Laplacian on an Irregular Lattice – Ken 19Dec2017

Suppose we have a lattice where the spacing varies from region to region but is a multiple of some fine spacing s. If we are computing the Laplacian at a point $\vec{r}=\vec{0}$, then we can gather neighbor points out to some distance and fit them with a quadratic equation.

$$f\left(\vec{r}\right)=a+\sum_{\alpha=0}^{\alpha<d} b_\alpha r_\alpha+\sum_{\alpha=\beta=0,\alpha\le\beta}^{\beta<d} c_{\alpha\beta} r_\alpha r_\beta$$

Points are on the fine lattice, so we can rewrite this with $r_\alpha=sn_\alpha$ where n is a vector of integers. The fine spacing s into b and c yielding

$$f\left(\vec{n}\right)=a+\sum_{\alpha=0}^{\alpha<d} b_\alpha n_\alpha+\sum_{\alpha=\beta=0,\alpha\le\beta}^{\beta<d} c_{\alpha\beta} n_\alpha n_\beta$$

Now suppose we have a set of N samples of the function f at a set of points $n_{i\alpha}$. A slightly modified residual is given by

$$R^2=\sum_i w_i\left(f_i-\left(a+\sum_{\alpha<d} b_\alpha n_{i\alpha}+\sum_{\alpha\le\beta<d} c_{\alpha\beta} n_{i\alpha} n_{i\beta}\right)\right)^2$$

The weight $w_i=1/\left|\vec{n}\right|$ is chosen to reflect the distance from the point at which the Laplacian is to be calculated. This weight comes from a study of constructing Laplacians that are more rotationally invariant from samples on a uniform lattice.

The residual is minimized by setting the derivatives to 0.

$$\frac{\partial R^2}{\partial a}=-2\sum_i w_i\left(f_i-\left(a+\sum_{\alpha<d} b_\alpha n_{i\alpha}+\sum_{\alpha\le\beta<d} c_{\alpha\beta} n_{i\alpha} n_{i\beta}\right)\right)=0$$

$$\frac{\partial R^2}{\partial b_\gamma}=-2\sum_i w_i\left(f_i-\left(a+\sum_{\alpha<d} b_\alpha n_{i\alpha}+\sum_{\alpha\le\beta<d} c_{\alpha\beta} n_{i\alpha} n_{i\beta}\right)\right)n_{i\gamma}=0$$

$$\frac{\partial R^2}{\partial c_{\gamma\chi}}=-2\sum_i w_i\left(f_i-\left(a+\sum_{\alpha<d} b_\alpha n_{i\alpha}+\sum_{\alpha\le\beta<d} c_{\alpha\beta} n_{i\alpha} n_{i\beta}\right)\right)n_{i\gamma} n_{i\chi}=0,\qquad \gamma\le\chi$$

In 3 dimensions this is 10 equations with $c_{\gamma\chi}$ symmetric. Reorganizing:

$$\begin{aligned}
a:&\quad \sum_i w_i f_i &&=a\sum_i w_i &&+\sum_\alpha b_\alpha\sum_i w_i n_{i\alpha} &&+\sum_{\alpha\beta} c_{\alpha\beta}\sum_i w_i n_{i\alpha} n_{i\beta}\\
b_\gamma:&\quad \sum_i w_i f_i n_{i\gamma} &&=a\sum_i w_i n_{i\gamma} &&+\sum_\alpha b_\alpha\sum_i w_i n_{i\alpha} n_{i\gamma} &&+\sum_{\alpha\beta} c_{\alpha\beta}\sum_i w_i n_{i\alpha} n_{i\beta} n_{i\gamma}\\
c_{\gamma\chi}:&\quad \sum_i w_i f_i n_{i\gamma} n_{i\chi} &&=a\sum_i w_i n_{i\gamma} n_{i\chi} &&+\sum_\alpha b_\alpha\sum_i w_i n_{i\alpha} n_{i\gamma} n_{i\chi} &&+\sum_{\alpha\beta} c_{\alpha\beta}\sum_i w_i n_{i\alpha} n_{i\beta} n_{i\gamma} n_{i\chi}
\end{aligned}$$

One possibility that make sense is to fix $a = f(0)$ so that the quadratic is an exact match at the origin. This is what the Taylor's series expansion would have if we knew the derivatives instead of just trying to fit them from the samples.

In matrix form the left hand sides become a result vector

$$y = \left\{ \sum_i w_i f_i, \sum_i w_i f_i n_{i\gamma}, \sum_i w_i f_i n_{i\gamma} n_{i\chi} \right\} = \sum_i w_i f_i \left\{ 1, n_{i\gamma}, n_{i\gamma} n_{i\chi} \right\}$$

If we are fixing a then we will use $\left(y - az \right)$ where

$$y = \sum_i w_i f_i \left\{ n_{i\gamma}, n_{i\gamma} n_{i\chi} \right\},\ z = \sum_i w_i \left\{ n_{i\gamma}, n_{i\gamma} n_{i\chi} \right\}$$

A second vector is formed from the parameters

$$p = \left\{ a, b_\alpha, c_{\alpha\beta} \right\} \quad \text{or} \quad p = \left\{ b_\alpha, c_{\alpha\beta} \right\}$$

And a matrix is formed from the rest of the right hand side

$$M = \begin{bmatrix} \sum_i w_i & \sum_i w_i n_{i\alpha} & \sum_i w_i n_{i\alpha} n_{i\beta} \\ \sum_i w_i n_{i\gamma} & \sum_i w_i n_{i\alpha} n_{i\gamma} & \sum_i w_i n_{i\alpha} n_{i\beta} n_{i\gamma} \\ \sum_i w_i n_{i\gamma} n_{i\chi} & \sum_i w_i n_{i\alpha} n_{i\gamma} n_{i\chi} & \sum_i w_i n_{i\alpha} n_{i\beta} n_{i\gamma} n_{i\chi} \end{bmatrix}$$

Alternatively if a is fixed to f(0)

$$M = \begin{bmatrix} \sum_i w_i n_{i\alpha} n_{i\gamma} & \sum_i w_i n_{i\alpha} n_{i\beta} n_{i\gamma} \\ \sum_i w_i n_{i\alpha} n_{i\gamma} n_{i\chi} & \sum_i w_i n_{i\alpha} n_{i\beta} n_{i\gamma} n_{i\chi} \end{bmatrix}$$

In the vectors and matrix, expand vertically over the values of α and β and horizontally over the values of γ and χ to make dimension $\left(1 + d + d\left(d+1\right)/2\right)$ vectors and matrix. Subtract 1 if a is fixed to f(0). This yields the equation

$$y = Mp \quad \Rightarrow \quad p = M^{-1} y$$

If a is fixed, then

$$\left(y - az \right) = Mp \quad \Rightarrow \quad p = M^{-1} y - a M^{-1} z$$

The idea here is to track the contribution of the central point separately.

The Laplacian is then $\nabla^2 f\left(\vec{r}\right)\Big|_{\vec{r}=0} \approx \frac{2}{s^2} Tr\left[c_{\alpha\beta} \right]$.

The trace is simply the sum of d elements of p corresponding to $c_{00}, c_{11}, \ldots, c_{d-1,d-1}$.