Connecting SOC with RL – Importance sampling

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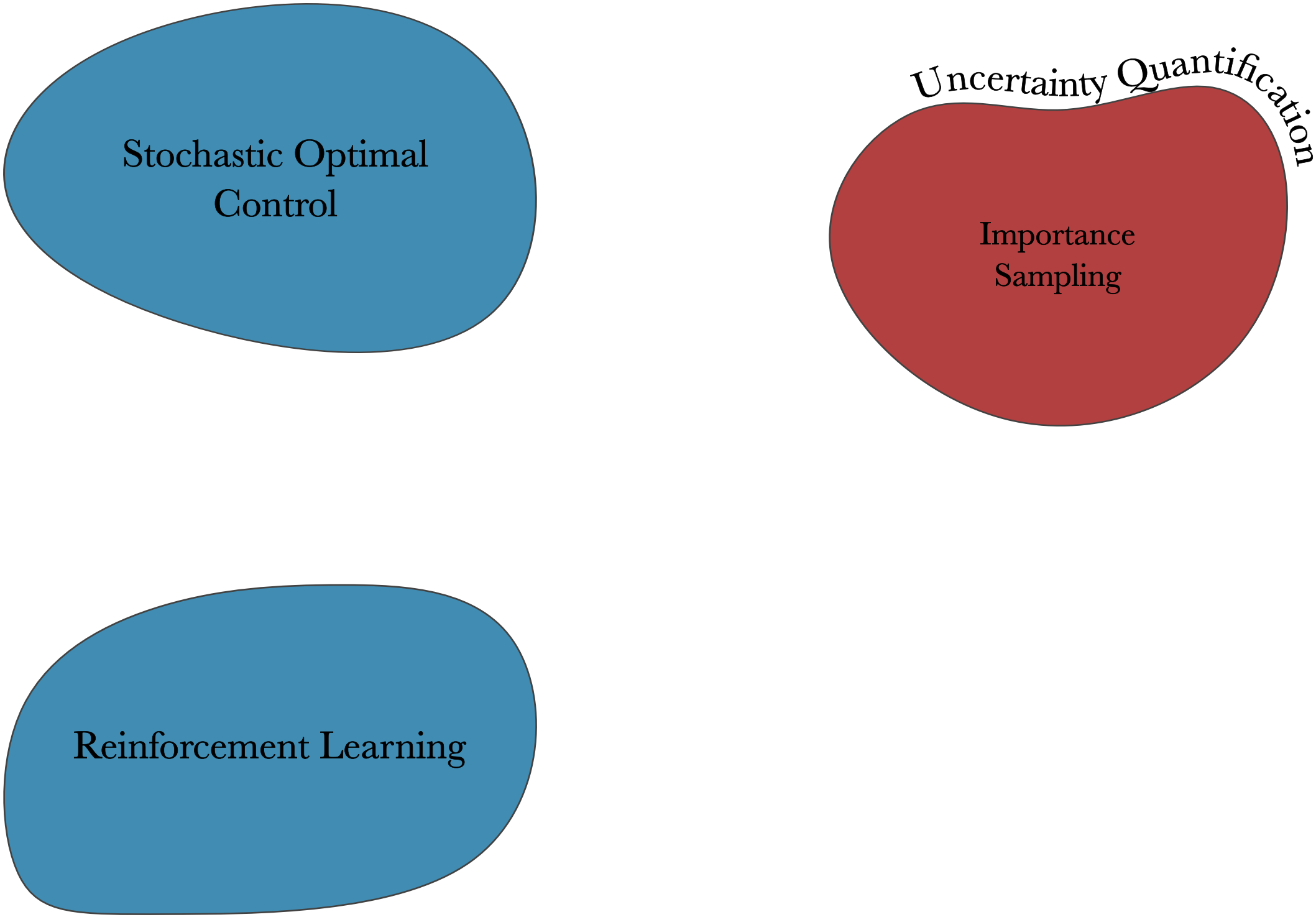
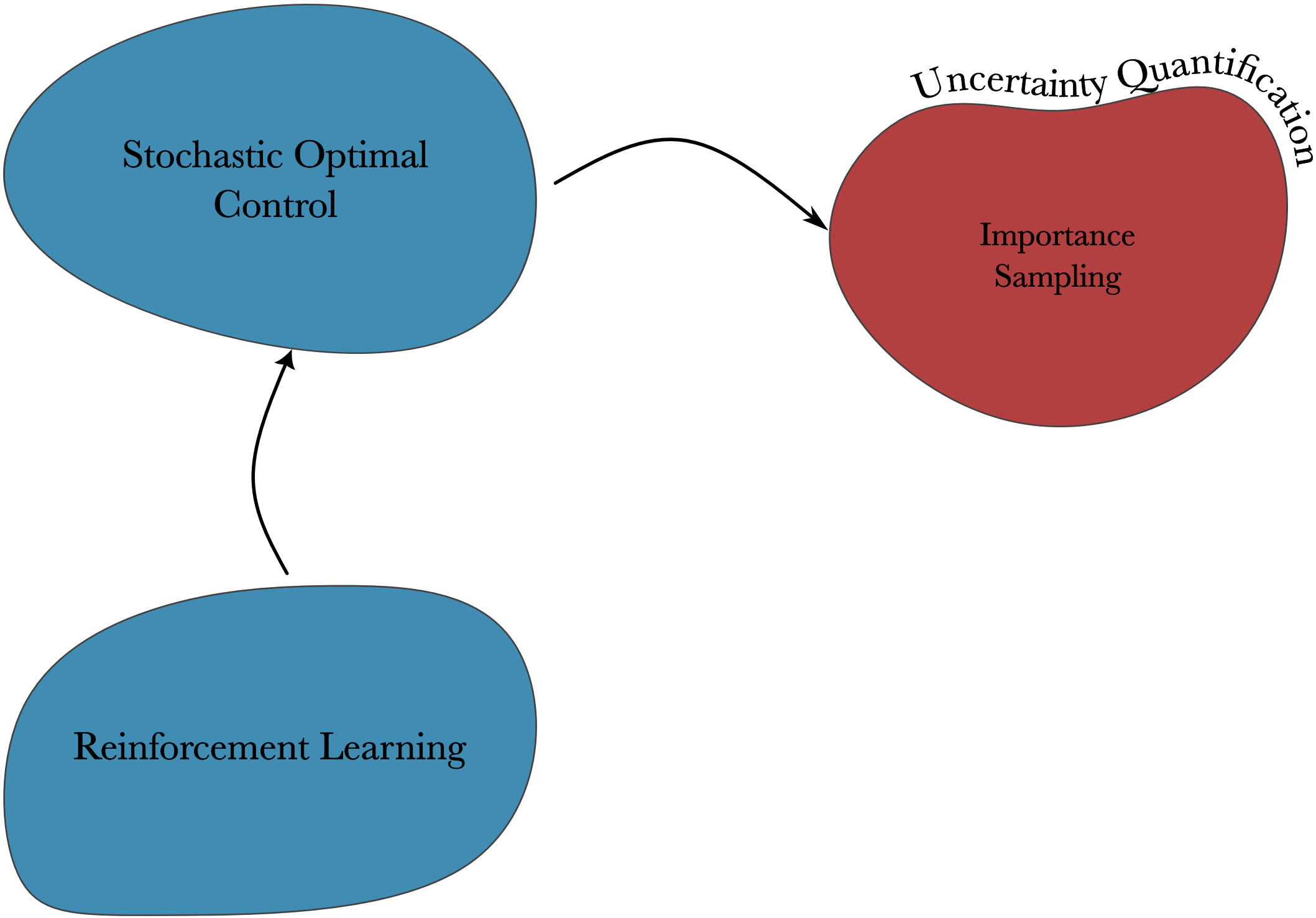

Stochastic Optimal Control
Uncertainty Quantification
Importance Sampling
Reinforcement Learning

Speaker notes

What optimization models have we seen in the seminar so far?


Stochastic Optimal Control
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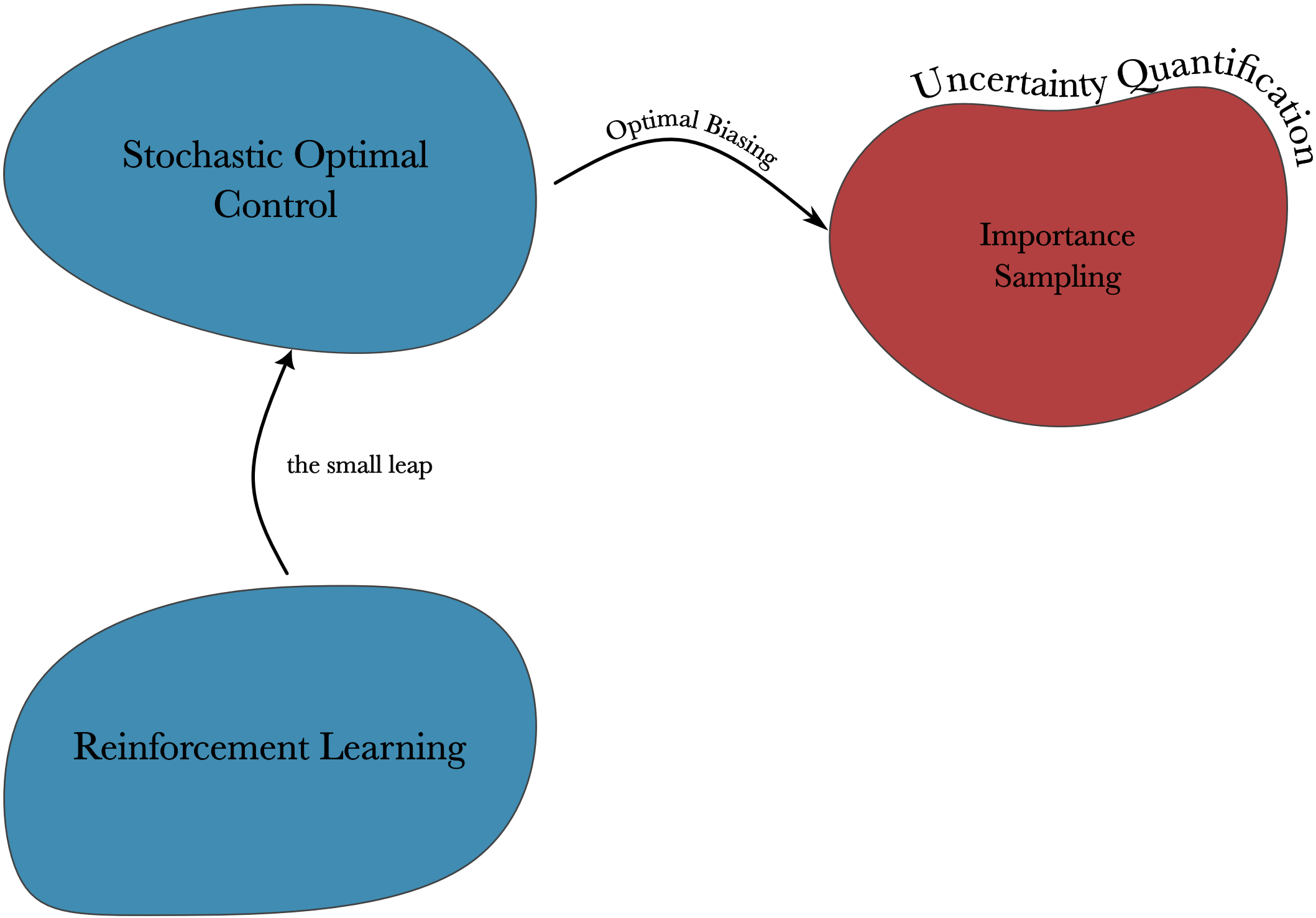

Stochastic Optimal Control
Optimal Biasing
Uncertainty Quantification
Importance Sampling
the small leap
Reinforcement Learning

Speaker notes

- So far we've seen RL as a fancy tool to explore complicated spaces. Today, we're going to think of how the discipline of RL as a whole introduces new ideas to other areas of mathematics and creates new fertile ground.
- Instead of finding ways of computing faster, we're looking for avenues to come up with entirely new ways of posing problems that allow us to use all of the work that was already invested in "AI"

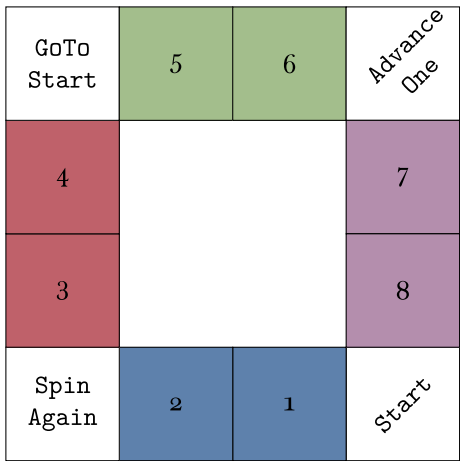
Outline

1. *Crash* course on RL
2. What is importance sampling

   - The connection to optimization
   - Optimal biasing

4. Optimal biasing as an RL problem
5. SOC ≠ RL

Crash course on Reinforcement Learning



A miniopoly board

Speaker notes

- I’m training a robot to become the best Miniopoly player
- The rules:
  - Players play in turns
  - They move a number of squares determined by a 4-sided dice roll
  - After completing a lap, it gets a reward of x dollars
  - The trap squares do what it says on the square
  - They can buy property and hotels in the squares.
    - If they land of a square someone owns, they pay
    - If someone lands on their square, they charge rent
  - The game ends when someone runs out of money

- The game has a state at turn t denoted s_t
- At a turn t players roll the dice
- The change in money after buying/paying rent/charging rent is recorded as a reward r_t

Important

We train our robot to maximize the rewards as it takes actions exploring the space of states

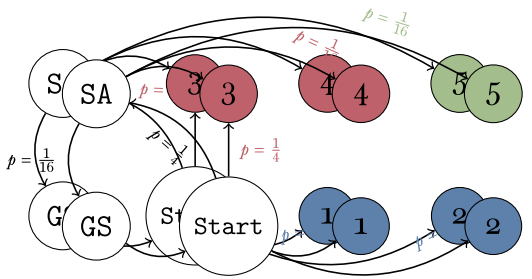
Speaker notes

- The state of the game an any given time is information like, who owns what squares, how much money they have, in what positions each playe is, and so on.
- Once a player lands in another square, they can choose to buy it if available. If it’s not, we carry out the accounting of how much rent is, and let the player know how much it won/lost and to what square this is connected.

Can you describe the state space?

How does it *look*

It’s hard to describe the state space, but we can study the dynamics



What if we don’t know how square transitions work?

- We calculated transition probability *with* the knowledge of the dice

5 minutes to think

- What is a reasonable way of guessing transition probabilities?
- Can I be sure to observe even improbable but still possible states?

The right answers are:

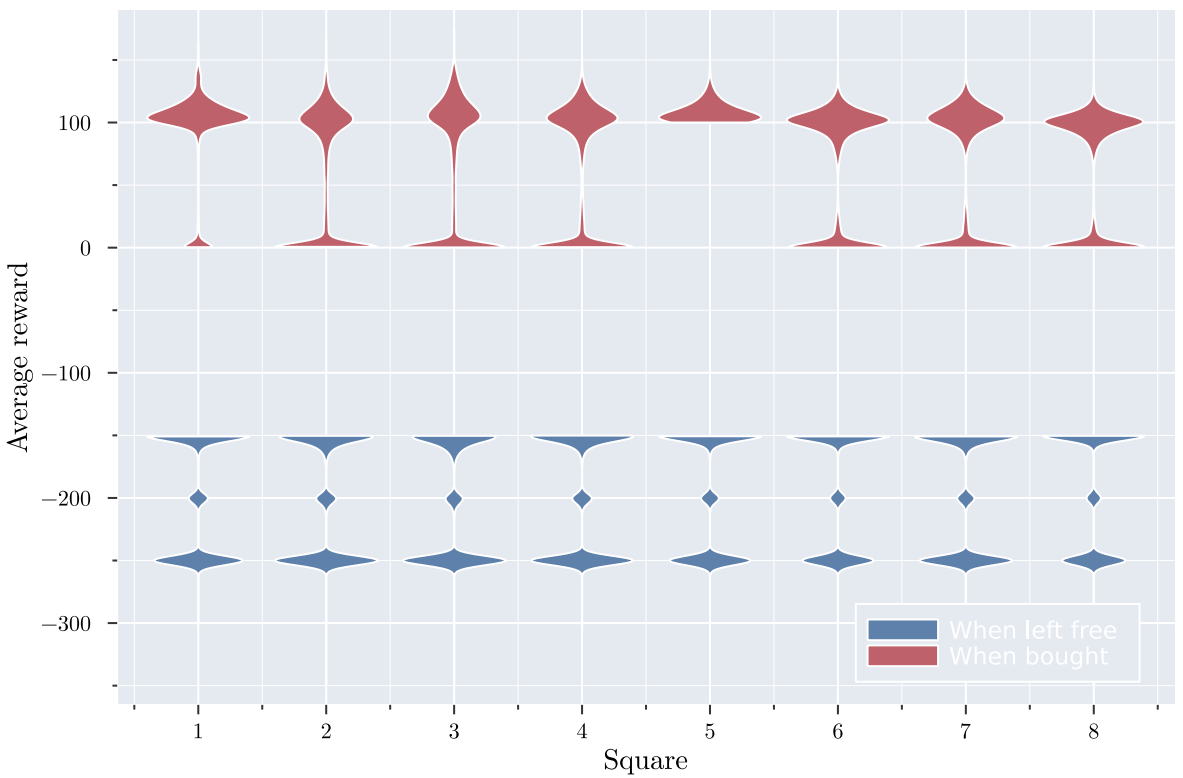
- By simulating the transitions and get empirical estimates
- No

Speaker notes

- Without knowledge of the dice, we would be left to guess.

Markov Chain Monte Carlo

- We let the robot roam around and buy squares as it pleases
  - For any square, it can either buy it or not



Speaker notes

- Graph:
  - This is a violin plot. It shows the estimated probability densities of observing…
  - The x axis shows the different squares
  - The y axis shows the estimated rewards. i.e. money
  - The red distributions correspond to the expected reward when buying a square, while the blue the expected loss when not buying them
  - i.e. When we buy squares we expect to profit from them, but clearly not all squares are as profitable, look at the different shapes of the distributions. On the other hand, it looks like losing any given square leads to the same expected loss

Importance Sampling

- We wanted to compute the expected reward of the robot after the entire game
- Not every problem is this well behaved
- This property is called *metastability*
- Importance sampling aims to remedy this

> **Important**
>
> The general idea of importance sampling is to draw random variables from another probability measure and subsequently weight them back in order to still have an unbiased estimator of the desired quantity of interest

Speaker notes

- We **estimated** this quantity by observing and measuring an empirical average. But our approximation for extremely unlikely states will always be bad by virtue of how little samples we have.
- Many problems, like molecular dynamics, chemical reactions, etc… have extremely like states, and other extremely unlikely states. If we were to use MCMC, we would need impractical amounts of time to simulate it and observe every state
- Metastability makes MCMC extremely hard to apply. The variance of our estimations is always going to be enourmous under these conditions
- We can aim to make sampling faster by reducing the inherent variance
- **After Callout** In the case of stochastic processes this change of measure corresponds to adding a control to the original process

- We want to explore space
  - We can’t make it to the other well
- The jumps are exponentially less probable w.r.t the height of the barrier

Speaker notes

- It turns out that there is an optimal way to design such a scheme, leading to substantially reduced mean hitting times which do not scale exponentially with the energy barrier anymore

More formally…

Speaker notes

- Where:
  - X_s is the position of our particle at time s
  - V is a “potential”
  - We assume there exists a unique strong solution that is ergodic
- Note that τ is a.s. finite
- Where $\mathcal{W}$ serving as a measure of “work” over a trajectory

Our main goal is to compute

$$\Psi(X) := \mathbb{E}^x[I(X)] := \mathbb{E}[I(X) \mid X_0 = x]$$

But…

- MCMC has terrible properties because of metastability
- No closed form exists

> **Tip**
>
> - We can “push” the particle adding force, as long as we account for it and correct for that bias
> - That “push” is achieved by adding a control u.

The new, controlled dynamics are now described as

$$\mathrm{d}X_s^u = (-\nabla V(X_s^u) + \sigma(X_s^u)\, u(X_s^u))\mathrm{d}s + \sigma(X_s^u)\mathrm{d}W_s,$$

Via Girsanov, we can relate our QoI to the original as such:

$$\mathbb{E}^x\left[I(X)\right] = \mathbb{E}^x\left[I(X^u)M^u\right],$$

where the exponential martingale

$$M^u := \exp\left(-\int_0^{\tau^u} u(X_s^u)\cdot \mathrm{d}W_s - \frac{1}{2}\int_0^{\tau^u} |u(X_s^u)|^2 \mathrm{d}s\right)$$

corrects for the bias the pushing introduces.

Important

The previous relationship always holds. But the variance of the estimator depends *heavily* on the choice of u.

Clearly, we aim to achieve the smallest possible variance through on *optimal control* u^*

$$\mathrm{Var}\left(I(X^{u^*})M^{u^*}\right) = \inf_{u\in\mathcal{U}}\{\mathrm{Var}(I(X^u)M^u)\}$$

Speaker notes

- Where:
  - X_s^u is the position of our particle at time s under control u
  - The potential u is an Itô integrable function satisfying a linear growth condition
- Note that τ is a.s. finite
- Where $\mathcal{W}$ serving as a measure of “work” over a trajectory

Connection to optimization

It turns out [1] that the problem of minimizing variance corresponds to a problem in optimal control

The cost functional J to find the variance minizing control is

$$J(u;x) := \mathbb{E}^x \left[\mathcal{W}(X^u) + \frac{1}{2} \int_0^{\tau^u} |u(X_s^u)|^2 \mathrm{d}s \right],$$

So that

$$\Phi(x) = \inf_{u \in \mathcal{U}} J(u;x).$$

Important

The optimal bias achieves zero variance:

$$\mathrm{Var}\left(I(X^{u^*})M^{u^*}\right) = 0.$$

Optimal biasing through RL

- Let's reconsider the SOC problem (excuse the change in notation)
- We discretize with Euler–Marujama

$$\boldsymbol{s}_{t+1} = \boldsymbol{s}_t + (-\nabla V(\boldsymbol{s}_t) + \sigma u(\boldsymbol{s}_t))\Delta t + \sigma\sqrt{\Delta t}\,\eta_{t+1}$$
$$\boldsymbol{s}_0 = x$$

Speaker notes

- Sorry for the slightly different notation
- Where
  - Our state is now represented by s
  - We have the same potential V
  - The difussion term is σ again
  - Δt is the length of the time step
  - The term $\sqrt{\Delta t}\eta_{t+1}$ is a Brownian increment, $\eta_t \sim N(0, 1)$

The time-discretized objective function is given by

$$J(u;x) := \mathbb{E}^x \left[g(s_{T_u}) + \sum_{t=0}^{T_{u-1}} f(s_t)\Delta t + \frac{1}{2} \sum_{t=0}^{T_{u-1}} |u(s_t)|^2 \Delta t \right.$$

- Our stopping time τ is now denoted T_u

Some formalities

- The state space $\mathcal{S}$ is all possible $s \in \mathbb{R}^d$
- The action space $\mathcal{A}$ is the codomain of all possible controls $\mathbb{R}^d$
- The stopping time T_u for the controlled process is a.s. finite

- We'll approximate the control with Galerkin projections u_θ
- We still need to derive probability transition and reward functions

- The return we want to optimize depends on a rewards function

$$r_t = r(\boldsymbol{s}_t, a_t) := \begin{cases} -f(\boldsymbol{s}_t)\Delta t - \frac{1}{2}|a_t|^2 \Delta t & \text{if } \boldsymbol{s}_t \notin \mathcal{T} \\ -g(\boldsymbol{s}_t) & \text{if } \quad \boldsymbol{s}_t \in \mathcal{T} \end{cases}$$

Speaker notes

- The reward function is defined such that the corresponding return along a trajectory equals the negative term inside the expectation of the time-discretized cost functional
- Notice that the reward signal is in general not sparse since the agent receives feedback at each time step but the choice of the running cost f and the final cost g can influence this statement.

Future work

References

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