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November 13, 2018
Predator-Prey model (Lotka-Volterra system)

Stochastic model as continuous-time Markov chain
A simple Predator-Prey model

- Populations of $X$ prey molecules and $Y$ predator molecules

- Three possible reactions (events)
  1) Prey reproduction: $X \rightarrow 2X$
  2) Prey consumption to generate predator: $X + Y \rightarrow 2Y$
  3) Predator death: $Y \rightarrow \emptyset$

- Each prey reproduces at rate $\alpha$
  $\Rightarrow$ Population of $X$ preys $\Rightarrow \alpha X = \text{rate of first reaction}$

- Prey individual consumed by predator individual on chance encounter
  $\Rightarrow \beta = \text{Rate of encounters between prey and predator individuals}$
  $\Rightarrow X$ preys and $Y$ predators $\Rightarrow \beta XY = \text{rate of second reaction}$

- Each predator dies off at rate $\gamma$
  $\Rightarrow$ Population of $Y$ predators $\Rightarrow \gamma Y = \text{rate of third reaction}$
The Lotka-Volterra equations

- Study population dynamics ⇒ $X(t)$ and $Y(t)$ as functions of time $t$

- **Conventional approach**: model via system of differential eqs.
  ⇒ **Lotka-Volterra (LV) system of differential equations**

- Change in prey ($dX(t)/dt$) = Prey generation - Prey consumption
  ⇒ Prey is generated when it reproduces (rate $\alpha X(t)$)
  ⇒ Prey consumed by predators (rate $\beta X(t)Y(t)$)

$$\frac{dX(t)}{dt} = \alpha X(t) - \beta X(t)Y(t)$$

- Predator change ($dY(t)/dt$) = Predator generation - consumption
  ⇒ Predator is generated when it consumes prey (rate $\beta X(t)Y(t)$)
  ⇒ Predator consumed when it dies off (rate $\gamma Y(t)$)

$$\frac{dY(t)}{dt} = \beta X(t)Y(t) - \gamma Y(t)$$
Solution of the Lotka-Volterra equations

- LV equations are non-linear but can be solved numerically

- Prey reproduction rate $\alpha = 1$
- Predator death rate $\gamma = 0.1$
- Predator consumption of prey $\beta = 0.1$
- Initial state $X(0) = 4$, $Y(0) = 10$
- Boom and bust cycles

- Start with prey reproduction $> \text{consumption} \Rightarrow \text{prey } X(t) \text{ increases}$
- Predator production picks up (proportional to $X(t)Y(t)$)
- Predator production $> \text{death} \Rightarrow \text{predator } Y(t) \text{ increases}$
- Eventually prey reproduction $< \text{consumption} \Rightarrow \text{prey } X(t) \text{ decreases}$
- Predator production slows down (proportional to $X(t)Y(t)$)
- Predator production $< \text{death} \Rightarrow \text{predator } Y(t) \text{ decreases}$
- Prey reproduction $> \text{consumption}$ (start over)
State-space diagram

- **State-space diagram** ⇒ plot \( Y(t) \) versus \( X(t) \)

⇒ Constrained to single orbit given by initial state \((X(0), Y(0))\)

**Buildup:** Prey increases fast, predator increases slowly (move right and slightly up)

**Boom:** Predator increases fast depleting prey (move up and left)

**Bust:** When prey is depleted predator collapses (move down almost straight)
Two observations

▶ Too much regularity for a natural system (exact periodicity forever)

▶ $X(t), Y(t)$ modeled as continuous but actually discrete. Is this a problem?

▶ If $X(t), Y(t)$ large can interpret as concentrations (molecules/volume)
  ⇒ Often accurate (millions of molecules)

▶ If $X(t), Y(t)$ small does not make sense
  ⇒ We had 7/100 prey at some point!

▶ There is an extinction event we are missing
Things deterministic model explains (or does not)

- Deterministic model is useful $\Rightarrow$ **Boom and bust cycles**
  $\Rightarrow$ Important property that the model predicts and explains

- But it does not capture some aspects of the system
  $\Rightarrow$ Non-discrete population sizes (unrealistic fractional molecules)
  $\Rightarrow$ No random variation (unrealistic regularity)

- Possibly *missing important phenomena* $\Rightarrow$ **Extinction**

- Shortcomings most pronounced when number of **molecules is small**
  $\Rightarrow$ **Biochemistry at cellular level** (1 $\sim$ 5 molecules typical)

- Address these shortcomings through a **stochastic model**
Stochastic model as CTMC

Predator-Prey model (Lotka-Volterra system)

Stochastic model as continuous-time Markov chain
Stochastic model

- Three possible reactions (events) occurring at rates $c_1$, $c_2$ and $c_3$
  1) Prey reproduction: $X \xrightarrow{c_1} 2X$
  2) Prey consumption to generate predator: $X + Y \xrightarrow{c_2} 2Y$
  3) Predator death: $Y \xrightarrow{c_3} \emptyset$

- Denote as $X(t)$, $Y(t)$ the number of molecules by time $t$

- Can model $X(t)$, $Y(t)$ as continuous time Markov chains (CTMCs)?

- Large population size argument not applicable
  $\Rightarrow$ Interest in systems with small number of molecules/individuals
Consider system with 1 prey molecule $x$ and 1 predator molecule $y$

Let $T_2(1, 1)$ be the time until $x$ reacts with $y$

⇒ Time until $x, y$ meet, and $x$ and $y$ move randomly around

⇒ Reasonable to model $T_2(1, 1)$ as memoryless

$$P (T_2(1, 1) > s + t \mid T_2(1, 1) > s) = P (T_2(1, 1) > t)$$

$T_2(1, 1)$ is exponential with parameter (rate) $c_2$
Suppose now there are $X$ preys and $Y$ predators

⇒ There are $XY$ possible predator-prey reactions

Let $T_2(X, Y)$ be the time until the first of these reactions occurs

⇒ Min. of exponential RVs is exponential with summed parameters

⇒ $T_2(X, Y)$ is exponential with parameter $c_2 XY$

Likewise, time until first reaction of type 1 is $T_1(X) \sim \exp(c_1 X)$

Time until first reaction of type 3 is $T_3(Y) \sim \exp(c_3 Y)$
CTMC model

- If reaction times are exponential can model as CTMC
  \[ \Rightarrow \text{CTMC state } (X, Y) \text{ with nr. of prey and predator molecules} \]

Transition rates

- \((X, Y) \rightarrow (X + 1, Y)\): Reaction 1 = \(c_1 X\)
- \((X, Y) \rightarrow (X - 1, Y + 1)\): Reaction 2 = \(c_2 XY\)
- \((X, Y) \rightarrow (X, Y - 1)\): Reaction 3 = \(c_3 Y\)
- State-dependent rates
Use CTMC model to simulate predator-prey dynamics
- Initial conditions are $X(0) = 50$ preys and $Y(0) = 100$ predators

- Prey reproduction rate $c_1 = 1$ reactions/second
- Rate of predator consumption of prey $c_2 = 0.005$ reactions/second
- Predator death rate $c_3 = 0.6$ reactions/second

⇒ Boom and bust cycles still the dominant feature of the system
⇒ But random fluctuations are apparent
CTMC model in state space

- Plot $Y(t)$ versus $X(t)$ for the CTMC $\Rightarrow$ state-space representation

- No single fixed orbit as before
  $\Rightarrow$ Randomly perturbed version of deterministic orbit
Effect of different initial population sizes

- Chance of extinction captured by CTMC model (top plots)

(Notice that Y-axis scales are different)
Conclusions and the road ahead

- Deterministic vs. stochastic (random) modeling
  - Deterministic modeling is simpler
    ⇒ Captures dominant features (boom and bust cycles)
  - CTMC-based stochastic simulation more complex
    ⇒ Less regularity (all runs are different, state orbit not fixed)
    ⇒ Captures effects missed by deterministic solution (extinction)
- Gillespie’s algorithm. Optional reading in class website
  ⇒ CTMC model for every system of reactions is cumbersome
  ⇒ Impossible for hundreds of types and reactions
  ⇒ Q: Simulation for generic system of chemical reactions?