M A D
Math and Data

NYU COURANT INSTITUTE OF MATHEMATICAL SCIENCES
NYU CENTER FOR DATA SCIENCE

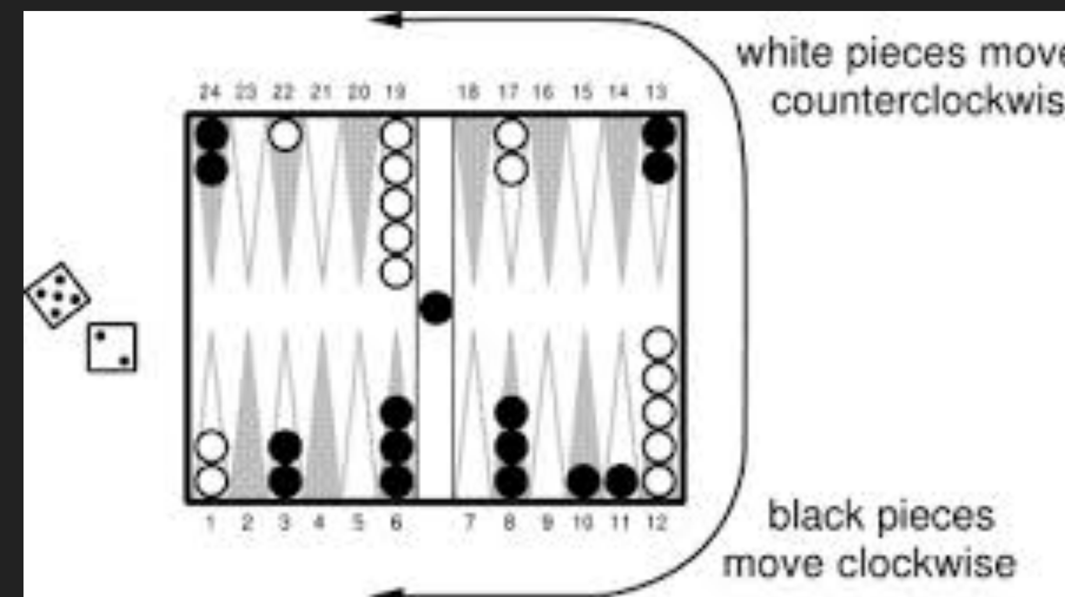
JOAN BRUNA

GEOMETRIC INSIGHTS FOR NONLINEAR TD CONVERGENCE

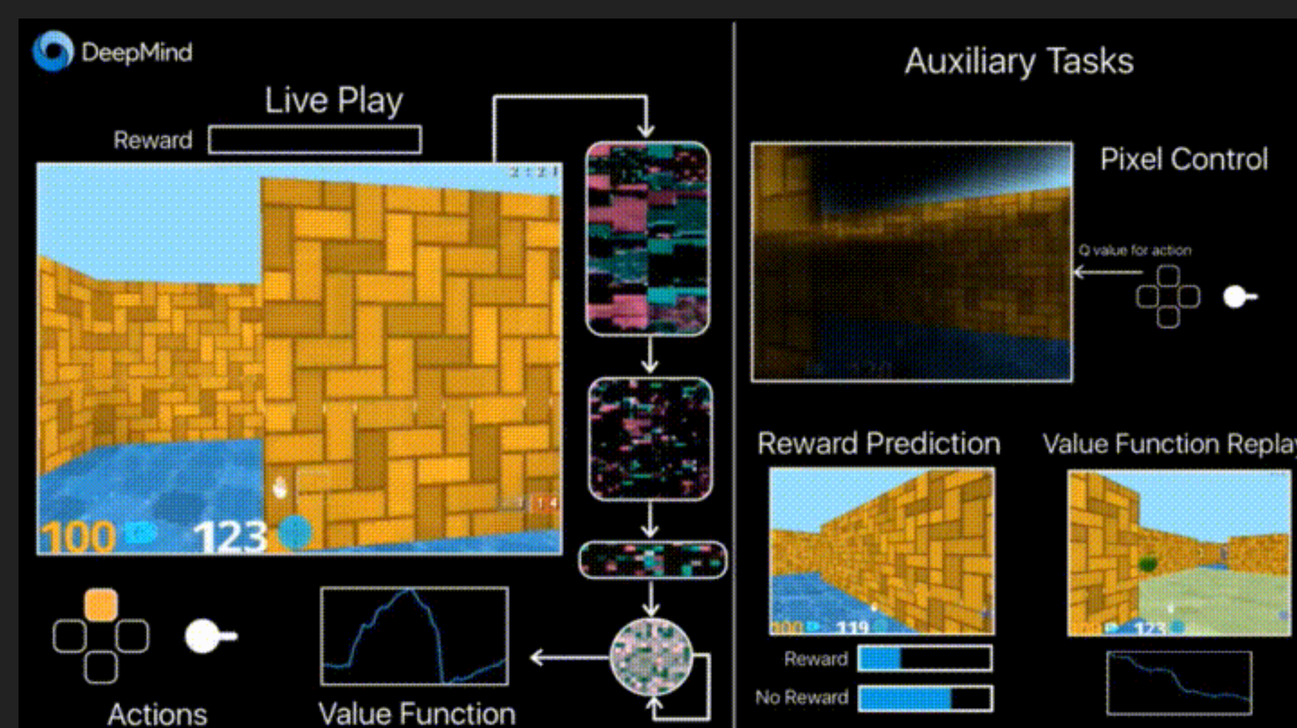
joint work with David Brandfonbrener

- General framework to learn how to interact in complex, high-dimensional environments.

Deepmind'16

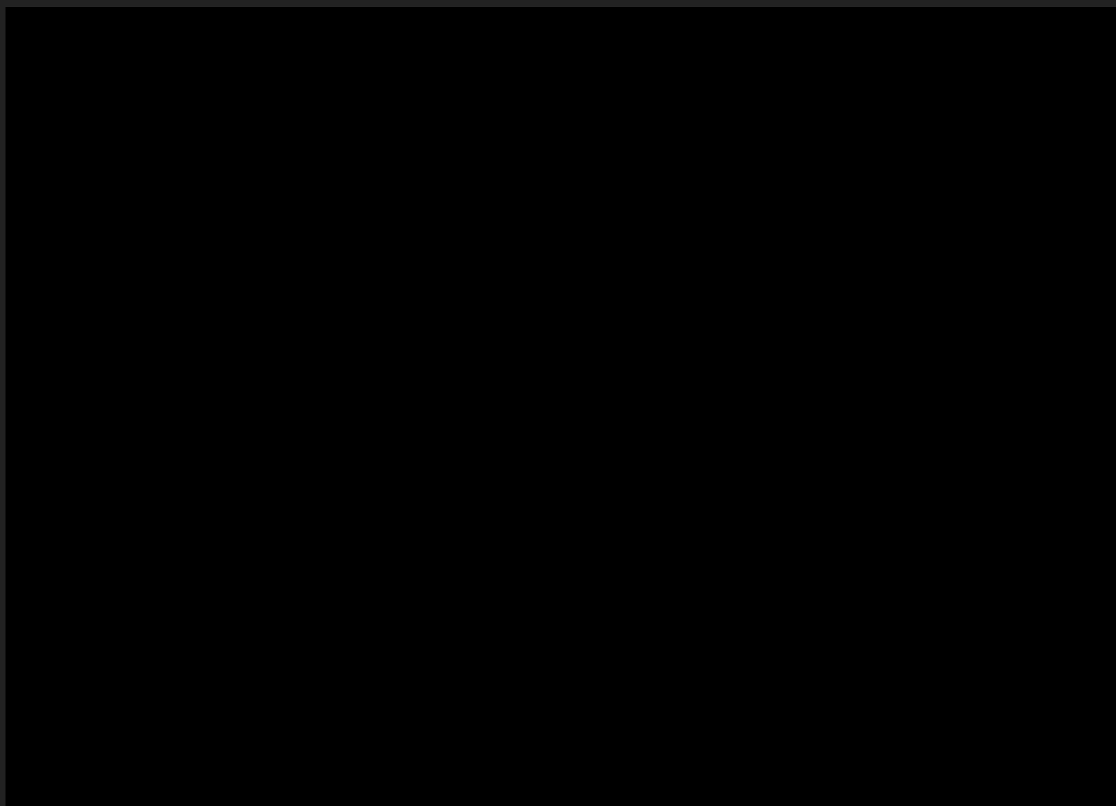


TD-Gammon, Tesauro'92



Deepmind'17

REINFORCEMENT LEARNING



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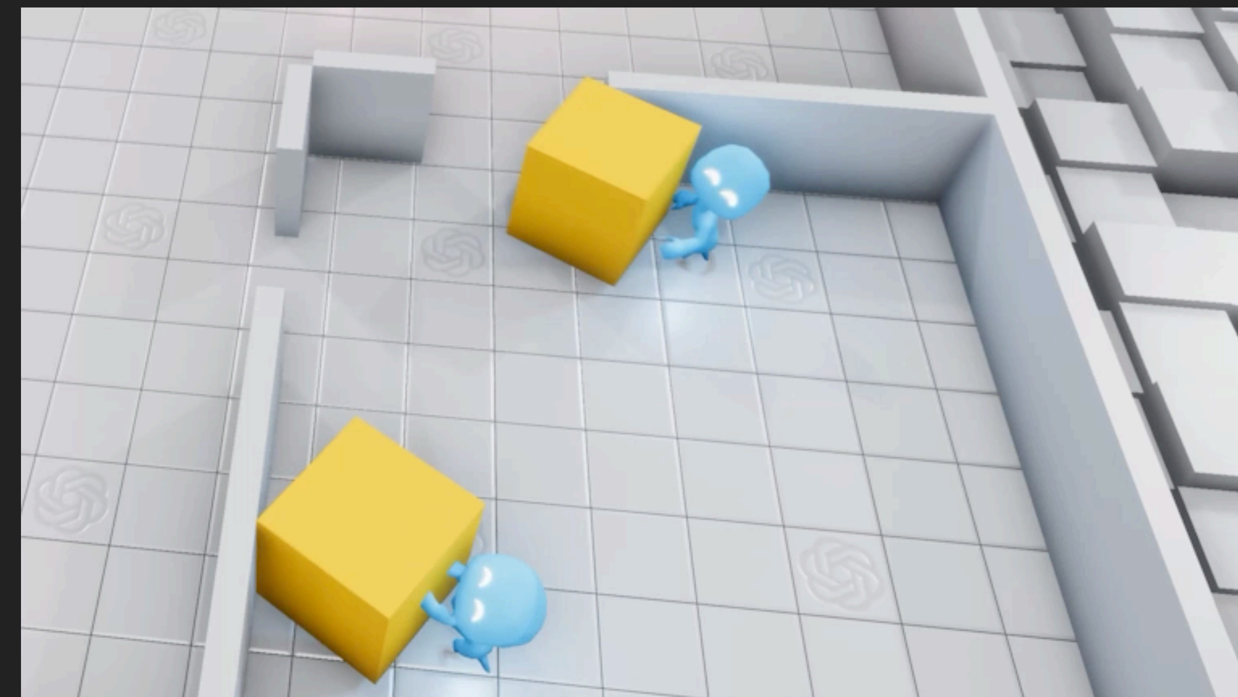
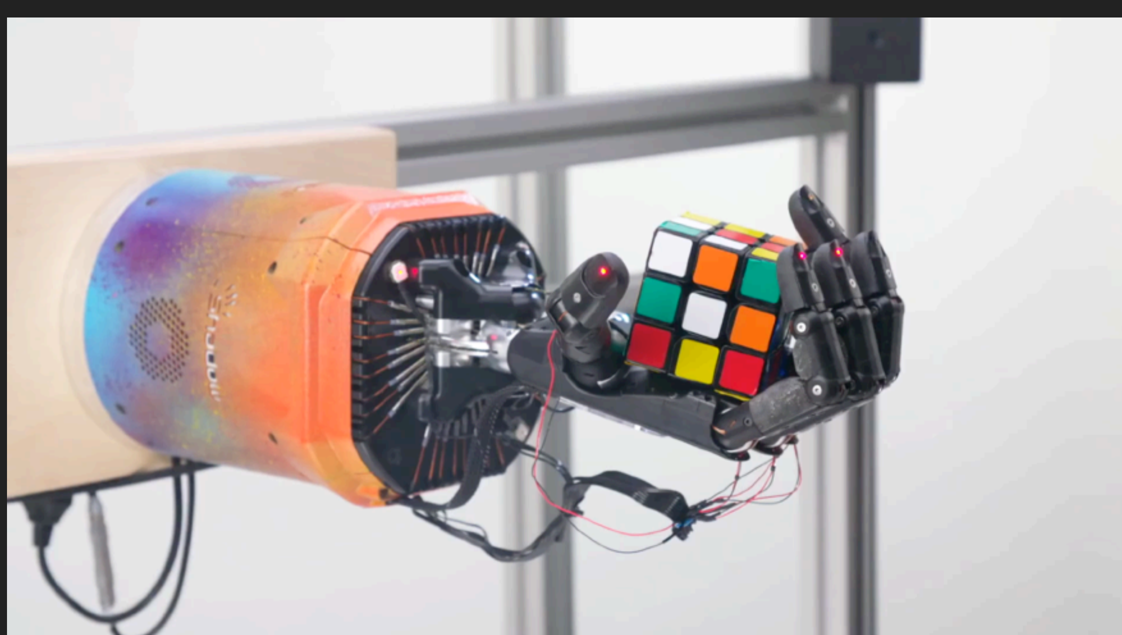


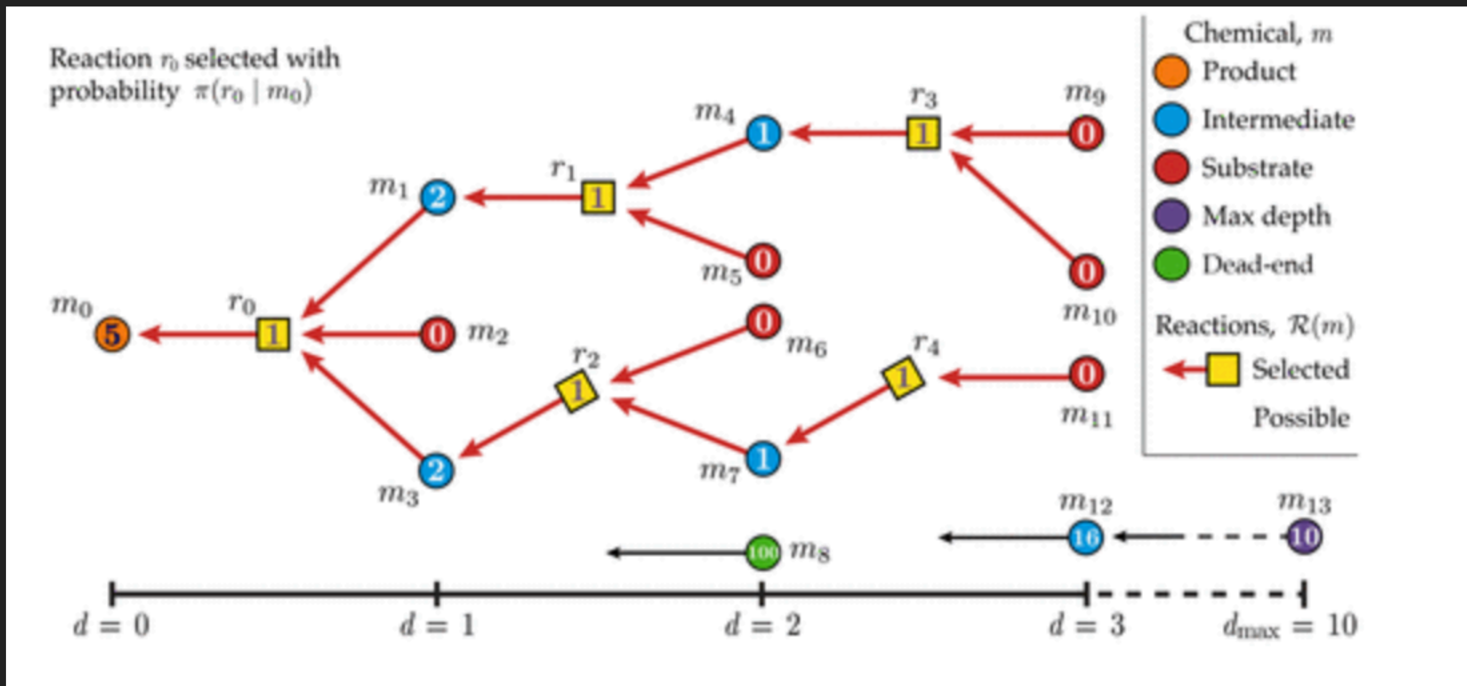
Hide and Seek, OpenAI'19



OpenAI'19

Alphastar, Deepmind'19

REINFORCEMENT LEARNING



Chemical Retrosynthesis, Shreck et al.

Quantum Control

ARTICLE OPEN

Universal quantum control through deep reinforcement learning

Murphy Yuezhen Niu[1,2], Sergio Boixo[2], Vadim N. Smelyanskiy[2] and Hartmut Neven[2]

Reinforcement Learning for Integer Programming: Learning to Cut

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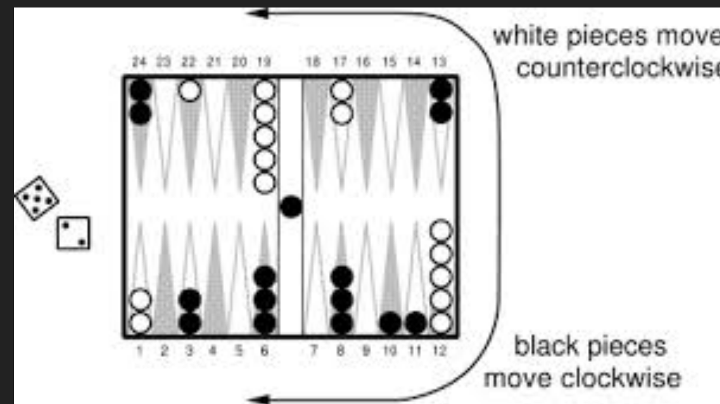
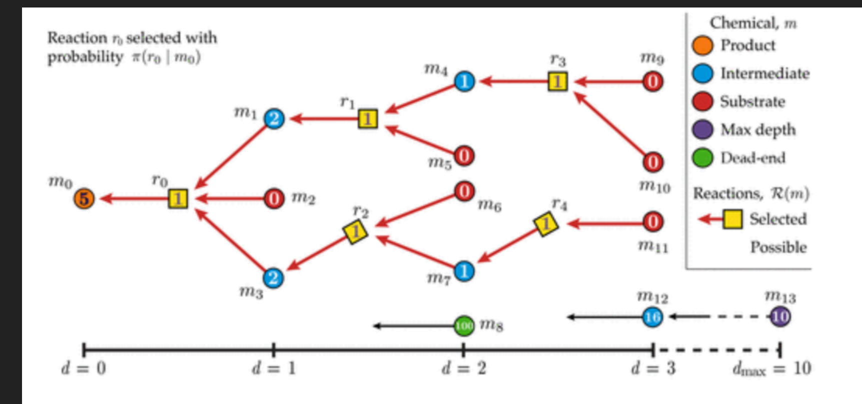
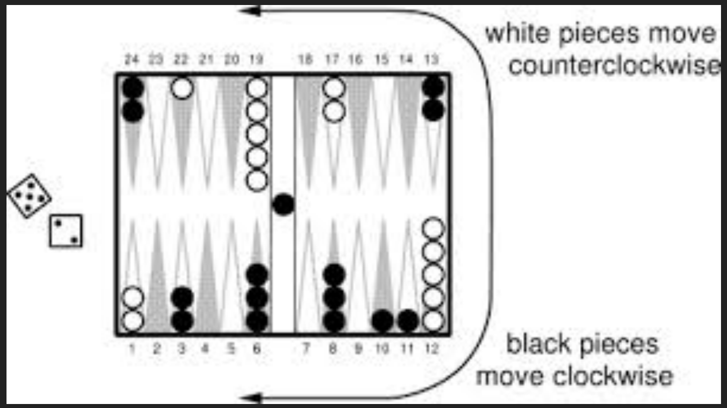
Integer Programming

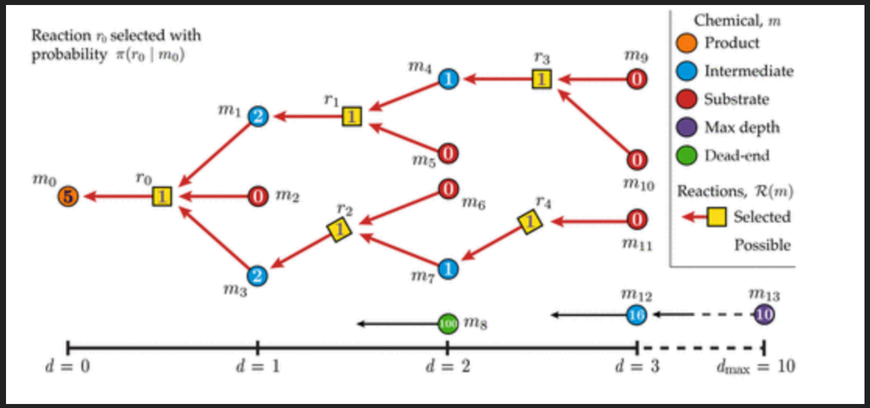
RL TODAY





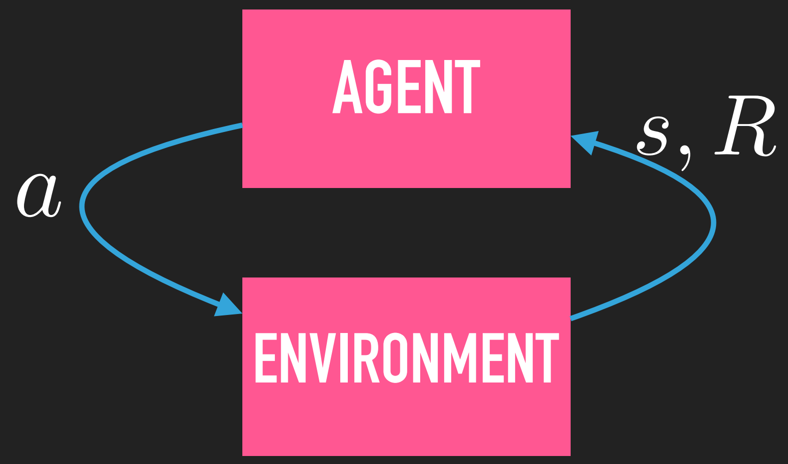
- Remarkable ability to discover useful policies in large environments.
- High-dimensional, noisy, observations.





- Remarkable ability to discover useful policies in large environments.
- High-dimensional, noisy, observations.
- Yet, with
  - poor sample efficiency.
  - limited theoretical guarantees.

- Mathematical Setup: $\mathcal{M} = (\mathcal{S}, \mathcal{A}, \mathcal{P}, R, \gamma, \rho)$
  - $\mathcal{S}$: state space (might be discrete or continuous).
  - $\mathcal{A}$: space of actions (assumed the same for all states).
  - $\mathcal{P}(s' \mid s, a)$: Markov transition probability kernel.
  - ρ : initial state distribution.
  - $R(s, a)$: instantaneous reward.
  - γ : discount factor, assume $0 \leq \gamma < 1$.



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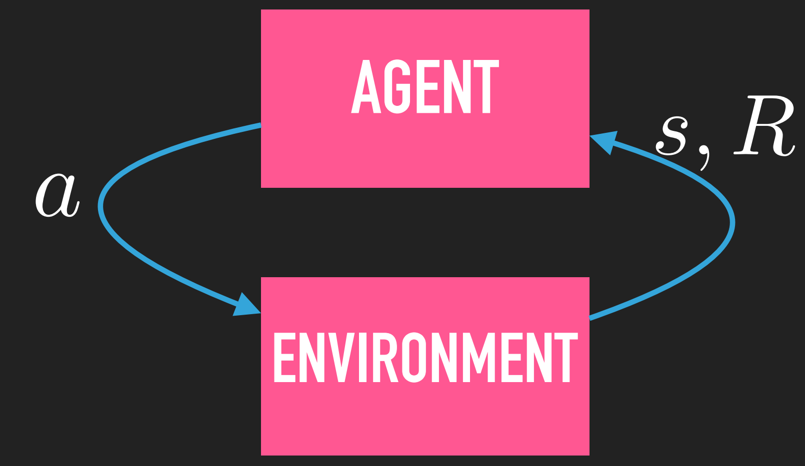
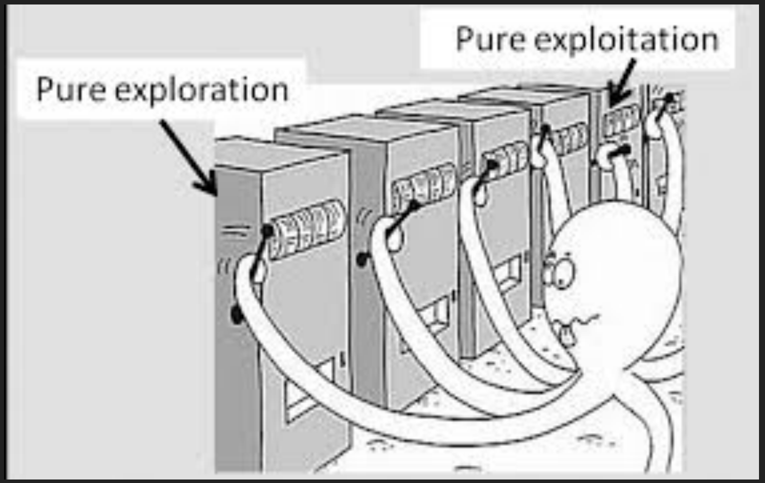


- Goal: Find a *policy* $\pi : \mathcal{S} \to \mathcal{A}$ that maximizes expected sum of discounted rewards:

$$\max_{\pi} \mathbb{E}_{\rho,\mathcal{P}} \sum_k \gamma^k R(s_k, a_k) \text{ subject to } \begin{aligned} & s_{k+1} \sim \mathcal{P}(s'|s_k, a_k) \\ & s_0 \sim \rho \\ & a_k = \pi(s_k) \end{aligned}$$

- Exploration/Exploitation tradeoff:
    - Unknown environment, need to uncover potential rewards while exploiting known good strategies.



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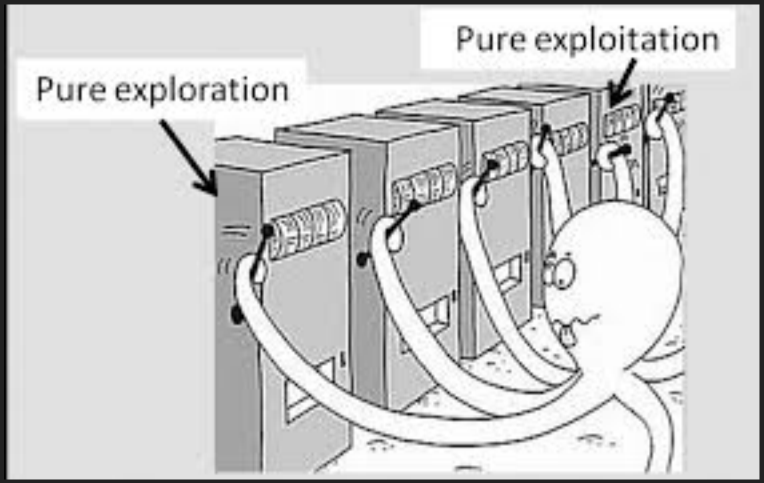

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    - Valid strategies may pay off at later stages.

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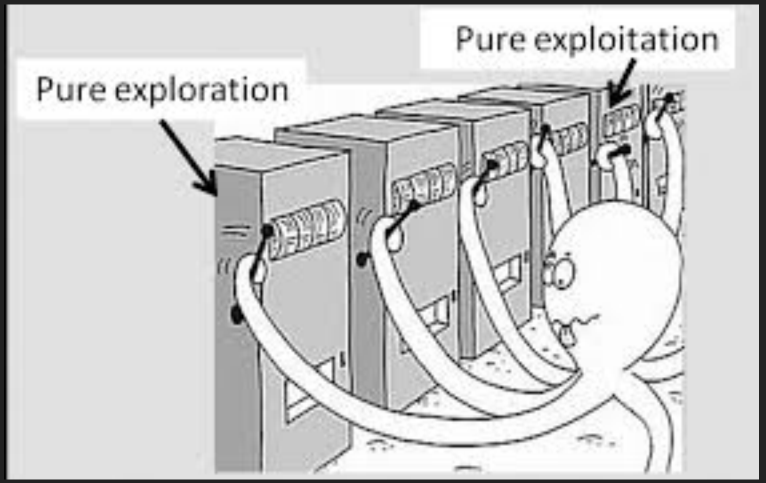

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- High-dimensional, complex observations.
  - Need to learn good state representations.

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- *Approximate Dynamic Programming:* Exploit recurrence structure in optimal policy (Q-learning):
  - Estimation: Given a policy π, compute the *Value* of a state *s:*

$$V^{\pi}(s) := \mathbb{E} \sum_k \gamma^k R(s_k, a_k); s_0 = s, a_k = \pi(s_k).$$

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  - Control: Modify π greedily from estimated value functions.
- *Policy gradient:* Bypass both model and value, optimize directly over parameters of policy. *Essentially a derivative-free method.*

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- How to learn with guarantees using nonlinear approx?

- Focus on Value estimation with non-linear function approximation: convergence of non-linear TD learning.
- Interplay between MDP and function approximation geometry: we establish convergence conditions.
- Key geometric properties of function approximation:
  - Homogeneity
  - “Includes” linear functions –> Residual architecture.

- Recall the value function associated to a current policy:

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- The most popular algorithm to estimate it is *Temporal-Difference learning* [Sutton, Samuel].
  - Given transition $(s, \bar{R}(s), s')$ and step-size α_k

$$V^{(k+1)}(s) = V^{(k)}(s) + \alpha_k \left(R(s,a) + \gamma V^{(k)}(s') - V^{(k)}(s) \right).$$

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  - Under appropriate conditions, we have $V^{(k)} \to V$ as $k \to \infty$.

[Robbins & Munro,50s]

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    - as $\alpha_k \to 0$, the *expected* dynamics of TD become

$$\dot{V}(s) = \mu(s)\left(\bar{R}(s) + \gamma \mathbb{E}_{s' \sim \mathcal{P}(.|s)}[V(s')] - V(s)\right)$$

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  - In matrix form, using Bellman equation $V^\pi = \bar{R} + \gamma \mathcal{P} V^\pi$,

$$\dot{V} = D_\mu(\bar{R} + \gamma \mathcal{P} V - V) = -A(V - V^\pi), \text{ with}$$
$$A := D_\mu(I - \gamma \mathcal{P}),\ D_\mu = \mathrm{diag}(\mu).$$

- Fact: A is a "positive-definite", non-symmetric, matrix, ie $x^\top A x > 0 \text{ when } \|x\| > 0.$ [Sutton,'88]

CONSISTENCY OF TD-LEARNING: TABULAR CASE

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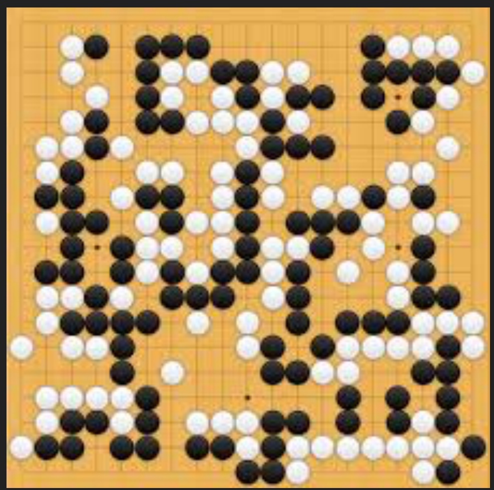
- Infeasible in any typical large-scale scenario.



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- TD(0) "semi-gradient" algorithm [Sutton]:

$$\theta^{(k+1)} = \theta^{(k)} + \alpha_k \nabla_\theta V_{\theta^{(k)}}(s) \left(\bar{R}(s) + \gamma V_{\theta^{(k)}}(s') - V_{\theta^{(k)}}(s) \right).$$

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- Such update approximates the stochastic gradient of the squared Bellman error $\Delta(\theta) := \|V_\theta - \bar{R} - \gamma \mathcal{P} V_\theta\|^2$
  - Problem: an unbiased estimator of $\nabla_\theta \Delta(\theta)$ requires two samples s' from the environment ("*double-sample*" problem):

$$\nabla_\theta \Delta(\theta) := 2(V_\theta - \bar{R} - \gamma \mathcal{P} V_\theta) \cdot (\nabla_\theta V_\theta - \gamma \mathcal{P} \nabla_\theta V_\theta)$$

  - This breaks convergence guarantees of stochastic optimization.

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- Alternative Strategies to TD to ensure convergence:
  - "Two-time-scale" algorithms [Dai et al., Borkar et al, Chung et al]

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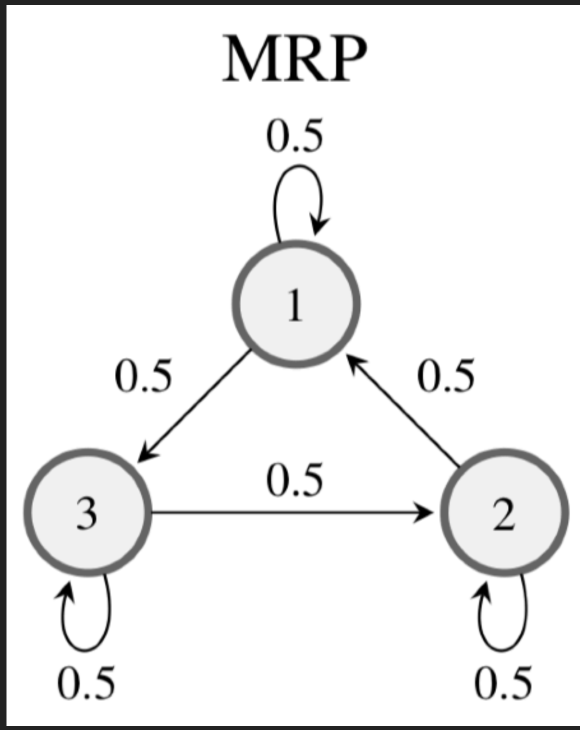
- Divergence example from [Tsitsiklis & van Roy]:



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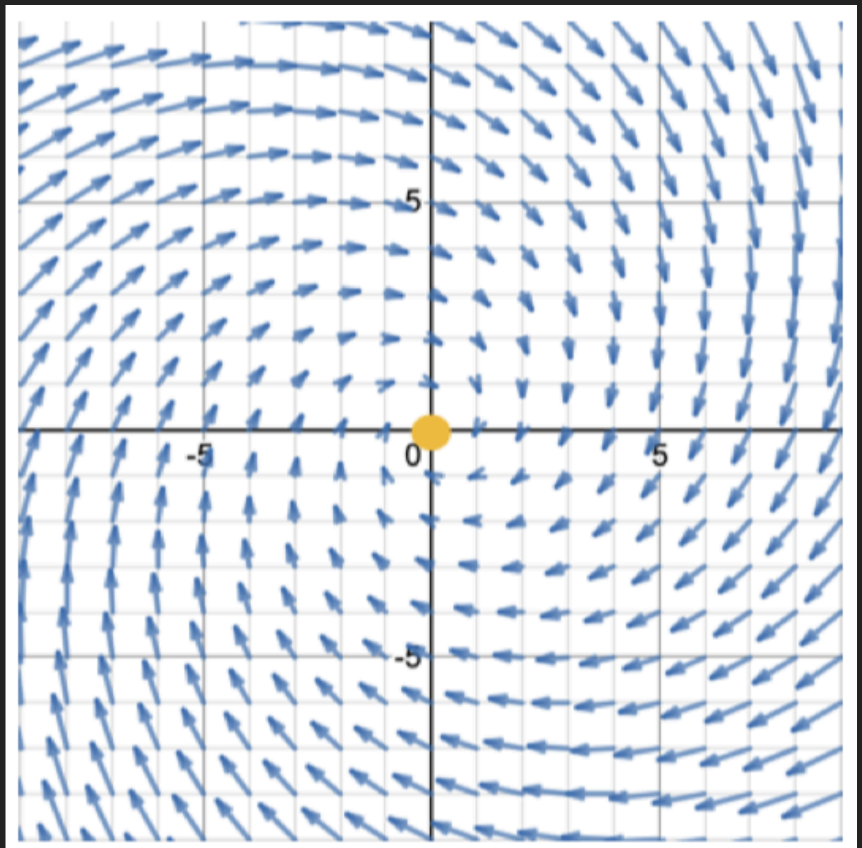
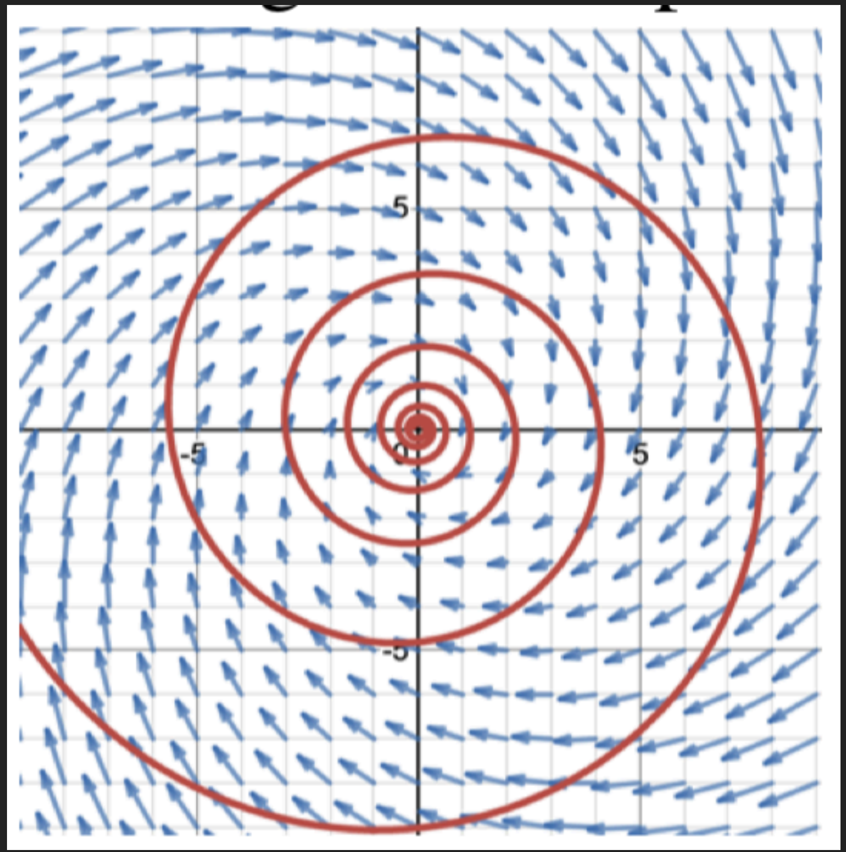
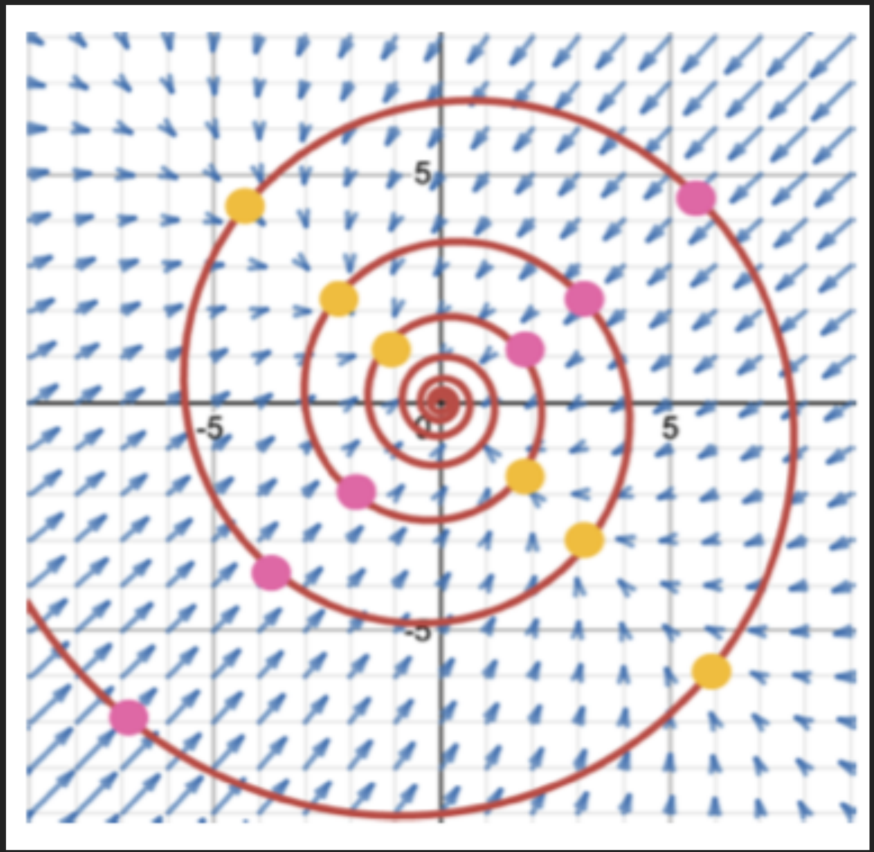


Nonlinear Function Approximation



Reversible Case



- $f : \mathbb{R}^k \to \mathbb{R}^m$ is *h*-homogenous for $h \in \mathbb{R}$ if

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Theorem [BB'19]: Let $\theta \mapsto V(\theta)$ be h-homogeneous and l-Holder. Then for each $\epsilon > 0$ and any initial θ_0, we have

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  - In the worst case, homogeneous TD is not worse than using the 0 function baseline: $\|0 - V^*\|_\mu \simeq \frac{\|\bar{R}\|_\mu}{1-\gamma}$
  - Stronger baseline?

- $f : \mathbb{R}^{k_1} \times \mathbb{R}^{k_2} \to \mathbb{R}^m$ is *residual-homogeneous* if $f(x_1, x_2) = \Phi x_1 + g(x_2),\ \text{with } g \text{ homogeneous.}$

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- Generically, no global convergence. Role of overparametrisation?

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- Global convergence with well-conditioned function approximation:

Theorem [BB'19]: Assume that $\kappa(\nabla V(\theta)\nabla V(\theta)^\top) < \rho(\mathcal{P})$ for all θ. Then $V(\theta(t)) \to V^\pi$ as $t \to \infty$.

- Recall that reversible dynamics result in gradient descent [Ollivier'18]. Can we leverage this property?
- **Definition:** The reversibility coefficient of a Markov Chain $\mathcal{P}$ is
$$\rho(\mathcal{P}) = \inf_{v \in \mathbb{R}^n \setminus \{0\}} \frac{\|S_A v\|^2 + \|Av\|^2}{\|R_A v\|^2}, \text{ with}$$
$$A = D_\mu(I - \gamma\mathcal{P}), S_A = (A + A^\top)/2, R_A = (A - A^\top)/2.$$
- Global convergence with well-conditioned function approximation:

Theorem [BB'19]: Assume that $\kappa(\nabla V(\theta) \nabla V(\theta)^\top) < \rho(\mathcal{P})$ for all θ. Then $V(\theta(t)) \to V^\pi$ as $t \to \infty$.

  - Observe that $\kappa(\nabla V(\theta) \nabla V(\theta)^\top) < \infty$ requires $d > |\mathcal{S}|$.
  - Open: underparametrised case with extra smoothness?

BEYOND CONVERGENCE

- Convergence of Value Estimation is the weakest possible guarantee.
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- Rate of convergence currently only known for linear models [Bandhari et al.'18]. Non-linear case?
- Preliminary analysis: does not measure sample efficiency.
- Sample Complexity of "model-free" RL
  - Tabular Case [Jin et al.'18], [Azar et al.'17], [Brunskill et al.].
  - Linear Function Approximation [Jin et al.'19], [Brandfonbrener et al.'19]
  - Policy Gradients [Argawal et al.'19]

CONCLUSIONS

- Analysis of TD-learning using nonlinear function approximation.
- Interplay between geometry of function approximation (homogeneity, conditioning, linear baseline) and environment (reversibility).
- Learning with guarantees under such conditions.
- Next: Further exploit regularity of reward/environment to reduce overparametrisation.
- Next: From of value estimation to policy update, tighter link between environment and network parametrisation.

Thanks!

Reference:

“Geometric Insights into the convergence of nonlinear TD learning”, D. Brandfonbrener and J. Bruna, *submitted*, https://arxiv.org/abs/1905.12185