Notes on the error bars for cross-spectral admittance estimates.

WHF Smith, 20 October 2004.

The question was raised by Joaquim Luis (jluis@ualg.pt) and further comment added by Marta Ghidella (Argentine Antarctic Institute, mghidella@dna.gov.ar). Both were looking at "gravfft", a supplement (by Joaquim, I think) built upon "grdfft", the FFT-based filter for 2-d grids in "GMT" (http://gmt.soest.hawaii.edu). This caused me to take a second look at how error bars are done in the 1-d GMT program "spectrum1d" also, because the expressions in "grdfft" are built upon "spectrum1d" with some further assumptions generalizing the 1-d case to the 2-d case (more on that below). In turn, "spectrum1d" is built upon foundations in Bendat and Piersol (hearafter B&P), *Random Data*, 2nd edition, John Wiley and Sons, New York, 1986. B&P do not give an expression for the expected error in an admittance estimate, and so I will try to derive one here, after laying out the problem in B&P notation.

True values, estimated values, and estimation errors

B&P use symbols without overlying marks (e.g. A) to indicate true values, an overlying tilde (e.g. $\tilde{A}$) to indicate a estimate obtained from a single sample realization, and an overlying circumflex (e.g. $\hat{A}$) to indicate an estimate made by averaging of several $\tilde{A}$ values obtained from statistically independent samples. Let $E\{\ \}$ denote the statistical operation of taking the expectation. The variance of an estimate is the expected (mean) squared error of the estimate: $\mathrm{var}\left\{\tilde{A}\right\} = E\left\{\left(\tilde{A} - A\right)^2\right\} = E\left\{\tilde{A}^2\right\} - 2AE\left\{\tilde{A}\right\} + A^2$. If $E\left\{\tilde{A}\right\} = A$, then the estimate $\tilde{A}$ is unbiased, and $\mathrm{var}\left\{\tilde{A}\right\} = E\left\{\tilde{A}^2\right\} - A^2$. The covariance of two estimates is $\mathrm{cov}\left\{\tilde{A},\tilde{B}\right\} = E\left\{\left(\tilde{A} - A\right)\left(\tilde{B} - B\right)\right\}$, and if both estimates are unbiased, $\mathrm{cov}\left\{\tilde{A},\tilde{B}\right\} = E\left\{\tilde{A}\tilde{B}\right\} - AB$. Note that $\mathrm{var}\left[\hat{A}\right] = \left(\mathrm{var}\left[\tilde{A}\right]\right)/N$, where N is the number of statistically independent realizations that are used to obtain an "ensemble average", $\hat{A}$, and that $\hat{A}$ is unbiased when $\tilde{A}$ is unbiased.

Auto- and cross-spectra

B&P define the cross-spectrum G_{xy} in terms of the Fourier transforms $X(f)$ and $Y(f)$ of two time series $x(t)$ and $y(t)$ as

$$G_{xy} = X^* Y . \tag{1}$$

The auto-spectra

$$G_{xx} = X^* X \tag{2x}$$

$$G_{yy} = Y^* Y \tag{2y}$$

can be viewed as special cases of (1). Auto-spectra are real-valued functions, but the cross-spectrum is, in general, complex; it can be expressed in terms of a pair of real functions in either of two ways:

$$G_{xy} = \left|G_{xy}\right| \exp\left(-j\theta_{xy}\right), \tag{3}$$

$$G_{xy} = C_{xy} - jQ_{xy}, \tag{4}$$

with $j = \sqrt{-1}$ in B&P notation. $\left|G_{xy}\right|$ is the cross-spectral amplitude and θ_{xy} is the cross-spectral phase. $C_{xy} = \mathrm{Re}\left\{G_{xy}\right\}$ is called the co-spectrum and characterizes the in-phase covariance of x and y, while $Q_{xy} = -\mathrm{Im}\left\{G_{xy}\right\}$ is called the "quadrature spectrum" and characterizes the out-of-phase covariance. From (1), $G_{yx} = Y^* X = \left(X^* Y\right)^* = G_{xy}^*$, so that $Q_{yx} = -Q_{xy}$ and $\theta_{yx} = -\theta_{xy}$ while $C_{yx} = C_{xy}$ and $\left|G_{yx}\right| = \left|G_{xy}\right|$; thus reversing the roles of x and y reverses the sense of phase and quadrature while leaving the co-spectrum and cross-spectral amplitude unchanged.

Estimates of auto- and cross-spectra

B&P show (section 9.1 at page 293) that estimates $\tilde{G}_{xx}$, $\tilde{G}_{yy}$, $\tilde{C}_{xy}$, and $\tilde{Q}_{xy}$ at discrete transform frequencies can be formed in the usual and intuitively obvious way by ensemble averaging of combinations of the real and imaginary, or cosine and sine, coefficients in the discrete Fourier transform of discrete equidistant samples of $x(t)$ and

$y(t)$. These estimates will be unbiased if the length of each transformed segment is long enough that the resolution bias error is negligible. This assumption is made by B&P in Chapter 9 where they derive the variance and covariance of estimated spectral quantities.

Since the $\tilde{C}_{xy}$ and $\tilde{Q}_{xy}$ estimates are straightforward, the error analysis of $\hat{C}_{xy}$ and $\hat{Q}_{xy}$ follows directly. The error analysis for other cross-spectral quantity estimators is not so straightforward, and one must follow the error propagation through the estimation process. Suppose for example, sample estimates of $\left|\tilde{G}_{xy}\right|$ and $\tilde{\theta}_{xy}$ are obtained via $\left|\tilde{G}_{xy}\right| = \sqrt{\tilde{C}_{xy}^2 + \tilde{Q}_{xy}^2}$ and $\tilde{\theta}_{xy} = \tan^{-1}\left(\tilde{Q}_{xy} / \tilde{C}_{xy}\right)$ from each of many independent sample realizations, and these sample estimates are then averaged; the results will not be equal to $\sqrt{\hat{C}_{xy}^2 + \hat{Q}_{xy}^2}$ and $\tan^{-1}\left(\hat{Q}_{xy} / \hat{C}_{xy}\right)$ because the square root and arctangent operations do not commute with the averaging operation: $E\left\{\left|\tilde{G}_{xy}\right|\right\} \neq \left|\hat{G}_{xy}\right| = \sqrt{\hat{C}_{xy}^2 + \hat{Q}_{xy}^2}$ and $E\left\{\tilde{\theta}_{xy}\right\} \neq \hat{\theta}_{xy} = \tan^{-1}\left(\hat{Q}_{xy} / \hat{C}_{xy}\right)$. Thus one must be careful to perform error analysis of an estimator following precisely the data processing recipe that defines the estimator.

Cross-spectral coherency

The cross-spectral coherence function is defined thus:

$$\gamma_{xy}^2 = \frac{\left|G_{xy}\right|^2}{G_{xx} G_{yy}}. \tag{5}$$

B&P follow most authors in calling this the "coherency" for brevity; a few authors call it the squared coherency for clarity in contexts where $\left|\gamma_{xy}\right| = \sqrt{\gamma_{xy}^2}$ also appears. I will call (5) the coherency. Note that $\gamma_{xy}^2 = \gamma_{yx}^2$; coherency is a real-valued function and symmetric with respect to reversal of the roles of *x* and *y*. It is the cross-spectral analogue of a linear correlation coefficient; $-1 \le \gamma_{xy}^2 \le 1$ is the linear correlation coefficient between *X* and *Y* as a function of frequency, and measures the extent to which *x* and *y* are related by a convolution-type operator.

Estimation of the cross-spectral coherency requires that one first ensemble-average the components separately and then form the coherency estimate. To see this, define the single-estimate and ensemble-estimate values thus:

$$\tilde{\gamma}_{xy}^2 = \frac{\left|\tilde{G}_{xy}\right|^2}{\tilde{G}_{xx}\tilde{G}_{yy}}, \qquad \hat{\gamma}_{xy}^2 = \frac{\left|\hat{G}_{xy}\right|^2}{\hat{G}_{xx}\hat{G}_{yy}}. \tag{6}$$

If each sample of x and y contains some random fluctuation in either x or y or both, then these fluctuations will cause the ensemble-averaging to yield $-1 < \hat{\gamma}_{xy}^2 < 1$, indicating the lack of perfect correlation between x and y. However, inspection of the algebra involved in $\tilde{\gamma}_{xy}^2$ shows that it is identically equal to 1 at all frequencies for any single realization of the data, and so an average of several independent $\tilde{\gamma}_{xy}^2$ values cannot yield the correct estimate of coherency; $E\left\{\tilde{\gamma}_{xy}^2\right\} = 1$, regardless of the true value of γ_{xy}^2. When the true coherency is ± 1, so that x and y are exactly correlated and are also both noise-free, then $\hat{\gamma}_{xy}^2$ will equal ± 1 as it should.

When the number of independent samples N is large, or when $\left|\gamma_{xy}^2\right|$ is near one, then the bias error in $\hat{\gamma}_{xy}^2$ is negligible, provided that the delay is also small (B&P, section 9.2.1). A $\left|\gamma_{xy}^2\right|$ near one implies that x and y are approximately related by a convolution-type operator, which could include a delay operation, e.g. $y(t) = x(t-\tau)$. The ensemble-averaged coherency has negligible bias only if any delay is small compared to the length of the x and y samples that are Fourier transformed to do the analysis. If $\hat{\gamma}_{xy}^2$ has negligible bias, then

$$\mathrm{var}\left[\hat{\gamma}_{xy}^2\right] \approx \frac{2\gamma_{xy}^2\left(1-\gamma_{xy}^2\right)}{N} \tag{7}$$

(B&P, equation 9.81).

In "spectrum1d", the coherency is estimated by the ensemble average formula on the right in (6) above, using $\left|\hat{G}_{xy}\right|^2 = \hat{C}_{xy}^2 + \hat{Q}_{xy}^2$. The error estimate is made using (7) but substituting $\hat{\gamma}_{xy}^2$ for γ_{xy}^2 on the right hand side. This substitution is approximately valid under the assumption that $\hat{\gamma}_{xy}^2$ is unbiased.

Input-output relationships

Suppose $x(t)$ is the noise-free "input" to a linear process with impulse response $h(t)$, so that $v(t) = x(t) * h(t)$ would be the "output" of this process in the absence of noise, with the symbol indicating convolution. Suppose that we can obtain realizations of

noise-free samples of $x(t)$ but we cannot sample $v(t)$; only noisy realizations $y(t) = v(t) + e(t)$ are available, with $e(t)$ a random noise process and uncorrelated with $v(t)$. Suppose we don't know $h(t)$ but wish to estimate it from samples of *x* and *y* by minimizing the expected mean square error

$$S^2 = E\left\{\sum_t \left[y(t) - h * x(t)\right]^2 = \sum_f \left|Y(f) - H(f)X(f)\right|^2\right\}, \tag{8}$$

where the expectation is taken over realizations of *x* and *y*. It turns out that the best estimator of $h(t)$ is obtained in terms of its transfer function $H(f)$ via the ensemble-averaged estimator

$$\hat{H}_{xy} = \frac{\hat{G}_{xy}}{\hat{G}_{xx}}. \tag{9}$$

The ensemble-averaged estimator is required for much the same reason that the cross-spectral coherency cannot be found from a single estimator: only by averaging many samples can one hope to separate the effects of *h* and *e* in *y*.

In the absence of noise, the filter's output would have an auto-spectral density given by

$$G_{vv} = \left|H_{xy}X\right|^2 = \left|H_{xy}\right|^2 G_{xx} = \gamma_{xy}^2 G_{yy} \tag{10a}$$

and since the output signal and noise are uncorrelated, their auto-spectral densities combine as $G_{vv} + G_{ee} = G_{yy}$, and so

$$G_{ee} = \left(1 - \gamma_{xy}^2\right)G_{yy}. \tag{11a}$$

G_{vv} and G_{ee} are real-valued functions known as the coherent output spectrum and the noise spectrum, respectively; in "spectrum1d" they are estimated as

$$\hat{G}_{vv} = \hat{\gamma}_{xy}^2 \hat{G}_{yy} \tag{10b}$$

and

$$\hat{G}_{ee} = \left(1 - \hat{\gamma}^2_{xy}\right)\hat{G}_{yy}. \tag{11b}$$

These estimators are assumed to be unbiased, following the previous assumptions and results, and the variance of these estimators is (B&P, equations 9.70 and 9.72)

$$\mathrm{var}\left[\hat{G}_{vv}\right] = G^2_{vv}\frac{2 - \gamma^2_{xy}}{N\gamma^2_{xy}}, \tag{10c}$$

$$\mathrm{var}\left[\hat{G}_{ee}\right] = \frac{G^2_{ee}}{N}. \tag{11c}$$

In "spectrum1d" the ensemble-estimated values are substituted for the true values on the right hand sides in (10c) and (11c), which is approximately correct since the estimators are approximately unbiased.

In posing the least-squares problem for the optimal estimate of $\hat{H}_{xy}$, no symmetry constraints on $h(t)$ are imposed, so that, in general, $\hat{H}_{xy}$ is complex; thus one also expresses the filter transfer function in terms of a gain factor estimate,

$$\left|\hat{H}_{xy}\right| = \frac{\left|\hat{G}_{xy}\right|}{\hat{G}_{xx}} \tag{12a}$$

and a phase factor estimate,

$$\hat{\phi}_{xy} = \tan^{-1}\left[\frac{\hat{Q}_{xy}}{\hat{C}_{xy}}\right]. \tag{13b}$$

These estimators are again approximately unbiased, and have variances given by

$$\mathrm{var}\left[\left|\hat{H}_{xy}\right|\right] \approx \left|\hat{H}_{xy}\right|^2 \frac{1 - \gamma^2_{xy}}{2N\gamma^2_{xy}} \tag{12b}$$

$$\mathrm{var}\left[\hat{\phi}_{xy}\right] \approx \frac{1 - \gamma^2_{xy}}{2N\gamma^2_{xy}} \tag{13b}$$

(B&P, from equations 9.89 and 9.91). Again, "spectrum1d" uses these expressions, and again substituting estimates for true values on the right hand side of the error expressions.

Admittance

In the geophysical literature on isostasy, the term admittance is used to describe the cross-spectral estimate of a linear filter operation relating an "input" topography to an output "gravity". The topography is assumed noise-free and the gravity is assumed to have "noise". The literature often defines the admittance as

$$\hat{Z} = \frac{\langle XY^* \rangle}{\langle XX^* \rangle} \tag{14}$$

with the bent brackets indicating ensemble averaging and the asterisk indicating complex conjugation, and x the topography and y the gravity. This is almost analogous to the input/output model above, but for a few peculiarities.

First, the order of the conjugation in (10) is the reverse of (1). This is of no consequence for the denominator of (14), which is real-valued in any case, but it gives the complex conjugate of (1) in the numerator, so that we have in effect

$$\hat{Z} = \hat{H}^*_{xy}. \tag{15}$$

This means that $\mathrm{Re}\left\{\hat{Z}\right\} = \mathrm{Re}\left\{\hat{H}_{xy}\right\}$ but $\mathrm{Im}\left\{\hat{Z}\right\} = -\mathrm{Im}\left\{\hat{H}_{xy}\right\}$, and consequently the sense of the phase angle of the filter will be reversed.

Second, and more important, because it renders the first point somewhat moot, is that the literature doesn't mean what it says when it writes (14). It really means

$$\hat{Z} = \frac{\mathrm{Re}\left\{\langle XY^* \rangle\right\}}{\langle XX^* \rangle} = \frac{\hat{C}_{xy}}{\hat{G}_{xx}}, \tag{16}$$

which is a purely real, zero phase filter. The reason that this is the intent is that the filtered output signal v is the gravitational attraction of the topography (or compensation of the topography, or both) and so the filter's impulse response must be a symmetric

function; the gravitational attraction of a point mass is symmetric around the mass. By imposing this constraint, the "noise" in the gravity is not merely that which cannot be correlated with a linear operation on the topography, but rather that which cannot be correlated with a *symmetric* linear operation on the topography.

The GMT program "spectrum1d" estimates admittance as the ratio of ensemble-averaged co-spectra and input auto-spectra, as in (16). B&P do not discuss admittance estimates of any kind, and so do not give an expression for the error in the estimate.

Expected error in the admittance estimate

Following a scheme used by B&P for other quantities, set $Z = C_{xy} / G_{xx}$ and differentiate:

$$dZ = \left[G_{xx}\left(dC_{xy}\right) - C_{xy}\left(dG_{xx}\right)\right] \Big/ G_{xx}^2 . \tag{17}$$

Now associate each differential with an error quantity, e.g. $dZ = \tilde{Z} - Z$:

$$\tilde{Z} - Z = \left[G_{xx}\left(\tilde{C}_{xy} - C_{xy}\right) - C_{xy}\left(\tilde{G}_{xx} - G_{xx}\right)\right] \Big/ G_{xx}^2 . \tag{18}$$

Taking expectations of both sides and using the fact that $\tilde{C}_{xy}$ and $\tilde{G}_{xx}$ are unbiased shows that

$$E\left\{\tilde{Z} - Z\right\} = 0, \tag{19}$$

that is, $\tilde{Z} = \tilde{C}_{xy} / \tilde{G}_{xx}$ is an unbiased estimator of *Z*.

Using (18), the expected mean square error in $\tilde{Z}$ is expressed as

$$E\left\{\left(\tilde{Z} - Z\right)^2\right\} = \left\{G_{xx}^2 \operatorname{var}\left[\tilde{C}_{xy}\right] - 2C_{xy}G_{xx} \operatorname{cov}\left[\tilde{C}_{xy}, \tilde{G}_{xx}\right] + C_{xy}^2 \operatorname{var}\left[\tilde{G}_{xx}\right]\right\} \Big/ G_{xx}^4 . \tag{20}$$

B&P give $\operatorname{var}\left[\tilde{G}_{xx}\right] = G_{xx}^2$ (their equation 9.24) and $\operatorname{cov}\left[\tilde{C}_{xy}, \tilde{G}_{xx}\right] = C_{xy}G_{xx}$ (their equation 9.37), and with these substitutions (20) reduces to

$$E\left\{\left(\tilde{Z}-Z\right)^2\right\}=\mathrm{var}\left[\tilde{Z}\right]=\left\{\mathrm{var}\left[\tilde{C}_{xy}\right]-C_{xy}^2\right\}\Big/G_{xx}^2. \tag{21}$$

B&P give $\mathrm{var}\left[\tilde{C}_{xy}\right]=\frac{1}{2}\left(G_{xx}G_{yy}+C_{xy}^2-Q_{xy}^2\right)$ (their equation 9.25) and substituting this in (21) and using $C_{xy}^2+Q_{xy}^2=\left|G_{xy}\right|^2=\gamma_{xy}^2G_{xx}G_{yy}$ one then obtains

$$\mathrm{var}\left[\tilde{Z}\right]=\frac{G_{yy}}{2G_{xx}}\left(1-\gamma_{xy}^2\right). \tag{22}$$

Since this is the expected variance in a single realization, the variance in an ensemble average of *N* statistically independent realizations is expected to be

$$\mathrm{var}\left[\hat{Z}\right]=\frac{G_{yy}}{2NG_{xx}}\left(1-\gamma_{xy}^2\right). \tag{23}$$

Expressions (22) and (23) imply that the error in the admittance estimate is zero when the coherency is 1, i.e., complete absence of noise, and perfect correlation between *x* and *y*. This makes intuitive sense. Conversely, when there is complete absence of coherency, equation (22) says that the variance in the one-sample admittance estimate will be half of the ratio of the *y* and *x* power spectral densities. This also makes intuitive sense, as when there is a complete absence of correlation, the correct answer is $Z = 0$ but *x* and *y* should be in phase and in quadrature each about 1/2 the time, so that the one sample estimate $\tilde{Z}$ will be wrong by about half of G_{yy}/G_{xx}.

Alternative approach to admittance error

Suppose that the admittance was not estimated by (16) but instead by

$$\hat{Z}=\left|\hat{H}\right|\cos\hat{\phi}. \tag{24}$$

In this case an error analysis using the approach similar to (17) thru (23) would obtain

$$\mathrm{var}\left[\hat{Z}\right]=\mathrm{var}\left[\left|\hat{H}\right|\right]\cos^2\phi-2\sin\phi\cos\phi\,\mathrm{cov}\left[\left|\hat{H}\right|,\hat{\phi}\right]+\left|\hat{H}\right|^2\sin^2\phi\,\mathrm{var}\left[\hat{\phi}\right]. \tag{25}$$

B&P do not discuss $\mathrm{cov}\left[\left|\hat{H}\right|,\hat{\phi}\right]$ but all other related expressions they show have zero expected covariance. Assuming the covariance term in (25) is zero, and substituting for the variance terms in (12b) and (13b), one obtains

$$\mathrm{var}\left[\tilde{Z}\right] \approx \left|\hat{H}_{xy}\right|^2 \frac{1-\gamma_{xy}^2}{2N\gamma_{xy}^2}, \tag{26}$$

which appears identical in form to (12b).

Are expressions (23) and (26) equal, or equally useful?

Equation (26) gives the expected mean square error in an admittance estimate made by (24), while equation (23) applies to the estimate made by (16); I see no reason why we should expect these to be equal, since the estimators are formulated differently. However, by squaring expression (12a) and also using (5), one can show that the right hand sides of (26) and (23) are equivalent. This implies that the two recipes for estimating admittance, (16) and (24), are equally good, or equally erroneous, or that the error analysis is equally inadequate in both cases.

Expression (23) makes very clear that $0 \le \mathrm{var}\left[\hat{Z}\right] \le G_{yy}/\left(2NG_{xx}\right)$ and that $\mathrm{var}\left[\hat{\hat{Z}}\right]$ is a decreasing function of γ_{xy}^2. The behavior of expression (26) as $\gamma^2 \to 0$ is not so clear, as it will depend on the limiting form of Z^2/γ^2. Knowing that (23) and (26) are equivalent, one can say that admittance decreases as coherency decreases in such a way that Z^2/γ^2 remains bounded as $\gamma^2 \to 0$.

In practice, one doesn't know the true values of the quantities on the right hand sides and one must substitute estimated quantities. In that case I think (23) is to be preferred, as it clearly will yield a stable result as $\hat{\gamma}_{xy}^2 \to 0$.

Expressions in the literature

Joaquim Luis pointed out to me that G. D. Karner and A. B. Watts ("On isostasy at Atlantic-type continental margins", *J. Geophys. Res.*. vol. 87, no. B-4, pp. 2923-2948, April 10, 1982) give an expression in the caption to Figure 6 of their paper (at page

2934): They say "the standard deviation of each estimate is computed assuming a normal probability distribution for the ratio of true-sample admittance:

$$\sigma = \sqrt{\left(\gamma^{-2} - 1\right) / (2N)}, \tag{27}$$

where N is the number of independent estimates of the admittance and γ^2 is the coherence or correlation coefficient between true and sample admittance." I have changed their symbol p to my N for convenience of comparing the expressions; otherwise, this is a direct quote. I am not sure I know what it means. They do not cite any reference for it, or describe it in any further detail than the quote given here.

Marta Ghidella pointed out to me that M. Maia, M. Diament, and M. Recq ("Isostatic response of the lithosphere beneath the Mozambique Ridge (SW Indian Ocean) and geodynamic implications", *Geophys. J. Int.*, vol 100, pp. 337-348, 1990) state (their equation 10) that

$$\mathrm{var}\left[\hat{Z}\right] = Z^2 \frac{1 - \gamma^2}{2N\gamma^2} \tag{28}$$

and they claim, without derivation, that this follows from an expression in B&P for the variance in the coherency.

Algebraic manipulation of (27) yields $\sigma = \sqrt{\left(1 - \gamma^2\right) / \left(2N\gamma^2\right)}$, which is the square root of the second factor in (28). Thus if Karner and Watts meant to give the one-sigma expected error in the ratio $\hat{Z}/Z$, then Karner and Watts appear to be saying the same thing that Maia et al. are saying. I think this is a reasonable interpretation of Karner and Watts.

Comparing these expressions

Expression (28) from Maia et al. has the same form as my (26) except that a substitution $Z^2 = \left|H_{xy}\right|^2$ has been made. My intuition is that this is not correct, since $Z = C_{xy}/G_{xx} = \left|H_{xy}\right| \cos\phi_{xy}$. If the true filter H really is zero phase at all frequencies, then $\cos\phi_{xy} = 1$ and the substitution is valid, but in the general case, this will not be so, and substituting Z^2 for $\left|H_{xy}\right|^2$ will underestimate the error in the admittance.

In gravity work the admittance functions are used to investigate isostasy, or depth to a source, or other operations. Theoretical expressions for the admittance of the operations of isostatic compensation or upward continuation are zero-phase (in 1-d, and radially symmetric in 2-d). The assumption is then made that the gravity:topography (output:input) relationship will be entirely zero phase. However, this will be true only if gravity signals due to other phenomena have been entirely removed, which is unlikely to be the case in practice. Therefore I expect that in actual practice the optimal filter will have non-zero phase at some frequencies, and therefore that the admittance error will be underestimated by the error expression in the literature.

Error bars for spectrum1d

The GMT program "spectrum1d" currently estimates the error bar using the expression (28), which I am now convinced is wrong. I believe it should be replaced by (23), since this appears more stable than (26) and is also derived directly from consideration of the way that spectrum1d estimates admittance: $\hat{Z} = \hat{C}_{xy} / \hat{G}_{xx}$.

What about the 2-d case?

The above discussion assumes time series data, which depend on one scalar variable, time, and so have Fourier transforms depending on one scalar variable, frequency. The above also assumes that a long-enough data set is available that many independent samples can be obtained for ensemble averaging. (The idea that subsets of a data set will give statistically equivalent spectra also requires an assumption of ergodicity.) For one-dimensional profiles through space, time and frequency can of course be replaced by scalar distance and scalar wavenumber.

In the 2-d case we have data that are functions of two coordinates and their Fourier transforms are functions of two wavenumbers. If we have the luxury of having enough data to form multiple independent subsets, then all the above approach applies. In the GMT program "grdfft", however, we try to extract the full range of information from only one sample. Auto-spectra are formed in the row (or column) dimension by averaging the results obtained from each row (or column), and using the above expressions with N taken as the number of rows (or columns). This isn't quite correct, as it assumes that each row (or column) is an independent sample; however, correlation in

the orthogonal direction will reduce the independence. Thus the row and column direction auto-spectra error bars are probably under-estimated.

A radially symmetric auto-spectrum estimate is also available in "grdfft". It takes the auto-spectra values at discrete points in the 2-d wavenumber plane and averages these in annuli, taking N as a number representing the number of independent samples in an average. This also is rather ad hoc.

I don't know what Joaquim's routine "gravfft" does. For my 2003 Fall AGU talk I did some 2-d optimal least-squares filtering, with the unknown filter to be determined having a constraint of radial symmetry, which is the 2-d analog of the constraint in 1-d of a zero-phase filter. Given input A and output B I found the best least-squares filter H such that

$$S^2 = \sum_{u,v} \left| B(u,v) - H(q) A(u,v) \right|^2 \tag{29}$$

was minimized, with u,v the spatial wavenumbers in the two directions for the 2-d functions A and B, and $q = \sqrt{u^2 + v^2}$ the radial wavenumber. In this approach, $H(q)$ is the Hankel transform of the optimal, radially-symmetric filter.