Loss function for a Poisson 2D inverse problem of finding a constant unknown forcing

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1 The Problem

Find the function $u : \Omega \to \mathbb{R}$ and constant f such that

$$\begin{aligned} -\nabla^2 u(x,y) &= f && \text{for } (x,y) \text{ in } \Omega \\ u(x,y) &= 0.3(1-x^2-y^2) && \text{for } (x,y) \text{ on } \partial\Omega \\ u(x_d,y_d) &= 0.3(1-x_d^2-y_d^2) \end{aligned}$$

where $\Omega = (-1,1)\times(-1,1)$ and (x_d, y_d) is an internal data point in Ω. The solution for this problem is

$$\begin{aligned} u &= 0.3(1-x^2-y^2) \\ f &= 1.2 \end{aligned}$$

We wish to solve this class of inverse problems in the FEM framework using ML techniques.

2 The loss function

We will be working with a 3 node triangular mesh over the domain Ω. The input for the loss function would be

1. the vector u_{out} where the indices are the value of u at each node, which would be the output of a GCN,
2. f_{val}, a guess for the unknown constant f, which would be a trainable parameter,
3. the stiffness matrix $K \in \mathbb{R}^{n\times n}$,
4. data forcing vector $f_d \in \mathbb{R}^n$,
5. and forcing vector $f_0 \in \mathbb{R}^n$ assuming a forcing of unity, that is $f = 1$.

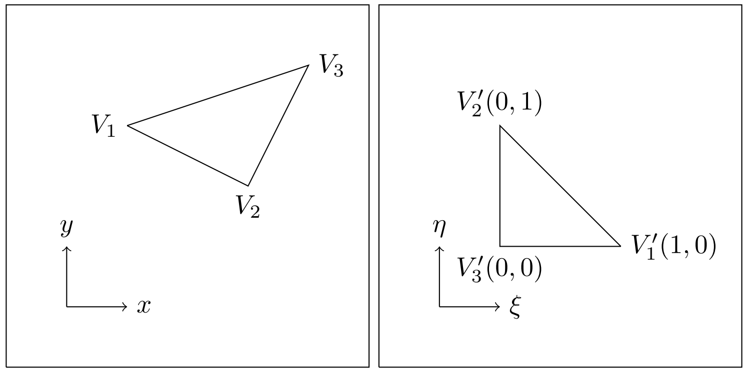

Figure 1: The triangular element T in the computaional domain is shown on the left while its reference element T' is shown on the right.

where n is the degree of freedom, that is the number of nodes on which the value of u is unknown. If we have $N \times N$ total nodes, $n = N^2 - 4N + 3$, as there are $4(N-2)+4$ boundary data points and 1 internal data point.

The loss function we consider is the following.

$$r = Ku_{out} + f_d - f_{val} f_0 \tag{1}$$

$$Loss = \sum_i r_i^2 \tag{2}$$

The derivation can be found in the following sections.

3 Algebraic equations for one element

Consider the triangular element T as seen in figure 1. Given a point $O(x,y)$ inside the triangle $V_1V_2V_3$, we define ξ and η, the barycentric coordinates.

$$\xi = \frac{\text{area}(OV_2V_3)}{\text{area}(V_1V_2V_3)}$$

$$\eta = \frac{\text{area}(OV_1V_3)}{\text{area}(V_1V_2V_3)}$$

Let the value of the trial function $u(x,y)$ at the vertices V_1, V_2 and V_3 be u_1, u_2 and u_3 respectively. Similarly, let the value of the test function $v(x,y)$ at the vertices V_1, V_2 and V_3 be v_1, v_2 and v_3 respectively. Now, the points inside or on the triangle are easily parameterised by ξ and η in the following manner.

$$x = N_1x_1 + N_2x_2 + N_3x_3 \tag{3}$$

$$y = N_1y_1 + N_2y_2 + N_3y_3 \tag{4}$$

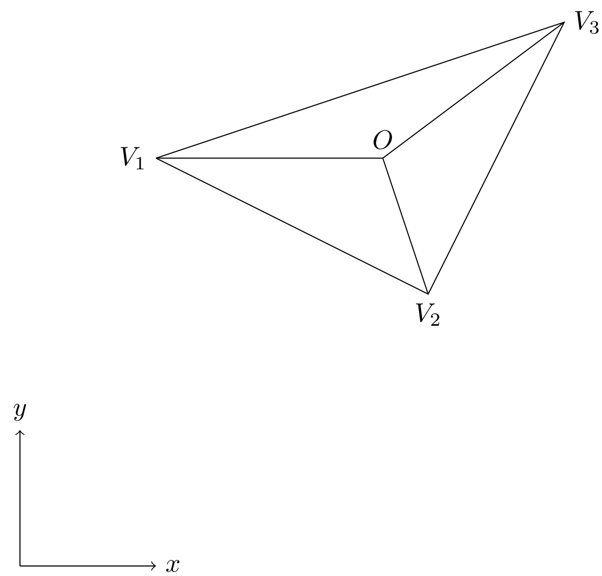

Figure 2: To define parameters ξ and η we form three triangles OV_2V_3, OV_3V_1, and OV_1V_2 which put together form the triangle $V_1V_2V_3$.

where

$$N = \begin{bmatrix} N_1 & N_2 & N_3 \end{bmatrix}$$
$$N_1, N_2, N_3 = \xi, \eta, 1 - \xi - \eta$$

Assuming V_1, V_2 and V_3 to be free nodes, the finite dimensional weak formulation for the Poisson's problem in two dimensions for the triangular element T is to find $\hat{u} = \begin{bmatrix} u_1 & u_2 & u_3 \end{bmatrix}^\mathsf{T}$ such that

$$\int_T \frac{\partial v}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\frac{\partial u}{\partial y} dxdy = \int_T fvdxdy \tag{5}$$

for all $\hat{v} = \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix}^\mathsf{T}$, where,

$$u(x(\xi, \eta), y(\xi, \eta)) = N\hat{u}$$
$$v(x(\xi, \eta), y(\xi, \eta)) = N\hat{v}$$

Following standard procedure, to find algebraic equations for the element, we start from

$$
\begin{aligned}
\begin{bmatrix}\partial u/\partial \xi \\ \partial u/\partial \eta\end{bmatrix} &= J \begin{bmatrix}\partial u/\partial x \\ \partial u/\partial y\end{bmatrix} \qquad\qquad J = \begin{bmatrix}x_1 - x_3 & y_1 - y_3 \\ x_2 - x_3 & y_2 - y_3\end{bmatrix} \\
\implies \begin{bmatrix}\partial u/\partial x \\ \partial u/\partial y\end{bmatrix} &= J^{-1} \begin{bmatrix}\partial u/\partial \xi \\ \partial u/\partial \eta\end{bmatrix} \\
&= J^{-1} \begin{bmatrix}u_1 - u_3 \\ u_2 - u_3\end{bmatrix}
\end{aligned}
$$

Therefore,

$$
\begin{bmatrix}\partial u/\partial x \\ \partial u/\partial y\end{bmatrix} = B\hat{u} \tag{6}
$$

$$
\begin{bmatrix}\partial v/\partial x \\ \partial v/\partial y\end{bmatrix} = B\hat{v} \tag{7}
$$

$$
\tag{8}
$$

where,

$$
B = \frac{1}{\det J} \begin{bmatrix}y_2 - y_3 & y_3 - y_1 \\ x_3 - x_2 & x_1 - x_3\end{bmatrix} \begin{bmatrix}1 & 0 & -1 \\ 0 & 1 & -1\end{bmatrix}
$$

So, the LHS of equation 5 is the following.

$$
\begin{aligned}
&\int_T (B\hat{v})^\mathsf{T} (B\hat{u}) dxdy \\
=&\hat{v}^\mathsf{T} B^\mathsf{T} B\hat{u} \int_T dxdy \\
=&\hat{v}^\mathsf{T} K_e \hat{u}
\end{aligned}
$$

where,

$$
K_e = \frac{\det J}{2} B^\mathsf{T} B
$$

The RHS of equation 5 is the following.

$$
\begin{aligned}
&\int_T f\hat{v}^\mathsf{T} \begin{bmatrix}N_1 \\ N_2 \\ N_3\end{bmatrix} \det J d\xi d\eta \\
=&f\hat{v}^\mathsf{T} \hat{f}_e
\end{aligned}
$$

where $\hat{f}_e = \det J/6 \begin{bmatrix}1 & 1 & 1\end{bmatrix}^\mathsf{T}$.

Therefore, under the assumption that V_1, V_2 and V_3 are free nodes, the finite dimensional weak form boils down to finding $\hat{u}$ such that

$$
\hat{v}^\mathsf{T} K_e \hat{u} = f\hat{v}^\mathsf{T} \hat{f}_e \tag{9}
$$

for all $\hat{v} \in \mathbb{R}^3$.

4 Assembly

Upon assembling the equations obtained by the above mentioned treatment, we get the following larger system of equations to be solved.

$$\bar{v}^\top \bar{K}\bar{u} = f\bar{v}^\top \bar{f}$$

where,

1. the total number of nodes are N^2,
2. $\bar{u} \in \mathbb{R}^{N^2}$ and $\bar{u}_i$ is the value of u at the i-th node,
3. similarly, $\bar{v} \in \mathbb{R}^{N^2}$ and $\bar{v}_i$ is the value of v at the i-th node
4. $\bar{K} \in \mathbb{R}^{N^2 \times N^2}$ and

   $$\bar{K}_{ij} = \sum_{\{i',j',e|e(i')=i\&e(j')=j\}} K_e(i',j')$$

   note that an element e is defined by three node indices, so if nodes i_1, i_2 and i_3 form the element e, $e(k) = i_k$ for $k = 1$, 2 and 3.
5. $\bar{f} \in \mathbb{R}^{N^2}$ and its i-th entry

   $$\bar{f}_i = \sum_{\{i',e|e(i')=i\}} \hat{f}_e(i')$$

We know the value of u on $\partial\Omega$ and the data point on (x_d, y_d). As discussed earlier there are $n = N^2 - 4N + 3$ free nodes $\mathcal{F} = [i_1, i_2, \ldots, i_n]$ and $n' = 4N - 3$ data nodes $\mathcal{D} = [i'_1, i'_2, \ldots, i'_{n'}]$ From the variational form, the value of the test function on the data nodes is zero and arbitrary on the free nodes, therefore,

$$K\tilde{u} + K'\tilde{u}' = ff_0 \tag{10}$$

$$\Longrightarrow K\tilde{u} + f_d = ff_0 \tag{11}$$

where,

1. the values at the free nodes is $\tilde{u} \in \mathbb{R}^n$, the k-th entry $\tilde{u}_k = \bar{u}_{i_k}$ for $\mathcal{F}(k) = i_k$, the k-th free node
2. the values at the data nodes is $\tilde{u}' \in \mathbb{R}^{n'}$, the k-th entry $\tilde{u}'_k = \bar{u}_{i'_k}$ for $\mathcal{D}(k) = i'_k$, the k-th data node
3. the vector $f_0 \in \mathbb{R}^n$, the k-th entry is $\bar{f}_{i_k}$ for $\mathcal{F}(k) = i_k$, the k-th free node
4. the matrix $K \in \mathbb{R}^{n \times n}$, such that $K_{ij} = \bar{K}_{i'j'}$, i' and j' are the i-th and j-th free nodes, that is $\mathcal{F}(i) = i'$ and $\mathcal{F}(j) = j'$
5. the matrix $K' \in \mathbb{R}^{n' \times n'}$ such that $K'_{ij} = \bar{K}_{i'j'}$, i' is the i-th free node, that is $\mathcal{F}(i) = i'$, and j' is the j-th data node, that is $\mathcal{D}(j) = j'$

5 Justification for the loss

From equation 11 we form the residual r and use its squared sum as the loss as seen in equation 2.

$$r = Ku_{out} + f_d - f_{val} f_0$$
$$Loss = \sum_i r_i^2$$

6 Other alternatives