Regularization for Multi-Output Learning

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About this class

Goal In many practical problems, it is convenient to model the object of interest as a function with multiple outputs.
In machine learning, this problem typically goes under the name of multi-task or multi-output learning. We present some concepts and algorithms to solve this kind of problems.

Plan

- Examples and Set-up
- Tikhonov regularization for multiple output learning
- Regularizers and Kernels
- Vector Fields
- Multiclass
- Conclusions

Costumers Modeling

Costumers Modeling

the goal is to model buying preferences of several people based on previous purchases.

borrowing strength

People with similar tastes will tend to buy similar items and their buying history is related.
The idea is then to predict the consumer preferences for all individuals **simultaneously** by solving a multi-output learning problem.

Each consumer is modelled as a task and its previous preferences are the corresponding training set.

Multi-task Learning

We are given T scalar tasks.

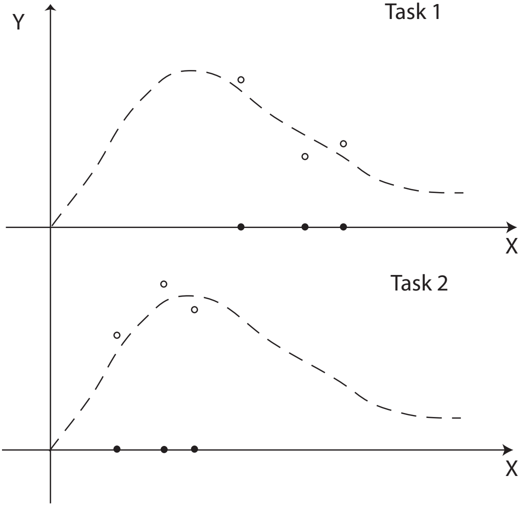
For each task $j = 1, \ldots, T$, we are given a set of examples

$$S_j = (x_i^j, y_i^j)_{i=1}^{n_j}$$

sampled i.i.d. according to a distribution P_t.
The goal is to find

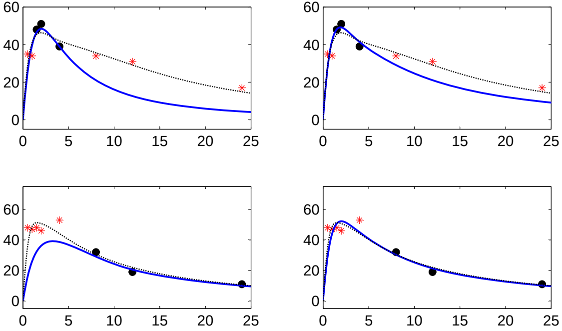
$$f^t(x) \sim y \quad t = 1, \ldots, T.$$

Multi-task Learning



Pharmacological Data

Blood concentration of a medicine across different times. Each task is a patient.



Single-task

Multi-task

Red dots are test and black dots are training points.

(pics from Pillonetto et al. 08)

Names and Applicatons

Related problems:

- conjoint analysis
- transfer learning
- collaborative filtering
- 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)

Multi-task Learning: Remarks

The framework is very general.

- The input spaces can be different.
- The output space can be different.
- The hypotheses spaces can be different

How Can We Design an Algorithm?

In all the above problems one can think of improving performances, by exploiting relation among the different outputs.

A possible way to do this is penalized empirical risk minimization

$$\min_{f^1,\dots,f^T} ERR[f_1,\dots,f_T] + \lambda PEN(f^1,\dots,f^T)$$

Typically

- The error term is the sum of the empirical risks.
- The penalty term enforces similarity among the tasks.

Error Term

We are going to choose the square loss to measure errors.

$$ERR[f^1, \ldots, f^T] = \sum_{j=1}^{T} \frac{1}{n_j} \sum_{i=1}^{n} (y_i^j - f^j(x_i^j))^2$$

MTL

Let $f^j : X \to \mathbb{R}, \quad j = 1, \dots T$ then

$$ERR[f^1, \dots, f^T] = \sum_{j=1}^{T} I_{S_j}[f^j]$$

with

$$I_S[f] = \frac{1}{n} \sum_{i=1}^{n} (y_i - f(x_i))^2$$

Building Regularizers

We assume that input, output and hypotheses spaces are the same, i.e.

$$X_j = X,$$

$$Y_j = Y,$$

and

$$\mathcal{H}_j = \mathcal{H},$$

for all $j = 1, \ldots, T$.
We also assume $\mathcal{H}$ to be a RKHS with kernel K.

Regularizers: Mixed Effect

For each component/task the solution is the same function plus a component/task specific component.

$$PEN(f_1, \dots, f_T) = \lambda \sum_{j=1}^{T} \|f^j\|_K^2 + \gamma \sum_{j=1}^{T} \|f^j - \sum_{s=1}^{T} f^s\|_K^2$$

We can define a regularizer that, in addition to a standard regularization on the single components, forces stronger or weaker similarity through a $T \times T$ positive weight matrix M:

$$PEN(f_1, \dots, f_T) = \gamma \sum_{\ell,q=1}^{T} \|f^\ell - f^q\|_K^2 M_{\ell q} + \lambda \sum_{\ell=1}^{T} \|f^\ell\|_K^2 M_{\ell\ell}$$

Regularizers: cluster

The components/tasks are partitioned into c clusters: components in the same cluster should be similar.
Let

- m_r, $r = 1, \dots, c$, be the cardinality of each cluster,
- $I(r)$, $r = 1, \dots, c$, be the index set of the components that belong to cluster c.

$$PEN(f_1, \dots, f_T) = \gamma \sum_{r=1}^{c} \sum_{l \in I(r)} ||f^l - \bar{f}_r||_K^2 + \lambda \sum_{r=1}^{c} m_r ||\bar{f}_r||_K^2$$

where $\bar{f}_r$, , $r = 1, \dots, c$, is the mean in cluster c.

How can we find a the solution?

We have to solve

$$\min_{f_1,\dots,f_T}\{\frac{1}{n}\sum_{j=1}^{T}\sum_{i=1}^{n}(y_i^j - f^j(x_i))^2 + \lambda\sum_{j=1}^{T}\|f^j\|_K^2 + \gamma\sum_{j=1}^{T}\|f^j - \sum_{s=1}^{T} f^s\|_K^2\}$$

(we considered the first regularizer as an example).
The theory of RKHS gives us a way to do this using what we already know from the scalar case.

Tikhonov Regularization

We now show that for al the above penalties we can define a suitable RKHS with kernel Q (and re-index the sums in the error term), so that

$$\min_{f_1,\dots,f_T} \{ \sum_{j=1}^{T} \frac{1}{n_j} \sum_{i=1}^{n} (y_i^j - f^j(x_i))^2 + \lambda PEN(f_1, \dots, f_T) \}$$

can be written as

$$\min_{f \in \mathcal{H}} \{ \frac{1}{n_T} \sum_{i=1}^{n_T} (y_i - f(x_i, t_i))^2 + \lambda \|f\|_Q^2 \}$$

Kernels at Rescue

Consider a (joint) kernel $Q : (X, \Pi) \times (X, \Pi) \to \mathbb{R}$, where $\Pi = 1, \ldots T$ is the index set of the output components.
A function in the space is

$$f(x,t) = \sum_i Q((x,t),(x_i,t_i))c_i,$$

with norm

$$\|f\|_Q^2 = \sum_{i,j} Q((x_j,t_j),(x_i,t_i))c_i c_j.$$

A Useful Class of Kernels

Let A be a $T \times T$ positive definite matrix and K a scalar kernel. Consider a kernel $Q : (X, \Pi) \times (X, \Pi) \to \mathbb{R}$, defined by

$$Q((x,t),(x',t')) = K(x,x')A_{t,t'}.$$

Then the norm of a function is

$$\|f\|_Q^2 = \sum_{i,j} K(x_i,x_j)A_{t_i t_j} c_i c_j.$$

Regularizers and Kernels

If we fix t then $f_t(x) = f(t, x)$ is one of the task. The norm $\|\cdot\|_Q$ can be related to the scalar products among the tasks.

$$\|f\|_Q^2 = \sum_{s,t} A^\dagger_{s,t} \langle f_s, f_t \rangle_K$$

This implies that :

- A regularizer of the form $\sum_{s,t} A^\dagger_{s,t} \langle f_s, f_t \rangle_K$ defines a kernel Q.
- The norm induced by a kernel Q of the form $K(x, x')A$ can be seen as a regularizer.

The matrix A encodes relations among outputs.

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Regularizers and Kernels

We sketch the proof of

$$\|f\|_Q^2 = \sum_{s,t} A^{\dagger}_{s,t} \langle f_s, f_t \rangle_K$$

Recall that

$$\|f\|_Q^2 = \sum_{ij} K(x_i, x_j) A_{t_i t_j} c_i c_j$$

and note that if $f_t(x) = \sum_i K(x, x_i) A_{t,t_i} c_i$, then

$$\langle f_s, f_t \rangle_K = \sum_{i,j} K(x_i, x_j) A_{s,t_i} A_{t,t_j} c_i c_j.$$

We need to multiply by $A^{-1}_{s,t}$ (or rather $A^{\dagger}_{s,t}$) the last equality.

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Examples I

Let $\mathbf{1}$ be the $T \times T$ matrix whose entries are all equal to 1 and $\mathbf{I}$ the d-dimensional identity matrix.
The kernel

$$Q((x,t)(x',t')) = K(x,x')(\omega\mathbf{1} + (1-\omega)\mathbf{I})_{t,t'}$$

induces a penalty:

$$A_\omega \left(B_\omega \sum_{\ell=1}^{T} ||f^\ell||_K^2 + \omega T \sum_{\ell=1}^{T} ||f^\ell - \frac{1}{T}\sum_{q=1}^{T} f^q||_K^2 \right)$$

where $A_\omega = \frac{1}{2(1-\omega)(1-\omega+\omega T)}$ and $B_\omega = (2 - 2\omega + \omega T)$.

Examples II

The penalty

$$\frac{1}{2}\sum_{\ell,q=1}^{T}||f^{\ell}-f^{q}||_K^2 M_{\ell q}+\sum_{\ell=1}^{T}||f^{\ell}||_K^2 M_{\ell\ell}$$

can be rewritten as:

$$\sum_{\ell,q=1}^{T} < f^{\ell}, f^{q} >_K L_{\ell q}$$

where $L = D - M$, with $D_{\ell q} = \delta_{\ell q}(\sum_{h=1}^{T} M_{\ell h} + M_{\ell q})$.
The kernel is $Q((x,t)(x',t')) = K(x,x')L^{\dagger}_{t,t'}$.

Examples III

The penalty

$$\epsilon_1 \sum_{c=1}^{r} \sum_{l \in I(c)} ||f^l - \bar{f}_c||_K^2 + \epsilon_2 \sum_{c=1}^{r} m_c ||\bar{f}_c||_K^2$$

induces a kernel $Q((x,t)(x',t')) = K(x,x')G^{\dagger}_{t,t'}$ with

$$G_{lq} = \epsilon_1 \delta_{lq} + (\epsilon_2 - \epsilon_1) M_{lq}.$$

The $T \times T$ matrix M is such that $M_{lq} = \frac{1}{m_c}$ if components l and q belong to the same cluster c, and m_c is its cardinality ($M_{lq} = 0$ otherwise).

Tikhonov Regularization

Given the above penalties and re-indexing the sums in the error term

$$\min_{f_1,\dots,f_T}\{\sum_{j=1}^{T}\frac{1}{n_j}\sum_{i=1}^{n}(y_i^j - f^j(x_i))^2 + \lambda PEN(f_1,\dots,f_T)\}$$

can be written as

$$\min_{f\in\mathcal{H}}\{\frac{1}{n_T}\sum_{i=1}^{n_T}(y_i - f(x_i,t_i))^2 + \lambda\|f\|_Q^2\}$$

where $\mathcal{H}$ is the RKHS with kernel Q and we consider a training set $(x_1,y_1,t_1),\dots,(x_{n_T},y_{n_T},t_{n_T})$ with $n_T = \sum_{j=1}^{T} n_j$.

Representer Theorem

A representer theorem can be proved using the same technique of the standard case

$$f(x,t) = f_t(x) = \sum_{i=1}^{n} Q((x,t),(x_i,t_i))c_i,$$

where the coefficients are given by

$$(\mathbf{Q} + \lambda I)\mathbf{C} = \mathbf{Y}.$$

where $\mathbf{C} = (c_1, \ldots, c_n)^T$, $\mathbf{Q}_{ij} = Q((x_i,t_i),(x_j,t_j))$ and $\mathbf{Y} = (y_1, \ldots, y_n)^T$.

L_2 Boosting

Note that we can write the empirical risk as,

$$\frac{1}{n_T}\|\mathbf{Y} - \mathbf{QC}\|_{n_T}^2$$

The minimization with gradient descent show that the coefficients can be found by setting $\mathbf{C}^0 = 0$ and considering for $i = 1, \ldots, t-1$ the following iteration

$$\mathbf{C}^i = \mathbf{C}^{i-1} + \eta(\mathbf{Y} - \mathbf{QC}^{i-1}),$$

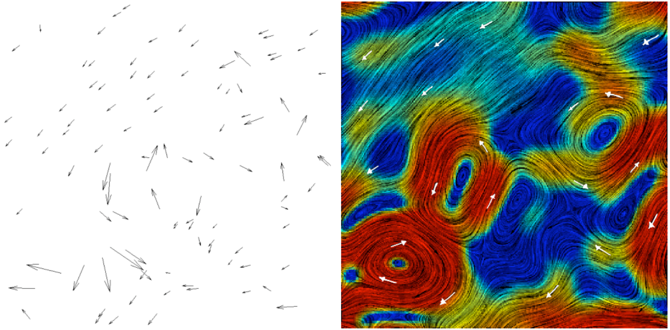
where η the step size.
Regularization can be achieved by early stopping.

Remarks

- The effect of MTL is especially evident when few examples are available for each task.
- The complexity of Tikhonov regularization can be reduced when some (all) input points are the same (Dinuzzo et al. 09, Baldassarre et al. 09).
- The design of efficient kernel is a considerably more difficult problem than in the scalar case.

Learning Vector Fields: Example

We sample the velocity fields of an incompressible fluid and want to recover the whole velocity field.



To each point in the space we associate a velocity vector.

(figures from Macêdo and Castro 08)

It is the most natural extension of the scalar setting.

We are given a training set of points
$S = \{(x_1, y_1), \ldots, (x_n, y_n)\}$,where

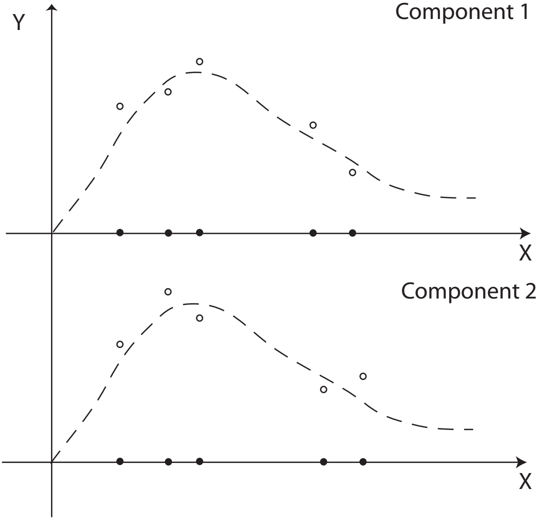
- $x_1, \ldots, x_n \in \mathbb{R}^p$
- $y_1, \ldots, y_n \in \mathbb{R}^T$

As usual the point are assumed to be sampled (i.i.d.) according to some probability distribution P.
The goal is to find

$$f(x) \sim y,$$

where y is a vector.

Vector fields Learning



Error Term for Vector fields

Note that

$$ERR[f^1, \ldots, f^T] = \frac{1}{n} \sum_{j=1}^{T} \sum_{i=1}^{n} (y_i^j - f^j(x_i^j))^2$$

can be written as

VFL

$$ERR[f] = \frac{1}{n} \sum_{i=1}^{n} \|y_i - f(x_i)\|_T^2, \quad \|y - f(x)\|_T^2 = \sum_{j=1}^{T} (y^j - f^j(x))^2$$

with $f : X \to \mathbb{R}^T$ and $f = f^1, \ldots f^T$.

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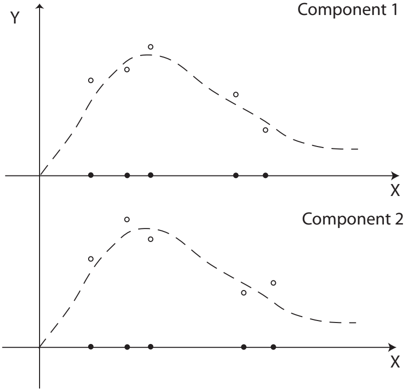
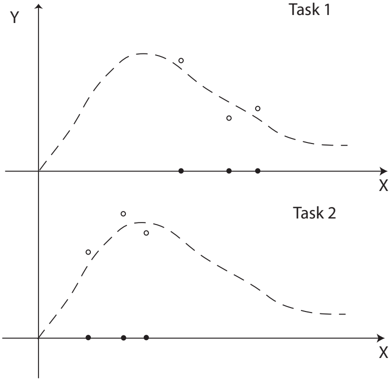
Vector fields vs Multi-task Learning





Vector fields vs Multi-task Learning

The two problems are clearly related.

- Tasks can be seen as components of a vector fields and viceversa
- In multitask we might sample each task in a different way, so that when we consider the tasks together we are essentially augmenting the number of sample available for each individual task.

Multi-class and Multi-label

Multiclass

In multi-category classification each input can be assigned to one of T classes. We can think of encoding each class with a vector, for example: class one can be $(1, 0 \ldots, 0)$, class 2 $(0, 1 \ldots, 0)$ etc.

Multilabel

Images contain at most T objects each input image is associate to a vector

$$(1, 0, 1 \ldots, 0)$$

where $1/0$ indicate presence/absence of the an object.

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Consider the coding where class 1 is $(1, -1, \dots, -1)$, class 2 is $(-1, 1, \dots, -1)$ ...

One can easily check that the problem

$$\min_{f_1,\dots,f_T} \{\frac{1}{n}\sum_{j=1}^{T}\sum_{i=1}^{n}(y_i^j - f^j(x_i))^2 + \lambda\sum_{j=1}^{T}\|f^j\|_K^2$$

is exactly the one versus all scheme with regularized least squares.

One Versus All

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is exactly the one versus all scheme with regularized least squares.

Final Remarks

Kernel Methods and regularization can be used in a many situations when the object of interest is a multi output function.

Kernel/Regularizer choice is crucial

Recently other approaches based on regularization and sparsity were proposed.

Sparsity Across Tasks

Assume that each task is of the form

$$f^t(x) = \sum_{j=1}^{p} \phi_j(x) c_j^t$$

where $\phi_1, \ldots, \phi_p$ are the same features for all tasks.

A penalization can be written as

$$\sum_j \|\mathbf{c}_j\|_T$$

where $\mathbf{c}_j = (c_j^1, \ldots, c_j^T)$ are the coefficients corresponding to the $j-th$ feature across the various tasks.

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