University of Idaho
Bioinformatics and Computational Biology Program

Solving Biological Stochastic Optimal Control Problems Using Physics Informed Neural Networks

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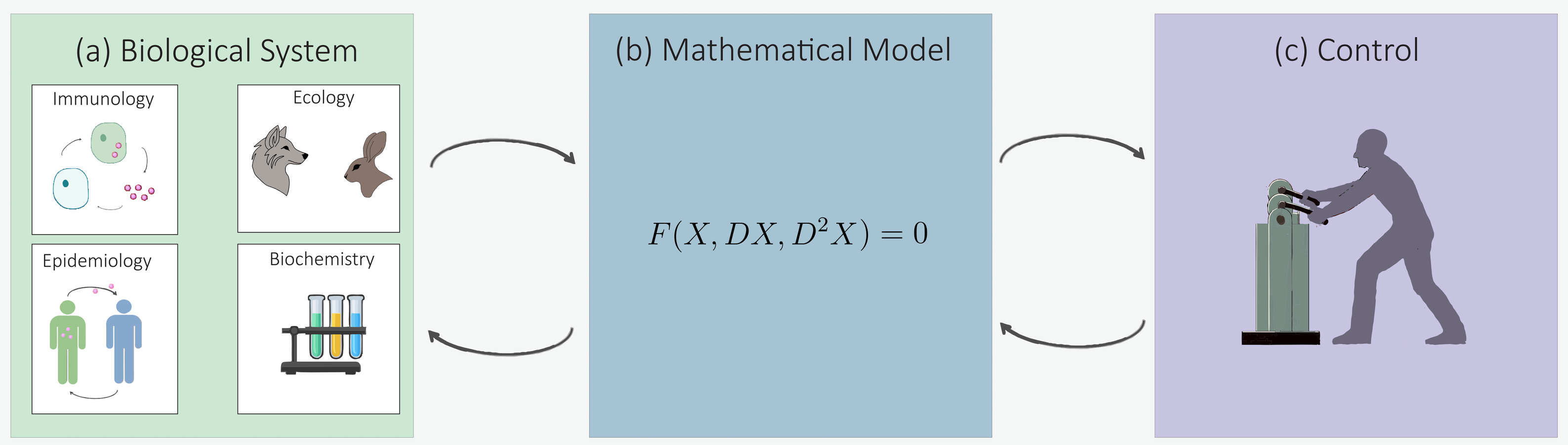
Introduction



(a) There are many natural systems of interest.

(b) We develop models to better understand these systems.

(c) Understanding these systems allows us to influence them.

Mathematical modeling better allows us to influence our environment.

Methods

Mathematics for Optimal Control of Stochastic Systems

(a)

$$d\mathbf{X}_t = \mathbf{f}(t, \mathbf{X}_t, \mathbf{u}_t)dt + \boldsymbol{\sigma}(t, \mathbf{X}_t, \mathbf{u}_t)d\mathbf{W}_t$$

Stochastic system dynamics are incorporated into a constrained optimization problem to find the control policy.

(b)

$$\inf_{\mathbf{u}_t} \mathbb{E}\left[\int_0^T L(t, \mathbf{X}_t, \mathbf{u}_t)dt + \phi(\mathbf{X}_T)\right]$$
$$\text{s.t. } d\mathbf{X}_t = \mathbf{f}(t, \mathbf{X}_t, \mathbf{u}_t)dt + \boldsymbol{\sigma}(t, \mathbf{X}_t, \mathbf{u}_t)d\mathbf{W}_t$$

The stochastic optimization problem is rewritten as a nonlinear partial differential equation by Bellman's principle of optimality.

(c)

$$-V_t(t, \mathbf{X}_t) = L(t, \mathbf{X}_t, \mathbf{u}_t^*) + \langle V_{\mathbf{X}_t}(t, \mathbf{X}_t), \mathbf{f}(t, \mathbf{X}_t, \mathbf{u}_t^*)\rangle + \langle \frac{1}{2}\mathrm{tr}(\boldsymbol{\sigma}\boldsymbol{\sigma}^T(t, \mathbf{X}_t, \mathbf{u}_t^*)), \nabla^2_{\mathbf{X}_t} V\rangle$$

The optimal feedback control is derived as a function of the solution of the partial differential equation.

(d)

$$\mathbf{u}_t^* = G(t, \mathbf{X}_t, \mathbf{f}, \boldsymbol{\sigma}, L, V, \nabla_{\mathbf{X}_t} V)$$

(a) We assume that the system of interest can be represented adequately by a drift-diffusion process.

(b) We write the optimal control problem for a drift-diffusion process in this form. Note the use of expectation to maintain a real-valued objective.

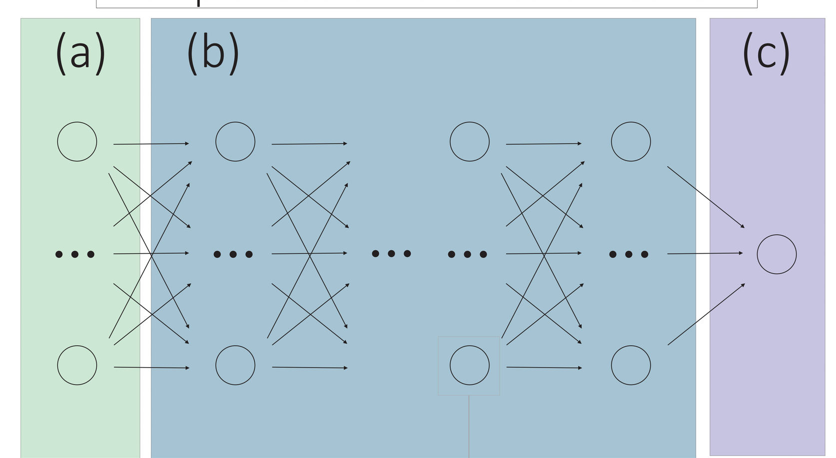
(c) The resulting Hamilton-Jacobi-Bellman equation is a generally nonlinear second order partial differential equation.

(d) We solve for the optimal feedback given the solution to the nonlinear partial differential equation.

Solution of the Hamilton-Jacobi-Bellman equation provides the optimal feedback control policy, but is a difficult procedure generally.

Anatomy of a Neural Network

Example Feedforward Neural Network



Typical Hidden Layer Nueron

(d)

$$\mathbf{y}(\mathbf{x}|\mathbf{a}, b) = \sigma\left(b + \sum_{i=1}^{n} a_i \mathbf{x}_i\right)$$

σ - Neuron activation function

$\mathbf{y}$ - Neuron output

$\mathbf{x}$ - Neuron input

$\mathbf{a}$ - Input weight parameters

b - Input bias parameter

Neural networks are common tools in modern applied mathematics. Commonly, neural networks are used to represent and approximate complex relationships.

(a) The network input layer. Often, this layer scales the inputs to a small range of values

(b) The hidden layers of a neural network represent are where the approximation occurs. Combinations and compositions of neurons allow the network to represent complex relations

(c) The network output layer. Often, this layer rescales the outputs

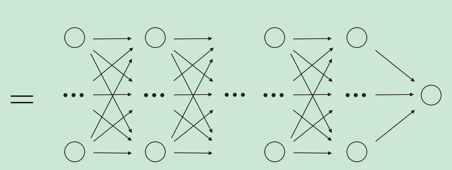
(d) A hidden layer neuron. Each neuron is typically a simple nonlinear function of the previous layer outputs

Neural networks can approximate complex mathematical functions

Physics Informed Neural Networks

(a)

$$V \approx \hat{V} =$$



We use a neural network to represent V, and we train the network against the degree to which it satisfies the partial differential equation.

(b)

$$-V_t(t, \mathbf{X}_t) = L(t, \mathbf{X}_t, \mathbf{u}_t^*) + \langle V_{\mathbf{X}_t}(t, \mathbf{X}_t), \mathbf{f}(t, \mathbf{X}_t, \mathbf{u}_t^*)\rangle + \langle \frac{1}{2}\mathrm{tr}(\boldsymbol{\sigma}\boldsymbol{\sigma}^T(t, \mathbf{X}_t, \mathbf{u}_t^*)), \nabla^2_{\mathbf{X}_t} V\rangle$$

We can then recover the optimal control using autodifferentiation facilities present in modern machine learning software tools.

(c)

$$\hat{\mathbf{u}}_t^* = G(t, \mathbf{X}_t, \mathbf{f}, \boldsymbol{\sigma}, L, \hat{V}, \nabla_{\mathbf{X}_t} \hat{V})$$

(a) We can represent the solution V to the Hamilton-Jacobi-Bellman equation using a neural network.

(b) We can then use the approximated V to solve the Hamilton-Jacobi-Bellman equation.

(c) We can use the approximate solution to derive the optimal feedback control policy.

We can use neural networks to solve the Hamilton-Jacobi-Bellman equation for the optimal feedback control policy

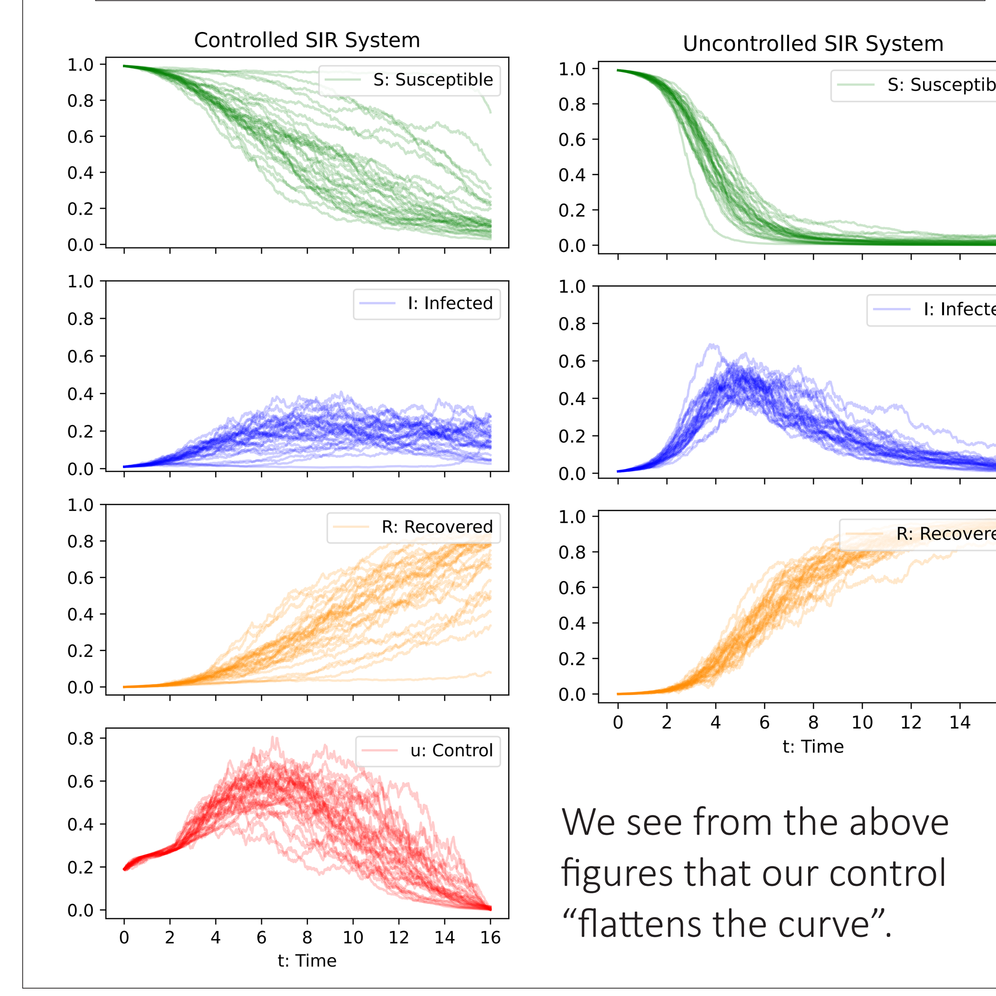
Results

Example Problem: Controlled SIR

$$\inf_{u} \mathbb{E}\left[\int_0^T (c_1 I_t^2 + c_2 u_t^2)\, dt\right]$$
$$\text{s.t. } dS_t = [-(1-u_t)\beta S_t I_t]\, dt - \sigma_\beta S_t I_t dW_{t,\beta} + \sigma_S S_t dW_{t,S}$$
$$dI_t = [(1-u_t)\beta S_t I_t - \gamma I_t]\, dt + \sigma_\beta S_t I_t dW_{t,\beta} - \sigma_\gamma I_t dW_{t,\gamma} + \sigma_I I_t dW_{t,I}$$
$$dR_t = [\gamma I_t]\, dt + -\sigma_\gamma I_t dW_{t,\gamma} + \sigma_R R_t dW_{t,R}$$

We consider control of the stochastic SIR model.

Stochasticity is assumed to enter the system parameters and states.



We see from the above figures that our control "flattens the curve".

Note, the values of parameters c_1 and c_2 which represent the cost of infected population size and control magnitude at any point have a meaningful impact on the resulting solutions.

We trained our model on mid range consumer hardware (RTX 4060 in a 6 year old mid-range desktop). Training took about 3 hours.

We can successfully apply our method to deriving stochastic optimal feedback controls for biological systems.

Future Work

1. Investigate the application of pairing filtering methods and transfer learning to apply this technique to real time problems.

2. Apply this methodology to solve differential game problems, which involve systems of Hamilton-Jacobi-Bellman equations.

Acknowledgments

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References

Materials for this poster can be found on GitHub using the above QR code