Random Features, Density Estimate and Simultaneous Localization and Mapping

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Kernel Trick

- Data set

$$(\mathbf{X}, \mathbf{y}) = \{(x_1, y_1), \dots, (x_n, y_n)\} \in \mathcal{X} \times \mathbb{R}, \quad y_i = f(x_i) + \varepsilon_i, \quad \varepsilon \sim \mathcal{N}(0, \sigma^2)$$

- Let $\phi(x) : \mathcal{X} \to \mathbb{R}^d$ be some feature map
- Suppose that $y = \beta^\top \phi(x)$, then prediction is given by

$$\hat{f}(x^*) = \phi(x^*)^\top \left(\phi(\mathbf{X})^\top \phi(\mathbf{X}) + \lambda \mathbf{I}\right)^{-1} \phi(\mathbf{X})^\top \mathbf{y}, \qquad \mathcal{O}(d^3)$$

- Let $k(x, x') = \langle \phi(x), \phi(x') \rangle$ be a *kernel function*. Then prediction can be rewritten as

$$\hat{f}(x^*) = \mathbf{k}_*^\top \left(\mathbf{K} + \lambda \mathbf{I}\right)^{-1} \mathbf{y}, \qquad \mathcal{O}(n^3)$$

where $\mathbf{k}_* = (k(x^*, x_1), \dots, k(x^*, x_n))$, $\mathbf{K}_{ij} = k(x_i, x_j)$.

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Random Fourier Features (RFF)

Theorem (Bochner)

A continuous kernel $k(x, x') = k(x - x')$ on $\mathbb{R}^d$ is positive definite if and only if $k(\delta)$ is a Fourier transform of a non-negative measure

$$k(x, x') = \int_{\Omega} p(w) e^{j w^{\top}(x - x')} dw$$

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RFF idea

Idea: use Monte-Carlo to approximate the integral[1]

$$k_{RFF}(x, x') = \frac{1}{D}\sum_{i=1}^{D} \cos(w_i^\top (x - x')) = \psi_{\mathbf{W}}(x)^T \psi_{\mathbf{W}}(x'),$$

where

- $w_i \sim p(w)$
- $\mathbf{W} = (w_1^\top, \dots, w_D^\top)^\top$
- $\psi_{\mathbf{w}}(x) = 1/\sqrt{D}(\cos(w_1^\top x), \sin(w_1^\top x), \dots, \cos(w_D^\top x), \sin(w_D^\top x))^\top$

$$\widehat{\mathbf{K}} = \Psi\Psi^T, \quad \Psi = \|\psi_{\mathbf{w}}(x_i)^\top\|_{i=1}^n$$

$\rightarrow$ Go back to linear model with $\psi_{\mathbf{W}}(x)$ features

[1] Rahimi, A., Recht, B. (2008). Random features for large-scale kernel machines.

Related works

- Quasi Monte-Carlo (QMC)[2]
- Gaussian Quadrature [3]
- Orthogonal Random Features (ORF)[4]
- Random Orthogonal Matrices (ROM)[5]
- Ridge Leverage Score based Features [6]

[2] Yang, et al. (2016). Quasi-Monte Carlo feature maps for shift-invariant kernels.
[3] Dao et al. (2017). Gaussian quadrature for kernel features.
[4] Felix, X. Yu, et al. (2016). Orthogonal random features.
[5] Choromanski, et al. (2016). Recycling randomness with structure for sublinear time kernel expansions.
[6] Avron, et al. (2017). Random Fourier features for kernel ridge regression: A pproximation bounds and statistical guarantees.

Integral representation of kernel function

$$k(x, x') = \int_{\Omega} \psi(w, x)\psi(w, x')p(w)dw = \int_{\Omega} f_{xx'}(w)p(w)dw,$$

where $p(w)$ is $\mathcal{N}(0, \sigma_p^2 \mathbf{I})$ – density associated with the kernel and $\psi(\cdot, x)$ is a feature map.

Quadrature rules

1. Change variables to spherical-radial coordinates $(w = r\mathbf{z}, \mathbf{z}^\top \mathbf{z} = 1, w^\top w = r)$

$$k(x, x') = \frac{(2\pi)^{-\frac{d}{2}}}{2} \int\limits_{U_d} \int\limits_{-\infty}^{\infty} e^{-\frac{r^2}{2}} |r|^{d-1} f_{xx'}(r\mathbf{z}) dr d\mathbf{z},$$

   where U_d is a d-dimensional unit sphere.
2. Use stochastic radial-spherical rules.

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Stochastic spherical-radial rules

- **Spherical-radial rules**[6] of degree (n, p)

$$SR_{\mathbf{Q},\rho}^{(n,p)}(f) = \sum_{j=1}^{p} \widetilde{w}_j \sum_{i=1}^{n} \frac{w_i}{2} \left(f(-\rho_i \mathbf{Q}\mathbf{z}_j) + f(\rho_i \mathbf{Q}\mathbf{z}_j) \right)$$

- Let $p = 2n + 1$. Then the weights are chosen such that the rule is exact for polynomials of degree $2n + 1$.

[6] Genz, A., & Monahan, J. (1998). Stochastic integration rules for infinite regions.

Examples

- Degree 1 rule

$$SR^{(1,1)}_{\mathbf{Q},\rho}(f) = \frac{f_{xx'}(\rho\mathbf{Q}\mathbf{z}) + f_{xx'}(-\rho\mathbf{Q}\mathbf{z})}{2},$$

where
  - $\rho \sim \chi(d)$, $\mathbf{Q}$ – random orthogonal matrix,
  - $\mathbf{z}$ – point on unit sphere.

$\rightarrow$ Classical Random Fourier Features

- Degree $(1,3)$ rule

$$SR_{\mathbf{Q},\rho}(f)^{(1,3)} = \sum_{i=1}^{d} \frac{f_{xx'}(-\rho\mathbf{Q}\mathbf{e}_i) + fxx'(\rho\mathbf{Q}\mathbf{e}_i)}{2d},$$

where $\mathbf{e}_i = (0,\ldots,0,1,0,\ldots,0)^\top$ with 1 in the i-th position.

$\rightarrow$ Orthogonal Random Features!

Degree $(3,3)$ rule

Degree $(3,3)$ rule

$$k_{QBF}(x,x') = \left(1 - \frac{1}{d+1}\sum_{j=1}^{d+1}\frac{d}{\rho_j^2}\right) f_{xx'}(\mathbf{0}) + \\ + \frac{d}{d+1}\sum_{j=1}^{d+1}\left[\frac{f_{xx'}(-\rho_j \mathbf{Q}\mathbf{v}_j) + f_{xx'}(\rho_j \mathbf{Q}\mathbf{v}_j)}{2\rho_j^2}\right],$$

where

- $\rho_j \sim \chi(d+2)$
- $\mathbf{v}_j$ is the j'th vertex of unit d-simplex $\mathbf{V}$
- $\mathbf{Q}$ is a random $d \times d$ orthogonal matrix.

Use structured $\mathbf{Q}$ matrix to speed up feature generation

Empirical results

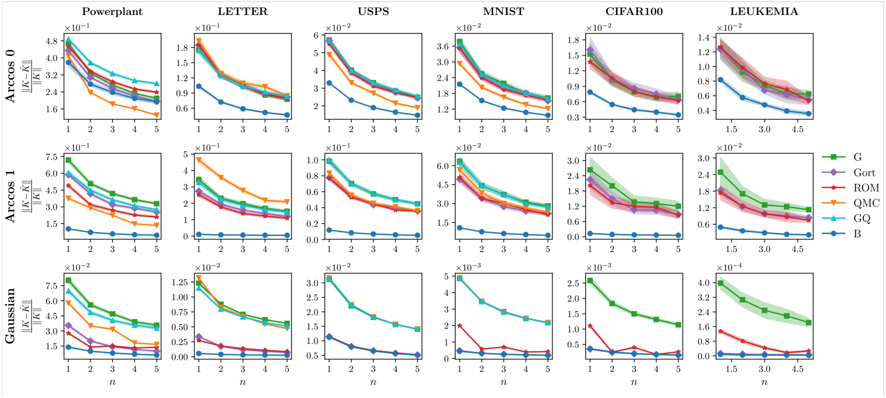

Figure: Error of kernel approximation on different datasets

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Empirical results

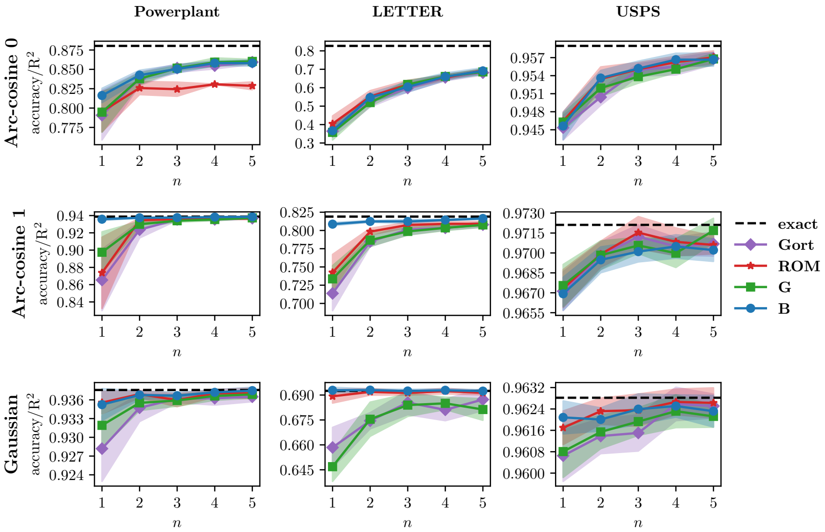

Figure: Error of regression/classification on different datasets

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Score Matching

- Given a data set $\{\mathbf{x}_i\}_{i=1}^n,\ \mathbf{x}_i \sim p_0(\mathbf{x})$, estimate unknown density $p_0(\mathbf{x})$.
- Find $p_\theta(\mathbf{x}) \in \mathcal{P}$ that minimizes Fisher divergence

$$J(p_0 \| p_\theta) = \frac{1}{2} \int p_0(\mathbf{x}) \|\nabla \log p_\theta(\mathbf{x}) - \nabla \log p_0(\mathbf{x})\|_2^2 d\mathbf{x}$$

- Equivalent **score matching** objective

$$J_{SM}(p_0 \| p_\theta) = \mathbb{E}_{p_0} \left[\Delta \log p_\theta(\mathbf{x}) + \frac{1}{2} \|\nabla \log p_\theta(\mathbf{x})\|_2^2 \right]$$

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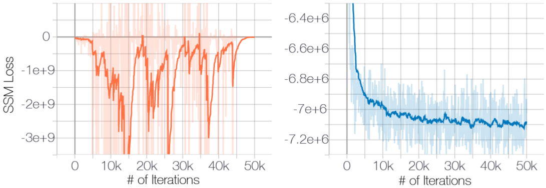
Issues

- Need to compute second derivatives
- $\text{supp } p_0 \neq \text{supp } p_\theta$



Song, Y., Ermon, S. (2019). Generative modeling by estimating gradients of the data distribution.

Figure: **Left**: original and PCA reconstructions of images. **Middle**: score matching loss. **Right**: score matching loss with noisy data

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Kernel Exponential Family and Score Matching

- Consider distributions that satisfy

$$\log p_\theta(\mathbf{x}) = f(\mathbf{x}) + \log q_0(\mathbf{x}), \quad f \in \mathcal{H},$$

  where $\mathcal{H}$ is an RKHS with kernel k, q_0 is some generating density.
- Solution

$$f(\mathbf{x}) = -\frac{\xi}{\lambda} + \sum_{a=1}^{n}\sum_{i=1}^{d} \beta_{(\alpha-1)d+i}\partial_i k(\mathbf{x}_a, \cdot),$$

$$\xi = \frac{1}{n}\sum_{a=1}^{n}\sum_{i=1}^{d}\left(\partial_i k(\mathbf{x}_a, \cdot)\partial_i \log q_0(\mathbf{x}_a) + \partial_i^2 k(\mathbf{x}_a, \cdot)\right),$$

$$\left(\mathbf{G} + n\lambda\mathbf{I}\right)\beta = \frac{1}{\lambda}\mathbf{h},$$

$$\mathbf{G}_{(a-1)d+i,(b-1)d+j} = \partial_i\partial_{j+d}k(\mathbf{x}_a, \mathbf{x}_b),$$

$$\mathbf{h} = \langle \xi, \partial_i k(\mathbf{x_a}, \cdot)\rangle_{\mathcal{H}}$$

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Denoising score matching

Adding noise to input data is equivalent to convolution of the loss with noise distribution:

$$
\begin{aligned}
&\mathbb{E}_{p_\varepsilon}\mathbb{E}_{p_0}\left[\Delta \log p_\theta(\mathbf{x}+\boldsymbol{\varepsilon}) + \frac{1}{2}\|\nabla \log p_\theta(\mathbf{x}+\boldsymbol{\varepsilon})\|^2\right] \\
&= \mathbb{E}_{p_0}\left[\left(\left(\Delta \log p_\theta(\cdot) + \frac{1}{2}\|\nabla \log p_\theta(\cdot)\|^2\right) * p_\varepsilon\right)(\mathbf{x})\right]
\end{aligned}
$$

Solution derived only for Random Features

$$
\hat{f}(\mathbf{x}) = \frac{1}{\lambda}\boldsymbol{\phi}(\mathbf{x})^\top (\boldsymbol{H} + n\lambda \mathbf{I})^{-1}\boldsymbol{H}\boldsymbol{h} - \frac{1}{\lambda}\boldsymbol{\phi}(\mathbf{x})^\top \boldsymbol{h},
$$

where

$$
\boldsymbol{H} = \int p_\varepsilon(\mathbf{y})\partial\boldsymbol{\Phi}_y^\top \partial\boldsymbol{\Phi}_y d\mathbf{y}, \quad \boldsymbol{h} = \frac{1}{n}(\partial^2\boldsymbol{\Phi}_z * p(\mathbf{z}))^\top \mathbf{1},
$$

and

$$
[\partial\boldsymbol{\Phi}_y]_{(a-1)d+i} = \partial_i \boldsymbol{\phi}^\top(\boldsymbol{W}(\mathbf{x}_a + \mathbf{y}))
$$

Denoising Score Matching with Random Features

- Regularization:

$$\boldsymbol{h}_i \sim e^{-\sigma_\varepsilon^2 \|\mathbf{w}_i\|_2^2},$$

  i.e. small weights for high-frequency components

- Explicit dependence on noise parameters $\rightarrow$ easier to tune them
- We learn $p_0 * p_\varepsilon \rightarrow$ trade-off between
  - stability of convergence
  - closeness to p_0

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Experimental setup

- Adjust kernel parameters on training set using Denoising Score Matching
- Adjust noise variance on hold-out set using Score Matching
- Compare 3 models: proposed approach (**DSM RFF**), score matching with RFF (**SM RFF**), score matching with Nyström approximation (**Nyström**)
- Datasets
  - synthetic 2D data sets: Cosine, Uniform, Banana, Funnel, Rings
  - UCI: RedWine, WhiteWine, MiniBoone
- Metrics:
  - Log-likelihood
  - Wasserstein distance
  - Fisher divergence (for synthetic datasets)

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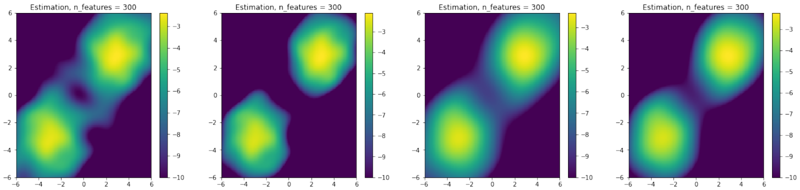
Mixtures



(a) SM RFF, narrow kernel

(b) DSM RFF, narrow kernel

(c) SM RFF, wider kernel

(d) DSM RFF, wider kernel

Figure: Mixture of Gaussians

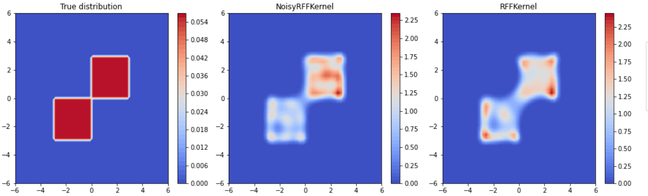


Figure: Mixture of Uniforms

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Experiments

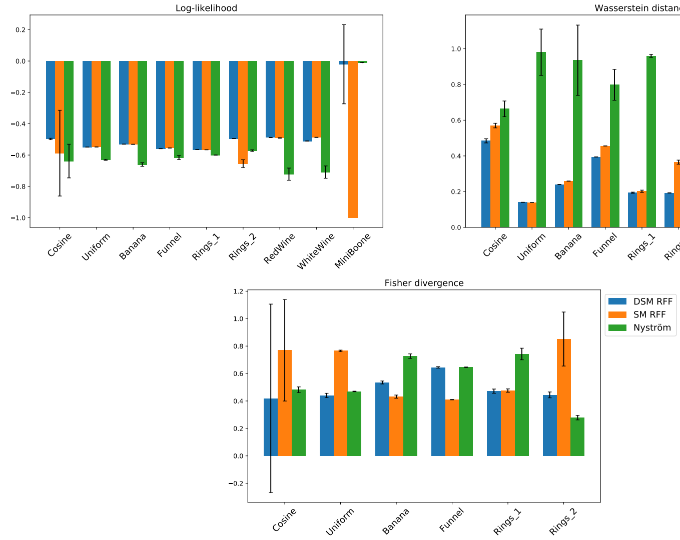


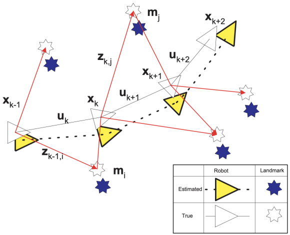
Figure: Comparison on synthetic and UCI data sets

Simultaneous Localization and Mapping (SLAM)

- Consider mobile robot moving in an environment.
- At each time step t_i we obtain measurements $\mathbf{z}_i$ corresponding to some **landmarks** $\boldsymbol{l} = \begin{bmatrix} \boldsymbol{l}_1 \\ \dots \\ \boldsymbol{l}_M \end{bmatrix}$

$$\mathbf{z}_i = \mathbf{h}(\mathbf{x}(t_i), \boldsymbol{l}) + \mathbf{n}_i, \quad \mathbf{n}_i \sim \mathcal{N}(0, \mathbf{R}_i).$$

- Control variables $\mathbf{u}_i$ (maybe missing or given at different timestamps)
- We want to estimate both the robot trajectory $\mathbf{x}(t_1), \dots, \mathbf{x}(t_T)$ and landmarks $\boldsymbol{l}$.
- Time-continuous SLAM: estimate trajectory as a function of time $\mathbf{x}(t)$.



Durrant-Whyte, H., Bailey, T. (2006)

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GP based SLAM

- Assumptions

$$\boldsymbol{x}(t) \sim \mathcal{GP}(\boldsymbol{\mu}_x, \boldsymbol{k}(t, t'))$$
$$\boldsymbol{l} \sim \mathcal{N}(\boldsymbol{\mu}_l, \mathbf{L})$$

- Let us denote $\boldsymbol{\theta} = \begin{bmatrix} \boldsymbol{x}(t) \\ \boldsymbol{l} \end{bmatrix}$. We want to maximize the posterior

$$p(\boldsymbol{\theta}|\boldsymbol{z}) \propto p(\boldsymbol{z}|\boldsymbol{\theta})p(\boldsymbol{\theta}) = -\frac{1}{2}\left(\sum_{i=1}^{T} \|\boldsymbol{z}_i - \boldsymbol{h}(\boldsymbol{\theta}(t_i))\|^2_{\mathbf{R}_i} + \|\boldsymbol{\theta} - \boldsymbol{\mu}\|^2_{\mathbf{P}}\right) = -J$$

RFF SLAM

- Random Features for locations

$$\boldsymbol{x}(t) = \begin{bmatrix} x(t) \\ y(t) \\ \alpha(t) \end{bmatrix} = \boldsymbol{\psi}(t)^\top \boldsymbol{b} + \varepsilon, \quad \begin{matrix} \boldsymbol{b} \in \mathbb{R}^{D\times 3}, i = \overline{1,3} \\ \boldsymbol{b} \sim \mathcal{N}(\boldsymbol{\mu}_b, \mathbf{B}) \end{matrix}$$

  where $\boldsymbol{\psi}(t)$ – random features, $\mathbf{B}$ is block-diagonal covariance matrix.

- Gauss-Newton method

$$(\delta\boldsymbol{b}^*, \delta\boldsymbol{l}) = \underset{\delta\boldsymbol{b}, \delta\boldsymbol{l}}{\operatorname{argmin}} \sum_{i=1}^{T} \|\boldsymbol{z}_i - \boldsymbol{h}(\boldsymbol{\psi}(t_i)\bar{\boldsymbol{b}}, \boldsymbol{l}) - \mathbf{H}_i \Psi_i \delta\boldsymbol{b}\|^2_{\mathbf{R}_i} + \|\bar{\boldsymbol{b}} + \delta\boldsymbol{b} - \boldsymbol{\mu}_b\|^2_{\mathbf{B}} + \|\bar{\boldsymbol{l}} + \delta\boldsymbol{l} - \boldsymbol{\mu}_l\|^2_{\mathbf{L}},$$

  where $\bar{\boldsymbol{b}}$ is current solution.

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Related works

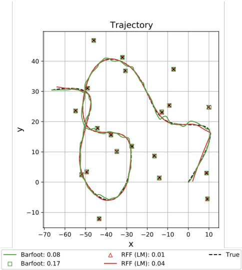
- A lot of works that use splines
- State-space model [7]

$$\dot{\mathbf{x}}(t) = \mathbf{A}(t)\mathbf{x}(t) + \mathbf{v}(t) + \mathbf{F}(t)\mathbf{w}(t),$$

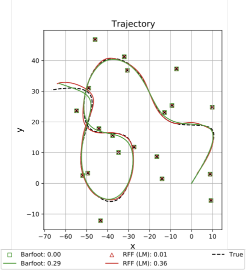
  - $\mathbf{A}(t), \mathbf{F}(t)$ are time-dependent system matrices,
  - $\mathbf{w}(t) \sim \mathcal{GP}(0, \mathbf{Q}_C \delta(t - t'))$
- Solution is GP with block-tridiagonal inverse $\mathbf{K}$ matrix.
- Assumes Markovian-trajectories.
- RBF kernel can better in some cases (like noisy observations)

[7] Barfoot et al. (2014). Batch Continuous-Time Trajectory Estimation as Exactly Sparse Gaussian Process Regression

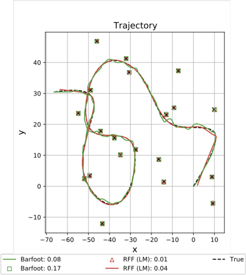
Synthetic trajectories



(a) Bearing only



(b) Range only



(c) Range-Bearing

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Synthetic trajectories

		Pos.	Rot.	Landmarks
RangeBearing	RFF	**0.033**	0.0018	**0.019**
	Barfoot	0.096	0.0013	0.191
Range	RFF	0.309	0.0197	0.004
	Barfoot	**0.208**	0.0114	0.001
Bearing	RFF	**0.036**	0.0016	**0.018**
	Barfoot	0.096	0.0013	0.191

Table: Relative Pose Errors

Relative position errors don't take into account drift:

$$\mathrm{RPE} = \sum_{i=1}^{T} \|\delta\hat{\mathbf{x}}_i \ominus \delta\mathbf{x}_i\|$$

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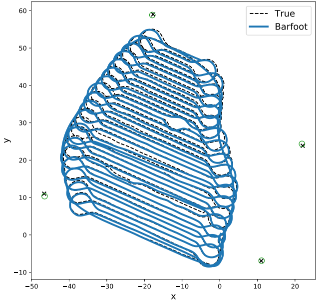
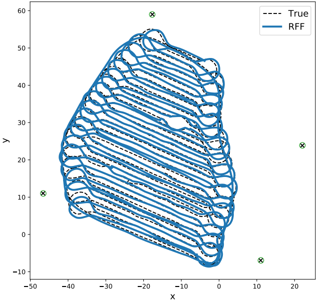
Autonomous Lawn-Mower

Range only data set



(a) State-Space Model



(b) Random Features based

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Summary

Random Features

- proposed Quadrature-based Features
- accurate kernel approximation
- in downstream tasks benefit is smaller

Score Matching

- exact solution for Denoising Score Matching with RFF was proposed
- Natural regularization
- Faster than N yström-type approximation

SLAM

- Random Features give dense covariance $\rightarrow$ better accuracy in case of noisy data
- Random Features can oscillate

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