On Uniform Error Bounds for Kernel Regression under Non-Gaussian Noise

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Learning and Uncertainty Quantification via Kernel Regression

Data-generating process

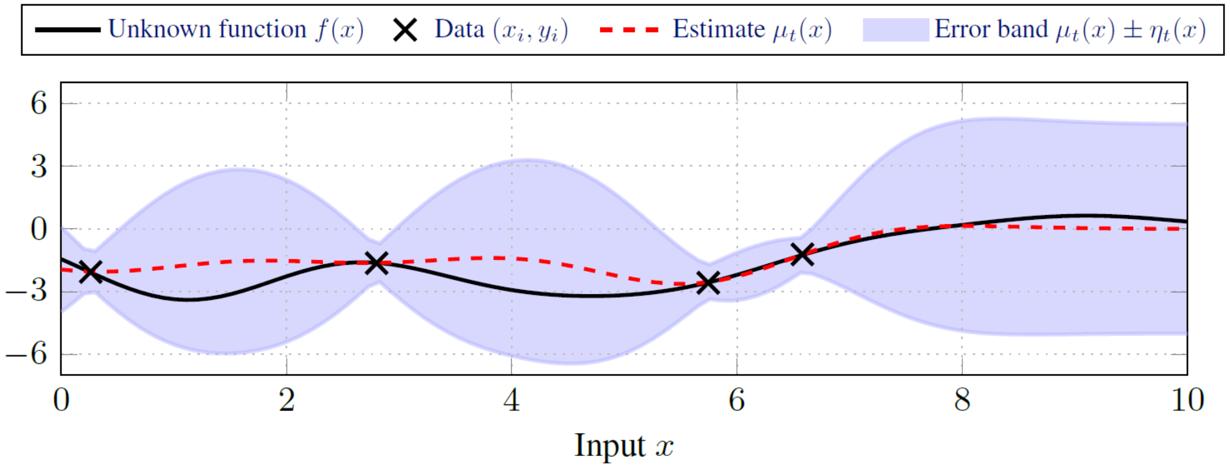
$$y_i = f(x_i) + m_i$$

Kernel regression[1]

- Unknown function $f \in \mathcal{H}_k$
  - RKHS $\mathcal{H}_k$
  - Kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_{\geq 0}$
  - Norm bound $\|f\|_{\mathcal{H}_k} \leq B$
- Noise realization m_i
- Input/Output data (x_i, y_i)

Function estimate + Probabilistic uniform error bound

$$\mathbb{P}\left[\forall x \in \mathcal{X}, t \in \mathbb{N}: \quad |f(x) - \mu_t(x)| \leq \eta_t(x)\right] \geq 1 - \delta$$



Relevance: Safe Bayesian optimization[2], reinforcement learning[3], robot control[4], …

Availability and tightness of uniform error bounds is **essential** for **safety and performance**!

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Challenges and Key Idea

RKHS norm bound

Gaussian Process[8] posterior variance

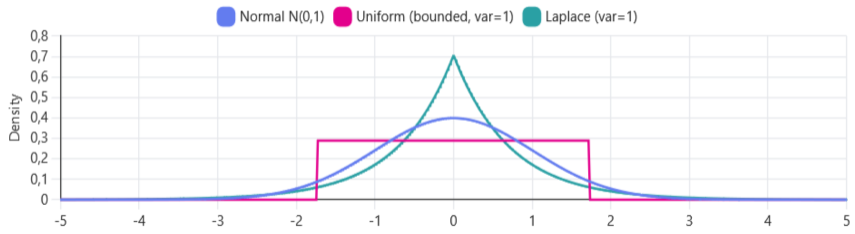
$$\eta_t(x) = (B + \beta(\delta))\, \sigma_t(x)$$

Scaling due to noise

Issues with existing uniform error bounds:[5,6,7]

(1) Overly conservative

(2) Limited to sub-Gaussian noise



$$\sigma_t^2(x) = k(x,x) - \mathbf{k}_t(x)^\top \mathbf{h}_t(x)$$

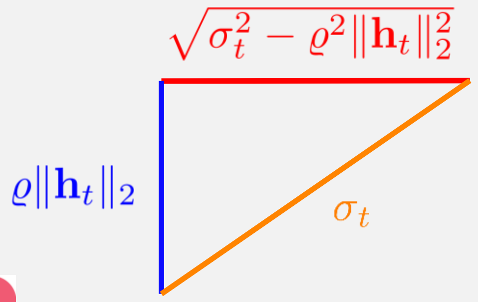
$$\mathbf{h}_t(x) = \left(\mathbf{K}_t + \varrho^2 \mathbf{I}_t\right)^{-1} \mathbf{k}_t(x)$$

Key Idea of Proposed Work

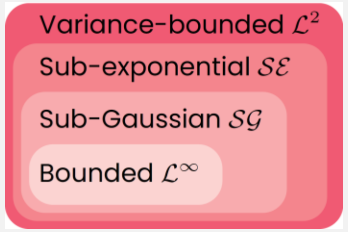
(1) Separation of uncertainty:

$$\text{Uncertainty} = \text{Lack of RKHS exploration} + \text{Noise in data}$$

$$\sigma_t^2 = \left(\sqrt{\sigma_t^2 - \varrho^2 \|\mathbf{h}_t\|_2^2}\right)^2 + \varrho^2 \|\mathbf{h}_t\|_2^2$$



(2) Generalization to various noise distribution classes:



[5] Srinivas, N., Krause, A., Kakade, S. M., and Seeger, M. Gaussian process optimization in the bandit setting: No regret and experimental design. In Proceedings of the 27th ICML, pp. 1015–1022.
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[7] Chowdhury, S. R. and Gopalan, A. On kernelized multi-armed bandits. In Proceedings of the 34th ICML, volume 70, pp. 844–853. PMLR, 2017.
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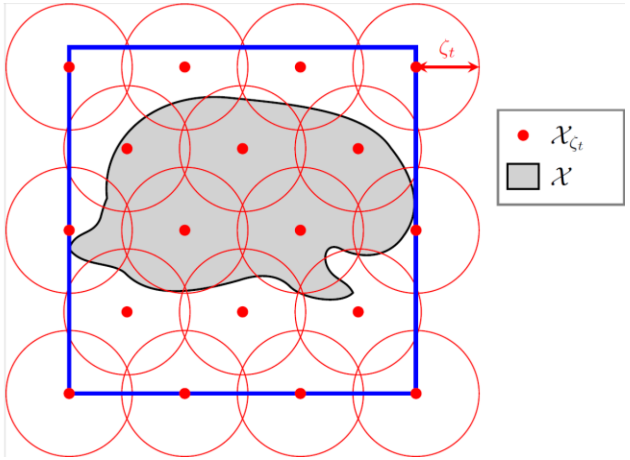
Method Overview

Proposed Uniform Error Bounds:

$$\mathbb{P}\left[\forall x \in \mathcal{X}, t \in \mathbb{N} : \quad |f(x) - \mu_t(x)| \leq \eta_t(x) = B\tilde{\sigma}_t(x) + \eta_t^M(x)\right] \geq 1 - \delta$$



Components:

- Bound on lack of exploration of the RKHS
- Bound on noise term
  - Utilize concentration inequalities
    $\rightarrow$ for sub-Gaussian noise: $\eta_t^M(x) = \beta_t^{\mathcal{SG}}(\delta, \zeta_t)\ \|\mathbf{h}_t(x)\|_2 + \Delta_t^{\mathcal{SG}}(\delta, \zeta_t)$
  - Uniform $\forall t \in \mathbb{N}$ due to Boole: $\delta \leftarrow \delta / \pi_t$, with $\sum_{t=1}^{\infty} \pi_t^{-1} = 1$
  - Uniform $\forall x \in \mathcal{X}$ due to …
    … discretization of input domain $\mathcal{X}$ with grid parameter ζ_t
    … Hölder continuity of kernel $k(x, x')$

$$\#\text{Grid points} \leq \left(1 + \frac{\sqrt{n_x}\max_{x,x' \in \mathcal{X}} \|x - x'\|_\infty}{2\zeta_t}\right)^{n_x}$$

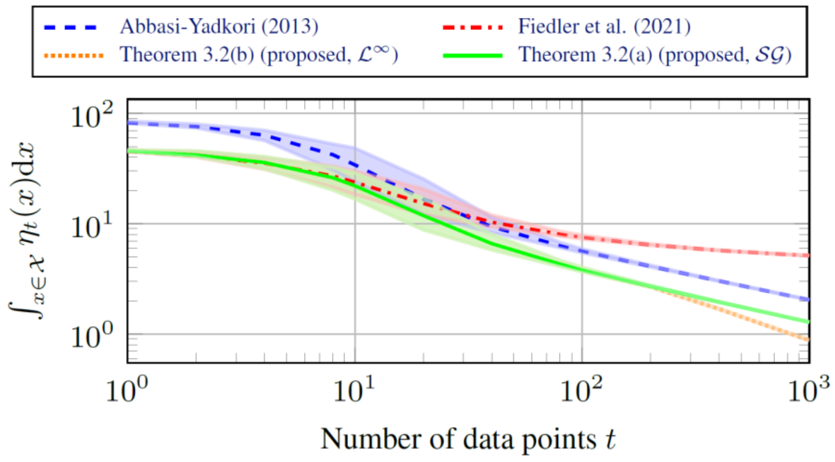
The proposed bound can be tailored to the available noise properties!

Numerical Evaluation

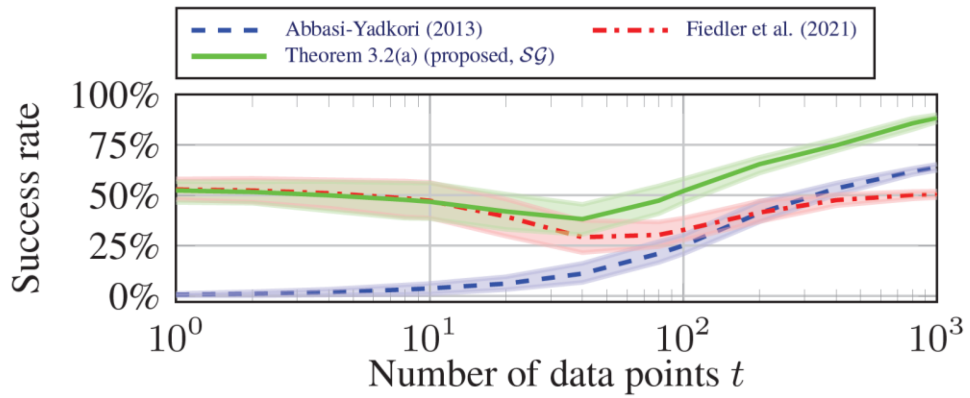
Evaluation of the proposed error bounds:

- Comparison with related bound from the literature[6,9,10]
- Evaluation of learning error $\int_{x\in\mathcal{X}} \eta_t(x)\mathrm{d}x$ and application in safe control
- Analysis of different noise classes and hyperparameters

$\rightarrow$ **Learning error:**



$\rightarrow$ **Safe control:**



The proposed bound are less conservative over a wide range of scenarios $\Longrightarrow$ **higher success rate!**

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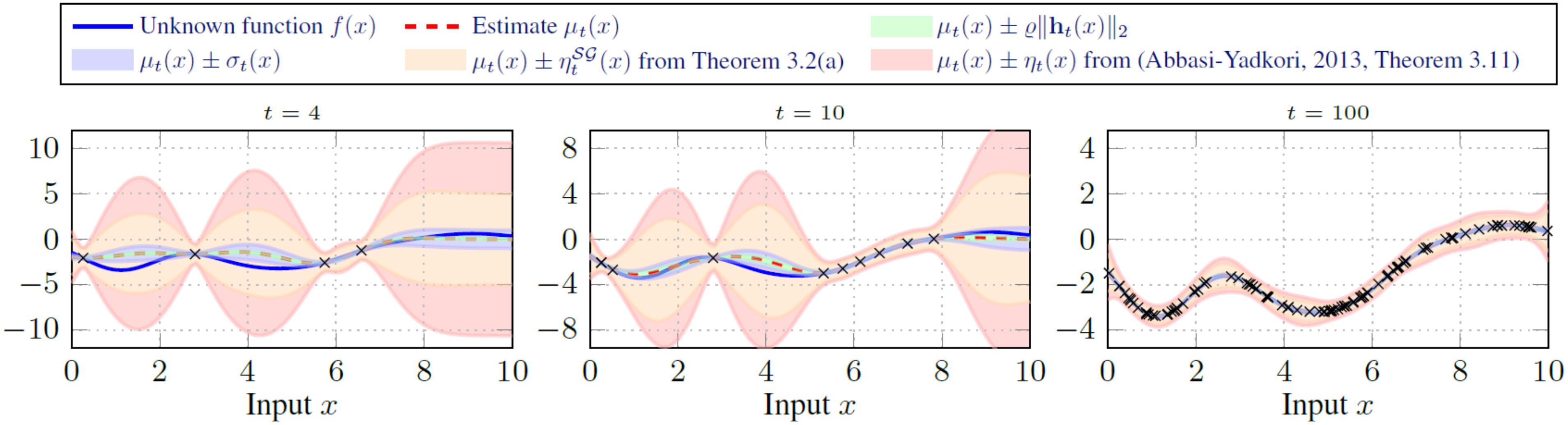
Conclusion

Probabilistic uniform error bounds under non-Gaussian noise:

- Tailored to the available/known noise properties
  $\Longrightarrow$ widening field of applications

- Competitive against existing bounds from related works
  $\Longrightarrow$ less conservative, thus improved performance



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