RegML 2020
Class 4
Regularization for multi-task learning

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Supervised learning so far

- Regression $f : X \to Y \subseteq \mathbb{R}$
- Classification $f : X \to Y = \{-1, 1\}$

What next?

- Vector-valued $f : X \to Y \subseteq \mathbb{R}^T$
- Multiclass $f : X \to Y = \{1, 2, \ldots, T\}$
- ...

Multitask learning

Given

$$S_1 = (x_i^1, y_i^1)_{i=1}^{n_1}, \dots, S_T = (x_i^T, y_i^T)_{i=1}^{n_T}$$

find

$$f_1 : X_1 \to Y_1, \dots, f_T : X_T \to Y_T$$

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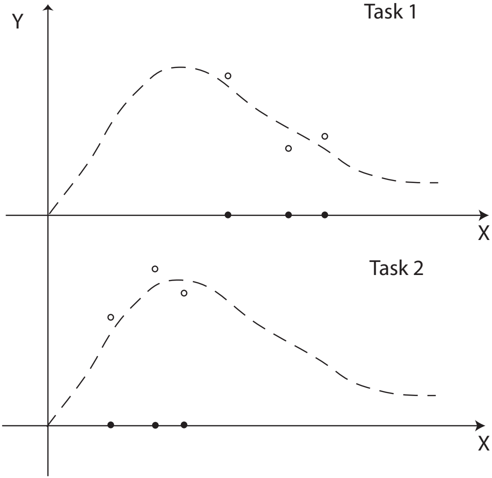
- vector valued regression,

  $$S_n = (x_i, y_i)_{i=1}^n, \quad x_i \in X, \quad y_i \in \mathbb{R}^T$$

  MTL with equal inputs! Output coordinates are "tasks"
- multiclass

  $$S_n = (x_i, y_i)_{i=1}^n, \quad x_i \in X, \quad y_i \in \{1, \dots, T\}$$

Why MTL?



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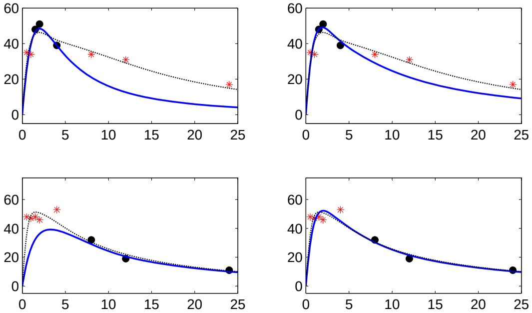


Real data!

Why MTL?

Related problems:

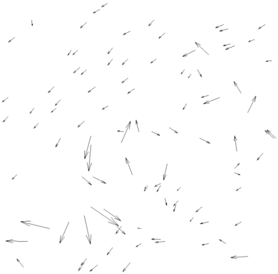
- conjoint analysis
- transfer learning
- collaborative filtering
- co-kriging

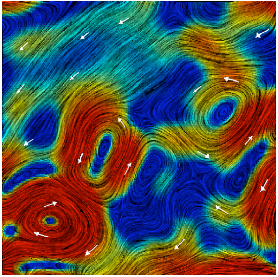
Examples of applications:

- geophysics
- music recommendation (Dinuzzo 08)
- pharmacological data (Pillonetto at el. 08)
- binding data (Jacob et al. 08)
- movies recommendation (Abernethy et al. 08)
- HIV Therapy Screening (Bickel et al. 08)

Why MTL?

VVR, e.g. vector fields estimation





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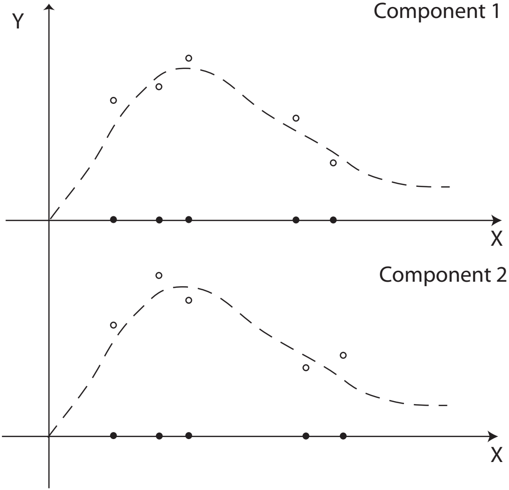

Penalized regularization for MTL

$$\mathrm{err}(w_1, \dots, w_T) \quad + \quad \mathrm{pen}(w_1, \dots, w_T)$$

We start with linear models

$$f_1(x) = w_1^\top x, \dots, f_T(x) = w_T^\top x$$

Empirical error

$$\widehat{\mathcal{E}}(w_1, \dots, w_T) = \sum_{i=1}^{T} \frac{1}{n_i} \sum_{j=1}^{n_i} (y_j^i - w_i^\top x_j^i)^2$$

- could consider other losses
- could try to "couple" errors

Least squares error

We focus on vector valued regression (VVR)

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$$\frac{1}{n} \sum_{t=1}^T \sum_{i=1}^n (y_i^t - w_t^\top x_i)^2 = \frac{1}{n} \| \underbrace{\hat{X}}_{n \times d} \underbrace{W}_{d \times T} - \underbrace{\widehat{Y}}_{n \times T} \|_F^2$$

$$\|W\|_F^2 = \mathrm{Tr}(W^\top W), \quad W = (w_1, \dots, w_T), \quad \widehat{Y}_{it} = \hat{y}_i^t \;\; i = 1 \dots n \;\; t = 1 \dots T$$

MTL by regularization

$$\mathrm{pen}(w_1 \dots w_T)$$

- Coupling task solutions by regularization
- Borrowing strength
- Exploit structure

Regularizations for MTL

$$\mathsf{pen}(w_1, \dots, w_T) = \sum_{t=1}^{T} \|w_t\|^2$$

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Single tasks regularization!

$$\min_{w_1,\dots,w_T} \frac{1}{n} \sum_{t=1}^{T} \sum_{i=1}^{n} (y_i^t - w_t^\top x_i)^2 + \lambda \sum_{t=1}^{T} \|w_t\|^2 =$$

$$\sum_{t=1}^{T} (\min_{w_t} \frac{1}{n} \sum_{i=1}^{n} (y_i^t - w_t^\top x_i)^2 + \lambda \|w_t\|^2)$$

Regularizations for MTL

- Isotropic coupling

$$(1-\alpha)\sum_{j=1}^{T}\|w_j\|^2 \quad + \quad \alpha\sum_{j=1}^{T}\left\|w_j \; - \; \frac{1}{T}\sum_{i=1}^{T} w_i\right\|^2$$

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- Graph coupling - Let $M \in \mathbb{R}^{T\times T}$ an adjacency matrix, with $M_{ts} \geq 0$

$$\sum_{t=1}^{T}\sum_{s=1}^{T} M_{ts}\|w_t - w_s\|^2 + \gamma\sum_{t=1}^{T}\|w_t\|^2$$

special case: output divided in clusters

A general form of regularization

All the regularizers so far are of the form

$$\sum_{t=1}^{T} \sum_{s=1}^{T} A_{ts} w_t^\top w_s$$

for a suitable positive definite matrix A

MTL regularization revisited

- Single tasks $\sum_{j=1}^{T} \|w_j\|^2 \quad \Longrightarrow \quad A = I$

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$$\Longrightarrow \quad A = I - \frac{\alpha}{T}\mathbf{1}$$

MTL regularization revisited

- Single tasks $\sum_{j=1}^{T} \|w_j\|^2 \quad \Longrightarrow \quad A = I$
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$$\Longrightarrow \quad A = I - \frac{\alpha}{T}\mathbf{1}$$

- Graph coupling

$$\sum_{t=1}^{T}\sum_{s=1}^{T} M_{ts}\|w_t - w_s\|^2 + \gamma\sum_{t=1}^{T}\|w_t\|^2$$

$$\Longrightarrow \quad A = L + \gamma I,$$

where L graph Laplacian of M

$$L = D - M, \quad D = \text{diag}(\sum_j M_{1,j}, \ldots, \sum_j M_{T,j},)$$

A general form of regularization

Let $W = (w_1, \dots, w_T), \quad A \in \mathbb{R}^{T \times T}$

Note that

$$\sum_{t=1}^{T} \sum_{s=1}^{T} A_{ts} w_t^\top w_s = \mathrm{Tr}(WAW^\top)$$

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Indeed

$$\mathrm{Tr}(WAW^\top) = \sum_{i=1}^{d} {W_i}^\top A W_i = \sum_{i=1}^{d} \sum_{t,s=1}^{T} A_{ts} W_{it} W_{is}$$

$$= \sum_{t,s=1}^{T} A_{ts} \sum_{i=1}^{d} W_{is} W_{ir} = \sum_{t,s=1}^{T} A_{ts} w_t^\top w_s$$

Computations

$$\frac{1}{n}\|\widehat{X}W - \widehat{Y}\|_F^2 + \lambda \mathrm{Tr}(WAW^\top)$$

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Consider the SVD $A = U\Sigma U^\top$, $\Sigma = \mathsf{diag}(\sigma_1, \dots, \sigma_T)$

Computations

$$\frac{1}{n}\|\widehat{X}W - \widehat{Y}\|_F^2 + \lambda \mathrm{Tr}(WAW^\top)$$

Consider the SVD $A = U\Sigma U^\top$, $\Sigma = \mathrm{diag}(\sigma_1, \dots, \sigma_T)$ let

$$\tilde{W} = WU, \qquad \tilde{Y} = \widehat{Y}U$$

then we can rewrite the above problem as

$$\frac{1}{n}\|\widehat{X}\tilde{W} - \tilde{Y}\|_F^2 + \lambda \mathrm{Tr}(\tilde{W}\Sigma\tilde{W}^\top)$$

Computations (cont.)

Finally, rewrite

$$\frac{1}{n}\|\widehat{X}\tilde{W} - \tilde{Y}\|_F^2 + \lambda \mathrm{Tr}(\tilde{W}\Sigma\tilde{W}^\top)$$

as

$$\sum_{t=1}^{T}(\frac{1}{n}\sum_{i=1}^{n}(\tilde{y}_i^t - \tilde{w}_t^\top x_i)^2 + \lambda\sigma_t\|\tilde{w}_t\|^2)$$

and use $W = \tilde{W}U^\top$

Compare to single task regularization...

Computations (cont.)

$$\mathcal{E}_\lambda(W) = \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|_F^2 + \lambda \mathrm{Tr}(WAW^\top)$$

Alternatively

$$\nabla\mathcal{E}_\lambda(W) = \frac{2}{n}\widehat{X}^\top(\widehat{X}W - \widehat{Y}) + 2\lambda WA$$

$$W_{t+1} = W_t - \gamma\nabla\mathcal{E}_\lambda(W_t)$$

Trivially extends to other loss functions.

Beyond Linearity

$$f_t(x) = w_t^\top \Phi(x), \quad \Phi(x) = (\phi_1(x), \dots, \phi_p(x))$$

$$\mathcal{E}_\lambda(W) = \frac{1}{n} \|\widehat{\Phi} W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(W A W^\top),$$

with $\widehat{\Phi}$ matrix with rows $\Phi(x_1), \dots, \Phi(x_n)$

Nonparametrics and kernels

$$f_t(x) = \sum_{i=1}^{n} K(x, x_i) C_{it}$$

with

$$C_{\ell+1} = C_\ell - \gamma \left(\frac{2}{n} \widehat{K} C_\ell - \widehat{Y} + 2\lambda C_\ell A \right)$$

- $C_\ell \in \mathbb{R}^{n \times T}$
- $\widehat{K} \in \mathbb{R}^{n \times n}$, $\widehat{K}_{ij} = K(x_i, x_j)$
- $\widehat{Y} \in \mathbb{R}^{n \times T}$, $\widehat{Y}_{ij} = y_i^j$

Spectral filtering for MTL

Beyond penalization

$$\min_{W} \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WAW^\top),$$

other forms of regularizations can be considered

- projection
- early stopping

Multiclass and MTL

$$Y = \{1, \ldots, T\}$$

From Multiclass to MTL

Encoding For $j = 1, \dots, T$

$$j \mapsto e_j$$

canonical vector of $\mathbb{R}^T$

the problem reduces to vector valued regression

Decoding For $f(x) \in \mathbb{R}^T$

$$f(x) \mapsto \operatorname*{argmax}_{t=1,\dots t} e_t^\top f(x) = \operatorname*{argmax}_{t=1,\dots t} f_t(x)$$

Single MTL and OVA

Write

$$\min_{W} \frac{1}{n} \|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WW^\top),$$

as

$$\sum_{t=1}^{T} \min_{w_t} \frac{1}{n} \sum_{i=1}^{n_t} (w_t^\top x_i^t - y_i^t)^2 + \lambda \|w_t\|^2$$

This is known as one versus all (OVA)

Beyond OVA

Consider

$$\min_{W} \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WAW^\top),$$

that is

$$\sum_{t=1}^{T} \min_{\tilde{w}_t} \sum_{t=1}^{T} (\frac{1}{n} \sum_{i=1}^{n} (\tilde{y}_i^t - \tilde{w}_t^\top x_i)^2 + \lambda \sigma_t \|\tilde{w}_t\|^2)$$

Class relatedness encoded in A

Back to MTL

$$\sum_{t=1}^{T} \frac{1}{n_t} \sum_{j=1}^{n_t} (y_j^t - w_i^\top x_j^t)^2$$

$$\Downarrow$$

$$\|(\underbrace{\hat{X}}_{n\times d} \underbrace{W}_{d\times T} - \underbrace{\overline{Y}}_{n\times T}) \odot \underbrace{M}_{n\times T}\|_F^2, \qquad n = \sum_{t=1}^{T} n_t$$

- $\odot$ Hadamard product
- M mask
- $\overline{Y}$ having one non-zero value for each row

Computations

$$\min_{W} \|(\hat{X}W - \overline{Y}) \odot M\|_F^2 + \lambda \mathrm{Tr}(WAW^\top)$$

- can be rewritten using tensor calculus
- computation for vector valued regression easily extended
- sparsity of M can be exploited

From MTL to matrix completion

Special case Take $d = n$ and $X = I$

$$\|(\hat{X}W - \overline{Y}) \circ M\|_F^2$$

$$\Downarrow$$

$$\sum_{t=1}^{T}\sum_{i=1}^{n}(w_{ij} - \bar{y}_{ij})^2 M_{ij}$$

Summary so far

A regularization framework for

- VVR
- Multiclass
- MTL
- Matrix completion

if the structure of the "tasks" is known.

What if it is not?

The structure of MTL

Consider

$$\min_W \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WAW^\top),$$

the matrix A encodes structure.

Can we learn it?

Learning structure of MTL

Consider

$$\min_{W,A} \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WAW^\top) + \gamma \mathsf{pen}(A)$$

Estimate a positive definite matrix A using a regularizer $\mathsf{pen}(A)$

Regularizers for MTL

For example consider

$$\min_{W,A} \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WAW^\top) + \gamma \mathrm{Tr}(A^{-2})$$

using the same change of coordinates as before we have

$$\min_{\tilde{w}_1,\dots,w_T,\quad \sigma_1,\dots,\sigma_t} \sum_{t=1}^{T} \sum_{t=1}^{T} \frac{1}{n} \sum_{i=1}^{n} (\tilde{y}_i^t - \tilde{w}_t^\top x_i)^2 + \lambda \sigma_t \|\tilde{w}_t\|^2 + \gamma \sum_{t=1}^{T} \left(\frac{1}{\sigma_t^2}\right)$$

we avoid each task having too little weight

Alternating minimization

Solving

$$\min_{W,A} \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WAW^\top) + \gamma \mathsf{pen}(A)$$

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Solving

$$\min_{W,A} \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WAW^\top) + \gamma \mathsf{pen}(A)$$

- Fix $A = A_0$
- Compute W_1 solving

$$\min_{W} \frac{1}{n}\|\widehat{X}W - \widehat{Y}\|^2 + \lambda \mathrm{Tr}(WA_0W^\top)$$

- Compute A_1 solving

$$\min_{A} \lambda \mathrm{Tr}(W_1AW_1^\top) + \gamma \mathsf{pen}(A)$$

- Repeat...

This class

- Why MTL?
- Regularization for MTL to exploit structure
- MTL and other problems
- Learning tasks AND their structure

Next class

Sparsity!