1 Canonical Adjoint Problem

Adjointize Poisson Equation *We will start with Poisson equation;*

$$-\nabla^2 u = f \quad \text{in} \quad \Omega$$
$$u = 0 \quad \text{on} \quad \partial\Omega$$

Find f subject to $u \approx u^*$, where u^* is analytical solution or experimental data.

Solution. Let's start with defining functional J;

$$J = \int_\Omega \frac{1}{2}(u - u^*)^2 d\Omega$$

Now we could define Lagrangian L;

$$L(u, v, f) = J + \int_\Omega v(-\nabla^2 u - f) d\Omega$$

where v is adjoint variable(also Lagrangian multiplier). We know that;

$$\frac{\partial L}{\partial u} = \frac{\partial L}{\partial v} = \frac{\partial L}{\partial f} = 0$$

We are starting with getting variational formulation of L with respect to u;

$$\delta L = \int_\Omega (u - u^*)\delta u d\Omega + \int_\Omega v(-\nabla^2 \delta u - f) d\Omega \tag{1}$$

$$\delta L = \int_\Omega (u - u^*)\delta u d\Omega - \int_{\partial\Omega} v\nabla\delta u d\Omega + \int_\Omega \nabla v \nabla \delta u d\Omega \tag{2}$$

$$\delta L = \int_\Omega (u - u^*)\delta u d\Omega - \int_{\partial\Omega} v\nabla\delta u d\Omega + \int_{\partial\Omega} \nabla v \delta u d\Omega - \int_\Omega \nabla^2 v \delta u d\Omega \tag{3}$$

We impose that our adjoint variable is zero on boundary, $\partial\Omega$. So second and third integrals become zero. Now we are in a position that we can derive $\partial L/\partial u = 0$, by moving δu to the left hand side;

$$\frac{\delta L}{\delta u} = \frac{\partial L}{\partial u} = \int_\Omega |u - u^*| d\Omega - \int_\Omega \nabla^2 v d\Omega = 0 \tag{4}$$

Then adjoint problem becomes;

$$\nabla^2 v = |u - u^*| \quad \text{in} \quad \Omega \tag{5}$$

$$v = 0 \quad \text{on} \quad \partial\Omega \tag{6}$$

Now let's move on to the second derivative, $\partial L/\partial v = 0$;

$$\frac{\partial L}{\partial v} = \int_\Omega (-\nabla^2 u - f) d\Omega = 0 \tag{7}$$

It is obvious that this is our PDE. Lastly, we are going to derive variation expression for δL with respect to control variable f;

$$\delta L = \frac{\partial J}{\partial f}\delta f + \int_\Omega -v\delta f d\Omega \tag{8}$$

$$\frac{\delta L}{\delta f} = \frac{\partial J}{\partial f} - \int_\Omega v d\Omega = 0 \tag{9}$$

Hence, we can calculate the gradient;

$$\frac{\partial J}{\partial f} = \int_\Omega v d\Omega \tag{10}$$

Now we can use the gradient to find next f;

$$f_{next} = \frac{\partial J}{\partial f}\alpha + f_{current} \tag{11}$$

where α is the step size.

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So general workflow of the adjoint based optimization problem;

1. Solve the PDE
2. Solve the Adjoint PDE
3. Calculate the gradient using (16)
4. Update f

This process can be done until match the u and u^*.

1.1 Weak form of the Direct PDE and Adjoint PDE

The canonical Poisson equation was;

$$-\nabla^2 u = f \quad \text{in} \quad \Omega$$
$$u = 0 \quad \text{on} \quad \partial\Omega$$

Now, we need to multiply both sides of the PDE by test function p and integrate over the domain yields;

$$\int_\omega (-\nabla^2 up)dx = \int_\omega fpdx \tag{12}$$

General aim is to reduce the order of derivatives as small as possible. So we integrate the left-hand side by parts;

$$\int_\omega (-\nabla^2 up)dx = -\int_{\partial\Omega} u\nabla pdx + \int_\Omega \nabla u \cdot \nabla pdx = \int_\omega fpdx \tag{13}$$

Since the control variable u is 0 on the boundaries, the boundary integral vanishes.

This system is ready for *assembling* process, hence we can write variational formulation $a(u,p) = L(p)$;

Weak form for direct Poisson equation

$$\int_\Omega \nabla u \cdot \nabla pdx = a(u,p) \tag{14a}$$

$$\int_\Omega fpdx = L(p) \tag{14b}$$

If we repeat the same steps for the adjoint Poisson equation (6) by selecting the test function as q, the weak for of adjoint Poisson equation can be derived as;

Weak form for adjoint Poisson equation

$$-\int_\Omega \nabla v \cdot \nabla qdx = a_{adjoint}(v,q) \tag{15a}$$

$$\int_\Omega (u-u^*)qdx = L_{adjoint}(q) \tag{15b}$$

It is easy to recognize that the solution of direct problem u appears in the left hand side of the variational formulation.

We will use these weak form for solving the Poisson equation using finite element method.

1.2 Numerical Example

We will consider the Poisson equation again;

$$
\begin{aligned}
-\nabla^2 u = f \quad \text{in} \quad \Omega \\
u = 0 \quad \text{on} \quad \partial\Omega
\end{aligned}
$$

We want to find f such that it satisfies the analytical solution of

$$u^* = u(x, y) = 1 + x^2 + y^2$$

when $f = -6$.

Solution. We want to find f which satisfies the anayltical solution of (1.2) for $f = 6$. In other words, we need to get this plot below for certain f;

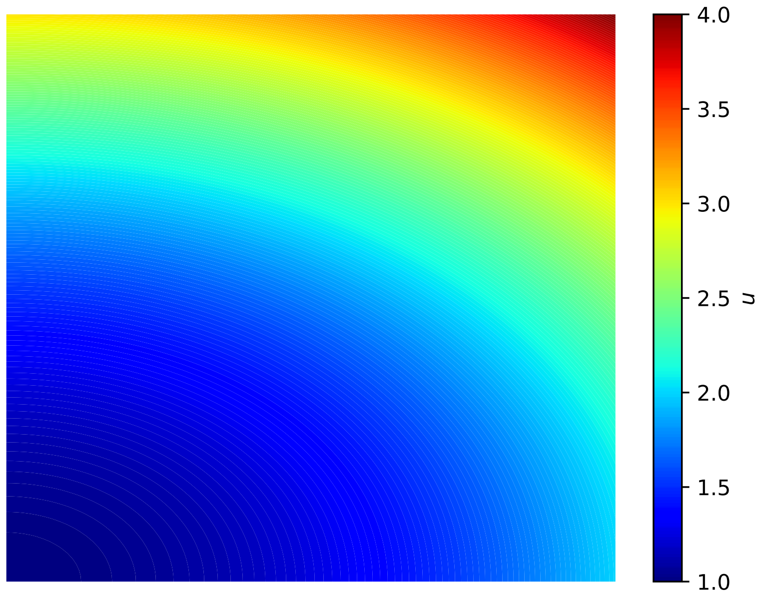

Figure 1: Analytical solution of $u(x, y) = 1 + x^2 + y^2$ for $f = -6$

So the steps are;

1. Start with random f and calculate the direct u
2. Calculate the adjoint u
3. find $\dfrac{\partial J}{\partial f} = \int_\Omega v d\Omega$
4. update f

1.2.1 Start with random f and calculate the direct u

Let's start with $f = 5$. We need to solve direct system by using (14) for $f = 5$. The finite element method is used for solving the system. FenicsX framework is very suitable for this problem. The solution of (14) then becomes;

Figure 2: Direct solution of u

As we can see from Figure 2, solution is not as same as in Figure 1. So we need to change f, but in which direction?

The answer is starts by solving adjoint problem as it is derived in (15). To solve adjoint equation, we have u and u^*, which is analytical solution (Figure 1)

1.2.2 Calculate the adjoint u

For adjoint equation the boundary values are all zero, as stated in (15). If we solve the system with Fenicsx again, we will get this plot;

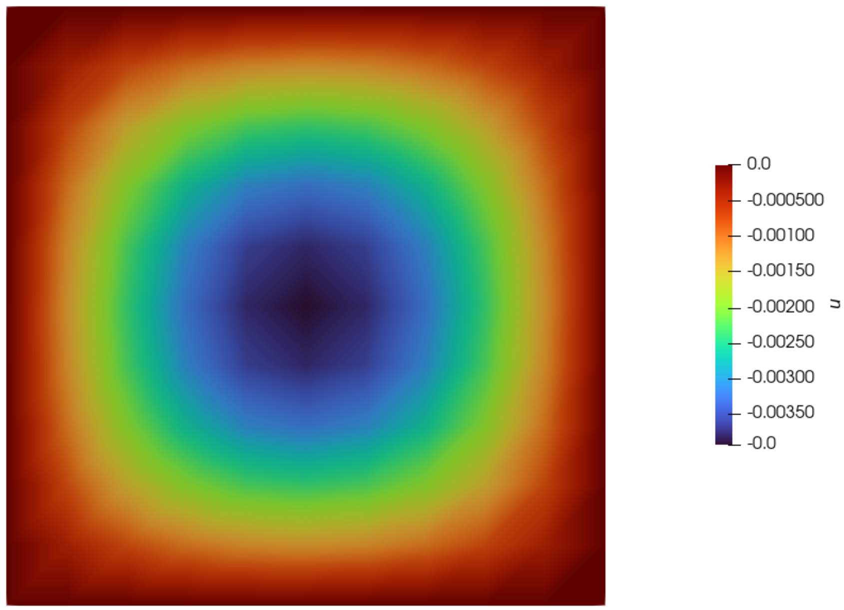

Figure 3: Adjoint solution of u

Figure 3 does not tell anything physically. But this solution is very important for calculating the gradient of functional with respect to f.

1.2.3 Find $\frac{\partial J}{\partial f}$

We will recall the equation of

$$\frac{\partial J}{\partial f} = \int_{\Omega} v d\Omega \tag{16}$$

We can determine the (16) by using the calculated adjoint solution. If we substitute the adjoint solution in 16;

$$\frac{\partial J}{\partial f} = \int_{\Omega} v d\Omega = -0.0016 \tag{17}$$

The found gradient tells that we need to update f such that its value should change in negative direction. For this, we can define new f as;

$$f_{next} = \frac{\partial J}{\partial f}\alpha + f_{current} \tag{18}$$

If we specify α as $1e3$, then new f becomes $f_{new} = -0.0016 * 1e3 + 5 = 3.4$.

Now, as our solution is $f = -6$, we are moving towards right direction now. So we will repeat the steps above. Figure 4 shows that the value f is converged to -6 after 50 iterations.

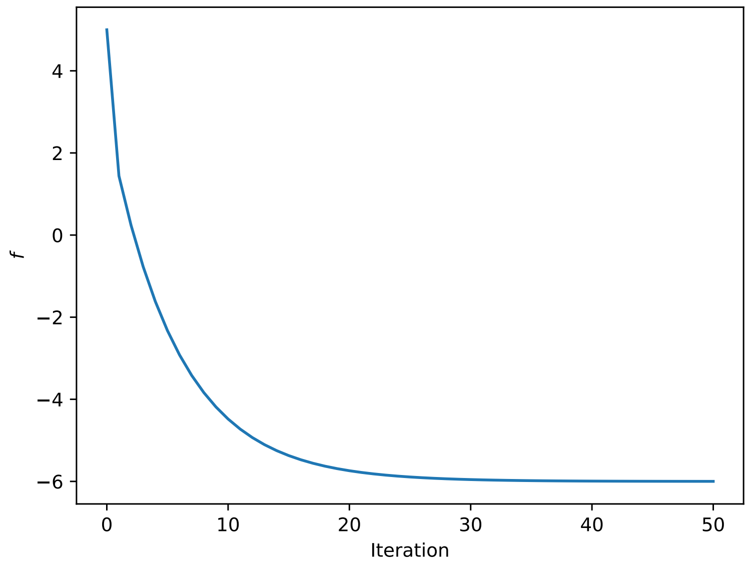

Figure 4: change of value f through 50 iterations

Direct solution of u for $f = -6$ is;

Figure 5: FEM simulation of direct Poisson problem for f=-6

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