Pico.jl Implementation Notes

Aaron Trowbridge

Contents

0 Introduction

The goal of QOC is to generate a *pulse* $\mathbf{a}(t)$ that minimizes some cost between

$$|\psi(T)\rangle = U(T,0)\,|\psi\rangle_{\text{init}} \tag{1}$$

where

$$U(T,0) = \mathcal{T}\exp\left(\frac{-i}{\hbar}\int_0^T dt\ H(\mathbf{a}(t),t)\right) \tag{2}$$

and $|\psi\rangle_{\text{goal}}$. This cost is typically defined to be the infidelity:

$$\ell(|\psi(T)\rangle) = 1 - \left|\langle\psi(T)|\psi\rangle_{\text{goal}}\right|^2 \tag{3}$$

The QOC optimization problem can then be defined as finding the pulse that minimizes the infidelity; this is accomplished by discretizing the trajectory of $|\psi(t)\rangle$ and $\mathbf{a}(t)$, with a time step Δt and solving the following optimization problem:

$$\begin{aligned}
\hat{\mathbf{a}}_{1:T-1} = \arg\min_{\mathbf{a}_{1:T-1}} \quad & \ell(|\psi(T)\rangle) \\
\text{s.t.} \quad & |\psi(T)\rangle = \prod_{t=1}^{T-1}\exp\left(\frac{-i}{\hbar}\ H(\mathbf{a}_t,t)\ \Delta t\right)|\psi\rangle_{\text{init}}
\end{aligned}$$

1 Problem Formulation

Given a quantum system with a Hamiltonian of the form

$$H(\mathbf{a}(t),t) = H_{\text{drift}} + \sum_{j=1}^{c} a^j(t) H^j_{\text{drive}}$$

we solve the constrained optimization problem

$$\begin{aligned}
\underset{\mathbf{x}_{1:T},\ \mathbf{u}_{1:T-1}}{\text{minimize}} \quad & \frac{1}{2}\sum_{t=1}^{T-1}\left(\mathbf{a}_t^\top R_{\mathbf{a}}\mathbf{a}_t + \dot{\mathbf{a}}_t^\top R_{\dot{\mathbf{a}}}\dot{\mathbf{a}}_t + \mathbf{u}_t^\top R_{\mathbf{u}}\mathbf{u}_t\right) + Q\cdot\ell(\tilde{\psi}^i_T) \\
\text{subject to} \quad & \mathbf{f}(\mathbf{x}_{t+1},\mathbf{x}_t,\mathbf{u}_t) = \mathbf{0} \\
& \tilde{\psi}^i_1 = \tilde{\psi}^i_{\text{init}} \\
& \tilde{\psi}^1_T = \tilde{\psi}^1_{\text{goal}} \quad \text{if } \mathsf{pin_first_qstate} = \mathsf{true} \\
& \textstyle\int \mathbf{a}_1 = \mathbf{a}_1 = \mathrm{d}_t\mathbf{a}_1 = \mathbf{0} \\
& \textstyle\int \mathbf{a}_T = \mathbf{a}_T = \mathrm{d}_t\mathbf{a}_T = \mathbf{0} \\
& \left|a^j_t\right| \le a^j_{\text{bound}}
\end{aligned}$$

The *state* vector $\mathbf{x}_t$ contains both the n (nqstates) quantum isomorphism states $\tilde{\psi}^i_t$ (each of dimension isodim = 2*ketdim) and the augmented control states $\int\mathbf{a}_t$, $\mathbf{a}_t$, and $\mathrm{d}_t\mathbf{a}_t$ (the number of augmented state vector is augdim). The *action* vector $\mathbf{u}_t$ contains the second derivative of the *control* vector $\mathbf{a}_t$, which has dimension ncontrols. Thus, we have:

$$\mathbf{x}_t = \begin{pmatrix} \tilde{\psi}^1_t \\ \vdots \\ \tilde{\psi}^n_t \\ \int\mathbf{a}_t \\ \mathbf{a}_t \\ \mathrm{d}_t\mathbf{a}_t \end{pmatrix} \quad \text{and} \quad \mathbf{u}_t = \left(\mathrm{d}_t^2\mathbf{a}_t\right) \tag{4}$$

In summary,

$$\begin{aligned}\dim(\mathbf{x}_t) &= \mathsf{nstates} = \mathsf{nqstates} \text{ * } \mathsf{isodim} + \mathsf{ncontrols} \text{ * } \mathsf{augdim} \\ \dim(\mathbf{u}_t) &= \mathsf{ncontrols}\end{aligned}$$

Additionally the cost function ℓ can be chosen somewhat liberally, the default is currently

$$\ell(\tilde{\psi}, \tilde{\psi}_{\text{goal}}) = 1 - |\langle\psi|\psi_{\text{goal}}\rangle|^2$$

2 Dynamics

Finally, $\mathbf{f}(\mathbf{x}_{t+1}, \mathbf{x}_t, \mathbf{u}_t)$ describes the dynamics of all the variables in the system, where the controls' dynamics are trivial and formally $\tilde{\psi}_t^i$ satisfies a discretized version of the isomorphic Schröedinger equation:

$$\frac{\mathrm{d}\tilde{\psi}^i}{\mathrm{d}t} = \widetilde{(-iH)}(\mathbf{a}(t), t)\tilde{\psi}^i$$

I will the use the notation $G(H)(\mathbf{a}(t), t) = \widetilde{(-iH)}(\mathbf{a}(t), t)$, to describe this operator (the Generator of time translation), which acts on the isomorphic quantum state vectors

$$\tilde{\psi} = \begin{pmatrix} \psi^{\mathrm{Re}} \\ \psi^{\mathrm{Im}} \end{pmatrix}$$

It can be shown that

$$G(H) = -\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \otimes H^{\mathrm{Re}} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes H^{\mathrm{Im}}$$

where $\otimes$ is the Kronecker product. We then have the linear isomorphism dynamics equation:

$$\frac{\mathrm{d}\tilde{\psi}}{\mathrm{d}t} = G(\mathbf{a}(t), t)\tilde{\psi}$$

where

$$G(\mathbf{a}(t), t) = G(H_{\mathrm{drift}}) + \sum_j a^j(t) G(H^j_{\mathrm{drive}})$$

The implicit dynamics constraint function $\mathbf{f}$ can be decomposed as follows:

$$\mathbf{f}(\mathbf{x}_{t+1}, \mathbf{x}_t, \mathbf{u}_t) = \begin{pmatrix} \mathbf{P}^{(m)}(\tilde{\psi}^1_{t+1}, \tilde{\psi}^1_t, \mathbf{a}_t) \\ \vdots \\ \mathbf{P}^{(m)}(\tilde{\psi}^n_{t+1}, \tilde{\psi}^n_t, \mathbf{a}_t) \\ \int \mathbf{a}_{t+1} - (\int \mathbf{a}_t + \mathbf{a}_t \cdot \Delta t_t) \\ \mathbf{a}_{t+1} - (\mathbf{a}_t + \mathrm{d}_t\mathbf{a}_t \cdot \Delta t_t) \\ \mathrm{d}_t\mathbf{a}_{t+1} - (\mathrm{d}_t\mathbf{a}_t + \mathbf{u}_t \cdot \Delta t_t) \end{pmatrix}$$

2.1 Padé integrators

We define (and implement) just the $m \in \{2, 4\}$ order Padé integrators $\mathbf{P}^{(m)}$:

$$
\begin{aligned}
\mathbf{P}^{(2)}(\tilde{\psi}^i_{t+1}, \tilde{\psi}^i_t, \mathbf{a}_t) &= \left(I - \frac{\Delta t}{2} G(\mathbf{a}_t)\right) \tilde{\psi}^i_{t+1} - \left(I + \frac{\Delta t}{2} G(\mathbf{a}_t)\right) \tilde{\psi}^i_t \\
\mathbf{P}^{(4)}(\tilde{\psi}^i_{t+1}, \tilde{\psi}^i_t, \mathbf{a}_t) &= \left(I - \frac{\Delta t}{2} G(\mathbf{a}_t) + \frac{(\Delta t)^2}{9} G(\mathbf{a}_t)^2\right) \tilde{\psi}^i_{t+1} \\
&\quad - \left(I + \frac{\Delta t}{2} G(\mathbf{a}_t) + \frac{(\Delta t)^2}{9} G(\mathbf{a}_t)^2\right) \tilde{\psi}^i_t
\end{aligned}
$$

Where again

$$G(\mathbf{a}_t) = G_{\text{drift}} + \mathbf{a}_t \cdot \mathbf{G}_{\text{drive}}$$

with $\mathbf{G}_{\text{drive}} = (G^1_{\text{drive}}, \ldots, G^c_{\text{drive}})^\top$, where $c = \mathsf{ncontrols}$

3 Differentiation

Our problem consists of $Z_{\text{dim}} = (\textsf{nstates} + \textsf{ncontrols}) \times \textsf{T}$ total variables, arranged into a vector

$$\mathbf{Z} = \begin{pmatrix} \mathbf{x}_1 \\ \mathbf{u}_1 \\ \vdots \\ \mathbf{x}_T \\ \mathbf{u}_T \end{pmatrix} = \begin{pmatrix} \mathbf{z}_1 \\ \vdots \\ \mathbf{z}_T \end{pmatrix} \tag{5}$$

where $\mathbf{z}_t = \begin{pmatrix} \mathbf{x}_t \\ \mathbf{u}_t \end{pmatrix}$ is referred to as a *knot point* and has dimension

$$z_{\text{dim}} = \textsf{vardim} = \textsf{nstates} + \textsf{ncontrols}.$$

Also, as of right now, $\mathbf{u}_T$ is included in $\mathbf{Z}$ but is ignored in calculations.

3.1 Objective Gradient

Given the objective

$$J(\mathbf{Z}) = Q \sum_{i=1}^{n} \ell(\tilde{\psi}_T^i, \tilde{\psi}_{\text{goal}}^i) + \frac{R}{2} \sum_{t=1}^{T-1} \mathbf{u}_t^2 \tag{6}$$

we arrive at the gradient

$$\boldsymbol{\nabla}_{\mathbf{Z}} J(\mathbf{Z}) = \begin{pmatrix} \mathbf{0}_{x_{\text{dim}}} \\ R \cdot \mathbf{u}_1 \\ \vdots \\ \mathbf{0}_{x_{\text{dim}}} \\ R \cdot \mathbf{u}_t \\ \vdots \\ \mathbf{0}_{x_{\text{dim}}} \\ R \cdot \mathbf{u}_{T-1} \\ Q \cdot \boldsymbol{\nabla}_{\tilde{\psi}^1} \ell^1 \\ \vdots \\ Q \cdot \boldsymbol{\nabla}_{\tilde{\psi}^n} \ell^n \\ \mathbf{0} \end{pmatrix} \tag{7}$$

where $\ell^i = \ell(\tilde{\psi}_T^i, \tilde{\psi}_{\text{goal}}^i)$. $\boldsymbol{\nabla}_{\tilde{\psi}^i} \ell^i$ is currently not calculated by hand, but at compile time via Symbolics.jl.

3.2 Dynamics Jacobian

Writing, $\mathbf{f}(\mathbf{z}_t, \mathbf{z}_{t+1}) = \mathbf{f}(\tilde{\psi}_{t+1}^i, \tilde{\psi}_t^i, \mathbf{a}_t)$, we can arrange the dynamics constraints into a vector

$$\mathbf{F} = \begin{pmatrix} \mathbf{f}(\mathbf{z}_1, \mathbf{z}_2) \\ \vdots \\ \mathbf{f}(\mathbf{z}_{T-1}, \mathbf{z}_T) \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \vdots \\ \mathbf{f}_{T-1} \end{pmatrix} \tag{8}$$

where we have defined $\mathbf{f}_t = \mathbf{f}(\mathbf{z}_t, \mathbf{z}_{t+1})$.

The dynamics Jacobian matrix $\frac{\partial \mathbf{F}}{\partial \mathbf{Z}}$ then has dimensions

$$F_{\text{dim}} \times Z_{\text{dim}} = (f_{\text{dim}} \cdot (T-1)) \times (z_{\text{dim}} \cdot T)$$

This matrix has a block diagonal structure:

$$\frac{\partial \mathbf{F}}{\partial \mathbf{Z}} = \begin{pmatrix} \frac{\partial \mathbf{f}_1}{\partial \mathbf{z}_1} & \frac{\partial \mathbf{f}_1}{\partial \mathbf{z}_2} & & & & \\ & \ddots & \ddots & & & \\ & & \frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_t} & \frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_{t+1}} & & \\ & & & \ddots & \ddots & \\ & & & & \frac{\partial \mathbf{f}_T}{\partial \mathbf{z}_{T-1}} & \frac{\partial \mathbf{f}_T}{\partial \mathbf{z}_T} \end{pmatrix} \tag{9}$$

We just need the $f_{\text{dim}} \times z_{\text{dim}}$ Jacobian matrices $\frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_t}$ and $\frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_{t+1}}$.

$\mathbf{f}_t$ Jacobian expressions

With $\mathbf{P}_t^{(m),i} = \mathbf{P}^{(m)}(\tilde{\psi}_{t+1}^i, \tilde{\psi}_t^i, \mathbf{a}_t)$, we first have

$$\frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_t} = \begin{pmatrix} \ddots & & & \vdots & & & \\ & \frac{\partial \mathbf{P}_t^{(m),i}}{\partial \tilde{\psi}_t^i} & & \frac{\partial \mathbf{P}_t^{(m),i}}{\partial \mathbf{a}_t} & & & \\ & & \ddots & \vdots & & & \\ & & -I_c^{\int \mathbf{a}_t} & -\Delta t I_c^{\mathbf{a}_t} & & & \\ & & & -I_c^{\mathbf{a}_t} & -\Delta t I_c^{\mathrm{d}_t \mathbf{a}_t} & & \\ & & & & \ddots & \ddots & \\ & & & & & -I_c^{\mathrm{d}_t^{c-1} \mathbf{a}_t} & -\Delta t I_c^{\mathbf{u}_t} \end{pmatrix} \tag{10}$$

where, $c =$ ncontrols, and the diagonal dots in the bottom right indicate that the number of $-I_c$ blocks on the diagonal should equal augdim, which is set to 3 by default.

Lastly,

$$\frac{\partial \mathbf{f}_t}{\partial \mathbf{z}_{t+1}} = \begin{pmatrix} \frac{\partial \mathbf{P}_t^{(m),1}}{\partial \tilde{\psi}_{t+1}^1} & & & \\ & \ddots & & \\ & & \frac{\partial \mathbf{P}_t^{(m),n}}{\partial \tilde{\psi}_{t+1}^n} & \\ & & & I_{c\cdot \mathsf{augdim}} \end{pmatrix} \tag{11}$$

$\mathbf{P}_t^{(m),i}$ Jacobian expressions

For the $\tilde{\psi}^i$ components, we have, for $m = 2$,

$$\frac{\partial \mathbf{P}_t^{(2),i}}{\partial \tilde{\psi}_t^i} = -\left(I + \frac{\Delta t}{2} G(\mathbf{a}_t)\right) \tag{12}$$

$$\frac{\partial \mathbf{P}_t^{(2),i}}{\partial \tilde{\psi}_{t+1}^i} = I - \frac{\Delta t}{2} G(\mathbf{a}_t) \tag{13}$$

and, for $m = 4$,

$$\frac{\partial \mathbf{P}_t^{(4),i}}{\partial \tilde{\psi}_t^i} = -\left(I + \frac{\Delta t}{2} G(\mathbf{a}_t) + \frac{(\Delta t)^2}{9} G(\mathbf{a}_t)^2\right) \tag{14}$$

$$\frac{\partial \mathbf{P}_t^{(4),i}}{\partial \tilde{\psi}_{t+1}^i} = I - \frac{\Delta t}{2} G(\mathbf{a}_t) + \frac{(\Delta t)^2}{9} G(\mathbf{a}_t)^2. \tag{15}$$

Now, for the $\mathbf{a}_t$ components, we have, for $m = 2$,

$$\frac{\partial \mathbf{P}_t^{(2),i}}{\partial a_t^j} = \frac{-\Delta t}{2} G_{\text{drive}}^j \left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i\right) \tag{16}$$

and, for $m = 4$,

$$\frac{\partial \mathbf{P}_t^{(4),i}}{\partial a_t^j} = \frac{-\Delta t}{2} G_{\text{drive}}^j \left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i\right) + \frac{(\Delta t)^2}{9} \left\{G_{\text{drive}}^j, G(\mathbf{a}_t)\right\} \left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i\right) \tag{17}$$

where $\{A, B\} = AB + BA$ is the anticommutator.

3.3 Hessian of the Lagrangian

The Lagrangian function is defined to be

$$\mathscr{L}(\mathbf{Z}; \sigma, \boldsymbol{\mu}) = \sigma \cdot J(\mathbf{Z}) + \boldsymbol{\mu} \boldsymbol{\cdot} \mathbf{F}(\mathbf{Z}) \tag{18}$$

where $\boldsymbol{\mu}$ is a Z_{dim}-dimensional vector provided by the solver.

For the Hessian we have

$$\nabla^2 \mathscr{L} = \sigma \cdot \nabla^2 J + \boldsymbol{\mu} \boldsymbol{\cdot} \nabla^2 \mathbf{F}. \tag{19}$$

We will look at $\nabla^2 J$ and $\boldsymbol{\mu} \boldsymbol{\cdot} \nabla^2 \mathbf{F}$ separately.

Objective Hessian

With $\ell^i = \ell(\tilde{\psi}^i_T, \tilde{\psi}^i_{\text{goal}})$, we have

$$\nabla^2 J(\mathbf{Z}) = \begin{pmatrix} \ddots & & & & & & & \\ & \mathbf{0} & & & & & & \\ & & R_t I_c & & & & & \\ & & & \ddots & & & & \\ & & & & \ddots & & & \\ & & & & & Q \cdot \nabla^2 \ell^i & & \\ & & & & & & \ddots & \\ & & & & & & & \mathbf{0} \end{pmatrix} \tag{20}$$

where $\nabla^2 \ell^i$ is again calculated using Symbolics.jl.

Dynamics Hessian

With $\boldsymbol{\mu} = (\vec{\mu}_1, \ldots, \vec{\mu}_T)$, $\vec{\mu}_t = \left(\mu_t^1, \ldots, \mu_t^{z_{\text{dim}}}\right)$, and using

$$\vec{\mu}_t^{\tilde{\psi}^i} = \left(\mu_t^{(i-1)\cdot\tilde{\psi}_{\text{dim}}+1}, \ldots, \mu_t^{i\cdot\tilde{\psi}_{\text{dim}}}\right)$$

we have

$$\boldsymbol{\mu} \cdot \nabla^2 \mathbf{F} = \begin{pmatrix} & \vdots & & & & \\ & \left(\frac{\partial^2 \mathbf{P}_t^{(m),i}}{\partial \tilde{\psi}_t^i \partial a_t^j}\right)^\top \vec{\mu}_t^{\tilde{\psi}^i} & & & & \\ & \vdots & & & & \\ \ddots & \mathbf{0} & & & & \\ & \sum_{i=1}^n \vec{\mu}_t^{\tilde{\psi}^i} \cdot \frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial a_t^k \partial a_t^j} & \mathbf{0} & \ldots & \left(\vec{\mu}_t^{\tilde{\psi}^i}\right)^\top \frac{\partial^2 \mathbf{P}_t^{(m),i}}{\partial a_t^k \partial \tilde{\psi}_{t+1}^i} & \ldots \\ & & \ddots & & & \end{pmatrix} \tag{21}$$

with

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial a_t^k \partial a_t^j} = \frac{(\Delta t)^2}{9} \left\{ G_{\text{drive}}^j, G_{\text{drive}}^k \right\} \left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i \right) \tag{22}$$

with, again, $\{A, B\} = AB + BA$, being the anticommutator.

since

$$x \cdot (Ay) = x^\top A y = (A^\top x)^\top y$$

For the mixed partials we have:

$$\frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \tilde{\psi}_t^i \partial a_t^j} = \frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \tilde{\psi}_{t+1}^i \partial a_t^j} = -\frac{\Delta t}{2} G_{\text{drive}}^j \tag{23}$$

and

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \tilde{\psi}_t^i \partial a_t^j} = -\frac{\Delta t}{2} G_{\text{drive}}^j - \frac{(\Delta t)^2}{9} \left(\left\{ G_{\text{drive}}^j, G_{\text{drift}} \right\} + \mathbf{a}_t \cdot \left\{ G_{\text{drive}}^j, \mathbf{G}_{\text{drive}} \right\} \right) \tag{24}$$

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \tilde{\psi}_{t+1}^i \partial a_t^j} = -\frac{\Delta t}{2} G_{\text{drive}}^j + \frac{(\Delta t)^2}{9} \left(\left\{ G_{\text{drive}}^j, G_{\text{drift}} \right\} + \mathbf{a}_t \cdot \left\{ G_{\text{drive}}^j, \mathbf{G}_{\text{drive}} \right\} \right) \tag{25}$$

4 Minimum Time Problem

Once a solution has been found for a given *time horizon*, we can solve the time minimization problem below, initialized with the given solution.

$$\begin{aligned} \underset{\substack{\mathbf{x}_{1:T},\ \mathbf{u}_{1:T-1} \\ \Delta t_{1:T-1}}}{\text{minimize}} \quad & \sum_t \Delta t_t + \frac{1}{2} \sum_t \mathbf{u}_t^\top R_u \mathbf{u}_t + \frac{R_s}{2} \sum_t (\mathbf{u}_{t+1} - \mathbf{u}_t)^2 \\ \text{subject to} \quad & \mathbf{f}(\mathbf{x}_{t+1}, \mathbf{x}_t, \mathbf{u}_t, \Delta t_t) = \mathbf{0} \\ & \mathbf{x}_T = \mathbf{x}_T^{\text{nominal}} \end{aligned}$$

For this problem we will define, with $\mathbf{Z}$ as defined before

$$\Delta \mathbf{t} = \begin{pmatrix} \Delta t_1 \\ \vdots \\ \Delta t_{T-1} \end{pmatrix} \quad \text{and} \quad \bar{\mathbf{Z}} = \begin{pmatrix} \mathbf{Z} \\ \Delta \mathbf{t} \end{pmatrix}$$

4.1 Objective Gradient

Let's write the objective function as

$$J = J_{\Delta t} + J_u + J_s \tag{26}$$

then

$$\nabla_{\bar{\mathbf{Z}}} J = \begin{pmatrix} \nabla_{\mathbf{Z}} J \\ \nabla_{\mathbf{\Delta t}} J \end{pmatrix} = \begin{pmatrix} \nabla_{\mathbf{Z}} J_u + \nabla_{\mathbf{Z}} J_s \\ \nabla_{\mathbf{\Delta t}} J_{\Delta t} \end{pmatrix} \tag{27}$$

where

$$\nabla_{\mathbf{Z}} J_u = \begin{pmatrix} \vdots \\ \mathbf{0} \\ R_u \mathbf{u}_t \\ \vdots \end{pmatrix}, \qquad \nabla_{\mathbf{Z}} J_s = \begin{pmatrix} \mathbf{0} \\ R_s(\mathbf{u}_1 - \mathbf{u}_2) \\ \vdots \\ \mathbf{0} \\ R_s(-\mathbf{u}_{t-1} + 2\mathbf{u}_t - \mathbf{u}_{t+1}) \\ \vdots \\ \mathbf{0} \\ R_s(-\mathbf{u}_{T-2} + \mathbf{u}_{T-1}) \end{pmatrix}, \tag{28}$$

and

$$\nabla_{\mathbf{\Delta t}} J_{\Delta t} = \mathbf{1}_{T-1} \tag{29}$$

4.2 Dynamics Jacobian

We then have, with $\mathbf{F}$ defined as before (but taking the corresponding Δt_t):

$$\frac{\partial \mathbf{F}}{\partial \bar{\mathbf{Z}}} = \begin{pmatrix} \frac{\partial \mathbf{F}}{\partial \mathbf{Z}} & \frac{\partial \mathbf{F}}{\partial \mathbf{\Delta t}} \end{pmatrix} \tag{30}$$

where

$$\frac{\partial \mathbf{F}}{\partial \mathbf{\Delta t}} = \begin{pmatrix} \frac{\partial \mathbf{f}_1}{\partial \Delta t_1} & & \\ & \ddots & \\ & & \frac{\partial \mathbf{f}_{T-1}}{\partial \Delta t_{T-1}} \end{pmatrix} \tag{31}$$

with

$$\frac{\partial \mathbf{f}_t}{\partial \Delta t_t} = \begin{pmatrix} \vdots \\ \frac{\partial \mathbf{P}_t^{(n),i}}{\partial \Delta t_t} \\ \vdots \\ -\mathbf{a}_t \\ -\dot{\mathbf{a}}_t \\ -\mathbf{u}_t \end{pmatrix} \tag{32}$$

and

$$\begin{aligned} \frac{\partial \mathbf{P}_t^{(4),i}}{\partial \Delta t_t} &= \left(-\frac{1}{2}G(\mathbf{a}_t) + \frac{2\Delta t_t}{9}G(\mathbf{a}_t)^2\right)\tilde{\psi}_{t+1}^i - \left(\frac{1}{2}G(\mathbf{a}_t) + \frac{2\Delta t_t}{9}G(\mathbf{a}_t)^2\right)\tilde{\psi}_t^i \\ &= -\frac{1}{2}G(\mathbf{a}_t)\left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i\right) + \frac{2\Delta t_t}{9}G(\mathbf{a}_t)^2\left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i\right) \end{aligned} \tag{33}$$

$$\frac{\partial \mathbf{P}_t^{(2),i}}{\partial \Delta t_t} = -\frac{1}{2}G(\mathbf{a}_t)\left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i\right) \tag{34}$$

4.3 Hessian of the Lagrangian

As before we will first define the objective Hessian and then the dynamics Lagrangian Hessian

Objective Hessian

Decomposing as before, we have

$$\nabla^2_{\tilde{\mathbf{Z}}} J = \begin{pmatrix} \nabla^2_{\mathbf{Z}} J_u + \nabla^2_{\mathbf{Z}} J_s & \\ & \nabla^2_{\mathbf{\Delta t}} J_{\Delta t} \end{pmatrix} = \begin{pmatrix} \nabla^2_{\mathbf{Z}} J_u + \nabla^2_{\mathbf{Z}} J_s & \\ & \mathbf{0}_{T-1\times T-1} \end{pmatrix}$$

where

$$\nabla^2_{\mathbf{Z}} J_u = \begin{pmatrix} \ddots & & & \\ & \mathbf{0} & & \\ & & R_u I & \\ & & & \ddots \end{pmatrix} \tag{35}$$

and, showing the upper triangular structure of the Hessian,

$$\nabla^2_{\mathbf{Z}} J_s = \begin{pmatrix} \mathbf{0} & & \mathbf{0} & & & & & \\ & R_s I & & -R_s I & & & & \\ & & \mathbf{0} & & \mathbf{0} & & & \\ & & & 2R_s I & & -R_s I & & \\ & & & & \mathbf{0} & & \ddots & \\ & & & & & 2R_s I & & -R_s I \\ & & & & & & \ddots & \\ & & & & & & & R_s I \end{pmatrix} \tag{36}$$

Hessian of the Dynamics Lagrangian

Defining

$$\mathcal{L}_f = \boldsymbol{\mu} \cdot \mathbf{F}$$

we want to compute

$$\nabla^2_{\tilde{\mathbf{Z}}} \mathcal{L}_f = \begin{pmatrix} \nabla^2_{\mathbf{Z}} \mathcal{L}_f & \nabla^\top_{\mathbf{\Delta t}} \nabla_{\mathbf{Z}} \mathcal{L}_f \\ \nabla^\top_{\mathbf{Z}} \nabla_{\mathbf{\Delta t}} \mathcal{L}_f & \nabla^2_{\mathbf{\Delta t}} \mathcal{L}_f \end{pmatrix}$$

we have already computed $\nabla^2_{\mathbf{Z}} \mathcal{L}_f$ above, so we then have

$$\nabla^2_{\mathbf{\Delta t}} \mathcal{L}_f = \begin{pmatrix} \ddots & & \\ & \vec{\mu}_t \cdot \dfrac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t^2} & \\ & & \ddots \end{pmatrix} \tag{37}$$

where

$$\vec{\mu}_t \cdot \frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t^2} = \vec{\mu}_t \cdot \begin{pmatrix} \vdots \\ \dfrac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t^2} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} = \sum_i \vec{\mu}_t^{\tilde{\psi}_i} \cdot \frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t^2} \tag{38}$$

with

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \Delta t_t^2} = \frac{2}{9} G(\mathbf{a}_t)^2 \left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i\right) \tag{39}$$

$$\frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \Delta t_t^2} = \mathbf{0} \tag{40}$$

We also have

$$\nabla_{\Delta \mathbf{t}}^\top \nabla_{\mathbf{Z}} \mathcal{L}_f = \begin{pmatrix} \ddots & & & \\ & \left(\frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t \partial \mathbf{z}_t}\right)^\top \vec{\mu}_t & & \\ & \left(\frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t \partial \mathbf{z}_{t+1}}\right)^\top \vec{\mu}_t & \left(\frac{\partial^2 \mathbf{f}_{t+1}}{\partial \Delta t_{t+1} \partial \mathbf{z}_{t+1}}\right)^\top \vec{\mu}_{t+1} & \\ & & \left(\frac{\partial^2 \mathbf{f}_{t+1}}{\partial \Delta t_{t+1} \partial \mathbf{z}_{t+2}}\right)^\top \vec{\mu}_{t+1} & \\ & & & \ddots \end{pmatrix} \tag{41}$$

where

$$\left(\frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t \partial \mathbf{z}_t}\right)^\top \vec{\mu}_t = \begin{pmatrix} \vdots \\ \left(\frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t \partial \tilde{\psi}_t^i}\right)^\top \vec{\mu}_t^{\tilde{\psi}^i} \\ \vdots \\ \mathbf{0} \\ -\vec{\mu}_t^{\int \mathbf{a}} + \sum_i \left(\frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t \partial \mathbf{a}_t}\right)^\top \vec{\mu}_t^{\tilde{\psi}^i} \\ -\vec{\mu}_t^{\mathbf{a}} \\ -\vec{\mu}_t^{\dot{\mathbf{a}}} \end{pmatrix} \tag{42}$$

and

$$\left(\frac{\partial^2 \mathbf{f}_t}{\partial \Delta t_t \partial \mathbf{z}_{t+1}}\right)^\top \vec{\mu}_t = \begin{pmatrix} \vdots \\ \left(\frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t \partial \tilde{\psi}_{t+1}^i}\right)^\top \vec{\mu}_t^{\tilde{\psi}^i} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \tag{43}$$

with

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \Delta t_t \partial \tilde{\psi}_t^i} = -\left(\frac{1}{2} G(\mathbf{a}_t) + \frac{2\Delta t_t}{9} G(\mathbf{a}_t)^2\right) \tag{44}$$

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \Delta t_t \partial \tilde{\psi}_{t+1}^i} = -\frac{1}{2} G(\mathbf{a}_t) + \frac{2\Delta t_t}{9} G(\mathbf{a}_t)^2 \tag{45}$$

and

$$\frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \Delta t_t \partial \tilde{\psi}_t^i} = \frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \Delta t_t \partial \tilde{\psi}_{t+1}^i} = -\frac{1}{2} G(\mathbf{a}_t) \tag{46}$$

and for the jth column of $\frac{\partial^2 \mathbf{P}_t^{(n),i}}{\partial \Delta t_t \partial \mathbf{a}_t}$ we have

$$\frac{\partial^2 \mathbf{P}_t^{(4),i}}{\partial \Delta t_t \partial a_t^j} = -\frac{1}{2} G_{\text{drive}}^j \left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i \right) + \frac{2\Delta t_t}{9} \left\{ G_{\text{drive}}^j, G(\mathbf{a}_t) \right\} \left(\tilde{\psi}_{t+1}^i - \tilde{\psi}_t^i \right) \tag{47}$$

and

$$\frac{\partial^2 \mathbf{P}_t^{(2),i}}{\partial \Delta t_t \partial a_t^j} = -\frac{1}{2} G_{\text{drive}}^j \left(\tilde{\psi}_{t+1}^i + \tilde{\psi}_t^i \right) \tag{48}$$

5 Unitary Implementation

5.1 Definitions

$$\text{isovec}(I_2 \otimes A + \text{Im} \otimes B) = \begin{pmatrix} \text{vec}(A) \\ \text{vec}(B) \end{pmatrix}$$

$$B(\mathbf{a}_t, h_t) = I_2 \otimes B^{\text{R}} + \text{Im} \otimes B^{\text{I}}$$

$$\begin{aligned} B^{\text{R}} &= I - \frac{h_t}{2} H^{\text{I}} + \frac{h_t^2}{9}\Big(\big(H^{\text{I}}\big)^2 - \big(H^{\text{R}}\big)^2\Big) \\ B^{\text{I}} &= \frac{h_t}{2} H^{\text{R}} - \frac{h_t^2}{9}\big\{H^{\text{R}}, H^{\text{I}}\big\} \end{aligned}$$

$$F(\mathbf{a}_t, h_t) = I_2 \otimes F^{\text{R}} - \text{Im} \otimes F^{\text{I}}$$

$$\begin{aligned} F^{\text{R}} &= I + \frac{h_t}{2} H^{\text{I}} + \frac{h_t^2}{9}\Big(\big(H^{\text{I}}\big)^2 - \big(H^{\text{R}}\big)^2\Big) \\ F^{\text{I}} &= \frac{h_t}{2} H^{\text{R}} + \frac{h_t^2}{9}\big\{H^{\text{R}}, H^{\text{I}}\big\} \end{aligned}$$

$$\begin{aligned} f(\vec{\widetilde{U}}_t, \mathbf{a}_t, h_t, \vec{\widetilde{U}}_{t+1}) &= \text{isovec}\Big(\mathbf{P}(\widetilde{U}_{t+1}, \widetilde{U}_t, \mathbf{a}_t, h_t)\Big) \\ &= \text{isovec}\Big(B(\mathbf{a}_t, h_t)\widetilde{U}_{t+1} - F(\mathbf{a}_t, h_t)\widetilde{U}_t\Big) \\ &= \hat{B}(\mathbf{a}_t, h_t)\vec{\widetilde{U}}_{t+1} - \hat{F}(\mathbf{a}_t, h_t)\vec{\widetilde{U}}_t \end{aligned}$$

where

$$\begin{aligned} \hat{B}(\mathbf{a}_t, h_t) &= (I_2 \otimes I_N) \otimes B^{\text{R}} + (\text{Im} \otimes I_N) \otimes B^{\text{I}} \\ \hat{F}(\mathbf{a}_t, h_t) &= (I_2 \otimes I_N) \otimes F^{\text{R}} - (\text{Im} \otimes I_N) \otimes F^{\text{I}} \end{aligned}$$

5.2 Derivatives

Jacobian

For the states we have

$$\frac{\partial f}{\partial \vec{\tilde{U}}_t} = -\hat{F} \quad \text{and} \quad \frac{\partial f}{\partial \vec{\tilde{U}}_{t+1}} = \hat{B}$$

For the drives we have

$$\begin{aligned}
\frac{\partial f}{\partial a_t^j} &= \frac{\partial \hat{B}}{\partial a_t^j}\vec{\tilde{U}}_{t+1} - \frac{\partial \hat{F}}{\partial a_t^j}\vec{\tilde{U}}_t \\
&= \left((I_2 \otimes I_N) \otimes \frac{\partial B^{\mathrm{R}}}{\partial a_t^j} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial B^{\mathrm{I}}}{\partial a_t^j} \right) \vec{\tilde{U}}_{t+1} \\
&\quad - \left((I_2 \otimes I_N) \otimes \frac{\partial F^{\mathrm{R}}}{\partial a_t^j} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial F^{\mathrm{I}}}{\partial a_t^j} \right) \vec{\tilde{U}}_t
\end{aligned}$$

where, writing $\partial_{a_t^j} H = H_j$, we have

$$\begin{aligned}
\frac{\partial B^{\mathrm{R}}}{\partial a_t^j} &= -\frac{h_t}{2} H_j^{\mathrm{I}} + \frac{h_t^2}{9}\left(\{H^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H^{\mathrm{R}}, H_j^{\mathrm{R}}\}\right) \\
&= -\frac{h_t}{2} H_j^{\mathrm{I}} + \frac{h_t^2}{9}\left(\{H_0^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H_0^{\mathrm{R}}, H_j^{\mathrm{R}}\} + \sum_{i=0}^{d} a_t^i \left(\{H_i^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H_i^{\mathrm{R}}, H_j^{\mathrm{R}}\}\right) \right) \\
\frac{\partial B^{\mathrm{I}}}{\partial a_t^j} &= \frac{h_t}{2} H_j^{\mathrm{R}} - \frac{h_t^2}{9}\left(\{H^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H^{\mathrm{I}}, H_j^{\mathrm{R}}\}\right) \\
&= \frac{h_t}{2} H_j^{\mathrm{R}} - \frac{h_t^2}{9}\left(\{H_0^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H_0^{\mathrm{I}}, H_j^{\mathrm{R}}\} + \sum_{i} a_t^i \left(\{H_i^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H_i^{\mathrm{I}}, H_j^{\mathrm{R}}\}\right) \right)
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial F^{\mathrm{R}}}{\partial a_t^j} &= \frac{h_t}{2} H_j^{\mathrm{I}} + \frac{h_t^2}{9}\left(\{H^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H^{\mathrm{R}}, H_j^{\mathrm{R}}\}\right) \\
&= \frac{h_t}{2} H_j^{\mathrm{I}} + \frac{h_t^2}{9}\left(\{H_0^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H_0^{\mathrm{R}}, H_j^{\mathrm{R}}\} + \sum_{i} a_t^i \left(\{H_i^{\mathrm{I}}, H_j^{\mathrm{I}}\} - \{H_i^{\mathrm{R}}, H_j^{\mathrm{R}}\}\right) \right) \\
\frac{\partial F^{\mathrm{I}}}{\partial a_t^j} &= \frac{h_t}{2} H_j^{\mathrm{R}} + \frac{h_t^2}{9}\left(\{H^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H^{\mathrm{I}}, H_j^{\mathrm{R}}\}\right) \\
&= \frac{h_t}{2} H_j^{\mathrm{R}} + \frac{h_t^2}{9}\left(\{H_0^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H_0^{\mathrm{I}}, H_j^{\mathrm{R}}\} + \sum_{i} a_t^i \left(\{H_i^{\mathrm{R}}, H_j^{\mathrm{I}}\} + \{H_i^{\mathrm{I}}, H_j^{\mathrm{R}}\}\right) \right)
\end{aligned}$$

For the timestep h_t we have

$$\begin{aligned}
\frac{\partial f}{\partial h_t} &= \frac{\partial \hat{B}}{\partial h_t}\vec{\tilde{U}}_{t+1} - \frac{\partial \hat{F}}{\partial h_t}\vec{\tilde{U}}_t \\
&= \left((I_2 \otimes I_N) \otimes \frac{\partial B^{\mathrm{R}}}{\partial h_t} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial B^{\mathrm{I}}}{\partial h_t} \right) \vec{\tilde{U}}_{t+1} \\
&\quad - \left((I_2 \otimes I_N) \otimes \frac{\partial F^{\mathrm{R}}}{\partial h_t} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial F^{\mathrm{I}}}{\partial h_t} \right) \vec{\tilde{U}}_t
\end{aligned}$$

where

$$\frac{\partial B^{\mathrm{R}}}{\partial h_t} = -\frac{1}{2}H^{\mathrm{I}} + \frac{2h_t}{9}\left(\left(H^{\mathrm{I}}\right)^2 - \left(H^{\mathrm{R}}\right)^2\right)$$
$$\frac{\partial B^{\mathrm{I}}}{\partial h_t} = \frac{1}{2}H^{\mathrm{R}} - \frac{2h_t}{9}\left\{H^{\mathrm{R}}, H^{\mathrm{I}}\right\}$$

and

$$\frac{\partial F^{\mathrm{R}}}{\partial h_t} = \frac{1}{2}H^{\mathrm{I}} + \frac{2h_t}{9}\left(\left(H^{\mathrm{I}}\right)^2 - \left(H^{\mathrm{R}}\right)^2\right)$$
$$\frac{\partial F^{\mathrm{I}}}{\partial h_t} = \frac{1}{2}H^{\mathrm{R}} + \frac{2h_t}{9}\left\{H^{\mathrm{R}}, H^{\mathrm{I}}\right\}.$$

So we then have, with $z_t = \begin{pmatrix}\vec{\tilde{U}}_t & \mathbf{a}_t & h_t\end{pmatrix}^\top$

$$\partial_{z_t:z_{t+1}} f = \begin{pmatrix}\partial_{z_t} f & \partial_{z_{t+1}} f\end{pmatrix} = \begin{pmatrix}-\hat{F} & \partial_{\mathbf{a}_t} f & \partial_{h_t} f & \hat{B} & \mathbf{0} & \mathbf{0}\end{pmatrix}$$

Hessian of the Lagrangian

$$\mathcal{L} = \boldsymbol{\mu}^\top \mathbf{F}(\mathbf{Z}) = \sum_t \mu_t^\top f(z_t, z_{t+1}) = \sum_t \mathcal{L}_t$$

$$\mathcal{L}_t = \mu_t^\top f(z_t, z_{t+1})$$

$$\partial^2_{z_t:z_{t+1}} \mathcal{L}_t = \begin{pmatrix}\partial^2_{z_t}\mathcal{L}_t & \partial_{z_{t+1}}\partial_{z_t}\mathcal{L}_t \\ \ddots & \mathbf{0}\end{pmatrix}$$

$$\partial^2_{z_t}\mathcal{L}_t = \begin{pmatrix}\mathbf{0} & \partial_{\mathbf{a}_t}\partial_{\vec{\tilde{U}}_t}\mathcal{L}_t & \partial_{h_t}\partial_{\vec{\tilde{U}}_t}\mathcal{L}_t \\ & \partial^2_{\mathbf{a}_t}\mathcal{L}_t & \partial_{h_t}\partial_{\mathbf{a}_t}\mathcal{L}_t \\ & & \partial^2_{h_t}\mathcal{L}_t\end{pmatrix}$$

$$\partial_{z_{t+1}}\partial_{z_t}\mathcal{L}_t = \begin{pmatrix}\mathbf{0} & \partial_{\vec{\tilde{U}}_{t+1}}\partial_{\mathbf{a}_t}\mathcal{L}_t & \partial_{\vec{\tilde{U}}_{t+1}}\partial_{h_t}\mathcal{L}_t \\ & \mathbf{0} & \mathbf{0} \\ & & \mathbf{0}\end{pmatrix}$$

$$\begin{aligned}\frac{\partial^2\mathcal{L}_t}{\partial a_t^j \partial\vec{\tilde{U}}_t} &= \frac{\partial}{\partial a_t^j}\frac{\partial\mathcal{L}_t}{\partial\vec{\tilde{U}}_t} \\ &= \frac{\partial}{\partial a_t^j}\left(-\hat{F}^\top\mu_t\right) \\ &= -\left(\frac{\partial\hat{F}}{\partial a_t^j}\right)^\top \mu_t \\ &= -\left((I_2\otimes I_N)\otimes\frac{\partial F^{\mathrm{R}}}{\partial a_t^j} - (\mathrm{Im}\otimes I_N)\otimes\frac{\partial F^{\mathrm{I}}}{\partial a_t^j}\right)^\top \mu_t\end{aligned}$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial a_t^j \partial \vec{\vec{U}}_{t+1}} &= \frac{\partial}{\partial a_t^j} \frac{\partial \mathcal{L}_t}{\partial \vec{\vec{U}}_{t+1}} \\
&= \frac{\partial}{\partial a_t^j} \left(\hat{B}^\top \mu_t \right) \\
&= \left(\frac{\partial \hat{B}}{\partial a_t^j} \right)^\top \mu_t \\
&= \left((I_2 \otimes I_N) \otimes \frac{\partial B^{\mathrm{R}}}{\partial a_t^j} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial B^{\mathrm{I}}}{\partial a_t^j} \right)^\top \mu_t
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial a_t^i \partial a_t^j} &= \mu_t^\top \frac{\partial^2 f_t}{\partial a_t^i \partial a_t^j} \\
&= \mu_t^\top \left(\frac{\partial^2 \hat{B}}{\partial a_t^i \partial a_t^j} \vec{\vec{U}}_{t+1} - \frac{\partial^2 \hat{F}}{\partial a_t^i \partial a_t^j} \vec{\vec{U}}_t \right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \hat{B}}{\partial a_t^i \partial a_t^j} &= (I_2 \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{R}}}{\partial a_t^i \partial a_t^j} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{I}}}{\partial a_t^i \partial a_t^j} \\
\frac{\partial^2 \hat{F}}{\partial a_t^i \partial a_t^j} &= (I_2 \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{R}}}{\partial a_t^i \partial a_t^j} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{I}}}{\partial a_t^i \partial a_t^j}
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 B^{\mathrm{R}}}{\partial a_t^i \partial a_t^j} &= \frac{h_t^2}{9} \left(\left\{ H_i^{\mathrm{I}}, H_j^{\mathrm{I}} \right\} - \left\{ H_i^{\mathrm{R}}, H_j^{\mathrm{R}} \right\} \right) \\
\frac{\partial^2 B^{\mathrm{I}}}{\partial a_t^i \partial a_t^j} &= -\frac{h_t^2}{9} \left(\left\{ H_i^{\mathrm{R}}, H_j^{\mathrm{I}} \right\} + \left\{ H_i^{\mathrm{I}}, H_j^{\mathrm{R}} \right\} \right)
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial^2 F^{\mathrm{R}}}{\partial a_t^i \partial a_t^j} &= \frac{h_t^2}{9} \left(\left\{ H_i^{\mathrm{I}}, H_j^{\mathrm{I}} \right\} - \left\{ H_i^{\mathrm{R}}, H_j^{\mathrm{R}} \right\} \right) \\
\frac{\partial^2 F^{\mathrm{I}}}{\partial a_t^i \partial a_t^j} &= \frac{h_t^2}{9} \left(\left\{ H_i^{\mathrm{R}}, H_j^{\mathrm{I}} \right\} + \left\{ H_i^{\mathrm{I}}, H_j^{\mathrm{R}} \right\} \right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial h_t \partial \vec{\vec{U}}_t} &= \frac{\partial}{\partial h_t} \frac{\partial \mathcal{L}_t}{\partial \vec{\vec{U}}_t} \\
&= \frac{\partial}{\partial h_t} \left(-\hat{F}^\top \mu_t \right) \\
&= -\left(\frac{\partial \hat{F}}{\partial h_t} \right)^\top \mu_t \\
&= -\left((I_2 \otimes I_N) \otimes \frac{\partial F^{\mathrm{R}}}{\partial h_t} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial F^{\mathrm{I}}}{\partial h_t} \right)^\top \mu_t
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial h_t \partial \vec{\tilde{U}}_{t+1}} &= \frac{\partial}{\partial h_t} \frac{\partial \mathcal{L}_t}{\partial \vec{\tilde{U}}_{t+1}} \\
&= \frac{\partial}{\partial h_t} \left(\hat{B}^\top \mu_t \right) \\
&= \left(\frac{\partial \hat{B}}{\partial h_t} \right)^\top \mu_t \\
&= \left((I_2 \otimes I_N) \otimes \frac{\partial B^{\mathrm{R}}}{\partial h_t} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial B^{\mathrm{I}}}{\partial h_t} \right)^\top \mu_t
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial h_t \partial a_t^j} &= \mu_t^\top \frac{\partial^2 f_t}{\partial h_t \partial a_t^j} \\
&= \mu_t^\top \left(\frac{\partial^2 \hat{B}}{\partial h_t \partial a_t^j} \vec{\tilde{U}}_{t+1} - \frac{\partial^2 \hat{F}}{\partial h_t \partial a_t^j} \vec{\tilde{U}}_t \right) \\
&= \mu_t^\top \Bigg(\left((I_2 \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{R}}}{\partial h_t \partial a_t^j} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{I}}}{\partial h_t \partial a_t^j} \right) \vec{\tilde{U}}_{t+1} \\
&\quad - \left((I_2 \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{R}}}{\partial h_t \partial a_t^j} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{I}}}{\partial h_t \partial a_t^j} \right) \vec{\tilde{U}}_t \Bigg)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 B^{\mathrm{R}}}{\partial h_t \partial a_t^j} &= -\frac{1}{2} H_j^{\mathrm{I}} + \frac{2h_t}{9} \left(\{ H^{\mathrm{I}}, H_j^{\mathrm{I}} \} - \{ H^{\mathrm{R}}, H_j^{\mathrm{R}} \} \right) \\
\frac{\partial^2 B^{\mathrm{I}}}{\partial h_t \partial a_t^j} &= \frac{1}{2} H_j^{\mathrm{R}} - \frac{2h_t}{9} \left(\{ H^{\mathrm{R}}, H_j^{\mathrm{I}} \} + \{ H^{\mathrm{I}}, H_j^{\mathrm{R}} \} \right)
\end{aligned}
$$

and

$$
\begin{aligned}
\frac{\partial^2 F^{\mathrm{R}}}{\partial h_t \partial a_t^j} &= \frac{1}{2} H_j^{\mathrm{I}} + \frac{2h_t}{9} \left(\{ H^{\mathrm{I}}, H_j^{\mathrm{I}} \} - \{ H^{\mathrm{R}}, H_j^{\mathrm{R}} \} \right) \\
\frac{\partial^2 F^{\mathrm{I}}}{\partial h_t \partial a_t^j} &= \frac{1}{2} H_j^{\mathrm{R}} + \frac{2h_t}{9} \left(\{ H^{\mathrm{R}}, H_j^{\mathrm{I}} \} + \{ H^{\mathrm{I}}, H_j^{\mathrm{R}} \} \right)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial^2 \mathcal{L}_t}{\partial h_t^2} &= \mu_t^\top \frac{\partial^2 f_t}{\partial h_t^2} \\
&= \mu_t^\top \left(\frac{\partial^2 \hat{B}}{\partial h_t^2} \vec{\tilde{U}}_{t+1} - \frac{\partial^2 \hat{F}}{\partial h_t^2} \vec{\tilde{U}}_t \right) \\
&= \mu_t^\top \Bigg(\left((I_2 \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{R}}}{\partial h_t^2} + (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 B^{\mathrm{I}}}{\partial h_t^2} \right) \vec{\tilde{U}}_{t+1} \\
&\quad - \left((I_2 \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{R}}}{\partial h_t^2} - (\mathrm{Im} \otimes I_N) \otimes \frac{\partial^2 F^{\mathrm{I}}}{\partial h_t^2} \right) \vec{\tilde{U}}_t \Bigg)
\end{aligned}
$$

where

$$\begin{aligned}
\frac{\partial^2 B^{\mathrm{R}}}{\partial h_t^2} &= \frac{2}{9}\Big(\big(H^{\mathrm{I}}\big)^2 - \big(H^{\mathrm{R}}\big)^2\Big) \\
\frac{\partial^2 B^{\mathrm{I}}}{\partial h_t^2} &= -\frac{2}{9}\big\{H^{\mathrm{R}}, H^{\mathrm{I}}\big\}
\end{aligned}$$

and

$$\begin{aligned}
\frac{\partial^2 F^{\mathrm{R}}}{\partial h_t^2} &= \frac{2}{9}\Big(\big(H^{\mathrm{I}}\big)^2 - \big(H^{\mathrm{R}}\big)^2\Big) \\
\frac{\partial^2 F^{\mathrm{I}}}{\partial h_t^2} &= \frac{2}{9}\big\{H^{\mathrm{R}}, H^{\mathrm{I}}\big\}
\end{aligned}$$