Least Squares, Equidistribution and Conservation

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Abstract

Let $\mathbf{F}$ be a vector valued function which is piecewise conforming on a partition of a polygonal region Ω into triangles, with a prescribed flux across the boundary $\partial\Omega$. Then minimisation of the l_2 norm of the *fluctuation* of $\mathbf{F}$ over the internal nodes of the partition is equivalent to minimisation of the l_2 norm of the *differences* in the fluctuations of $\mathbf{F}$ over all the elements of the partition. In this sense l_2 minimisation is equivalent to an l_2 measure of equidistribution. The result is also true for the l_2 norm of the *local average residuals*, i.e. the fluctuations weighted by the reciprocal areas of the elements.

The particular case $\mathbf{F} = U\mathbf{a}$, where U is a piecewise linear function prescribed on $\partial\Omega$ and $\mathbf{a}$ is divergence-free, is considered in detail.

The result extends to the *local average vorticity* as well as to norms combining both the residual and the vorticity, as for example in the case of the Cauchy-Riemann equations.

1 Introduction

There are two main approaches to the problem of generating an irregular mesh on which to approximately solve a differential equation. A popular criterion has been that of equidistribution, in which the grid is determined by a monitor function whose integral is the same in each interval [1],[2],[3]. Another approach is to use direct minimisation of a suitable functional of the equation [3],[4],[5] in which the grid participates in the minimisation. Each of these methods has advantages and disadvantages but comparisons have been impeded by the absence of any link between them. In this report we demonstrate that, provided that the boundary values are fixed, direct minimisation of a discrete least squares error over internal variations of the function and the nodes is equivalent to minimising a corresponding measure of equidistribution.

2 Fluctuations and Residuals

Consider the first order conservation law

$$div\mathbf{f} = 0 \tag{1}$$

in a polygonal region Ω and let $\mathbf{f}$ be approximated by a conforming approximation $\mathbf{F}$ on a triangulation $\{T\}$ of Ω. Then, following Roe [7], on each triangle T we may define the *fluctuation*

$$\phi_T = -\int_T div\mathbf{F}d\Omega. \tag{2}$$

We may also define an *local average residual* on the triangle T

$$\overline{R}_T = \frac{1}{S_T}\int_T div\mathbf{F}d\Omega, \tag{3}$$

where S_T is the area of the triangle, so that

$$\overline{R}_T = -\frac{\phi_T}{S_T}. \tag{4}$$

If $\mathbf{F} = U\mathbf{a}$ where U is piecewise linear and $\mathbf{a}$ is divergence-free we have

$$div\mathbf{F} = \mathbf{a}.\nabla U \tag{5}$$

and the fluctuation is

$$\phi_T = -\int_T \mathbf{a}.\nabla U d\Omega = -\left(\int_T \mathbf{a}d\Omega\right).(\nabla U)_T = -S_T\,(\overline{\mathbf{a}}.\nabla U)_T \tag{6}$$

where $\overline{\mathbf{a}}$ is the centroid value of $\mathbf{a}$. In that case we may define the *average residual* to be

$$\overline{R}_T = (\overline{\mathbf{a}}.\nabla U)_T = -\frac{\phi_T}{S_T} \tag{7}$$

in each triangle, using (6). If a is constant we may define the unique *residual*

$$R_T = (div\mathbf{F})_T = (\mathbf{a}.\nabla U)_T. \tag{8}$$

These definitions also hold in higher dimensions with S_T replaced by the volume of the appropriate simplex and Ω by the union of the simplexes.

3 A Zero Residual Property

In the case where **a** is constant it has been pointed out in [7] that if two of the vertices of a triangle T lie on a characteristic, i.e. a line in the direction of **a** on which U is constant, then the fluctuation ϕ_T (and therefore the residual R_T) vanishes. This follows from (5) since any line joining two vertices of T on which U is constant is a level line of the locally linear function U and therefore perpendicular to ∇U. Similarly, in higher dimensions, if any two vertices of a simplex lie on a characteristic then the fluctuation ϕ_T and the residual R_T vanish by the same argument.

We give an algebraic proof of this result in two dimensions which also serves to introduce some notation. Let the vertices (X_i, Y_i) of the triangle T be numbered $i = 1, 2, 3$ in an anticlockwise sense. Then in triangle T

$$\nabla U = \frac{1}{S_T}\left(\sum Y_1(U_2 - U_3), \;\; -\sum X_1(U_2 - U_3)\right) \tag{9}$$

where the sum is taken cyclically over the vertices of the triangle. In the same notation the area S_T of the triangle is

$$S_T = \sum X_1(Y_2 - Y_3) = -\sum Y_1(X_2 - X_3). \tag{10}$$

It follows that

$$\phi_T = -S_T\mathbf{a}.\nabla U = -\sum(aY_1 - bX_1)(U_2 - U_3) \tag{11}$$

where $\mathbf{a} = (a, b)$ which, if $U_2 = U_3$, reduces to

$$\begin{aligned}\phi_T &= -(aY_2 - bX_2)(U_3 - U_1) - (aY_3 - bX_3)(U_1 - U_2)\\ &= (-a(Y_2 - Y_3) + b(X_2 - X_3))(U_2 - U_1).\end{aligned} \tag{12}$$

The right hand side vanishes when the vector $(X_2 - X_3, Y_2 - Y_3)$ is in the direction of **a**.

4 Fluctuation Equidistribution

Consider now the identity

$$\phi_1^2 + \phi_2^2 \equiv \frac{1}{2}(\phi_1 + \phi_2)^2 + \frac{1}{2}(\phi_1 - \phi_2)^2 \tag{13}$$

which may readily be generalised to

$$\sum_{i=1}^{N} \phi_i^2 \equiv \frac{1}{N}\left(\sum_{i=1}^{N}\phi_i\right)^2 + \frac{1}{2N}\sum_{i=1}^{N}\sum_{j=1}^{N}\left(\phi_i - \phi_j\right)^2. \tag{14}$$

Let ϕ_i be the fluctuation ϕ_T in triangle T_i as defined in section 1 and let N be the number of triangles in Ω. The first term in brackets on the right hand side of (14) may then be written

$$\sum_{i=1}^{N}\phi_i = -\sum_{i=1}^{N}\int_{T_i} div\mathbf{F}d\Omega = -\sum_{i=1}^{N}\int_{\partial T_i}\mathbf{F}.ds \tag{15}$$

where ∂T_i is the boundary of T_i. Since $\mathbf{F}$ is conforming (15) reduces to

$$-\int_{\partial\Omega}\mathbf{F}.ds \tag{16}$$

over the boundary $\partial\Omega$ of Ω. The quantity in (16) is fixed when the flux of $\mathbf{F}$ across the outer boundary is preserved. In the original conservation law problem only the contribution to (16) from the inflow is prescribed but the least squares minimisation procedure described below also demands an outflow condition, in which case (16) is fully prescribed.

It then follows from (14) that, if (16) is fixed, then under variations of the internal values of $\mathbf{F}$ and the internal grid points, the l_2 norm of ϕ_{T_i} is least when the final term in (14) vanishes. If the ϕ_{T_i} are equal for all i then the minimum is achieved and equidistribution is equivalent to least squares minimisation. If this condition is unattainable the result is restricted to the observation that the two norms

$$\sum_{i=1}^{N}\phi_i^2 \quad \text{and} \quad \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\phi_i - \phi_j\right)^2 \tag{17}$$

are minimised simultaneously. The second of these is a measure of the equidistribution of ϕ_T over the triangles.

The result generalises to any number of dimensions.

When $\mathbf{F} = U\mathbf{a}$ with U piecewise linear and a divergence-free ϕ_T is given by

$$\phi_T = -S_T\bar{\mathbf{a}}.\nabla U \tag{18}$$

(cf. (11)) which in two dimensions has the form

$$\phi_T = -\sum(\bar{a}Y_1 - \bar{b}X_1)(U_2 - U_3). \tag{19}$$

In that case minimisation of the norm

$$\sum_{i=1}^{N}\phi_i^2 = \sum_{i=1}^{N}(S_T\bar{\mathbf{a}}.\nabla U)^2 = \sum_{i=1}^{N}\left(\sum(\bar{a}Y_1 - \bar{b}X_1)(U_2 - U_3)\right)^2 \tag{20}$$

is equivalent to minimisation of the l_2 norm of the *differences* between the ϕ_T's of (19) provided that the boundary quantity in (16) is held constant.

5 Residual Equidistribution

From (7) we have

$$\phi_T = -S_T\overline{R}_T \tag{21}$$

so that the norms in (17) become

$$\sum_{i=1}^{N}\left(S_T\overline{R}_T\right)_i^2 \quad \text{and} \quad \sum_{i=1}^{N}\sum_{j=1}^{N}\left((S_T R_T)_i - (S_T R_T)_j\right)^2. \tag{22}$$

Another useful norm, used in [7], is the l_2 norm of the residual $\overline{R}_T$ weighted by the triangle area, i.e.

$$\sum_{i=1}^{N} S_T\overline{R}_{T_i}^2 \tag{23}$$

(cf. (22)). In that case we may consider a generalisation of the identity (14), in the form

$$\sum_{i=1}^{N} S_i \sum_{i=1}^{N}\left(\frac{\phi_i}{S_i}\right)^2 \equiv \left(\sum_{i=1}^{N}\phi_i\right)^2 + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j\left\{\frac{\phi_i}{S_i} - \frac{\phi_j}{S_j}\right\}^2 \tag{24}$$

where $S_i = S_{T_i}$ or, equivalently,

$$\sum_{i=1}^{N} S_i \sum_{i=1}^{N}\overline{R}_i \equiv \left(\sum_{i=1}^{N}\phi_{T_i}\right)^2 + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j\left(\overline{R}_i - \overline{R}_j\right)^2 \tag{25}$$

(see (4)). Clearly

$$\sum_{i=1}^{N} S_i = \int_{T_i} d\Omega_{T_i} = \Omega \tag{26}$$

is a constant equal to the total area of the domain while

$$\sum_{i=1}^{N}\phi_i = -\sum_{i=1}^{N}\int_{\partial T_i} div\mathbf{F}d\Omega = -\int_{\partial\Omega}\mathbf{F}.ds, \tag{27}$$

independent of the internal values of **F** and the internal grid locations as before.

We may thus write (25) as

$$\sum_{i=1}^{N} S_i\overline{R}_i^2 \equiv \frac{1}{\Omega}\left(\int_{\partial\Omega}\mathbf{F}.ds\right)^2 + \frac{1}{2\Omega}\sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j\left(\overline{R}_i - \overline{R}_j\right)^2 \tag{28}$$

from which it follows that, provided (27) is held constant, the weighted l_2 norm (23), when minimised over internal values of U and the internal grid points, is least when the average residual $\overline{R}_{T_i}$ is equidistributed. If this property is not attainable we still have the result that the two norms

$$\sum_{i=1}^{N} S_i \overline{R}_i^2 \quad \text{and} \quad \sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_i \left(\overline{R}_i - \overline{R}_j\right)^2 \tag{29}$$

are minimised simultaneously.

Once again the result hold in higher dimensions.

When $\mathbf{F} = U\mathbf{a}$ where U is piecewise linear and $\mathbf{a}$ is divergence-free $\overline{R}_T$ is given by

$$\overline{R}_T = \overline{\mathbf{a}}.\nabla U \tag{30}$$

(cf. (11)) which in two dimensions takes the form

$$\overline{R}_T = \frac{\sum(\overline{a}Y_1 - \overline{b}X_1)(U_2 - U_3)}{S_T}. \tag{31}$$

In that case minimisation of the norm

$$\sum_{i=1}^{N} S_i \overline{R}_i^2 = \sum_{i=1}^{N} S_i \left(\overline{\mathbf{a}}.\nabla U\right)_i^2 = \sum_{i=1}^{N} \frac{\left(\sum(\overline{a}Y_1 - \overline{b}X_1)(U_2 - U_3)\right)_i^2}{\sum X_1(Y_2 - Y_3)_i} \tag{32}$$

is equivalent to minimisation of the norm of the difference in the residuals

$$\sum_{i=1}^{N}\sum_{j=1}^{N} \left(\overline{R}_i - \overline{R}_j\right)^2, \tag{33}$$

again provided that (16) is held constant.

6 An Example of Residual Minimisation

An example in two dimensions, quoted in [7], for which $\overline{R}_{T_i}$ and $\overline{R}_{T_j}$ are equal to a high degree of approximation, is as follows. Let Ω be the rectangular box $|x| < 1, y > 1$ and let $\mathbf{a} = (-y, x)$ so that $div\mathbf{a} = 0$. Then from (6) and (7)

$$\phi_T = -S_T(-\overline{Y}U_x + \overline{X}U_y)_T \tag{34}$$

and

$$\overline{R}_T = -(-\overline{Y}U_x + \overline{X}U_y)_T \tag{35}$$

where $\overline{x}, \overline{y}$ are the centroid values of x, y. Let the inflow conditions be prescribed as zero except at two points on the boundary where U takes the value 1 (see figure 1) and suppose that outflow conditions are also prescribed as zero except at the two 'mirror' points on the boundary where U is also taken to be 1.

The weighted l_2 norm of the residual is now minimised over both nodal U values and nodal locations, giving the variational equations

$$\sum_{i=1}^{N} \frac{1}{2}\overline{R}_i \left(-\overline{Y}(Y_3 - Y_2) + \overline{X}(X_3 - X_2)\right) = 0, \tag{36}$$

$$\sum_{i=1}^{N} \left(-\frac{b}{2}\overline{R}_i(U_3 - U_2) + \frac{1}{4}\overline{R}_i^2(Y_3 - Y_2)\right) = 0 \tag{37}$$

and

$$\sum_{i=1}^{N} \left(\frac{a}{2}\overline{R}_i(U_3 - U_2) - \frac{1}{4}\overline{R}_i^2\,(X_3 - X_2)\right) = 0 \tag{38}$$

where node i is also node 1 of the cyclic trio of nodes $1, 2, 3$ and $\overline{R}_T$ is given by (35).

The resulting grid is shown in figure 1. The nodes move into positions for which the residuals are small and, in accordance with the discussion in section 4, the sides of the triangles attempt to line up with the characteristics. Moreover, by the result in section 5, the l_2 norm of the *differences* in the residuals is also minimised, leading to approximate equidistribution.

7 Systems

A generalisation of the underlying identity (25) to systems has been given by Roe [8]. If $\underline{g}_i$ is a column vector and Q is a matrix of constant values we have the identity

$$\sum_{i=1}^{N} S_i \sum_{i=1}^{N} S_i \underline{g}_i^t Q \underline{g}_i$$

$$\equiv \left(\sum_{i=1}^{N} S_i \underline{g}_i\right)^t Q \left(\sum_{i=1}^{N} S_i \underline{g}_i\right) + \sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j \left(\underline{g}_i - \underline{g}_j\right)^t Q \left(\underline{g}_i - \underline{g}_j\right). \tag{39}$$

With $\underline{g}_i = \underline{\overline{R}}_i$ the first sum in brackets on the right hand side is

$$\sum_{i=1}^{N} S_i \underline{\overline{R}}_i = \sum_{i=1}^{N} \int_{\Omega_i} div \underline{\mathbf{F}} d\Omega = \sum_{i=1}^{N} \int_{\partial\Omega_i} \underline{\mathbf{F}}.ds = \int_{\partial\Omega} \underline{\mathbf{F}}.ds, \tag{40}$$

(independent of internal values of $\mathbf{F}$ or internal grid locations). Hence, from (39), provided that (40) is held fixed the minimum of the weighted least squares norm of the residuals

$$\sum_{i=1}^{N} S_i \underline{\overline{R}}_i^t Q \underline{\overline{R}}_i \tag{41}$$

is achieved when the weighted norm of the residual *differences*

$$\sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j \left(\underline{\overline{R}}_i - \underline{\overline{R}}_j\right)^t Q \left(\underline{\overline{R}}_i - \underline{\overline{R}}_j\right) \tag{42}$$

is also minimised. The result is true in any number of dimensions.

Although the problem of solving $\overline{R}_i = \overline{R}_j$ is overdetermined in general the result shows, in the case of a vector residual for a conservative system, that there is a close connection between equidistribution and minimisation of the weighted least squares norm of the average residual in the sense that a weighted least squares norm of the average residual differences is minimised.

8 Vorticity

The self-cancelling property of (15) applies also to

$$\int_{\partial T_i} \mathbf{F} \times \mathbf{ds} = \int_{\partial T_i} curl\mathbf{F} d\Omega \tag{43}$$

so that defining

$$\underline{\overline{\omega}} = \frac{1}{S_i} \int curl\mathbf{F} d\Omega \tag{44}$$

as the *average local vorticity* in triangle T_i, we have, using (39) with $\mathbf{g} = \underline{\overline{\omega}}$ and $Q = I$ that

$$\sum_{i=1}^{N} S_i \sum_{i=1}^{N} S_i \left|\underline{\overline{\omega}}_i\right|^2$$

$$= \left|\sum_{i=1}^{N} S_i \underline{\overline{\omega}}_i\right|^2 + \sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j \left|\underline{\overline{\omega}}_i - \underline{\overline{\omega}}_j\right|^2. \tag{45}$$

Now

$$\sum_{i=1}^{N} S_i \underline{\overline{\omega}}_i = \sum_{i=1}^{N} \int_{T_i} curl\mathbf{F} d\Omega = \sum_{i=1}^{N} \int_{\partial T_i} \mathbf{F} \times d\mathbf{s} = \int_{\partial\Omega} \mathbf{F} \times d\mathbf{s} \tag{46}$$

which is independent of internal values of $\mathbf{F}$ and internal grid points. Hence if (46) is held fixed we have from (45) that the weighted l_2 norm of $\underline{\overline{\omega}}$ is minimised when the weighted l_2 norm of the differences in $\underline{\overline{\omega}}$ is also minimised.

Combining (45) with (28) we have

$$\sum_{i=1}^{N} S_i \left(\sum_{i=1}^{N} S_i \left(\overline{R}_i^2 + \gamma \left|\underline{\overline{\omega}}_i\right|^2\right)\right)$$

$$= \left(\int_{\partial\Omega} \mathbf{F}.d\mathbf{s}\right)^2 + \gamma \left|\int_{\partial\Omega} \mathbf{F} \times d\mathbf{s}\right|^2$$

$$+ \sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j \left(\left(\overline{R}_i - \overline{R}_j\right)^2 + \gamma \left|\underline{\overline{\omega}}_i - \underline{\overline{\omega}}_j\right|^2\right) \tag{47}$$

for any constant γ. Then if the boundary values of $\mathbf{F}$ and its grid are held fixed it follows that the norms

$$\sum_{i=1}^{N} S_i \left(\overline{R}_i^2 + \gamma \left|\underline{\overline{\omega}}_i\right|^2\right) \tag{48}$$

and

$$\sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j \left(\left(\overline{R}_i - \overline{R}_j \right)^2 + \gamma \left| \overline{\boldsymbol{\omega}}_i - \overline{\boldsymbol{\omega}}_j \right|^2 \right) \tag{49}$$

are minimised simultaneously. Hence (48) is least when both the average residuals and vorticities are equidistributed.

If $curl\mathbf{F} = \mathbf{0}$ and there exists a potential function ψ such that $div\mathbf{F} = \nabla^2\psi$ and

$$\overline{R}_i = \frac{1}{S_i}\int_{T_i} \nabla^2 \psi d\Omega = \frac{1}{S_i}\int_{\partial T_i} \frac{\partial \psi}{\partial n} ds \tag{50}$$

in two dimensions. Of course if $div\mathbf{F}$ is also zero then ψ is harmonic.

9 Cauchy-Riemann Equations

An application of the result of the previous section is to the Cauchy-Riemann equations

$$div\mathbf{F} = 0, \qquad curl\mathbf{F} = \mathbf{0} \tag{51}$$

in two dimensions, i.e.

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \qquad \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = 0. \tag{52}$$

Defining

$$\begin{aligned} \overline{R}_i &= \frac{1}{S_i}\int_{T_i} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) d\Omega \\ \overline{\omega}_i &= \frac{1}{S_i}\int_{T_i} \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) d\Omega, \end{aligned} \tag{53}$$

approximate solutions may be obtained by minimising the least squares norm

$$\sum_{i=1}^{N} S_i \left(\overline{R}_i^2 + \overline{\omega}_i^2 \right) \tag{54}$$

over internal values of u, v and x, y. By the result in (48),(49) the norm

$$\sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j \left(\left(\overline{R}_i - \overline{R}_j \right)^2 + \left(\overline{\omega}_i - \overline{\omega}_j \right)^2 \right) \tag{55}$$

is also minimised, indicating approximate equidistribution of both $\overline{R}_i$ and $\overline{\omega}_i$.

In [7] Roe also considers the system

$$(1 - M^2)\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0, \qquad \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = 0 \tag{56}$$

where $M^2 > 1$ corresponds to a hyperbolic system and $M^2 < 1$ to an elliptic system (see also [9]). The norm minimised is

$$\sum_{i=1}^{N} S_i \left(\overline{R}_i^2 + \left|M^2 - 1\right| \overline{\omega}_i^2\right) \tag{57}$$

correponding to (47) with $\gamma = |M^2 - 1|$. Minimisation of (57) over internal parameters thus implies minimisation of

$$\sum_{i=1}^{N}\sum_{j=1}^{N} S_i S_j \left(\left(\overline{R}_i - \overline{R}_j\right)^2 + \left|M^2 - 1\right| (\overline{\omega}_i - \overline{\omega}_j)^2\right), \tag{58}$$

which indicates the extent to which $\overline{R}_i$ and $\overline{\omega}_i$ are approximately equidistributed.

10 Acknowledgement

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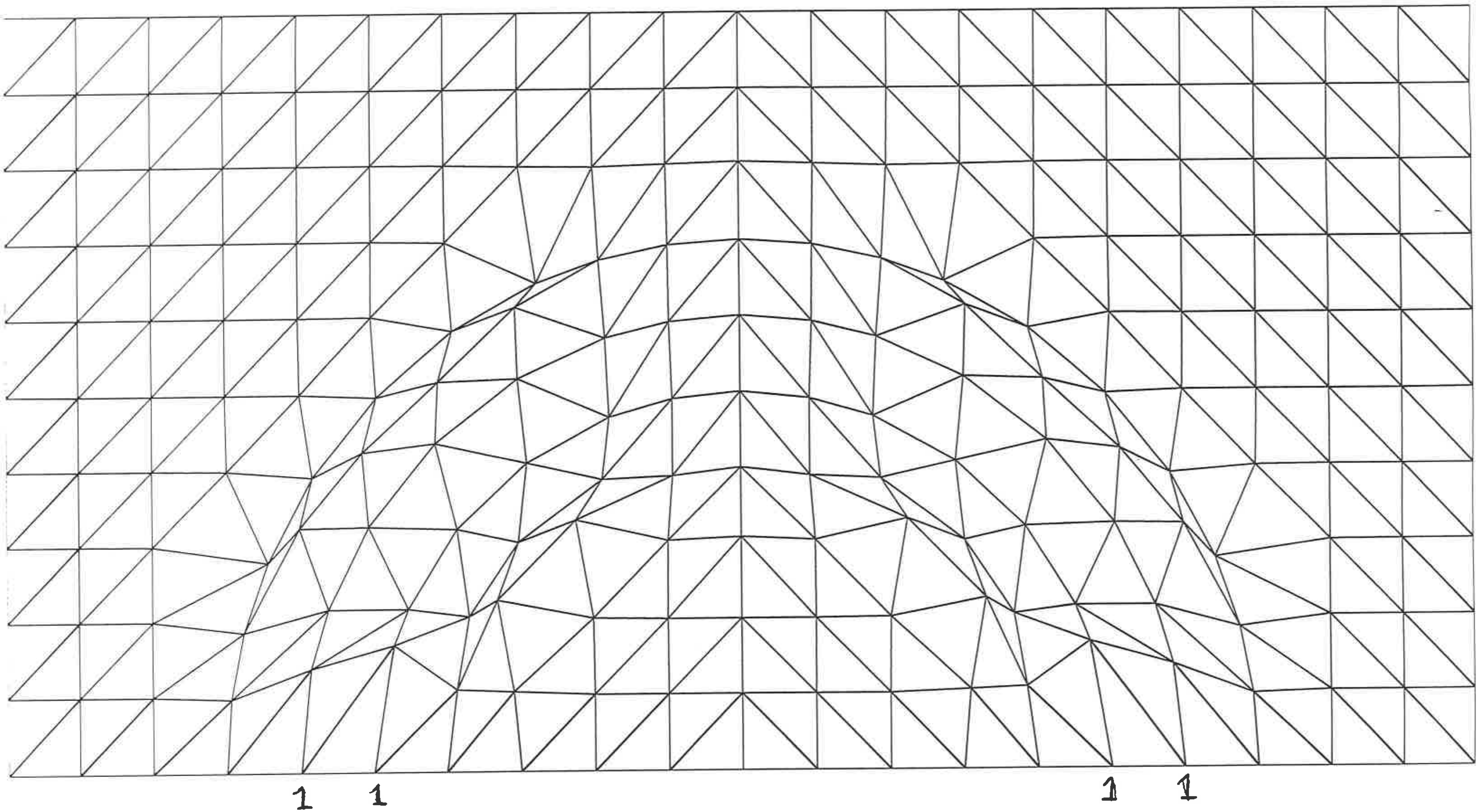

Fig-1