Multi-output Polynomial Networks
and Factorization Machines

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Abstract

Factorization machines and polynomial networks are supervised polynomial models based on an efficient low-rank decomposition. We extend these models to the multi-output setting, i.e., for learning vector-valued functions, with application to multi-class or multi-task problems. We cast this as the problem of learning a 3-way tensor whose slices share a common decomposition and propose a convex formulation of that problem. We then develop an efficient conditional gradient algorithm and prove its global convergence, despite the fact that it involves a non-convex hidden unit selection step. On classification tasks, we show that our algorithm achieves excellent accuracy with much sparser models than existing methods. On recommendation system tasks, we show how to combine our algorithm with a reduction from ordinal regression to multi-output classification and show that the resulting algorithm outperforms existing baselines in terms of ranking accuracy.

1 Introduction

Interactions between features play an important role in many classification and regression tasks. Classically, such interactions have been taken advantage of either explicitly, by mapping features to their products (as in polynomial regression), or implicitly, through the use of the kernel trick. While fast linear model solvers have been engineered for the explicit approach [9, 28], they are typically limited to small numbers of features or low-order feature interactions, due to the fact that the number of parameters that they need to learn scales as \(O(d^t)\), where \(d\) is the number of features and \(t\) is the order of interactions considered. Models kernelized with the polynomial kernel do not suffer from this problem; however, the cost of storing and evaluating these models grows linearly with the number of training instances, a problem sometimes referred to as the curse of kernelization [30].

Factorization machines (FMs) [25] are a more recent model that can use pairwise feature interactions efficiently even in very high-dimensional data. The key idea of FMs is to model the weights of feature interactions using a low-rank matrix. While this idea offers clear benefits in terms of model compression in comparison to classical approaches, the main application for which this idea has proved instrumental is the modeling of interactions between categorical variables, converted to binary features via a one-hot encoding. Such binary features are usually so sparse that many interactions are never observed in the training set, preventing classical approaches from capturing their relative importance. By imposing a low rank on the feature interaction weight matrix, FMs encourage shared parameters between interactions, allowing to estimate their weights even if they never occurred in the training set. This property has been used in recommender systems to model interactions between user variables and item variables, and is the basis of several industrial successes of FMs [32, 17].

Originally motivated as neural networks with a polynomial activation (instead of the classical sigmoidal or rectifier activations), polynomial networks (PNs) [20] have been shown to be intimately related to FMs and to only subtly differ in the non-linearity they use [5]. PNs have been shown to
achieve better performance than rectifier networks on pedestrian detection [20] and on dependency parsing [10], and to outperform kernel approximations such as the Nyström method [5]. However, existing PN and FM works have been limited to single-output models, i.e., they are designed to learn scalar-valued functions, which restricts them to regression or binary classification problems.

**Our contributions.** In this paper, we generalize FM and PNs to multi-output models, i.e., for learning vector-valued functions, with application to multi-class or multi-task problems.

1) We cast learning multi-output FMs and PNs as learning a 3-way tensor, whose slices correspond to $\sigma$ where $w$ we propose to cast it as learning an infinite-dimensional but row-wise sparse matrix. We show that (a.k.a. Frank-Wolfe) algorithm [11, 15], which repeats the following two steps: i) select a new hidden vector, $H$ using a tensor network (a.k.a. tensor train) instead of the canonical polyadic (CP) decomposition.

2) To solve the obtained optimization problem, we develop a variant of the conditional gradient (a.k.a. Frank-Wolfe) algorithm [11, 15], which repeats the following two steps: i) select a new hidden unit to add to the model and ii) refit the model over the current hidden units. (§4) We prove the global convergence of this algorithm (Theorem 1), despite the fact that the hidden unit selection step is more challenging in the shared decomposition setting and in fact non-convex. (§5)

3) On multi-class classification tasks, we show that our algorithm achieves comparable accuracy to kernel SVMs but with much more compressed models than the Nyström method. On recommender system tasks, where kernelized models cannot be used (since they do not generalize to unseen user-item pairs), we demonstrate how our algorithm can be combined with a reduction from ordinal regression to multi-output classification and show that the resulting algorithm outperforms existing single-output PNs and FMs both in terms of root mean squared error (RMSE) and ranking accuracy, as measured by nDCG (normalized discounted cumulative gain) scores. (§6)

### 2 Background and related work

**Notation.** We denote the set $\{1, \ldots, m\}$ by $[m]$. Given a vector $v \in \mathbb{R}^k$, we denote its elements by $v_r \in \mathbb{R}$ $\forall r \in [k]$. Given a matrix $V \in \mathbb{R}^{k \times m}$, we denote its rows by $v_r \in \mathbb{R}^m$ $\forall r \in [k]$ and its columns by $v_{r, c} \in \mathbb{R}$ $\forall c \in [m]$. We denote the $l_p$ norm of $V$ by $\|V\|_p := \|\text{vec}(V)\|_p$ and its $l_p/l_q$ norm by $\|V\|_{p,q} := \left(\sum_{i=1}^k \|v_r\|_q^p\right)^{1/p}$. The number of non-zero rows of $V$ is denoted by $\|V\|_{0,\infty}$. 

**Factorization machines (FMs).** Given an input vector $x \in \mathbb{R}^d$, FMs predict a scalar output by

$$\hat{y}_{\text{FM}} := w^T x + \sum_{i<j} w_{i,j} x_i x_j,$$

where $w \in \mathbb{R}^d$ contains feature weights and $W \in \mathbb{R}^{d \times d}$ is a low-rank matrix that contains pairwise feature interaction weights. To obtain a low-rank $W$, [25] originally proposed to use a change of variable $W = H^T H$, where $H \in \mathbb{R}^{k \times d}$ (with $k \in \mathbb{N}_+$ a rank parameter) and to learn $H$ instead. Noting that this quadratic model results in a non-convex problem in $H$, [4, 31] proposed to convexify the problem by learning $W$ directly but to encourage low rank using a nuclear norm on $W$. For learning, [4] proposed a conditional gradient like approach with global convergence guarantees.

**Polynomial networks (PNs).** PNs are a recently-proposed form of neural network where the usual activation function is replaced with a squared activation. Formally, PNs predict a scalar output by

$$\hat{y}_{\text{PN}} := w^T x + v^T \sigma(Hx) = w^T x + \sum_{r=1}^k v_r \sigma(h_r^T x),$$

where $\sigma(a) := a^2$ (evaluated element-wise) is the squared activation, $v \in \mathbb{R}^k$ is the output layer vector, $H \in \mathbb{R}^{k \times d}$ is the hidden layer matrix and $k$ is the number of hidden units. Because the r.h.s term can be rewritten as $x^T W x = \sum_{i,j=1}^d w_{i,j} x_i x_j$ if we set $W = H^T \text{diag}(v) H$, we see that PNs are clearly a minor variant of FMs and that learning $(v, H)$ can be recast as learning a low-rank matrix $W$. Based on this observation, [20] proposed to use GECO [26], a greedy algorithm for convex optimization with a low-rank constraint, similar to the conditional gradient algorithm. [13] proposed a learning algorithm for PNs with global optimality guarantees but their theory imposes non-negativity on the network parameters and they need one distinct hyper-parameter per hidden unit to avoid trivial models. Other low-rank polynomial models were recently introduced in [29][23] but using a tensor network (a.k.a. tensor train) instead of the canonical polyadic (CP) decomposition.
Figure 1: Our multi-output PNs / FMs learn a tensor whose slices share a common basis \( \{ h_r \}_{r=1}^k \).

## 3 A convex formulation of multi-output PNs and FMs

In this section, we generalize PNs and FMs to multi-output problems. For the sake of concreteness, we focus on PNs for multi-class classification. The extension to FM is straightforward and simply requires to replace \( \sigma(h^T x) = (h^T x)^2 \) by \( \sigma_{\text{ANOVA}}(h, x) := \sum_{i<j} x_i h_i x_j h_j \), as noted in [5].

The predictions of multi-class PNs can be naturally defined as \( \hat{y}_{\text{MPN}} := \text{argmax}_{c \in [m]} w_c^T x \). 

We focus on PNs for multi-class classification. The extension to FM is straightforward and simply requires to replace \( \sigma(h^T x) = (h^T x)^2 \) by \( \sigma_{\text{ANOVA}}(h, x) := \sum_{i<j} x_i h_i x_j h_j \), as noted in [5].

Penalties make solving (1) challenging, since they make classes (outputs) inter-dependent. Although \( \ell_1 \) (group lasso) and \( \ell_2 \) penalties for multi-output PNs and FM, we can rescale the output layer appropriately. We therefore denote the set of hidden units by \( \Omega \) according to shared \( \Omega \) (group lasso) or global \( \ell_2 \) regularization, as noted in [5].

Our key idea is to cast the problem of learning a multi-output PN as that of learning an infinite but sparse matrix. Without loss of generality, we assume that hidden units lie in the unit ball (if not the case, we can rescale the output layer appropriately). We therefore denote the set of hidden units by \( \Omega \) and share a common basis (hidden units) amounts to encouraging the rows of \( U \) to be either dense or entirely sparse. This can be naturally achieved using group-sparsity inducing penalties. Intuitively, \( V \) can be thought as \( U \) restricted to its row support. Define the training set by \( X \in \mathbb{R}^{n \times d} \) and \( y \in \mathbb{R}^m \). We then propose to solve the convex problem

\[
\min_{U \in \mathbb{R}^{\Omega \times \Omega}} F(U) := \sum_{i=1}^n \ell (y_i, o(x_i; U)) + \lambda \| U \|_{1,2} + \| U \|_{1,\infty},
\]

where \( \ell \) is a smooth and convex multi-class loss function (cf. Appendix A for three common examples), \( \Omega \) is a sparsity-inducing penalty and \( \tau > 0 \) is a hyper-parameter. In this paper, we focus on the \( \ell_1 \) (lasso), \( \ell_1/\ell_2 \) (group lasso) and \( \ell_1/\ell_\infty \) penalties for \( \Omega \), cf. Table 1. However, \( \ell_1/\ell_2 \) and \( \ell_1/\ell_\infty \) penalties make solving (1) challenging, since they make classes (outputs) inter-dependent. Although this formulation is based on an infinite view, we next show that \( U^* \) has finite row support.

**Proposition 1** Finite row support of \( U^* \) for multi-output PNs and FM

Let \( U^* \) be an optimal solution of (1), where \( \Omega \) is one of the penalties in Table 1. Then, \( \| U^* \|_{0,\infty} \leq \text{nm} + 1 \). If \( \Omega(\cdot) = \| \cdot \|_1 \), we can tighten this bound to \( \| U^* \|_{0,\infty} \leq \min(n, \text{m} + 1, dm) \).

Proof is in Appendix B.1. It is open whether we can tighten this result when \( \Omega = \| \cdot \|_1 \) or \( \| \cdot \|_{\infty} \).
where we see that $\Delta \sigma$ is the gradient of $\ell \circ (\hat{\Delta}, \Gamma, h)$ w.r.t. $h$. We therefore cast hidden unit selection as a continuous optimization problem w.r.t. $h$. As shown in Table 1, elements of $H$ that achieve that maximum, i.e., $\Delta^*$ is obtained by solving a linear approximation of the objective around the current iterate $U(t)$:

$$\Delta^* = \arg\min_{\Omega(\Delta) \leq \tau} \nabla F(U(t)) = \tau \cdot \arg\max_{\Omega(\Delta) \leq 1} \nabla F(U(t)) \cdot \Omega(\Delta).$$

Let us denote the negative gradient $-\nabla F(U)$ by $G \in \mathbb{R}^{\mathcal{H} \times m}$ for short. Its elements are defined by

$$g_{h,c} = -\sum_{i=1}^{n} \sigma(h^T x_i) \nabla \ell(y_i, o(x_i; U))_c,$$

where $\nabla \ell(y, o) \in \mathbb{R}^m$ is the gradient of $\ell$ w.r.t. $o$ (cf., Appendix A). For ReLu activations, solving (2) even approximately is known to be NP-hard [1]. Here, we focus on quadratic activations, for which we will be able to provide approximation guarantees. Plugging the expression of $\sigma$, we get

$$g_{h,c} = -h^T \Gamma_c h \text{ where } \Gamma_c := X^T D_c X \text{ (PN) or } \Gamma_c := \frac{1}{2} \left( X^T D_c X - D_c \sum_{i=1}^{n} \text{diag}(x_i)^2 \right) \text{ (FM)}$$

and $D_c \in \mathbb{R}^{n \times n}$ is a diagonal matrix such that $(D_c)_{i,i} := \nabla \ell(y_i, o(x_i; U))_c$. Let us recall the definition of the dual norm of $\Omega$:

$$\Omega(\Delta) := \max_{\nabla F(U) \in \mathbb{R}^{\mathcal{H} \times m}} \langle \Omega(\Delta), \nabla F(U) \rangle.$$

By comparing this equation to (2), we see that $\Delta^*$ is the argument that achieves the maximum in the dual norm $\Omega^*(G)$, up to a constant factor $\tau$. It is easy to verify that any element in the subdifferential of $\Omega^*(G)$, which we denote by $\partial \Omega^*(G) \subseteq \mathbb{R}^{\mathcal{H} \times m}$, achieves that maximum, i.e., $\Delta^* \in \tau \cdot \partial \Omega^*(G)$.

**Hidden unit selection.** As shown in Table 1, elements of $\Omega^*(G)$ (subgradients) are $|\mathcal{H}| \times m$ matrices with a single non-zero row indexed by $h^*$, where $h^*$ is an optimal hidden unit selected by

$$h^* = \arg\max_{h \in \mathcal{H}} \|g_h\|_p,$$

and where $p = \infty$ when $\Omega = \| \cdot \|_1$, $p = 2$ when $\Omega = \| \cdot \|_{1,2}$ and $p = 1$ when $\Omega = \| \cdot \|_{1,\infty}$. We call (3) a hidden unit selection criterion. Although this selection criterion was derived from the linearization of the objective, it is fairly natural: it chooses the hidden unit with largest “optimality violation”, as measured by the $l_p$ norm of the negative gradient row $g_h$.

**Multiplicative approximations.** The key challenge in solving (2) or equivalently (3) arises from the fact that $G$ has infinitely many rows $g_h$. We therefore cast hidden unit selection as a continuous optimization problem w.r.t. $h$. Surprisingly, although the entire objective (1) is convex, (3) is not. Instead of the exact maximum, we will therefore only require to find a $\hat{\Delta} \in \mathbb{R}^{\mathcal{H} \times m}$ that satisfies

$$\Omega(\hat{\Delta}) \leq \tau \text{ and } \langle \hat{\Delta}, G \rangle \geq \nu \langle \Delta^*, G \rangle,$$

where $\nu \in (0, 1]$ is a multiplicative approximation (higher is better). It is easy to verify that this is equivalent to replacing $h^*$ by an $\hat{h} \in \mathcal{H}$ that satisfies $\|g_{\hat{h}}\|_p \geq \nu \|g_{h^*}\|_p$.

| $\Omega(U)$ | $\Omega^*(G)$ | $\Delta^* \in \tau \cdot \partial \Omega^*(G)$ | Subproblem | $\nu$ |
|---|---|---|---|---|
| $l_1$ (lasso) | $\|U\|_1$ | $\|G\|_\infty$ | $\tau \cdot \arg\max_{h \in \mathcal{H}, c \in [m]} \|g_{h,c}\|$ | $1 - \epsilon$ |
| $l_1/l_2$ (group lasso) | $\|U\|_{1,2}$ | $\|G\|_{1,2}$ | $\tau e_{h,c} \|g_{h,c}\|_2$ | $\|g_{h,c}\|_2$ | $\frac{1 - \epsilon}{\sqrt{m}}$ |
| $l_1/l_\infty$ | $\|U\|_{1,\infty}$ | $\|G\|_{1,\infty}$ | $\tau e_{h,c} \text{sign}(g_{h,c})^T$ | $\|g_{h,c}\|_1$ | $\frac{1 - \epsilon}{m}$ |

Table 1: Sparsity-inducing penalties considered in this paper. With some abuse of notation, we denote by $e_{h,c}$ and $e_{c}$ standard basis vectors of dimension $|\mathcal{H}|$ and $m$, respectively. Selecting the optimal hidden unit $h^*$ to add is a non-convex optimization problem. The constant $\epsilon \in (0, 1)$ is the tolerance parameter used for the power method and $\nu$ is the multiplicative approximation we guarantee.
Sparse case. When $\Omega(\cdot) = \| \cdot \|_1$, we need to solve
\[
\max_{h \in \mathcal{H}} \|gh\|_\infty = \max_{h \in \mathcal{H}} \max_{c \in \{1, \ldots, m\}} |h^T \Gamma_c h| = \max_{c \in \{1, \ldots, m\}} \max_{h \in \mathcal{H}} |h^T \Gamma_c h|.
\]
It is well known that the optimal solution of $\max_{h \in \mathcal{H}} |h^T \Gamma_c h|$ is the dominant eigenvector of $\Gamma_c$. Therefore, we simply need to find the dominant eigenvector $h_c$ of each $\Gamma_c$ and select $\hat{h}$ as the $h_c$ with largest singular value $|\hat{h}^T \Gamma_c \hat{h}|$. Using the power method, we can find an $h_c$ that satisfies
\[
|h^T \Gamma_c h_c| \geq (1 - \epsilon) \max_{h \in \mathcal{H}} |h^T \Gamma_c h|,
\]
for some tolerance parameter $\epsilon \in (0, 1)$. The procedure takes $O(N_c \log(d)/\epsilon)$ time, where $N_c$ is the number of non-zero elements in $\Gamma_c$. Taking the maximum w.r.t. $c \in \{1, \ldots, m\}$ on both sides of (4) leads to $\|gh\|_\infty \geq \nu \|gh\|_\infty$, where $\nu = 1 - \epsilon$. However, using $\Omega = \| \cdot \|_1$ does not encourage selecting an $\hat{h}$ that is useful for all outputs (it is equivalent to independent nuclear norms on $W_1, \ldots, W_m$).

Group-sparse cases. When $\Omega(\cdot) = \| \cdot \|_{1,2}$ or $\Omega(\cdot) = \| \cdot \|_{1,\infty}$, we need to solve
\[
\max_{h \in \mathcal{H}} \|gh\|_2^2 = \max_{h \in \mathcal{H}} f_2(h) := \sum_{c=1}^{m} (h^T \Gamma_c h)^2 \quad \text{or} \quad \max_{h \in \mathcal{H}} \|gh\|_1 = \max_{h \in \mathcal{H}} f_1(h) := \sum_{c=1}^{m} |h^T \Gamma_c h|,
\]
respectively. Unlike the $l_1$-constrained case, we are clearly selecting the hidden unit with largest violation across all outputs. However, we are now faced with a more difficult non-convex optimization problem. Our strategy is to first choose an initialization $h^{(0)}$ which guarantees a certain multiplicative approximation $\nu$, and then refine the solution using a monotonic iterative procedure.

Initialization. We simply choose $h^{(0)}$ as the approximate solution of the $\Omega = \| \cdot \|_1$ case, i.e., we have
\[
\|gh^{(0)}\|_\infty \geq (1 - \epsilon) \max_{h \in \mathcal{H}} \|gh\|_\infty.
\]
Now, using $\sqrt{m} \|x\|_\infty \geq \|x\|_2 \geq \|x\|_\infty$ and $m \|x\|_\infty \geq \|x\|_1 \geq \|x\|_\infty$, this immediately implies
\[
\|gh^{(0)}\|_p \geq \nu \max_{h \in \mathcal{H}} \|gh\|_p
\]
with $\nu = \frac{1 - \epsilon}{\sqrt{m}}$ if $p = 2$ and $\nu = \frac{1 - \epsilon}{m}$ if $p = 1$.

Refining the solution. We now apply another instance of the conditional gradient algorithm to solve the subproblem $\max_{\|h\|_2 \leq 1} f_p(h)$ itself, leading to the following iterates:
\[
h^{(t+1)} = (1 - \eta_t)h^{(t)} + \eta_t \frac{\nabla f_p(h^{(t)})}{\|\nabla f_p(h^{(t)})\|_2},
\]
where $\eta_t \in [0, 1]$. Following [3 Section 2.2.2], if we use the Armijo rule to select $\eta_t$, every limit point of the sequence $\{h^{(t)}\}$ is a stationary point of $f_p$. In practice, we observe that $\eta_t = 1$ is almost always selected. Note that when $\eta_t = 1$ and $m = 1$ (i.e., single-output case), our refining algorithm recovers the power method. Generalized power methods were also studied for structured matrix factorization [16, 21], but with different objectives and constraints. Since the conditional gradient algorithm assumes a differentiable function, in the case $p = 1$, we replace the absolute function with the Huber function $|x| \approx \frac{1}{2}x^2$ if $|x| \leq 1$, $|x| - \frac{1}{2}$ otherwise.

Corrective refitting step. After $t$ iterations, $U^{(t)}$ contains at most $t$ non-zero rows. We can therefore always store $U^{(t)}$ as $V^{(t)}$ in $\mathbb{R}^{1 \times m}$ (the output layer matrix) and $H^{(t)}$ in $\mathbb{R}^{d \times k}$ (the hidden units added so far). In order to improve accuracy, on iteration $t$, we can then refit the objective $F_t(V, H) := \sum_{i=1}^n \ell(y_i, \sum_{r=1}^t \sigma(h_{r}^T x_i)v_{r})$. We consider two kinds of corrective steps, a convex one that minimizes $F_t(V, H)$ w.r.t. $V \in \mathbb{R}^{1 \times m}$ and an optional non-convex one that minimizes $\Omega(V) \leq \tau$ w.r.t. both $V \in \mathbb{R}^{1 \times m}$ and $H \in \mathbb{R}^{d \times x}$. Refitting allows to remove previously-added bad hidden units, thanks to the use of sparsity-inducing penalties. Similar refitting procedures are commonly used in matching pursuit [22].

The entire procedure is summarized in Algorithm 1 and implementation details are given in Appendix D.
5 Analysis of Algorithm 1

The main difficulty in analyzing the convergence of Algorithm 1 stems from the fact that we cannot solve the hidden unit selection subproblem globally when $\Omega = \| \cdot \|_{1,2}$ or $\| \cdot \|_{1,\infty}$. Therefore, we need to develop an analysis that can cope with the multiplicative approximation $\nu$. Multiplicative approximations were also considered in [13] but the condition they require is too stringent (cf. Appendix B.2 for a detailed discussion). The next theorem guarantees the number of iterations needed to output a multi-output network that achieves as small objective value as an optimal solution of (1).

**Theorem 1.** Convergence of Algorithm 1

Assume $F$ is smooth with constant $\beta$. Let $U^{(t)}$ be the output after $t$ iterations of Algorithm 1 run with constraint parameter $\zeta$. Then, $F(U^{(t)}) - \min_{\Omega(U) \leq \tau} F(U) \leq \epsilon, \forall t \geq \frac{8\epsilon^2\beta}{\epsilon \nu^2} - 2$.

In [20], single-output PNs were trained using GECO [26], a greedy algorithm with similar $O\left(\frac{\epsilon^2\beta}{\epsilon \nu^2}\right)$ guarantees. However, GECO is limited to learning infinite vectors (not matrices) and it does not constrain its iterates like we do. Hence GECO cannot remove bad hidden units. The proof of Theorem 1 and a detailed comparison with GECO are given in Appendix B.2. Finally, we note that the infinite dimensional view is also key to convex neural networks [2]. However, to our knowledge, we are the first to give an explicit multiplicative approximation guarantee for a non-linear multi-output network.

6 Experimental results

6.1 Experimental setup

**Datasets.** For our multi-class experiments, we use four publicly-available datasets: segment (7 classes), vowel (11 classes), satimage (6 classes) and letter (26 classes) [12]. Quadratic models substantially improve over linear models on these datasets. For our recommendation system experiments, we use the MovieLens 100k and 1M datasets [14]. See Appendix E for complete details.

**Model validation.** The greedy nature of Algorithm 1 allows us to easily interleave training with model validation. Concretely, we use an outer loop (embarrassingly parallel) for iterating over the range of possible regularization parameters, and an inner loop (Algorithm 1, sequential) for increasing the number of hidden units. Throughout our experiments, we use 50% of the data for training, 25% for validation, and 25% for evaluation. Unless otherwise specified, we use a multi-class logistic loss.

6.2 Method comparison for the hidden unit selection subproblem

As we mentioned previously, the linearized subproblem (hidden unit selection) for the $l_1/l_2$ and $l_1/l_\infty$ constrained cases involves a significantly more challenging non-convex optimization problem. In this section, we compare different methods for obtaining an approximate solution $\hat{h}$. We focus on the $\ell_1/\ell_\infty$ case, since we have a method for computing the true global solution $h^*$, albeit with exponential complexity in $m$ (cf., Appendix C). This allows us to report the empirically observed multiplicative approximation factor $\hat{\nu} := f_1(\hat{h})/f_1(h^*)$.

**Compared methods.** We compare $l_1$ init + refine (proposed), random init + refine, $l_1$ init (without refine), random init and best data: $\hat{h} = \arg\max_{i \in [n]} x_i / \|x_i\|_2$.

**Results.** We report $\hat{\nu}$ in Figure 2. $l_1$ init + refine achieves nearly the global maximum on both datasets and outperforms random init + refine, showing the effectiveness of the proposed initialization and that (5) can get stuck in a bad local minimum if initialized badly. On the other hand, $l_1$ init + refine outperforms $l_1$ init alone, showing the importance of iteratively refining the solution. Best data, a heuristic similar to that of approximate kernel SVMs [7], is not competitive.
6.3 Sparsity-inducing penalty comparison

In this section, we compare the $l_1$, $l_1/l_2$ and $l_1/l_\infty$ penalties for the choice of $\Omega$, when varying the maximum number of hidden units. Figure 4 indicates test set accuracy when using output layer refitting. We also include linear logistic regression, kernel SVMs and the Nyström method as baselines. For the latter two, we use the quadratic kernel $(x_i^T x_j + 1)^2$. Hyper-parameters are chosen so as to maximize validation set accuracy.

Results. On the vowel (11 classes) and letter (26 classes) datasets, $l_1/l_2$ and $l_1/l_\infty$ penalties outperform $l_1$ norm starting from 20 and 75 hidden units, respectively. On satimage (6 classes) and segment (7 classes), we observed that the three penalties are mostly similar (not shown). We hypothesize that $l_1/l_2$ and $l_1/l_\infty$ penalties make a bigger difference when the number of classes is large. Multi-output PNs substantially outperform the Nyström method with comparable number of hidden units (basis vectors). Multi-output PNs reach the same test accuracy as kernel SVMs with very few hidden units on vowel and satimage but appear to require at least 100 hidden units to reach good performance on letter. This is not surprising, since kernel SVMs require 3,208 support vectors on letter, as indicated in Table 2 below.

6.4 Multi-class benchmark comparison

Compared methods. We compare the proposed conditional gradient algorithm with output layer refitting only and with both output and hidden layer refitting; projected gradient descent (FISTA) with random initialization; linear and kernelized models; one-vs-rest PNs (i.e., fit one PN per class). We focus on PNs rather than FMs since they are known to work better on classification tasks [5].

Results are included in Table 2. From these results, we can make the following observations and conclusions. When using output-layer refitting on vowel and letter (two datasets with more than 10 classes), group-sparse inducing penalties lead to better test accuracy. This is to be expected, since these penalties select hidden units that are useful across all classes. When using full hidden layer and output layer refitting, $l_1$ catches up with $l_1/l_2$ and $l_1/l_\infty$ on the vowel and letter datasets. Intuitively, the hidden unit selection becomes less important if we make more effort at every iteration by refitting the hidden units themselves. However, on vowel, $l_1/l_2$ is still substantially better than $l_1$ (89.57 vs. 87.83).

Compared to projected gradient descent with random initialization, our algorithm (for both output and full refitting) is better on $\mathcal{H}_1 (l_1)$, $\mathcal{H}_4 (l_1/l_2)$ and $\mathcal{H}_4 (l_1/l_\infty)$ of the datasets. In addition, with our algorithm, the best model (chosen against the validation set) is substantially sparser. Multi-output PNs substantially outperform OvR PNs. This is to be expected, since multi-output PNs learn to share hidden units across different classes.

6.5 Recommender system experiments using ordinal regression

A straightforward way to implement recommender systems consists in training a single-output model to regress ratings from one-hot encoded user and item indices [25]. Instead of a single-output PN or FM, we propose to use ordinal McRank, a reduction from ordinal regression to multi-output binary classification, which is known to achieve good nDCG (normalized discounted cumulative gain) scores [19]. This reduction involves training a probabilistic binary classifier for each of the $m$
relevance levels (for instance, \( m = 5 \) in the MovieLens datasets). The expected relevance of \( x \) (the concatenation of the one-hot encoded user and item indices) is then computed by

\[
\hat{y} = \sum_{c=1}^{m} c \cdot p(y = c \mid x) = \sum_{c=1}^{m} c \left[ p(y \leq c \mid x) - p(y \leq c - 1 \mid x) \right],
\]

where we use the convention \( p(y \leq 0 \mid x) = 0 \). Thus, all we need to do to use ordinal McRank is to train a probabilistic binary classifier \( p(y \leq c \mid x) \) for all \( c \in [m] \). We can also use a similar approach to compute the variance of the predicted relevance and use it as a measure of uncertainty.

Our key proposal is to use a multi-output model to learn all \( m \) classifiers simultaneously, i.e., in a multi-task fashion. Let \( n \) be the number of user-item pair \( x_i \), for which we have a rating \( y_i \). Concretely, we form a \( n \times m \) matrix \( Y \) such that \( y_{i,c} = +1 \) if \( y_i \leq c \) and \(-1\) otherwise, and solve

\[
\min_{\Omega(U) \leq \epsilon} \sum_{i=1}^{n} \sum_{c=1}^{m} \ell \left( y_{i,c} \cdot \sum_{h \in H} \sigma_{\text{ANOVA}}(h, x_i) u_{h,c} \right),
\]

where \( \ell \) is set to the binary logistic loss, in order to be able to produce probabilities. After running Algorithm 1 on that objective for \( k \) iterations, we obtain \( H \in \mathbb{R}^{k \times d} \) and \( V \in \mathbb{R}^{k \times m} \). Because \( H \) is shared across all outputs, the only small overhead of using the ordinal McRank reduction, compared to a single-output regression model, therefore comes from learning \( V \in \mathbb{R}^{k \times m} \) instead of \( v \in \mathbb{R}^{k} \).

In this experiment, we focus on multi-output factorization machines (FMs), since FMs usually work better than PNs for one-hot encoded data \cite{3}. We indicate RMSE and nDCG truncated at 1 and 5 when varying \( k \) (the maximum number of hidden units) in Figure 4.

**Results.** When combined with the ordinal McRank reduction, we found that \( l_1/l_2 \) and \( l_1/l_\infty \)-constrained multi-output FMs substantially outperform single-output FMs and PNs on both RMSE and nDCG measures. For instance, on MovieLens 100k and 1M, \( l_1/l_\infty \)-constrained multi-output FMs achieve an nDCG@1 of 0.75 and 0.76, respectively, while single-output FMs only achieve 0.71 and 0.75. Similar trends are observed with nDCG@5. We believe that this reduction is more robust to ranking performance measures such as nDCG thanks to its modelling of the expected relevance.

### 7 Conclusion and future directions

In this paper, we defined the problem of learning multi-output PNs and FMs as that of learning a 3-way tensor whose slices share a common decomposition. To obtain a convex optimization objective, we reformulated that problem as learning an infinite but row-wise sparse matrix. To learn that matrix, we developed a conditional gradient algorithm with corrective refitting, and were able to provide convergence guarantees, despite the non-convexity of the hidden unit selection step.

Although not considered in this paper, our algorithm and its analysis can be modified to make use of stochastic gradients. An open question remains whether a conditional gradient algorithm with provable guarantees can be developed for training deep polynomial networks or factorization machines. However, this would require the introduction of a new functional analysis framework.

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**Figure 4:** Recommender system experiment: RMSE (lower is better) and nDCG (higher is better).
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Appendix

A Convex multi-class loss functions

Table 3: Examples of convex multi-class loss functions \( \ell(y, o) \in \mathbb{R} \), where \( y \in [m] \) is the correct label and \( o \in \mathbb{R}^m \) is a vector of predicted outputs.

| Loss                        | \( \ell(y, o) \)                                                                 | \( \rho_o(y, o) \)                                                                 |
|-----------------------------|----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------|
| Multi-class logistic        | \( \log(1 + \sum_{c \neq y} \exp(o_c - o_y)) \)                                | \( \frac{\exp(o_c - o_y)}{\sum_{c \neq y} \exp(o_c - o_y)} \)                    |
| Smoothed multi-class hinge  | \( \log(1 + \sum_{c \neq y} \exp(1 + o_c - o_y)) \)                            | \( \frac{\exp(1 + o_c - o_y)}{\sum_{c \neq y} \exp(1 + o_c - o_y)} \)           |
| Multi-class squared hinge   | \( \sum_{c \neq y} \max(1 + o_c - o_y, 0)^2 \)                                | \( 2 \max(1 + o_c - o_y, 0) \)                                                  |

The gradient w.r.t. \( o \), denoted \( \nabla \ell(y, o) \in \mathbb{R}^m \), can be computed by

\[
\nabla \ell(y, o) = \sum_{c \neq y} \rho_o(y, o)(e_c - e_y),
\]

where \( e_c \in \mathbb{R}^m \) is a vector whose \( c^{th} \) element is 1 and other elements are 0. For the smoothed multi-class hinge loss and the multi-class squared hinge loss, see [27] and [6], respectively.

B Proofs

B.1 Finite support of an optimal solution (Proposition 1)

General case. We first state a result that holds for arbitrary activation function \( \sigma \) (sigmoid, ReLu, etc...). The main idea is to use the fact that the penalties considered in Table 2 are atomic [8]. Then, we can equivalently optimize (1) over the convex hull of a set of atoms and invoke Carathéodory’s theorem for convex hulls.

Let \( \phi_h(X) \) be an \( n \)-dimensional vector whose \( i^{th} \) element is \( \sigma(h^T x_i) \). Let us define the sets

\[
\mathcal{A} := \{e_h v^T : h \in \mathcal{H}, v \in \mathcal{V}\} \subset \mathbb{R}^{|\mathcal{H}| \times m} \quad \text{and} \quad \mathcal{B} := \{\phi_h(X)v^T : h \in \mathcal{H}, v \in \mathcal{V}\} \subset \mathbb{R}^{n \times m},
\]

where we define the set \( \mathcal{V} \) as follows:

- \( l_1 \) case: \( \mathcal{V} := \{s e_c : s \in \{-1, 1\}, c \in [m]\} \)
- \( l_1/l_2 \) case: \( \mathcal{V} := \{v \in \mathbb{R}^m : \|v\|_2 = 1\} \)
- \( l_1/\infty \) case: \( \mathcal{V} := \{-1, 1\}^m \).

Then (1) is equivalent to

\[
\min_{U \in \mathbb{R}^{|\mathcal{H}| \times m}} \sum_{i=1}^n \ell \left( y_i, \sum_{h \in \mathcal{H}} \phi_h(X) e_h u_h \right) \quad \text{s.t.} \quad \Omega(U) \leq \tau
\]

\[
= \min_{U \in \mathbb{R}^{|\mathcal{H}| \times m}} \sum_{i=1}^n \ell \left( y_i, \sum_{h \in \mathcal{H}} \phi_h(X) e_h u_h \right) \quad \text{s.t.} \quad U \in \tau \cdot \text{conv} (\mathcal{A})
\]

\[
= \min_{O \in \mathbb{R}^{n \times m}} \sum_{i=1}^n \ell \left( y_i, o_i \right) \quad \text{s.t.} \quad O \in \tau \cdot \text{conv} (\mathcal{B}),
\]

where \( \text{conv}(\mathcal{S}) \) is the convex hull of the set \( \mathcal{S} \). The matrices \( U \) and \( O \) are related to each other by

\[
U = \sum_{h \in \mathcal{H}} \sum_{v \in \mathcal{V}} \theta_{h,v} e_h v^T \quad \text{and} \quad O = \sum_{h \in \mathcal{H}} \sum_{v \in \mathcal{V}} \theta_{h,v} \phi_h(X)v^T,
\]
We focus on constrained optimization problems of the form
\[
\min_{x \in \mathbb{R}^d} f(x),
\]
where \( f \) is convex and \( \beta \)-smooth w.r.t. \( \Omega \) and \( \mathcal{D} := \{ x : \Omega(x) \leq \tau \} \).

**Curvature and smoothness constants.** The convergence analysis depends on the following standard curvature constant
\[
C_{f, \mathcal{D}} := \sup_{x, y \in \mathcal{D}} \frac{2}{\gamma^2} \left( f(y) - f(x) - \langle y - x, \nabla f(x) \rangle \right).
\]
Intuitively, this is a measure of non-linearity of \( f \): the maximum deviation between \( f \) and its linear approximations over \( \mathcal{D} \). The assumption of bounded \( C_{f, \mathcal{D}} \) is closely related to a smoothness assumption on \( f \). Following [15] Lemma 7, for any choice of norm \( \Omega \), \( C_{f, \mathcal{D}} \) can be upper-bounded by the smoothness constant \( \beta \) as
\[
C_{f, \mathcal{D}} \leq \text{diam}_\Omega(\mathcal{D})^2 \beta.
\]
Using \( \mathcal{D} = \{ x : \Omega(x) \leq \tau \} \), we obtain
\[
\text{diam}_\Omega(\mathcal{D}) = \sup_{x, y \in \mathcal{D}} \Omega(x - y) \leq \sup_{x, y \in \mathcal{D}} \Omega(x) + \Omega(y) \leq 2\tau
\]
and therefore
\[
C_{f, \mathcal{D}} \leq 4\tau^2 \beta. \tag{6}
\]

**Linear duality gap.** Following [15], we define the linear duality gap
\[
g_D(x) := \max_{s \in \mathcal{D}} \langle x - s, \nabla f(x) \rangle.
\]
Since $f$ is convex and differentiable, we have that
\[ f(s) \geq f(x) + \langle s - x, \nabla f(x) \rangle. \] (7)

Let us define the primal error
\[ h_D(x) := f(x) - \min_{x \in D} f(x). \]

Minimizing (7) w.r.t. $s \in D$ on both sides we obtain
\[ g_D(x) \geq h_D(x). \]
Hence $g_D(x)$ can be used as a certificate of optimality about $x$.

**Bounding progress.** Let $x \in D$ be the current iterate and $y = x + \gamma(s - x)$ be our update. The definition of $C_{f,D}$ implies
\[ f(y) \leq f(x) + \gamma \langle s - x, \nabla f(x) \rangle + \frac{\gamma^2}{2} C_{f,D}. \]

We now use that $s$ is obtained by an exact linear minimization oracle (LMO)
\[ s = \arg\min_{s \in D} \langle s, \nabla f(x) \rangle \]
and therefore $\langle s - x, \nabla f(x) \rangle = -g_D(x)$. Combined with $g_D(x) \geq h_D(x)$, we obtain
\[ f(y) \leq f(x) - \gamma h_D(x) + \frac{\gamma^2}{2} C_{f,D}. \]
Subtracting $\min_{x \in D} f(x)$ on both sides, we finally get
\[ h_D(y) \leq (1 - \gamma) h_D(x) + \frac{\gamma^2}{2} C_{f,D}. \]

**Primal convergence.** Since we use a fully-corrective variant of the conditional gradient method, our algorithm enjoys a convergence rate at least as good as the variant with fixed step size. Following [15, Theorem 1] and using (6), for every $t \geq 1$, the iterates satisfy
\[ f(x^{(t)}) - \min_{x \in D} f(x) \leq \frac{2 C_{f,D}}{t + 2} \leq \frac{8 \tau^2 \beta}{t + 2}. \]

Thus, we can obtain an $\epsilon$-accurate solution if we run the algorithm for $t \geq \frac{8 \tau^2 \beta}{\epsilon} - 2$ iterations.

**Linear minimization with multiplicative approximation.** We now extend the analysis to the case of approximate linear minimization. Given $x \in D$, we assume that an approximate LMO outputs a certain $s \in D$ such that
\[ \langle -s, \nabla f(x) \rangle \geq \nu \max_{s' \in D} \langle -s', \nabla f(x) \rangle, \]
for some multiplicative factor $\nu \in (0, 1]$ (higher is more accurate). Since $x$ and $y = x + \gamma(s - x)$ are in $D$, we have like before
\[ f(y) \leq f(x) + \gamma \langle s - x, \nabla f(x) \rangle + \frac{\gamma^2}{2} C_{f,D}. \]
Following the same trick as [11, Appendix B], we now absorb the multiplicative factor $\nu$ in the constraint
\[ \langle -s, \nabla f(x) \rangle \geq \max_{s' \in D'} \langle -s', \nabla f(x) \rangle, \]
where we defined $D' := \{ x : \Omega(x) \leq \tau \nu \}$ (i.e., the ball is shrunk by a factor $\nu$). We therefore obtain $\langle s - x, \nabla f(x) \rangle \leq -g_D'(x)$. Similarly as before, this implies that
\[ f(y) \leq f(x) - \gamma h_D'(x) + \frac{\gamma^2}{2} C_{f,D}. \]
Subtracting $\min_{x \in D'} f(x)$ on both sides, we get
\[ h_D'(y) \leq (1 - \gamma) h_D'(x) + \frac{\gamma^2}{2} C_{f,D}. \]
We thus get that iterate \( x^{(t)} \) satisfies \( x^{(t)} \in D \) and
\[
f(x^{(t)}) \leq \min_{x \in D} f(x) + \frac{8\tau^2 \beta}{t + 2}.
\]
We can therefore obtain an \( x^{(t)} \in D \) such that \( f(x^{(t)}) - \min_{x \in D} f(x) \leq \epsilon \) if we run our algorithm for \( t \geq \frac{8\tau^2 \beta}{\epsilon} - 2 \) iterations with constraint parameter \( \tau \) and multiplicative factor \( \nu \). Put differently, we can obtain an \( x^{(t)} \in \frac{1}{\nu} D \) such that \( f(x^{(t)}) - \min_{x \in D} f(x) \leq \epsilon \) if we run our algorithm for \( t \geq \frac{8\tau^2 \beta}{\nu^2 \epsilon} - 2 \) iterations with constraint parameter \( \frac{\tau}{\nu} \) and multiplicative factor \( \nu \).

**Comparison with the analysis of GECO.** GECO [26] is a greedy algorithm with fully-corrective refitting steps for learning a sparse vector from possibly infinitely-many features, similarly to our algorithm. However, unlike our algorithm, GECO does not constrain the norm of its iterates (i.e., there is no parameter \( \tau \)), which can lead to severe overfitting in practice. Following [26, Theorem 1], GECO was used to learn single-output polynomial networks in [20]. Combining (8) together with \( \|x\|_\infty \|x\|_0 \geq \|x\|_1 \), it was shown that GECO can learn the parameters \( x^{(t)} \) (unbounded) of a single-output polynomial network with \( l_\infty \) unit ball constraint and squared activation such that
\[
f(x^{(t)}) - \min_{\|x\|_\infty \leq 1} f(x) \leq \epsilon \quad \forall x, \forall t \geq \frac{2\|x\|_1^2 \beta}{\epsilon \nu^2} - 1.
\]
However, if we run our algorithm with an \( l_1 \) constraint, it can learn an \( x^{(t)} \) such that \( \|x^{(t)}\|_1 \leq \frac{1}{\nu} \)
and
\[
f(x^{(t)}) - \min_{\|x\|_\infty \leq 1} f(x) \leq f(x^{(t)}) - \min_{\|x\|_1 \leq 1} f(x) \leq \epsilon \quad \forall t \geq \frac{8\beta}{\nu^2} - 2.
\]
Clearly, our algorithm with an \( l_1 \) constraint uses fewer iterations than GECO for learning polynomial networks with \( l_\infty \) unit ball constraint and more than \( \|x\|_0 = 3 \) hidden units.

**Comparison with the analysis of Block-FW.** [18] analyze a block Frank-Wolfe method with “multiplicative” approximations in the linear minimization oracle. However, they require a different condition, namely:
\[
\langle x - s, \nabla f(x) \rangle \geq \kappa \cdot \max_{s' \in D} \langle x - s', \nabla f(x) \rangle
\]
\[
\iff \langle -s, \nabla f(x) \rangle \geq \kappa \cdot \max_{s' \in D} \langle -s', \nabla f(x) \rangle + \langle x, \nabla f(x) \rangle (\kappa - 1),
\]
for some \( \kappa \in (0, 1] \). Under this condition, they show that the algorithm converges to an \( \epsilon \)-approximate solution in \( O\left(\frac{1}{\epsilon}\right) \) iterations. A disadvantage of the above condition is that it contains an additive term that depends on the current iterate \( x \) and so it is difficult to give guarantees on \( \kappa \) in general.

**C Computing an optimal solution of the linearized subproblem (\( l_1/l_\infty \) case)**

We describe how to compute an optimal hidden unit \( h^* \) in the \( l_1/l_\infty \) case, albeit with exponential complexity in \( m \). Because of its exponential complexity in \( m \) (the number of outputs), clearly, this method should only be used to evaluate other (polynomial-time) algorithms.

Recall that we want to solve
\[
\max_{h \in H} f_1(h) = \sum_{c=1}^m |h^T \Gamma_c h|,
\]
for some \( \kappa \in (0, 1] \). Under this condition, they show that the algorithm converges to an \( \epsilon \)-approximate solution in \( O\left(\frac{1}{\epsilon}\right) \) iterations. A disadvantage of the above condition is that it contains an additive term that depends on the current iterate \( x \) and so it is difficult to give guarantees on \( \kappa \) in general.

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Recall that we want to solve
\[
\max_{h \in H} f_1(h) = \sum_{c=1}^m |h^T \Gamma_c h|,
\]
Now, if we knew the sign $s_c := \text{sign}(h^T \Gamma_c h^*)$, we could rewrite the problem as

$$\max_{h \in H} f_1(h) = \sum_{c=1}^m s_c h^T \Gamma_c h = h^T \left( \sum_{c=1}^m s_c \Gamma_c \right) h,$$

whose optimal solution is the dominant eigenvector of the symmetric matrix $\sum_{c=1}^m s_c \Gamma_c$. The idea is then simply to find the dominant eigenvector for all possible $2^m$ sign vectors and choose the eigenvector that achieves largest objective value.

### D Implementation details

In practice, penalized formulations are more convenient to handle than constrained ones. Here, we discuss why we can safely replace constrained formulations by penalized formulations in the refitting step. We use the output layer refitting objective as an example. It is well known that there exists $\lambda > 0$ such that this objective is equivalent to

$$\min_{V \in \mathbb{R}^{t \times m}} F(V, H^{(t)}) + \lambda \Omega(V).$$

Unfortunately, the relation between $\tau$ and $\lambda$ is a priori unknown. However, it is easy to see that the constant factor $\tau$ in (2) is absorbed by the output layer in our refitting step. This means that we need to know the actual value of $\tau$ for the refitting step but not for the hidden unit selection step. As long as we compute a full regularization path, we may therefore use a penalized formulation in a practical implementation. We do so for both refitting objectives we discussed.

For both refitting objectives, we use FISTA, an accelerated projected gradient method with $O(1/t^2)$ convergence rate, where $t$ is the iteration number. We set the maximum number of iterations to 1000 and the stopping criterion’s tolerance to $10^{-3}$.

### E Datasets

For our multi-class experiments, we used the following four publicly available datasets [12].

| Name    | $n$   | $d$ | $m$ |
|---------|-------|-----|-----|
| segment | 2,310 | 19  | 7   |
| vowel   | 528   | 10  | 11  |
| satimage| 4,435 | 36  | 6   |
| letter  | 15,000| 16  | 26  |

For recommender system experiments, we used the following two publicly available datasets [14].

| Name            | $n$           | $d$                      | $m$          |
|-----------------|---------------|--------------------------|--------------|
| Movielens 100k  | 100,000 (ratings) | 2,625 = 943 (users) + 1,682 (movies) | 5            |
| Movielens 1M    | 1,000,209 (ratings) | 9,940 = 6,040 (users) + 3,900 (movies) | 5            |

The task is to predict ratings between 1 and 5 given by users to movies, i.e., $y \in \{1, \ldots, 5\}$. The design matrix $X$ was constructed following [25]. Namely, for each rating $y_i$, the corresponding $x_i$ is set to the concatenation of the one-hot encodings of the user and item indices. Hence the number of samples $n$ is the number of ratings and the number of features is equal to the sum of the number of users and items. Each sample contains exactly two non-zero features. It is known that factorization machines are equivalent to matrix factorization when using this representation [25].
F Additional experimental results

F.1 Multi-class squared hinge loss results

We also compared the multi-class logistic (ML) loss to the multi-class squared hinge (MSH) loss. The MSH loss achieves comparable test accuracy to the ML loss. However, it can often be much faster to train, since it does not require expensive exponential and logarithm calculations.

Table 4: Comparison between multi-class squared hinge (MSH) and logistic (ML) losses.

| Constraint | Loss | Conditional gradient (full refitting) | Conditional gradient (output-layer refitting) |
|------------|------|--------------------------------------|-----------------------------------------------|
|            |      | segment | vowel | satimage | letter | segment | vowel | satimage | letter | segment | vowel | satimage | letter | segment | vowel | satimage | letter |
| $l_1$ (#units) | MSH | 96.01 | 87.83 | 89.98 | 92.03 | (21) | (8) | (22) | (130) | 95.67 | 79.13 | 88.99 | 91.25 | (21) | (25) | (21) | (149) |
|            | ML | 96.71 | 87.83 | 89.80 | 92.29 | (41) | (12) | (25) | (150) | 97.05 | 80.00 | 89.71 | 91.01 | (20) | (21) | (40) | (139) |
| $l_1/l_2$ (#units) | MSH | 96.01 | 86.96 | 90.25 | 91.57 | (15) | (8) | (12) | (94) | 95.67 | 85.22 | 89.98 | 92.03 | (25) | (19) | (50) | (149) |
|            | ML | 96.71 | 89.57 | 89.08 | 91.81 | (40) | (15) | (18) | (106) | 96.36 | 85.22 | 89.71 | 92.24 | (21) | (15) | (50) | (150) |
| $l_1/l_\infty$ (#units) | MSH | 95.84 | 85.22 | 89.80 | 92.27 | (16) | (16) | (29) | (149) | 97.05 | 86.09 | 88.99 | 91.20 | (28) | (33) | (24) | (119) |
|            | ML | 96.71 | 86.96 | 88.99 | 92.35 | (24) | (15) | (20) | (149) | 96.19 | 86.96 | 89.35 | 91.68 | (16) | (41) | (41) | (128) |

F.2 Full vs. output layer refitting comparison

In this experiment, we compare output layer refitting with full refitting of both the hidden and output layers. Empirically, we observe that full refitting does not always outperform output layer refitting in terms of objective value but it does so in terms of test accuracy.

Figure 5: Relative objective difference from best (top) and multi-class test set accuracy values (bottom) when performing output layer refitting (dashed) and full, non-convex refitting (solid), optimizing a penalized $l_1/l_2$ objective with $\lambda = 0.1$. 

Multi-output Polynomial Networks and Factorization Machines