Slepian functions on the sphere:
Applications in cosmology and geophysics

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## WMAP \& Cosmic Background Radiation - 1



## WMAP \& Cosmic Background Radiation - 2



## WMAP \& Cosmic Background Radiation - 3



## GRACE \& Earth's Gravity Field - 1



## GRACE \& Earth's Gravity Field - 2



## GRACE \& Earth's Gravity Field - 3



## CHAMP \& Earth's Magnetic Field — 1



## CHAMP \& Earth's Magnetic Field — 2



## Common problems - 1

Scalar data $d(\mathbf{r})$ modeled on a unit sphere $\Omega$ parameterized as $\mathbf{r}=(\theta, \phi)$ :


Spherical harmonics $Y_{l m}(\mathbf{r})$ form an orthonormal basis on $\Omega$ :

$$
\int_{\Omega} Y_{l m}^{*} Y_{l^{\prime} m^{\prime}} d \Omega=\delta_{l l^{\prime}} \delta_{m m^{\prime}}
$$

$\| \leftarrow$ a delta function

## Common problems - 2

The domain of data availability or the region of interest is $R \in \Omega$.


The spherical harmonics $Y_{l m}(\mathbf{r})$ are not orthogonal on $R$ :

$$
\int_{R} Y_{l m}^{*} Y_{l^{\prime} m^{\prime}} d \Omega=D_{l m, l^{\prime} m^{\prime}}
$$

$\| \leftarrow$ not a delta function

The spatiospectral localization kernel $\mathbf{D}$ is not sparse, but it is blocky (order $m$ is a good quantum number) for axially symmetric $R$.

## Slepian's problem

Eigenvectors of $D$ are expansion coefficients of Slepian functions,

$$
g(\mathbf{r})=\sum_{l m}^{L} g_{l m} Y_{l m}(\mathbf{r})
$$

They satisfy the spherical concentration problem to the region $R$ of area $A$ :

$$
\lambda=\int_{R} g^{2} d \Omega / \int_{\Omega} g^{2} d \Omega=\text { maximum }
$$

The Slepian functions $g_{\alpha}(\mathbf{r})$, designed for any region $R$, are still orthonormal over the whole sphere $\Omega$ but now they are also orthogonal over the region $R$ :

$$
\int_{R} g_{\alpha} g_{\beta} d \Omega=\lambda_{\alpha} \delta_{\alpha \beta} \quad \text { and } \quad \int_{\Omega} g_{\alpha} g_{\beta} d \Omega=\delta_{\alpha \beta} .
$$

They are a doubly orthogonal bandlimited basis for localized and global signals.

## Slepian functions for abitrary regions $(L=60)$



## Slepian functions for cosmology


$\lambda=0.000007$

$\lambda=0.000136$
$\lambda=0.000336$

$\lambda=0.004188$

$\lambda=0.038757$


## Common problems - 3

Signal estimation:
Problem 1
Given $d(\mathbf{r})$ and $\left\langle n(\mathbf{r}) n\left(\mathbf{r}^{\prime}\right)\right\rangle$, estimate the signal $s(\mathbf{r})$ at source level:
realizing that the estimate $\hat{s}(\mathbf{r})$ is always bandlimited to $0 \leq L<\infty$.

Spectral estimation:
Problem 2
Given $d(\mathbf{r})$ and $\left\langle n(\mathbf{r}) n\left(\mathbf{r}^{\prime}\right)\right\rangle$, and assuming the signal behaves as
estimate the power spectral density $S_{l}$, for $0 \leq l<\infty$.

## Common problems - 3

Signal estimation:
Problem 1
Given $d(\mathbf{r})$ and $\left\langle n(\mathbf{r}) n\left(\mathbf{r}^{\prime}\right)\right\rangle$, estimate the signal $s(\mathbf{r})$ at source level:

$$
\hat{s}(\mathbf{r})=\sum_{l m}^{L} \hat{s}_{l m} Y_{l m}(\mathbf{r})
$$

realizing that the estimate $\hat{s}(\mathbf{r})$ is always bandlimited to $0 \leq L<\infty$.

Spectral estimation:
Problem 2
Given $d(\mathbf{r})$ and $\left\langle n(\mathbf{r}) n\left(\mathbf{r}^{\prime}\right)\right\rangle$, and assuming the signal behaves as

$$
\left\langle s_{l m}\right\rangle=0 \quad \text { and } \quad\left\langle s_{l m} s_{l^{\prime} m^{\prime}}^{*}\right\rangle=S_{l} \delta_{l l^{\prime}} \delta_{m m^{\prime}}
$$

estimate the power spectral density $S_{l}$, for $0 \leq l<\infty$.

## Why we solve Problem 1



Chen, Wilson \& Tapley, Science (2006):
Spatial leakage effects are also evident, because of filtering applied to suppress the noise in high-degree and high- order spherical harmonics.


## Problem 1 - Finding the signal

Construct a bandlimited estimate in the spherical harmonic basis by minimizing the quadratic misfit to the data over $R$. The optimal solution depends on $\mathrm{D}^{-1}$ :

$$
\hat{s}_{l m}=\sum_{l^{\prime} m^{\prime}}^{L} D_{l m, l^{\prime} m^{\prime}}^{-1} \int_{R} d Y_{l^{\prime} m^{\prime}}^{*} d \Omega
$$

Finding $\mathrm{D}^{-1}$ is tough, so construct a truncated-Slepian basis estimate instead:

The solution depends on the localization eigenvalue $\lambda_{\alpha}$ at the same rank:

Truncation prevents the blowup of the low eigenvalues.

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$$
\hat{s}(\mathbf{r})=\sum_{\alpha}^{J} \hat{s}_{\alpha} g_{\alpha}(\mathbf{r})
$$

The solution depends on the localization eigenvalue $\lambda_{\alpha}$ at the same rank:

$$
\hat{s}_{\alpha}=\lambda_{\alpha}^{-1} \int_{R} d g_{\alpha} d \Omega
$$

Truncation prevents the blowup of the low eigenvalues.


## Slepian estimation of gravity field changes - 2 <br> 19/49



## Slepian estimation of gravity field changes - $3 \quad 2049$







To assess the quality of our spectral estimates $\hat{S}_{l}$, we calculate:

$$
\begin{align*}
\text { variance: } \quad v_{l} & =\left\langle\hat{S}_{l}^{2}\right\rangle-\left\langle\hat{S}_{l}\right\rangle^{2}  \tag{1}\\
\text { bias: } \quad b_{l} & =\left\langle\hat{S}_{l}\right\rangle-S_{l}  \tag{2}\\
\text { error: } \quad \epsilon_{l} & =\hat{S}_{l}-S_{l}  \tag{3}\\
\text { mse: }\left\langle\epsilon_{l}^{2}\right\rangle & =v_{l}+b_{l}^{2} . \tag{4}
\end{align*}
$$

A good estimator is unbiased and/or minimizes the mse.

The industry-standard maximum-likelihood method via the iterative, nonlinear, Newton-Raphson algorithm returns the minimum-variance unbiased estimate of the power spectral density - but the estimation variance is quite high!:

$$
\begin{equation*}
\left\langle\hat{S}_{l}^{\mathrm{ML}}\right\rangle=S_{l} \tag{5}
\end{equation*}
$$

## Finding the spectrum, the multitaper way

Use the Slepian functions as data tapers, with weights be chosen iteratively to minimize the mse of the multitaper estimate (Wieczorek \& Simons, JFAA, 2007). Dahlen \& Simons, GJI (2008) choose the eigenvalues of D:

$$
\hat{S}_{l}^{\mathrm{MT}}=\frac{1}{K} \sum_{\alpha} \lambda_{\alpha}\left(\frac{1}{2 l+1} \sum_{m}\left|\int_{\Omega} g_{\alpha}(\mathbf{r}) d(\mathbf{r}) Y_{l m}^{*}(\mathbf{r}) d \Omega\right|^{2}\right)
$$

Bias (degree coupling) depends only on the bandwidth $L$ of the Slepian windows, and variance is almost exactly $K$ times smaller than the periodogram variance when their (effective) bandwidths are similar, as it is in the 1-D case!

Spectral and spatial concentration trade off via the Shannon number, which is the sole parameter to be chosen by the analyst:I

$$
K=\sum_{\alpha}^{(L+1)^{2}} \lambda_{\alpha}=(L+1)^{2} \frac{A}{4 \pi}
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# Spectral estimation on a sphere in geophysics and cosmology 

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#### Abstract

SUMMARY We address the problem of estimating the spherical-harmonic power spectrum of a statistically isotropic scalar signal from noise-contaminated data on a region of the unit sphere. Three different methods of spectral estimation are considered: (i) the spherical analogue of the onedimensional (1-D) periodogram, (ii) the maximum-likelihood method and (iii) a spherical analogue of the 1-D multitaper method. The periodogram exhibits strong spectral leakage, especially for small regions of area $A \ll 4 \pi$, and is generally unsuitable for spherical spectral analysis applications, just as it is in 1-D. The maximum-likelihood method is particularly useful in the case of nearly-whole-sphere coverage, $A \approx 4 \pi$, and has been widely used in cosmology to estimate the spectrum of the cosmic microwave background radiation from spacecraft observations. The spherical multitaper method affords easy control over the fundamental trade-off between spectral resolution and variance, and is easily implemented regardless of the region size, requiring neither non-linear iteration nor large-scale matrix inversion. As a result, the method is ideally suited for most applications in geophysics, geodesy or planetary science, where the objective is to obtain a spatially localized estimate of the spectrum of a signal from noisy data within a pre-selected and typically small region.


Key words: Time series analysis; Fourier analysis; Inverse theory; Spatial analysis.

## Whole-sphere spectral estimate

Assuming isotropy, add the power from all orders and subtract noise term:

$$
\hat{S}_{l}^{\mathrm{WS}}=\frac{1}{2 l+1} \sum_{m}\left|\int_{\Omega} d(\mathbf{r}) Y_{l m}^{*}(\mathbf{r}) d \Omega\right|^{2}-N_{l}
$$

This estimate is unbiased:

$$
\begin{equation*}
b_{l}^{\mathrm{WS}}=0, \tag{6}
\end{equation*}
$$

and its variance, our gold standard, can be calculated from elementary statistics:

$$
\begin{equation*}
v_{l}^{\mathrm{WS}}=\frac{2}{2 l+1}\left(S_{l}+N_{l}\right)^{2}, \tag{7}
\end{equation*}
$$

In the absence of noise, the nonzero sampling variance is termed cosmic.

The problem is that we do not have whole-sphere data.

## Cut-sphere spectral estimate (periodogram)

Simply work with the available data - i.e. use a gain-adjusted boxcar window:

$$
\hat{S}_{l}^{\mathrm{SP}}=\left(\frac{4 \pi}{A}\right) \frac{1}{2 l+1} \sum_{m}\left|\int_{R} d(\mathbf{r}) Y_{l m}^{*}(\mathbf{r}) d \Omega\right|^{2}-\text { noise correction. }
$$

This estimate is biased (unless $S_{l}=S$ or $R=\Omega$ ):

$$
\begin{equation*}
b_{l}^{\mathrm{SP}}=\sum_{l^{\prime}}\left[\left(\frac{4 \pi}{A}\right) \frac{1}{2 l+1} \sum_{m m^{\prime}}\left|D_{l m, l^{\prime} m^{\prime}}\right|^{2}-\delta_{l l^{\prime}}\right] S_{l^{\prime}}, \tag{8}
\end{equation*}
$$

and the variance is:

$$
\begin{equation*}
v_{l}^{\mathrm{SP}}=\left.\left.\frac{2(4 \pi / A)^{2}}{(2 l+1)^{2}} \sum_{m m^{\prime}}\left|\sum_{p q}\left(S_{p}+N_{p}\right)\right| D_{l m, p q}\right|^{2}\right|^{2} \tag{9}
\end{equation*}
$$

The appearance of the spatiospectral localization kernel D in these expressions has been known since at least the work of Peebles and Hauser (1973).

## The periodogram coupling matrix

The periodogram coupling matrix shows the leakage from untargeted degrees:

$$
K_{l l^{\prime}}=\left(\frac{4 \pi}{A}\right) \frac{1}{2 l+1} \sum_{m m^{\prime}}\left|D_{l m, l^{\prime} m^{\prime}}\right|^{2}
$$

It shows us the contributions of adjacent $l^{\prime}$ when we seek the power at $l$.


This coupling is neither bandlimited nor very well localized in the spectrum... we can do much better!

## Single-taper spectral estimate

Use one of the Slepian functions as data window:

$$
\begin{equation*}
\hat{S}_{l}^{\alpha}=\frac{1}{2 l+1} \sum_{m}\left|\int_{\Omega} g_{\alpha}(\mathbf{r}) d(\mathbf{r}) Y_{l m}^{*}(\mathbf{r}) d \Omega\right|^{2}-\text { noise correction } \tag{10}
\end{equation*}
$$

to obtain a biased estimate controlled by a coupling matrix

$$
M_{l l^{\prime}}^{\alpha}=\left(\frac{2 l^{\prime}+1}{4 \pi}\right) \sum_{p q}\left|g_{\alpha, p q}\right|^{2}\left(\begin{array}{lll}
l & p & l \\
0 & 0 & 0
\end{array}\right)^{2}
$$

which shows the resulting estimate is a bandlimited and well-localized average of the spectral power within a certain bandwidth.

Spectral and spatial concentration trade off via the Shannon number, which is the sole parameter to be chosen by the analyst.

As with the periodogram, the Slepian functions can be normalized to yield an unbiased estimate of a white power spectrum.

## Multiple-taper spectral estimate

Single-tapers are good, but weighted averaging the estimates made with many different tapers reduces the estimation variance without increasing the bias.

$$
\begin{equation*}
\hat{S}_{l}^{\mathrm{MT}}=\sum_{\alpha} c_{\alpha} \hat{S}_{l}^{\alpha} \quad \text { where } \quad \sum_{\alpha} c_{\alpha}=1 \tag{11}
\end{equation*}
$$

Two tapers $\alpha$ and $\beta$ have a covariance that behaves almost as if both estimates were statistically uncorrelated:

$$
\begin{equation*}
v_{l}^{\alpha \beta}=\text { diagonally dominant } \tag{12}
\end{equation*}
$$

thus the multitaper estimation variance

$$
\begin{equation*}
v_{l}^{\mathrm{MT}}=\sum_{\alpha \beta} c_{\alpha} v_{l}^{\alpha \beta} c_{\beta} \tag{13}
\end{equation*}
$$

is reduced by the addition of estimates made with subsequent tapers.

## The multitaper coupling matrix

The weights $c_{\alpha}$ can be chosen iteratively to minimize the mean-squared error of the multitaper estimate. However, a logical choice are the eigenvalues of $D$. Then the multitaper coupling matrix is

$$
M_{l l^{\prime}}=\frac{2 l^{\prime}+1}{(L+1)^{2}} \sum_{p}^{L}(2 p+1)\left(\begin{array}{lll}
l & p & l^{\prime} \\
0 & 0 & 0
\end{array}\right)^{2}
$$

which — amazingly — depends only upon the chosen bandwidth $L$.


## Quadratic spectral estimators

Maximum-likelihood ... very cumbersome, unbiased, high variancel
Whole-sphere ... unattainable

$$
\begin{equation*}
\hat{S}_{l}^{\mathrm{WS}}=\frac{1}{2 l+1} \sum_{m}\left|\int_{\Omega} d(\mathbf{r}) Y_{l m}^{*}(\mathbf{r}) d \Omega\right|^{2}-\text { noise correction. } \tag{14}
\end{equation*}
$$

Periodogram ... broadband bias, high variance

$$
\begin{equation*}
\hat{S}_{l}^{\mathrm{SP}}=\left(\frac{4 \pi}{A}\right) \frac{1}{2 l+1} \sum_{m}\left|\int_{R} d(\mathbf{r}) Y_{l m}^{*}(\mathbf{r}) d \Omega\right|^{2}-\text { noise correction. } \tag{15}
\end{equation*}
$$

Single-taper ... bandlimited bias

$$
\begin{equation*}
\hat{S}_{l}^{\alpha}=\frac{1}{2 l+1} \sum_{m}\left|\int_{\Omega} g_{\alpha}(\mathbf{r}) d(\mathbf{r}) Y_{l m}^{*}(\mathbf{r}) d \Omega\right|^{2}-\text { noise correction. } \tag{16}
\end{equation*}
$$

Multiple-taper ... bandlimited bias, lower variance, easily implemented

$$
\begin{equation*}
\hat{S}_{l}^{\mathrm{MT}}=\frac{1}{K} \sum_{\alpha} \lambda_{\alpha} \hat{S}_{l}^{\alpha} \tag{17}
\end{equation*}
$$

## Appraisal of performance

We study the performance of the various estimators by forming the variance ratios

$$
\left(\sigma_{l}^{2}\right)^{\mathrm{XX}}=v_{l}^{\mathrm{XX}} / v_{l}^{\mathrm{WS}}
$$

where XX stands for any of the acronyms SP, DP, ML or MT.
The deconvolved periodogram

$$
\begin{equation*}
\hat{S}_{l}^{\mathrm{DP}}=\sum_{l^{\prime}} K_{l l^{\prime}}^{-1} \hat{S}_{l^{\prime}}^{\mathrm{SP}} \tag{18}
\end{equation*}
$$

where $K$ is the periodogram coupling matrix, is unbiased $\left\langle\hat{S}_{l}^{\mathrm{DP}}\right\rangle=S_{l}$.
For white signal and noise, $S_{l}=S$ and $N_{l}=N$, the deconvolved periodogram concides with the maximum likelihood estimator.

Since $\left(\sigma_{l}^{2}\right)^{\mathrm{ML}}=\left(\sigma_{l}^{2}\right)^{\mathrm{DP}}=\left(\frac{4 \pi}{A}\right) K_{l l}^{-1}$, we can compute the maximum-likelihood variance ratio without actually forming the maximum-likelihood estimate.

## Maximum-likelihood / Whole-sphere variance



## Periodogram / Whole-sphere variance



## Multitaper / Whole-sphere variance



## Multitaper / Whole-sphere variance at large I




## Conclusions

1. Each the discussed estimators is quadratic in the data: a common framework allows us to study their relative merits.
2. The maximum-likelihood estimate provides the best unbiased estimate of the spectrum. However, its calculation is cumbersome, and requires an iterative procedure and the inversion of very large matrices.
3. The periodogram estimate is generally unsuitable for power spectral estimation on the sphere, much like it is in one dimension.
4. The Slepian multitaper method yields a smoothed and thus biased estimate of the spectrum, but it requires neither iteration nor large-scale matrix inversion. Its variance is much lower than that of any other method, and the only parameter that needs to be specified by the analyst is the Shannon number, or the space-bandwidth product diagnostic of the spatiospectral concentration.

## Review: Scalar Slepian functions

Eigenvectors of D expand to bandlimited Slepian functions:
that satisfy Slepian's concentration problem to the region $R$ of area $A$ :

The Shannon number, or sum of the eigenvalues,
is the effective dimension of the space for which the bandlimited $g$ are a basis.

## Review: Scalar Slepian functions

Eigenvectors of $\mathbf{D}$ expand to bandlimited Slepian functions:

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g=\sum_{l m}^{L} g_{l m} Y_{l m}
$$

that satisfy Slepian's concentration problem to the region $R$ of area $A$ :

$$
\lambda=\int_{R} g^{2} d \Omega / \int_{\Omega} g^{2} d \Omega=\text { maximum } .
$$

The Shannon number, or sum of the eigenvalues,

$$
K=(L+1)^{2} \frac{A}{4 \pi},
$$

 both spatially and spectrally, to a new basis with only about $K$ functions, $g$.

## Vector spherical harmonics



## New: Vectorial Slepian functions - 1

Let $g$ be a spectrally bandlimited vector field:
and maximize the spatial concentration inside of the region of interest:

The vector Shannon number, or sum of the eigenvalues,
is the effective dimension space for which the vector $g$ are a basis.

## New: Vectorial Slepian functions - 1

Let $\mathbf{g}$ be a spectrally bandlimited vector field:

$$
\mathrm{g}=\mathbf{g}^{r}+\mathbf{g}^{t}=\sum_{l=0}^{L} \sum_{m=-l}^{m} U_{l m} \mathbf{P}_{l m}+V_{l m} \mathbf{B}_{l m}+W_{l m} \mathbf{C}_{l m}
$$

and maximize the spatial concentration inside of the region of interest:

$$
\lambda=\frac{\int_{R} \mathrm{~g} \cdot \mathrm{~g} d \Omega}{\int_{\Omega} \mathrm{g} \cdot \mathrm{~g} d \Omega}=\text { maximum }
$$

The vector Shannon number, or sum of the eigenvalues,

$$
K=\left[3(L+1)^{2}-2\right] \frac{A}{4 \pi},
$$

is the effective dimension of the space for which the vector $\mathbf{g}$ are a basis.

## Vectorial Slepian functions - 2



## Inverse problems in a vector Slepian basis - 1

## Signal:

NGDC720 V3 (Maus, 2010)
$L=72$
Data points:
2292 equal-area-random
points over Africa

## Noise:

Gaussian random values
$\mu=0$,
$\sigma^{2}=2.5 \%$ of signal energy


## Inverse problems in a vector Slepian basis - 2 49/49


$a=800 \mathrm{~km}$
$J=291$


Relative mse=2.4\%


Relative $\mathrm{mse}=18 \%$

