Appendix B

Invariant Regions

B.1 Definition

Definition B.1 ([6], page 12) *Let Σ be a domain enclosed by a simple curve*[1] *$\partial\Sigma$ in the phase space. Then Σ is an invariant set for the two-component system*

$$\begin{aligned} \frac{du}{dt} &= \mathbf{f}(u,v)\,, \\ \frac{dv}{dt} &= \mathbf{g}(u,v)\,. \end{aligned} \tag{B.1}$$

if any solution of the system with initial conditions in Σ remains in Σ for all $t > 0$. (This definition generalises to higher dimensional phase spaces in the obvious way.)

Lemma B.1 ([6], page 12) *If*

$$\mathbf{f}(\mathbf{u}) \cdot \mathbf{n}(\mathbf{u}) < 0 \tag{B.2}$$

for all $\mathbf{n}(\mathbf{u}) \in \partial\Sigma$, where $\mathbf{n}(\mathbf{u})$ is the unit outward normal at $\mathbf{u} \in \partial\Sigma$, then Σ is an invariant set. (If $\mathbf{f}$ and σ are sufficiently smooth, this may be extended to $\mathbf{f} \cdot \mathbf{n} \leq 0$.)

Proof $\mathbf{f} \cdot \mathbf{n} = \dot{\mathbf{u}} \cdot \mathbf{n} < 0$. But $\dot{\mathbf{u}}$ points along the solution trajectory of (B.1) and therefore this trajectory points to the interior of Σ. Thus, no trajectory may leave Σ, and Σ is invariant. □

Lemma B.1 can be applied to domains containing points where $\mathbf{f} \cdot \mathbf{n} = 0$ or where the normal vector $\mathbf{n}$ is undefined provided that at these points the direction of the derivative vector does not point out of the invariant set.

In many practical problems there is a restriction that $u \geq 0$ and $v \geq 0$. For example, the concentrations of a chemical or a population denisty can not become negative. For such systems the positive quadrant must be invariant. This situation is shown in figure B.1 along with the corresponding outward normal vectors. Along the line $(u, 0)$ the unit outward normal is $(0, -1)$ and we must show that $-g(u, 0) < 0$. Similarly along the line $(0, v)$ the unit outward normal is $(-1, 0)$ and thus we must show that $-f(0, u) < 0$. At the corner point of the positive quadrant, $(u, v) = (0, 0)$, the unit outward normal vector is undefined. At this point we must show that the derivative vector does not point out of the positive quadrant 'by hand'.

Example B.1 ([11]) *Show that the rectangle defined by $\left(0 \leq S^* \leq 1 + \frac{E_0^*}{q^* S_0^*}, 0 \leq \theta_S \leq 1\right)$, is invariant for the*

[1] A curve is simple if it does not cross itself.

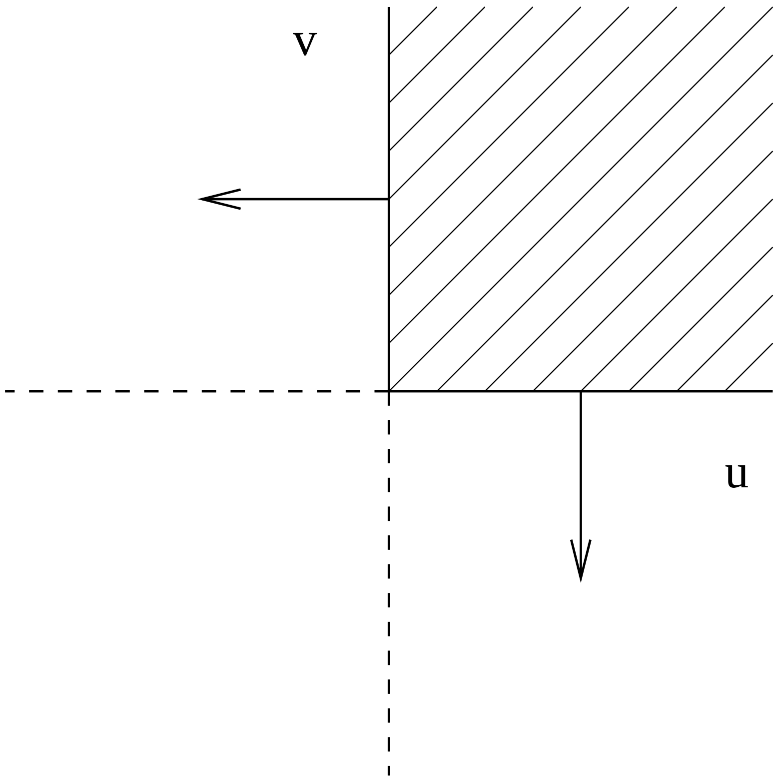

Figure B.1: The unit outward normals when the postive quadrant ($u \geq 0$, $v \geq 0$) is invariant.

system

$$\frac{dS^*}{dt^*} = q^* \left(1 - S^*\right) + \frac{E_0^*}{S_0^*}\theta_S - E_0^* \left(1 - \theta_S\right) S^*, \tag{B.3}$$

$$\frac{d\theta_S}{dt^*} = S_0^* \left(1 - \theta_S\right) S^* - \left(1 + k_2^*\right) \theta_S. \tag{B.4}$$

You may assume that the parameters (E_0^*, k_2^*, q^*, S_0^*) are strictly positive.

Proof We must confirm that $\mathbf{f} \cdot \mathbf{n} = \dot{\mathbf{u}} \cdot \mathbf{n} < 0$ along the four sides of the invariant region and check the direction of the derivative vector at the four corner points of the invariant region.

Edge 1. Consider the edge $0 \leq S^* \leq 1 + \frac{E_0^*}{q^* S_0^*}$ with $\theta_S = 0$. The unit outward normal is the vector $(0, -1)$ and we have

$$\begin{aligned} \mathbf{f}\left(\mathbf{u}\right) \cdot \mathbf{n}\left(\mathbf{u}\right) &= -S_0^* \left(1 - \theta_S\right) S^* + \left(1 + k_2^*\right) \theta_S, \\ &= -S_0 S^* \quad \text{as } \theta_S = 0 \text{ by assumption,} \\ &< 0 \quad \text{by assumption that } S^* \geq 0 \text{ except at the point } S^* = 0 \end{aligned}$$

Note that lemma B.1 fails at the point $(S^*, \theta_S) = (0.0)$ — one of the four corner points.

Edge 2. Consider the edge $S^* = 0$ with $0 \leq \theta_S \leq 1$.

Left for the student to do.

Edge 3 Consider the edge $0 \leq S^* \leq 1 + \frac{E_0^*}{q^* S_0^*}$ with $\theta_S = 1$. The unit outward normal is the vector $(0, 1)$ and we have

$$\begin{aligned} \mathbf{f}\left(\mathbf{u}\right) \cdot \mathbf{n}\left(\mathbf{u}\right) &= S_0^* \left(1 - \theta_S\right) S^* - \left(1 + k_2^*\right) \theta_S, \\ &= -\left(1 + k_2^*\right) \quad \text{as } \theta_S = 1 \text{ by assumption,} \\ &< 0 \quad \text{by assumption that } k_2^* > 0 \end{aligned}$$

Edge 4. Consider the edge $S^* = 1 + \dfrac{E_0^*}{q^* S_0^*}$ with $0 \leq \theta_S \leq 1$.

Left for the student to do.

Point 1. Consider the direction of the derivative vector at the point $(S^*, \theta_S) = (0, 0)$. At this point we have

$$\left(\dot{S^*}, \dot{\theta_S}\right) = (q^*, 0)$$

which points along the boundary of the invariant set. Thus it does not point out of the invariant set.

Point 2. Consider the direction of the derivative vector at the point $(S^*, \theta_S) = (0, 1)$.

Left for the student to do.

Point 3. Consider the direction of the derivative vector at the point $(S^*, \theta_S) = \left(1 + \frac{E_0^*}{q^* S_0^*}, 1\right)$. At this point we have

$$\left(\dot{S^*}, \dot{\theta_S}\right) = (0, -1 - k_2^*)$$

which points along the boundary of the invariant set. Thus it does not point out of the invariant set.

Point 4. Consider the direction of the derivative vector at the point $(S^*, \theta_S) = \left(1 + \dfrac{E_0^*}{q^* S_0^*}, 0\right)$.

Left for the student to do. □

Question B.1 *Complete the proof of example B.1 by considering edges 2 & 4 and points 2 & 4.*