

MAS212 Scientific Computing and Simulation

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Today's lecture

- Scientific computing modules:
 - numpy
 - matplotlib
 - **scipy**
- **Differential equations:**
Phase diagrams; equilibria; limit cycles.
- **Non-linear ODEs:** 3 examples:
 - 1 Logistic equation (1D)
 - 2 Predator-prey equation (2D autonomous conservative)
 - 3 van der Pol equation (2nd-order)

SciPy

What is SciPy?

SciPy is a collection of mathematical algorithms and convenience functions built on the Numpy extension of Python.

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> import scipy as sp
```

- Tutorial:

<http://docs.scipy.org/doc/scipy-dev/reference/tutorial/index.html>

- Various useful modules in the `scipy` package:
 - `sp.special` : special functions (Bessel, Legendre, Hypergeometric, etc).
 - `sp.integrate` : for integrating functions and sets of ODEs
 - `sp.optimize` : curve fitting, minimization, etc.
 - `sp.interpolate` : interpolation, splines, etc.
 - `sp.fftpack` : Fourier transforms.
 - `sp.linalg` : Linear algebra.
- We will solve differential equations with `scipy.integrate.odeint`

Ordinary differential equations

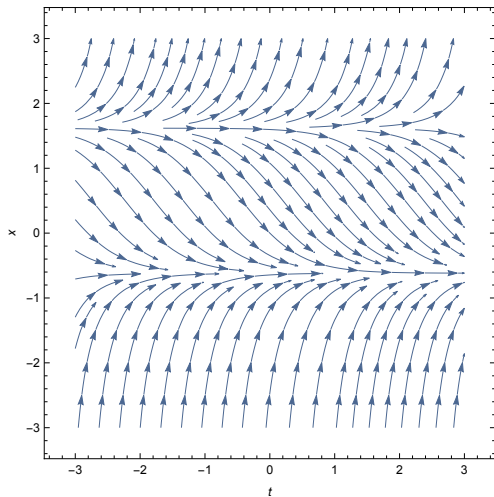
- Here is an example of an **ordinary differential equation** (ODE):

$$\frac{dx}{dt} = x^2 - x - 1$$

- x is the dependent variable, and t is the **independent** variable.
- a specific solution $x(t)$ is an **integral curve** of the ODE.
- to find an integral curve, we specify an **initial condition**, e.g.

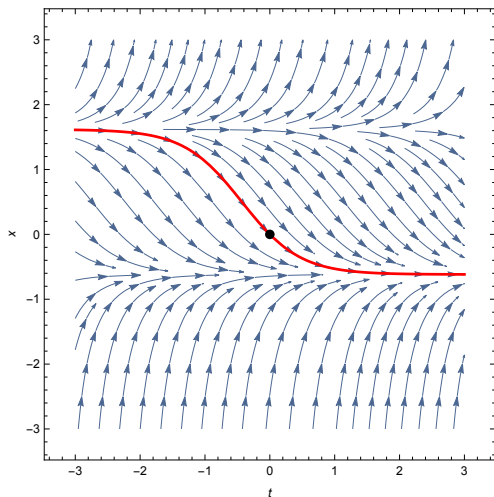
$$x(t = 0) = 3$$

Ordinary differential equations



- Here is the gradient field $\frac{dx}{dt}$ at each point in the flow

Ordinary differential equations



- Here is an **integral curve** with initial condition $x(0) = 0$

Ordinary differential equations (ODEs)

- ODEs have **one** independent variable, t say
- There may be several dependent variables
 $x_i = \{x_1(t), x_2(t), \dots\}$.
- A set of functions F_j relating x and its derivatives,

$$F_j(x_i, \dot{x}_i, \ddot{x}_i, \dots; t) = 0$$

where $\dot{x}_i = \frac{dx_i}{dt}$, $\ddot{x}_i = \frac{d^2x_i}{dt^2}$, etc.

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- **Order** refers to highest derivative: k th order $\Leftrightarrow \frac{d^k x}{dt^k}$
- **Dimension** refers number of dependent variables $\mathbf{x} = [x_1 \dots x_d]$, and the number of independent equations.
- **Autonomous** $\Leftrightarrow F_j$ have no explicit dependence on t
- **Linear** if F_j has only linear dependence on x_i, \dot{x}_i, \dots and their combinations. Otherwise it is **non-linear**.
- **Linear** \Rightarrow superposition principle \Rightarrow 'Easy'.

Ordinary differential equations

$$\frac{dx}{dt} = x^2 - x - 1$$

This example is ...

- ... **first-order**, as dx/dt is the highest derivative
- ... **one-dimensional**, as x is the only dependent variable
- ... **autonomous**, as the rate of change dx/dt does not depend on the independent variable t
- ... **non-linear**, because of the non-linear term x^2 on the right-hand side.

1D autonomous equation

- Consider the 1st-order autonomous case:

$$\boxed{\frac{dx}{dt} = f(x)}$$

- Solution typically found by **separation of variables**
- Divide by $f(x)$ and integrate

$$\int \frac{dx}{f(x)} = t + c$$

- Some cases can be solved exactly, e.g.,

$$f(x) = x \quad \Rightarrow \ln(x) = t + c \quad \Rightarrow x(t) = Ae^t$$

- What if integral can't be found analytically?
- Integrate numerically and invert to find $x(t)$? **No.**
- Numerically solve the differential equation with odeint.

1D autonomous equation: example

- The **Logistic Equation** is a 1st order autonomous ODE:

$$\frac{dx}{dt} = x(1 - x), \quad x(0) = x_0$$

- It has the exact solution (**show**):

$$x(t) = \frac{1}{1 + Ae^{-t}}.$$

(Here $A = 1/x_0 - 1$)

1D autonomous equation: example

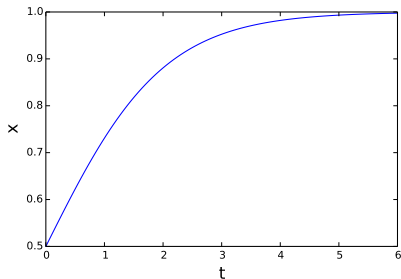
$$\frac{dx}{dt} = x(1 - x), \quad x(0) = x_0$$

```
import matplotlib.pyplot as plt
from scipy.integrate import odeint
def logistic(x, t):
    """dx/dt for the logistic equation"""
    return x*(1 - x)

ts = np.linspace(0.0, 10.0, 100) # values of independent variable
x0 = 0.5 # initial condition, x(0) = x0
xs = odeint(logistic, x0, ts) # integrates the ODE
# 'odeint' returns an array of 'x' values, at the times in ts.
plt.xlabel('t', fontsize=16); plt.ylabel('x', fontsize=16)
plt.plot(ts, xs)
```

1D autonomous equation: example

$$\frac{dx}{dt} = x(1 - x), \quad x(0) = x_0$$



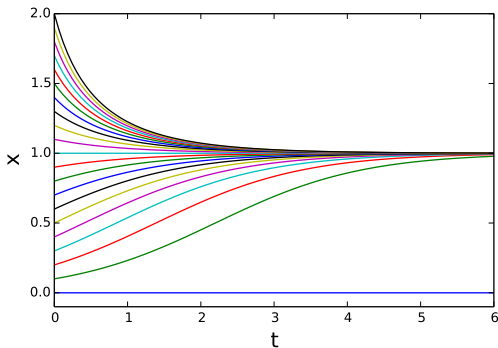
- Here $x_0 = 0.5$. Not very interesting ...
- Let's plot curves for several initial conditions ...

1D autonomous equation: example

$$\frac{dx}{dt} = x(1 - x), \quad x(0) = x_0$$

```
# Plot curves for several initial conditions  
ics = np.arange(0.0, 2.01, 0.1) # a list of initial conditions  
for x0 in ics:  
    xs = odeint(logistic, x0, ts)  
    plt.plot(ts, xs)
```

1D autonomous equation: example



- Two equilibrium positions: $x = 0$ and $x = 1$.
- $x = 0$ is an **unstable** equilibrium
- $x = 1$ is a **stable** equilibrium

2D autonomous equations

- Now consider a first order system with two dependent variables, x and y ,

$$\begin{aligned}\frac{dx}{dt} &= f(x, y; t), \\ \frac{dy}{dt} &= g(x, y; t).\end{aligned}$$

- System is **autonomous** iff f and g do not depend on t
- **Example:** Modelling the populations of rabbits and foxes

2D autonomous equations: example

Predator-prey equations

Also known as *Lotka-Volterra equations*, the predator-prey equations are a pair of coupled first-order non-linear ordinary differential equations.

They represent a simplified model of the change in populations of two species which interact via predation. For example, foxes (predators) and rabbits (prey). Let x and y represent rabbit and fox populations, respectively. Then

$$\begin{aligned}\frac{dx}{dt} &= ax - bxy \\ \frac{dy}{dt} &= -cy + dxy\end{aligned}$$

Here a , b , c and d are parameters, which are assumed to be positive.

Predator-prey equations

$$\frac{dx}{dt} = ax - bxy$$

$$\frac{dy}{dt} = -cy + dxy$$

```
a,b,c,d = 1,1,1,1 # set parameters to 1 for this example
def dx_dt(x, t):
    """Computes rate of change of prey and predator populations.
    x[0] = prey; x[1] = predator population; a,b,c,d = parameters."""
    return [x[0]*(a - b*x[1]), -x[1]*(c - d*x[0])]

ts = np.linspace(0, 12, 100)
x0 = [1.5, 1.0] # initial conditions
xs = odeint(dx_dt, x0, ts)
prey = xs[:,0]
predators = xs[:,1]
```

Predator-prey equations

$$\frac{dx}{dt} = ax - bxy$$

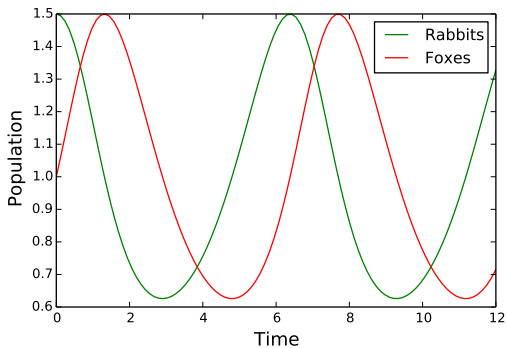
$$\frac{dy}{dt} = -cy + dxy$$

```
# Let's plot 'rabbit' and 'fox' populations as a function of time  
plt.plot(ts, prey, "+", label="Rabbits")  
plt.plot(ts, predators, "x", label="Foxes")  
plt.xlabel("Time", fontsize=14)  
plt.ylabel("Population", fontsize=14)  
plt.legend();
```

Predator-prey equations

$$\frac{dx}{dt} = ax - bxy$$

$$\frac{dy}{dt} = -cy + dxy$$

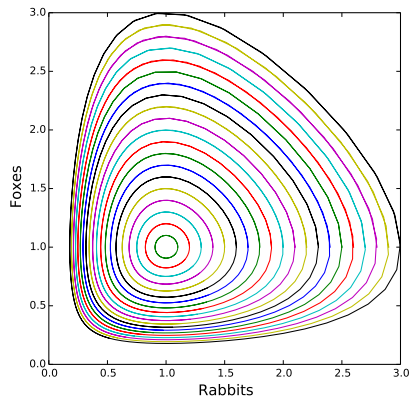


Predator-prey equations: Phase plot

- The ODEs are autonomous: no explicit dependence on t
- **Phase plot:** Plot x vs y (instead of x, y vs t).
- One curve for each initial condition
- Curves will not cross, in general

```
fig = plt.figure()
fig.set_size_inches(6,6) # Square plot, 1:1 aspect ratio
ics = np.arange(1.0, 3.0, 0.1)
for r in ics:
    x0 = [r, 1.0]
    xs = odeint(dx_dt, x0, ts)
    plt.plot(xs[:,0], xs[:,1], "-")
plt.xlabel("Rabbits", fontsize=14)
plt.ylabel("Foxes", fontsize=14)
```

Predator-prey equations: Phase plot



- Curves do not cross
- Closed curves \Leftrightarrow **Periodic** solutions
- Equilibrium at $x = y = 1 \Rightarrow \dot{x} = \dot{y} = 0$

Predator-prey equations: A conservation law

Exercise: Show that h is **constant** along an integral curve of the Lotka-Volterra equations, where

$$h = a \ln y - by + c \ln x - dx$$

$$\frac{dx}{dt} = ax - bxy$$

$$\frac{dy}{dt} = -cy + dxy$$

The Van der Pol oscillator

The (undriven) Van der Pol oscillator is a non-conservative oscillator with non-linear damping, satisfying

$$\ddot{x} - a(1 - x^2)\dot{x} + x = 0$$

- Second-order ODE with one parameter a
 - $|x| > 1$: loses energy
 - $|x| < 1$: absorbs energy
-
- Originally, a model for an electric circuit with a vacuum tube
 - Used to model biological processes such as heart beat, circadian rhythms, biochemical oscillators, and pacemaker neurons.

Van der Pol oscillator

$$\ddot{x} - a(1 - x^2)\dot{x} + x = 0$$

First-order reduction:

Any second-order equation can be written as two coupled first-order equations, by introducing a new variable

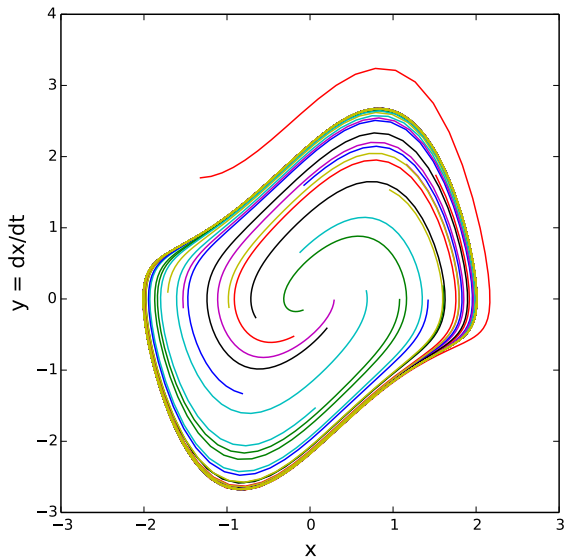
- Let $y = \dot{x}$. Then

$$\begin{aligned}\dot{x} &= y \\ \dot{y} &= a(1 - x^2)y - x\end{aligned}$$

- (Not unique: we could make another choice, such as $z = \dot{x} + x$.)

$$\begin{aligned}\dot{x} &= y \\ \dot{y} &= a(1-x^2)y - x\end{aligned}$$

```
def dx_dt(x, t, a = 1.0):
    return [x[1], a*(1-x[0]**2)*x[1] - x[0]]
def random_ic(scalefac=2.0): # generate initial condition
    return scalefac*(2.0*np.random.rand(2) - 1.0)
ts = np.linspace(0.0, 40.0, 400)
nlines = 20
for ic in [random_ic() for i in range(nlines)]:
    xs = odeint(dx_dt, ic, ts)
    plt.plot(xs[:,0], xs[:,1])
plt.xlabel("x", fontsize=14)
plt.ylabel("y = dx/dt", fontsize=14)
```



- All curves tend towards a **limit cycle**

Van der Pol oscillator: Limit cycles

- Investigate how limit cycle varies with a

```
avals = np.arange(0.2, 2.0, 0.2) # parameters
minpt = int(len(ts) / 2) # look at late-time behaviour
for a in avals:
    xs = odeint(dx_dt, random_ic(), ts)
    plt.plot(xs[minpt:,0], xs[minpt:,1])
```

