Implementation specification: optimization on z ODE system of order 1

Xiaorong Zou (xiaorong.zou@bofa.com)
Global Market Risk Analytic, Bank of America

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Abstract. This is the implementation specification for the algorithm in [2].

1. Trigonometric Interpolation on Solutions of d dimensional Non-Linear ODE System

In this section, we aim to develop an algorithm on numerical solution of a general first order ODE: Let $\mathbf{y} = (y_1, \cdots, y_d)$,

$$\begin{aligned} y'_\alpha(x) &= f_\alpha(x, \mathbf{y}), \quad 1 \le \alpha \le d, \quad x \in [s, e] && (1)\\ \mathbf{y}(s) &= (\xi_1, \ldots, \xi_d) =: \xi, && (2)\\ H(\mathbf{y}) &= 0, && (3) \end{aligned}$$

where $f_\alpha(x, \mathbf{y})$ is continuously differential on the range $[s-\delta, e+\delta] \times R^d$ [1] and the constrain H is a differential d-dim function. Replacing $f(x, \mathbf{y})$ by $f(x + o, \mathbf{y})$ if needed, we assume that $o := s - \delta = 0$ and denote $h(x)$ as the cut-off function defined in Section **??**. Apply h to extend $f(x, \mathbf{y})$ as follows [2]:

$$\mathbf{F}_\alpha(x, \mathbf{u}) = \begin{cases} f_\alpha(x, \mathbf{u})h(x) & \text{if } x \in [0, b], \\ -f_\alpha(-x, \mathbf{u})h(-x) & \text{if } x \in [-b, 0]. \end{cases} \tag{4}$$

We shall search numerical solution for the extended ODE:

$$\begin{aligned} u'_\alpha(x) &= F_\alpha(x, \mathbf{u}), \quad 1 \le \alpha \le d, \quad x \in [-b, b], && (5)\\ \mathbf{u}(s) &= \xi. && (6)\\ H(\mathbf{u}) &= 0, && (7) \end{aligned}$$

Since $(u_\alpha(x) - u_\alpha(-x))' \equiv 0$, $u_\alpha(x)$ is even and its derivative $z_\alpha(x) := u'_\alpha(x)$ is odd. It is clear that u_α can be smoothly extended to even periodic function with period $2b$ and $u_\alpha(x)|_{[s,e]}$ solves Eq. (1)- (2). Let $\{(x_k, z_{\alpha,k})\}_{0 \le k < N}$ be a grid set of $z_\alpha(x)$:

$$\begin{aligned} x_k &= -b + \frac{2b}{N}k, \qquad k = 0, 1, \cdots, N-1, \\ z_{\alpha,0} &= 0, \quad z_{\alpha,N-k} = -z_{\alpha,k}, \qquad 1 \le k < M, \end{aligned}$$

[1] double check solution should be unique with references
[2] We use $\mathbf{u}$ to denote the periodic extension of $\mathbf{y}$.

and

$$z_{\alpha,M}(x) = \sum_{0\le j<M} b_{\alpha,j} \sin \frac{j\pi x}{b} \tag{8}$$

be the interpolant of $z(x)$ with

$$b_{\alpha,j} = \frac{2}{N}\sum_{k=0}^{N-1}(-1)^j z_{\alpha,k} \sin\frac{2\pi jk}{N} = \frac{4}{N}\sum_{k=0}^{M-1}(-1)^j z_{\alpha,k} \sin\frac{2\pi jk}{N}. \tag{9}$$

It is clear

$$\frac{\partial b_{\alpha,j}}{\partial z_{\alpha,k}} = \frac{4}{N}(-1)^j \sin\frac{2\pi jk}{N}, \quad 0\le j,k<M.$$

u_α can be approximated based on Eq. (8) by

$$\tilde{u}_{\alpha,M}(x) = \sum_{0\le j<M} a_{\alpha,j}\cos\frac{j\pi x}{b}, \quad a_{\alpha,j} = -\frac{b b_{\alpha,j}}{j\pi}, \quad 1\le j<M,$$

and $a_{\alpha,0}$ can be solved by the initial condition $u_\alpha(-s) = u_\alpha(x_{m+n}) = \xi_\alpha$

$$a_{\alpha,0} = \xi_\alpha - \sum_{1\le j<M}(-1)^j a_{\alpha,j}\cos\frac{2\pi j(m+n)}{N}.$$

Let 0_M be the M-dim zero vector and define $\frac{1}{0} := 0$. The following notations will be adopted in the rest of this subsection. Let $w_\beta > 0$ be some weights assigned to β component of ODE system.

$$\begin{aligned}
J &= (0, 1, \frac{1}{2}, \ldots, \frac{1}{M-1}, 0_M),\\
u_{\alpha,k} &= \tilde{u}_{\alpha,M}(x_k), \quad \mathbf{u}_k = (u_{1,k}, \cdots, u_{d,k}), \quad U_\alpha = (u_{\alpha,0}, \cdots, u_{\alpha,M-1}),\\
h_k &= H(\mathbf{u_k}), \quad \mathbf{h} = (h_0, \cdots, h_{M-1}), \quad DH_{\alpha,k} = \frac{\partial H}{\partial u_\alpha}(\mathbf{u_k})\\
Z_\alpha &= (z_{\alpha,0}, \cdots, z_{\alpha,M-1}), \quad Z = (Z_1, \cdots, Z_d),\\
F_{\alpha,k} &= F_\alpha(x_k, \mathbf{u}_k), \quad DF^\beta_{\alpha,k} = \frac{\partial F_\beta}{\partial u_\alpha}(x_k, \mathbf{u}_k),\\
F_\alpha &= (F_{\alpha,k})_{0\le k<M}, \quad DF^\beta_\alpha = (DF^\beta_{\alpha,k})_{0\le k<M},\\
\Phi &= (\frac{1}{k}\cos\frac{2\pi k(m+n)}{N})_{k=0}^{M-1}, \quad \Phi_N = (\Phi, 0_M),\\
\psi_{\alpha,k} &= \sum_{1\le\beta\le d}(z_{\beta,k} - F_{\beta,k})DF^\beta_{\alpha,k} - w_k H_k DH_{\alpha,k}, \quad \Psi_\alpha = (\psi_{\alpha,k})_{0\le k<M},\\
\Psi_{\alpha,N} &= (\Psi_\alpha, 0_M), \qquad I_\alpha = sum(\Psi_\alpha).
\end{aligned}$$

ODE (5)-(6) can be solved by minimizing the following error function:

$$\begin{aligned}\phi((z_{\alpha,k})_{1\le\alpha\le d,0\le k<M}) &= \frac{1}{2dM}\sum_{1\le\beta\le d}\sum_{0\le k<M}(z_{\beta,k}-F_{\beta,k})^2\\ &+ \frac{1}{2dM}\sum_{0\le k<M} w_k H_k^2. \end{aligned} \tag{10}$$

where $w_k = 1$ if $-e \le x_k \le -s$ and $w_k = 0$ otherwise. We need an effective way to calculate its gradient $\frac{\partial\phi}{\partial Z}$ when M, the number of variables of ϕ, is not small. Note that $\{u_{\alpha,k}\}_{0\le k<M}$ is uniquely determined by $\{z_{\alpha,k}\}_{0\le k<M}$ and does not depend on $\{z_{\beta,k}\}_{0\le k<M}$ for $\beta\ne\alpha$.

$$\begin{aligned} dM\frac{\partial\phi}{\partial z_{\alpha,t}} &= \sum_{1\le\beta\le d}\sum_{0\le k<M}(z_{\beta,k}-F_{\beta,k})(\delta_{\alpha=\beta,k=t}-\frac{\partial F_\beta(x_k,\mathbf{u}_k)}{\partial z_{\alpha,t}})\\ &+ \sum_{0\le k<M} w_k H_k DH_{\alpha,k}\frac{\partial u_{\alpha,k}}{\partial z_{\alpha,t}}\\ &= (z_{\alpha,t}-F_{\alpha,t}) - \sum_{1\le\beta\le d} w_\beta \sum_{0\le k<M}(z_{\beta,k}-F_{\beta,k})\frac{\partial F_\beta}{\partial u_\alpha}(x_k,\mathbf{u}_k)\frac{\partial u_{\alpha,k}}{\partial z_{\alpha,t}}\\ &+ \sum_{0\le k<M} w_k H_k DH_{\alpha,k}\frac{\partial u_{\alpha,k}}{\partial z_{\alpha,t}}\\ &= (z_{\alpha,t}-F_{\alpha,t}) - \sum_{1\le\beta\le d}\sum_{0\le k<M}(z_{\beta,k}-F_{\beta,k})DF^{\beta}_{\alpha,k}\frac{\partial u_{\alpha,k}}{\partial z_{\alpha,t}}\\ &+ \sum_{0\le k<M} w_k H_k DH_{\alpha,k}\frac{\partial u_{\alpha,k}}{\partial z_{\alpha,t}}\\ &= (z_{\alpha,t}-F_{\alpha,t}) - \sum_{0\le k<M}(\psi_{\alpha,k}-w_kH_kDH_{\alpha,k})\frac{\partial u_{\alpha,k}}{\partial z_{\alpha,t}} \end{aligned}\tag{11}$$

To copy with $\frac{\partial U_\alpha}{\partial Z_\alpha}$ in Eq. (11), we need express U_α in term of Z_α. By Eq (9) and $z_{\alpha,0} = z_{\alpha,M}$, we obtain for $0\le k<N$

$$\begin{aligned} u_{\alpha,k} &= a_{\alpha,0} - \sum_{0\le j<M}(-1)^j\frac{bb_{\alpha,j}}{j\pi}\cos\frac{2\pi jk}{N}\\ &= a_{\alpha,0} - \frac{2b}{\pi N}\sum_{0\le j<M}\frac{1}{j}\cos\frac{2\pi jk}{N}\sum_{0\le l<N} z_{\alpha,l}\sin\frac{2\pi jl}{N}\\ &= a_{\alpha,0} - \frac{2b}{\pi N}\sum_{0\le l<N} z_{\alpha,l}\sum_{0\le j<M}\frac{1}{j}\cos\frac{2\pi jk}{N}\sin\frac{2\pi jl}{N} \end{aligned}\tag{12}$$

$$= a_{\alpha,0} - \frac{4b}{\pi N} \sum_{0\le l<M} z_{\alpha,l} \sum_{0\le j<M} \frac{1}{j} \cos\frac{2\pi jk}{N} \sin\frac{2\pi jl}{N}. \quad (13)$$

The last step is due to $z_{\alpha,l} \sin\frac{2\pi jl}{N} = z_{\alpha,N-1} \sin\frac{2\pi j(N-l)}{N}$. One can rewrite (12) in term of ifft as follows:

$$U\alpha = a_{\alpha,0} - \frac{2bN}{\pi} Re\{ifft(J \circ Im\{ifft(Z\alpha)\})\}, \quad (14)$$

where $\circ$ denotes the Hadamard product, which applies the element-wise product to two metrics of same dimension. $a_{\alpha,0}$ in (13) can be further interpreted by Z_α as follows:

$$\begin{aligned} a_{\alpha,0} &= \xi_\alpha - \sum_{1\le j<M} (-1)^j a_{\alpha,j} \cos\frac{2\pi j(m+n)}{N} \\ &= \xi_\alpha + \frac{b}{\pi} \sum_{1\le j<M} (-1)^j \frac{b_{\alpha,j}}{j} \cos\frac{2\pi j(m+n)}{N} \\ &= \xi_\alpha + \frac{2b}{\pi N} \sum_{1\le j<M} \frac{1}{j} \cos\frac{2\pi j(m+n)}{N} \sum_{k=0}^{N-1} z_k \sin\frac{2\pi jk}{N}, \quad (15) \end{aligned}$$

which implies

$$\frac{\partial a_{\alpha,0}}{\partial z_k} = \frac{4b}{\pi N} \sum_{0\le j<M} \frac{1}{j} \cos\frac{2\pi j(m+n)\pi}{N} \sin\frac{2\pi jk}{N}, \quad 0 \le k < M (16)$$

Combining (13) and (16), we obtain

$$\begin{aligned} \frac{\partial u_{\alpha,k}}{\partial z_{\alpha,t}} &= \frac{4b}{\pi N} \sum_{0\le j<M} \frac{1}{j} \cos\frac{2\pi j(m+n)}{N} \sin\frac{2\pi jt}{N} \\ &- \frac{4b}{\pi N} \sum_{0\le j<M} \frac{1}{j} \cos\frac{2\pi jk}{N} \sin\frac{2\pi jt}{N}. \end{aligned} \quad (17)$$

We are ready to attack the non-trivial term in Eq. (11). Define

$$w_{\alpha,t} := \sum_{0\le k<M} \psi_{\alpha,k} \frac{\partial u_{\alpha,k}}{\partial z_{\alpha,t}}.$$

By (17),

$$\frac{\pi N}{4b} w_{\alpha,t} = \sum_{0\le j<M} \frac{I_\alpha}{j} \cos\frac{2\pi j(m+n)\pi}{N} \sin\frac{2\pi jt}{N}$$

$$
\begin{aligned}
& - \sum_{0\le j,k<M} \frac{\psi_{\alpha,k}}{j} \sin\frac{2\pi jt}{N}\cos\frac{2\pi jk}{N} \\
&= I_\alpha \sum_{0\le j<M} \Phi_j \sin\frac{2\pi jt}{N} - \sum_{0\le j,k<M} J_j \psi_{\alpha,k} \sin\frac{2\pi jt}{N}\cos\frac{2\pi jk}{N}.
\end{aligned}
$$

Define

$$
W_\alpha = \frac{4bI_\alpha}{\pi} Im(ifft(\Phi_{\alpha,N})) - \frac{4bN}{\pi} Im\{ifft(J \circ Re[ifft(\Psi_{\alpha,N})])\}. \tag{18}
$$

The gradient vector (11) can be formulated by FFT as follows:

$$
\frac{\partial\phi}{\partial Z_\alpha} = \frac{1}{dM}((Z_\alpha - F_\alpha) - W_\alpha[0:M-1]), \tag{19}
$$

$$
\frac{\partial\phi}{\partial Z} = (\frac{\partial\phi}{\partial Z_1}, \cdots, \frac{\partial\phi}{\partial Z_d}) \tag{20}
$$

2. The numerical performance assessments

Consider ODE (1-2) with $d = 3$ and following f_α over $[s, e] = [1, 3] \times R^3$.

$$
\begin{aligned}
f_1(x, y_1, y_2, y_3) &= r_1(x) + p_1 y_2^2 + q_1 y_1, \\
f_2(x, y_1, y_2, y_3) &= r_2(x) + p_2 y_3^2 + q_2 y_2, \\
f_3(x, y_1, y_2, y_3) &= r_3(x) + p_3 y_1^2 + q_3 y_3,
\end{aligned}
$$

where $(p_i, q_i)_{1\le i\le 3}$ are constant and $(r_i(x), \xi_i)_{1\le i\le 3}$ are determined in the way such that

$$
\hat{y}_1(x) = \sin(\theta x), \quad \hat{y}_1(x) = \sin(\theta x), \quad \hat{y}_1(x) = x
$$

solve ODE (1-2). Specifically,

$$
\begin{aligned}
r_1(x) &= \hat{y}_1'(x) - (p_1\hat{y}_2^2 + q_1\hat{y}_1), \\
r_2(x) &= \hat{y}_2(x) - (p_2\hat{y}_3^2 + q_2\hat{y}_2), \\
r_3(x) &= \hat{y}_3'(x) - (p_3\hat{y}_1^2 + q_3\hat{y}_3), \\
\xi_\alpha &= \hat{y}_\alpha(s), \quad 1 \le \alpha \le 3.
\end{aligned}
$$

For all the tests conducted in this section, we set $p_\alpha = q_\alpha = 0.1$ for all $1 \le \alpha \le 3$.

References

1. X. Zou, *On Trigonometric Interpolation and Its Applications* https://arxiv.org/pdf/2505.02330, May, 2025
2. K. Liu, B. Wang, X. Wu, X. Zou *On Application of Trigonometric Interpolation Based Optimization solving d dim Non-Linear ODE System*, To be appeared