USAGE NOTES FOR PACKAGE CHEBPOL

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Abstract. Here are some examples of how package **chebpol** is used, with description of differences between the methods.

1. Introduction

Interpolating a function f means to find a reasonably behaved function, an interpolant g which agrees with f on some points. I.e. given $N \in \mathbb{N}$ we have $\{x_i\}_{i=1}^N$ in the domain of f, and the interpolant g satisifies $g(x_i) = f(x_i)$ for $1 \leq i \leq N$. The points x_i are often referred to as *knots*.

We limit ourselves to functions $\mathbb{R}^n \mapsto \mathbb{R}$, or even compactly supported functions $[-1,1]^n \mapsto \mathbb{R}$.

Which method to use depends first and foremost on one thing. Can we choose the points x_i freely? If $n > 1$, can we choose the points as a grid, i.e. a Cartesian product of single-dimension points?

Say we have a function $f(x,y)$ defined in a square, i.e. for $\{(x,y) \,|\, -1 \leq x \leq 1 \text{ and } -1 \leq y \leq 1\}$. Can we pick our knots exactly as we wish, e.g. as a Cartesian grid $X \times Y = \{(x,y) \,|\, x \in X \text{ and } y \in Y\}$ for some X and Y?

If we want our interpolant g to be a polynomial, there is a canonical way to do this. The knots should preferably be the Cartesian product of Chebyshev knots. The Chebyshev knots are not uniform, but a special set of knots which cluster near the end points.

If we are not free to choose the knots as we wish, but say we must stick to uniformly spaced knots, say $X = \{-1, -0.9, -0.8, \ldots, 0.8, 0.9, 1.0\}$, it is not particularly wise to interpolate with a polynomial. The reason is that polynomial interpolants can get gradually worse as the number of knots increases.

Some functions can, for some reason or the other, only be evaluated in irregular grids, or should have a denser grid near certain areas. Some functions can't be evaluated at all, they only come as values in some scattered points. Here are typical examples in two dimensions.

```
library(chebpol)
par(mfrow=c(2,2))
grid <- list(x=seq(-1,1,length.out=12), y=seq(-1,1,length.out=10))
plot(y~x,data=expand.grid(grid),typ='p',col='blue',main='Uniform 2d-grid')
grid <- chebknots(c(x=12,y=10))
plot(y ~ x, data=expand.grid(grid), typ='p',col='blue',main='Chebyshev 2d-grid')
grid <- list(x=seq(-1,1,length.out=12)^3L, y=sort(c(0,runif(10,-1,1),1)))
plot(y ~ x, data=expand.grid(grid), typ='p',col='blue',main='Irregular 2d-grid')
data <- cbind(x=runif(120,-1,1),y=runif(120,-1,1))
plot(y ~ x, data=data, typ='p', col='blue', main='Scattered data')
```

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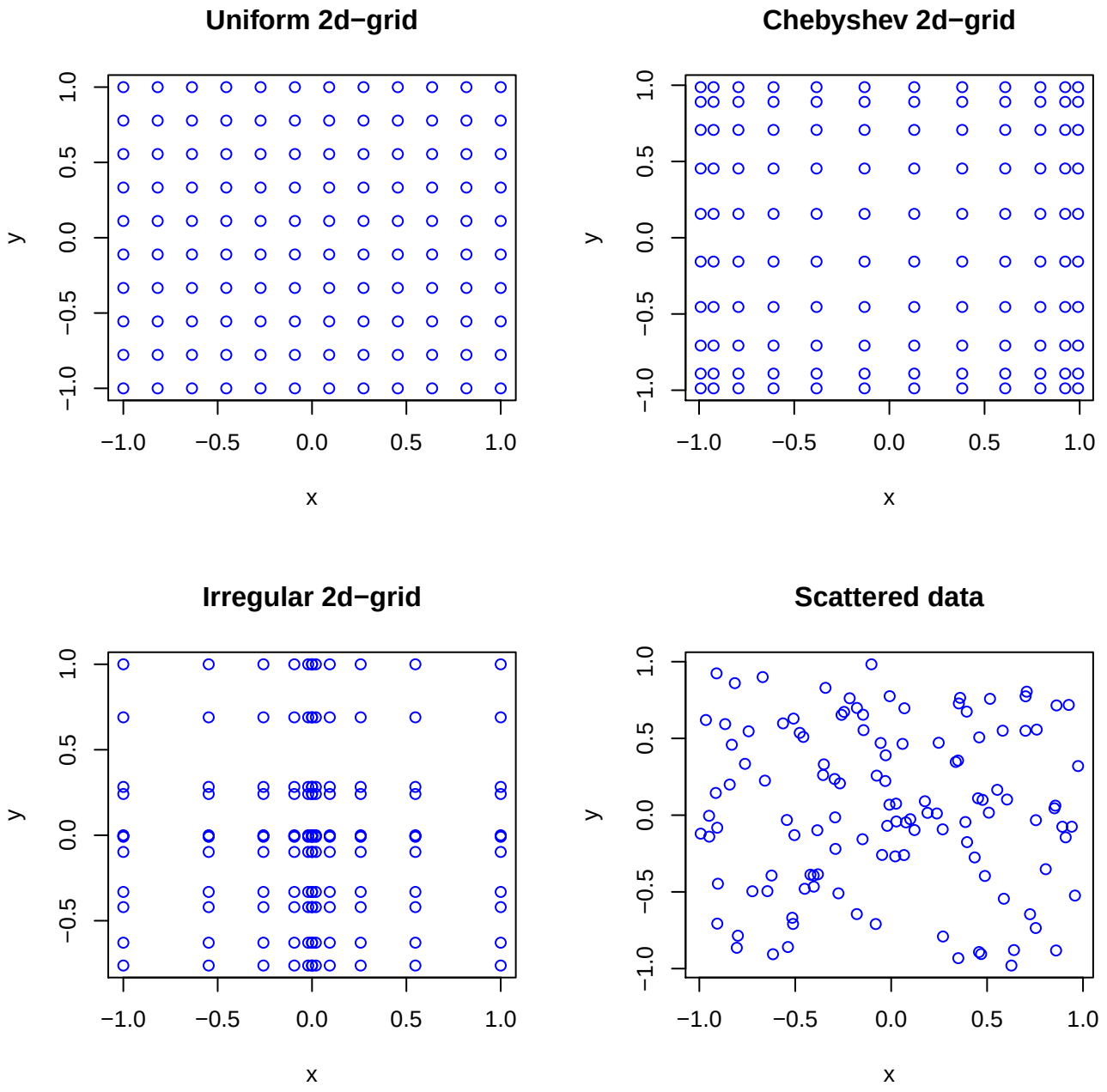
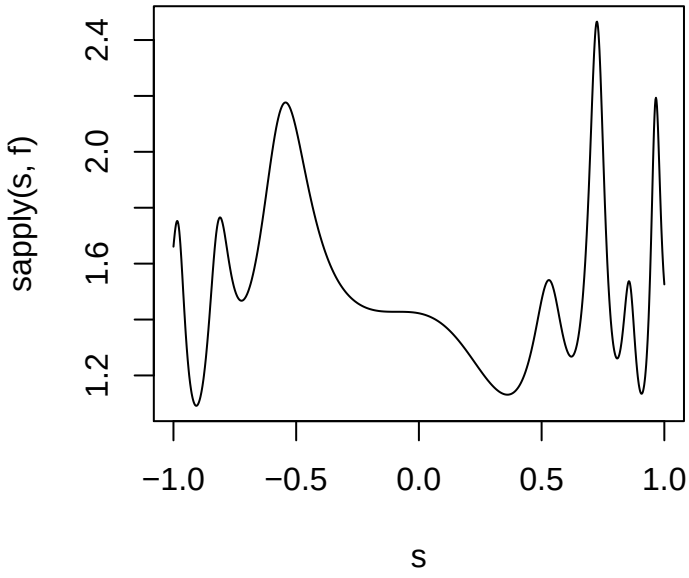


2. The chebpol package

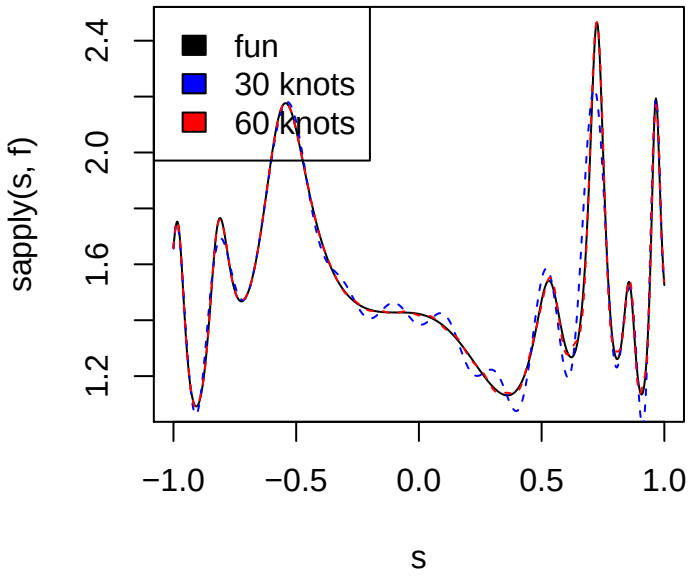
Since the generalization to multiple dimensions is fairly straightforward, we focus on the one-dimensional case. I.e. functions $[-1,1] \mapsto \mathbb{R}$. We use the following function:

```
f <- function(x) 1/mean(log1p(0.5 + sin(0.8+2.3*pi*c(0.6,1.4)*(x+0.09)^3)^2))
s <- seq(-1, 1, length.out=1000)
plot(s, sapply(s,f), typ='l')
```



Since this is a toy function, we can illustrate all sorts of knots. The first one out is the traditional Chebyshev interpolation. The oscillations are typical for polynomial interpolation with too few knots, that's how polynomials are.

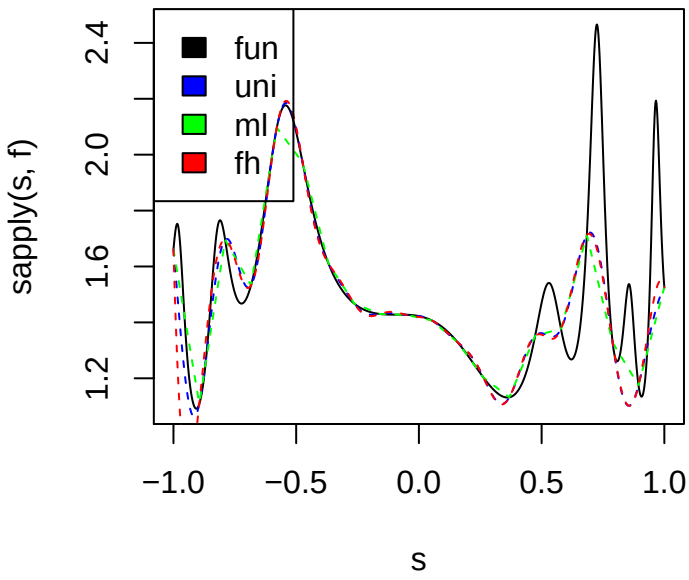
```
ch30 <- ipol(f, dims=30, method='cheb')
ch60 <- ipol(f, dims=60, method='cheb')
plot(s, sapply(s,f), typ='l')
lines(s, ch30(s), col='blue', lty=2)
lines(s, ch60(s), col='red', lty=2)
legend('topleft',c('fun','30 knots','60 knots'),fill=c('black','blue','red'))
```



We see that with 60 knots we follow the peaks quite well. There is another thing to note also. We can't evaluate the function `f` in all points at once, with `f(s)`, we must `sapply(s, f)`. However, the interpolants produced by package **chebpol** can evaluate in a series of points. It is even able to parallelize the evaluation, if you have more than one CPU in your computing contraption. It's just to feed it a `threads=` argument.

Then, what if we can't pick Chebyshev knots, but for some reason have to stick to uniformly spaced knots, say 20 or 40 of them. We then have a couple of methods to choose from. One is called `"uniform"` and is a trigonometric mapping of the uniformly spaced knots into Chebyshev knots. Another is piecewise linear. Then there is the Floater-Hormann rational interpolation from [1]. The F.H. interpolation comes with an integer parameter which is the degree of certain blending polynomials. In theory it works with any degree below the number of knots, but in practice high degrees introduce round off errors, so we better keep it small. We see some of the methods here:

```
plot(s, sapply(s,f), typ='l')
uni <- ipol(f, dims=20, method='uniform')
grid <- seq(-1,1,len=20)
ml <- ipol(f, grid=grid, method='multilinear')
fh <- ipol(f, grid=grid, method='fh', k=3)
lines(s, uni(s), col='blue', lty=2)
lines(s, ml(s), col='green', lty=2)
lines(s, fh(s, threads=4), col='red', lty=2)
legend('topleft',c('fun','uni','ml','fh'),fill=c('black','blue','green','red'))
```



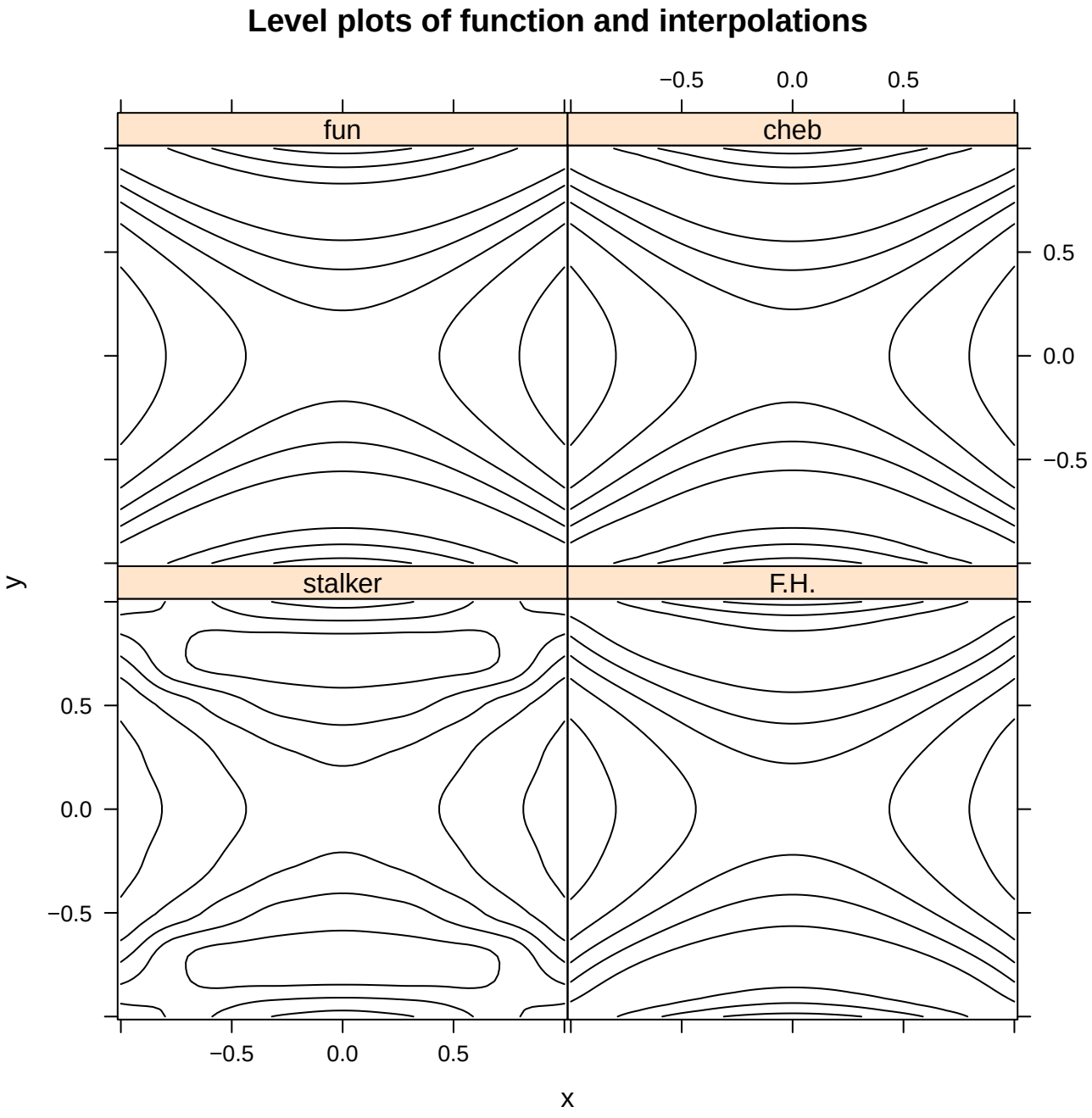
3. Multidimensional data

All of the above methods work with more than one dimension via a standard tensor product construction, but that presupposes that the function can be evaluated on a Cartesian grid. The Chebyshev and uniform methods use particular grids. The method `"general"` is similar to `"uniform"` in that it transforms an arbitrary Cartesian grid into a Chebyshev grid by means of a monotonic spline in each dimension. The multilinear and Floater-Hormann methods also work on arbitrary Cartesian grids.

To illustrate how this works, here is a quite nice function on $[-1,1]^2$ and contour plots of it and the 9×9 Chebyshev interpolation, a homegrown "stalker" spline (described in a vignette) and the Floater-Hormann methods on a uniform 9×9 grid.

```
f1 <- function(x) 1.5/log(5+sin(pi/2*(x[1]^2-2*x[2]^2)))
ch1 <- ipol(f1, dims=c(9,9), method='cheb')
igrid <- list(x=seq(-1,1,len=9), y=seq(-1,1,len=9))
st1 <- ipol(f1, grid=igrid, method='hstalker')
```

```
fh1 <- ipol(f1, grid=igrid, method='fh', k=3)
y <- x <- seq(-1,1,len=70)
testset <- expand.grid(list(x=x,y=y))
data <- cbind(testset,fun= apply(testset,1,f1), cheb=ch1(t(testset)),
              stalker=st1(t(testset)), F.H.=fh1(t(testset)))

lattice::contourplot(stalker+F.H.+fun+cheb ~ x+y, data=data, cuts=10,
          labels=FALSE, layout=c(2,2),
          main='Level plots of function and interpolations')
```

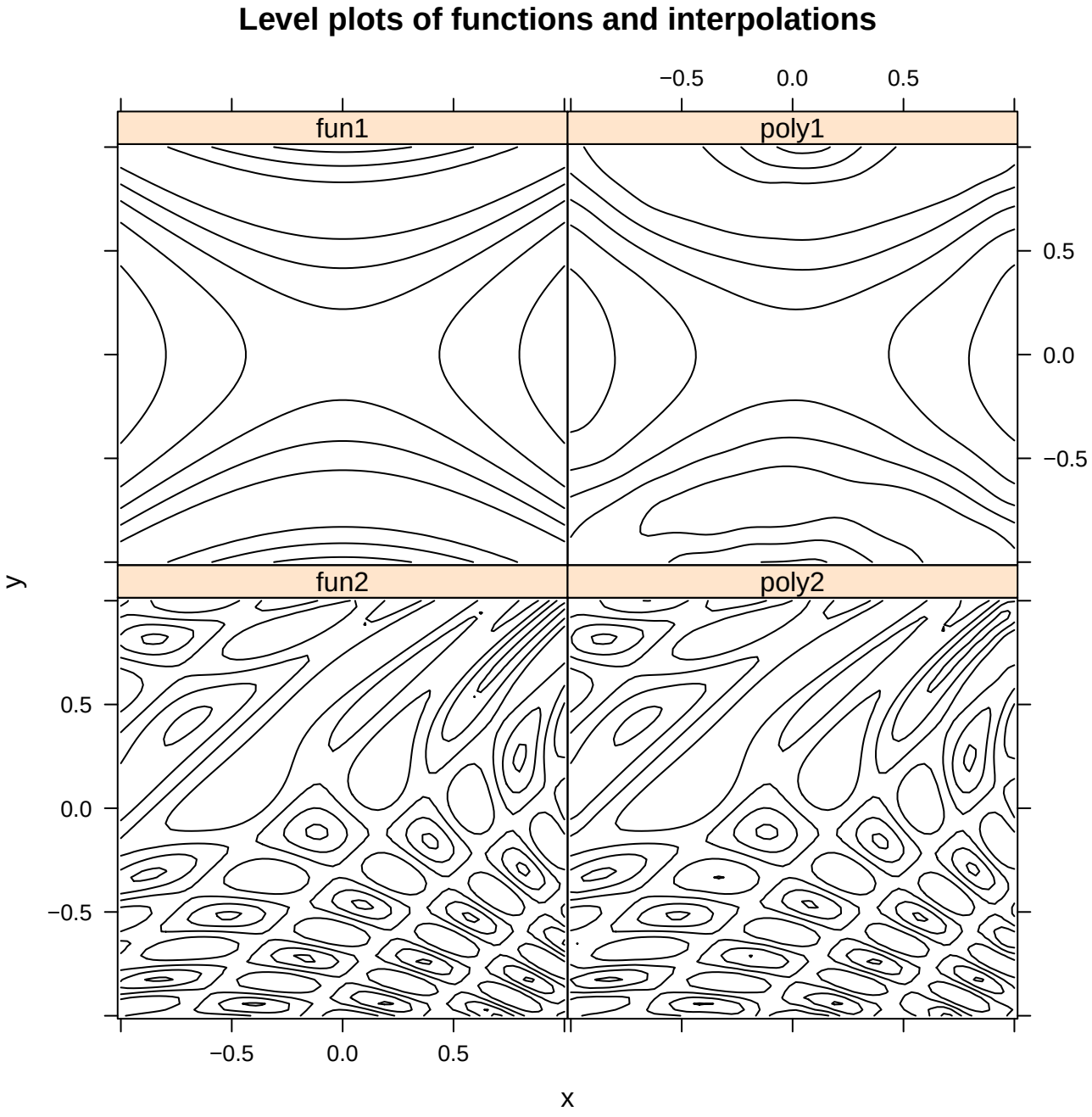


The stalker spline is not designed for smooth surfaces, but for following first order features (monotonicity and local extrema) along the grid lines.

There are two interpolation methods we have not mentioned yet. If the data are scattered in two or more dimensions, none of the methods above will work. They need a Cartesian product grid. The **chebpol** package contains two methods for scattered data also, the most versatile being the polyharmonic spline (see [2]). It is parametric with an integer $k \in \mathbb{N}$. For free we also throw in a Gaussian radial basis function interpolation for negative $k \in \mathbb{R}^-$. Here we create

two functions and plot level plots of them and their polyharmonic interpolations. One of the functions is quite smooth, the other is quite wobbly and requires a lot of scattered points.

```
f2 <- function(x) 1.2/mean(log(3.1 + sin(0.7+1.8*pi*(x+0.39*x[1]^2-x[2]^2))^2))
ph1 <- ipol(f1, knots=matrix(runif(200,-1,1),2), method='polyharmonic', k=2)
ph2 <- ipol(f2, knots=matrix(runif(4000,-1,1),2), method='polyharmonic', k=3)
data <- cbind(testset,fun1= apply(testset,1,f1), poly1=ph1(t(testset)),
              fun2=apply(testset,1,f2), poly2=ph2(t(testset)))

lattice::contourplot(fun2+poly2+fun1+poly1 ~ x+y, data=data, cuts=10,
          labels=FALSE, layout=c(2,2),
          main='Level plots of functions and interpolations')
```




```
# compute L2-error (rmse)
sqrt(cubature::hcubature(function(x) as.matrix((ph2(x)-apply(x,2,f2))^2), rep(-1,2), rep(1,2),
          vectorInterface=TRUE, absError=1e-6)$integral/4)
```

```
## [1] 0.002618839
```

The polyharmonic spline method is quite slow. It requires solving a $K \times K$ dense linear system, where K is the number of knots. It helps a lot to use a tuned and parallel BLAS with R, such as Intel's MKL.

In Figure 1 are various interpolated 3d-pictures of the Maungawhau volcano (Mt. Eden, Auckland, New Zealand). We illustrate the other method which works on scattered data, it is piecewise linear on triangles (more generally on simplices).

```
data(volcano)
volc <- volcano[seq(1,nrow(volcano),3),seq(1,ncol(volcano),3)]/10 #low res volcano
grid <- list(x=as.numeric(seq_len(nrow(volc))), y=as.numeric(seq_len(ncol(volc))))
fh <- ipol(volc, grid=grid, method='fh', k=0)
knots <- t(expand.grid(grid))
sl <- ipol(volc, knots=knots, method='simplex')
ph <- ipol(volc, knots=knots, method='poly')
g <- list(x=seq(1,nrow(volc), len=50), y=seq(1,ncol(volc),len=50))
par(mar=rep(0,4)); col <- 'green'
light <- list(specular=0.2,ambient=0.0,diffuse=0.6)
plot3D::persp3D(grid$x, grid$y, volc, colvar=NULL, lighting=light,
        theta=135, ltheta=90, lphi=40, col=col, axes=FALSE, bty='n',scale=FALSE)
for(f in list(ph, fh, sl)) {
plot3D::persp3D(g$x, g$y, evalongridV(f,grid=g), colvar=NULL, lighting=light,
        theta=135, ltheta=90, lphi=40, col=col, axes=FALSE, bty='n', scale=FALSE)
}
```

4. Radial basis functions with compact support (ALGLIB)

The ALGLIB library (`http://www.alglib.net/interpolation/fastrbf.php`) contains an implementation of compact support radial basis function interpolation on scattered data. It is available with `ipol(..., method='crbf')` if ALGLIB was available at build time.

By default, this is not true for Windows. However if ALGLIB is available, **chebpol** can be built with it from source by editing the file `src/Makevars.win`. The library must be put into the make variable `PKG_LIBS` as something like `-LC:/somewhere/libs -lalglib`, and the compiler must be told where to find ALGLIB's include file by inserting something like `-IC:/somewhere/include -DHAVE_ALGLIB` in the `PKG_CPPFLAGS`.

On linux and other unix-variants, ALGLIB should be put into the `pkg-config` database so that the command `pkg-config --libs alglib` reports the link and compiler flags. This amounts to creating a file `alglib.pc` in the search path of `pkg-config` with the necessary content (`Libs:` and `Cflags:`) The author has put ALGLIB in `/usr/local`, and `alglib.pc` contains:

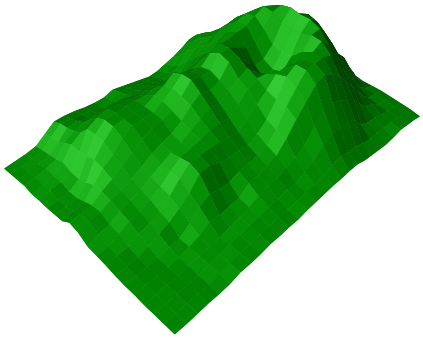
```
prefix=/usr/local
exec_prefix=${prefix}
libdir=${prefix}/lib
includedir=${prefix}/include/alglib

Name: ALGLIB
Description: Various numerical mathematics
Version: 3.14.0
Libs: -L${libdir} -lalglib
Cflags: -I${includedir}
```

When this works, **chebpol** will be built with ALGLIB when you do an `install.packages('chebpol')`.

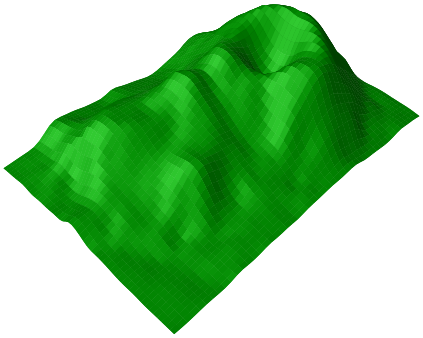
5. Speed considerations

There are two parts to interpolation. Creating the interpolant, and using it. Both of these take some time. The time depends on the method, as well as the dimension r of the problem, and the number of grid points n along a dimension, or the number of knots K. For the Cartesian grids, the number of knots is n^r.

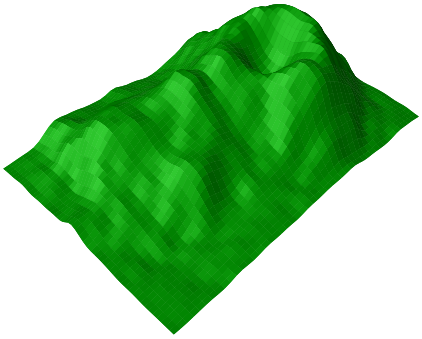
Traditionally, Chebyshev interpolation has been favoured for two reasons. The Chebyshev interpolation is the right way to do polynomial interpolation, due to certain analytical facts. The Chebyshev coefficients can also be calculated by a (possibly multi dimensional) Fast Fourier Transform (FFT). This is much faster than solving a large linear system which is the pedestrian approach for finding polynomial interpolants. **chebpol** uses the FFT from the software package FFTW, if it was available during compilation. Otherwise a slower matrix method is used. Creation with FFT typically



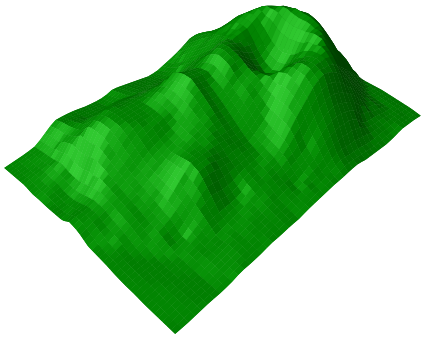
(A) low resolution



(B) polyharmonic



(C) Floater-Hormann



(D) simplex

FIGURE 1. Volcanoes

takes of the order $O(n^r \log n)$. The evaluation of Chebyshev interpolants is not particularly fast, **chebpol** uses the Clenshaw algorithm, which is a variant of Horner's method for evaluating polynomials. It typically goes in time n for each dimension, but they must be combined, so $O(n^r)$.

The multilinear interpolation is the fastest in **chebpol**. Creating the interpolant takes little time at all, the grid and function values are saved, *as is*, that's all. Evaluation consists of computing a convex combination of the function values in the corners of the surrounding hypercube. Typically an $O(\log n)$ task for each dimension, but there are 2^r corners for an r-dimensional problem, so $O(r2^r + r \log n)$.

The stalker and hyperbolic stalker interpolations are also local methods which are quite fast, both to create and to evaluate. They have the same complexity as the multi linear, but slower by some constant.

Creation of the Floater-Hormann interpolation requires calculating the weights, roughly an $O(rn^2)$ task. Evaluation is $O(n^r)$. Quite similar to the Chebyshev method.

The polyharmonic spline method is the most demanding. Creation requires calculating some weights which amounts to solving a dense $K \times K$ linear system, an $O(K^3)$ task (or $O(n^{3r})$ to compare with the grid methods). Evaluation is faster, of the order $O(Kr)$ (or $O(rn^r)$).

Creation of the simplex linear interpolation requires calculation of the Delaunay triangulation of the knots. This is usually quite fast, using the `qhull` library (`http://www.qhull.org`) available through package **geometry**. Evaluation requires finding the enclosing simplex of the point, this is done linearly by filtering out bounding boxes which does not include the point, this is quite fast, and then for the remaining simplices, by verifying that the barycentric coordinates of the point are in $[0, 1]$. It works reasonably fast for a few thousand knots and dimension below 4-5. With more knots, or higher dimensions, both creation and evaluation is markedly slower due to exceedingly high numbers of simplices.

The compact radial basis functions approach of ALGLIB in `method='crbf'` *requires* tuning. The three parameters is the base radius (`rbase`), the number of layers (`layers`), and a smoothing parameter (`lambda`). The ALGLIB docs says that the base radius should be larger than the typical Euclidean distance between the knots. Each layer halves the radius, and the final radius should be smaller than the minimal distance, to capture the most rapid changes. The smoothing parameter λ defaults to 0, but typical values can be around 10^{-6} or 10^{-5}. The default in `ipol` is $(2, 5, 0)$, but this may be a very bad choice for your data. A commercial variant of ALGLIB is available, with parallelization and instruction-level optimizations, the author has not tried it.

To alleviate speed problems, parts of **chebpol** has been parallelized with OpenMP. The number of threads is taken from `getOption("chebpol.threads")` which is initialized from the environment variable `CHEBPOL_THREADS`. It defaults to 1. Some of the creation routines use parallelization, however the polyharmonic spline does not. It depends on the underlying BLAS for solving the system, of course it helps if it is optimized and parallel.

Evaluation of the interpolants are parallelized if one evaluates more than one point. I.e. the interpolants can take a matrix of column vectors, and may calculate values in parallel:

```
m <- matrix(runif(2*6,-1,1),2)
print(m)
##            [,1]       [,2]       [,3]       [,4]       [,5]      [,6]
## [1,] -0.9711147  0.04088274 -0.2114722 -0.3162226 -0.1854045 0.1936394
## [2,] -0.1570820 -0.52174500 -0.9379660 -0.1015732  0.6033676 0.6767862
print(ph2(m, threads=3))
## [1] 0.9369171 0.9713621 0.9770991 0.9693429 0.9133033 0.9146778
```

This means that even if one has a function available in R, it might be faster to use an interpolant since it's automatically parallelized. Even if one does not have more than one CPU, it is worthwile to use the matrix interface if more than one point is to be evaluated (such as in the vector interface of package **cubature**), it is a lot faster with `ph2(m)` than with `apply(m,2,ph2)`.

```
f <- ipol(sin, grid=seq(-pi,pi,length.out=1000), method='hstalker')
a <- runif(1e6)
system.time(sin(a))
##    user  system elapsed
##   0.073   0.000   0.073
system.time(f(a,threads=8))
##    user  system elapsed
##   0.250   0.011   0.042
```

References

1. Michael S. Floater and Kai Hormann, *Barycentric rational interpolation with no poles and high rates of approximation*, Numerische Mathematik **107** (2007), no. 2, 315–331.
2. Thomas Hangelbroek and Jeremy Levesley, *On the density of polyharmonic splines*, Journal of Approximation Theory **167** (2013), 94–108.

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