# Symplectic Runge-Kutta Schemes for Adjoint Equations

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# Introduction

This presentation is mainly a reading of 2 papers, and a book chapter, with a few other things mixed in:

- Sanz-Serna, J. M. (2016). Symplectic Runge–Kutta Schemes for Adjoint Equations, Automatic Differentiation, Optimal Control, and More. SIAM Review, 58(1), 3–33.
- G. J. COOPER (1987). Stability of Runge-Kutta Methods for Trajectory Problems, IMA Journal of Numerical Analysis, Volume 7, Issue 1, 1–13.
- Atkinson, K. E. (1989). An Introduction to Numerical Analysis. New York: John Wiley  Sons.
- All examples I came up with myself to help with explanation.

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# RK Methods (why?)

Mostly from Kendall Atkinson "Numerical Analysis":

- Self starting, unlike multi-step methods.
- Less memory than multi-step methods.
- Easier implementations of adaptive time-stepping

# RK Methods

$s$ stage RK method is specified by $s^2 + 2s$ numbers:

$$a_{ij}, b_i, c_i \qquad i, j = 1, \ldots s$$

and approximates $u(t_n)$ as $u_n$ for $n = 0, 1 \ldots N$ with step length $h_n = t_{n+1} - t_n$ as:

$$u_{n+1} = u_n + h_n \sum_{i=1}^{s} b_i K_{n,i} = u_n + h_n F(u_n, t_n, a, b, c)$$

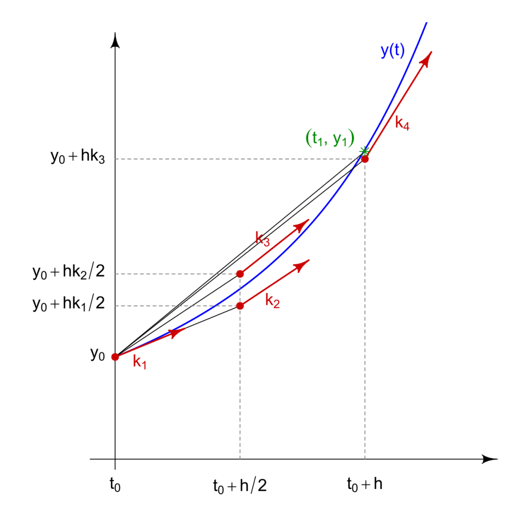
with slopes $K_{n,i}$:

$$K_{n,i} = f(R_{n,i}, t_n + c_i h_n), \qquad i = 1 \ldots, s$$

and interial stages $R_{n,i}$:

$$R_{n,i} = u_n + h_n \sum_{j=1}^{s} a_{ij} K_{n,j}, \qquad i = 1, \ldots s$$

# RK4 - example

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butcher tableau:

$$
\begin{array}{c|cccc}
c_1 & & & & \\
c_2 & a_{21} & & & \\
\vdots & \vdots & a_{32} & & \\
c_s & a_{s1} & \dots & a_{ss} & \\
\hline
 & b_1 & b_2 & \dots & b_s
\end{array}
$$

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
1 & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}
$$

Weighted average of the samples of the vector field $f$.
Explicit methods have lower triangular $a$.

# RK - accuracy conditions continued

For higher order methods this matching gets disgusting, interestingly determining the coefficients of the RK method can be reduced to a problem involving recursively attaching rooted trees to eachother. Appendix H of Richard Palais "Differential Equations, Mechanics, and Computation" has an explanation.

# Symplectic Integrators

Going back to our system of equations:

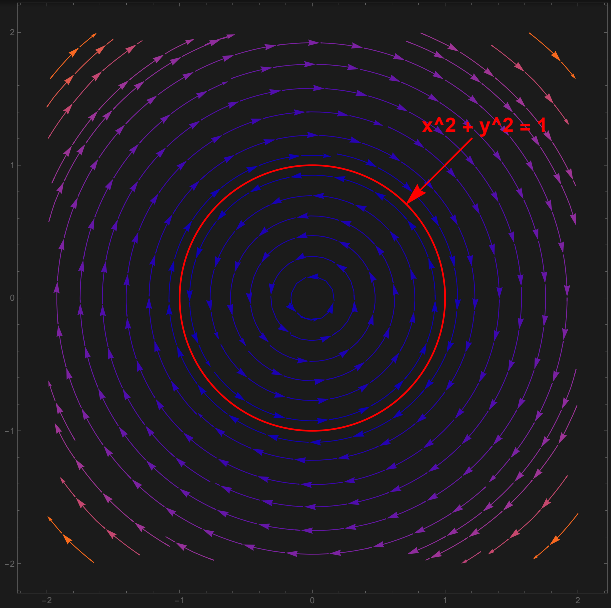
$$\dot{u} = f(u, t)$$

Many systems we care about conserve some quantity in phase space. For instance, harmonic oscillators, predator-prey models, etc. These conserved quantities appear as orbits in phase space and if the conserved quantity is quadratic it takes the form:

$$Q(u) = u^T C u = c$$

where $C$ is positive definite, and the value that $Q(u)$ takes on for a single solution is determined by the initial condition $u(t_0)$.*

# Symplectic Integrators

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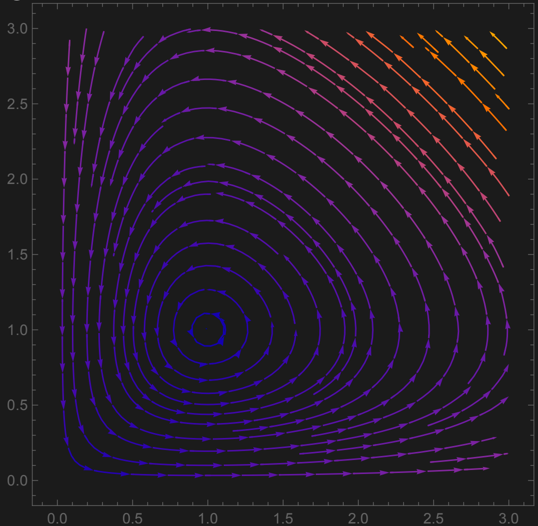
# Symplectic Integrators

Lotka-Volterra conserving growth-rate and competition:




Not necessarily conserved, because not a quadratic invariant. *

# Symplectic Integrators

Mostly from G.J. Cooper, "Stability of Runge-kutta Methods for Trajectory Problems"
Symplectic integrators conserve quadratic invariants. Quadratic conservation is a necessary but not sufficient condition for Symplecticness (Symplecticness is defined in terms of Hamiltonian systems, which we won't worry about).

# Symplectic Integrators

What kind of orbital stability do we want to impose?

1. Stability on the first integral curve itself. i.e. a solution and its perturbation stay close together on the first integral curve.
2. Stability close to the solution but not necessarily on the first integral. A different surface is then stable if it stays near the trajectory of a solution. When the dimension is 2 these definitions are the same.
3. An RK method is orbitally stable if for initial condition $u_n$, and solution step $u_{n+1}$:

$$u_{n+1}^T C u_{n+1} = u_n^T C u_n$$

This suppose to discretely mimick 2.

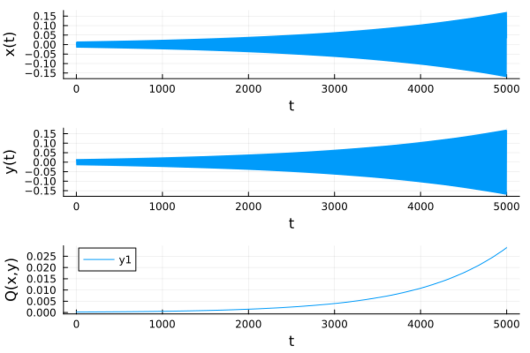
# Symplectic Integrators

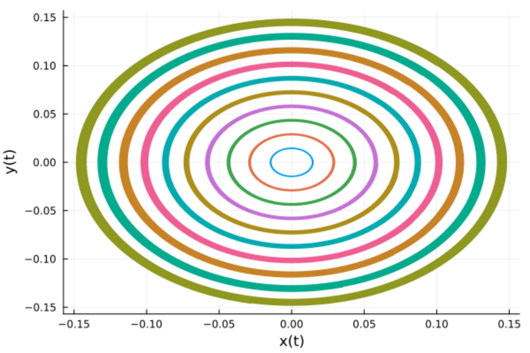
Conditions for orbital stability and what is called a Symplectic RK method are:

$$b_i a_{ij} + b_j a_{ij} - b_i b_j = 0 \qquad i, j = 1 \ldots s$$

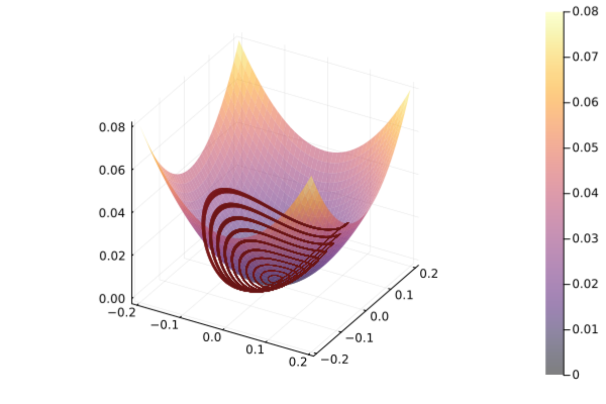
Proof in Cooper (1987). *

# Symplectic Integrators: Euler method

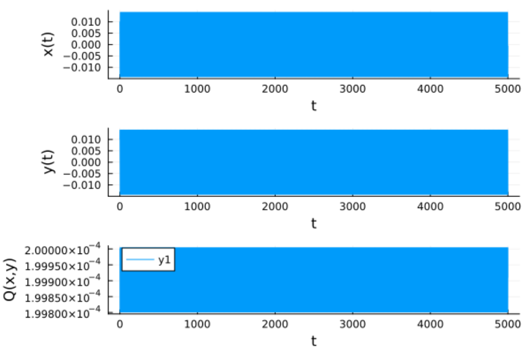


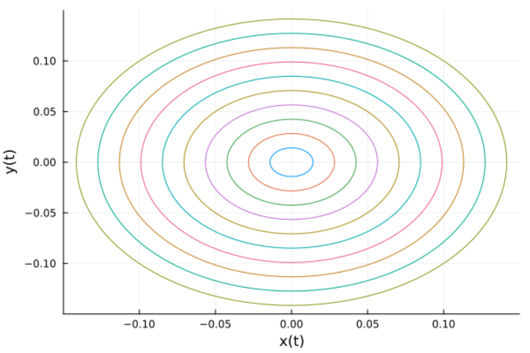



# Symplectic Integrators: Euler method

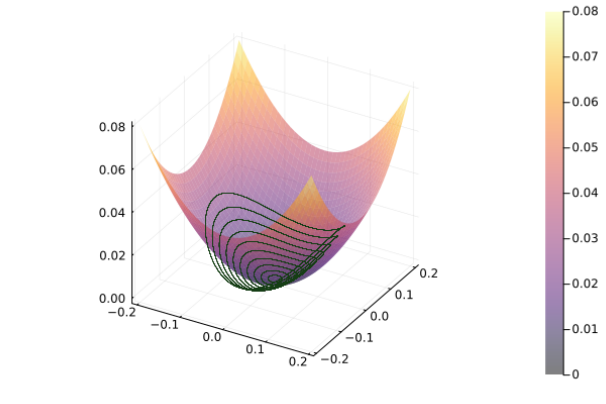


# Symplectic Integrators: Semi-implicit Euler method



# Symplectic Integrators: Semi-implicit Euler method

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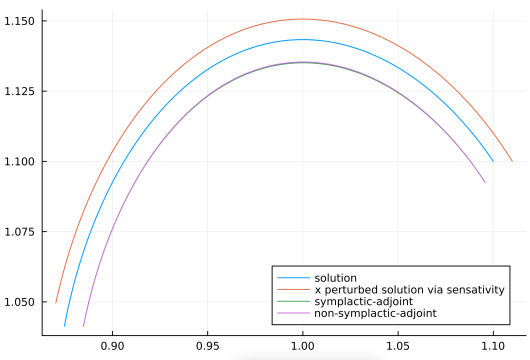
# Adjoint and perturbations

Lotka–Volterra equations:




$$w = [.01, 0]$$

$$w^T \delta(t0 + T) = -4.4607354 * 10^{-5}$$

explicit euler: $\lambda(t_0)^T \eta = -4.249682 * 10^{-5}$

semi-implicit euler: $\lambda(t_0)^T \eta = -4.461427 * 10^{-5}$

explicit euler: $\dfrac{\lambda(t_0)^T \eta - w^T \delta(t0 + T)}{w^T \delta(t0 + T)} = -0.047313$

explicit euler: $\dfrac{\lambda(t_0)^T \eta - w^T \delta(t0 + T)}{w^T \delta(t0 + T)} = -0.000155$