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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

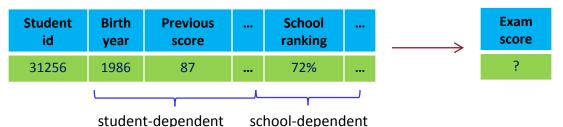
Examination Scores Prediction¹ (Argyriou et. al.'08)

School 1 - Alverno High School

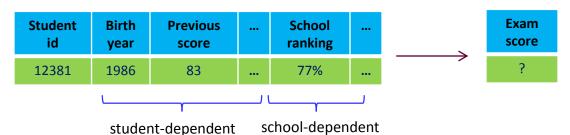
Student id	Birth year	Previous score		School ranking		→	Exam score		
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student-dependent school-dependent									



School 138 - Jefferson Intermediate School



School 139 - Rosemead High School

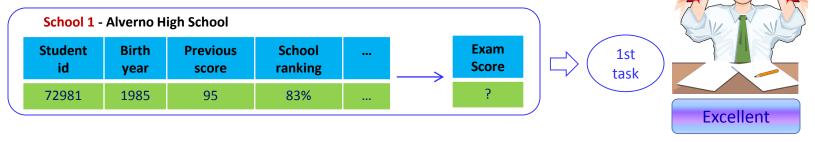


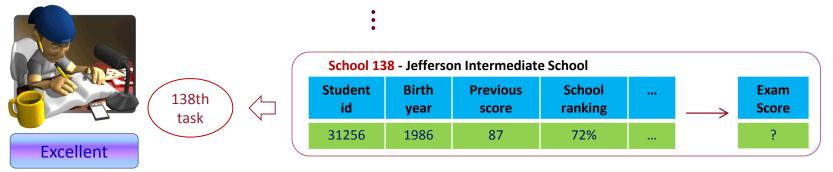
¹The Inner London Education Authority (ILEA) 2016/11/5

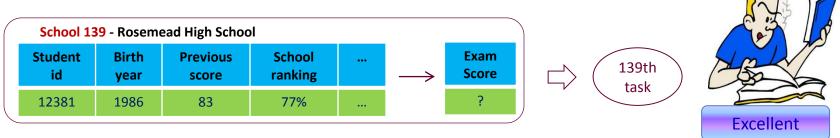
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Learning Multiple Tasks

Learning each task independently





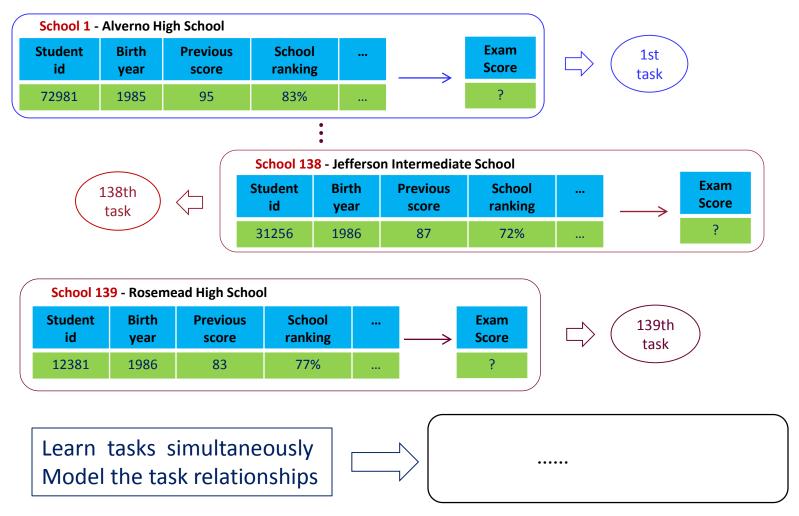


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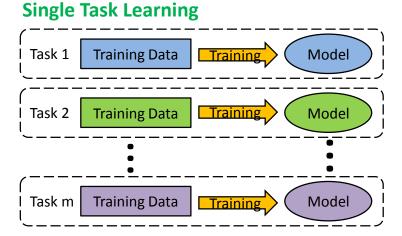
Learning Multiple Tasks

Learning multiple tasks simultaneously

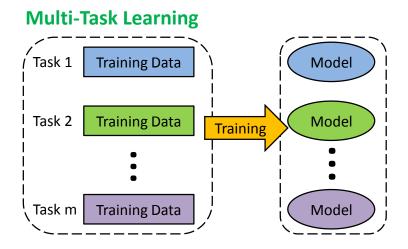


Multi-Task Learning

Different from single task learning



 Training multiple tasks simultaneously to exploit task relationships



Exploiting Task Relationships

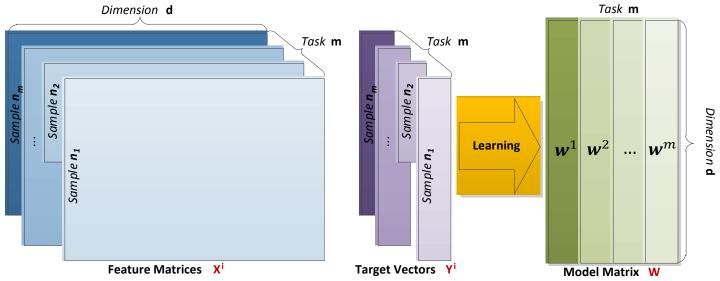
Key challenge in multi-task learning:

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:
$$Y^i \sim X^i w^i$$

 $X^i \in \mathbb{R}^{n_i \times d}, Y^i \in \mathbb{R}^{n_i \times 1}, W = [w^1, w^2, ..., w^m] \in \mathbb{R}^{d \times m}$

Generic framework

$$\min_{W} \sum_{i} Loss(W, X^{i}, Y^{i}) + \lambda Reg(W)$$

Impose various types of relations on tasks with Reg(W)

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Learning with outlier tasks

MTL Methods: Mean-Regularized MTL

Evgeniou & Pontil, 2004 KDD

<u>Assumption:</u> 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

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

14

MTL Methods: Joint Feature Learning

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

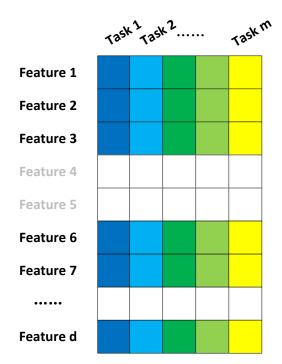
<u>Assumption:</u> models of all tasks share a common set of features

– 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

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



MTL Methods: Low-Rank MTL

Ji et. al. 2009 ICML

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

Regularization - Rank minimization formulation $\min_{W} Loss(W) + \lambda \cdot \operatorname{rank}(W)$

- Rank minimization is NP-Hard for general loss functions
- Convex relaxation: nuclear norm minimization $\min_{W} Loss(W) + \lambda ||W||_*$ ($||W||_*$: sum of singular values of W)

How Tasks Are Related?

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MTL Methods: Clustered MTL

Zhou et. al. 2011 NIPS

<u>Assumption:</u> 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

$$\min_{W,F:F^TF=I_k} Loss(W) + \alpha \frac{[\mathrm{tr}(W^TW) - \mathrm{tr}(F^TW^TWF)]}{[\mathrm{capture cluster structures}]} + \beta \frac{\mathrm{tr}(W^TW)}{[\mathrm{Improves generalization performance}]}$$

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?

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Learning with outlier tasks

MTL Methods: Robust MTL

Chen et. al. 2011 KDD

Assumption: models share the same low-rank subspace

+ outlier tasks

$$W = P + Q$$

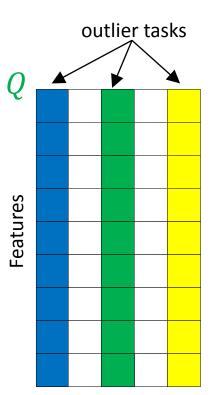
Regularization

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

$$\min_{W} Loss(W) + \alpha ||P||_{*} + \beta ||Q||_{2,1}$$

$$||P||_{*} + \beta ||Q||_{2,1}$$

$$||Q||_{2,1}$$



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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Recap: How Tasks Are Related?

- All tasks are related
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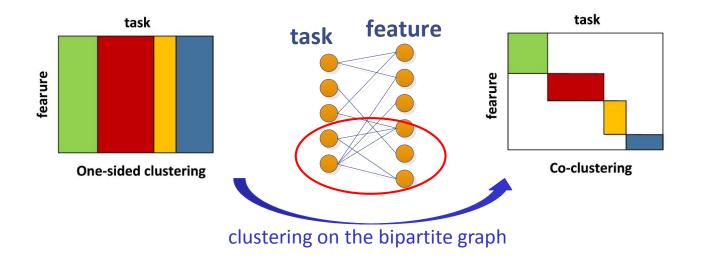
How Tasks are Related

 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 $\min_{W} Loss(W) + \lambda_1 \; \Omega_1(P) + \lambda_2 \; \Omega_2(Q)$

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

K-means Clustering with Spectral Relaxation:

$$\min_{H^TH=I} \left\{ tr(Z^TZ) - tr(H^TZ^TZH) \right\}$$

- Z: data matrix.

task

2016/11

- H: indicating matrix.

clustering on the bipartite graph

Co-clustering Scenario:

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

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

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

CoCMTL: Model

• Decomposition model: W=P+Q $\min_{W} Loss(W) + \lambda_1 \; \Omega_1(P) + \lambda_2 \; \Omega_2(Q)$

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 $F = (\mathbf{u}_1, \ldots, \mathbf{u}_k)$, $G = (\mathbf{v}_1, \ldots, \mathbf{v}_k)$, 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 $\sigma_1(Q) \geq \sigma_2(Q) \geq \cdots \geq \sigma_{\min(d,m)}(Q) \geq 0$ are the singular values of Q.

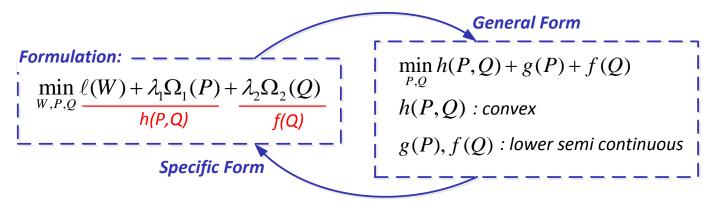
$$\Omega_2(Q) = \sum_{i=k+1}^{\min(d,m)} \sigma_i^2(Q)$$

non-convex

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

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.

$$\begin{cases} P_r = \arg\min_{P} \frac{\gamma_r}{2} \|P - C_P\|_F^2 & \arg\min_{Q} \frac{\gamma_r}{2} \|Q - C_Q\|_F^2 \\ Q_r = \arg\min_{Q} \frac{\gamma_r}{2} \|Q - C_Q\|_F^2 + \lambda_2 \Omega_2(Q) \end{cases}$$
 arg min $\frac{\gamma_r}{2} \|Q - C_Q\|_F^2$
$$+ \lambda_2 tr(F_*^T Q Q^T F_*)$$
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
- Convex relaxation: nuclear norm minimization $\min_{W} Loss(W) + \lambda \|W\|_{*}$ ($\|W\|_{*}$: sum of singular values of W)

More on Nuclear Norm

Rank minimization formulation

$$\min_{W} Loss(W) + \lambda \cdot \operatorname{rank}(W)$$

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

$$\min_{W} Loss(W) + \lambda \sum_{i} p_{i} \sigma_{i}(W)$$

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

Idea: Weighted Nuclear Norm

$$\min_{W} Loss(W) + \lambda \sum_{i} p_{i} \sigma_{i}(W)$$

$$p_{i}^{k} = \frac{r}{(\sigma_{i}(W^{k}) + \epsilon)^{1-r}}$$

$$\min_{W} Loss(W) + \lambda \sum_{i} (\sigma_{i}(W) + \epsilon)^{r}$$
Enhances low rank approximation
$$\rightarrow \operatorname{rank}(W) \text{ when } \epsilon \rightarrow 0, r \rightarrow 0$$

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

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

- —
 On-convex proximal operator problem
- ③ 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 < \overline{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
       k = k + 1 Barzilai Borwein (BB) rule update t^k
        make t^k \in [t_{\min}, t_{\max}]
         while true do
            update X^{k+1}
            if line search criterion is satisfied then
               Break;
 9:
10:
            end if
        t^k = \rho t^k
                               decrease the step size
         end while
12:
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

<u>Theorem.</u> 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)

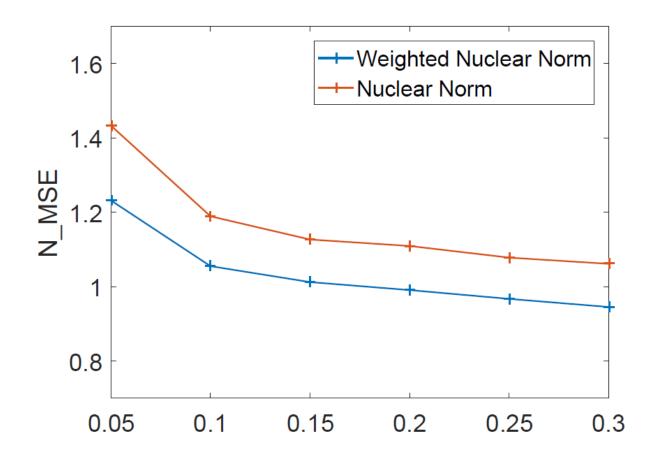
Sublinear convergence rate

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

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

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

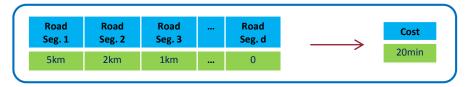


Trajectory Regression: Problem

Given a set consisting of *N* trajectory-cost pairs:

$$D \equiv \{(x_i, y_i) | i = 1, 2, ..., N\}, x_i \in \mathbb{R}_d$$

— Each feature of x_i corresponds to a link — distance traveled along the link



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

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



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

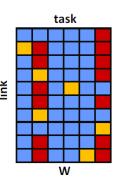
- Divide D into m disjoint subsets ordered by time
- Multi-task learning framework: each time slot corresponds to a task
 - leverage the inherent relations of tasks to enhance the predictive performance, especially when the data samples are insufficient

Trajectory Regression

$$\min_{\mathbf{W}} \sum_{i} Loss(\mathbf{W}, \mathbf{X}^{i}, \mathbf{Y}^{i}) + \lambda \operatorname{Reg}(\mathbf{W}) = \min_{\mathbf{W}} \sum_{i} ||\mathbf{Y}^{i} - \mathbf{X}^{i} \mathbf{w}^{i}|| + \lambda \operatorname{Reg}(\mathbf{W})$$

W Structure in the trajectory regression problem

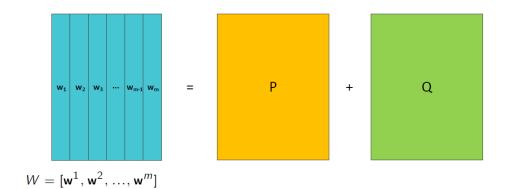
- Global temporal smoothness:
 - Link costs change smoothly most of the time
- Global spatial smoothness:
 - Costs are similar if the two corresponding links are close to each other
- Local temporal patterns:
 - Significant temporal changes in rush hours



Trajectory Regression - Additive Model

$$\min_{\mathbf{W}} \sum_{i} Loss(\mathbf{W}, \mathbf{X}^{i}, \mathbf{Y}^{i}) + \lambda \operatorname{Reg}(\mathbf{W}) = \min_{\mathbf{W}} \sum_{i} ||\mathbf{Y}^{i} - \mathbf{X}^{i} \mathbf{w}^{i}|| + \lambda \operatorname{Reg}(\mathbf{W})$$

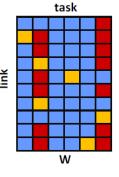
$$W = P + Q$$



- 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

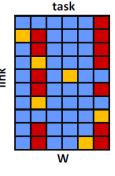
Global temporal smoothness

$$\Omega_1 = \sum_{t=1}^m \left\| P_{:,t} - \frac{1}{m} \sum_{r=1}^m P_{:,r} \right\|_2^2 = tr(PL_1P^T) \qquad L_1 = I - \frac{1}{m} \mathbf{1} \mathbf{1}'$$

 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

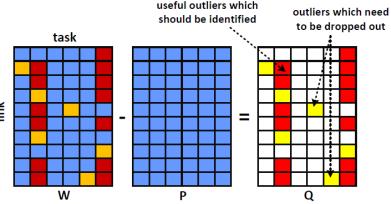
$$\Omega_2 = \sum_{i,j=1}^{d} S_{ij} || P_{i,:} - P_{j,:} ||_2^2 = tr(P^T L_2 P)$$

- 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" $\stackrel{\$}{=}$

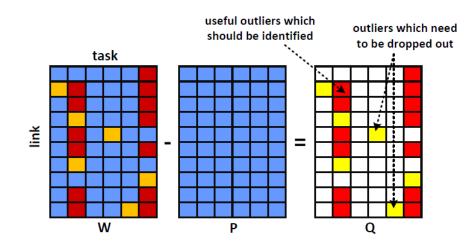


Local significant temporal transitions

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

- $||Z||_{\infty,1} = \sum_{j} ||Z_{:,j}||_{\infty}$, $||Z_{:,j}||_{\infty} = \max_{i} |Z_{ij}|$
- 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



$$\min_{W} \sum_{i=1}^{m} \|Y^{i} - X^{i} \mathbf{w}^{i}\|_{2}^{2} + \lambda_{1} tr(PL_{1}P^{T}) + \lambda_{2} tr(P^{T}L_{2}P) + \lambda_{3} \|Q\|_{\infty,1}$$

Trajectory Regression - Optimization

$$\min_{W} \sum_{i=1}^{m} \|Y^{i} - X^{i} \mathbf{w}^{i}\|_{2}^{2} + \lambda_{1} tr(PL_{1}P^{T}) + \lambda_{2} tr(P^{T}L_{2}P) + \lambda_{3} \|Q\|_{\infty,1}$$

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

$$\min_{W} \{F(W) + R(W)\} \begin{cases} F(W) = L(W) + \lambda_1 tr(PL_1 P^T) + \lambda_2 tr(P^T L_2 P) \\ R(W) = \lambda_3 ||Q||_{\infty, 1} \end{cases}$$

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

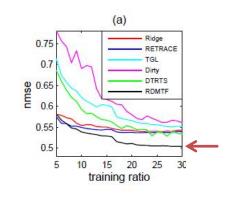
$$Q_r = arg \min_{Q} \frac{\gamma_r}{2} \|Q - C_Q(Q_{r-1})\|_F^2 + \lambda_3 \|Q\|_{\infty,1}$$

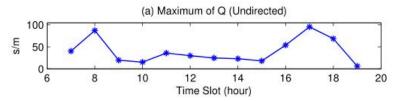
$$\min_{\boldsymbol{q}^i} \frac{1}{2} \|\boldsymbol{q}^i - \boldsymbol{c}^i\|_2^2 + \lambda \|\boldsymbol{q}^i\|_{\infty} \xrightarrow{Moreau \ Decomposition} \min_{\boldsymbol{q}^i} \left\{ \boldsymbol{c}^i - \left(\frac{1}{2} \|\boldsymbol{q}^i - \boldsymbol{c}^i\|_2^2 + \lambda \|\boldsymbol{q}^i\|_1 \right) \right\}$$

Trajectory Regression - Results

- Suzhou Traffic Data
 - Contains 59593 trajectory records of 4797 taxies 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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