Lesson 2: Exercises on Simulation of Stochastic Dynamic Models

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This document contains worked solutions to the exercises from Lesson 2 on simulation of stochastic dynamic models, implemented using `pypomp`.

Import Required Packages

```
import jax.numpy as jnp
import jax
import pandas as pd
import numpy as np
import pypomp as pp
import matplotlib.pyplot as plt
import io
import requests
```

Load the Consett Measles Data

```python
# Download and prepare data
meas = (pd.read_csv(
          "https://kingaa.github.io/sbied/stochsim/Measles_Consett_1948.csv")
          .loc[:, ["week", "cases"]]
          .rename(columns={"week": "time", "cases": "reports"})
          .set_index("time")
          .astype(float))

ys = meas.copy()
ys.columns = pd.Index(["reports"])
```

Define Helper Functions

```python
def nbinom_logpmf(x, k, mu):
    """Log PMF of NegBin(k, mu) that is robust when mu == 0."""
    x = jnp.asarray(x)
    k = jnp.asarray(k)
    mu = jnp.asarray(mu)
    # Handle mu == 0 separately
    logp_zero = jnp.where(x == 0, 0.0, -jnp.inf)
    safe_mu = jnp.where(mu == 0.0, 1.0, mu)  # Dummy value, ignored
    core = (jax.scipy.special.gammaln(k + x)
            - jax.scipy.special.gammaln(k)
            - jax.scipy.special.gammaln(x + 1)
            + k * jnp.log(k / (k + safe_mu))
            + x * jnp.log(safe_mu / (k + safe_mu)))
    return jnp.where(mu == 0.0, logp_zero, core)

def rnbinom(key, k, mu):
    """Sample from NegBin(k, mu) via Gamma-Poisson mixture."""
    key_g, key_p = jax.random.split(key)
    lam = jax.random.gamma(key_g, k) * (mu / k)
    return jax.random.poisson(key_p, lam)
```

Problem Statement

What is the link between little o notation and the derivative? Explain why

$$f(x+\delta) = f(x) + \delta\, g(x) + o(\delta)$$

is the same statement as

$$\frac{df}{dx} = g(x).$$

What considerations might help you choose which of these notations to use?

Solution I

We combine the equation

$$f(x+\delta) = f(x) + \delta\, g(x) + o(\delta),$$

with the definition that $h(\delta) = o(\delta)$ means

$$\lim_{\delta \to 0} \frac{h(\delta)}{\delta} = 0.$$

Rearranging, we see that

$$\lim_{\delta \to 0} \frac{f(x+\delta) - f(x)}{\delta} = g(x)$$

which, by definition, implies that $df(x)/dx = g(x)$.

Solution II

Key Insight: Little-o notation is compact, and so is useful for simplifying complex expressions.

When to use which notation:

- Use derivative notation ($\frac{df}{dx} = g(x)$) when working with deterministic, continuous dynamics
- Use little-o notation when working with stochastic processes, particularly Markov chains, where discrete transitions happen over small time intervals δ

Problem Statement I

A widely used exact simulation method for continuous-time Markov chains is Gillespie's algorithm. We do not emphasize it here. **Why?**

When would you prefer an implementation of Gillespie's algorithm to an Euler solution?

Solution I

Why we don't emphasize Gillespie's algorithm:

For reasons explained in the lesson, scientific conclusions may not hinge on the extent to which numerical approximations agree with exact solutions of the equations defining a continuous-time model.

For constant-rate compartmental models, the Gillespie algorithm gives an **exact** solution at the expense of additional computation time. We may on occasion want an exact simulator, and in that case Gillespie can be used.

Solution II

When to prefer Gillespie's algorithm:

1. When population sizes are **small** (Gillespie is exact but slow for large populations)
2. When event rates are **low** (fewer events to simulate)
3. When **exact** stochastic realizations are scientifically important
4. When you need to avoid **discretization artifacts** from Euler methods

Solution III

When to prefer Euler methods:

1. **Large populations**: Gillespie becomes impractically slow
2. **Environmental stochasticity**: Euler handles this naturally, Gillespie does not
3. **Observation times**: Euler naturally aligns with fixed observation intervals
4. **Computational efficiency**: Euler is generally faster for practical applications
5. **Tau-leaping**: A variant that bridges both approaches

Numerically, Gillespie's algorithm is often approximated using so-called tau-leaping methods, which are closely related to Euler's approach.

Problem Statement

Fiddle with the parameters to see if you can find a model for which the data are a more plausible realization.

Baseline SIR Model Setup I

First, let's set up the baseline SIR model from the lesson:

Baseline SIR Model Setup II

```
def rinit(theta_, key, covars, t0):
    """Initial state simulator for SIR model."""
    N = theta_["N"]
    eta = theta_["eta"]
    S0 = jnp.round(N * eta)
    I0 = 1.0
    R0 = jnp.round(N * (1 - eta)) - 1.0
    H0 = 0.0  # Accumulator for true incidence
    return {"S": S0, "I": I0, "R": R0, "H": H0}

def rproc(X_, theta_, key, covars, t, dt):
    """Process simulator for SIR model with Euler-binomial scheme."""
    S, I, R, H = X_["S"], X_["I"], X_["R"], X_["H"]
    Beta = theta_["Beta"]
    mu_IR = theta_["mu_IR"]
    N = theta_["N"]

    p_SI = 1.0 - jnp.exp(-Beta * I / N * dt)
    p_IR = 1.0 - jnp.exp(-mu_IR * dt)

    key_SI, key_IR = jax.random.split(key)
    dN_SI = jax.random.binomial(key_SI, n=S.astype(jnp.int32), p=p_SI)
    dN_IR = jax.random.binomial(key_IR, n=I.astype(jnp.int32), p=p_IR)
```

Helper Function for Simulation and Plotting

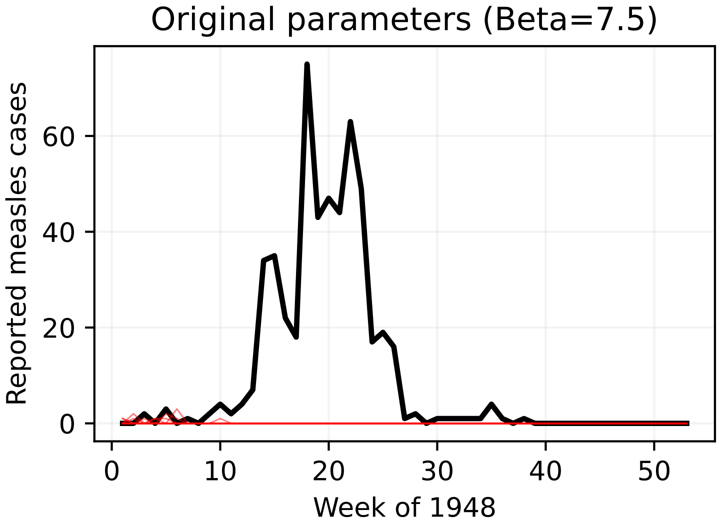
```python
def run_simulation_and_plot(theta, title="SIR simulation", n_sims=20):
    """Create SIR model, run simulations, and plot results."""

    statenames = ["S", "I", "R", "H"]

    sir_obj = pp.Pomp(
        rinit=rinit,
        rproc=rproc,
        dmeas=dmeas,
        rmeas=rmeas,
        ys=ys,
        theta=theta,
        statenames=statenames,
        t0=0.0,
        nstep=7,
        accumvars=(3,),
        ydim=1,
        covars=None
    )

    key = jax.random.key(42)
    X_sims, Y_sims = sir_obj.simulate(key=key, nsim=n_sims)

    sim_df = Y_sims.pivot_table(
```

Attempt 1: Original Parameters I

The original parameters from the lesson produce simulations where the outbreak is too small and dies out too quickly:

```
theta_original = {
    "Beta": 7.5,       # Transmission rate (per week)
    "mu_IR": 0.5,      # Recovery rate (per week)
    "N": 38000.0,      # Population size
    "eta": 0.03,       # Initial susceptible fraction
    "rho": 0.5,        # Reporting probability
    "k": 10.0          # Overdispersion parameter
}

_ = run_simulation_and_plot(theta_original, "Original parameters (Beta=7.5)")
```

Attempt 1: Original Parameters II

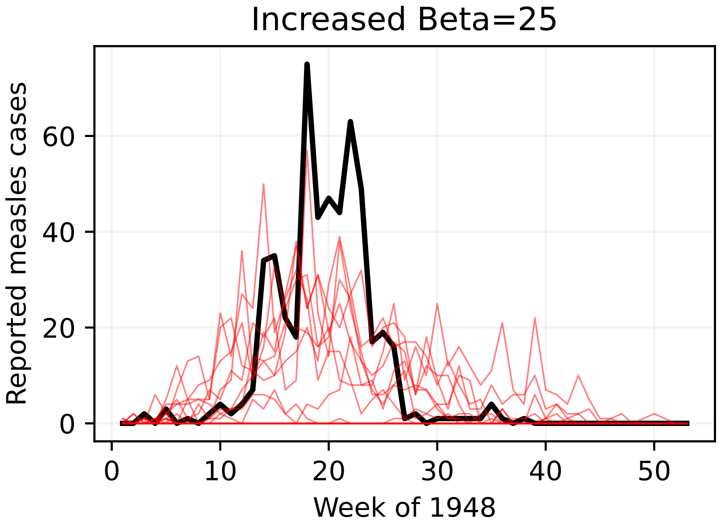


Attempt 2: Increase Force of Infection I

Let's try increasing β to increase the overall incidence:

```
theta_test1 = {
    "Beta": 25.0,     # Increased transmission rate
    "mu_IR": 0.5,
    "N": 38000.0,
    "eta": 0.03,
    "rho": 0.5,
    "k": 10.0
}

_ = run_simulation_and_plot(theta_test1, "Increased Beta=25")
```

Attempt 2: Increase Force of Infection II



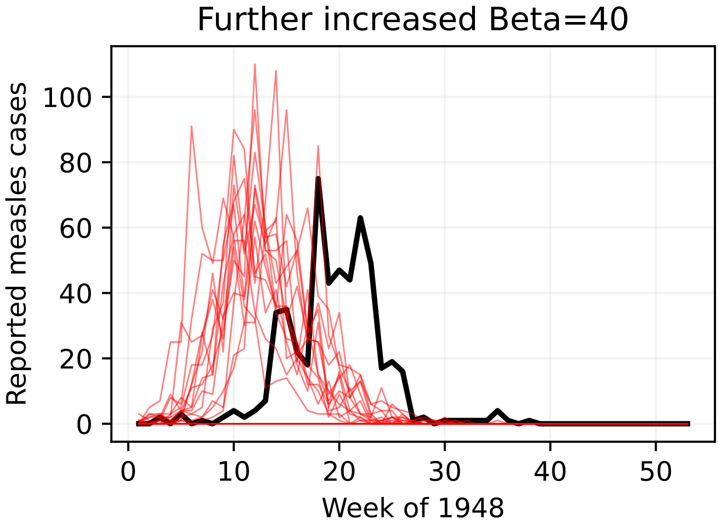
Attempt 2: Increase Force of Infection III

This produces larger outbreaks, but they may still be too short.

Attempt 3: Further Increase Beta I

```python
theta_test2 = {
    "Beta": 40.0,    # Further increased transmission rate
    "mu_IR": 0.5,
    "N": 38000.0,
    "eta": 0.03,
    "rho": 0.5,
    "k": 10.0
}

_ = run_simulation_and_plot(theta_test2, "Further increased Beta=40")
```

Attempt 3: Further Increase Beta II

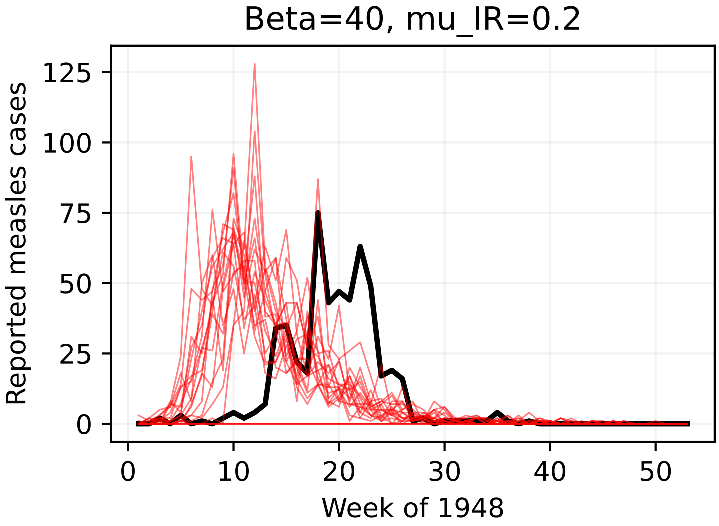


Attempt 4: Adjust Recovery Rate I

Let's try decreasing μ_{IR} (longer infectious period):

```python
theta_test3 = {
    "Beta": 40.0,
    "mu_IR": 0.2,    # Decreased recovery rate (longer infectious period)
    "N": 38000.0,
    "eta": 0.03,
    "rho": 0.5,
    "k": 10.0
}

_ = run_simulation_and_plot(theta_test3, "Beta=40, mu_IR=0.2")
```

Attempt 4: Adjust Recovery Rate II

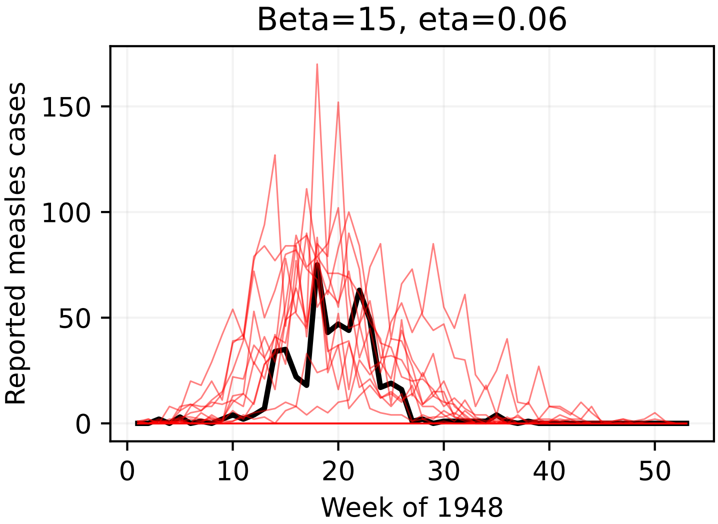


Attempt 5: Increase Susceptible Fraction I

Let's try increasing the initial susceptible fraction η:

```
theta_test4 = {
    "Beta": 15.0,
    "mu_IR": 0.5,
    "N": 38000.0,
    "eta": 0.06,     # Doubled susceptible fraction
    "rho": 0.5,
    "k": 10.0
}

_ = run_simulation_and_plot(theta_test4, "Beta=15, eta=0.06")
```

Attempt 5: Increase Susceptible Fraction II



Summary of Exploration

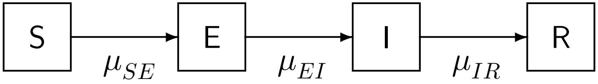
Different parameter combinations affect the outbreak dynamics:

Parameter	Effect of Increasing
β (Beta)	Faster spread, higher peak, shorter duration
μ_{IR}	Faster recovery, shorter outbreaks
η	More susceptibles, larger outbreaks
ρ	More cases reported (observation only)
k	Less overdispersion in observations

Finding parameters that match the data well requires systematic fitting methods (covered in later lessons).

Problem Statement I

Below is a diagram of the so-called SEIR model. This differs from the SIR model in that infected individuals must pass a period of latency before becoming infectious.



$$\begin{tikzcd} \boxed{S} \arrow[r, "\mu_{SE}"'] & \boxed{E} \arrow[r, "\mu_{EI}"'] & \boxed{I} \arrow[r, "\mu_{IR}"'] & \boxed{R} \end{tikzcd}$$

Problem Statement II

Task: Modify the codes above to construct a `Pomp` object containing the Consett measles data and an SEIR model. Perform simulations as above and adjust parameters to get a sense of whether improvement is possible by including a latent period.

SEIR Model Components I

First, we define the initial state simulator for the SEIR model:

```python
def seir_rinit(theta_, key, covars, t0):
    """Initial state simulator for SEIR model."""
    N = theta_["N"]
    eta = theta_["eta"]
    S0 = jnp.round(N * eta)
    E0 = 0.0   # No initial exposed individuals
    I0 = 1.0   # Start with one infectious
    R0 = jnp.round(N * (1 - eta)) - 1.0
    H0 = 0.0   # Accumulator for true incidence
    return {"S": S0, "E": E0, "I": I0, "R": R0, "H": H0}
```

SEIR Model Components II

Now the process simulator, which includes the additional E (exposed) compartment:

SEIR Model Components III

```
def seir_rproc(X_, theta_, key, covars, t, dt):
    """Process simulator for SEIR model with Euler-binomial scheme."""
    # Unpack state
    S, E, I, R, H = X_["S"], X_["E"], X_["I"], X_["R"], X_["H"]

    # Unpack parameters
    Beta = theta_["Beta"]
    mu_EI = theta_["mu_EI"]  # Rate of leaving E (1/latent period)
    mu_IR = theta_["mu_IR"]  # Rate of leaving I (1/infectious period)
    N = theta_["N"]

    # Transition probabilities (exponential form)
    p_SE = 1.0 - jnp.exp(-Beta * I / N * dt)  # S -> E
    p_EI = 1.0 - jnp.exp(-mu_EI * dt)         # E -> I
    p_IR = 1.0 - jnp.exp(-mu_IR * dt)         # I -> R

    # Draw transitions
    key_SE, key_EI, key_IR = jax.random.split(key, 3)
    dN_SE = jax.random.binomial(key_SE, n=S.astype(jnp.int32), p=p_SE)
    dN_EI = jax.random.binomial(key_EI, n=E.astype(jnp.int32), p=p_EI)
    dN_IR = jax.random.binomial(key_IR, n=I.astype(jnp.int32), p=p_IR)

    # Update state
    S_new = S - dN_SE
```

Helper Function for SEIR Simulations I

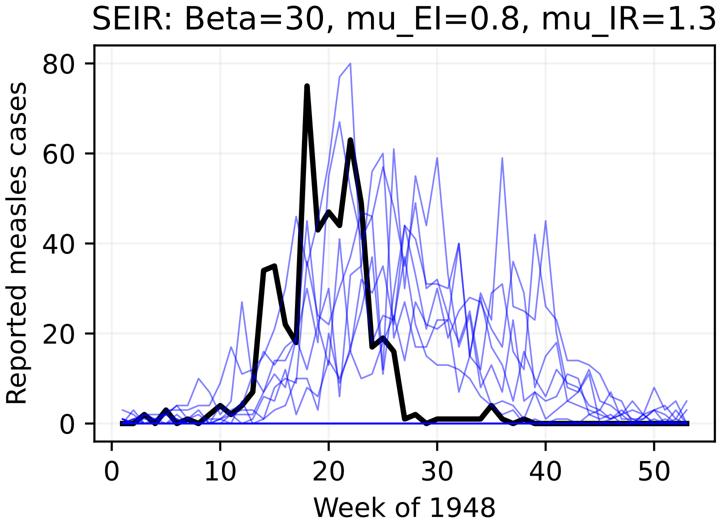
Helper Function for SEIR Simulations II

```python
def run_seir_simulation_and_plot(theta, title="SEIR simulation", n_sims=20):
    """Create SEIR model, run simulations, and plot results."""

    statenames = ["S", "E", "I", "R", "H"]

    seir_obj = pp.Pomp(
        rinit=seir_rinit,
        rproc=seir_rproc,
        dmeas=seir_dmeas,
        rmeas=seir_rmeas,
        ys=ys,
        theta=theta,
        statenames=statenames,
        t0=0.0,
        nstep=7,                # 7 sub-steps per week (daily steps)
        accumvars=(4,),         # Index of H in statenames
        ydim=1,
        covars=None
    )

    key = jax.random.key(42)
    X_sims, Y_sims = seir_obj.simulate(key=key, nsim=n_sims)

    sim_df = Y_sims.pivot_table(
```

SEIR Simulation: Attempt 1 I

```
theta_seir1 = {
    "Beta": 30.0,     # Transmission rate
    "mu_EI": 0.8,     # 1/latent period (~ 1.25 weeks latent)
    "mu_IR": 1.3,     # 1/infectious period (~ 0.77 weeks infectious)
    "N": 38000.0,
    "eta": 0.06,
    "rho": 0.5,
    "k": 10.0
}

_ = run_seir_simulation_and_plot(theta_seir1, "SEIR: Beta=30, mu_EI=0.8, mu_IR=1.3"
```

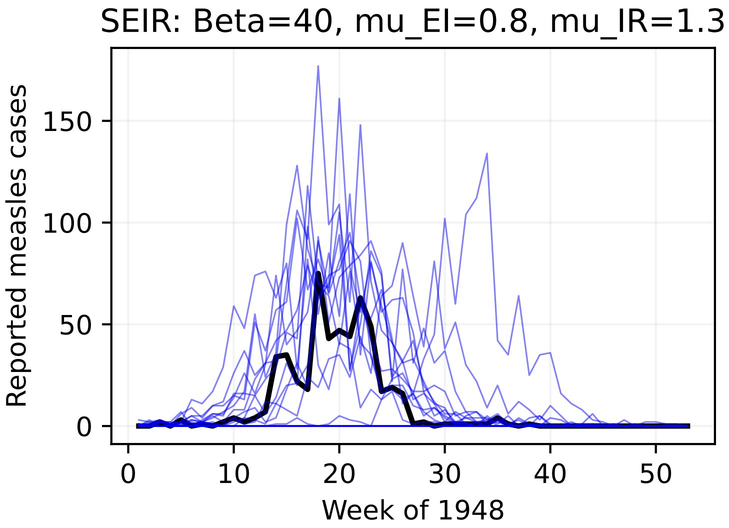
SEIR Simulation: Attempt 1 II



SEIR Simulation: Attempt 2 I

```
theta_seir2 = {
    "Beta": 40.0,    # Increased transmission
    "mu_EI": 0.8,
    "mu_IR": 1.3,
    "N": 38000.0,
    "eta": 0.06,
    "rho": 0.5,
    "k": 10.0
}

_ = run_seir_simulation_and_plot(theta_seir2, "SEIR: Beta=40, mu_EI=0.8, mu_IR=1.3"
```

SEIR Simulation: Attempt 2 II



Comparison: SIR vs SEIR

The SEIR model introduces a **latent period** (time in the E compartment before becoming infectious), which can affect:

1. **Outbreak timing**: Delayed onset due to latent period
2. **Peak timing**: Later peak as infections take longer to develop
3. **Outbreak shape**: More gradual rise and fall

For measles, realistic parameters might be:

- Latent period ($1/\mu_{EI}$): ~8-13 days
- Infectious period ($1/\mu_{IR}$): ~4-8 days

The SEIR model provides a more biologically realistic representation of measles epidemiology.

Key Takeaways

1. **Little-o notation** provides a compact way to express derivatives and is especially useful for continuous-time Markov chains
2. **Euler vs Gillespie**: Euler methods are preferred for computational efficiency and handling large populations; Gillespie provides exact simulations but is slower
3. **Parameter exploration**: Finding good parameters requires systematic experimentation and ultimately formal fitting methods
4. **SEIR vs SIR**: The SEIR model's latent period can better capture the epidemiology of diseases like measles

References I