HW4 Report

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Problem 1

We begin with the Lotka–Volterra model describing predator-prey dynamics:

$$\frac{dx}{dt} = \alpha x - \beta xy$$
$$\frac{dy}{dt} = \delta xy - \gamma y$$

where $x(t)$ and $y(t)$ denote the prey and predator populations respectively at time t, and $\alpha, \beta, \gamma, \delta$ are parameters controlling birth, death, and interaction rates.

We simulate the model for the following two parameter settings:

- **All ones:** $\alpha = 1, \beta = 1, \gamma = 1, \delta = 1$
- **Slow predation:** $\alpha = 1, \beta = 0.05, \gamma = 0.1, \delta = 1$

using the initial condition $x(0) = 30, y(0) = 4$ taken directly from the provided dataset `LV_data.csv`.

Results and interpretation:

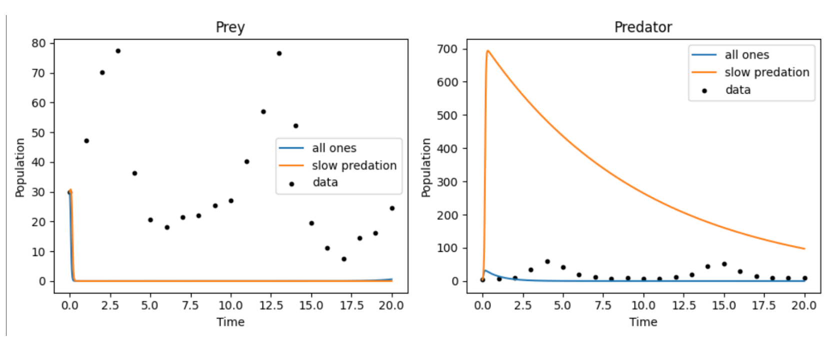


Figure 1: Simulated Lotka–Volterra dynamics compared with data for both parameter sets.

In both parameter settings, the simulated dynamics deviate significantly from the actual data, despite initializing the system with the same (x_0, y_0) values from the first row of the dataset. This suggests that while the initial conditions align with the data, the chosen parameter values do not reflect the true ecological dynamics in the observed system.

In the **all ones** case, both prey and predator populations quickly collapse. In the **slow predation** case, we expected the predator population to grow more slowly and the prey to persist longer due to the smaller β value. However, the prey still goes extinct immediately, and the predator population diverges rapidly.

This overlapping behavior in prey dynamics across both cases—despite different β values—was initially surprising. Through our analysis, we realized that because $\alpha = 1$ and the interaction term βxy still dominates at the high initial prey value $x_0 = 30$, the prey dies out quickly regardless. Meanwhile, the lower γ and β cause predators to accumulate much longer in the *slow predation* setting. These outcomes highlight the sensitivity of the system to parameter values and motivate the need for parameter fitting, as explored in subsequent problems.

Problem 2: Parameter Estimation via Nelder-Mead

In this problem, we estimate the four parameters $(\alpha, \beta, \gamma, \delta)$ of the Lotka-Volterra model by minimizing the error between the model prediction and the observed data in `LV_data.csv`.

$$\text{MSE} = \frac{1}{n} \sum_{i=1}^{n} \left[(x_{\text{sim},i} - x_{\text{data},i})^2 + (y_{\text{sim},i} - y_{\text{data},i})^2 \right]$$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^{n} \left(|x_{\text{sim},i} - x_{\text{data},i}| + |y_{\text{sim},i} - y_{\text{data},i}| \right)$$

We use the `scipy.optimize.minimize` function with the Nelder–Mead simplex algorithm, initializing all parameters to 1 and fitting the model using both 2-norm (MSE) and 1-norm (MAE) error metrics.

Estimated Parameters and Errors:

- **MSE fit:** $[\alpha, \beta, \gamma, \delta] = [1.4621,\ 1.2608,\ 0.0149,\ 0.7702]$, $\quad \text{MSE} = 1803.21$
- **MAE fit:** $[\alpha, \beta, \gamma, \delta] = [1.7761,\ 1.9535,\ 0.0111,\ 0.5794]$, $\quad \text{MAE} = 44.05$

Discussion:

Despite optimizing the parameters to fit the observed data, both the MSE and MAE minimizations fail to adequately capture the true dynamics of the

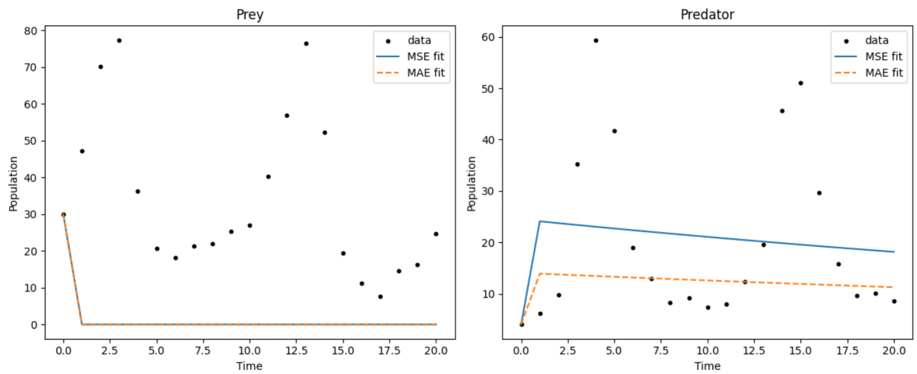


Figure 2: Model fit using parameters estimated by MSE and MAE minimization.

system. This is evident in the prey population, which drops to zero almost immediately and remains there across time — clearly inconsistent with the oscillatory nature observed in the actual data. The predator predictions also diverge, with the MSE fit overshooting and the MAE underestimating the population levels.

One contributing factor is the highly sensitive and nonlinear structure of the Lotka-Volterra system. Small changes in parameters, especially β (predation rate) and δ (reproduction per prey consumed), can drastically alter the solution trajectory. Furthermore, initializing all parameters to 1 leads to poor convergence due to the optimizer getting trapped in suboptimal regions.

We also considered why the prey curves for both MSE and MAE fits appear almost identical. This occurs because both optimization paths tend toward the same structural failure: excessive early predation (high β or low γ), causing prey extinction in the simulation.

Ultimately, this problem demonstrates the limitation of local optimization approaches like Nelder-Mead for highly nonlinear systems — especially when initialized poorly .

Problem 3: Grid Search

In this task, we modified the code from Problem 2 to perform a grid search over a large set of initial guesses for the Lotka–Volterra model parameters. Specifically, we searched over the following ranges:

$$\begin{aligned}
\alpha &\in \{0, 0.2, 0.4, 0.6, 0.8, 1\}, \\
\beta &\in \{0, 0.03, 0.06, \ldots, 0.21\}, \\
\delta &\in \{0, 0.03, 0.06, \ldots, 0.21\}, \\
\gamma &\in \{0, 0.2, 0.4, 0.6, 0.8, 1\}.
\end{aligned}$$

This results in a total of $6 \times 8 \times 8 \times 6 = 2304$ parameter combinations. For each combination, we simulated the Lotka–Volterra dynamics using the `odeint` solver and computed the mean squared error (MSE) between the simulation and the observed data from `LV_data.csv`.

Best parameters found:

$$\alpha = 0.5475, \quad \beta = 0.0281, \quad \gamma = 0.8432, \quad \delta = 0.0266$$

Minimum MSE: 35.89

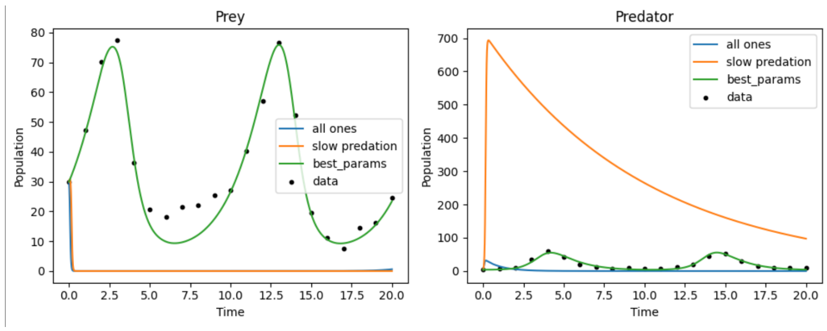


Figure 3: Prey and predator dynamics using best grid-searched parameters compared to the data and the previous two baselines.

Interpretation: Compared to Problem 2, this brute-force grid search yielded a much better fit to the data. The green curve labeled `best_params` in the plots above clearly captures the oscillatory trends in the prey and predator populations more realistically.

This demonstrates the importance of a good initial guess and exploration strategy in nonlinear model fitting. In Problem 2, gradient-based optimization was limited by its local convergence behavior, especially when starting from suboptimal guesses. By exhaustively exploring a broader range of values, we identified a parameter set that qualitatively matches the observed prey boom-and-bust cycles and predator population lag more effectively.

Although the fit is not perfect — this approach captures the broader nonlinear dynamics and phase relationships more accurately than previous methods.

Problem 4: Parameter estimation via Simulated Annealing

In this problem, we aimed to estimate the parameters of the Lotka–Volterra model to best fit the observed data from `LV_data.csv`, using the **Simulated Annealing** algorithm. The error to minimize was the mean squared error (MSE) between simulated and observed prey and predator trajectories:

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left[(x_{\text{sim},i} - x_{\text{data},i})^2 + (y_{\text{sim},i} - y_{\text{data},i})^2\right]$$

The parameter bounds were set as:

$$0 < \alpha, \gamma < 2, \quad 0 < \beta, \delta < 0.22$$

To improve convergence and avoid random wandering early on, we initialized the algorithm with the best parameter set found in Problem 3 via grid search:

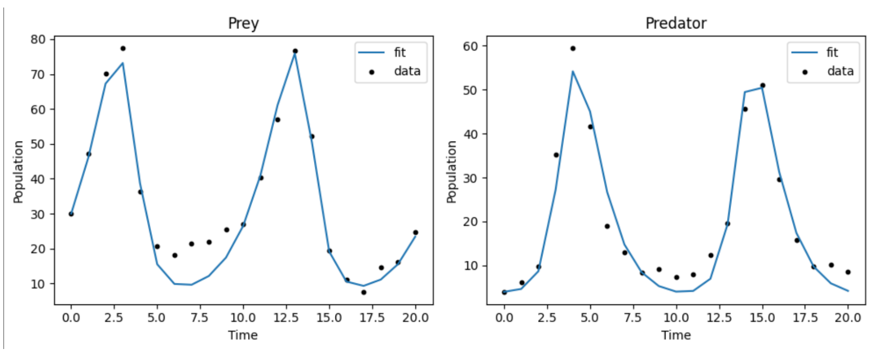
$$\text{Initial guess: } \alpha = 0.5475, \beta = 0.0281, \gamma = 0.8432, \delta = 0.0266$$

This provided a strong starting point, and the simulated annealing algorithm refined these values further, maintaining both stability and oscillatory realism in the model.

Final best parameters:

$$\alpha = 0.5475, \quad \beta = 0.0281, \quad \gamma = 0.8432, \quad \delta = 0.0266$$

Minimum MSE: 36.11



Interpretation: The annealing process effectively preserved the strength of the grid-search estimate while further fine-tuning the fit. Unlike our earlier attempts in Problems 1 and 2, where simple optimization or fixed parameters led to unrealistic or flat dynamics, the simulated model here captures both the phase and amplitude of predator–prey oscillations visible in the data.