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User's Manual

Version 1.1

MALSAR: Multi-tAsk Learning via StructurAl Regularization

Version 1.1

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1 Introduction

1.1 Multi-Task Learning

In many real-world applications we deal with multiple related classification/regression/clustering tasks. For example, in the prediction of therapy outcome (Bickel et al., 2008), the tasks of predicting the effectiveness of several combinations of drugs are related. In the prediction of disease progression, the prediction of outcome at each time point can be considered as a task and these tasks are temporally related (Zhou et al., 2011b). A simple approach is to solve these tasks independently, ignoring the task relatedness. In multi-task learning, these related tasks are learnt simultaneously by extracting and utilizing appropriate shared information across tasks. Learning multiple related tasks simultaneously effectively increases the sample size for each task, and improves the prediction performance. Thus multi-task learning is especially beneficial when the training sample size is small for each task. Figure 1 illustrates the difference between traditional single task learning (STL) and multi-task learning (MTL). In STL, each task is considered to be independent and learnt independently. In MTL, multiple tasks are learnt simultaneously, by utilizing task relatedness.

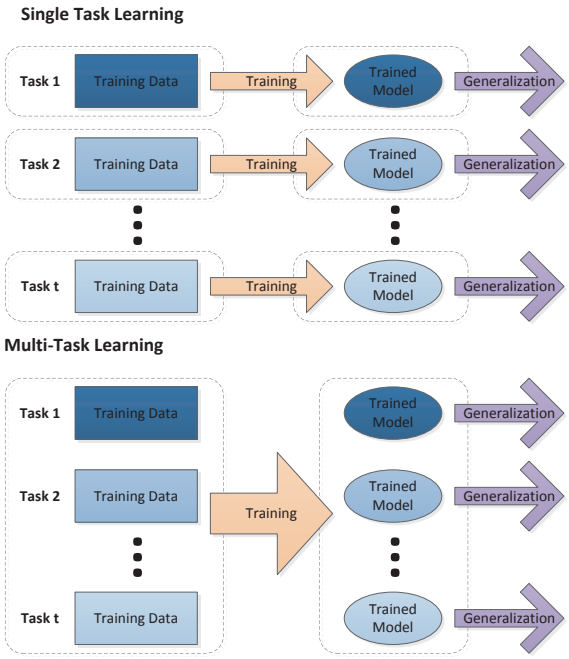

Figure 1: Illustration of single task learning (STL) and multi-task learning (MTL). In single task learning (STL), each task is considered to be independent and learnt independently. In multi-task learning (MTL), multiple tasks are learnt simultaneously, by utilizing task relatedness.

In data mining and machine learning, a common paradigm for classification and regression is to minimize the penalized empirical loss:

$$\min_{W} \mathcal{L}(W) + \Omega(W), \tag{1}$$

where W is the parameter to be estimated from the training samples, $\mathcal{L}(W)$ is the empirical loss on the training set, and $\Omega(W)$ is the regularization term that encodes task relatedness. Different assumptions on task relatedness lead to different regularization terms. In the field of multi-task learning, there are many prior work that model relationships among tasks using novel regularizations (Evgeniou & Pontil, 2004; Ji & Ye,

2009; Abernethy et al., 2006; Abernethy et al., 2009; Argyriou et al., 2008a; Obozinski et al., 2010; Chen et al., 2010; Argyriou et al., 2008b; Agarwal et al., 2010). The formulations implemented in the MALSAR package is summarized in Table 1. The notations used in this manual (unless otherwise specified) are given in Table 2. Note, for some formulations, only certain loss versions are included (e.g., squared loss for dirty model, multi-stage multi-task feature learning). In most cases this is because a theory is associated with the loss function provided. However, practically, other loss functions can be used. One can always modify the code according to existing ones to use other loss.

Table 1: Formulations included in the MALSAR package of the following form: $\min_W \mathcal{L}(W) + \Omega(W)$.

Name	Loss function $\mathcal{L}(W)$	Regularization $\Omega(W)$	Main Reference
Lasso	Least Squares, Logistic	$\rho_1\|W\|_1$	(Tibshirani, 1996)
Mean Regularized	Least Squares, Logistic	$\rho_1 \sum_{t=1}^{T} \|W_t - \frac{1}{T}\sum_{s=1}^{T} W_s\| = \rho_1\|WR\|_F^2$	(Evgeniou & Pontil, 2004)
Joint Feature Selection	Least Squares, Logistic	$\lambda\|W\|_{1,2}$	(Argyriou et al., 2007)
Dirty Model	Least Squares	$\rho_1\|P\|_{1,\infty} + \rho_2\|Q\|_1$	(Jalali et al., 2010)
Graph Structure	Least Squares, Logistic	$\rho_1\|WR\|_F^2 + \rho_2\|W\|_1$	
Low Rank	Least Squares, Logistic	$\rho_1\|W\|_*$	(Ji & Ye, 2009)
Sparse+Low Rank	Least Squares	$\gamma\|P\|_1$, s.t. $W = P+Q, \|Q\|_* \leq \tau$	(Chen et al., 2010)
Relaxed Clustered MTL	Least Squares, Logistic	$\rho_1\eta(1+\eta)$tr $\left(W(\eta I + M)^{-1}W^T\right)$ s.t. tr $(M) = k, M \preceq I, M \in S_+^t, \eta = \frac{\rho_2}{\rho_1}$	(Zhou et al., 2011a)
Relaxed ASO	Least Squares, Logistic	$\rho_1\eta(1+\eta)$tr $\left(W^T(\eta I + M)^{-1}W\right)$ s.t. tr $(M) = k, M \preceq I, M \in S_+^d, \eta = \frac{\rho_2}{\rho_1}$	(Chen et al., 2009)
Robust MTL	Least Squares	$\rho_1\|P\|_* + \rho_2\|Q\|_{1,2}$, s.t. $W = P + W$	(Chen et al., 2011)
Robust Feature Learning	Least Squares	$\rho_1\|P\|_{2,1} + \rho_2\|Q\|_{1,2}$, s.t. $W = P + Q$	(Gong et al., 2012b)
Temporal Group Lasso	Least Squares, Logistic	$\rho_1\|W\|_F^2 + \rho_2\|WR\|_F^2 + \rho_3\|W\|_{2,1}$	(Zhou et al., 2011b)
Fused Sparse Group Lasso	Least Squares, Logistic	$\rho_1\|W\|_1 + \rho_2\|WR\|_1 + \rho_3\|W\|_{2,1}$, $\rho_1 \sum_{i=1}^{d} \sqrt{\|\mathbf{w}_i\|_1} + \rho_2\|RW^T\|_1$, $\rho_1 \sum_{i=1}^{d} \sqrt{\|R\mathbf{w}_i^T\|_1 + \rho_2\|\mathbf{w}_i\|_1}$	(Zhou et al., 2012)
Incomplete Multi-Source	Least Squares, Logistic	$\rho_1 \sum_{s=1}^{S} \sum_{k=1}^{p_s} \left\|W_{G(s,k)}\right\|_2$	(Yuan et al., 2012)
Multi-Stage Feat. Learn.	Least Squares	$\rho_1 \sum_{j=1}^{d} \min(\|\mathbf{w}_i\|_1, \theta)$	(Gong et al., 2012a)
Multi-Task Clustering	Sum of Squared Error	$\sum_{i=1}^{t} \|W^T X_i - M P_i^T\|_F^2$	(Gu & Zhou, 2009)

1.2 Optimization Algorithm

In the MALSAR package, most optimization algorithms are implemented via the accelerated gradient methods (AGM) (Nemirovski, ; Nemirovski, 2001; Nesterov & Nesterov, 2004; Nesterov, 2005; Nesterov, 2007). The AGM differs from the traditional gradient method in that every iteration it uses a linear combination of previous two points as the search point, instead of only using the latest point. The AGM has the convergence speed of $O(1/k^2)$, which is the optimal among first order methods. The key subroutine in AGM is to compute the proximal operator:

$$W^* = \operatorname*{argmin}_W \mathcal{M}_{\gamma,S}(W) = \operatorname*{argmin}_W \frac{\gamma}{2}\|W - (S - \frac{1}{\gamma}\nabla\mathcal{L}(W))\|_F^2 + \Omega(W) \tag{2}$$

Table 2: A list of notations and corresponding Matlab variables (if applicable) used in this manual. Other usages of the notations may exist and are specified in the context.

Math Notation	Meaning	Matlab Variable	Size
S_+	symmetric positive semi-definite		
$\|\cdot\|_1$	ℓ_1-norm		
$\|\cdot\|_\infty$	ℓ_∞-norm		
$\|\cdot\|_F$	ℓ_2-norm (Frobenius norm)		
$\|\cdot\|_*$	trace-norm (sum of singular values)		
$\|\cdot\|_{1,2}$	$\ell_{1,2}$-norm (row grouped ℓ_1)		
$\|\cdot\|_{1,\infty}$	$\ell_{1,\infty}$-norm (row grouped ℓ_1)		
$\|\cdot\|_{2,1}$	$\ell_{2,1}$-norm (column grouped ℓ_1)		
t	task number		
d	dimensionality		
n_i	sample size of task i		
ρ	formulation parameters i		
$\mathcal{L}$	loss function		
Ω	regularization terms		
X	data (attributes, features)	`X`	t by 1 cell array
Y	target (response, label)	`Y`	t by 1 cell array
W	model (weight, parameter)	`W`	d by t matrix
P, Q, M	model components	`P, Q, M`	d by t matrix
R	structure variable	`R`	matrix of varying size
I	identity matrix	`I`	matrix of varying size
$\mathbf{c}$	model bias (in logistic loss)	`c, C`	1 by t vector
X_i	the data of the task i	`X{ i }`	n_i by d matrix
Y_i	the target of the task i	`Y{ i }`	n_i by 1 vector
W_i	the model of the task i	`W(:,i)`	d by 1 vector
$\mathbf{w}_i$	the model at i-th feature of all tasks		1 by t vector
$\mathbf{c}_i$	the model bias of the task i (in logistic loss)	`c, C`	scalar
$X_{i,j}$	the data of the j-th sample of the task i	`X{ i }(i,:)`	1 by d vector
$Y_{i,j}$	the target of the j-th sample of the task i	`Y{ i }(i,:)`	scalar
	optimization options	`opts`	struct variable
	objective function value	`funcVal`	a vector of varying size

where $\Omega(W, \lambda)$ is the non-smooth regularization term, γ is the step size, $\nabla\mathcal{L}(\cdot)$ is the gradient of $\mathcal{L}(\cdot)$, S is the current search point.

2 Package and Installation

The MALSAR package is currently only available for MATLAB[1]. The user needs MATLAB with 2011a or higher versions. If you are using lower versions, some functions (such as `rng` the random number generator settings may not work properly)

After MATLAB is correctly installed, download the MALSAR package from the software homepage[2], and unzip to a folder. If you are using a Unix-based machines or Mac OS, there is an additional step to build C libraries: Open MATLAB, navigate to package folder, and run `INSTALL.M`. A step-by-step installation guide is given in Table 3.

Table 3: Installation of MALSAR

Step	Comment
1. Install MATLAB 2010a or later	Required for all functions.
2. Download MALSAR and uncompress	Required for all functions.
3. In MATLAB, go to the MALSAR folder, run `INSTALL.M` in command window	Required for non-Windows machines.

The folder structure of MALSAR package is:

- `manual`. The location of the manual.
- `MALSAR`. This is the folder containing main functions and libraries.
  - `utils`. This folder contains opts structure initialization and some common libraries. The folder should be in MATLA path.
  - `functions`. This folder contains all the MATLAB functions and are organized by categories.
  - `c_files`. All c files are in this folder. It is not necessary to compile one by one. For Windows users, there are precompiled binaries for i386 and x64 CPU. For Mac OS X users, binaries for Intel x64 are included. For Unix users and other Mac OS users, you can perform compilation all together by running `INSTALL.M`.
- `examples`. Many examples are included in this folder for functions implemented in MALSAR. If you are not familiar with the package, this is the perfect place to start with.
- `data`. Popular multi-task learning datasets, currently we have included the School data and a part of the 20 Newsgroups.

[1] http://www.mathworks.com/products/matlab/

[2] http://www.public.asu.edu/∼jye02/Software/MALSAR

3 Interface Specification

3.1 Input and Output

All functions implemented in MALSAR follow a common specification. For a multi-task learning algorithm NAME, the input and output of the algorithm are in the following format:

```
[MODEL_VARS, func_val, OTHER_OUTPUT] = ...
    LOSS_NAME(X, Y, ρ1, ..., ρp, [opts])
```

where the name of the loss function is LOSS, and MODEL_VARS is the model variables learnt.

In the input fields, X and Y are two t-dimensional cell arrays. Each cell of X contains a n_i-by-d matrix, where n_i is the sample size for task i and d is the dimensionality of the feature space. Each cell of Y contains the corresponding n_i-by-1 response. The relationship among X, Y and W is given in Figure 2. $\rho_1 \dots \rho_p$ are algorithm parameters (e.g., regularization parameters). opts is the optional optimization options that are elaborated in Sect 3.2.

In the output fields, **MODEL_VARS** are model variables that can be used for predicting unseen data points. Depending on different loss functions, the model variables may be different. Specifically, the following format is used under the least squares loss:

```
[W, func_val, OTHER_OUTPUT ] = Least_NAME (X, Y, ρ1, ..., ρp [opts])
```

where W is a d-by-t matrix, each column of which is a d dimensional parameter vector for the corresponding task. For a new input $\mathbf{x}$ from task i, the prediction y is given by

$$y = \mathbf{x}^T \cdot W(:, i).$$

The following format is used under the logistic loss:

```
[W, c, func_val, OTHER_OUTPUT ] = ...
Logistic_NAME (X, Y, ρ1, ..., ρp [opts])
```

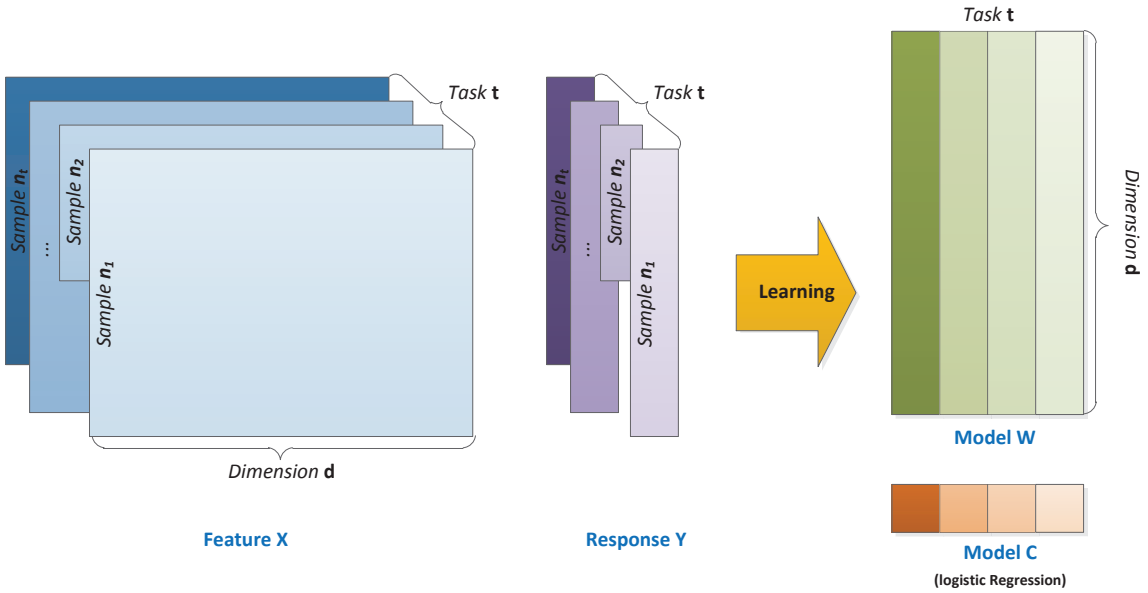

Figure 2: The main input and output variables.

where W is a d-by-t matrix, each column of which is a d dimensional parameter vector for the corresponding task, and $\mathbf{c}$ is a t-dimensional vector. For a new input $\mathbf{x}$ from task i, the binary prediction y is given by

$$y = \text{sign}(\mathbf{x}^T \cdot W(:, i) + \mathbf{c}(i)).$$

These two loss functions are available for most of the algorithms in the package. The output func_val is the objective function values at all iterations of the optimization algorithms. In some algorithms, there are other output variables that are not directly related to the prediction. For example in convex relaxed ASO, the optimization also gives the shared feature mapping, which is a low rank matrix. In some scenarios the user may be interested in such variables. The variables are given in the field %OTHER_OUTPUT%.

3.2 Optimization Options

All optimization algorithms in our package are implemented using iterative methods. Users can use the optional *opts* input to specify starting points, termination conditions, tolerance, and maximum iteration number. The input *opts* is a structure variable. To specify an option, user can add corresponding fields. If one or more required fields are not specified, or the opts variable is not given, then default values will be used. The default values can be changed in `init_opts.m` in `\MALSAR\utils`.

- **Starting Point .init**. Users can use the field to specify different starting points.
  - `opts.init = 0`. If 0 is specified then the starting points will be initialized to a guess value computed from data. For example, in the least squares loss, the model `W(:, i)` for i-th task is initialized by `X{i} * Y{i}`.
  - `opts.init = 1`. If 1 is specified then `opts.W0` is used. Note that if value 1 is specified in .init but the field .W0 is not specified, then .init will be forced to the default value.
  - `opts.init = 2 (default)`. If 2 is specified, then the starting point will be a zero matrix.
- **Termination Condition .tFlag and Tolerance .tol**. In this package, there are 4 types of termination conditions supported for all optimization algorithms.
  - `opts.tFlag = 0`.
  - `opts.tFlag = 1 (default)`.
  - `opts.tFlag = 2`.
  - `opts.tFlag = 3`.
- **Maximum Iteration .maxIter**. When the tolerance and/or termination condition is not properly set, the algorithms may take an unacceptable long time to stop. In order to prevent this situation, users can provide the maximum number of iterations allowed for the solver, and the algorithm stops when the maximum number of iterations is achieved even if the termination condition is not satisfied.

  For example, one can use the following code to specify the maximum iteration number of the optimization problem:

  ```
  opts.maxIter = 1000;
  ```

  The algorithm will stop after 1000 iteration steps even if the termination condition is not satisfied.

4 Multi-Task Learning Formulations

4.1 Sparsity in Multi-Task Learning: ℓ_1-norm Regularized Problems

The ℓ_1-norm (or Lasso) regularized methods are widely used to introduce sparsity into the model and achieve the goal of reducing model complexity and feature learning (Tibshirani, 1996). We can easily extend the ℓ_1-norm regularized STL to MTL formulations. A common simplification of Lasso in MTL is that the parameter controlling the sparsity is shared among all tasks, assuming that different tasks share the same sparsity parameter. The learnt model is illustrated in Figure 3.

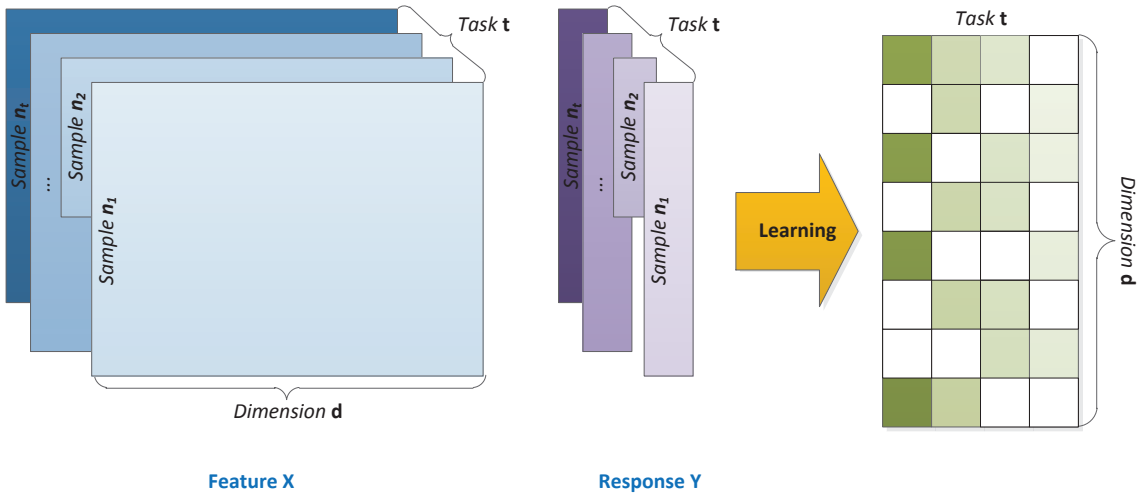

Figure 3: Illustration of multi-task Lasso.

4.1.1 Multi-Task Lasso with Least Squares Loss (`Least_Lasso`)

The function

```
[W, funcVal] = Least_Lasso(X, Y, ρ1, [opts])
```

solves the ℓ_1-norm (and the squared ℓ_2-norm) regularized multi-task least squares problem:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \|W\|_1 + \rho_{L2} \|W\|_F^2, \tag{3}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, the regularization parameter ρ_1 controls sparsity, and the optional ρ_{L2} regularization parameter controls the ℓ_2-norm penalty. Note that both ℓ_1-norm and ℓ_2-norm penalties are used in elastic net.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`
- Regularization: `opts.rho_L2`

4.1.2 Multi-Task Lasso with Logistic Loss (`Logistic_Lasso`)

The function

`[W, c, funcVal] =` **`Logistic_Lasso`**`(X, Y,` ρ_1`, [opts])`

solves the ℓ_1-norm (and the squared ℓ_2-norm) regularized multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \sum_{i=1}^{t} \sum_{j=1}^{n_i} \log(1 + \exp\left(-Y_{i,j}(W_j^T X_{i,j} + \mathbf{c}_i)\right)) + \rho_1 \|W\|_1 + \rho_{L2} \|W\|_F^2, \tag{4}$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model for task i, the regularization parameter ρ_1 controls sparsity, and the optional ρ_{L2} regularization parameter controls the ℓ_2-norm penalty.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`, `opts.C0`
- Termination: `opts.tFlag`, `opts.tol`
- Regularization: `opts.rho_L2`

4.2 Joint Feature Selection: $\ell_{2,1}$-norm Regularized Problems

One way to capture the task relatedness from multiple related tasks is to constrain all models to share a common set of features. This motivates the group sparsity, i.e. the ℓ_1/ℓ_2-norm regularized learning (Argyriou et al., 2007; Argyriou et al., 2008a; Liu et al., 2009; Nie et al., 2010):

$$\min_W \mathcal{L}(W) + \lambda \|W\|_{1,2}, \tag{5}$$

where $\|W\| = \sum_{t=1}^{T} \|W_t\|_2$ is the group sparse penalty. Compared to Lasso, the $\ell_{2,1}$-norm regularization results in grouped sparsity, assuming that all tasks share a common set of features. The learnt model is illustrated in Figure 4.

4.2.1 $\ell_{2,1}$-Norm Regularization with Least Squares Loss (`Least_L21`)

The function

`[W, funcVal] =` **`Least_L21`**`(X, Y,` ρ_1`, [opts])`

solves the $\ell_{2,1}$-norm (and the squared ℓ_2-norm) regularized multi-task least squares problem:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \|W\|_{2,1} + \rho_{L2} \|W\|_F^2, \tag{6}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, the regularization parameter ρ_1 controls group sparsity, and the optional ρ_{L2} regularization parameter controls ℓ_2-norm penalty.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`
- Regularization: `opts.rho_L2`

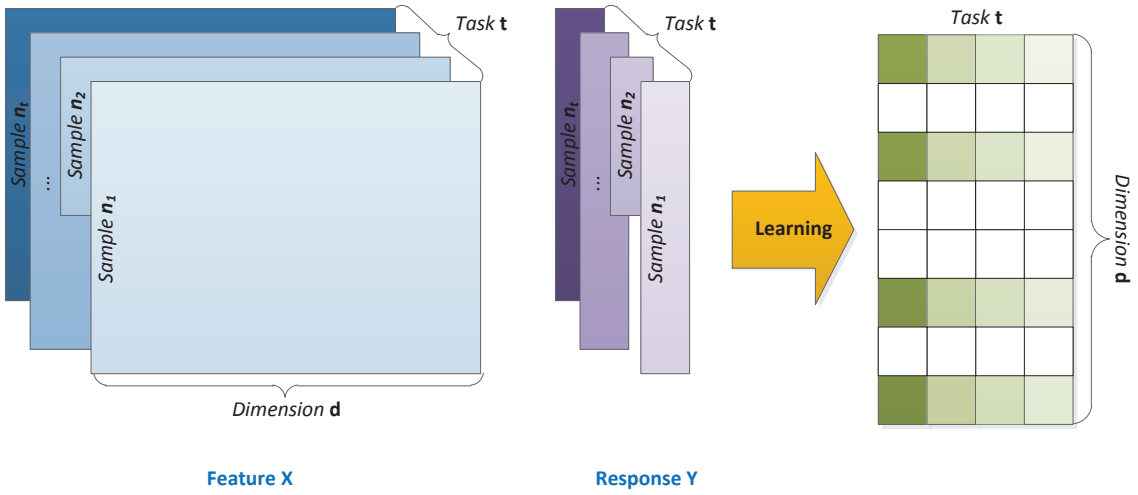

Figure 4: Illustration of multi-task learning with joint feature selection based on the $\ell_{2,1}$-norm regularization.

4.2.2 $\ell_{2,1}$-Norm Regularization with Logistic Loss (`Logistic_L21`)

The function

$$\texttt{[W, c, funcVal] = Logistic\_L21(X, Y, } \rho_1 \texttt{, [opts])}$$

solves the $\ell_{2,1}$-norm (and the squared ℓ_2-norm) regularized multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \sum_{i=1}^{t} \sum_{j=1}^{n_i} \log(1 + \exp\left(-Y_{i,j}(W_j^T X_{i,j} + \mathbf{c}_i)\right)) + \rho_1 \|W\|_{2,1} + \rho_{L2} \|W\|_F^2, \tag{7}$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model for task i, the regularization parameter ρ_1 controls group sparsity, and the optional ρ_{L2} regularization parameter controls ℓ_2-norm penalty.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`, `opts.C0`
- Termination: `opts.tFlag`, `opts.tol`
- Regularization: `opts.rho_L2`

4.3 The Dirty Model for Multi-Task Learning

The joint feature learning using ℓ_1/ℓ_q-norm regularization performs well in idea cases. In practical applications, however, simply using the ℓ_1/ℓ_q-norm regularization may not be effective for dealing with dirty data which may not fall into a single structure. To this end, the dirty model for multi-task learning is proposed (Jalali et al., 2010). The key idea in the dirty model is to decompose the model W into two components P and Q, as shown in Figure 5.

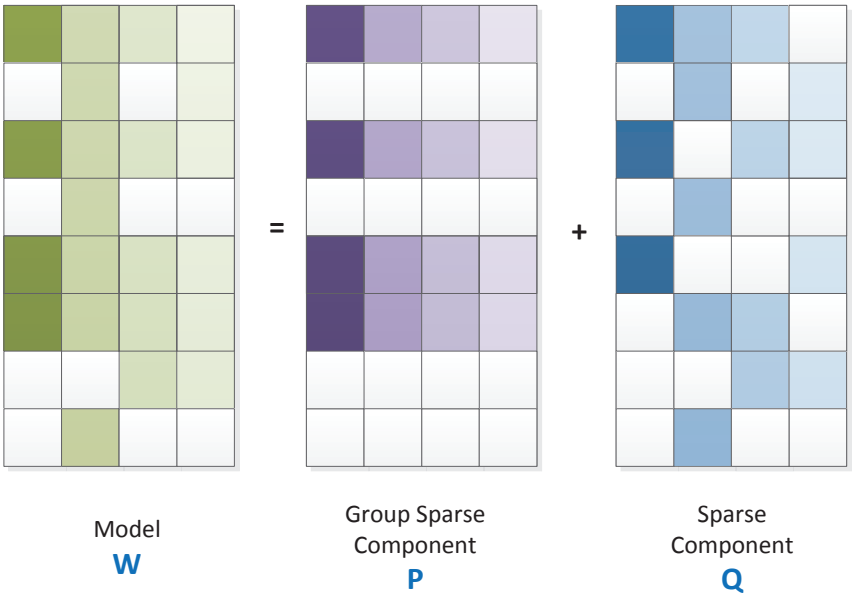

Figure 5: Illustration of dirty model for multi-task learning.

4.3.1 A Dirty Model for Multi-Task Learning with the Least Squares Loss (`Least_Dirty`)

The function

```
[W, funcVal, P, Q] = Least_Dirty(X, Y, ρ1, ρ2, [opts])
```

solves the dirty multi-task least squares problem:

$$\min_{W} \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \|P\|_{1,\infty} + \rho_2 \|Q\|_1, \tag{8}$$

$$\text{subject to:} W = P + Q \tag{9}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, P is the group sparsity component and Q is the elementwise sparse component, ρ_1 controls the group sparsity regularization on P, and ρ_2 controls the sparsity regularization on Q.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.P0`, `opts.Q0` (set `opts.W0` to any non-empty value)
- Termination: `opts.tFlag`, `opts.tol`
- Initial Lipschiz Constant: `opts.lFlag`

4.4 Encoding Graph Structure: Graph Regularized Problems

In some applications, the task relationship can be represented using a graph where each task is a node, and two nodes are connected via an edge if they are related. Let $\mathcal{E}$ denote the set of edges, and we denote edge i as a vector $\mathbf{e}^{(i)} \in \mathbb{R}^t$ defined as follows: $\mathbf{e}_x^{(i)}$ and $\mathbf{e}_y^{(i)}$ are set to 1 and -1 respectively if the two nodes x and

y are connected. The complete graph is encoded in the matrix $R = [\mathbf{e}^{(1)}, \mathbf{e}^{(2)}, \ldots, \mathbf{e}^{(\|\mathcal{E}\|)}] \in \mathbb{R}^{t \times \|\mathcal{E}\|}$. The following regularization penalizes the differences between all pairs connected in the graph:

$$\|WR\|_F^2 = \sum_{i=1}^{\|\mathcal{E}\|} \|We^{(i)}\|_2^2 = \sum_{i=1}^{\|\mathcal{E}\|} \|W_{e_x^{(i)}} - W_{e_y^{(i)}}\|_2^2, \tag{10}$$

which can also be represented in the following matrix form:

$$\|WR\|_F^2 = \text{tr}\left((WR)^T(WR)\right) = \text{tr}\left(WRR^TW^T\right) = \text{tr}\left(W\mathcal{L}W^T\right), \tag{11}$$

where $\mathcal{L} = RR^T$, known as the Laplacian matrix, is symmetric and positive definiteness. In (Li & Li, 2008), the network structure is defined on the features, while in MTL the structure is on the tasks.

In the multi-task learning formulation proposed by (Evgeniou & Pontil, 2004), it assumes all tasks are related in the way that the models of all tasks are close to their mean:

$$\min_W \mathcal{L}(W) + \lambda \sum_{t=1}^{T} \|W_t - \frac{1}{T}\sum_{s=1}^{T} W_s\|, \tag{12}$$

where $\lambda > 0$ is penalty parameter. The regularization term in Eq.(12) penalizes the deviation of each task from the mean $\frac{1}{T}\sum_{s=1}^{T} W_s$. This regularization can also be encoded using the structure matrix R by setting `R = eye(t) - ones(t)/t`.

4.4.1 Sparse Graph Regularization with Logistic Loss (`Least_SRMTL`)

The function

```
[W, funcVal] = Least_SRMTL(X, Y, R, ρ1, ρ2, [opts])
```

solves the graph structure regularized and ℓ_1-norm (and the squared ℓ_2-norm) regularized multi-task least squares problem:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \|WR\|_F^2 + \rho_2 \|W\|_1 + \rho_{L2} \|W\|_F^2, \tag{13}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, the regularization parameter ρ_1 controls sparsity, and the optional ρ_{L2} regularization parameter controls ℓ_2-norm penalty.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`
- Regularization: `opts.rho_L2`

4.4.2 Sparse Graph Regularization with Logistic Loss (`Logistic_SRMTL`)

The function

```
[W, c, funcVal] = Logistic_SRMTL(X, Y, R, ρ1, ρ2, [opts])
```

solves the graph structure regularized and ℓ_1-norm (and the squared ℓ_2-norm) regularized multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \sum_{i=1}^{t} \sum_{j=1}^{n_i} \log(1 + \exp\left(-Y_{i,j}(W_j^T X_{i,j} + \mathbf{c}_i)\right)) + \rho_1 \|WR\|_F^2 + \rho_2 \|W\|_1 + \rho_{L2} \|W\|_F^2, \qquad (14)$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model for task i, the regularization parameter ρ_1 controls sparsity, and the optional ρ_{L2} regularization parameter controls ℓ_2-norm penalty.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`, `opts.C0`
- Termination: `opts.tFlag`, `opts.tol`
- Regularization: `opts.rho_L2`

4.5 Low Rank Assumption: Trace-norm Regularized Problems

One way to capture the task relationship is to constrain the models from different tasks to share a low-dimensional subspace, i.e., W is of low rank, resulting in the following rank minimization problem:

$$\min \mathcal{L}(W) + \lambda \text{rank}(W).$$

The above problem is in general NP-hard (Vandenberghe & Boyd, 1996). One popular approach is to replace the rank function (Fazel, 2002) by the trace norm (or nuclear norm) as follows:

$$\min \mathcal{L}(W) + \lambda \|W\|_*, \qquad (15)$$

where the trace norm is given by the sum of the singular values: $\|W\|_* = \sum_i \sigma_i(W)$. The trace norm regularization has been studied extensively in multi-task learning (Ji & Ye, 2009; Abernethy et al., 2006; Abernethy et al., 2009; Argyriou et al., 2008a; Obozinski et al., 2010).

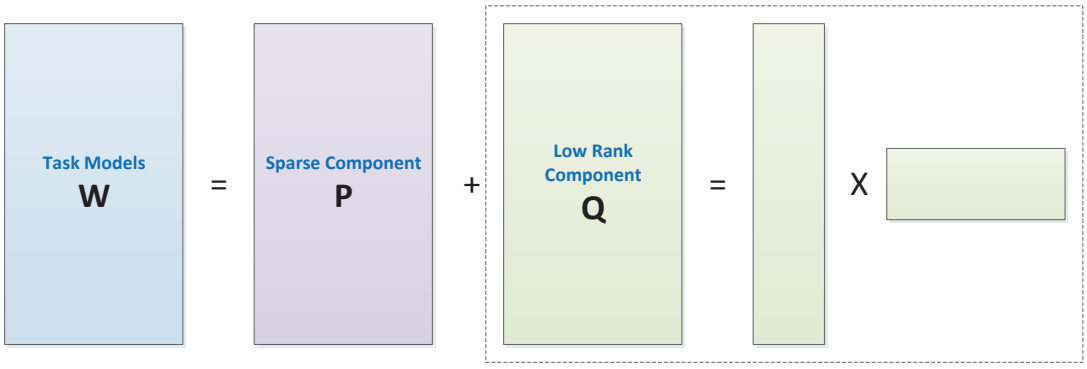

Figure 6: Learning Incoherent Sparse and Low-Rank Patterns form Multiple Tasks.

The assumption that all models share a common low-dimensional subspace is restrictive in some applications. To this end, an extension that learns incoherent sparse and low-rank patterns simultaneously was

proposed in (Chen et al., 2010). The key idea is to decompose the task models W into two components: a sparse part P and a low-rank part Q, as shown in Figure 6. It solves the following optimization problem:

$$\min_W \mathcal{L}(W) + \gamma\|P\|_1$$
$$\text{subject to: } W = P + Q, \|Q\|_* \leq \tau.$$

4.5.1 Trace-Norm Regularization with Least Squares Loss (`Least_Trace`)

The function

```
[W, funcVal] = Least_Trace(X, Y, ρ1, [opts])
```

solves the trace-norm regularized multi-task least squares problem:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1\|W\|_*, \tag{16}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, and the regularization parameter ρ_1 controls the rank of W.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`

4.5.2 Trace-Norm Regularization with Logistic Loss (`Logistic_Trace`)

The function

```
[W, c, funcVal] = Logistic_Trace(X, Y, ρ1, [opts])
```

solves the trace-norm regularized multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \sum_{i=1}^{t} \sum_{j=1}^{n_i} \log(1 + \exp\left(-Y_{i,j}(W_j^T X_{i,j} + \mathbf{c}_i)\right)) + \rho_1\|W\|_*, \tag{17}$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model for task i, and the regularization parameter ρ_1 controls the rank of W.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`, `opts.C0`
- Termination: `opts.tFlag`, `opts.tol`

4.5.3 Learning with Incoherent Sparse and Low-Rank Components (`Least_SparseTrace`)

The function

```
[W, funcVal, P, Q] = Least_SparseTrace(X, Y, ρ1, ρ2, [opts])
```

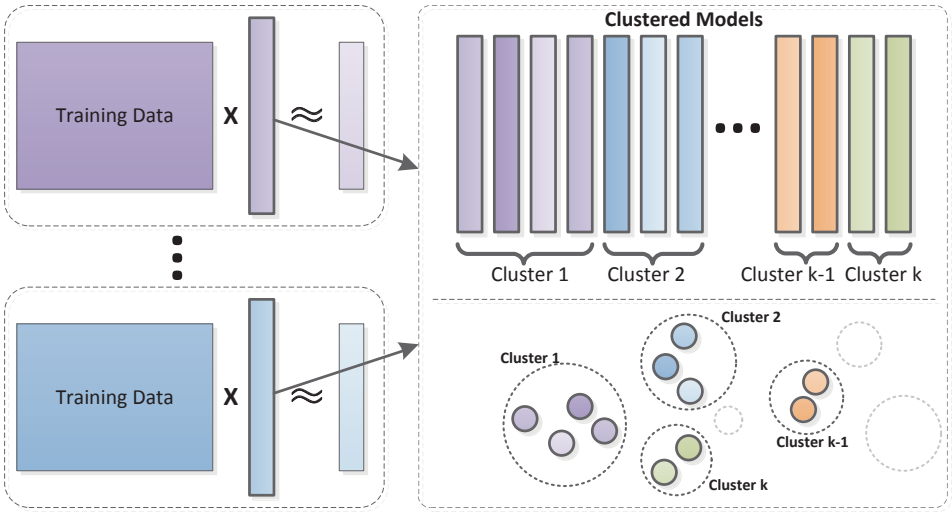

Figure 7: Illustration of clustered tasks. Tasks with similar colors are similar with each other.

solves the incoherent sparse and low-rank multi-task least squares problem:

$$\min_{W} \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \|P\|_1 \tag{18}$$

$$\text{subject to: } W = P + Q, \|Q\|_* \leq \rho_2 \tag{19}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, the regularization parameter ρ_1 controls sparsity of the sparse component P, and the ρ_2 regularization parameter controls the rank of Q.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.P0`, `opts.Q0` (set `opts.W0` to any non-empty value)
- Termination: `opts.tFlag`, `opts.tol`

4.6 Discovery of Clustered Structure: Clustered Multi-Task Learning

Many multi-task learning algorithms assume that all learning tasks are related. In practical applications, the tasks may exhibit a more sophisticated group structure where the models of tasks from the same group are closer to each other than those from a different group. There have been many work along this line of research (Thrun & O'Sullivan, 1998; Jacob et al., 2008; Wang et al., 2009; Xue et al., 2007; Bakker & Heskes, 2003; Evgeniou et al., 2006; Zhang & Yeung, 2010), known as clustered multi-task learning (CMTL). The idea of CMTL is shown in Figure 7.

In (Zhou et al., 2011a) we proposed a CMTL formulation which is based on the spectral relaxed k-means clustering (Zha et al., 2002):

$$\min_{W,F:F^TF=I_k} \mathcal{L}(W) + \alpha \left(\text{tr}W^TW - \text{tr}F^TW^TWF\right) + \beta \text{tr}(W^TW). \tag{20}$$

where k is the number of clusters and F captures the relaxed cluster assignment information. Since the formulation in Eq. (20) is not convex, a convex relaxation called cCMTL is also proposed. The formulation

of cCMTL is given by:

$$\min_W \mathcal{L}(W) + \rho_1 \eta (1+\eta) \text{tr}\left(W(\eta I + M)^{-1} W^T\right)$$
$$\text{subject to: } \text{tr}\,(M) = k, M \preceq I, M \in S_+^t, \eta = \frac{\rho_2}{\rho 1}$$

There are many optimization algorithms for solving the cCMTL formulations (Zhou et al., 2011a). In our package we include an efficient implementation based on Accelerated Projected Gradient.

4.6.1 Convex Relaxed Clustered Multi-Task Learning with Least Squares Loss (`Least_CMTL`)

The function

```
[W, funcVal, M] = Least_CMTL(X, Y, ρ1, ρ2, k, [opts])
```

solves the relaxed k-means clustering regularized multi-task least squares problem:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \eta (1+\eta) \text{tr}\left(W(\eta I + M)^{-1} W^T\right), \tag{21}$$
$$\text{subject to: } \text{tr}\,(M) = k, M \preceq I, M \in S_+^t, \eta = \frac{\rho_2}{\rho 1} \tag{22}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, and ρ_1 is the regularization parameter. Because of the equality constraint $\text{tr}\,(M) = k$, the starting point of M is initialized to be $M_0 = k/t \times I$ satisfying $\text{tr}\,(M_0) = k$.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`

4.6.2 Convex Relaxed Clustered Multi-Task Learning with Logistic Loss (`Logistic_CMTL`)

The function

```
[W, c, funcVal, M] = Logistic_CMTL (X, Y, ρ1, ρ2, k, [opts])
```

solves the relaxed k-means clustering regularized multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \sum_{i=1}^{t} \sum_{j=1}^{n_i} \log(1 + \exp\left(-Y_{i,j}(W_j^T X_{i,j} + \mathbf{c}_i)\right)) + \rho_1 \eta (1+\eta) \text{tr}\left(W(\eta I + M)^{-1} W^T\right), \tag{23}$$
$$\text{subject to: } \text{tr}\,(M) = k, M \preceq I, M \in S_+^t, \eta = \frac{\rho_2}{\rho 1} \tag{24}$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model for task i, and ρ_1 is the regularization parameter. Because of the equality constraint $\text{tr}\,(M) = k$, the starting point of M is initialized to be $M_0 = k/t \times I$ satisfying $\text{tr}\,(M_0) = k$.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`, `opts.C0`
- Termination: `opts.tFlag`, `opts.tol`

4.7 Discovery of Shared Feature Mapping: Alternating Structure Optimization

The basic idea of alternating structure optimization (ASO) (Ando & Zhang, 2005) is to decompose the predictive model of each task into two components: the task-specific feature mapping and task-shared feature mapping, as shown in Figure 8. The ASO formulation for linear predictors is given by:

$$\begin{aligned} \min_{\{v_t,w_t\},\Theta} \quad & \sum_{t=1}^{T}\left(\frac{1}{n_t}\mathcal{L}(w_t)+\alpha\|w_t\|^2\right) \\ \text{subject to} \quad & \Theta\Theta^T=I, \quad w_t=u_t+\Theta^T v_t, \end{aligned} \tag{25}$$

where Θ is the low dimensional feature map across all tasks. The predictor f_t for task t can be expressed as:

$$f_t(x)=w_t^T x=u_t^T x+v_t^T\Theta x.$$

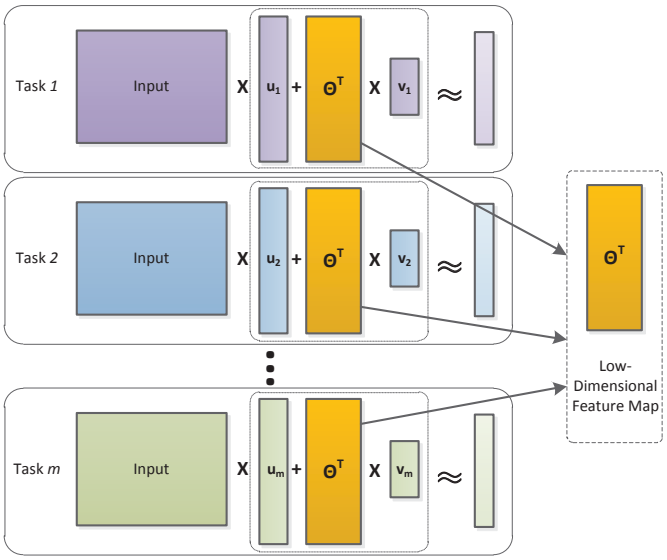

Figure 8: Illustration of Alternating Structure Optimization. The predictive model of each task includes two components: the task-specific feature mapping and task-shared feature mapping.

The formulation in Eq.(12) is not convex. A convex relaxation of ASO called cASO is proposed in (Chen et al., 2009):

$$\begin{aligned} \min_{\{w_t\},M} \quad & \sum_{t=1}^{T}\left(\frac{1}{n_t}\sum_{i=1}^{n_t}\mathcal{L}(w_t)\right)+\alpha\eta(1+\eta)\text{tr}\left(W^T(\eta I+M)^{-1}W\right) \\ \text{subject to} \quad & \text{tr}(M)=h, M\preceq I, M\in S_+^d \end{aligned} \tag{26}$$

It has been shown in (Zhou et al., 2011a) that there is an equivalence relationship between clustered multi-task learning in Eq. (20) and cASO when the dimensionality of the shared subspace in cASO is equivalent to the cluster number in cMTL.

4.7.1 cASO with Least Squares Loss (`Least_CASO`)

The function

```
[W, funcVal, M] = Least_CASO(X, Y, ρ1, ρ2, k, [opts])
```

solves the convex relaxed alternating structure optimization (ASO) multi-task least squares problem:

$$\min_{W} \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \eta(1+\eta) \text{tr}\left(W^T(\eta I + M)^{-1} W\right), \tag{27}$$

$$\text{subject to: } \text{tr}\,(M) = k, M \preceq I, M \in S_+^d, \eta = \frac{\rho_2}{\rho 1} \tag{28}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, and ρ_1 is the regularization parameter. Due to the equality constraint $\text{tr}\,(M) = k$, the starting point of M is initialized to be $M_0 = k/t \times I$ satisfying $\text{tr}\,(M_0) = k$.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`

4.7.2 cASO with Logistic Loss (`Logistic_CASO`)

The function

```
[W, c, funcVal, M] = Logistic_CASO(X, Y, ρ1, ρ2, k, [opts])
```

solves the convex relaxed alternating structure optimization (ASO) multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \sum_{i=1}^{t} \sum_{j=1}^{n_i} \log(1 + \exp\left(-Y_{i,j}(W_j^T X_{i,j} + \mathbf{c}_i)\right)) + \rho_1 \eta(1+\eta) \text{tr}\left(W^T(\eta I + M)^{-1} W\right), \tag{29}$$

$$\text{subject to: } \text{tr}\,(M) = k, M \preceq I, M \in S_+^d, \eta = \frac{\rho_2}{\rho 1} \tag{30}$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model for task i, and ρ_1 is the regularization parameter. Due to the equality constraint $\text{tr}\,(M) = k$, the starting point of M is initialized to be $M_0 = k/t \times I$ satisfying $\text{tr}\,(M_0) = k$.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`, `opts.C0`
- Termination: `opts.tFlag`, `opts.tol`

4.8 Dealing with Outlier Tasks: Robust Multi-Task Learning

Most multi-task learning formulations assume that all tasks are relevant, which is however not the case in many real-world applications. Robust multi-task learning (RMTL) is aimed at identifying irrelevant (outlier) tasks when learning from multiple tasks.

One approach to perform RMTL is to assume that the model W can be decomposed into two components: a low rank structure L that captures task-relatedness and a group-sparse structure S that detects outliers (Chen et al., 2011). If a task is not an outlier, then it falls into the low rank structure L with its corresponding column in S being a zero vector; if not, then the S matrix has non-zero entries at the corresponding column. The following formulation learns the two components simultaneously:

$$\min_{W=L+S} \mathcal{L}(W) + \rho_1 \|L\|_* + \beta \|S\|_{1,2} \tag{31}$$

The predictive model of RMTL is illustrated in Figure 9.

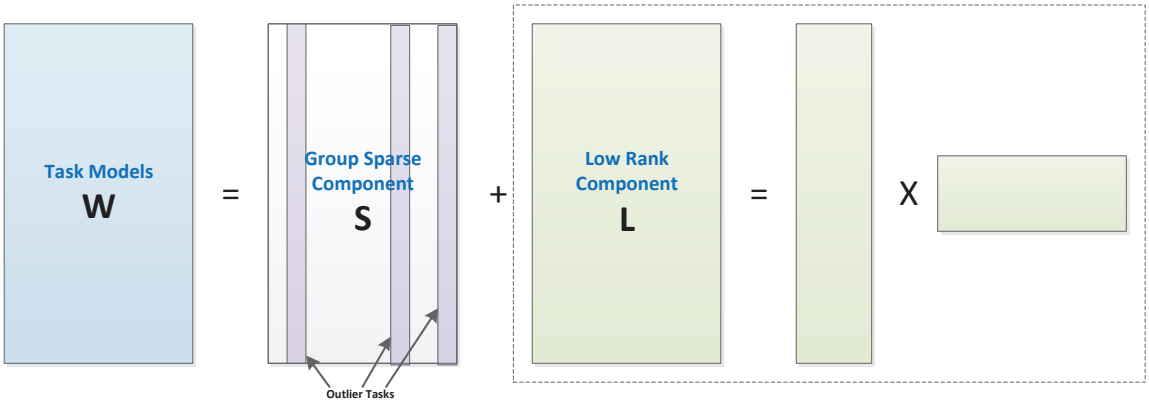

Figure 9: Illustration of robust multi-task learning. The predictive model of each task includes two components: the low-rank structure L that captures task relatedness and the group sparse structure S that detects outliers.

4.8.1 RMTL with Least Squares Loss (`Least_RMTL`)

The function

$$\texttt{[W, funcVal, L, S] = Least\_RMTL(X, Y, } \rho_1\texttt{, } \rho_2\texttt{, [opts])}$$

solves the incoherent group-sparse and low-rank multi-task least squares problem:

$$\min_{W} \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \|L\|_* + \rho_2 \|S\|_{1,2} \tag{32}$$

$$\text{subject to: } W = L + S \tag{33}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, the regularization parameter ρ_1 controls the low rank regularization on the structure L, and the ρ_2 regularization parameter controls the $\ell_{2,1}$-norm penalty on S.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.L0`, `opts.S0` (set `opts.W0` to any non-empty value)
- Termination: `opts.tFlag`, `opts.tol`

4.9 Joint Feature Learning with Outlier Tasks: Robust Multi-Task Feature Learning

The joint feature learning formulation in 4.2 selects a common set of features for all tasks. However, it assumes there is no outlier task, which may not the case in practical applications. To this end, a robust multi-task feature learning (rMTFL) formulation is proposed in (Gong et al., 2012b). rMTFL assumes that the model W can be decomposed into two components: a shared feature structure P that captures task-relatedness and a group-sparse structure Q that detects outliers. If the task is not an outlier, then it falls into the joint feature structure P with its corresponding column in Q being a zero vector; if not, then the Q matrix has non-zero entries at the corresponding column. The following formulation learns the two components simultaneously:

$$\min_{W=P+Q} \mathcal{L}(W) + \rho_1 \|P\|_{2,1} + \beta \|Q^T\|_{2,1} \tag{34}$$

The predictive model of rMTFL is illustrated in Figure 10.

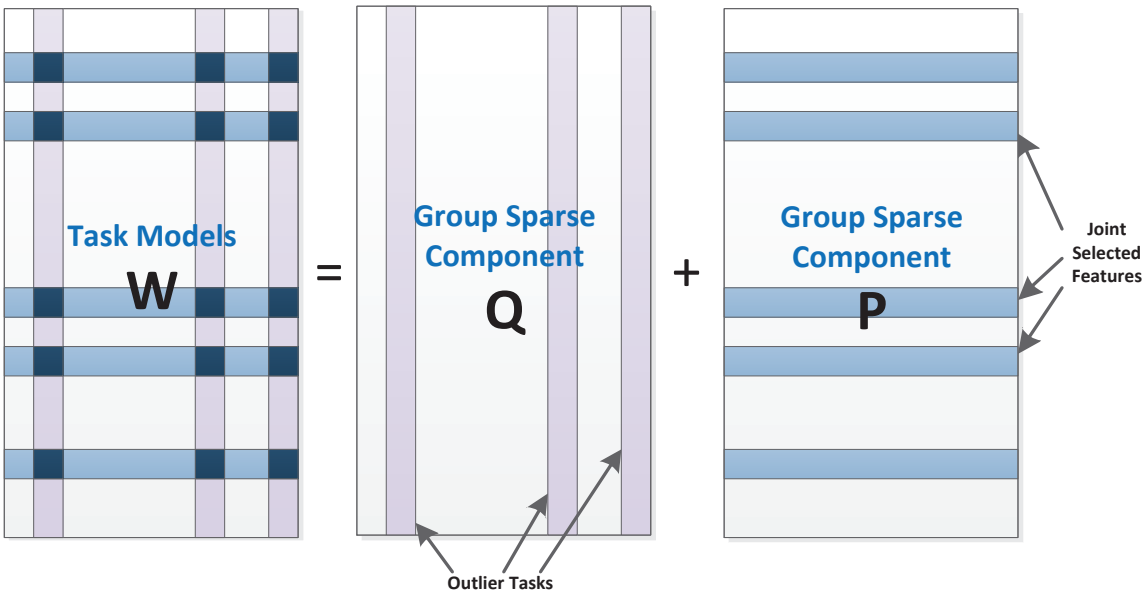

Figure 10: Illustration of robust multi-task feature learning. The predictive model of each task includes two components: the joint feature selection structure P that captures task relatedness and the group sparse structure Q that detects outliers.

4.9.1 RMTL with Least Squares Loss (`Least_rMTFL`)

The function

```
[W, funcVal, Q, P] = Least_rMTFL(X, Y, ρ1, ρ2, [opts])
```

solves the problem of robust multi-task feature learning with least squares loss:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \|P\|_{2,1} + \rho_2 \|Q^T\|_{2,1} \tag{35}$$

$$\text{subject to: } W = P + Q \tag{36}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the model for task i, the regularization parameter ρ_1 controls the joint feature learning, and the regularization parameter ρ_2 controls the columnwise group sparsity on Q that detects outliers.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.L0`, `opts.S0` (set `opts.W0` to any non-empty value)
- Termination: `opts.tFlag`, `opts.tol`
- Initial Lipschitz constant: `opts.lFlag`

4.10 Encoding Temporal Information: Disease Progression Models

Disease progression can be modeled using multi-task learning (Zhou et al., 2011b). In many longitudinal study of diseases, subjects are followed over a period of time and asked to visit the hospital repeatedly.

Each visit a variety of biomarkers (e.g. imaging, plasma panels) and disease status (e.g. scores that reflect cognitive status) are measured from patients. One important task is to build predictive models of future disease status given biomarker measurements at one or more time points. The prediction of the value of the disease status at one time point is considered as a task, the prediction models at different time points may be similar because that they are temporally related. The model encodes the temporal information using regularization terms. Specifically, the formulation is given by:

$$\min_W \mathcal{L}(W) + \rho_1 \|W\|_F^2 + \rho_2 \sum_{i=1}^{t-1} \|W_i - W_{i+1}\|_F^2 + \rho_3 \|W\|_{2,1},$$

where the first penalty controls the complexity of the model; the second penalty couples the neighbor tasks, encouraging every two neighbor tasks to be similar (temporal smoothness); and the third penalty induces the grouped sparsity, which performs the joint feature selection on the tasks at different time points (longitudinal feature selection, see Figure 11).

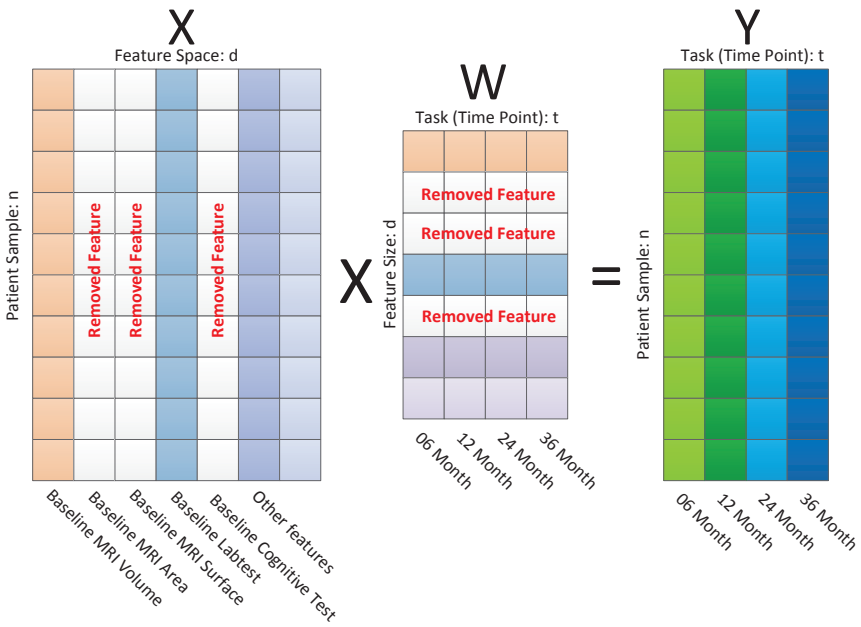

Figure 11: Illustration of the temporal group Lasso (TGL) disease progression model.

We can understand the temporal information as a type of graph regularization, where neighbor tasks are coupled via edges. The structure variable R can be defined as:

```
R = zeros(t, t-1); R(1:(t+1):end) = 1; R(2:(t+1):end) = -1;
```

and the formulation can be written in a simple form:

$$\min_W \mathcal{L}(W) + \rho_1 \|W\|_F^2 + \rho_2 \|WR\|_F^2 + \rho_3 \|W\|_{2,1}, \tag{37}$$

Note that the implementation of TGL algorithm can deal with general graph structure in the structure variable `R`, but not limited to temporal regularization. Please refer Section 4.4 for specification of the structure variable `R`.

One advantage of TGL formulation in Eq. (37) is that the regularization terms are simple to solve and thus can be efficiently solved. However, the formulation assumes that a biomarker is either selected or is

not selected at all time points. The convex fused sparse group Lasso (cFSGL) formulations are proposed to overcome this issue (Zhou et al., 2012):

$$\min_W \mathcal{L}(W) + \rho_1\|W\|_1 + \rho_2\|RW^T\|_1 + \rho_3\|W\|_{2,1}, \tag{38}$$

where the fused structure R is defined in the same way as in TGL. In cFSGL , we aim to select task-shared and task-specific features using the sparse group Lasso penalty. However, the sparsity-inducing penalties are known to lead to biased estimates. The paper also discussed two non-convex multi-task regression formulations for modeling disease progression (Zhou et al., 2012):

$$\text{[nFSGL1]} \quad \min_W \mathcal{L}(W) + \rho_1 \sum_{i=1}^{d} \sqrt{\|\mathbf{w}_i\|_1} + \rho_2\|RW^T\|_1, \tag{39}$$

$$\text{[nFSGL2]} \quad \min_W \mathcal{L}(W) + \rho_1 \sum_{i=1}^{d} \sqrt{\|R\mathbf{w}_i^T\|_1 + \rho_2\|\mathbf{w}_i\|_1}, \tag{40}$$

where the second term is the summation of the squared root of ℓ_1-norm of $\mathbf{w}_i$ ($\mathbf{w}_i$ is the ith row of W). For a detailed discussion and comparison among different disease progression models, the reader is referred to the paper (Zhou et al., 2012). In the package, we have included all algorithms for the disease progression models discussed above.

4.10.1 Temporal Group Lasso with Least Squares Loss (`Least_TGL`)

The function

```
[W, funcVal] = Least_TGL (X, Y, R, ρ1, ρ2, [opts])
```

solves the temporal smoothness regularized (and the squared ℓ_2-norm) regularized multi-task least squares problem:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1\|W\|_F^2 + \rho_2\|WR\|_F^2 + \rho_3\|W\|_{2,1}, \tag{41}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the task model for task i, ρ_2 is the regularization parameter that controls temporal smoothness, the regularization parameter ρ_3 controls group sparsity for joint feature selection, and the ρ_1 regularization parameter controls ℓ_2-norm penalty and can be set to prevent overfitting.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`

4.10.2 Temporal Group Lasso with Logistic Loss (`Logistic_TGL`)

The function

```
[W, c, funcVal] = Logistic_TGL (X, Y, R, ρ1, ρ2, [opts])
```

solves the temporal smoothness regularized (and the squared ℓ_2-norm) regularized multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \sum_{i=1}^{t} \sum_{j=1}^{n_i} \log(1 + \exp\left(-Y_{i,j}(W_j^T X_{i,j} + \mathbf{c}_i)\right)) + \rho_1 \|W\|_F^2 + \rho_2 \|WR\|_F^2 + \rho_3 \|W\|_{2,1}, \qquad (42)$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model parameters for task i, ρ_2 is the regularization parameter for temporal smoothness the regularization parameter ρ_3 controls group sparsity for joint feature selection , and the ρ_1 regularization parameter controls ℓ_2-norm penalty and can be set to prevent overfitting.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`, `opts.C0`
- Termination: `opts.tFlag`, `opts.tol`

4.10.3 Convex Sparse Fused Group Lasso (cFSGL) with Least Squares Loss (`Least_CFGLasso`)

The function

`[W, funcVal] =` **`Least_CFGLasso`** `(X, Y,` ρ_1`,` ρ_2`,` ρ_3`, [opts])`

solves the convex fused sparse group Lasso regularized multi-task least squares problem:

$$\min_{W} \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \|W\|_1 + \rho_2 \|RW^T\|_1 + \rho_3 \|W\|_{2,1}, \qquad (43)$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the task model for task i, the regularization parameter ρ_3 controls group sparsity for joint feature selection, ρ_1 and ρ_2 are the parameters for the fused Lasso. Specifically, ρ_1 controls element-wise sparsity and ρ_2 controls the fused regularization.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`

4.10.4 Convex Sparse Fused Group Lasso (cFSGL) with Logistic Loss (`Logistic_CFGLasso`)

`[W, c, funcVal] =` **`Logistic_CFGLasso`** `(X, Y,` ρ_1`,` ρ_2`,` ρ_3`, [opts])`

solves the convex fused sparse group Lasso regularized multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \sum_{i=1}^{t} \sum_{j=1}^{n_i} \log(1 + \exp\left(-Y_{i,j}(W_j^T X_{i,j} + \mathbf{c}_i)\right)) + \rho_1 \|W\|_1 + \rho_2 \|RW^T\|_1 + \rho_3 \|W\|_{2,1}, \qquad (44)$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model parameters for task i, the regularization parameter ρ_3 controls group sparsity for joint feature selection, ρ_1 and ρ_2 are the parameters for the fused Lasso. Specifically, ρ_1 controls element-wise sparsity and ρ_2 controls the fused regularization.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`, `opts.C0`
- Termination: `opts.tFlag`, `opts.tol`

4.10.5 Non-Convex Sparse Fused Group Lasso Formulation 1 (nFSGL1) (`Least_NCFGLassoF1`)

The function

```
[W, funcVal] = Least_NCFGLassoF1 (X, Y, ρ1, ρ2, [opts])
```

solves the non-convex fused sparse group Lasso (nFSGL1) regularized multi-task least squares problem:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \sum_{i=1}^{d} \sqrt{\|\mathbf{w}_i\|_1} + \rho_2 \|RW^T\|_1 \tag{45}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the task model for task i, the regularization parameter ρ_1 controls the group sparsity for joint feature selection and also the element-wise sparsity, ρ_2 controls the fused regularization. Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`
- Outer Loop Max Iteration: `opts.max_iter`
- Outer Loop Tolerance: `opts.tol_funcVal`

Note that this is a multi-stage optimization problem, it is suggested that the outer loop need NOT to converge to a high precision. Typically a very small max iteration (e.g. 10) is used.

4.10.6 Non-Convex Sparse Fused Group Lasso Formulation 2 (nFSGL2) (`Logistic_NCFGLassoF2`)

The function

```
[W, funcVal] = Least_NCFGLassoF2 (X, Y, ρ1, ρ2, [opts])
```

solves the non-convex fused sparse group Lasso (nFSGL2) regularized multi-task least squares problem:

$$\min_W \sum_{i=1}^{t} \|W_i^T X_i - Y_i\|_F^2 + \rho_1 \sum_{i=1}^{d} \sqrt{\|R\mathbf{w}_i^T\|_1 + \rho_2 \|\mathbf{w}_i\|_1}, \tag{46}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the task model for task i, the regularization parameter ρ_1 controls the group sparsity for joint feature selection and also fused regularization, ρ_2 controls the element-wise sparsity.

Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`
- Outer Loop Max Iteration: `opts.max_iter`
- Outer Loop Tolerance: `opts.tol_funcVal`

Note that this is a multi-stage optimization problem, it is suggested that the outer loop need NOT to converge to a high precision. Typically a very small max iteration (e.g. 10) is used.

4.11 The Multi-Task Feature Learning Framework for Incomplete Multi-Source Data Fusion (iMSF)

In some learning problems that involve multiple data sources, though all data sources consist of different features for the same set of samples, it is common that each data source has some missing samples that are different from each other. When one wants to build predictive models that involve features from more than one data sources, a common way is to remove the the samples that are missing in any of these data sources. However, this approach removes too much information that can be potentially useful in the learning. Recently, a multi-task learning framework for incomplete multi-source data fusion (iMSF) has been proposed to solve this problem (Yuan et al., 2012). Considering a data set with three sources (CSF, MRI, PET) and assuming all samples have MRI measures, we first partition the samples into multiple blocks (4 in this case), one for each combination of data sources available: (1) PET, MRI; (2) PET, MRI, CSF; (3) MRI, CSF; and (4) MRI. We then build four models, one for each block of data, resulting in four prediction tasks (Figure 12).

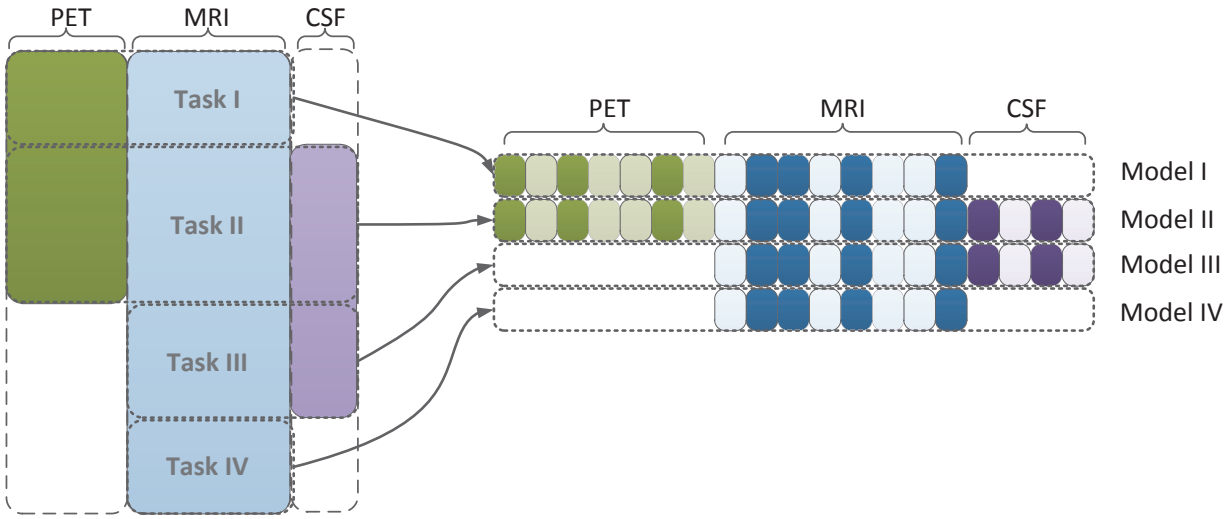

Figure 12: Illustration of the multi-task feature learning framework for incomplete multi-source data fusion (iMSF). In the proposed framework, we first partition the samples into multiple blocks (four blocks in this case), one for each combination of data sources available: (1) PET, MRI; (2) PET, MRI, CSF; (3) MRI, CSF; (4) MRI. We then build four models, one for each block of data, resulting in four prediction tasks. We use a joint feature learning framework that learns all models simultaneously. Specifically, all models involving a specific source are constrained to select a common set of features for that particular source.

Assume that we have a total of S data sources, and the feature dimensionality of the s-th source is denoted as p_s. For notational convenience, we introduce an index function $G(s,k)$ as follows: $W_{G(s,k)}$ denotes all the model parameters corresponding to the k-th feature in the s-th data source. The iMSF formulation is:

$$\mathcal{L}(W) + \rho_1 \sum_{s=1}^{S} \sum_{k=1}^{p_s} \left\| W_{G(s,k)} \right\|_2 \tag{47}$$

where $\mathcal{L}(\cdot)$ is the loss function.

4.11.1 Incomplete Multi-Source Fusion (iMSF) with Least Squares Loss (`Least_iMSF`)

The function

```
[W, funcVal] = Least_iMSF (X, Y, ρ1, [opts])
```

solves the convex fused sparse group Lasso regularized multi-task least squares problem:

$$\min_W \frac{1}{t}\sum_{i=1}^{t}\frac{1}{n_i}\|W_i^T X_i - Y_i\|_F^2 + \rho_1 \sum_{s=1}^{S}\sum_{k=1}^{p_s}\left\|W_{G(s,k)}\right\|_2 \tag{48}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the task model for task i, the regularization parameter ρ_1 controls group sparsity. Currently, this function supports the following optional fields:

- Termination: `opts.tFlag`, `opts.tol`

4.11.2 Incomplete Multi-Source Fusion (iMSF) with Logistic Loss (`Logistic_iMSF`)

```
[W, c, funcVal] = Logistic_iMSF (X, Y, ρ1, [opts])
```

solves the convex fused sparse group Lasso regularized multi-task logistic regression problem:

$$\min_{W,\mathbf{c}} \frac{1}{t}\sum_{i=1}^{t}\frac{1}{n_i}\sum_{j=1}^{n_i}\log(1+\exp\left(-Y_{i,j}(W_j^T X_{i,j}+\mathbf{c}_i)\right)) + \rho_1 \sum_{s=1}^{S}\sum_{k=1}^{p_s}\left\|W_{G(s,k)}\right\|_2 \tag{49}$$

where $X_{i,j}$ denotes sample j of the i-th task, $Y_{i,j}$ denotes its corresponding label, W_i and $\mathbf{c}_i$ are the model parameters for task i, the regularization parameter ρ_1 controls group sparsity. Currently, this function supports the following optional fields:

- Termination: `opts.tFlag`, `opts.tol`

4.12 Multi-Stage Multi-Task Feature Learning (MSMTFL)

In many recent studies of sparse learning, capped vector norms are shown to enjoy better theoretical properties and better empirical performance than the classic sparsity inducing norms (Zhang, 2010). More recently the capped norm is used in multi-task feature learning and is shown to possess both theoretical and empirical improvements on feature learning (Gong et al., 2012a). The method is called multi-stage multi-task feature learning (MSMTFL), which simultaneously learn the features specific to each task as well as the common features shared among tasks. The non-convex MSMTFL solves the following formulation

$$\min_W \left\{ L(W) + \rho_1 \sum_{j=1}^{d} \min(\|\mathbf{w}_j\|_1, \theta) \right\},$$

where $\mathbf{w}_j$ is the j-th row the model W. Using the difference of convex procedures, the optimization of MSMTFL is to iteratively solve ℓ_1-regularized convex problems.

4.12.1 Multi-Stage Feature Learning (MSMTFL) with Least Squares Loss (`Least_msmtfl_capL1`)

The function

```
[W, funcVal] = Least_msmtfl_capL1 (X, Y, ρ1, θ, [opts])
```

solves the multi-stage multi-task feature learning problem:

$$\min_W \frac{1}{t}\sum_{i=1}^{t}\frac{1}{n_i}\|W_i^T X_i - Y_i\|_F^2 + \rho_1 \sum_{j=1}^{d}\min(\|\mathbf{w}_j\|_1, \theta), \tag{50}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding label, W_i is the task model for task i, $\mathbf{w}_j$ is the j-th row the model W, the regularization parameter ρ_1 controls group sparsity, and θ is the parameter for the capped ℓ_1. Currently, this function supports the following optional fields:

- Starting Point: `opts.init`, `opts.W0`
- Termination: `opts.tFlag`, `opts.tol`

4.13 Learning the Shared Subspace for Multi-Task Clustering (LSSMTC)

Most of the multi-task learning algorithms in the literature fall in the field of supervised learning. However, multi-task learning can also be used in the unsupervised learning, i.e., clustering (Gu & Zhou, 2009). One may get confused between the clustered multi-task learning (CMTL) and multi-task clustering (MTC). In CMTL, the objects to be clustered are model vectors, i.e., columns of the model matrix W (refer Section for detailed information). In MTC, the objects to be clustered are samples, i.e., rows of the design matrix X.

One way to model task relatedness in the MTC is to assume that the data matrix share a common subspace, and data points from each task forms cluster in the subspace. In (Gu & Zhou, 2009), an algorithm for learning the shared subspace for multi-task clustering (LSSMTC) is proposed to address the MTC with shared subspace. Assume there are t clustering tasks, and each task clusters the samples into c clusters, the formulation of LSSMTC is given by:

$$\begin{aligned}&\min_{M,P,W} \rho_1 \sum_{i=1}^{t}\|X_i - M_i P_i^T\|_F^2 + (1-\rho_1)\sum_{i=1}^{t}\|W^T X_i - M P_i^T\|_F^2\\ &\text{subject to: } W^T W = I, P_i \geq 0\end{aligned}$$

where $M_i \in \mathbb{R}^{d\times c}$ is the matrix for cluster centers of task i, $P_i \in \mathbb{R}^{n_i \times c}$ is the relaxed cluster assignment of task i, $W \in \mathbb{R}^{d\times l}$, and l is the dimensionality of the shared subspace. The first term is the objective of relaxed k-means and the second the term is the objective of the relaxed k-means in the shared subspace.

4.13.1 Learning Shared Subspace for Multi-Task Clustering (`LSSMTC`)

The function

```
[W, M, P, funcVal, Acc, NMI] = LSSMTC (X, Y, c, l, ρ1, [opts])
```

solves the following multi-task clustering formulation:

$$\min_{M,P,W} \rho_1 \sum_{i=1}^{t}\|X_i - M_i P_i^T\|_F^2 + (1-\rho_1)\sum_{i=1}^{t}\|W^T X_i - M P_i^T\|_F^2 \tag{51}$$

$$\text{subject to: } W^T W = I, P_i \geq 0 \tag{52}$$

where X_i denotes the input matrix of the i-th task, Y_i denotes its corresponding clustering label (the input is not mandatory, it is only required if the evaluation metric accuracy `Acc` and/or normalized mutual information `NMI` are needed), W is the shared subspace, P_i is the partition matrix for task i, M_i is the matrix that consists of the centers of clusters of task i, c is the cluster number, l is the dimension of the shared subspace, and the regularization parameter ρ_1 controls the importance of the clustering quality in the shared space and in the original space. Currently, this function supports the following optional fields:

- Termination: `opts.tFlag`, `opts.tol`

5 Examples

In this section we provide some running examples for some representative multi-task learning formulations included in the MALSAR package. All figures in these examples can be generated using the corresponding MATLAB scripts in the `examples` folder.

5.1 Code Usage and Optimization Setup

The users are recommended to add paths that contains necessary functions at the beginning:

```
addpath('/MALSAR/functions/Lasso/');  % load function
addpath('/MALSAR/utils/');            % load utilities
addpath(genpath('/MALSAR/c_files/')); % load c-files
```

An alternative is to add the entire MALSAR package:

```
addpath(genpath('/MALSAR/'));
```

The users then need to setup optimization options before calling functions (refer to Section 3.2 for detailed information about `opts`):

```
opts.init = 0;        % compute start point from data.
opts.tFlag = 1;       % terminate after relative objective
                      % value does not changes much.
opts.tol = 10^-5;     % tolerance.
opts.maxIter = 1500; % maximum iteration number of optimization.
[W funcVal]  = Least_Lasso(data_feature, data_response, lambda, opts);
```

Note: For efficiency consideration, it is important to set proper tolerance, termination conditions and most importantly, maximum iterations, especially for large-scale problems.
Note: In many of the following examples we use the following command to control random generator:

```
rng('default');      % reset random generator.
```

This command is only available on MATLAB 2011 and later version. If you are using earlier versions, another command can achieve the same goal `reset`. Please use the MATLAB help to get more information about the command.

5.2 Training and Testing in Multi-Task Learning

In multi-task learning (MTL), a set of related tasks are learnt simultaneously by extracting and utilizing appropriate shared information among tasks. In the supervised multi-task learning, each task has its own training data and testing data. Though in the training (inference) stage, the training data for all tasks are inputed in MTL algorithms simultaneously, the algorithms give one model for each task (in our package the model for task i is given by the i-th column of W). The evaluation of each task is independently performed on its testing data using the model for the task.

In this example we show the training, testing and model selection using the benchmark dataset - School data[3]. In the School data there are 15362 students and their exam scores, and the students are described by 27 attributes (features). Our goal is to build regression models to predict the exam score of students

[3] http://www.cs.ucl.ac.uk/staff/A.Argyriou/code/

from the attributes. The students come from one of the 139 secondary schools, and we build one regression model for each school because the regression models are likely to be different for different schools (e.g., different textbooks may be used). Therefore we have 139 tasks, and each task is the exam score prediction for students from one school.

We use the trace-norm regularized multi-task learning formulation in this example (for a detailed example designed for understanding this particular formulation, see Sect. 5.5). This formulation has one data-dependent parameter (the regularization parameter for the trace norm penalty), and we also show how to estimate the parameter on the training data via cross validation, this process is also known as the model selection (Kohavi, 1995). The code for this example is included in the example file `test_script.m` in the `train_and_test` subfolder. Firstly we load the School data:

```
load_data = load('../../data/school.mat');% load sample data.
X = load_data.X;
Y = load_data.Y;
```

The data file is already prepared in the cell format (for details about input and output format, the users are referred to Section 3.1). We then perform z-score to normalize `X` and add a bias column to the data for each task to learn the bias. Alternatively, one can choose to normalize the target `Y` in the training data, and apply the reverse transformation on the predicted values during testing.

```
for t = 1: length(X)
    X{t} = zscore(X{t});                  % normalization
    X{t} = [X{t} ones(size(X{t}, 1), 1)]; % add bias.
end
```

We specify a training percentage to randomly split the data of each task to the training and testing part:

```
training_percent = 0.3;
[X_tr, Y_tr, X_te, Y_te] = mtSplitPerc(X, Y, training_percent);
```

The next step is to perform model selection and estimate the best regularization parameter from the data. In order to perform cross validation, one must specify a criterion for evaluating the parameters. In multi-task regression, a commonly used criterion is root mean squared error (MSE) given by

$$\frac{\sum_{i=1}^{t} \sqrt{\sum_{j=1}^{n_i} (X_{i,j} * W_i - Y_{i,j})^2} * n_i}{\sum_{i=1}^{t} n_i}.$$

We use 5-fold cross validation to estimate the trace norm regularization parameter:

```
% the function used for evaluation.
eval_func_str = 'eval_MTL_mse';
higher_better = false;  % mse is lower the better.
% cross validation fold
cv_fold = 5;
% optimization options
opts = [];
opts.maxIter = 100;
% model parameter range
param_range = [0.001 0.01 0.1 1 10 100 1000 10000];
% cross validation
best_param = CrossValidation1Param( X_tr, Y_tr, 'Least_Trace', opts, param_range, ...
    cv_fold, eval_func_str, higher_better);
```

We have included the code for computing MSE and 1-parameter cross validation `CrossValidation1Param` in the example folder. After the best parameter is obtained, we can build models using the parameter and compute performance:

```
W = Least_Trace(X_te, Y_te, best_param, opts);
final_performance = eval_MTL_mse(Y_te, X_te, W);
```

5.3 Sparsity in Multi-Task Learning: ℓ_1-norm regularization

In this example, we explore the sparsity of prediction models in ℓ_1-norm regularized multi-task learning using the School data. To use school data, first load it from the `data` folder.

```
load('../data/school.mat'); % load sample data.
```

Define a set of regularization parameters and use pathwise computation:

```
lambda = [1 10 100 200 500 1000 2000];
sparsity = zeros(length(lambda), 1);
log_lam  = log(lambda);
for i = 1: length(lambda)
    [W funcVal] = Least_Lasso(X, Y, lambda(i), opts);
    % set the solution as the next initial point.
    % this gives better efficiency.
    opts.init = 1;
    opts.W0 = W;
    sparsity(i) = nnz(W);
end
```

The algorithm records the number of non-zero entries in the resulting prediction model W. We show the change of the `sparsity` variable against the logarithm of regularization parameters in Figure 13. Clearly, when the regularization parameter increases, the sparsity of the resulting model increases, or equivalently, the number of non-zero elements decreases. The code that generates this figure is from the example file `example_Lasso.m`.

5.4 Joint Feature Selection: $\ell_{2,1}$-norm regularization

In this example, we explore the $\ell_{2,1}$-norm regularized multi-task learning using the School data from the `data` folder:

```
load('../data/school.mat'); % load sample data.
```

Define a set of regularization parameters and use pathwise computation:

```
lambda = [200 :300: 1500];
sparsity = zeros(length(lambda), 1);
log_lam  = log(lambda);

for i = 1: length(lambda)
    [W funcVal] = Least_L21(X, Y, lambda(i), opts);
    % set the solution as the next initial point.
    % this gives better efficiency.
```

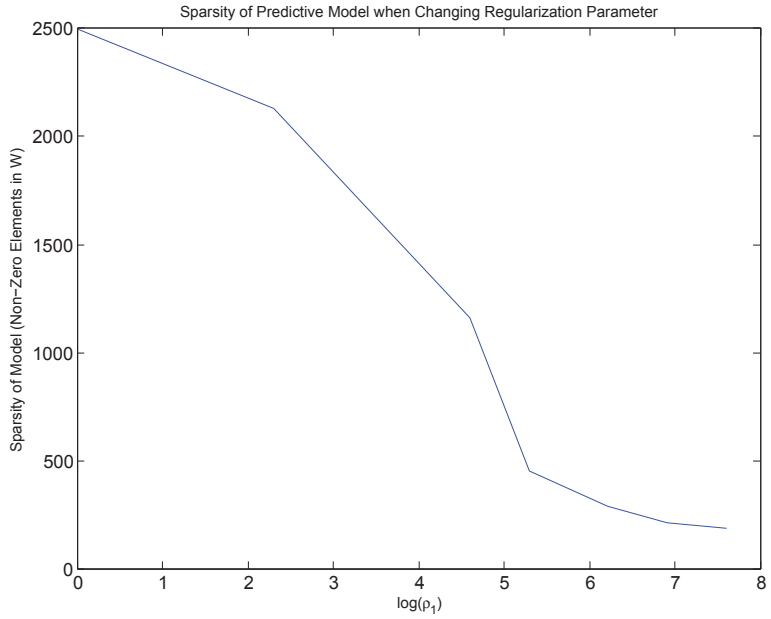

Figure 13: Sparsity of the model Learnt from ℓ_1-norm regularized MTL. As the parameter increases, the number of non-zero elements in W decreases, and the model W becomes more sparse.

```
    opts.init = 1;
    opts.W0 = W;
    sparsity(i) = nnz(sum(W,2 )==0)/d;
end
```

The statement `nnz(sum(W,2 )==0)` computes the number of features that are not selected for all tasks. We can observe from Figure 14 that when the regularization parameter increases, the number of selected features decreases. The code that generates this result is from the example file `example_L21.m`.

5.5 Low-Rank Structure: Trace norm Regularization

In this example, we explore the trace-norm regularized multi-task learning using the School data from the `data` folder:

```
load('../data/school.mat'); % load sample data.
```

Define a set of regularization parameters and use pathwise computation:

```
tn_val = zeros(length(lambda), 1);
rk_val = zeros(length(lambda), 1);
log_lam  = log(lambda);

for i = 1: length(lambda)
    [W funcVal] = Least_Trace(X, Y, lambda(i), opts);
    % set the solution as the next initial point.
    % this gives better efficiency.
    opts.init = 1;
    opts.W0 = W;
```

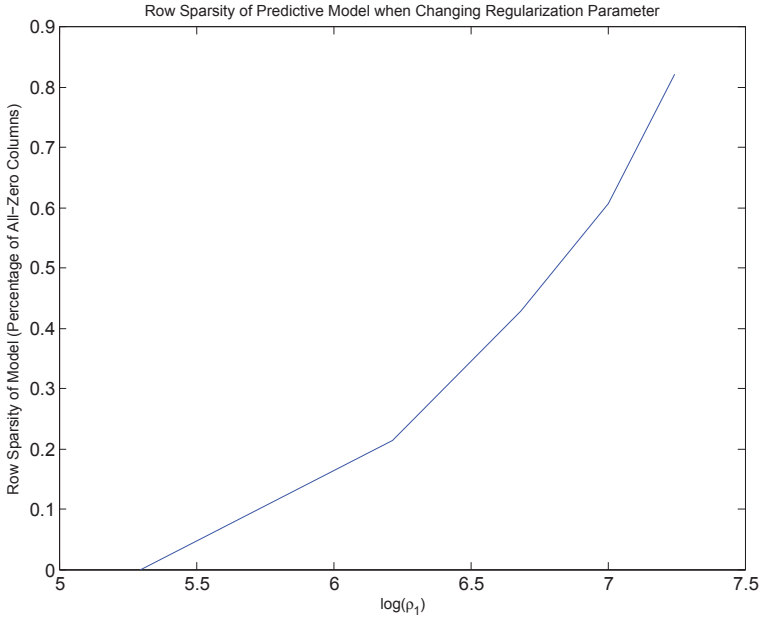

Figure 14: Joint feature learning via the $\ell_{2,1}$-norm regularized MTL. When the regularization parameter increases, the number of selected features decreases.

```
    tn_val(i) = sum(svd(W));
    rk_val(i) = rank(W);
end
```

In the code we compute the value of trace norm of the prediction model as well as its rank. We gradually increase the penalty and the results are shown in Figure 15. The code `sum(svd(W))` computes the trace norm (the sum of singular values).

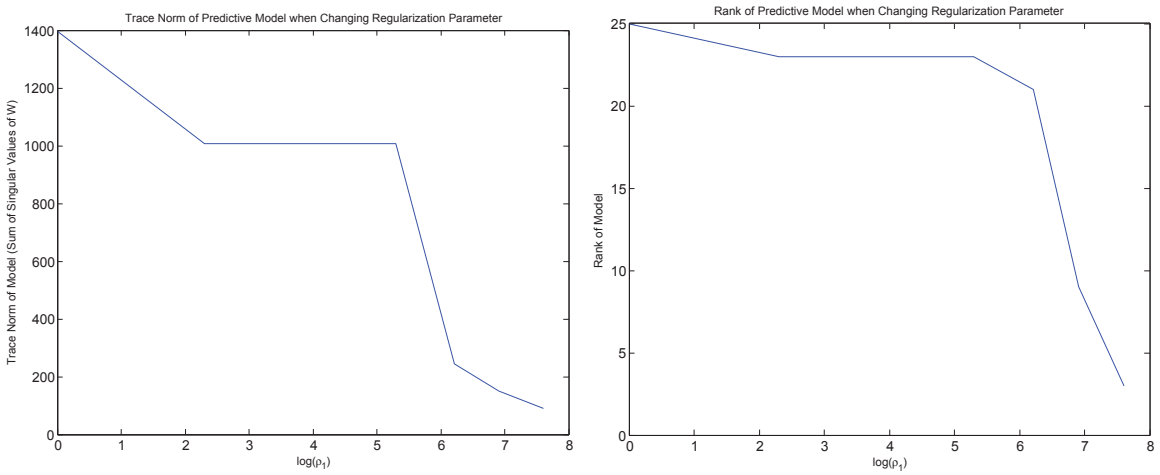

Figure 15: The trace norm and rank of the model learnt from trace norm regularized MTL.

As the trace-norm penalty increases, we observe the monotonic decrease of the trace norm and rank. The code that generates this result is from the example file `example_Trace.m`.

5.6 Graph Structure: Graph Regularization

In this example, we show how to use graph regularized multi-task learning using the `SRMTL` functions. We use the School data from the `data` folder:

```
load('../data/school.mat'); % load sample data.
```

For a given graph, we first construct the graph variable `R` to encode the graph structure:

```
% construct graph structure variable.
R = [];
for i = 1: task_num
    for j = i + 1: task_num
        if graph (i, j) ≠0
            edge = zeros(task_num, 1);
            edge(i) = 1;
            edge(j) = -1;
            R = cat(2, R, edge);
        end
    end
end
[W_est funcVal] = Least_SRMTL(X, Y, R, 1, 20);
```

The code that generates this result is from `example_SRMTL.m` and `example_SRMTL_spcov.m`.

5.7 Learning with Outlier Tasks: RMTL

In this example, we show how to use robust multi-task learning to detect outlier tasks using synthetic data:

```
dimension = 500;
sample_size = 50;
task = 50;
X = cell(task ,1);
Y = cell(task ,1);
for i = 1: task
    X{i} = rand(sample_size, dimension);
    Y{i} = rand(sample_size, 1);
end
```

To generate reproducible results, we reset the random number generator before we use the `rand` function. We then run the following code:

```
opts.init = 0;       % guess start point from data.
opts.tFlag = 1;      % terminate after relative objective value does not changes much.
opts.tol = 10^-6;    % tolerance.
opts.maxIter = 1500; % maximum iteration number of optimization.
rho_1 = 10;%    rho1: low rank component L trace-norm regularization parameter
rho_2 = 30; %    rho2: sparse component S L1,2-norm sprasity controlling parameter
[W funcVal L S] = Least_RMTL(X, Y, rho_1, rho_2, opts);
```

We visualize the matrices `L` and `S` in Figure 16. In the figure, the dark blue color corresponds to a zero entry. The matrices are transposed since the dimensionality is much larger than the task number. After transpose, each row corresponds to a task. We see that for the sparse component `S` has non-zero rows, corresponding to the outlier tasks. The code that generates this result is from the example file `example_Robust.m`.

5.8 Joint Feature Learning with Outlier Tasks: rMTFL

In this example, we show how to use robust multi-task learning to detect outlier tasks using synthetic data:

```
dimension = 500;
sample_size = 50;
task = 50;
X = cell(task ,1);
Y = cell(task ,1);
for i = 1: task
    X{i} = rand(sample_size, dimension);
    Y{i} = rand(sample_size, 1);
end
```

To generate reproducible results, we reset the random number generator before we use the `rand` function. We then run the following code:

```
opts.init = 0;       % guess start point from data.
opts.tFlag = 1;      % terminate after relative objective value does not changes much.
opts.tol = 10^-6;    % tolerance.
opts.maxIter = 500; % maximum iteration number of optimization.
rho_1 = 90;%   rho1: joint feature learning
rho_2 = 280; %   rho2: detect outlier
[W funcVal P Q] = Least_rMTFL(X, Y, rho_1, rho_2, opts);
```

We visualize the matrices `P` and `Q` in Figure 17. The code that generates this result is from the example file `example_rMTFL.m`.

5.9 Learning with Dirty Data: Dirty MTL Model

In this example, we show how to use dirty multi-task learning using synthetic data:

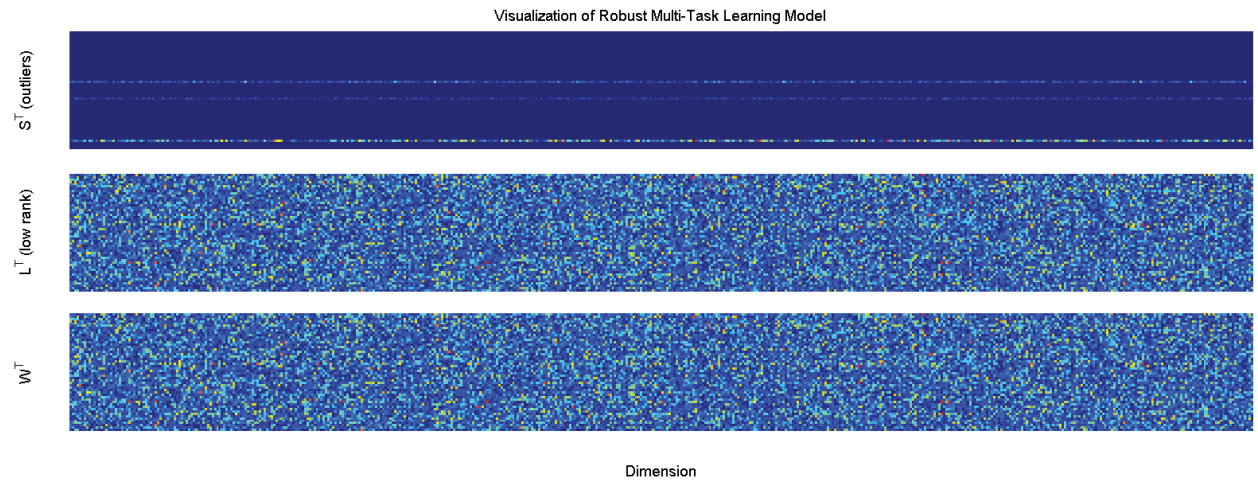

Figure 16: Illustration of RMTL. The dark blue color corresponds to a zero entry. The matrices are transposed since the dimensionality is much larger than the task number. After transpose, each row corresponds to a task. We see that for the sparse component `S` has non-zero rows, corresponding to the outlier tasks.

```
dimension = 500;
sample_size = 50;
task = 50;
X = cell(task ,1);
Y = cell(task ,1);
for i = 1: task
    X{i} = rand(sample_size, dimension);
    Y{i} = rand(sample_size, 1);
end
```

We then run the following code:

```
opts.init = 0;       % guess start point from data.
opts.tFlag = 1;      % terminate after relative objective value does not changes much.
opts.tol = 10^-4;    % tolerance.
opts.maxIter = 500; % maximum iteration number of optimization.
rho_1 = 350;%   rho1: group sparsity regularization parameter
rho_2 = 10;%   rho2: elementwise sparsity regularization parameter
[W funcVal P Q] = Least_Dirty(X, Y, rho_1, rho_2, opts);
```

We visualize the non-zero entries in `P`, `Q` and `R` in Figure 18. The figures are transposed for better visualization. We see that matrix `P` has a clear group sparsity property and it captures the joint-selected features. The features that do not fit into the group sparsity structure is captured in matrix `Q`. The code that generates this result is from the example file `example_Dirty.m`.

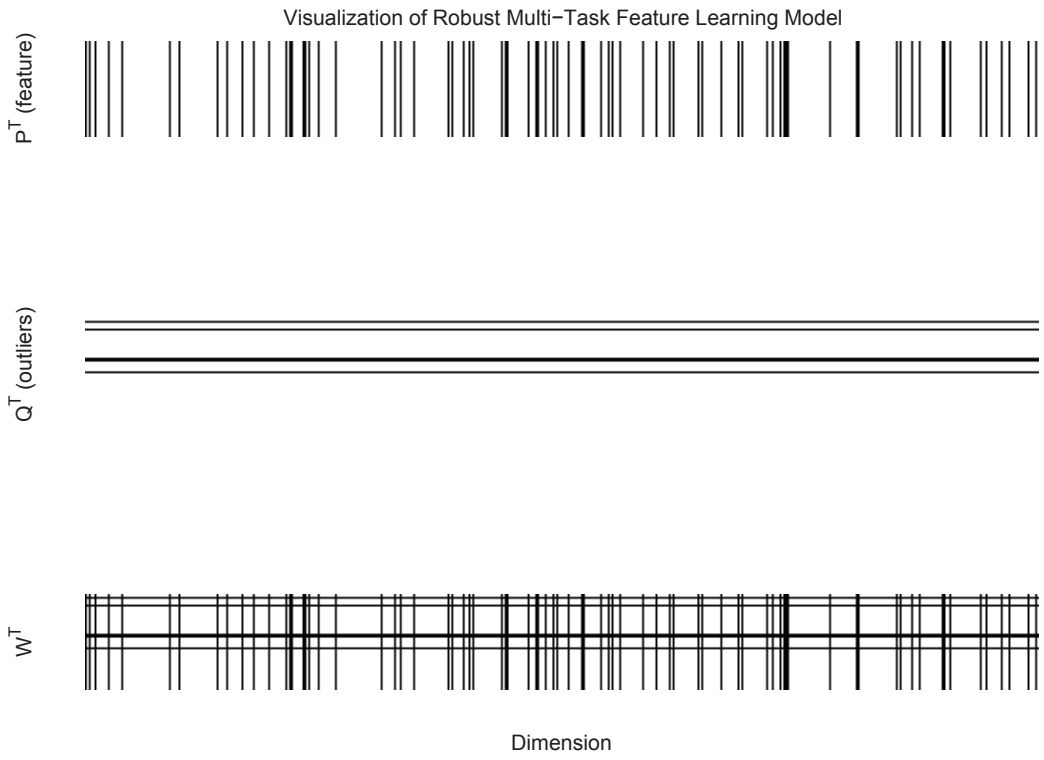

Figure 17: Illustration of outlier tasks detected by rMTFL. Black means non-zero entries. The matrices are transposed because that dimension number is larger than the task number. After transpose, each row denotes a task.

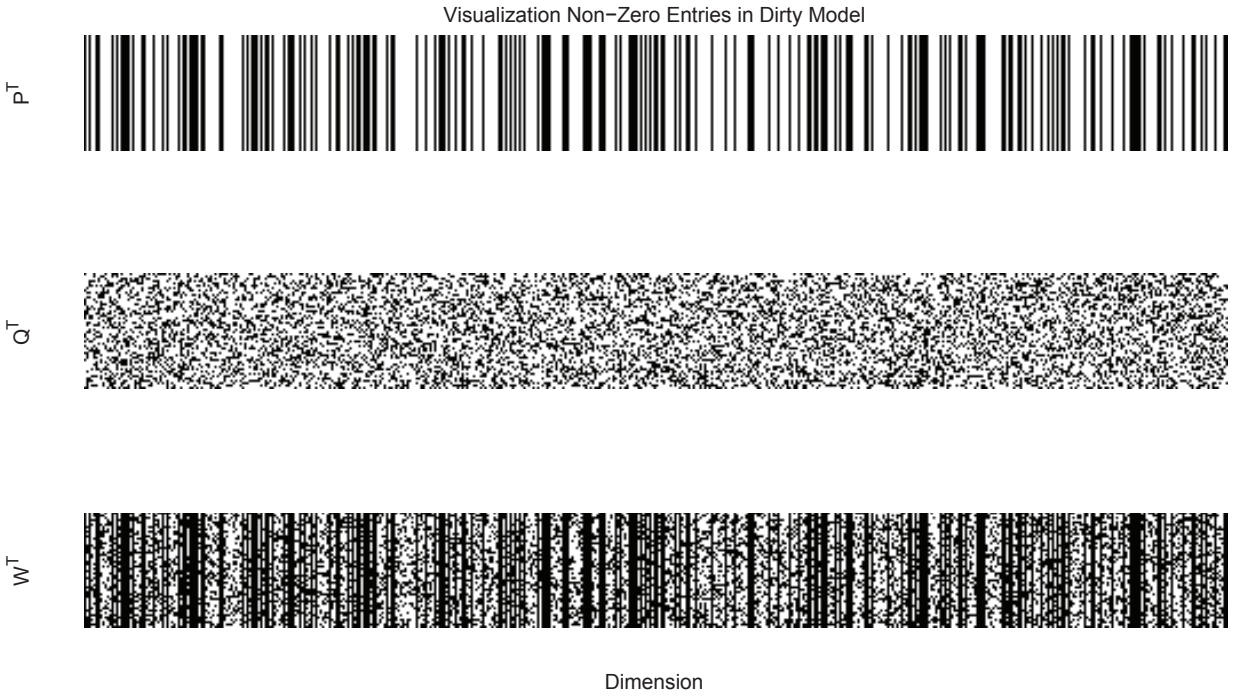

Figure 18: The dirty prediction model `W` learnt as well as the joint feature selection component `P` and the element-wise sparse component `Q`.

5.10 Learning with Clustered Structures: CMTL

In this example, we show how to use clustered multi-task learning (CMTL) functions. we use synthetic data generated as follows:

```
clus_var = 900;  % cluster variance
task_var = 16;   % inter task variance
nois_var = 150;  % variance of noise
clus_num = 2;                          % clusters
clus_task_num = 10;                    % task number of each cluster
task_num = clus_num * clus_task_num; % total task number.
sample_size = 100;
dimension   = 20;         % total dimension
comm_dim    = 2;          % independent dimension for all tasks.
clus_dim    = floor((dimension - comm_dim)/2); % dimension of cluster
% generate cluster model
cluster_weight = randn(dimension, clus_num) * clus_var;
for i = 1: clus_num
    cluster_weight (randperm(dimension-clus_num)≤clus_dim, i) = 0;
end
cluster_weight (end-comm_dim:end, :) = 0;
W = repmat (cluster_weight, 1, clus_task_num);
cluster_index = repmat (1:clus_num, 1, clus_task_num)';
% generate task and intra-cluster variance
W_it = randn(dimension, task_num) * task_var;
for i = 1: task_num
    W_it(cat(1, W(1:end-comm_dim, i)==0, zeros(comm_dim, 1))==1, i) = 0;
end
W = W + W_it;
```

```
% apply noise;
W = W + randn(dimension, task_num) * nois_var;
% Generate Data Sets
X = cell(task_num, 1);
Y = cell(task_num, 1);
for i = 1: task_num
    X{i} = randn(sample_size, dimension);
    xw   = X{i} * W(:, i);
    xw   = xw + randn(size(xw)) * nois_var;
    Y{i} = sign(xw);
end
```

We generate a set of tasks as follows: We firstly generate 2 cluster centers with between cluster variance $\mathcal{N}(0, 900)$, and for each cluster center we generate 10 tasks with intra-cluster variance $\mathcal{N}(0, 16)$. We thus generate a total of 20 task models `W`. We generate data points with variance $\mathcal{N}(0, 150)$. After we generate the data set, we run the following code to learn the CMTL model:

```
opts.init = 0;       % guess start point from data.
opts.tFlag = 1;      % terminate after relative objective value does not changes much.
opts.tol = 10^-6;    % tolerance.
opts.maxIter = 1500; % maximum iteration number of optimization.
rho_1 = 10;
rho_2 = 10^-1;
W_learn = Least_CMTL(X, Y, rho_1, rho_2, clus_num, opts);
% recover clustered order.
kmCMTL_OrderedModel = zeros(size(W));
OrderedTrueModel = zeros(size(W));
for i = 1: clus_num
    clusModel = W_learn         (:, i:clus_num:task_num );
    kmCMTL_OrderedModel         (:, (i-1)* clus_task_num + 1: i* clus_task_num ) = ...
        clusModel;

    clusModel = W               (:, i:clus_num:task_num );
    OrderedTrueModel            (:, (i-1)* clus_task_num + 1: i* clus_task_num ) = ...
        clusModel;
end
```

We visualize the models in Figure 19. We see that the clustered structure is captured in the learnt model. The code that generates this result is from the example file `example_CMTL.m`.

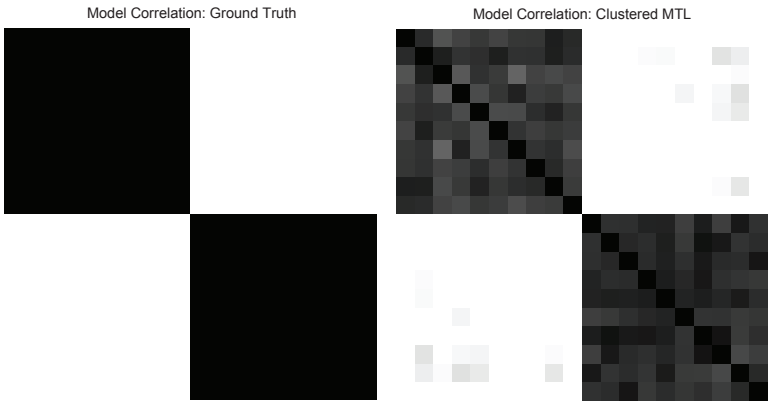

Figure 19: Illustration of the cluster Structure Learnt from CMTL.

5.11 Learning with Incomplete Data: Incomplete Multi-Source Fusion (iMSF)

In this example we show how to use incomplete multi-source fusion (iMSF). First, we import the path necessary for running iMSF.

```
addpath('../MALSAR/utils/')
addpath('../MALSAR/functions/iMSF')
```

Next, we construct 3 data sources that are block-wise missing. In total there are 50 samples, and the dimensions of the three data sources are 45, 55, 50 respectively. In the first data source, we suppose that the last 20% samples are missing, in the second data source, the first 20% samples are missing, and in the third data source there are 30% samples are missing. The missing patterns of the data sources are illustrated in Figure 20. Note that using this dataset for training the iMSF gives 4 models, one for each missing pattern (and the dimensions of these models are 95, 150, 100,105 respectively).

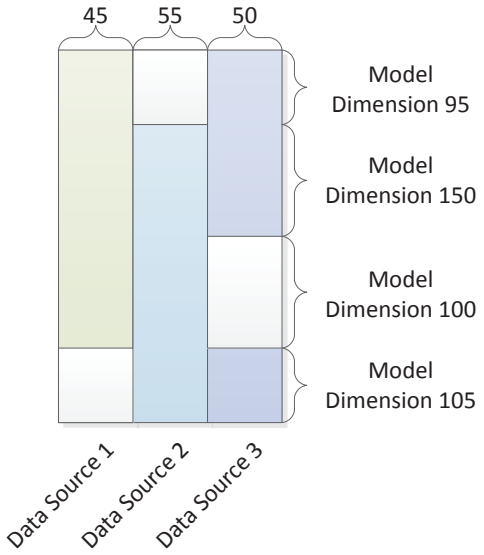

Figure 20: Illustration the block-wise missing patterns in the incomplete multi-source fusion.

We use the following code to construct these data sources and block-wise missing patterns:

```
n = 50; p1 = 45; p2 = 55; p3 = 50;
X1 = randn(n, p1); X2 = randn(n, p2); X3 = randn(n, p3);
X1(round(0.8 * n):end, :) = nan;
X2(1:round(0.2 * n), :) = nan;
X3(round(0.5 * n):round(0.8 * n), :) = nan;
Y = sign(randn(n, 1));
X_Set{1} = X1; X_Set{2} = X2; X_Set{3} = X3;
```

After the data sets are constructed, one can use the iMSF with logistic loss (or least squares loss) to build the models.

```
opts.tol = 1e-6;
opts.maxIter = 5000;
lambda = 0.1;
```

```
[logistic_Sol, logistic_funVal] = Logistic_iMSF(X_Set, Y, lambda, opts);
```

5.12 Towards Better Multi-Task Feature Learning: Multi-Stage Multi-Task Feature Learning

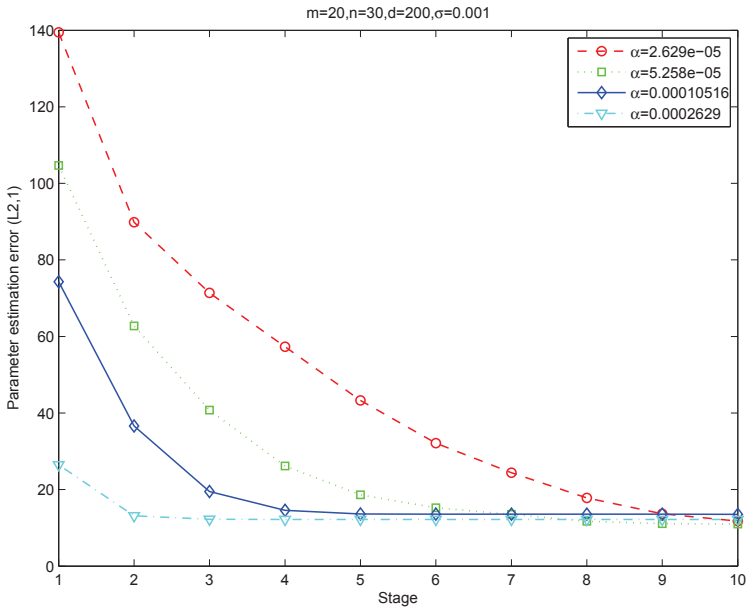

Figure 21: The parameter estimation error ($\ell_{2,1}$) of multi-stage feature learning with different number of stages.

In this example we explore the effectiveness of multi-stages methods in the multi-task feature learning. We generate data randomly from a given distribution and vary the parameters of the algorithm to demonstrate the effectiveness of the algorithm evaluated by $\ell_{2,1}$-norm between the ground truth and the model estimated from synthetic data.

We firstly load directories for the function and dependent utilities:

```
addpath('../MALSAR/functions/msmtfl/'); % load function
addpath('../MALSAR/utils/'); % load utilities
```

and specify experimental settings:

```
% problem size
m = 20; % task number
n = 30; % number of samples for each task
samplesize = n*ones(m,1);
d = 200; % dimensionality
repeat_num = 10; % repeat the experiment for 10 times
maxstep = 10;    % compare different parameters up to 10 stages.
% distribution for model and data
zerorow_percent = 0.9;
restzero_percent = 0.8;
noiselevel = 0.001;
```

```
% algorithm property
opts.tol = 1e-5;
opts.lFlag = 0;
opts.init = 1;
opts.W0 = randn(d,m);
opts.tFlag = 1;
% algorithm parameter settings.
scale = 50;
para = [0.00005; 0.0001; 0.0002; 0.0005]*sqrt(log(d*m)/n);
para_num = length(para);
```

In the experiment, we repeat the following experiments for 10 times and evaluate the average performance. We generate synthetic model and data from the given distribution

```
% generate model
W = rand(d,m)*20 - 10;
permnum = randperm(d);
zerorow = permnum(1:round(d*zerorow_percent));
nonzerorow = permnum(round(d*zerorow_percent)+1:end);
W(zerorow,:) = 0;
Wtemp = W(nonzerorow,:);
permnum = randperm(length(nonzerorow)*m);
Wtemp(permnum(1:round(length(nonzerorow)*m*restzero_percent))) = 0;
W(nonzerorow,:) = Wtemp;
% genetate data
X = cell(m,1);
Y = cell(m,1);
for ii = 1:m
    X{ii} = normrnd(0,1,samplesize(ii),d);
    X{ii} = normalize(X{ii},samplesize(ii));
    Y{ii} = X{ii} * W(:, ii) + noiselevel*normrnd(0,1,samplesize(ii),1);
end
```

and we study for each given maximum step (stage), the performance of different λ and the performance.

```
opts.maxIter = ii; % given (maximum) stage number.
lambda = para(1)*m*n;
theta = scale(1)*m*lambda;
[W_ms1,¬] = Least_msmtfl_capL1(X,Y,lambda,theta,opts);
```

and evaluate the performance using the $\ell_{2,1}$-norm:

```
Werror_ms1_21(ii,jj) = norm(sum(abs(W_ms1 - W),2));
```

A comparison of the performance of different settings is shown in the Figure 21. The code used to generate the figure can be found in the script `example_msmtfl.m` in the example folder of the package.

5.13 Unsupervised Multi-Task Learning: Learning Shared Subspace in Multi-Task Clustering (LSSMTC)

In this example we show how to learn shared subspace in multi-task clustering (LSSMTC). We use the 20 Newsgroup data [4], which is a collection of approximately 20k newsgroup documents, partitioned across 20 different newsgroups nearly evenly. In the `Data` folder we include two cross domain data sets (Rec. vs.

[4] http://people.csail.mit.edu/jrennie/20Newsgroups

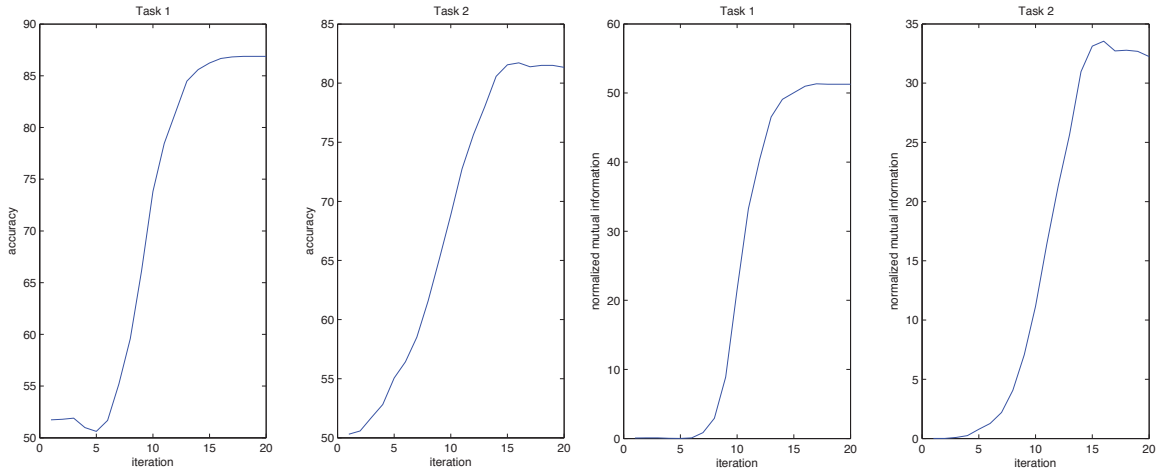

Figure 22: The accuracy and normalized mutual information for multi-task clustering on the 20 Newsgroups *Computer vs Science* dataset.

Talk and Comp. vs. Sci.). We demonstrate the LSSMTC algorithm on Computer vs Science dataset. Firstly we add paths necessary for running LSSMTC:

```
addpath('../MALSAR/functions/mutli-task clustering/');
addpath('../MALSAR/utils/');
```

We then load the clustering tasks into proper data structures:

```
m = 2; % there are two tasks in this dataset.
cellX = cell(m,1); cellgnd = cell(m,1);
for i=1:m
    task_data = load([path 'Task' num2str(i)]);
    cellX{i} = task_data.fea';
    cellgnd{i} = task_data.gnd;
end
```

Note that we need the label information only for the computation of performance metric (accuracy and/or normalized mutual information). In applications where ground truth is unknown, one may set `cellgnd=[]`. And then we can perform LSSMTC:

```
opts.tFlag = 2; % termination: run maximum iteration.
opts.maxIter = 20; % maximum iteration.
c = length(unique(cellgnd{1})); % cluster number
l = 2; % subspace dimension
lambda = 0.75; % multi-task regulariation paramter
[W cellM cellP residue cellAcc cellNMI] = LSSMTC(cellX,cellgnd,c,l,lambda,opts);
```

Note that for the purpose of illustration, for the cluster number `c` we use the ground truth, in real applications, however, the number (and also the dimension of the subspace l) should be estimated from data via cross validation. The accuracy and normalized mutual information for the two tasks are given in Figure 22. It can be seen from the results that the multi-task clustering improves the clustering performance for both tasks.

6 Revision, Citation and Acknowledgement

Revision

- Version 1.0 was released on April, 2012.
- Version 1.1 was released on December, 2012. There are several improvements and new features:
  1. Improved algorithm performance.
  2. Added disease progression models (Zhou et al., 2011b; Zhou et al., 2012).
  3. Added the incomplete multi-source fusion (iMSF) models (Yuan et al., 2012).
  4. Added the multi-stage multi-task feature learning (Gong et al., 2012a).
  5. Added the learning shared subspace for multi-task clustering (LSSMTC) algorithm (Gu & Zhou, 2009).
  6. Added an example to illustrate training, testing and model selection in multi-task learning.

Citation

In citing MALSAR in your papers, please use the following reference:

[Zhou 2012] J. Zhou, J. Chen, and J. Ye. MALSAR: Multi-tAsk Learning via StructurAl Regularization. Arizona State University, 2012. `http://www.MALSAR.org`

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References

Abernethy, J., Bach, F., Evgeniou, T., & Vert, J. (2006). Low-rank matrix factorization with attributes. *Arxiv preprint cs/0611124*.

Abernethy, J., Bach, F., Evgeniou, T., & Vert, J. (2009). A new approach to collaborative filtering: Operator estimation with spectral regularization. *The Journal of Machine Learning Research*, *10*, 803–826.

Agarwal, A., Daumé III, H., & Gerber, S. (2010). Learning multiple tasks using manifold regularization. .

Ando, R., & Zhang, T. (2005). A framework for learning predictive structures from multiple tasks and unlabeled data. *The Journal of Machine Learning Research*, *6*, 1817–1853.

Argyriou, A., Evgeniou, T., & Pontil, M. (2007). Multi-task feature learning. *Advances in neural information processing systems*, *19*, 41.

Argyriou, A., Evgeniou, T., & Pontil, M. (2008a). Convex multi-task feature learning. *Machine Learning*, *73*, 243–272.

Argyriou, A., Micchelli, C., Pontil, M., & Ying, Y. (2008b). A spectral regularization framework for multi-task structure learning. *Advances in Neural Information Processing Systems*, *20*, 25–32.

Bakker, B., & Heskes, T. (2003). Task clustering and gating for bayesian multitask learning. *The Journal of Machine Learning Research*, *4*, 83–99.

Bickel, S., Bogojeska, J., Lengauer, T., & Scheffer, T. (2008). Multi-task learning for hiv therapy screening. *Proceedings of the 25th international conference on Machine learning* (pp. 56–63).

Chen, J., Liu, J., & Ye, J. (2010). Learning incoherent sparse and low-rank patterns from multiple tasks. *Proceedings of the 16th ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 1179–1188).

Chen, J., Tang, L., Liu, J., & Ye, J. (2009). A convex formulation for learning shared structures from multiple tasks. *Proceedings of the 26th Annual International Conference on Machine Learning* (pp. 137–144).

Chen, J., Zhou, J., & Ye, J. (2011). Integrating low-rank and group-sparse structures for robust multi-task learning. *Proceedings of the tenth ACM SIGKDD international conference on Knowledge discovery and data mining*.

Evgeniou, T., Micchelli, C., & Pontil, M. (2006). Learning multiple tasks with kernel methods. *Journal of Machine Learning Research*, *6*, 615.

Evgeniou, T., & Pontil, M. (2004). Regularized multi–task learning. *Proceedings of the tenth ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 109–117).

Fazel, M. (2002). *Matrix rank minimization with applications*. Doctoral dissertation, PhD thesis, Stanford University.

Gong, P., Ye, J., & Zhang, C. (2012a). Multi-stage multi-task feature learning. *Advances in Neural Information Processing Systems*.

Gong, P., Ye, J., & Zhang, C. (2012b). Robust multi-task feature learning. *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*. New York, NY, USA: ACM.

Gu, Q., & Zhou, J. (2009). Learning the shared subspace for multi-task clustering and transductive transfer classification. *Data Mining, 2009. ICDM'09. Ninth IEEE International Conference on* (pp. 159–168).

Jacob, L., Bach, F., & Vert, J. (2008). Clustered multi-task learning: A convex formulation. *Advances in Neural Information Processing Systems*.

Jalali, A., Ravikumar, P., Sanghavi, S., & Ruan, C. (2010). A dirty model for multi-task learning. *Proceedings of the Conference on Advances in Neural Information Processing Systems (NIPS)*.

Ji, S., & Ye, J. (2009). An accelerated gradient method for trace norm minimization. *Proceedings of the 26th Annual International Conference on Machine Learning* (pp. 457–464).

Kohavi, R. (1995). A study of cross-validation and bootstrap for accuracy estimation and model selection. *International joint Conference on artificial intelligence* (pp. 1137–1145).

Li, C., & Li, H. (2008). Network-constrained regularization and variable selection for analysis of genomic data. *Bioinformatics*, *24*, 1175–1182.

Liu, J., Ji, S., & Ye, J. (2009). Multi-task feature learning via efficient l 2, 1-norm minimization. *Proceedings of the Twenty-Fifth Conference on Uncertainty in Artificial Intelligence* (pp. 339–348).

Nemirovski, A. Efficient methods in convex programming. *Lecture Notes*.

Nemirovski, A. (2001). Lectures on modern convex optimization. *Society for Industrial and Applied Mathematics (SIAM*.

Nesterov, Y. (2005). Smooth minimization of non-smooth functions. *Mathematical Programming*, *103*, 127–152.

Nesterov, Y. (2007). Gradient methods for minimizing composite objective function. *ReCALL*, *76*.

Nesterov, Y., & Nesterov, I. (2004). *Introductory lectures on convex optimization: A basic course*, vol. 87. Springer.

Nie, F., Huang, H., Cai, X., & Ding, C. (2010). Efficient and robust feature selection via joint l21-norms minimization. .

Obozinski, G., Taskar, B., & Jordan, M. (2010). Joint covariate selection and joint subspace selection for multiple classification problems. *Statistics and Computing*, *20*, 231–252.

Thrun, S., & O'Sullivan, J. (1998). Clustering learning tasks and the selective cross-task transfer of knowledge. *Learning to learn*, 181–209.

Tibshirani, R. (1996). Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society. Series B (Methodological)*, 267–288.

Vandenberghe, L., & Boyd, S. (1996). Semidefinite programming. *SIAM review*, 49–95.

Wang, F., Wang, X., & Li, T. (2009). Semi-supervised multi-task learning with task regularizations. *2009 Ninth IEEE International Conference on Data Mining* (pp. 562–568).

Xue, Y., Liao, X., Carin, L., & Krishnapuram, B. (2007). Multi-task learning for classification with dirichlet process priors. *The Journal of Machine Learning Research*, *8*, 35–63.

Yuan, L., Wang, Y., Thompson, M., Narayan, A. V., & Ye, J. (2012). Multi-source learning for joint analysis of incomplete multi-modality neuroimaging data. *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*. New York, NY, USA: ACM.

Zha, H., He, X., Ding, C., Gu, M., & Simon, H. (2002). Spectral relaxation for k-means clustering. *Advances in Neural Information Processing Systems*, *2*, 1057–1064.

Zhang, T. (2010). Analysis of multi-stage convex relaxation for sparse regularization. *The Journal of Machine Learning Research*, *11*, 1081–1107.

Zhang, Y., & Yeung, D. (2010). A convex formulation for learning task relationships in multi-task learning. *Proceedings of the 26th Conference on Uncertainty in Artificial Intelligence (UAI)* (pp. 733–742).

Zhou, J., Chen, J., & Ye, J. (2011a). Clustered multi-task learning via alternating structure optimization. *Advances in Neural Information Processing Systems*.

Zhou, J., Liu, J., Narayan, A. V., & Ye, J. (2012). Modeling disease progression via fused sparse group lasso. *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*. New York, NY, USA: ACM.

Zhou, J., Yuan, L., Liu, J., & Ye, J. (2011b). A multi-task learning formulation for predicting disease progression. *Proceedings of the 17th ACM SIGKDD international conference on Knowledge discovery and data mining* (pp. 814–822). New York, NY, USA: ACM.