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:

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

See 4.1 for motivation of the gradient flow equation.

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 4.2 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

$$
\begin{aligned}
d\mathcal{E}_D|_f(u) &= -\langle \Delta f, u\rangle_{L^2} && (23)\\
&= -\langle f, \Delta u\rangle_{L^2} && (24)\\
&= -\langle \Delta^{-1} f, u\rangle_{H^2} && (25)
\end{aligned}
$$

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*. 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 4.2.1.

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 $\mu \coloneqq \frac{\Delta t}{(\Delta x)^4}$. 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 Motivation of Gradient Flow

Recall the gradient flow equation:

$$\frac{d}{dt} f = -\operatorname{grad} \mathcal{E}(f) \tag{40}$$

Compare this with the original gradient method used for solving the optimization problem: $\min_{\mathbf{x}} f(\mathbf{x})$

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n \nabla f(\mathbf{x}_n) \tag{41}$$

We may use this to motivate the gradient flow equation, which is for solving the optimization problem: $\min_f \mathcal{E}(f)$. Note that the standard gradient descent method (41) suggests that we may analogously write:

$$f_{n+1} = f_n - \alpha_n \operatorname{grad} \mathcal{E}(f_n) \tag{42}$$

Suppose $\alpha_n \equiv 1$, and divide by the time step Δt, then take the limit as $\Delta t \to 0$ to arrive at the gradient flow equation

4.2 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:

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

Computing the differential with boundary terms:

$$\begin{aligned}
d\mathcal{E}_D|_f(u) &= \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(\mathcal{E}(f + \epsilon u) - \mathcal{E}(f) \right) && (43) \\
&= \frac{1}{2} \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_\Omega \left(|\nabla f + \epsilon \nabla u|^2 - |\nabla f|^2 \right) \mathrm{d}x && (44) \\
&= \frac{1}{2} \lim_{\epsilon \to 0} \frac{1}{\epsilon} \int_\Omega \left(2\epsilon \nabla f \cdot \nabla u + \epsilon^2 |\nabla u|^2 \right) \mathrm{d}x && (45) \\
&= \int_\Omega \nabla f \cdot \nabla u \, \mathrm{d}x && (46)
\end{aligned}$$

4.2.1 L^2

We continue from (46)

$$\begin{aligned}
d\mathcal{E}_D|_f(u) &= \int_\Omega \nabla f \cdot \nabla u \, \mathrm{d}x && (47) \\
&= \int_\Omega \left(\nabla \cdot (u \nabla f) - u \Delta f \right) \mathrm{d}x && (48) \\
&= \langle -\Delta f, u \rangle_{L^2} + \underbrace{\oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \, \mathrm{d}s}_{\text{Boundary Term}} && (49)
\end{aligned}$$

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

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

4.2.2 H^1

Note, from (46),

$$d\mathcal{E}_D|_f(u) = \int_\Omega \nabla f \cdot \nabla u \,\mathrm{d}x \tag{50}$$
$$= \langle f, u\rangle_{H^1} \tag{51}$$

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

4.2.3 H^{-1}

We continue from (49). Define $g \coloneqq \Delta f$ and $v \coloneqq \Delta^{-1} u$

$$d\mathcal{E}_D|_f(u) = \langle -\Delta f, u\rangle_{L^2} + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \,\mathrm{d}s \tag{52}$$
$$= \langle -g, \Delta v\rangle_{L^2} + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \,\mathrm{d}s \tag{53}$$
$$= -\int_\Omega g \nabla^2 v \,\mathrm{d}x + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \,\mathrm{d}s \tag{54}$$
$$= -\int_\Omega \left(\nabla \cdot (g \nabla v) - \nabla g \cdot \nabla v\right) \,\mathrm{d}x + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \,\mathrm{d}s \tag{55}$$
$$= \int_\Omega \nabla g \cdot \nabla v \,\mathrm{d}x - \oint_{\partial\Omega} g \nabla v \cdot \mathbf{n} ds + \oint_{\partial\Omega} u \nabla f \cdot \mathbf{n} \,\mathrm{d}s \tag{56}$$
$$= \int_\Omega \nabla (\Delta f) \cdot \nabla \left(\Delta^{-1} u\right) \,\mathrm{d}x + \underbrace{\oint_{\partial\Omega} \left(u \nabla f - (\Delta f) \nabla \left(\Delta^{-1} u\right)\right) \cdot \mathbf{n} \,\mathrm{d}s}_{\text{Boundary Terms}} \tag{57}$$