Note for NODE Approach to the MQCD Phase Diagram via Holography Yao Zhang

1 Deduction

Assume a vector field representation of the governing equations:

$$\vec{\Theta}(z) = \begin{bmatrix} \Phi(z) \\ F(z) \\ \Sigma(z) \\ A(z) \\ G(z) \end{bmatrix} \triangleq \begin{bmatrix} u_1(z) \\ u_2(z) \\ u_3(z) \\ u_4(z) \\ u_5(z) \end{bmatrix}$$
(1)

Further assume the system dynamics are governed by:

$$\frac{d\vec{\Theta}(z)}{dz} = \begin{bmatrix} \frac{d}{dz}\Phi(z) \\ \frac{d}{dz}F(z) \\ \frac{d}{dz}\Delta(z) \\ \frac{d}{dz}A(z) \\ \frac{d}{dz}G(z) \end{bmatrix} \triangleq \frac{d\vec{u}}{dz} = \begin{bmatrix} \frac{du_1(z)}{dz} \\ \frac{du_2(z)}{dz} \\ \frac{du_3(z)}{dz} \\ \frac{du_4(z)}{dz} \\ \frac{du_5(z)}{dz} \end{bmatrix} = \vec{f}\left(\vec{u}; \vec{Z}\left(z\Phi\left(z; \vec{\xi}\right)\right), \frac{\partial \vec{Z}\left(z\Phi\left(z; \vec{\xi}\right)\right)}{\partial z\Phi\left(z; \vec{\xi}\right)}\right)$$

$$= \vec{f}\left(\vec{u}; u_6\left(x; \vec{\xi}\right), u_7\left(x; \vec{\xi}\right)\right) = \begin{bmatrix} f_1\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), \frac{\partial u_6(x; \vec{\xi})}{\partial x}\right) \\ f_2\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), \frac{\partial u_6(x; \vec{\xi})}{\partial x}\right) \\ f_3\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), \frac{\partial u_6(x; \vec{\xi})}{\partial x}\right) \\ f_4\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), \frac{\partial u_6(x; \vec{\xi})}{\partial x}\right) \\ f_5\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), \frac{\partial u_6(x; \vec{\xi})}{\partial x}\right)$$

where $u_6\left(x;\vec{\xi}\right)=\widehat{Z}\left(z\Phi\left(z\right);\vec{\xi}\right)$ with $x=z\Phi\left(z\right),$ under the assumption that $\frac{\partial u_6\left(x;\vec{\xi}\right)}{\partial x}=u_7\left(x;\vec{\xi}\right).$

The constrained optimization problem seeks to minimize:

$$\min_{\vec{\xi}} J\left(\vec{u}(z); \vec{\xi}\right), \quad s.t. \quad \vec{f}\left(z, \vec{u}(z); u_6\left(x; \vec{\xi}\right), u_7\left(x; \vec{\xi}\right)\right) - \frac{d\vec{u}}{dz} = \vec{0},\tag{3}$$

with the loss functional defined as:

$$J(\vec{u}) = \int_{z_0}^{z_T} g(\vec{u}) dz + J_1(\vec{u}(z_T)). \tag{4}$$

The corresponding Lagrangian functional is constructed as:

$$L(\vec{u}, \vec{\lambda}) = J_{1}(\vec{u}(z_{T})) + \int_{z_{0}}^{z_{T}} g(\vec{u}) dz + \int_{z_{0}}^{z_{T}} \vec{\lambda}^{T} \left(\vec{f}(z; \vec{u}, u_{6}, u_{7}) - \frac{d\vec{u}}{dz} \right) dz$$

$$= J_{1}(\vec{u}(z_{T})) + \int_{z_{0}}^{z_{T}} \left[g(\vec{u}) + \vec{\lambda}^{T} \left(\vec{f}(z; \vec{u}, u_{6}, u_{7}) - \frac{d\vec{u}}{dz} \right) \right] dz,$$
(5)

Taking the total derivative with respect to the parameter vector $\vec{\xi}$ yields:

$$\frac{dL}{d\vec{\xi}} = \left. \frac{\partial J_1}{\partial \vec{u}} \frac{d\vec{u}}{d\vec{\xi}} \right|_{z=z_T} + \int_{z_0}^{z_T} \left[\frac{\partial g}{\partial \vec{u}} \frac{d\vec{u}}{d\vec{\xi}} + \vec{\lambda}^T \left(\frac{\partial \vec{f}}{\partial \vec{u}} \frac{d\vec{u}}{d\vec{\xi}} + \frac{\partial \vec{f}}{\partial u_6} \frac{du_6}{d\vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7} \frac{du_7}{d\vec{\xi}} - \frac{d}{d\vec{\xi}} \left(\frac{d\vec{u}}{dz} \right) \right) \right] dz, \tag{6}$$

where $\frac{\partial \vec{f}}{\partial \vec{u}} = \begin{bmatrix} \frac{\partial \vec{f}}{\partial u_1} & \frac{\partial \vec{f}}{\partial u_2} & \frac{\partial \vec{f}}{\partial u_3} & \frac{\partial \vec{f}}{\partial u_4} & \frac{\partial \vec{f}}{\partial u_5} \end{bmatrix}$, $\frac{\partial u_6}{\partial \xi} = \begin{bmatrix} \frac{\partial u_6}{\partial \xi_1} & \frac{\partial u_6}{\partial \xi_2} & \cdots & \cdots & \frac{\partial u_6}{\partial \xi_p} \end{bmatrix}^T$ and other terms follow analogously. Applying integration by parts to the term $\frac{d}{d\vec{\xi}} \left(\frac{d\vec{u}}{dz} \right)$:

$$\int_{z_0}^{z_T} -\vec{\lambda}^T \frac{d}{d\vec{\xi}} \left(\frac{d\vec{u}}{dz} \right) dz = \int_{z_0}^{z_T} -\vec{\lambda}^T \frac{d}{dz} \left(\frac{d\vec{u}}{d\vec{\xi}} \right) dz = -\left[\vec{\lambda}^T \frac{d\vec{u}}{d\vec{\xi}} \right]_{z_0}^{z_T} + \int_{z_0}^{z_T} \left(\frac{d\vec{\lambda}}{dz} \right)^T \frac{d\vec{u}}{d\vec{\xi}} dz$$

$$= \left(\vec{\lambda} (z_0) \right)^T \frac{d\vec{u}}{d\vec{\xi}} \Big|_{z=z_0} - \left(\vec{\lambda} (z_T) \right)^T \frac{d\vec{u}}{d\vec{\xi}} \Big|_{z=z_T} + \int_{z_0}^{z_T} \left(\frac{d\vec{\lambda}}{dz} \right)^T \frac{d\vec{u}}{d\vec{\xi}} dz = -\left(\vec{\lambda} (z_T) \right)^T \frac{d\vec{u}}{d\vec{\xi}} \Big|_{z=z_T} + \int_{z_0}^{z_T} \left(\frac{d\vec{\lambda}}{dz} \right)^T \frac{d\vec{u}}{d\vec{\xi}} dz. \tag{7}$$

where we assume $\left.\frac{d\vec{t}}{d\vec{\xi}}\right|_{z=z_0}=\vec{0}$ due to initial condition independence.

Substituting equation (7) into (6) yields:

$$\frac{dL}{d\vec{\xi}} = \frac{\partial J_1}{\partial \vec{u}} \frac{d\vec{u}}{d\vec{\xi}} \Big|_{z=z_T} + \int_{z_0}^{z_T} \left[\frac{\partial g}{\partial \vec{u}} \frac{d\vec{u}}{d\vec{\xi}} + \vec{\lambda}^T \left(\frac{\partial \vec{f}}{\partial \vec{u}} \frac{d\vec{u}}{d\vec{\xi}} + \frac{\partial \vec{f}}{\partial u_6} \frac{\partial u_6}{\partial \vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7} \frac{\partial u_7}{\partial \vec{\xi}} \right) + \left(\frac{d\vec{\lambda}}{dz} \right)^T \frac{d\vec{u}}{d\vec{\xi}} \Big|_{z=z_T} \\
= \int_{z_0}^{z_T} \left[\left[\frac{\partial g}{\partial \vec{u}} + \vec{\lambda}^T \frac{\partial \vec{f}}{\partial \vec{u}} + \left(\frac{d\vec{\lambda}}{dz} \right)^T \right] \frac{d\vec{u}}{d\vec{\xi}} + \vec{\lambda}^T \left(\frac{\partial \vec{f}}{\partial u_6} \frac{\partial u_6}{\partial \vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7} \frac{\partial u_7}{\partial \vec{\xi}} \right) \Big|_{z=z_T} dz + \left(\frac{\partial J_1}{\partial \vec{u}} - \left(\vec{\lambda} (z_T) \right)^T \right) \frac{d\vec{u}}{d\vec{\xi}} \Big|_{z=z_T}, \tag{8}$$

To address the computational challenges posed by $\frac{d\vec{u}}{d\vec{\xi}}$ and $\frac{d\vec{u}}{d\vec{\xi}}\Big|_{z=z_T}$ in (8), we enforce the adjoint system:

$$\begin{cases} \frac{\partial g}{\partial \vec{u}} + \vec{\lambda}^T \frac{\partial \vec{f}}{\partial \vec{u}} + \left(\frac{d\vec{\lambda}}{dz}\right)^T = \vec{0}, \\ \vec{\lambda}(z_T) = \frac{\partial J_1}{\partial \vec{u}}(z_T). \end{cases}$$
(9)

It yields the simplified sensitivity expression through the equivalence $\frac{dL}{d\vec{\xi}} = \frac{dJ}{d\vec{\xi}}$:

$$\frac{dJ}{d\vec{\xi}} = \int_{z_0}^{z_T} \vec{\lambda}^T \left(\frac{\partial \vec{f}}{\partial u_6} \frac{\partial u_6}{\partial \vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7} \frac{\partial u_7}{\partial \vec{\xi}} \right) dz. \tag{10}$$

In summary:

1. Initial value problem: Solve forward

$$\begin{cases} \frac{d\vec{u}}{dz} = f\left(z; \vec{u}, u_6\left(x; \vec{\xi}\right), u_7\left(x; \vec{\xi}\right)\right) \\ \vec{u}\left(z = 1\right) = \vec{u}_0 \end{cases}$$
(11)

This system can be expanded as:

This system is solved by determining u_1 through u_5 via NDSolve, with u_6 and u_7 are provided by the neural network.

2. Terminal value problem: Solve backward

$$\begin{cases} \frac{\partial g}{\partial \vec{u}} + \vec{\lambda}^T \frac{\partial \vec{f}}{\partial \vec{u}} + \left(\frac{d\vec{\lambda}}{dz}\right)^T = \vec{0}, \\ \vec{\lambda} \left(z = z_T = 0\right) = \frac{\partial J_1}{\partial \vec{u}} \left(z_T\right), \end{cases}$$
(13)

for $\vec{\lambda}(z)$.

Now, in detail, we have the following system of equations:

$$\begin{bmatrix}
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5}
\end{bmatrix} + \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda_3 & \lambda_4 & \lambda_5 \end{bmatrix} \begin{bmatrix}
\frac{\partial f_1}{\partial u_1} & \frac{\partial f_1}{\partial u_2} & \frac{\partial f_1}{\partial u_3} & \frac{\partial f_1}{\partial u_4} & \frac{\partial f_1}{\partial u_5} \\
\frac{\partial f_2}{\partial u_1} & \frac{\partial g_2}{\partial u_2} & \frac{\partial g_2}{\partial u_3} & \frac{\partial g_2}{\partial u_4} & \frac{\partial g_2}{\partial u_5}
\end{bmatrix} + \cdots \\
= \begin{bmatrix} \frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_1} & \frac{\partial g}{\partial u_2} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_3} & \frac{\partial g}{\partial u_4} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{\partial u_5} \\
\frac{\partial g}{\partial u_5} & \frac{\partial g}{$$

That is,

$$\frac{\partial g}{\partial u_1} + \left[\lambda_1 \frac{\partial f_1}{\partial u_1} + \lambda_2 \frac{\partial f_2}{\partial u_1} + \dots + \lambda_5 \frac{\partial f_5}{\partial u_1} \right] + \frac{\partial \lambda_1}{\partial z} = 0,$$

$$\frac{\partial g}{\partial u_2} + \left[\lambda_1 \frac{\partial f_1}{\partial u_2} + \lambda_2 \frac{\partial f_2}{\partial u_2} + \dots + \lambda_5 \frac{\partial f_5}{\partial u_2} \right] + \frac{\partial \lambda_2}{\partial z} = 0,$$

$$\vdots$$

$$\frac{\partial g}{\partial u_7} + \left[\lambda_1 \frac{\partial f_1}{\partial u_5} + \lambda_2 \frac{\partial f_2}{\partial u_5} + \dots + \lambda_7 \frac{\partial f_7}{\partial u_5} \right] + \frac{\partial \lambda_5}{\partial z} = 0.$$
(15)

In other words, we can express the system as:

$$\frac{\partial g}{\partial u_i} + \sum_{j=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_i} + \frac{\partial \lambda_i}{\partial z} = 0, \quad i \in [1, 5].$$
 (16)

Finally, the system in (13) becomes:

$$\begin{cases}
\frac{\partial g}{\partial u_i} + \sum_{j=1}^{7} \lambda_j \frac{\partial f_j}{\partial u_i} + \frac{\partial \lambda_i}{\partial z} = 0, \\
\lambda_i (z = 0) = \frac{\partial J_1}{\partial u_i},
\end{cases} \qquad i \in [1, 7]. \tag{17}$$

3. Evaluate

$$\frac{dJ}{d\vec{\xi}} = \int_{z_0}^{z_T} \vec{\lambda}^T \left(\frac{\partial \vec{f}}{\partial u_6} \frac{\partial u_6}{\partial \vec{\xi}} + \frac{\partial \vec{f}}{\partial u_7} \frac{\partial u_7}{\partial \vec{\xi}} \right) dz$$

$$= \int_{1}^{0} \left[\lambda_1 \quad \lambda_2 \quad \lambda_3 \quad \lambda_4 \quad \lambda_5 \right] \left[\begin{bmatrix} \frac{\partial f_1}{\partial u_6} \\ \frac{\partial f_2}{\partial u_6} \\ \frac{\partial f_3}{\partial u_6} \\ \frac{\partial f_3}{\partial u_6} \end{bmatrix} \frac{\partial u_6}{\partial \vec{\xi}} + \begin{bmatrix} \frac{\partial f_1}{\partial u_7} (x; \vec{\xi}) \\ \frac{\partial f_3}{\partial u_7} (x; \vec{\xi}) \\ \frac{\partial f_3}{\partial u_7} (x; \vec{\xi}) \end{bmatrix} \frac{\partial u_7}{\partial \vec{\xi}} dz$$

$$= \int_{1}^{0} \left[\left(\sum_{i=1}^{5} \lambda_i \frac{\partial f_i}{\partial u_6} \right) \frac{\partial u_6}{\partial \vec{\xi}} + \left(\sum_{i=1}^{5} \lambda_i \frac{\partial f_i}{\partial u_7} (x; \vec{\xi}) \right) \frac{\partial u_7}{\partial \vec{\xi}} (x; \vec{\xi}) \right] dz$$

$$= \int_{1}^{0} \left[\left(\sum_{i=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_6} \right) \frac{\partial u_6}{\partial \vec{\xi}} + \left(\sum_{i=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_7} (x; \vec{\xi}) \right) \frac{\partial u_7}{\partial \vec{\xi}} (x; \vec{\xi}) \right] dz$$

$$= \int_{1}^{0} \left[\left(\sum_{i=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_6} \right) \frac{\partial u_6}{\partial \vec{\xi}} + \left(\sum_{i=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_7} (x; \vec{\xi}) \right) \frac{\partial u_7}{\partial \vec{\xi}} (x; \vec{\xi}) \right] dz$$

$$= \int_{1}^{0} \left[\left(\sum_{i=1}^{5} \lambda_i \frac{\partial f_j}{\partial u_6} \right) \frac{\partial u_6}{\partial \vec{\xi}} + \left(\sum_{i=1}^{5} \lambda_j \frac{\partial f_j}{\partial u_7} (x; \vec{\xi}) \right) \frac{\partial u_7}{\partial \vec{\xi}} (x; \vec{\xi}) \right] dz$$

2 Implement

To solve this problem using a system of first-order differential equations, we introduce auxiliary variables $\Phi_2(z)$ and $G_2(z)$, defined as $\Phi_2(z) = \Phi'(z)$ and $G_2(z) = G'(z)$, respectively. Consequently, $\vec{\Theta}(z)$ can be expressed as:

$$\vec{\Theta}(z) = \begin{bmatrix} \Phi_{2}(z) \\ G_{2}(z) \\ \Phi(z) \\ G(z) \\ \Sigma(z) \\ F(z) \end{bmatrix} = \begin{bmatrix} u_{1}(z) \\ u_{2}(z) \\ u_{3}(z) \\ u_{4}(z) \\ u_{5}(z) \\ u_{6}(z) \end{bmatrix} = \vec{u}(z),$$
(19)

with the system dynamics:

$$\frac{d\vec{\Theta}(z)}{dz} = \begin{bmatrix}
\frac{d}{dz}\Phi_{2}(z) \\
\frac{d}{dz}G_{2}(z) \\
\frac{d}{dz}\Phi(z) \\
\frac{d}{dz}G(z) \\
\frac{d}{dz}E(z) \\
\frac{d}{dz}E(z) \\
\frac{d}{dz}E(z)
\end{bmatrix} = \vec{f}(\vec{u}; u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) = \begin{bmatrix}
f_{1}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{2}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{3}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{4}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{5}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{5}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{6}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi}))
\end{bmatrix}, (20)$$

where $u_7\left(x;\vec{\xi}\right)=\widehat{Z}\left(z\Phi\left(z\right);\vec{\xi}\right)$ with $x=z\Phi\left(z\right),$ and assume that $\frac{\partial u_7\left(x;\vec{\xi}\right)}{\partial x}=u_8\left(x;\vec{\xi}\right).$

1. Solve forward

$$\begin{bmatrix}
\frac{du_{1}}{dz} \\
\frac{du_{2}}{dz} \\
\frac{du_{3}}{dz} \\
\frac{du_{4}}{dz} \\
\frac{du_{5}}{dz} \\
\frac{du_{6}}{dz}
\end{bmatrix} = \begin{bmatrix}
f_{1}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{2}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{3}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{4}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{5}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi})) \\
f_{6}(z; \vec{u}, u_{7}(x; \vec{\xi}), u_{8}(x; \vec{\xi}))
\end{bmatrix}, (21)$$

with the initial values:

$$\begin{bmatrix} u_{1}(z=1) \\ u_{2}(z=1) \\ u_{3}(z=1) \\ u_{4}(z=1) \\ u_{5}(z=1) \\ u_{6}(z=1) \end{bmatrix} = \begin{bmatrix} u_{10} \\ u_{20} \\ u_{30} \\ u_{40} \\ u_{50} \\ u_{60} \end{bmatrix}.$$
 (22)

The system will be solved using NDSolve, with u_7 and u_8 are provided by the neural network.

2. Solve backward

$$\begin{cases}
\frac{\partial \lambda_{i}}{\partial z} + \sum_{j=1}^{6} \lambda_{j} \frac{\partial f_{j}}{\partial u_{i}} + \frac{\partial g}{\partial u_{i}} = 0, \\
\lambda_{i}(z=0) = \frac{\partial J_{1}}{\partial u_{i}},
\end{cases} (23)$$

for λ_i , $i \in [1, 6]$.

3. Evaluate

$$\frac{dJ}{d\vec{\xi}} = \int_{1}^{0} \left[\left(\sum_{j=1}^{8} \lambda_{j} \frac{\partial f_{j}}{\partial u_{7}(x; \vec{\xi})} \right) \frac{\partial u_{7}(x; \vec{\xi})}{\partial \vec{\xi}} + \left(\sum_{j=1}^{8} \lambda_{j} \frac{\partial f_{j}}{\partial u_{8}(x; \vec{\xi})} \right) \frac{\partial u_{8}(x; \vec{\xi})}{\partial \vec{\xi}} \right] dz. \tag{24}$$

```
NDSolve[((class["$2eom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Geom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Geom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Geom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Geom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eeom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B → class["B"]) == 0 // SetAccuracy[#, 100] &, (class["Eoom"] /. B
```

Fig. 1: Incomplete codes for (21).

Fig. 2: Incomplete codes for (23).

```
class["zlist"] = Table[i, {i, 1/100, 99/100, 1/1000}];
class["dz"] = 1 / 1000;
(*实际上Z函数及其导数里面的参数总是z Φ[z], 所以做出z Φ[z]的表格以供神经网络使用*)
 class["zint_pd_list"] = \textbf{Table}[backequ["zint'"] \ /. \ z \rightarrow class["zlist"] \ [i]] \ /. \ class["backfun"] \ /. \ class["date_IRtoUV"] \ /. \ B \rightarrow class["B"], 
  {i, 1, Length[class["zlist"]]}];
class["zint_pd_2_list"] = Table[backequ["zint''"] /. z → class["zlist"][i]] /. class["backfun"] /. class["date_IRtoUV"] /. B → class["B"],
  {i, 1, Length[class["zlist"]]}];
 {\tt class["nn_B"] = class["dz"] \times Sum[backequ["B"] /. z \rightarrow class["zlist"][i]] /. class["backfun"] /. class["date_IRtoUV"] /. B \rightarrow class["B"], } 
   {i, 1, Length[class["zlist"]]}];
(*反向传播到神经网络*)
Module[{nni}, For[nni = 1, nni ≤ Length[class["zlist"]], nni++,
  (*这里将z的导数导数通过1/10000的步长拆分成z函数进行反向传播*)
  zintforward1[class["nn_zlist"][[nni]]];
 class["g"] = class["zint_pd_list"] [[nni]] - 1000 class["zint_pd_2_list"] [[nni]];
  class["g"] = class["dz"] x class["g"];
 Gnet["back"][class["g"]];
  addGnet["func"];
  zintforward1[class["nn_zlist"][nni] + 1 / 1000];
 class["g"] = 1000 class["zint_pd_2_list"][nni];
  class["g"] = class["dz"] x class["g"];
```

Fig. 3: Incomplete codes for (24).