

Dirichlet Energy in Different Spaces

December 18, 2022

1 Relevant Definitions

Definition 1 (Gradient Flow). Given an energy (functional) $\mathcal{E}(f)$, *gradient flow* is:

$$\frac{d}{dt}f = -\text{grad } \mathcal{E}(f) \quad (1)$$

Definition 2 (Differential). *Differential* $d\mathcal{E}$ describes change in \mathcal{E} due to¹ u : f

$$d\mathcal{E}|_f(u) = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} (\mathcal{E}(f + \epsilon u) - \mathcal{E}(f)) \quad (2)$$

Definition 3 (Gradient). Given a space X , *gradient* of \mathcal{E} is the unique function $\text{grad}_X \mathcal{E}$ such that,

$$\langle \text{grad}_X \mathcal{E}, u \rangle_X = d\mathcal{E}(u) \quad \forall u \in X \quad (3)$$

2 Dirichlet Energy Example

Definition 4 (Dirichlet Energy). Dirichlet Energy is defined as:

$$\mathcal{E}_D(f) := \frac{1}{2} \int_{\Omega} |\text{grad } f(x)|^2 dx = \frac{1}{2} \langle \nabla f, \nabla f \rangle_{L^2} = -\frac{1}{2} \langle \Delta f, f \rangle_{L^2} \quad (4)$$

where the last equality comes from IBP.

Computing the differential $d\mathcal{E}_D|_f(u)$ of Dirichlet energy using (2),

$$d\mathcal{E}_D|_f(u) = -\frac{1}{2} \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} (\langle \Delta(f + \epsilon u), f + \epsilon u \rangle_{L^2} - \langle \Delta f, f \rangle_{L^2}) \quad (5)$$

$$= -\frac{1}{2} \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} (\epsilon \langle \Delta f, u \rangle_{L^2} + \epsilon \langle \Delta u, f \rangle_{L^2} + \epsilon^2 \langle u, u \rangle_{L^2}) \quad (6)$$

$$= -\frac{1}{2} (\langle \Delta f, u \rangle_{L^2} + \langle \Delta u, f \rangle_{L^2}) \quad (7)$$

$$= -\frac{1}{2} (\langle \Delta f, u \rangle_{L^2} + \langle \Delta f, u \rangle_{L^2}) \quad (8)$$

$$= -\langle \Delta f, u \rangle_{L^2} \quad (9)$$

where the step from (7) to (8) is by integration by parts².

¹analogous in traditional vector space would be “in the direction of” u

²This trick will be used all over the place when constructing gradients and forming **natural boundary condition**. See 4.1 in the Appendix

2.1 Gradient Flow in L^2

By (3), we may spot from (9) that the gradient can be written as

$$\text{grad } \mathcal{E}_{L^2} = -\Delta f \quad (10)$$

Hence, the gradient flow equation (1) can be written as:

$$\frac{d}{dt}f = \Delta f \quad (11)$$

which is the heat equation.

2.2 Gradient Flow in H^1

We may express the differential (9) as

$$d\mathcal{E}_D|_f(u) = -\langle \Delta f, u \rangle_{L^2} \quad (12)$$

$$= \langle \nabla f, \nabla u \rangle_{L^2} \quad (13)$$

$$= \langle f, u \rangle_{H^1} \quad (14)$$

So by (3), the gradient in H^1 can be written as

$$\text{grad } \mathcal{E}_{H^1} = f \quad (15)$$

The gradient flow equation (1) can be written as

$$\frac{d}{dt}f = -f \quad (16)$$

which describes exponential decay.

2.3 Gradient Flow in H^{-1}

We may express the differential (9) as

$$d\mathcal{E}_D|_f(u) = -\langle \Delta f, u \rangle_{L^2} \quad (17)$$

$$= \langle \nabla (\Delta f), \nabla (\Delta^{-1}u) \rangle_{L^2} \quad (18)$$

$$= \langle \Delta f, \Delta^{-1}u \rangle_{H^1} \quad (19)$$

$$= \langle \Delta^2 f, u \rangle_{H^{-1}} \quad (20)$$

So by (3), the gradient in H^{-1} can be written as

$$\text{grad } \mathcal{E}_{H^{-1}} = \Delta^2 f \quad (21)$$

The gradient flow equation (1) can be written as

$$\frac{d}{dt}f = -\Delta^2 f \quad (22)$$

2.4 Gradient Flow in H^2

We may express the differential (9) as

$$d\mathcal{E}_D|_f(u) = -\langle \Delta f, u \rangle_{L^2} \quad (23)$$

$$= -\langle f, \Delta u \rangle_{L^2} \quad (24)$$

$$= -\langle \Delta^{-1} f, u \rangle_{H^2} \quad (25)$$

So by (3), the gradient in H^2 can be written as

$$\text{grad } \mathcal{E}_{H^2} = -\Delta^{-1} f \quad (26)$$

The gradient flow equation (1) can be written as

$$\frac{d}{dt} f = \Delta^{-1} f \quad (27)$$

3 Numerically Solving Gradient Flow Equations

3.1 Gradient Flow in L^2

For L^2 , given the gradient flow equation (11), we may write down explicit Euler scheme:

$$\frac{f_j^{m+1} - f_j^m}{\Delta t} = \frac{f_{j+1}^m - 2f_j^m + f_{j-1}^m}{(\Delta x)^2} \quad (28)$$

which can be rewritten as

$$f_j^{m+1} = f_j^m + \mu (f_{j+1}^m - 2f_j^m + f_{j-1}^m) \quad (29)$$

where $\mu := \frac{\Delta t}{(\Delta x)^2}$ is called the *CFL number*.

3.1.1 Boundary Conditions

For *periodic boundary condition*, we impose:

$$f_0^m = f_J^m \quad \forall m$$

For *natural boundary condition*, we impose:

$$\begin{cases} f_{-1}^m = f_0^m \\ f_J^m = f_{J+1}^m \end{cases} \quad \forall m$$

where this comes from Neumann BC as derived at subsection 4.1.1.

3.1.2 Consistency Error

This method is known to have consistency error

$$T_j^m = \mathcal{O}\left((\Delta x)^2 + \Delta t\right) \quad (30)$$

3.2 Gradient Flow in H^1

Given the gradient flow equation (16), we may write down explicit Euler scheme:

$$\frac{f_j^{m+1} - f_j^m}{\Delta t} = -f_j^m \quad (31)$$

which can be rewritten as

$$f_j^{m+1} = f_j^m - (\Delta t)f_j^m \quad (32)$$

3.3 Gradient Flow in H^{-1}

Given the gradient flow equation (22), we may write down explicit Euler scheme:

$$\frac{f_j^{m+1} - f_j^m}{\Delta t} = -\frac{f_{j+2}^m - 4f_{j+1}^m + 6f_j^m - 4f_{j-1}^m + f_{j-2}^m}{(\Delta x)^4} \quad (33)$$

3.4 Gradient Flow in H^2

Given the gradient flow equation (27), it can be rewritten as

$$\frac{d}{dt}\Delta f = f \quad (34)$$

we may write down explicit Euler scheme:

$$\frac{1}{\Delta t} \left(\frac{f_{j+1}^{m+1} - 2f_j^{m+1} + f_{j-1}^{m+1}}{(\Delta x)^2} - \frac{f_{j+1}^m - 2f_j^m + f_{j-1}^m}{(\Delta x)^2} \right) = f_j^m \quad (35)$$

which can be rewritten as

$$\begin{pmatrix} 1 & -2 & 1 \end{pmatrix} \begin{pmatrix} f_{j-1}^{m+1} \\ f_j^{m+1} \\ f_{j+1}^{m+1} \end{pmatrix} = \begin{pmatrix} 1 & -2 + \Delta t(\Delta x)^2 & 1 \end{pmatrix} \begin{pmatrix} f_{j-1}^m \\ f_j^m \\ f_{j+1}^m \end{pmatrix} \quad (36)$$

Assuming Dirichlet boundary condition $f_0^m = a$ and $f_J^m = b$, we may write this as a matrix equation:

$$\begin{pmatrix} -2 & 1 & & & & & & \\ 1 & -2 & 1 & & & & & \\ & 1 & -2 & 1 & & & & \\ \vdots & & & & & & & \\ & & & & 1 & -2 & 1 & \\ & & & & & 1 & -2 & \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{J-4} \\ f_{J-3} \\ f_{J-2} \\ f_{J-1} \end{pmatrix}^{m+1} = \begin{pmatrix} -2 + \Delta t(\Delta x)^2 & 1 & & & & & & \\ 1 & -2 + \Delta t(\Delta x)^2 & 1 & & & & & \\ & 1 & -2 + \Delta t(\Delta x)^2 & 1 & & & & \\ \vdots & & & & & & & \\ & & & & 1 & -2 + \Delta t(\Delta x)^2 & 1 & \\ & & & & & 1 & -2 & \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{J-4} \\ f_{J-3} \\ f_{J-2} \\ f_{J-1} \end{pmatrix}^m$$

It might be worth noting that

$$A_n^{-1} := \underbrace{\begin{pmatrix} -2 & 1 & 0 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & \cdots & 0 & 1 & -2 \end{pmatrix}}_{n \times n}^{-1} = -\frac{1}{n+1} \underbrace{\begin{pmatrix} n & (n-1) & (n-2) & \cdots & 1 \\ (n-1) & 2(n-1) & 2(n-2) & \cdots & 2 \\ (n-2) & 2(n-2) & 3(n-2) & \cdots & 3 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & 2 & 3 & \cdots & n \end{pmatrix}}_{\text{Symmetric Matrix}} \quad (37)$$

In terms of practical computation, it might be worth investigating how the condition number grows as the size of A_n^{-1} (which is equivalent to the condition number of A_n) grows. To do this, we could investigate eigenvalues³ A (potentially) useful fact about this matrix is that the characteristic equation can be written recursively.

$$\begin{cases} |A_n - \lambda I| =: J_n = -\delta J_{n-1} - J_{n-2} \\ J_1 = -\delta \\ J_2 = \delta^2 - 1 \end{cases} \quad (38)$$

where $\delta := \lambda + 2$.⁴

This method has consistency error

$$T_j^m = \mathcal{O}\left((\Delta x)^2 + \Delta t\right) \quad (39)$$

³Analytically, solutions to the characteristic equation.

⁴The term *continuant* might be interesting to look at

4 Appendix

4.1 Natural Boundary Condition

We pay more attention to the boundary terms in the process of integrating by parts.

Starting from (4), we compute the differential $d\mathcal{E}_D|_f(u)$ again, but with boundary terms. Recall that the Dirichlet energy is given by:

$$\mathcal{E}_D(f) := \frac{1}{2} \int_{\Omega} |\nabla f(x)|^2 dx = \frac{1}{2} \langle \nabla f, \nabla f \rangle_{L^2}$$

Computing the differential with boundary terms:

$$d\mathcal{E}_D|_f(u) = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} (\mathcal{E}(f + \epsilon u) - \mathcal{E}(f)) \quad (40)$$

$$= \frac{1}{2} \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \int_{\Omega} (|\nabla f + \epsilon \nabla u|^2 - |\nabla f|^2) dx \quad (41)$$

$$= \frac{1}{2} \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \int_{\Omega} (2\epsilon \nabla f \cdot \nabla u + \epsilon^2 |\nabla u|^2) dx \quad (42)$$

$$= \int_{\Omega} \nabla f \cdot \nabla u dx \quad (43)$$

4.1.1 L^2

We continue from (43)

$$d\mathcal{E}_D|_f(u) = \int_{\Omega} \nabla f \cdot \nabla u dx \quad (44)$$

$$= \int_{\Omega} (\nabla \cdot (u \nabla f) - u \Delta f) dx \quad (45)$$

$$= \langle -\Delta f, u \rangle_{L^2} + \underbrace{\oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} ds}_{\text{Boundary Term}} \quad (46)$$

So for L^2 , the we can take the natural boundary condition to be

$$\nabla f \cdot \mathbf{n} \equiv 0 \quad \text{on } \partial\Omega$$

4.1.2 H^1

Note, from (43),

$$d\mathcal{E}_D|_f(u) = \int_{\Omega} \nabla f \cdot \nabla u dx \quad (47)$$

$$= \langle f, u \rangle_{H^1} \quad (48)$$

So for H^1 , there is no need to take a natural boundary condition.

4.1.3 H^{-1}

We continue from (46). Define $g := \Delta f$ and $v := \Delta^{-1}u$

$$d\mathcal{E}_D|_f(u) = \langle -\Delta f, u \rangle_{L^2} + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \, ds \quad (49)$$

$$= \langle -g, \Delta v \rangle_{L^2} + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \, ds \quad (50)$$

$$= - \int_{\Omega} g \nabla^2 v \, dx + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \, ds \quad (51)$$

$$= - \int_{\Omega} (\nabla \cdot (g \nabla v) - \nabla g \cdot \nabla v) \, dx + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \, ds \quad (52)$$

$$= \int_{\Omega} \nabla g \cdot \nabla v \, dx - \oint_{\partial\Omega} g \nabla v \cdot \mathbf{n} \, ds + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \, ds \quad (53)$$

$$= \int_{\Omega} \nabla (\Delta f) \cdot \nabla (\Delta^{-1}u) \, dx + \underbrace{\oint_{\partial\Omega} (u \nabla f - (\Delta f) \nabla (\Delta^{-1}u)) \cdot \mathbf{n} \, ds}_{\text{Boundary Terms}} \quad (54)$$