

Bregman Deviations of Generic Exponential Families

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Confidence sets

Let $X_1, \dots, X_t$ i.i.d random variables distributed as $X \sim \nu \in \mathcal{P}(\mathbb{R}^d)$.

Where is  $= \mathbb{E}[X]$?

t=3

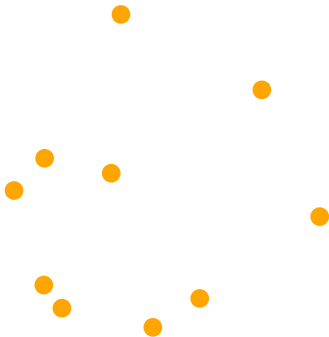


Confidence sets

Let $X_1, \dots, X_t$ i.i.d random variables distributed as $X \sim \nu \in \mathcal{P}(\mathbb{R}^d)$.

Where is  $= \mathbb{E}[X]$?

t=10

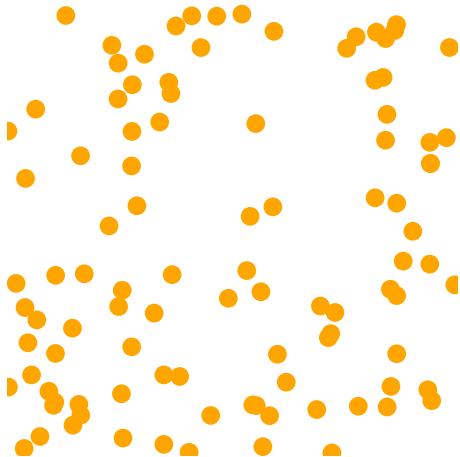


Confidence sets

Let $X_1, \dots, X_t$ i.i.d random variables distributed as $X \sim \nu \in \mathcal{P}(\mathbb{R}^d)$.

Where is  $= \mathbb{E}[X]$?

t=100

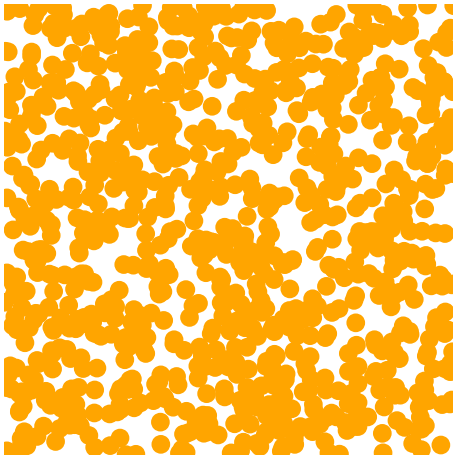


Confidence sets

Let $X_1, \dots, X_t$ i.i.d random variables distributed as $X \sim \nu \in \mathcal{P}(\mathbb{R}^d)$.

Where is  $= \mathbb{E}[X]$?

t=1000

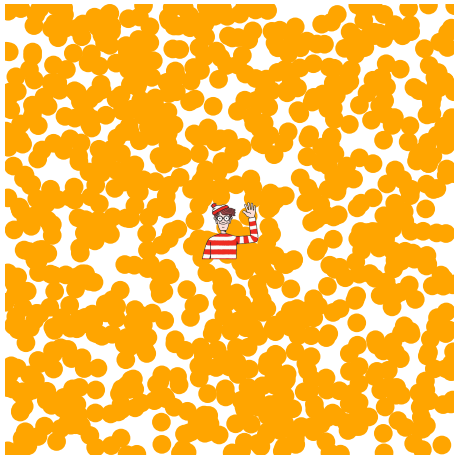


Confidence sets

Let $X_1, \dots, X_t$ i.i.d random variables distributed as $X \sim \nu \in \mathcal{P}(\mathbb{R}^d)$.

Where is  = $\mathbb{E}[X]$?

t=1000



Confidence sets

We want **confidence sets**, not just estimation!

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For $\delta \in (0, 1)$ and $t \in \mathbb{N}$, we need a set $\mathcal{C}_t^\delta$ such that $\mathbb{P}(\mu \in \mathcal{C}_t^\delta) \geq 1 - \delta$.

Asymptotically:

$$\mathcal{C}_t^\delta = \left[\hat{\mu}_t - \frac{\sigma^2}{\sqrt{t}} \Phi^{-1}(1 - \delta/2), \hat{\mu}_t + \frac{\sigma^2}{\sqrt{t}} \Phi^{-1}(1 - \delta/2) \right]$$

is such that

$$\lim_{t \rightarrow +\infty} \mathbb{P}(\mu \in \mathcal{C}_t^\delta) = 1 - \delta,$$

where $\hat{\mu}_t = \frac{1}{t} \sum_{s=1}^t X_s$.

✗ Does not tell us anything about the small sample size regime...

Nonasymptotic confidence sets

We need some assumptions...

Sub- ψ distributions:

$$\forall \lambda \in \mathcal{I} \subseteq \mathbb{R}_+, \log \mathbb{E}_{X \sim \nu} \left[e^{\lambda(X - \mu)} \right] \leq \psi(\lambda).$$

Proposition (Chernoff bound)

$$\mathbb{P} \left(\hat{\mu}_t - \mu \geq \psi_*^{-1} \left(\frac{1}{t} \log \frac{1}{\delta} \right) \right) \leq \delta,$$

where $\psi_*(u) = \sup_{\lambda \in \mathcal{I}} \lambda u - \psi(\lambda)$ is the Fenchel-Legendre conjugate of ψ .

Examples:

- $\nu = \mathcal{N}(\mu, \sigma^2)$, $\psi(\lambda) = \sigma^2 \lambda^2 / 2$.
- ν has bounded support, $\psi(\lambda) = \text{diam}(\text{Supp}(\nu))^2 \lambda^2 / 8$.
- $\nu = \chi^2(k)$, $\psi(\lambda) = (1 - 2\lambda)^{-k/2}$, $\mathcal{I} = (0, \frac{1}{2})$.

Nonasymptotic confidence sets

Proof:

$$\begin{aligned}\mathbb{P}\left(\sum_{s=1}^t X_s - \mu \geq tu\right) &= \mathbb{P}\left(\prod_{s=1}^t e^{\lambda(X_s - \mu)} \geq e^{t\lambda u}\right) \\ &\leq e^{-t\lambda u} \mathbb{E}\left[\prod_{s=1}^t e^{\lambda(X_s - \mu)}\right], \quad (\text{Markov}) \\ &= e^{-t\lambda u} \prod_{s=1}^t \mathbb{E}\left[e^{\lambda(X_s - \mu)}\right] \quad (\text{independence}) \\ &\leq e^{-t\lambda u + t\psi(\lambda)} \quad (\text{sub-}\psi),\end{aligned}$$

then optimise in $\lambda \in \mathcal{I}$.



Nonasymptotic confidence sets

Other possible assumptions:

- **Fully parametric**

- ▶ If you know the quantiles, use them!

- **Bounded**

- ▶ With control of moments:
Bennett, Bernstein [Boucheron et al. \[2013\]](#), [Bentkus \[2004\]](#),
- ▶ With empirical estimators of moments:
Bernstein [Maurer and Pontil \[2009\]](#),
Bentkus [Kuchibhotla and Zheng \[2021\]](#).
- ▶ With only boundedness: [Phan et al. \[2021\]](#).

- **Self-normalised sums**

- ▶ [Bercu et al. \[2015\]](#), [Bercu and Touati \[2019\]](#)

Is this all for mean estimation?

Detour: stochastic bandit



(a) 15% chance to win 10€



(b) 5% chance to win 10€



The casino does not tell you which one is the winner!

Optimism in face of uncertainty

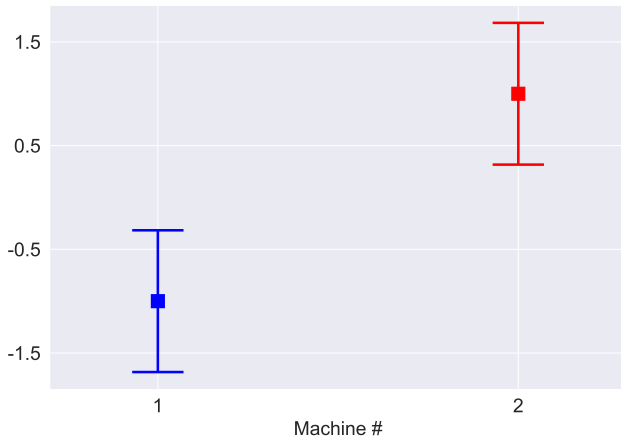
- **Optimism:** play the machine with highest *plausible* reward.
- More formally:
 - ▶ play $\operatorname{argmax}_{k=1,2} U_{\tau_k}^k(\delta)$,
 - ▶ τ_k : number of pulls to machine k (random stopping time),
 - ▶ $U_{\tau_k}^k(\delta)$ is a measurable function of τ_k samples from machine k such that

$$\mathbb{P}(\mu \geq U_{\tau_k}^k(\delta)) \leq \delta.$$



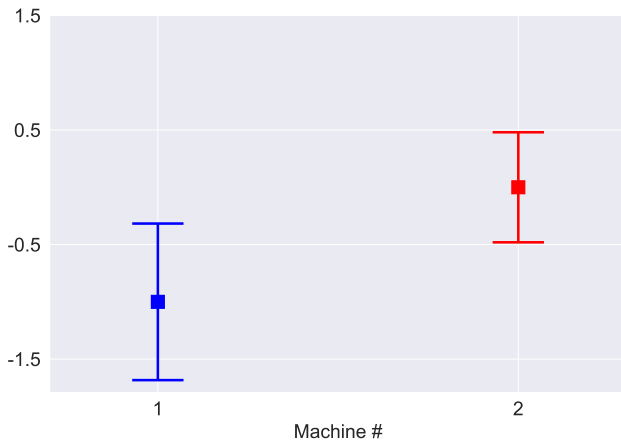
Concentration bound for sample of **random** size!

Optimism in face of uncertainty



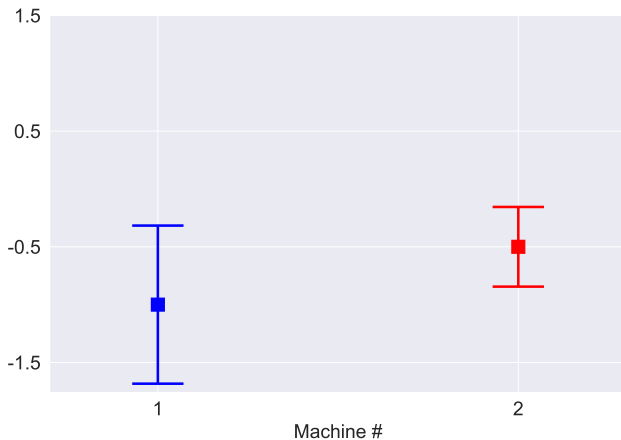
Machine 1: 5 pulls. Machine 2: 5 pulls.

Optimism in face of uncertainty



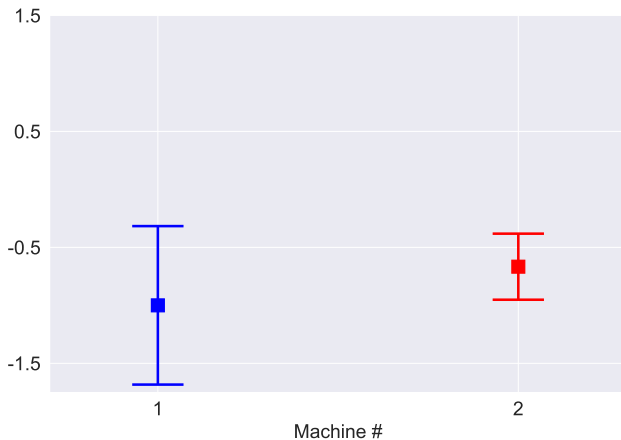
Machine 1: 5 pulls. Machine 2: 10 pulls.

Optimism in face of uncertainty



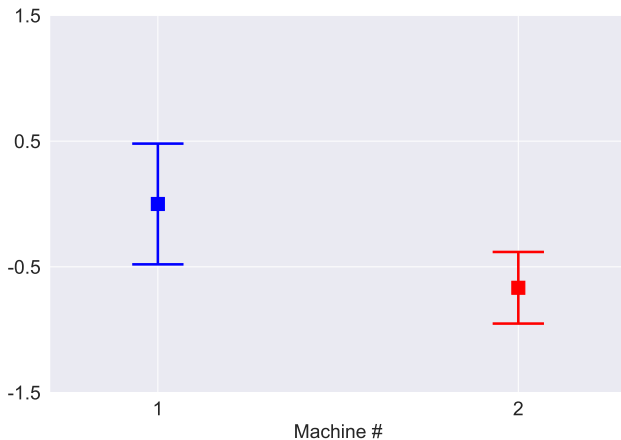
Machine 1: 5 pulls. Machine 2: 20 pulls.

Optimism in face of uncertainty



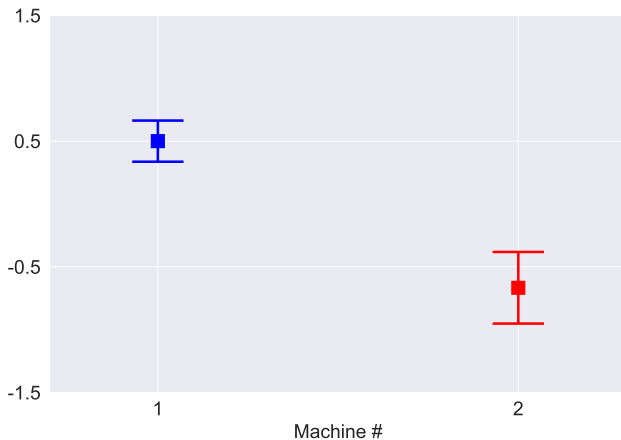
Machine 1: 5 pulls. Machine 2: 30 pulls.

Optimism in face of uncertainty



Machine 1: 10 pulls. Machine 2: 30 pulls.

Optimism in face of uncertainty



Machine 1: 100 pulls. Machine 2: 30 pulls.

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Martingale and stopping time

🔴 Stopping times are hard to deal with...

👤 ... but go well with martingales!

For $t \in \mathbb{N}$, assume we know an invertible, nondecreasing $F_t: \mathbb{R} \rightarrow \mathbb{R}_+$ s.t

(i) $M_t = F_t(S_t)$ defines a supermartingale adapted to the filtration $\mathcal{F}_t = \sigma(X_s, s \leq t)$, with $S_t = \sum_{s=1}^t X_s - \mu$;

(ii) $\mathbb{E}[M_0] \leq 1$.

Then for any $\mathcal{F}$ -stopping time τ ,

$$\begin{aligned} \mathbb{P}\left(S_\tau \geq F_\tau^{-1}\left(\frac{1}{\delta}\right)\right) &= \mathbb{P}\left(M_\tau \geq \frac{1}{\delta}\right) \\ &\leq \delta \mathbb{E}[M_\tau] \quad (\text{Markov}) \\ &\leq \delta \mathbb{E}[M_0] \quad (\text{Doob}) \\ &\leq \delta. \end{aligned}$$

To find a martingale

The sub- ψ assumption is really a martingale condition:

$\forall \lambda \in \mathcal{I}, M^\lambda = \left(e^{\lambda S_t - t\psi(\lambda)} \right)_{t \in \mathbb{N}}$ is a nonnegative supermartingale.

Proposition

For any $\mathcal{F}$ -stopping time τ ,

$$\forall \lambda \in \mathcal{I}, \mathbb{P} \left(\hat{\mu}_\tau - \mu \geq \frac{1}{\lambda} \left(\frac{1}{\tau} \log \frac{1}{\delta} + \psi(\lambda) \right) \right) \leq \delta.$$



Cannot optimise in λ for all values of τ !
(optimising for a fixed time t_0 recovers the Fenchel-Legendre formula).

To find a good martingale

For any mixture density $q(\lambda)$ over $\mathcal{I}$,

$$M = \left(\int_{\mathcal{I}} e^{\lambda S_t - t\psi(\lambda)} q(\lambda) d\lambda \right)_{t \in \mathbb{N}} \text{ is also a nonnegative supermartingale.}$$

Proposition (Chernoff-Laplace mixture bound (sub-Gaussian))

If $\psi(\lambda) = \frac{\sigma^2 \lambda^2}{2}$, then for any $\mathcal{F}$ -stopping time τ and any $c > 0$,

$$\mathbb{P} \left(\hat{\mu}_{\tau} - \mu \geq \sigma \sqrt{\frac{2 \left(1 + \frac{c}{\tau}\right) \log \left(\frac{\sqrt{\frac{\tau}{c} + 1}}{\delta} \right)}{\tau}} \right) \leq \delta.$$

Remark: this corresponds to the mixture distribution $\mathcal{N}(0, \frac{1}{c})$.

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Exponential families

Parametric family indexed by $\theta \in \Theta$ (open set) of distributions ν_θ over $\mathbb{R}^d$ given by

$$\frac{d\nu_\theta}{d\nu_{\theta_0}}(x) = h(x)e^{\langle \theta, F(x) \rangle - \mathcal{L}(\theta)} .$$

- F : feature function (of $x \in \mathbb{R}^d$),
- $\mathcal{L}$: log-partition function (of $\theta \in \Theta$), convex, twice differentiable.
 - ▶ Assume $\det \nabla^2 \mathcal{L}(\theta) > 0$ for all $\theta \in \Theta$.

Bregman divergence:

$$\begin{aligned} \mathcal{B}_{\mathcal{L}}(\theta', \theta) &= \mathcal{L}(\theta') - \mathcal{L}(\theta) - \langle \theta' - \theta, \nabla \mathcal{L}(\theta) \rangle \\ &= KL(\nu_\theta \| \nu_{\theta'}) . \end{aligned}$$

Examples

Gaussian $\mathcal{N}(\mu, \sigma^2)$ **with known variance** σ^2

$$\theta = \mu, \Theta = \mathbb{R},$$

$$\mathcal{B}_{\mathcal{L}}(\theta', \theta) = \frac{(\theta' - \theta)^2}{2\sigma^2}$$

Gaussian $\mathcal{N}(\mu, \sigma^2)$

$$\theta = \left(\frac{\mu}{\sigma^2}, -\frac{1}{2\sigma^2} \right)^{\top}, \Theta = \mathbb{R} \times \mathbb{R}_-^*,$$

$$\mathcal{B}_{\mathcal{L}}(\theta', \theta) = \frac{1}{2} \log \frac{\theta_2}{\theta'_2} + \frac{\theta'_2}{2\theta_2} - \theta'_2 \left(\frac{\theta'_1}{2\theta'_2} - \frac{\theta_1}{2\theta_2} \right)^2 - \frac{1}{2}.$$

Bernoulli $\mathcal{B}(p)$

$$\theta = p, \Theta = (0, 1),$$

$$\mathcal{B}_{\mathcal{L}}(\theta', \theta) = \theta \log \frac{\theta}{\theta'} + (1 - \theta) \log \frac{1 - \theta}{1 - \theta'}$$

Bregman supermartingale

Lemma

For $\theta \in \Theta$ and λ s.t. $\theta + \lambda \in \Theta$,

$$\log \mathbb{E}_{\theta} \left[e^{\langle \lambda, F(X) - \mathbb{E}_{\theta}[F(X)] \rangle} \right] = \mathcal{B}_{\mathcal{L}}(\theta + \lambda, \theta).$$

Consequence: let $\hat{\mu}_t = \frac{1}{t} \sum_{s=1}^t F(X_s)$ and $\mu = \mathbb{E}_{\theta}[F(X)]$, then

$\forall \lambda, M^{\lambda} = \left(e^{\langle \lambda, t(\hat{\mu}_t - \mu) \rangle - t\mathcal{B}_{\mathcal{L}}(\theta + \lambda, \theta)} \right)_{t \in \mathbb{N}}$ is a nonnegative (super)martingale.

Mixture: for $c > 0$,

$$q_{\theta}(\lambda|c) \propto e^{\langle \theta + \lambda, c \nabla \mathcal{L}(\theta) \rangle - c \mathcal{L}(\theta)},$$

$$M_t = \int M_t^{\lambda} q_{\theta}(\lambda|c) d\lambda.$$

Bregman-Laplace confidence set

Regularised parameter estimate:

$$\hat{\theta}_{t,c}(\theta) = \nabla \mathcal{L}^{-1} \left(\frac{t}{t+c} \hat{\mu}_t + \frac{c}{t+c} \mathcal{L}(\theta) \right).$$

Bregman information gain:

$$\gamma_{t,c}(\theta) = \log \frac{\int_{\Theta} e^{-c \mathcal{B}_{\mathcal{L}}(\theta', \theta)} d\theta'}{\int_{\Theta} e^{-(t+c) \mathcal{B}_{\mathcal{L}}(\theta', \hat{\theta}_{t,c}(\theta))} d\theta'}.$$

Theorem (Bregman-Laplace mixture bound for exponential families)

For any $\mathcal{F}$ -stopping time τ and any $c > 0$,

$$\mathbb{P} \left((\tau + c) \mathcal{B}_{\mathcal{L}} \left(\theta, \hat{\theta}_{\tau,c}(\theta) \right) \geq \log \frac{1}{\delta} + \gamma_{\tau,c}(\theta) \right) \leq \delta$$

Remarks

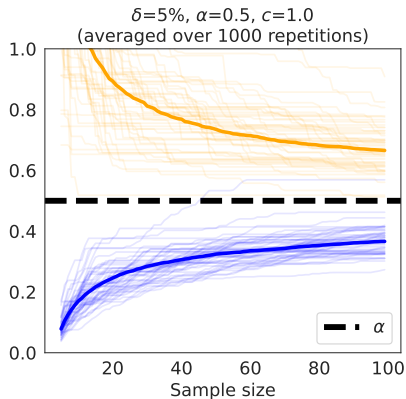
$$\mathbb{P} \left((\tau + c) \mathcal{B}_{\mathcal{L}} \left(\theta, \hat{\theta}_{\tau, c}(\theta) \right) \geq \log \frac{1}{\delta} + \gamma_{\tau, c}(\theta) \right) \leq \delta$$

- Laplace's method for approximating integrals: when $t \rightarrow +\infty$,

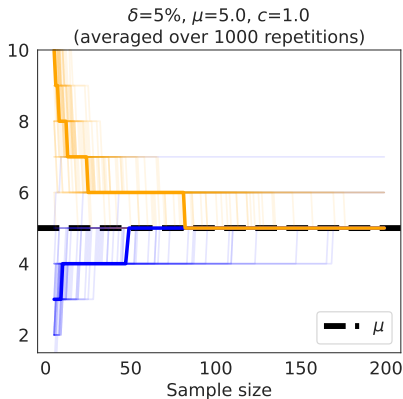
$$\gamma_{t, c}(\theta) = \frac{\dim \Theta}{2} \log \left(1 + \frac{t}{c} \right) + \mathcal{O}(1).$$

- Implicit confidence set...
 - ▶ ...but convex: easy numerical solution.

Numerical experiments



(a) Pareto



(b) Chi-square

Numerical experiments

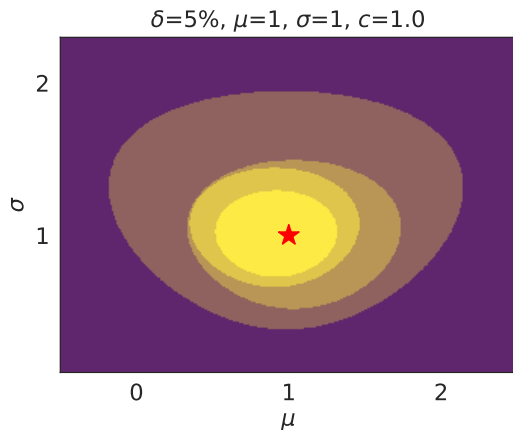
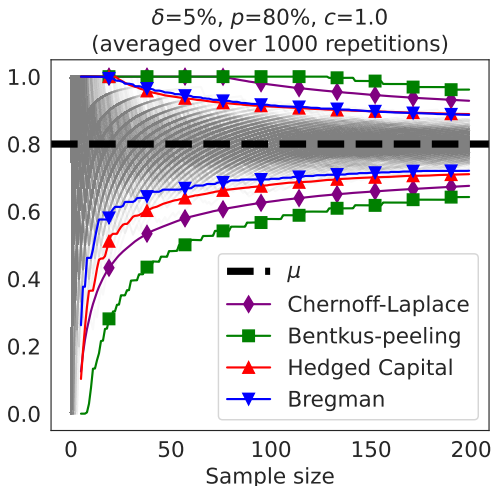


Figure: Gaussian (mean and variance) for $t \in \{10, 25, 50, 100\}$ observations

Numerical experiments



Comparison of median confidence envelopes around the mean for $\mathcal{B}(0.8)$. Grey lines are trajectories of empirical means $\hat{\mu}_n$.

Examples

Table 2: Summary of Bregman confidence sets given by Theorem 3.2 for representative families
Throughout, the following notations are used:

$$S_n = \sum_{t=1}^n X_t, \hat{\mu}_n = \frac{S_n}{n}, Z_n(\mu, \sigma) = \frac{1}{\sigma^2} \sum_{t=1}^n (X_t - \mu)^2,$$

$$S_n^{(k)} = \sum_{t=1}^n X_t^k, L_n = \sum_{t=1}^n \log X_t, K_n = \sum_{t=1}^n \log X_t/2,$$

$$I(a, b) = \int_{-\infty}^{+\infty} e^{-ae^b + b\theta} d\theta,$$

$$J(a, b) = \int_0^\infty \exp(-a \log \Gamma(\frac{k}{2}) + b \frac{k}{2}) dk \quad (\text{if } k \in \mathbb{R}_+),$$

$$J(a, b) = \sum_{k'=1}^\infty \exp(-a \log \Gamma(\frac{k'}{2}) + b \frac{k'}{2}) \quad (\text{if } k \in \mathbb{N}).$$

Gamma	$\lambda \in \mathbb{R}_+$	$\frac{S_n}{\lambda} - ((n+c)k+1) \log(\frac{S_n}{\lambda} + ck)$ $\leq \log \frac{1}{\delta} + \log \frac{\Gamma(c)}{\Gamma((n+c)k)} - \log((n+c)k) - ck \log ck$
Weibull	$\lambda \in \mathbb{R}_+$	$\frac{S_n^{(k)}}{\lambda^k} - (n+c+1) \log(\frac{S_n^{(k)}}{\lambda^k} + c)$ $\leq \log \frac{1}{\delta} + \log \frac{\Gamma(c)}{\Gamma(n+c)} - \log(n+c) - c \log c$
Pareto	$\alpha \in \mathbb{R}$	$\alpha L_n - (n+c+1) \log(\alpha L_n + c)$ $\leq \log \frac{1}{\delta} + \log \frac{\Gamma(c)}{\Gamma(n+c)} - \log(n+c) - c \log c$
Poisson	$\lambda \in \mathbb{R}_+$	$n\lambda - S_n \log \lambda$ $\leq \log \frac{1}{\delta} + \log I(c, c\lambda) - \log I(n+c, S_n + c\lambda)$
Chi-square	$k \in \mathbb{N}$ or $k \in \mathbb{R}_+$	$n \log \Gamma(\frac{k}{2}) - \frac{k}{2} K_n - \log J(c, c\psi_0(\frac{k}{2}))$ $+ \log J(n+c, K_n + c\psi_0(\frac{k}{2})) \leq \log \frac{1}{\delta}$

Name	Parameters	Formula
Gaussian	$\mu \in \mathbb{R}$	$\frac{1}{n+c} \frac{(S_n - n\mu)^2}{2\sigma^2} \leq \log \frac{1}{\delta} + \frac{1}{2} \log \frac{n+c}{c}$
Gaussian	$\sigma \in \mathbb{R}_+$	$\frac{Q_n(\mu)}{2\sigma^2} - (\frac{n+c}{2} + 1) \log(\frac{Q_n(\mu)}{2\sigma^2} + \frac{c}{2})$ $\leq \log \frac{1}{\delta} + \log \frac{\Gamma(\frac{c}{2})}{\Gamma(\frac{n+c}{2})} - \log(\frac{n+c}{2}) - \frac{c}{2} \log \frac{c}{2}$
Gaussian	$\mu \in \mathbb{R}$ $\sigma \in \mathbb{R}_+$	$\frac{1}{2} Z_n(\mu, \sigma) - \frac{n+c+3}{2} \log(\frac{n+c}{n+c} Z_n(\hat{\mu}_n, \sigma) + \frac{c}{n+c} Z_n(\mu, \sigma) + c)$ $\leq \log \frac{1}{\delta} - \frac{n}{2} \log 2 - (\frac{c}{2} + 2) \log c + \frac{1}{2} \log(n+c)$ $+ \log \Gamma(\frac{n+c}{2}) - \log \Gamma(\frac{n+c+3}{2})$
Bernoulli	$\mu \in [0, 1]$	$S_n \log \frac{1}{\mu} + (n - S_n) \log \frac{1}{1-\mu} + \log \frac{\Gamma(S_n + c\mu) \Gamma(n - S_n + c(1-\mu))}{\Gamma(c\mu) \Gamma(c(1-\mu))}$ $\leq \log \frac{1}{\delta} + \log \frac{\Gamma(n+c)}{\Gamma(c)}$
Exponential	$\mu \in \mathbb{R}_+$	$\frac{S_n}{\mu} - (n+c+1) \log(\frac{S_n}{\mu} + c)$ $\leq \log \frac{1}{\delta} + \log \frac{\Gamma(c)}{\Gamma(n+c)} - \log(n+c) - c \log c$

Questions?



References I

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- 4 Time-uniform concentration: other methods

A bad idea: union bound

Say we have:

$$\forall t \in \{1, \dots, T\}, \mathbb{P}(\mu \in \mathcal{C}_t^\delta) \geq 1 - \delta.$$

Then:

$$\begin{aligned} \mathbb{P}(\forall t \in \{1, \dots, T\}, \mu \in \mathcal{C}_t^\delta) &= 1 - \mathbb{P}\left(\bigcup_{t=1}^T \{\mu \notin \mathcal{C}_t^\delta\}\right) \\ &\geq 1 - \sum_{t=1}^T \mathbb{P}(\mu \notin \mathcal{C}_t^\delta) \\ &\geq 1 - T\delta. \end{aligned}$$

A bad idea: union bound

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Then:

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Proposition (Union bound)

$(\mathcal{C}_t^{\delta/T})_{t=1}^T$ is a uniform confidence sequence at level δ .

Turning a bad idea into a good one: time-peeling

Proposition (Doob's maximal inequality)

Let $(S)_{t \in \mathbb{N}}$ be a **nonnegative supermartingale** w.r.t a filtration $(\mathcal{F}_t)_{t \in \mathbb{N}}$. Then for all $p \geq 1$ and $\epsilon > 0$, it holds for all $T_0 < T$ that

$$\mathbb{P} \left(\max_{T_0 \leq t \leq T} S_t \geq \epsilon \right) \leq \frac{\mathbb{E} [S_{T_0}^p]}{\epsilon^p}.$$

Idea: apply union bound over a geometric grid $(t_k)_{k \in \mathbb{N}}$ with $t_k = (1 + \eta)^k$.

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Idea: apply union bound over a geometric grid $(t_k)_{k \in \mathbb{N}}$ with $t_k = (1 + \eta)^k$.

Proposition (Geometric time-peeling)

Let τ a $(\mathcal{F}_t)_{t \in \mathbb{N}}$ -stopping time. Then for $\eta > 0$ and $\delta \in (0, 1)$,

$$\mathbb{P} \left(\hat{\mu}_\tau - \mu \geq \psi_*^{-1} \left(\frac{1+\eta}{\tau} \log \left(\frac{\log(\tau) \log((1+\eta)\tau)}{\delta \log^2(1+\eta)} \right) \right) \right) \leq \delta$$