Computational Modelling
Moment closures and central limit approximation

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Outline

1. Fluid Equation and Moments
2. System-Size Expansion

VAN KAMPEN

3. Linear Noise Approximation

Population CTMC: definitions

Master equation

$$\frac{dP(\mathbf{x},t)}{dt} = \sum_{\eta \in \mathcal{T}} r_\eta(\mathbf{x}-\mathbf{v}_\eta) P(\mathbf{x}-\mathbf{v}_\eta, t) - \sum_{\eta \in \mathcal{T}} r_\eta(\mathbf{x}) P(\mathbf{x},t)$$

Drift

$$F(\mathbf{x}) = \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta r_\eta(\mathbf{x})$$

Diffusion matrix

$n \times n$, $n \equiv$ #species

$$D_{ik}(\mathbf{x}) = \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta[i]\mathbf{v}_\eta[k] r_\eta(\mathbf{x})$$

$v_\eta[1]^2$

First-order approximation

Differential equation for the average of a PCTMC

$$\frac{d\mathbb{E}[X_i]_t}{dt} = \mathbb{E}[F_i(\mathbf{X})]_t$$

Taylor expansion of $\boxed{\mathbb{E}[F_i(\mathbf{X})]_t}$

$$\mathbb{E}[F_i(\mathbf{X})]_t \approx F_i(\mathbb{E}[\mathbf{X}]_t) + \frac{1}{2}\sum_{h,k=1}^{|\mathbf{Y}|} \partial^2_{hk} F_i(\mathbb{E}[\mathbf{X}]_t) \cdot COV[X_h X_k]_t$$

First-order equation for the average

$$\frac{d\mathbb{E}[X_i]_t}{dt} = F_i(\mathbb{E}[\mathbf{X}]_t)$$

Second-Order Approximation

Exact equation for covariance

$$\frac{dCOV\left[X_i X_k\right]_t}{dt} = \mathbb{E}\left[D_{ik}(\mathbf{X})\right]_t + \mathbb{E}\left[(X_i - \mathbb{E}\left[X_i\right]_t)F_k(\mathbf{X})\right]_t + \mathbb{E}\left[(X_k - \mathbb{E}\left[X_k\right]_t)F_i(\mathbf{X})\right]_t$$

Second-order equations for average and covariance

$$\frac{d\mathbb{E}\left[X_i\right]_t}{dt} = F_i(\mathbb{E}\left[\mathbf{X}\right]_t) + \frac{1}{2}\sum_{h,k=1}^{|T(N)|} \partial^2_{hk} F_i(\mathbb{E}\left[\mathbf{X}\right]_t) \cdot COV\left[X_h X_k\right]_t$$

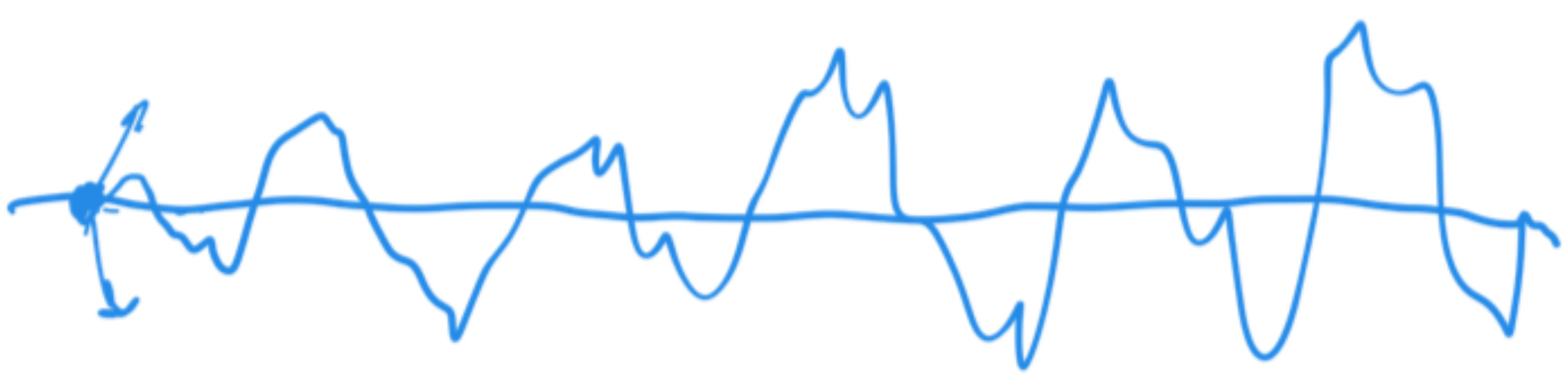
$$\frac{dCOV\left[X_i X_k\right]_t}{dt} = D_{ik}(\mathbb{E}\left[\mathbf{X}\right]_t) + \sum_{h=1}^{|\mathbf{X}|} \partial_h F_k(\mathbb{E}\left[\mathbf{Y}\right]_t) \cdot COV\left[X_i X_h\right]_t + \sum_{h=1}^{|\mathbf{X}|} \partial_h F_i(\mathbb{E}\left[\mathbf{X}\right]_t) \cdot COV\left[X_k X_h\right]_t$$

RANDOM WALK

One variable $X \in \mathbb{Z}$.
Transitions: $(inc, \top, X' = X + 1, k)$, $(dec, \top, X' = X - 1, k)$

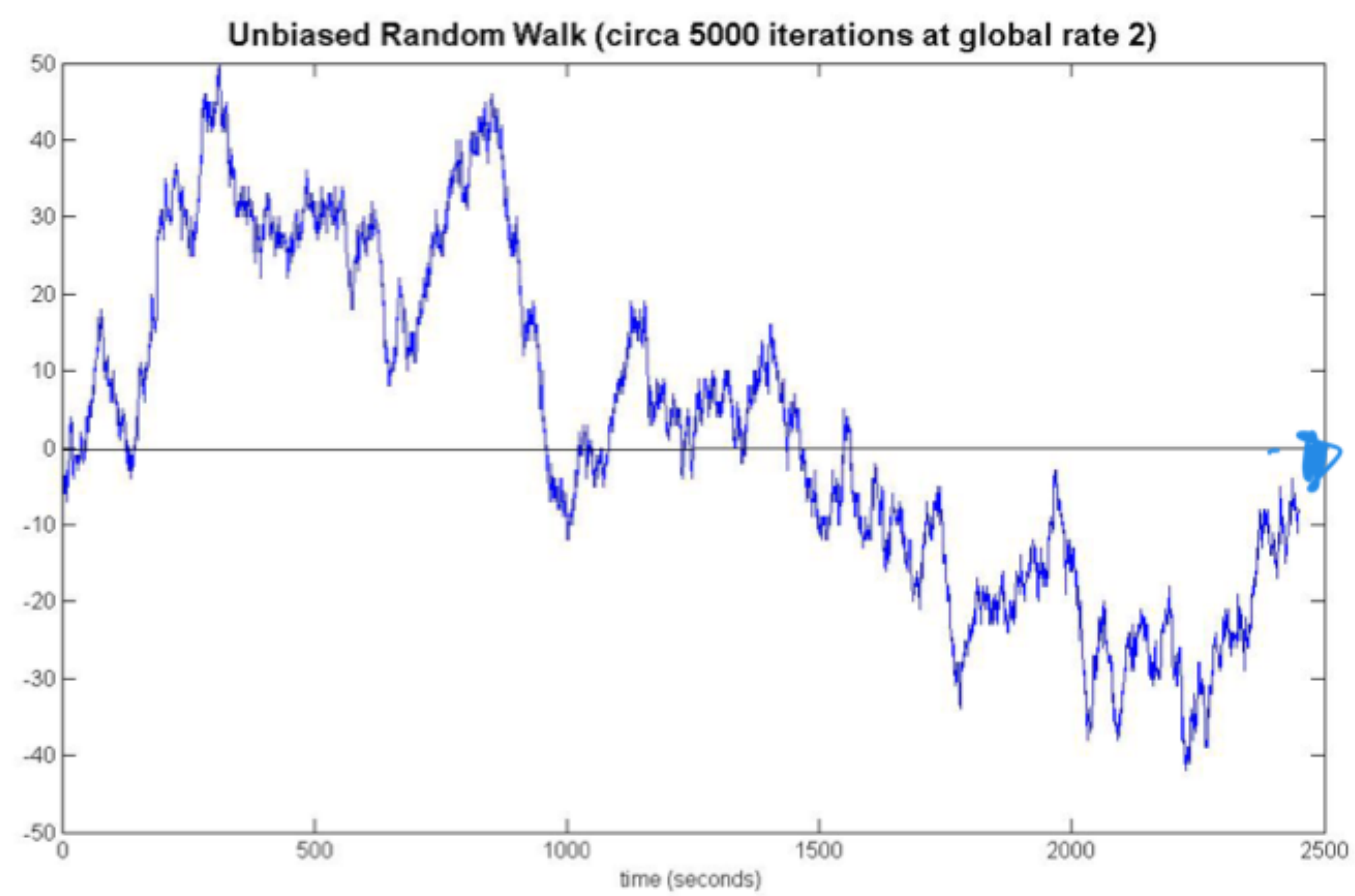
$$F(X) = 0$$
$$D(X) = 2k$$

$$\begin{cases} \mathbb{E}[\dot{X}] = F(\mathbb{E}[X]) + \frac{1}{2} COV\left[X^2\right] \partial^2_{XX} F(\mathbb{E}[X]) = 0 \\ \dot{COV}[X^2] = D(\mathbb{E}[X]) + 2 COV\left[X^2\right] \partial_X F(\mathbb{E}[X]) = 2k \end{cases}$$



$$\mathbb{E}[X]_t = X_0$$

$$COV\left[X^2\right]_t = 2kt + COV\left[X_0^2\right]$$



Outline

PARAMETER ESTIMATION WITH MOMENTS

1) → MOMENT MATCHING
2) → DISTRIBUTION RECONSTRUCTION + ML
3) → (GENERALIZED) METHOD OF MOMENTS ←

1) Moment Matching

•) Estimate moments from observations $x_1, \dots, x_N$ (at time t)

→ $\hat{\mu}_t = \frac{1}{N} \sum x_i(t)$, $\hat{\sigma}_t^2 = \frac{1}{N-1} \sum (x_i - \hat{\mu}_t)^2$, other moments.

Take a model $X(t, \vartheta)$

Compute $\mathbb{E}[X(t,\vartheta)] = \mu_t(\vartheta)$, $\mathrm{VAR}[X(t,\vartheta)] = \sigma_t^2(\vartheta)$ ...

using moment closure.

$$\hat{\vartheta} = \arg\min_{\vartheta} \underbrace{\left[(\mu_t(\vartheta) - \hat{\mu}_t)^2 + (\sigma_t^2(\vartheta) - \hat{\sigma}_t^2)^2 + \dots \right]}_{\| \|_2^2 \text{ of moments } \vec{\mu}_t(\vartheta) \text{ and } \hat{\mu}_t \text{ (estimated moments)}}$$

2) DISTRIBUTION RECONSTRUCTION

$X(t,\theta)$ $\quad P(x|t,\theta)$ density

Se conosco $\mu_t^{(j)} = \mathbb{E}[X^j(t,\theta)]$, $\underbrace{\mu_t^{(0)} = 1, \dots, \mu_t^{(k)}}_{\text{li ottengo da moment closure.}}$

posso approssimare $P(x|t,\theta)$?

Ci sono infinite $P(x)$ che hanno momenti $\underline{\mu_t^{(0)}, \dots, \mu_t^{(k)}}$

ENTROPIA di SHANNON

$$H[X] = \mathbb{E}_{p(x)}[-\log(p(x))] \quad \text{or} \quad \underline{H[p]} = \mathbb{E}_p[-\log(p(x))]$$

$$= \int -p(x) \log p(x)\, dx$$

(informazione media / incertezza di p)

Criterio: SCEGLI $p(x)$ CHE MASSIMIZZA L'ENTROPIA

NELLA CLASSE $\mathcal{G} = \{ g(x) \mid \mathbb{E}_g[X^j] = \mu^{(j)}, \forall j = 0, \dots, k \}$

$$\boxed{p^* = \underset{g \in \mathcal{G}}{\arg\max}\, H[g]}$$

maximum entropy <=> maximum uncertainty

"least committal".

$$f(g,\underline{\lambda}) = H[g] - \sum_{j=0}^{K} \lambda_j \Big[\underbrace{\int x^j g(x)\,dx - \mu^{(j)}}_{=0} \Big]$$

A λ fissato, $g_\lambda = \exp\underbrace{\Big(-1 - \sum_{j=0}^{K} \lambda_j x^j\Big)}_{\in \text{ exponential family}}$

$\underline{\psi(\lambda)} = f(g_\lambda, \lambda)$

K+1 dimensionale

$$\lambda^* = \arg\min_{\lambda} \psi(\lambda)$$

DUAL FORMULATION OF A CONSTRAINED OPTIMIZATION PROBLEM.

$$p^*(x) = \exp\Big(-1 - \sum_{j=0}^{K} \lambda_j^* x^j\Big)$$

[Se conosco solo $\mu^{(0)}, \mu^{(1)}, \mu^{(2)}$ $\Longrightarrow$ $p^*(x) = \mathcal{N}(\mu^{(1)}, \mu^{(2)} - \mu^{(1)2})$]

- ϑ, calcolo $\mu^{(j)}(\vartheta)$, $j=0,\dots,K$ con M.C., calcolo $p^*(x|\vartheta)$

calcolo likelihood $\prod_i p^*(x_i|\vartheta) = L(D,\vartheta)$, maximize L wrt ϑ.

Generalized method of moments

$\downarrow$

vedi moodle!

THE LINEAR NOISE ANSATZ

Fluctuations around the counting process are of order $N^{\frac{1}{2}}$. We assume that the PCTMC at level N fluctuates around the solution of the fluid equation:

$$\mathbf{X}^{(N)}(t) \approx N\mathbf{x}(t) + N^{\frac{1}{2}}\xi,$$

where ξ is a continuous random variable. This means that

$$\hat{\mathbf{X}}^{(N)}(t) \approx \mathbf{x}(t) + N^{-\frac{1}{2}}\xi$$

DERIVING THE EQUATIONS

One proceeds as follows

1. Write the master equation in terms of normalized variables;
2. Apply the Ansatz $\hat{X}^N(t) = x(t) + \frac{1}{\sqrt{N}}\xi(t)$
3. Expand probability and propensity functions around $\mathbf{x}(t)$. This makes sense if $N^{-\frac{1}{2}}\xi$ is small.
4. Introduce a new probability density $\Pi(\mathbf{x}, t)$ for the noise term ξ
5. Collect terms in order $\frac{1}{2}$ of N to get the fluid equation for $\mathbf{x}(t)$, and in order 0 of N to get the PDE equation for Π.

LINEAR NOISE APPROXIMATION

DRIFT, JACOBIAN, DIFFUSION MATRIX

$$F(\mathbf{x}) = \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta f_\eta(\mathbf{x})$$

$$J_{ij}(t) = \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta[i] \partial_j f_\eta(\mathbf{x}(t))$$

$$D_{ik}(\mathbf{x}) = \sum_{\eta \in \mathcal{T}} \mathbf{v}_\eta[i] \mathbf{v}_\eta[k] f_\eta(\mathbf{x})$$

NOISE: LINEAR FOKKER-PLANK EQUATION

$$\frac{\partial \Pi(\mathbf{x}, t)}{\partial (t)} = \sum_{i,j} J_{i,j}(t) \partial_i (\xi_j \Pi(\mathbf{x}, t)) + \frac{1}{2} \sum_{i,j} D_{ij} \partial_{ij} \Pi(\mathbf{x}, t).$$

LINEAR NOISE APPROXIMATION

LINEAR FOKKER-PLANK EQUATION

Linear Fokker-Plank equations have solutions which are Gaussian Processes! We can obtain the equations for average and variance from Π, and solve them to fully determine the noise term $\xi(t)$.

AVERAGE

$\frac{d\mathbb{E}[\xi(t)]}{dt} = J\mathbb{E}[\xi(t)]$, So if $\mathbb{E}[\xi(0)] = 0$, then $\mathbb{E}[\xi(t)] = 0$.

COVARIANCE MATRIX C

J, D valutati lungo x(t)

$$\frac{dC}{dt} = JC + CJ^T + D$$

$D = D(t) = D(x(t))$

SOLUTION TO THE SYSTEM

COVARIANCE + FLUID EQUATION

$\hat{\mathbf{X}}^{(N)}(t) \approx \mathbf{x}(t) + N^{-\frac{1}{2}}\xi(t)$ is a Gaussian Process.
At time t, it is a multivariate Gaussian distribution with mean $\mathbf{x}(t)$ and covariance $N^{-1}C$.

CENTRAL LIMIT THEOREM

We can look at the linear noise approximation from a limit theorem point of view.

$$\mathbf{X}^{(N)}(t) = N\mathbf{x}(t) + N^{\frac{1}{2}}\xi^{(N)}(t),$$

where we defined

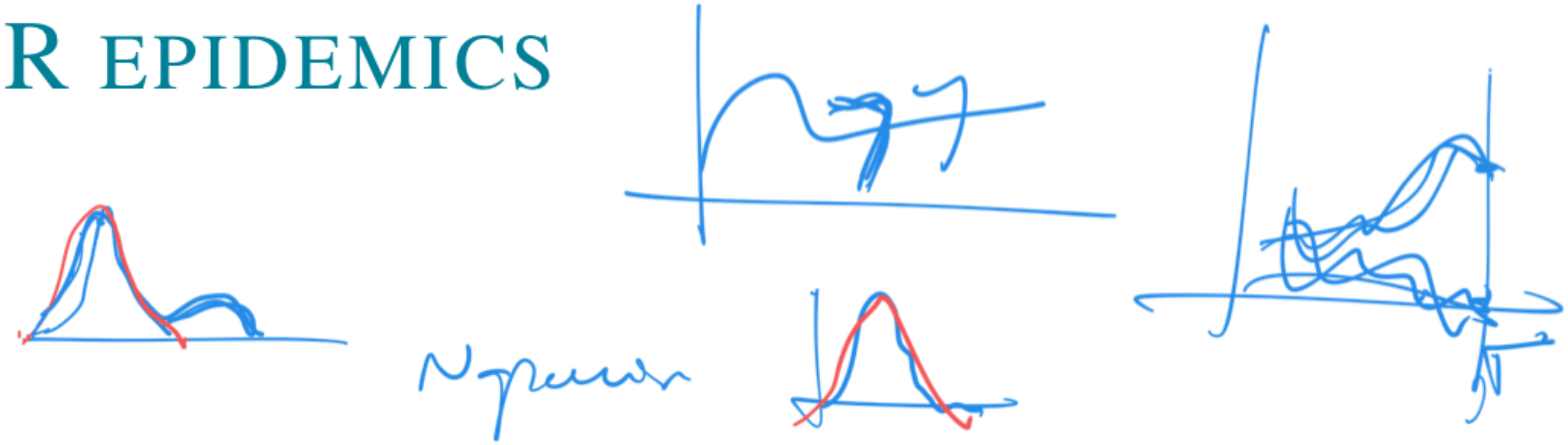
$$\xi^{(N)}(t) = N^{-\frac{1}{2}}(\mathbf{X}^{(N)}(t) - N\mathbf{x}(t))$$

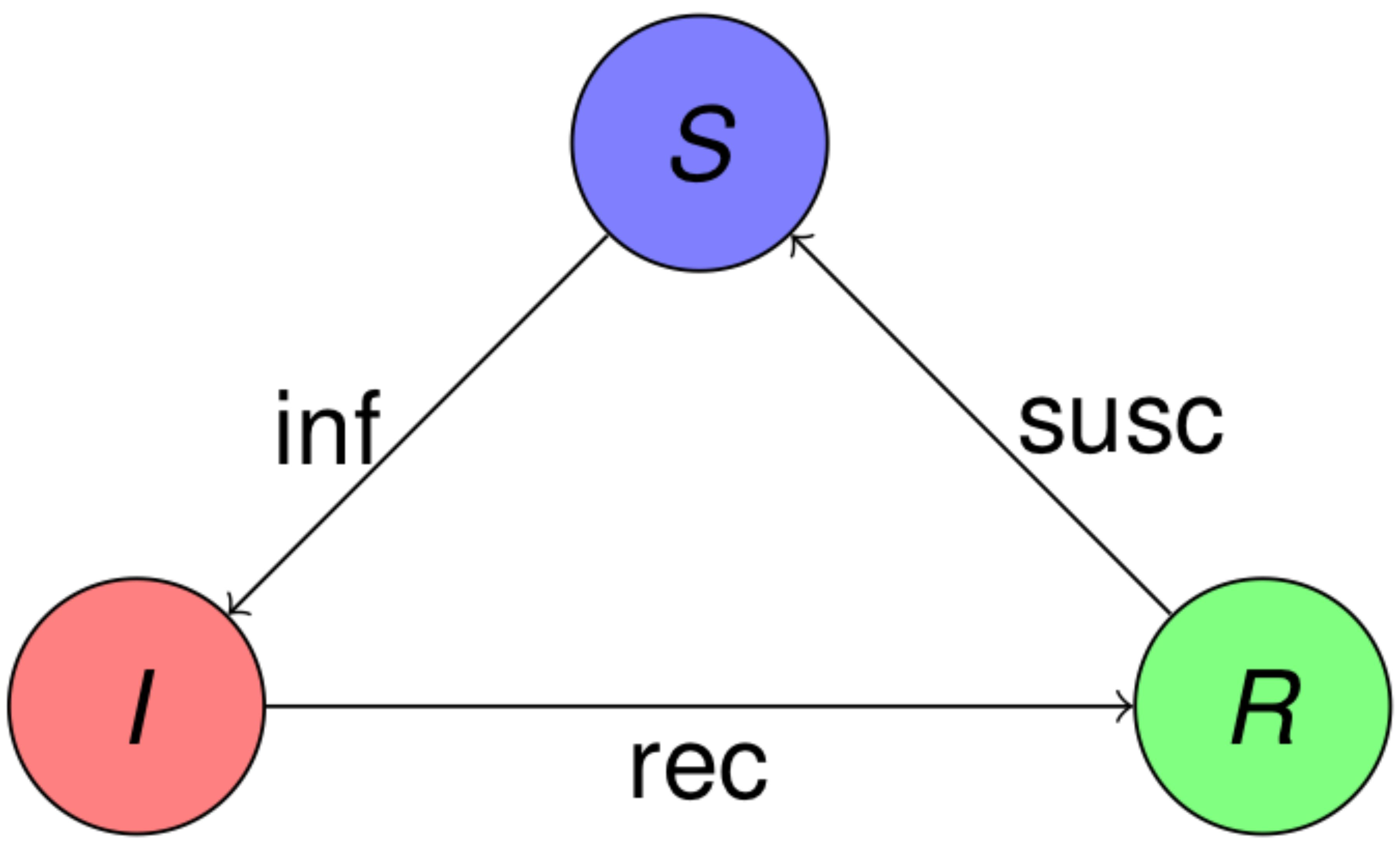
CENTRAL LIMIT THEOREM (KURTZ)

If rate functions are of class C^1, then

$$\xi^{(N)} \Rightarrow \xi \text{ (weakly)}$$

EXAMPLE: SIR EPIDEMICS





Three variables: X_S, X_I, X_R.
State space:
$\mathcal{D} = \{(n_1, n_2, n_3) \mid n_1 + n_2 + n_3 = N\} \subset \{0, \ldots, N\}^3$.

Transitions:

- $(inf, \top, (-1, 1, 0) k_I \frac{X_I}{N} X_S)$
- $(rec, \top, (0, -1, 1), k_R X_I)$
- $(susc, \top, (1, 0, -1), k_S X_R)$

EXAMPLE: SIR EPIDEMICS

REDUCE THE SYSTEM DIMENSION

As $X_R = N - X_S - X_I$, we can reduce to two dimensions: $x_S = x$ and $x_I = y$. Call also $u = VAR(\xi_S)$, $v = VAR(\xi_I)$, $c = COV(\xi_S, \xi_I)$

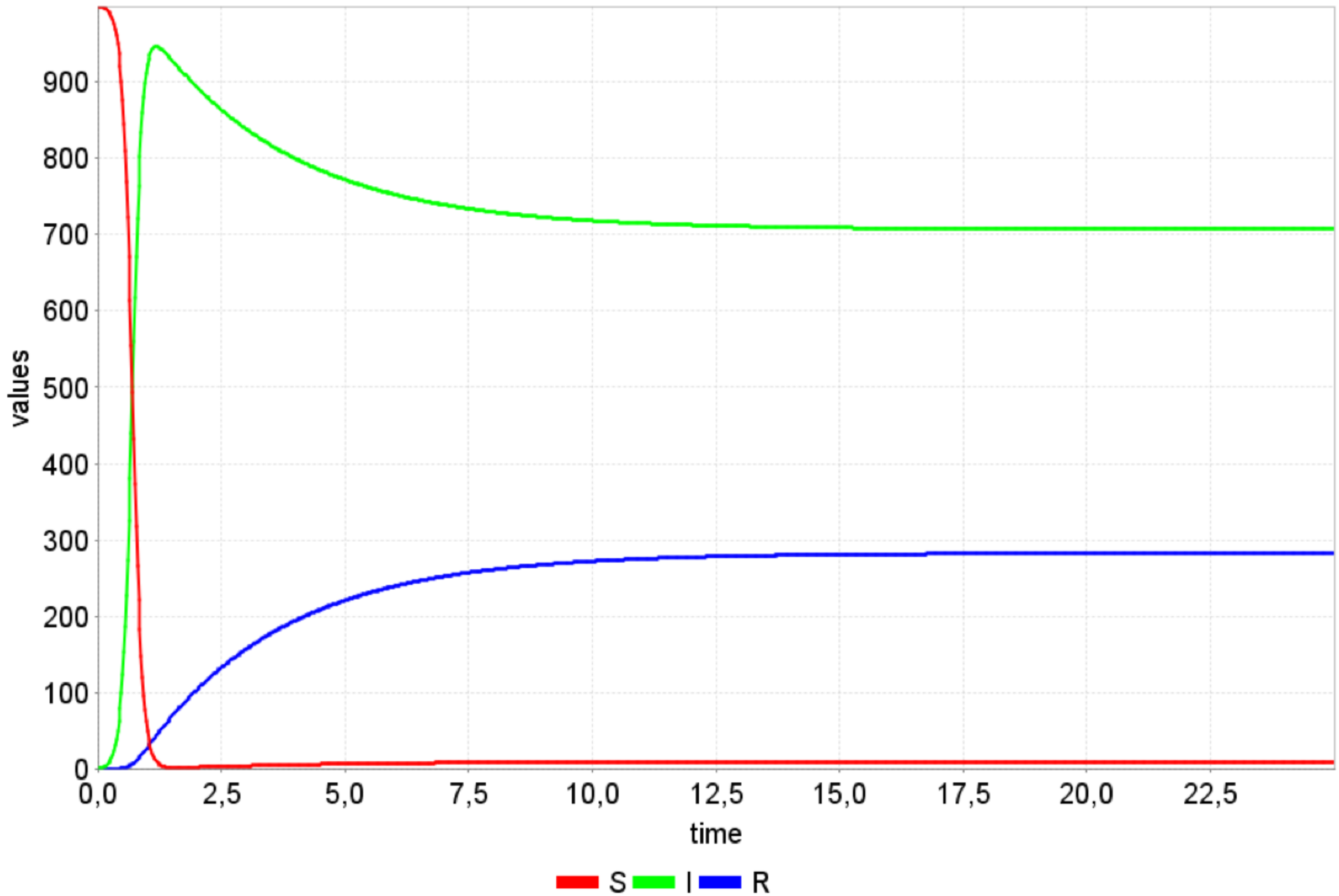
AVERAGE: FLUID EQUATIONS

$$\frac{dx}{dt} = -k_I xy + k_S(1 - x - y)$$
$$\frac{dy}{dt} = k_I xy - k_R y$$

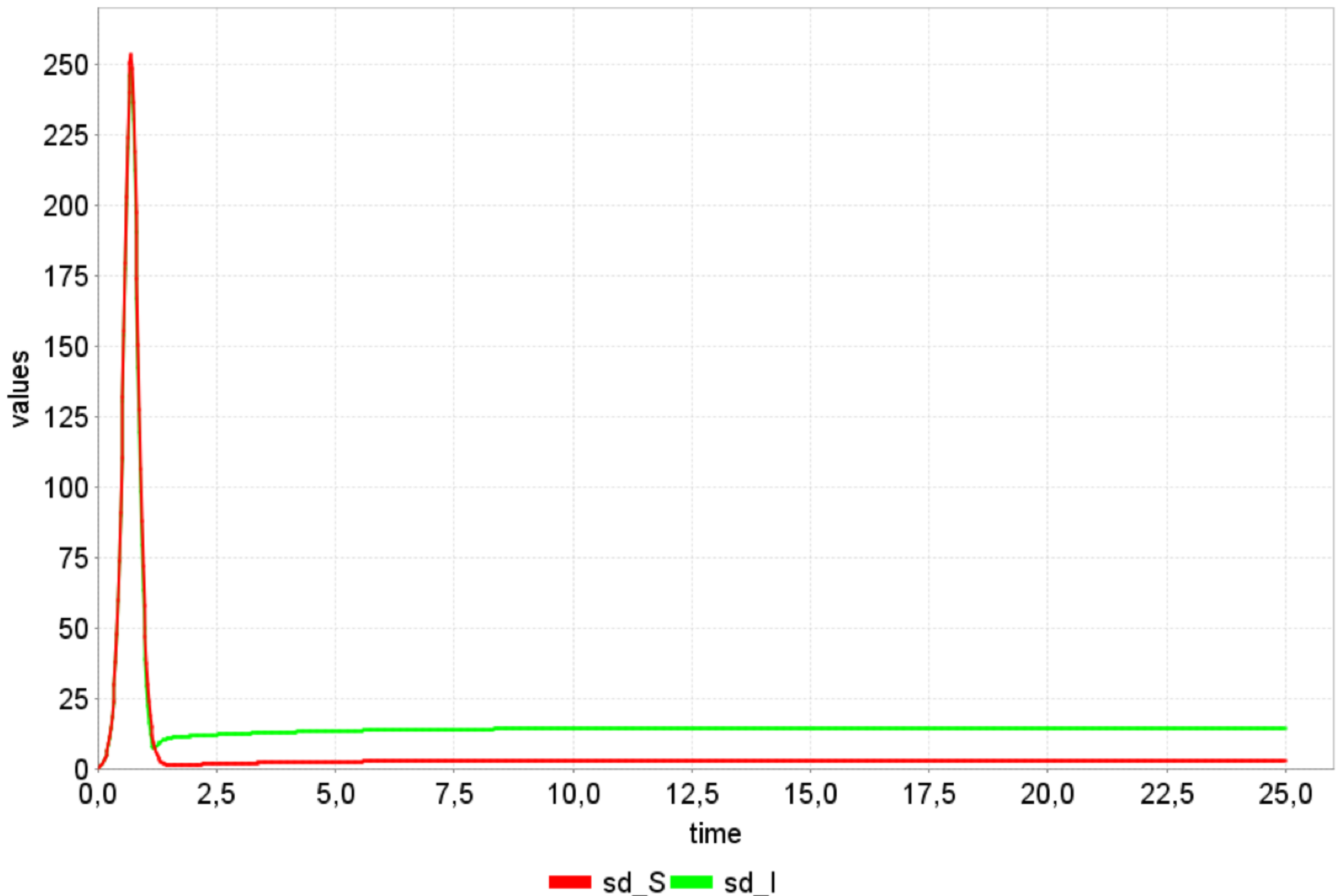
VARIANCE u OF x, v OF y, COVARIANCE c

$$\frac{du}{dt} = -2u(k_i y + k_s) - 2c(k_i x + k_s) + k_i xy + k_s(1 - x - y)$$
$$\frac{dv}{dt} = 2c(k_i y) + 2v(k_i x - kr) + kixy + k_r y$$
$$\frac{dc}{dt} = -c(k_i y + k_s) - v(k_i x + k_s) + k_i yu + c(k_i x - k_r) - k_i xy$$

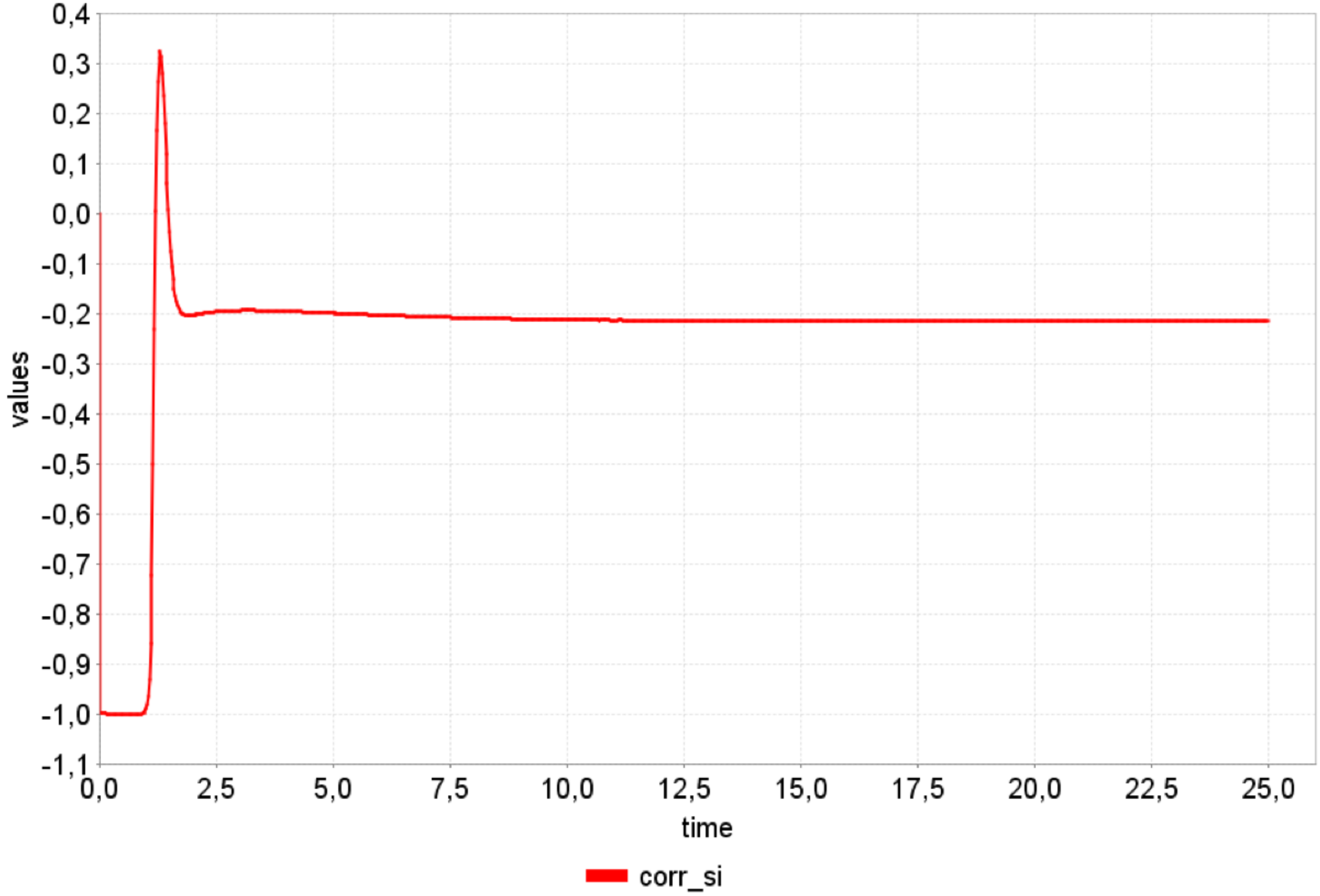
SIR EPIDEMICS: FLUID EQUATIONS



SIR EPIDEMICS: LN ESTIMATED STANDARD DEVIATION OF S AND I

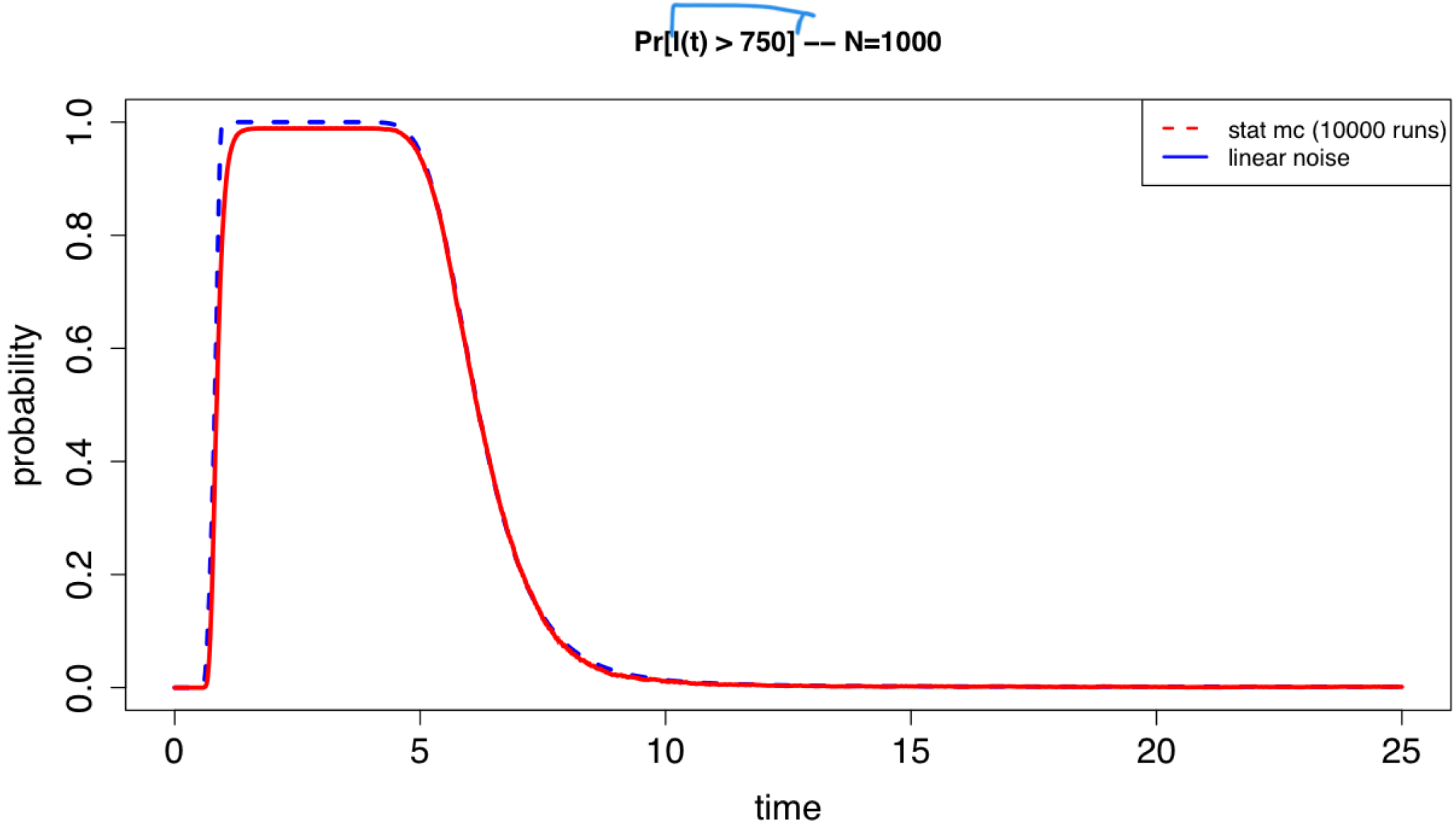


SIR EPIDEMICS: LN ESTIMATED CORRELATION OF S AND I



SIR EPIDEMICS: LN ESTIMATED $\mathbb{P}\{I(t) \geq 750\}$

N: 1000



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