Wavelet Methods for Time Series Analysis

Part III: Wavelet-Based Signal Extraction and Denoising

- overview of key ideas behind wavelet-based approach
- description of four basic models for signal estimation
- discussion of why wavelets can help estimate certain signals
- simple thresholding & shrinkage schemes for signal estimation
- wavelet-based thresholding and shrinkage
- discuss some extensions to basic approach

Wavelet-Based Signal Estimation: I

- DWT analysis of $\mathbf{X}$ yields $\mathbf{W} = \mathcal{W}\mathbf{X}$
- DWT synthesis $\mathbf{X} = \mathcal{W}^T\mathbf{W}$ yields multiresolution analysis by splitting $\mathcal{W}^T\mathbf{W}$ into pieces associated with different scales
- DWT synthesis can also estimate 'signal' hidden in $\mathbf{X}$ if we can modify $\mathbf{W}$ to get rid of noise in the wavelet domain
- if $\mathbf{W}'$ is a 'noise reduced' version of $\mathbf{W}$, can form signal estimate via $\mathcal{W}^T\mathbf{W}'$

Wavelet-Based Signal Estimation: II

- key ideas behind simple wavelet-based signal estimation
  - certain signals can be efficiently described by the DWT using
    - all of the scaling coefficients
    - a small number of 'large' wavelet coefficients
  - noise is manifested in a large number of 'small' wavelet coefficients
  - can either 'threshold' or 'shrink' wavelet coefficients to eliminate noise in the wavelet domain
- key ideas led to wavelet thresholding and shrinkage proposed by Donoho, Johnstone and coworkers in 1990s

Models for Signal Estimation: I

- will consider two types of signals:
  1. $\mathbf{D}$, an N dimensional deterministic signal
  2. $\mathbf{C}$, an N dimensional stochastic signal; i.e., a vector of random variables (RVs) with covariance matrix $\Sigma_{\mathbf{C}}$
- will consider two types of noise:
  1. $\boldsymbol{\epsilon}$, an N dimensional vector of independent and identically distributed (IID) RVs with mean 0 and covariance matrix $\Sigma_{\boldsymbol{\epsilon}} = \sigma_\epsilon^2 I_N$
  2. $\boldsymbol{\eta}$, an N dimensional vector of non-IID RVs with mean 0 and covariance matrix $\Sigma_{\boldsymbol{\eta}}$
     - one form: RVs independent, but have different variances
     - another form of non-IID: RVs are correlated

Models for Signal Estimation: II

- leads to four basic 'signal + noise' models for $\mathbf{X}$
  1. $\mathbf{X} = \mathbf{D} + \boldsymbol{\epsilon}$
  2. $\mathbf{X} = \mathbf{D} + \boldsymbol{\eta}$
  3. $\mathbf{X} = \mathbf{C} + \boldsymbol{\epsilon}$
  4. $\mathbf{X} = \mathbf{C} + \boldsymbol{\eta}$
- in the latter two cases, the stochastic signal $\mathbf{C}$ is assumed to be independent of the associated noise

Signal Representation via Wavelets: I

- consider deterministic signals $\mathbf{D}$ first
- signal estimation problem is simplified if we can assume that the important part of $\mathbf{D}$ is in its large values
- assumption is not usually viable in the original (i.e., time domain) representation $\mathbf{D}$, but might be true in another domain
- an orthonormal transform $\mathcal{O}$ might be useful because
  - $\mathbf{O} = \mathcal{O}\mathbf{D}$ is equivalent to $\mathbf{D}$ (since $\mathbf{D} = \mathcal{O}^T\mathbf{O}$)
  - we might be able to find $\mathcal{O}$ such that the signal is isolated in $M \ll N$ large transform coefficients
- Q: how can we judge whether a particular $\mathcal{O}$ might be useful for representing $\mathbf{D}$?

Signal Representation via Wavelets: II

- let O_j be the jth transform coefficient in $\mathbf{O} = \mathcal{O}\mathbf{D}$
- let $O_{(0)}, O_{(1)}, \ldots, O_{(N-1)}$ be the O_j's reordered by magnitude:

$$|O_{(0)}| \geq |O_{(1)}| \geq \cdots \geq |O_{(N-1)}|$$

- example: if $\mathbf{O} = [-3, 1, 4, -7, 2, -1]^T$, then $O_{(0)} = O_3 = -7$, $O_{(1)} = O_2 = 4$, $O_{(2)} = O_0 = -3$ etc.
- define a normalized partial energy sequence (NPES):

$$C_{M-1} \equiv \frac{\sum_{j=0}^{M-1} |O_{(j)}|^2}{\sum_{j=0}^{N-1} |O_{(j)}|^2} = \frac{\text{energy in largest } M \text{ terms}}{\text{total energy in signal}}$$

- let $\mathcal{I}_M$ be $N \times N$ diagonal matrix whose jth diagonal term is 1 if $|O_j|$ is one of the M largest magnitudes and is 0 otherwise

Signal Representation via Wavelets: III

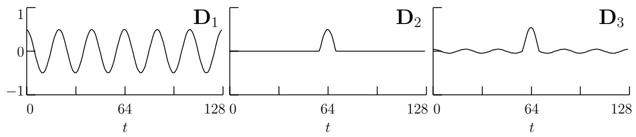
- form $\widehat{\mathbf{D}}_M \equiv \mathcal{O}^T\mathcal{I}_M\mathbf{O}$, which is an approximation to $\mathbf{D}$
- when $\mathbf{O} = [-3, 1, 4, -7, 2, -1]^T$ and $M = 3$, we have

$$\mathcal{I}_3 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \text{ and thus } \widehat{\mathbf{D}}_M = \mathcal{O}^T \begin{bmatrix} -3 \\ 0 \\ 4 \\ -7 \\ 0 \\ 0 \end{bmatrix}$$

- one interpretation for NPES:

$$C_{M-1} = 1 - \frac{\|\mathbf{D} - \widehat{\mathbf{D}}_M\|^2}{\|\mathbf{D}\|^2} = 1 - \text{relative approximation error}$$

Signal Representation via Wavelets: IV



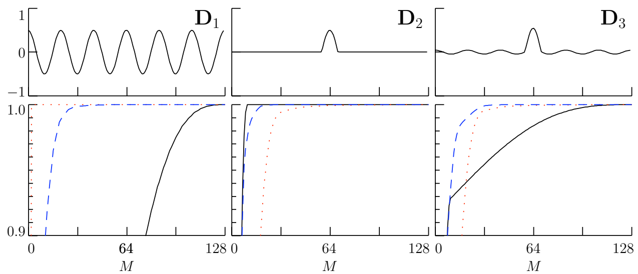
- consider three signals plotted above
- $\mathbf{D}_1$ is a sinusoid, which can be represented succinctly by the discrete Fourier transform (DFT)
- $\mathbf{D}_2$ is a bump (only a few nonzero values in the time domain)
- $\mathbf{D}_3$ is a linear combination of $\mathbf{D}_1$ and $\mathbf{D}_2$

Signal Representation via Wavelets: V

- consider three different orthonormal transforms
  - identity transform I (time)
  - the orthonormal DFT $\mathcal{F}$ (frequency), where $\mathcal{F}$ has (k,t)th element $\exp(-i2\pi tk/N)/\sqrt{N}$ for $0 \le k,t \le N-1$
  - the LA(8) DWT $\mathcal{W}$ (wavelet)
- # of terms M needed to achieve relative error $< 1\%$:

	$\mathbf{D}_1$	$\mathbf{D}_2$	$\mathbf{D}_3$
DFT	2	29	28
identity	105	9	75
LA(8) wavelet	22	14	21

Signal Representation via Wavelets: VI

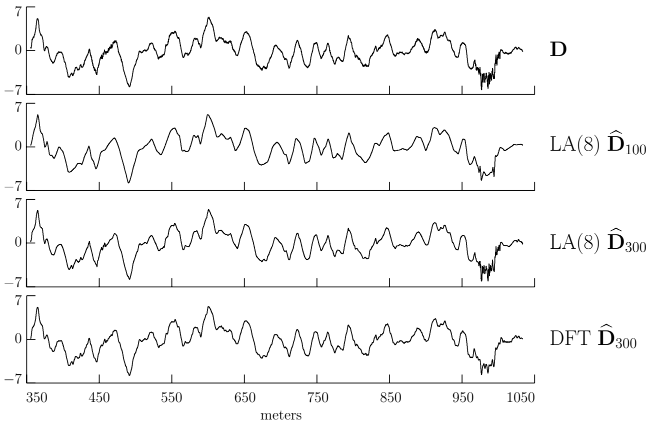


- use NPESs to see how well these three signals are represented in the time, frequency (DFT) and wavelet (LA(8)) domains
- time (solid curves), frequency (dotted) and wavelet (dashed)

Signal Representation via Wavelets: VII

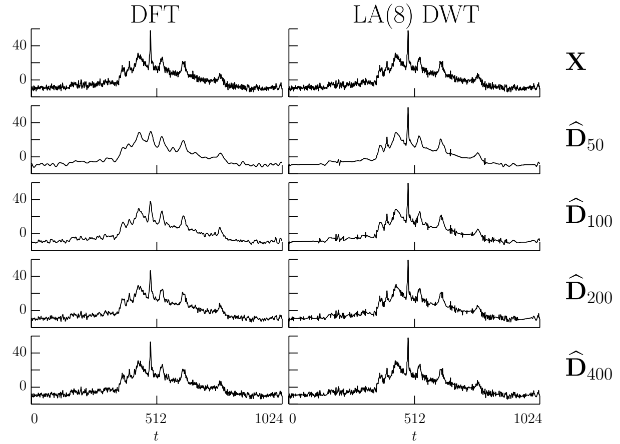
- example: vertical ocean shear time series
  - has 'frequency-domain' fluctuations
  - also has 'time-domain' turbulent activity
- next overhead shows
  - the signal $\mathbf{D}$ itself
  - its approximation $\widehat{\mathbf{D}}_{100}$ from 100 LA(8) DWT coefficients
  - $\widehat{\mathbf{D}}_{300}$ from 300 LA(8) DWT coefficients, giving $C_{299} \doteq 0.9983$
  - $\widehat{\mathbf{D}}_{300}$ from 300 DFT coefficients, giving $C_{299} \doteq 0.9973$
- note that 300 coefficients is less than 5% of $N = 6784$!

Signal Representation via Wavelets: VIII



- need 123 additional ODFT coefficients to match C_{299} for DWT

Signal Representation via Wavelets: IX



- 2nd example: DFT $\widehat{\mathbf{D}}_M$ (left-hand column) & $J_0 = 6$ LA(8) DWT $\widehat{\mathbf{D}}_M$ (right) for NMR series $\mathbf{X}$ (A. Maudsley, UCSF)

Signal Estimation via Thresholding: I

- assume model of deterministic signal plus IID noise: $\mathbf{X} = \mathbf{D} + \boldsymbol{\epsilon}$
- let $\mathcal{O}$ be an $N \times N$ orthonormal matrix
- form $\mathbf{O} = \mathcal{O}\mathbf{X} = \mathcal{O}\mathbf{D} + \mathcal{O}\boldsymbol{\epsilon} \equiv \mathbf{d} + \mathbf{e}$
- component-wise, have $O_l = d_l + e_l$
- define signal to noise ratio (SNR):

$$\frac{\|\mathbf{D}\|^2}{E\{\|\boldsymbol{\epsilon}\|^2\}} = \frac{\|\mathbf{d}\|^2}{E\{\|\mathbf{e}\|^2\}} = \frac{\sum_{l=0}^{N-1} d_l^2}{\sum_{l=0}^{N-1} E\{e_l^2\}}$$

- assume that SNR is large
- assume that $\mathbf{d}$ has just a few large coefficients; i.e., large signal coefficients dominate $\mathbf{O}$

Signal Estimation via Thresholding: II

- recall simple estimator $\widehat{\mathbf{D}}_M \equiv \mathcal{O}^T \mathcal{I}_M \mathbf{O}$ and previous example:

$$\widehat{\mathbf{D}}_M = \mathcal{O}^T \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} O_0 \\ O_1 \\ O_2 \\ O_3 \\ O_4 \\ O_5 \end{bmatrix} = \mathcal{O}^T \begin{bmatrix} O_0 \\ 0 \\ O_2 \\ O_3 \\ 0 \\ 0 \end{bmatrix}$$

- let $\mathcal{J}_m$ be a set of m indices corresponding to places where jth diagonal element of $\mathcal{I}_m$ is 1
- in example above, we have $\mathcal{J}_3 = \{0, 2, 3\}$
- strategy in forming $\widehat{\mathbf{D}}_M$ is to keep a coefficient O_j if $j \in \mathcal{J}_m$ but to replace it with 0 if $j \notin \mathcal{J}_m$ ('kill' or 'keep' strategy)

Signal Estimation via Thresholding: III

- can pose a simple optimization problem whose solution
  1. is a 'kill or keep' strategy (and hence justifies this strategy)
  2. dictates that we use coefficients with the largest magnitudes
  3. tells us what M should be (once we set a certain parameter)
- optimization problem: find $\widehat{\mathbf{D}}_M$ such that
$$\gamma_m \equiv \|\mathbf{X} - \widehat{\mathbf{D}}_m\|^2 + m\delta^2$$
  is minimized over all possible $\mathcal{I}_m$, $m = 0, \ldots, N$
- in the above δ^2 is a fixed parameter (set *a priori*)

Signal Estimation via Thresholding: IV

- $\|\mathbf{X} - \widehat{\mathbf{D}}_m\|^2$ is a measure of 'fidelity'
  - rationale for this term: under our assumption of a high SNR, $\widehat{\mathbf{D}}_m$ shouldn't stray too far from $\mathbf{X}$
  - fidelity increases (the measure decreases) as m increases
  - in minimizing γ_m, consideration of this term alone suggests that m should be large
- $m\delta^2$ is a penalty for too many terms
  - rationale: heuristic says $\mathbf{d}$ has only a few large coefficients
  - penalty increases as m increases
  - in minimizing γ_m, consideration of this term alone suggests that m should be small
- optimization problem: balance off fidelity & parsimony

Signal Estimation via Thresholding: V

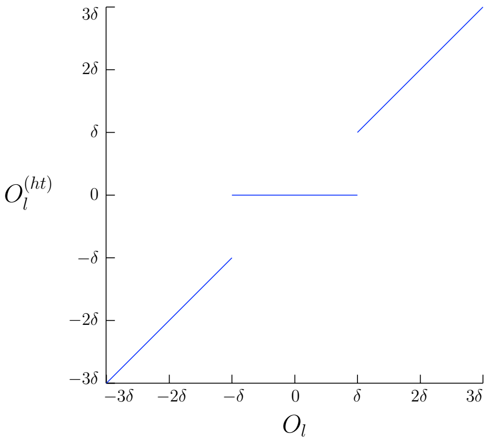
- claim: $\gamma_m = \|\mathbf{X} - \widehat{\mathbf{D}}_m\|^2 + m\delta^2$ is minimized when m is set to the number of coefficients O_j such that $O_j^2 > \delta^2$
- proof of claim: since $\mathbf{X} = \mathcal{O}^T\mathbf{O}$ & $\widehat{\mathbf{D}}_m \equiv \mathcal{O}^T\mathcal{I}_m\mathbf{O}$, have
$$\begin{aligned}\gamma_m = \|\mathbf{X} - \widehat{\mathbf{D}}_m\|^2 + m\delta^2 &= \|\mathcal{O}^T\mathbf{O} - \mathcal{O}^T\mathcal{I}_m\mathbf{O}\|^2 + m\delta^2\\ &= \|\mathcal{O}^T(I_N - \mathcal{I}_m)\mathbf{O}\|^2 + m\delta^2\\ &= \|(I_N - \mathcal{I}_m)\mathbf{O}\|^2 + m\delta^2\\ &= \sum_{j \notin \mathcal{J}_m} O_j^2 + \sum_{j \in \mathcal{J}_m} \delta^2\end{aligned}$$
- for any given j, if $j \notin \mathcal{J}_m$, we contribute O_j^2 to first sum; on the other hand, if $j \in \mathcal{J}_m$, we contribute δ^2 to second sum
- to minimize γ_m, we need to put j in $\mathcal{J}_m$ if $O_j^2 > \delta^2$, thus establishing the claim

Thresholding Functions: I

- more generally, thresholding schemes involve
  1. computing $\mathbf{O} \equiv \mathcal{O}\mathbf{X}$
  2. defining $\mathbf{O}^{(t)}$ as vector with lth element
$$O_l^{(t)} = \begin{cases} 0, & \text{if } |O_l| \le \delta;\\ \text{some nonzero value}, & \text{otherwise,}\end{cases}$$
     where nonzero values are yet to be defined
  3. estimating $\mathbf{D}$ via $\widehat{\mathbf{D}}^{(t)} \equiv \mathcal{O}^T\mathbf{O}^{(t)}$
- simplest scheme is 'hard thresholding' ('kill/keep' strategy):
$$O_l^{(ht)} = \begin{cases} 0, & \text{if } |O_l| \le \delta;\\ O_l, & \text{otherwise.}\end{cases}$$

Thresholding Functions: II

- plot shows mapping from O_l to $O_l^{(ht)}$



Thresholding Functions: III

- alternative scheme is 'soft thresholding:'

$$O_l^{(st)} = \text{sign}\,\{O_l\}\,(|O_l| - \delta)_+\,,$$

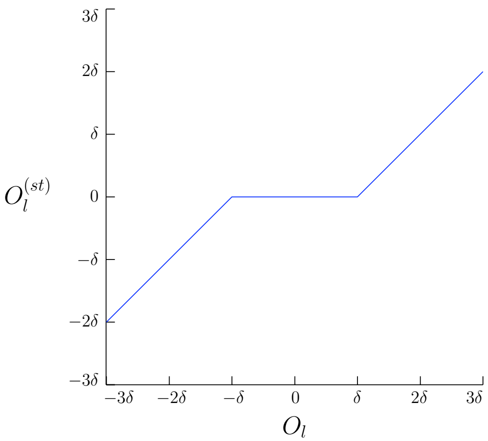
where

$$\text{sign}\,\{O_l\} \equiv \begin{cases} +1, & \text{if } O_l > 0; \\ 0, & \text{if } O_l = 0; \\ -1, & \text{if } O_l < 0. \end{cases} \quad \text{and} \quad (x)_+ \equiv \begin{cases} x, & \text{if } x \geq 0; \\ 0, & \text{if } x < 0. \end{cases}$$

- one rationale for soft thresholding is that it fits into Stein's class of estimators (will discuss later on)

Thresholding Functions: IV

- here is the mapping from O_l to $O_l^{(st)}$



Thresholding Functions: V

- third scheme is 'mid thresholding:'

$$O_l^{(mt)} = \text{sign}\,\{O_l\}\,(|O_l| - \delta)_{++}\,,$$

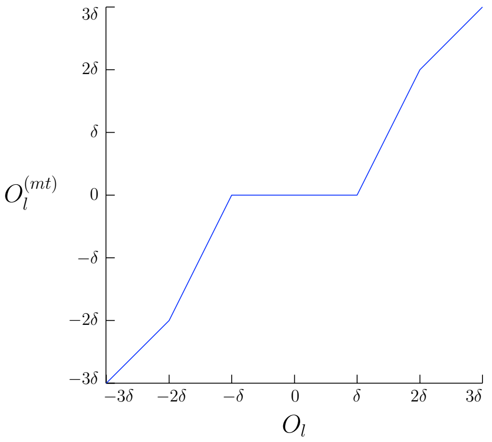
where

$$(|O_l| - \delta)_{++} \equiv \begin{cases} 2(|O_l| - \delta)_+, & \text{if } |O_l| < 2\delta; \\ |O_l|, & \text{otherwise} \end{cases}$$

- provides compromise between hard and soft thresholding

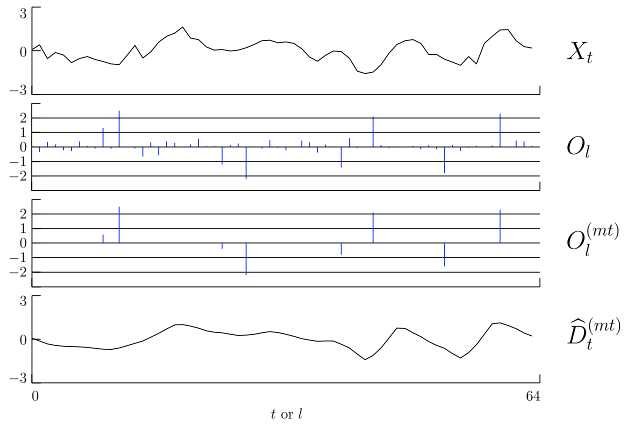
Thresholding Functions: VI

- here is the mapping from O_l to $O_l^{(mt)}$



Thresholding Functions: VII

- example of mid thresholding with $\delta = 1$



Universal Threshold: I

- Q: how do we go about setting δ?
- specialize to IID Gaussian noise $\boldsymbol{\epsilon}$ with covariance $\sigma_\epsilon^2 I_N$
- can argue $\mathbf{e} \equiv \mathcal{O}\boldsymbol{\epsilon}$ is also IID Gaussian with covariance $\sigma_\epsilon^2 I_N$
- Donoho & Johnstone (1995) proposed $\delta^{(u)} \equiv \sqrt{[2\sigma_\epsilon^2 \log(N)]}$ ('log' here is 'log base e')
- rationale for $\delta^{(u)}$: because of Gaussianity, can argue that

$$\mathbf{P}\left[\max_l\{|e_l|\} > \delta^{(u)}\right] \leq \frac{1}{\sqrt{[4\pi \log{(N)}]}} \to 0 \text{ as } N \to \infty$$

and hence $\mathbf{P}\left[\max_l\{|e_l|\} \leq \delta^{(u)}\right] \to 1$ as $N \to \infty$, so no noise will exceed threshold in the limit

Universal Threshold: II

- suppose $\mathbf{D}$ is a vector of zeros so that $O_l = e_l$
- implies that $\mathbf{O}^{(ht)} = 0$ with high probability as $N \to \infty$
- hence will estimate correct $\mathbf{D}$ with high probability
- critique of $\delta^{(u)}$:
  - consider lots of IID Gaussian series, $N = 128$: only 13% will have *any* values exceeding $\delta^{(u)}$
  - $\delta^{(u)}$ is slanted toward eliminating vast majority of noise, but, if we use, e.g., hard thresholding, any nonzero signal transform coefficient of a fixed magnitude will eventually get set to 0 as $N \to \infty$
- nonetheless: $\delta^{(u)}$ works remarkably well

Minimum Unbiased Risk: I

- second approach for setting δ is data-adaptive, but only works for selected thresholding functions
- assume model of deterministic signal plus non-IID noise: $\mathbf{X} = \mathbf{D} + \boldsymbol{\eta}$ so that $\mathbf{O} \equiv \mathcal{O}\mathbf{X} = \mathcal{O}\mathbf{D} + \mathcal{O}\boldsymbol{\eta} \equiv \mathbf{d} + \mathbf{n}$
- component-wise, have $O_l = d_l + n_l$
- further assume that n_l is an $\mathcal{N}(0, \sigma_{n_l}^2)$ RV, where $\sigma_{n_l}^2$ is assumed to be known, but we allow the possibility that n_l's are correlated
- let $O_l^{(\delta)}$ be estimator of d_l based on a (yet to be determined) threshold δ
- want to make $E\{(O_l^{(\delta)} - d_l)^2\}$ as small as possible

Minimum Unbiased Risk: II

- Stein (1981) considered estimators restricted to be of the form

$$O_l^{(\delta)} = O_l + A^{(\delta)}(O_l),$$

  where $A^{(\delta)}(\cdot)$ must be 'weakly differentiable' (basically, piecewise continuous plus a bit more)
- since $O_l = d_l + n_l$, above yields $O_l^{(\delta)} - d_l = n_l + A^{(\delta)}(O_l)$, so

$$E\{(O_l^{(\delta)} - d_l)^2\} = \sigma_{n_l}^2 + 2E\{n_l A^{(\delta)}(O_l)\} + E\{[A^{(\delta)}(O_l)]^2\}$$

- because of Gaussianity, can reduce middle term:

$$E\{n_l A^{(\delta)}(O_l)\} = \sigma_{n_l}^2 E\left\{ \frac{d}{dx} A^{(\delta)}(x)\bigg|_{x=O_l} \right\}$$

Minimum Unbiased Risk: III

- practical scheme: given realizations o_l of O_l, find δ minimizing estimate of

$$E\left\{ \sum_{l=0}^{N-1} (O_l^{(\delta)} - d_l)^2 \right\},$$

  which, in view of

$$E\{(O_l^{(\delta)} - d_l)^2\} = \sigma_{n_l}^2 + 2\sigma_{n_l}^2 E\left\{ \frac{d}{dx} A^{(\delta)}(x)\bigg|_{x=O_l} \right\} + E\{[A^{(\delta)}(O_l)]^2\},$$

  is

$$\sum_{l=0}^{N-1} \mathcal{R}(\sigma_{n_l}, o_l, \delta) \equiv \sum_{l=0}^{N-1} \sigma_{n_l}^2 + 2\sigma_{n_l}^2 \frac{d}{dx} A^{(\delta)}(o_l) + [A^{(\delta)}(o_l)]^2$$

- for a given δ, above is Stein's unbiased risk estimator (SURE)

Minimum Unbiased Risk: IV

- example: if we set

$$A^{(\delta)}(O_l) = \begin{cases} -O_l, & \text{if } |O_l| < \delta; \\ -\delta \operatorname{sign}\{O_l\}, & \text{if } |O_l| \geq \delta, \end{cases}$$

  we obtain $O_l^{(\delta)} = O_l + A^{(\delta)}(O_l) = O_l^{(st)}$, i.e., soft thresholding
- for this case, can argue that

$$\mathcal{R}(\sigma_{n_l}, O_l, \delta) = O_l^2 - \sigma_{n_l}^2 + (2\sigma_{n_l}^2 - O_l^2 + \delta^2) 1_{[\delta^2,\infty)}(O_l^2),$$

  where

$$1_{[\delta^2,\infty)}(x) \equiv \begin{cases} 1, & \text{if } \delta^2 \leq x < \infty; \\ 0, & \text{otherwise.} \end{cases}$$

- only the last term depends on δ, and, as a function of δ, SURE is minimized when last term is minimized

Minimum Unbiased Risk: V

- data-adaptive scheme is to replace O_l with its realization, say o_l, and to set δ equal to the value, say $\delta^{(S)}$, minimizing
$$\sum_{l=0}^{N-1}(2\sigma_{n_l}^2 - o_l^2 + \delta^2)1_{[\delta^2,\infty)}(o_l^2),$$
- must have $\delta^{(S)} = |o_l|$ for some l, so minimization is easy
- if n_l have a common variance, i.e., $\sigma_{n_l}^2 = \sigma_0^2$ for all l, need to find minimizer of the following function of δ:
$$\sum_{l=0}^{N-1}(2\sigma_0^2 - o_l^2 + \delta^2)1_{[\delta^2,\infty)}(o_l^2),$$
(in practice, σ_0^2 is usually unknown, so later on we will consider how to estimate this also)

Signal Estimation via Shrinkage

- so far, we have only considered signal estimation via thresholding rules, which will map some O_l to zeros
- will now consider shrinkage rules, which differ from thresholding only in that nonzero coefficients are mapped to nonzero values rather than exactly zero (but values can be *very* close to zero!)
- there are three approaches that lead us to shrinkage rules
  1. linear mean square estimation
  2. conditional mean and median
  3. Bayesian approach
- will only consider 1 and 2, but one form of Bayesian approach turns out to be identical to 2

Linear Mean Square Estimation: I

- assume model of stochastic signal plus non-IID noise: $\mathbf{X} = \mathbf{C} + \boldsymbol{\eta}$ so that $\mathbf{O} = \mathcal{O}\mathbf{X} = \mathcal{O}\mathbf{C} + \mathcal{O}\boldsymbol{\eta} \equiv \mathbf{R} + \mathbf{n}$
- component-wise, have $O_l = R_l + n_l$
- assume $\mathbf{C}$ and $\boldsymbol{\eta}$ are multivariate Gaussian with covariance matrices $\Sigma_{\mathbf{C}}$ and $\Sigma_{\boldsymbol{\eta}}$
- implies $\mathbf{R}$ and $\mathbf{n}$ are also Gaussian RVs, but now with covariance matrices $\mathcal{O}\Sigma_{\mathbf{C}}\mathcal{O}^T$ and $\mathcal{O}\Sigma_{\boldsymbol{\eta}}\mathcal{O}^T$
- assume that $E\{R_l\} = 0$ for any component of interest and that R_l & n_l are uncorrelated
- suppose we estimate R_l via a simple scaling of O_l:
$$\widehat{R}_l \equiv a_l O_l, \quad \text{where } a_l \text{ is a constant to be determined}$$

Linear Mean Square Estimation: II

- let us select a_l by making $E\{(R_l - \widehat{R}_l)^2\}$ as small as possible, which occurs when we set
$$a_l = \frac{E\{R_l O_l\}}{E\{O_l^2\}}$$
- because R_l and n_l are uncorrelated with 0 means and because $O_l = R_l + n_l$, we have
$$E\{R_l O_l\} = E\{R_l^2\} \text{ and } E\{O_l^2\} = E\{R_l^2\} + E\{n_l^2\},$$
yielding
$$\widehat{R}_l = \frac{E\{R_l^2\}}{E\{R_l^2\} + E\{n_l^2\}}O_l = \frac{\sigma_{R_l}^2}{\sigma_{R_l}^2 + \sigma_{n_l}^2}O_l$$
- note: ‘optimum’ a_l shrinks O_l toward zero, with shrinkage increasing as the noise variance increases

Background on Conditional PDFs: I

- let X and Y be RVs with probability density functions (PDFs) $f_X(\cdot)$ and $f_Y(\cdot)$
- let $f_{X,Y}(x,y)$ be their joint PDF at the point (x,y)
- $f_X(\cdot)$ and $f_Y(\cdot)$ are called marginal PDFs and can be obtained from the joint PDF via integration:

$$f_X(x) = \int_{-\infty}^{\infty} f_{X,Y}(x,y)\,dy$$

- the conditional PDF of Y given $X = x$ is defined as

$$f_{Y|X=x}(y) = \frac{f_{X,Y}(x,y)}{f_X(x)}$$

(read '|' as 'given' or 'conditional on')

Background on Conditional PDFs: II

- by definition RVs X and Y are said to be independent if

$$f_{X,Y}(x,y) = f_X(x)f_Y(y),$$

in which case

$$f_{Y|X=x}(y) = \frac{f_{X,Y}(x,y)}{f_X(x)} = \frac{f_X(x)f_Y(y)}{f_X(x)} = f_Y(y)$$

- thus X and Y are independent if knowing X doesn't allow us to alter our probabilistic description of Y
- $f_{Y|X=x}(\cdot)$ is a PDF, so its mean value is

$$E\{Y|X=x\} = \int_{-\infty}^{\infty} y f_{Y|X=x}(y)\,dy;$$

the above is called the conditional mean of Y, given X

Background on Conditional PDFs: III

- suppose RVs X and Y are related, but we can only observe X
- suppose we want to approximate the unobservable Y based on some function of the observable X
- example: we observe part of a time series containing a signal buried in noise, and we want to approximate the unobservable signal component based upon a function of what we observed
- suppose we want our approximation to be the function of X, say $U_2(X)$, such that the mean square difference between Y and $U_2(X)$ is as small as possible; i.e., we want

$$E\{(Y - U_2(X))^2\}$$

to be as small as possible

Background on Conditional PDFs: IV

- solution is to use $U_2(X) = E\{Y|X\}$; i.e., the conditional mean of Y given X is our best guess at Y in the sense of minimizing the mean square error (related to fact that $E\{(Y-a)^2\}$ is smallest when $a = E\{Y\}$)
- on the other hand, suppose we want the function $U_1(X)$ such that the mean absolute error $E\{|Y - U_1(X)|\}$ is as small as possible
- the solution now is to let $U_1(X)$ be the conditional median; i.e., we must solve

$$\int_{-\infty}^{U_1(x)} f_{Y|X=x}(y)\,dy = 0.5$$

to figure out what $U_1(x)$ should be when $X = x$

Conditional Mean and Median Approach: I

- assume model of stochastic signal plus non-IID noise:
  $\mathbf{X} = \mathbf{C} + \boldsymbol{\eta}$ so that $\mathbf{O} = \mathcal{O}\mathbf{X} = \mathcal{O}\mathbf{C} + \mathcal{O}\boldsymbol{\eta} \equiv \mathbf{R} + \mathbf{n}$
- component-wise, have $O_l = R_l + n_l$
- because $\mathbf{C}$ and $\boldsymbol{\eta}$ are independent, $\mathbf{R}$ and $\mathbf{n}$ must be also
- suppose we approximate R_l via $\widehat{R}_l \equiv U_2(O_l)$, where $U_2(O_l)$ is selected to minimize $E\{(R_l - U_2(O_l))^2\}$
- solution is to set $U_2(O_l)$ equal to $E\{R_l|O_l\}$, so let's work out what form this conditional mean takes
- to get $E\{R_l|O_l\}$, need the PDF of R_l given O_l, which is

$$f_{R_l|O_l=o_l}(r_l) = \frac{f_{R_l,O_l}(r_l,o_l)}{f_{O_l}(o_l)}$$

Conditional Mean and Median Approach: II

- joint PDF of R_l and O_l related to the joint PDF $f_{R_l,n_l}(\cdot,\cdot)$ of R_l and n_l via

$$f_{R_l,O_l}(r_l,o_l) = f_{R_l,n_l}(r_l, o_l - r_l) = f_{R_l}(r_l) f_{n_l}(o_l - r_l),$$

  with the 2nd equality following since R_l & n_l are independent
- marginal PDF for O_l can be obtained from joint PDF $f_{R_l,O_l}(\cdot,\cdot)$ by integrating out the first argument:

$$f_{O_l}(o_l) = \int_{-\infty}^{\infty} f_{R_l,O_l}(r_l,o_l)\,dr_l = \int_{-\infty}^{\infty} f_{R_l}(r_l) f_{n_l}(o_l - r_l)\,dr_l$$

- putting all these pieces together yields the conditional PDF

$$f_{R_l|O_l=o_l}(r_l) = \frac{f_{R_l,O_l}(r_l,o_l)}{f_{O_l}(o_l)} = \frac{f_{R_l}(r_l) f_{n_l}(o_l - r_l)}{\int_{-\infty}^{\infty} f_{R_l}(r_l) f_{n_l}(o_l - r_l)\,dr_l}$$

Conditional Mean and Median Approach: III

- mean value of $f_{R_l|O_l=o_l}(\cdot)$ yields estimator $\widehat{R}_l = E\{R_l|O_l\}$:

$$\begin{aligned} E\{R_l|O_l = o_l\} &= \int_{-\infty}^{\infty} r_l f_{R_l|O_l=o_l}(r_l)\,dr_l \\ &= \frac{\int_{-\infty}^{\infty} r_l f_{R_l}(r_l) f_{n_l}(o_l - r_l) dr_l}{\int_{-\infty}^{\infty} f_{R_l}(r_l) f_{n_l}(o_l - r_l)\,dr_l} \end{aligned}$$

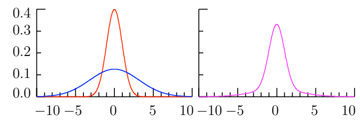
- to make further progress, we need a model for the wavelet-domain representation R_l of the signal
- heuristic that signal in the wavelet domain has a few large values and lots of small values suggests a Gaussian mixture model

Conditional Mean and Median Approach: IV

- let $\mathcal{I}_l$ be an RV such that $\mathbf{P}[\mathcal{I}_l = 1] = p_l$ & $\mathbf{P}[\mathcal{I}_l = 0] = 1 - p_l$
- under Gaussian mixture model, R_l has same distribution as

$$\mathcal{I}_l \mathcal{N}(0, \gamma_l^2 \sigma_{G_l}^2) + (1 - \mathcal{I}_l)\mathcal{N}(0, \sigma_{G_l}^2)$$

  where $\mathcal{N}(0,\sigma^2)$ is a Gaussian RV with mean 0 and variance σ^2
  - 2nd component models small # of large signal coefficients
  - 1st component models large # of small coefficients ($\gamma_l^2 \ll 1$)
- example: PDFs for case $\sigma_{G_l}^2 = 10$, $\gamma_l^2 \sigma_{G_l}^2 = 1$ and $p_l = 0.75$



Conditional Mean and Median Approach: V

- to complete model, let n_l obey a Gaussian distribution with mean 0 and variance $\sigma^2_{n_l}$
- conditional mean estimator of the signal RV R_l is given by

$$E\{R_l|O_l = o_l\} = \frac{a_l A_l(o_l) + b_l B_l(o_l)}{A_l(o_l) + B_l(o_l)} o_l,$$

where

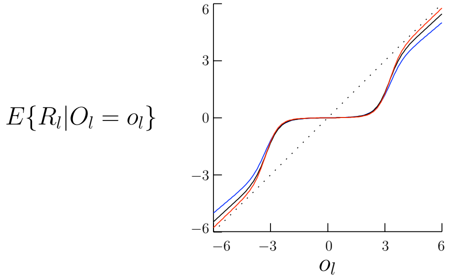
$$\begin{aligned} a_l &\equiv \frac{\gamma_l^2 \sigma^2_{G_l}}{\gamma_l^2 \sigma^2_{G_l} + \sigma^2_{n_l}} \text{ and } b_l \equiv \frac{\sigma^2_{G_l}}{\sigma^2_{G_l} + \sigma^2_{n_l}} \\ A_l(o_l) &\equiv \frac{p_l}{\sqrt{(2\pi[\gamma_l^2 \sigma^2_{G_l} + \sigma^2_{n_l}])}} e^{-o_l^2/[2(\gamma_l^2 \sigma^2_{G_l} + \sigma^2_{n_l})]} \\ B_l(o_l) &\equiv \frac{1 - p_l}{\sqrt{(2\pi[\sigma^2_{G_l} + \sigma^2_{n_l}])}} e^{-o_l^2/[2(\sigma^2_{G_l} + \sigma^2_{n_l})]} \end{aligned}$$

Conditional Mean and Median Approach: VI

- let's simplify to a 'sparse' signal model by setting $\gamma_l = 0$; i.e., large # of small coefficients are all zero
- distribution for R_l same as $(1 - \mathcal{I}_l)\mathcal{N}(0, \sigma^2_{G_l})$
- conditional mean estimator becomes $E\{R_l|O_l = o_l\} = \frac{b_l}{1+c_l} o_l$, where

$$c_l = \frac{p_l \sqrt{(\sigma^2_{G_l} + \sigma^2_{n_l})}}{(1 - p_l)\sigma_{n_l}} e^{-o_l^2 b_l/(2\sigma^2_{n_l})}$$

Conditional Mean and Median Approach: VII



- conditional mean shrinkage rule for $p_l = 0.95$ (i.e., $\approx$ 95% of signal coefficients are 0); $\sigma^2_{n_l} = 1$; and $\sigma^2_{G_l} = 5$ (curve furthest from dotted diagonal), 10 and 25 (curve nearest to diagonal)
- as $\sigma^2_{G_l}$ gets large (i.e., large signal coefficients increase in size), shrinkage rule starts to resemble mid thresholding rule

Conditional Mean and Median Approach: VIII

- now suppose we estimate R_l via $\widehat{R}_l = U_1(O_l)$, where $U_1(O_l)$ is selected to minimize $E\{|R_l - U_1(O_l)|\}$
- solution is to set $U_1(o_l)$ to the median of the PDF for R_l given $O_l = o_l$
- to find $U_1(o_l)$, need to solve for it in the equation

$$\int_{-\infty}^{U_1(o_l)} f_{R_l|O_l=o_l}(r_l)\, dr_l = \frac{\int_{-\infty}^{U_1(o_l)} f_{R_l}(r_l) f_{n_l}(o_l - r_l)\, dr_l}{\int_{-\infty}^{\infty} f_{R_l}(r_l) f_{n_l}(o_l - r_l)\, dr_l} = \frac{1}{2}$$

Conditional Mean and Median Approach: IX

- simplifying to the sparse signal model, Godfrey & Rocca (1981) show that

$$U_1(O_l) \approx \begin{cases} 0, & \text{if } |O_l| \le \delta; \\ b_l O_l, & \text{otherwise,} \end{cases}$$

where

$$\delta = \sigma_{n_l}\left[2\log\left(\frac{p_l \sigma_{G_l}}{(1-p_l)\sigma_{n_l}}\right)\right]^{1/2} \quad \text{and} \quad b_l = \frac{\sigma_{G_l}^2}{\sigma_{G_l}^2 + \sigma_{n_l}^2}$$

- above approximation valid if $p_l/(1-p_l) \gg \sigma_{n_l}^2/(\sigma_{G_l}\delta)$ and $\sigma_{G_l}^2 \gg \sigma_{n_l}^2$
- note that $U_1(\cdot)$ is approximately a hard thresholding rule

Wavelet-Based Thresholding

- assume model of deterministic signal plus IID Gaussian noise with mean 0 and variance σ_ϵ^2: $\mathbf{X} = \mathbf{D} + \boldsymbol{\epsilon}$
- using a DWT matrix $\mathcal{W}$, form $\mathbf{W} = \mathcal{W}\mathbf{X} = \mathcal{W}\mathbf{D} + \mathcal{W}\boldsymbol{\epsilon} \equiv \mathbf{d} + \mathbf{e}$
- because $\boldsymbol{\epsilon}$ IID Gaussian, so is $\mathbf{e}$
- Donoho & Johnstone (1994) advocate the following:
  - form partial DWT of level J_0: $\mathbf{W}_1, \ldots, \mathbf{W}_{J_0}$ and $\mathbf{V}_{J_0}$
  - threshold $\mathbf{W}_j$'s but leave $\mathbf{V}_{J_0}$ alone (i.e., administratively, all $N/2^{J_0}$ scaling coefficients assumed to be part of $\mathbf{d}$)
  - use universal threshold $\delta^{(u)} = \sqrt{[2\sigma_\epsilon^2 \log(N)]}$
  - use thresholding rule to form $\mathbf{W}_j^{(t)}$ (hard, etc.)
  - estimate $\mathbf{D}$ by inverse transforming $\mathbf{W}_1^{(t)}, \ldots, \mathbf{W}_{J_0}^{(t)}$ and $\mathbf{V}_{J_0}$

MAD Scale Estimator: I

- procedure assumes σ_ϵ is know, which is not usually the case
- if unknown, use median absolute deviation (MAD) scale estimator to estimate σ_ϵ using $\mathbf{W}_1$

$$\hat{\sigma}_{(\text{mad})} \equiv \frac{\text{median}\,\{|W_{1,0}|, |W_{1,1}|, \ldots, |W_{1,\frac{N}{2}-1}|\}}{0.6745}$$

  - heuristic: bulk of $W_{1,t}$'s should be due to noise
  - '0.6745' yields estimator such that $E\{\hat{\sigma}_{(\text{mad})}\} = \sigma_\epsilon$ when $W_{1,t}$'s are IID Gaussian with mean 0 and variance σ_ϵ^2
  - designed to be robust against large $W_{1,t}$'s due to signal

MAD Scale Estimator: II

- example: suppose $\mathbf{W}_1$ has 7 small 'noise' coefficients & 2 large 'signal' coefficients (say, a & b, with $2 \ll |a| < |b|$):

$$\mathbf{W}_1 = [1.23, -1.72, -0.80, -0.01, a, 0.30, 0.67, b, -1.33]^T$$

- ordering these by their magnitudes yields

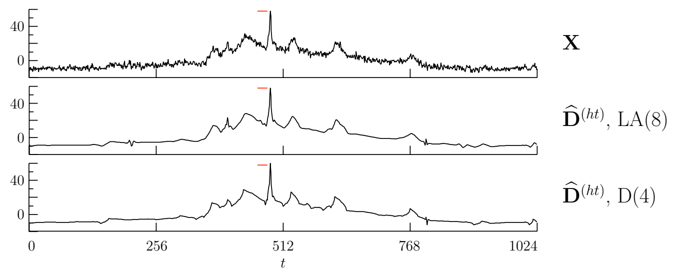
$$0.01, 0.30, 0.67, 0.80, 1.23, 1.33, 1.72, |a|, |b|$$

- median of these absolute deviations is 1.23, so

$$\hat{\sigma}_{(\text{mad})} = 1.23/0.6745 \doteq 1.82$$

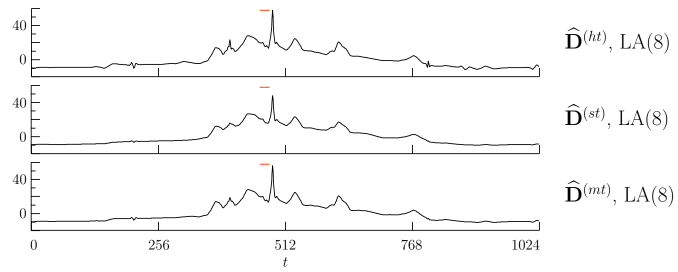
- $\hat{\sigma}_{(\text{mad})}$ not influenced adversely by a and b; i.e., scale estimate depends largely on the many small coefficients due to noise

Examples of DWT-Based Thresholding: I



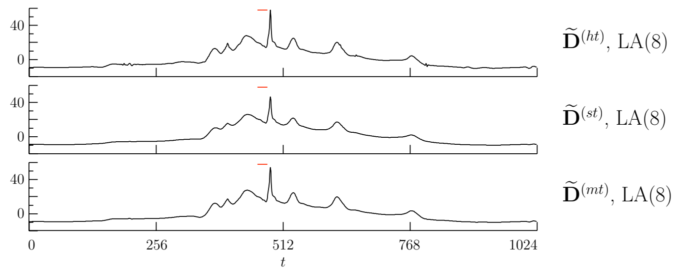
- top plot: NMR spectrum $\mathbf{X}$
- middle: signal estimate using $J_0 = 6$ partial LA(8) DWT with hard thresholding and universal threshold level estimated by $\hat{\delta}^{(u)} = \sqrt{[2\hat{\sigma}^2_{(\mathrm{mad})} \log(N)]} \doteq 6.13$
- bottom: same, but now using D(4) DWT with $\hat{\delta}^{(u)} \doteq 6.49$

Examples of DWT-Based Thresholding: II



- top: signal estimate using $J_0 = 6$ partial LA(8) DWT with hard thresholding (repeat of middle plot of previous overhead)
- middle: same, but now with soft thresholding
- bottom: same, but now with mid thresholding

Examples of MODWT-Based Thresholding

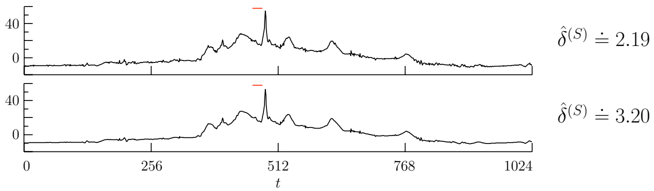


- as in previous overhead, but using MODWT rather than DWT
- because of MODWT filters are normalized differently, universal threshold must be adjusted for each level:
$$\tilde{\delta}^{(u)}_j \equiv \sqrt{[2\tilde{\sigma}^2_{(\mathrm{mad})} \log(N)/2^j]} \doteq 6.50/2^{j/2}$$
- results are identical to what 'cycle spinning' would yield

VisuShrink

- Donoho & Johnstone (1994) recipe with soft thresholding is known as 'VisuShrink' (but really thresholding, not shrinkage)
- rather than using the universal threshold, can also determine δ for VisuShrink by finding value $\hat{\delta}^{(S)}$ that minimizes SURE, i.e.,
$$\sum_{j=1}^{J_0} \sum_{t=0}^{N_j-1} (2\hat{\sigma}^2_{(\mathrm{mad})} - W^2_{j,t} + \delta^2) 1_{[\delta^2,\infty)}(W^2_{j,t}),$$
as a function of δ, with σ^2_ϵ estimated via MAD

Examples of DWT-Based Thresholding: III



- top: VisuShrink estimate based upon level $J_0 = 6$ partial LA(8) DWT and SURE with MAD estimate based upon $\mathbf{W}_1$
- bottom: same, but now with MAD estimate based upon $\mathbf{W}_1$, $\mathbf{W}_2, \ldots, \mathbf{W}_6$ (the common variance in SURE is assumed common to all wavelet coefficients)
- resulting signal estimate of bottom plot is less noisy than for top plot

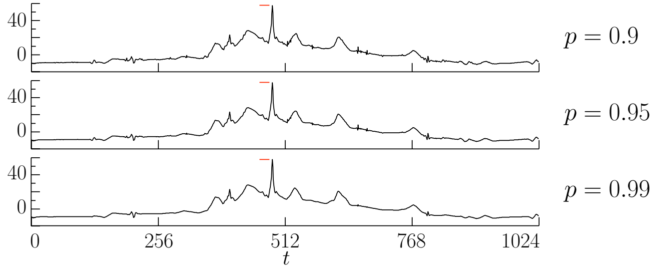
Wavelet-Based Shrinkage: I

- assume model of stochastic signal plus Gaussian IID noise: $\mathbf{X} = \mathbf{C} + \boldsymbol{\epsilon}$ so that $\mathbf{W} = \mathcal{W}\mathbf{X} = \mathcal{W}\mathbf{C} + \mathcal{W}\boldsymbol{\epsilon} \equiv \mathbf{R} + \mathbf{e}$
- component-wise, have $W_{j,t} = R_{j,t} + e_{j,t}$
- form partial DWT of level J_0, shrink $\mathbf{W}_j$'s, but leave $\mathbf{V}_{J_0}$ alone
- assume $E\{R_{j,t}\} = 0$ (reasonable for $\mathbf{W}_j$, but not for $\mathbf{V}_{J_0}$)
- use a conditional mean approach with the sparse signal model
  - $R_{j,t}$ has distribution dictated by $(1 - \mathcal{I}_{j,t})\mathcal{N}(0, \sigma_G^2)$, where
  $$\mathbf{P}\left[\mathcal{I}_{j,t} = 1\right] = p \text{ and } \mathbf{P}\left[\mathcal{I}_{j,t} = 0\right] = 1 - p$$
  - $R_{j,t}$'s are assumed to be IID
  - model for $e_{j,t}$ is Gaussian with mean 0 and variance σ_ϵ^2
  - note: parameters do not vary with j or t

Wavelet-Based Shrinkage: II

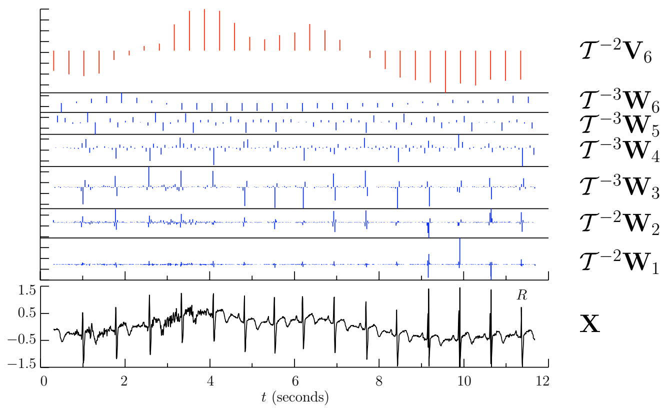
- model has three parameters σ_G^2, p and σ_ϵ^2, which need to be set
- let σ_R^2 and σ_W^2 be variances of RVs $R_{j,t}$ and $W_{j,t}$
- have relationships $\sigma_R^2 = (1-p)\sigma_G^2$ and $\sigma_W^2 = \sigma_R^2 + \sigma_\epsilon^2$
  - set $\hat{\sigma}_\epsilon^2 = \hat{\sigma}_{(\text{mad})}^2$ using $\mathbf{W}_1$
  - let $\hat{\sigma}_W^2$ be sample mean of all $W_{j,t}^2$
  - given p, let $\hat{\sigma}_G^2 = (\hat{\sigma}_W^2 - \hat{\sigma}_\epsilon^2)/(1-p)$
  - p usually chosen subjectively, keeping in mind that p is proportion of noise-dominated coefficients (can set based on rough estimate of proportion of 'small' coefficients)

Examples of Wavelet-Based Shrinkage



- shrinkage signal estimates of the NMR spectrum based upon the level $J_0 = 6$ partial LA(8) DWT and the conditional mean with $p = 0.9$ (top plot), 0.95 (middle) and 0.99 (bottom)
- as $p \to 1$, we declare there are proportionately fewer significant signal coefficients, implying need for heavier shrinkage

Comments on 'Next Generation' Denoising: I



- 'classical' denoising looks at each $W_{j,t}$ alone; for 'real world' signals, coefficients often cluster within a given level and persist across adjacent levels (ECG series offers an example)

Comments on 'Next Generation' Denoising: II

- here are some 'next generation' approaches that exploit these 'real world' properties:
  - Crouse *et al.* (1998) use hidden Markov models for stochastic signal DWT coefficients to handle clustering, persistence and non-Gaussianity
  - Huang and Cressie (2000) consider scale-dependent multiscale graphical models to handle clustering and persistence
  - Cai and Silverman (2001) consider 'block' thesholding in which coefficients are thresholded in blocks rather than individually (handles clustering)
  - Dragotti and Vetterli (2003) introduce the notion of 'wavelet footprints' to track discontinuities in a signal across different scales (handles persistence)

Comments on 'Next Generation' Denoising: III

- 'classical' denoising also suffers from problem of overall significance of multiple hypothesis tests
- 'next generation' work integrates idea of 'false discovery rate' (Benjamini and Hochberg, 1995) into denoising (see Wink and Roerdink, 2004, for an applications-oriented discussion)
- for more recent developments (there are a lot!!!), see
  - review article by Antoniadis (2007)
  - Chapters 3 and 4 of book by Nason (2008)
  - October 2009 issue of *Statistica Sinica*, which has a special section entitled 'Multiscale Methods and Statistics: A Productive Marriage'

References

- A. Antoniadis (2007), 'Wavelet Methods in Statistics: Some Recent Developments and Their Applications,' *Statistical Surveys*, **1**, pp. 16–55
- Y. Benjamini and Y. Hochberg (1995), 'Controlling the False Discovery Rate: A Practical and Powerful Approach to Multiple Testing,' *Journal of the Royal Statistical Society, Series B*, **57**, pp. 289–300
- T. Cai and B. W. Silverman (2001), 'Incorporating Information on Neighboring Coefficients into Wavelet Estimation,' *Sankhya Series B*, **63**, pp. 127–48
- M. S. Crouse, R. D. Nowak and R. G. Baraniuk (1998), 'Wavelet-Based Statistical Signal Processing Using Hidden Markov Models,' *IEEE Transactions on Signal Processing*, **46**, pp. 886–902
- P. L. Dragotti and M. Vetterli (2003), 'Wavelet Footprints: Theory, Algorithms, and Applications,' *IEEE Transactions on Signal Processing*, **51**, pp. 1306–23
- H.–C. Huang and N. Cressie (2000), 'Deterministic/Stochastic Wavelet Decomposition for Recovery of Signal from Noisy Data,' *Technometrics*, **42**, pp. 262–76
- G. P. Nason (2008), *Wavelet Methods in Statistics with R*, Springer, Berlin

- A. M. Wink and J. B. T. M. Roerdink (2004), 'Denoising Functional MR Images: A Comparison of Wavelet Denoising and Gaussian Smoothing,' *IEEE Transactions on Medical Imaging*, **23**(3), pp. 374–87