Differential equation modelling

S J Eglen

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Outline

1st order: Euler

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y)$$

For a fixed time-step h we Taylor expand to first order.

$$y(x+h) = y(x) + h\frac{\mathrm{d}y}{\mathrm{d}x} + h.o.t.$$

$$y(x+h) = y(x) + hf(x, y)$$

Making time-steps too small could cause accumulation of round-off error (Strogatz).

2nd order: midpoint method

Taylor expand to 2nd order; avoid calculating $f'()$ by chain rule, and equate coefficients.

$$\begin{aligned} k_0 &= hf(x, y(x)) \\ k_1 &= hf(x + h/2, y(x) + \frac{1}{2}k_0) \\ y(x+h) &= y(x) + k_1 \end{aligned}$$

- More evaluations, but better accuracy than Euler.

- Make a guess at an initial step
- Or take principled approach to get family of solvers for different coefficients (4 unknown with 3 equations)

4th order Runge-Kutta formula (fixed step size)

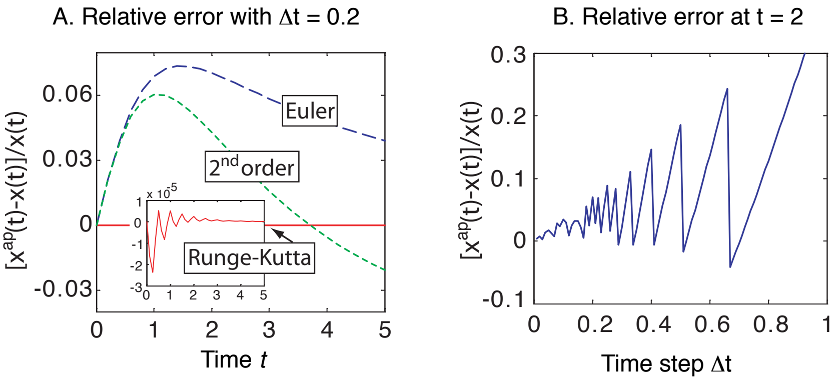
$$
\begin{aligned}
k_0 &= hf(x, y(x)) \\
k_1 &= hf(x + h/2, y(x) + \frac{1}{2}k_0) \\
k_2 &= hf(x + h/2, y(x) + \frac{1}{2}k_1) \\
k_3 &= hf(x + h, y(x) + k_2) \\
y(x + h) &= y(x) + \frac{k_0}{6} + \frac{k_1}{3} + \frac{k_2}{3} + \frac{k_3}{6}
\end{aligned}
$$

- f() may be expensive to compute.
- good trade off: computations performed vs accurary

Comparing solutions on problem with known solution

$$\frac{\mathrm{d}x}{\mathrm{d}t} = t - x + 1 \qquad x(0) = 1$$

$$\Rightarrow x(t) = t + e^{-t}$$



http://web.cs.dal.ca/~tt/fundamentals/figures/Appendices/

Adaptive step size solvers

- Compare accurary of one big jump (x+2h), with two jumps of size h.
- Cost: 11 f() evaluations, compared with 8 f() evaluations for two small jumps; e.g. figure 17.2.1 of NR.
- Adjust h to ensure that $\Delta \equiv y_2 - y_1$ within tolerance.
- popular solver: ode45
- More efficient step-size methods now available.

tolerance on error. *rk45* popular.

- Step-size increases when solution smooth.
- Stiff systems are a problem. (One component changing rapidly comparing to others.)
- Use industrial-strength solvers, e.g. LSODA.

Framework for integration

- Code up function that returns derivatives at any time, given params.
- See DMB guide for examples.

Example: van der Pol oscillator

IVP (initial value problems) e.g. van der Pol oscillator:

$$y'' - \mu(1 - y^2)y' + y = 0$$

Reduce to 1st order system ("normal form"):

$$\begin{aligned} x &= y' \\ x' - \mu(1 - y^2)x + y &= 0 \end{aligned}$$

If we regard our state vector as $\begin{pmatrix} y \\ x \end{pmatrix}$ then we have:

$$\begin{pmatrix} y' \\ x' \end{pmatrix} = \begin{pmatrix} x \\ \mu(1 - y^2)x - y \end{pmatrix}$$

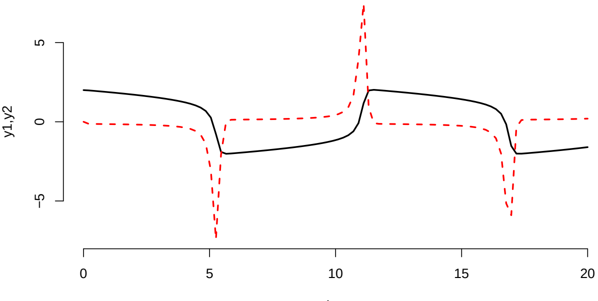
Calling the solver

```
library(deSolve)
vanderpol = function(t, y, parms) {
  ## T = current time
  ## Y = current state vector
  ## PARMS = vector of parameters for system.
  mu = parms[1]
  derivs = c( y[2], mu*(1-y[1]^2)*y[2] - y[1])
  ## Return
  list(derivs)
}

init.cond = c(2, 0);
times = seq(from=0, to=20, length=100)
parms = c(mu=5.0)
out = lsoda(init.cond, times, vanderpol, parms)
pdf(file='vanderpol.pdf', width=8, height=5); par(bty='n')
matplot(out[,1], out[,-1], type='l',xlab='time',
ylab='y1,y2',lwd=2)
```

Output

```
> out[1:5,]
  time         1           2
[1,] 0.0000000 2.000000  0.0000000
[2,] 0.2020202 1.981466 -0.1279646
[3,] 0.4040404 1.954426 -0.1371399
[4,] 0.6060606 1.926339 -0.1408267
[5,] 0.8080808 1.897523 -0.1444858
```



Limitations

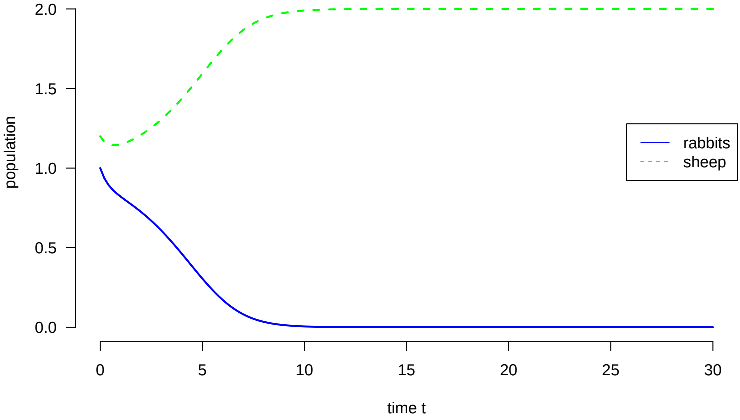
- How to add spikes into framework, if just returning derivative?
- or more generally, sudden changes to variables?
- how to debug?

Example: rabbits vs sheep (Strogatz, p155)

$$\frac{\mathrm{d}r}{\mathrm{d}t} = r(3 - r - 2s)$$
$$\frac{\mathrm{d}s}{\mathrm{d}t} = s(2 - r - s)$$

1. Compute trajectory over time
2. Plot phase planes
3. Nullclines
4. Examining stability

1. Computing any trajectory over time, as before.

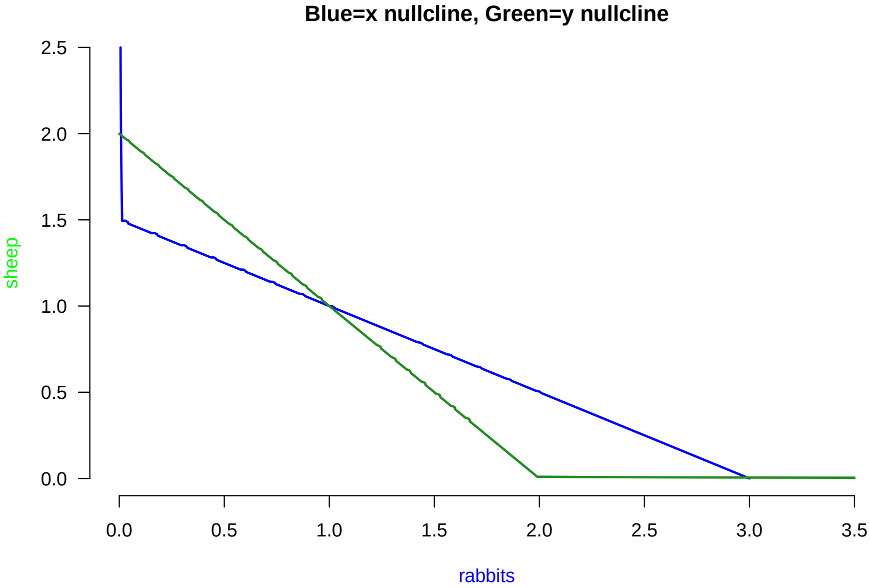


i.e. use numerical integration

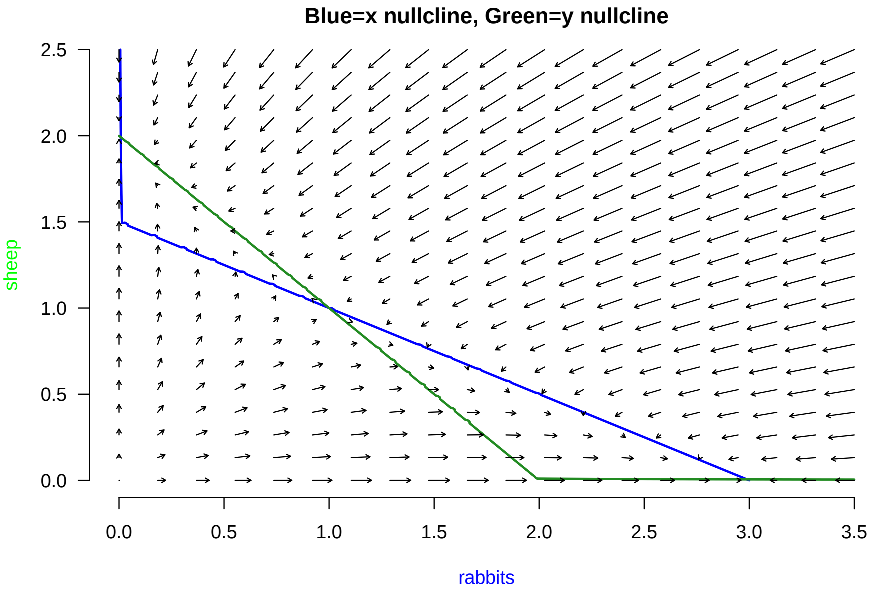
Finding nullclines and steady-states

- A nullcline for a variable x is where its DE $\frac{dx}{dt}$ is zero.
- For a two-variable system x and y, steady-states are found where the two nullclines intersect.

Poor-man's phase space: check either side of nullclines.



2. Phase-plane and 3. Nullclines



Steady-states: intersection of nullclines

Careful: not all nullclines are drawn on the previous page. This is an implementation issue with *contour()* for finding zeros.

- Find the steady-states
  1.
  2.
  3.
  4.

Classification of steady-states

Why take the Jacobian around the steady-state?

$$J(r,s) = \begin{pmatrix} 3-2r-2s & -2r \\ -s & 2-r-2s \end{pmatrix}$$

Recall: for a 2x2 matrix:

- Tr(J) = sum of eigenvalues
- Det(J) = product of eigenvalues.

Starting points

- deSolve package
- phase planes and nullclines (DMBpplane.r from DMB site, modified from Daniel Kaplan)
- integrate() – quadrature
- D() – symbolic differentiation
- optimize() (1d) and optim() (n-d)
- Steven Strogatz. Nonlinear dynamics and chaos.
- NR: William Press et al. Numerical Recipes in C/C++