An overview of psd: Adaptive sine multitaper power spectral density estimation in R

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Abstract

This vignette provides an overview of some features included in the package psd, designed to compute estimates of power spectral density (PSD) for a univariate series in a sophisticated manner, with very little tuning effort. The sine multitapers are used, and the number of tapers varies with spectral shape, according to the optimal value proposed by Riedel and Sidorenko (1995). The adaptive procedure iteratively refines the optimal number of tapers at each frequency based on the spectrum from the previous iteration. Assuming the adaptive procedure converges, this produces power spectra with significantly lower spectral variance relative to results from less-sophisticated estimators. Sine tapers exhibit excellent leakage suppression characteristics, so bias effects are also reduced. Resolution and uncertainty vary with the number of tapers, which means we do not need to resort to either (1) windowing methods, which inherently degrade resolution at low-frequency (e.g. Welch's method); or (2) smoothing kernels, which can badly distort important features without careful tuning (e.g. the Daniell kernel in stats::spectrum). In this regards psd is best suited for data having large dynamic range and some mix of narrow and wide-band structure, features typically found in geophysical datasets.

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1 Quick start: A minimal example.

First, we load the package into the namespace:

```
library(psd)

## Loading required package: fftw

## Loaded psd (0.5.0) - Adaptive multitaper spectrum estimation
```

For a series to analyze, we can use magnet, included in psd, which represents along-track measurements of horizontal magnetic-field strength from a gimbaled, airborne magnetometer. These data are a small subset of the full Project MAGNET series (Coleman, 1992), which has provided insight into the history of the Earth's oceanic crust (Parker and O'Brien, 1997; O'Brien et al., 1999; Korte et al., 2002). The sampling interval is once every kilometer (km), so the data will represent crustal magnetization with wavelengths longer than 2 km.

```
data(magnet)
```

The format of the data set is a data.frame with four sets of information:

```
names(magnet)
## [1] "km" "raw" "clean" "mdiff"
```

The raw and clean names represent raw and edited intensities respectively, expressed in units of nanotesla; mdiff is the difference between them. The difference between them is a matter of just a few points attributable to instrumental malfunction.

```
subset(magnet, abs(mdiff) > 0)

## km raw clean mdiff
## 403 402 209.1 -3.6355 -212.7355
## 717 716 -248.7 -9.7775 238.9225
```

These deviations can, as we will see, adversely affect the accuracy of any PSD estimate, multitaper or otherwise.

We can find power spectral density (PSD) estimates for the two series quite simply with pspectrum:

```
psdr <- pspectrum(magnet$raw)

## Stage 0 est. (pilot)
## environment ** .psdEnv ** refreshed

## detrending (and demeaning)
## tap c A 1 1024

## [1] 14

## f creation

## cpp 1:2048 1024 1025 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeec77e600</pre>
```

```
## cpp 4:1024
## cpp 5:(0)0 14 -1011.58 -16.7858
## cpp 5:(0)1 14 -98.1488 300.164
## cpp 5:(0)2 14 815.278 617.114
## cpp 5:(0)3 14 1329.47 -911.147
## cpp 5:(0)4 14 -387.976 -1489.23
## [1] 22.1659
## [1] 58.44037
## [1] -36.27447
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeec5b3200
## cpp 4:1024
## cpp 5:(0)0 42 -1.25056e-12 0
## cpp 5:(0)1 43 -98.1488 300.164
## cpp 5:(0)2 44 815.278 617.114
## cpp 5:(0)3 45 1329.47 -911.147
## cpp 5:(0)4 46 -387.976 -1489.23
## [1] 22.1659
## [1] 58.32732
## [1] -36.16142
## Stage 1 est. (Ave. S.V.R. -18.8 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeea0fea00
## cpp 4:1024
## cpp 5:(0)0 106 -1.25056e-12 0
## cpp 5:(0)1 105 -98.1488 300.164
## cpp 5:(0)2 104 815.278 617.114
## cpp 5:(0)3 103 1329.47 -911.147
## cpp 5:(0)4 102 -387.976 -1489.23
## [1] 22.1659
## [1] 58.28626
## [1] -36.12036
## Stage 2 est. (Ave. S.V.R. -23.6 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeeab81200
## cpp 4:1024
## cpp 5:(0)0 162 -1.25056e-12 0
## cpp 5:(0)1 163 -98.1488 300.164
## cpp 5:(0)2 164 815.278 617.114
## cpp 5:(0)3 165 1329.47 -911.147
## cpp 5:(0)4 166 -387.976 -1489.23
```

```
## [1] 22.1659
## [1] 58.25526
## [1] -36.08936
## Stage 3 est. (Ave. S.V.R. -24.2 dB)
## Normalized single-sided PSD (PSD) to single-sided PSD for sampling-freq. 1
psdc <- pspectrum(magnet$clean)</pre>
## Stage 0 est. (pilot)
## environment ** .psdEnv ** refreshed
## detrending (and demeaning)
## tap c A 1 1024
## [1] 14
## f creation
## cpp 1:2048 1024 1025 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeeaa1be00
## cpp 4:1024
## cpp 5:(0)0 14 -791.427 -115.093
## cpp 5:(0)1 14 -93.2315 227.168
## cpp 5:(0)2 14 604.964 569.429
## cpp 5:(0)3 14 1159.71 -664.567
## cpp 5:(0)4 14 -296.747 -1156.83
## [1] 20.53588
## [1] 56.77368
## [1] -36.2378
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeeac1e400
## cpp 4:1024
## cpp 5:(0)0 51 2.41585e-13 0
## cpp 5:(0)1 50 -93.2315 227.168
## cpp 5:(0)2 49 604.964 569.429
## cpp 5:(0)3 48 1159.71 -664.567
## cpp 5:(0)4 47 -296.747 -1156.83
## [1] 20.53588
## [1] 56.69873
## [1] -36.16285
## Stage 1 est. (Ave. S.V.R. -15.1 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeeb268800
## cpp 4:1024
## cpp 5:(0)0 91 2.41585e-13 0
```

```
## cpp 5:(0)1 90 -93.2315 227.168
## cpp 5:(0)2 89 604.964 569.429
## cpp 5:(0)3 88 1159.71 -664.567
## cpp 5:(0)4 87 -296.747 -1156.83
## [1] 20.53588
## [1] 56.67791
## [1] -36.14202
## Stage 2 est. (Ave. S.V.R. -22.6 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeed0d4200
## cpp 4:1024
## cpp 5:(0)0 175 2.41585e-13 0
## cpp 5:(0)1 176 -93.2315 227.168
## cpp 5:(0)2 177 604.964 569.429
## cpp 5:(0)3 177 1159.71 -664.567
## cpp 5:(0)4 176 -296.747 -1156.83
## [1] 20.53588
## [1] 56.61941
## [1] -36.08353
## Stage 3 est. (Ave. S.V.R. -26.8 dB)
## Normalized single-sided PSD (PSD) to single-sided PSD for sampling-freq.
```

Each application of pspectrum calculates a pilot PSD, followed by niter iterations of refinement. With each iteration the number of tapers is adjusted based on the proposed optimal number from Riedel and Sidorenko (1995), which depends on spectral shape; we use quadratically weighted spectral derivatives (Prieto et al., 2007) to estimate this shape. By default, a multipanel summary plot of the final PSD compared to the raw periodogram estimate is shown after the final iterative stage. Note that if the user forgets to assign the results of pspectrum to the global environment, this can be done with the psd_envGet function:

```
psdc_recovered <- psd_envGet("final_psd")
all.equal(psdc, psdc_recovered)
## [1] TRUE</pre>
```

In general, spectral variance is reduced with sequential refinements¹, but is not necessarily guaranteed to converge. Note that in the example the sampling frequency of both series is 1 km⁻¹, the assumed value.

Figure 1 compares the power spectra for the raw and clean series². We expect the Project MAGNET data to be linear in the space of linear-frequencies and logarithmic-power; we see a clear improvement in spectral shape between the two series, simply because the large outliers have been removed. The PSD of the clean series shows a very "red" spectrum typical of geophysical processes (Agnew, 1992), and a rolloff in signal for 10 kilometer wavelengths and longer; whereas, the PSD for the raw series looks somewhat unrealistic at higher wavelengths—features which could be difficult to judge if the spectral variance was higher.

¹ Messages are given by default; ones with "Ave. S.V.R." are in reference to "average spectral-variance reduction", which is the variance of the double-differenced spectra at each stage, relative to the pilot estimate's variance.

² Note that pspectrum returns an object with class spec, so we have access to methods within stats, including plot.spec.

2 Comparisons with other methods

As we have shown in the Project MAGNET example, improved understanding of the physics behind the signals in the data is of great concern. Assuming a sample is free of non-physical points, how do PSD estimates from psd compare with other methods? Unfortunately the suite of extensions with similar functionality is relatively limited, but hopefully we have summarized most, if not all, the available functions in Table 1.

Table 1: A comparison of power spectral density estimators in R, excluding extensions which only estimate raw-periodograms. Normalizations are shown as either "single" or "double" for either single- or double-sided spectra, and "various" if there are multiple, optional normalizations. A (*) denotes the default for a function having an option for either single or double.

Function	Namespace	SINE M.T.?	Adaptive?	Norm.	Reference
bspec	bspec	No	No	single*	Röver et al. (2011)
mtapspec	RSEIS	Yes	No	various	Lees and Park (1995)
pspectrum	psd	Yes	Yes	single	Barbour and Parker (2014, 2015)
spectrum	stats	No	No	double	R Core Team (2013)
spec.mtm	multitaper	Yes	Yes	double	Rahim and Burr (2013)
SDF	sapa	Yes	No	$single^*$	Percival and Walden (1993)

We compare results from psd with those from a few of the methods in Table 1, using the same data: the cleaned Project MAGNET series.

2.1 stats::spectrum

Included in the core distribution of R is stats::spectrum, which accesses stats::spec.ar or stats::spec.pgram for either parametric and non-parametric estimation, respectively. The user can optionally apply a single cosine taper, and/or a smoothing kernel. Our method is non-parametric; hence, we will compare to the latter.

Included in psdcore is an option to compare the results with a 20% cosine-tapered periodogram, found with the following command:

```
spec.pgram(X, pad = 1, taper = 0.2, detrend = FALSE, demean = FALSE, plot = FALSE)
```

Within psdcore the comparison is made with the logical argument preproc passed to spec.pgram, which is TRUE by default.

As a matter of bookkeeping and good practice, we should consider the working environment accessed by psd functions. To ensure psdcore does not access any inappropriate information leftover from the previous calculations, we can set refresh=TRUE. We can then re-calculate the multitaper PSD and the raw periodogram with plotpsd=TRUE; these results are shown in Figure 2.

2.2 RSEIS::mtapspec

In RSEIS the spectrum estimation tool is mtapspec, which calls the program of Lees and Park (1995). There are numerous optional tuning parameters, including flags for normalization and taper averaging. For our purpose the correct normalization for mtapspec is found by using MTP=list(kind=2, inorm=3) and scaling the results by 2 (to convert double-sided spectra to single-sided spectra).

We assume mtapspec doesn't remove a mean and trend from the input series. We can do this easily with the prewhiten methods:

```
require(RSEIS)
## Loading required package: RSEIS
dt = 1 \# km
# prewhiten the data after adding a linear trend + offset
summary(prewhiten(mc <- (ts(magnet$clean + 1000, deltat = dt) + seq_along(magnet$clean)),</pre>
   plot = FALSE))
## detrending (and demeaning)
          Length Class Mode
## lmdfit
          12 lm
                       list
## ardfit
          O -none- NULL
## prew_lm 2048 ts numeric
## prew_ar 0 -none- NULL
## imputed
           1 -none- logical
```

Although the default operation of **prewhiten** is to fit a linear model of the form $f(x) = \alpha x + \beta + \epsilon$ using ordinary linear least squares, setting AR.max higher than zero to fit an auto-regressive (AR) model to the data³. This fit uses the Akaike infomation criterion (AIC) to select the highest order appropriate for the data.

```
summary(atsar <- prewhiten(mc, AR.max = 100, plot = FALSE))</pre>
## detrending (and demeaning)
## autoregressive model fit (returning innovations)
          Length Class Mode
          12 lm
## lmdfit
                       list
## ardfit 14 ar
                       list
## prew_lm 2048 ts
                       numeric
## prew_ar 2048 ts
## imputed 1 -none- logical
print(atsar$ardfit)
##
## Call:
## ar.yw.default(x = tser_prew_lm, aic = TRUE, order.max = AR.max,
                                                                 demean = TRUE)
##
## Coefficients:
   1 2
                         3
                                           5
##
                                  4
## 1.5134 -1.1037 0.6723 -0.3880 0.2108 -0.0786
## Order selected 6 sigma^2 estimated as 19.46
ats_lm <- atsar$prew_lm</pre>
ats_ar <- atsar$prew_ar</pre>
```

³Note that the linear trend fitting is removed from the series prior to AR estimation, and the residuals from this fit are also returned

We didn't necessarily need to deal with the sampling information since it is just 1 per km; but, supposing the sampling information was based on an interval, we could have used a negative value for X.frq, with which psdcore would interpret as an interval (instead of a frequency). A quick example highlights the equivalency:

```
a \leftarrow rnorm(32)
all.equal(psdcore(a, 1)$spec, psdcore(a, -1)$spec)
## tap c A 1 16
## 'tapers' object: num. tapers applied by index
## head: 1
## ...
## tail: 1
## f creation
## cpp 1:32 16 17 32
## cpp 2:64 16
## cpp 3:0x7ffeec71b158
## cpp 4:16
## cpp 5:(0)0 1 1.32153 0.915948
## cpp 5:(0)1 1 0.309161 -0.0926227
## cpp 5:(0)2 1 -0.703206 -1.10119
## cpp 5:(0)3 1 0.117808 2.44293
## cpp 5:(0)4 1 4.82892 -2.99637
## [1] 0.7412527
## [1] 17.72907
## [1] -16.98782
## tap c A 1 16
## 'tapers' object: num. tapers applied by index
## head: 1
## ...
## tail: 1
## f creation
## cpp 1:32 16 17 32
## cpp 2:64 16
## cpp 3:0x7ffeec744e00
## cpp 4:16
## cpp 5:(0)0 1 1.32153 0.915948
## cpp 5:(0)1 1 0.309161 -0.0926227
## cpp 5:(0)2 1 -0.703206 -1.10119
## cpp 5:(0)3 1 0.117808 2.44293
## cpp 5:(0)4 1 4.82892 -2.99637
## [1] 0.7412527
## [1] 17.72907
## [1] -16.98782
## [1] TRUE
```

Returning the the RSEIS comparison, we first estimate the PSD from mtapspec with 10 tapers:

where nwin is the number of tapers taken and npi is, from the documentation, the "number of Pi-prolate functions" (we leave it out for the sake of comparison). Note that the object returned is not of class spec:

```
str(Mspec)
## List of 12
## $ dat
           : ts [1:2048, 1] -16.23 -14.56 -12.02 -7.21 -3.13 ...
    ..- attr(*, "dimnames")=List of 2
    ....$ : NULL
##
    ....$ : NULL
##
   ..- attr(*, "tsp")= num [1:3] 1 2048 1
##
## $ dt
            : num 1
## $ spec : num [1:4096] 528 557 600 595 615 ...
## $ dof : num [1:4096] 20 20 20 20 20 20 20 20 20 ...
            : num [1:4096] 4.45e-20 4.78e-02 5.36e-01 1.54 1.15 ...
## $ Rspec : num [1:2049, 1:10] 1.86e-07 -9.32e+01 6.05e+02 1.16e+03 -2.97e+02 ...
## $ Ispec : num [1:2049, 1:10] 0 -227 -569 665 1157 ...
## $ freq
             : num [1:2049] 0 0.000244 0.000488 0.000732 0.000977 ...
## $ df
            : num 0.000244
## $ numfreqs: num 2049
## $ klen : num 4096
## $ mtm
            :List of 4
   ..$ kind : num 2
##
##
   ..$ nwin : num 10
## ..$ npi : num 0
## ..$ inorm: num 3
```

We will calculate the comparative spectra from

- 1. spectrum (20% cosine taper),
- 2. psdcore (with fixed tapers), and
- 3. pspectrum (allowing adaptive taper refinement)

and we will need to correct for normalization factors, as necessary, with normalize. Note that by default the normalization is set within pspectrum (with normalize) once the adaptive procedure is finished.

```
## cpp 1:2048 1024 1025 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeed0fa600
## cpp 4:1024
## cpp 5:(0)0 10 -791.427 -115.093
## cpp 5:(0)1 10 -93.2315 227.168
## cpp 5:(0)2 10 604.964 569.429
## cpp 5:(0)3 10 1159.71 -664.567
## cpp 5:(0)4 10 -296.747 -1156.83
## [1] 20.53588
## [1] 56.80048
## [1] -36.2646
Aspec <- pspectrum(ats_lm, dt, tapinit, plot = FALSE)
## Stage 0 est. (pilot)
## environment ** .psdEnv ** refreshed
\#\# detrending (and demeaning)
## tap c A 1 1024
## [1] 1
## f creation
## cpp 1:2048 1024 1025 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeed611600
## cpp 4:1024
## cpp 5:(0)0 1 -791.427 -115.093
## cpp 5:(0)1 1 -93.2315 227.168
## cpp 5:(0)2 1 604.964 569.429
## cpp 5:(0)3 1 1159.71 -664.567
## cpp 5:(0)4 1 -296.747 -1156.83
## [1] 20.53588
## [1] 56.63675
## [1] -36.10087
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeed66e400
## cpp 4:1024
## cpp 5:(0)0 3 2.13163e-14 0
## cpp 5:(0)1 2 -93.2315 227.168
## cpp 5:(0)2 2 604.964 569.429
## cpp 5:(0)3 2 1159.71 -664.567
## cpp 5:(0)4 3 -296.747 -1156.83
## [1] 20.53588
## [1] 56.84493
## [1] -36.30904
## Stage 1 est. (Ave. S.V.R. -11.2 dB)
## f creation
```

```
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeed5dcc00
## cpp 4:1024
## cpp 5:(0)0 5 2.13163e-14 0
## cpp 5:(0)1 5 -93.2315 227.168
## cpp 5:(0)2 5 604.964 569.429
## cpp 5:(0)3 6 1159.71 -664.567
## cpp 5:(0)4 7 -296.747 -1156.83
## [1] 20.53588
## [1] 56.79174
## [1] -36.25586
## Stage 2 est. (Ave. S.V.R. -20.4 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeed5d9800
## cpp 4:1024
## cpp 5:(0)0 18 2.13163e-14 0
## cpp 5:(0)1 18 -93.2315 227.168
## cpp 5:(0)2 17 604.964 569.429
## cpp 5:(0)3 18 1159.71 -664.567
## cpp 5:(0)4 19 -296.747 -1156.83
## [1] 20.53588
## [1] 56.76308
## [1] -36.2272
## Stage 3 est. (Ave. S.V.R. -33.3 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeec7d4600
## cpp 4:1024
## cpp 5:(0)0 58 2.13163e-14 0
## cpp 5:(0)1 58 -93.2315 227.168
## cpp 5:(0)2 57 604.964 569.429
## cpp 5:(0)3 56 1159.71 -664.567
## cpp 5:(0)4 55 -296.747 -1156.83
## [1] 20.53588
## [1] 56.69992
## [1] -36.16404
## Stage 4 est. (Ave. S.V.R. -41.6 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeed535200
## cpp 4:1024
## cpp 5:(0)0 85 2.13163e-14 0
```

```
## cpp 5:(0)1 84 -93.2315 227.168
## cpp 5:(0)2 83 604.964 569.429
## cpp 5:(0)3 82 1159.71 -664.567
## cpp 5:(0)4 81 -296.747 -1156.83
## [1] 20.53588
## [1] 56.6447
## [1] -36.10882
## Stage 5 est. (Ave. S.V.R. -47.0 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeed0d9800
## cpp 4:1024
## cpp 5:(0)0 143 2.13163e-14 0
## cpp 5:(0)1 142 -93.2315 227.168
## cpp 5:(0)2 141 604.964 569.429
## cpp 5:(0)3 140 1159.71 -664.567
## cpp 5:(0)4 139 -296.747 -1156.83
## [1] 20.53588
## [1] 56.64201
## [1] -36.10612
## Stage 6 est. (Ave. S.V.R. -58.8 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeee09d400
## cpp 4:1024
## cpp 5:(0)0 163 2.13163e-14 0
## cpp 5:(0)1 162 -93.2315 227.168
## cpp 5:(0)2 162 604.964 569.429
## cpp 5:(0)3 161 1159.71 -664.567
## cpp 5:(0)4 161 -296.747 -1156.83
## [1] 20.53588
## [1] 56.61591
## [1] -36.08002
## Stage 7 est. (Ave. S.V.R. -69.9 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeee07fc00
## cpp 4:1024
## cpp 5:(0)0 164 2.13163e-14 0
## cpp 5:(0)1 164 -93.2315 227.168
## cpp 5:(0)2 164 604.964 569.429
## cpp 5:(0)3 164 1159.71 -664.567
## cpp 5:(0)4 164 -296.747 -1156.83
## [1] 20.53588
```

```
## [1] 56.61834
## [1] -36.08246
## Stage 8 est. (Ave. S.V.R. -73.0 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeee29a400
## cpp 4:1024
## cpp 5:(0)0 166 2.13163e-14 0
## cpp 5:(0)1 166 -93.2315 227.168
## cpp 5:(0)2 166 604.964 569.429
## cpp 5:(0)3 166 1159.71 -664.567
## cpp 5:(0)4 166 -296.747 -1156.83
## [1] 20.53588
## [1] 56.62527
## [1] -36.08939
## Stage 9 est. (Ave. S.V.R. -74.1 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeec7d4600
## cpp 4:1024
## cpp 5:(0)0 166 2.13163e-14 0
## cpp 5:(0)1 166 -93.2315 227.168
## cpp 5:(0)2 166 604.964 569.429
## cpp 5:(0)3 167 1159.71 -664.567
## cpp 5:(0)4 167 -296.747 -1156.83
## [1] 20.53588
## [1] 56.63289
## [1] -36.09701
## Stage 10 est. (Ave. S.V.R. -71.9 dB)
## Normalized single-sided PSD (PSD) to single-sided PSD for sampling-freq. 1
# Correct for double-sidedness of spectrum and mtapspec results
class(Mspec)
## [1] "list"
Mspec <- normalize(Mspec, dt, "spectrum")</pre>
## Normalized double-sided PSD (SPECTRUM) to single-sided PSD for sampling-freq. 1
nt <- 1:Mspec$numfreqs</pre>
mspec <- Mspec$spec[nt]</pre>
class(Xspec)
## [1] "spec"
Xspec <- normalize(Xspec, dt, "spectrum")</pre>
{\it \#\# Normalized double-sided PSD (SPECTRUM) to single-sided PSD for sampling-freq. \ 1}
```

These estimates are shown on the same scale in Figure 4.

Because we did not specify the length of the FFT in mtapspec we end up with different length spectra. So, to form some statistical measure of the results, we can interpolate PSD levels onto the psd-based frequencies (or reciprocally):

```
library(signal, warn.conflicts = FALSE)
pltpi <- interp1(pltf, pltp, Pspec$freq)</pre>
```

We regress the spectral values from mtapspec against the psdcore results because we have used them to produce uniformly tapered spectra with an equal number of sine tapers.

```
df <- data.frame(x = dB(Pspec$spec), y = pltpi, tap = unclass(Aspec$taper))</pre>
summary(dflm <- lm(y ~ x + 0, df))
##
## Call:
## lm(formula = y \sim x + 0, data = df)
##
## Residuals:
      Min
               1Q Median
                                30
##
## -2.2466 -0.3368 0.1776 0.9687 5.5773
##
## Coefficients:
## Estimate Std. Error t value Pr(>|t|)
## x 0.992488 0.002047 484.9 <2e-16 ***
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.196 on 1023 degrees of freedom
## Multiple R-squared: 0.9957, Adjusted R-squared: 0.9957
## F-statistic: 2.352e+05 on 1 and 1023 DF, p-value: < 2.2e-16
df$res <- residuals(dflm)</pre>
```

We show the regression residuals in Figure 5. The structure visible at low power levels might be from curvature bias in the mtapspec results, which manifests at short wavelengths in Figure 4.

2.3 multitaper::spec.mtm

The function with the highest similarity to psd is spec.mtm in the multitaper package: it uses the sine multitapers, and can adaptively refine the spectrum. In fact, this function calls source code of a Fortran equivalent to psd authored by R.L. Parker (2013) to do these operations.

There are some notable differences, though. By default spec.mtm uses the Discrete Prolate Spheroidal Sequences (dpss) of Thomson (1982), which can have very good spectral leakage suppression (assuming the number of tapers used is appropriate for the desired resolution, which varies inversely with the time-bandwidth product). Spectral analyses using dpss can have superior results if the series is relatively short (e.g. N < 1000), or has inherent spectra with sharply changing features or deep wells. Improper usage of the dpss, however, can lead to severe bias. Thus, considerable care should be given to parameter choices, which translates practicably to having many more knobs to turn.

2.4 sapa::SDF

As of this writing, the package has no maintainer; lest we end up discussing deprecated and archived functions, we will not compare it to psd.

2.5 bspec::bspec

An intriguing method for producing power spectral density estimates using Bayesian inference is presented by Röver et al. (2011) and included in the bspec package. Simplistically, the method uses a *Student's t* likelihood function to estimate the distribution of spectral densities at a given frequency. We will use the spectra from the previous calculation to compare with bspec results. For this comparison we use the default settings for the *a priori* distribution scale and degrees of freedom. In Figure 6 we have used the plot.bspec method and overlain the results found previously by psdcore.

```
library(bspec)
## Attaching package: 'bspec'
##
## The following object is masked from 'package:stats':
##
##
      acf
##
## The following object is masked from 'package:base':
##
##
      sample
print(Bspec <- bspec(ts(magnet$clean)))</pre>
    'bspec' posterior spectrum (one-sided).
##
## frequency range : 0--0.5
## number of parameters: 1025
  finite expectations : none
   finite variances
                        : none
   call: bspec.default(x = ts(magnet$clean))
```

3 Can AR prewhitening improve the spectrum?

This question must be addressed on a case-by-base basis; but, if there is significant auto-regressive structure in the series then the answer is likely YES. The MAGNET dataset is an example where the structure of the series is nicely represented by an AR model with a random noise component.

Recall the results of the prewhitening in Section 2.2. While AR.max was set relatively high, only an AR(6) model was fit significantly, according to the AIC requirements. The estimated variance of the innovations is about 20 nT². If the innovation spectrum is flat (as we expect), this variance translates to power levels of about 16 decibels for a 1 km sampling interval.

```
ntap <- 7
psd_ar <- psdcore(ats_ar, ntaper = ntap, refresh = TRUE)</pre>
```

```
## tap c A 1 1024
## [1] 7
## f creation
## cpp 1:2048 1024 1025 2048
## cpp 2:4096 1024
## cpp
       3:0x7ffeef29b800
       4:1024
## cpp
## cpp 5:(0)0 7 -152.395 -8.20045
## cpp 5:(0)1 7 -17.311 47.8793
## cpp 5:(0)2 7 117.773 103.959
## cpp 5:(0)3 7 206.522 -110.781
## cpp 5:(0)4 7 -35.875 -199.514
## [1] 12.81241
## [1] 49.03806
## [1] -36.22565
dB(mean(psd_ar$spec))
## [1] 15.82778
```

In Figure 7 we have used pilot_spec to model the spectral response of the AR component of the series (solid black line). The non-AR component (labelled "AR-innovations") contributes approximately ± 3 dB to the original spectrum. Overlain on these series is the adaptive spectrum found previously.

4 Assessing spectral properties

4.1 Spectral uncertainties

It is important to place bounds on the uncertainties associated with a spectral estimate. In a multitaper algorithm the uncertainty is distributed as a χ^2_{ν} variate where ν is the number of degrees of freedom, which is twice the number of tapers applied. A proxy for this is simply $1/\sqrt{\nu-1}$. Using $\nu=2*K$ we can approximate the distribution of uncertainties from the tapers alone; however, a more rigorous estimate comes from evaluating the appropriate distribution for a coverage probability (e.g. p=0.95). Among other calculations, spectral_properties returns the χ^2_{ν} based confidence intervals for p=0.95, as well as the approximate uncertainties.

To illustrate, we plot the uncertainties for an integer sequence⁴ of tapers [0,50], shown in Figure 8. The benefits of having more than just a few tapers becomes obvious, though the spectral uncertainty is asymptotically decreasing with taper numbers and yields only slight improvements with logarithmic number of tapers.

Returning to the Project MAGNET spectra, we will compare the spectral uncertainties from psd to the those from bspec, the Bayesian method, for a coverage probability of 95%. Figure 9 shows the uncertainties as bounded polygons, which we calculate here:

```
spp <- spectral_properties(Pspec$taper, db.ci = TRUE)</pre>
```

⁴ Note the χ^2_{ν} distribution is defined for non-negative, non-integer degrees of freedom, but we cannot apply fractions of tapers.

```
## Error in UseMethod("spectral_properties"): no applicable method for 'spectral_properties' applied
to an object of class "c('integer', 'numeric')"
spa <- spectral_properties(Aspec$taper, db.ci = TRUE)</pre>
## Error in UseMethod("spectral_properties"): no applicable method for 'spectral_properties' applied
to an object of class "c('integer', 'numeric')"
str(spa)
## Error in str(spa): object 'spa' not found
create_poly <- function(x, y, dy, from.lower = FALSE) {</pre>
    xx \leftarrow c(x, rev(x))
    if (from.lower) {
        yy \leftarrow c(y, rev(y + dy))
        yy \leftarrow c(y + dy, rev(y - dy))
    return(data.frame(xx = xx, yy = yy))
}
psppu <- create_poly(Pspec$freq, dB(Pspec$spec), spp$stderr.chi.upper)</pre>
## Error in create_poly(Pspec$freq, dB(Pspec$spec), spp$stderr.chi.upper): object 'spp' not found
pspau <- create_poly(Aspec$freq, dB(Aspec$spec), spa$stderr.chi.upper)</pre>
## Error in create_poly(Aspec$freq, dB(Aspec$spec), spa$stderr.chi.upper): object 'spa' not found
# and the Bayesian spectrum 95% limits
pspb <- create_poly(Bspec_plt$freq, Bspec_plt$spectrum[, 1], Bspec_plt$spectrum[,</pre>
  3], from.lower = TRUE)
```

4.2 Spectral resolution

There is an inherent tradeoff between the number of tapers applied and the spectral resolution (effectively, the spectral bandwidth). In general, the greater the number of tapers applied, the lower the spectral resolution. We can use the information returned from **spectral_properties** to visualize the actual differences in resolution for the Project MAGNET PSD estimates; these are shown in Figure 10.

4.3 Visualizing the adaptive history

One might be curious to study how the uncertainties change with each iteration. pspectrum saves an array of "historical" data in its working environment. Specifically, it saves the frequencies, spectral values, and number of tapers at each stage of the adaptive procedure, accessible with get_adapt_history. To ensure a fresh calculation and to add a few more iterations to visualize, we repeat the adaptive spectral analysis, and then bring the stage history into the .GlobalEnv environment:

```
pspectrum(ats_lm, niter = 4, plot = FALSE)

## Stage 0 est. (pilot)
## environment ** .psdEnv ** refreshed
```

```
## detrending (and demeaning)
## tap c A 1 1024
## f creation
## f creation
## Stage 1 est. (Ave. S.V.R. -16.0 dB)
## f creation
## Stage 2 est. (Ave. S.V.R. -27.2 dB)
## f creation
```

```
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeecb04800
## cpp 4:1024
## cpp 5:(0)0 175 2.13163e-14 0
## cpp 5:(0)1 176 -93.2315 227.168
## cpp 5:(0)2 177 604.964 569.429
## cpp 5:(0)3 177 1159.71 -664.567
## cpp 5:(0)4 176 -296.747 -1156.83
## [1] 20.53588
## [1] 56.61905
## [1] -36.08317
## Stage 3 est. (Ave. S.V.R. -41.1 dB)
## f creation
## cpp 1:2048 1024 1024 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeee7d6200
## cpp 4:1024
## cpp 5:(0)0 164 2.13163e-14 0
## cpp 5:(0)1 164 -93.2315 227.168
## cpp 5:(0)2 164 604.964 569.429
## cpp 5:(0)3 164 1159.71 -664.567
## cpp 5:(0)4 164 -296.747 -1156.83
## [1] 20.53588
## [1] 56.59701
## [1] -36.06112
## Stage 4 est. (Ave. S.V.R. -43.4 dB)
## Normalized single-sided PSD (PSD) to single-sided PSD for sampling-freq. 1
str(AH <- get_adapt_history())</pre>
## List of 3
## $ freq : num [1:1024] 0 0.000489 0.000978 0.001466 0.001955 ...
## $ stg_kopt:List of 5
## ..$ :Class 'tapers' atomic [1:1025] 14 14 14 14 14 14 14 14 14 14 ...
## ..... attr(*, "n_taper_limits")= num [1:2] 1 14
## ..... attr(*, "taper_positions")= logi NA
   .. .. ..- attr(*, "span_was_set")= logi TRUE
    ..... attr(*, "n_taper_limits_orig")= num [1:2] 1 14
    ..$: int [1:1024] 52 51 50 49 48 47 46 45 44 43 ...
##
    ..$: int [1:1024] 92 91 90 89 88 87 86 85 84 83 ...
##
    ..$: int [1:1024] 174 175 176 177 177 176 175 174 173 172 ...
##
##
    ## $ stg_psd :List of 5
##
    ..$ : num [1:1024] 1309 1698 1241 1075 1112 ...
##
   ..$ : num [1:1024] 1185 1190 1193 1192 1193 ...
## ..$ : num [1:1024] 1310 1307 1304 1300 1295 ...
## ..$: num [1:1024] 1277 1277 1277 1277 1277 ...
## ..$: num [1:1024] 1285 1286 1286 1286 1286 ...
```

Followed by some trivial manipulation:

```
Freqs <- (AH$freq)
Dat <- AH$stg_psd
numd <- length(Freqs)
numit <- length(Dat)
StgPsd <- dB(matrix(unlist(Dat), ncol = numit))
Dat <- AH$stg_kopt
StgTap <- matrix(unlist(Dat), ncol = numit)

## Warning in matrix(unlist(Dat), ncol = numit): data length [5121] is not a sub-multiple or multiple of the number of rows [1025]</pre>
```

We can plot these easily with matplot or other tools. We show the adaptive history in Figure 11. It may be informative to investigate cross correlation coefficients between the stages; but, in this case, only the PSD estimates are significantly correlated:

```
suppressWarnings(symnum(cP <- cor(StgPsd)))

##
## [1,] 1
## [2,] B 1
## [3,] B B 1
## [4,] B B B 1
## [5,] B B B B 1
## attr(,"legend")
## [1] 0 ' ' 0.3 '.' 0.6 ',' 0.8 '+' 0.9 '*' 0.95 'B' 1</pre>
```

5 Call overview

Shown in Figure 12 is a flow chart highlighting the essential functions involved in the adaptive estimation process. The primary function is pspectrum.

Session Info

```
utils::sessionInfo()
## R version 3.1.2 (2014-10-31)
## Platform: x86_64-apple-darwin13.4.0 (64-bit)
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
## attached base packages:
               graphics grDevices utils
## [1] stats
                                          datasets methods
## [7] base
##
## other attached packages:
## [1] bspec_1.4 ggplot2_1.0.0
                                           signal_0.7-4
## [4] RColorBrewer_1.1-2 RSEIS_3.3-3
                                           psd_0.5-0
## [7] fftw_1.0-3
                       knitr_1.9
##
## loaded via a namespace (and not attached):
## [1] colorspace_1.2-4 digest_0.6.8 evaluate_0.5.5
## [4] formatR_1.0
                      grid_3.1.2
                                      gtable_0.1.2
## [7] highr_0.4 labeling_0.3 lattice_0.5 munsell_0.4.2 plyr_1.8.1
                      labeling_0.3 lattice_0.20-29
## [13] proto_0.3-10 Rcpp_0.11.4
                                      reshape2_1.4.1
## [16] RPMG_2.1-5 Rwave_2.2
                                       scales_0.2.4
                      tools_3.1.2
## [19] stringr_0.6.2
                                       zoo_1.7-11
```

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Raw and Clean Project MAGNET power spectral density

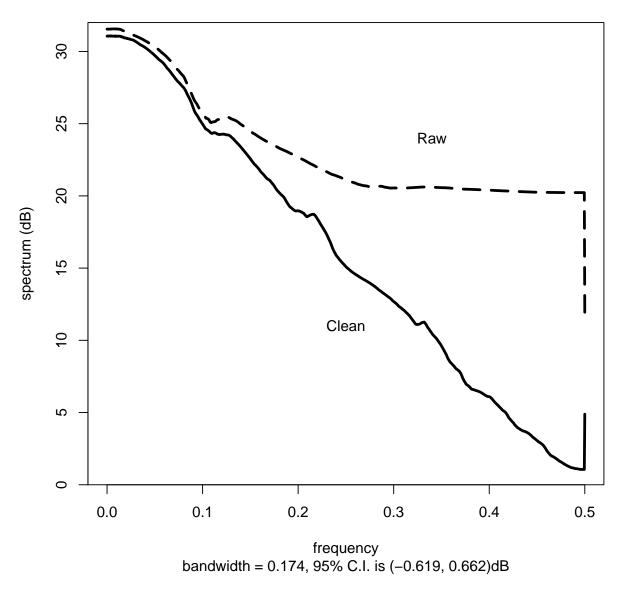
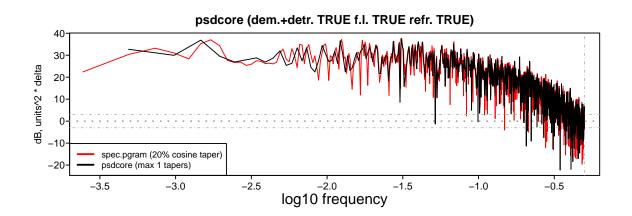


Figure 1: Power spectral density estimates for the raw and cleaned Project MAGNET data bundled with psd. Note that because the class is 'spec' we have utilized existing methods in the stats namespace.

```
ntap <- psdc$taper
psdcore(magnet$clean, ntaper = ntap, refresh = TRUE, plotpsd = TRUE)
                                            ## tap c B
                                           ## f creation
## cpp 1:2048 1024 1 2048
## cpp 2:4096 1024
        ## Warning in resample_fft_rcpp(fftz, kseq, verbose = verbose): forced taper length
## cpp 3:0x7ffeebdf7a00
## cpp 4:1024
## cpp 5:(0)0 1 -791.427 -115.093
## cpp 5:(0)1 1 -93.2315 227.168
## cpp 5:(0)2 1 604.964 569.429
## cpp 5:(0)3 1 1159.71 -664.567
## cpp 5:(0)4 1 -296.747 -1156.83
## [1] 20.53588
## [1] 56.63675
## [1] -36.10087
           ## Error in xy.coords(x, y, xlabel, ylabel, log): 'x' and 'y' lengths differ
```



```
plot(ts.union(orig.plus.trend = mc, linear = ats_lm, ar = ats_ar), yax.flip = TRUE,
    main = sprintf("Prewhitened Project MAGNET series"))
mtext(sprintf("linear and linear+AR(%s)", atsar$ardfit$order), line = 1.1)
```

Prewhitened Project MAGNET series linear and linear+AR(6) 3000 orig.plus.trend 2000 1000 30 -10 -30 15 ä -15 0 500 1000 1500 2000

Figure 3: Pre-whitening of the Project MAGNET series (with a synthetic linear model superimposed on it) assuming linear and linear-with-AR models.

Time

PSD Comparisons

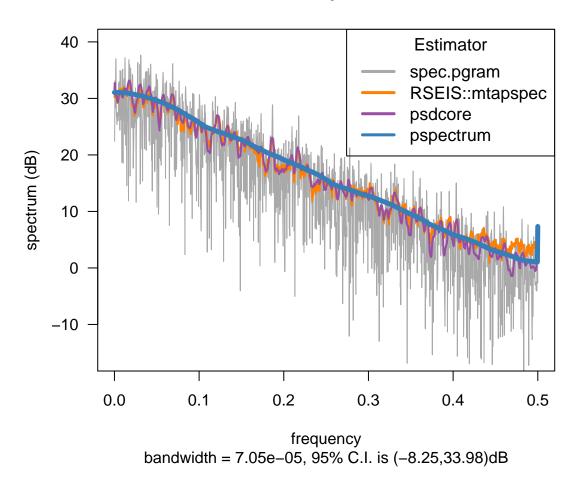


Figure 4: Comparisons of estimations of Project MAGNET power spectral densities.

```
library(ggplot2)
gr <- ggplot(df, aes(x = x, y = res)) + geom_abline(intercept = 0, slope = 0,
    size = 2, color = "salmon") + geom_point(aes(color = tap))
print(gr + theme_bw() + ggtitle("Regression residuals, colored by optimized tapers") +
    xlab("Power levels, dB") + ylab(""))</pre>
```

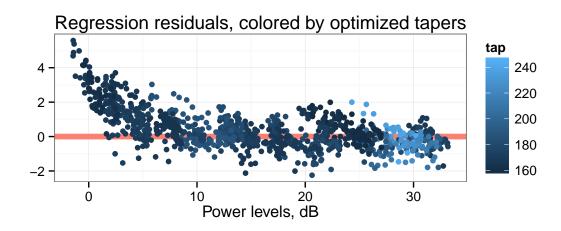


Figure 5: Linear regression residuals of mtapspec against psdcore for Project MAGNET PSD estimates.

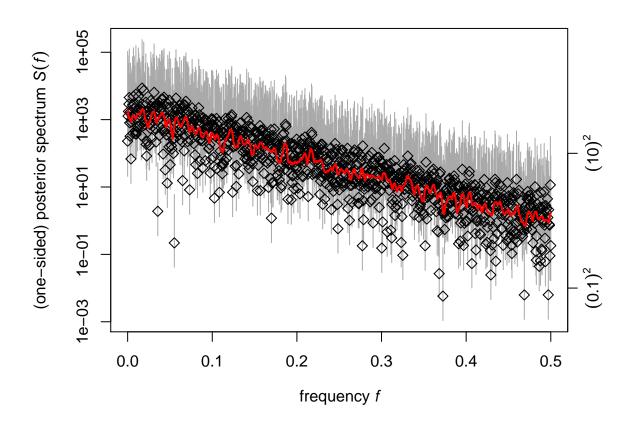
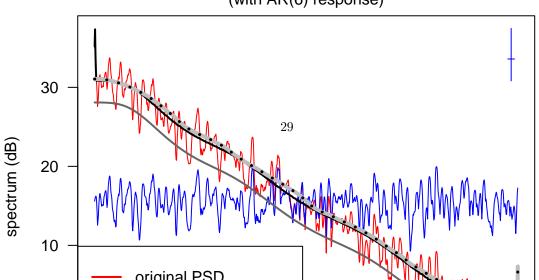


Figure 6: Project MAGNET PSD estimates from bapec, a Bayesian method, compared to the padcore results shown in Figure 4.

```
pilot_spec(ats_lm, ntap = ntap, remove.AR = 100, plot = TRUE)
                                         ## tap c A 1 1024
## [1] 7
                                           ## f creation
## cpp 1:2048 1024 1025 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeef042600
## cpp 4:1024
## cpp 5:(0)0 7 13.2137 0
## cpp 5:(0)1 7 -11.9169 39.4713
## cpp 5:(0)2 7 117.779 99.7275
## cpp 5:(0)3 7 207.127 -113.584
## cpp 5:(0)4 7 -35.8685 -201.63
## [1] 12.81242
## [1] 49.03509
## [1] -36.22267
                                         ## tap c A 1 1024
## [1] 7
                                           ## f creation
## cpp 1:2048 1024 1025 2048
## cpp 2:4096 1024
## cpp 3:0x7ffeef89ce00
## cpp 4:1024
## cpp 5:(0)0 7 -791.427 -115.093
## cpp 5:(0)1 7 -93.2315 227.168
## cpp 5:(0)2 7 604.964 569.429
## cpp 5:(0)3 7 1159.71 -664.567
## cpp 5:(0)4 7 -296.747 -1156.83
## [1] 20.53588
## [1] 56.93057
## [1] -36.39469
plot(Aspec, log = "dB", add = TRUE, col = "grey", lwd = 4)
plot(Aspec, log = "dB", add = TRUE, lwd = 3, lty = 3)
spec.ar(ats_lm, log = "dB", add = TRUE, lwd = 2, col = "grey40")
```

Pilot spectrum estimation

(with AR(6) response)



Spectral uncertainties

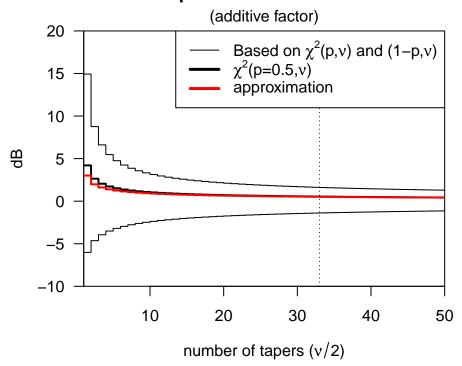


Figure 8: Additive spectral uncertainties by number of tapers needed to create 95% confidence intervals. These quantized curves are found by evaluating the χ^2_{ν} distribution, where ν is the number of degrees of freedom (two per taper). The thick, red line shows an approximation to these uncertainties based on $1/\sqrt{\nu-1}$, which is accurate to within a few percent in most cases. The vertical dotted-line shows the number of tapers need to make the width less than 3 decibels.

Project MAGNET Spectral Uncertainty (p > 0.95)

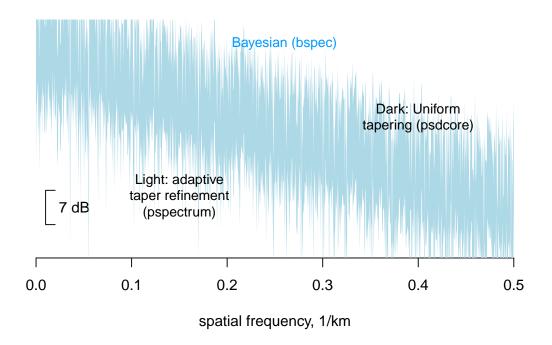
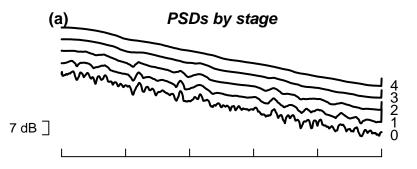


Figure 9: Project MAGNET spectral uncertainties for 95% coverage probability. The filled regions encompass the spectral uncertainties values based on the upper χ^2_{ν} curve shown in Figure 8, light and dark for PSDs with and without adaptive taper optimization, respectively. The results from Figure 6 (Bayesian method) are shown in blue.

```
frq <- Aspec$freq
relp <- (spa$resolution - spp$resolution)/spp$resolution
                   ## Error in eval(expr, envir, enclos): object 'spa' not found
par(las = 1, oma = rep(0, 4), omi = rep(0, 4), mar = c(4, 3, 2, 0))
layout(matrix(c(1, 2), 1, 2, byrow = TRUE), heights = c(2, 2), widths = c(3, 2)
    0.5), respect = TRUE)
plot(frq, relp, main = "Percent change in spectral resolution", col = "light grey",
    ylim = yl <- range(pretty(relp)), type = "h", xaxs = "i", ylab = "dB",</pre>
    xlab = "frequency, 1/km")
             ## Error in xy.coords(x, y, xlabel, ylabel, log): object 'relp' not found
lines(frq, relp)
                        ## Error in xy.coords(x, y): object 'relp' not found
text(0.25, 45, "Adaptive relative to fixed", cex = 0.9)
## Error in text.default(0.25, 45, "Adaptive relative to fixed", cex = 0.9): plot.new has not been
                                             called yet
par(mar = c(4, 0, 2, 2))
# empirical distribution of values
boxplot(relp, range = 0, main = sprintf("%.01f", median(relp)), axes = FALSE,
    ylim = yl, yaxs = "i", notch = TRUE)
  ## Error in boxplot(relp, range = 0, main = sprintf("%.01f", median(relp)), : object 'relp' not
                                                found
axis(4)
                       ## Error in axis(4): plot.new has not been called yet
```

Figure 10: Relative changes in resolution of the adaptive method relative to the fixed multitaper method, plotted as a function of spatial frequency in units of percent. The non-zero median value implies the pilot spectrum was found using too-few tapers, according to the optimization algorithm. Positive values indicate broadening resolution bandwidth.

Adaptive estimation history



```
## Error in xy.coords(x, y, xlabel, ylabel, log): 'x' and 'y' lengths differ
## Error in mtext("(b)", font = 2, adj = 0, line = 0.5): plot.new has not been called yet
## Error in mtext("Tapers by stage", line = 0.5, font = 4): plot.new has not been called yet
```

```
## Error in data.frame(xx = xx, yy = yy): arguments imply differing number of rows: 2048, 2050
## Error in mtext("(c)", font = 2, adj = 0, line = 0.6): plot.new has not been called yet
## Error in plot.xy(xy.coords(x, y), type = type, ...): plot.new has not been called yet
## Error in text.default(-0.06, -3.5 - 10, "7 dB", cex = 0.8): plot.new has not been called yet
## Error in mtext("Uncertainties by stage", line = 0.6, font = 4): plot.new has not been called
yet
## Error in mtext("Spatial frequency, 1/km", side = 1, line = 2.3): plot.new has not been called
yet
## Error in text.default(0.25, -14.5, "(pilot spectrum - uniform tapers)", : plot.new has not been
called yet
```

Figure 11: Adaptive spectral estimation history. (A) PSD series for each stage of the adaptive method, offset by a few decibels for visualization purposes. Filled polygons are shown in (B) for the number of tapers at each stage, and (C) the relative uncertainties of the PSDs.

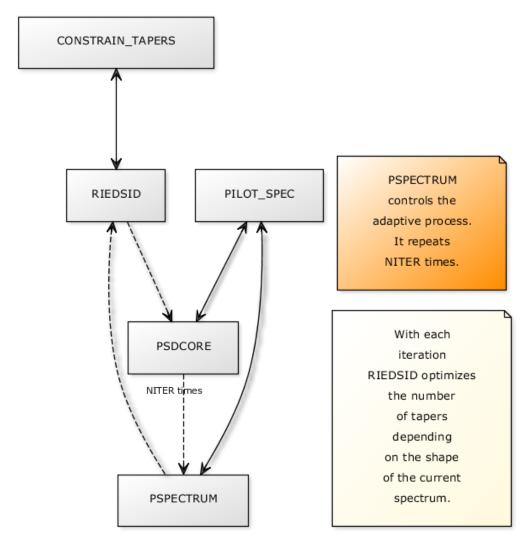


Figure 12: Simplified call graph for psd. The dashed lines show a simplified circuit which the spectra and its tapers make during the iterative process.