Scalable Gaussian Processes with Billions of Inducing Inputs via Tensor Train Decomposition

Pavel Izmailov pi49@cornell.edu

Alexander Novikov sasha.v.novikov@gmail.com

Dmitry Kropotov dmitry.kropotov@gmail.com

Summary

- Gaussian processes are powerful and elegant models, but exact inference requires $\mathcal{O}(n^3)$ computations, where n is the number of training data
- We propose the Tensor Train GP (TT-GP) framework with linear complexity $\mathcal{O}(n)$
- TT-GP allows to build flexible posterior approximations and train expressive deep kernels by using billions of inducing points for datasets containing millions of data points of dimensionality up to 10
- TT-GP achieves state-of-the-art results on several important benchmarks both with RBF and deep kernels

Inducing Inputs and Structured Kernel Interpolation

- Inducing inputs are imaginary data points that allow to speed up GP inference
- SKI (Wilson and Nickisch, 2015): set inducing points on a multi-dimensional grid

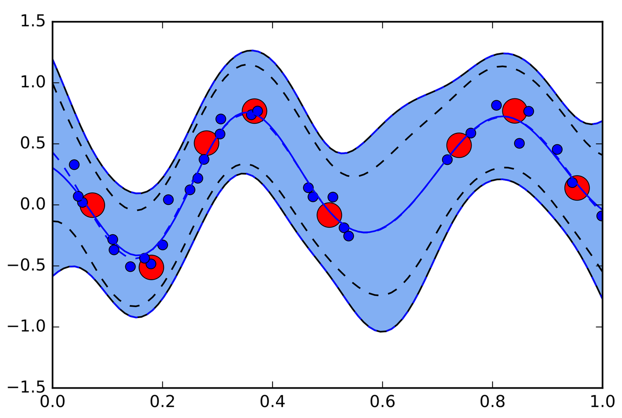
$$Z = Z^1 \times Z^2 \times \ldots \times Z^D.$$

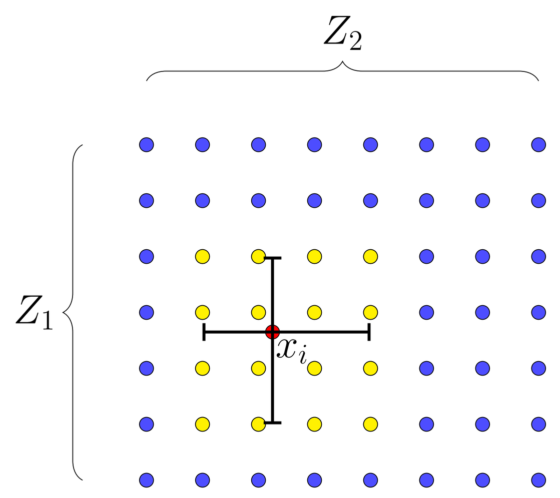
- Assume the kernel decomposes as

$$k(x, x') = k^1(x^1, x'^1) \cdot k^2(x^2, x'^2) \cdot \ldots \cdot k^D(x^D, x'^D)$$

Covariance matrix $K_{mm} \in \mathbb{R}^{m \times m}$ computed at the inducing points takes form

$$K_{mm} = K^1_{m_1 m_1} \otimes K^2_{m_2 m_2} \otimes \ldots \otimes K^D_{m_D m_D}$$





- $\det(K_{mm})$ and K_{mm}^{-1} can be computed efficiently
- Inducing points can be considered as inteprolation points for the kernel

$$k_i \approx K_{mm} w_i,$$

where $k_i \in \mathbb{R}^m$ is the vector of covariances between the i-th training object and the inducing points, $w_i \in \mathbb{R}^m$ is the vector of interpolation coefficients
- KISS-GP uses cubic convolutional interpolation for which

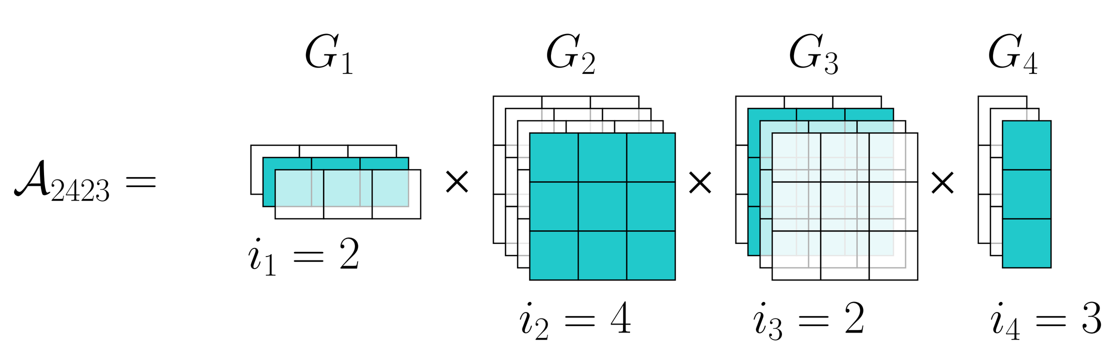
$$w_i = w_i^1 \otimes w_i^2 \otimes \ldots \otimes w_i^D$$

Tensor Train Format

Tensor $\mathcal{A}$ is said to be represented in Tensor Train (Oseledets, 2011) format if:

$$\mathcal{A}_{i_1 \ldots i_d} = \underbrace{G_1[i_1]}_{1 \times r} \underbrace{G_2[i_2]}_{r \times r} \ldots \underbrace{G_d[i_d]}_{r \times 1}$$

An example of computing one element of a 4-dimensional tensor:



- TT-format uses $O\left(dnr^2\right)$ memory to approximate a tensor with n^d elements
- Allows for efficient implementation of linear algebra operations

Gaussian Process ELBO

Evidence Lower Bound (Hensman et al., 2013) with KISS-GP approximation of k_i:

$$\log p(y) \geq \sum_{i=1}^{n} \left(\log \mathcal{N}(y_i | w_i^T \mu, \sigma^2) - \frac{1}{2\sigma^2}(\text{var}_i + w_i^T K_{mm} w_i) - \frac{1}{2\sigma^2}\text{tr}(w_i^T \Sigma w_i) \right)$$
$$- \frac{1}{2}\left(\log \frac{\det(K_{mm})}{\det(\Sigma)} - m + \text{tr}(K_{mm}^{-1}\Sigma) + \mu^T K_{mm}^{-1} \mu \right)$$

where
- σ^2 is the noise variance
- $\mu \in \mathbb{R}^m$, $\Sigma \in \mathbb{R}^{m \times m}$ variational parameters
- $\tilde{K}_{ii} = \text{var} - k_i^T K_{mm}^{-1} k_i$, where var is the prior variance of the process at any point

TT-GP

- Set inducing points Z on a grid in the feature space
- Restrict Σ to be in a Kronecker product format

$$\Sigma = \Sigma^1 \otimes \Sigma^2 \otimes \ldots \otimes \Sigma^D$$

- Represent μ as a d-dimensional tensor, restrict to be in TT format with TT-ranks r
- Maximize ELBO with respect to TT-cores of μ, Kronecker factors of Σ using SGD

Properties

- Linear computational complexity in the size of the data $\mathcal{O}(nDm^{1/D}r^2 + Dm^{1/D}r^3 + Dm^{3/D})$. TT-ranks are in general on the scale of $r \approx 10$.
Here $m = m_0^D$
- TT-GP can be applied for very large n and m

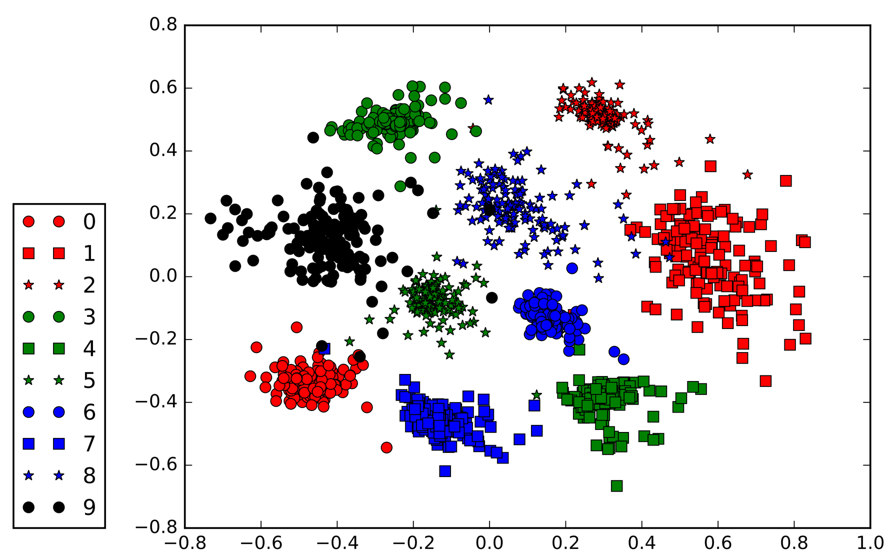
RBF Kernel Experiments

Comparison with SVI-GP (Hensman et al., 2013) on regression and classification tasks:

Dataset			SVI-GP / KLSP-GP			TT-GP			
Name	n	D	acc.	m	t (s)	acc.	m	d	t (s)
Powerplant	7654	4	0.94	200	10	**0.95**	35^4	-	5
Protein	36584	9	0.50	200	45	**0.56**	30^9	-	40
YearPred	$463K$	90	0.30	1000	597	**0.32**	10^6	6	105
Airline	$6M$	8	0.665*	-	-	**0.694**	20^8	-	5200
svmguide1	3089	4	0.967	200	4	**0.969**	20^4	-	1
EEG	11984	14	**0.915**	1000	18	0.908	12^{10}	10	10
covtype bin	465K	54	0.817	1000	320	**0.852**	10^6	6	172

Deep Kernel Experiments

Embedding learned by TT-GP with a deep kernel on *digits* dataset:



Comparison with SV-DKL (Wilson et al., 2016) and stand-alone DNN:

Dataset		SV-DKL	DNN		TT-GP		
Name	n	acc.	acc.	t (s)	acc.	d	t (s)
Airline	$6M$	0.781	0.780	1055	$\mathbf{0.788 \pm 0.002}$	2	1375
CIFAR-10	$50K$	–	**0.915**	166	0.908 ± 0.003	9	220
MNIST	$60K$	–	0.993	23	$\mathbf{0.9936 \pm 0.0004}$	10	64

References

J. Hensman, N. Fusi, and N. D. Lawrence. Gaussian processes for big data. In *Proceedings of the Twenty-Ninth Conference on Uncertainty in Artificial Intelligence*, pages 282–290. AUAI Press, 2013.

I. V. Oseledets. Tensor-train decomposition. *SIAM Journal on Scientific Computing*, 33(5):2295–2317, 2011.

A. G. Wilson and H. Nickisch. Kernel interpolation for scalable structured gaussian processes (kiss-gp). In *International Conference on Machine Learning*, pages 1775–1784, 2015.

A. G. Wilson, Z. Hu, R. Salakhutdinov, and E. P. Xing. Stochastic variational deep kernel learning. In *Advances in Neural Information Processing Systems*, pages 2586–2594, 2016.