Exercise 2.3.2

(Autocatalysis) Consider the model chemical reaction

$$A + X \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} 2X$$

in which one molecule of X combines with one molecule of A to form two molecules of X. This means that the chemical X stimulates its own production, a process called *autocatalysis*. This positive feedback process leads to a chain reaction, which eventually is limited by a "back reaction" in which $2X$ returns to $A + X$.

According to the *law of mass action* of chemical kinetics, the rate of an elementary reaction is proportional to the product of the concentrations of the reactants. We denote the concentrations by lowercase letters $x = [X]$ and $a = [A]$. Assume that there's an enormous surplus of chemical A, so that its concentration a can be regarded as constant. Then the equation for the kinetics of x is

$$\dot{x} = k_1 a x - k_{-1} x^2$$

where k_1 and k_{-1} are positive parameters called *rate constants*.

a) Find all the fixed points of this equation and classify their stability.

b) Sketch the graph of $x(t)$ for various initial values x_0.

Solution

The concentration of X is governed by

$$\dot{x} = k_1 a x - k_{-1} x^2.$$

Fixed points occur where $\dot{x} = 0$.

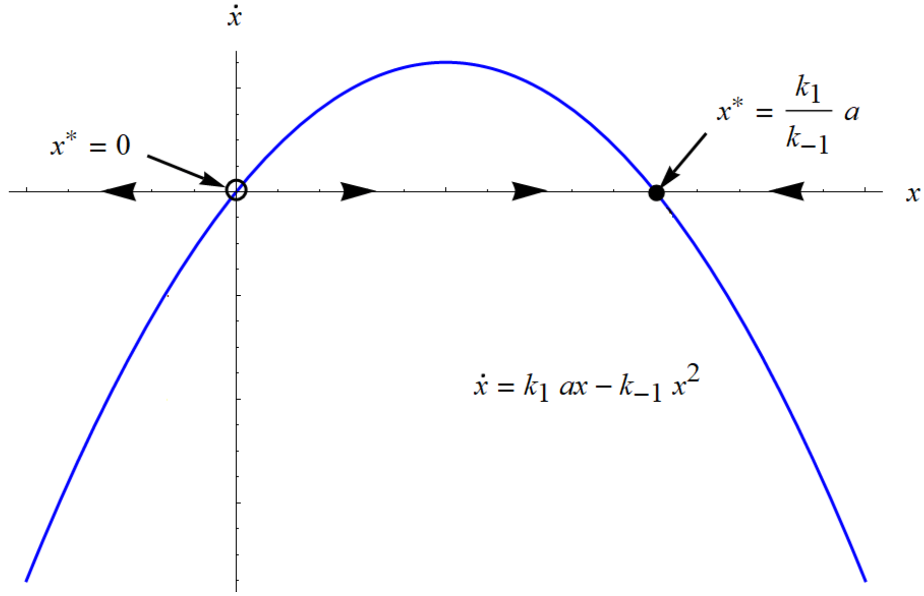
$$k_1 a x^* - k_{-1} x^{*2} = 0$$

$$x^*(k_1 a - k_{-1} x^*) = 0$$

$$x^* = 0 \quad \text{or} \quad k_1 a - k_{-1} x^* = 0$$

$$x^* = 0 \quad \text{or} \quad x^* = \frac{k_1}{k_{-1}} a$$

Plot $\dot{x}$ versus x in order to determine the stability of these fixed points.



When the function is negative the flow is to the left, and when the function is positive the flow is to the right. Therefore,

$$x^* = 0 \text{ is locally unstable.}$$

$$x^* = \frac{k_1}{k_{-1}} a \text{ is locally stable.}$$

Below is a qualitative sketch of x versus t for various initial conditions.