ODE parameter estimation

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Content

Introduction

We have a model which is governed by this equation :

$$\boxed{dX_t = f(t, X_t, \theta)dt},$$

and the question is **how to find the parameter θ using the observations ?**

Introduction

From this model we have the function f, the time t and some observations Y which are modelised with some noise (that we may don't know). That's why I transform the equation in :

$$\boxed{dX_t = f(t, X_t, \theta)dt + \sigma dB_t}$$

The unknown is θ and maybe σ too.

An example : the Lotka Volterra model

$$\boxed{dX_t = f(t, X_t, \theta)dt}$$

The problem that I used to test the theory is the Lotka-Volterra model :

$$\boxed{\begin{cases} \frac{dS}{dt} = S(\alpha - \beta W) \\ \frac{dW}{dt} = -W(\delta - \gamma S). \end{cases}}$$

So here the unknow are $\theta = (\alpha, \beta, \gamma, \delta)$, $X = (S, W)$ and f does not depend on t.

Likelihood

So we are working with :

$$\boxed{dX_t = f(t, X_t, \theta)dt + \sigma dB_t}$$

$$L(\theta) = p(x_{t_0}, t_0; \theta) \prod_{i=1}^{n} p(x_{t_i}, t_i \mid x_{t_{i-1}}, t_{i-1}; \theta)$$

where p is the probability to obtain x_{t_i} at t_i knowing $x_{t_{i-1}}$ when f is paramtrisezd by θ. So its log-likelihood becomes :

$$\boxed{l(\theta) = \log(p(x_{t_0}, t_0; \theta)) + \sum_{i=1}^{n} \log(p(x_{t_i}, t_i \mid x_{t_{i-1}}, t_{i-1}; \theta))}$$

Likelihood

We will use this formula :

$$\boxed{l(\theta) = \log(p(x_{t_0}, t_0; \theta)) + \sum_{i=1}^{n} \log(p(x_{t_i}, t_i \mid x_{t_{i-1}}, t_{i-1}; \theta))}$$

and we are looking for the maximum likelihood estimator

$$\widehat{\theta}_n = \underset{\theta \in \Theta}{\arg\max}\ l(\theta).$$

Likelihood

To find $\widehat{\theta}_n$ we need to simplify a little bit the log-likelihood. To do so we need to do quite simple approximations : Euler approximation :

$$X_{t_{i+1}} = X_{t_i} + f(t_i, X_{t_i}, \theta)(t_{i+1} - t_1) + \sigma(B_{t_{i+1}} - B_{t_i}).$$

So we can find p (B is a brownian motion) :

$$p(x_{t_i}, t_i \mid x_{t_{i-1}}, t_{i-1}; \theta) \sim \mathcal{N}(x_{t_{i-1}} + f(t_{i-1}, X_{t_{i-1}}, \theta)(t_i - t_{i-1}),\ (\sigma\, {}^t\sigma)(t_i - t_{i-1}))$$

and the log-likelihood becomes

$$l(\theta) = -\frac{1}{2}\sum_{i=1}^{n}\left(\frac{(x_{t_i} - x_{t_{i-1}} - f(t_{i-1}, x_{t_{i-1}}, \theta)(t_i - t_{i-1}))^2}{\sigma^2(t_i - t_{i-1})} + \log(2\pi\sigma^2(t_i - t_{i-1}))\right).$$

Likelihood

Now I did a hypothesis, I supposed that $\exists \Delta t \; \forall i, \;\; t_i - t_{i-1} = \Delta t$ so that the log-likelihood becomes :

$$l(\theta) = -\frac{1}{2} \sum_{i=1}^{n} \left(\frac{\|\sigma^{-1}(x_{t_i} - x_{t_{i-1}} - f(t_{i-1}, x_{t_{i-1}}, \theta)(t_i - t_{i-1}))\|_2^2}{(t_i - t_{i-1})} \right.$$
$$\left. + \log((2\pi)^n \det(\sigma)^2 (t_i - t_{i-1})) \right) .$$

So to maximize the log-likelihood is to maximises the previous equation.

Likelihood

So the new problem is how to minimise :

$$\boxed{S(\theta) = \sum_{i=1}^{n} \|\sigma^{-1}(x_{t_i} - x_{t_{i-1}} - f(t_{i-1}, x_{t_{i-1}}, \theta)(\Delta t))\|_2^2.}$$

and this is much more easy.

Remark : So, in our case, the max-likelihood estimator is the least squared estimator.

The Gauß-Newton method

The main idea of this method is to apply a Newton method to the derivate of S.

$$\theta^{(k+1)} = \theta^{(k)} - \mathrm{Hess}_{\theta^{(k)}}(S)^{-1}\mathrm{Jac}_{\theta^{(k)}}(S)$$

This isn't the relation that we can found on Wikipedia when we search "Gauß-Newton method", so we rewrite S as $S(\theta) = \sum_{i=1}^{n} r_i^2(\theta)$ we found :

$$\mathrm{Hess}_{\theta^{(k)}}(S)_{i,j} = \sum_k 2r_k \frac{\partial^2 r_k}{\partial x_i \partial x_j} + 2\frac{\partial r_k}{\partial x_i}\frac{\partial r_k}{\partial x_j}.$$

The Gauß-Newton method

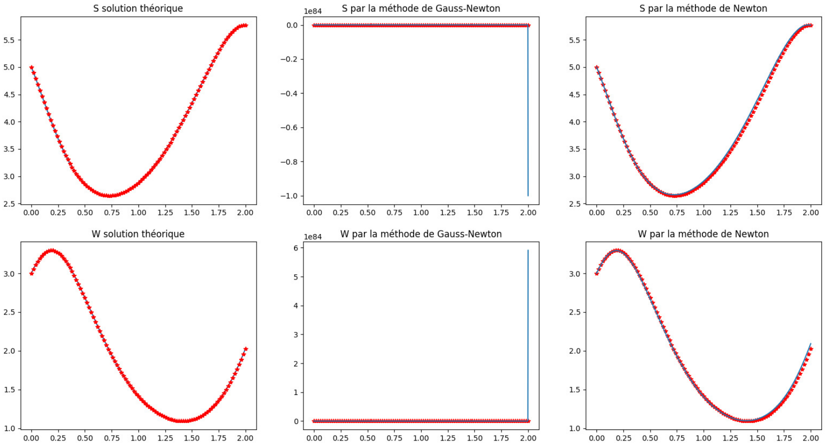
The formula that we found need the approximation (I have no main argument to justify it)

$$\left| r_k \frac{\partial^2 r_k}{\partial x_i \partial x_j} \right| \lll \left| \frac{\partial r_k}{\partial x_i} \frac{\partial r_k}{\partial x_j} \right| .$$

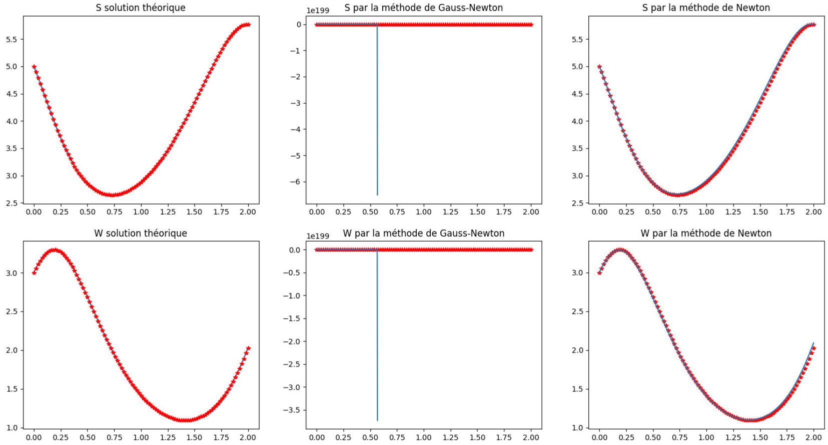
So the formula, which describes the Gauß-Newton method is :

$$\boxed{\theta^{(k+1)} = \theta^{(k)} - \left({}^t\mathrm{Jac}_{\theta^{(k)}}(\mathbf{r})\mathrm{Jac}_{\theta^{(k)}}(\mathbf{r})\right)^{-1}\mathrm{Jac}_{\theta^{(k)}}(\mathbf{r})\mathbf{r}}$$

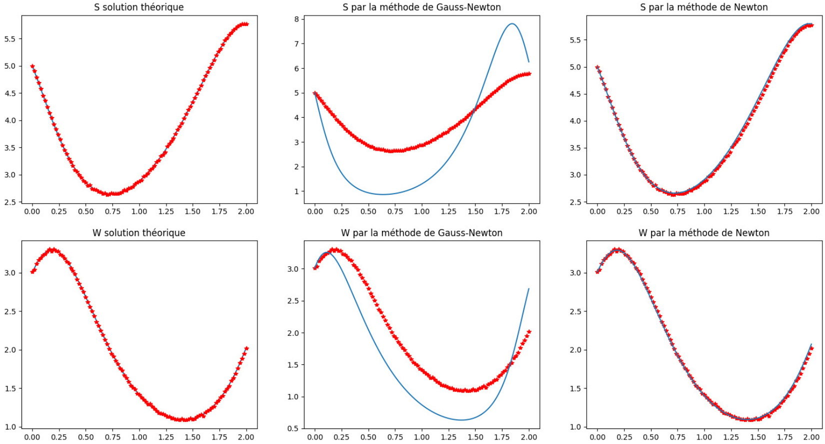
The Lotka-Volterra model without noise



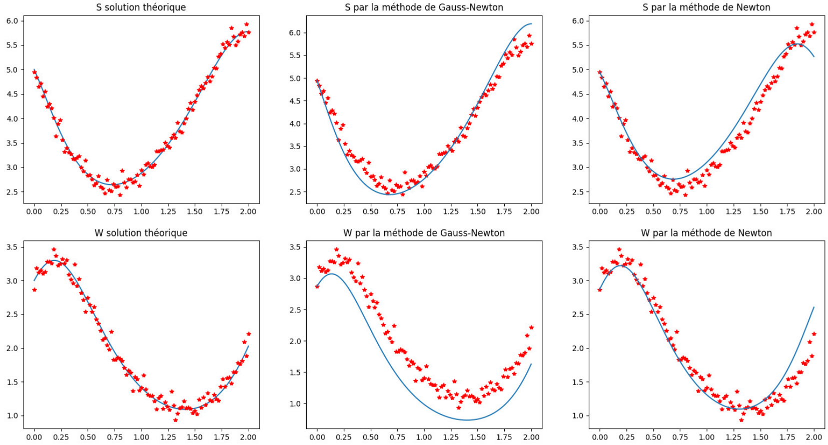
The Lotka-Volterra model with very small noise (0,001)



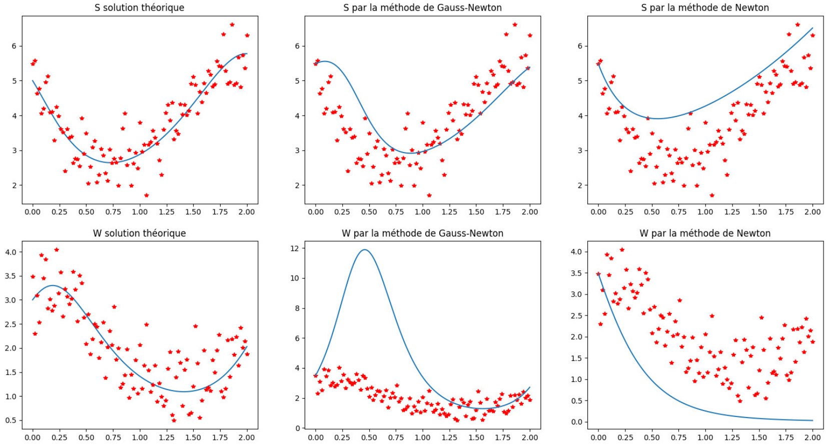
The Lotka-Volterra model with small noise (0,01)



The Lotka-Volterra model with noise (0,1)



The Lotka-Volterra model with noise (0,5)



The Gradient descent method

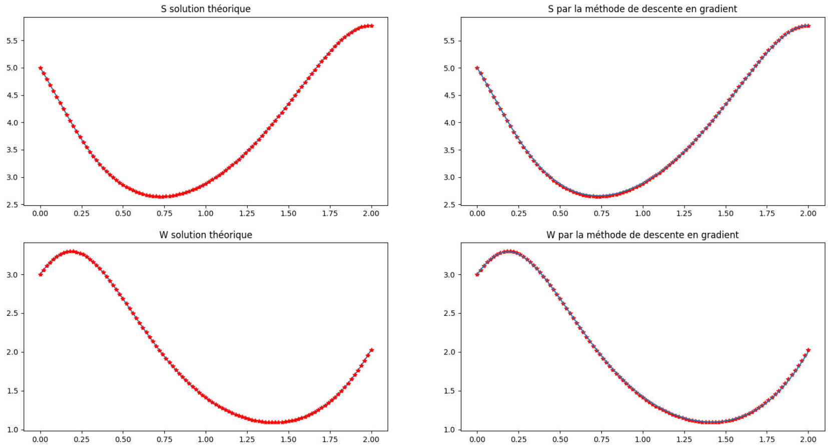
This algorithm uses this formula :

$$\boxed{\theta^{(k+1)} = \theta^{(k)} - \alpha_k \nabla_{\theta^{(k)}} S}$$

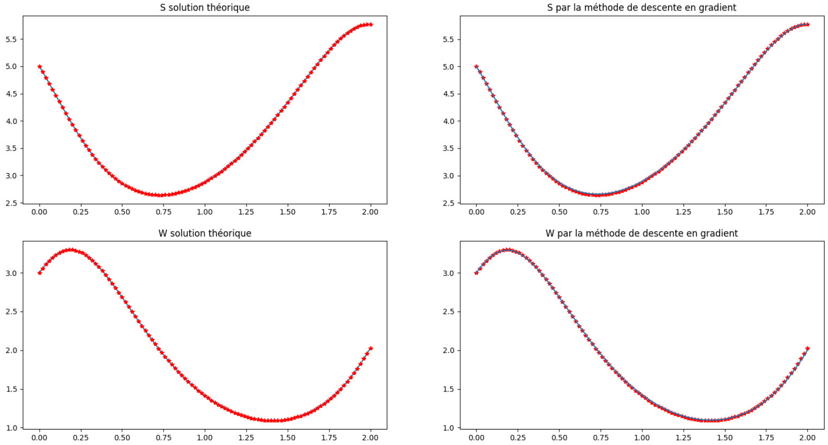
where $\nabla_{\theta^{(k)}} S$ is the gradient of S at $\theta^{(k)}$ and α_k need to be determined. We choose α_k such that :

$$\alpha_k = \arg\min_{\alpha \in \mathbb{R}} \{S(\theta^{(k)} - \alpha \nabla_{\theta^{(k)}} S)\}$$

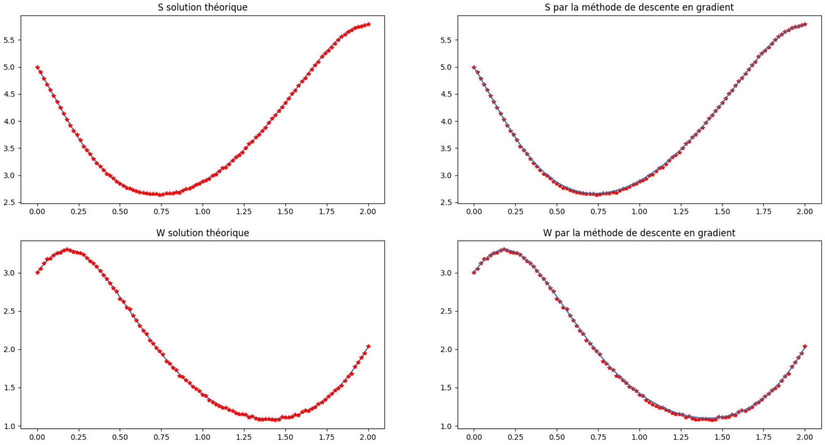
The Lotka-Volterra model without noise



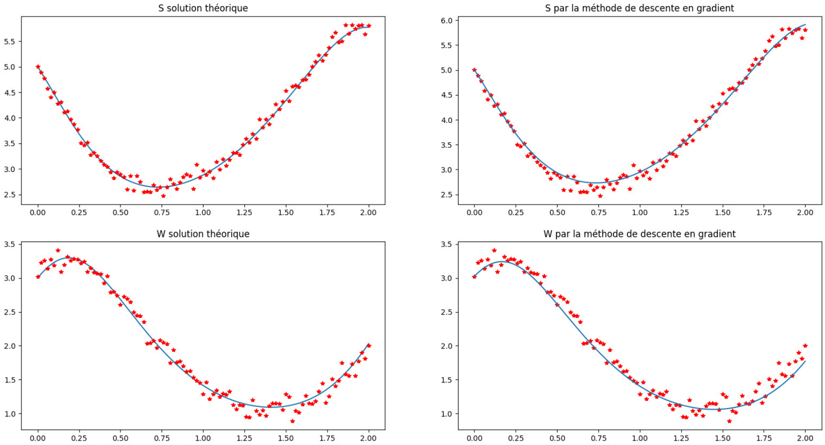
The Lotka-Volterra model with very small noise (0,001)



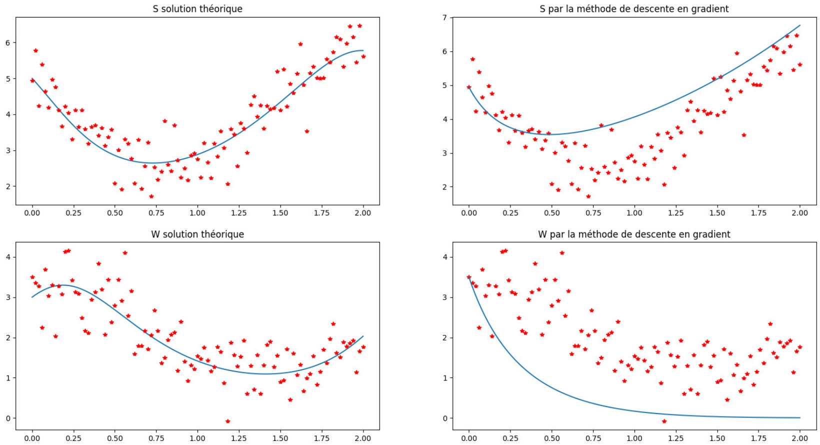
The Lotka-Volterra model with small noise (0,01)



The Lotka-Volterra model with noise (0,1)



The Lotka-Volterra model with noise (0,5)



The Levenberg-Marquardt method

If we come back to the Gauß-Newton formula and if we note $F = X - f(t, X; \theta)$ we have :

$$({}^t\mathrm{Jac}_{\theta^{(k)}}(F)\mathrm{Jac}_{\theta^{(k)}}(F))(\theta^{(k+1)} - \theta^{(k)}) = \mathrm{Jac}_{\theta^{(k)}}(F)(X - F).$$

To make the notations easier we will replace $\mathrm{Jac}_{\theta^{(k)}}(F)$ by $\mathbf{J}$. The Levenberg-Marquardt method consists to add a term (and there are two possibles) :

$$({}^t\mathbf{J}\mathbf{J} - \lambda \mathrm{Id})(\theta^{(k+1)} - \theta^{(k)}) = \mathbf{J}(X - F)$$
$$({}^t\mathbf{J}\mathbf{J} - \lambda \mathrm{diag}({}^t\mathbf{J}\mathbf{J}))(\theta^{(k+1)} - \theta^{(k)}) = \mathbf{J}(X - F)$$