Gradient Flow to Continuous Optimization via Fourier Series

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

$$\mathcal{E}(\boldsymbol{\gamma}) := \int_{C_{\boldsymbol{\gamma}}} \int_{C_{\boldsymbol{\gamma}}} k\left(\boldsymbol{\gamma}_1, \boldsymbol{\gamma}_2\right) \mathrm{d}\boldsymbol{\gamma}_1 \, \mathrm{d}\boldsymbol{\gamma}_2 \tag{1}$$

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

Note that we assume $\boldsymbol{\gamma}$ to be a periodic function of period 2π.

1 Multidimensional Fourier Series

1.1 1D Fourier Series

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

$$\begin{aligned} f(x) &= \frac{a_0}{2} + \sum_{n=1}^{\infty} \left(a_n \cos(nx) + b_n \sin(nx)\right) && (2) \\ &= \sum_{n=-\infty}^{\infty} c_n e^{inx} && (3) \end{aligned}$$

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

$$\begin{aligned} a_n &= \frac{1}{\pi} \int_0^{2\pi} f(x) \cos(nx) \, \mathrm{d}x && \in \mathbb{R} && (4) \\ b_n &= \frac{1}{\pi} \int_0^{2\pi} f(x) \sin(nx) \, \mathrm{d}x && \in \mathbb{R} && (5) \\ c_n &= \frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-inx} \, \mathrm{d}x && \in \mathbb{C} && (6) \end{aligned}$$

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]

[1] Lecture 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 $\mathbf{f} : \mathbb{R} \to \mathbb{R}^N$, we write its Fourier series as:

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

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

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

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

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

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

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

2 Gradient Flow to Continuous Optimization I

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

$$\frac{\partial \mathcal{E}}{\partial t} = -\operatorname{grad}_X E \tag{12}$$

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 $\boldsymbol{\gamma}(t)$ as a 3D Fourier series as:

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

One could approximate this to J terms:

$$\boldsymbol{\gamma}_N(t) = \sum_{n=-J}^{J} \mathbf{c}_n e^{-int} \tag{14}$$

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

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 $\mathcal{E}(\gamma_J) : \mathbb{R}^{3(2J+1)} = \mathbb{R}^{6J+3} \to \mathbb{R}$ where the parameters are the Fourier coefficients in 3D. The idea is now to consider this a standard optimiation problem:

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

which can be attempted by standard techniques such as SDM, bArmijo linesearch, 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, 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).

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

$$\mathcal{F}_l\left(g\right)\left(\omega\right) \coloneqq \int_{\mathbb{R}} g(t) e^{-\mathbf{j}2\pi\omega t} \,\mathrm{d}t \tag{16}$$

with its inverse

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

$$\begin{aligned} g(t) &= \mathcal{F}_l^{-1}\left[\mathcal{F}_l(g)\right](t) && (17)\\ &= \int_{\mathbb{R}} \mathcal{F}_l(g)(\omega) e^{\mathbf{j}2\pi\omega y} \,\mathrm{d}\omega && (18) \end{aligned}$$

[2]Bahri (2019)