# **Reinforcement Learning:** Dynamic Programming and Monte-Carlo Methods The Bellman Equations

Andrei Cozma and Landon Harris

### **Test Questions**

- 1. What does the "model" refer to in the terms "model-based" and "model-free"?
- 2. What are some of the limitations of Dynamic Programming methods?
- 3. How can you handle the exploration/exploitation trade-off in Monte Carlo methods?

# Presenters - Andrei Cozma

### Program: Computer Science M.S. (maybe PhD)

- Intelligent Systems & Machine Learning
- Advisor: Dr. Hairong Qi
- AICIP Lab Group



Undergraduate Degree:

- Computer Science B.S., May 2022
- Minors: Cybersecurity & Business Administration

### Interests

- Machine Learning & Deep Learning
  - Computer Vision
  - Natural Language Processing
  - Reinforcement Learning
- Signal & Information Processing

### Goals

- Publish some papers summer or fall
- Build a strong network of connections

### Presenters - Andrei Cozma

### • Deva, Romania



### Hendersonville, TN

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# Presenters - Andrei Cozma

- Traveling
- Exploring
- Photography
- Music & Concerts
  - Rock, Alternative, Blues, etc etc.
- Ice Skating, Biking, Swimming



















# Presenters – Landon Harris

### Program: Computer Science M.S.

- Advisor: Dr. Hairong Qi
- AICIP Lab Group

### Undergraduate Degree:

- Computer Science B.S., May 2022
- Minors: Mathematics

#### Interests

- Machine Learning & Deep Learning
  - Computer Vision
  - Reinforcement Learning
- Foundational AI
  - Dynamical Systems analysis
  - Training Policies / Continual Learning



### Presenters – Landon Harris

• Hometown: Franklin, TN













### Presenters – Landon Harris

- Traveling
- Hiking
- Music











# Outline

- 1. Terms & Overview
- 2. History
- 3. Background
- 4. Algorithms
  - Dynamic Programming
  - Monte Carlo
- 5. Applications
- 6. Implementation
- 7. Open Issues
- 8. Discussion

### Overview - Part 1

### **Reinforcement Learning (RL)**

- Subfield of Machine Learning
- Agents learn optimal actions through interaction with an environment.

### Markov Decision Process (MDP)

- Mathematical framework for modeling decision-making processes in stochastic, discrete-time, and finite-state environments
- <u>Markov Property</u>: future states depend only on the current state, not on the sequence of past states.

### **Model-Based Methods**

• Methods that use knowledge of the environment's dynamics

### **Model-Free Methods**

• Learn directly from experience, no model required

(more on these later)



Agent-environment interaction in a MDP

### **Applications:**

- Robotics
- Game Al
- Recommendation Systems
- Finance, Healthcare, etc

### Overview – Part #2

### Policy $(\pi)$ Defining the agent's behavior: mapping from state to action Stochastic: $\pi(a|s)$ is the probability of choosing action a while in state s Deterministic: $\pi(s)$ is the <u>action</u> taken while in <u>state s</u> Return (G) We try to maximize the <u>sum of all future rewards</u> • This holds for episodic/terminal (finite duration) problems 00

$${
m G}_{
m t} = \sum_{\{t=t+1\}}^T R_t \ = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \dots = \sum_{\{i=0\}}^\infty \gamma^i R_{t+i+1}$$



starting position

**Discounted Returns:** 

- For non-episodic problems, exploit the concept of discounting
- Gamma,  $0 < \gamma < 1$ , is the discount rate

recursive form:  $\mathbf{G}_{\mathrm{t}} = R_{t+1} + \gamma \mathbf{G}_{\mathrm{t}+1}$ 

### Overview – Part #3

Almost all Reinforcement Learning algorithms are based on estimating Value Functions

#### • Expected Return -> Value Functions

- Value of a state is the expected return when starting in that state and then following policy  $\pi$  thereafter
- $\circ$  Can only be calculated given a policy  $\pi$

### $V(s) = E\left[G_t \mid S_t = s ight]$

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#### State-Value Function

- *How good* is it to be in a <u>given state</u>?
- Maintain an average of actual returns for each state.
- Avg. will converge to the state's value.

$$V^{\pi}(s) = E_{\pi}\left[\mathrm{G_{t}} \mid \mathrm{S_{t}} = \mathrm{s}
ight] = -\mathrm{E}_{\pi}\left[\sum_{k=0}^{\infty}\gamma^{k}R_{t+k+1} \mid S_{t} = s
ight], orall s \in \mathcal{S}$$

#### Action-Value Function

- *How good* is it to take a <u>specific action</u> while in a <u>given state</u>?
- Maintain separate averages for each action taken in a state
- Avgs. will converge to the state-action values.

$$Q^{\pi}(s,a) = E_{\pi}\left[\mathrm{G_t} \mid \mathrm{S_t} = \mathrm{s}, A_t = a
ight] = ext{ } \mathrm{E_{\pi}}\left[\sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \mid S_t = s, A_t = a
ight], orall s \in \mathcal{S} ext{ } 12$$

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# History

### Early Beginnings: Pioneering Ideas (1950s-1960s)

- Bellman Introduced Dynamic Programming, Optimal Control, Markov Decision Processes (MDPs), and Value Functions (1957)
- Samuel Developed a checkers-playing program that learned value functions through approximation (1959)
- Howard Proposed the Policy Iteration method for solving MDPs (1960)
- Minsky Established the connection between DP and RL. Discussed <u>Trial-and-Error Learning</u>, Prediction, and Expectation. (1961)
- Michie, Chambers Early use of Monte Carlo methods in RL (1968)

#### Golden Age of Theoretical Foundations (1970s-1980s)

- Witten Published the earliest work on a <u>Temporal-Difference (TD) Learning</u> rule (1977)
- Barto, Sutton, Anderson Developed the Actor-Critic Architecture for combining TD learning with trial-and-error learning (1981)
- Narendra, Wheeler Introduced the Every-Visit Monte Carlo method (1986)
- Sutton Separated TD learning from control, introduced the  $\underline{TD}(\lambda)$  algorithm, and proved some of its convergence properties (1988)
- Watkins Developed <u>Q-Learning</u>, which extended and integrated prior work in RL research (1989)

# History

### Model-Based and Model-Free Era (1990s-2000s)

- Tesauro Developed <u>TD-Gammon</u>, a successful Backgammon player using TD-Learning (1992)
- Williams Policy Gradient methods gain popularity, optimizing policy directly (1992)
- Rummery, Niranjan <u>SARSA</u>: On-policy TD Control (1994)
- John Expected SARSA: Off-policy TD Control (1994)
- Bradtke, Barto Developments on Sample-Based Learning with Monte Carlo methods (1996)
- Sutton, Barto Popular RL book with a comprehensive overview of Model-Free and Model-Based methods (1998)

### **Revolutionary Breakthroughs (2010s-Present)**

- DeepMind <u>Deep Q-Network (DQN)</u> capable of learning from high-dimensional sensory inputs (2013)
- DeepMind DQN demonstrates human-level performance in Atari games (2015)
- DeepMind <u>AlphaGo</u>, combines Deep Neural Networks and <u>Monte Carlo Tree Search</u> (MCTS), defeats world champion (2016)
- OpenAI Proximal Policy Optimization (PPO) sample-efficiency and balances exploration and exploitation (2017)
- DeepMind <u>AlphaStar</u> achieves grandmaster level in StarCraft II (2019)

# Algorithms Intro - The Bellman Equations

From the definitions of <u>Value Function</u>:  $V(s) = E[G_t \mid S_t = s]$  and <u>Return</u>:  $G_t = R_{t+1} + \gamma G_{t+1}$ 

We can derive:  $V^{\pi}(s) = E_{\pi} \left[ R_{t+1} + \gamma G_{t+1} \mid S_t = s 
ight]$ 

### 

### Algorithms Intro – Optimal Policy & Value Functions

1. A **policy**  $\pi^*$  is defined to be better than or equal to a **policy**  $\pi$  if <u>for all states</u>, its <u>expected return is greater than or equal</u> to <u>that of  $\pi$ </u>

 $\pi^* \geq \pi \quad \Leftrightarrow \quad V^{\pi^*}(s) \geq V^{\pi}(s) \quad orall s \in S$ 

2. There is always at least one policy (a.k.a optimal policy) that is better than or equal to all other policies

$$egin{aligned} V^*(s) &= \max_{\pi} V^{\pi}(s) \quad orall s \in S \ V^*(s) &= \max_{a} E\left[r_{t+1} + \gamma V^*\left(s_{t+1}
ight) \mid S_t = s, A_t = a
ight] &= \max_{a} \sum_{s',r} p\left(s',r \mid s,a
ight) \left[r + \gamma V^*\left(s'
ight)
ight] \ Q^*(s,a) &= \max_{\pi} Q^{\pi}(s,a) \quad orall s \in S, a \in A(s) \ Q^*(s,a) &= \mathrm{E}\left[\mathrm{r}_{t+1} + \gamma V^*\left(s_{t+1}
ight) \mid s_t = s, a_t = a
ight] &= \sum_{s',r} p\left(s',r \mid s,a
ight) \left[r + \gamma \max_{a'} Q^*\left(s',a'
ight)
ight] \end{aligned}$$

Intuitively, it expresses the fact that <u>the value of a state under an optimal policy</u> **must equal** the <u>expected return for the best action from that state.</u>

### Algorithms Intro - Bellman Optimality Equations

- 1. Since V\*(s) and Q\*(s, a) are value functions for a policy, they must satisfy the Bellman Equation.
  - a. Any policy which is greedy with respect to the optimal value function, is an optimal policy.
  - <u>Principle of Optimality</u>: "An optimal policy has the property that whatever the initial state and initial decision are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision." (Bellman, 1957)
- 2. Given V\*(s), one-step-ahead search produces the long-term optimal actions

a. This is a deterministic policy 
$$\pi^*(s) = rgmax_{a \in A} \sum_{s',r} p\left(s',r \mid s,a
ight) \left[r + \gamma V^*\left(s'
ight)
ight]$$

3. Given **Q\*(s, a)**, the agent does not even need to do a one-step-ahead search  $\pi^*(s) = \operatorname*{argmax}_{a \in A} Q^*(s, a)$ 



# Algorithms – Dynamic Programming (DP)

A theoretically optimal method to compute an optimal policy  $\pi^*$ 

• Done by solving the Bellman Optimality Equations

Requires:

- An accurate model of the environment (e.g. transition probabilities)
- The environment maintains the Markov property
- Enough space & time to perform the computation

Usually have to settle for approximation, offering several advantages:

- learn more effectively
- feature extraction can reduce noise
- can address relatively large scale problems

# Algorithms – DP – Policy Evaluation

Task: finding the state-value function

Given: the current policy

### Steps:

- 1. Choose an arbitrary  $V_0$
- 2. At each step you use the update rule:

$$V_{k+1}^{\pi}(s) = \sum_{a} \pi(a \mid s) \sum_{s',r} p(s',r \mid s,a) \left[r + \alpha V_{k}^{\pi}(s')\right]$$
$$V_{0} \rightarrow V_{1} \rightarrow V_{2} \rightarrow \cdots \rightarrow V_{k} \rightarrow V_{k+1} \rightarrow \cdots \rightarrow V^{\pi}$$

- 3. Can be proven to converge to  $V^{\pi}$  as  $k \rightarrow \infty$
- 4. In each iteration all states are updated
  - a. scheme can be computationally heavy
- 5. When to stop?
  - a. Since we cannot do infinite iterations, do until largest update is smaller then some threshold

 $\max s \in S \left| V_{k+1}(s) - V_k(s) \right|$ 

# Algorithms – DP – Policy Improvement

Task: Update the policyGiven: the current state-value function

### Steps:

- 1. Suppose we've computed the state-value function (using Policy Evaluation) for some policy  $\pi$
- 2. Let  $\pi'$  be a deterministic policy that:
  - Selects an action *a* for each state *s* to maximize the first-step value

$$\pi'(s) = rgmax_{a} \sum_{s',r} p\left(s',r \mid s,a
ight) \left[r + \gamma V^{\pi}\left(s'
ight)
ight]$$

3. What is the value if we first choose action *a* which is not necessarily  $\pi(s)$ ?

$$Q^{\pi}(s,a) = \sum_{s',r} p\left(s',r \mid s,a
ight) \left[r + lpha V^{\pi}\left(s'
ight)
ight]$$

- If this is higher than  $V^{\pi}(s)$ , then it should be better to select action *a* and then follow  $\pi$ .
- Should we change the policy? Yes
- 4. <u>Policy Improvement Theorem</u>:
  - $\circ \qquad ext{if:} \qquad Q^{\pi}\left(s,\pi'(s)
    ight) \geq \mathrm{V}^{\pi}(s) \quad orall s \in S$
  - $\circ$  then:  $\mathrm{V}^{\pi'}(s) \geq \mathrm{V}^{\pi}(s)$

# Algorithms – DP – Policy Iteration

Technique for obtaining the optimal policy

- Two complementary steps:
  - a. <u>Policy Evaluation</u>: Finding the value function under a given policy
    - Updating the value function makes the policy not greedy anymore
  - b. <u>Policy Improvement</u>: Updating the policy given the current value function
    - Finding a greedy policy for  $V^{\pi}_{i}$  makes the value function incorrect

Yet together they drive each other to the optimal solution:  $\pi^*$  ,  $V^{\pi*}$ 

$$\pi_0 \stackrel{E}{\rightarrow} V_{\pi_0} \stackrel{I}{\rightarrow} \pi_1 \stackrel{E}{\rightarrow} V_{\pi_1} \stackrel{I}{\rightarrow} \pi_2 \stackrel{E}{\rightarrow} \ldots \stackrel{I}{\rightarrow} \pi_* \stackrel{E}{\rightarrow} V_{\pi_*}$$

It can be shown that π' is at least as good as π
 a. if they are equal they are both the optimal policy.



### Algorithms – DP – Value Iteration



# Algorithms – DP – Conclusions

### Key Takeaways

- Requires a complete model of the environment to compute state values (model-based)
  - State-transition probabilities
- Uses Bellman Equations to compute state-values for each time step, until convergence
- May not be practical for large problems
  - Today, we can get away with millions of states
- Dynamic programming is still more efficient than exhaustive search
  - DP is guaranteed to find the optimal policy in less than some polynomial combination of |A| and |S|
  - Exhaustive search is  $|A|^{|S|}$

# Algorithms – Monte Carlo (MC) Methods

A complete model of the environment is not always available.

### Learning through experience (sample-based)

- Online interaction with an environment
  - do not require prior knowledge (state transition probabilities)
- Simulated interactions
  - technically require a kind of model of the environment, but not probability distributions as required for DP
  - sometimes it's easier to only get samples!

Typically applied to <u>episodic tasks</u> (incremental in an episode-by-episode manner)

- In contrast, DP method focused on one-step transitions (step-by-step scheme)
- If task is not episodic, make it episodic (e.g. forced termination by max number of steps)

# Algorithms – Monte Carlo – Control

Generate an episode that follows policy  $\pi$ :

 $s_0, a_0, r_1, s_1, a_1, r_2, \dots, s_{T-1}, a_{T-1}, r_T$ 

### **Policy Iteration**

- Policy Evaluation
  - averaging sample returns over many outcomes to update value function
- Policy Improvement
  - selecting greedy actions to get the new policy
- Alternating between Evaluation and Improvement *each episode*.
  - Only calculating returns and new policy at the end of an episode

Converge to optimal policy over infinitely many episodes

• In practice, update only to a threshold desired level of performance (same as DP)



# Algorithms – MC – Policy Evaluation

Generate an episode that follows policy  $\pi$ :

 $s_0, a_0, r_1, s_1, a_1, r_2, \dots, s_{T-1}, a_{T-1}, r_T$ 

### Estimating $V^{\pi}(s)$ from experience

- Simply average many returns observed after visiting a certain state *s* 
  - After each occurrence of state *s* in an episode
- A state's value is the expected return
  - So, this average can become a good approximation to the expected value

### Two Types:

- First Visit: averaging only the returns following first visits to state s
- <u>Every Visit</u>: averaging returns <u>following all the visits to state s</u>

Use the same MC approach. The agent records the rewards received after taking action *a* at state *s* 

# Algorithms – MC – Policy Improvement

So we have discussed a way find  $V^{\pi}(s)$ 

Problem?

- We do not have the model of the environment (transition probabilities)
- Thus cannot easily do policy improvement (finding the new greedy policy  $\pi$ )

$$\pi'(s) = rg\max_{a} \sum_{s',r} \overbrace{p\left(s',r \mid s,a
ight)} [r + lpha V^{\pi}\left(s'
ight)]$$

• Instead we should estimate  $Q^{\pi}(s, a)$  directly:

$$\pi'(s) = rgmax_{a \in A} Q^{\pi}(s,a)$$

$$\pi_0 \stackrel{E}{
ightarrow} Q_{\pi_0} \stackrel{I}{
ightarrow} \pi_1 \stackrel{E}{
ightarrow} Q_{\pi_1} \stackrel{I}{
ightarrow} \pi_2 \stackrel{E}{
ightarrow} \dots \stackrel{I}{
ightarrow} \pi_* \stackrel{E}{
ightarrow} Q_{\pi_*}$$

# Algorithms – MC – Exploration Trade–Off

$$\pi_0 \stackrel{E}{
ightarrow} Q_{\pi_0} \stackrel{I}{
ightarrow} \pi_1 \stackrel{E}{
ightarrow} Q_{\pi_1} \stackrel{I}{
ightarrow} \pi_2 \stackrel{E}{
ightarrow} \dots \stackrel{I}{
ightarrow} \pi_* \stackrel{E}{
ightarrow} Q_{\pi_*}$$

#### Now we have another problem:

- Need to force exploration or some actions will never be chosen.
- How can we fix this?

#### Some ways...

- Exploring starts (MC-ES)
  - Each state-action pair at the beginning of an episode has a non zero probability.
    - But cannot always be done.
- <u>Soft policies</u> (e.g.: ε-greedy)
  - Most of the time choose an action that has maximal estimated action value
  - With probability epsilon instead select an action at random
- Off-Policy learning

 $\pi'(s) = \operatorname*{argmax}_{a \in A} Q^{\pi}(s,a)$ 

# Algorithms – MC – On–Policy vs Off–Policy



**On-policy:** Policy being evaluated and improved is also used to generate episode (e.g.:  $\epsilon$ -greedy) **Off-policy:** Separate <u>target policy</u> (greedy) and <u>behavior policy</u> ( $\epsilon$ -greedy)

# Algorithms – MC – Conclusions

### Key Takeaways

- Can learn directly from interaction with the environment
  - No need for full models
- No need to learn about all states
  - Computational complexity of updating one node is independent of |S|
  - So, optimal policy trajectory corresponds to a small state subset
  - Even if the environment's dynamics are known, MC is often more efficient than DP

### One issue to watch out for: maintaining sufficient exploration

- Exploring starts, Soft policies.
- Off-Policy Methods

# Algorithms - DP vs. MC Backup Diagrams



# Applications

### Robotics

- Robotic grasping and manipulation tasks
- Navigation in complex dynamic environments
- Autonomous driving, Industrial automation

#### Game Al

- Playing complex games like chess, Go, and poker
- Game AI for non-player characters (NPCs)
- Procedural content generation

#### **Recommendation systems**

- Personalized content recommendation
- Improving search engine results
- Dynamic pricing and demand forecasting

#### Finance

- Trading and portfolio optimization
- Fraud detection and prevention
- Risk management and forecasting

#### Healthcare

- Drug discovery and development
- Patient diagnosis and treatment planning
- Personalized medicine and treatment recommendations

# Implementation – Dynamic Programming

•	• •
	<pre>def train(self):</pre>
	delta = 0
	V_prev = np.copy(self.V)
	<pre>for state in range(self.env.observation_space.n):</pre>
	Q = np.zeros(self.env.action_space.n)
	<pre>for action in range(self.env.action_space.n):</pre>
	expected_value = 0
	<pre>for probability, next_state, reward, done in self.env.P[state][action]:</pre>
	expected_value += probability * (reward + self.gamma * self.V[next_state])
	Q[action] = expected_value
	action, value = np.argmax(Q), np.max(Q)
	<pre>self.V[state] = value</pre>
	delta = max(delta, abs(V_prev[state] - self.V[state]))
	if delta < self.theta:

#### Example Q-Table:



Resulting Policy:

# Implementation - Monte Carlo

# 

#### 🔴 🔴 🥘

def <b>update_first_visit</b> (self, episode_hist):			
for t in range(len(episode_hist) - 1, -1, -1):			
if (state, action) not in [(x[0], x[1]) for x in episode_hist[:t]]:			
<pre>self.R[state][action].append(G)</pre>			
<pre>self.Q[state, action] = np.mean(self.R[state][action])</pre>			
<pre>self.Pi[state] = np.full(self.n_actions, self.epsilon / self.n_actions)</pre>			
<pre>self.Pi[state, np.argmax(self.Q[state])] = (</pre>			

#### Example Q-Table:



# Implementation – Evaluation Environments

### Gymnasium - CliffWalking-v0

- **# States:** 48
- **# Actions:** 4
- Rewards:
  - -100 falling into cliff
  - 1 for reaching goal
  - -1 otherwise



# Implementation – Evaluation Environments

### Gymnasium - FrozenLake-v1

- **# States:** n^2 (variable)
- **# Actions:** 4
- Rewards:
  - 100 for reaching goal
  - -10 for falling into hole
  - -1 otherwise



# Implementation – Evaluation Environments

### Gymnasium - Taxi-v3

- # States: 500 (404 reachable)
  - 25 taxi positions
  - 5 passenger locations
  - 4 destinations
- # **Actions:** 6
- Rewards:
  - 20 for delivering passengers
  - -10 for illegal pickup/dropoff
  - -1 otherwise



### Implementation – Dynamic Programming Results

#### **Environment: FrozenLake-v1**

- Gammas tested: [0.95, 0.9, 0.8, 0.7, 0.6, 0.5, 0.1]
- Successful Gammas: [0.95, 0.9]



# Implementation – Monte Carlo Results



#### Environment: CliffWalking-v0

- Gammas tested: [1.0, 0.98, 0.96, 0.94]
- Epsilons tested: [0.1, 0.2, 0.3, 0.4, 0.5]
- $\leftarrow$  Average of 10 runs for each combination

Final Results → with Gamma=1.0 and Epsilon=0.4



# Implementation – Monte Carlo Results





#### **Environment: FrozenLake-v1**

- Gammas tested: [1.0, 0.98, 0.96, 0.94]
- Epsilons tested: [0.1, 0.2, 0.3, 0.4, 0.5]
- $\leftarrow$  Average of 10 runs for each combination

Final Results → with Gamma=1.0 and Epsilon=0.4



# Implementation – Monte Carlo Results



#### **Environment: Taxi-v3**

- Gammas tested: [1.0, 0.98, 0.96, 0.94]
- Epsilons tested: [0.1, 0.2, 0.3, 0.4, 0.5]
- $\leftarrow$  Average of 10 runs for each combination

Final Results → with Gamma=1.0 and Epsilon=0.5



# Implementation – Compare and Contrast

Number of Environment Samples*				
	Dynamic Programming	Monte Carlo		
FrozenLake	<u>3,328</u>	24,193		
CliffWalking	440,256	120,046		
TaxiCab	3,894,000	<u>1,055,934</u>		

# Implementation – Live Demo!

Hosted on HuggingFace Spaces: <u>https://huggingface.co/spaces/acozma/CS581-Algos-Demo</u>

GitHub Repository: https://github.com/andreicozma1/CS581-Algorithms-Project

# **Open Issues**

### • Exploration vs Exploitation

- Exploit (Act Greedily) with respect to what it has already experienced to maximize reward.
- Explore (Act Non-Greedily) or take actions which don't have the maximum expected reward in order to learn about new states
- Stochastic Tasks
  - Each action must be tried many times to gain a reliable estimate of its expected reward.
- Delayed Reward
  - Agents must consider more than the immediate reward because acting greedily may result in less future reward.
- Sample Efficiency
  - Some algorithms (like DP) require many environment samples which can be slow and inefficient

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### Discussion

# Test Questions (Revisited)

- 1. What does the "model" refer to in the terms "model-based" and "model-free"?
- 2. What are some of the limitations of Dynamic Programming methods?
- 3. How can you handle the exploration/exploitation trade-off in Monte Carlo methods?