CS4400
DEEP REINFORCEMENT LEARNING

Lecture 8: Exploration

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Content of this lecture

8.1

Exploration

Exploration

Recap: exploration so far

- Uninformed ϵ-greedy exploration

$$\pi_\theta^\epsilon(a|s) \quad := \quad (1-\epsilon)\,\pi_\theta(a|s) + \epsilon\,\frac{1}{|\mathcal{A}|}$$

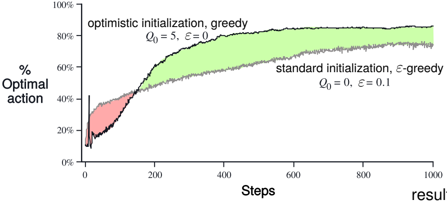
- Uninformed Boltzmann exploration

$$\pi_\theta^\beta(a|s) \quad := \quad \frac{\exp(\beta Q_\theta(s,a))}{\sum_{a'} \exp(\beta Q_\theta(s,a'))}$$

- Maximum entropy regularization/reward

$$\mathcal{L}^\alpha[\theta] \quad := \quad \mathcal{L}[\theta] \;+\; \alpha\,\mathbb{E}\Big[\ln \pi_\theta(a|s)\,\Big|\, a \sim \pi_\theta(\cdot|s)\Big]$$

$$r_t^\alpha \quad := \quad r(s_t, a_t) \;-\; \alpha\,\ln \pi(a_t|s_t)$$

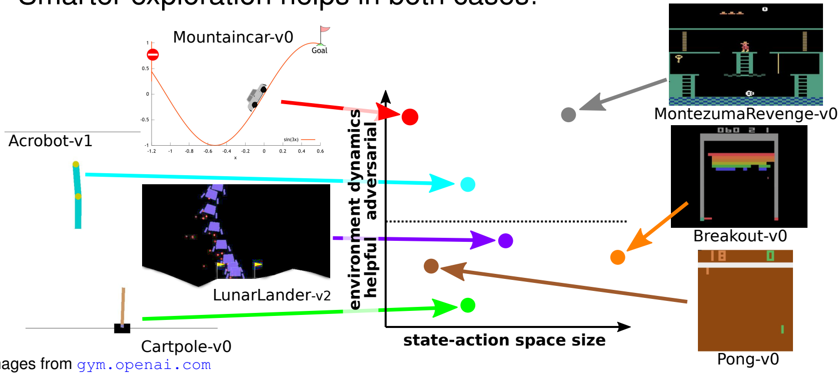


$P(r\,|\,\mathbf{a}_1) = 0.2 \qquad P(r\,|\,\mathbf{a}_2) = 0.8$

results for a 2-armed bandit task from Sutton and Barto (2018)

8.1 What makes exploration hard?

- Large state-action spaces $\rightarrow$ more episodes/generalization
  - random exploration is normal distributed, e.g. in navigation
  - many similar states easy to approximate, e.g. in Breakout
- Adversarial dynamics $\rightarrow$ more/longer episodes
- Smarter exploration helps in both cases!



images from gym.openai.com

8.1 How can we explore in a smart way?

- Choose actions with high observed reward more often
  - ϵ-greedy and Boltzman exploration
  - \+ exploration "around" exploitation policy
  - \- over-commits to easily reachable reward

this article by Lilian Weng gives a good overview over various exploration methods in deep RL

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  - \+ varying returns $\rightarrow$ uncertain future decision?
  - \- might be irreducible *aleatoric uncertainty*

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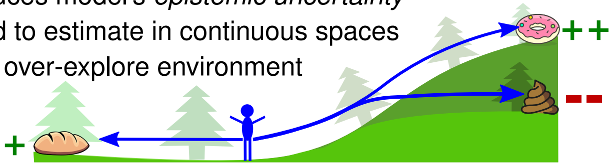
- Choose actions with uncertain returns
  - + varying returns $\rightarrow$ uncertain future decision?
  - - might be irreducible *aleatoric uncertainty*
- Choose actions you have not tried yet
  - + reduces model’s *epistemic uncertainty*
  - - hard to estimate in continuous spaces
  - - can over-explore environment



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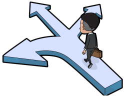
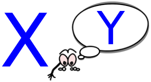
8.1 The many faces of uncertainty

- Aleatoric uncertainty
  - stochastic environment, irreducible
- Epistemic uncertainty
  - unknown environment, reducible
- Model-bias
  - wrong model, irreducible





assignment sheet 3

image sources: www.wikipedia.org, www.wikipedia.org, openclipart.org

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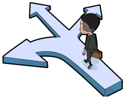

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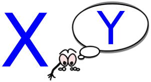

- Example: MSE regression on $\mathcal{D}$, $x \sim \rho(\cdot), y \sim \mathcal{N}\big(\,\cdot\,|\mu(x), \sigma^2(x)\big)$
  - only one possible definition of epistemic uncertainty!

$$\mathbb{E}_{\mathcal{D}}\Big[\underbrace{\mathbb{E}\big[\big(y - f_{\mathcal{D}}(x)\big)^2 \big| \mathcal{D}\big]}_{\text{generalization error}}\Big] = \underbrace{\mathbb{E}[\sigma^2(x)]}_{\text{aleatoric}} + \underbrace{\mathbb{E}\big[\mathbb{V}_{\mathcal{D}}[f_{\mathcal{D}}(x)|x]\big]}_{\text{epistemic}} + \underbrace{\mathbb{E}\big[\big(\mathbb{E}_{\mathcal{D}}[f_{\mathcal{D}}(x)|x] - \mu(x)\big)^2\big]}_{\text{model-bias}}$$

assignment sheet 3

image sources: www.wikipedia.org, www.wikipedia.org, openclipart.org

8.1 Summary

- Some environments are hard to explore randomly
- Agents should reduce the epistemic uncertainty
- Model-bias and aleatoric uncertainty are irreducible

Learning Objectives

LO8.1: Identify which environments are harder to explore
LO8.2: Explain the different types of uncertainties

8.2

Exploration
Thompson sampling

Thompson sampling

- Bayesian perspective: learn a posterior over models
  - another possible definition of epistemic uncertainty

$$\mathbb{P}(\theta|\mathcal{D}) \quad = \quad \frac{\mathbb{P}(\mathcal{D}|\theta)\,\mathbb{P}(\theta)}{\int \mathbb{P}(\mathcal{D}|\theta)\,\mathbb{P}(\theta)\,d\theta}$$

- Choose actions proportional to their optimality under $\mathbb{P}$

$$\pi(a|s) \quad = \quad \int \mathbb{P}(\theta|\mathcal{D})\,\delta\Big(Q_\theta(s,a) = \max_{a'\in\mathcal{A}} Q_\theta(s,a')\Big)\,d\theta$$

- Efficient implementation by sampling

$$a_t = \arg\max_{a\in\mathcal{A}} Q_\theta(s_t,a)\,, \qquad \theta \sim \mathbb{P}(\cdot|\mathcal{D})$$

assignment sheet 3

see Chapelle and Li (2011) for a recent survey on Thompson sampling (original Thompson, 1933) and Wang and Yeung (2020) for a recent survey on Bayesian deep learning

Question: posteriors over neural networks

- Thompson sampling requires $\mathbb{P}(\theta|\mathcal{D})$
  - how do we represent this posterior with a neural net?
  - how do we sample Q-value functions $q_\theta(s, a)$ from it?
  - try to think out of the box!

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- No spoilers!

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Bayes by backpropagation

- How to train a neural-net posterior $\mathbb{P}(\theta|\mathcal{D})$?
  - no analytical solution for Bayes update of neural network:

$$\mathbb{P}(\theta|\mathcal{D}) \quad = \quad \frac{\mathbb{P}(\mathcal{D}|\theta)\,\mathbb{P}(\theta)}{\int \mathbb{P}(\mathcal{D}|\theta')\,\mathbb{P}(\theta')\,d\theta'}$$

for some more information see Blundell et al. (2015) and Fortunato et al. (2019)

8.2 Bayes by backpropagation

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$$\mathbb{P}(\theta|\mathcal{D}) \quad = \quad \frac{\mathbb{P}(\mathcal{D}|\theta)\,\mathbb{P}(\theta)}{\int \mathbb{P}(\mathcal{D}|\theta')\,\mathbb{P}(\theta')\,d\theta'}$$

- Approximate the posterior distribution $\mathbb{P}(\theta|\mathcal{D}) \approx p_\phi(\theta)$
  - approximation only as good as the model class of p_ϕ
  - likelihood based on loss $\mathbb{P}(\mathcal{D}|\theta) \propto \exp(-\mathcal{L}_{[\theta]})$

$$\min_\phi D_{\mathsf{KL}}\big(p_\phi(\cdot)\big\|\mathbb{P}(\cdot|\mathcal{D})\big) \quad \equiv \quad \min_\phi \mathbb{E}\Big[\mathcal{L}_{[\theta]}\,\Big|\,\theta\sim p_\phi(\cdot)\Big] + D_{\mathsf{KL}}\big(p_\phi(\cdot)\big\|\mathbb{P}(\cdot)\big)$$

see Lecture 7.2 for the reparametrization trick, for some more information see Blundell et al. (2015) and Fortunato et al. (2019)

8.2 Bayes by backpropagation

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  - likelihood based on loss $\mathbb{P}(\mathcal{D}|\theta) \propto \exp(-\mathcal{L}_{[\theta]})$
  - reparameterization trick $\theta =: f_\phi(\epsilon) \sim p_\phi(\cdot)\,, \quad \epsilon \sim p'(\cdot)$

$$\begin{aligned}
\min_\phi D_{\mathsf{KL}}\big(p_\phi(\cdot)\big\|\mathbb{P}(\cdot|\mathcal{D})\big) \quad &\equiv \quad \min_\phi \mathbb{E}\Big[\mathcal{L}_{[\theta]}\,\Big|\,\theta\sim p_\phi(\cdot)\Big] + D_{\mathsf{KL}}\big(p_\phi(\cdot)\big\|\mathbb{P}(\cdot)\big) \\
&= \quad \min_\phi \mathbb{E}\Big[\mathcal{L}_{[f_\phi(\epsilon)]}\,\Big|\,\epsilon\sim p'(\cdot)\Big] + D_{\mathsf{KL}}\big(p_\phi(\cdot)\big\|\mathbb{P}(\cdot)\big)
\end{aligned}$$

- Minimize average loss $\mathbb{E}\Big[\mathcal{L}_{[\theta]}\,\Big|\,\theta\sim q_\phi(\cdot)\Big]$ with gradient descend of ϕ

see Lecture 7.2 for the reparametrization trick, for some more information see Blundell et al. (2015) and Fortunato et al. (2019)

Parameterizable posteriors

- Gaussian posterior over network parameters (Noisy Nets)
  - mean $\boldsymbol{\mu} \in \mathbb{R}^{|\boldsymbol{\theta}|}$ and diagonal covariance matrix $\boldsymbol{\Sigma} = \text{diag}(\boldsymbol{\sigma}^2)$
  - does not model correlations between parameters
  - e.g. linear layer: $g(\boldsymbol{x})_i = \sum_j \underbrace{(\mu_{ij} + \epsilon_{ij}|\sigma_{ij}|)}_{\theta_{ij} \sim \mathbb{P}} x_j \,,\; \epsilon_{ij} \sim \mathcal{N}(\cdot|\mathbf{0}, \mathbf{I})$

Fortunato et al. (2018) use Noisy Nets, and Gal et al. (2017) use dropout (Srivastava et al., 2014) for exploration

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- Dropout learns a distribution over robust networks
  - by 'dropping' parameters with probability $p \in [0, 1)$
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- Minimizing average loss drives posterior variance to zero
  - D_{KL} keeps it from collapsing completely

  $\Rightarrow$ terrible for detecting novel state-actions

Fortunato et al. (2018) use Noisy Nets, and Gal et al. (2017) use dropout (Srivastava et al., 2014) for exploration

8.2 Ensemble posterior

- Ensembles model posterior as set $\phi := \{\boldsymbol{\theta}^k\}_{k=1}^m$
  - initialize each $\boldsymbol{\theta}^k$ randomly like any neural net
  - Thompson sampling by selecting $k \sim$ Uniform$(1, \ldots, m)$
  - Bayes-by-backprop, similar to *particle filters*

$$\min_{\boldsymbol{\theta}^k} \mathbb{E}\big[\mathcal{L}_{[\boldsymbol{\theta}]} | \boldsymbol{\theta} \sim p_\phi\big] + D_{\mathsf{KL}}[p_\phi \| \mathbb{P}] \quad \equiv \quad \min_{\boldsymbol{\theta}^k} \mathcal{L}_{[\boldsymbol{\theta}^k]} + \tfrac{1}{2\sigma^2} \|\boldsymbol{\theta}^k\|_2^2 \,, \forall k$$

here we use $p_\phi(\boldsymbol{\theta}) = \frac{1}{m} \sum_{k=1}^m \delta(\boldsymbol{\theta} = \boldsymbol{\theta}^k)$ and $\mathbb{P}(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta} | \mathbf{0}, \sigma^2 \mathbf{I})$; en.wikipedia.org/wiki/Particle_filter

Ensemble posterior

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- Ensembles work more by accident than by design
  - reasonable m are much to small to represent posterior
  - but $\boldsymbol{\theta}^k$ converge to different local minima of $\mathcal{L}$

  $\rightarrow$ predictions coincide on training set $\mathcal{D}$

  $\rightarrow$ predictions often diverge outside $\mathcal{D}$

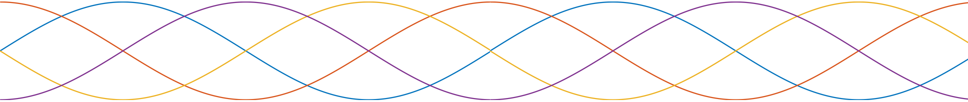
$\Rightarrow$ suitable to detect novel state-actions!

see Lu and Van Roy (2017) for ensemble sampling for exploration

8.2 Ensemble extensions

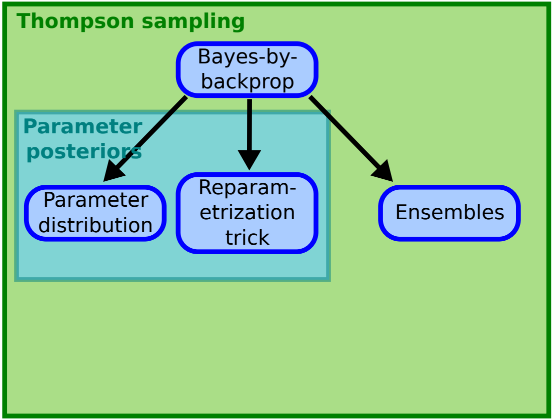
- Bootstrapped ensembles vary the data each model trains on
  - by using random masks on the mini-batches of each model
  - minor effect in comparison to different local minima

- Randomized prior functions make sure predictions diverge
  - define set of m functions g^k such that $\forall \boldsymbol{x}$:
    $\|\boldsymbol{g}(\boldsymbol{x}) - \boldsymbol{g}(\boldsymbol{x}')\| > \epsilon, \forall \boldsymbol{x}' \in \big\{\boldsymbol{x}' \big| \|\boldsymbol{x}' - \boldsymbol{x}\| > \epsilon' \big\}$
  - g^k is prior function of model $\boldsymbol{\theta}^k$, e.g.: $f(\boldsymbol{x})_i = \sum_j \theta^k_{ij} x_j + g^k(\boldsymbol{x})_i$
  - models learn to compensate for priors on training set $\mathcal{D}$
  - outside $\mathcal{D}$ priors guarantee divergent predictions



Osband et al. (2016) use bootstrapped ensembles and Osband et al. (2018) use randomized priors for exploration

Overview Thompson sampling



8.2 Summary

- Thompson sampling reduces epistemic uncertainty
- Posteriors are learned with Bayes-by-backpropagation
- Gaussian and dropout posteriors do not work well
- Ensemble posteriors work well, but only by accident
- Randomized prior functions improve ensembles

Learning Objectives

LO8.3: Explain Thompson sampling
LO8.4: Explain and derive Bayes-by-backpropagation
LO8.5: Explain why ensembles detect out-of-distribution samples

8.3

Exploration
Optimistic exploration

Optimistic exploration

- Upper confidence bounds (UCB) from multi-armed bandits
  - after $N(s,a)$ executions of a in s
  - variance of average $\mathbb{V}[\frac{1}{N(s,a)} \sum_{t=1}^{n} r_t \, \delta(s_t = s) \, \delta(a_t = a)] \propto \frac{1}{N(s,a)}$
  - act *optimistically* with confidence-parameter C
  - guaranteed to converge to optimum (constant regret)

$$a_t^* \quad := \quad \arg\max_{a \in \mathcal{A}} \Big(Q_\theta(s_t, a) + C \underbrace{\sqrt{\frac{\log \sum_{a'} N(s_t,a')}{N(s_t,a)}}}_{\text{bonus } \eta(s_t,a)} \Big)$$

for $\mathbb{V} \propto \frac{1}{N}$ see exercise sheet 1

see Auer et al. (2002) for UCB1

8.3 Optimistic exploration

- Upper confidence bounds (UCB) from multi-armed bandits
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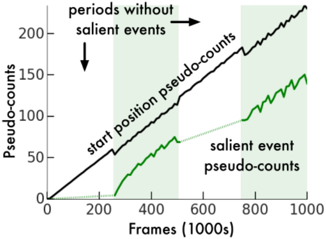
- Works decently well in tabular reinforcement learning
  - confidence bonus diminishes over time
  - special case of optimistic initialization
  - how do counts generalize to continuous spaces?

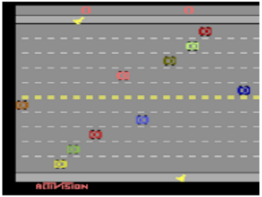
other bonuses exist, e.g. Rashid et al. (2020) add the bonus $\eta(s,a) = N(s,a)^{-m}$ to the Q-values

8.3 Visitation counts

- Counting visitations $N(s,a)$ impossible in continuous spaces
- Pseudo-counts are based on estimated density model $p(s,a)$
  - after observing n samples in s: $p(s,a) = \frac{N(s,a)}{n}$
  - after observing (s,a) again: $p'(s,a) = \frac{N(s,a)+1}{n+1}$

  $\Rightarrow \; N(s,a) = \frac{p(s,a)\,(1-p'(s,a))}{p'(s,a)-p(s,a)}$
  - perform gradient descent and compare density before and after





see Bellemare et al. (2016, image source) with a weak density model; and Ostrovski et al. (2017) with auto-regressive model

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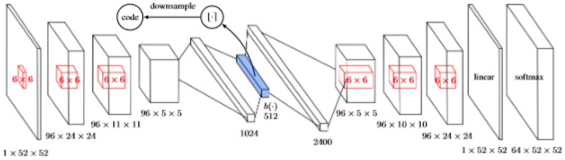
  $\Rightarrow \quad N(s,a) = \frac{p(s,a)\,(1-p'(s,a))}{p'(s,a)-p(s,a)}$
  - perform gradient descent and compare density before and after
- Random hash functions can divide state-action space
  - e.g. Gaussian hash $h(s,a) = \delta(\mathbf{A}^\top \boldsymbol{b}(s,a) > 0)\,, \quad A_{ij} \sim \mathcal{N}(\cdot|0,1)$
  - quality depends very much on hash function



hash counting by Tang et al. (2017)

8.3 Novelty measures

- UCB can use *any* novelty measure bonus that decays to 0
  - no theoretical motivation, but works in practice
- Random network distillation (RND)
  - two differently initialized neural nets, $\boldsymbol{f}_\phi, \boldsymbol{f}_\psi : \mathcal{S} \times \mathcal{A} \to \mathbb{R}^m$
  - keep ψ fixed and train $\min_\phi \mathbb{E}\big[\|\boldsymbol{f}_\phi(s,a) - \boldsymbol{f}_\psi(s,a)\|^2\big]$
  - distance $\eta(s,a) := \|\boldsymbol{f}_\phi(s,a) - \boldsymbol{f}_\psi(s,a)\|^2$ is novelty measure
  - ensemble without the interpretation as posterior variance

assignment sheet 4

random network distillation by Burda et al. (2019)

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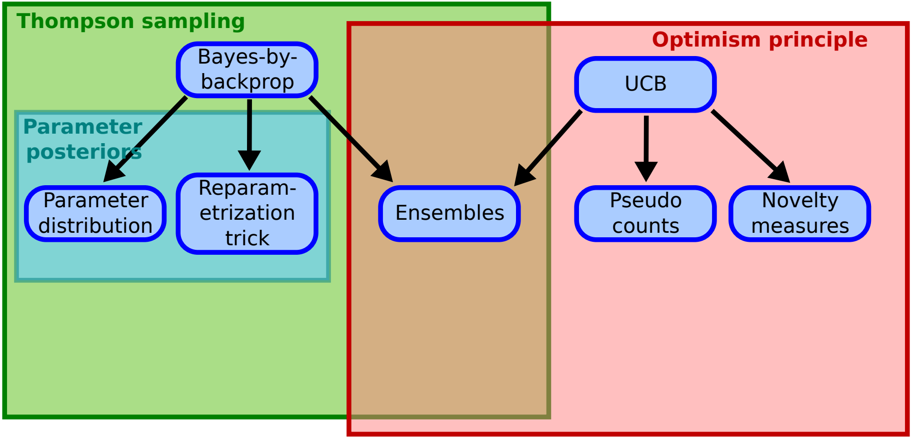
  - distance $\eta(s,a) := \|\boldsymbol{f}_\phi(s,a) - \boldsymbol{f}_\psi(s,a)\|^2$ is novelty measure
  - ensemble without the interpretation as posterior variance
- Many other novelty measures exist
  - predicting the next state or reward
  - cosine-similarity to training samples
- Novelty measures are scale-free
  - no interpretation like variance of values
  - hyper-parameter selection even harder

novelty based on state prediction e.g. in Pathak et al. (2017), cosine-similarity in O'Donoghue et al. (2018); Böhmer et al. (2019)

8.3 Overview optimism principle



8.3 Summary

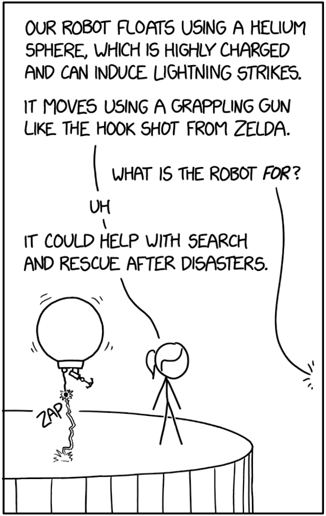
- Optimistic exploration gives bonus for uncertain actions
- Pseudo-counts and hash functions generalize visitations
- Novelty measure estimate uncertainty without interpretation

Learning Objectives

LO8.6: Explain optimistic exploration
LO8.7: Explain and compare visitation counts and novelty estimation

8.3 Next lecture

- Next lecture: **offline RL**!
- Don't forget assignment 3!
- Questions? Ask them here: `answers.ewi.tudelft.nl`



"IT COULD HELP WITH SEARCH AND RESCUE" IS ENGINEER-SPEAK FOR "WE JUST REALIZED WE NEED A JUSTIFICATION FOR OUR COOL ROBOT."

image source: xkcd.com

References I

Peter Auer, Nicolò Cesa-Bianchi, and Paul Fischer. Finite-time analysis of the multiarmed bandit problem. *Machine Learning*, 47(2–3):235–256, 2002. ISSN 0885-6125.

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