Tensor Train Kernel Learning for Gaussian Process Regression

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Gaussian Process Regression

Goal: learn approximation f of a function

$$\Phi\colon \Omega \longrightarrow \mathbb{R}, \qquad \Omega = [a,b]^d \subset \mathbb{R}^d,$$

based on N realizations of random variables

- $\mathbf{X} = [x^{(1)}, \ldots, x^{(N)}]$ with $x^{(i)} \in \Omega$, $x^{(i)} \sim \rho$,
- $\mathbf{y} = [y^{(1)}, \ldots, y^{(N)}]$ with $y^{(i)} = \Phi(x^{(i)})$

for $i = 1, \ldots, N$.

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A Gaussian Process (GP) prior

$$f_0(x) \sim \mathcal{GP}(m_0(x), k_0(x, x'))$$

over f is characterised by

- a mean function $m_0 \colon \mathbb{R}^d \to \mathbb{R}$
- a spd covariance function $k_0 \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

Gaussian Process Regression

For a finite number of inputs, the function values of the GP prior have a joint Gaussian distribution

$$f_0(\mathbf{X}) = [f_0(x^{(1)}), \dots, f_0(x^{(N)})] \sim \mathcal{N}(m_0(\mathbf{X}), k_0(\mathbf{X}, \mathbf{X})),$$

with

- mean vector $m_0(\mathbf{X}) = [m_0(x^{(1)}), \dots, m_0(x^{(N)})]$
- and covariance matrix $(k_0(\mathbf{X}, \mathbf{X}))_{ij} = k_0(x^{(i)}, x^{(j)})$ for $i, j = 1, \dots, N$

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To predict at new points $\mathbf{X}_* = (x_*^{(1)}, \ldots, x_*^{(M)})$ we condition the GP on the data, yielding the posterior

$$f_*(\mathbf{X}_*) \sim \mathcal{N}(m_*(\mathbf{X}_*), k_*(\mathbf{X}_*, \mathbf{X}_*))$$

with

$$m_*(\mathbf{X}_*) = m_0(\mathbf{X}_*) - k_0(\mathbf{X}_*, \mathbf{X}) k_0(\mathbf{X}, \mathbf{X})^{-1}(m_0(\mathbf{X}) - \mathbf{y})),$$
$$k_*(\mathbf{X}_*, \mathbf{X}_*) = k_0(\mathbf{X}_*, \mathbf{X}_*) - k_0(\mathbf{X}_*, \mathbf{X}) k_0(\mathbf{X}, \mathbf{X})^{-1} k_0(\mathbf{X}, \mathbf{X}_*).$$

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with

$$\begin{aligned} m_*(\mathbf{X}_*) &= m_0(\mathbf{X}_*) - k_0(\mathbf{X}_*, \mathbf{X}) k_0(\mathbf{X}, \mathbf{X})^{-1} (m_0(\mathbf{X}) - \mathbf{y})), \\ k_*(\mathbf{X}_*, \mathbf{X}_*) &= k_0(\mathbf{X}_*, \mathbf{X}_*) - k_0(\mathbf{X}_*, \mathbf{X}) k_0(\mathbf{X}, \mathbf{X})^{-1} k_0(\mathbf{X}, \mathbf{X}_*). \end{aligned}$$

From now on we assume $m_0 \equiv 0$.

Gaussian Process Regression

The covariance function k_0 usually depends on some set of hyper-parameters $\boldsymbol{\theta}$, i.e.

$$k_0(x, x') = k_0(x, x' | \boldsymbol{\theta}).$$

For the RBF kernel

$$k_{\mathrm{RBF}}(x, x') = \sigma_f^2 \exp\left(-\frac{1}{2\ell}\|x - x'\|^2\right)$$

we have

- the prior standard deviation σ_f, i.e. signal variance
- the lengthscale ℓ, determining correlation decay rate with increasing distance between inputs

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With the noise variance σ_n, the set of hyper-parameters is given by $\boldsymbol{\theta} = \{\sigma_f, \ell, \sigma_n\}$.

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With the noise variance σ_n, the set of hyper-parameters is given by $\boldsymbol{\theta} = \{\sigma_f, \ell, \sigma_n\}$.
GP training: maximise marginal (log-)likelihood of targets over $\boldsymbol{\theta}$:

$$\log\ p(\mathbf{y}|X, \boldsymbol{\theta}) \propto -\mathbf{y}^\intercal K_{\boldsymbol{\theta}}^{-1}\mathbf{y} - \log|K_{\boldsymbol{\theta}}|$$

with $K_{\boldsymbol{\theta}} = k_0(\mathbf{X}, \mathbf{X})$.

Feature Extraction for GPs

Let

$$f_W : \mathbb{R}^d \to \mathcal{Z}$$

denote a feature extractor with parameters W mapping to a latent space $\mathcal{Z}$.

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Now, assume the composite kernel

$$k(x, x'|\boldsymbol{\theta}) \coloneqq \hat{k}(f_W(x), f_W(x')|\theta),$$

where

$$\hat{k}\colon \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$$

is a base kernel with hyper-parameters θ, e.g. RBF or linear kernel, and

$$\boldsymbol{\theta} \coloneqq \{W, \theta\}$$

are the joint hyper-parameters.

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Possible feature extractors:

- Deep neural networks, W are the weights $\hookrightarrow$ DKL [WHSX16]
- Tensorized function spaces, W is the coefficient tensor $\hookrightarrow$ TTKL

Tensor Kernel Learning

Consider the case $\mathcal{Z} = \mathbb{R}$.
Start with a set of basis functions

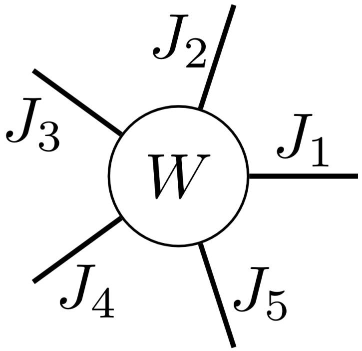
$$P_{\alpha_i} : \mathbb{R} \to \mathbb{R}, \qquad \alpha_i = 1, \dots, J_i, \qquad J_i \in \mathbb{N}, \qquad i = 1, \dots, d$$

and set for all $x = (x_1, \dots, x_d) \in \Omega$

$$f_W(x) = \sum_{\alpha_1=1}^{J_1} \cdots \sum_{\alpha_d=1}^{J_d} W_{\alpha_1,\dots,\alpha_d} \prod_{i=1}^{d} P_{\alpha_i}(x_i) \tag{1}$$

with coefficient tensor

$$W \in \mathbb{R}^{J_1 \times \dots \times J_d}.$$



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Remarks:

- Potentially high expressive power (think of P_{α_i} as polynomials up to degree $d-1$)
- For $J_i \equiv J$, W has storage complexity of $J^d \hookrightarrow$ *curse of dimensionality*

Alleviating the curse of dimensionality: Tensor Trains

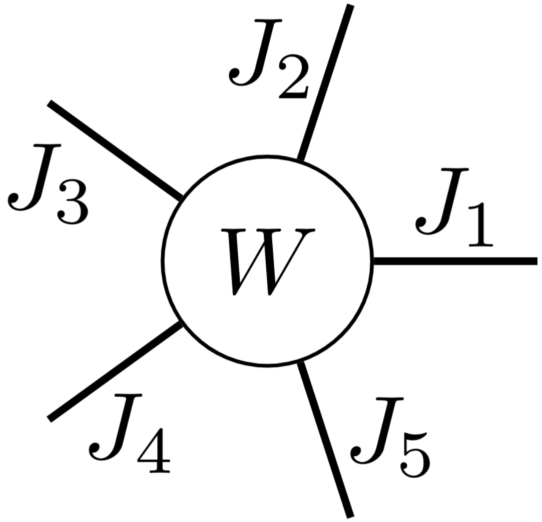

Figure: A full tensor W of order 5

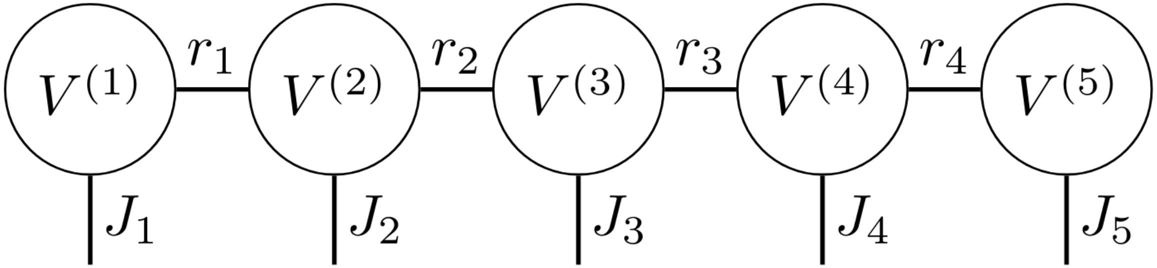

Figure: A Tensor Train (TT) decomposition of W with TT ranks (r_1, r_2, r_3, r_4)

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Recall

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A low-rank TT compression of the coefficient tensor W reads

$$W_{\alpha_1,\ldots,\alpha_d} \approx \sum_{k_0=1}^{r_0} \cdots \sum_{k_d=1}^{r_d} \prod_{i=1}^{d} V^{(i)}_{k_{i-1},\alpha_i,k_i} \tag{3}$$

with

- $V^{(i)} \in \mathbb{R}^{r_{i-1}\times J_i \times r_i}$, $i = 1,\ldots,d$,
- $r_0 = r_d = 1$
- TT ranks $r_1,\ldots,r_{d-1}$ determining accuracy of the compression.

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For every W, there exist TT-ranks such that equality holds in (3) [Ose11].

In our work: Optimise W only on a manifold of fixed TT rank.

Alleviating the curse of dimensionality: Tensor Trains

With $J_i \equiv J$, the coefficient tensor W of a fully tensorized function

$$f_W(x) = \sum_{\alpha_1,\ldots,\alpha_d} W_{\alpha_1,\ldots,\alpha_d} \prod_i P_{\alpha_i}(x_i) \tag{4}$$

has storage complexity $\mathcal{O}(J^d)$.

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On the other hand, the *coefficient Tensor Train* V of

$$f_V(x) = \sum_{\alpha_1,\dots,\alpha_d} \sum_{k_0,\dots,k_d} \prod_i V^{(i)}_{k_{i-1},\alpha_i,k_i} P_{\alpha_i}(x_i) \tag{5}$$

has storage complexity $\mathcal{O}(Jdr^2)$, where $r = \max_{i=1,\dots,d-1}\{r_i\}$.

The set of Tensor Trains with fixed TT-rank $\mathbf{r} = (r_1 \dots, r_d)$ is usually denoted $\mathcal{M}_{\mathbf{r}}$.

Pre-training with the Alternating Linear Scheme

The loss functional of the risk minimisation

$$L(f) := \int_{\Omega} (\Phi(x) - f(x))^2 \ \rho(\mathrm{d}x) \tag{6}$$

is approximated by the empirical risk minimisation for a set of iid realisations

$$x^{(n)} \sim \rho, \qquad y_n = \Phi(x^{(n)}),$$

for $n = 1, \dots, N$, i.e.

$$L(f) \approx \frac{1}{N} \sum_{n=1}^{N} \left(y^{(n)} - f(x^{(n)}) \right)^2 . \tag{7}$$

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To reduce over-fitting, we introduce regularisation, minimising

$$\hat{L}(f) = \sum_{n=1}^{N} \left(y^{(n)} - f(x^{(n)}) \right)^2 + \delta \|f\|_{\mathcal{F}}^2, \tag{8}$$

for $\delta > 0$ and $\mathcal{F} \coloneqq H^1_{\text{mix}}(\Omega) = \bigotimes_{i=1}^{d} H^1([a, b])$.

Pretraining with the Alternating Linear Scheme

The minimisation problem reads

$$\min_{f_V} \hat{L}(f_V) = \sum_{n=1}^{N} \left(y^{(n)} - f_V(x^{(n)}) \right)^2 + \delta \| f_V \|_{\mathcal{F}}^2. \tag{9}$$

for f_V parametrised by a Tensor Train $V \in \mathcal{M}_{\mathbf{r}}$.

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for f_V parametrised by a Tensor Train $V \in \mathcal{M}_{\mathbf{r}}$.

Choosing the basis functions P_{α_i} as $H^1([a,b])$-orthonormal polynomials, the tensor structure and Parseval's identity yield

$$\| f_V \|_{\mathcal{F}}^2 = \| V \|_F^2,$$

where $\|.\|_F$ denotes the Frobenius-norm in full tensor space.

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$$\| f_V \|_{\mathcal{F}}^2 = \| V \|_F^2,$$

where $\|.\|_F$ denotes the Frobenius-norm in full tensor space.

Hence, we arrive at the finite dimensional minimisation problem

$$\min_{V \in \mathcal{M}_{\mathbf{r}}} \hat{L}(f_V) = \min_{V \in \mathcal{M}_{\mathbf{r}}} \frac{1}{N} \sum_{n=1}^{N} \left(y^{(n)} - f_V(x^{(n)}) \right)^2 + \delta \| V \|_F^2, \tag{10}$$

Pretraining with the Alternating Linear scheme (ALS)

Idea of ALS [HRS11]: Sweep back and forth over the tensor network, sequentially performing

$$\min_{V^{(j)}} \frac{1}{N} \sum_{n=1}^{N} \Big(\Phi(x^{(n)}) - f_V(x^{(n)}) \Big)^2 + \delta \|V^{(j)}\|_F^2, \tag{11}$$

where $V^{(i)}$ is fixed for all $i \neq j$.

ALS optimization monotincally decreases continuously differentiable cost functionals.

Intermediate Recap: Tensor Train Kernel Learning

We train a GP with composite kernel

$$k(x, x'|\boldsymbol{\theta}) := \hat{k}(f_V(x), f_V(x')|\theta),$$

where

$$\hat{k} \colon \mathcal{Z} \times \mathcal{Z} \to \mathbb{R}$$

is a base kernel with hyper-parameters θ, e.g. RBF, and

$$f_V \colon \mathbb{R}^d \longrightarrow \mathcal{Z}$$

is a TT function with H^1-orthonormal basis functions and coefficient tensor V.

The totality of hyperparameters is absorbed into $\boldsymbol{\theta}$.

Numerical Experiments - Overview

Following models[1] compared on three synthetic and six real-world (UCI) data sets:

- TTKL
- TT model
- Sparse GP
- Fully-connected deep neural network (DNN)
- DKL with DNN as feature extractor
- Canonical-Polyadic model from [KLM21] (CPKL)

We use random search [BB12] together with advanced early-stopping [LJR+20] for hyper-parameter optimisation. Additionally, we repeat model evaluation six times with randomly selected seeds and report the resulting mean and standard deviation.

[1] All models were implemented with the PyTorch [PGM+19] and GPyTorch [GPB+18] frameworks. Distributed model selection and evaluation were facilitated by means of Ray [MNW+18] and Tune [LLN+18].

Numerical Experiments - TTKL Set-up

- H^1-orthonormal polynomials P_{α_i} for fixed degree $\alpha_i = 1, \dots, J$
- TT rank uniformly constrained to r
- Base kernel $\hat{k} = k_{RBF}$
- ALS solved using LU factorisation
- Sparse variational inference (VI) [LDJD21] with mean-field Gaussian
- Individual learning rates for TT components, RBF kernel and VI hyper-parameters
- ADAM [KB15] with default hyper-parameters, except for the initial learning rates

Numerical Experiments - Results

Table 1: Log-likelihood (higher is better) and one standard deviation for all probabilistic models on three synthetic and six real-world data sets.

Data set	N	d	Test LL			
			TTKL (ours)	CPKL	DKL	GP
HighDimSin (Synthetic)	100 000	30	$\mathbf{2.46 \pm 9.51 \times 10^{-1}}$	$-1.94 \pm 6.90 \times 10^{-4}$	$2.43 \times 10^{-2} \pm 7.84 \times 10^{-2}$	$-3.43 \pm 7.15 \times 10^{-2}$
Friedman (Synthetic)	100 000	5	$\mathbf{3.06 \pm 3.05 \times 10^{-2}}$	$2.50 \pm 1.28 \times 10^{-1}$	$1.33 \times 10^{-1} \pm 6.66 \times 10^{-2}$	$1.53 \pm 9.32 \times 10^{-2}$
Grid (Synthetic)	65 536	2	$\mathbf{2.54 \pm 8.21 \times 10^{-2}}$	$1.88 \pm 5.52 \times 10^{-1}$	$1.34 \pm 9.02 \times 10^{-2}$	$\pm$
Kegg (Real)	48 827	22	$\mathbf{6.40 \times 10^{-1} \pm 5.11 \times 10^{-1}}$	$-1.74 \pm 2.72 \times 10^{-5}$	$3.56 \times 10^{-1} \pm 1.11 \times 10^{-1}$	$3.41 \times 10^{-1} \pm 1.38 \times 10^{-2}$
Skillcraft (Real)	3338	19	$-1.53 \pm 4.39 \times 10^{-1}$	$-7.20 \times 10^{-1} \pm 2.58 \times 10^{-1}$	$\mathbf{-2.95 \times 10^{-1} \pm 3.14 \times 10^{-2}}$	$-3.05 \times 10^{-1} \pm 7.30 \times 10^{-3}$
Elevators (Real)	16 599	18	$\mathbf{8.17 \times 10^{-1} \pm 3.51 \times 10^{-2}}$	$-8.04 \times 10^{-2} \pm 8.30 \times 10^{-2}$	$7.16 \times 10^{-2} \pm 1.18 \times 10^{-2}$	$7.61 \times 10^{-2} \pm 1.80 \times 10^{-3}$
Housing (Real)	506	13	$\mathbf{-9.46 \times 10^{-1} \pm 2.78 \times 10^{-1}}$	$-3.98 \pm 8.89 \times 10^{-2}$	$-3.54 \pm 1.77 \times 10^{-1}$	$-5.50 \pm 3.04 \times 10^{-1}$
Protein (Real)	45 730	9	$\mathbf{1.11 \times 10^{-1} \pm 4.17 \times 10^{-2}}$	$-1.17 \pm 7.00 \times 10^{-5}$	$-7.49 \times 10^{-1} \pm 1.94 \times 10^{-1}$	$-1.18 \pm 1.94 \times 10^{-2}$
Kin40K (Real)	40 000	8	$\mathbf{2.15 \pm 1.34 \times 10^{-1}}$	$3.11 \times 10^{-1} \pm 9.27 \times 10^{-1}$	$7.92 \times 10^{-1} \pm 2.89 \times 10^{-2}$	$-2.78 \times 10^{-2} \pm 1.72 \times 10^{-3}$

Numerical Experiments - Results

Table 3: Mean squared error, one standard deviation and number of trainable parameters for all models on three synthetic and six real-world data sets.

Data set	N	d	TTKL (ours)	CPKL	DKL	DNN	TT	GP
			Test MSE / Num Params					
HighDimSin (Synthetic)	100 000	30	2.54×10^{-4} $\pm 3.75 \times 10^{-4}$ 26 609	2.83 $\pm 2.77 \times 10^{-4}$ 40 767	2.77×10^{-2} $\pm 5.97 \times 10^{-3}$ 58 007 943	3.34×10^{-2} $\pm 3.47 \times 10^{-3}$ 42 575 956	$\mathbf{2.69 \times 10^{-14}}$ $\mathbf{\pm 1.87 \times 10^{-15}}$ 252 600	2.11×10^{-2} $\pm 2.94 \times 10^{-4}$ 18 512
Friedman (Synthetic)	100 000	5	9.00×10^{-6} $\pm 9.42 \times 10^{-7}$ 4308	1.20×10^{-4} $\pm 3.12 \times 10^{-5}$ 3746	1.14×10^{-2} $\pm 2.74 \times 10^{-3}$ 50 820 695	1.23×10^{-2} $\pm 1.88 \times 10^{-3}$ 2 052 701	$\mathbf{2.34 \times 10^{-16}}$ $\mathbf{\pm 1.25 \times 10^{-16}}$ 1020	1.73×10^{-3} $\pm 2.85 \times 10^{-4}$ 2572
Grid (Synthetic)	65 536	2	4.99×10^{-6} $\pm 8.29 \times 10^{-7}$ 2182	1.12×10^{-3} $\pm 1.48 \times 10^{-3}$ 1394	1.06×10^{-3} $\pm 3.36 \times 10^{-4}$ 2 695 770	1.29×10^{-3} $\pm 1.97 \times 10^{-4}$ 2 614 358	$\mathbf{9.02 \times 10^{-8}}$ $\mathbf{\pm 7.66 \times 10^{-12}}$ 52	2.65×10^{-6} $\pm 4.61 \times 10^{-7}$ 1030
Kegg (Real)	48 827	22	$\mathbf{1.93 \times 10^{-3}}$ $\mathbf{\pm 3.85 \times 10^{-4}}$ 1469	1.89 $\pm 2.66 \times 10^{-5}$ 25 258	2.22×10^{-2} $\pm 1.60 \times 10^{-3}$ 2 999 434	1.76×10^{-2} $\pm 8.90 \times 10^{-4}$ 57 336 262	3.23×10^{-2} $\pm 2.78 \times 10^{-3}$ 19 448	2.39×10^{-2} $\pm 2.52 \times 10^{-4}$ 17 844
Skillcraft (Real)	3338	19	$\mathbf{3.61 \times 10^{-2}}$ $\mathbf{\pm 1.21 \times 10^{-2}}$ 14 457	1.51×10^{-1} $\pm 1.12 \times 10^{-5}$ 18 318	8.18×10^{-2} $\pm 1.52 \times 10^{-3}$ 9 530 027	1.14×10^{-1} $\pm 5.76 \times 10^{-2}$ 57 292 606	3.18×10^{-1} $\pm 5.44 \times 10^{-2}$ 12 350	9.78×10^{-2} $\pm 1.92 \times 10^{-3}$ 6709
Elevators (Real)	16 599	18	1.14×10^{-2} $\pm 1.64 \times 10^{-3}$ 2366	6.31×10^{-2} $\pm 2.18 \times 10^{-6}$ 7400	4.91×10^{-2} $\pm 3.82 \times 10^{-4}$ 12 513 644	4.86×10^{-2} $\pm 3.23 \times 10^{-4}$ 14 920 122	$\mathbf{9.07 \times 10^{-3}}$ $\mathbf{\pm 1.74 \times 10^{-4}}$ 52 200	4.99×10^{-2} $\pm 2.15 \times 10^{-4}$ 7346
Housing (Real)	506	13	$\mathbf{1.62 \times 10^{-1}}$ $\mathbf{\pm 6.75 \times 10^{-2}}$ 2116	8.17×10^{1} $\pm 4.76 \times 10^{-1}$ 21 023	1.88×10^{1} ± 1.22 89 226 791	2.82×10^{1} ± 1.16 2 982 619	1.42×10^{1} $\pm 1.54 \times 10^{-1}$ 3770	3.83×10^{1} ± 2.62 1835
Protein (Real)	45 730	9	$\mathbf{5.18 \times 10^{-2}}$ $\mathbf{\pm 7.96 \times 10^{-3}}$ 4754	6.04×10^{-1} $\pm 1.04 \times 10^{-5}$ 18 974	4.00×10^{-1} $\pm 2.04 \times 10^{-1}$ 7 557 785	2.06×10^{-1} $\pm 1.02 \times 10^{-2}$ 26 561 968	6.70×10^{-1} $\pm 7.70 \times 10^{-2}$ 1170	6.00×10^{-1} $\pm 1.08 \times 10^{-3}$ 6185
Kin40K (Real)	40 000	8	$\mathbf{3.49 \times 10^{-4}}$ $\mathbf{\pm 1.84 \times 10^{-4}}$ 9916	1.82×10^{-2} $\pm 1.78 \times 10^{-2}$ 11 090	9.74×10^{-3} $\pm 5.09 \times 10^{-4}$ 9 466 377	1.13×10^{-2} $\pm 3.55 \times 10^{-4}$ 2 631 074	1.96×10^{-3} $\pm 6.43 \times 10^{-5}$ 3600	4.00×10^{-2} $\pm 4.62 \times 10^{-4}$ 7738

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Numerical Experiments - Ablations

Table 2: Mean squared error and one standard deviation for ablation experiments (vanilla, extended and full TTKL model) on three synthetic data sets.

Data set	N	d	Test MSE				
			Vanilla	H^1	Pre-Train	Opt	Full
HighDimSin	100 000	30	2.84 $\pm 1.04 \times 10^{-2}$	1.62×10^{-2} $\pm 4.75 \times 10^{-2}$	4.48×10^{-5} $\pm 1.92 \times 10^{-5}$	2.89 $\pm 7.92 \times 10^{-2}$	2.54×10^{-4} $\pm 3.75 \times 10^{-4}$
Friedman	100 000	5	1.92 ± 2.84	3.76×10^{-2} $\pm 8.59 \times 10^{-3}$	1.40×10^{-2} $\pm 1.71 \times 10^{-5}$	1.54×10^{-2} $\pm 1.91 \times 10^{-2}$	9.00×10^{-6} $\pm 9.42 \times 10^{-7}$
Grid	65 536	2	8.39×10^{-5} $\pm 2.77 \times 10^{-5}$	4.58×10^{-5} $\pm 2.91 \times 10^{-5}$	5.15×10^{-6} $\pm 1.60 \times 10^{-6}$	1.15×10^{-4} $\pm 5.26 \times 10^{-5}$	4.99×10^{-6} $\pm 8.29 \times 10^{-7}$

Numerical Experiments - Data Sets

Grid:

- $\Omega = [0,1]^2$
- $\Phi(x) = \sum_{i=1}^{2} \sin(2\pi i x_i) + \epsilon$ with $\epsilon \sim \mathcal{N}(0, 0.1)$
- $65\,536$ total data points (equidistant grid with 256 vertices)

Friedman [Fri91]:

- $\Omega = [0,1]^5$
- $\rho = \bigotimes_{i=1}^{5} \mathcal{U}(0,1)$
- $\Phi(x) = 10\sin(\pi x_1 x_2) + 20(x_3 - 0.5)^2 + 10x_4 + 5x_5$
- $100\,000$ data points

HighDimSine:

- $\Omega = [0,1]^{30}$
- $\rho = \bigotimes_{i=1}^{30} \mathcal{U}(0,1)$
- $\Phi(x) = \sum_{i=1}^{30} \sin(\pi x_i)$
- $100\,000$ data points

UCI Machine Learning Repository:

- Physicochemical Properties of Protein Tertiary Structure
- KEGG Metabolic Relation Network (Directed)
- Kin40k
- SkillCraft1 Master
- Housing

Hyper-Parameters

TTKL:

- Tensor-Train ranks: $r \sim \mathcal{U}(2, 15)$,
- H^1 polynomial degree: $J \sim \mathcal{U}(2, 14)$,
- ALS regularisation coefficient: $\delta_1 = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-10}), \log(1 \times 10^{-1}))$
- orthogonalisation of TT after pre-training with equal probability
- latents dimensionality: $L \sim \mathcal{U}(1, d)$
- number of inducing points: $M \sim \mathcal{U}(10, 1000)$
- TT regularisation during end-to-end training with equal probability
- TT regularisation coefficient during end-to-end training: $\delta_2 = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-10}), \log(1 \times 10^{-1}))$
- initial TT learning rate: $\eta_1 = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-5}), \log(1 \times 10^{-1}))$
- initial RBF hyper-parameters learning rate: $\eta_2 = 10^b$,
  $b \sim \mathcal{U}(\log(1 \times 10^{-4}), \log(1 \times 10^{-1}))$
- initial VI related hyper-parameters learning rate: $\eta_3 = 10^b$,
  $b \sim \mathcal{U}(\log(1 \times 10^{-3}), \log(1 \times 10^{-1}))$
- data batch size: $S \sim \mathcal{U}(4, 1024)$

Hyper-Parameters

CPKL:

- Canonical-Polyadic rank: $r \sim \mathcal{U}(2, 15)$,
- polynomial degree: $J \sim \mathcal{U}(2, 20)$,
- latents dimensionality: $L \sim \mathcal{U}(1, d)$
- number of inducing points: $M \sim \mathcal{U}(10, 1000)$
- CP regularisation during end-to-end training with equal probability
- CP regularisation coefficient during end-to-end training: $\delta_2 = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-10}), \log(1 \times 10^{-1}))$
- initial CP learning rate: $\eta_1 = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-5}), \log(1 \times 10^{-1}))$
- initial RBF hyper-parameters learning rate: $\eta_2 = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-4}), \log(1 \times 10^{-1}))$
- initial VI related hyper-parameters learning rate: $\eta_3 = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-3}), \log(1 \times 10^{-1}))$
- data batch size: $S \sim \mathcal{U}(4, 1024)$

Hyper-Parameters

DNN:

- output dimension of first and second hidden layer: $h_{1,2} \sim \mathcal{U}(1000, 10\,000)$
- output dimension of third hidden layer: $h_3 \sim \mathcal{U}(100, 1000)$
- output dimension of fourth hidden layer: $h_4 \sim \mathcal{U}(10, 100)$
- hidden layer's non-linearity is with equal probability either ReLU, Tanh or quadratic
- data batch size: $S \sim \mathcal{U}(4, 1024)$
- initial learning rate: $\gamma = 10^a$, $a \sim \mathcal{U}(\log(1 \times 10^{-5}), \log(1 \times 10^{-1}))$
- regularisation is either applied or not with equal probability
- regularisation coefficient: $\delta = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-10}), \log(1 \times 10^{-1}))$

Hyper-Parameters

TT:

- Tensor-Train rank: $r \sim \mathcal{U}(2, 15)$,
- H^1 polynomial degree: $J \sim \mathcal{U}(2, 14)$,
- regularisation coefficient: $\delta = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-10}), \log(1 \times 10^{-1}))$.

Hyper-Parameters

GP:

- Number inducing points: $M \sim \mathcal{U}(100, 1000)$
- initial learning rate: $\gamma = 10^b$, $b \sim \mathcal{U}(\log(1 \times 10^{-3}), \log(1 \times 10^{-1}))$
- Batch size: $S \sim \mathcal{U}(4, 1024)$.

Hyper-Parameters

DKL:

- latents dimensionality: $L \sim \mathcal{U}(1, d)$
- number of inducing points for sparse VI: $M \sim \mathcal{U}(10, 1000)$
- initial learning rate GP: $\gamma_1 = 10^a$, $a \sim \mathcal{U}(\log(1 \times 10^{-3}), \log(1 \times 10^{-1}))$
- initial RBF hyper-parameters learning rate: $\gamma_2 = 10^a$, $a \sim \mathcal{U}(\log(1 \times 10^{-4}), \log(1 \times 10^{-1}))$
- initial DNN learning rate: $\gamma_3 = 10^a$, $a \sim \mathcal{U}(\log(1 \times 10^{-5}), \log(1 \times 10^{-1}))$
- data batch size: $S \sim \mathcal{U}(4, 1024)$