SUPERVISED CLUSTERING IN THE DATA CUBE

VINCENT ROULET, FAJWEL FOGEL, ALEXANDRE D’ASPREMONT, AND FRANCIS BACH

ABSTRACT. We study a supervised clustering problem seeking to cluster either features, tasks or sample points using losses extracted from supervised learning problems. We formulate a unified optimization problem handling these three settings and derive algorithms whose core iteration complexity is concentrated in a k-means clustering step, which can be approximated efficiently. We test our methods on both artificial and realistic data sets extracted from movie reviews and 20NewsGroup.

1. INTRODUCTION

Using information from a supervised problem like regression or classification, supervised clustering seeks to discover hidden clusters of features, tasks or samples that both help inference, and provide additional structural insights on the data.

In the classical multi-task setting, clustering predictors of related tasks often helps prediction. In computer vision for instance, classifiers associated with different species of cats should be quite similar, but well separated from classifiers associated with cars, and incorporating this structural information at the training stage should improve performance. This problem has been well studied in the multi-task learning literature [1, 2, 3].

Similarly, when there exists some groups of highly correlated features, reducing dimensionality by assigning the same weights to some groups of features can be beneficial both in terms of prediction and interpretation [4]. This often occurs in text classification, where it is natural to group together words having the same meaning for a given task [5, 6].

Finally, in some settings, it can be valuable to cluster sample points, with each cluster having its own distinct prediction function [7]. This last problem may have applications in the context of privacy learning, where the group information of an individual may not be revealed because of confidentiality issues.

Here, we present a unified and flexible framework for supervised clustering over the “data cube” of either tasks, features or sample points (a representation introduced by [8]). We directly formulate supervised clustering as an optimization problem on the clustered predictors, where clustering is either a hard constraint or a soft regularization penalty, and losses are adapted to the application at hand (classification or regression, clustering tasks, features or sample points). We propose several optimization schemes to solve these problems efficiently. While the original optimization problem is non-convex, we show that the core non-convexity is concentrated in a subproblem similar to k-means, which we solve using classical approximation techniques [9]. In the particular case of feature clustering for regression, the k-means steps are performed in dimension one, and can therefore be solved exactly by dynamic programming [10, 11]. Our formulation is then an explicit convex relaxation which can be solved efficiently using the conditional gradient algorithm [12, 13]. We describe experiments on both synthetic and real datasets involving large corpora of text where our method compares favorably with standard benchmarks.

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The two first authors contributed equally.
2. Supervised clustering of features, tasks or samples

We write supervised clustering as a clustering problem penalized by a supervised learning loss. We let \( n \) be the number of training examples in the dataset, \( d \) the number of features (i.e. the ambient dimension) and \( K \) the number of tasks. For regression or binary classification \( K = 1 \), while for multi-classification \( K \) corresponds to the number of classes (using one-versus-all majority vote, training one binary classifier per class vs all others). For simplicity, we consider only square or logistic losses for linear predictors.

Our main variable is a matrix of predictors with one column per task, written \( W = [w_1, \ldots, w_K] \in \mathbb{R}^{d \times K} \). We let \( Q \) be the desired number of clusters and \( m \) the number of items to cluster. When clustering \( Q, m = K \) and we are grouping the predictors associated with each task, i.e. the columns of \( W \). When clustering features, \( m = d \) and we are clustering the predictors associated with each feature, i.e. the rows of \( W \). Finally, when clustering sample points, \( m = n \) and we introduce individual predictor vectors \( W^{(i)} \) for each sample point \( i \), which we cluster together to obtain \( Q \) distinct predictors associated with a partition of the points into \( Q \) groups. Hence, the term “predictors” either refers to columns of \( W \), rows of \( W \), or individual predictor vectors \( W^{(i)} \), depending on which dimension of the data cube (tasks, features or sample points) the clustering is performed. A summary of these settings is given in Table 1. In the following we use the generic notations \( U \) and \( V \) to designate predictors.

A clustering can be seen as a partition \( C_1 \cup C_2 \cup \cdots \cup C_Q = [1, m] \) of predictors, to which corresponds an assignment matrix \( Z \in \{0, 1\}^{m \times Q} \) such that \( Z_{ij} = 1 \) if item \( i \) is in cluster \( C_j \). As in k-means, we define a matrix of centroids \( C = [c_1, \ldots, c_Q] \), with each centroid \( c_j \) equal to the mean of predictors in cluster \( j \). This information is summarized in the matrix \( V = CZ^T \), which we call matrix of individual centroids (MIC), whose columns \( v_i \) are such that \( v_i = c_j \) if predictor \( i \) is in cluster \( C_j \).

Given a supervised learning loss \( L(\cdot) \) and a regularizing penalty \( \Omega(\cdot) \) on predictors, we formulate the supervised clustering problem as an optimization problem over the set of MIC matrix \( V \). Enforcing the hard constraint that predictors are exactly confounded with centroids, we get the following hard supervised clustering problem (HSC)

\[
\begin{align*}
\text{minimize} & \quad L(V) + \Omega(V) \\
\text{subject to} & \quad V = CZ^T, \quad Z \in \{0, 1\}^{m \times Q}, \quad Z1 = 1.
\end{align*}
\]

If instead we want to allow predictors \( w_i \) to deviate from their assigned centroid \( v_i \), we can relax the hard clustering constraint using a regularizer \( \Omega_{SC}(U, V) \) described below. This yields the soft supervised clustering problem (SSC)

\[
\begin{align*}
\text{minimize} & \quad L(U) + \Omega_{SC}(U, V) + \Omega(V) \\
\text{subject to} & \quad V = CZ^T, \quad Z \in \{0, 1\}^{m \times Q}, \quad Z1 = 1.
\end{align*}
\]

Given \( Q \) clusters \( C_q \), we let \( s_q = |C_q| \) be the size of the \( q \)th cluster, with \( s = Z^T1 \) the corresponding vector. We write \( \Pi = I - \frac{1}{m}11^T \) the centering matrix. As in [2], the clustering penalty \( \Omega_{SC}(W, V) \) can be decomposed into three separable terms as follows (see Figure 1 for an illustration).

- A measure of how large the barycenter of the centers \( \bar{c} = \frac{1}{m} \sum_{q=1}^Q s_q c_q \) is

\[
\Omega_{\text{mean}}(V) = \lambda_m \frac{m}{2} ||\bar{c}||_2^2 = \frac{\lambda_m}{2} \text{Tr}(V(I - \Pi)V^T).
\]

- A measure of the variance between clusters

\[
\Omega_{\text{between}}(V) = \frac{\lambda_b}{2} \sum_{q=1}^Q s_q ||v_q - \bar{c}||_2^2 = \frac{\lambda_b}{2} \text{Tr}(VIV^T).
\]

- A measure of the variance within clusters

\[
\Omega_{\text{within}}(U, V) = \frac{\lambda_w}{2} \sum_{q=1}^Q \sum_{i \in C_q} ||u_i - c_q||_2^2 = \frac{\lambda_w}{2} ||U - V||_F^2.
\]
Within between mean 0

Figure 1. Decomposed clustering penalty on $m$ items.

We then simply add a penalty with parameter $\mu$ on the Frobenius norm of $V$, i.e. the norm of the centroids weighted by the number of items in each cluster $s_q$

$$\Omega(V) = \frac{\mu}{2} \sum_{q=1}^{Q} s_q \|c_q\|^2 = \frac{\mu}{2} \text{Tr}(V^TV).$$

We now detail the losses associated with each dimension of the data cube: tasks, features or sample points. Input samples are given by the matrix $X = [x_1, \ldots, x_n]^T \in \mathbb{R}^{n \times d}$, labels by $(y_1, \ldots, y_n)$, and $x^{(j)}$ refers to the $j^{th}$ coordinate of $x$.

2.1. Clustering features. Given a regression or classification task, we want to reduce dimensionality by grouping together features which have a similar influence on the output. We present the linear regression case [4], which can be extended to logistic regression and classification. Imposing that all predictor coefficients within a cluster with (scalar) centroid $c_q$ are identical means the prediction function can be written $f : x \rightarrow \sum_{q=1}^{Q} c_q \sum_{j \in C_q} x^{(j)}$, which leads to the following loss

$$L(V) = \frac{1}{n} \sum_{i=1}^{n} l \left( y_i, \sum_{q=1}^{Q} c_q \sum_{j \in C_q} x_i^{(j)} \right) = \frac{1}{n} \sum_{i=1}^{n} l \left( y_i, \sum_{j=1}^{d} \sum_{q=1}^{Q} Z_{jq} c_q x_i^{(j)} \right),$$

in the variable $V = \sum_{q=1}^{Q} Z_{jq} c_q = CZ^T \in \mathbb{R}^d$ of predictor coefficients, quantized over $Q$ values. In this case, if we relax the hard clustering by imposing a soft clustering penalty, we lose the benefit of dimensionality reduction.

2.2. Clustering tasks. Given a set of $K$ supervised tasks like regression or binary classification, multitask learning aims at jointly solving these tasks, hoping that each task can benefit from the information given by other tasks [1, 2, 3]. For simplicity, we illustrate the case of multi-classification, which can be extended to the general multitask setting. When performing classification with one-versus-all majority vote, we train one binary classifier for each class vs all others. We define the total empirical loss as

$$L(U) = \frac{1}{n} \sum_{k=1}^{K} \sum_{i=1}^{n} l(y_i, u_k^T x_i).$$

in the matrix variable $U \in \mathbb{R}^{d \times K}$ of classifier vectors (one per task).

2.3. Clustering sample points. Imagine for instance that we are interested in measuring the effect of two treatments, e.g. a medicine and a placebo, on uniformly distributed patients. Clearly, the regression function varies a lot between the groups of patients that have a different treatment. Now suppose that we do not know to which patients different treatments were given. Since patients are uniformly distributed, the groups cannot be predicted without supplementary information. We will use the effect of treatments to simultaneously retrieve the groups of patients and the associated regression functions. Note that this setting is different
from a mixture of experts model in the sense that the latent cluster assignment variable \( Z \) can only be estimated once \( y \) is known and cannot be deduced from the input features \( X \) (cf. figure 2).

**Figure 2. Learning multiple diverse predictors (left), mixture of experts model (right).**

Given a regression or multi-classification task, we want to find \( Q \) groups of sample points to maximize the within-group prediction performance using a group specific predictor. This amounts to producing \( Q \) diverse answers per sample point, considering only the best one. We thus learn \( Q \) predictors, each predictor having low error rate on some cluster of points. For simplicity, we illustrate the case of regression, which can be extended to multi-classification. We minimize the loss incurred by the best linear predictor \( f_q : \mathbf{x} \rightarrow c_q^T \mathbf{x} \) for each point, i.e.

\[
L(V) = L(CZ^T) = \frac{1}{n} \sum_{i=1}^{n} \min_{q \in \{1, \ldots, Q\}} l(y_i, c_q^T \mathbf{x}_i) = \frac{1}{n} \sum_{i=1}^{n} \left( y_i, \sum_{q=1}^{Q} Z_{iq} c_q^T \mathbf{x}_i \right),
\]

in the matrix variable \( V \in \mathbb{R}^{d \times n} \) of predictor vectors (one per sample point), where \( C \in \mathbb{R}^{d \times Q} \) and \( Z \in \{0,1\}^{n \times Q} \) are the centroid and assignment matrices defined above.

**Table 1.** Summary of the presented supervised clustering settings.

<table>
<thead>
<tr>
<th>Features</th>
<th>Loss</th>
<th>Dim. ( U, V )</th>
<th>Predictors</th>
<th>Goal</th>
</tr>
</thead>
<tbody>
<tr>
<td>Samples</td>
<td>( \frac{1}{n} \sum_{i=1}^{n} l \left( \sum_{q=1}^{Q} Z_{iq} c_q^T \mathbf{x}_i \right) )</td>
<td>( d \times n )</td>
<td>( W^{(i)} )</td>
<td>regression</td>
</tr>
<tr>
<td>Tasks</td>
<td>( \frac{1}{n} \sum_{k=1}^{K} \sum_{i=1}^{n} l(w_k^T \mathbf{x}_i) )</td>
<td>( d \times K )</td>
<td>( )</td>
<td>classification</td>
</tr>
<tr>
<td>Features</td>
<td>( \frac{1}{n} \sum_{i=1}^{n} l \left( \sum_{q=1}^{Q} Z_{iq} c_q \right) )</td>
<td>( 1 \times d )</td>
<td>rows of ( W )</td>
<td>regression</td>
</tr>
</tbody>
</table>

3. **Algorithms**

We now present optimization strategies to solve these supervised clustering problems. We begin by simple greedy procedures, then propose a non-convex projected gradient descent scheme and finally a more refined convex relaxation solved using conditional gradient and approximations to k-means.

3.1. **Simple strategies.** A straightforward strategy is to first minimize on predictors, as in a classical supervised learning problem, and then cluster predictors together using k-means. The procedure can be repeated in the case of a soft clustering penalty. In the same spirit, when clustering sample points, one can alternate minimization on the predictors of each group and assignment of each point to the group where its loss is smallest. These methods are fast but very dependent on the initialization. Alternating minimization can optionally be used to refine the solution of the more robust algorithms proposed below.

3.2. **Projected gradient descent.** A natural strategy is to do a projected gradient descent on the non-convex problems (HSC) or (SSC). The projection of a matrix \( V \) is made by finding

\[
\text{argmin}_{Z,C} \| V - CZ^T \|^2_F = \text{argmin} \sum_{q=1}^{Q} \sum_{i \in C_q} \| v_i - c_q \|^2_2,
\]
where the minimum is taken over centroids $c_i$ and partitions $(C_1, \ldots, C_Q)$. This can be solved with the k-means++ algorithm which performs alternate minimization on the assignments and the centroids. Although it is a non-convex problem, k-means++ gives general approximation bounds on its solution [9].

Writing k-means++$(V, Q)$ the approximate solution of the projection. Writing $\phi$ the objective function and using a backtracking line search for the stepsize $\alpha_t$, the full procedure is summarized in Algorithms 1 and 2. Details of gradient computations for each setting are given in the appendix.

**Algorithm 1** Proj. Gradient Descent (SSC)

**Input:** $X, y, Q, \epsilon, \lambda_b, \lambda_w, \lambda_m, \mu$

Initialize $W_0 = V_0 = 0$

while $|\phi(W_t, V_t) - \phi(W_{t-1}, V_{t-1})|\geq \epsilon$

$W_{t+1} = W_t - \alpha_t(\nabla L(W_t) + \nabla \Omega_{S,C}(V_t, W_t))$

$V_{t+\frac{1}{2}} = V_t - \alpha_t\nabla \Omega_{S,C}(V_t, W_t)$

$[Z_{t+1}, C_{t+1}] = \text{k-means++}(V_{t+\frac{1}{2}}, Q)$

$V_{t+1} = C_{t+1}Z_{t+1}^T$

end while

$Z^*$ and $C^*$ are given through Kmeans++

**Output:** $W^*, V^*, Z^*, C^*$

**Algorithm 2** Proj. Gradient Descent (HSC)

**Input:** $X, y, Q, \epsilon, \mu$

Initialize $V_0 = 0$

while $|\phi(V_t) - \phi(V_{t-1})|\geq \epsilon$

$V_{t+\frac{1}{2}} = V_t - \alpha_t(\nabla L(V) + \nabla \Omega(V))$

$[Z_{t+1}, C_{t+1}] = \text{k-means++}(V_{t+\frac{1}{2}}, Q)$

$V_{t+1} = C_{t+1}Z_{t+1}^T$

end while

$Z^*$ and $C^*$ are given through Kmeans++

**Output:** $V^*, Z^*, C^*$

3.3. Convex relaxation using approximate conditional gradient. Another algorithmic approach to the supervised clustering problem is to minimize with respect to the assignment matrix $Z$ using the Frank-Wolfe algorithm (a.k.a. conditional gradient, [12, 13]). Considering the squared loss $l(f(x), y) = \frac{1}{2}(y - f(x))^2$, we use the analytic form of the minimization in $(W, V)$ or $V$ to rewrite the problem. The clustering is then captured in terms of the equivalence matrix $M = Z(Z^TZ)^{-1}Z^T$, which satisfies $M_{ij} = 1/|C_q|$ if item $i$ and $j$ are in the same cluster $q$ and $M_{ij} = 0$ otherwise.

We describe here the simple case of supervised clustering of features in a regression task, introduced in §2.1. Detailed computations and explicit procedures for all settings are given in the appendix. When clustering features, we optimize over the coefficients associated with each feature and the k-means step can be performed exactly using dynamic programming [10, 11].

The loss $L$ can be written here

$$L(V) = L(CZ^T) = \frac{1}{2n} \sum_{i=1}^{n} \left( y_i - \sum_{j=1}^{d} \sum_{q=1}^{Q} Z_{jq}c_qx_i^{(j)} \right)^2,$$

where $C = [c_1, \ldots, c_Q] \in \mathbb{R}^{1 \times Q}$, hence the regularized loss becomes

$$\phi(C, Z) = \frac{1}{2n} \sum_{i=1}^{n} \left( y_i - CZ^T x_i \right)^2 + \frac{\mu}{2} \|CZ^T\|_2^2$$

$$= \frac{1}{2n} \text{Tr}(y^Ty) + \frac{1}{2n} \text{Tr}(CZ^TX^TXZC^T) - \frac{1}{n} \text{Tr}(CZ^TX^Ty) + \frac{\mu}{2} \text{Tr}(CZ^TZC^T).$$
Minimizing in $C$ and using the Sherman-Woodbury-Morrison formula we get

$$G(M) := \min_C L(CZ^T) + \frac{\mu}{2} \|CZ^T\|^2_2$$

$$= \frac{1}{2n} (yy^T (I - XZ(Z^TXZ + \mu n Z^T Z)^{-1} Z^T X^T y))$$

$$= \frac{1}{2n} \text{Tr} \left( yy^T \left( I + \frac{1}{n\mu} XMX^T \right)^{-1} \right).$$

Defining $\mathcal{M}$ as the set of equivalence matrices of the form

$$M = Z(Z^TZ)^{-1} Z^T,$$

for $Z$ an assignment matrix, each iteration of the conditional gradient method requires solving an affine minimization subproblem over $\text{hull}(\mathcal{M})$. The set $\mathcal{M}$ being discrete, we have

$$\arg\min_{M \in \text{hull}(\mathcal{M})} \text{Tr}(MG(M)) = \arg\min_{M \in \mathcal{M}} \text{Tr}(MG(M)).$$

Writing $P = -\nabla G(M)$, we get

$$P = \frac{1}{2n^2 \mu} X^T \left( I + \frac{1}{n\mu} XMX^T \right)^{-1} yy^T \left( I + \frac{1}{n\mu} XMX^T \right)^{-1} X,$$

which is always semidefinite positive. Writing $P^{\frac{1}{2}}$ the matrix square root of $P$ we have

$$\arg\min_{M \in \mathcal{M}} \text{Tr}(MG(M)) = \arg\min_{M \in \mathcal{M}} -\text{Tr}(MP^{\frac{1}{2}} P^{\frac{1}{2}} T)$$

$$= \arg\min_{M \in \mathcal{M}} \text{Tr} ((I - M)P^{\frac{1}{2}} P^{\frac{1}{2}} T))$$

$$= \arg\min_{M \in \mathcal{M}} \|P^{\frac{1}{2}} - M P^{\frac{1}{2}}\|_F^2$$

$$= \arg\min_{Z} \|P^{\frac{1}{2}} - Z C^T\|_F^2,$$

where we recognize the k-means problem defined above. In fact, in this particular case, the k-means subproblem is one-dimensional and can be solved exactly using dynamic programming \cite{10, 11}. We use the classical stepsize for conditional gradient $\alpha_k = \frac{2}{k+2}$ and Frank-Wolfe rounding. The procedure is summarized in Algorithm 3.

**Algorithm 3** Conditional gradient on the equivalence matrix

**Input:** $X, y, Q, \epsilon$

Initialize $M_0 \in \mathcal{M}$

while $|G(M_k) - G(M_{k-1})| \geq \epsilon$ do

Compute the matrix square root $P^{\frac{1}{2}}$ of $-\nabla G(M_k)$

Get oracle $\Delta_k = \text{k-means}(P^{\frac{1}{2}}, Q)$

$M_{k+1} = M_k + \alpha_k (\Delta_k - M_k)$

end while

Use Frank Wolfe rounding to get a solution $M^* \in \mathcal{M}$

$Z^*$ is given by k-means

$C^*$ is given by the analytic solution of the minimization for $Z^*$ fixed

**Output:** $C^*, Z^*, M^*$

3.4. **Complexity.** The core complexity of Algorithms 1 and 2 is concentrated in the inner k-means subproblem, which standard alternating minimization approximates in $O(tQS)$, where $t$ is the number of alternating steps, $Q$ is the number of clusters, and $S$ is the product of the dimensions of $V$ (see Table 1). Using a proper conditioning of the gradient, the number of iterations before convergence is typically below 100, which
make Algorithms 1 and 2 both fast and scalable. For Algorithm 3, we also need to compute a matrix square root of the gradient at each iteration, which can slow down computations for large datasets. The choice of the number of clusters can be done given an a priori on the problem (e.g. if we know the hierarchical structure of classes in a classification problem), or cross-validation, idem for the other regularization parameters.

4. NUMERICAL EXPERIMENTS

4.1. Synthetic dataset.
Supervised clustering of sample points. We generate \( n \) data points \((x_i, y_i)\) for \( i = 1, \ldots, n \) with \( x_i \in \mathbb{R}^d \) and \( y_i \in \mathbb{R} \), divided in two clusters corresponding to regression tasks with weights \( w_1 \) and \( w_2 \). Regression labels for points \( x_i \) in cluster \( q \) are given by \( y_i = w_q^T x_i + \eta \), where \( \eta \sim \mathcal{N}(0, \sigma^2) \). We test the robustness of the algorithms to noise dimensions, i.e. we complete \( x_i \) with \( d_n \) dimensions of noise \( \eta_d \sim \mathcal{N}(0, \sigma_d) \). The results are reported in Table 2.

Here, the intrinsic dimension is 10. “Oracle” refers to the least square fit given the true assignments. It can be seen as the best error rate that can be achieved. PGK refers to projected gradient, OM refers to conditional gradient on \( M \), AM refers to alternate minimization. PGK and OM were followed by AM refinement. 200 points were used for training, 200 for testing. The regularization parameter was set to \( \lambda = 10^{-2} \) for all experiments. Noise on labels and added dimensions \( \sigma_y = \sigma_d = 2 \times 10^{-1} \). Results were averaged over 100 experiments, figures after the sign ± correspond to one standard deviation.

<table>
<thead>
<tr>
<th></th>
<th>dim-noise=0</th>
<th>dim-noise=100</th>
<th>dim-noise=300</th>
<th>dim-noise=900</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Oracle</strong></td>
<td>4.2±0.5</td>
<td>29.5±7.0</td>
<td>17.3±6.2</td>
<td>81.6±30.0</td>
</tr>
<tr>
<td><strong>PGK</strong></td>
<td>5.8±15.1</td>
<td>251.0±154.4</td>
<td>187.5±98.7</td>
<td>275.2±167.2</td>
</tr>
<tr>
<td><strong>OM</strong></td>
<td>4.3±0.5</td>
<td>254.4±144.6</td>
<td>209.2±93.5</td>
<td>220.9±93.0</td>
</tr>
<tr>
<td><strong>AM</strong></td>
<td>50.4±121.1</td>
<td>897.0±456.1</td>
<td>445.3±207.1</td>
<td>455.4±192.3</td>
</tr>
</tbody>
</table>

Table 2. Supervised clustering of sample points.

It appears that that PGK and OM give very similar results, significantly improving on the naive alternating minimization scheme. In view of standard deviations, OM seems more robust.

Supervised clustering of features. We generate \( n \) data points \((x_i, y_i)\) for \( i = 1, \ldots, n \) with \( x_i \in \mathbb{R}^d \) and \( y_i \in \mathbb{R} \). Regression weights have only 10 different values \( w_q \) for \( q = 1, \ldots, 10 \), uniformly distributed around 0. Regression labels are given by \( y_i = w^T x_i + \eta \), where \( \eta \sim \mathcal{N}(0, \sigma^2) \). We test the robustness of the algorithms to the number of learning examples, i.e. the size of the training set \( n \). We measure the \( l_2 \) norm of the difference between the true vector of weights and the estimated ones.

We compare in Table 3 the proposed algorithms to OSCAR [4], Ridge, Lasso and Ridge followed by k-means on the weights (using associated centroids as predictors). “Oracle” refers to the mean square fit given the true assignments of features. It can be seen as the best error rate that can be achieved. PGK refers to projected gradient and was initialized with the solution of Ridge followed by k-means, OM refers to conditional gradient on \( M \) and was followed by PGK. Noise on labels is set to \( \sigma = 10^{-1} \). Algorithm parameters were all cross-validated using a logarithmic grid. Results were averaged over 30 experiments and figures after the sign ± correspond to one standard deviations. Results were multiplied by 100 to shorten the table.

PGK and OM appear to give significantly better results than other methods and even reach the performance of the Oracle for \( n > d \), while for \( n \leq d \) results are in the same range. Note that contrary to OSCAR, Lasso and Ridge, reduction of dimensionality is guaranteed (the number of clusters is fixed).

4.2. Real data.
### Table 3. Supervised clustering of features.

<table>
<thead>
<tr>
<th>Method</th>
<th>n=50</th>
<th>n=75</th>
<th>n=100</th>
<th>n=150</th>
<th>n=200</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oracle</td>
<td>3.3±1.2</td>
<td>2.6±0.9</td>
<td>2.2±0.5</td>
<td>1.8±0.4</td>
<td>1.5±0.4</td>
</tr>
<tr>
<td>PGK</td>
<td>72.9±2.7</td>
<td>58.0±2.7</td>
<td>41.6±12.1</td>
<td>1.9±1.0</td>
<td>1.5±0.4</td>
</tr>
<tr>
<td>OM+PGK</td>
<td>73.1±2.5</td>
<td>55.9±3.5</td>
<td>43.5±7.9</td>
<td>4.6±7.4</td>
<td>1.5±0.4</td>
</tr>
<tr>
<td>Ridge+Kmeans</td>
<td>72.1±1.6</td>
<td>58.6±2.7</td>
<td>46.9±20.6</td>
<td>7.7±4.1</td>
<td>2.4±1.0</td>
</tr>
<tr>
<td>OSCAR</td>
<td>80.3±7.5</td>
<td>65.9±1.4</td>
<td>32.8±4.2</td>
<td>14.0±1.9</td>
<td>9.9±0.9</td>
</tr>
<tr>
<td>Lasso</td>
<td>91.2±0.6</td>
<td>81.9±4.2</td>
<td>56.1±30.5</td>
<td>13.9±1.7</td>
<td>10.0±1.0</td>
</tr>
<tr>
<td>Ridge</td>
<td>69.9±0.5</td>
<td>58.0±0.8</td>
<td>33.0±5.8</td>
<td>14.0±1.6</td>
<td>10.1±0.9</td>
</tr>
</tbody>
</table>

4.2.1. **20NewsGroup classification.** We perform classification on 2800 documents extracted from the publicly available 20NewsGroup dataset, which contains 20 different newsgroups, each one corresponding to a different topic. Some of the newsgroups are very closely related to each other (e.g. comp.sys.ibm.pc.hardware and comp.sys.mac.hardware), while others are highly unrelated (e.g. misc.forsale and soc.religion.christian). Our goal is to retrieve clusters of related newsgroups, while performing competitive classification. We used a dictionary of 5000 words chosen by tf-idf and took the empirical distribution over words as covariates for each document.

In Table 4, we compare our approach to other classical regularizations such as the Frobenius norm and the trace norm, as implemented in [3], using either a ridge or a logistic loss. As the projected gradient descent scheme is not convex we initialize it by the solution given by the logistic loss non regularized. All algorithms were 5-fold cross-validated on 80% of the data then tested on the remaining 20%. The number of clusters was set to 5, as suggested by the names of newsgroups. Figures after the sign ± correspond to one standard deviation when varying the training and test sets. As reported in Table 4, it appears that the clustering regularization helps prediction on topics.

<table>
<thead>
<tr>
<th>Method</th>
<th>Frobenius Logistic</th>
<th>Trace Ridge</th>
<th>OM Ridge</th>
<th>PGK Logistic</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5.8±2.0</td>
<td>4.3±0.8</td>
<td>4.9±0.8</td>
<td>2.6±1.5</td>
</tr>
</tbody>
</table>

Table 4. 100 × mean absolute errors for predicting topics on 20NewsGroup dataset.

4.2.2. **Predicting ratings associated with reviews using groups of words.** We perform “sentiment” analysis of newspaper movie reviews. We use the publicly available dataset introduced in [14] which contains movie reviews paired with star ratings. We treat it as a regression problem, taking log-responses for y in (0, 1) and the empirical distribution over words as covariates. With a 5000 term vocabulary chosen by tf-idf, the corpus contains 5006 documents and comprises 1.6M words. We evaluate our algorithms for regression with clustered features against standard regression approaches: Lasso, Ridge, and Ridge followed by k-means on predictors. All algorithms were 5-fold cross-validated on 80% of the dataset and then tested on the remaining 20%. The number of clusters was arbitrarily set to 10, though we did not notice significant changes when varying it. Results are reported in Table 5, figures after the sign ± correspond to one standard deviation when varying the training and test sets. While all methods including ours give 10% mean absolute errors on the test set (up to 0.5% accuracy), our approach has the additional benefit of providing clusters of words which have a similar influence. Moreover we noticed that the clusters with highest absolute weights are also the ones with smallest number of words, which confirms the intuition that only a few words are very discriminative. We illustrate this in Table 6, listing words of the first and last clusters.

5. **Discussion**

We have developed a unified framework for supervised clustering over tasks, features or samples and provided two robust algorithms for solving the associated optimization problems. Results on synthetic and
| Cluster 1 (negative) size 47 | stupidity, shred, inept, sophomoric, sit, drivel, uninteresting, clue, ludicrous, tedious, single, remotely, crass, tolerable, bland, predictable, devoid, waste, fail, embarrassing, mess, idea, inane, lifeless, abysmal, badly, disgusting, bearable, poorly, care, leaden, annoying, turkey, attempt, interesting, problem, lame, lack, worse, unfunny, watchable, worst, ridiculous, flat, dull, boring, awful, suppose, bad |
| Cluster 10 (positive) size 87 | perfect, fascinating, great, powerful, hilarious, fine, brilliant, delightful, strongly, easy, rare, wonderfully, recommendation, mature, nomination, simple, perfectly, good-spirited, masterpiece, strong, potent, marvelous, excellent, fortunately, world, intelligent, memorable, unique, send, small, funniest, unexpected, carefully, academy, superbly, important, life, poignancy, speak, wonderful, outstanding, mesmerizing, man, imaginative, simplicity, confidence, delightfully, delight, touching, nuanced, study, melville, brilliance, work, picture, honest, oscar, classification, masterfully, favorite, effective, masterful, intense, bind, unrated, surprisingly, superb, triumph, flawless, move, lyrical, gem, devastate, intricate, highly, subtle, power, accomplishment, keen, uplifting, empathize, element, quibble, minor, love, finest, criss |

Table 5. 100 × mean absolute errors for predicting movie ratings associated with reviews.

Table 6. Supervised clustering of words on movie reviews.

realistic text datasets suggest that our method is competitive against standard regression and classification methods, while having the additional benefit of providing clusters of tasks, features or samples. Similarly as in compressed sensing, optimization is made on a union of subspaces, hence in analogy with RIP conditions for iterative hard thresholding [15], it would be interesting to see under which assumptions our algorithms can recover the optimal solution to the supervised clustering problem.

6. APPENDIX

We give here detailed computations of the function $G$ corresponding to the convex relaxation defined in 3.3 in all settings.

We always suppose $Z^T Z$ invertible i.e. $\forall q, s_q \neq 0$ (there is no empty cluster). For any integer $p$, we let $1_p \in \mathbb{R}^p$ be the vector whose coordinates are all ones, $I_p$ the identity matrix in $\mathbb{R}^{p \times p}$, $\Gamma_p = \frac{1_p 1_p^T}{p}$ and $\Pi_p = I_p - \Gamma_p$ the corresponding centering matrix.

For all settings input samples are represented by the matrix $X = (x_1, ..., x_n)^T \in \mathbb{R}^{n \times d}$ and their respective labels by $y = (y_1, ..., y_n) \in \mathcal{Y}$. For regression problems $\mathcal{Y} = \mathbb{R}$. Classification problems are casted into the multitask setting, each class corresponding to a task. We denote by $y^k = (y^k_1, ..., y^k_n)$ the vector of binary labels corresponding to the class $k \in [1, K]$ and $Y = (y^1, ..., y^K)$.

6.1. Minimization in $C$ for Soft Clustering Problems. For soft supervised clustering problems, the minimization in the variable $C$ for $W, Z$ fixed can be made without assumptions on the specific loss $L$. We let $(\delta, m)$ be the dimensions of the predictors of interest, such that $W \in \mathbb{R}^{d \times m}, C \in \mathbb{R}^{\delta \times Q}$ and $Z \in \{0, 1\}^{m \times Q}$. We denote by $\lambda_W, \lambda_B, \lambda_M$ the weights associated respectively to the within, between and mean penalties. Minimization in $C$ is then given by

$$H(W, Z) := \min_{C \in \mathbb{R}^{\delta \times Q}} \frac{\lambda_W}{2} \|W - CZ^T\|_F^2 + \frac{\lambda_B}{2} \text{Tr}(CZ^T \Pi_m Z C^T) + \frac{\lambda_M}{2} \text{Tr}(CZ^T \Gamma_m Z C^T)$$

$$= \min_{C \in \mathbb{R}^{\delta \times Q}} \frac{\lambda_W}{2} \|W\|_F^2 + \frac{1}{2} \text{Tr} \left( C \left( (\lambda_W + \lambda_B)Z^T Z + (\lambda_M - \lambda_B)Z^T \Gamma_m Z \right) C^T \right) - \lambda_W \text{Tr}(C^T W Z)$$

$$= \frac{\lambda_W}{2} \text{Tr}(WW^T) - \frac{\lambda_W^2}{2} \text{Tr} \left( WZ \left( (\lambda_W + \lambda_B)ZZ^T + (\lambda_M - \lambda_B)Z^T \Gamma_m Z \right)^{-1} Z^T W \right).$$
Let \( s = Z^T 1_m \in \mathbb{R}^Q \) be the vector whose coordinates \( s_q \) are the sizes of the clusters, denoting by \( s_1^2 \) the vector whose coordinates are \( \sqrt{s_q} \), and by \( s_1^2 \) the vector whose coordinates are \( \frac{1}{\sqrt{s_q}} \), we can derive the inversion in the precedent formula,

\[
J^{-1} = ((\lambda_W + \lambda_B)ZZ^T + (\lambda_M - \lambda_B)Z^T \Gamma_m Z)^{-1} \\
= \left( (\lambda_W + \lambda_B) \text{diag}(s) + (\lambda_M - \lambda_B) \frac{ss^T}{m} \right)^{-1} \\
= \frac{1}{\lambda_W + \lambda_B} \text{diag}(s^{-\frac{1}{2}}) \left( I_Q + \frac{\lambda_M - \lambda_B}{\lambda_W + \lambda_B} \frac{s_1^2 s_1^2^T}{m} \right)^{-1} \text{diag}(s^{-\frac{1}{2}}) \\
= \frac{1}{\lambda_W + \lambda_B} \text{diag}(s^{-\frac{1}{2}}) \left( I_Q - \frac{\lambda_M - \lambda_B}{\lambda_W + \lambda_M} \frac{s_1^2 s_1^2^T}{m} \right) \text{diag}(s^{-\frac{1}{2}}) \\
= \frac{1}{\lambda_W + \lambda_B} \left( (Z^T Z)^{-1} - \frac{1}{\lambda_W + \lambda_M} \frac{1_Q 1_Q^T}{m} \right) + \frac{1}{\lambda_W + \lambda_M} \frac{1_Q 1_Q^T}{m},
\]

where we used that \( p = \frac{s_1^2 s_1^2^T}{m} = \frac{s_1^2 s_1^2^T}{\|s^2\|_2^2} \) is a projector and therefore \((I + \alpha p)^{-1} = I - \frac{\alpha}{\alpha + 1} p\), added to the fact that \( \text{diag}(s) = Z^T Z \).

Now introducing the equivalence matrix \( M = Z(Z^T Z)^{-1} Z^T \), and using that \( Z \frac{1_Q 1_Q^T}{m} Z^T = \Gamma_m \), we finally obtain

\[
H(W, Z) = \frac{\lambda_W}{2} \text{Tr}(WW^T) - \frac{\lambda_M^2}{2} \text{Tr} \left( W \left( \frac{1}{\lambda_W + \lambda_B} (M - \Gamma_m) + \frac{1}{\lambda_W + \lambda_M} \Gamma_m \right) W^T \right) \\
= \frac{\lambda_W}{2} \text{Tr} \left( W (I_m - \alpha (M - \Gamma_m) - \beta \Gamma_m) W^T \right),
\]

where \( \alpha = \frac{\lambda_W}{\lambda_W + \lambda_M} \) and \( \beta = \frac{\lambda_W}{\lambda_W + \lambda_M} \).

Denoting \( P = I_m - \alpha (M - \Gamma_m) - \beta \Gamma_m \), one can also use Kronecker’s formula:

\[
H(W, Z) = \frac{\lambda_W}{2} \text{Vec}(W)^T (P \otimes I_d) \text{Vec}(W).
\]

### 6.2. Clustered Multitask Learning

We derive here the computation of \( G \) when clustering tasks. We restrict ourselves to the case of multiclass setting cast as a multitask problem such that each task shares the same input data. Given \( K \) classes, we denote by \( W = (w_1, ..., w_K) \in \mathbb{R}^{d \times K} \) the matrix of linear predictors. Using a squared loss \( l(f(x), y) = \frac{1}{2} (y - f(x))^2 \) the empirical loss is given by:

\[
L(W) = \frac{1}{2n} \sum_{i=1}^{n} \sum_{k=1}^{K} (y_i^k - w_k^T x_i)^2.
\]

Using Kronecker’s product formula, we get
\[ L(W) = \frac{1}{2n} \sum_{k=1}^{K} w_k^T X^T X w_k - \frac{1}{n} \sum_{k=1}^{K} w_k^T X^T y^k + \frac{1}{2n} \| y \|_2^2 \]

\[ = \frac{1}{2n} \sum_{k=1}^{K} e_k^T W^T X W e_k - \frac{1}{n} \text{Tr}(W X Y) + \frac{1}{2n} \| y \|_2^2 \]

\[ = \frac{1}{2n} \text{Vec}(W)^T (I_K \otimes X^T X) \text{Vec}(W) - \frac{1}{n} \text{Vec}(W)^T \text{Vec}(X^T Y) + \frac{1}{2n} \| y \|_2^2. \]

Using the expression found by minimizing in \( C \) the regularization penalty, we get an expression for \( G \):

\[ G(M) = \min_W L(W) + H(W, Z) \]

\[ = \min_W \frac{1}{2n} \text{Vec}(W)^T (I_K \otimes X^T X + P \otimes I_d) \text{Vec}(W) - \frac{1}{n} \text{Vec}(W)^T \text{Vec}(X^T Y) + \frac{1}{2n} \| y \|_2^2 \]

\[ = -\frac{1}{2n} \text{Vec}(X^T Y)^T (I_K \otimes X^T X + \lambda_W n P \otimes I_d)^{-1} \text{Vec}(X^T Y) + \frac{1}{2n} \| y \|_2^2 \]

Denote \((v_1, ..., v_d) \in \mathbb{R}^{d \times d}, (\lambda_1, ..., \lambda_d) \in \mathbb{R}^d\) and \((u_1, ..., u_s) \in \mathbb{R}^{S \times S}, (\mu_1, ..., \mu_S) \in \mathbb{R}^S\) the eigenvectors and corresponding eigenvalues respectively of matrices \( X^T X \) and \( P = (I_K - \alpha (M - \Gamma_K)) + \beta \Gamma_K \). The eigenvectors and corresponding eigenvalues of \( I_K \otimes X^T X + \lambda_W n P \otimes I_d \) are \((u_i \otimes v_j)_{i \in [1, n]} \) and \((\lambda_W n \mu_i + \lambda_j)_{j \in [1, d]} \). The inversion in the expression of \( G \) is then given by

\[ J^{-1} = (I_K \otimes X^T X + \lambda_W n P \otimes I_d)^{-1} = \sum_{i=1}^{n} \sum_{j=1}^{d} \frac{1}{\lambda_W n \mu_i + \lambda_j} u_i u_i^T \otimes v_j v_j^T. \]

Then we note that the set of eigenvectors of \( P \) can be decomposed into three sets. Indeed the matrices \( I_K - M, M - \Gamma_K \) and \( \Gamma_K \) are orthogonal projectors on orthogonal subspaces spanning the entire space. Denote by \( \mathcal{I}_W, \mathcal{I}_B, \mathcal{I}_M \) the sets of eigenvectors corresponding respectively to \( I_K - M, M - \Gamma_K \) and \( \Gamma_K \), their corresponding eigenvalues in \( P \) can easily be computed and we obtain

\[ P = I_K - M + (1 - \alpha)(M - \Gamma_K) + (1 - \beta) \Gamma_K \]

\[ = \sum_{i \in \mathcal{I}_W} u_i u_i^T + (1 - \alpha) \sum_{i \in \mathcal{I}_W} u_i u_i^T + (1 - \beta) \sum_{i \in \mathcal{I}_M} u_i u_i^T. \]

This decomposition can be used for the inversion:
\[
J^{-1} = \sum_{i \in I_W} \sum_{j=1}^{d} \frac{1}{\lambda_W n + \lambda_j} u_i u_i^T \otimes v_j v_j^T 
+ \sum_{i \in I_B} \sum_{j=1}^{d} \frac{1}{\lambda_W n(1-\alpha) + \lambda_j} u_i u_i^T \otimes v_j v_j^T 
+ \sum_{i \in I_W} \sum_{j=1}^{d} \frac{1}{\lambda_W n(1-\beta) + \lambda_j} u_i u_i^T \otimes v_j v_j^T 
= (I_K - M) \otimes (X^T X + n\lambda_W I_d)^{-1} + (M - \Gamma_K) \otimes (X^T X + n\lambda_W (1-\alpha) I_d)^{-1} 
+ \Gamma_K \otimes (X^T X + n\lambda_W (1-\beta) I_d)^{-1}.
\]

Finally, \( G \) can be simplified using properties of the Kronecker product:

\[
G(M) = -\frac{1}{2n} \text{Vec}(X^T Y)^T ((I_K - M) \otimes (X^T X + n\lambda_W I_d)^{-1}) \text{Vec}(X^T Y) 
- \frac{1}{2n} \text{Vec}(X^T Y)^T ((M - \Gamma_K) \otimes (X^T X + n\lambda_W (1-\alpha) I_d)^{-1}) \text{Vec}(X^T Y) 
- \frac{1}{2n} \text{Vec}(X^T Y)^T (\Gamma_K \otimes (X^T X + n\lambda_W (1-\beta) I_d)^{-1}) \text{Vec}(X^T Y) + \frac{1}{2n} \|Y\|_F^2 
= -\frac{1}{2n} \text{Tr}(Y^T X (X^T X + n\lambda_W I_d)^{-1} X^T Y (I_K - M)) 
- \frac{1}{2n} \text{Tr}(Y^T X (X^T X + n\lambda_W (1-\alpha) I_d)^{-1} X^T Y (M - \Gamma_K)) 
- \frac{1}{2n} \text{Tr}(Y^T X (X^T X + n\lambda_W (1-\beta) I_d)^{-1} X^T Y \Gamma_K) + \frac{1}{2n} \|Y\|_F^2.
\]

Therefore \( G \) is a linear function of \( M \) whose gradient is given by

\[
\nabla G(M) = \frac{1}{2n} Y^T X \left( (X^T X + n\lambda_W I_d)^{-1} - (X^T X + n\lambda_W (1-\alpha) I_d)^{-1} \right) X^T Y.
\]

As \( 1 \geq \alpha \geq 0 \), we get that \(-\nabla G(M) \succeq 0\).

For a fixed \( M, W \) is given using precedent computations and Kronecker’s formula by

\[
W_M = (X^T X + n\lambda_W I_d)^{-1} X^T Y (I_K - M) 
+ (X^T X + n\lambda_W (1-\alpha) I_d)^{-1} X^T Y (M - \Gamma_K) 
+ (X^T X + n\lambda_W (1-\beta) I_d)^{-1} X^T Y \Gamma_K.
\]

6.3. **Learning with clustered features.** For more generality we cast the problem of learning clustered features in the multiclass learning setting. We restrict here to the soft supervised clustering problem as the hard one has already be done. We keep notations introduced in section 6.2 though we now have \( W = \)

\((\mathbf{w}_1, \ldots, \mathbf{w}_K)^T \in \mathbb{R}^{K \times d}\). The empirical loss is given by

\[
L(W) = \frac{1}{2n} \sum_{i=1}^{n} \sum_{k=1}^{K} (y_i^k - \mathbf{w}_k^T \mathbf{x}_i)^2.
\]

\[
= \frac{1}{2n} \sum_{k=1}^{K} \mathbf{w}_k^T X^T X \mathbf{w}_k - \frac{1}{n} \sum_{k=1}^{K} \mathbf{w}_k^T X^T Y^k + \frac{1}{2n} \|Y\|_F^2
\]

\[
= \frac{1}{2n} \sum_{k=1}^{K} \text{Tr}(W^T W X^T X) - \frac{1}{n} \text{Tr}(W X^T Y) + \frac{1}{2n} \|Y\|_F^2.
\]

Adding the regularization penalty and minimizing in \(C\) we obtain

\[
G(M) = \min_{W} \frac{1}{2n} \sum_{k=1}^{K} \text{Tr} \left( W^T W (X^T X + \lambda_n P) \right) - \frac{1}{n} \text{Tr}(W X^T Y) + \frac{1}{2n} \|Y\|_F^2
\]

\[
= \frac{1}{2n} \|Y\|_F^2 - \frac{1}{2n} \left( Y^T X (X^T X + \lambda_n P)^{-1} X^T Y \right)
\]

\[
= \frac{1}{2n} \text{Tr} \left( Y Y^T (I_n - X (X^T X + \lambda_n P)^{-1} X^T) \right)
\]

\[
= \frac{1}{2n} \text{Tr} \left( Y Y^T (I_n + \frac{1}{\lambda M} X P^{-1} X^T)^{-1} \right)
\]

As detailed before, the inverse of \(P\) can be found analytically by observing that it is composed of orthogonal projectors on orthogonal subspaces spanning the entire space. Hence we have \(P^{-1} = I_d - M + \frac{1}{1 - \alpha} (M - \Gamma_d) + \frac{1}{1 - \beta} \Gamma_d\). We now get

\[
G(M) = \frac{1}{2n} \text{Tr} \left( Y Y^T (I_d + \frac{1}{n \lambda_B} X (M - \Gamma_d) X^T + \frac{1}{n \lambda M} X \Gamma_d X^T) \right)
\]

Note that we still have \(-\nabla G(M) \succeq 0\). For a fixed \(M\), \(W\) is given analitically by

\[
W_M = Y^T X (X^T X + \lambda_n (I_d - \alpha (M - \Gamma_d) - \beta \Gamma_d))^{-1}.
\]

### 6.4. Learning multiple predictors.

In the setting of learning multiple predictors, we denote by \(C_q\) the set of points whose best linear predictor is \(w_q\), having therefore \(C_1, \ldots, C_Q\) a partition of \([1, n]\). Let us as above \(s_q\) be the cardinal of the set \(C_q\), \(X_q \in \mathbb{R}^{s_q \times d}\) is the matrix whose columns are the points belonging to the cluster \(q\), and \(y_q\) is the column vector of labels corresponding to cluster \(q\). We use a squared loss \(l(f(x), y) = \frac{1}{2} (y - f(x))^2\).

For \(C_1, \ldots, \tilde{C}_Q\) fixed (or equivalently \(Z\) fixed), we can compute \(G\) using the Sherman-Woodbury-Morrison formula as

\[
G(M) = \min_{w_1, \ldots, w_Q} \frac{1}{2n} \sum_{q=1}^{Q} \sum_{i \in C_q} (y_i - w_q^T x_i)^2 + \frac{\mu}{2} \sum_{q=1}^{Q} s_q \|w_q\|_2^2
\]

\[
= \sum_{q=1}^{Q} \frac{1}{2n} y_q^T \left( \frac{1}{s_q \lambda_n} X_q X_q^T + I_n \right)^{-1} y_q.
\]
We define $E \in \mathbb{R}^{n \times n}$ the permutation matrix permuting order of points such that

$$
Ey = \begin{pmatrix}
y_{c_1} \\
\vdots \\
y_{c_Q}
\end{pmatrix}
$$

$$
EX = \begin{pmatrix}
X_1 \\
\vdots \\
X_Q
\end{pmatrix}.
$$

We denote for $q \in [1, Q]$, $R_q = \sum_{p=1}^{q} \sum_{p=1}^{n} e_i e_j^T$ orthogonal projectors on the ordered sets of points belonging to cluster $q$ such that

$$
\begin{pmatrix}
X_1X_1^T & 0 & 0 \\
0 & \ddots & 0 \\
0 & 0 & X_QX_Q^T
\end{pmatrix} = \text{diag}(EXX^TE^T) = \sum_{q=1}^{Q} R_q EXX^TE^T R_q.
$$

Thus we get

$$
G(M) = \frac{1}{2n} y^T E^T \left( \sum_{q=1}^{Q} \frac{1}{s_q \mu n} R_q EXX^TE^T R_q + I_n \right)^{-1} Ey
$$

$$
= \frac{1}{2n} y^T \left( \sum_{q=1}^{Q} \frac{1}{s_q \mu n} E^TR_qEXX^TE^TR_qE + I_n \right)^{-1} y.
$$

Then we notice that $E^TR_qE = \text{diag}(Z_q)$ i.e. the projector on the set of points belonging to cluster $q$, and that $\sum_{q=1}^{Q} \frac{1}{s_q} \text{diag}(Z_Q)XX^T \text{diag}(Z_q) = M \circ XX^T$, where $\circ$ denotes the Hadamard product. Hence we finally get

$$
G(M) = \frac{1}{2n} y^T \left( \frac{1}{\mu n} XX^T \circ M + I_n \right)^{-1} y.
$$

Its gradient is given by

$$
2n \nabla G(M) = \frac{1}{\mu n} XX^T \circ \left( I_n + \frac{1}{\mu n} XX^T \circ M \right)^{-1} y y^T \left( I_n + \frac{1}{\mu n} XX^T \circ M \right)^{-1},
$$

for which we have $-\nabla G(M) \succeq 0$.

For a fixed $Z$, denoting by $X_q = Z_q^T X$ the set of points belonging to cluster $q$, the linear predictors $w_q$ for each cluster of points are given by

$$
w_q = \left( n \mu s_q I_d + X_q^T X_q \right)^{-1} X_q^T y_q.
$$

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REFERENCES


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