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:

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

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:

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

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

$$\begin{aligned}
d\mathcal{E}_D|_f(u) &= -\frac{1}{2} \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(\langle \Delta(f + \epsilon u), f + \epsilon u \rangle_{L^2} - \langle \Delta f, f \rangle_{L^2}\right) && (5) \\
&= -\frac{1}{2} \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(\epsilon \langle \Delta f, u \rangle_{L^2} + \epsilon \langle \Delta u, f \rangle_{L^2} + \epsilon^2 \langle u, u \rangle_{L^2}\right) && (6) \\
&= -\frac{1}{2} (\langle \Delta f, u \rangle_{L^2} + \langle \Delta u, f \rangle_{L^2}) && (7) \\
&= -\frac{1}{2} (\langle \Delta f, u \rangle_{L^2} + \langle \Delta f, u \rangle_{L^2}) && (8) \\
&= -\langle \Delta f, u \rangle_{L^2} && (9)
\end{aligned}$$

where the last step is by integration by parts [2].

[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. 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

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

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

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

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 $\mu \coloneqq \frac{\Delta t}{(\Delta x)^2}$ 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

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

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

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

[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.

From (7), we use IBP while assuming for conditons that eliminates the boundary terms.

4.1.1 L^2

Starting from (7),

$$
\begin{aligned}
-2d\mathcal{E}_D|_f(u) - \langle \Delta f, u \rangle_{L^2} &= \langle \Delta u, f \rangle_{L^2} && (40)\\
&= \int_R f \nabla^2 u \, \mathrm{d}V && (41)\\
&= \int_R u \nabla^2 f + \nabla \cdot (f \nabla u - u \nabla f) \, \mathrm{d}V && (42)\\
&= \int_R u \nabla^2 f + \oint_{\partial R} (f \nabla u - u \nabla f) \cdot \mathbf{n} \, \mathrm{d}s && (43)\\
&= \langle \Delta f, u \rangle_{L^2} + \oint_{\partial R} \underbrace{(f \nabla u - u \nabla f) \cdot \mathbf{n}}_{\text{Boundary Terms}} \, \mathrm{d}s && (44)
\end{aligned}
$$

4.1.2 H^1

Starting from (7),

$$
\begin{aligned}
-2d\mathcal{E}_D|_f(u) &= (\langle \Delta f, u \rangle_{L^2} + \langle \Delta u, f \rangle_{L^2}) && (45)\\
&= \int_R \left(u \nabla^2 f + f \nabla^2 u \right) \, \mathrm{d}V && (46)\\
&= \int_R \nabla \cdot \left(u \nabla^2 f \right) - \nabla u \cdot \nabla f \, \mathrm{d}V + \int_R \nabla \cdot \left(f \nabla^2 u \right) - \nabla u \cdot \nabla f \, \mathrm{d}V && (47)\\
&= -2 \int_R \nabla u \cdot \nabla f \, \mathrm{d}V + \oint_{\partial R} \left(u \nabla^2 f + f \nabla^2 u \right) \cdot \mathbf{n} \, \mathrm{d}s && (48)\\
&= -2 \langle \nabla u, \nabla f \rangle_{H^1} + \oint_{\partial R} \underbrace{\left(u \nabla^2 f + f \nabla^2 u \right) \cdot \mathbf{n}}_{\text{Boundary Terms}} \, \mathrm{d}s && (49)
\end{aligned}
$$