

Multi-Task Learning: Theory, Algorithms, and Applications

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The Twelfth SIAM Information Conference on Data Mining, April 27, 2012



Tutorial Goals

- Understand the basic concepts in multi-task learning
- Understand different approaches to model task relatedness
- Get familiar with different types of multi-task learning techniques
- Introduce multi-task learning applications
- Introduce the multi-task learning package: MALSAR



Tutorial Road Map

- Part I: Multi-task Learning (MTL) background and motivations
- Part II: MTL formulations
- Part III: Case study of real-world applications
 - Incomplete Multi-Source Fusion
 - Drosophila Gene Expression Image Analysis
- Part IV: An MTL Package (MALSAR)
- Current and future directions



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ARIZONA STATE UNIVERSITY

Multiple Tasks

• Examination Scores Prediction¹ (Argyriou *et. al.*'08)

School 1 - Alverno High School





School 138 - Jefferson Intermediate School





School 139 - Rosemead High School



¹The Inner London Education Authority (ILEA)

-



Learning Multiple Tasks

• Learning each task independently

School 1 -	Alverno H	igh School					
Student id	Birth year	Previous score	School ranking	 \longrightarrow	Exam Score	task 1st	
72981	1985	95	83%		?		
							Excellent



School 139	- Rosem	ead High Sch	nool				
Student id	Birth year	Previous score	School ranking	 \rightarrow	Exam Score	task 139th	1 Sol
12381	1986	83	77%		?		
						/	Excellent



Learning Multiple Tasks

• Leaning multiple tasks simultaneously











Performance of MTL

- Evaluation on the *School* data:
 - Predict exam scores for 15362 students from 139 schools
 - Describe each student by 27 attributes
 - Compare single task learning approaches (Ridge Regression, Lasso) and one multi-task learning approach (trace-norm regularized learning)



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Multi-Task Learning

- Multi-task Learning is different from single task learning in the training (induction) process.
- Inductions of multiple tasks are performed simultaneously to capture intrinsic relatedness.





Learning Methods



- o Multi-task Learning
 - Model the task relatedness
 - Learn all tasks simultaneously
 - Tasks may have different data/features
- o Multi-label Learning
 - Model the label relatedness
 - Learn all labels simultaneously
 - Labels share the same data/features
- Multi-class Learning
 - Learn the classes independently
 - All classes are exclusive



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Web Pages Categorization

Chen et. al. 2009 ICML

- Classify documents into categories
- The classification of each category is a task
- The tasks of predicting different categories may be latently related



Home U.S.	World	Politics	Business	Sports	Entertainment	Health	Tech & science	Travel	Local	Weather	
Gadhafi vows 'lo	ng war' aft	er US, allies	strike		Video		Africa		World Blog		
Joy in rebel stronghold after Western attack					indicat	Pentagon: 'No indications of	Americas	Americas		Behind the Wall	
Japan reports pro	ogress at le	eaking nucle	ear complex		civiliar	a casualties'	Europe		Wonderful V	Norld	
Mullen: Chance (Gadhafi co	uld cling to	power		Slides		Mideast & N. Afr	ica	Weather		
Egypt: Voters OK constitution changes				The second		The Week in Pictures	Asia-Pacific		PhotoBlog		
Woman, grandso	on found ur	nder rubble i	in Japan			11111111111111111111111111111111111111	South & Central	Asia	The Windso	or Knot	
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MTL for HIV Therapy Screening

Bickel *et. al.* ICML 08

- Hundreds of possible combinations of drugs, some of which use similar biochemical mechanisms
- The samples available for each combination are limited.
- For a patient, the prediction of using one combination is a task
- Use the similarity information by multiple task learning







Other Applications

- Portfolio selection [Ghosn and Bengio, NIPS'97]
- Collaborative ordinal regression [Yu et. al. NIPS'06]
- Web image and video search [Wang *et. al.* CVPR'09]
- Disease progression modeling [Zhou *et. al.* KDD'11]
- Disease prediction [Zhang *et. al.* NeuroImage 12]



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How Tasks Are Related



Assumption: All tasks are related

Methods

- Mean-regularized MTL
- Joint feature learning
- Trace-Norm regularized MTL
- Alternating structural optimization (ASO)
- Shared Parameter Gaussian Process



How Tasks Are Related



Assumption: There are outlier tasks

- Assume all tasks are related may be too strong for practical applications.
- There are some irrelevant (outlier) tasks.



How Tasks Are Related



Methods

- Clustered MTL
- Tree MTL
- Network MTL





Multi-Task Learning Methods

- Regularization-based MTL
 - All tasks are related
 - regularized MTL, joint feature learning, low rank MTL, ASO
 - Learning with outlier tasks: robust MTL
 - Tasks form groups/graphs/trees
 - clustered MTL, network MTL, tree MTL
- Other Methods
 - Shared Hidden Nodes in Neural Network
 - Shared Parameter Gaussian Process



Regularization-based Multi-Task Learning

- All tasks are related
 - Mean-Regularized MTL
 - MTL in high dimensional feature space
 - Embedded Feature Selection
 - Low-Rank Subspace Learning
- Clustered MTL
- MTL with Tree/Graph structure



Notation



• We focus on linear models: $Y_i = X_i \times W_i$ $X_i \in \mathbb{R}^{n_i \times d}, Y_i \in \mathbb{R}^{n_i \times 1}, W = [W_1, W_2, ..., W_m]$



Mean-Regularized Multi-Task Learning

Evgeniou & Pontil, 2004 KDD

- Assumption: task parameter vectors of all tasks are close to each other.
 - Advantage: simple, intuitive, easy to implement
 - Disadvantage: may not hold in real applications.

Regularization

penalizes the deviation of each task from the mean

$$\min_{W} \frac{1}{2} \|XW - Y\|_{F}^{2} + \lambda \sum_{i=1}^{m} \left\| W_{i} - \frac{1}{m} \sum_{s=1}^{m} W_{s} \right\|_{2}^{2}$$





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Multi-Task Learning with High Dimensional Data

- In practical applications, we may deal with high dimensional data.
 - Gene expression data, biomedical image data
- Curse of Dimensionality
- Dealing with high dimensional data in multi-task learning
 - Embedded feature selection: L_1/L_q Group Lasso
 - Low-rank subspace learning: low-rank assumption ASO, Trace-norm regularization



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Multi-Task Learning with Joint Feature Learning

- One way to capture the task relatedness from multiple related tasks is to constrain all models to share a common set of features.
- For example, in school data, the scores from different schools may be determined by a similar set of features.





Multi-Task Learning with Joint Feature Learning

Obozinski et. al. 2009 Stat Comput, Liu et. al. 2010 Technical Report

- Using group sparsity: ℓ_1/ℓ_q -norm regularization
- When q>1 we have group sparsity.



$$\min_{W} \frac{1}{2} \|XW - Y\|_{F}^{2} + \lambda \|W\|_{1,q}$$



Writer-Specific Character Recognition

Obozinski, Taskar, and Jordan, 2006

• Each task is a classification between two letters for one writer.

	pixels: error (%)							
Task	ℓ_1/ℓ_2	ℓ_1/ℓ_1	$\mathrm{id}.\ell_1$	pool				
c/e	4.0	8.5	9.0	4.5				
g/y	11.4	16.1	17.2	18.6				
g/s	4.4	10.0	10.3	6.9				
m/n	2.5	6.3	6.9	4.1				
a/g	1.3	3.6	4.1	3.6				
i/j	12.0	14.0	14.0	11.3				
a/o	2.8	4.8	5.2	4.2				
f/t	5.0	6.7	6.1	8.2				
h/n	3.2	14.3	18.6	5.0				

Dirty Model for Multi-Task Learning

Jalali et. al. 2010 NIPS

• In practical applications, it is too restrictive to constrain all tasks to share a single shared structure.





Robust Multi-Task Learning

Most Existing MTL Approaches
Robust MTL Approaches





Robust Multi-Task Feature Learning

Gong et. al. 2012 Submitted

• Simultaneously captures a common set of features among relevant tasks and identifies outlier tasks.



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Trace-Norm Regularized MTL

Capture task relatedness via a shared low-rank structure





• Assume we have a rank 2 model matrix:



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Ji et. al. 2009 ICML

- Rank minimization formulation
 - $-\min_{W} \text{Loss}(W) + \lambda \times \text{Rank}(W)$
 - Rank minimization is NP-Hard for general loss functions
- Convex relaxation: trace norm minimization
 - $\min_{W} \text{Loss}(W) + \lambda \times ||W||_{*}$ $||W||_{*}$: sum of singular values of W
 - The trace norm is theoretically shown to be a good approximation for rank function (Fazel et al., 2001).



- Evaluation on the *School* data:
 - Predict exam scores for 15362 students from 139 schools
 - Describe each student by 27 attributes
 - Compare Ridge Regression, Lasso, and Trace Norm (for inducing a low-rank structure)




Alternating Structure Optimization (ASO)

Ando and Zhang, 2005 JMRL

• ASO assumes that the model is the sum of two components: a task specific one and a shared low dimensional subspace.





Alternating Structure Optimization (ASO)



• Empirical loss function for i-th task

$$\mathcal{L}_{i}(X_{i}(\Theta v_{i} + w_{i}), y_{i}) = ||X_{i}(\Theta v_{i} + w_{i}) - y_{i}||^{2}$$

• ASO simultaneously learns *models* and the *shared structure*:

$$\begin{split} & \min_{\boldsymbol{\theta}, \{v_i, w_i\}} \sum_{i=1}^m \{ \mathcal{L}_i(X_i(\boldsymbol{\theta} v_i + w_i), y_i) + \alpha \| w_i \|^2 \} \\ \text{subject to} & \boldsymbol{\theta}^T \boldsymbol{\theta} = \mathbf{I} \end{split}$$



iASO Formulation

Chen et al., 2009 ICML

 \circ iASO formulation

$$\min_{\substack{\boldsymbol{\theta}, \{v_i, w_i\}\\ \boldsymbol{\theta} \in \mathbf{I}}} \sum_{i=1}^{m} \{ \mathcal{L}_i(X_i(\boldsymbol{\theta} v_i + w_i), y_i) + \alpha \| \boldsymbol{\theta} v_i + w_i \|^2 + \beta \| w_i \|^2 \}$$
subject to
$$\begin{array}{l} \prod_{i=1}^{m} \{\mathcal{L}_i(X_i(\boldsymbol{\theta} v_i + w_i), y_i) + \alpha \| \boldsymbol{\theta} v_i + w_i \|^2 + \beta \| w_i \|^2 \} \\ = 1 \end{array}$$

- control both *model complexity* and task relatedness
- subsume ASO (Ando et al.'05) as a special case
- naturally lead to a convex relaxation (Chen et al., 09, ICML)
- Convex relaxed ASO is equivalent to iASO under certain mild conditions



Capture task relatedness

Incoherent Low-Rank and Sparse Structures

Chen *et. al.* 2010 KDD

• ASO uses L2-norm on task-specific component, we can also use L1-norm to learn task-specific features.

Task-specific features



W





Robust Low-Rank in MTL

Chen et. al. 2011 KDD

• Simultaneously perform low-rank MTL and identify outlier tasks.





al al sub-training an

Summary

- All multi-task learning formulations discussed above can fit into the **W=P+Q** schema.
 - Component P: shared structure
 - Component Q: information not captured by the shared structure

Embedded Feature Selection	Shared Structure P	Component Q
L1/Lq	Feature Selection (L1/Lq Norm)	0
Dirty	Feature Selection (L1/Lq Norm)	L1-norm
rMTFL	Feature Selection (L1/Lq Norm)	Outlier (column-wise L1/Lq Norm)
Low-Rank Subspace Learning		
Trace Norm	Low-Rank (Trace Norm)	0
ISLR	Low-Rank (Trace Norm)	L1-norm
ASO	Low-Rank (Shared Subspace)	L2-norm on independent comp.
RMTL	Low-Rank (Trace Norm)	Outlier (column-wise L1/Lq Norm)



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Multi-Task Learning with Clustered Structures

- Most MTL techniques assume all tasks are related
- Not true in many applications
- Clustered multi-task learning assumes
 - the tasks have a group structure
 - the models of tasks from the same group are closer to each other than those from a different group



e.g. tasks in the yellow group are predictions of heart related diseases and in the blue group are brain related diseases.



Clustered Multi-Task Learning

Jacob et. al. 2008 NIPS, Zhou et. al. 2011 NIPS

• Use regularization to capture clustered structures.



Clustered Multi-Task Learning

Zhou et. al. 2011 NIPS

 Capture structures by minimizing sumof-square error (SSE) in K-means clustering:

$$\min_{I} \sum_{j=1}^{k} \sum_{v \in I_{j}} \left\| w_{v} - \overline{w}_{j} \right\|_{2}^{2}$$

$$I_{j} \text{ index set of } j^{\text{th}} \text{ cluster}$$

$$\min_{F} \operatorname{tr}(W^{T}W) - \operatorname{tr}(F^{T}W^{T}WF)$$

 $F: m \times k$ orthogonal cluster indicator matrix $F_{i,j} = 1/\sqrt{n_j}$ if $i \in I_j$ and 0 otherwise



task number m > cluster number k



Clustered Multi-Task Learning

Zhou et. al. 2011 NIPS

 Directly minimizing SSE is hard because of the non-linear constraint on F:

$$\min_F \operatorname{tr}(W^T W) - \operatorname{tr}(F^T W^T W F)$$

 $F: m \times k$ orthogonal cluster indicator matrix $F_{i,j} = 1/\sqrt{n_j}$ if $i \in I_j$ and 0 otherwise

$$\min_{F:F^T F=I_k} \operatorname{tr}(W^T W) - \operatorname{tr}(F^T W^T W F)$$

Zha et. al. 2001 NIPS



task number m > cluster number k



Cluster k-1

Clustered Multi-Task Learning

Zhou et. al. 2011 NIPS

• Clustered multi-task learning (CMTL) formulation

$$\min_{W,F:F^{T}F=I_{k}} \text{Loss}(W) + \alpha[\text{tr}(W^{T}W) - \text{tr}(F^{T}W^{T}WF)] + \beta \text{tr}(W^{T}W)$$

$$\text{capture cluster structures}$$

$$\lim_{Cluster 1} Cluster 2$$

- CMTL has been shown to be equivalent to ASO
 - Given the dimension of the shared low-rank subspace in ASO and the cluster number in clustered multi-task learning (CMTL) are the same.



Convex Clustered Multi-Task Learning

Zhou et. al. 2011 NIPS





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- In some applications, the tasks may be equipped with a tree structure:
 - The tasks belonging to the same node are similar to each other
 - The similarity between two nodes is related to the depth of the 'common' tree node





Kim and Xing 2010 ICML

• Tree-Guided Group Lasso





- In real applications, tasks involved in MTL may have graph structures
 - The two tasks are related if they are connected in a graph, i.e. the connected tasks are similar
 - The similarity of two related tasks can be represented by the weight of the connecting edge.





- A simple way to encode graph structure is to penalize the difference of two tasks that have an edge between them
- Given a set of edges E, we thus penalize: $\sum_{i=1}^{|E|} \left\| W_{e_{\{i,1\}}} - W_{e_{\{i,2\}}} \right\|_2^2 = \|WR^T\|_F^2 \quad R \in \mathbb{R}^{|E| \times m}$
- The graph regularization term can also be represented in the form of Laplacian term

 $\|WR^{T}\|_{F}^{2} = tr((WR^{T})^{T}WR^{T}) = tr(WR^{T}RW^{T}) = tr(W\mathcal{L}W^{T})$



- How to obtain graph information
 - External domain knowledge
 - protein-protein interaction (PPI) for microarray
 - Discover task relatedness from data
 - Pairwise correlation coefficient
 - Sparse inverse covariance (Friedman et. al. 2008 Biostatistics)





Sparse Inverse Covariance Graph (lambda=0.10, #edge = 1620)





Chen et. al. 2011 UAI, Kim et. al. 2009 Bioinformatics

• Graph-guided Fused Lasso





Kim et. al. 2009 Bioinformatics

- In some applications, we know not only which pairs are related, but also **how** they are related.
- Graph-Weighted Fused Lasso.



$$\min_{W} \operatorname{Loss}(W) + \lambda \|W\|_{1} + \gamma \sum_{e=(m,l)\in E} \tau(r_{ml}) \sum_{j=1}^{J} |W_{jm} - sign(r_{ml})W_{jl}|$$

Added weight information!



Practical Guideline

• MTL versus STL

 MTL is preferred when dealing with multiple related tasks with small number of training samples

• Shared features versus shared subspace

- Identifying shared features is preferred When the data dimensionality is large
- Identifying a shared subspace is preferred when the number of tasks is large



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Case Study I: Incomplete Multi-Source Data Fusion

- In many applications, multiple data sources may contain a considerable amount of missing data.
- In ADNI, over half of the subjects lack CSF measurements; an independent half of the subjects do not have FDG-PET.





Overview of iMSF

Yuan et. al. 2012 NeuroImage





iMSF: Performance

Yuan et. al. 2012 NeuroImage







Case Study II: *Drosophila* Gene Expression Image Analysis

- *Drosophila* (fruit fly) is a favorite model system for geneticists and developmental biologists studying embryogenesis.
 - The small size and short generation time make it ideal for genetic studies.
- In situ hybridization allows us to generate images showing when and where individual genes were active.
 - The analysis of such images can potentially reveal gene functions and gene-gene interactions.





Drosophila gene expression pattern images





stage 4-6

stage 7-8

Comparative image analysis

Twist



anterior endoderm AISN trunk mesoderm AISN subset cellular blastoderm mesoderm AISN



dorsal ectoderm AISN procephalic ectoderm AISN subset cellular blastoderm mesoderm AISN

stumps

anterior endoderm AISN trunk mesoderm AISN

head mesoderm AISN



trunk mesoderm PR head mesoderm PR anterior endoderm anlage



trunk mesoderm PR head mesoderm PR



yolk nuclei trunk mesoderm PR head mesoderm PR anterior endoderm anlage

We need the spatial and temporal annotations of expressions

[Tomancak et al. (2002) Genome Biology; Sandmann et al. (2007) Genes & Dev.]



Challenges of manual annotation





Method outline

Ji et. al. 2008 Bioinformatics; Ji et. al. 2009 BMC Bioinformatics; Ji et. al. 2009 NIPS





Low rank multi-task learning model

Ji et. al. 2009 BMC Bioinformatics



Graph-based multi-task learning model





Closed-form solution



Center for Evolutionary Medicine and Informatics

Spatial annotation performance



- 50% data for training and 50% for testing and 30 random trials are generated
- Multi-task approaches outperform single-task approaches



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MULTI-TASK LEARNING VIA STRUCTURAL REGULARIZATION JIAYU ZHOU, JIANHUI CHEN, JIEPING YE

- A multi-task learning package
- Encode task relationship via structural regularization
- www.public.asu.edu/~jye02/Software/MALSAR/



MTL Algorithms in MALSAR 1.0

- Mean-Regularized Multi-Task Learning
- MTL with Embedded Feature Selection
 - Joint Feature Learning
 - Dirty Multi-Task Learning
 - Robust Multi-Task Feature Learning
- MTL with Low-Rank Subspace Learning
 - Trace Norm Regularized Learning
 - Alternating Structure Optimization
 - Incoherent Sparse and Low Rank Learning
 - Robust Low-Rank Multi-Task Learning
- Clustered Multi-Task Learning
- Graph Regularized Multi-Task Learning



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Trends in Multi-Task Learning

- **Develop efficient algorithms** for large-scale multitask learning.
- Semi-supervised and unsupervised MTL
- Learn task structures automatically in MTL
- Asymmetric MTL
- Cross-Domain MTL
 - The features may be different



The relationship is not mutual



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