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

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Abstract

We propose a new method (TT-GP) for approximate inference in Gaussian process models. We build on previous results on scalable GPs including stochastic variational inference based on inducing inputs, kernel interpolation and structure exploiting algebra. We also utilize the Tensor Train decomposition which allows us to efficiently train GP models with billions of inducing inputs and improve the results of previous GP models on several benchmark datasets. Further, our approach allows us to train kernels based on deep neural networks without any modifications of the underlying GP model. Our model allows end-to-end training of both GP and Neural Network parameters without pretraining through maximization of GP marginal likelihood. In this approach DNN learns a multidimensional embedding for the data, which is used by the GP to make the final prediction. We show the efficiency of the proposed approach on several widely used classification benchmark datasets including CIFAR10, MNIST and Airline.

1 Introduction

Gaussian processes (GP) provide a prior over functions and allow finding complex regularities in data. The ability of GPs to adjust the complexity of the model to the size of the data makes them appealing to use for big datasets. Unfortunately, standard methods for GP regression and classification scale as $\mathcal{O}(n^3)$ with the size of the data n and can not be applied when n exceeds several thousands.

Numerous approximate inference methods have been proposed in the literature. Many of these methods are based on the concept of inducing inputs (**?**], **?**], **?**]). These methods build a smaller set Z of m points that serve to approximate the true posterior of the process and reduce the complexity to $\mathcal{O}(nm^2 + m^3)$. **?**] proposed to consider the values u of the Gaussian process at the inducing inputs as latent variables and derived a variational inference procedure to approximate the posterior distribution of these variables. **?**] and **?**] extended this framework by using stochastic optimization to scale up the method and generalized it to classification problems.

Inducing input methods allowed to use Gaussian processes on datasets containing million of examples. However, these methods are still limited with the number of inducing points m they can use. **?**] proposed the KISS-GP framework, which exploits the Kronecker product structure in covariance matrices for inducing points placed on a multidimensional grid in the feature space. KISS-GP has complexity $\mathcal{O}(n + Dm^{1+1/D})$, where D is the dimensionality of the feature space. Note however, that m is the number of points in a D-dimensional grid and grows exponentially with D, which makes the method inapplicable when the number of features D is larger than 4.

In this paper we propose a method TT-GP, that can use billions of inducing inputs and is applicable to high-dimensional feature spaces. We achieve this by combining kernel interpolation and Kronecker algebra of KISS-GP with a scalable variational inference procedure. We restrict the family of

Submitted to 31st Conference on Neural Information Processing Systems (NIPS 2017). Do not distribute.

variational distributions from **?**] to have parameters in special formats. Specifically, we use Kronecker product format for the covariance matrix Σ and Tensor Train format (**?**]) for the expectation μ of the variational distribution over the values u of the process at inducing inputs Z.

The proposed TT-GP method naturally allows to train expressive kernel functions on big datasets. **?**] and **?**] demonstrated the efficiency of Gaussian processes with kernels based on deep neural networks. They used subsets of the outputs of a neural network as inputs for the Gaussian process. As the authors were using KISS-GP, they were limited to using low dimensional Gaussian processes and had to pretrain the network before adding the GP layer. The proposed TT-GP method allows us to learn multidimensional embeddings and train the model end-to-end.

2 Background

2.1 Gaussian Processes

A Gaussian process is a collection of random variables, any finite number of which have a joint normal distribution. A GP f taking place in $\mathbb{R}^D$ is fully defined by its mean $m : \mathbb{R}^D \to \mathbb{R}$ and covariance $k : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$ functions. For every $x_1, x_2, \ldots, x_n \in \mathbb{R}^D$

$$f(x_1), f(x_2), \ldots, f(x_n) \sim \mathcal{N}(m, K),$$

where $m = (m(x_1), m(x_2), \ldots, m(x_n))^T \in \mathbb{R}^n$, and $K \in \mathbb{R}^{n \times n}$ is the covariance matrix with $K_{ij} = k(x_i, x_j)$. Below we will use notation $K(A, B)$ for the matrix of pairwise values of covariance function k on points from sets A and B.

Consider a regression problem. The dataset consists of n objects $X = (x_1, \ldots, x_n)^T \in \mathbb{R}^{n \times D}$, and target values $y = (y_1, y_2, \ldots, y_n)^T \in \mathbb{R}^n$. We assume that the data is generated by a latent zero-mean Gaussian process f plus independent Gaussian noise:

$$p(y, f|X) = p(f|X) \prod_{i=1}^{n} p(y_i|f_i),\ p(y_i|f_i) = \mathcal{N}(y_i|f_i, \nu^2 I),\ p(f) = \mathcal{N}(f|0, K(X, X)), \quad (1)$$

where $f_i = f(x_i)$ is the value of the process at data point x_i and ν^2 is the noise variance.

Assume that we want to predict the values of the process f_* at a set of test points X_*. As the joint distribution of y and f_* is Gaussian, we can analytically compute the conditional distribution $p(f_*|y, X, X_*) = \mathcal{N}(f_*|\hat{m}, \hat{K})$ with analytical formulas for $\hat{m}$ and $\hat{K}$. The complexity of this calculation is $\mathcal{O}(n^3)$ since it involves calculation of the inverse of the covariance matrix K.

Popular covariance functions usually have a set of hyper-parameters θ. For example, the RBF kernel

$$k_{\text{RBF}}(x, x') = \sigma_f^2 \exp\left(-0.5\|x - x'\|^2 / l^2\right)$$

has two hyper-parameters l and σ_f. In order to fit the model to the data, we can maximize the marginal likelihood of the process $p(y|X)$ with respect to these parameters. In case of GP regression this marginal likelihood is calculated analytically. The computational complexity of this marginal likelihood is again $\mathcal{O}(n^3)$.

For two-class classification problem we use the same model (**??**) with $p(y_i|f_i) = 1/(1+\exp(-y_i f_i))$, where $y_i \in \{-1, +1\}$. In this case both predictive distribution and marginal likelihood are intractable. For detailed description of GP regression and classification see **?**].

2.2 Inducing Inputs

A number of approximate methods were developed to scale up Gaussian processes. **?**] proposed a variational lower bound that factorizes over observations for Gaussian process marginal likelihood. We rederive this bound here.

Consider a set $Z \in \mathbb{R}^{m \times D}$ of m inducing points in the feature space and latent variables $u \in \mathbb{R}^m$ representing the values of the Gaussian process at these points. Consider the augmented model

$$p(y, f, u) = p(y|f)p(f|u)p(u) = \prod_{i=1}^{n} p(y_i|f_i)p(f|u)p(u)$$

with

$$p(f|u) = \mathcal{N}(f|K_{nm}K_{mm}^{-1}u, K_{nn} - K_{nm}K_{mm}^{-1}K_{mn}),$$
$$p(u) = \mathcal{N}(u|0, K_{mm}), \tag{2}$$

where $K_{nn} = K(X, X), K_{nm} = K(X, Z), K_{mn} = K(Z, X) = K_{nm}^T, K_{mm} = K(Z, Z)$.

The standard variational lower bound is given by

$$\log p(y) \geq \mathbb{E}_{q(u,f)} \log \frac{p(y, f, u)}{q(u, f)} = \mathbb{E}_{q(f)} \log \prod_{i=1}^{n} p(y_i|f_i) - \text{KL}(q(u, f)||p(u, f)), \tag{3}$$

where $q(u, f)$ is the variational distribution over latent variables. Consider the following family of variational distributions

$$q(u, f) = p(f|u)\mathcal{N}(u|\mu, \Sigma), \tag{4}$$

where $\mu \in \mathbb{R}^m$ and $\Sigma \in \mathbb{R}^{m\times m}$ are variational parameters. Then the marginal distribution over f can be computed analytically

$$q(f) = \mathcal{N}\left(f|K_{nm}K_{mm}^{-1}\mu, K_{nn} + K_{nm}K_{mm}^{-1}(\Sigma - K_{mm})K_{mm}^{-1}K_{mn}\right).$$

We can then rewrite (2) as

$$\log p(y) \geq \sum_{i=1}^{n} \mathbb{E}_{q(f_i)} \log p(y_i|f_i) - \text{KL}(q(u)||p(u)). \tag{5}$$

Note that the lower bound (4) factorizes over observations and thus stochastic optimization can be applied to maximize this bound with respect to both kernel hyper-parameters θ and variational parameters μ and Σ. In case of regression we can rewrite (4) in the closed form

$$\begin{aligned}\log p(y) \geq \sum_{i=1}^{n} \left(\log \mathcal{N}(y_i|k_i^T K_{mm}^{-1}\mu, \nu^2) - \frac{1}{2\nu^2}\tilde{K}_{ii} - \frac{1}{2\nu^2}\text{tr}(k_i^T K_{mm}^{-1}\Sigma K_{mm}^{-1}k_i)\right) - \\ -\frac{1}{2}\left(\log\frac{|K_{mm}|}{|\Sigma|} - m + \text{tr}(K_{mm}^{-1}\Sigma) + \mu^T K_{mm}^{-1}\mu\right),\end{aligned} \tag{6}$$

where $k_i \in \mathbb{R}^m$ is the i-th column of K_{mn} matrix and $\tilde{K} = K_{nn} - K_{nm}K_{mm}^{-1}K_{mn}$.

At prediction time we can use the variational distribution as a substitute for posterior

$$p(f_*|y) = \int p(f_*|f, u)p(f, u|y)df du \approx \int p(f_*|f, u)q(f, u)df du = \int p(f_*|u)q(u)du.$$

The complexity of computing the bound (5) is $\mathcal{O}(nm^2 + m^3)$. **?**] proposes to use Gauss-Hermite quadratures to approximate the expectation term in (4) for binary classification problem to obtain the same computational complexity $\mathcal{O}(nm^2 + m^3)$. This complexity allows to use Gaussian processes in tasks with millions of training samples, but these methods are limited to use small numbers of inducing points m, which hurts the predictive performance and doesn't allow to learn expressive kernel functions.

2.3 KISS-GP

?] noted that the covariance matrices computed at points on a multidimensional grid in the feature space can be represented as a Kronecker product if the kernel function factorizes over dimensions

$$k(x, x') = k_1(x^1, x'^1) \cdot k_2(x^2, x'^2) \cdot \ldots \cdot k_D(x^D, x'^D). \tag{7}$$

Note, that many popular covariance functions, including RBF, belong to this class. Kronecker structure of covariance matrices allows to perform efficient inference for full Gaussian processes with inputs X on a grid.

?] proposed to set inducing inputs Z on a grid:

$$Z = Z^1 \times Z^2 \times \ldots \times Z^D, \quad Z^i \in \mathbb{R}^{m_i} \quad \forall i = 1, 2, \ldots, D.$$

The number m of inducing points is then given by $m = \prod_{i=1}^{D} m_i$.

Let the covariance function satisfy (6). Then the covariance matrix K_{mm} can be represented as a Kronecker product over dimensions

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

where

$$K^i_{m_i m_i} = K_i(Z_i, Z_i) \in \mathbb{R}^{m_i \times m_i} \quad \forall i = 1, 2, \ldots, D.$$

Kronecker products allow efficient computation of matrix inverse and determinant:

$$(A_1 \otimes A_2 \otimes \ldots \otimes A_D)^{-1} = A_1^{-1} \otimes A_2^{-1} \otimes \ldots \otimes A_D^{-1},$$
$$|A_1 \otimes A_2 \otimes \ldots \otimes A_D| = |A_1|^{c_1} \cdot |A_2|^{c_2} \cdot \ldots \cdot |A_D|^{c_D},$$

where $A_i \in \mathbb{R}^{k_i \times k_i}$, $c_i = \prod_{j \neq i} k_j, \forall i = 1, 2, \ldots, D$.

Another major idea of KISS-GP is to use interpolation to approximate K_{mn}. Considering inducing inputs as interpolation points for the function $k(\cdot, z_i)$ we can write

$$K_{mn} \approx K_{mm} W, \quad k_i \approx K_{mm} w_i, \tag{8}$$

where $W \in \mathbb{R}^{m \times n}$ contains the coefficients of interpolation, and w_i is it's i-th column. Authors of KISS-GP suggest using cubic convolutional interpolation (**?**]), in which case the interpolation weights w_i can be represented as a Kronecker product over dimensions

$$w_i = w_i^1 \otimes w_i^2 \otimes \ldots \otimes w_i^D, \qquad w_i \in \mathbb{R}^{m_i} \quad \forall i = 1, 2, \ldots, D.$$

?] combine these ideas with SOR (**?**]) in the KISS-GP method with $\mathcal{O}(n + Dm^{1+1/D})$ computational complexity. This complexity allows to use KISS-GP with a large number (possibly greater than n) of inducing points. Note, however, that m grows exponentially with the dimensionality D of the feature space, and the method becomes impractical when $D \gg 4$.

2.4 Tensor Train Decomposition

Tensor Train (TT) decomposition, proposed in **?**], allows to efficiently store tensors (multidimensional arrays of data), large matrices and vectors. For matrices and vectors in TT-format linear algebra operations can be implemented efficiently. TT format was successfully applied for different machine learning tasks (see **?**], **?**]).

Consider a D-dimensional tensor $\mathcal{A} \in \mathbb{R}^{k_1 \times k_2 \times \ldots \times k_D}$. $\mathcal{A}$ is said to be in the Tensor Train format if

$$\mathcal{A}(i_1, i_2, \ldots, i_d) = G_1[i_1] \cdot G_2[i_2] \cdot \ldots \cdot G_D[i_D], \quad i_k \in \{1, 2, \ldots, n_k\} \ \forall k, \tag{9}$$

where $G_k[i_k] \in \mathbb{R}^{r_k \times r_{k+1}} \ \forall k, i_k, \ r_0 = r_{D+1} = 1$. Matrices G_k are called TT-cores, and numbers r_k are called TT-ranks of tensor $\mathcal{A}$.

In order to represent a vector in TT-format, it is reshaped to a multidimensional tensor (possibly with zero padding) and then format (8) is used. We will use TT-format for the vector μ of expectations of the values u of the Gaussian process in points Z placed on a multidimensional grid. In this case, μ is naturally represented as a D-dimensional tensor.

For matrices TT format is given by

$$M(i_1, i_2, \ldots, i_d; j_1, j_2, \ldots, j_D) = G_1[i_1, j_1] \cdot G_2[i_2, j_2] \cdot \ldots \cdot G_D[i_D, j_D],$$

where $G_k[i_k, j_k] \in \mathbb{R}^{r_k \times r_{k+1}} \ \forall k, i_k, j_k, \ r_0 = r_{D+1} = 1$. Note, that Kronecker product format is a special case of TT for TT-ranks $r_1 = r_2 = \ldots = r_{D+1} = 1$.

Let $u, v \in \mathbb{R}^{n_1 \cdot n_2 \cdot \ldots \cdot n_D}$ be vectors in TT-format with TT-ranks not greater than r. Let A and B be represented as a Kronecker product

$$A = A_1 \otimes A_2 \otimes \ldots \otimes A_D, \quad A_k \in \mathbb{R}^{n_k \times n_k} \ \forall k,$$

and the same for B. Let $n = \max_k n_k$. Then the computational complexity of computing the quadratic form $u^T A v$ and $\text{tr}(AB)$ is $\mathcal{O}(Dnr^3)$ and $\mathcal{O}(Dn^2)$ correspondingly. We will need these two operations below.

3 TT-GP

In the previous section we described several methods for GP regression and classification. All these methods have different limitations. Standard methods can not be applied for big datasets, KISS-GP requires small dimensionality of the feature space and other methods based on inducing points are limited to use a small number m of these points. In this section we propose the TT-GP method that can be used with big datasets and can incorporate billions of inducing inputs. TT-GP can naturally be used for training expressive deep kernels to work with structured data (e.g. images).

3.1 Variational Parameters Approximation

In section 2.2 we derived the variational lower bound of **?**]. We will place the inducing inputs Z on a multidimensional grid in the feature space and we will assume the the covariance function satisfies (6). Let the number of inducing points in each dimension be m_0. Then

$$m = m_0^D.$$

As shown in section 2.3, in this case K_{mm} matrix can be rewritten as a Kronecker product over dimensions. Substituting the approximation (7) into the lower bound (5), we obtain

$$\begin{aligned}\log p(y) \geq \sum_{i=1}^{n} \left(\log \mathcal{N}(y_i | w_i^T \mu, \nu^2) - \frac{1}{2\nu^2} \tilde{K}_{ii} - \frac{1}{2\nu^2} \text{tr}(w_i^T \Sigma w_i) \right) - \\ - \frac{1}{2} \left(\log \frac{|K_{mm}|}{|\Sigma|} - m + \text{tr}(K_{mm}^{-1} \Sigma) + \mu^T K_{mm}^{-1} \mu \right),\end{aligned} \tag{10}$$

where $\tilde{K}_{ii} = k(x_i, x_i) - w_i^T K_{mm} w_i$.

Note that K_{mm}^{-1} and $|K_{mm}|$ can be computed with $\mathcal{O}(Dm_0^3) = \mathcal{O}(Dm^{3/D})$ operations due to the Kronecker product structure. Now the most computationally demanding terms are those containing variational parameters μ and Σ.

Let us restrict the family of variational distributions (3). Let Σ be a Kronecker product over dimensions, and μ be in TT-format with TT-ranks not greater than r. Then, according to section 2.4, we can then compute the lower bound with $\mathcal{O}(nDm_0r^2 + Dm_0r^3 + Dm_0^3) = \mathcal{O}(nDm^{1/D}r^2 + Dm^{1/D}r^3 + Dm^{1/D})$.

Thus, the proposed TT-GP method has linear complexity with respect to dimensionality D of the feature space, despite the exponential growth of the number of inducing inputs. Lower bound (9) can be maximized with respect to kernel hyper-parameters θ, TT-cores of μ and Kronecker multipliers of Σ. Note that stochastic optimization can be applied, as the bound (9) factorizes over data points. The total number of optimized parameters is $\mathcal{O}(\sharp\theta + Dm^{1/D} + Dm^{2/D})$, where $\sharp\theta$ is the number of kernel hyper-parameters.

3.2 Classification

In this section we describe a generalization of the proposed method for multiclass classification. In this case the dataset consists of features $X = (x_1, x_2, \ldots, x_n)^T \in \mathbb{R}^{n \times D}$ and target values $y = (y_1, y_2, \ldots, y_n)^T \in \{1, 2, \ldots, C\}^n$, where C is the number of classes.

Consider C Gaussian processes taking place in $\mathbb{R}^D$. Each process corresponds to it's own class. We will place $m = m_0^D$ inducing points Z on a grid in the feature space, and they will be shared between all processes. Each process has it's own set of latent variables representing the values of the process at data points $f^c \in \mathbb{R}^n$, and inducing inputs $u^c \in \mathbb{R}^m$. We will use the following model

$$p(y, f, u) = \prod_{i=1}^{n} p(y_i | f_i^{1,2,\ldots,C}) \prod_{c=1}^{C} p(f^c | u^c) p(u^c),$$

where $p(f^c|u^c)$ and $p(u^c)$ are defined as in (1). For $p(y_i|f_i^{1,2,\ldots,C})$ we will use discrete distribution with probabilities

$$p(y_i = c | f_i^{1,2,\ldots,C}) = \frac{\exp(f_i^c)}{\sum_{j=1}^{C} \exp(f_i^j)}.$$

We will use variational distributions of form

$$q(f^1, f^2, \ldots, f^C, u^1, u^2, \ldots, u^C) = q(f^1, u^1) \cdot q(f^2, u^2) \cdot \ldots \cdot q(f^C, u^C),$$

where

$$q(f^c, u^c) = p(f^c|u^c)\mathcal{N}(u^c|\mu^c, \Sigma^c) \quad c = 1, 2, \ldots, C,$$

where all μ^c are represented in TT-format with TT-ranks not greater than r, and Σ^c are represented as Kronecker products over dimensions. Similarly to (4), we obtain

$$\log p(y) \geq \sum_{i=1}^{n} \mathbb{E}_{q(f_i^{1,2,\ldots,C})} \log p(y_i|f_i^{1,2,\ldots,C}) - \sum_{c=1}^{C} \mathrm{KL}(q(u_c)||p(u_c)) \tag{11}$$

The second term in (10) can be computed analytically as a sum of KL-divergences between normal distributions. The first term is intractable. In order to approximate the first term we will use a lower bound. Let y_i belong to class c. Then, we can rewrite

$$\mathbb{E}_{q(f_i^{1,2,\ldots,C})} \log p(y_i|f_i^{1,2,\ldots,C}) = \mathbb{E}_{q(f_i^c)} f_i^c - \mathbb{E}_{q(f_i^{1,2,\ldots,C})} \log \left(\sum_{j=1}^{C} \exp(f_i^j) \right), \tag{12}$$

where

$$q(f_i^{1,2\ldots,C}) = \mathcal{N}(f^1|m_i^1, s_i^1) \cdot \mathcal{N}(f^2|m_2, s_i^2) \cdot \ldots \cdot \mathcal{N}(f^C|m_i^C, s_i^C).$$

The first term in (11) is obviously tractable, while the second term has to be approximated. **?**] discusses several lower bounds for expectations of this type. Below we derive one of these bounds, which we use in TT-GP.

Concavity of logarithm implies

$$\log(\sum_{j=1}^{C} \exp(f_i^j)) \leq \log \frac{1}{\varphi} + \varphi \left(\sum_{j=1}^{C} \exp(f_i^j) - \frac{1}{\varphi} \right) = \varphi \sum_{j=1}^{C} \exp(f_i^j) - \log \varphi - 1,$$

where the right hand side is the linearization of the logarithm at $\frac{1}{\varphi}$. Taking expectation of both sides of the inequality and minimizing with respect to φ, we obtain

$$\mathbb{E}_{q(f_i^{1,2,\ldots,C})} \log \left(\sum_{j=1}^{C} \exp(f_i^j) \right) \leq \log \left(\sum_{j=1}^{C} \exp \left(m_i^j + \frac{1}{2} s_i^j \right) \right). \tag{13}$$

Substituting (12) back into (10) we obtain a tractable lower bound for multiclass classification task, that can be maximized with respect to kernel hyper-parameters θ^c, TT-cores of μ^c and Kronecker factors of Σ^c. The complexity of the method is C times higher, than in regression case.

3.3 Deep kernels

?] and **?**] showed the efficiency of using expressive kernel functions based on deep neural networks with Gaussian processes on a variety of tasks. The proposed TT-GP method is naturally compatible with this idea.

Consider a covariance function k (satisfying (6)) and a neural network (or in fact any parametric transform) net. We can define a new kernel as follows

$$k_{net}(x, x') = k(net(x), net(x')).$$

We can train the neural network weights through maximization of GP marginal likelihood, the same way, as we normally train kernel hyper-parameters θ. This way, the network learns a multidimensional embedding for the data, and the GP is making the prediction working with this embedding. **?**] trained one-dimensional GPs on different outputs of the network. TT-GP allows us to train Gaussian processes on all network outputs, and train the whole model end-to-end without pretraining.

Table 1: Results of experiments with UCI, LIBSVM and Airline datasets. In the table acc. stands for r^2 for regression and accuracy for classification tasks. Here and below n is the size of the training set, and D is the dimensionality of the feature space; m is the number of inducing inputs used by the methods, r is TT-ranks of μ for TT-GP; t is the time per one pass over the data (epoch) in seconds; where provided, d is the dimensionality of linear embedding.
* for KLSP-GP on Airline we provide results from the original article where the accuracy is given as a plot, and detailed information about experiment setup is not availible.

Dataset			SVI-GP / KLSP-GP			TT-GP				
Name	n	D	acc.	m	t (s)	acc.	m	r	d	t (s)
Powerplant	7654	4	0.94	200	10	0.95	35^4	30	-	5
Protein	36584	9	0.50	200	45	0.56	30^9	25	-	40
YearPred	$463K$	90	0.30	1000	597	0.32	10^6	10	6	105
Airline	$6M$	8	0.665^*	-	-	0.694	20^8	15	-	5200
svmguide1	3089	4	0.967	200	4	0.969	20^4	15	-	1
EEG	11984	14	0.915	1000	18	0.908	12^{10}	15	10	10
covtype bin	465K	54	0.817	1000	320	0.852	10^6	10	6	172

4 Experiments

In this section we evaluate the proposed TT-GP method in different settings and compare it with existing approaches. We first compare our method with SVI-GP (**?**]) on regression tasks and KLSP-GP (**?**]) on binary classification tasks using standard RBF kernel functions. Then, we test the ability of our method to learn expressive deep kernel functions and compare it with SV-DKL (**?**]). For TT-GP we use our implementation availible at `https://anonimized-link`.

4.1 Standard Kernels

For testing our method with standard covariance functions we used a range of classification and regression tasks from UCI and LIBSVM archives and the Airline dataset, that is popular for testing scalable GP models (**?**], **?**], **?**], **?**]) .

To obtain the Airline dataset we used the scripts[1] provided with **?**]. In UCI and LIBSVM datasets we randomly split the data with 80:20 proportions for train and test samples, unless test data is availible explicitly. For all datasets we first normalize the features X. For regression we also normalize the target variables y.

For SVI-GP and KLSP-GP we used the implementations provided in GPfLow (**?**]). For Airline dataset we provide results reported in the original paper (**?**]).

For our experiments we use a cluster of Intel Xeon E5-2698B v3 CPUs having 16 cores and 230 GB of RAM.

For YearPred, EEG and covtype datasets we used a d-dimensional linear embedding inside the RBF kernel for TT-GP, as the number D of features makes it impractical to set inducing inputs on a grid in a D-dimensional space in this case. On all other datasets we used the RBF kernel on initial features. For KLSP-GP and SVI-GP we used RBF kernel in all cases.

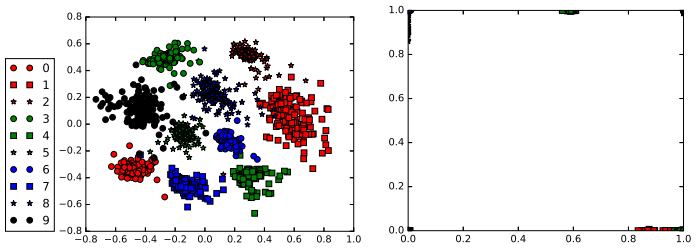
Table 1 shows the results on different regression and classification tasks. We can see, that TT-GP is able to achieve better predictive quality on all datasets except EEG. We also note that the method is able to achieve good predictive performance with linear embedding, which makes it practical for a wide range of datasets.

[1] `https://people.orie.cornell.edu/andrew/code/#SVDKL`

4.2 Deep Kernels

4.2.1 Representation learning

We first explore the representation our model learns for data on the small Digits[2] dataset containing $n = 1797$ 8×8 images of handwritten digits. We used a TT-GP with a kernel based on a small fully-connected neural network with two hidden layers with 50 neurons each and $d = 2$ neurons in the output layer to obtain a 2-dimensional embedding. We trained the model to classify the digits to 10 classes corresponding to different digits. Fig. 1a shows the learned embedding. We also trained the same network standalone, adding another layer with 10 outputs and softmax activations. The embedding for this network is shown in fig. 1b.



(a) DNN with TT-GP (b) Plain DNN

Figure 1: Learned representation for Digits dataset

We can see that the stand-alone DNN with linear classifiers is unable to learn a good 2-dimensional embedding. On the other hand, using a flexible GP classifier our model learns to group objects of the same class into compact regions.

4.2.2 Classification tasks

To test our model with deep kernels we used Airline, CIFAR10 (**?**]) and MNIST (**?**]) datasets.

We will use the following notation to describe DNN architecture. fc(h) means a fully-connected layer with h neurons; conv($h \times w$, f) means a convolutional layer with f $h \times w$ filters; maxpool($h \times w$) means max-pooling with $h \times w$ kernel; ReLU means rectified linear unit activation function; BN means batch normalization (**?**]).

For the Airline dataset we used a DNN with 5 fully-connected layers with architecture fc(1000)-ReLU-fc(1000)-ReLU-fc(500)-ReLU-fc(50)-ReLU-fc(2). The same architecture was used in **?**] on this task.

On MNIST we used a convolutional DNN with the following architecture: conv(5×5, 32)-ReLU-maxpool(2×2)-conv(5×5, 64)-ReLU-maxpool(2×2)-fc(1024)-ReLU-fc(4).

On CIFAR10 we used an 9-layer convolutional neural network with the following architecture: conv(3×3, 128)-BN-ReLU-conv(3×3, 128)-BN-ReLU-maxpool(3×3)-conv(3×3, 256)-BN-ReLU-conv(3×3, 256)-BN-ReLU-maxpool(3×3)-conv(3×3, 256)-BN-ReLU-conv(3×3, 256)-BN-ReLU-maxpool(3×3)-fc(1536)-BN-ReLU-fc(512)-BN-ReLU-fc(9). We also use standard data augmentation techniques on this dataset with random cropping of 24×24 parts of the image, horizontal flipping, randomly adjusting brightness and contrast.

In all experiments we also add a BN without trainable mean and variance after the DNN output layer to project the outputs into the region where inducing inputs are placed. We use $m_0 = 10$ inducing inputs per dimension and set TT-ranks of μ to $r = 10$ for all three datasets.

For experiments with convolutional neural networks (on MNIST and CIFAR10), we used Nvidia Tesla K80 GPUs to train the model.

[2] `http://scikit-learn.org/stable/auto_examples/datasets/plot_digits_last_image.html`

Table 2 shows the results of the experiments for our TT-GP with DNN kernel and SV-DKL. Note, that the comparison is not absolutely fair on CIFAR10 and MNIST datasets, as we didn't use the same exact architecture and preprocessing as **?**]. On Airline we used the same exact architecture and preprocessing as SV-DKL, and TT-GP achieves a higher accuracy on this dataset.

We also provide results of stand-alone DNNs for comparison. We used the same networks that were used in TT-GP kernels with the last linear layers replaced by layers with C outputs and softmax activations. Overall, we can see, that our model is able to achieve good predictive performance, improving the results of standalone DNN on Airline and MNIST.

Table 2: Results of experimetns with deep kernels. Here acc. is classification accuracy; C is the number of classes; d is the dimensionality of embedding learned by the model; t is the time per one pass over data (epoch) in seconds.

Dataset				SV-DKL	DNN		TT-GP		
Name	n	D	C	acc.	acc.	t (s)	acc.	d	t (s)
Airline	$6M$	8	2	0.781	0.780	1055	0.784	2	1375
CIFAR10	$50K$	$32\times32\times3$	10	0.770	0.915	166	0.909	9	220
MNIST	$60K$	28×28	10	0.992	0.993	23	0.994	10	64

We train all the models from random initialization without pretraining. We also tried using pretrained DNNs as initialization for our TT-GP model's kernel, which sometimes leads to faster convergence, but does not improve the final accuracy.

5 Discussion

We proposed TT-GP method for scalable inference in Gaussian process models for regression and classification. The proposed method is capable of using billions of inducing inputs, which is impossible for existing method. This allows us to improve the performance over state-of-the-art methods both with standard and deep kernels on several important benchmark datasets. Further, we believe, that our model provides a more natural and straightforward way of learning deep kernel functions, than the existing approaches.

Our preliminary experiments showed, that TT-GP is inferior in terms of uncertainty quatification compared to existing methods. We suspect that the reason for this is that we use covariance matrices Σ represented as Kronecker products over dimensions, which is rather restricting. We hope to alleviate this limitation by using Tensor Train format for Σ, and using approximations to compute it's inverse and determinant.

As a promissing direction for future work we also consider training TT-GP with deep kernels incrementally, using the variational approximation of posterior distribution as a prior for new data. We also find it interesting to try using the low-dimensional (compared to embeddings learned by standard DNNs) embeddings learned by our model for transfer learning. Finally, we want to explore the performance of our model in different practical applications including hyper-parameter optimization.