PARAMETER ESTIMATION

- PARAMETRIC FAMILY OF MODELS $\circledast$ M_ϑ , $\vartheta = (\vartheta_1, \dots, \vartheta_K)$
- OBSERVATIONS $y^{(j)}(t_i)$ $j: 1, \dots, N$ indep. , t_i , $i: 0, \dots, m$ time points
- PROBABILISTIC MODEL OF OBSERVATIONS

$y^{(j)}(t) = (y_1^{(j)}, \dots, y_n^{(j)})(t)$

$$\Rightarrow p\left(y^{(j)}(t_0), \dots, y^{(j)}(t_m) \mid M_\vartheta\right) \leftarrow$$

$\circledast$ MODELS $\equiv$ (STOCHASTIC) DYNAMICAL SYSTEMS
($\Rightarrow$ Random. VARIABLES OVER TRAJECTORIES)

MAXIMUM LIKELIHOOD ESTIMATION

$$\boxed{\vartheta_{ML} = \underset{\vartheta}{\operatorname{argmax}}\, f(\vartheta)}$$

$$f(\vartheta) = \log \mathcal{L}(\vartheta) = \log \prod_{j=1}^{N} p\left(y^{(j)}(t_0), \dots, y^{(j)}(t_m) \mid \overset{M_\vartheta}{\vartheta}\right)$$

$$= \sum_j \log p\left(y^{(j)}(t_0), \dots, y^{(j)}(t_m) \mid \vartheta\right)$$

• MODELS M_θ = ODE (e.g. mean field)

$$\frac{d}{dt}x(t) = \underbrace{F(x(t))}_{F(x_1(t),\, \theta)} \qquad x(0) = x_0 .$$

dependency on model parameters

SIS
$$\begin{cases} \dfrac{dx_S}{dt} = -k_I x_S x_I + k_R x_I \\ \dfrac{dx_I}{dt} = k_I x_S x_I - k_R x_I \end{cases}$$

$F(x, \theta)$

$\theta = (k_I, k_R, x_S(0), x_I(0))$

• DATA (N = 1 TRAJECTORIES AT m time points)

$\rightarrow\ y(t_1) \ \text{—}\ y(t_m)$ $\qquad y(t) = x(t, \theta) + \varepsilon \quad \varepsilon \sim \mathcal{N}(0, \sigma^2)$

$$p(y(t_1), \dots y(t_m) \mid \theta) = \prod_i p(y(t_i) \mid \theta) \Rightarrow f(\theta) \propto \underbrace{-\sum_i [y(t_i) - x(t_i, \theta)]^2}_{-\text{SUM of SQUARE}}$$

IDENTIFIABILITY

$\emptyset \longrightarrow X \quad , \quad k_1$

$X \longrightarrow \emptyset \quad , \quad k_2 \cdot X$

$\frac{dx}{dt}$

$\dot{x} = k_1 - k_2 x$

$x(t,\theta) \xrightarrow{t \to \infty} \frac{k_1}{k_2}$

$y(t)$, for t large , $t \approx \infty$

$$L(\theta) = -\left(\frac{k_1}{k_2} - y(t) \right)^2$$

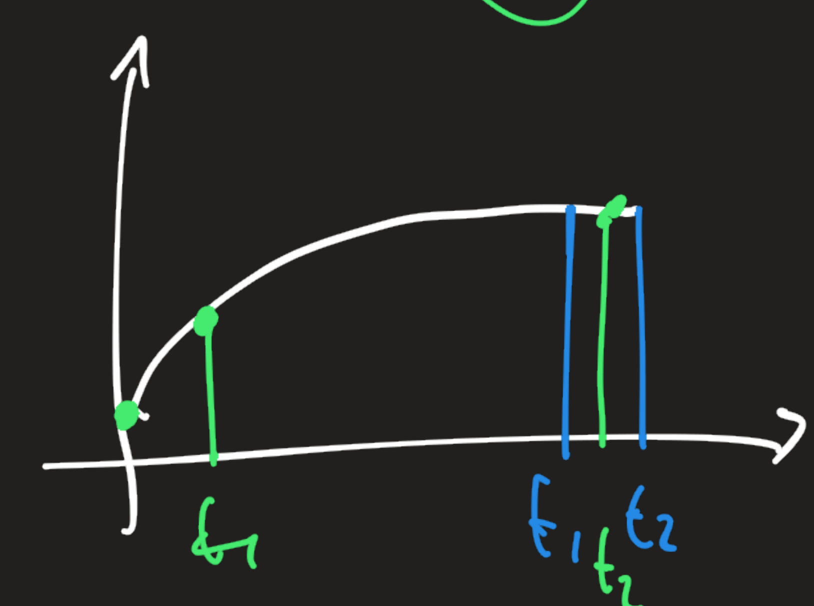
$$\frac{k_1}{k_2} = \gamma \Rightarrow k_1 = \gamma k_2$$

$$\bar{k}_1 = \alpha \gamma, \quad \bar{k}_2 = \alpha \Rightarrow \frac{\bar{k}_1}{\bar{k}_2} = \gamma$$

$\Rightarrow$ we cannot identify both k_1 and k_2

IF we have two observations at times t_1, t_2

s.t. $\|y(t_1) - y(t_2)\| > \delta$



- WE OBSERVE THE MEAN AT TIMES $t_1, \dots, t_m$ (SAMPLE MEAN)

    a) MEAN FIELD / MOMENT CLOSURE

    b) ESTIMATE MEAN OF $X(t)$ by SIMULATION $\Big\}$ USE A GAUSSIAN LIKELIHOOD

- WE OBSERVE INDIVIDUAL RUNS AT TIMES $t_1, \dots, t_m$

    - OBSERVATIONS AT TIMES $t_1 \to t_m$ are independent

$$p(y^{(j)}(t_1), \dots, y^{(j)}(t_m) \mid \vartheta) = \prod_i \boxed{p(y^{(j)}(t_i) \mid \vartheta)}$$

    - OBSERVATIONS AT TIMES $t_1 \to t_m$ ARE FROM the SAME TRAJECTORY

$$\left(p(y^{(j)}(t_1), \dots, y^{(j)}(t_m) \mid \vartheta) \right) \underbrace{\mathcal{N}(x(t_1, \vartheta), \dots, x(t_m, \vartheta), \sigma^2)}_{=\,P(y^{(j)}(t_1), \dots, y^{(j)}(t_m) \mid x(t_i, \vartheta)_{i=1,\dots,m})}$$

$$= \underbrace{\int dx(t_1) \cdots dx(t_m)\, P(x(t_1), \dots, x(t_m) \mid \vartheta) \cdot P(y^{(j)}(t_1), \dots, y^{(j)}(t_m) \mid x(t_i, \vartheta)_{i=1,\dots,m})}_{\mathbb{E}_{x(t_1) \dots x(t_m)}\left[P(y^{(j)}(t_1), \dots, y^{(j)}(t_m) \mid x(t_1) \dots x(t_m)) \right]}$$

$$f(\vartheta) = \sum_{j=1}^{N} \mathbb{E}_{X(t_1)\dots X(t_n)}\left[\sum_i \left(y^{(j)}(t_i) - X(t_i,\vartheta)\right)^2\right]$$

$X^{(k)}(t_1) \dots X^{(k)}(t_m)$ = simulation, trajectory $k = 1 \dots K$

$$\approx \underbrace{\sum_{j=1}^{N} \frac{1}{K}\sum_{k=1}^{K}\sum_{i=1}^{m}\left(y^{(j)}(t_i) - X^{(k)}(t_i,\vartheta)\right)^2}$$

→ RUN K SIMULATIONS, evaluate

OPTIMIZE $f(\vartheta)$ w.r.t. ϑ, use a gradient-free method.

(evolutionary algorithms)

(nelder-mead)