Monte Carlo with Differential Equations for Fun and Profit

Monte Carlo Methods Reading Course - Final Project

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Contents

Introduction

This project provides an overview of Monte Carlo methods as applied to the field of ordinary differential equations. Monte Carlo methods are a broad class of numerical techniques. Generally speaking, they are unified by the fact that they leverage randomness [1]. Monte Carlo methods are used for Markov Chain simulation, global optimization problems, and integration problems. They are highly preferred by physicists and statisticians because of their conceptual similarity to statistical modelling.

We study two model problems which fall under the Monte Carlo umbrella: fitting parameters to a model given noisy input data by using simulated annealing, and numerically solving the realizations of a harmonic oscillator with a stochastic spring constant (an SDE). The problems chosen are meant to demonstrate the versatility and applicability of Monte Carlo to real-world problems.

Simulated Annealing

Simulated annealing algorithms are stochastic methods that are used for global optimization problems. They require very little information from the function to be optimized: only an evaluation method is needed, in contrast to gradient-descent based methods, which require a jacobian. As such, they can be used to fit parameters to models given a set of data, via the minimization of a cost function which measures the difference between the model predictions and input data.

The convergence rates of simulated annealing are not well-studied, although it is known that the basic forms of the algorithm do converge to a global optimum [2]. Simulated annealing algorithms remain highly popular in biology and other fields, precisely because of their versatility [1], [3]. They are known to perform well on problems with a high number of parameters, especially in contrast to Nonlinear Least-Squares.

In Part 1 of this project, we study the effectiveness of simulated annealing algorithms on fitting parameters for models of systems governed by differential equations. To this end we study a system of N coupled harmonic oscillators, as well as a system of N coupled Van der Pol oscillators. We derive and numerically solve the systems for fixed spring constants k_i and damping constants μ_i using an adaptive ODE solver, then artificially inject noise to the solutions. Then, we use simulated annealing to fit the generated data and compare its performance to a competitor algorithm (Nonlinear Least-Squares). We find that simulated annealing performs better than Nonlinear Least-Squares for a threshold value of $N > N_{\text{cutoff}}$, demonstrating the power of annealing for large sets of parameters.

Stochastic Differential Equations (SDEs)

SDEs are differential equations which express how a quantity changes when it depends on a random process. A model SDE is the geometric Brownian motion, which is given by

$$dX = \mu(t)Xdt + \sigma(t)XdB,$$

and has an exact solution given by

$$X(0)\exp\left(\mu t - \frac{\sigma^2}{2}t + \sigma W(t)\right).$$

SDEs are popular in finance, where they are used to model the rise and fall of stock prices and the valuation of portfolios [4]. In spite of their popularity, finding the analytic solution to many SDEs remains challenging. As such, computer simulation is a versatile first step to understanding the quantitative behaviour of a given SDE.

In Part 2 of this project, we study the numerically generated realizations of the stochastic harmonic oscillator. This is the equation of a simple harmonic oscillator whose spring constant k is a function of a Brownian motion $B(t)$ and has mean $\mu = 1$. We simulate the SDE using a form of Euler-Maruyama timestepping, a low-order numerical method whose realizations are known to converge to the true distribution in a formal sense.

We find that the resulting solution paths resemble the solution of a simple harmonic oscillator with constant $k = 1$. We also try to sample a set of paths from our SDE and to fit an SDE model with an unknown mean and standard deviation to the generated paths. We use dual annealing to fit our model, as in Part 1. To our surprise, the model is fit to the original parameters with a reasonable order-of-magnitude degree of accuracy, even with a naive implementation. The results appear to suggest that it is reasonable to fit the distribution parameters of an SDE using global optimization.

Fitting a Model of Van der Pol Oscillators with Noisy Data.

In this section we study the problem of fitting a model to data generated by a system of coupled harmonic oscillators. The generated data is inexact because it is assumed that the measurement apparatus has some uncertainty associated with it.

Derivation of the System

Suppose there are N masses with unit mass and coupled to each other by springs. When the masses are distance d apart from each other, the system is in rest position, ie. no force is exerted by any of the springs. Two boards with fixed positions $x_0 = 0$ and $x_{N+1} = (N + 1)d$ hold the system of masses in place, and there are N masses and $N + 1$ springs in total. The spring constants k_i of the ith spring may or may not be uniform.

Now consider an initial condition on the spring system where the first mass is displaced from its rest position. Then because the masses are coupled, all masses experience a force caused by the displacement of the leftmost mass. Labelling the masses $1, \ldots, i, \ldots, N$, the springs $0, \ldots, i, \ldots, N + 1$, and letting Δx_i, $F(i)$ be the displacement from rest position and force felt by mass i respectively, we find

$$F(i) = -k_{i-1} \left(\Delta x_i - \Delta x_{i-1}\right) + k_i \left(\Delta x_{i+1} - \Delta x_i\right)$$

.

For convenience we define $\Delta x_0 = \Delta x_{N+1} = 0$, which also agrees with our model if we think of the left and rightmost boards as the 0th and $N + 1$th masses, respectively. Since $F(i) = \partial_{tt} \Delta x$ is the acceleration felt by mass i we are left with a linear system of second-order ODEs.

A fairly standard transformation $x_i'' = f(t, x_i) \to [x_i' = v_i, v_i' = f(t, x)]$ converts each second-order ODE into a set of two first-order ODEs, with the independent variable being time and the dependent variables being the displacement x_i and the velocity v_i. The resulting system can then be plugged into a standard numerical ODE solver; for instance `scipy`'s `solve_ivp` method, which uses Runge-Kutta 4(5) by default [5].

The Python code for this system contains possibly too much Python-specific trivia to be of use to MATLAB users, but is available on request. Figure 1 shows a few frames of a simulation for a system of 5 masses with a uniform spring constant. In the initial condition both masses 1 and 2 are perturbed.

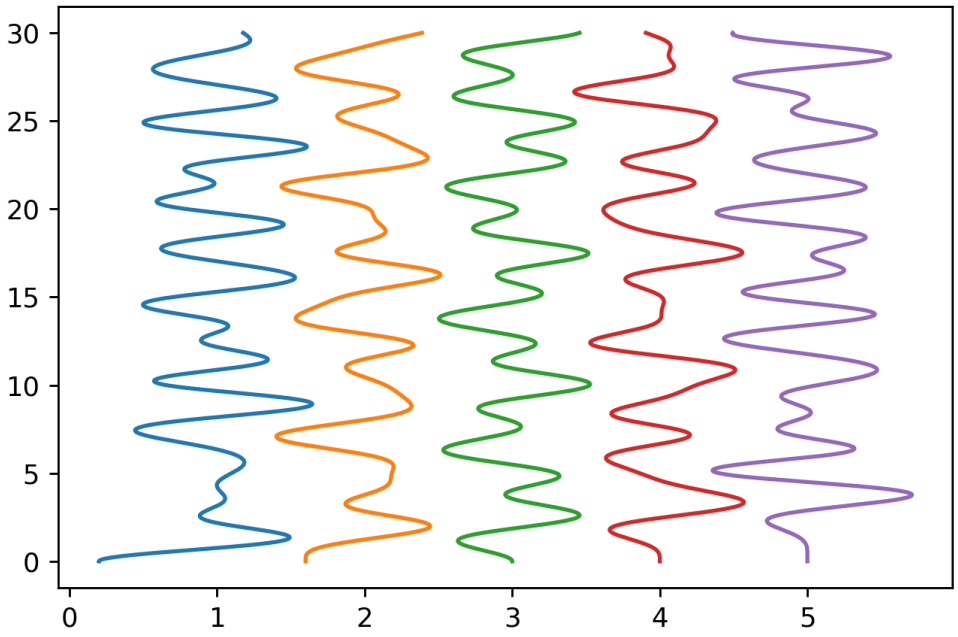


Figure 1: 5 coupled harmonic oscillators. Time is plotted on the vertical axis and the position of each mass is plotted as a curve on the horizontal axis.

The choice to use this system was inspired in part by a problem in Trefethen's *Numerical Linear Algebra* [6].

Finite Differences and the Method of Lines

As a fun fact, we notice that if the spring constants k_i are all equal to k, then the equation for the force on mass i reduces to

$$F(i) = k\left(\Delta x_{i+1} - 2\Delta x_i + \Delta x_{i-1}\right)$$

which may look similar to the second-order finite difference operator for a second derivative,

$$\partial_{xx} u(x) \approx \frac{u(x+h) - 2u(x) + u(x-h)}{(\Delta x)^2}.$$

Thus with an appropriate scaling the system of coupled springs and masses with uniform spring constants k is simply a method-of-lines approximation to the wave equation $u_{tt} = u_{xx}$ [7].

The Van der Pol Oscillator

The Van der Pol oscillator is a close relative of the simple harmonic oscillator and is often used as a first example of an ordinary differential equation with nonlinear damping [8]. In particular, the equation of a single oscillator takes the form

$$u'' - \mu(1 - u^2)u' + u = 0$$

we can compare this with the equation of the damped harmonic oscillator,

$$u'' + \mu u' + u = 0.$$

For the latter equation we know that $\mu u'$ is a damping term that causes the mass to lose energy over time, proportional to the current speed of the mass. In contrast, the nonlinear damping term $\mu(1 - u^2)$ in the Van der Pol oscillator changes sign when $u = 1$. For $u' > 1$, the system is damped, but for $u < 1$, the term actually acts as a *forcing term*, increasing the acceleration felt by the mass. For this reason, the typical long-term solutions of a Van der Pol oscillator will be a periodic wave. Experimentally, it appears that the amplitude of this wave is around 2.

In Figure 2 we show profiles of the phase plane for the damped harmonic oscillator and Van der Pol oscillator. While the damped harmonic oscillator tends towards the origin, typical trajectories of the Van der Pol oscillator tend towards a stable *limit cycle*.

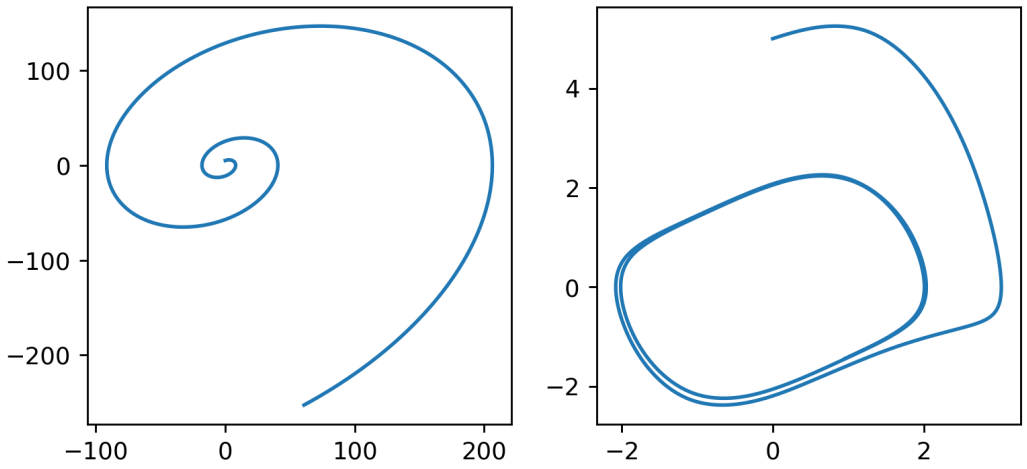


Figure 2: Phase trajectories for a damped harmonic oscillator (left) and Van der Pol oscillator (right) for an initial condition $(x, x') = (0, 5)$ and damping constant $\mu = 0.5$.

We can couple together Van der Pol oscillators in a way similar to our previous derivation for a set of coupled harmonic oscillators. Essentially, we add the nonlinear damping term to each mass in our coupled system, so that the force felt by a mass now becomes

$$F(i) = -k_{i-1}\left(\Delta x_i - \Delta x_{i-1}\right) + k_i\left(\Delta x_{i+1} - \Delta x_i\right) - \mu_i(1 - \Delta x^2)\Delta x'$$

.

Figure {3 shows the evolution of a system of coupled masses governed by the Van der Pol equation.

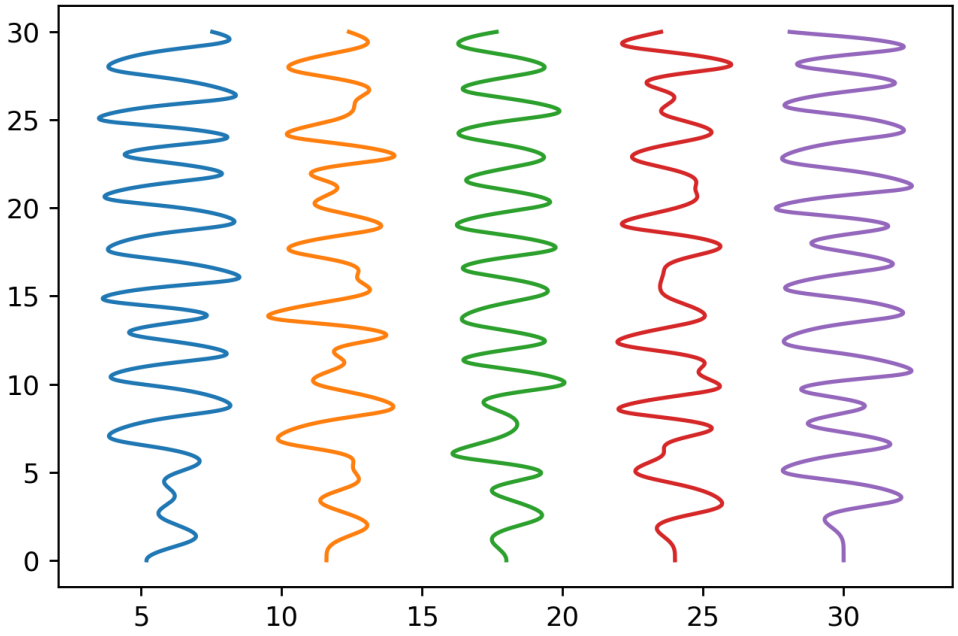


Figure 3: Initial condition for a system of coupled Van der Pol oscillators

It's worth asking whether the solution to a system of coupled Van der Pol oscillators is well-posed, i.e. whether perturbing the initial conditions drastically changes the trajectory of the solution. Finding a formal $\epsilon - \delta$ bound for this problem is beyond the scope of this project, but we can directly simulate the paths of the masses for an ϵ-ball of initial conditions around our original initial condition in the phase plane. Figure 4 shows the results of the simulation.

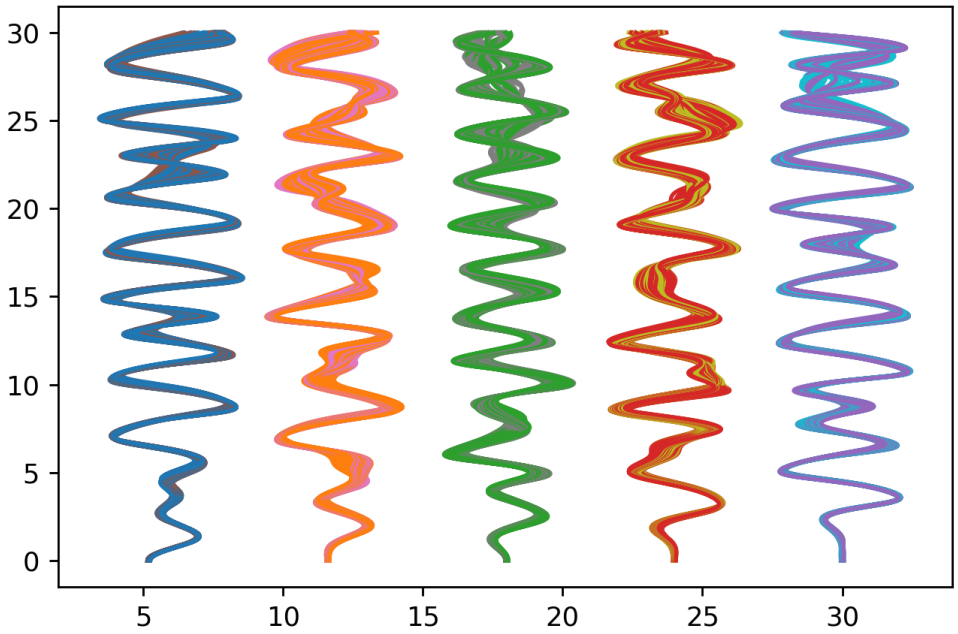


Figure 4: Plot of perturbed values for the system of Van der Pol oscillators. Here $\epsilon = 0.05$.

Our results give us confidence that it is sensible to try to fit parameters to data generated by a system of coupled Van der Pol oscillators.

Using Simulated Annealing to Fit VdP Oscillators

Now we try to fit data which has been generated from a system of Van der Pol oscillators by using simulated annealing. We use 2 types of annealing: a naive implementation of simulated annealing, and `scipy`'s dual annealing algorithm [9]. As a comparison method, we use Nonlinear Least-Squares.

The Naive Annealing Algorithm

Our Naive Annealing algorithm performs a random walk over the search space to minimize a cost function $C(x)$. Given a current position x, and a randomly sampled neighbouring state y, the probability that the annealing algorithm jumps to state y is

$$P(T, x, y) = e^{-\frac{\delta(x,y)}{T}}$$

where $\delta(x, y)$ is the (clamped) increase in cost for jumping to state y, relative to the cost at state x:

$$\delta(x, y) = \min\left(\frac{C(y) - C(x)}{C(x)}, 0\right)$$

The temperature T decays exponentially over time. The rate of decay is given by $\beta = 0.999$, and when the temperature is 0.0001, it is reset to 1. As the temperature decays, the annealing becomes more selective.

The neighbouring states are generated by sampling from a normal distribution with standard deviation 0.05. It's assumed that states are a vector in $\mathbb{R}^n$, and that Euclidean distance is a reasonable indicator of nearness. The choice of acceptance function $P(T, x, y)$ and temperature schedule were based on the exposition in Kalos and Whitlock [1].

We tested the Naive Annealing algorithm on fitting the spring constant to a harmonic oscillator with spring constant $k = 1$. The cost function, `cost(k)`, is the sum-of-squares difference between the exact solution of the ODE and the numerical solution. We use both the position and velocity data in this difference. The domain of time integration is $[0, 2\pi]$, and we take the sum-of-squares difference at 50 times uniformly spaced over the interval (the actual value of Δt for the time-marching method is small enough as to be negligible).

We summarize our results for some sample executions. A fixed number of steps $n = 2^14$ was used for each run.

Initial k	Final k	Cost	Execution Time (s)
3	0.9994	1e-5	21.3
50	10.5	70.6	65
50	38.7	72.1	102
50	27.3	71.8	94

We can discern a few things from the results: annealing finds the correct value of k with high accuracy when the initial k is nearby. The annealing seems to get stuck at local optima when the initial value of k is very far away from the true value. This might be remedied by making the 'next state' sampler more likely to choose farther away points, but doing so might also be detrimental for other problems and other initial ks. Surprisingly, the execution time seems to vary somewhat widely for the $k = 50$ runs even though the number of steps is fixed.

Based on the results above, we decided not to try using the Naive Annealing algorithm to fit our model of coupled Van der Pol oscillators.

The Coupled Van der Pol Oscillators

We simulated a system of 5 coupled Van der Pol oscillators. The spring constants for the system were chosen to be

$$k_1, \ldots, k_5 = 2.\dot{7}, 1.\dot{4}, 1.\dot{1}, 1.\dot{7}, 5.\dot{4}$$

The damping coefficients μ_i were chosen to be uniformly equal to 0.5. The system was simulated from an initial time $t = 0$ to a terminal time of $t = 8$. After solving this system numerically, we perturbed the solution using normally-distributed noise with standard deviation 0.2. The noisy data plotted in Figure 5 was the input data for the annealing algorithm.

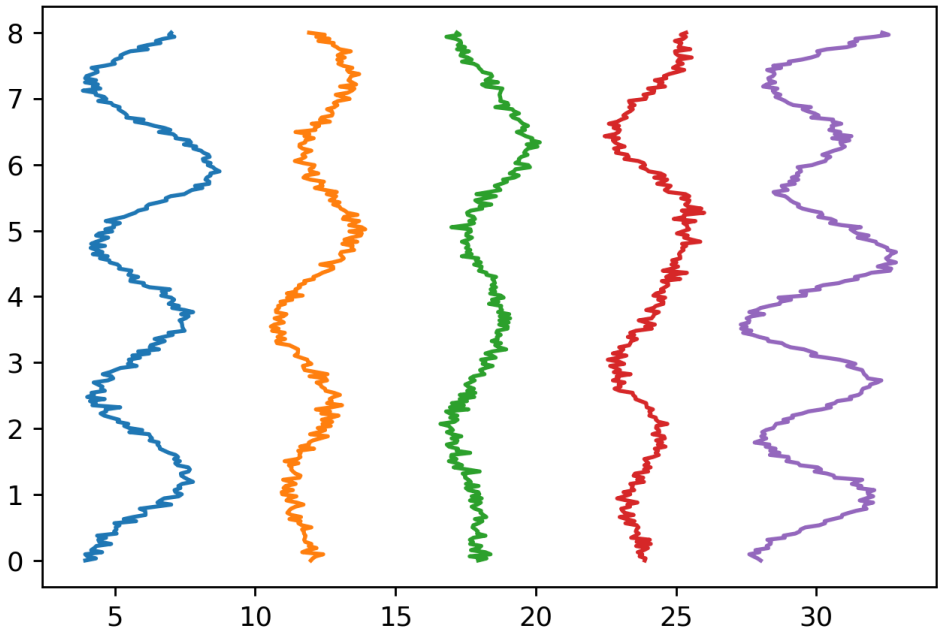


Figure 5: Input data for the optimization algorithms. Normally-distributed noise modelling measurement error has been added to the data.

The optimization algorithms were asked to fit the spring constants to the input data (the damping coefficients were given). The cost function was defined as the sum-of-squares distance between the data and the numerical solution for the candidate spring constants.

Note that it is still sensible to use the sum-of-squares distance to fit the data using annealing, even though there is no value of $k_1, \ldots, k_5$ which fits the noisy data exactly.

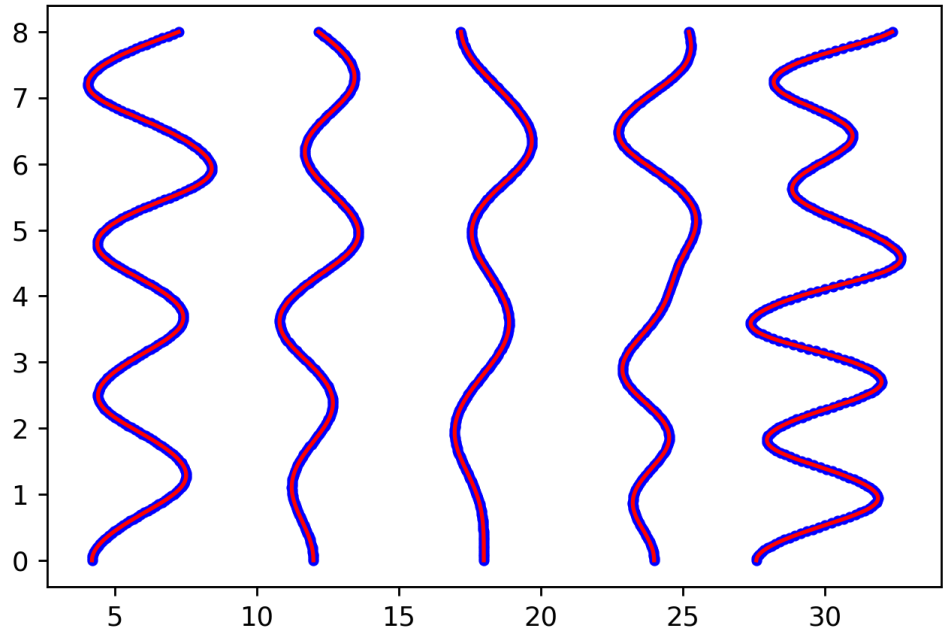
Results for Dual Annealing

Dual annealing is meant to be an accelerated version of simulated annealing, and combines performance characteristics from a 'fast' and 'slow' variant of simulated annealing. Below we present our results for 4 sample runs of using `scipy`'s dual annealing. Unlike the Naive Annealing, the `scipy` implementation of dual annealing does not require an initial state to be specified. However, upper and lower bounds for the parameters for the model must be provided. We specified that the spring constants k_i must all lie in $[0, 50]$, and that the maximum number of iterations for the algorithm was 100.

Run	k1	k2	k3	k4	k5	Error (sup norm)	Execution time
0	2.77954	1.43923	1.1143	1.77685	5.44766	0.00521917	1 min 8s
1	2.77742	1.4422	1.11535	1.77471	5.44791	0.00424044	1 min 58s
2	3.19587	0.661927	1.88541	1.96975e-06	6.06968	1.77778	4 min 5s
3	2.77818	1.44113	1.11442	1.77541	5.44777	0.00332224	3min 50s

In 3 out of 4 runs, the exact values of k_i are found with two decimal places of accuracy (in the

sup norm). In 1 out of 4 runs, a different set of k_i are found. The run time is variable between executions, although all runs used the full 100 iterations.



The exact solution (red) is overlaid onto the solution found by dual annealing (blue).

Results for Nonlinear Least-Squares

Nonlinear Least-Squares (NLS) is another optimization method, used for nonlinear cost functions. NLS finds a local optimum, and can be used repeatedly with different starting states to find a global optimum. NLS is known to be faster than annealing algorithms for low-dimensional search spaces.

We test whether finding 5 spring constants is a low enough dimension for NLS to outperform dual annealing. We present our results for 2 representative runs. The `scipy` default implementation for NLS requires an upper and lower bound for the parameters to be passed in. In the first sample run, we use the same bounds as in the dual annealing runs, $k_i \in [0, 50]$. In the second run, we use a reduced set of bounds, $k_i \in [0, 10]$. In each run, we generate an initial guess for the k_i uniformly at random, and pass this in as an argument to NLS. We do this for 10 different initial guesses, and take the best result from all 10 runs.

Run	k1	k2	k3	k4	k5	Error	Upper bound	Exec. Time
0	8.73992	24.0767	7.08632	5.30664	0.0920452	22.6322	50	3m 1s
1	2.6071	6.5433	4.59483	0.350083	5.90575	5.09885	10	1m 41

The execution time of NLS for 10 different initial guesses, with an upper bound of 50 is on the same order of magnitude as for the simulated annealing. However, NLS is not able to find a suitable set of k_i in the larger parameter space, given a similar time budget. When the search space is reduced by decreasing the upper bound on k_i, NLS is able to find a better choice of k_i.

However, the error in the sup norm for the k_i is still very high. It's worth wondering if NLS was able to find a choice of k_i that was different from the true k_i, but produced similar data. This does not appear to be so; see Figure 6 below.

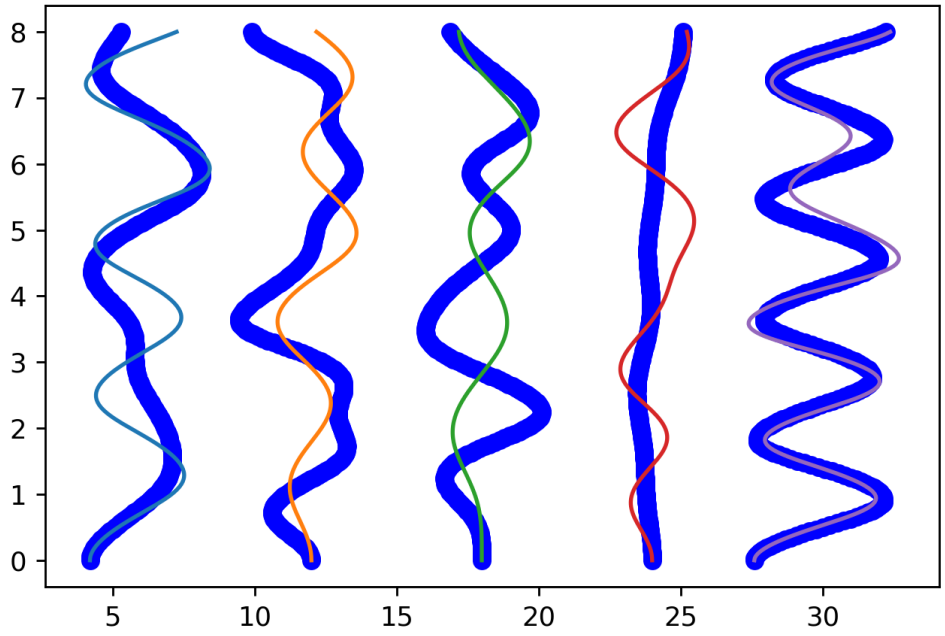


Figure 6: The exact solution to the coupled Van der Pol system (various colours) is shown along with the better solution found by NLS (thick blue).

Discussion

The results show clearly that for our modest parameter-fitting problem, dual annealing already outperforms Nonlinear Least-Squares. Dual annealing is able to find the exact values of k_i for noisy input data and a large search space with a high degree of accuracy. Nonlinear Least-Squares does much more poorly, being unable to find the exact k_i on a much smaller search space.

The fact that dual annealing found an incorrect set of k_i during one of the runs seems like a cause for alarm at first, since in an experimental setting we would not have the true values of the k_i to compare our results to. However, we can still use the cost function, as well as qualitative inspection of the resulting model, to assess the goodness of the model found by annealing.

Summary

In this section we compared the performance of dual annealing and Nonlinear Least-Squares on a parameter-fitting problem for data generated by a system of coupled Van der Pol oscillators. We found that dual annealing outperforms Nonlinear Least-Squares and is able to find the spring constants of the system to 2 decimal places of accuracy. We also profiled the performance of Naive Annealing on fitting a single spring constant for a harmonic oscillator, and derived the equations for the system of Van der Pol oscillators.

The Stochastic Harmonic Oscillator

In this section we consider the equation of a stochastic harmonic oscillator. The equation of the oscillator is given by

$$u'' = -ku$$

where the spring constant, k is now a function of a Brownian motion, such that

$$k(0) = 1,$$

$$dk = \sigma dB(t)$$

Here σ represents the 'drift' of the stochastic process governing k. We choose $\sigma = 0.1$, which is small relative to $k(0)$.[1]

Making k stochastic turns this differential equation into a *stochastic* differential equation, or SDE. It is worth noting that this stochastic formulation of the harmonic oscillator has a good amount of literature on it [10], [11]. This is probably because the equation of the simple harmonic oscillator is a model equation in physics, and is very well understood. On the other hand, the stochastic equation is difficult to solve analytically without knowledge of advanced probability and stochastic processes [3]. Thus studying the stochastic oscillator can provide us valuable insight into the behaviour of SDEs.

Additionally, the equation has a physical interpretation. For example Borret et al. [10] write that it might be reasonable to make k stochastic in order to model the effects of weak gravitational or electrical fields which may be difficult to model otherwise.

In our formulation, the drift parameter σ is small relative to the initial value. Thus we expect that on small timescales, realizations of this SDE will behave like the solutions to the equation of the simple harmonic oscillator when $k = 1$. As we increase the time of observation, however, the standard deviation of k also increases; at time t, the standard deviation of $k(t)$ is given by $0.1\sqrt{t}$. Thus for large enough t, the realizations of this SDE will begin to diverge.

The Euler-Maruyama Method

Since we don't have the tools at our disposal to perform an analytical solution for the stochastic oscillator, we turn to numerical simulations.

The Euler-Maruyama method is a time-stepping method for numerically generating realizations of an SDE. It roughly fits under the Monte Carlo class of methods because it uses random sampling. It is closely related to the forward Euler method for ODEs and has the main difference that variables which depend on the brownian motion $B(t)$ should be updated by sampling from a normal distribution with standard deviation $\sqrt{\Delta t}$.

We present Python code used to solve the equation of the harmonic oscillator below. Notice that the numerical value y_{n+1} is updated with the value of k_n, and not the value of k_{n+1}; or equivalently, the value of k is updated after updating y.

[1] We actually clamp the value of k so that it is always non-negative, making this a non-ideal Brownian motion. However the drift values and timescales we simulate on are small enough as to be negligible.

```python
def euler_maruyama(y0, t_eval, kmean, damping):
    # y0 : initial condition
    # t_eval : times to evaluate
    # kmean, damping: mean and drift of k
    y = y0
    k = kmean
    dt = t_eval[1] - t_eval[0]

    for i in range(len(t_eval)):
        f = lambda x: np.array([x[1], - k * x[0] ])
        y = y + dt * f(y) # forward Euler update

        k += damping * np.random.randn() * np.sqrt(dt)
    return y
```

As the size of the timesteps goes to 0, the Euler-Maruyama method produces realizations which are identical in distribution to the true distribution of the SDE. Higher-order methods also exist for solving SDEs, and are derived from higher-order ODE methods. However, 'higher-order' has a different meaning in numerical SDEs.

Realizations of the Stochastic Harmonic Oscillator

We plot 20 realizations of the SDE using the Euler-Maruyama time stepping method. A terminal time of $t = 10$ is used, using $10(2^10)$ timesteps ($\Delta t \approx 9.76e - 5$).

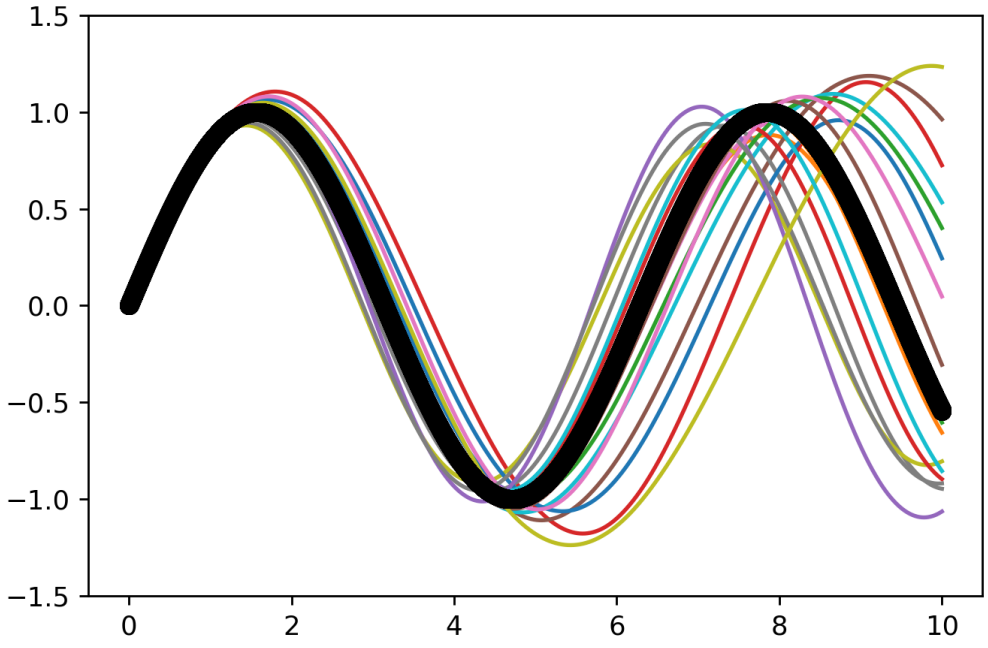


Figure 7: 20 realizations of the stochastic harmonic oscillator. The solution to the corresponding simple harmonic oscillator is in black.

If we increase the terminal time to $t = 100$, but use the same number of timesteps, some of the

realizations ‘blow up’ – the amplitude increases.

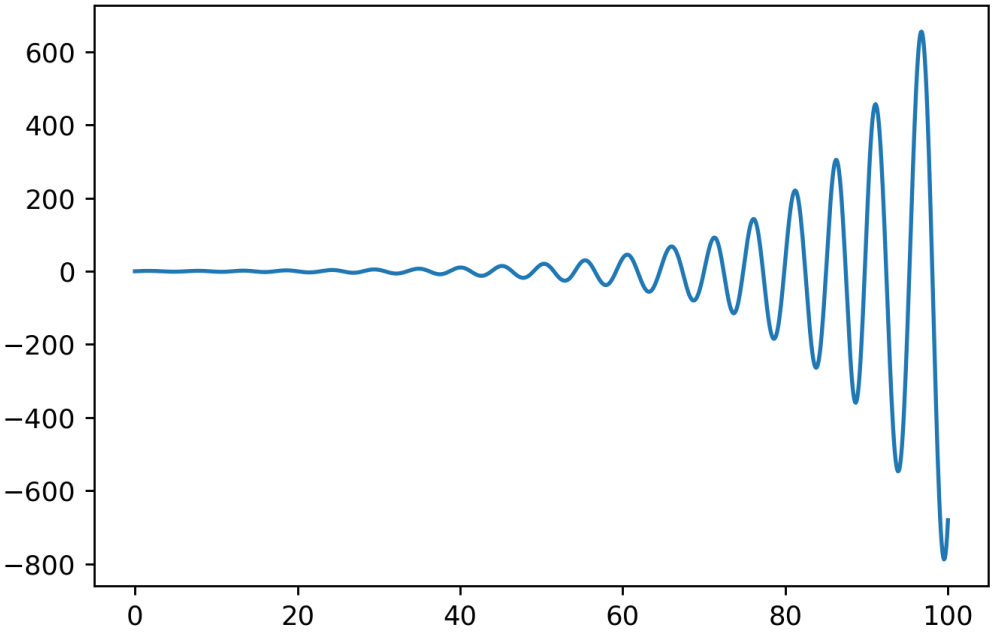


Figure 8: Realization of stochastic harmonic oscillator with terminal time 100. The amplitude of the solution increases due to numerical error.

Since k controls the *frequency* of the oscillator in the equation of the simple harmonic oscillator, and not the amplitude, we don’t expect the realizations of the SDE to blow up in amplitude. Prof. Stinchcombe notes that this may be occuring because of the instability of the forward Euler method, since we are now using larger values of Δt. If we increase the number of timesteps so that $\Delta t \approx 9.76e-5$, then we do not see the blow-up in the realizations.

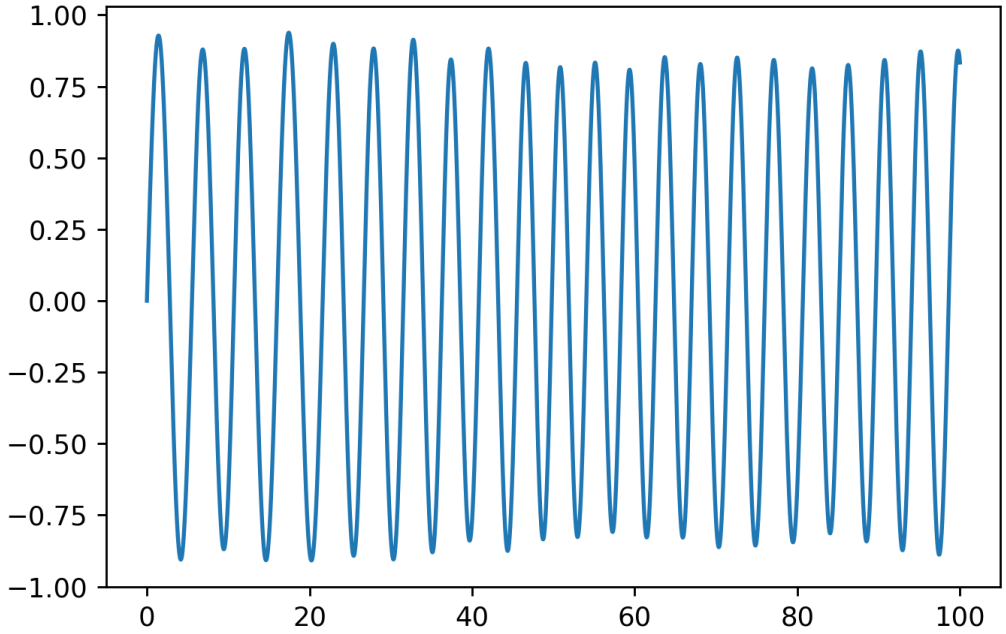


Figure 9: Realization of stochastic harmonic oscillator with terminal time 100.

Using Simulated Annealing to Fit the SDE

Bringing both parts of the project together, we try to fit the mean and drift of the spring constant k by using dual annealing. To do this, we define a cost function with the following procedure:

1. Sample 20 realizations of the SDE for a k with mean 1 and standard deviation 0.10.
2. For each candidate value k': 2i. Sample 32 realizations of the SDE with spring constant k', with mean μ and drift σ. 2ii. Compute the cost as the sum-of-squares difference between each of the 32 sampled solutions for k' with each of the 20 sampled solutions for k.
3. Use (2) as the cost function for dual annealing.

Results

Our results for 3 runs of dual annealing are presented below. We use a modest computational budget of 20 iterations for the annealing; however, we restrict the search space as well, specifying $\mu \in [0, 2]$ and $\sigma \in [0, 1]$.

Run	μ	σ	Error in μ	Error in σ	Execution time
0	1.01936	0.0114919	0.0193628	0.0885081	5min 6s
1	0.998614	0.0227675	0.0013859	0.0772325	2min 42s
2	0.976937	0.108667	0.0230635	0.00866725	2min 59s

Surprisingly, annealing finds values of μ with 1 decimal place of accuracy. The estimate of σ is considerably worse.

Discussion

In spite of our cost function being *ad hoc*, simulated annealing performs reasonably well at fitting μ. It does worse at fitting σ, and seems to be biased towards fitting smaller values of σ. We could try sampling more realizations of the true SDE and also of the SDEs used in the evaluation of the cost function to get better results.

Summary

In this section we have studied the equation of a harmonic oscillator with stochastic spring constant. We computed numerical realizations to the SDE, and some of the pitfalls associated with using the Euler-Maruyama method to do so. We examined the qualitative behaviour of realizations to the equation and found that they are similar to the solution to the simple harmonic oscillator. Finally, we attempted to fit the mean and standard deviation of k for an SDE model using dual annealing. Much to our surprise, we found that dual annealing worked reasonably well.

Conclusions

Monte Carlo methods are a broad and powerful class of methods which incorporate random sampling. Although introducing randomness can make it more difficult to reason about these methods, their versatility and ease-of-use makes them highly appealing. In this project, we have found that Monte Carlo methods can fit parameters to models extremely well, even when the input data is noisy or the model is stochastic in nature. Additionally, Monte Carlo methods allow us to derive insights about stochastic differential equations experimentally. We conclude that Monte Carlo methods should be seriously considered for experimental data fitting problems, and are a valuable addition to any applied mathematician's toolkit.

Implementation Notes

The code for this project was written in Python 3. Benchmarks were performed on an X1 Carbon laptop with a modern multi-threaded processor and 16GiB of memory.

Acknowledgements

This project would not have been possible without the advice and support of Professor Adam Stinchcombe, who agreed to be my advisor for this reading course. Thanks are also to Belal and Gonzalo, who sat in the course with me.

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