Advanced concepts of Reinforcement learning

a practical guide

Simon Hirlaender IDA LAB <u>simon.hirlaender@plus.ac.at</u>

Artificial intelligence and Human Interfaces Digital and Analytical Sciences University of Salzburg







What's the goal

Learn how to make good decisions under uncertainty









Goals of today

- We don't necessarily develop new algorithms!
- Learn how to:
 - identify and set up RL problems
 - apply RL appropriately
 - deal with common problems
- RL is not easy, don't expect to understand or solve things immediately









Stop, Think, Apply!

- Pick the right problems!
 - Ask: does this have a chance of solving an important problem? Does my optimization problem have a chance to be solved? Do I solve the right problem?









RL - what is it today?

- What is addressed by RL: position in AI, community of researchers applying tools, data-driven dynamic programming
- Little knowledge of probabilistic mechanism how data and rewards change over time
- Probe and learn dynamics to find control

B. Recht, 2018





Al and optimization viewpoint







How to approach RL

- Pick the right problems (important and solvable)!
 - ➡ What is my goal?
 - What are my observables and my actions?
- Model the problem appropriately
- Training and evaluation of RL
- Are there better alternatives?







The entire problem

SB: 1, 3, 10, 17





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The entire problem

Markov decision process - MDP









Common set-up

Partially observable Markov decision process - POMDP









Wellcome to POMDPs





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Problem design - capture the right thing

- We want to solve an SDM problem: Information→Decision→Information→Decision→…
- Such problems are generally be stochastic!
- Consequently we build a feedback system not planing too far in the future:
 - We define a <u>state</u> $s_t = h_t(o_t, a_{t-1}, o_{t-1}, a_{t-2}, o_{t-2}...)$, as a function holding <u>sufficient statistics</u> until time step *t* for a decision (example pong)
 - We look for a decision based on s_t via: a_t = π_t(s_t) the policy optimise an expected aggregate of future rewards



• Rarely the observation *o* is the state *s*, the world state is, but often we assume it is!

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Generally POMDP - today MDPs!





POMDPs and non stationarity

- POMDP generally P-Space hard (not on average)
- To find a proper state we have to solve the additional prediction problem $s_t = h_t(o_t, a_{t-1}, o_{t-1}, a_{t-2}, o_{t-2}...)$
- In the non-stationary, finite horizon formulation the MDP has the form $(S, A, \{P\}_h, \{r\}_h, H, \rho_0) \Rightarrow$ Value-functions $Q_h(s, a)$ get time depended \Rightarrow similar form of Bellman equations
- We can incorporate time into state e.g. $\tilde{s} = (s, h) \Rightarrow$ standard MDP
- Generally Bellman equation nice in discounted, stationary formulation ⇒ this is what we usually see and most libraries build on this formulation





Remarks on MDPs

- Mainly we have POMDPs
 - Try to find a state which provides sufficient statistics to solve your problem (internal representation of the agent) - not world state
- Why is MDP so popular?
 - ➡ It always possible to make an MDP by including sufficient information
 - What if not Markov?
 - What happens? Q-learning example
 - Montecarlo No need for Markov assumption
 - History inclusion RNNs, LSTMs
- Extreme: Bandits \rightarrow no states (little knowledge about state)





The problem modelling









MDP - the ingredients

- MDP discounted version: (S, A, R, P, ρ_0 , γ)
 - → $P(s', r | s, a) = \mathbb{P}(S_t = s', R_t = r | S_{t-1} = s, A_{t-1} = a)$ dynamics function
 - Mainly defined by system (and my state and reward definition)
- What do I want to solve? What's the objective function? How to reach the goal? The expectation of reward in the future!







RL and optimization

- All said falls into the domain of optimization:
 - An optimiser tries to find the arguments of a function to maximise the function value (optimization is greedy!)
 - RL algorithms look to find a mapping (the policy) from states to actions maximising the expected cumulative reward rather than just a single optimal function value
 - If parametric function approximation is used, we try to find the values of the parameters of the approximated function (either a value function or the policy directly) to obtain this mapping (this a classical optimisation problem).
- RL is comparable to calculus of variation (its origin is in classical mechanics - HJB equation) instead of function optimization

Optimization

maximise_{A_i}
$$\sum_{t=0}^{T} R(S_t, A_t, W_t)$$

subject to: $S_{t+1} = f(S_t, A_t, W_t)$

 $\begin{aligned} & \text{maximise}_{\pi_t} \mathbb{E}_{W_t} [\sum_{t=0}^T R_t(S_t, A_t, W_t)] \\ & \text{subject to: } S_{t+1} = f(S_t, A_t, W_t) \\ & A_t = \pi_t(S_t, S_{t-1}, \ldots) \end{aligned}$

RL

Feedback structure takes noise into account

Often optimization is performed only for one step horizon: maximise_{*a*} $R(\cdot, a, W_t)$





Episodic training: we probe the system



- The system generates noisy trajectories: $\tau_i = o_{0,i}, a_{0,i}, o_{1,i}, r_{1,i}, a_{1,i}, o_{2,i}, r_{2,i}, \dots$
- From these probes we learn, but how?





Learning from episodes

- Rarely we have a full online learning problem
- The problem either is naturally episodic or we train in an episodic manner and are reset (adding absorbing state): $\tau_i = o_{0,i} \sim \rho_0, a_{0,i}, o_{1,i}, r_{1,i}, a_{1,i}, o_{2,i}, r_{2,i}, \dots$
- Design the episodic training:
 - → Is it an infinite horizon problem \rightarrow stability forever?
 - ➡ Is it a finite horizon problem with stationary dynamics?
- What is the role of ρ_0 ?
- What is the role of a finite maximum length?
- Exploration (finite time in infinite problem) not part of the problem

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• $(S, A, R, P, \rho_0, \gamma)$



Reward design and shaping

• (*S*, *A*, *R*, *P*,
$$\rho_0$$
, γ)

- The reward includes the goal and how to reach the goal!
- There is an equivalence class of problem formulations leading to the same goal → differences in algorithmic efficiency
 - Example: Negative/Positive/Normalised Reward
- Generally probabilistic: $P(r \mid s, a, s') = \sum_{s'} P(r, s' \mid S_t = s, A_t = a)$
- Can be formulated in dependence of s and a or given as a direct feedback signal
- To improve exploration or to solve sparse reward problems reward shaping during training!





The discounting γ - a hyperparameter?

- (*S*, *A*, *R*, *P*, ρ_0 , γ)
- Generally we don't need discounting
- Introduced due to mathematical convenience: convergence of cumulative sum of rewards as N

alternative to mean reward:

$$\sum_{t}^{N} \gamma^{t} R_{t} \leq \frac{1}{1 - \gamma}, \text{ when }$$

 R_t is bounded in [0,1]

- Can be used influence training performance
- Not needed in naturally episodic problems!







- Capture the right problem
- Formulate the MDP appropriately
- (Problem equivalent) Design has impact on RL algorithm
- Problem I solve = Designed MDP + Reward objective









The entire problem







About Machine Learning

SB: 9









RL and decision theory

 $\text{Information} \rightarrow \text{decision} \rightarrow \text{Information} \rightarrow \text{decision} \rightarrow \text{Information} \rightarrow \dots$



- One step horizon offline RL \Rightarrow Prediction $\mathbb{P}(Y_i | X_i)$ pattern recognition or supervised learning (SL)
- One step horizon RL \Rightarrow active Learning e.g. system identification
- RL is a multi step optimization problem we learn about the dynamics of the world







Prediction

• Function approximation (FA):

- → Parametric compact approximation of a function using a parametrised representation $f(x) \approx \hat{f}(x, \bar{\theta})$, where $\bar{\theta}$ are parameters to be adapted
 - Fixed representational power
 - Constant computationally complexity fixed set of parameters
 - Example: Artificial neural networks (ANNs), linear approximations...
- Non-parametric memory based:

$$f(x) \approx \hat{f}(x, \textcircled{D}) = \sum_{x' \in \mathscr{D}} \underbrace{k(x, x')}_{\text{Kernel Weight}}$$

- No fixed representational power
- Parameters are not learned directly
- Computationally complexity grows with data
- Example: Gaussian processes, Kernel-based methods,...







Problem



Solving the problem







Most common issues RL - algorithmic side

- Sample efficiency
- Stability
- Run time
- Hyperparameter tuning
- Exploration







Remarks on RL

- Trial and error
- Only rewards (labels of visited state, actions)
- Policy decides what we learn usually censored
- Only valid estimates of things sufficiently learned







Special cases

- We know $P(s', r \mid s, a)$ and the MDP is finite frame work of dynamic problem can be used (Bellman update is exact):
 - ➡ Good theoretic properties
 - Playground of classical control theory
 - ➡ If large, we use sampling: approximative dynamic programming
- If P(s', r | s, a) is known, the dynamics is linear and we design a quadratic dependence of s and a of the reward: analytical solutions (the popular Linear Quadratic Regulator -LQR).
 Stationary dynamics → Bellman → Ricatti equation static state feedback.

- Alternative solution methods?
 - ➡ E.g. linear programming







Hidden Markov Models - POMDPs

- Linear POMDP: believe state $O_t = h_t(S_t, A_t, W_t)$
 - Static output feedback is NP hard (linear in O and dynamics)
 - General POMDPs are PSPACE hard
- There are ways out separation principle:
 - → Filtering $\hat{s}_t = f(\{o_t\})$ prediction problem
 - Action based on certainty equivalence
 - Optimal filtering if dynamics are linear and noise is Gaussian Kalman filtering - general belief propagation - LQG

- Kalman filtered state duality between estimation and control
- Estimate state with prediction $S_t = h(\tau_t)$, τ_t are time lags





General cases

- $P(s', r \mid s, a)$ unknown \rightarrow approximative methods
- MDP finite: approximative dynamic programming
- General MDPs: Continuous A, S spaces
 - Value function approximated with FA

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- Policy approximated with FA
- ➡ Model of the MDP (learn from data or from simulator) use certainty equivalence
- Trained in a stochastic fashion







Policy based





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Direct policy search

- RL as derivative free optimization:
 - → maximise_{$z \in \mathbb{R}^d$} R(z) ⇒ maximise_{p(z)} $\mathbb{E}_p[R(z)]$
 - → Parametrise a distribution $p(z; \theta) \Rightarrow \text{maximise}_{p(\theta)} \mathbb{E}_{p(z; \theta)}[R(z)]$
 - Likelihood trick estimate the derivative:

$$\nabla_{\theta} J(\theta) = \int R(z) \nabla_{\theta} p(z;\theta) dz = \int R(z) \frac{\nabla_{\theta} p(z;\theta)}{p(z;\theta)} p(z|\theta) dz$$

$$= \int R(z) \nabla_{\theta} \log p(z;\theta) p(z|\theta) dz = \mathbb{E}_{p(z;\theta)} [R(z) \frac{\text{Score function}}{\nabla_{\theta} \log p(z;\theta)}]$$

• Unbiased gradient estimate of *J*, if sample efficiently from $p(z; \theta)$ and $\log p(z; \theta)$

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• High variance



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Probabilistic trajectories

- Objective if episodic: $J(\theta) = V^{\pi_{\theta}}(s_0) := V(\theta)$
 - Stochastic search: pure random search, Simplex, Bayesian optimization



- Sampling of $A_t \sim p(\cdot | \tau_t; \theta)$
 - Handle probabilistic policies (example)
 - High dimensional and continuous action spaces
 - Reinforce algorithm considers temporal structure
- Finite difference approximation $\hat{=}$ Reinforce algorithm









Value based



The value-function is introduced to compare policies



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Basis of Q-Learning - Temporal difference (TD) learning

 If one had to identify one idea as central and novel to reinforcement learning, it would undoubtedly be temporal-difference learning. (Sutton and Barto, p.113)

•
$$V^{\pi}(s) = \mathbb{E}_{\pi}\left[\sum_{t} \gamma^{t} R_{t+1} | S_{t} = s\right] = \mathbb{E}_{\pi}[R_{t+1} + \gamma V(s') | S_{t} = s]$$

- Estimated via sampling: TD(0) error
- $\hat{V}(S_t) \leftarrow \hat{V}(S_t) \alpha[R_{t+1} + \gamma \hat{V}(S_{t+1}) \hat{V}(S_t)]$ Bootstrapping = Learn rate Bootstrapping =
- Can be used in episodic an non-episodic scenarios
- Immediate update of the estimator
- If probabilities known exact update





Q-learning - issues

 $\begin{array}{l} \text{Bellman equation:}\\ Q^*(s,a) = \mathbb{E}[R_t + \max_{a'} Q^*(s',a')]]\\ \text{Bellman-operator is a contraction operator }(L^2\text{norm}) \text{ - converges to a fixed point}\\ \text{Here - stochastic approximation:}\\ \hat{Q}(s,a) \approx \hat{Q}(s,a) + \alpha[R_t - \max_{a'} \hat{Q}(s',a')] \end{array}$

•
$$\pi(s) = \operatorname{argmax}_a Q(s, a)$$

- Two immediate consequences:
 - Maximisation bias (expectation and maximisation don't commute)

- ➡ Bias through bootstrapping
- Inefficient update (compare to e.g. SL)
- If FA is used contraction property might lost
- Might diverge **deadly triad**:
 - ⇒ FA
 - Bootstrapping
 - ➡ Off-policy







Deep approximate dynamic programming

- Value dominated
- Tries to mitigate maximisation bias (double networks)
- Stabilises training of networks trough tricks (random batches from replay buffer, target network, action noise) - (DDPG, TD3)
- More recent: distributional learning (D4PG), truncating trajectories (TQC)









Modern algorithms

- Interplay of Bias and Variance
- Policy dominated: add baseline the critic!
- DDPG: maximisation operator in Bellman equation is approximated - the actor!









Modern landscape

- Bias-Variance trade-off
- Regulated via Policy based and Value based methods
- Policy gradient regulated via update-length of value function











Value vs policy dominated



- SAC Soft Q learning stochastic
- D4PG Distributional Q-Learning
- MPO





Summary

- Value based: Approximate bellman updates biased
- Policy based: high variance but stable
- Modern actor critic algorithms: bias-variance tradeoff







Model of the MDP



Separation heuristics

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Modelling the MDP

- We can have a **simulation** $\hat{P}(r, s' | s, a)$ which models the real (true) MPD P(r, s' | s, a)
- We can learn the MDP from real data using FA
- During training the RL algorithm we use $\hat{P}(r, s' | s, a)$ as it would be P(r, s' | s, a) and hope to solve the problem (certainty equivalence)
- We can use a mixture of both
- Deal with consequences, try to learn $\hat{P}(r, s' | s, a)$ as accurate as possible (system identification)







Train a good MDP

- What degrees of freedom to excite to learn the control problem?
- Model the uncertainties appropriately
 - ➡ Learn a model capturing the epistemic and aleatoric uncertainty (the noise)

- ➡ Take the epistemic uncertainty appropriately into account
- ➡ Examples: ensembles of ANNs, Bayesian ANNs, GPs...
- Having a model allows for planning
 - ➡ Horizon is critical!
 - Safety constrains can be taken into account







AWAKE Simulation Benchmark



Correctors (magnets)

•
$$R = -(\sum_{i} \Delta x_{i}^{2})^{\frac{1}{2}}$$

• 10 magnets = {
$$k_1, k_2, \dots, k_{10}$$
}

• 10 positions = { $\Delta x_1, \Delta x_2...\Delta x_{10}$ }



Target: trajectory steering - correct the trajectory in as little steps as possible.







Example: Model based policy optimization

- Dyna style algorithm
- Model: Bayesian ANN bootstrapped ensemble
- RL algorithm: SAC
- Short roll-outs from real interactions
- Monotonic behaviour

Dynamics Model

• Many hyper-parameters

https://arxiv.org/abs/1906.08253

Ground Tru Bootstrap 1

 Bootstrap 2 Training Date Real

AWAKE simulation 250 o 120 keps 120 keps inlati cumm 50 10 20 30 40 50 30 ep_length 20 30 40 50 0.0 ep_reward -0.2 -0.4-0.6 20 30 40 50 10 #episodes Trajectory Propagation c'''

Adapted from https://arxiv.org/abs/1805.12114



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Example: Model predictive control (MPC)

- If convergence quickly no long term planning needed - solve infinite horizon problem with short term planning (open loop)
- Plans action sequence (optimisation) and takes first action only then replan
- Might retrain MDP model each step













• Solves the infinite optimization problem (W_t =random variable):

$$\begin{split} \text{maximise}_{\pi_t} \mathbb{E}[\sum_{t=0}^{\infty} R_t(S_t, A_t, W_t)] \\ & \underset{t=0}{\overset{t=0}{\text{Optimise finite horizon}}} \\ \approx \text{maximise}_{\pi_t} \mathbb{E}_{W_t}[\sum_{t=0}^{T} R_t(S_t, A_t, W_t)] + \frac{V(S_{T+1})}{V(S_{T+1})}] \\ & \text{subject to: } S_{t+1} = f(S_t, A_t, W_t) \\ & A_t = \pi_t(S_t, S_{t-1}, \dots), \qquad S_0 = s \end{split}$$





MPC with Gaussian Processes

- Data-Efficient Reinforcement Learning with Probabilistic Model Predictive Control
- Few shot RL learning on AWAKE



Summary

- Modelling the MDP certainty equivalence
- Modelling epistemic and and aleatoric error
- Short horizons and feedbacks avoid model bias
- With a model safety concerns can be considered







General comments on RL











Exploration/Exploitation

- You only can estimate things you have sufficiently learned!
- Finite MDP: ε greedy, what does this mean?
- Gaussian noise continuous actions
- Boltzmann exploration
- Theory: Bandit algorithms to study trade-offs (Book)





Sample-Complexity





ALZBURG

Use existing data?

• On-policy, off-policy, offline training



https://arxiv.org/format/2005.01643







Some training tips

- How to measure the performance of RL algorithms?
 - ➡ Take different seeds!
 - Return per episode on validation during training
 - Episode length
- How to set up your algorithmic environment?
 - Only start to implement, if there is no established library
 - Debugging is tricky in Monte-Carlo experiments, start simple and slowly increase complexity

- More in our tutorial
- The solution is on <u>MDP + objective function</u>







Limitations

- Stability
- Safety
- Sample-efficiency
- Sufficient observability
- Interpretability
- •







Summary

- Exploration/Exploitation
- Sample-efficiency
- On-policy, off-policy, offline RL
- Training
- Limitations







Advanced topics - outlook









Beyond the classical MDP



Contextual MDPs

Multi task RL

Meta RL





Common learning can Accelerates learning improve sample efficiency enormously



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Example: Meta-RL

- Awake simulation, varying quads
- Few shot stable adaption
- TRPO with some guarantees

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Further advanced topics

- Meta RL
- Multi task RL
- Contextual RL
- Multi-agent RL
- Hierarchical RL
- Distributional RL
- Inverse RL/Imitation learning







Summary

- Overview of designing correct problem
- Function approximation
- Different RL solution approaches: Value, Policy, MDP-model

- RL algorithmic challenges
- Beyond classical RL







Selected Literature

General:



M Reinforcement Learning: An Introduction http://incompleteideas.net/book/the-book-2nd.html



Deep Reinforcement Learning: Fundamentals, Research and Applications https://link.springer.com/book/10.1007/978-981-15-4095-0



https://rltheorybook.github.io/

POMDPs:



Algorithms for Decision Making https://algorithmsbook.com/



Decision Making Under Uncertainty: Theory and Application: http://web.stanford.edu/group/sisl/public/dmu.pdf



Markov Decision Processes: Discrete Stochastic Dynamic Programming: https://onlinelibrary.wiley.com/doi/book/10.1002/9780470316887



Reinforcement Learning and Stochastic Optimization: A Unified Framework for Sequential Decisions: https://onlinelibrary.wiley.com/doi/book/10.1002/9781119815068





