

Bayesian Lower Bounds for Regret Minimization

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Introduction

Paper: Regret Lower Bound [Lai, 1987]



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ADAPTIVE TREATMENT ALLOCATION AND THE MULTI-ARMED BANDIT PROBLEM¹

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A class of simple adaptive allocation rules is proposed for the problem (often called the "multi-armed bandit problem") of sampling x_1,\ldots,x_N sequentially from k populations with densities belonging to an exponential family, in order to maximize the expected value of the sum $S_N=x_1+\cdots+x_N$. These allocation rules are based on certain upper confidence bounds, which are developed from boundary crossing theory, for the k population parameters. The rules are shown to be asymptotically optimal as $N\to\infty$ from both Bayesian and frequentist points of view. Monte Carlo studies show that they also perform very well for moderate values of the horizon N.

Motivation



Today we discuss unstructured multi-armed bandit problems (MAB). We will talk about:

- 1. Deriving asymptotic instance-dependent regret lower bounds in the Bayesian setting [Lai, 1987, Atsidakou et al., 2023]).
- 2. Possible extensions and some considerations on this topic

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Today we discuss unstructured multi-armed bandit problems (MAB). We will talk about:

- 1. Deriving asymptotic instance-dependent regret lower bounds in the Bayesian setting [Lai, 1987, Atsidakou et al., 2023]).
- 2. Possible extensions and some considerations on this topic.



Consider a MAB problem with a = 1, ..., K arms:











- ▶ Sequential: In round t the learner pulls arm $a_t \in [K]$ and receives the reward $r_t \sim \theta_{a_t}$.
 - Each arm a is characterized by a density function $f(r; \theta_a)$ with respect to the Lebesgue measure, and $\theta_a \in \Theta$ is an unknown parameter that belongs to some open set $\Theta \subset \mathbb{R}$.
 - ▶ (Integrability) For all $\theta \in \Theta$ we assume that $\mu_a(\theta) := \mathbb{E}_{\theta_a}[|R|] = \int_{\mathbb{R}} |r|f(r;\theta_a) dr < \infty$.
- ▶ (Bayesian Prior) We denote by $H = (H_1, ..., H_K)$ a factorized prior distribution on Θ^K , with density $h(\theta) = \prod_a h_a(\theta_a)$ (note that each h_a may be different).
- ▶ We indicate by $\mu^*(\theta) \coloneqq \max_a \mu_a(\theta)$ the value of the best arm.

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Problems Considered









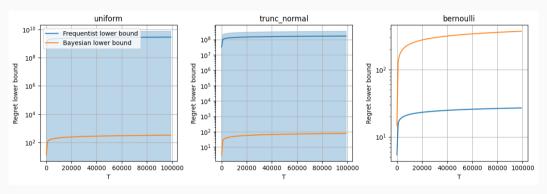




- **Regret Minimization**: Minimize the regret incurred in not choosing the best arm in each time-step over an horizon T.
- ▶ Best Arm Identification objective: quickly find the optimal arm with confidence at-least $1 \delta, \delta \in (0, 1/2)$.

Bayesian vs Frequentist Regret Lower Bound

▶ Can we just compute the average frequentist lower bound over many different problems?



Average computed over 3000000 sampled MAB problems. Shaded areas indicate the 95% C.I.

The frequentist lower bound simply explodes with continuous priors.



We consider $f(r; \theta_a)$ to belong to the single-parameter exponential family $f(r; \theta_a)$

$$f_a(r;\theta) = \exp(\theta_a r - \psi(\theta_a)),$$

where $\psi(\theta_a)$ is the cumulant generating function².

- \triangleright θ_a is called natural parameter.
- $\dot{\psi}(\theta_a) = \frac{\mathrm{d}\psi}{\mathrm{d}\theta_a} = \mu_a(\theta) \text{ is the mean value and } \ddot{\psi}(\theta_a) = \mathbb{E}_{r \sim \theta_a}[(r \dot{\psi}(\theta_a))^2] \text{ is the variance.}$ We also have that $\dot{\psi}$ is increasing in θ_a , and we let $\theta^\star = \max_a \theta_a$.
- ► Kullback-Leibler (KL) Divergence defined as

$$\underline{D(\theta_a, \theta_a') = (\theta_a - \theta_a')\dot{\psi}(\theta_a) - (\psi(\theta_a) - \psi(\theta_a'))} = \int_{\theta_a}^{\theta_a} (t - \theta_a) \dot{\psi}(t) dt$$

¹Includes Bernoulli, Poisson, Gaussian distribution with known variance, etc. [Efron, 2022].

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Observation. For the single-parameter exponential distribution family we have that for y>x, with $x,y\in [a,b]$, $\exists c_1,c_2>0$ such that

$$c_1(y-x) \geq \underbrace{[\dot{\psi}(y) - \dot{\psi}(x)]}_{\text{mean values}} \geq 2c_2\frac{D(x,y)}{(y-x)} > 0.$$

Proof.

- 1. By the mean value theorem $\exists \xi \in (x,y) \colon \dot{\psi}(y) \dot{\psi}(x) = \ddot{\psi}(\xi)(y-x) \ge \min_{z \in [a,b]} \ddot{\psi}(z)(y-x)$ (the upper bound follows similarly).
- 2. Then, recall $D(x,y)=(x-y)\dot{\psi}(x)-(\psi(x)-\psi(y))=\int_x^y(t-x)\ddot{\psi}(t)\mathrm{d}t$
- 3. We use that $\dot{\psi}$ is increasing and differentiable $\Rightarrow \ddot{\psi} > 0$. Thus $D(x,y) \leq \frac{\max_{z \in [a,b]} \dot{\psi}(z)}{2} (x-y)^2$.

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Regret Minimization: lower

bound

Sampling rule or allocation rule

Denote by $\pi = (\pi_t)_{t \ge 1}$ the sampling rule of the learner (a.k.a. allocation rule). Concretely

 $ightharpoonup \pi$ is a sequence of measurable functions, each of which associates past data with an arm, namely

$$a_{t+1} = \pi_t(I_t)$$
, where $I_t = (u_0, a_1, r_1, u_1, \dots, a_t, r_t, u_t)$, $I_0 = u_0$

and $(u_t)_{t\geq 0}$ is a sequence of iid uniform noise, such that u_t is independent of I_{t-1} and (a_t, r_t) . Thus $a_t \in \mathcal{F}_{t-1} := \sigma(I_{t-1})$.

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Bayesian Regret (Bayes Risk):
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$$\mathrm{Reg}(T) = \int_{\Theta^K} \mathrm{Reg}(T;\theta) \mathrm{d}H(\theta)$$
 vs Frequentist Regret $\mathrm{Reg}(T;\theta)$

- Note that people have applied Bayesian algorithms to the Frequentist regret: Posterior sampling helps with exploration (epistemic uncertainty).
- ► Similarly, UCB-designs have been used to find rules that are efficient in the Bayesian regret sense.
- ▶ In this work we study the Bayesian regret.

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Optimal solutions

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- ▶ Bernoulli bandits with uniform prior on the means. The posterior is a Beta distribution $\text{Beta}(S_a(t)+1,N_a(t)-S_a(t)+1)$, where $N_a(t)=|\{t\in [K]:a_t=a\}|$ and $S_a(t)=|\{t:r_{a_t}=1\}.$
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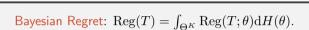
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We now derive an asymptotic instance-dependent lower bound for the Bayesian Regret.

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Wrong! We need to integrate and then take the limit. Need to be careful, since the lower bound needs to have some form of uniformity in θ !

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Uniformly fast convergent strategies. A strategy π is uniformly fast convergent if for all models θ , for all sub-optimal arms a we have $\mathbb{E}_{\theta}[N_a(T)] = o(T^{\alpha})$ for all $\alpha \in (0,1)$.

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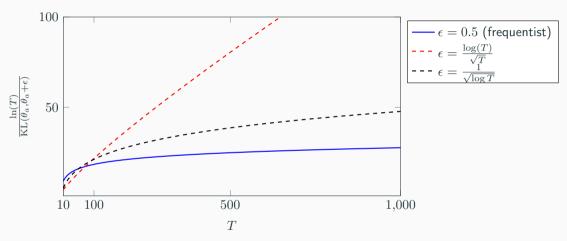
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Remark: Just saying that π is *uniformly fast convergent strategy* is not enough. We need to guarantee uniform convergence across different values of θ .

Notation.

- For an arm a and vector θ , denote by $\frac{\theta_{\backslash a}}{\theta_{\backslash a}} = (\theta_1, \dots, \theta_{a-1}, \theta_{a+1}, \dots, \theta_K)$ the vector θ without θ_a . Similarly, we also define $H_{\backslash a}$.
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- Also recall that $\mu_a(\theta) = \dot{\psi}(\theta_a)$, which is increasing in θ_a . Hence θ^* corresponds to the parameter of the best arm.

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Uniform Boundary Crossing Problem

To our help comes Prof. Lai [Lai, 1987]. With a single parameter, he noted that UCB methods (based on the KL divergence⁵) satisfy the following:



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, then, as $T\to\infty$
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 ${}^5\mathrm{UCB}(n) = \inf\{\theta: \theta \geq \hat{\theta}_n, nD(\hat{\theta}_n, \theta) \geq \log(n/T) + \xi \log\log(n/T)\} \text{ for some } \xi \in \mathbb{R} \text{ and } \hat{\theta}_n \text{ is the MLE in round } n.$

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Bayesian Regret Lower Bound: Assumptions on the Sampling Policy



Using this intuition, [Lai, 1987] derived the following sampling condition ⁶.

Let
$$\xi, \gamma \in (0,1)$$
. π is a Bayes-uniformly fast convergent strategy if
$$\lim_{T \to \infty, \epsilon \to 0, T\epsilon^2 \to \infty} \int_{\Theta^{K-1}} \mathbb{P}_{\theta} \left(N_a(T) \le (1-\gamma) \frac{\log T\epsilon^2}{D(\theta_a, \theta_{\setminus a}^\star + \xi\epsilon)} \right) h_a(\theta_a) \mathrm{d}H(\theta_{\setminus a}) = 0$$
 with $\theta_a = \theta_{\setminus a}^\star - \epsilon$.

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$$\theta_a = \theta^{\star}_{\backslash a} - \epsilon$$

The probability that we under-sample over regions with small gaps tends to 0.

⁶Recall from the previous slide that we need a sampling rate $\approx \log(T\epsilon^2)/\epsilon^2$. Since $\theta_a = \theta_{\setminus a}^{\star} - \epsilon$ we have $D(\theta_a, \theta_{\setminus a}^{\star} + \xi \epsilon) \approx (1 + \xi)^2 \epsilon^2$.

$$\int_{\theta \in \Theta^K: \theta_a < \theta^*} \Delta_a(\theta) \mathbb{E}_{\theta}[N_a(T)] dH(\theta) = \int_{\theta \in \Theta^K: \theta_a < \theta^*_{\setminus a}} \Delta_a(\theta) \mathbb{E}_{\theta}[N_a(T)] dH(\theta) = (*)$$

The idea is to consider $\theta_a=\theta^\star_{\backslash a}-\epsilon$, with ϵ belonging to a small region around the maximum. We consider an open set $\mathcal{E}_T\subset\mathbb{R}_+$ such that $\mathcal{E}_T\to\{0\}$ (more details on this later).

$$\begin{split} (*) &= \int_{\theta \in \Theta^{K-1}} \int_{\theta_a < \theta_{\backslash a}^{\star}} \Delta_a(\theta) \mathbb{E}_{\theta}[N_a(T)] \mathrm{d}H_a(\theta_a) \; \mathrm{d}H_{\backslash a}(\theta_{\backslash a}), \\ &\geq \int_{\theta \in \Theta^{K-1}} \int_{\theta_{\backslash a}^{\star} - \theta_a \in \mathcal{E}_T} \Delta_a(\theta) \mathbb{E}_{\theta}[N_a(T)] \; \mathrm{d}H_a(\theta_a) \mathrm{d}H_{\backslash a}(\theta_{\backslash a}), \\ &= \int_{\theta \in \Theta^{K-1}} \int_{\mathcal{E}_T} (\dot{\psi}(\theta_{\backslash a}^{\star}) - \dot{\psi}(\theta_{\backslash a}^{\star} - \epsilon)) \mathbb{E}_{\theta}[N_a(T)] h_a(\theta_{\backslash a}^{\star} - \epsilon) \; \mathrm{d}\epsilon \; \mathrm{d}H_{\backslash a}(\theta_{\backslash a}), \end{split}$$

where we used that $\Delta_a(\theta) = \max_j \mu_j(\theta) - \mu_a(\theta) = \max_j \dot{\psi}(\theta_j) - \dot{\psi}(\theta_a)$ and performed a change of variable $\theta_a = \theta_{\setminus a}^* - \epsilon, \epsilon \in \mathcal{E}_T$.

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Let $\gamma \in (0,1)$. Use that

1.
$$p_{\theta}(T, \epsilon) = \mathbb{P}_{\theta}\left(N_a(T) \leq (1 - \gamma) \frac{\log T \epsilon^2}{D(\theta_{\lambda}^{\star} - \epsilon, \theta_{\lambda}^{\star} + \xi \epsilon)}\right)^{7}$$
 implies

$$\mathbb{E}[N_a(\theta)] \ge (1 - \frac{p_{\theta}(T, \epsilon)}{D(\theta_{\setminus a}^* - \epsilon, \theta_{\setminus a}^* + \xi \epsilon)}]$$

by Markov's inequality. Note also that $D(\theta^\star_{\backslash a} - \epsilon, \theta^\star_{\backslash a} + \xi\epsilon) \leq c'(1+\xi)^2\epsilon^2/2$

- 2. By continuity, for ϵ small we can say $h_a(\theta_{\backslash a}^{\star} \epsilon) \approx h_a(\theta_{\backslash a}^{\star})$
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Recal

Let $\xi, \gamma \in (0,1)$. π is a Bayes-uniformly fast convergent strategy if

$$\lim_{T \to \infty, \epsilon \to 0, T\epsilon^2 \to \infty} \int_{\Theta^{K-1}} \mathbb{P}_{\theta} \left(N_a(T) \le (1 - \gamma) \frac{\log T\epsilon^2}{D(\theta_{\backslash a}^{\star} - \epsilon, \theta_{\backslash a}^{\star} + \xi\epsilon)} \right) h_a(\theta_{\backslash a}^{\star}) dH(\theta_{\backslash a}) = 0$$

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Discussion

Congrats for reaching this point!

- ▶ What is the intuition behind the lower bound?
- ▶ Show how the condition on $p_{\theta}(T, \epsilon)$ makes $\int \int p_{\theta}(T, \epsilon) \to 0$ (see appendix).
- ▶ Why $\inf \mathcal{E}_T = N^{-(1-\gamma)/2}$ (We will not discuss this)
- ► How is the definition of a Bayes-uniformly fast convergent strategy derived? (We will not discuss this) .
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- ► The regret is only characterized by the complexity of the priors!
- ▶ K_a^{\star} denotes the complexity for arm a: large K_a^{\star} implies a larger likelihood that a is close to optimality (if $h_a(\theta_{\backslash a}^{\star})$ is large, then it becomes harder to distinguish between a and the other good arm).

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$$\liminf_{T \to \infty} \frac{\operatorname{Reg}(T)}{\log^2 T} \ge \sum_a \underbrace{\frac{1}{2} \int_{\Theta^{K-1}} h_a(\theta_{\backslash a}^{\star}) \mathrm{d} H_{\backslash a}(\theta_{\backslash a})}_{=:K_a^{\star}}, \qquad K^{\star} \coloneqq \sum_a K_a^{\star}.$$

Assume i.i.d. $(\theta_a)_a$ (i.i.d. priors) with $h_a \equiv h \ \forall a$ (sim. $H_a \equiv H$). Then $H_{\backslash a} = H^{K-1}$, implying

$$\mathbb{P}_{H}(\theta_{\backslash a}^{\star} \leq x) = \mathbb{P}_{H}(\theta_{1} \leq x, \dots, \theta_{a-1} \leq x, \theta_{a+1} \leq x, \dots, \theta_{K} \leq x) = H^{K-1}(x).$$

$$\Rightarrow K^* = \frac{K}{2} \int_{\Theta} h(\theta) \mathrm{d}H^{K-1}(\theta)$$

Since $\mathrm{d}H^{K-1}(\theta)=(K-1)H^{K-2}(\theta)\mathrm{d}H(\theta)$ and $\mathrm{d}H(\theta)=h(\theta)\mathrm{d}\theta$

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Connections to order statistics

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there is actually a connection to order statistics.

Order statistics. Given a random vector $\theta = (\theta_1, \dots, \theta_K)$, sort the components into a vector $(\theta_{(1)}, \dots, \theta_{(K)})$ satisfying

$$\theta_{(1)} \le \theta_{(2)} \le \dots \le \theta_{(K)}$$

This vector is called the order statistics of θ .

▶ The joint pdf f of (θ_{K-1}, θ_K) (with cdf F) is [Casella and Berger, 2024]

$$f(x,y) = K(K-1)f(x)f(y)F^{K-2}(x)$$

Letting $x \to y$ we find $\lim_{x \to y} f(x,y) = K(K-1)f^2(y)F^{K-2}(y)$. This is the limiting contribution when the two upper-most samples almost tie.

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Other interpreation

Since $\lim_{x\to y} f(x,y) = K(K-1)f^2(y)F^{K-2}(y)$, another connection is to see the overall integral as the chance that the top two samples fall into it a tiny interval

$$\begin{split} \mathbb{P}(|\theta_{(K)} - \theta_{(K-1)}| < \epsilon) &= K(K-1) \int_{\Theta} \int_{0}^{\epsilon} h(\theta) h(\theta + \epsilon) H^{K-2}(\theta) \, d\epsilon \, d\theta, \\ &= 2K^{*}\epsilon + o(\epsilon) \end{split}$$

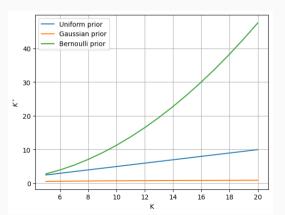
Thus

$$\frac{\mathbb{P}(|\theta_{(K)} - \theta_{(K-1)}| < \epsilon)}{\epsilon} \xrightarrow[\epsilon \to 0]{} 2K^{\star}.$$

Scaling of K^{\star}

Scaling of K^* vs K, with: (1) $H = \mathcal{U}([0,1])$; (2) $H = \mathcal{N}(0,1)$ and (3) $H = \mathrm{Ber}(0.5)$ (uniform, Gaussian, Bernoulli).

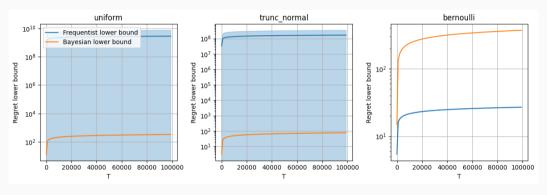
We consider a MAB problem with K arms and Gaussian rewards $\mathcal{N}(\theta_a,1)$, with θ_a drawn iid from the prior.



Examples

Bayesian vs Frequentist Regret Lower Bound

▶ Can we just compute the average frequentist lower bound over many different problems?



Same setting as in the previous slide, with K=5. Average computed over 3000000 sampled MAB problems. Shaded areas indicate the 95% C.I.

The frequentist lower bound simply explodes with continuous priors.

Algorithm Design

Can we use the lower bound to design asymptotically optimal algorithms? Probably. I believe the intuition is to solve the following problem

$$\inf_{\eta} \sum_{a} \int \eta_{a} \Delta_{a}(\theta) \mathrm{d}H(\theta) \text{ s.t. } \int_{\Theta^{K-1}} \eta_{a} D(\theta_{a}, \theta_{\backslash a}^{\star}) h_{a}(\theta_{a}) \mathrm{d}H_{\backslash a}(\theta_{\backslash a}) \geq 1$$

where $\eta \in \Delta(K)$ represents the proportion of times we should play each arm $^{\mathfrak{l}}$

Algorithm design 33/36

⁸This is probably incorrect, but the true problem should vaguely resemble this one.

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Possible extensions:

- ▶ Optimal algorithms based on the lower bound.
- ▶ Bayesian regret lower bounds for MDPs.
- A more comprehensive analysis of Bayesian BAI.

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Appendix

Condition on $p_{\theta}(T, \epsilon)$

We need to show that

$$(*) = \int_{\Theta^{K-1}} h_a(\theta_{\backslash a}^{\star}) \int_{\mathcal{E}_T} p_{\theta}(T, \epsilon) d\epsilon dH_{\backslash a}(\theta_{\backslash a}) \to 0,$$

where $(\mathcal{E}_T)_T$ is a sequence of open sets, satisfying such that $\lambda(\mathcal{E}_T) < \infty$ (Lebesgue measure) for all T, with $\sup E_T \leq \sup E_{T-1}, \inf \mathcal{E}_T \leq \inf \mathcal{E}_{T-1}$ and $\mathcal{E}_T \underset{T \to \infty}{\longrightarrow} \{0\}.$

Note

$$(*) \leq \lambda(\mathcal{E}_T) \int_{\Theta^{K-1}} [\sup_{\epsilon \in \mathcal{E}_T} p_{\theta}(T, \epsilon)] h_a(\theta_{\backslash a}^*) dH_{\backslash a}(\theta_{\backslash a})$$

We show how we can rewrite the original condition in this form

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We show how we can rewrite the original condition in this form.

$$\lim_{T \to \infty, \epsilon \to 0, T\epsilon^2 \to \infty} \underbrace{\int_{\Theta^{K-1}} p_{\theta}(T, \epsilon) h_a(\theta^*_{\backslash a}) dH(\theta_{\backslash a})}_{g_T(\epsilon)} = 0$$

This limit also implies that

$$\forall \delta > 0 \; \exists T_{\delta} \in \mathbb{N}, \alpha_{\delta}, K_{\delta} \in \mathbb{R}_{+} : g_{T}(\epsilon) < \delta \; \text{ whenever } \; (T, \epsilon) \in \{T, \epsilon : T \geq T_{\delta}, \epsilon \leq \alpha_{\delta}, T\epsilon^{2} \geq K_{\delta}\}.$$

Consider the set $\mathcal{E}_T = (1/T^{(1-\gamma)/2}, \log^{-1} T)$. Then

- $\blacktriangleright \ \forall \alpha_{\delta} \ \exists T'_{\delta} : \ \log^{-1} T \leq \alpha_{\delta} \ \text{whenever} \ T \geq T'_{\delta}.$

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