

Bounding Estimation Performance in Inverse Problems via Conformal Prediction

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Inverse problems

Inverse problems:

- Unknown quantity $\mathbf{x}_0 \in \mathbb{R}^d$
- Masked/noisy/distorted measurements $\mathbf{y} = \mathbf{h}(\mathbf{x}_0)$
 - Communications examples: wireless device localization, CSI estimation, RF tomography
 - Imaging examples: MRI, CT, inpainting, deblurring, super-resolution, phase retrieval
- Estimate $\hat{\mathbf{x}} = \mathbf{r}(\mathbf{y})$

Challenge:

- Typically ill-posed: many hypotheses of $\mathbf{x}_0$ form good explanations of $\mathbf{y}$

Subject of this talk:

- We want to quantify the uncertainty of the estimate $\hat{\mathbf{x}}$
- In particular, we want rigorous probabilistic bounds on the accuracy of $\hat{\mathbf{x}}$

Example: Wireless transmitter localization

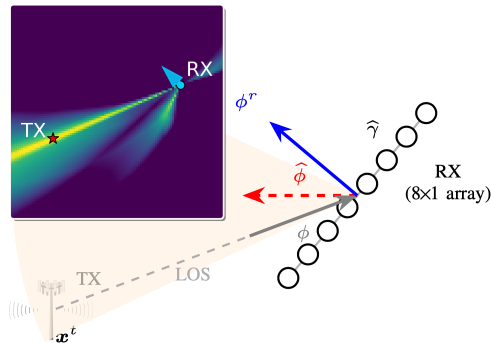
- We'd like to estimate the 2D Tx location $\mathbf{x}_0$ from a pilot signal and Rx array measurements $\mathbf{y}$
- Ill-posed due to noise, multipath fading, array ambiguities, non-ideal antenna elements, etc
- The posterior $p(\mathbf{x}_0|\mathbf{y})$ is shown on the right:
- For a user-chosen error-rate $\alpha \in (0, 1)$ and arbitrary estimator $\hat{\mathbf{x}} = \mathbf{r}(\mathbf{y})$, can we construct an upper bound $\beta(\mathbf{y})$ such that

$$\Pr \{ \|\hat{\mathbf{x}} - \mathbf{x}_0\| \leq \beta(\mathbf{y}) \} \geq 1 - \alpha ?$$

Beyond Point Estimates: Likelihood-Based Full-Posterior Wireless Localization

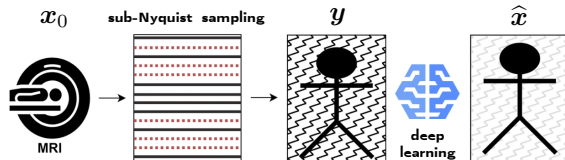
Haozhe Lei¹, Hao Guo^{1,2}, Tommy Svensson², and Sundee Rangan¹

arXiv:2509.25719

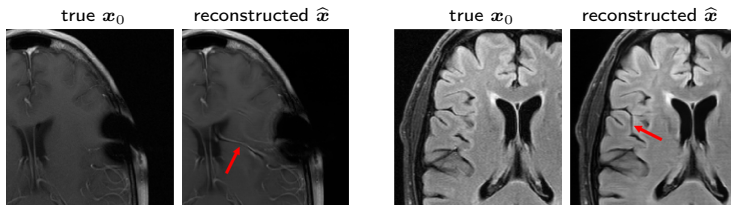


Example: Accelerated MRI

- x_0 is the true image
- y are $\frac{1}{R}$ sub-Nyquist measurements
- $\hat{x} = r(y)$ is the reconstructed image



Problem: modern recovery methods can **hallucinate**, i.e., generate clean but inaccurate $\hat{x}$. For example:¹



¹Muckley et al.'21

Probabilistic bounds on estimation accuracy

- We'd like to know the **accuracy** of $\hat{\mathbf{x}}_0$ relative to the true $\mathbf{x}_0$
 - From now on, subscript "0" indicates "test" quantity vs calibration quantity
- To quantify accuracy, we'll use an arbitrary metric $z_0 = m(\hat{\mathbf{x}}_0, \mathbf{x}_0)$, such as
 - $m(\hat{\mathbf{x}}_0, \mathbf{x}_0) = -\|\hat{\mathbf{x}}_0 - \mathbf{x}_0\|_p$ for wireless localization
 - $m(\hat{\mathbf{x}}_0, \mathbf{x}_0) =$ PSNR or SSIM or LPIPS or DISTS for images
- Is it possible to **guarantee the accuracy** of $\hat{\mathbf{x}}_0$, i.e., construct a lower bound $\beta_0(\mathbf{y}_0)$ such that

$$\Pr\{Z_0 \geq \beta_0(\mathbf{Y}_0)\} \geq 1 - \alpha$$

for some chosen error rate α ? (Here, capital letters denote random variables)

What if we had a perfect posterior sampler?

- Suppose we had a **perfect posterior sampler** generating n_{post} independent samples $\{\tilde{\mathbf{x}}_0^{(j)}\}_{j=1}^{n_{\text{post}}}$

$$\{\tilde{\mathbf{x}}_0^{(1)}, \dots, \tilde{\mathbf{x}}_0^{(n_{\text{post}})}\} \sim p_{\mathbf{X}_0 | \mathbf{Y}_0}(\cdot | \mathbf{y}_0)$$

- Define the corresponding **accuracy samples** $\tilde{z}_0^{(j)} \triangleq m(\hat{\mathbf{x}}_0, \tilde{\mathbf{x}}_0^{(j)})$:

$$\{\tilde{z}_0^{(1)}, \dots, \tilde{z}_0^{(n_{\text{post}})}\} \sim p_{Z_0 | \mathbf{Y}_0}(\cdot | \mathbf{y}_0)$$

- We can construct a lower bound β_0 that obeys $\Pr\{Z_0 \geq \beta_0 | \mathbf{Y}_0 = \mathbf{y}_0\} = 1 - \alpha$ using an **empirical quantile** using asymptotically many samples:

$$\beta_0 = \lim_{n_{\text{post}} \rightarrow \infty} \hat{\beta}_{0, n_{\text{post}}} \quad \text{with} \quad \hat{\beta}_{0, n_{\text{post}}} \triangleq \text{EmpQuant}(\alpha, \{\tilde{z}_0^{(j)}\}_{j=1}^{n_{\text{post}}})$$

- Okay, but can we make this practical?

A useful tool: split conformal prediction

- Given an estimate $\hat{z}_0$ of the true $z_0 \in \mathbb{R}$, **split conformal prediction**¹ can construct a set $\mathcal{C}_\lambda(\hat{z}_0)$ that contains z_0 with high probability. Here, $|\mathcal{C}_\lambda(\cdot)|$ grows with $\lambda \in \mathbb{R}$
- Given a user-chosen error rate $\alpha \in (0, 1)$, it computes a $\hat{\lambda}_\alpha \in \mathbb{R}$ using **calibration data** $d_{\text{cal}} = \{(z_i, \hat{z}_i)\}_{i=1}^{n_{\text{cal}}}$ of size n_{cal}
- The prediction set guarantees **marginal coverage**

$$\Pr \{Z_0 \in \mathcal{C}_{\hat{\lambda}_\alpha(D_{\text{cal}})}(\hat{Z}_0)\} \geq 1 - \alpha$$

when the test & calibration pairs $\{(Z_0, \hat{Z}_0), (Z_1, \hat{Z}_1), \dots, (Z_{n_{\text{cal}}}, \hat{Z}_{n_{\text{cal}}})\}$ are **statistically exchangeable**

¹Vovk, Gammerman, Shafer'05, ²Lei, G'Sell, Rinaldo, Tibshirani, Wasserman'18

Approximate posterior sampling & conformal prediction

Recall we want to lower-bound the accuracy $z_0 = m(\hat{\mathbf{x}}_0, \mathbf{x}_0)$ of estimate $\hat{\mathbf{x}}_0 = \mathbf{r}(\mathbf{y}_0)$ of unknown $\mathbf{x}_0$

- Assume we have **calibration samples** $\{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1}^{n_{\text{cal}}}$ in addition to the test measurements $\mathbf{y}_0$
- Generate **approximate posterior samples** $\{\tilde{\mathbf{x}}_i^{(j)}\}_{j=1}^{n_{\text{post}}}$ from $\mathbf{y}_i$ for each $i = 0, \dots, n_{\text{cal}}$.
- Compute the **accuracy samples** $\tilde{z}_i^{(j)} = m(\hat{\mathbf{x}}_i, \tilde{\mathbf{x}}_i^{(j)})$ for all $i = 0, \dots, n_{\text{cal}}$ and $j = 1, \dots, n_{\text{post}}$
- Construct **approximate bounds** $\hat{\beta}_i = \text{EmpQuant}(\alpha, \{\tilde{z}_i^{(j)}\}_{j=1}^{n_{\text{post}}})$ for $i = 0, \dots, n_{\text{cal}}$
- Construct **bound-violation scores** $s_i = \hat{\beta}_i - z_i$ for $i = 1, \dots, n_{\text{cal}}$ (positive when bound is violated)
- Compute the **bound calibration term**

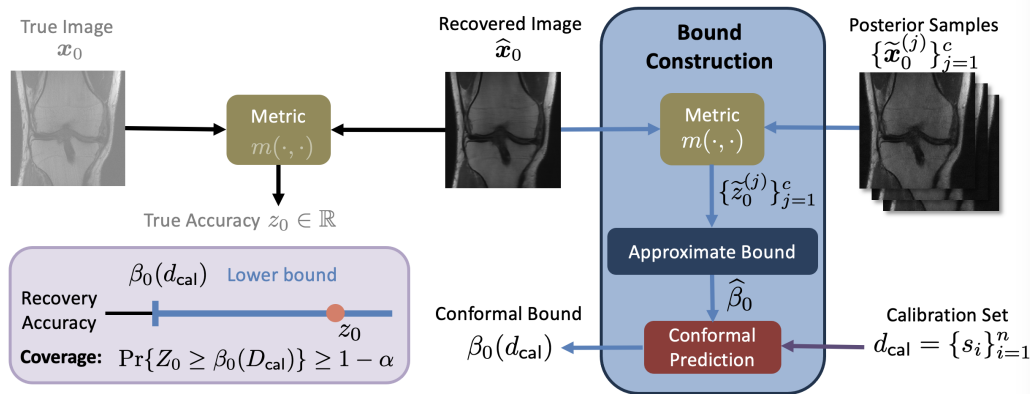
$$\hat{\lambda}_\alpha(d_{\text{cal}}) = \text{EmpQuant}\left(\frac{\lceil (1-\alpha)(n_{\text{cal}}+1) \rceil}{n_{\text{cal}}}, \{s_i\}_{i=1}^{n_{\text{cal}}}\right), \quad \text{where } d_{\text{cal}} \triangleq \{s_i\}_{i=1}^{n_{\text{cal}}}$$

- Finally, form the **lower-bound** as $\beta_0(\mathbf{y}_0, d_{\text{cal}}) = \hat{\beta}_0(\mathbf{y}_0) - \hat{\lambda}_\alpha(d_{\text{cal}})$

If $\{S_0, S_1, \dots, S_n\}$ are statistically exchangeable, then we have the **marginal coverage guarantee**

$$\Pr\{Z_0 \geq \beta_0(\mathbf{Y}_0, D_{\text{cal}})\} \geq 1 - \alpha$$

Illustration of lower-bound procedure (for accelerated MRI)

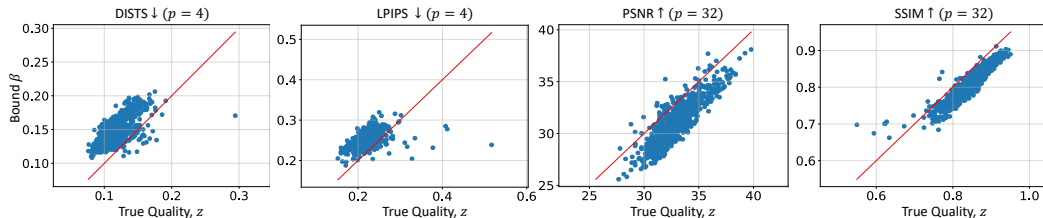


- This bounding methodology¹ works with any estimation problem, estimator, accuracy metric, and approximate posterior sampler

¹Wen, Ahmad, Schniter'25a

Example: Bounding recovery accuracy in MRI

- Scatter plots of (z_0, β_0) from **fastMRI knee** recovery @ acceleration $R = 8$ using a conditional normalizing flow¹:



The red line indicates where the bound would be exact

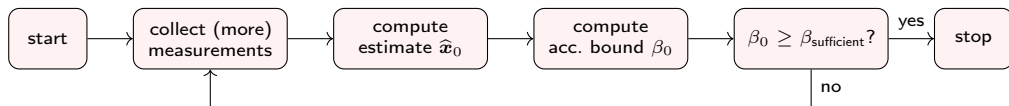
- Validation of marginal coverage using 10 000 Monte-Carlo trials (each with a random 70% test / 30% calibration split):

target coverage $1 - \alpha$	average empirical coverage
0.95	0.9504 ± 0.0001

¹Wen, Ahmad, S'23

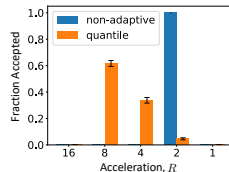
Leveraging the accuracy-bound for multi-round measurements

- Often, the estimate $\hat{x}_0$ can be improved by gathering more measurements y
 - wireless Tx localization: gather more pilot sequences
 - accelerated MRI: gather more k-space samples
- But often there's a cost to collecting more measurements
- Proposed idea: **Collect measurements until the accuracy lower-bound surpasses a threshold**



- Applied to MRI with $1-\alpha = 0.95$:

method	avg acceleration	empirical coverage
single-round	2.000 ± 0.0000	0.9505 ± 0.0001
multi-round	5.422 ± 0.0001	0.9461 ± 0.0001



Back to wireless transmitter localization

- Given the nature of the posterior, we may want to **separately bound the angle and the radius**
- This gives multiple accuracies to bound:

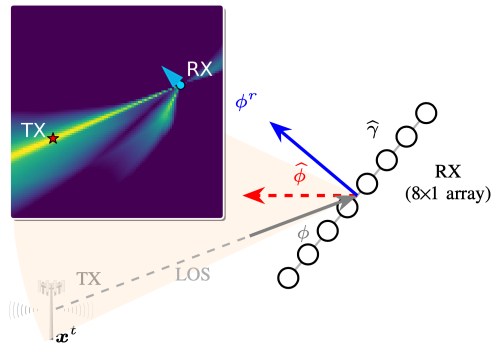
$$z_0 = \begin{bmatrix} -|\angle(\hat{\mathbf{x}}_0) - \angle(\mathbf{x}_0)| \\ -\|\hat{\mathbf{x}}_0\| - \|\mathbf{x}_0\| \end{bmatrix} \in \mathbb{R}^2$$

and requires extending our conformal bounding method to **multiple “targets”**

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Multi-target conformal prediction

- Say we have $K > 1$ scalar accuracies $\{z_{0,k}\}_{k=1}^K$ and we want to lower-bound each of them
- Our goal is to compute bounds $\{\beta_{0,k}\}_{k=1}^K$ that guarantee **joint marginal coverage**:

$$\Pr \left\{ \bigcap_{k=1}^K Z_{0,k} \geq \beta_{0,k}(\mathbf{Y}_0, D_{\text{cal}}) \right\} \geq 1 - \alpha,$$

which means that, with probability at least $1 - \alpha$, all bounds are *simultaneously* valid

- Several existing methods¹ accomplish this task, but they struggle with **uniformity across targets**: bounds for some targets are too loose while those for other targets are unnecessarily tight

¹Messoudi et al.'20, Sampson&Chan'24, Sun&Yu'24, Park&Cho'25

Proposed multi-target conformal prediction

- Since **looser bounds correspond to larger *single*-target coverages** $\Pr\{Z_{0,k} \geq \beta_{0,k}\}$, we propose to solve

$$\arg \min_{(\beta_{0,1}, \dots, \beta_{0,K})} \max_k \Pr\{Z_{0,k} \geq \beta_{0,k}\} \quad \text{s.t.} \quad \Pr\left\{\bigcap_{k=1}^K Z_{0,k} \geq \beta_{0,k}\right\} \geq 1 - \alpha$$

i.e., **minimize the maximum single-target coverage** subject to the joint-coverage constraint

- Forming the k th bound as $\beta_{0,k} = \hat{\beta}_{0,k}(\mathbf{y}_0) - \lambda_k$ and bound-violation score as $s_{0,k} = \hat{\beta}_{0,k}(\mathbf{y}_0) - z_{0,k}$, we have

$$\begin{aligned} \Pr\{Z_{0,k} \geq \beta_{0,k}\} &= \Pr\{S_{0,k} \leq \lambda_k\} = F_{S_{0,k}}(\lambda_k) \quad \text{with CDF } F_{S_{0,k}}(\cdot) \\ \& \Pr\left\{\bigcap_{k=1}^K Z_{0,k} \geq \beta_{0,k}\right\} &= \Pr\left\{\bigcap_{k=1}^K S_{0,k} \leq \lambda_k\right\} = \Pr\left\{\bigcap_{k=1}^K F_{S_{0,k}}(S_{0,k}) \leq F_{S_{0,k}}(\lambda_k)\right\} \end{aligned}$$

- Thus the **minimax** design problem can be rephrased as

$$\begin{aligned} &\min_{(\lambda_1, \dots, \lambda_K)} \max_k F_{S_{0,k}}(\lambda_k) \quad \text{s.t.} \quad \Pr\left\{\bigcap_{k=1}^K F_{S_{0,k}}(S_{0,k}) \leq F_{S_{0,k}}(\lambda_k)\right\} \geq 1 - \alpha \\ \Leftrightarrow &\min_{(\zeta_1, \dots, \zeta_K)} \max_k \zeta_k \quad \text{s.t.} \quad \Pr\left\{\bigcap_{k=1}^K F_{S_{0,k}}(S_{0,k}) \leq \zeta_k\right\} \geq 1 - \alpha \quad \text{via } \zeta_k \triangleq F_{S_{0,k}}(\lambda_k) \\ \Leftrightarrow &\min_{\zeta} \zeta \quad \text{s.t.} \quad \Pr\left\{\bigcap_{k=1}^K F_{S_{0,k}}(S_{0,k}) \leq \zeta\right\} \geq 1 - \alpha \quad \text{via } \zeta \triangleq \max_k \zeta_k \end{aligned}$$

Proposed multi-target conformal prediction (cont.)

- If we knew the joint statistics of the bound violation scores $\mathbf{S}_0 \triangleq [S_{0,1}, \dots, S_{0,K}]$, we could solve for

$$\zeta_* = \arg \min_{\zeta} \zeta \quad \text{s.t.} \quad \Pr \left\{ \bigcap_{k=1}^K F_{S_{0,k}}(S_{0,k}) \leq \zeta \right\} \geq 1 - \alpha$$

and then form the k th bound as $\beta_{0,k} = \hat{\beta}_{0,k}(\mathbf{y}_0) - \lambda_k$ with $\lambda_k = F_{S_{0,k}}^{-1}(\zeta_*)$

- But we don't know the statistics of $\mathbf{S}_0$. So we propose to compute an empirical CDF $\hat{F}_{S_k}(\cdot)$ using a **tuning set** $d_{\text{tune},k} = \{s_{i,k}\}_{i=n_{\text{cal}}+1}^{n_{\text{cal}}+n_{\text{tune}}}$ of size n_{tune}

- Next we compute **transformed calibration scores** $u_{i,k} \triangleq \hat{F}_{S_k}(s_{i,k})$ from $d_{\text{cal},k} = \{s_{i,k}\}_{i=1}^{n_{\text{cal}}}$, and then

$$\hat{\zeta}(d_{\text{cal}}) = \text{EmpQuant} \left(\left\lceil \frac{(1-\alpha)(n_{\text{cal}}+1)}{n_{\text{cal}}} \right\rceil; \{u_i\}_{i=1}^{n_{\text{cal}}} \right) \quad \text{with} \quad u_i \triangleq \max_k u_{i,k},$$

and finally set the k th bound as $\beta_{0,k} = \hat{\beta}_{0,k}(\mathbf{y}_0) - \hat{\lambda}_k$ with $\hat{\lambda}_k = \hat{F}_{S_k}^{-1}(\hat{\zeta}(d_{\text{cal}}))$

Proposed multi-target conformal prediction (cont.)

We prove¹ the following about our proposed scheme:

- For any chosen error-rate $\alpha \in (0, 1)$, it **guarantees joint marginal coverage**, i.e.,

$$\Pr \left\{ \bigcap_{k=1}^K Z_{0,k} \geq \beta_{0,k}(\mathbf{Y}_0, D_{\text{cal}}) \right\} \geq 1 - \alpha,$$

as long as $\{\mathbf{S}_0, \mathbf{S}_1, \dots, \mathbf{S}_{n_{\text{cal}}}\}$ are statistically exchangeable

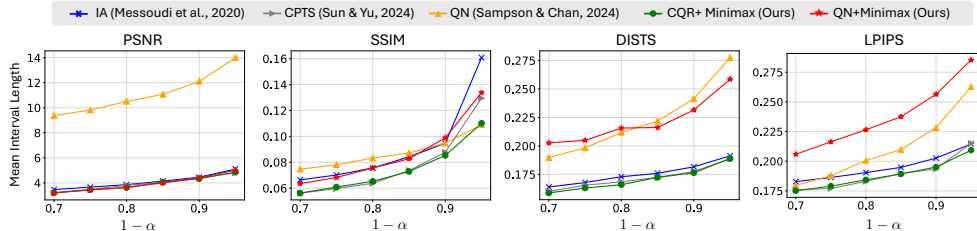
- It is **asymptotically minimax** in that

$$\hat{\zeta}(d_{\text{cal}}) \xrightarrow{a.s.} \zeta_* \quad \text{as } n_{\text{cal}}, n_{\text{tune}} \rightarrow \infty$$

¹Wen, Ahmad, Schniter'25b

Bounding multiple accuracy metrics in accelerated MRI

- Say we want to guarantee the performance of accelerated MRI simultaneously in PSNR, SSIM, LPIPS, and DISTS metrics (i.e., $K = 4$ targets)
- Among existing methods that guarantee joint marginal coverage, **ours** (green) provides tighter bounds across k :



Conclusion

- Due to the ill-posedness of many inverse problems, there's a need to **bound estimator accuracy**
- By combining **approximate posterior sampling** with **conformal prediction**, we proposed accuracy lower-bounds $\beta(\cdot)$ with probabilistic guarantees of the form

$$\Pr \{m(\hat{\mathbf{x}}, \mathbf{x}_0) \leq \beta(\mathbf{y}, d_{\text{cal}}, \alpha)\} \geq 1 - \alpha$$

that allow arbitrary estimators $\mathbf{r}(\cdot)$, accuracy metrics $m(\cdot)$, and error-rates $\alpha \in (0, 1)$, assuming exchangeable test & calibration scores

- Although our prior work focused on MRI imaging, the techniques are directly applicable to communications problems like **wireless device localization**, **CSI estimation**, and **RF tomography**

