

Gradient Flow to Continuous Optimization via Fourier Series

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We've been concerned about minimizing the energy functional of the form:

$$\mathcal{E}(\gamma) := \int_{C_\gamma} \int_{C_\gamma} k(\gamma_1, \gamma_2) \, d\gamma_1 \, d\gamma_2 \quad (1)$$

where $\gamma : E \rightarrow \mathbb{R}^3$ is a parameterization function of a closed curve on the interval $E = [0, 2\pi)$ (without loss of generality).

Note that we assume γ to be a periodic function of period 2π .

1 Multidimensional Fourier Series

1.1 1D Fourier Series

Given a continuous 1D 2π -periodic function $f : \mathbb{R} \rightarrow \mathbb{R}$ (where we only need to define f on $[0, 2\pi)$), there exists a Fourier series representation:

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} (a_n \cos(nx) + b_n \sin(nx)) \quad (2)$$

$$= \sum_{n=-\infty}^{\infty} c_n e^{inx} \quad (3)$$

where the coefficients $\{a_n\}, \{b_n\}, \{c_n\}$ are given by

$$a_n = \frac{1}{\pi} \int_0^{2\pi} f(x) \cos(nx) \, dx \quad \in \mathbb{R} \quad (4)$$

$$b_n = \frac{1}{\pi} \int_0^{2\pi} f(x) \sin(nx) \, dx \quad \in \mathbb{R} \quad (5)$$

$$c_n = \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-inx} \, dx \quad \in \mathbb{C} \quad (6)$$

Fourier convergence theorem states that the rate of convergence is $O\left(\frac{1}{n^{p+1}}\right)$ where f has the first jump discontinuity in the p^{th} derivative.¹

¹Lecture note

1.2 Multidimensional Extension

For a vector valued function of dimension N (which we will take $N = 3$ for our case), we have Fourier series representation in each of the coordinates.

For $\mathbf{f} : \mathbb{R} \rightarrow \mathbb{R}^N$, we write its Fourier series as:

$$\mathbf{f}(x) = \frac{1}{2} \begin{pmatrix} a_{1,0} \\ a_{2,0} \\ \vdots \\ a_{N,0} \end{pmatrix} + \sum_{n=1}^{\infty} \begin{pmatrix} a_{1,n} & b_{1,n} \\ a_{2,n} & b_{2,n} \\ \vdots & \vdots \\ a_{N,n} & b_{N,n} \end{pmatrix} \begin{pmatrix} \cos(nx) \\ \sin(nx) \end{pmatrix} \quad (7)$$

$$= \sum_{n=-\infty}^{\infty} \begin{pmatrix} c_{1,n} \\ c_{2,n} \\ \vdots \\ c_{N,n} \end{pmatrix} e^{-inx} \quad (8)$$

where the coefficients $\{a_{i,n}\}, \{b_{i,n}\}, \{c_{i,n}\}$ are given by

$$a_{i,n} = \frac{1}{\pi} \int_0^{2\pi} f_i(x) \cos(nx) dx \quad (9)$$

$$b_{i,n} = \frac{1}{\pi} \int_0^{2\pi} f_i(x) \sin(nx) dx \quad (10)$$

$$c_{i,n} = \frac{1}{2\pi} \int_0^{2\pi} f_i(x) e^{-inx} dx \quad (11)$$

for $i = 1, 2, \dots, N$

2 Gradient Flow to Continuous Optimization I

For minimization of \mathcal{E} , the original approach is to use the gradient flow equation:

$$\frac{\partial \mathcal{E}}{\partial t} = -\text{grad}_X E \quad (12)$$

where grad_X is gradient on inner product space X .

This is needed as a description of reduction of functional \mathcal{E} was needed. For a solution, one would could use a numerical method to solve the differential equation by sampling at different points on the curve.

However, consider expressing $\gamma(t)$ as a 3D Fourier series as:

$$\gamma(t) = \sum_{n=-\infty}^{\infty} \mathbf{c}_n e^{-int} \quad (13)$$

One could approximate this to J terms:

$$\gamma_N(t) = \sum_{n=-J}^J \mathbf{c}_n e^{-int} \quad (14)$$

(Noting $\|\gamma - \gamma_J\| = O\left(\frac{1}{J^{p+1}}\right)$)

Then now the reduction process of $\mathcal{E}(\gamma)$ can be approximated by the reduction process of $\mathcal{E}(\gamma_J)$. It is paramount to note that $\mathcal{E}(\gamma_J) : \mathbb{R}^{3(2J+1)} = \mathbb{R}^{6J+3} \rightarrow \mathbb{R}$ where the parameters are the Fourier coefficients in 3D. The idea is now to consider this a standard optimiation problem:

$$\min_{[\mathbf{c}_{-J}, \dots, \mathbf{c}_J]} \mathcal{E}(\gamma_J) \quad (15)$$

which can be attempted by standard techniques such as SDM, bArmijo line-search, etc.

2.1 Pro

An inherent benefit of this formulation is that there are more various robust methods that can be used for optimizing a function rather than a functional. Also one could use much less memory for computation as Fourier series expansion of the closed curve captures it to a very low error with only a few coefficients, whereas in the reduction-of-functional problem, one must store coordinates on the curve at a fine mesh.

One could even go further at using less memory by considering a quaternion version of Fourier theory to capture the curve with less variable, but it does not change the order of complexity.

2.2 Con

A drawback with this method is that the interpolation (at the preprocessing stage) is arbitrary in the sense that an ordered set of points in \mathbb{R}^3 can be placed (in order) in any spacing. In an interval domain, a potential choice would be placing the “output values” on Chebyshev points or Legendre points, but even this is a bit arbitrary. Should this become a problem, one could partially resolve this problem by spline interpolation, then taking Fourier series of that spline.

Another drawback is that this is inherently a method for closed curves, not all curves. For a nonclosed curve with two openings at infinity, one could map them to point at infinity, treating it like a closed curve (in this case, Fourier transform might be more appropriate than Fourier series). On the other hand, if it is a finite curve, then one could naïvely attempt Fourier analysis on discontinuous function.

2.3 Complexity (Scribble)

For a general approximation of $\mathcal{E}(\gamma_J)$,

- Evaluation of the energy functional $\mathcal{E}(\gamma_J)$ takes $O(J \log J)$ operations via FFT and possibly Clenshaw-Curtis quadrature (or just a Newton-Cotes quadrature, as it is a cyclic domain, although since the problem is posed in terms of restriction to an interval, maybe Clenshaw-Curtis is still better?).
- Other operations might be of lower order?

3 Gradient Flow to Continuous Optimization II

Instead of taking Fourier transform in three different coordinates, one may attempt to use quaternions.

First, note the definition of one-dimensional quaternion FT (qFT)²

Definition 1. 1-D QFT of g is given by

$$\mathcal{F}_l(g)(\omega) := \int_{\mathbb{R}} g(t) e^{-\mathbf{j}2\pi\omega t} dt \quad (16)$$

with its inverse

Definition 2. Inverse 1-D QFT corresponding to 1-D QFT is:

$$g(t) = \mathcal{F}_l^{-1}[\mathcal{F}_l(g)](t) \quad (17)$$

$$= \int_{\mathbb{R}} \mathcal{F}_l(g)(\omega) e^{\mathbf{j}2\pi\omega t} d\omega \quad (18)$$

²Bahri (2019)