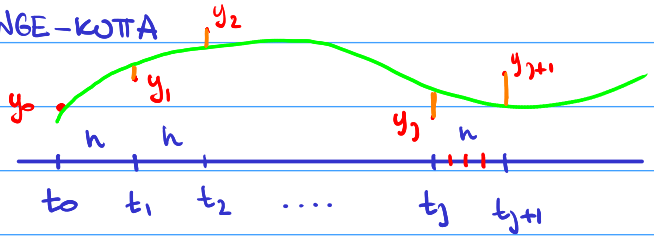
ODE integrators

This semester

- ·) Runge-Kutta schemes ⇝ One-step methods
- ·) LMM – Linear multistep methods
- ·) Geometric Integrators (Preservation of first integrals)
  Symplectic integrators

RUNGE-KUTTA



$y_j \cong y(t_j)$.

y_{j+1} determined only looking at t_j, y_j

Order of consistency / convergence p ⇒ err $\sim O(h^p)$

EULER ⇝ $p = 1$ (low-regularity is fine!)

RK 4/5 ⇝ $p = 4$ or 5 (high-regularity required)

RK 7,8,9 ⇝ less common

In these methods: error estimation is done by running two methods at once

RK 4/5 $\quad y_j^{(4)} \quad y_j^{(5)} \quad \varepsilon_j^{(4)} \quad y_j^{(4)} - y(t_j) \sim O(h^4)$

$\varepsilon_j^{(5)} \quad y_j^{(5)} - y(t_j) \sim O(h^5)$

If $h \ll 1$ ⇒ $|\varepsilon_j^{(4)} - \varepsilon_j^{(5)}| \cong |\varepsilon_j^{(4)}|$

$y_j^{(4)} - y_j^{(5)}$ → can be computed

Trick: Embedded RK to save computations

·) LMM: Use information from the past $t_{j-k+1} \dots t_j$ to find y_{j+1}.

CONS: Difficult to start / Difficult to adapt h

In both cases we have EXPLICIT and IMPLICIT methods

RK 4/5 is a good choice

·) EXPL.: y_{j+1} is obtained by a "formula" combining information from the past.

Both LMM and RK

·) IMPL.: y_{j+1} is def. by a formula that dep. on y_{j+1} ⇒ we need to solve a nonlinear equation to find y_{j+1}

LMM are more common: BDF are the most used

$y' = f(t,y)$ $\quad$ $y(t)$ is bounded or goes to 0 at $+\infty$; will my integrator do the same?

With explicit methods we may be forced to choose $h \ll 1$.

Not the case for implicit methods.

This problem only appears for **stiff** diff. eq.

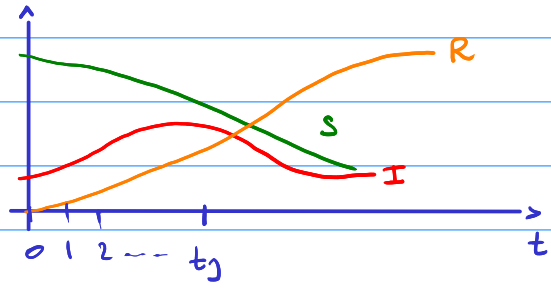
↳ $\| \frac{\partial f}{\partial y} \|$ large

=

SIR model from last time: $(\beta, \gamma) \longrightarrow [y_0, y_1 \dots y_N]$

discrete solution of the ODE

Task fit β, γ so that y_J matches the recorded infections / recoveries



Find suitable β, γ so that we can describe the behavior up to $t = t_J$

=> use the ODE to predict in the future.

$$F(\beta,\gamma) = \begin{bmatrix} y_0 \\ \vdots \\ y_N \end{bmatrix} \qquad \begin{bmatrix} \hat{y}_0 \\ \hat{y}_1 \\ \vdots \\ \hat{y}_N \end{bmatrix}$$

↳ computed data ↳ measured data

$\min_{x \in \mathbb{R}^n} f(x)$ $\quad$ In our case: $n = 2$

$$f(x) = \tfrac{1}{2} \| F\left(\begin{bmatrix} \beta \\ \gamma \end{bmatrix}\right) - \begin{bmatrix} \hat{y}_0 \\ \vdots \\ \hat{y}_N \end{bmatrix} \|_2^2$$

OPT. PROBLEM $\quad$ NONLINEAR LEAST SQUARES PROBLEM

Idea: Start with $x_0 \in \mathbb{R}^n$ and produce $\{x_k\}$ $x_k \to x^*$, with x^* a minimum of $f(x)$

How do I check if x^* is a minimum point?

-) $\nabla f(x^*) = 0$ (NECESSARY)
-) $\nabla^2 f$ is positive def. $\Rightarrow$ x^* is a local minimum

$\nabla^2 f$ INDEF $\Rightarrow$ saddle point

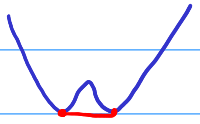
$\nabla^2 f$ NEG. DEF $\Rightarrow$ maximum point.

$$f(x) = f(x^*) + \nabla f(x^*)^T (x - x^*) + \tfrac{1}{2} (x - x^*)^T \nabla^2 f(x)(x - x^*) + O(\|x - x^*\|^3)$$

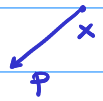
$$f(x+p) = f(x) + \underbrace{\nabla f(x)^T p}_{=0 \text{ at the st. point}} + \underbrace{\tfrac{1}{2} p^T \nabla^2 f(x) p}_{>0 \text{ if } p \neq 0,\ \nabla^2 f \text{ POS DEF}} + O(\|p\|^3)$$

If $f(x)$ is convex $\Rightarrow$ local minima are global

" " strictly convex $\Rightarrow$ unique minimum (both global & local)



If p: $\nabla f(x)^T p < 0$ $\Rightarrow$ p is a descent direction $\Leftrightarrow$ $f(x + tp) < f(x)$ for small t



$p = -\nabla f(x)$ $\rightsquigarrow$ steepest descent (gradient)