Dirichlet Energy in Different Spaces

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1 Relevant Definitions

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

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

Definition 2 (Differential). *Differential* $d\mathcal{E}$ *describes change in* $\mathcal{E}$ *due to[1]* u: f

$$d\mathcal{E}|_f(u) = \lim_{\epsilon \to 0}\frac{1}{\epsilon}\left(\mathcal{E}(f + \epsilon u) - \mathcal{E}(f)\right) \tag{2}$$

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

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

2 Dirichlet Energy Example

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

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

where the last equality comes from IBP.

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

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

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

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

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

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

where the step from (7) to (8) is by integration by parts [2].

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[1] analogous in traditional vector space would be "in the direction of" u

[2] This 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

$$\operatorname{grad} \mathcal{E}_{L^2} = -\Delta f \tag{10}$$

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

$$\frac{d}{dt} f = \Delta f \tag{11}$$

which is the heat equation.

2.2 Gradient Flow in H^1

We may express the differential (9) as

$$d\mathcal{E}_D|_f(u) = -\langle \Delta f, u \rangle_{L^2} \tag{12}$$
$$= \langle \nabla f, \nabla u \rangle_{L^2} \tag{13}$$
$$= \langle f, u \rangle_{H^1} \tag{14}$$

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

$$\operatorname{grad} \mathcal{E}_{H^1} = f \tag{15}$$

The gradient flow equation (1) can be written as

$$\frac{d}{dt} f = -f \tag{16}$$

which describes exponential decay.

2.3 Gradient Flow in H^{-1}

We may express the differential (9) as

$$d\mathcal{E}_D|_f(u) = -\langle \Delta f, u \rangle_{L^2} \tag{17}$$
$$= \langle \nabla (\Delta f), \nabla (\Delta^{-1} u) \rangle_{L^2} \tag{18}$$
$$= \langle \Delta f, \Delta^{-1} u \rangle_{H^1} \tag{19}$$
$$= \langle \Delta^2 f, u \rangle_{H^{-1}} \tag{20}$$

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

$$\operatorname{grad} \mathcal{E}_{H^{-1}} = \Delta^2 f \tag{21}$$

The gradient flow equation (1) can be written as

$$\frac{d}{dt} f = -\Delta^2 f \tag{22}$$

2.4 Gradient Flow in H^2

We may express the differential (9) as

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

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

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

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

$$\operatorname{grad} \mathcal{E}_{H^2} = -\Delta^{-1} f \tag{26}$$

The gradient flow equation (1) can be written as

$$\frac{d}{dt} f = \Delta^{-1} f \tag{27}$$

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:

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

which can be rewritten as

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

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

This method is known to have consistency error

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

3.2 Gradient Flow in H^1

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

$$\frac{f_j^{m+1} - f_j^m}{\Delta t} = -f_j^m \tag{31}$$

which can be rewritten as

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

3.3 Gradient Flow in H^{-1}

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

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

3.4 Gradient Flow in H^2

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

$$\frac{d}{dt}\Delta f = f \tag{34}$$

we may write down explicit Euler scheme:

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

which can be rewritten as

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

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

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

$$\tag{37}$$

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 eigenvalues[3] A (potentially) useful fact about this matrix is that the characteristic equation can be written recursively.

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

where $\delta := \lambda + 2$.[4]

This method has consistency error

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

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[3] Analytically, solutions to the characteristic equation.
[4] The 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:

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

Computing the differential with boundary terms:

$$d\mathcal{E}_D|_f(u) = \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(\mathcal{E}(f + \epsilon u) - \mathcal{E}(f) \right) \tag{40}$$

$$= \frac{1}{2} \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_\Omega \left(|\nabla f + \epsilon \nabla u|^2 - |\nabla f|^2 \right) \, \mathrm{d}x \tag{41}$$

$$= \frac{1}{2} \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_\Omega \left(2\epsilon \nabla f \cdot \nabla u + \epsilon^2 |\nabla u|^2 \right) \, \mathrm{d}x \tag{42}$$

$$= \int_\Omega \nabla f \cdot \nabla u \, \mathrm{d}x \tag{43}$$

4.1.1 L^2

We continue from (43)

$$d\mathcal{E}_D|_f(u) = \int_\Omega \nabla f \cdot \nabla u \, \mathrm{d}x \tag{44}$$

$$= \int_\Omega \left(\nabla \cdot (u \nabla f) - u \Delta f \right) \, \mathrm{d}x \tag{45}$$

$$= \langle -\Delta f, u \rangle_{L^2} + \underbrace{\oint_{\partial \Omega} u \nabla f \cdot \mathbf{n} \, \mathrm{d}s}_{\text{Boundary Term}} \tag{46}$$

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

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

4.1.2 H^1

Note, from (43),

$$d\mathcal{E}_D|_f(u) = \int_\Omega \nabla f \cdot \nabla u \, \mathrm{d}x \tag{47}$$

$$= \langle f, u \rangle_{H^1} \tag{48}$$

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