0.]$

Main Adaptivity Result for E-Bayes(A)

If $0 < p, q \leq 2, sq \leq A$, then for any $\Theta(C)$ in $\mathcal{R} \cup \mathcal{L} \cup \mathcal{C}$



 $r'' = \alpha - \sigma - (1/p - 1/q)_+ \ge \min(r, r'); \ 0 \le \nu \le 4.$

i.e. E-Bayes(A) attains optimal rate for full range of **smoothness** α and **losses** σ .



Reduction to Single Sequence Model

- Convert to noise level 1: $x_{jk} = N^{1/2}y_{jk}$ has mean $\mu_{jk} = N^{1/2}\theta_{jk}$, variance 1.
- ℓ_p balls reduction:

$$\theta \in B^{\alpha}_{p,\infty}(C) \quad \Leftrightarrow \qquad \|\theta_{\mathbf{j}}\|_{p} \leq C2^{-a\mathbf{j}} \quad \forall \mathbf{j}$$

$$\Leftrightarrow \quad 2^{-\mathbf{j}/p} \|\mu\|_{p} \leq \underbrace{CN^{1/2}2^{-(a+1/p)\mathbf{j}}}_{\eta_{\mathbf{j}}}$$

- As $\mathbf{j} \nearrow$, $\eta_{\mathbf{j}}$ crosses **dense**, sparse, v. sparse regions
- Singe sequence result (for all regions) \Rightarrow

$$\sup_{\|\boldsymbol{\theta}_{\mathbf{j}}\| \leq C2^{-a\mathbf{j}}} E\|\boldsymbol{\theta}_{\mathbf{j}}^{EB} - \boldsymbol{\theta}_{\mathbf{j}}\|_{q}^{q} \leq c \left[R_{p,q}^{SS}(CN^{1/2}2^{-a\mathbf{j}}, 2^{\mathbf{j}}) + \cdots\right]$$



$$\eta_j = CN^{1/2} 2^{-(a+1/p)j} > 1$$









- ℓ_p ball risk results for FDR, SURE each have limited range
- FDR (fine scales) combined with SURE (coarse scales) works for *R* (but not for *L*?)

Where we're been

• Presence of **phase changes**

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challenges good threshold selection in sequence model.

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- Some methods (E-Bayes, penalized least squares ...) can be shown to do so
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Take-away message

Minimax analysis, ℓ_p norms, function spaces, rates of convergence etc.,

deepen understanding of a key methodological problem,
by yielding

- emergent phenomena *(phase changes)*
- a searching discipline of anaylsis *(adaptation)*
- aligned with practical considerations (stability, reconstruction)

and, not least, available software, at

• www.stats.ox.ac.uk/~silverma/

Three Talks

1. Function Estimation & Classical Normal Theory

• $X_n \sim N_{p(n)}(\theta_n, I)$ $p(n) \nearrow$ with n (MVN)

- 2. The Threshold Selection Problem
 - In (MVN) with, say, $\hat{\theta}_i = X_i I\{|X_i| > \hat{t}\}$
 - How to select $\hat{t} = \hat{t}(X)$ "reliably"?

3. Large Covariance Matrices

- $X_n \sim N_{p(n)}(I \otimes \Sigma_{p(n)})$; especially $X_n = \begin{vmatrix} Y_n \\ Z_n \end{vmatrix}$
- spectral properties of $n^{-1}X_nX_n^T$
- PCA, CCA, MANOVA

FDR chooses large t in dense cases

- k = 500 of n = 1000 have $\mu_i = 3$, else 0 (10 reps).
- FDR at q = .01, .05, .1 chooses larger thresholds, with worse MSE, than E-Bayes at a = .2, .5, 1

