DETAILS OF CHEBPOL

SIMEN GAURE

ABSTRACT. **chebpol** is a package for multivariate interpolation using Chebyshev-polynomials. Interpolation means that the approximating function it produces matches the original function in prespecified points, and try to fill in between the gaps. Thus, it is not smoothing like the **mgcv** package. Indeed, the package also contains some other multivariate interpolation methods. This document outlines how **chebpol** works.

1. INTRODUCTION

We consider the problem of interpolating a continuous function $f : [-1, 1] \mapsto \mathbb{R}$ based on its values in n points $\{x_i\}_{i=1..n}$ called *knots*. I.e. we want to find a reasonably behaved function P_f^n defined on $[-1, 1]$ such that $P_f^n(x_i) = f(x_i)$ for $i = 1..n$.

A classical approach is to let P_f^n be a polynomial of degree $n - 1$ and find the coefficients by solving the linear system $P_f^n(x_i) = f(x_i)$ $(i = 1..n)$. However, high-degree polynomials do not always behave *reasonably*. In particular there is the Runge phenomenon: If the points x_i are uniformly spaced in $[-1, 1]$ and one tries to interpolate the Runge function $f : x \mapsto (1 + 25x^2)^{-1}$, there will be oscillations in P_f^n near the end-points. As n grows, the amplitude of these oscillations grow without bounds.

Most of the functionality in the package is reachable from the function `ipol`.

2. CHEBYSHEV INTERPOLATION

The classical solution to the Runge phenomenon is to use a particular set of knots, the Chebyshev knots $x_i^n = \cos(\pi(i-0.5)/n)$ for $i = 1..n$. This will ensure that P_f^n will converge uniformly to f as $n \to \infty$, provided f is uniformly continuous. In this case one uses a special basis for the space of polynomials of degree up to $n - 1$, the Chebyshev polynomials $\{T_i(x)\}_{i=0..n-1}$, which are orthogonal w.r.t to a suitable inner product. Due to a trigonometric identity, we have $T_i(x) = \cos(i \cos^{-1}(x))$. The coefficients for these polynomials may be computed by a variant of the DCT-II transform. Thus, the method is fast.

More modern methods use splines, where the idea is to glue pieces of simple functions together, either low-degree polynomials or rational functions, subject to various constraints. Splines are in many respects superior to Chebyshev-interpolation.

For the multivariate case, where $f : [-1, 1]^r \to \mathbb{R}$, the DCT-II transform, being a variant of the Fourier transform, factors over tensor-products, so a natural choice is to use this tensor-product transform in the multivariate case. The knots are the Cartesian product of one-dimensional knots. This is a classical way to interpolate multivariate real functions.

This procedure is available in package **chebpol**. Either we have the function to interpolate, or we have the values in the Chebyshev-knots. Given a function f we may compute its Chebyshev approximation and plot it:

```
f <- function(x) cos(3*pi*x)/(1+25*(x-0.25)^2)
ch <- ipol(f,dims=15,method='chebyshev')
s <- seq(-1,1,length.out=401)
plot(s, f(s),type='l')
lines(s, ch(s), col='red')
```

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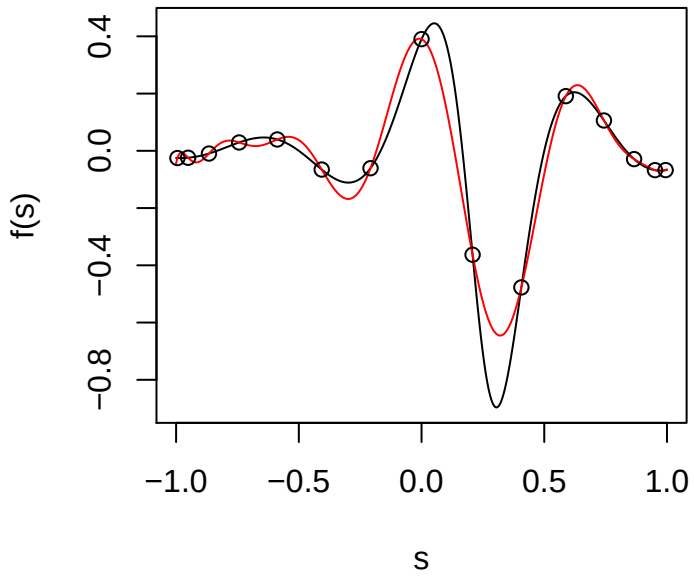
```
kn <- chebknots(15)[[1]]
points(kn,f(kn))
```



Even though there still are oscillations near the end points, their amplitude will diminish as n grows. The knots are the locations where the curves intersect.

In the multivariate case, the `dims` argument is a vector of integers, the number of knots in each dimension. If we have the values, not the function, we may pass those to `ipol` as an array with the `dim` attribute correctly set.

If you look at the function `ch` returned by `ipol`, you'll notice that it has two arguments. The first one, `x`, is the point at which you want to evaluate the function. This `x` can also be a matrix where each column is a point, the interpolation function can handle more than one point. In the special case with a single argument function, any vector argument is treated as a matrix with one row, i.e. a series of points, just like ordinary R-functions like `exp` or `sin`.

The second argument to `ch` is called `threads`, it defaults to `getOption('chebpol.threads')`, and is the number of parallel threads which should be used to compute the interpolations. Thus, above we could have written `lines(s, ch(s,8))` to compute the 401 points in `s` in 8 threads. There is nothing to gain from specifying more threads than there are CPUs in your computer, nor more than there are input vectors. The interpolants produced by **chebpol** has a `threads`-argument. The `chebpol.threads` option is initialized from the environment variable `CHEBPOL_THREADS` when the package is loaded.

3. Uniformly spaced grids

In some applications it is not feasible to evaluate the function f in the Chebyshev knots. Rather it may have to be evaluated on a uniformly spaced grid. To avoid the Runge phenomenon, **chebpol** transforms the domain of the function as follows.

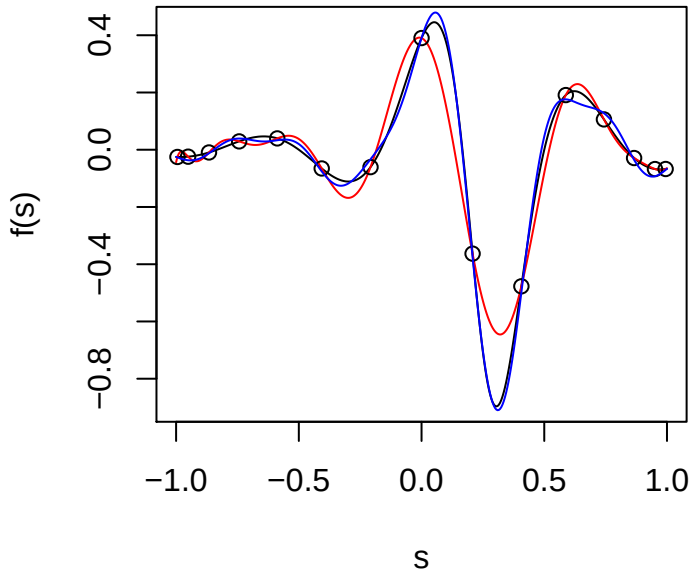
A fairly simple function exists which monotonically maps uniform grid points into Chebyshev knots. It's $g : x \mapsto \sin\left(\frac{\pi x(1-n)}{2n}\right)$. We omit the dependence on n to avoid clutter. This g has the property that for Chebyshev knots x_i^n and a uniform grid $y_i^n = -1 + 2(i-1)/(n-1)$ we have $g(y_i^n) = x_i^n$ for $i = 1..n$.

Thus, given a function f to interpolate on a uniform grid, we construct the function $h : x \mapsto f(g^{-1}(x))$. We then create the Chebyshev approximation P_h^n which requires h to be evaluated in the Chebyshev knots x_i^n, but $g^{-1}(x_i^n) = y_i^n$ are the uniform grid points, so f is evaluated there. We then use the function $Q^n : x \mapsto P_h^n(g(x))$ for interpolation.

It is readily verified that for $i = 1..n$ we have $Q^n(y_i^n) = f(y_i^n)$, thus Q^n agrees with the function f on the uniform grid. This is no longer a polynomial interpolation, so the Runge phenomenon is not necessarily present.

Continuing the former example, we have

```
plot(s,f(s),type='l')
lines(s,ch(s), col='red')
points(kn,f(kn))
uc <- ipol(f, dims=15, method='uniform')
lines(s,uc(s),col='blue')
```



For the multivariate case, a separate map function g is created for each dimension, which may have different number of knots. One could imagine a case where some dimensions are evaluated on Chebyshev grids, whereas other dimensions are evaluated on uniform grids. Although **chebpol** has no ready-made wrapper function to do this, it is not particularly difficult to achieve.

4. Non-standard hypercubes

Often, the domain of the function is not $[-1, 1]$, but rather some other interval $[a, b]$. This interval may be affinely mapped onto $[-1, 1]$ by $x \mapsto (2x - (a + b))/(b - a)$. For the multidimensional case this may

be done for each dimension separately. The functions in **chebpol** have an optional `intervals` argument, a list of such intervals, one for each dimension, to support such hyper-rectangles.

In principle, the same could be done with infinite intervals, with e.g. a mapping $(-\infty,\infty)\mapsto(-1,1)$ like $x\mapsto\frac{2}{\pi}\tan^{-1}(x)$, but **chebpol** does not implement it.

4.1. **A multivariate example.** Let f be the function $f:(x,y)\mapsto\log(x)\sqrt{y}/\log(x+y)$ defined on $[1,2]\times[15,20]$. Let's approximate it with 5 knots in x and 8 in y and see how it fares in a random point:

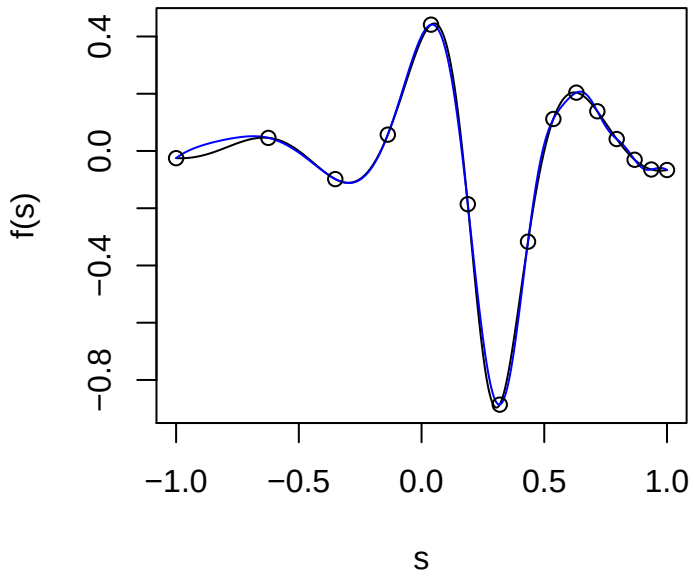
```
library(chebpol)
f <- function(x) log(x[[1]])*sqrt(x[[2]])/log(sum(x))
ch <- ipol(f, dims=c(5,8), intervals=list(c(1,2), c(15,20)), method='chebyshev')
uc <- ipol(f, dims=c(5,8), intervals=list(c(1,2), c(15,20)), method='uniform')
tp <- c(runif(1,1,2), runif(1,15,20))
cat('arg:',tp,'true:', f(tp), 'ch:', ch(tp), 'uc:',uc(tp),'\n')
## arg: 1.055284 15.78011 true: 0.07570634 ch: 0.07562689 uc: 0.05716209
```

5. Arbitrarily spaced grids

In some applications not even uniformly spaced grids are feasible. In this case we do something similar as in the uniformly spaced case. We have grid-points $\{y_i\}_{i=1..n}$ in ascending or descending order. We then use `splinefun` in package **stats** with `method='monoH.FC'` to create a monotone function g from the grid-points $\{y_i\}_{i=1..n}$ to the Chebyshev knots $\{x_i^n\}_{i=1..n}$. Otherwise, the same method as for uniform grids are used.

The method `"general"` performs this procedure. In the multivariate case, it is assumed that the grid in each dimension is arbitrary, but the multi-dimensional grid is still a Cartesian product of these. We may test this on a non-uniform grid.

```
f <- function(x) cos(3*pi*x)/(1+25*(x-0.25)^2)
gr <- log(seq(exp(-1),exp(1),length=15))
chg <- ipol(f, grid=gr, method='general')
plot(s, f(s), col='black', type='l')
lines(s, chg(s), col='blue')
points(gr,f(gr))
```



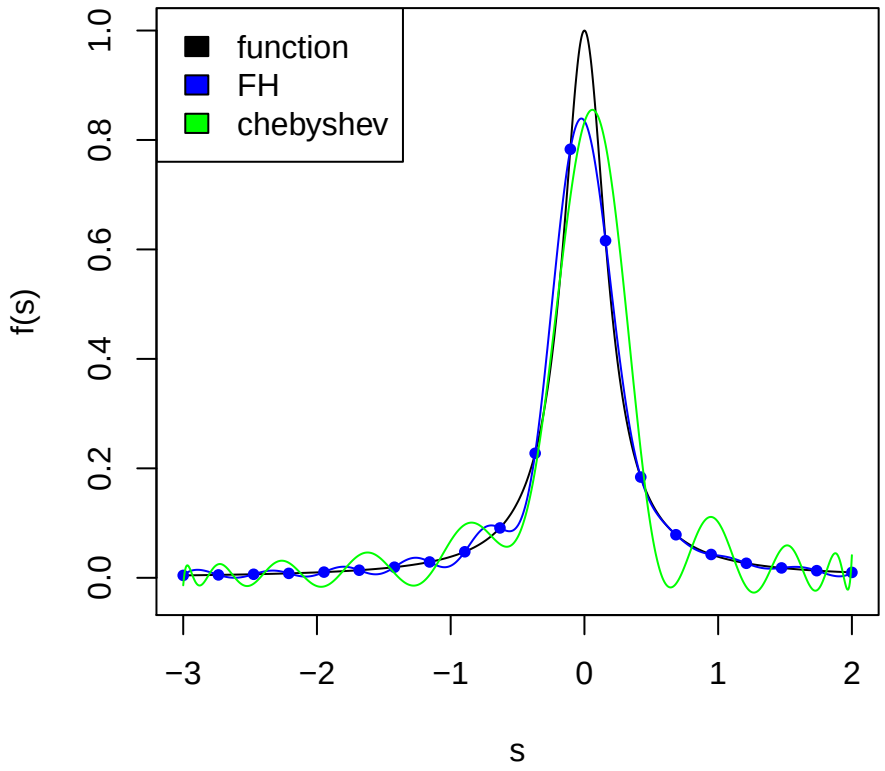
6. Floater-Hormann interpolation

An old interpolation method due to Lagrange is polynomial, but written so that one does not need to see any polynomial. Given function values $f_i = f(x_i)$ in some points $(x_i)_{i=0}^N$, the interpolant can be written in barycentric form:

$$L(x) = \frac{\sum_{i=0}^N f_i \frac{w_i}{(x-x_i)}}{\sum_{i=0}^N \frac{w_i}{(x-x_i)}},$$

where the w_i's are weights. It so happens that if the points x_i are $x_i = \cos(i\pi/N)$, the Chebyshev points of the second kind, the weights have alternating signs, with absolute values $|w_0| = |w_N| = 1$, and $|w_i| = 2$ for $0 < i < N$. See e.g. [1]. In [2] another set of weights which corresponds to certain blending polynomials in rational interpolants are found. This is used in method `"fh"`. Here is an example with a Runge function.

```
f <- function(x) 1/(1+25*x^2)
# Uniform grid:
unigrid <- list(seq(-3,2,length.out=20))
uni <- ipol(f, grid=unigrid, k=2, method='fh')
ch <- ipol(f, dims=20, intervals=c(-3,2), method='chebyshev')
s <- seq(-3,2,length.out=1000)
plot(s,f(s),ylim=range(uni(s),f(s),ch(s)),typ='l')
lines(s,uni(s),col='blue')
points(unigrid[[1]],uni(unigrid[[1]]),col='blue',pch=20)
lines(s,ch(s),col='green')
legend('topleft',c('function','FH','chebyshev'),fill=c('black','blue','green'))
```

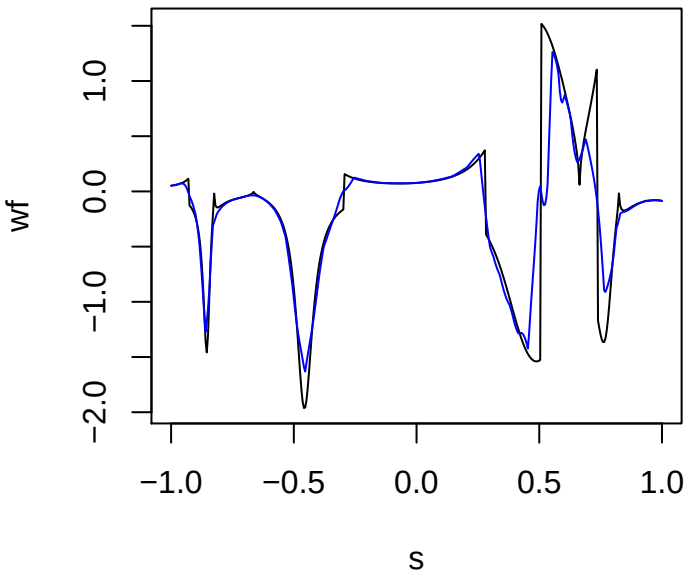


7. Multilinear interpolation

For demanding functions **chebpol** also contains a multilinear interpolation. A multilinear function is a function $f(x_1, x_2, ..., x_n)$ such that for each $i = 1..n$ the function $g_i(x) = f(x_1, ..., x_{i-1}, x, x_{i+1}, ..., x_n)$ is of the form $ax+b$ for every choice of the x_is. A typical example is $f(x, y, z) = xyz+xy+2yz-x+2$. The method `"multilinear"` may take either a function or function values as its first argument and create a piecewise multilinear interpolation. It is a straightforward implementation which interpolates a point by a convex combination of the function values in the corners of the surrounding hypercube. We try it out on an intricate function on $[-1, 1]^4$ and evaluate the result along an intricate parametric curve. Of course, if one is interested in this particular curve, one could interpolate along it instead. This is just an example of multilinear interpolation.

```
f <- function(x) sign(sum(x^3)-0.1)*
                  sqrt(abs(25*prod(x)-4))/
                  (1+25*sum(x)^2)
grid <- replicate(4,list(seq(-1,1,length=15)))
ml <- ipol(f, grid=grid, method='multilinear')
s <- seq(-1,1,length=400)
curve <- function(x) c(cos(1.2*pi*x),
                       sin(1.5*pi*x^3),
```

```
                        x^2, -x/(1+x^2))
wf <- sapply(s,function(x) f(curve(x)))
wml <- sapply(s,function(x) ml(curve(x)))
plot(s,wf,typ='l')  # function
lines(s,wml,col='blue') # multilinear interpolation
```



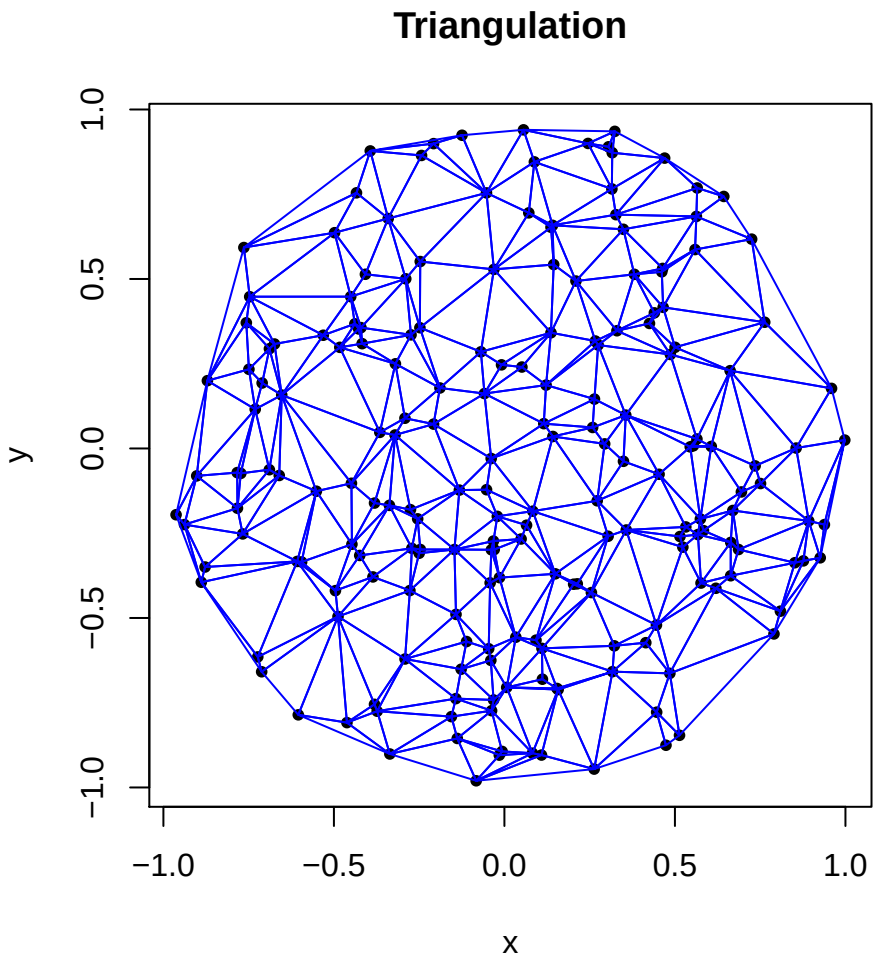
8. Scattered data

In some cases multidimensional data points are not organized in a grid, rather they are scattered. For this case, **chebpol** has two methods.

8.1. **Simplex linear interpolation.** The first one is linear in simplices. A Delaunay triangulation is created from the scattered data, i.e. a simplicial complex (a collection of triangles, tetrahedra, and their higher dimensional analogues). When evaluating the interpolant, the simplex enclosing the point is found, and the value in the point is a convex combination of the function values in the corners of the simplex, with the weights being the barycentric coordinates of the point. We create a function defined on the unit circle, and put some random knots in there, and see what the Delaunay triangulation looks like.

```
f <- function(x) sqrt(1-sum(x^2))
theta <- runif(200, 0, 2*pi)
r <- sqrt(runif(200))
knots <- rbind(r*cos(theta), r*sin(theta))
g <- ipol(f, knots=knots, method='simplexlinear')
# yank out the simplices for drawing
simp <- get('dtri', environment(get('fun', environment(g))))
drawtri <- function(pts,col) lines(c(pts[1,],pts[1,1]), c(pts[2,],pts[2,1]), col=col)
```

```
plot(knots[1,], knots[2,], typ='p', pch=20, xlab='x', ylab='y', main='Triangulation')
invisible(apply(simp,2,function(kn) drawtri(knots[,kn], col='blue')))
```




```
theta <- runif(7, 0, 2*pi)
r <- sqrt(runif(7))
test <- rbind(r*cos(theta), r*sin(theta))
rbind(true=apply(test,2,f), sl=g(test,epol=TRUE))
##           [,1]      [,2]      [,3]      [,4]      [,5]      [,6]      [,7]
## true 0.8573409 0.9569339 0.7836407 0.9354700 0.6468739 0.8716940 0.5273634
## sl   0.8482392 0.9502945 0.7746896 0.9315686 0.6292800 0.8657017 0.5065331
```

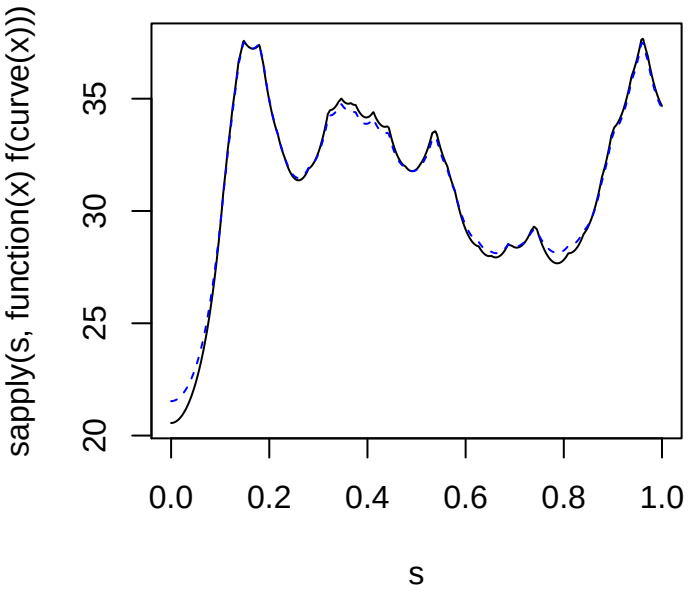
The main shortcoming of this method is visible in the Delaunay triangulation. Some of the triangles near the borders are very stretched out. This can happen even if we have a large number of knots. This is because the triangles must cover the convex hull, and there is no other way to do that. Such long simplices will lead to poor linear approximation if second derivatives there are large. Another shortcoming is that the entire triangulation is computed when the interpolant is created, not only the

parts needed for interpolating specific points. The number of simplices grows with the dimension d, typically as $d!$. This quickly gets out of hand when d grows.

By default, the interpolant will return `NA` for inputs which are outside the convex hull of the knots, but an extrapolation from the nearest simplex will be done if the argument `epol=TRUE` is specified.

8.2. **Polyharmonic splines.** The other scattered method is polyharmonic splines in the method `"polyharmonic"`. It accepts a function, or function values, and a matrix of centres (knots), one centre in each column. Here is a 20-dimensional example with 3000 randomly placed knots:

```
r <- runif(20)
r <- r/sum(r)
f <- function(x) 1/mean(log1p(r*x))
knots <- matrix(runif(60000), 20)
phs <- ipol(f, knots=knots, k=3, method='polyharmonic')
rr <- runif(20)
curve <- function(x) abs(cos(5*pi*rr*x))
s <- seq(0,1,length.out=1000)
plot(s,sapply(s,function(x) f(curve(x))),typ='l')
lines(s,sapply(s,function(x) phs(curve(x))),col='blue',lty=2)
```



The `"polyharmonic"` method fits a function of the form $P(x) = \sum_{i=1}^{n} w_i \phi(\|x - c_i\|) + L(x) + c$ such that $P(c_i) = f(c_i)$ for each i where the $c_i \in \mathbb{R}^d$ are the knots, $\|\cdot\|$ is the Euclidean norm on $\mathbb{R}^d$, $w_i \in \mathbb{R}$ are weights, L is linear $\mathbb{R}^d \mapsto \mathbb{R}$, and $c \in \mathbb{R}$ is a constant. ϕ is the function $\mathbb{R}^+ \mapsto \mathbb{R}$

$$\phi(x) = \begin{cases} x^k & \text{when } k \in \mathbb{N} \text{ is odd,} \\ x^k \log(x) & \text{when } k \in \mathbb{N} \text{ is even,} \\ \exp(kx^2) & \text{when } k < 0. \end{cases}$$

Note that this differs from some other expositions, which use $2m - d$ as exponent for a natural number m.

For $k = 2$, we get the thin plate spline. Note that the fitting may fail, in particular for $k < 0$ and irregular data. In this case a least squares fit is used, and a warning is issued. The k parameter then may need to be tuned for the problem at hand. Note that by default the knots and coordinates are transformed into a unit hypercube if any of the knots are outside, see the help entry for `polyh`. Note that for positive k the theory in [3, Proposition 6] says that there are enough splines even if we do not scale, but the numerics may be more favourable when we scale. There is more about polyharmonic splines in [4].

There do exist some acceleration schemes for low dimensions, but the current implementation does not use any. It is an entirely straightforward implementation which fits by solving a linear system, and evaluates the $P(x)$ directly.

References

1. J. Berrut and L. Trefethen, *Barycentric Lagrange Interpolation*, SIAM Review **46** (2004), no. 3, 501–517.
2. 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.
3. Thomas Hangelbroek and Jeremy Levesley, *On the density of polyharmonic splines*, Journal of Approximation Theory **167** (2013), 94 – 108.
4. Christophe Rabut, *Elementary m-harmonic cardinal B-splines*, Numerical Algorithms **2** (1992), no. 1, 39–61.

Ragnar Frisch Centre for Economic Research, Oslo, Norway