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:

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

where the last equality comes from IBP.

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 step from (7) to (8) 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 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

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

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*. For this explicit Euler scheme to be stable, it is needed that $\mu \leq \frac{1}{2}$

3.1.1 Boundary Conditions

For *periodic boundary condition*, we impose:

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

For *natural boundary condition*, we impose:

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

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

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

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:

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

Define an analogous quantity to CFL number by $\mu := \frac{\Delta t}{(\Delta x)^4}$. By discrete Fourier transform, we deduce that we can guarantee stability of the scheme by imposing condition $\mu \leq \frac{1}{8}$.

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.

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:

$$\begin{aligned}
d\mathcal{E}_D|_f(u) &= \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left(\mathcal{E}(f+\epsilon u) - \mathcal{E}(f)\right) &(40)\\
&= \frac{1}{2}\lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_\Omega \left(|\nabla f + \epsilon\nabla u|^2 - |\nabla f|^2\right)\,\mathrm{d}x &(41)\\
&= \frac{1}{2}\lim_{\epsilon\to 0}\frac{1}{\epsilon}\int_\Omega \left(2\epsilon\nabla f\cdot\nabla u + \epsilon^2|\nabla u|^2\right)\,\mathrm{d}x &(42)\\
&= \int_\Omega \nabla f\cdot\nabla u\,\mathrm{d}x &(43)
\end{aligned}$$

4.1.1 L^2

We continue from (43)

$$\begin{aligned}
d\mathcal{E}_D|_f(u) &= \int_\Omega \nabla f\cdot\nabla u\,\mathrm{d}x &(44)\\
&= \int_\Omega \left(\nabla\cdot(u\nabla f) - u\Delta f\right)\,\mathrm{d}x &(45)\\
&= \langle -\Delta f, u\rangle_{L^2} + \underbrace{\oint_{\partial\Omega} u\nabla f\cdot\mathbf{n}\,\mathrm{d}s}_{\text{Boundary Term}} &(46)
\end{aligned}$$

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),

$$\begin{aligned}
d\mathcal{E}_D|_f(u) &= \int_\Omega \nabla f\cdot\nabla u\,\mathrm{d}x &(47)\\
&= \langle f, u\rangle_{H^1} &(48)
\end{aligned}$$

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

4.1.3 H^{-1}

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

$$
\begin{aligned}
d\mathcal{E}_D|_f(u) &= \langle -\Delta f, u\rangle_{L^2} + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n}\, \mathrm{d}s && (49)\\
&= \langle -g, \Delta v\rangle_{L^2} + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n}\, \mathrm{d}s && (50)\\
&= -\int_{\Omega} g \nabla^2 v\, \mathrm{d}x + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n}\, \mathrm{d}s && (51)\\
&= -\int_{\Omega} \left(\nabla \cdot (g \nabla v) - \nabla g \cdot \nabla v\right) \mathrm{d}x + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n}\, \mathrm{d}s && (52)\\
&= \int_{\Omega} \nabla g \cdot \nabla v\, \mathrm{d}x - \oint_{\partial\Omega} g \nabla v \cdot \mathbf{n} ds + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n}\, \mathrm{d}s && (53)\\
&= \int_{\Omega} \nabla (\Delta f) \cdot \nabla \left(\Delta^{-1} u\right) \mathrm{d}x + \underbrace{\oint_{\partial\Omega} \left(u \nabla f - (\Delta f)\, \nabla \left(\Delta^{-1} u\right)\right) \cdot \mathbf{n}\, \mathrm{d}s}_{\text{Boundary Terms}} && (54)
\end{aligned}
$$