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Multi-Task Learning: Models, Optimization and Applications

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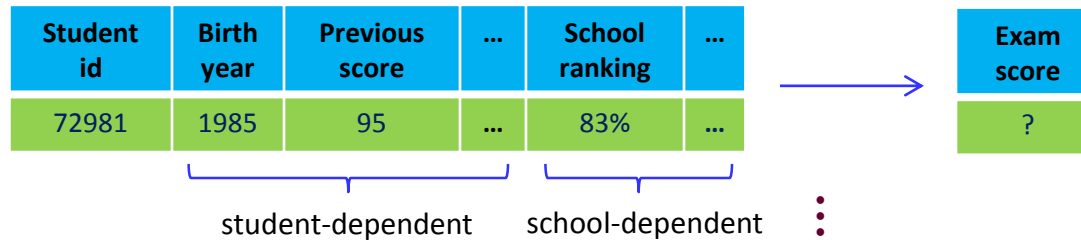
Outline

- Introduction to multi-task learning (MTL): problem and models
- Multi-task learning with task-feature co-clusters
- Low-rank optimization in multi-task learning
- Multi-task learning applied to trajectory regression

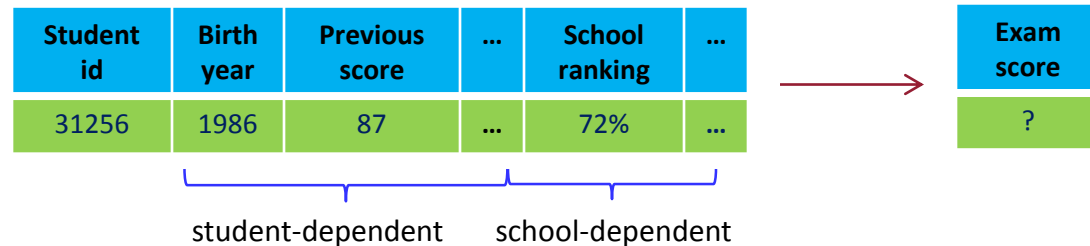
Multiple Tasks

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

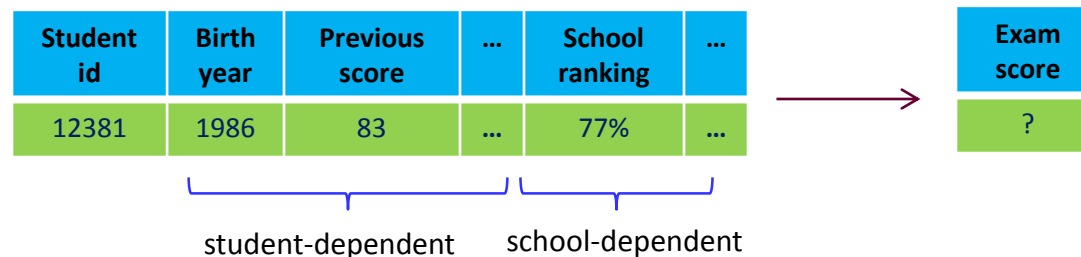
School 1 - Alverno High School



School 138 - Jefferson Intermediate School



School 139 - Rosemead High School



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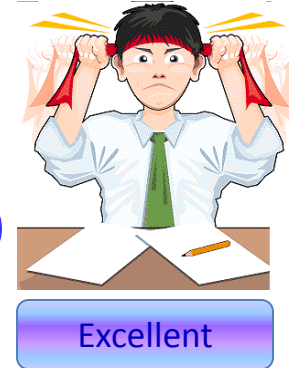
Learning Multiple Tasks

Learning each task independently

School 1 - Alverno High School

Student id	Birth year	Previous score	School ranking	...	Exam Score
72981	1985	95	83%	...	?

1st task



⋮

School 138 - Jefferson Intermediate School

Student id	Birth year	Previous score	School ranking	...	Exam Score
31256	1986	87	72%	...	?

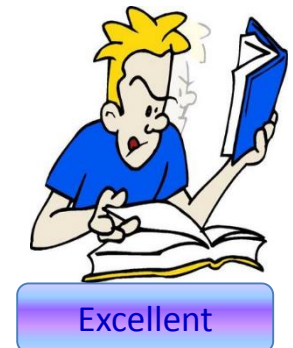
138th task



School 139 - Rosemead High School

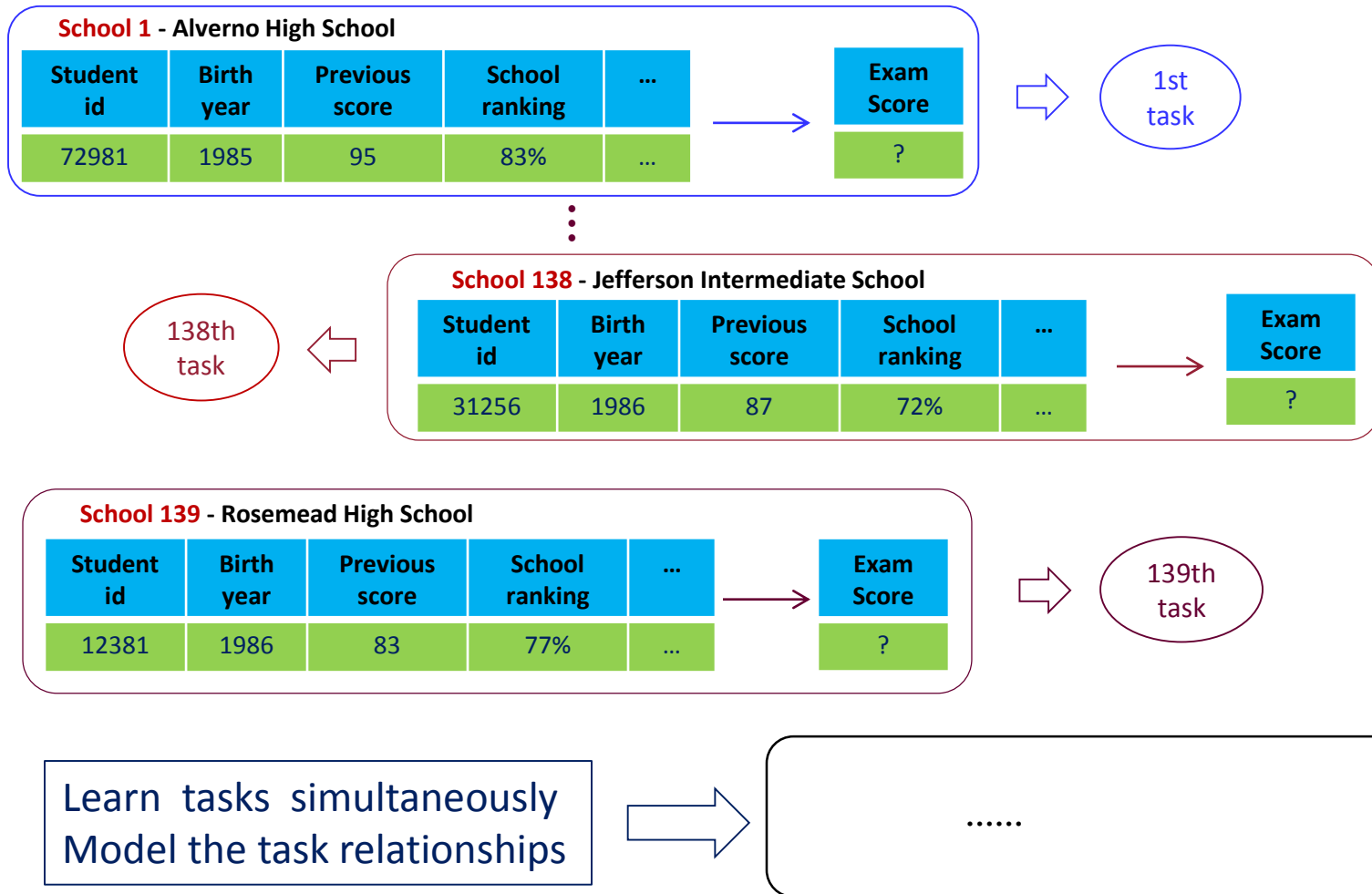
Student id	Birth year	Previous score	School ranking	...	Exam Score
12381	1986	83	77%	...	?

139th task



Learning Multiple Tasks

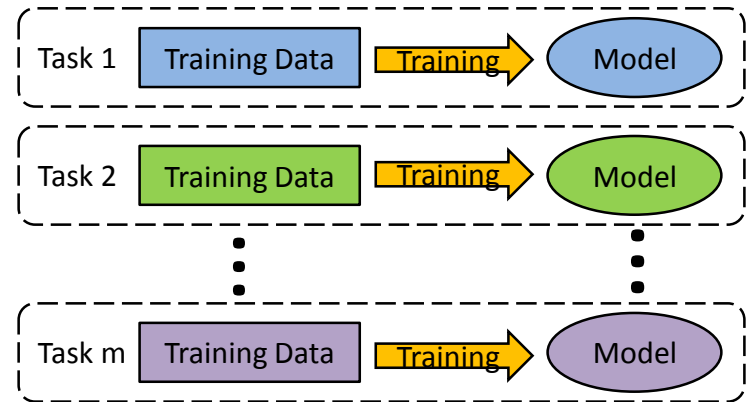
Learning multiple tasks simultaneously



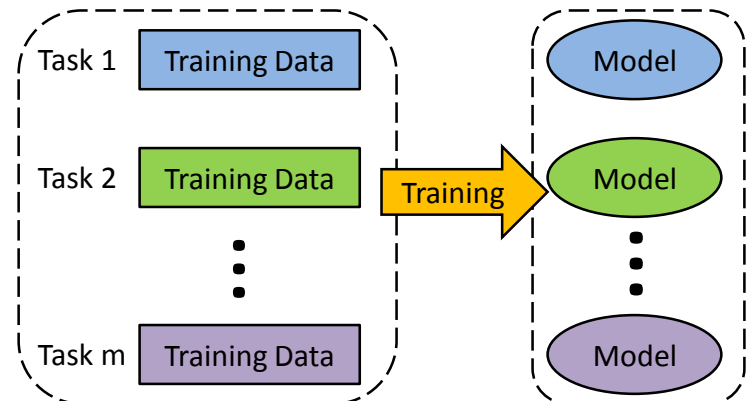
Multi-Task Learning

- Different from single task learning
- Training multiple tasks simultaneously to exploit task relationships

Single Task Learning



Multi-Task Learning



Exploiting Task Relationships

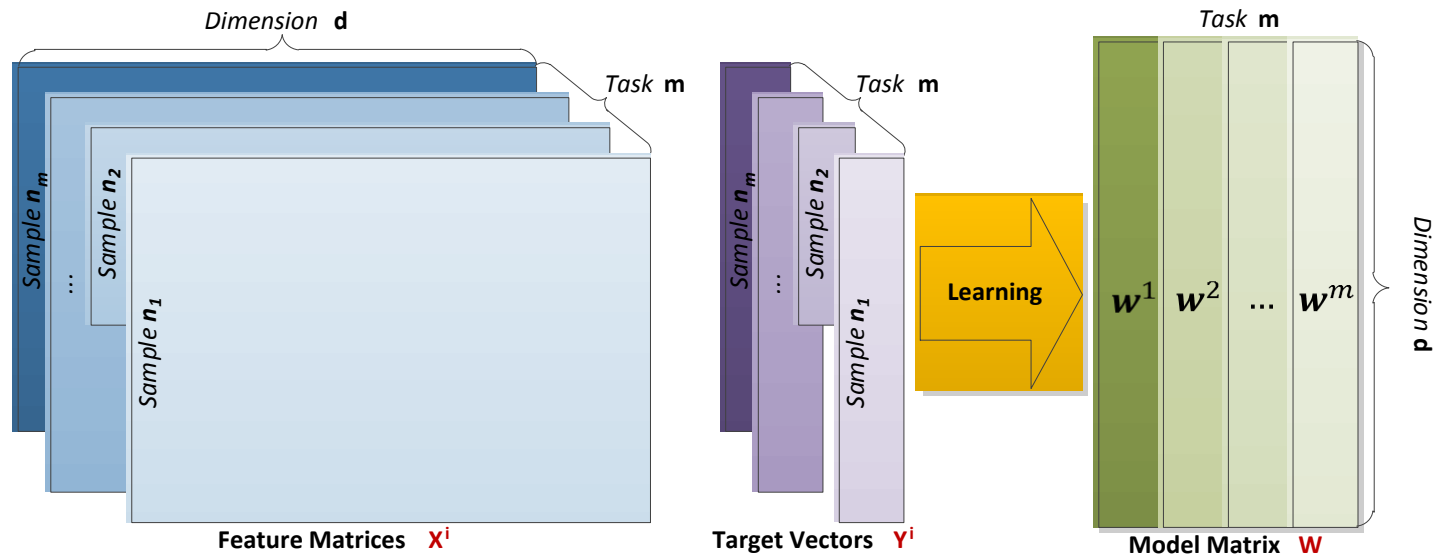
Key challenge in multi-task learning:

Exploiting (statistical) relationships between the tasks so as to improve individual and/or overall predictive accuracy (in comparison to training individual models)!

How Tasks Are Related?

- All tasks are related
 - Models of all tasks are close to each other;
 - Models of all tasks share a common set of features;
 - Models share the same low rank subspace
- Structure in tasks
 - clusters / graphs / trees
- Learning with outlier tasks

Regularization-based Multi-Task Learning



We focus on linear models: $Y^i \sim X^i w^i$
 $X^i \in \mathbb{R}^{n_i \times d}, Y^i \in \mathbb{R}^{n_i \times 1}, W = [w^1, w^2, \dots, w^m] \in \mathbb{R}^{d \times m}$

Generic framework

$$\min_W \sum_i \text{Loss}(W, X^i, Y^i) + \lambda \text{Reg}(W)$$

Impose various types of relations on tasks with $\text{Reg}(W)$

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MTL Methods: Mean-Regularized MTL

Evgeniou & Pontil, 2004 KDD

Assumption: model parameters of all tasks are close to each other.

- Advantage: simple, intuitive, easy to implement
- Disadvantage: **too simple**

Regularization

- Penalizes the deviation of each task from the mean

$$\min_W \text{Loss}(W) + \lambda \sum_{i=1}^m \left\| W^i - \frac{1}{m} \sum_{s=1}^m W^s \right\|_2^2$$

MTL Methods: Joint Feature Learning

Evgeniou *et al.* 2006 NIPS, Obozinski *et al.* 2009 Stat Comput, Liu *et al.* 2010 Technical Report

Assumption: models of all tasks share a common set of features

- Using group sparsity: $\ell_{1,q}$ -norm regularization

Regularization

- $\|W\|_{1,q} = \sum_{i=1}^d \|\mathbf{w}_i\|_q$
- When $q > 1$ we have group sparsity

$$\min_W \text{Loss}(W) + \lambda \|W\|_{1,q}$$

	Task 1	Task 2	Task m
Feature 1				
Feature 2				
Feature 3				
Feature 4				
Feature 5				
Feature 6				
Feature 7				
.....				
Feature d				

MTL Methods: Low-Rank MTL

Ji et. al. 2009 ICML

Assumption: in high dimensional feature space, the linear models share the same low-rank subspace

Regularization - Rank minimization formulation

$$\min_W \text{Loss}(W) + \lambda \cdot \text{rank}(W)$$

– Rank minimization is *NP-Hard* for general loss functions

- Convex relaxation: nuclear norm minimization

$$\min_W \text{Loss}(W) + \lambda \|W\|_*$$

($\|W\|_*$: sum of singular values of W)

How Tasks Are Related?

- All tasks are related
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MTL Methods: Clustered MTL

Zhou et. al. 2011 NIPS

Assumption: cluster structure in tasks - the models of tasks from the same group are closer to each other than those from a different group

Regularization - capture clustered structures

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

capture cluster structures

Improves
generalization
performance

Regularization-based MTL: Decomposition Framework

- In practice, it is too restrictive to constrain all tasks to share a single shared structure.
- Assumption: the model is the sum of two components $W = P + Q$
 - A shared low dimensional subspace and a task specific component (Ando and Zhang, 2005, JMLR)
 - A group sparse component and a task specific sparse component (Jalali et.al., 2010, NIPS)
 - A low rank structure among relevant tasks + outlier tasks (Gong et.al., 2011, KDD)

How Tasks Are Related?

- All tasks are related
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MTL Methods: Robust MTL

Chen *et. al.* 2011 KDD

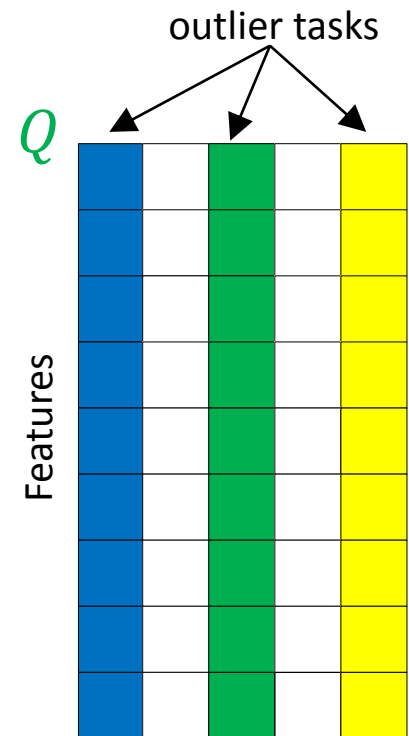
Assumption: models share the same low-rank subspace
+ outlier tasks

$$W = P + Q$$

Regularization

- $\|P\|_*$: nuclear norm
- $\|Q\|_{2,1} = \sum_{j=1}^m \|\mathbf{q}_{:,j}\|_2$

$$\min_W \text{Loss}(W) + \underbrace{\alpha \|P\|_*}_{\text{low rank}} + \underbrace{\beta \|Q\|_{2,1}}_{\text{column-sparse}}$$



Summary So Far...

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

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- Introduction to multi-task learning (MTL): problem and models
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Recap: How Tasks Are Related?

- All tasks are related
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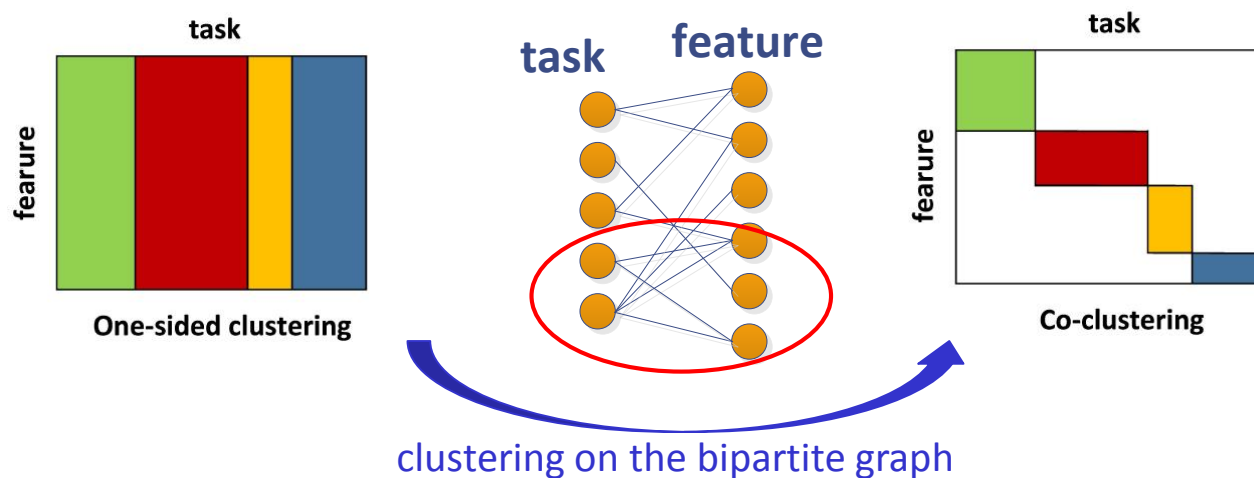
How Tasks are Related

- Existing methods consider the structure at a general **task-level**
- Restrictive assumption in practice:
 - In document classification: different tasks may be relevant to different sets of words
 - In a recommender system: two users with similar tastes on one feature subset may have totally different preference on another subset

CoCMTL: MTL with Task-Feature Co-Clusters

[Xu. et al, AAAI15]

- Motivation: feature-level groups



- Impose task-feature co-clustering structure with $Reg(W)$

CoCMTL: Model

- Decomposition model: $W = P + Q$

$$\min_W \text{Loss}(W) + \lambda_1 \Omega_1(P) + \lambda_2 \Omega_2(Q)$$

Global Similarities: $\Omega_1(P) = \sum_{i=1}^m \left\| p^i - \frac{1}{m} \sum_{j=1}^m p^j \right\|_2^2 = \text{tr}(PLP^T)$

Group Specific Similarities:

K-means Clustering with Spectral Relaxation:

$$\min_{H^T H = I} \left\{ \text{tr}(Z^T Z) - \text{tr}(H^T Z^T Z H) \right\}$$

- Z: data matrix.
- H: indicating matrix.

Co-clustering Scenario:

$$Z = \begin{pmatrix} 0 & Q \\ Q^T & 0 \end{pmatrix} \quad H = \begin{pmatrix} F \\ G \end{pmatrix} \quad \begin{matrix} F^T F = I \\ G^T G = I \end{matrix}$$

- F, G: indicating matrices for tasks and features.

$$\min_{F^T F = I, G^T G = I} \left\{ 2 \|Q\|_F^2 - \text{tr}(F^T Q Q^T F) - \text{tr}(G^T Q^T Q G) \right\}$$

task feature



clustering on the
bipartite graph

CoCMTL: Model

- Decomposition model: $W = P + Q$

$$\min_W \text{Loss}(W) + \lambda_1 \Omega_1(P) + \lambda_2 \Omega_2(Q)$$

non-convex

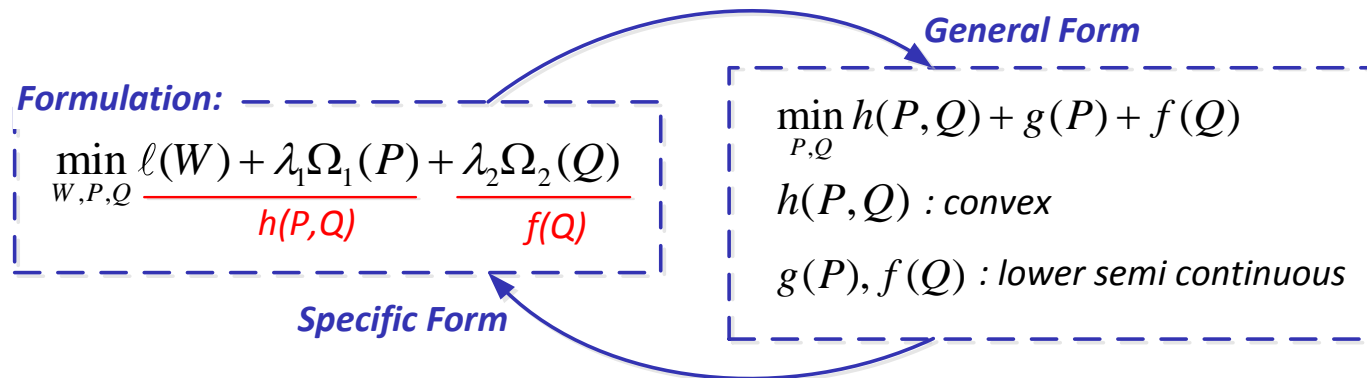
Theorem 1. For any given matrix $Q \in \mathbb{R}^{d \times m}$, any matrices $F \in \mathbb{R}^{d \times k}$, $G \in \mathbb{R}^{m \times k}$ and any nonnegative integer k , $k \leq \min(d, m)$, Problem (4) reaches its minimum value at $F = (\mathbf{u}_1, \dots, \mathbf{u}_k)$, $G = (\mathbf{v}_1, \dots, \mathbf{v}_k)$, where \mathbf{u}_i and \mathbf{v}_i are the i -th left and right singular vectors of Q respectively. The minimum value is $2 \sum_{i=k+1}^{\min(d,m)} \sigma_i^2(Q)$, where $\sigma_1(Q) \geq \sigma_2(Q) \geq \dots \geq \sigma_{\min(d,m)}(Q) \geq 0$ are the singular values of Q .

$$\Omega_2(Q) = \sum_{i=k+1}^{\min(d,m)} \sigma_i^2(Q)$$

$$\min_W \text{Loss}(W) + \lambda_1 \text{tr}(PLP^T) + \lambda_2 \sum_{i=k+1}^{\min(d,m)} \sigma_i^2(Q)$$

CoCMTL: Optimization

- We follow the ***Proximal Alternative Linear Method (PALM)*** to solve the non-convex problem.



In the r -th iteration, we get two sub-problems.

$$\begin{cases} P_r = \arg \min_P \frac{\gamma_r}{2} \|P - C_P\|_F^2 \\ Q_r = \arg \min_Q \frac{\gamma_r}{2} \|Q - C_Q\|_F^2 + \lambda_2 \Omega_2(Q) \end{cases}$$

$$\arg \min_Q \frac{\gamma_r}{2} \|Q - C_Q\|_F^2 + \lambda_2 \text{tr}(F_*^T Q Q^T F_*)$$

Alternative Optimization

CoCMTL: Results

School data: #Tasks 139, #Features 27, #Samples 15k

	Training Ratio	Ridge	L21	Low Rank	rMTL	rMTFL	Dirty	Flex-Clus	CMTL	CoCMTL
nMSE	10%	1.1031	1.0931	0.9693	0.9603	1.3838	1.1421	0.8862	0.9914	0.8114
	20%	0.9178	0.9045	0.8435	0.8198	1.0310	0.9436	0.7891	0.8462	0.7688
	30%	0.8511	0.8401	0.8002	0.7833	0.9103	0.8517	0.7634	0.8064	0.7515
aMSE	10%	0.2891	0.2867	0.2541	0.2515	0.3618	0.2983	0.2315	0.2593	0.2118
	20%	0.2385	0.2368	0.2207	0.2147	0.2702	0.2470	0.2062	0.2214	0.2009
	30%	0.2212	0.2197	0.2091	0.2049	0.2378	0.2225	0.1992	0.2107	0.1961
rMSE	10%	11.5321	11.5141	11.2000	11.1984	12.1233	11.6401	10.9991	11.2680	10.7430
	20%	10.7318	10.7011	10.5427	10.4866	10.9928	10.8033	10.3986	10.5500	10.3110
	30%	10.1831	10.1704	10.0663	10.0291	10.3338	10.1956	9.9767	10.0865	9.9221

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– Rank minimization is *NP-Hard* for general loss functions

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$$\min_W \text{Loss}(W) + \lambda \|W\|_*$$

($\|W\|_*$: sum of singular values of W)

More on Nuclear Norm

Rank minimization formulation

$$\min_W \text{Loss}(W) + \lambda \cdot \text{rank}(W)$$

- $\text{rank}(W) = \# \text{non-zero singular values}$
- $\|W\|_* = \sum \sigma_i(W)$: sum of singular values

- Limitation of $\|W\|_*$
 - Large singular values are penalized more heavily
 - Large singular values are dominant in determining the properties of a matrix

Idea: Weighted Nuclear Norm

[Zhong et al, AAAI15; Xu et al, ICDM16]


Non-convex

$$\min_W \text{Loss}(W) + \lambda \sum_i p_i \sigma_i(W)$$


- Intuition: penalize large singular values less
 - Non-descending weights p_i
- Reweighting strategy:
 - Given current weights \mathbf{p}^{k-1} , solve for W^{k-1}
 - Reweighting of \mathbf{p}
 - $p_i^k = \frac{r}{(\sigma_i(W^k) + \epsilon)^{1-r}}$, where $0 < r < 1, \epsilon > 0$
 - Each weight inversely proportional to the corresponding singular value

Idea: Weighted Nuclear Norm

$$\min_W \text{Loss}(W) + \lambda \sum_i p_i \sigma_i(W)$$


$$p_i^k = \frac{r}{(\sigma_i(W^k) + \epsilon)^{1-r}}$$

$$\min_W \text{Loss}(W) + \lambda \sum_i (\sigma_i(W) + \epsilon)^r$$



Enhances low rank approximation



→ rank(W) when $\epsilon \rightarrow 0, r \rightarrow 0$

Optimization: Proximal Operator

First-order approximation of $Loss(W)$, regularized by a proximal term

$$P_{t^k}(W, W^k) = Loss(W^k) + \langle W - W^k, \nabla Loss(W^k) \rangle + \frac{t^k}{2} \|W - W^k\|^2$$

Generate the sequence

$$W^k = \arg \min_W \frac{t^k}{2\lambda} \left\| W - \left(W^k - \frac{1}{t^k} \nabla Loss(W^k) \right) \right\|_F^2 + (p^k)^T \sigma(W)$$

- ☹ Non-convex proximal operator problem
- ☺ Has closed form solution by exploiting structure of the weighted nuclear norm (unitarily invariant property)

Theorem. Suppose that $A = U\Sigma V^T$, then, $W^* = UD(x^*)V^T$ is a global solution of the problem

$$\min_x \frac{\mu}{2} \|W - A\|_F^2 + p^T \sigma(W)$$


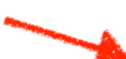

where x^* can be denoted as $x^* = \max\left(\sigma(A) - \frac{1}{\mu} p, 0\right)$

Optimization: Algorithm

Algorithm 1 Iterative Shrinkage-Thresholding and Reweighted Algorithm (ISTRA)

Input: $0 < t_{\min} < t_{\max}$, $0 < \tau < 1$, $0 < r < 1$, $\lambda > 0$,
 $\delta > 0$, $\epsilon > 0$, $\rho > 1$

Output: X^*

- 1: **Initialize:** $k = -1$, $w^0 = \mathbf{1}^T$, X^{-1} , X^0
 - 2: **repeat**
 - 3: $k = k + 1$  Barzilai Borwein (BB) rule
 - 4: update t^k
 - 5: make $t^k \in [t_{\min}, t_{\max}]$
 - 6: **while true do**
 - 7: update X^{k+1}
 - 8: **if** line search criterion **is satisfied then**
 - 9: **Break;**
 - 10: **end if**
 - 11: $t^k = \rho t^k$  decrease the step size
 - 12: **end while**
 - 13: update the weights w_i^{k+1} , $i = 1 \cdots q$  reweighting strategy
 - 14: **until** stop criterion $\|X^{k+1} - X^k\|^2 \leq \delta$ **is satisfied**
-

Convergence Analysis

- Critical points

Theorem. The sequence $\{W^k\}$ generated by the ISTRA algorithm makes the objective function monotonically decrease, and all accumulation points (i.e. the limit points of convergent subsequence in $\{W^k\}$) are critical points (i.e. 0 belongs to the subgradients)

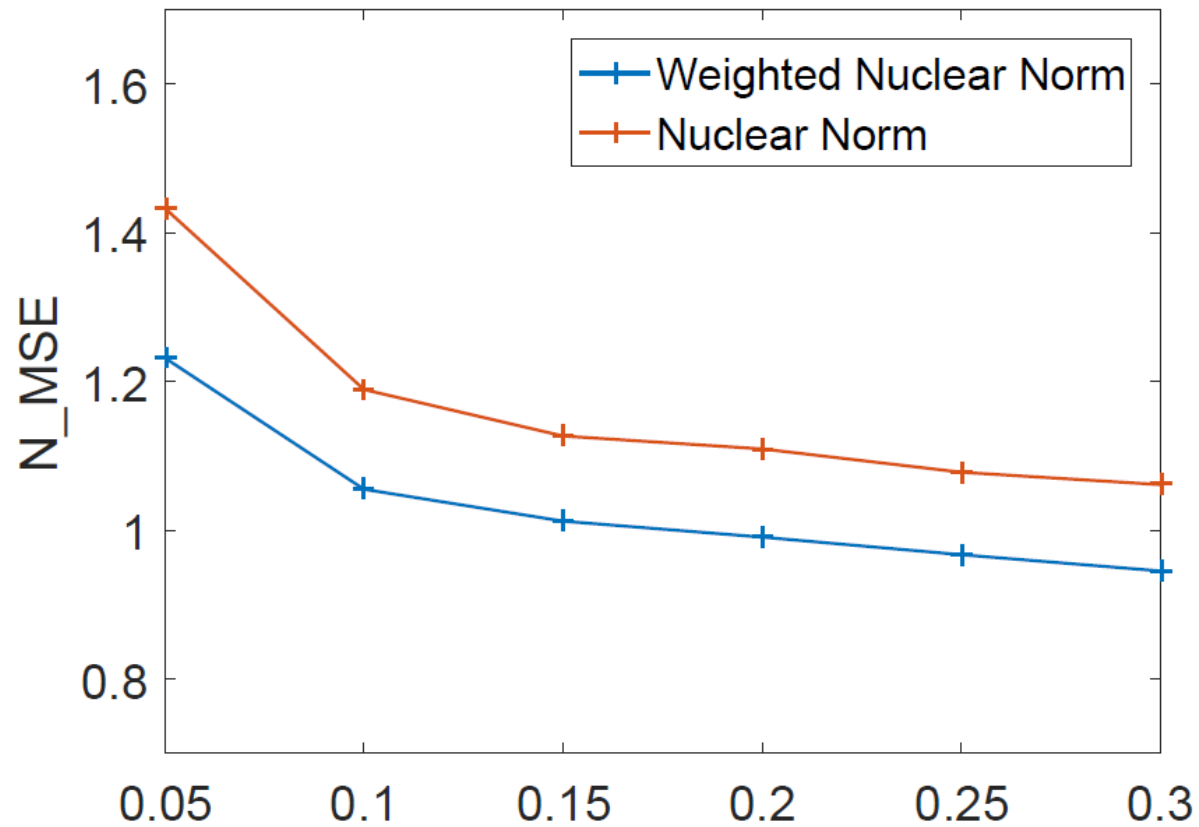
- Sublinear convergence rate

Theorem. Suppose that $\{W^k\}$ is the sequence generated by the ISTRA algorithm, and W^* is an accumulation point of $\{X^k\}$, then

$$\min_{0 \leq k \leq n} \|W^{k+1} - W^k\|^2 \leq 2(g(W^0) - g(W^*)) / n\tau t_{\min}$$

Results

School data



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Trajectory Regression: Problem

Trajectory:

A sequence of link (road segments),
where any two consecutive links
share an intersection

Goal:

Estimate the total travel time of an
arbitrary trajectory

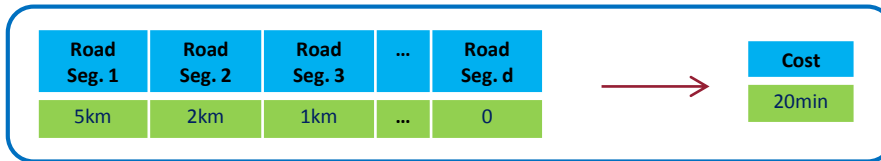


Trajectory Regression: Problem

Given a set consisting of N trajectory-cost pairs:

$$D \equiv \{(\mathbf{x}_i, y_i) | i = 1, 2, \dots, N\}, \mathbf{x}_i \in \mathbb{R}_d$$

- Each feature of \mathbf{x}_i corresponds to a link — distance traveled along the link



Goal: Learn the weights $\mathbf{w} \in \mathbb{R}_d$ that encode the cost per distance unit for each link

Single task learning: $\min_{\mathbf{w}} \|\mathbf{Y} - \mathbf{X}\mathbf{w}\|_2^2 + \beta \|\mathbf{w}\|_2^2$



Trajectory Regression: Key Challenges

- **Dynamic**: costs of road segments are not static over time
 - Cost of a road segment fluctuates smoothly most of the time
 - Costs can be abruptly different between peak periods and off-peak periods
- Trajectories are extremely **sparse**
 - A driving path spans just a small fraction of road segments
- **Insufficient** instances

Trajectory Regression: Idea

[Huang et al. ICDM14]

Dynamic trajectory regression in an MTL framework

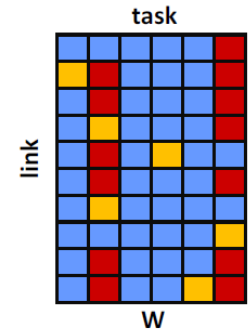
- Divide D into m disjoint subsets ordered by time
- Multi-task learning framework: each time slot corresponds to a task
 - leverage the inherent relations of tasks to enhance the predictive performance, especially when the data samples are insufficient

Trajectory Regression

$$\min_W \sum_i \text{Loss}(W, X^i, Y^i) + \lambda \text{Reg}(W) = \min_W \sum_i \|Y^i - X^i w^i\| + \lambda \text{Reg}(W)$$

W Structure in the trajectory regression problem

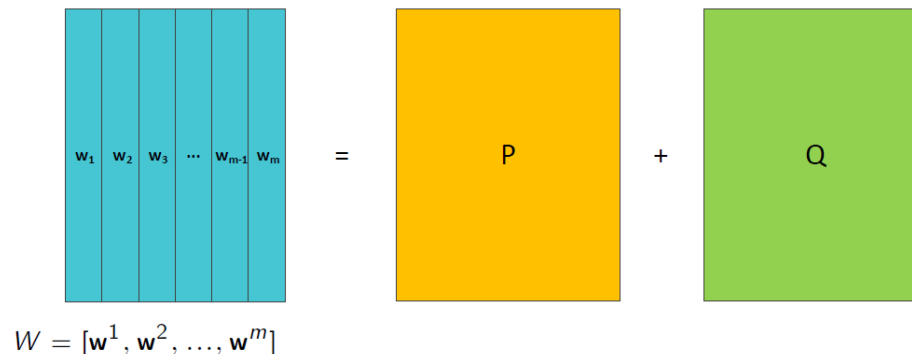
- **Global** temporal smoothness:
 - Link costs change smoothly most of the time
- **Global** spatial smoothness:
 - Costs are similar if the two corresponding links are close to each other
- **Local** temporal patterns:
 - Significant temporal changes in rush hours



Trajectory Regression - Additive Model

$$\min_W \sum_i \text{Loss}(W, X^i, Y^i) + \lambda \text{Reg}(W) = \min_W \sum_i \|Y^i - X^i \mathbf{w}^i\| + \lambda \text{Reg}(W)$$

$$W = P + Q$$

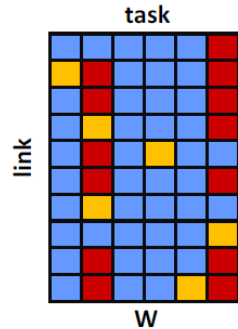


- P : models the global smoothness over links and time
- Q : captures the local “outliers” including rush hours

Trajectory Regression - Regularization

$$W = P + Q$$

- P : models the **global** smoothness over links and time



- **Global temporal smoothness**

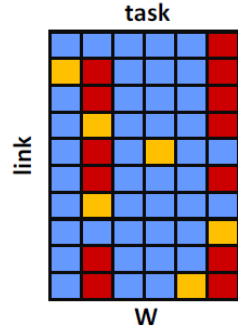
$$\Omega_1 = \sum_{t=1}^m \left\| P_{:,t} - \frac{1}{m} \sum_{r=1}^m P_{:,r} \right\|_2^2 = \text{tr}(P L_1 P^T) \quad L_1 = I - \frac{1}{m} \mathbf{1} \mathbf{1}'$$

- Enforces the columns of P or the tasks to be similar with some discrepancy

Trajectory Regression - Regularization

$$W = P + Q$$

- P : models the **global** smoothness over links and time



- **Global spatial smoothness**

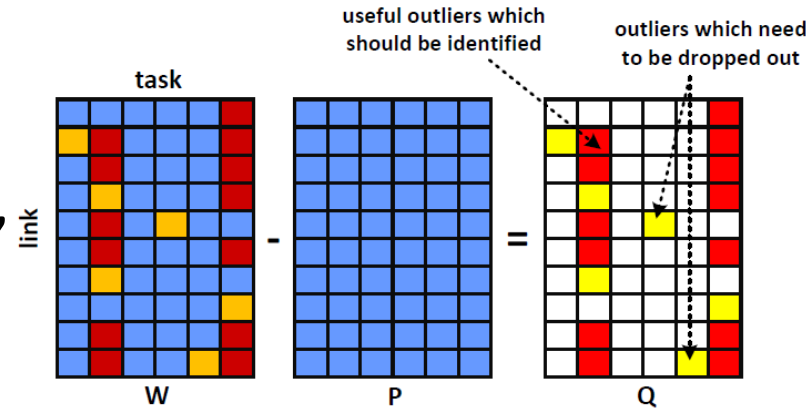
$$\Omega_2 = \sum_{i,j=1}^d S_{ij} \|P_{i,:} - P_{j,:}\|_2^2 = \text{tr}(P^T L_2 P)$$

- S measures the spatial closeness of links
- Costs are similar if the two corresponding links are close to each other

Trajectory Regression - Regularization

$$W = P + Q$$

- Q : captures the **local** “outliers”

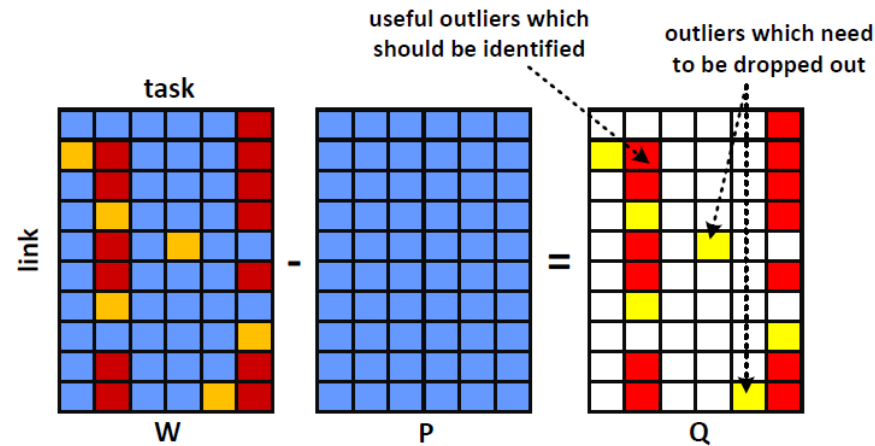


- **Local significant temporal transitions**

$$\Omega_3 = \|Q\|_{\infty,1}$$

- $\|Z\|_{\infty,1} = \sum_j \|Z_{:,j}\|_{\infty}, \quad \|Z_{:,j}\|_{\infty} = \max_i |Z_{ij}|$
- Enforces column sparsity to identify peak traffic
- The $\ell_{\infty,1}$ norm is only influenced by the maximum elements of the nonzero columns — the cost of a trajectory is mostly decided by the link with highest cost during traffic peaks
- Leaves out the outliers — **ROBUST**

Trajectory Regression - Model



$$\min_W \sum_{i=1}^m \|Y^i - X^i \mathbf{w}^i\|_2^2 + \lambda_1 \text{tr}(P L_1 P^T) + \lambda_2 \text{tr}(P^T L_2 P) + \lambda_3 \|Q\|_{\infty,1}$$

Trajectory Regression - Optimization

$$\min_W \sum_{i=1}^m \|Y^i - X^i \mathbf{w}^i\|_2^2 + \lambda_1 \text{tr}(P L_1 P^T) + \lambda_2 \text{tr}(P^T L_2 P) + \lambda_3 \|Q\|_{\infty,1}$$

Convex problem, but non-trivial for optimization due to the $\ell_{\infty,1}$ term

Proximal Method:

$$\min_W \{F(W) + R(W)\} \quad \begin{cases} F(W) = L(W) + \lambda_1 \text{tr}(P L_1 P^T) + \lambda_2 \text{tr}(P^T L_2 P) \\ R(W) = \lambda_3 \|Q\|_{\infty,1} \end{cases}$$

$$P_r = \arg \min_P \frac{\gamma_r}{2} \|P - C_P(P_{r-1})\|_F^2,$$

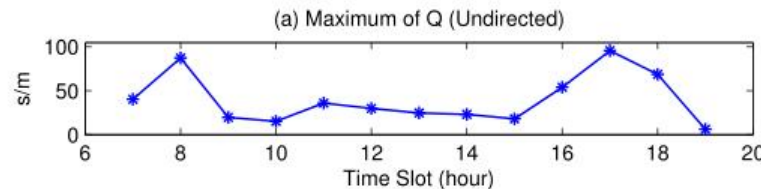
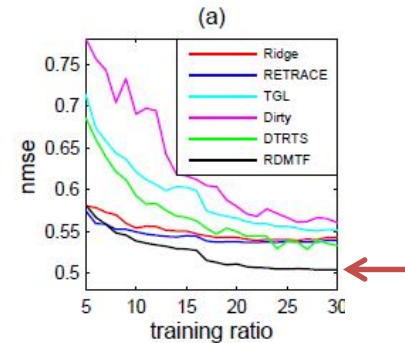
$$Q_r = \arg \min_Q \frac{\gamma_r}{2} \|Q - C_Q(Q_{r-1})\|_F^2 + \lambda_3 \|Q\|_{\infty,1}$$

$$\min_{\mathbf{q}^i} \frac{1}{2} \|\mathbf{q}^i - \mathbf{c}^i\|_2^2 + \lambda \|\mathbf{q}^i\|_{\infty} \xrightarrow[\mathbf{c} = \text{prox}_R(\mathbf{c}) + \text{prox}_{R^*}(\mathbf{c})]{\text{Moreau Decomposition}} \min_{\mathbf{q}^i} \left\{ \mathbf{c}^i - \left(\frac{1}{2} \|\mathbf{q}^i - \mathbf{c}^i\|_2^2 + \lambda \|\mathbf{q}^i\|_1 \right) \right\}$$

Trajectory Regression - Results

- Suzhou Traffic Data
 - Contains 59593 trajectory records of 4797 taxis from 7:00 to 19:59 in urban area of Suzhou during the first week in March, 2012

Training Ratio	20%(nmse)	30%(nmse)	40%(nmse)
Ridge	0.549 ± 0.013	0.547 ± 0.019	0.540 ± 0.025
STL-Ridge	0.617 ± 0.027	0.589 ± 0.040	0.560 ± 0.029
RETRACE	0.546 ± 0.013	0.545 ± 0.022	0.538 ± 0.027
STL-RETRACE	0.668 ± 0.035	0.628 ± 0.042	0.587 ± 0.036
TGL	0.570 ± 0.032	0.581 ± 0.063	0.538 ± 0.046
Dirty	0.626 ± 0.034	0.615 ± 0.056	0.590 ± 0.034
DTRTS	0.612 ± 0.051	0.596 ± 0.048	0.531 ± 0.022
L2.1	0.525 ± 0.024	0.562 ± 0.068	0.525 ± 0.049
RDMTF	0.494 ± 0.014	0.498 ± 0.040	0.481 ± 0.023



Summary

- Multi-task Learning (MTL)
 - MTL is preferred when dealing with multiple related tasks with small number of training samples
 - Key issue of MTL: Exploiting relationships among the tasks
- Optimization
 - General formulations, classical algorithms apply
 - Distributed optimization
- Applications
 - Task relationships are specific to the nature of the problem

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Thanks!

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