Smooth Spherical Interpolation –Theory–

Author

Peter M. Solfest

1 Introduction

Given a sparse set of data points around a sphere, it is convenient to have an analytical function fitting the data which allows for which to interpolate to any point on the sphere. Much work has been done representing a function in spherical harmonics, which can then be used for such interpolations.

Techniques using exact quadrature exist, but require data available on a regularly or gaussian spaced grid. For sparse real world data, this spacing is often not available. Thus techniques involving exact quadrature fail. Furthermore, it is not clear that an inexact quadrature scheme can be used given the arbitrary nature of real world locations.

Presented below is a method which fits arbitrary data to spherical harmonics of specified degree, minimizing a function involving terms measuring smoothness in addition to the least squares fitting. This smoothing not only allows for a determination of an arbitrarily large set of spherical harmonics, but also acts to minimize the large oscillations (gibbs phenomenon) introduced by spherically fitting data which may exhibit wide variations.

Furthermore, the final algorithm can be computed utilizing an iterative scheme involving only matvecs, saving the computational expense of solving a least squares problem.

2 Theory

Let there be s sample points, and b the number of basis functions used. Traditionally spherical harmonics are labeled $Y_{l,m}$, so an easy map for indices is $i = l(l+1)+m$, so $Y_{l,m} = Y_i$. Our data points will be labeled $f = f[j] = x_j$ for each sampled location x_j.

The goal is to find a set of coefficients c_i such that at an arbitrary point x:

$$f(x) = \sum_{i=0}^{(l+1)^2} c_i \cdot Y_i(x)$$

where $f(x_j) = f_j + \varepsilon$ for small ε is desired.

In order to do this, we need a vandermonde like matrix, $M \in \mathbb{R}^{s\times b}$, such that

$$M_{j,i} = Y_i(s_j)$$

Potentially the most straightforward way to form the coefficients c_i is by solving the least squares problem

$$Mc = f$$

This is equivalent to solving[1]

$$\min_c \|Mc - f\|$$

The problem with this is b can grow to infinity, creating increasingly overdetermined systems. Furthermore, if a bad data point at x_i is near x_j, but f_i is far from x_j, the least squares solution will match these incredibly well, leading to large oscillations.

To prevent this, we can choose a better objective function to minimize, namely

$$\min_c \left(\frac{1}{2}\| \triangle f\|^2 + \lambda\|Mc - f\|^2\right) \tag{1}$$

[1] $\|\cdot\| = \|\cdot\|_2$

Where $\lambda \in [0, \infty)$ determines what we are interested in, and the $\frac{1}{2}$ is introduced for convenience. Note that $\lambda = 0$ corresponds to a perfectly smooth function, namely the mean of f_j. Whereas $\lambda = \infty$ corresponds to the least squares solution.

One of the beauties of this is that spherical harmonics are eigenfunctions of the laplacians, so we get

$$\lambda f = Bc$$

where $B \in \mathbb{Z}^{b \times b}$ is a diagonal matrix such that $B_{i,i} = l_i^2 \cdot (l_i + 1)^2$, where l_i is the l corresponding to Y_i.

Thus equation 1 yields equation 2 when discretized.

$$\min_c \left(\frac{1}{2} c^t B c + \lambda (Mc - f)^T (Mc - f) \right) \tag{2}$$

This is a quadratic equation, so differentiating and setting equal to zero yields that the solution[2] is

$$Bc + 2\lambda M^T M c - 2\lambda M^T f = 0$$

Rearranging yields equation 3

$$\frac{1}{2\lambda} c = B^{-1} M^T f - B^{-1} M^T M c \tag{3}$$

3 Iteration

This arrangement immediately suggests an iterative technique for solving this problem. Namely,

$$c_i = 2\lambda \left(B^{-1} M^T f - B^{-1} M^T M c_{i-1} \right) \tag{4}$$

Also, define $c \cdot e_1 = \text{mean}(f_i)$. This lets our iterations ignore the $l = 0, m = 0$ term and only add it back in when reconstructing f. Also, B^{-1} is trivial to calculate since B is diagonal. Furthermore, the positive term on the right is constant, so only needs to be computed once, leaving a mere 2 matvecs per iteration in the solution. Thus a reasonable starting point is $c_0 = 0$, or equivalently $c_1 = 2\lambda B^{-1} M^T f$.

3.1 Convergence analysis

First, consider

$$\begin{aligned} \|c_{i+1} - c_i\| &= \|2\lambda B^{-1} M^T f - 2\lambda B^{-1} M^T M c_i - c_i\| && (5) \\ &= \|2\lambda B^{-1} M^T f - (I + 2\lambda B^{-1}) M^T M) c_i\| && (6) \end{aligned}$$

Furthermore,

$$\begin{aligned} \|c_{i+2} - c_{i+1}\| &= \|2\lambda B^{-1} M^T f - (I + 2\lambda B^{-1} M^T M) c_{i+1}\| && (7) \\ &= \|2\lambda B^{-1} M^T f - (I + 2\lambda B^{-1} M^T M) 2\lambda (B^{-1} M^T f - B^{-1} M^T M c_i)\| && (8) \\ &= \|2\lambda (B^{-1} M^T f - B^{-1} M^T f + B^{-1} M^T M c_i - 2\lambda B^{-1} M^T M B^{-1} M^T f + && (9) \\ & 2\lambda B^{-1} M^T M B^{-1} M^T M c_i)\| && (10) \\ &\leq 2\lambda \|B^{-1} M^T M\| \cdot \|2\lambda B^{-1} M^T f - (I + 2\lambda B^{-1} M^T M) c_i\| && (11) \\ &\leq 2\lambda \|B^{-1} M^T M\| \cdot \|c_{i+1} - c_i\| && (12) \end{aligned}$$

[2]Note that differentiating twice yields $B + 2\lambda M^T M$ which is positive definite. Thus it is indeed the minimum as the only solution.

Thus using that $\|B^{-1}\| = \frac{1}{4}$, since B is diagonal and it's smallest value is $1^2(1+1)^2$ since the sole $l = 0$ term has been eliminated by enforcing $c_0 = \text{mean}(f)$.

$$\frac{\|c_{i+2} - c_{i+1}\|}{\|c_{i+1} - c_i\|} \leq 2\lambda\|B^{-1}\|\|M^T M\| = \frac{\lambda}{2}\|M^T M\| = \frac{\lambda}{2}\|M\|^2 \tag{13}$$

Since convergence happens when

$$\frac{\|c_{i+2} - c_{i+1}\|}{\|c_{i+1} - c_i\|} < 1$$

convergence happens when

$$\|M\| < \sqrt{2/\lambda} \tag{14}$$

Recall that the smaller λ is, the smoother the fit is. So this places a lower limit on how smooth the fit must be.

3.2 A quick note on choosing λ

By definition, we have that

$$\|M\| = \|M^T\| \geq \frac{\|M^T x\|}{\|x\|} \quad \forall\, x$$

$$\|M\| \geq \frac{\|M^T f\|}{\|f\|}$$

So we can speculate that $\|M\| \approx \frac{1}{2}\frac{\|M^T f\|}{\|f\|}$ will suffice to serve the following purpose: Thus we can form an initial guess for a λ such that 5 by taking

$$\lambda = \frac{\|f\|^2}{\|M^T f\|} = \frac{1}{2}\frac{2 \cdot f^T f}{(M^T f)^T M^T f}$$

3.3 The algorithm

With a given scale factor $\alpha > 1$ and convergence tolerance ε, we can form an iterative algorithm as follows:

Input: α, ε, M, f
Output: c

$c_p \leftarrow 0$
$c_n \leftarrow 2\lambda B^{-1} M^T f$
$\lambda \leftarrow \dfrac{f^T f}{(M^T f)^T M^T f}$
$i \leftarrow 1$
$\Delta_n \leftarrow \|c_n - c_p\|^2$
while $\Delta_n \geq \varepsilon$ **do**
    $\Delta_p \leftarrow \Delta_n$
    $c_p \leftarrow c_n$
    $c_n \leftarrow 2\lambda \left(B^{-1} M^T f - B^{-1} M^T M c_p\right)$
    $\Delta_n \leftarrow \|c_n - c_p\|^2$

while $\Delta_n/\Delta_p \geq 1$ **do**
$\lambda \leftarrow \lambda/\alpha$
$c_n \leftarrow 2\lambda\left(B^{-1}M^T f - B^{-1}M^T M c_p\right)$
$\Delta_n \leftarrow \|c_n - c_p\|^2$
end while
end while
$c \leftarrow c_n$

Note that λ monotonically decreases by a factor of α each time the iteration 5 fails to get closer to the true answer. There are considerable variations available for how to shrink λ effectively, but the α shrinking outlined above should be sufficeint.

This will ultimately converge to the largest λ satisfying condition 14. Thus a smoother result could be arrived at via modifying how α behaves.

3.4 Implementation notes

3.4.1 Spherical harmonics

Let $k = l(l+1) + m$, then the spherical harmonics have

$$Y_k(\theta,\phi) = \begin{cases} \sqrt{2}\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-|m|)!}{(l+|m|)!}}P_l^{|m|}\left(\cos(\theta)\right)\sin(|m|\phi) & \text{if } m < 0 \\ \sqrt{\frac{2l+1}{4\pi}}P_l^0\left(\cos(\theta)\right) & \text{if } m = 0 \\ \sqrt{2}\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}P_l^m\left(\cos(\theta)\right)\cos(|m|\phi) & \text{if } m > 0 \end{cases}$$

Where $P_l^m\left(\cos(\theta)\right)$ can be formed using the following procedure

Input: L, θ
$P_0^0 \leftarrow 0$
for $l = 0, L-1$ **do**
$P_{l+1}^{l+1} \leftarrow -(2l+1)\sin(\theta)P_l^l$
for $m = 0, l$ **do**
$P_{l+1}^m \leftarrow \dfrac{(2l+1)\cos(\theta)P_l^m - (l+m)P_{l-1}^m}{l-m+1}$
end for
end for

Note that this must be done for each θ in the data set.