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.

Contents

1 Quick start: A minimal example.

First, we load the package into the namespace:

```
library(psd)

## Loaded psd (2.1.1) - Adaptive multitaper spectrum estimation; see ?pspectrum
```

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)
```

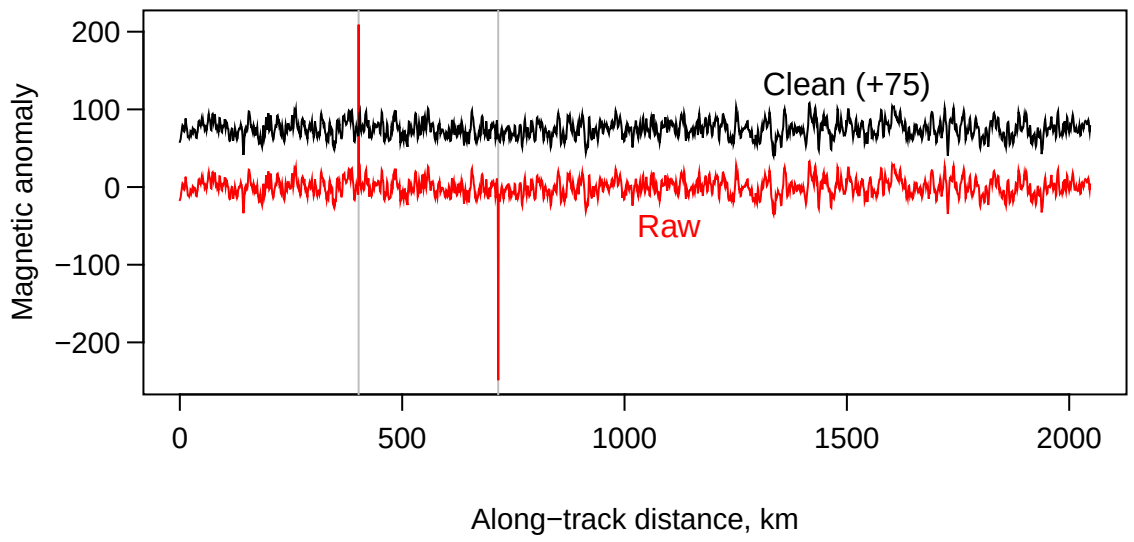
The format of the data set is a `data.frame` with four sets of information:

```
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; but, as we will see, the outliers adversely affect the accuracy of any type PSD estimate, regardless of the level of sophistication of the method.

```
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 are readily apparent in the timeseries:



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)
## Stage  1 est.  (Ave.  S.V.R. -13.0 dB)
## Stage  2 est.  (Ave.  S.V.R. -27.2 dB)
## Stage  3 est.  (Ave.  S.V.R. -44.4 dB)
## Normalized  single-sided  psd estimates ( psd ) for sampling-freq.   1

psdc <- pspectrum(magnet$clean)

## Stage  0 est.  (pilot)
## environment  ** .psdEnv **  refreshed
## detrending (and demeaning)
## Stage  1 est.  (Ave.  S.V.R. -13.1 dB)
## Stage  2 est.  (Ave.  S.V.R. -27.8 dB)
## Stage  3 est.  (Ave.  S.V.R. -44.9 dB)
## Normalized  single-sided  psd estimates ( psd ) for sampling-freq.   1
```

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. Note that if the user forgets to assign the results of `pspectrum` to the global environment, the result can be recovered with the `psd_envGet` function:

```
psdc_recovered <- psd_envGet("final_psd")
all.equal(psdc, psdc_recovered)

## [1] TRUE
```

In general, spectral variance is reduced with sequential refinements[1], but is not necessarily guaranteed to reduce monotonically.

Figure 1 compares power spectra for the `raw` and `clean` series produced by `stats::spectrum` and `pspectrum`[2] using default settings. We expect the Project MAGNET data to be linear in the space of linear-frequencies and logarithmic-power; in fact there is 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 the type of 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 shorter wavelengths – features which could be difficult to judge with high spectral variance.

[1] Messages are given by default; ones which read "Ave. S.V.R." are in reference to average spectral-variance reduction, which we define here as the variance of the double-differenced spectra at each stage, relative to the spectral variance in the pilot estimate.

[2] Note that `pspectrum` returns an object with class `spec` (and `amt`), so we have access to methods within `stats`, including `plot.spec`.

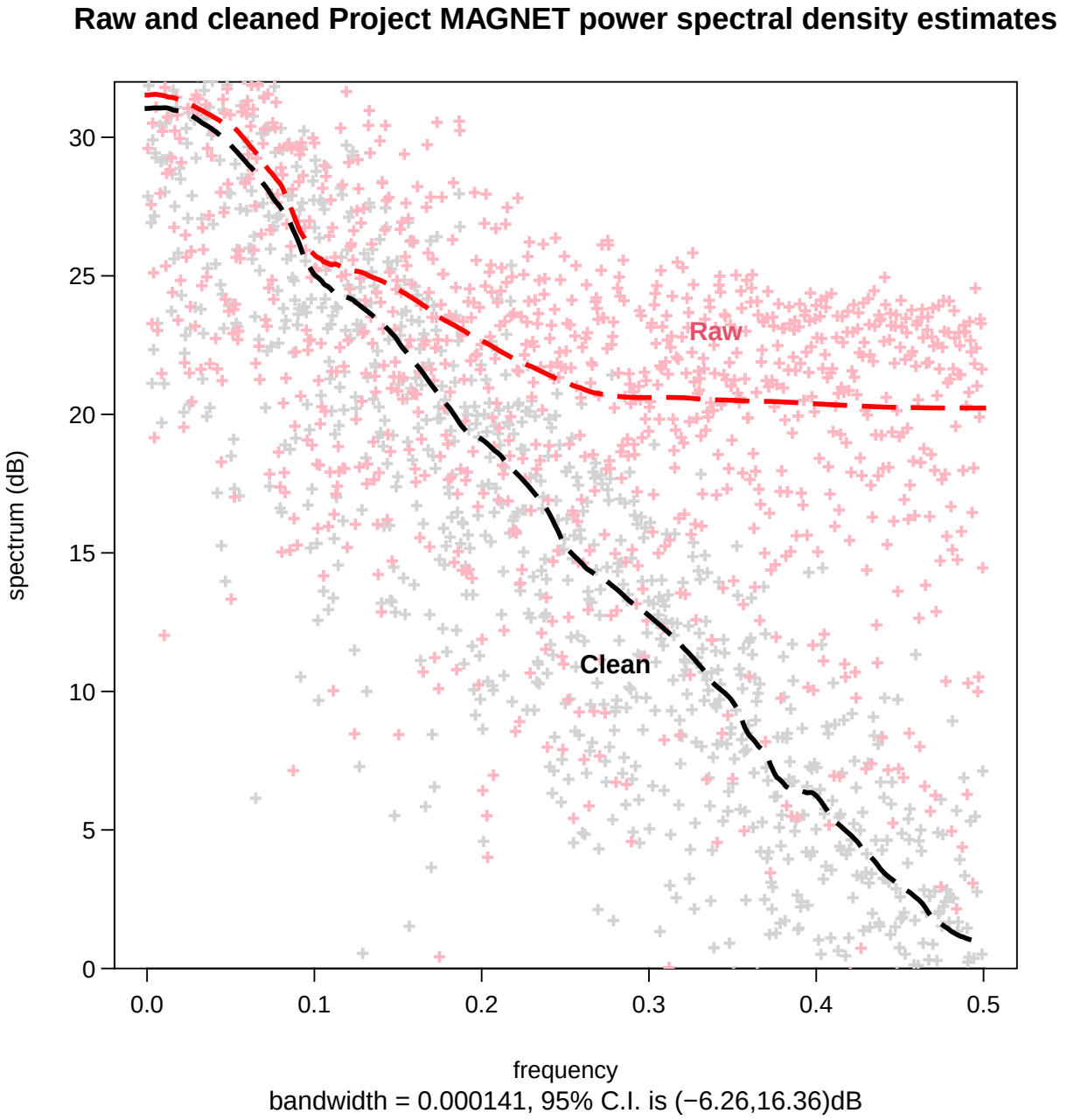


Figure 1: Power spectral density estimates for the raw and cleaned Project MAGNET data bundled with `psd`: see `?magnet`. Points are estimates produced by `spectrum` and dashed lines are estimates produced by `pspectrum`, using the default settings. *Note that because the objects class includes 'spec', we have utilized existing methods in the `stats` namespace. The bandwidth and confidence interval estimates are for the `spectrum`-based result.*

2 Comparisons with other methods

As we have shown in the Project MAGNET example, a more accurate estimate of the power spectrum can help improve understanding of the physics behind the signals in the data. But, 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); Barbour et al. (2020)
`spectrum`	`stats`	No	No	double	R Core Team (2014)
`spec.mtm`	`multitaper`	Yes	Yes	double	Rahim et al. (2014)
`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` (which was used for the estimates in Figure 1) 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 cosine-tapered periodogram, found with a command equivalent to this:

```
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 then re-calculate the multitaper PSD and the raw periodogram with `plot=TRUE`; these results are shown in Figure 2.

```r
ntap <- psdc[["taper"]]  # get the previous vector of tapers
psdcore(magnet$clean, ntaper = ntap, refresh = TRUE, plot = TRUE)
```

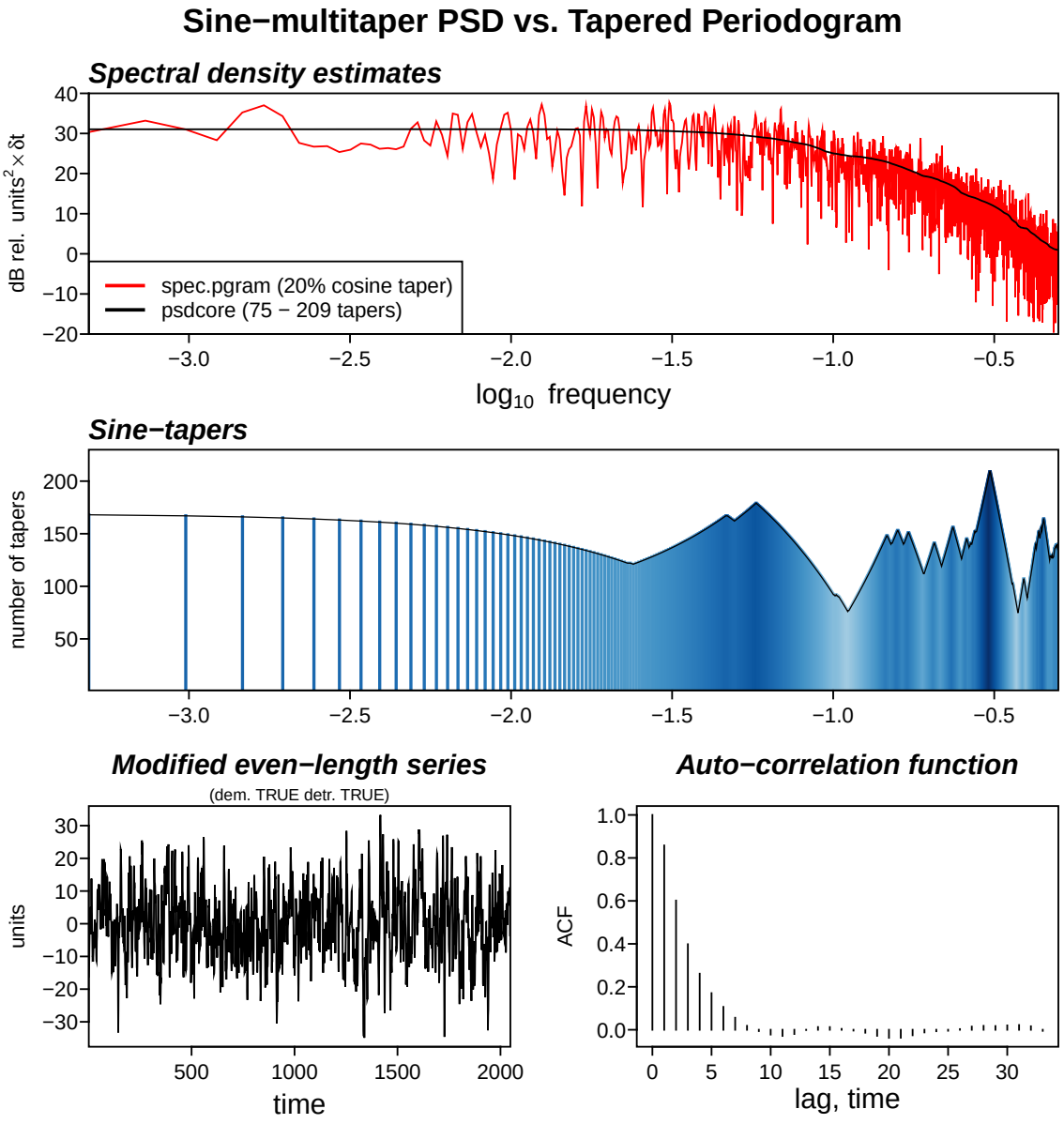


Figure 2: A summary plot produced by `psdcore` when `plot=TRUE`. Top: Comparison between PSD estimators for the cleaned Project MAGNET data. The frequency axis is in units of $\log_{10}$ km^{-1}, and power axis is in decibels. Middle: The number of tapers applied as a function of frequency from the `plot.tapers` method. Bottom: The spatial series used to estimate the PSDs and a subset of the full autocorrelation function.

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, but 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:

```
library(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),
    plot = FALSE))

## detrending (and demeaning)

##         Length Class  Mode
## lmdfit     0   -none- NULL
## ardfit     0   -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 data[3]. This fit uses the Akaike Information Criterion (AIC) to select the highest order appropriate for the data.

```
summary(atsar <- prewhiten(mc, AR.max = 100, plot = FALSE))

## detrending (and demeaning)
## autoregressive model fit (returning innovations)

##         Length Class  Mode
## lmdfit     0   -none- NULL
## ardfit    15   ar     list
## prew_lm 2048   ts     numeric
## prew_ar 2048   -none- numeric
## imputed    1   -none- logical

# linear model:
str(atsar[["lmdfit"]])

##  NULL

ats_lm <- atsar[["prew_lm"]]
# AR model:
str(atsar[["ardfit"]])
```

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

```
## List of 15
##  $ order       : int 6
##  $ ar          : num [1:6] 1.513 -1.104 0.672 -0.388 0.211 ...
##  $ var.pred    : num 19.5
##  $ x.mean      : num 4.49e-17
##  $ aic         : Named num [1:101] 3598.8 872.8 258.2 81 26.3 ...
##   ..- attr(*, "names")= chr [1:101] "0" "1" "2" "3" ...
##  $ n.used      : int 2048
##  $ n.obs       : int 2048
##  $ order.max   : num 100
##  $ partialacf  : num [1:100, 1, 1] 0.8579 -0.5099 0.2894 -0.1653 0.0925 ...
##  $ resid       : Time-Series [1:2048] from 1 to 2048: NA NA NA NA NA ...
##  $ method      : chr "Yule-Walker"
##  $ series      : chr "tser_prew_lm"
##  $ frequency   : num 1
##  $ call        : language ar.yw.default(x = tser_prew_lm, aic = TRUE, order.max = AR.max,      demean = TRUE)
##  $ asy.var.coef: num [1:6, 1:6] 0.000487 -0.000733 0.000526 -0.000304 0.000148 ...
##  - attr(*, "class")= chr "ar"

ats_ar <- atsar[["prew_ar"]]
```

```
plot(ts.union(orig.plus.trend = mc, linear = ats_lm, ar = ats_ar), yax.flip = TRUE,
    main = sprintf("Prewhitened Project MAGNET series"), las = 0)
mtext(sprintf("linear and linear+AR(%s)", atsar[["ardfit"]][["order"]]),
    line = 1.1)
```

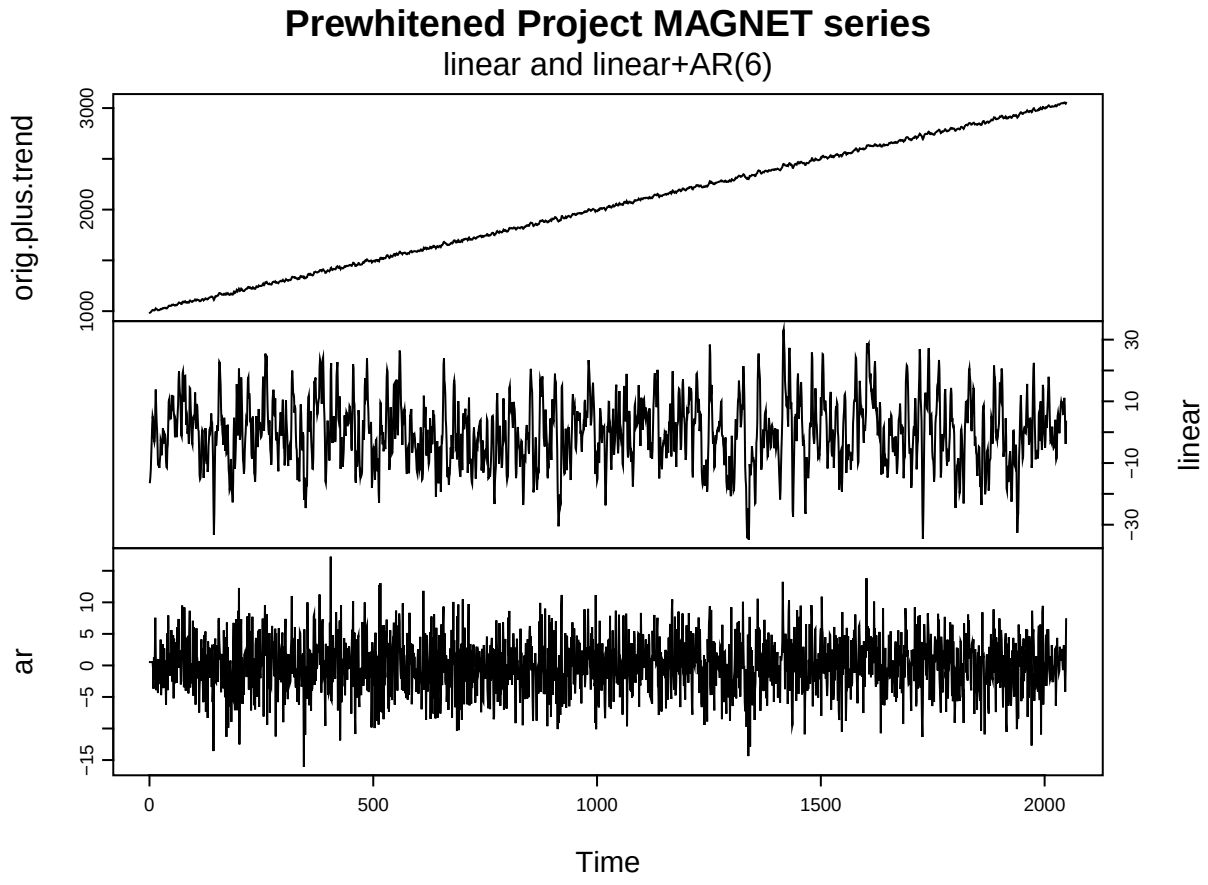


Figure 3: Pre-whitening of the Project MAGNET series (with a synthetic linear model superimposed on it) assuming linear and linear-with-AR models.

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 <- rnorm(32)
all.equal(psdcore(a, 1), psdcore(a, -1))

## [1] TRUE
```

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

```
tapinit <- 10
Mspec <- mtapspec(ats_lm, deltat(ats_lm), MTP = list(kind = 2, inorm = 3,
    nwin = tapinit, npi = 0))
```

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     : Time-Series [1:2048, 1] from 1 to 2048: -16.23 -14.56 -12.02 -7.21 -3.13 ...
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
##   .. ..$ : NULL
##  $ 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 20 ...
##  $ Fv      : 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.

```
Xspec <- spec.pgram(ats_lm, pad = 1, taper = 0.2, detrend = TRUE, demean = TRUE,
    plot = FALSE)
Pspec <- psdcore(ats_lm, ntaper = tapinit)
Aspec <- pspectrum(ats_lm, ntap.init = tapinit)

## Stage  0 est.  (pilot)
## environment  ** .psdEnv **  refreshed
## detrending (and demeaning)
## Stage  1 est.  (Ave.  S.V.R. -12.6 dB)
## Stage  2 est.  (Ave.  S.V.R. -28.3 dB)
## Stage  3 est.  (Ave.  S.V.R. -40.2 dB)
## Normalized  single-sided  psd estimates ( psd ) for sampling-freq.   1

# Correct for double-sidedness of spectrum and mtapspec results
class(Mspec)

## [1] "list"

Mspec <- normalize(Mspec, dt, "spectrum")

## Normalized  double-sided  psd estimates ( spectrum ) for sampling-freq.   1

nt <- seq_len(Mspec[["numfreqs"]])
mspec <- Mspec[["spec"]][nt]
class(Xspec)

## [1] "spec"

Xspec <- normalize(Xspec, dt, "spectrum")

## Normalized  double-sided  psd estimates ( spectrum ) for sampling-freq.   1
```

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

```
library(RColorBrewer)
cols <- c("dark grey", brewer.pal(8, "Set1")[c(5:4, 2)])
lwds <- c(1, 2, 2, 5)
plot(Xspec, log = "dB", ylim = 40 * c(-0.4, 1), ci.col = NA, col = cols[1],
    lwd = lwds[1], main = "PSD Comparisons")
pltf <- Mspec[["freq"]]
pltp <- dB(mspec)
lines(pltf, pltp, col = cols[2], lwd = lwds[2])
plot(Pspec, log = "dB", add = TRUE, col = cols[3], lwd = lwds[3])
plot(Aspec, log = "dB", add = TRUE, col = cols[4], lwd = lwds[4])
legend("topright", c("spec.pgram", "RSEIS::mtapspec", "psdcore", "pspectrum"),
    title = "Estimator", col = cols, lwd = lwds, bg = "grey95", box.col = NA,
    cex = 0.8, inset = c(0.02, 0.03))
```

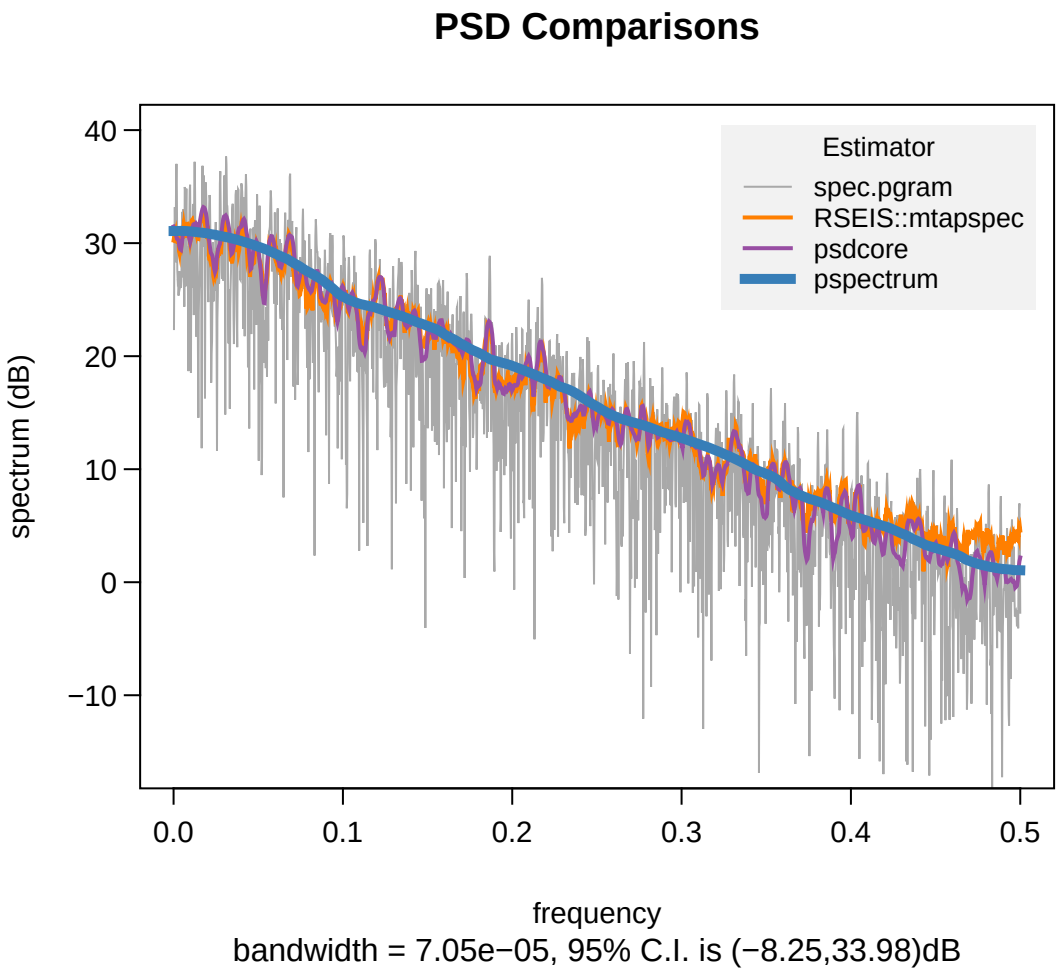


Figure 4: Comparisons of estimations of Project MAGNET power spectral densities.

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"]])
```

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"]]))
summary(dflm <- lm(y ~ x + 0, df))

##
## Call:
## lm(formula = y ~ x + 0, data = df)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -2.2855 -0.3041  0.1996  0.9356  5.5479
##
## Coefficients:
##   Estimate Std. Error t value Pr(>|t|)
## x 0.991899   0.002067   479.8   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.208 on 1023 degrees of freedom
## Multiple R-squared:  0.9956, Adjusted R-squared:  0.9956
## F-statistic: 2.302e+05 on 1 and 1023 DF,  p-value: < 2.2e-16

df$res <- residuals(dflm)
```

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.

```
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))
          ## Warning:  Using 'size' aesthetic for lines was deprecated in ggplot2 3.4.0.
                                ## i Please use 'linewidth' instead.
                           ## This warning is displayed once every 8 hours.
              ## Call 'lifecycle::last_lifecycle_warnings()' to see where this warning
                                       ## was generated.

print(gr + theme_bw() + ggtitle("Regression residuals, colored by optimized tapers") +
    xlab("Power levels, dB") + ylab(""))
```

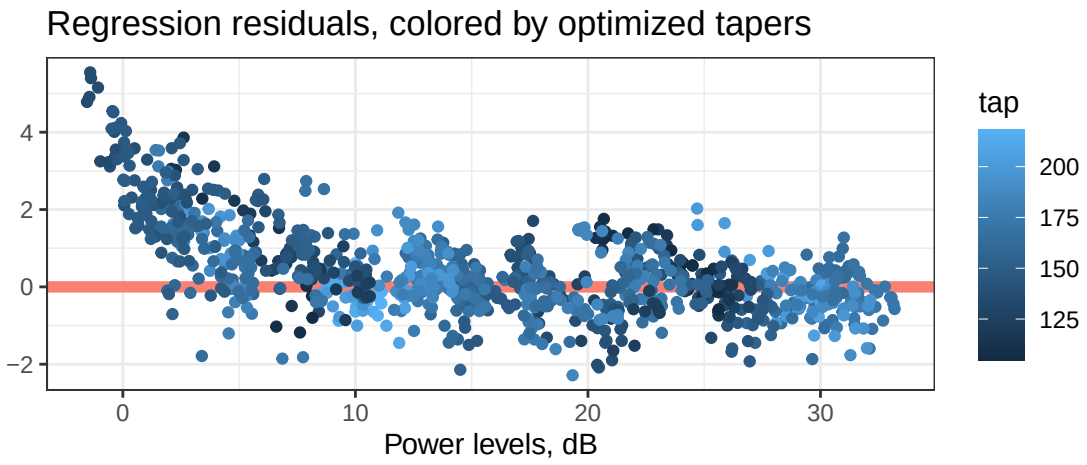


Figure 5: Linear regression residuals of `mtapspec` against `psdcore` for Project MAGNET PSD estimates.

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 (2015) 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

This package was previously orphaned but, as of this writing, the package has a new maintainer, so we may add a comparison in future versions of this document.

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)))

##  '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))
```

```r
par(las = 0)
Bspec_plt <- plot(Bspec)
with(Pspec, lines(freq, spec, col = "red", lwd = 2))
```

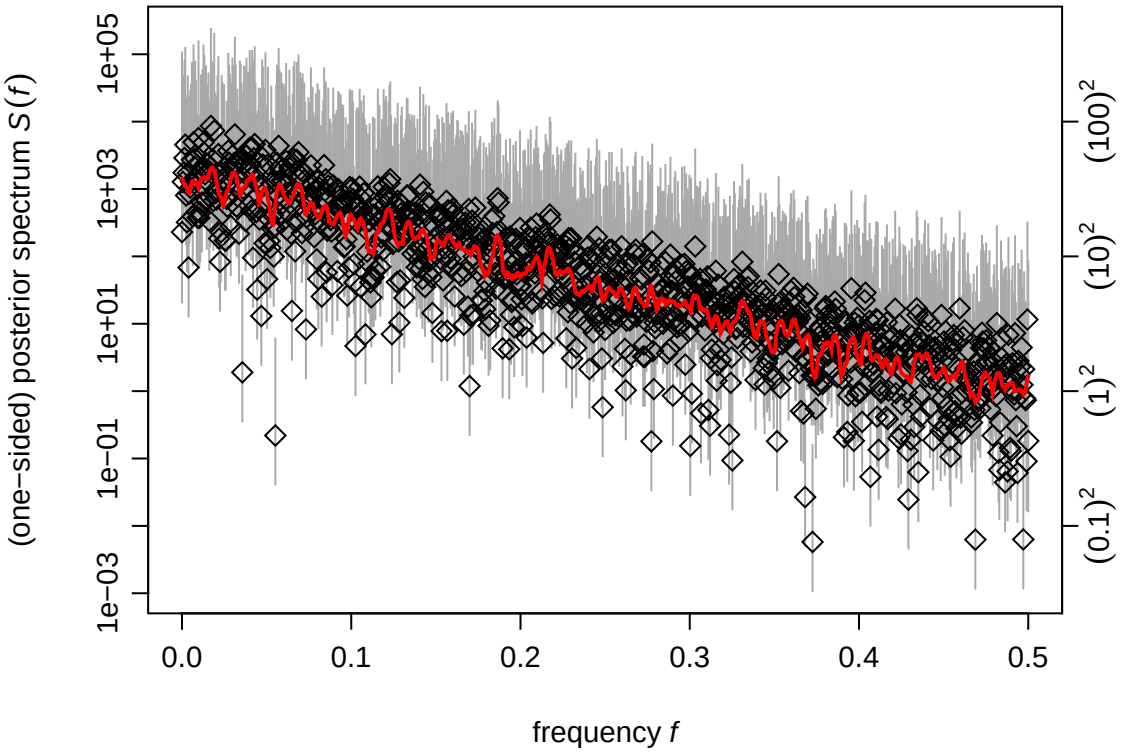


Figure 6: Project MAGNET PSD estimates from `bspec`, a Bayesian method, compared to the `psdcore` results shown in Figure 4.

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 nT^2. 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)
dB(mean(psd_ar$spec))

## [1] 15.82754
```

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 (labeled "AR-innovations") contributes approximately ±3 dB to the original spectrum. Overlain on these series is the adaptive spectrum found previously.

```
pilot_spec(ats_lm, ntap = ntap, remove.AR = 100, plot = TRUE)
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")
```

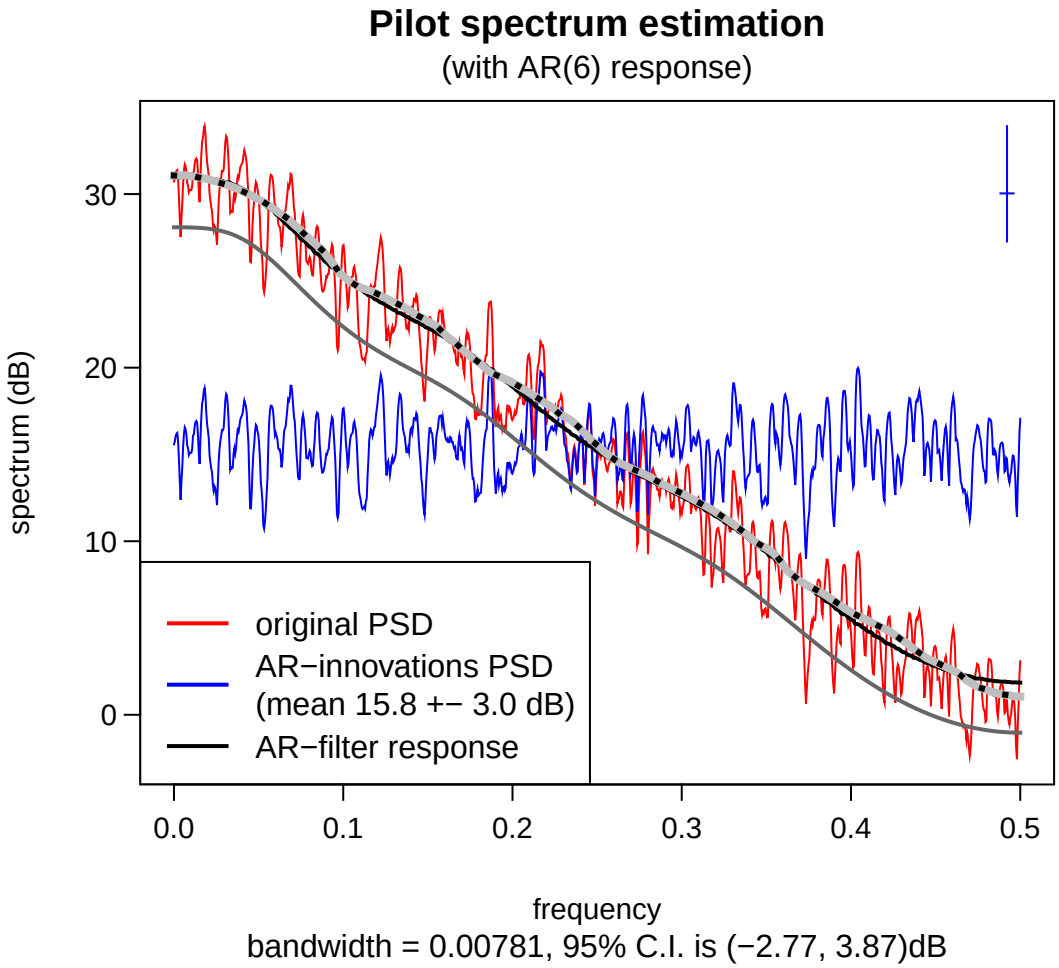


Figure 7: AR response spectrum for the MAGNET dataset produced by `pilot_spec`. Overlain on the figure is the adaptive estimation from Figure 4 (dotted line), and the results from `spec.ar` in dark grey; the shift is due to a normalization difference.

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 sequence[4] 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)
spa <- spectral_properties(Aspec[["taper"]], db.ci = TRUE)
str(spa)

## 'data.frame': 1024 obs. of  8 variables:
##  $ taper            : int  166 166 166 166 165 165 164 164 163 163 ...
##  $ stderr.chi.lower : num  -0.639 -0.639 -0.639 -0.639 -0.641 ...
##  $ stderr.chi.upper : num  0.684 0.684 0.684 0.684 0.686 ...
##  $ stderr.chi.median: num  0.233 0.233 0.233 0.233 0.233 ...
##  $ stderr.chi.approx: num  0.232 0.232 0.232 0.232 0.233 ...
##  $ resolution       : num  0.326 0.326 0.326 0.326 0.324 ...
##  $ dof              : num  332 332 332 332 330 330 328 328 326 326 ...
##  $ bw               : num  0.163 0.163 0.163 0.163 0.162 ...

psppu <- with(Pspec, create_poly(freq, dB(spec), spp$stderr.chi.upper))
pspau <- with(Aspec, create_poly(freq, dB(spec), spa$stderr.chi.upper))
# and the Bayesian spectrum 95% posterior distribution range
pspb <- with(Bspec_plt, create_poly(freq, spectrum[, 1], spectrum[, 3], from.lower = TRUE))
```

[4] Note the χ^2_ν distribution is defined for non-negative, non-integer degrees of freedom, but we cannot apply fractions of tapers.

```
sp <- spectral_properties(as.tapers(1:50), p = 0.95, db.ci = TRUE)
plot(stderr.chi.upper ~ taper, sp, type = "s", ylim = c(-10, 20), yaxs = "i",
    xaxs = "i", xlab = expression("number of tapers (" * nu/2 * ")"), ylab = "dB",
    main = "Spectral uncertainties")
mtext("(additive factors)", line = 0.3, cex = 0.8)
lines(stderr.chi.lower ~ taper, sp, type = "s")
lines(stderr.chi.median ~ taper, sp, type = "s", lwd = 2)
lines(stderr.chi.approx ~ taper, sp, type = "s", col = "red", lwd = 2)
# to reach 3 db width confidence interval at p=.95
abline(v = 33, lty = 3)
abline(h = 0, lty = 3)
legend("topright", c(expression("Based on " * chi^2 * "(p," * nu * ") and (1-p," *
    nu * ")"), expression("" * chi^2 * "(p=0.5," * nu * ")"), "approximation"),
    lwd = c(1, 3, 3), col = c("black", "black", "red"), bg = "white")
```

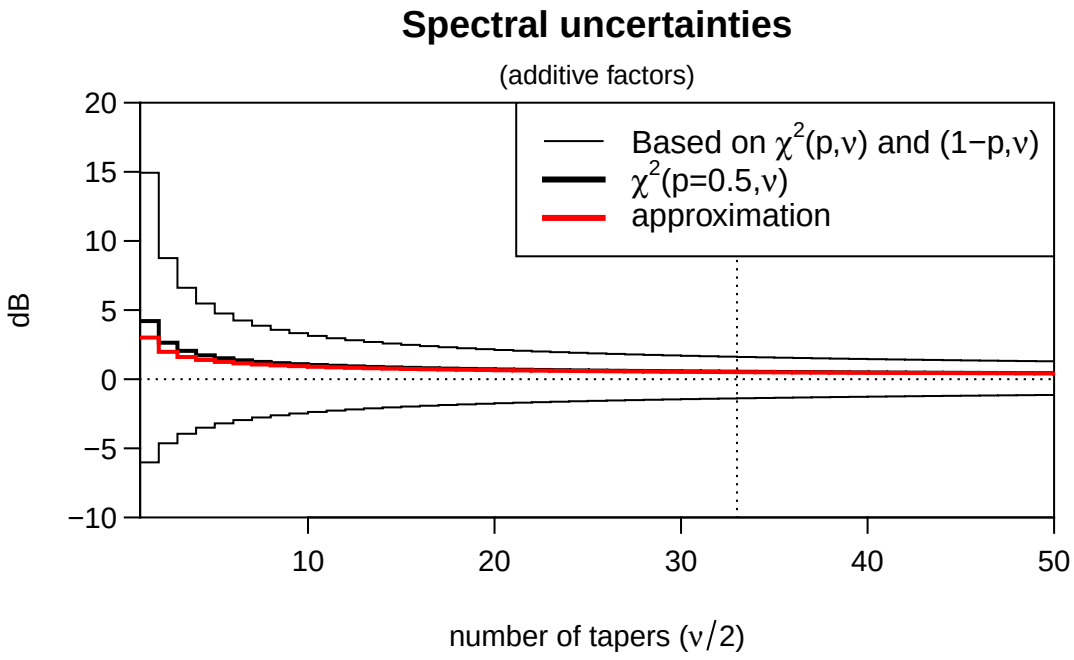


Figure 8: Additive spectral uncertainties by number of tapers needed to create 95% confidence intervals. These quantized curves are found by evaluating the χ^2_ν distribution, where ν is the number of degrees of freedom (two per taper). The thick, red line shows an approximation to these uncertainties 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.

```
plot(c(-0.005, 0.505), c(-5, 40), col = NA, xaxs = "i", main = "Project MAGNET Spectral Uncertainty (p > 0.95)",
    ylab = "", xlab = "spatial frequency, 1/km", yaxt = "n", frame.plot = FALSE)
lines(c(2, 1, 1, 2) * 0.01, c(0, 0, 7, 7))
text(0.04, 3.5, "7 dB")
with(pspb, polygon(x.x, dB(y.y), col = "light blue", border = NA))
text(0.26, 37, "Posterior distribution\n(bspec)", col = "#0099FF", cex = 0.8)
with(psppu, polygon(x.x, y.y, col = "dark grey", border = "black", lwd = 0.2))
text(0.15, 6, "Light: adaptive\ntaper refinement\n(pspectrum)", cex = 0.8)
with(pspau, polygon(x.x, y.y, col = "light grey", border = "black", lwd = 0.2))
text(0.4, 22, "Dark: Uniform\ntapering (psdcore)", cex = 0.8)
box()
```

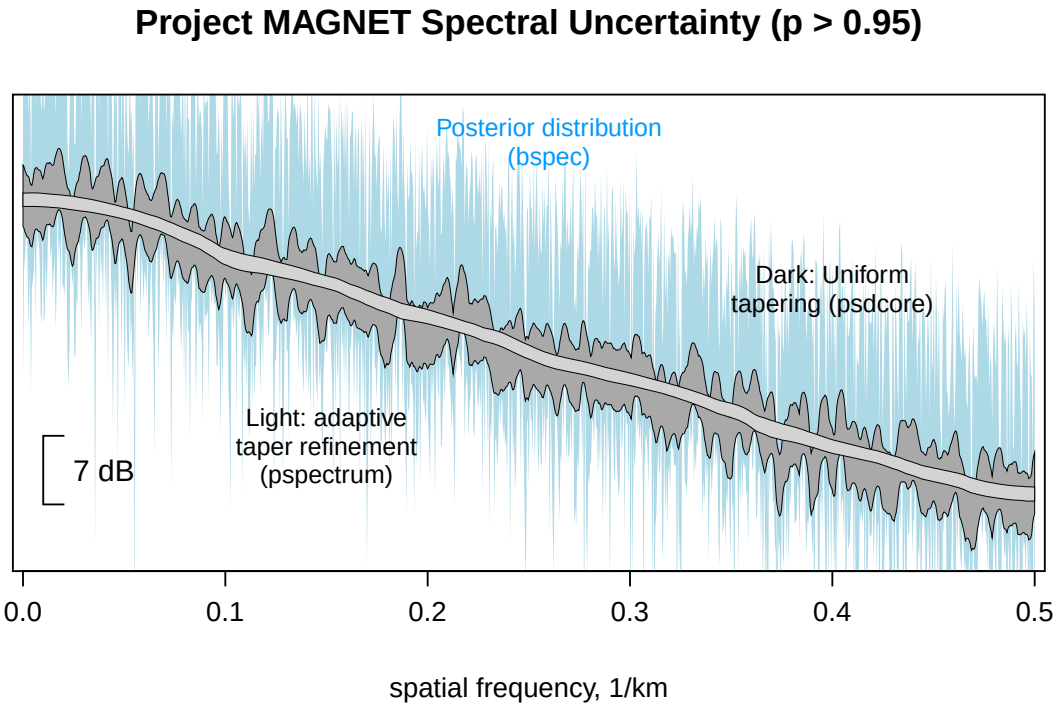


Figure 9: Project MAGNET spectral uncertainties for 95% coverage probability. The filled regions encompass the spectral uncertainties values based on the upper χ^2_ν curve shown in Figure 8, light and dark for PSDs with and without adaptive taper optimization, respectively. The results from Figure 6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

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.

```
frq <- Aspec[["freq"]]
relp <- (spa$resolution - spp$resolution)/spp$resolution
yl <- range(pretty(relp))
par(las = 1, oma = rep(0, 4), omi = rep(0, 4), mar = c(4, 3, 2, 0))
layout(matrix(c(1, 2), 1), heights = c(2, 2), widths = c(3, 0.5), respect = TRUE)
plot(frq, relp, main = "Percent change in spectral resolution", col = "light grey",
    ylim = yl, yaxs = "i", type = "h", ylab = "dB", xlab = "frequency, 1/km")
lines(frq, relp)
text(0.25, 45, "Adaptive relative to fixed", cex = 0.9)
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)
axis(4)
```

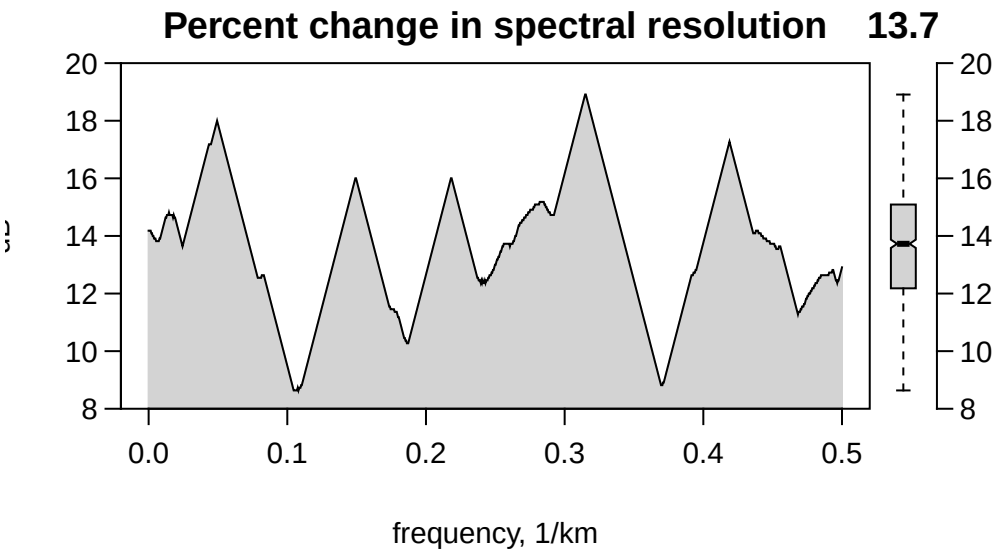


Figure 10: Relative changes in resolution of the adaptive method relative to the fixed multitaper method, plotted as a function of spatial frequency in units of percent. The non-zero median value implies the pilot spectrum was found using too-few tapers, according to the optimization algorithm. Positive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

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)
## Stage  1 est.  (Ave.  S.V.R. -13.1 dB)
## Stage  2 est.  (Ave.  S.V.R. -27.8 dB)
## Stage  3 est.  (Ave.  S.V.R. -44.9 dB)
## Stage  4 est.  (Ave.  S.V.R. -48.9 dB)
## Normalized  single-sided  psd estimates ( psd ) for sampling-freq.   1

str(AH <- get_adapt_history())

## List of 3
##  $ freq    : num [1:1024] 0 0.000489 0.000978 0.001466 0.001955 ...
##  $ stg_kopt:List of 5
##   ..$ : 'tapers' int [1:1024] 7 7 7 7 7 7 7 7 7 7 ...
##   .. ..- attr(*, "last_recorded")= logi NA
##   .. ..- attr(*, "n_taper_limits_orig")= num [1:2] 1 7
##   .. ..- attr(*, "taper_positions")= logi NA
##   .. ..- attr(*, "span_was_set")= logi FALSE
##   .. ..- attr(*, "n_taper_limits")= int [1:2] 7 7
##   ..$ : 'tapers' int [1:1024] 19 20 21 22 23 24 24 25 26 27 ...
##   .. ..- attr(*, "last_recorded")= logi NA
##   .. ..- attr(*, "n_taper_limits_orig")= num [1:2] 1 36
##   .. ..- attr(*, "taper_positions")= logi NA
##   .. ..- attr(*, "span_was_set")= logi FALSE
##   .. ..- attr(*, "n_taper_limits")= int [1:2] 14 36
##   ..$ : 'tapers' int [1:1024] 63 63 64 65 66 67 68 69 70 71 ...
##   .. ..- attr(*, "last_recorded")= logi NA
##   .. ..- attr(*, "n_taper_limits_orig")= num [1:2] 1 98
##   .. ..- attr(*, "taper_positions")= logi NA
##   .. ..- attr(*, "span_was_set")= logi FALSE
##   .. ..- attr(*, "n_taper_limits")= int [1:2] 29 98
##   ..$ : 'tapers' int [1:1024] 169 168 167 166 165 164 163 162 161 160 ...
##   .. ..- attr(*, "last_recorded")= logi NA
##   .. ..- attr(*, "n_taper_limits_orig")= num [1:2] 1 209
##   .. ..- attr(*, "taper_positions")= logi NA
##   .. ..- attr(*, "span_was_set")= logi FALSE
##   .. ..- attr(*, "n_taper_limits")= int [1:2] 75 209
##   ..$ : 'tapers' int [1:1024] 165 164 164 164 163 163 163 163 163 163 ...
##   .. ..- attr(*, "last_recorded")= logi NA
##   .. ..- attr(*, "n_taper_limits_orig")= num [1:2] 1 236
##   .. ..- attr(*, "taper_positions")= logi NA
```

```
##   .. ..- attr(*, "span_was_set")= logi FALSE
##   .. ..- attr(*, "n_taper_limits")= int [1:2] 136 236
##  $ stg_psd :List of 5
##   ..$ : num [1:1024] 1181 1228 1318 1363 1377 ...
##   ..$ : num [1:1024] 1138 1130 1133 1146 1165 ...
##   ..$ : num [1:1024] 1232 1231 1232 1237 1245 ...
##   ..$ : num [1:1024] 1271 1271 1272 1272 1273 ...
##   ..$ : num [1:1024] 1273 1274 1274 1274 1275 ...
```

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)
```

We can plot these easily with `matplot` or other tools. We show the adaptive history in Figure 11.

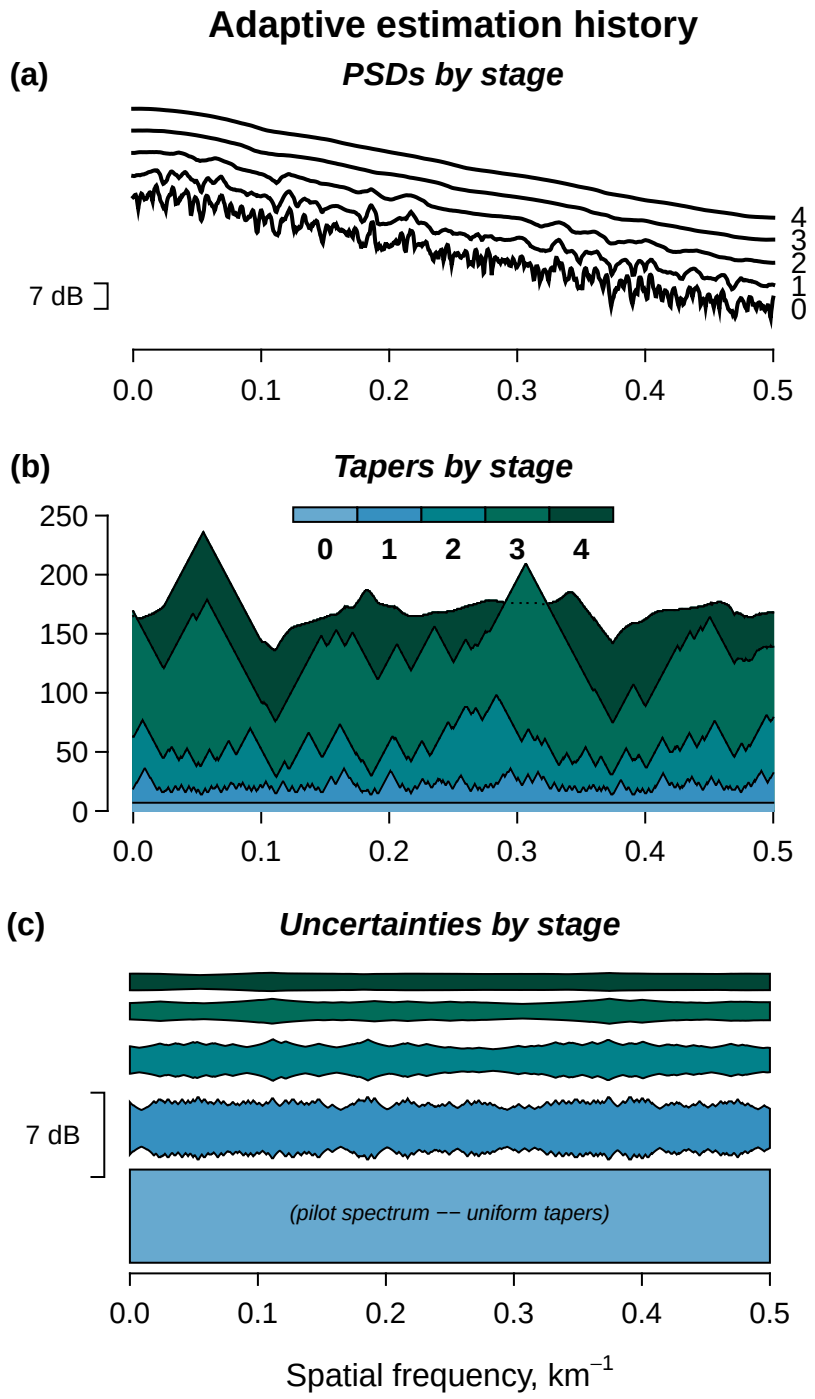


Figure 11: Adaptive spectral estimation history. (A) PSD series for each stage of the adaptive method, offset by a few decibels for visualization purposes. Filled polygons are shown in (B) for the number of tapers at each stage, and (C) the relative uncertainties of the PSDs.

Session Info

```
utils::sessionInfo()

## R version 4.4.1 (2024-06-14)
## Platform: x86_64-pc-linux-gnu
## Running under: Ubuntu 24.04.1 LTS
##
## Matrix products: default
## BLAS:   /usr/lib/x86_64-linux-gnu/openblas-pthread/libblas.so.3
## LAPACK: /usr/lib/x86_64-linux-gnu/openblas-pthread/libopenblasp-r0.3.26.so;  LAPACK version 3.12.0
##
## locale:
##  [1] LC_CTYPE=en_US.UTF-8       LC_NUMERIC=C
##  [3] LC_TIME=en_US.UTF-8        LC_COLLATE=C
##  [5] LC_MONETARY=en_US.UTF-8    LC_MESSAGES=en_US.UTF-8
##  [7] LC_PAPER=en_US.UTF-8       LC_NAME=C
##  [9] LC_ADDRESS=C               LC_TELEPHONE=C
## [11] LC_MEASUREMENT=en_US.UTF-8 LC_IDENTIFICATION=C
##
## time zone: Etc/UTC
## tzcode source: system (glibc)
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods
## [7] base
##
## other attached packages:
## [1] bspec_1.6          ggplot2_3.5.1      signal_1.8-1
## [4] RColorBrewer_1.1-3 RSEIS_4.2-4        psd_2.1.1
## [7] knitr_1.48
##
## loaded via a namespace (and not attached):
##  [1] gtable_0.3.5     compiler_4.4.1   highr_0.11       crayon_1.5.3
##  [5] Rcpp_1.0.13      scales_1.3.0     R6_2.5.1         labeling_0.4.3
##  [9] MASS_7.3-61      tibble_3.2.1     maketools_1.3.1  munsell_0.5.1
## [13] pillar_1.9.0     rlang_1.1.4      utf8_1.2.4       Rwave_2.6-5
## [17] xfun_0.48        sys_3.4.3        cli_3.6.3        withr_3.0.1
## [21] magrittr_2.0.3   formatR_1.14     grid_4.4.1       lifecycle_1.0.4
## [25] vctrs_0.6.5      evaluate_1.0.1   glue_1.8.0       farver_2.1.2
## [29] buildtools_1.0.0 fansi_1.0.6      colorspace_2.1-1 tools_4.4.1
## [33] pkgconfig_2.0.3  RPMG_2.2-7
```

References

Agnew, D. C. (1992). The time-domain behavior of power-law noises. *Geophysical Research Letters*, 19:333–336.

Barbour, A. J., Kennel, J., , and Parker, R. L. (2020). *psd: Adaptive, sine-multitaper power spectral density estimation*. R package version 2.0.

Barbour, A. J. and Parker, R. L. (2014). psd: Adaptive, sine multitaper power spectral density estimation for R. *Computers & Geosciences*, 63:1–8.

Coleman, R. J. (1992). Project Magnet high-level vector survey data reduction. In *Types and Characteristics of Data for Geomagnetic Field Modeling*, volume 3153, pages 215–248.

Korte, M., Constable, C., and Parker, R. (2002). Revised magnetic power spectrum of the oceanic crust. *Journal of Geophysical Research*, 107(B9):2205.

Lees, J. M. and Park, J. (1995). Multiple-taper spectral analysis: A stand-alone C-subroutine. *Computers & Geosciences*, 21(2):199–236.

O'Brien, M. S., Parker, R. L., and Constable, C. G. (1999). Magnetic power spectrum of the ocean crust on large scales. *Journal of Geophysical Research*, 104(B12):29189–29.

Parker, R. L. (2015). PSD. `http://igppweb.ucsd.edu/%7Eparker/Software/`. *Maintained software (last accessed March 2015)*.

Parker, R. L. and O'Brien, M. S. (1997). Spectral analysis of vector magnetic field profiles. *Journal of Geophysical Research*, 102(B11):24815–24.

Percival, D. and Walden, A. (1993). *Spectral analysis for physical applications*. Cambridge University Press.

Prieto, G. A., Parker, R. L., Thomson, D. J., Vernon, F. L., and Graham, R. L. (2007). Reducing the bias of multitaper spectrum estimates. *Geophysical Journal International*, 171(3):1269–1281.

R Core Team (2014). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. ISBN 3-900051-07-0.

Rahim, K. J., Burr, W. S., and Thomson, D. J. (2014). *Applications of Multitaper Spectral Analysis to Nonstationary Data*. PhD thesis, Queen's University. R package version 1.0-11.

Riedel, K. S. and Sidorenko, A. (1995). Minimum bias multiple taper spectral estimation. *IEEE Trans. SP*, 43(1):188–195.

Röver, C., Meyer, R., and Christensen, N. (2011). Modelling coloured residual noise in gravitational-wave signal processing. *Classical and Quantum Gravity*, 28(1):015010.

Thomson, D. J. (1982). Spectrum estimation and harmonic analysis. *Proceedings of the IEEE*, 70(9):1055–1096.