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

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Summary

- Gaussian processes are powerful and elegant models, but the 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 $\mathcal{O}(nD)$ w.r.t. the dataset size n and the dimensionality of the data D
- TT-GP supports billions of inducing inputs
- Can train TT-GP with neural network embeddings end-to-end
- TT-GP achieves state-of-the-art results on several benchmarks both with RBF and deep kernels

Inducing Inputs

- Inducing points (Z, u) are m imaginary points that compress information in data. The joint distribution of labels y, process values $f \in \mathbb{R}^n$ at data points and process values $u \in \mathbb{R}^m$ at inducing points is given by

$$p(y, f, u) = \prod_i p(y_i|f) \cdot p(f|u) \cdot p(u),$$

where $p(f|u) = \mathcal{N}(f|K_{nm}K_{mm}^{-1}u, K_{nn} - K_{nm}K_{mm}^{-1}K_{nm}^T)$, $p(u) = \mathcal{N}(u|0, K_{mm})$. Here $K_{mm} \in \mathbb{R}^{m\times m}$, $K_{nm} \in \mathbb{R}^{n\times m}$, $K_{nn} \in \mathbb{R}^{n\times n}$ are covariance matrices computed between Z and Z, X and Z, X and X respectively

- Using the variational distribution of the form $q(f, u) = p(f|u)q(u)$ with $q(u) = \mathcal{N}(u|\mu, \Sigma)$ we can derive the variational lower bound

$$\log p(y) \geq \sum_i \mathbb{E}_{q(f_i)} \log p(y_i|f_i) - \text{KL}\left(q(u)||p(u)\right)$$

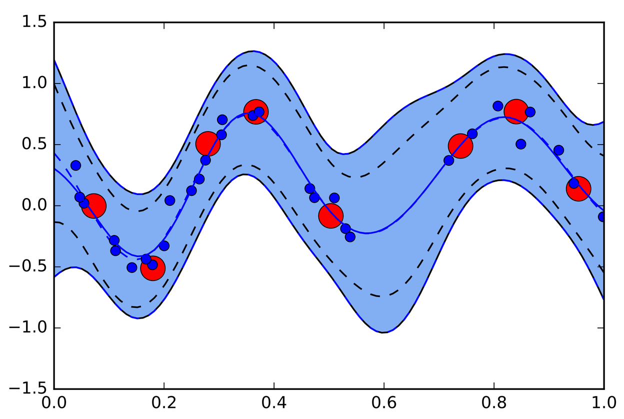
- The complexity of computing this bound is $\mathcal{O}(nm^2 + m^3)$

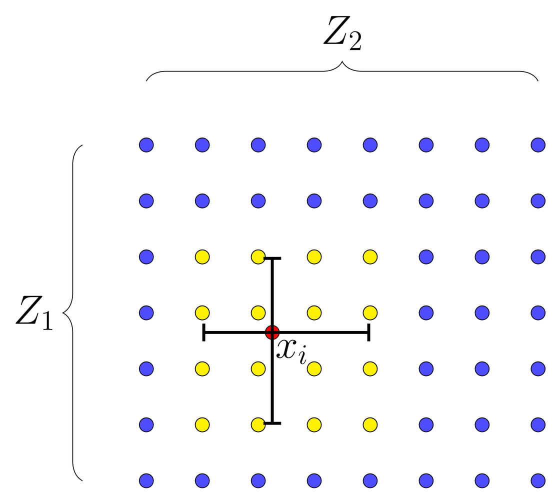
Structured Kernel Interpolation

- 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} 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 in $\mathcal{O}(Dm^{3/D})$
- 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

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

Gaussian Process ELBO

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

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

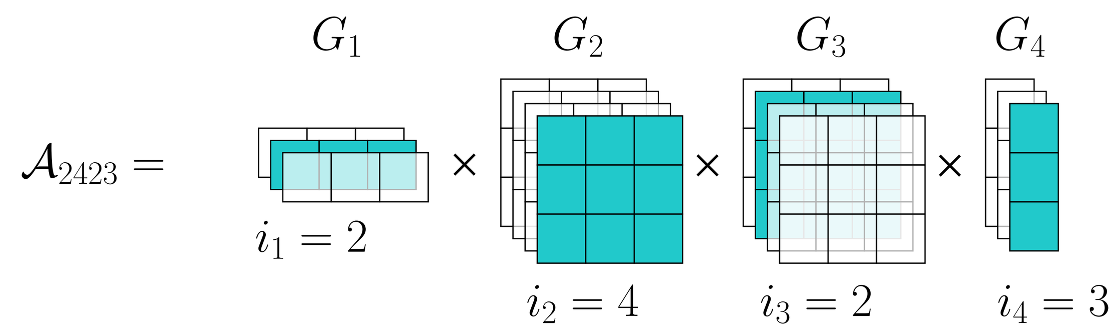
where σ^2 is the noise variance, δ is the prior variance of the process at any point and $\mu \in \mathbb{R}^m$, $\Sigma \in \mathbb{R}^{m\times m}$ are variational parameters

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

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, and kernel parameters using stochastic optimization

Properties

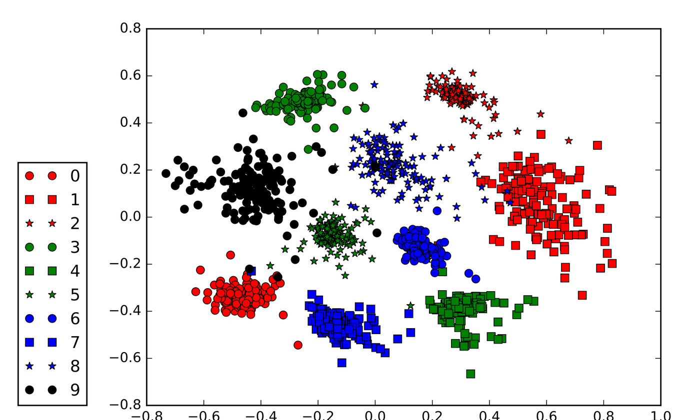
- Linear complexity $\mathcal{O}(nDm^{1/D}r^2 + Dm^{1/D}r^3 + Dm^{3/D})$ w.r.t. the dataset size n and dimensionality D. TT-ranks are in general on the scale of $r \approx 10$. Here $m = m_0^D$, where m_0 is the number of inducing points per dimension
- TT-GP can be applied for $n \approx 10^6$ and $m \approx 10^{10}$

RBF Kernel Experiments

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

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

Deep Kernel Experiments



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

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

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

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