# Regularization for Multi-Output Learning

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9.520 Class 11

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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.

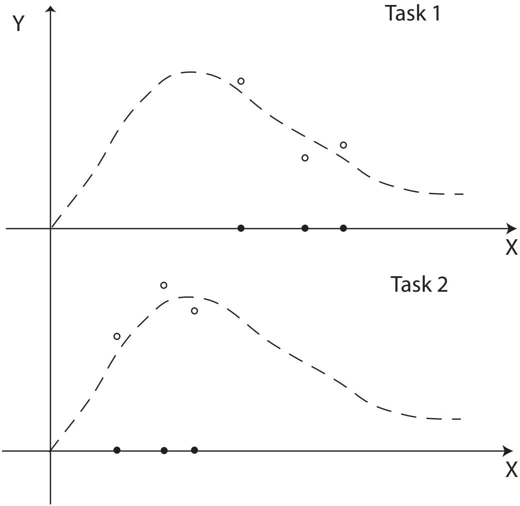
For each task $j = 1, \dots, T$, we are given a set of examples

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

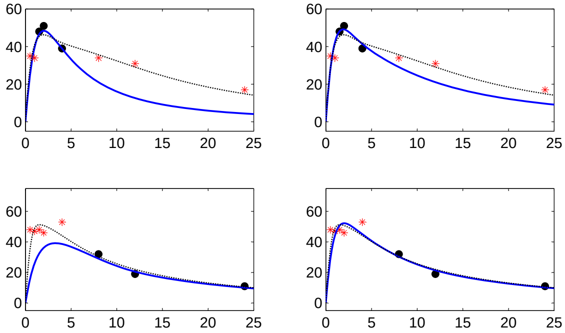
sampled i.i.d. according to a distribution $P_t$.
The goal is to find

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

# Multi-task Learning



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
- 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)

# 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.

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

# Regularizers: Graph Regularization

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

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

(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

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

# 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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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:

$$\sum_{\ell,q=1}^{T}\langle f^{\ell},f^{q}\rangle_K L_{\ell q}$$

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

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

can be written as

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

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

# $L_2$ 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

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

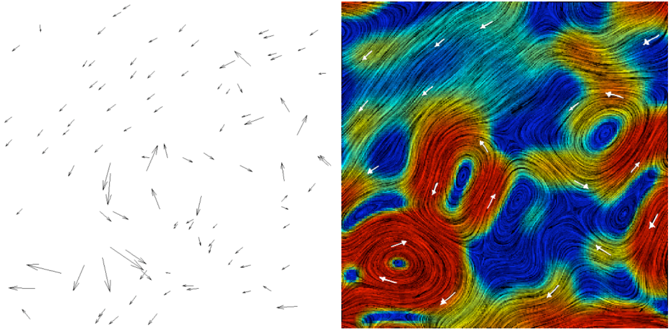
where $\eta$ the step size.
Regularization can be achieved by early stopping.

# 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)

# Learning Vector fields

It is the most natural extension of the scalar setting.

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

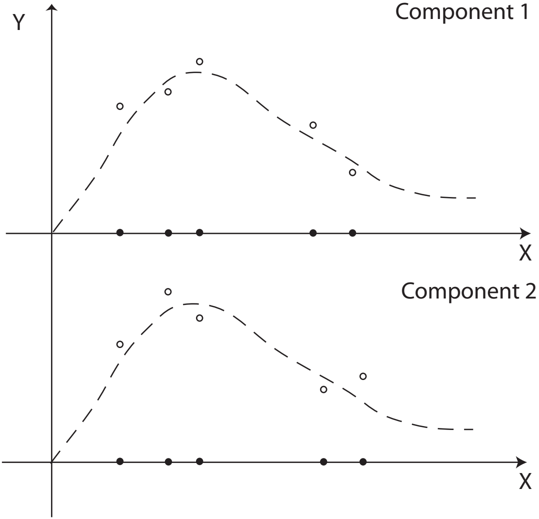
- $x_1, \dots, x_n \in \mathbb{R}^p$
- $y_1, \dots, y_n \in \mathbb{R}^T$

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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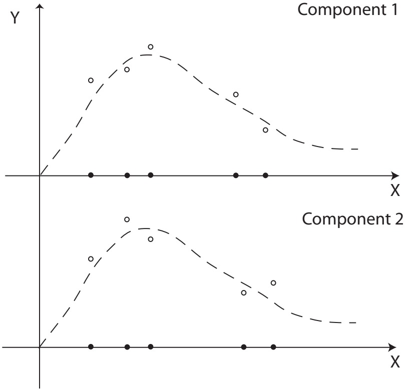
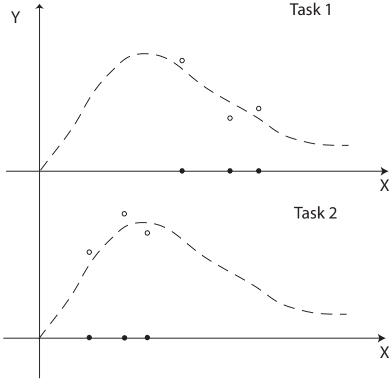
# Vector fields vs Multi-task Learning



# 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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# One Versus All

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

One can easily check that the problem

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

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

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# 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**

- Sparsity
- Manifold
- ????

# 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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