Learning High-Order Task Relationships in Multi-Task Learning

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Abstract

Multi-task learning is a way of bringing inductive transfer studied in human learning to the machine learning community. A central issue in multi-task learning is to model the relationships between tasks appropriately and exploit them to aid the simultaneous learning of multiple tasks effectively. While some recent methods model and learn the task relationships from data automatically, only pairwise relationships can be represented by them. In this paper, we propose a new model, called Multi-Task High-Order relationship Learning (MTHOL), which extends in a novel way the use of pairwise task relationships to high-order task relationships. We first propose an alternative formulation of an existing multi-task learning method. Based on the new formulation, we propose a high-order generalization leading to a new prior for the model parameters of different tasks. We then propose a new probabilistic model for multi-task learning and validate it empirically on some benchmark datasets.

1 Introduction

Most conventional machine learning problems consider the learning of a single task totally independent of some other activities, including the learning of some other possibly closely related tasks. For human learning, however, it is well accepted that learning to do a task can help us to acquire some generic knowledge that can be transferred to the learning of other related tasks, often referred to as learning to learn or inductive transfer. For example, the experience gained by learning to ride a bicycle can help a person greatly in learning to ride a tricycle. Such insights from cognitive science and psychology have inspired the development of a paradigm in machine learning called multi-task learning [Caruana, 1997; Baxter, 1997; Thrun, 1995]. An additional need for multi-task learning arises when the amount of labeled data in a single supervised learning task is scarce but there exist multiple related tasks. This scenario can be found in many applications. Multi-task learning can be very useful in this situation by leveraging useful information from multiple related tasks.

Over the past decade or so, many multi-task learning methods have been proposed both for general applications and for some domain-specific applications. Among the earliest methods are some layered neural network models which learn from multiple tasks a common data representation in the hidden layer of a neural network [Caruana, 1997]. Similar to neural network models but formulated under the regularization framework, multi-task feature learning [Argyriou *et al.*, 2006] learns a common data representation for multiple tasks. There are other regularized multi-task learning methods based on extending their single-task counterparts, e.g., extending support vector machines (SVM) [Evgeniou and Pontil, 2004; Evgeniou *et al.*, 2005], by incorporating new regularizers to encode the task relationships. Similar ideas have been extended to multi-task metric learning [Parameswaran and Weinberger, 2010] and boosting [Chapelle *et al.*, 2010]. Moreover, some regularized methods such as that in [Ando and Zhang, 2005] assume that the model parameters of different tasks share the same subspace, with possible extension to include random noise in the shared subspace [Chen *et al.*, 2010]. Another important approach to multi-task learning is the task clustering approach [Thrun and O'Sullivan, 1996; Bakker and Heskes, 2003; Xue *et al.*, 2007; Jacob *et al.*, 2008; Kumar and III, 2012]. It first groups the tasks into clusters by similarity and then learns the same or similar model parameters for all tasks within each cluster. Besides the methods formulated under the regularization framework, some Bayesian models have also been proposed for multi-task learning, e.g., Gaussian process (GP) in [Yu *et al.*, 2005], its robust counterpart, the t process, in [Yu *et al.*, 2007; Zhang and Yeung, 2010b], and sparse Bayesian models [Archambeau *et al.*, 2011; Titsias and Lázaro-Gredilla, 2011]. More recently, some methods based on the so-called task relationship learning approach have been proposed to discover the relationships between tasks automatically, e.g., GP in [Bonilla *et al.*, 2007] or a regularized method in [Zhang and Yeung, 2010a]. Using a task covariance matrix, this approach provides an effective way to characterize different types of pairwise task relationships. This approach has also been applied to multi-task feature selection [Zhang *et al.*, 2010] which generalizes previous settings by allowing the existence of dissimilar tasks and to transfer learning [Zhang and Yeung, 2010c; 2012].

The task relationship learning approach based on a task covariance matrix is a promising approach because it considers more general types of task relationships than those exploited by previous methods. Specifically, not only can two tasks be positively correlated or unrelated, but they can also be negatively correlated. Moreover, the task relationships are learned from data automatically but not prespecified and fixed based on possibly incorrect assumptions. Nevertheless, the existing task relationship learning methods [Bonilla *et al.*, 2007; Zhang and Yeung, 2010a; Zhang *et al.*, 2010] only model and learn pairwise task relationships. Some relationships between tasks found in real applications may be more complicated than what pairwise relationships can characterize. For example, it is possible for two tasks to appear uncorrelated when considering pairwise relationships, but their partial similarity can be revealed by considering high-order task relationships after incorporating a third task which is positively correlated with the two tasks. This motivates us to explore the use of high-order task relationships for multi-task learning.

We first briefly review an existing task relationship learning method and propose an alternative formulation of the model based on a matrix-variate probability distribution. The new formulation allows us to generalize, in a nontrivial way, the use of pairwise task relationships to high-order task relationships, leading to a new prior for the model parameters of different tasks. We then propose a new model which we refer to as Multi-Task High-Order relationship Learning (MTHOL). Experiments on some benchmark datasets demonstrate the effectiveness of our MTHOL method.

2 High-Order Task Relationship Learning

In this section, we present our method for modeling and learning high-order task relationships in the context of multi-task learning.

Let there be m supervised learning tasks and T_i denote the ith learning task. The training data for T_i is represented by a set of n_i independent and identically distributed (i.i.d.) input-output pairs $\left\{(\mathbf{x}_j^i, y_j^i)\right\}_{j=1}^{n_i}$ with each data point $\mathbf{x}_j^i \in \mathbb{R}^d$ and its corresponding output $y_j^i \in \mathbb{R}$ for a regression task and $y_j^i \in \{-1, 1\}$ for a binary classification task. For both regression and classification tasks, we consider linear functions in the form $f_i(\mathbf{x}) = \mathbf{w}_i^T\mathbf{x} + b_i$ for T_i.

2.1 Generalization of an Existing Method

All existing multi-task learning methods that learn the relationships between tasks only exploit pairwise relationships. We first briefly review a recently proposed method, called Multi-Task Relationship Learning (MTRL) [Zhang and Yeung, 2010a], which belongs to this category of multi-task learning methods. The brief review also serves the purpose of introducing the notation to be used later in the paper. We then propose a novel extension of MTRL for modeling and learning high-order task relationships.

Let the random matrix $\mathbf{W} = (\mathbf{w}_1, \ldots, \mathbf{w}_m)$ denote the model parameters for all m tasks. In MTRL, a matrix-variate normal prior is placed on $\mathbf{W}$:

$$\mathbf{W} \sim \mathcal{MN}_{d\times m}(\mathbf{0}, \mathbf{I}_d \otimes \mathbf{\Omega}), \tag{1}$$

where $\mathbf{0}$ denotes a zero matrix of appropriate size, $\mathbf{I}_d$ denotes a $d \times d$ identity matrix, $\otimes$ denotes the Kronecker product, and $\mathcal{MN}_{d\times m}(\mathbf{M}, \mathbf{A}\otimes\mathbf{B})$ denotes a matrix-variate normal distribution [Gupta and Nagar, 2000] with mean $\mathbf{M} \in \mathbb{R}^{d\times m}$, row covariance matrix $\mathbf{A} \in \mathbb{R}^{d\times d}$ and column covariance matrix $\mathbf{B} \in \mathbb{R}^{m\times m}$, and its probability density function is given by $p(\mathbf{X} \mid \mathbf{M}, \mathbf{A}, \mathbf{B}) = \frac{\exp\left\{-\frac{1}{2}\mathrm{tr}\left[\mathbf{A}^{-1}(\mathbf{X}-\mathbf{M})\mathbf{B}^{-1}(\mathbf{X}-\mathbf{M})^T\right]\right\}}{(2\pi)^{md/2}\,|\mathbf{A}|^{m/2}\,|\mathbf{B}|^{d/2}}$. Here $\mathrm{tr}(\mathbf{Z})$, $\mathbf{Z}^{-1}$ and $|\mathbf{Z}|$ denote the trace, inverse and determinant, respectively, of a square matrix $\mathbf{Z}$. In Eq. (1), the column covariance matrix $\mathbf{\Omega}$ models the pairwise correlation between different columns of $\mathbf{W}$ which are the model parameters for different tasks. Thus $\mathbf{\Omega}$ can be thought of as modeling the pairwise correlation between different tasks via the corresponding model parameters.

Based on the matrix-variate formulation of MTRL given in Eq. (1), we now proceed to propose a generalization which allows high-order task relationships to be modeled as well. Our point of departure is to exploit the close relationships between the matrix-variate normal distribution and the Wishart distribution [Gupta and Nagar, 2000]. It is easy to see that $\mathbf{W}^T$ has the following prior distribution

$$\mathbf{W}^T \sim \mathcal{MN}_{m\times d}(\mathbf{0}, \mathbf{\Omega} \otimes \mathbf{I}_d),$$

if $\mathbf{W}$ follows the prior distribution in Eq. (1). It thus follows that the square matrix $\mathbf{W}^T\mathbf{W}$ follows the Wishart distribution:

$$\mathbf{W}^T\mathbf{W} \sim \mathcal{W}_m(d, \mathbf{\Omega}), \tag{2}$$

where $\mathcal{W}_m(d, \mathbf{\Omega})$ denotes the Wishart distribution for an $m \times m$ positive definite matrix with d degrees of freedom and scale matrix $\mathbf{\Omega}$. Its density function is given by

$$p(\mathbf{X} \mid d, \mathbf{\Omega}) = \frac{|\mathbf{X}|^{\frac{d-m-1}{2}} \exp\left\{-\frac{1}{2}\mathrm{tr}[\mathbf{\Omega}^{-1}\mathbf{X}]\right\}}{2^{md/2}\,\Gamma_m(\frac{d}{2})\,|\mathbf{\Omega}|^{d/2}},$$

where $\Gamma_m(\cdot)$ is the multivariate gamma function. Here we assume that $d \geq m$ or otherwise it will degenerate into a singular distribution [Uhling, 1994]. As we will see later, this assumption is satisfied in our method and in most applications.

The Wishart prior on $\mathbf{W}^T\mathbf{W}$ can help us to understand the role played by the matrix $\mathbf{\Omega}$ better. From the properties of the Wishart distribution [Gupta and Nagar, 2000], we know that the mean and mode of $\mathbf{W}^T\mathbf{W}$ are $d\mathbf{\Omega}$ and $(d-m-1)\mathbf{\Omega}$, respectively, which both depend on $\mathbf{\Omega}$. Since each element of $\mathbf{W}^T\mathbf{W}$ is the dot product of the model parameter vectors of the corresponding tasks, it is a way to express the pairwise correlation between tasks. Thus $\mathbf{\Omega}$ is also related to pairwise task correlation.

We now propose a generalization of the above model for pairwise task relationships to high-order task relationships. We use the following prior distribution

$$(\mathbf{W}^T\mathbf{W})^t \sim \mathcal{W}_m(d, \mathbf{\Omega}), \tag{3}$$

where the integer $t \geq 1$ is called the degree and $\mathbf{X}^t = \mathbf{X}^{t-1}\mathbf{X}$ for a square matrix $\mathbf{X}$. Note that the prior in Eq. (2) is a special case of Eq. (3) when $t = 1$. We first investigate the physical meaning of each element in $(\mathbf{W}^T\mathbf{W})^t$. As discussed above, the (i, j)th element s_{ij} of $\mathbf{W}^T\mathbf{W}$ describes the pairwise similarity between the ith and jth tasks. Since the (i, j)th element s'_{ij} of $(\mathbf{W}^T\mathbf{W})^2$ is calculated as $s'_{ij} = \sum_{k=1}^m s_{ik}s_{jk}$, we can think of it as describing the similarity between the ith and jth tasks via other tasks from the perspective of graph theory. For example, if two tasks are partially similar which may not be reflected in pairwise similarity, then with the help of a third task which is similar to these two tasks, the intrinsic similarity of these two tasks can be found in $(\mathbf{W}^T\mathbf{W})^2$. Hence $(\mathbf{W}^T\mathbf{W})^t$ describes the similarity between any two tasks with the help of other tasks and it can be viewed as a way to model high-order task relationships.

However, Eq. (3) only gives us the prior distribution on $(\mathbf{W}^T\mathbf{W})^t$ but what we actually need is the distribution on $\mathbf{W}$. In what follows, we will show how to obtain the prior $p(\mathbf{W})$ based on Eq. (3).

2.2 Computation of the Prior $p(\mathbf{W})$

For notational simplicity, let us introduce the variable $\mathbf{S}$ to denote $\mathbf{W}^T\mathbf{W}$. Thus

$$\mathbf{S}^t \sim \mathcal{W}_m(d, \mathbf{\Omega}).$$

By using the Jacobian of the transformation from $\mathbf{S}^t$ to $\mathbf{S}$, we obtain the density function for $\mathbf{S}$ as

$$p(\mathbf{S}) = \frac{|\mathbf{S}|^{\frac{t(d-m-1)}{2}} \exp\left\{-\frac{1}{2}\mathrm{tr}[\mathbf{\Omega}^{-1}\mathbf{S}^t]\right\}}{2^{md/2}\,\Gamma_m(\frac{d}{2})\,|\mathbf{\Omega}|^{d/2}} J(\mathbf{S}^t \to \mathbf{S}).$$

where $J(\mathbf{A} \to \mathbf{B})$ denotes the Jacobian of the transformation from variable $\mathbf{A}$ to $\mathbf{B}$. The following lemma from [Mathai, 1997] tells us how to compute the Jacobian $J(\mathbf{S}^t \to \mathbf{S})$ needed for the computation of $p(\mathbf{S})$.

Lemma 1 *For an $m \times m$ square matrix $\mathbf{S}$, we have*

$$J(\mathbf{S}^t \to \mathbf{S}) = \prod_{i,j=1}^{m} F(\lambda_i, \lambda_j, t), \tag{4}$$

where λ_i is the ith largest eigenvalue of $\mathbf{S}$ and $F(\lambda_i,\lambda_j,t) = \sum_{k=0}^{t-1}\lambda_i^k\lambda_j^{t-1-k}$.

With this result, we can now compute $p(\mathbf{S})$ as

$$p(\mathbf{S}) = \frac{|\mathbf{S}|^{\frac{t(d-m-1)}{2}} \exp\left\{-\frac{1}{2}\mathrm{tr}[\mathbf{\Omega}^{-1}\mathbf{S}^t]\right\}\prod_{i,j=1}^{m} F(\lambda_i,\lambda_j,t)}{2^{md/2}\,\Gamma_m(\frac{d}{2})\,|\mathbf{\Omega}|^{d/2}}. \tag{5}$$

Based on $p(\mathbf{S})$ in Eq. (5), Theorem 1 below allows us to compute the density function of $\mathbf{W}$.

Theorem 1 *If a random matrix $\mathbf{S}$ has probability density function as expressed in Eq. (5) and $\mathbf{S} = \mathbf{W}^T\mathbf{W}$ with $\mathbf{W} \in \mathbb{R}^{d\times m}$, the probability density function of $\mathbf{W}$ can be computed as*

$$p(\mathbf{W}) = \frac{|\mathbf{W}^T\mathbf{W}|^{\frac{(t-1)\tilde{d}}{2}} \exp\left\{-\frac{1}{2}\mathrm{tr}[\mathbf{\Omega}^{-1}(\mathbf{W}^T\mathbf{W})^t]\right\}\prod_{i,j} F(\lambda_i,\lambda_j,t)}{(2\pi)^{md/2}\,|\mathbf{\Omega}|^{d/2}}, \tag{6}$$

where $\tilde{d} = d - m - 1$ and λ_i, for $i = 1,\ldots,m$, is the ith largest eigenvalue of $\mathbf{W}^T\mathbf{W}$ or, equivalently, the ith largest squared singular value of $\mathbf{W}$.

Proof: Since $\mathbf{S}$ is symmetric and positive definite, we can express it in terms of the (unique) Cholesky decomposition as $\mathbf{S} = \mathbf{C}\mathbf{C}^T$, where $\mathbf{C}$ is a lower triangular matrix with positive diagonal elements. We define an independent random matrix $\mathbf{L} \in \mathbb{R}^{m\times d}$ such that $\mathbf{L}\mathbf{L}^T = \mathbf{I}_m$, with density given by $\frac{\Gamma_m(\frac{d}{2})}{2^m\pi^{md/2}} g_{d,m}(\mathbf{L})$ where $g_{d,m}(\mathbf{L})$ is as defined in Eq. (1.3.26) in [Gupta and Nagar, 2000]. Then the joint density of $\mathbf{S}$ and $\mathbf{L}$ is

$$p(\mathbf{S},\mathbf{L}) = \frac{|\mathbf{S}|^{\frac{t\tilde{d}}{2}} \exp\left\{-\frac{1}{2}\mathrm{tr}[\mathbf{\Omega}^{-1}\mathbf{S}^t]\right\} g_{d,m}(\mathbf{L})\prod_{i,j} F(\lambda_i,\lambda_j,t)}{(2\pi)^{md/2}\,2^m\,|\mathbf{\Omega}|^{d/2}}.$$

Let us define $\tilde{\mathbf{W}} = \mathbf{L}^T\mathbf{C}^T$. It is easy to show that $\tilde{\mathbf{W}}^T\tilde{\mathbf{W}} = \mathbf{S}$. In order to compute the density of $\tilde{\mathbf{W}}$, we first calculate the Jacobian of the transformation from $\mathbf{S}$ to $\tilde{\mathbf{W}}$ as

$$\begin{aligned}
&J(\mathbf{S} \to \tilde{\mathbf{W}})\\
=&J(\mathbf{S} \to \mathbf{C})J(\mathbf{C},\mathbf{L} \to \tilde{\mathbf{W}}) \text{ (chain rule)}\\
=&\frac{J(\mathbf{S} \to \mathbf{C})}{J(\tilde{\mathbf{W}} \to \mathbf{C},\mathbf{L})} \text{ (property of Jacobian transformation)}\\
=&\frac{2^m\prod_{i=1}^m c_{ii}^{m-i+1}}{g_{d,m}(\mathbf{L})\prod_{i=1}^m c_{ii}^{d-i}} \text{ (property of Jacobian transformation)}\\
=&\frac{2^m}{g_{d,m}(\mathbf{L})\,|\tilde{\mathbf{W}}^T\tilde{\mathbf{W}}|^{\frac{\tilde{d}}{2}}}, \text{ (property of Cholesky decomposition)}
\end{aligned}$$

where c_{ij} is the (i,j)th element of $\mathbf{C}$. We can then get the density function of $\tilde{\mathbf{W}}$ as

$$p(\tilde{\mathbf{W}}) = \frac{|\tilde{\mathbf{W}}^T\tilde{\mathbf{W}}|^{\frac{(t-1)\tilde{d}}{2}} \exp\left\{-\frac{1}{2}\mathrm{tr}[\mathbf{\Omega}^{-1}(\tilde{\mathbf{W}}^T\tilde{\mathbf{W}})^t]\right\}\prod_{i,j} F(\lambda_i,\lambda_j,t)}{(2\pi)^{md/2}\,|\mathbf{\Omega}|^{d/2}}.$$

It is easy to show that $\tilde{\mathbf{W}} = \mathbf{P}\mathbf{W}$ for some orthogonal matrix $\mathbf{P} \in \mathbb{R}^{d\times d}$. Because $J(\tilde{\mathbf{W}} \to \mathbf{W}) = |\mathbf{P}|^d = 1$, we can get the density function of $\mathbf{W}$ in Eq. (6). Since λ_i is the ith largest eigenvalue of $\mathbf{S} = \mathbf{W}^T\mathbf{W}$, λ_i is also the ith largest squared singular value of $\mathbf{W}$. This completes the proof. ■

When $t = 1$, the density function in Eq. (6) will degenerate to the matrix-variate normal distribution used in the MTRL model [Zhang and Yeung, 2010a] since the first term in the numerator of Eq. (6) disappears and $F(\lambda_i,\lambda_j,t) = 1$. Hence the prior defined in Eq. (6) can be viewed as a generalization of the matrix-variate normal prior.

2.3 Properties of the Prior $p(\mathbf{W})$

We briefly present here some properties of the prior on $\mathbf{W}$ with the general form of the density function given in Eq. (6).

Theorem 2 $\mathbb{E}[\mathbf{W}] = \mathbf{0}$*, where $\mathbb{E}[\cdot]$ denotes the expectation operator.*

Proof: From the definition of expectation, $\mathbb{E}[\mathbf{W}] = \int \mathbf{W}p(\mathbf{W})d\mathbf{W}$. It is easy to show that $p(\mathbf{W}) = p(-\mathbf{W})$ implying $\mathbf{W}p(\mathbf{W}) + (-\mathbf{W})p(-\mathbf{W}) = \mathbf{0}$. So we can obtain

$$\mathbb{E}[\mathbf{W}] = \int \mathbf{W}p(\mathbf{W})d\mathbf{W} = \mathbf{0}$$

which is the conclusion. □

We may generalize the density of $\mathbf{W}$ in Eq. (6) by replacing $\mathbf{W}$ with $(\mathbf{W}-\mathbf{M})$ for any $\mathbf{M} \in \mathbb{R}^{d\times m}$ and then we can easily get $\mathbb{E}[\mathbf{W}] = \mathbf{M}$.

As a consequence of using the matrix-variate normal prior in MTRL, we note that the different rows of $\mathbf{W}$ under the prior in Eq. (1) are independent due to the fact that $p(\mathbf{W}) = \prod_{j=1}^{d} p(\mathbf{w}^{(j)})$ where $\mathbf{w}^{(j)}$ is the jth row of $\mathbf{W}$. So the prior in MTRL cannot capture the dependency between different features. For our method, it is easy to show that $p(\mathbf{W}) \neq \prod_{j=1}^{d} p(\mathbf{w}^{(j)})$ and hence our method can capture feature dependency to a certain extent. This capability is an extra advantage of our method over MTRL in addition to exploiting high-order task relationships.

From the properties of the Wishart distribution, we also have the following results.

Theorem 3 $\mathbb{E}[(\mathbf{W}^T\mathbf{W})^t] = d\mathbf{\Omega}$.

Theorem 4 $\text{Mode}[(\mathbf{W}^T\mathbf{W})^t] = (d-m-1)\mathbf{\Omega}$ *when* $d \geq m+1$, *where* $\text{Mode}[\cdot]$ *denotes the mode operator.*

2.4 Model Formulation and Learning

Eq. (6) defines the prior of $\mathbf{W}$. For the likelihood, we use the (univariate) normal distribution which corresponds to the squared loss:

$$y_j^i \mid \mathbf{x}_j^i, \mathbf{w}_i, \mathbf{b}_i \sim \mathcal{N}(\mathbf{w}_i^T\mathbf{x}_j^i + b_i, \sigma_i^2), \tag{7}$$

where $\mathcal{N}(\mu, \sigma^2)$ denotes the univariate normal distribution with mean μ and variance σ^2.

For computational efficiency, as in MTRL, we seek to find the *maximum a posteriori* (MAP) solution as a point estimate based on the prior in Eq. (6) and the likelihood in Eq. (7). The optimization problem can equivalently be formulated as the following minimization problem:

$$\begin{aligned}\min_{\mathbf{W},\mathbf{b},\boldsymbol{\sigma},\mathbf{\Omega}} L =& \sum_{i=1}^{m}\sum_{j=1}^{n_i}\left[\frac{(\mathbf{w}_i^T\mathbf{x}_j^i + b_i - y_j^i)^2}{2\sigma_i^2} + \ln\sigma_i\right] + \frac{d}{2}\ln|\mathbf{\Omega}| \\ &- \sum_{i,j=1}^{m}\ln F(\lambda_i,\lambda_j,t) - \frac{(t-1)\tilde{d}}{2}\ln|\mathbf{W}^T\mathbf{W}| \\ &+ \frac{1}{2}\text{tr}\left[\mathbf{\Omega}^{-1}(\mathbf{W}^T\mathbf{W})^t\right],\end{aligned} \tag{8}$$

where $\mathbf{b} = (\mathbf{b}_1, \ldots, \mathbf{b}_m)^T$ and $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_m)^T$. Since the problem (8) seems complicated, we make some simplification first. By setting the gradient of L with respect to $\mathbf{\Omega}^{-1}$ to zero, we can get

$$\frac{\partial L}{\partial \mathbf{\Omega}^{-1}} = \Big((\mathbf{W}^T\mathbf{W})^t - d\mathbf{\Omega}\Big) - \frac{1}{2}\Big((\mathbf{W}^T\mathbf{W})^t - d\mathbf{\Omega}\Big)\odot \mathbf{I}_m = 0,$$

where $\odot$ denotes the Hadamard product or equivalently the matrix elementwise product, which suggests an analytical solution for $\mathbf{\Omega}$ as

$$\mathbf{\Omega} = \frac{1}{d}(\mathbf{W}^T\mathbf{W})^t. \tag{9}$$

Plugging the solution of $\mathbf{\Omega}$ in Eq. (9) to the function L, we can reformulate L as follows by omitting some constant terms

$$\begin{aligned}\min_{\mathbf{W},\mathbf{b},\boldsymbol{\sigma}} L =& \sum_{i=1}^{m}\sum_{j=1}^{n_i}\left[\frac{(\mathbf{w}_i^T\mathbf{x}_j^i + b_i - y_j^i)^2}{2\sigma_i^2} + \ln\sigma_i\right] + \frac{\beta}{2}\ln|\mathbf{W}^T\mathbf{W}| \\ &- \sum_{i,j=1}^{m}\ln F(\lambda_i,\lambda_j,t),\end{aligned} \tag{10}$$

where $\beta = d + (m+1)(t-1)$. Note that problem (10) is non-convex and it is not easy to optimize with respect to all variables simultaneously. We use an alternating method instead.

Each iteration of the iterative learning procedure involves two steps. In the first step, $\mathbf{W}$ is held fixed while minimizing the objective function in (10) with respect to $\mathbf{b}$ and $\boldsymbol{\sigma}$. We compute the gradients of L with respect to b_i and σ_i as

$$\begin{aligned}\frac{\partial L}{\partial \sigma_i} &= \sum_{j=1}^{n_i}\left[-\frac{(\mathbf{w}_i^T\mathbf{x}_j^i + b_i - y_j^i)^2}{\sigma_i^3} + \frac{1}{\sigma_i}\right], \\ \frac{\partial L}{\partial b_i} &= \sum_{j=1}^{n_i}\frac{b_i + \mathbf{w}_i^T\mathbf{x}_j^i - y_j^i}{\sigma_i^2},\end{aligned}$$

and set them to 0 to obtain the analytical solutions for making the update:

$$\sigma_i^2 = \frac{1}{n_i}\sum_{j=1}^{n_i}(\mathbf{w}_i^T\mathbf{x}_j^i + b_i - y_j^i)^2,\ b_i = \frac{1}{n_i}\sum_{j=1}^{n_i}(y_j^i - \mathbf{w}_i^T\mathbf{x}_j^i)$$

In the second step of each iteration, optimization is done with respect to $\mathbf{W}$ while keeping all other variables fixed. Since there is no analytical solution for $\mathbf{W}$, we use the conjugate gradient method to find the solution using the following gradient

$$\begin{aligned}\frac{\partial L}{\partial \mathbf{W}} =& \sum_{i=1}^{m}\sum_{j=1}^{n_i}\frac{\mathbf{x}_j^i(\mathbf{x}_j^i)^T\mathbf{W}\mathbf{e}_i\mathbf{e}_i^T + (b_i - y_j^i)\mathbf{x}_j^i\mathbf{e}_i^T}{\sigma_i^2} \\ &- \sum_{i,j=1}^{m}\frac{\partial \ln F(\lambda_i,\lambda_j,t)}{\partial \mathbf{W}} + \beta\mathbf{W}(\mathbf{W}^T\mathbf{W})^{-1},\end{aligned}$$

where $\mathbf{e}_i$ is the ith column of the $m\times m$ identity matrix. The term $\frac{\partial \ln F(\lambda_i,\lambda_j,t)}{\partial \mathbf{W}}$ can be calculated as

$$\begin{aligned}&\frac{\partial \ln F(\lambda_i,\lambda_j,t)}{\partial \mathbf{W}} \\ &= \begin{cases}\frac{t-1}{\lambda_i}\frac{\partial \lambda_i}{\partial \mathbf{W}} & \text{if } \lambda_i = \lambda_j \\ \frac{t\left(\lambda_i^{t-1}\frac{\partial\lambda_i}{\partial \mathbf{W}} - \lambda_j^{t-1}\frac{\partial \lambda_j}{\partial \mathbf{W}}\right)}{\lambda_i^t - \lambda_j^t} - \frac{\frac{\partial\lambda_i}{\partial \mathbf{W}} - \frac{\partial\lambda_j}{\partial \mathbf{W}}}{\lambda_i - \lambda_j} & \text{otherwise}\end{cases}\end{aligned}$$

where, by using the chain rule, we can calculate $\frac{\partial \lambda_i}{\mathbf{W}}$ as

$$\frac{\partial\lambda_i}{\partial \mathbf{W}} = \frac{\partial\lambda_i}{\partial\rho_i}\frac{\partial\rho_i}{\partial \mathbf{W}} = \frac{\partial\rho_i^2}{\partial\rho_i}\frac{\partial\frac{1}{\alpha_i}\text{tr}(\mathbf{U}_i^T\mathbf{W}\mathbf{V}_i)}{\partial \mathbf{W}} = \frac{2\rho_i}{\alpha_i}\mathbf{U}_i\mathbf{V}_i^T \tag{11}$$

where $\mathbf{W} = \mathbf{U}\mathbf{D}\mathbf{V}^T$ is the thin singular value decomposition of $\mathbf{W}$ (since $d \geq m$) with orthogonal matrices $\mathbf{U} \in \mathbb{R}^{d\times m}$ and $\mathbf{V} \in \mathbb{R}^{m\times m}$ and the diagonal matrix $\mathbf{D}$ containing the singular values ρ_i, α_i is the repeatedness of ρ_i, and $\mathbf{U}_i \in \mathbb{R}^{d\times\alpha_i}$ and $\mathbf{V}_i \in \mathbb{R}^{m\times\alpha_i}$ are the left and right singular vectors or matrices corresponding to the singular value ρ_i. The second step of the above derivation (11) holds since $\mathbf{U}_i^T\mathbf{W}\mathbf{V}_i = \rho_i\mathbf{I}_{\alpha_i}$ and $\lambda_i = \rho_i^2$ due to the relation between the ith largest eigenvalue λ_i of $\mathbf{W}^T\mathbf{W}$ and the ith largest singular value of $\mathbf{W}$.

2.5 Kernel Extension

A natural question to ask is whether the method presented above can be extended to the general nonlinear case using the kernel trick.

Unlike MTRL [Zhang and Yeung, 2010a] and other kernel methods such as the support vector machine, using the higher-order form of $\mathbf{W}$ in our method does not allow us to use the dual form to facilitate kernel extension. However, kernel extension is still possible by adopting a different strategy used before by some Bayesian kernel methods such as the relevance vector machine [Tipping, 2001].

Specifically, the kernel information can be directly incorporated into the data representation by defining a new data representation as follows:

$$\tilde{\mathbf{x}}_j^i = \Big(k(\mathbf{x}_j^i, \mathbf{x}_1^1), \ldots, k(\mathbf{x}_j^i, \mathbf{x}_{n_m}^m)\Big)^T,$$

where $k(\cdot,\cdot)$ is some kernel function such as the linear kernel or RBF kernel. With the new representation, we can use the method presented in the previous section to learn a good model. It is easy to show that $\tilde{\mathbf{x}}_j^i \in \mathbb{R}^n$ where n is the total number of data points in all tasks. As a consequence, another benefit of this kernel extension scheme is that the dimensionality n of each data point is larger than the number of tasks m and hence satisfies the requirement of our new prior and the model. In case the dimensionality n of the new data representation is very high, we may first apply a dimensionality reduction method such as principal component analysis to find a lower-dimensional representation before model learning.

3 Experiments

We report the empirical studies in this section to compare MTHOL with several related methods. Since MTHOL generalizes MTRL [Zhang and Yeung, 2010a] by learning high-order task relationships, MTRL will be included in the comparative study. Moreover, we have also included the other methods considered in the comparative study of the MTRL paper, including a single-task learning (STL) method, multi-task feature learning (MTFL) method [Argyriou *et al.*, 2006] as well as multi-task GP (MTGP) method [Bonilla *et al.*, 2007] which, like MTRL, can learn task relationships. For fair comparison, the data we used for all methods adopt the new representation described in section 2.5 when a kernel is used.

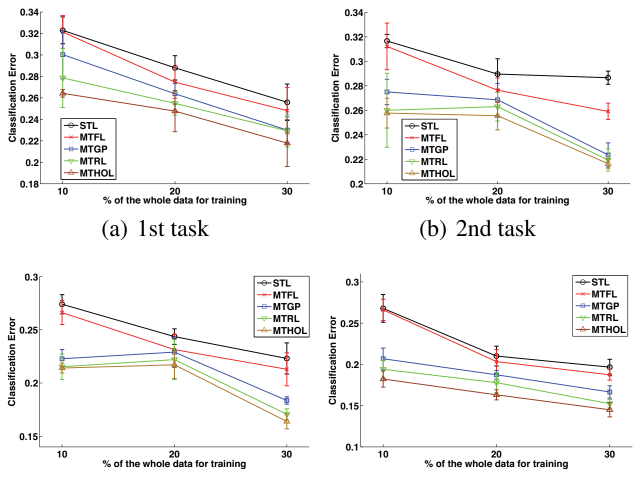
3.1 Robot Inverse Dynamics

This application[1] is on learning the inverse dynamics of a 7-DOF robot arm. The input consists of 21 features corresponding to the joint angles, velocities and accelerations of the seven joints, and the output consists of seven joint torques which are used for seven regression tasks. There are 2000 data points in each task. We use the normalized mean squared error (nMSE), the mean squared error divided by the variance of the ground-truth output, as the performance measure. Kernel ridge regression is used as the STL baseline for this data set.

We perform two sets of experiments on all the methods with different numbers of training data points. The first setting randomly selects 10% of the data for each task as the training set and the second setting selects 20%. Those not selected for training are used for testing. For all methods, the RBF kernel is adopted. For each setting, we report the mean and standard deviation of the performance measure over 10 random splits of the data. Table 1 depicts the results, with the best ones shown in bold. Paired t-test and ANOVA test at 5% significance level show that MTHOL with $t = 2$ is the best for some tasks and is comparable with the best for other tasks.

3.2 Multi-Domain Sentiment Application

The second one is a multi-domain sentiment classification application[2]. Four binary classification tasks correspond to four domains of products at Amazon.com, which include books, DVDs, electronics and kitchen appliances. For each domain, there are 1000 positive and 1000 negative product reviews corresponding to the two classes of the classification problem. The document representation for each review contains 473856 feature dimensions. Like the above experiments, we use training sets of different sizes for training, corresponding to 10%, 20% and 30% of the data for each task. Classification error is used as the performance measure. For the STL baseline, we use a linear SVM which has been demonstrated to perform well for such text classification applications with high feature dimensionality. For other compared methods, we also use the linear kernel. As above, we perform 10 random data splits and report the mean and standard deviation of the classification error in Figure 1(a) to Figure 1(d). Again, for all settings, MTHOL is either the best or among the best by using paired t-test and ANOVA significance test.



(a) 1st task (b) 2nd task

(c) 3rd task (d) 4th task

Figure 1: Performance of STL, MTFL, MTGP, MTRL and MTHOL on each task of the multi-domain sentiment application when the training set size is varied.

3.3 Examination Score Prediction

This application is a regression problem for predicting the examination scores of the students from 139 secondary schools (http://www.cs.ucl.ac.uk/staff/A.Argyriou/code/). There are

[1]http://www.gaussianprocess.org/gpml/data/

[2]http://www.cs.jhu.edu/∼mdredze/datasets/sentiment/

Table 1: Results on learning robot inverse dynamics. For each method and each task, the two rows report the mean and standard deviation of the nMSE over 10 trials. The upper (lower) table records the results of the setting with 10% (20%) of the data for the training set.

Method	1st	2nd	3rd	4th	5th	6th	7th
STL	0.1507	0.1920	0.1866	0.0283	0.3563	0.6454	0.0409
	0.0077	0.0087	0.0054	0.0038	0.0246	0.0202	0.0016
MTFL	0.1404	0.1953	0.1823	0.0221	0.3294	0.6497	0.0470
	0.0056	0.0079	0.0195	0.0127	0.0139	0.0118	0.0044
MTGP	0.0926	0.1471	0.1084	0.0116	0.3465	0.6833	0.0438
	0.0035	0.0076	0.0067	0.0013	0.0070	0.0109	0.0190
MTRL	0.0879	0.1358	**0.1030**	0.0098	0.3248	0.6223	**0.0387**
	0.0008	0.0038	0.0034	0.0017	0.0054	0.0034	0.0073
MTHOL	**0.0782**	**0.1242**	**0.1035**	**0.0082**	**0.3158**	**0.6032**	**0.0372**
(*t*=2)	0.0019	0.0048	0.0050	0.0015	0.0096	0.0094	0.0042

Method	1st	2nd	3rd	4th	5th	6th	7th
STL	0.1140	0.1714	0.1537	0.0141	0.2805	0.5501	0.0298
	0.0027	0.0032	0.0046	0.0005	0.0062	0.0161	0.0018
MTFL	0.1131	0.1800	0.1516	0.0187	0.2832	0.5596	0.0371
	0.0029	0.0050	0.0045	0.0014	0.0081	0.0142	0.0034
MTGP	0.0813	0.1208	**0.0893**	**0.0088**	0.2982	0.5453	0.0346
	0.0023	0.0058	0.0048	0.0004	0.0093	0.0252	0.0134
MTRL	0.0812	0.1122	0.0947	**0.0087**	0.2712	0.5429	0.0282
	0.0021	0.0032	0.0028	0.0013	0.0031	0.0060	0.0007
MTHOL	**0.0706**	**0.0980**	**0.0898**	**0.0078**	**0.1333**	**0.5243**	**0.0200**
(*t*=2)	0.0029	0.0034	0.0041	0.0016	0.0050	0.0077	0.0027

139 learning tasks corresponding to the 139 schools, with a total of 15362 data points. There are 27 input attributes representing information about both the schools and the students. Like the experiment setting on robot inverse dynamics, we use the nMSE as performance measure and kernel ridge regression as the STL baseline. We also use 10% and 20% of the data for training. Table 2 summarizes the results over 10 random data splits. We can see that MTHOL outperforms all other methods.

Table 2: Results (in mean±deviation) on examination score prediction for different training set sizes.

Method	10%	20%
STL	1.0744±0.0235	0.9549±0.0116
MTFL	0.8868±0.0235	0.7341±0.0077
MTGP	0.7267±0.0078	0.6282±0.0115
MTRL	0.7085±0.0160	0.5963±0.0194
MTHOL	**0.6889±0.0183**	**0.5717±0.0154**

3.4 Handwritten Letter Classification

The handwritten letter data set is another classification application (http://multitask.cs.berkeley.edu/). It consists of seven tasks each of which is a binary classification problem for two letters: c/e, g/y, m/n, a/g, a/o, f/t and h/n. The input for each data point consists of 128 features representing the pixel values of the handwritten letter. For each task, there are about 1000 positive and 1000 negative examples. Similar to the multi-domain sentiment classification problem, different settings correspond to 10%, 20% and 30% of the data for training and the performance measure is the classification error. From Table 3, MTHOL again gives very competitive results.

Table 3: Results (in mean±deviation) on handwritten letter classification for different training set sizes.

Method	10%	20%	30%
STL	0.0949±0.0016	0.0794±0.0035	0.0765±0.0010
MTFL	0.0843±0.0073	0.0758±0.0045	0.0734±0.0024
MTGP	0.0767±0.0039	0.0691±0.0068	0.0660±0.0020
MTRL	0.0733±0.0044	0.0615±0.0072	**0.0601±0.0033**
MTHOL	**0.0687±0.0057**	**0.0547±0.0040**	**0.0598±0.0034**

4 Conclusion

In this paper, we have proposed a novel, nontrivial generalization of an existing multi-task learning method by modeling and learning high-order task relationships.

Although our method can use different values for the degree t, its value has to be set in advance and fixed during model learning. One possible direction to extend the current method is to allow the degree t to be learned from data automatically. To address this issue in our future work, we plan to adopt the full Bayesian approach which may bring about further performance improvement by making model selection via hyperparameter learning as an integral part of model learning.

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