Solutions to Worksheet 1

Exercise 1:

- A Hamiltonian function is a map $H : \mathbb{R}^{2d} \mapsto \mathbb{R},\ z = (p, q) \mapsto H(z)$. Consequently, the gradient of H satisfies

$$\nabla_z H : \mathbb{R}^{2d} \mapsto \mathbb{R}^{2d},\ z \mapsto \begin{pmatrix} \partial_p H(z) \\ \partial_q H(z) \end{pmatrix}. \tag{0.1}$$

  Note that $p, q \in \mathbb{R}^d$ and thus $\partial_p H(z) = \begin{pmatrix} \partial_{p_1} H(z) \\ \vdots \\ \partial_{p_n} H(z) \end{pmatrix}$ resp. $\partial_q H(z) = \begin{pmatrix} \partial_{q_1} H(z) \\ \vdots \\ \partial_{q_n} H(z) \end{pmatrix}$.
  The associated Hamiltonian system is defined as $\dot{z} = \Omega^{-1}\nabla_z H(z)$ and $z(0) = z_0$. To show that the Hamiltonian flow of such a system is volume preserving we now calculate the divergence of the right hand side,

$$\text{div}[\Omega^{-1}\nabla_z H](z) = \text{div}[\begin{pmatrix} -\partial_q H(z) \\ \partial_p H(z) \end{pmatrix}]. \tag{0.2}$$

  Using the definition $\text{div}[f](x) = \sum_{i=1}^n \frac{\partial f_i}{\partial x_i}(x)$ we find

$$\begin{aligned} \text{div}[\Omega\nabla_z H](z) &= \sum_{i=1}^n \frac{\partial(-\partial q_i H)}{\partial_{p_i}}(z) + \sum_{i=1}^n \frac{\partial(\partial p_i H)}{\partial_{q_i}}(z) && (0.3)\\ &= \sum_{i=1}^n (-\partial_{p_i}\partial_{q_i} H(z) + \partial_{q_i}\partial_{p_i} H(z)) && (0.4)\\ &= 0 && (0.5) \end{aligned}$$

  since partial derivatives interchange if they are continuous due to Schwarz' theorem.

- Another way to show volume conservation is to use the Hamiltonian flow $\Phi_t : \mathbb{R}^{2d} \mapsto \mathbb{R}^{2d},\ z_0 \mapsto \Phi_t(z_0) = z(t, z_0)$ that is defined via the solution $z(t)$ of the Hamiltonian system.
  The flow map of a Hamiltonian system is always symplectic, see for example $LR, Theorem$ 1. The proof is based on the fact that $\partial_t \Phi_t = \Omega^{-1}\nabla_z H(z)$ and $\partial_z \Phi_0 = \text{Id}$.
  Recall that a map $\Psi : \mathbb{R}^d \mapsto \mathbb{R}^d$ is called symplectic, if its Jacobian $\Psi_x \in \mathbb{R}^{d\times d}$ satisfies $\Psi_x^T \Omega \Psi_x = \Omega$. In particular, every symplectic map Ψ satisfies $|\det(\Psi_x)| = 1$, since $\det(\Omega) = 1$ and thus

$$\det(\Psi_x^T \Omega \Psi_x) = \det(\Psi_x)^2 \det(\Omega) = 1.$$

  It suffices to use this implication to proof volume preservation.
  The volume of any domain $V \subset \mathbb{R}^{2d}$ is given by

$$\text{vol } V = \int_V 1 \ dz = \int_{\mathbb{R}^{2d}} \mathbf{1}_V(z) \ dz \tag{0.6}$$

where $\mathbf{1}_V$ denotes the indicator function of V, $\mathbf{1}_V(z) = \begin{cases} 1 & \text{for } z \in V \\ 0 & \text{else} \end{cases}$. Then the transported volume satisfies

$$\text{vol } \Phi_t(V) = \int_{\Phi_t(V)} 1 \, dz = \int_V 1 \cdot |\det(\partial_z \Phi_t)| \, dz. \tag{0.7}$$

So the volume is preserved if and only if $|\det(\partial_z \Phi_t)| = 1$, what holds true for the symplectic flow Φ_t.

- As a last step we give an example for a transform that is volume preserving but not symplectic. We choose as an easy example a linear map $f : \mathbb{R}^{2d} \mapsto \mathbb{R}^{2d}, \; z \mapsto Az$ where A is a square $2d \times 2d$-matrix. In this case

$$\text{div}[f] = \text{tr}(A) \tag{0.8}$$

and f being symplectic is equivalent to

$$A^T \Omega A = \Omega. \tag{0.9}$$

So we can choose any matrix A that has trace zero, but does not satisfy (0.9).
Take for example $d = 1$ and $A = \begin{pmatrix} 1 & 2 \\ 2 & -1 \end{pmatrix}$. Then, $f : \mathbb{R}^2 \mapsto \mathbb{R}^2, \; (x, y) \mapsto \begin{pmatrix} x + 2y \\ 2x - y \end{pmatrix}$. $\text{tr}(A) = 1 - 1 = 0$, but

$$A^T \Omega A = \begin{pmatrix} 0 & -5 \\ 5 & 0 \end{pmatrix}. \tag{0.10}$$

Exercise 3:

1. We start with differentiating the midpoint rule with respect to z^n. Let ∂_2 denote the derivative w.r.t. the second component. Then,

$$\frac{\partial z^{n+1}}{\partial z^n} = \text{Id} + h \cdot \frac{1}{2}\left(\frac{\partial z^n}{\partial z^n} + \frac{\partial z^{n+1}}{\partial z^n}\right)\partial_2 f\left(t_n + \frac{h}{2}, \frac{z^{n+1} + z^n}{2}\right) \tag{0.11}$$

$$\frac{\partial z^{n+1}}{\partial z^n} = \text{Id} + \frac{h}{2}\left(\text{Id} + \frac{\partial z^{n+1}}{\partial z^n}\right)\partial_2 f\left(t_n + \frac{h}{2}, \frac{z^{n+1} + z^n}{2}\right). \tag{0.12}$$

Moreover, we have $\partial_2 f(t, z) = \Omega^{-1} D^2 H(z)$ since the second component of f should approximate the change in the z value given by the Hamiltonian system and thus,

$$\frac{\partial z^{n+1}}{\partial z^n} = \text{Id} + \frac{h}{2}\left(\text{Id} + \frac{\partial z^{n+1}}{\partial z^n}\right)\Omega^{-1} D^2 H\left(\frac{z^{n+1} + z^n}{2}\right). \tag{0.13}$$

Introducing the notation $A := \frac{h}{2} D^2 H(\frac{z^{n+1}+z^n}{2})$ we end up with

$$\frac{\partial z^{n+1}}{\partial z^n} = \text{Id} + \left(\text{Id} + \frac{\partial z^{n+1}}{\partial z^n}\right)\Omega^{-1} A, \tag{0.14}$$

$$\frac{\partial z^{n+1}}{\partial z^n} = \text{Id} - \Omega A - \frac{\partial z^{n+1}}{\partial z^n}\Omega A \tag{0.15}$$

$$\frac{\partial z^{n+1}}{\partial z^n}(\text{Id} + \Omega A) = \text{Id} - \Omega A \tag{0.16}$$

and finally

$$\frac{\partial z^{n+1}}{\partial z^n} = (\mathrm{Id} - \Omega A)(\mathrm{Id} + \Omega A)^{-1} \tag{0.17}$$

2. On the one hand, we know from our first calculation that

$$X = (\mathrm{Id} - \Omega A)(\mathrm{Id} + \Omega A)^{-1} = -\Omega(A+\Omega)(\Omega(A-\Omega))^{-1} \tag{0.18}$$
$$= -\Omega(A+\Omega)(A-\Omega)^{-1}\Omega^{-1} = \Omega(A+\Omega)(A-\Omega)^{-1}\Omega. \tag{0.19}$$

   Using the hint and commuting the two factors we find on the other hand

$$X = (\mathrm{Id} + \Omega A)^{-1}(\mathrm{Id} - \Omega A) = (\Omega(A-\Omega))^{-1}\Omega^{-1}(A+\Omega) \tag{0.20}$$
$$= (A-\Omega)^{-1}\Omega^{-1}\Omega^{-1}(A+\Omega) = -(A-\Omega)^{-1}(A+\Omega). \tag{0.21}$$

   Note that $\Omega^{-1} = -\Omega$ and $\Omega\Omega = -\mathrm{Id}$.

3. We start with the second representation of X to show that

$$X^T = -(A+\Omega)^T(A-\Omega)^{-T} = -(A-\Omega)(A+\Omega)^{-1} \tag{0.22}$$

   since $A^T = A$ (note that Hessian matrices are symmetric) and $\Omega^T = -\Omega$ due to definition. Inserting this and the first representation of X into the symplecticity condition leads to

$$X^T\Omega X = -(A-\Omega)(A+\Omega)^{-1}\Omega\Omega(A+\Omega)(A-\Omega)^{-1}\Omega \tag{0.23}$$
$$= (A-\Omega)(A+\Omega)^{-1}(A+\Omega)(A-\Omega)^{-1}\Omega \tag{0.24}$$
$$= (A-\Omega)(A-\Omega)^{-1}\Omega \tag{0.25}$$
$$= \Omega. \tag{0.26}$$