Estimating High-dimensional Confidence Sets: A Robust Estimation Perspective

Vaidehi Srinivas

Northwestern University, Computer Science

Chao Gao

University of Chicago, Statistics

Liren Shan

Toyota Technological Institute, Chicago

Aravindan Vijayaraghavan

Northwestern University, Computer Science

COLT 2025 Workshop on Predictions and Uncertainty

High-dimensional Confidence Sets

Goal: Find a high-density region of an **arbitrary** distribution

Problem: Given samples drawn i.i.d. from an unknown distribution $\mathscr{D}$ over $\mathbb{R}^d$, and target **coverage rate** δ, fit the **smallest volume** confidence set S such that

$$\mathbb{P}_{y\sim\mathscr{D}}(y \in S) \geq \delta\,.$$

(Think of $\delta = 0.9$)

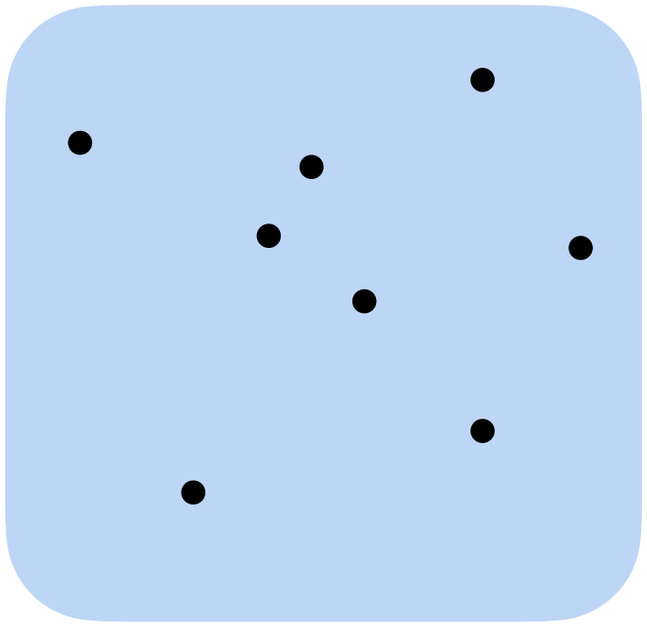
"Volume optimality"

Applications: Central problem in statistics

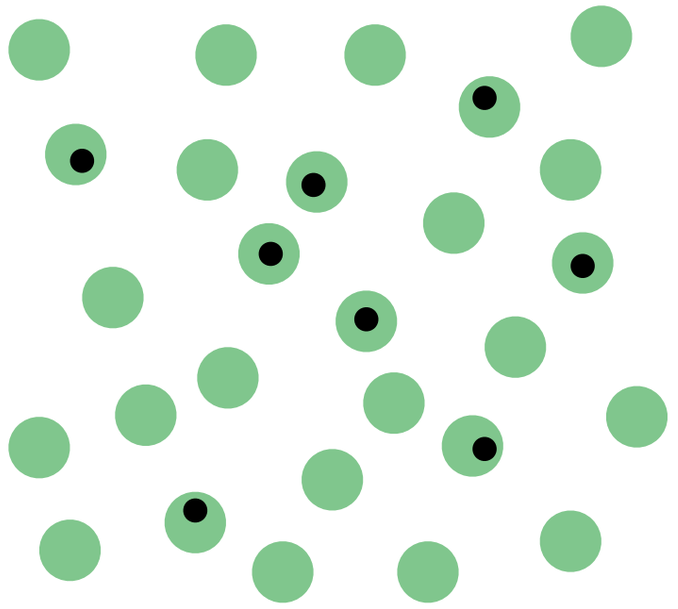
- Conformal prediction [Gao Shan S. Vijayaraghavan '25],
- Estimating density level sets [Garcia Kutalik Cho Wolkenhauer '03],
- Support estimation [Schölkopf Platt Shawe-Taylor Smola Williamson '01],
- Robust estimation [Rousseeuw '84, 85],
- and many more!

Trouble with Volume Optimality

Bad news: Impossible to achieve volume optimality in general!



$\mathscr{D}_1$
does not admit a small confidence set



$\mathscr{D}_2$
admits a small confidence set

Cannot distinguish between $\mathscr{D}_1$ and $\mathscr{D}_2$

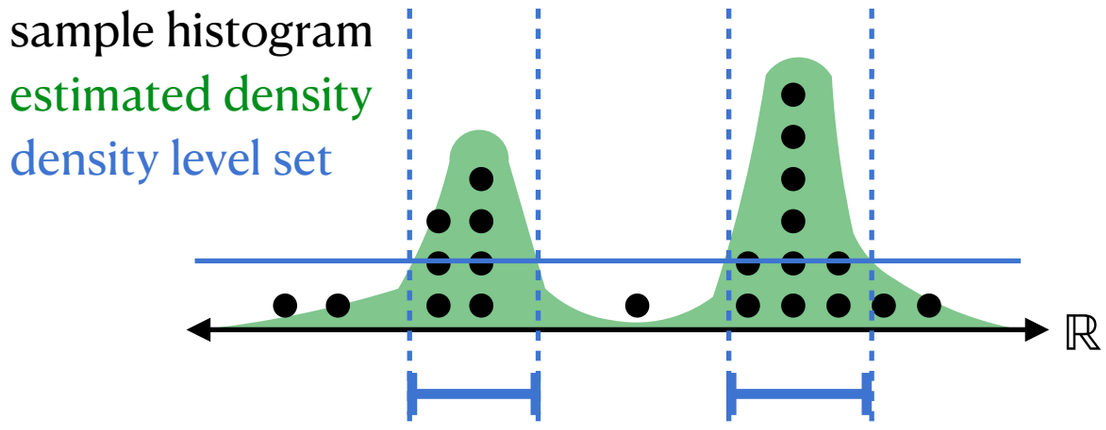
Forced to lose in either **coverage** or **volume**

(even in one dimension!)

Restricted Volume Optimality

Strategy 1: Restrict the class of distributions

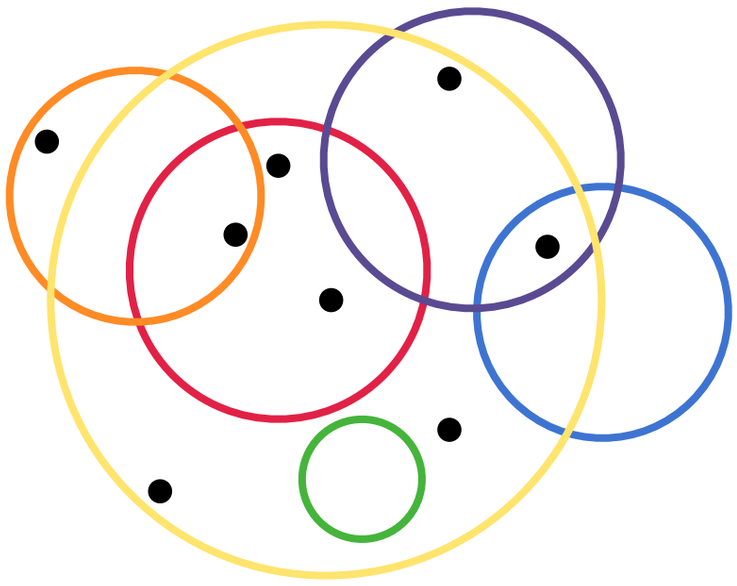
Example: density estimation [Lei, Robins, Wasserman '13], [Izbicki, Shimizu, Stern '22]



- Works for nicely-behaved distributions in one dimension
- Statistically intractable in high-dimensions

Strategy 2: Restrict the class of confidence sets [Scott Nowak '05][Gao, Shan, **S.**, Vijayaraghavan '25]

Examples: confidence intervals over $\mathbb{R}$, Euclidean balls over $\mathbb{R}^d$



- Set families of bounded VC-dimension exhibit **uniform convergence**
- Coverage of all balls simultaneously converge in $\text{poly}(d)$ samples $\Rightarrow$ **statistically tractable**!
- Aim to compete with best set in the family

Learning a Confidence Set

Focus: $\mathscr{S} = \mathscr{B}$ the set of Euclidean balls in $\mathbb{R}^d$.

Updated problem: Let $B^\star \in \mathscr{B}$ be the minimum volume set with coverage $\geq \delta$ over $\mathscr{D}$. Find a set $\widehat{S}$ with coverage $\geq \delta$ over $\mathscr{D}$, and

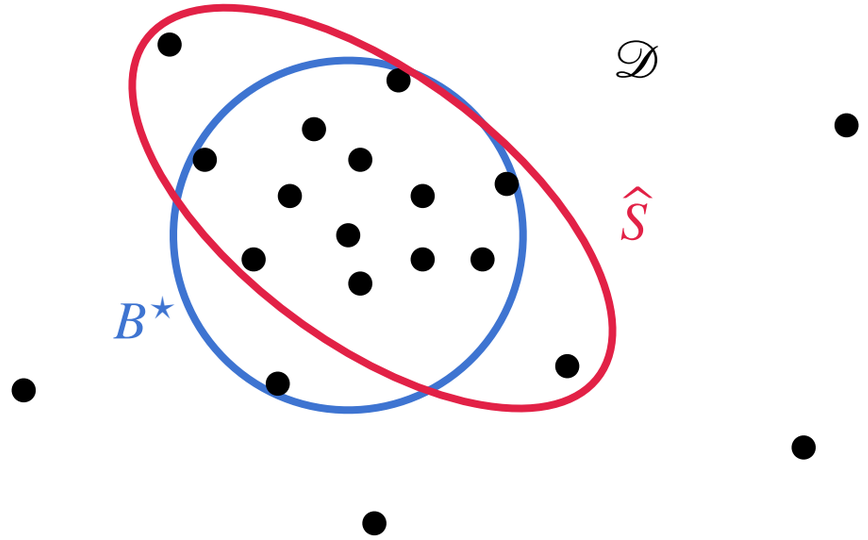
$$\mathrm{vol}(\widehat{S}) \lesssim \mathrm{vol}(B^\star).$$

(also natural to compare "radii": $\mathrm{vol}(\widehat{S})^{1/d} \lesssim \mathrm{vol}(B^\star)^{1/d}$)

$\rightarrow$ $\widehat{S}$ does not necessarily need to be in $\mathscr{B}$, similar to PAC learning

($\widehat{S} \in \mathscr{B}$ is **proper learning**)

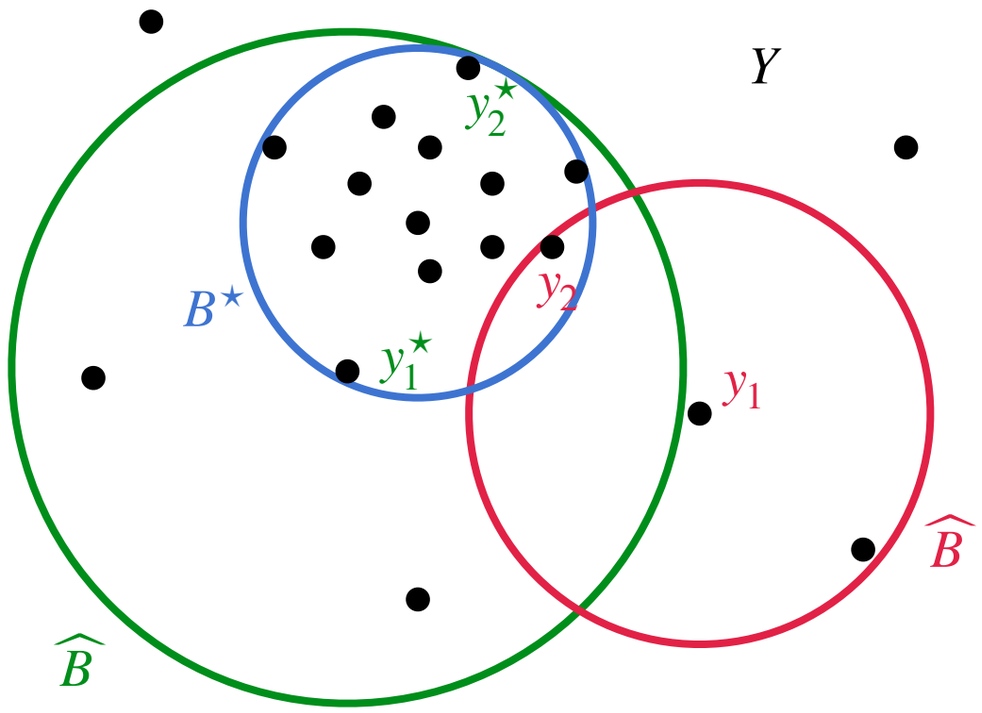
Arbitrary nature of $\mathscr{D}$ makes this is a **worst-case** problem (rather than average-case)



How to compute such an $\widehat{S}$ in polynomial time?

- Can find the min.-volume ball enclosing **all** samples in polynomial time (SDP)
- Capturing δ-fraction is more challenging, hope to achieve volume **approximation**

Simple Approximation



Sample set of points Y from $\mathscr{D}$

Algorithm:

- For every pair of points $y_1, y_2 \in Y$, construct a ball $\widehat{B}$ with center y_1 and farthest point y_2
- Search over all $\leq n^2$ possibilities, output smallest vol. such ball containing at least δ of Y

Analysis: Choose $y_1^\star, y_2^\star$ to be maximally distant points in the optimal solution $B^\star$ to cover all of $B^\star$ and get

$$\text{2-approx. in radius} \iff (2^d)\text{-approx. in volume.}$$

Strategies based on coresets can get volume approximations [Badoiu Har-Peled Indyk '02]

$$\exp\left(O(d/\text{polylog}(d))\right).$$

Proper learning!

Informal Result

Can we get a better approximation?

For any constant $\varepsilon > 0$, NP-**hard** to **properly** approximate min.-volume ball containing δ of $\mathscr{D}$ up to factor

$$(1 + 1/d^{\varepsilon}) \text{ in radius} \iff \exp(d^{1-\varepsilon}) \text{ in volume}$$

Can get much better approximation via improper learning!

Improper learning: Find confidence set that is an ellipsoid

Informal result: Given a polynomial number of samples from $\mathscr{D}$, in polynomial time it is possible to find an ellipsoid $\widehat{E}$ that achieves coverage $\approx \delta$, and has volume at most

$$\text{vol}(\widehat{E}) \leq \exp(\widetilde{O}(d^{1/2})) \cdot \text{vol}(B^{\star}),$$

where $B^{\star}$ is the optimal ball achieving coverage δ over $\mathscr{D}$.

via robust estimation!

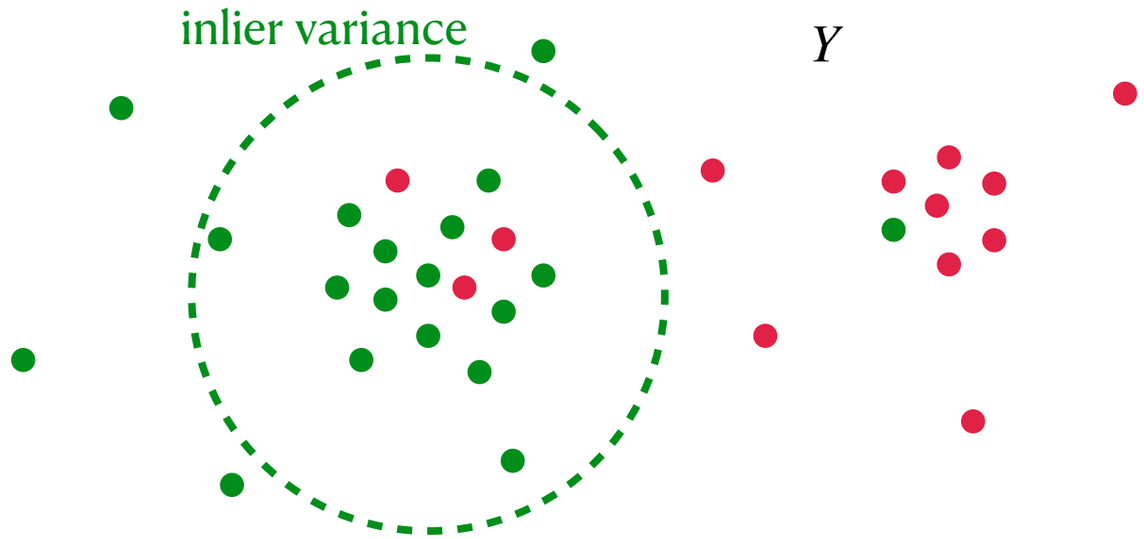
Robust High-dimensional Estimation

Goal: Estimate statistics of adversarially corrupted data

Example: Given samples Y from a distribution

$$\mathscr{D} = \delta\mathscr{D}_{\text{inlier}} + (1-\delta)\mathscr{D}_{\text{outlier}},$$

estimate the mean of $\mathscr{D}_{\text{inlier}}$.



Need to take advantage of structure in inlier distribution

→ for example: inliers have **bounded variance** in every direction

In polynomial time, have techniques to robustly estimate

- **median**: minimizes sum of distances to samples
- **mean**: minimizes sum of squared distances to samples

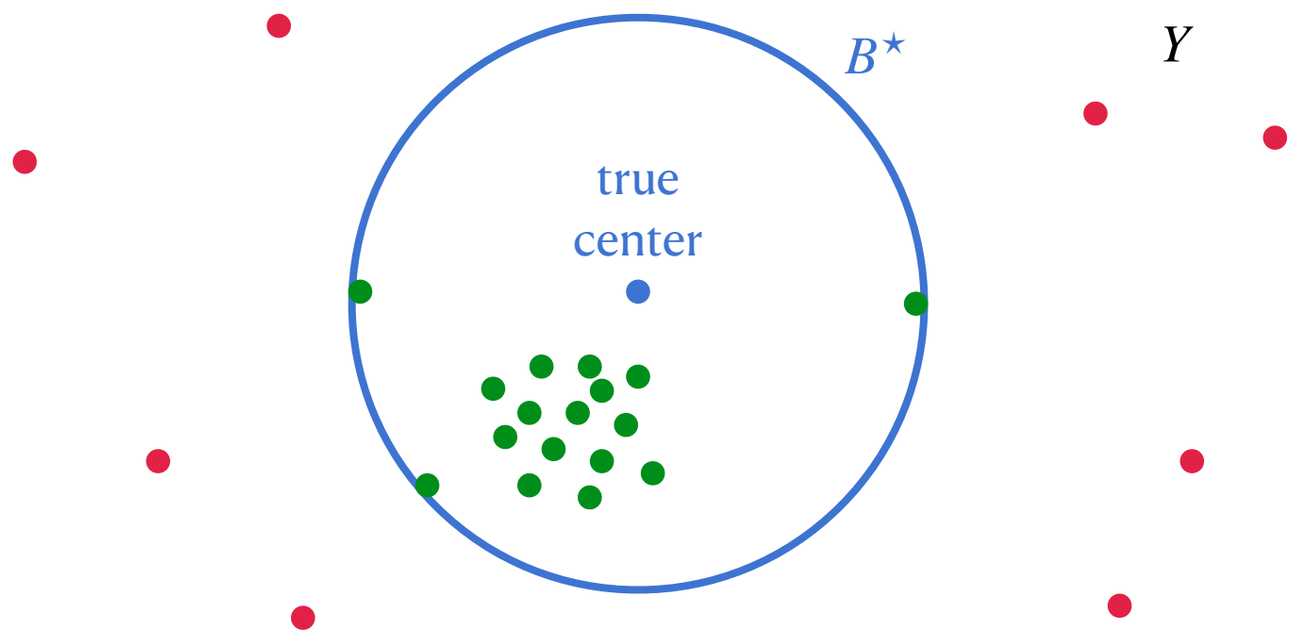
Can we robustly estimate the **center**?
(minimizes maximum distance to samples)

Connection to Confidence Sets

Volume optimality: Compete with $B^\star$, the optimal ball capturing δ-fraction of $\mathscr{D}$

Let $\mathscr{D}_{\text{inlier}}$ be the distribution in $B^\star$, $\mathscr{D}_{outlier}$ be the distribution outside $B^\star$, thus

$$\mathscr{D} = \delta\mathscr{D}_{\text{inlier}} + (1-\delta)\mathscr{D}_{\text{outlier}}.$$



Would like to estimate the **center** (minimize the maximum distance to points) of the inlier distribution $\mathscr{D}_{\text{inlier}}$.

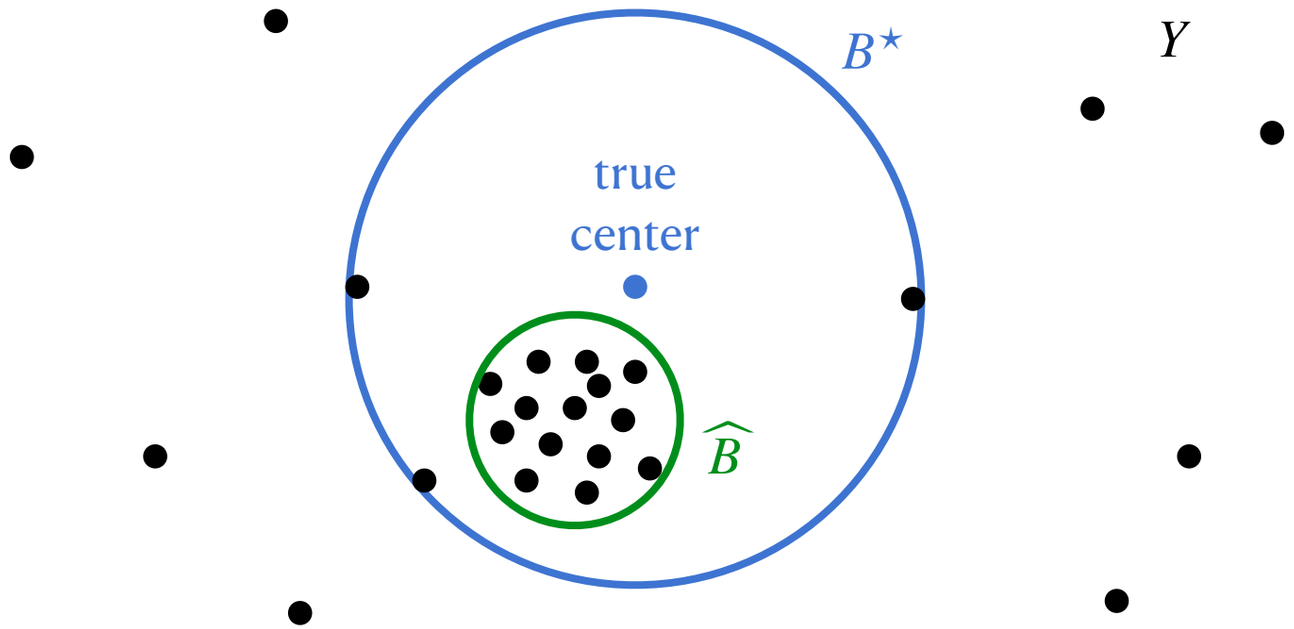
$\rightarrow$ would give the center of $B^\star$, easy to guess radius once we have the center

Any method that produces small confidence sets must be robust to outliers!

Robust Center Estimation?

In $\mathbb{R}^d$, the **center** only depends on $d+1$ points, so it is **not robustly estimatable**.

(cannot hope for robust estimation, even statistically)



Relaxation: compete with best ball that covers δ-fraction of Y, but only cover $(\delta-\gamma)$-fraction of Y, for small **coverage slack factor** $\gamma > 0$.

(Think of $\delta = 0.9, \gamma = 0.01, \delta - \gamma = 0.89$)

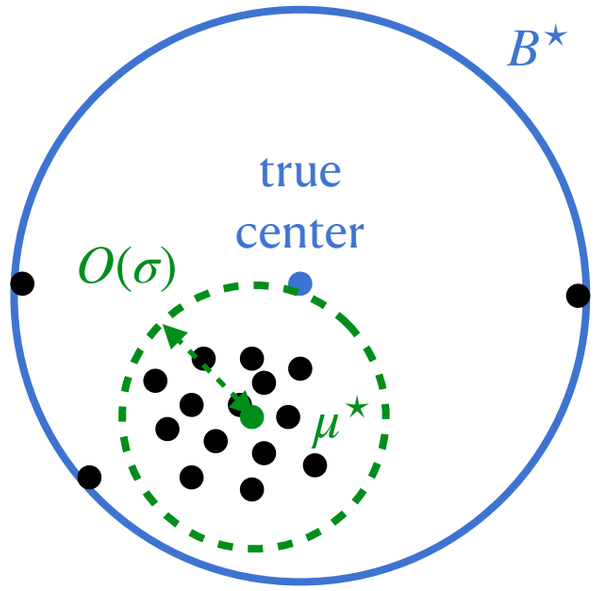
Coverage slack is relatively benign, and gives us a foothold in the algorithmic problem

Mean as Robust Proxy for Center

Chebyshev's inequality says most points in $B^\star$ (inliers) must be within a few **standard deviations**, σ, of the mean $\mu^\star$ of $B^\star$

$\Longrightarrow$ $\mu^\star$ is a proxy for the center of **most** of the points!

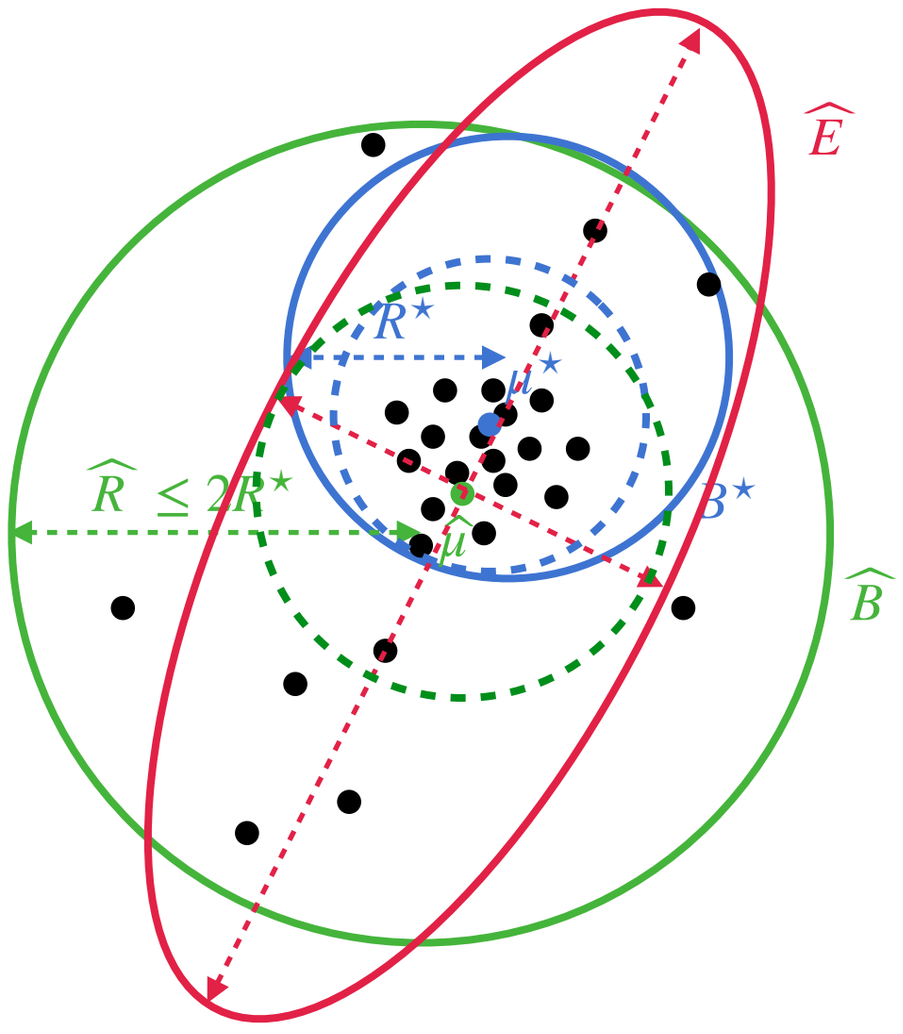
Can hope to robustly estimate $\mu^\star$



Requires bound on the variance of the points in $B^\star$

- to bound radius of ball around $\mu^\star$
- to accurately recover $\mu^\star$, the mean of inliers

Bootstrapping Variance Bound



Recall: Simple algorithm finds $\widehat{B}$ that contains all points in optimal $B^\star$, with at most $2 \times$ radius of $B^\star$

Because points are bounded in $\widehat{B}$, **on average** over directions their variance is low!

Centering a ball around $\mu^\star$, mean of $B^\star$, captures most of the mass in most directions

$\mu^\star$ is near $\widehat{\mu}$ since $B^\star$ contains at least δ mass, so can center ball at $\widehat{\mu}$, mean of $\widehat{B}$

There can only be a few directions in which the variance of points in $\widehat{B}$ is much higher than average, in which we expand our set

$\rightarrow$ log-concavity of volume means it is ok to expand a lot in a few directions

Algorithmic via PCA

Result

Theorem: We give a polynomial-time algorithm, that for a target coverage $\delta \in (0,1)$, and coverage slack $\gamma \in (0,1)$, given $n = \Omega(d^2/\gamma^2)$ samples drawn i.i.d. from an arbitrary $\mathscr{D}$, finds with high probability a set S such that

$$\mathbb{P}_{y\sim\mathscr{D}}[y \in S] \geq \delta,$$

and

$$\mathrm{vol}(S) \leq \mathrm{vol}(B^\star) \cdot \exp\left(O_{\delta,\gamma}(d^{1/2+o(1)})\right),$$

where $B^\star$ is the minimum volume ball that achieves $\delta + \gamma + O(\sqrt{d^2/n})$ coverage over $\mathscr{D}$.

- Combined with hardness for approximating balls with balls, gives a **separation between proper and improper learning** for a natural task
- Can use ideas to compete against sets that are unions of balls
- **Beyond-worst-case extension:** Can use **list-decodable mean estimation** as a black-box to get an $O(1)$ volume approximation factor for nicely-behaved distributions (inliers are approximately isotropic)

Conclusion

Problem: Estimating the high-density region of an **arbitrary** distribution

Application: Conformal prediction, and more!

Techniques: High-dimensional robust estimation toolkit

Results: Polynomial-time approximation algorithm, and separation between proper and improper learning

Future directions:

- Can we improve the approximation factor for balls, or prove hardness?
- Can we approximate other natural set families? Ex: ℓ_p balls for p other than 2
  [Braun Aolaritei Jordan Bach '25]
- Give a statistical characterization of tractability (i.e., bounded VC-dimension is sufficient, but is it necessary?)
- Online and/or streaming algorithms? [Angelopoulos Candes Tibshirani '23][**S.** '25]

Thanks!

vaidehi@u.northwestern.edu