Sparse Partially Linear Additive Models

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The generalized partially linear additive model (GPLAM) is a flexible and interpretable approach to building predictive models. It combines features in an additive manner, allowing each to have either a linear or nonlinear effect on the response. However, the choice of which features to treat as linear or nonlinear is typically assumed known. Thus, to make a GPLAM a viable approach in situations in which little is known a priori about the features, one must overcome two primary model selection challenges: deciding which features to include in the model and determining which of these features to treat non-linearly. We introduce the sparse partially linear additive model (SPLAM), which combines model fitting and both of these model selection challenges into a single convex optimization problem. SPLAM provides a bridge between the lasso and sparse additive models. Through a statistical oracle inequality and thorough simulation, we demonstrate that SPLAM can outperform other methods across a broad spectrum of statistical regimes, including the high-dimensional (p ≫ N) setting. We develop efficient algorithms that are applied to real datasets with half a million samples and over 45,000 features with excellent predictive performance. Supplementary materials for this article are available online.

Key Words: Classification; Generalized partially linear additive models; Group lasso; Regression; Sparsity.

1. INTRODUCTION

Generalized partially linear additive models (GPLAMs, Härdle and Liang 2007) provide an attractive middle ground between the simplicity of generalized linear models (GLMs, Nelder and Wedderburn 1972) and the flexibility of generalized additive models (GAMs, Hastie and Tibshirani 1990). Given a dataset \( \{ (x_i, y_i) \}_{i=1}^{N} \), a GPLAM relates the conditional mean of the response, \( y_i \), to the \( p \)-dimensional predictor vector, \( x_i \), using a known link function, \( g \):

\[
g(E[y_i|x_i]) = \sum_{j \in N} f_j(x_{ij}) + \sum_{j \in L} x_{ij}\theta_j.
\]
The features in $\mathcal{N}$ contribute to the model in a nonlinear fashion while the features in $\mathcal{L}$ contribute in a linear fashion. A GLM treats all features as being in $\mathcal{L}$ and may therefore be biased when nonlinear effects are present; on the other extreme, a GAM treats all features as being in $\mathcal{N}$, which incurs unnecessary variance for the features that should be treated as linear. GPLAMs are a popular tool for data analysis in multiple domains including economics (Engle et al. 1986; Green and Silverman 1993) and biology (Dinse and Lagakos 1983; Lian, Chen, and Yang 2012).

A major obstacle to using GPLAMs on large-scale datasets is that one rarely knows a priori which features should be assigned to $\mathcal{N}$ and $\mathcal{L}$. A further challenge is in deciding which features should be excluded from the model entirely. The goal of this article is to make GPLAMs a viable tool for building large-scale predictive models. To do so, we must overcome two model-selection challenges: automatically deciding which features are at all relevant in the model and deciding which of those features should be fit linearly versus nonlinearly.

In the context of GAMs (where $\mathcal{L}$ is taken to be empty), the sparse additive model (SpAM) is a useful framework for performing feature selection on $\mathcal{N}$ (Ravikumar et al. 2009). From the perspective of a GPLAM, SpAM takes an “all-in” or “all-out” approach to feature selection. In this work, we introduce the sparse partially linear additive model (SPLAM) that provides the finer-grained selection demanded by a GPLAM. SPLAMs build on the SpAM framework, providing a natural bridge between the $\ell_1$-penalized GLM and SpAM, thereby reaping many of the benefits enjoyed by both of these methods.

Failing to account for exactly linear features is disadvantageous in terms of interpretability and on statistical and computational grounds. As a motivating example, consider a situation in which $p = 1000$, $|\mathcal{N}| = 5$, and $|\mathcal{L}| = 295$. Assuming the correct set of features is selected, SpAM would include 300 features. From an interpretability standpoint, one would have to manually inspect the 300 nonparametric fits to reveal that only five features are effectively nonlinear. The other 295 of them would appear nearly, but not exactly, linear such as in Figure 1(d). Statistically, a price is paid in variance for the many nearly linear features; and, computationally, such a model is wasteful both in terms of memory and speed for making future predictions.

In the last several years, a number of methods have been proposed to address various aspects of this problem. In Chen, Liang, and Wang (2011), a bootstrap-based test is developed to determine the linearity of a component. In Huang, Wei, and Ma (2012), the authors
used a group minimax concave penalty (MCP) to decide which features should be linear versus nonlinear, but features may not be completely excluded from the model. In Du, Cheng, and Liang (2012), an algorithm is developed that iterates between two optimization problems: one that decides which nonlinear features should be made linear and the other that decides which linear features should be set to zero. An alternative approach to SpAM is the component selection and smoothing operator (COSSO) method, which uses unsquared reproducing kernel Hilbert space (RKHS) norm penalties (Lin and Zhang 2006). The linear and nonlinear discoverer extends COSSO to the GPLAM setting (Zhang, Cheng, and Liu 2011). Relationally, Lian, Chen, and Yang (2012) combined smoothness and sparsity SCAD-based penalties for a similar purpose. None of the above methods is geared toward high-dimensional data in terms of statistical theory or computation. Several other methods are geared toward the high-dimensional setting but do not perform both model selection tasks. For example, in Bunea (2004), Xie and Huang (2009), and Müller and van de Geer (2015), methods are developed to perform feature selection for the set \( L \) while assuming that the set \( N \) is known; Lian and Liang (2013) and Wang et al. (2014) performed feature selection on both \( L \) and \( N \) individually but assumed an initial partition of the features into those potentially in \( L \) and those potentially in \( N \).

By contrast, SPLAM is designed for large-scale datasets (e.g., we apply it to a dataset with \( p = 47, 236 \)). SPLAM is formulated through a single convex optimization problem that admits an efficient algorithm and strong theoretical properties even in the \( p \gg N \) setting.

In Section 2, we define the SPLAM estimator as the solution to a convex optimization problem, and, in Section 3, we discuss how this problem may be efficiently solved in large-scale contexts. Section 4 presents consistency results under weak assumptions and lends theoretical support to the conceptual difference in predictive performance between SPLAM and SpAM, its close relative. Section 5 provides an empirical study of SPLAM, including both a thorough simulation study and comparison of SPLAM to other methods on an array of large data examples.

## 2. THE SPLAM OPTIMIZATION

We approach the challenging model selection and fitting problem posed by a GPLAM through convex relaxation. For each feature \( x_j \), we perform an \( M \)-dimensional basis expansion \( b(x_j) = [b_1(x_j), \ldots, b_M(x_j)] \) in which \( b_1(x_j) = x_j \) and \( M \) is typically small. Our main requirement of the basis is that \( b_1(x_j) \) models the linear part and that \( [b_2(x_j), \ldots, b_M(x_j)] =: b_{-1}(x_j) \) models the nonlinear part. SPLAM estimates each \( f_j(\cdot) \) by a function in the space spanned by \( b(\cdot) \), that is, \( f_j(x_j) = b(x_j)\beta_j \), where \( \beta_j \in \mathbb{R}^M \) (for ease of exposition we ignore the intercept). We use \( \beta_{j1} \) and \( \beta_{j,-1} \) to denote the coefficients of the linear and nonlinear basis functions, respectively. Letting \( \beta = [\beta_1^T, \ldots, \beta_p^T]^T \in \mathbb{R}^{pM} \) and \( X = [b(x_1) : \ldots : b(x_p)] \in \mathbb{R}^{N \times pM} \) be the design matrix, we have

\[
X\beta = \sum_{j=1}^p \left[ \beta_{j1}x_j + \beta_{j,-1}b_{-1}(x_j) \right].
\]
Given a convex smooth loss function $L(y, X, \beta)$, SPLAM is formulated as the solution to the following convex program with hierarchical sparsity regularization:

**Optimization Problem 1.** SPLAM

$$
\min_{\beta} L(y, X, \beta) + \lambda \Omega^{\text{SPLAM}}(\beta),
$$

(2)

where $\Omega^{\text{SPLAM}}(\beta) = \sum_{j=1}^{p} \left[ \alpha \|\beta_j\|_2 + (1 - \alpha) \|\beta_j, -1\|_2 \right]$, $\lambda \geq 0$, and $\alpha \in [0, 1]$.

In this article, we focus on linear regression, in which $L(y, X, \beta) = \frac{1}{2N} \|y - X\beta\|_2^2$ and logistic regression, in which $L(y, X, \beta) = \frac{1}{N} \sum_i \log(1 + \exp[-y_i \sum_{k=1}^{pM} X_{ik} \beta_k])$, where $y_i \in \{-1, 1\}$. The penalty function $\Omega^{\text{SPLAM}}$ is convex and is an instance of the hierarchical group lasso (Zhao, Rocha, and Yu 2009; Jenatton et al. 2010). Its two terms address the two forms of model selection present in the GPLAM problem: the first term affects the overall number of predictors appearing in the fitted model; the second term controls the number of those features that are treated nonlinearly.

Just as GPLAMs generalize both GLMs and GAMs, it is useful to note that SPLAM includes the most common penalized estimators used for these two kinds of models.

- When $\alpha = 1$ and an orthogonal basis is used, Problem 1 becomes SpAM in group lasso form.
- When $\lambda = \tilde{\lambda}/\alpha$ and $\alpha$ is sufficiently small, SPLAM reduces to the lasso (Tibshirani 1996) applied to the linear features only.

In practice, we solve the SPLAM problem over a grid of $(\lambda, \alpha)$ pairs. Our strategy is to fix $\alpha$ and solve the problem pathwise starting from the smallest value of $\lambda$ for which $\hat{\beta}_j = 0$ for all $j = 1, \ldots, p$ and decreasing $\lambda$ exponentially. In Section 4.1, we prove that SPLAM is consistent under general conditions for $\alpha = (1 + \sqrt{6})/(1 + 2\sqrt{6})$ and suitably chosen $\lambda$.

After posting the initial draft of this article online, we learned of a similar method being developed independently and concurrently to ours (Chouldechova and Hastie 2015); their approach to the GPLAM problem also makes use of an overlapping group lasso penalty, but uses a different form of penalty known as the latent overlapping group lasso penalty (Obozinski, Jacob, and Vert 2011). Also, Petersen, Witten, and Simon (2016) in a recent preprint propose a method that combines feature selection and nonlinear, piecewise-constant modeling using a fused-lasso penalty.

### 3. COMPUTATION

The hierarchical group lasso can be solved efficiently by proximal gradient descent (Beck and Teboulle 2009) as described by Jenatton et al. (2010). The idea of this algorithm is to modify the standard gradient steps that one would take if simply minimizing $L$ and then apply the proximal operator of the nondifferentiable penalty, $\lambda \Omega^{\text{SPLAM}}(\cdot)$:

$$
\beta^{k+1} = \arg \min_{z \in \mathbb{R}^{pM}} \left\{ \frac{1}{2t^k} \|z - (\beta^k - t^k \nabla L(y, X, \beta^k))\|_2^2 + \lambda \Omega^{\text{SPLAM}}(z) \right\},
$$

(3)
where $t^k$ is a suitable step size. It is known that setting the step size to the reciprocal of the Lipschitz constant of $\nabla L$ guarantees convergence (Beck and Teboulle 2009). A key property of hierarchical penalties such as $\Omega^{\text{SPLAM}}$ is that the proximal operator can be very efficiently solved. In particular, Jenatton et al. (2010) showed that the dual of this problem can be solved in a single pass of block coordinate descent (and therefore has essentially a closed form). While the proximal gradient method as described above can be used to solve this problem, we observe that a closely related method, called block coordinate gradient descent, performs better in practice for solving the SPLAM problem in large-scale settings. Furthermore, in the regression setting, we develop an even more efficient approach that solves the problem by applying the proximal operator only once. Additional details about our implementation are given in the supplementary material.

### 3.1 Block Coordinate Gradient Descent

The block coordinate gradient descent (BCGD) method is a hybrid of blockwise coordinate descent (BCD) and a proximal method. A simple quadratic approximation of $L$ is used in each coordinate update. The particular form of BCDG we propose is to apply the proximal operator one block at a time, allowing each block update to use a distinct step size. We find that empirically this is more efficient than proximal gradient descent (this has been noted in a related problem by Qin, Scheinberg, and Goldfarb (2010), in which they call this method ISTA-BC.

We cycle through the blocks (taking each $\beta_j \in \mathbb{R}^M$ as a block), and on the $(k+1)$st pass, the update of block $j$ is given by

$$
\beta_{j}^{k+1} = P_{\beta_j}^j(\beta^k)
= : \arg \min_{z \in \mathbb{R}^M} \left\{ \frac{1}{2t_j} \| z - (\beta_j^k - t_j \nabla_{\beta_j} L(\beta^k)) \|_2^2 + \lambda \alpha \| z \|_2 + \lambda (1 - \alpha) \| z - 1 \|_2 \right\},
$$

(4)

where $t_j$ is the step size for block $j$.

This proximal problem has essentially a closed-form solution and therefore can be solved very efficiently, as shown in Jenatton et al. (2010). Let $g_j = \beta_j^k - t_j \nabla_{\beta_j} L(\beta^k)$ and consider its dual,

$$
\begin{align*}
\min_{\gamma_1 \in \mathbb{R}^M, \gamma_2 \in \mathbb{R}^{M-1}} \quad & \frac{1}{2} \| g_j - \gamma_1 - [0, \gamma_2^T]^T \|_2^2 \\
\text{s.t.} \quad & \| \gamma_1 \|_2 \leq t_j \lambda \alpha \quad \| \gamma_2 \|_2 \leq t_j \lambda (1 - \alpha).
\end{align*}
$$

(5)

Jenatton et al. (2010) showed that it can be solved in one pass of block coordinate descent,

$$
\begin{align*}
\hat{\gamma}_2 &= \Pi_{t_j \lambda (1 - \alpha)}(g_j, -1), \quad \hat{\gamma}_1 = \Pi_{t_j \lambda \alpha}(g_j - [0, \hat{\gamma}_2^T]^T),
\end{align*}
$$

(7)

where $\Pi_r(u)$ is the Euclidean projection of the vector $u$ onto the $\ell_2$-ball of radius $r$. Having solved the dual, we get $P_{\beta_j}^j(\beta^k) = g_j - \hat{\gamma}_1 - [0, \hat{\gamma}_2^T]^T$. 

We perform a backtracking line search until the following inequality holds to select $t_j$

\[ L(\tilde{\beta}) \leq L(\hat{\beta}) + (P_j^i(\beta^k) - \beta_j^k, \nabla_{\beta_j} L(\hat{\beta})) + \frac{1}{2t_j} \|P_j^i(\beta^k) - \beta_j^k\|_2^2, \]  

(8)

where

\[
\hat{\beta} = \left[ \beta_1^{k+1T}, \ldots, \beta_{j-1}^{k+1T}, \beta_j^k, \ldots, \beta_p^k, \beta_j^{kT} \right]^T \quad \text{and} \quad \tilde{\beta} = \left[ \beta_1^{k+1T}, \ldots, \beta_{j-1}^{k+1T}, P_j^i(\beta^k)^T, \ldots, \beta_p^k \right]^T.
\]

Computing the Lipschitz constant, $C_j$, of $\nabla_{\beta_j} L$ is relatively inexpensive since $X_j^T X_j$ is just an $M$-by-$M$ matrix, where $M$ is typically very small. Thus, in practice we can easily compute the minimum step size $1/C_j$, to avoid the step size $t_j$ going below this value.

Algorithm 1 summarizes our BCGD method. We cycle through each block (Line 5), solve the proximal operator for that block (Lines 7–10) and check if the step size is proper using a backtracking line search (Lines 11–14). In the supplementary material, we show that the proposed algorithm fits the framework of Tseng and Yun (2009) and therefore is guaranteed to converge.

Algorithm 1 SPLAM via BCGD (for general loss $L$)

1. $t_j = t_j^0$, for $j = 1, \ldots, p$
2. $k \leftarrow 0$
3. $\beta^0 \leftarrow 0$
4. while not converge do
5.   for $j = 1$ to $p$ do
6.     while true do
7.       $g_j \leftarrow \beta_j^k - t_j \nabla_{\beta_j} L(\beta^k)$
8.       $\hat{\gamma}_2 \leftarrow \Pi_{I_{t_j \lambda (1-\alpha)}}(g_{j,1})$
9.       $\hat{\gamma}_1 \leftarrow \Pi_{I_{t_j \lambda (1-\alpha)}}(g_j - [0, \hat{\gamma}_2^T]_T)$
10.      $\beta_j^{k+1} \leftarrow g_j - \hat{\gamma}_1 - [0, \hat{\gamma}_2^T]_T$
11.      if inequality (8) holds then
12.         break
13.      else
14.         $t_j \leftarrow \min(\eta t_j, 1/C_j)$
15.     $k \leftarrow k + 1$

3.2 Block Coordinate Descent

Although Algorithm 1 is applicable to any differentiable loss function $L$, in the special case of a quadratic loss, a more efficient solution strategy is available if we are willing to use an orthonormal basis expansion, $Q_j \in \mathbb{R}^{n \times M}$, of each feature $j$. Thus, in this section we assume that the design matrix $X = [Q_1 : \ldots : Q_p]$ and that $Q_j^T Q_j = I_M$. (We still require, as throughout this article, that the first column corresponds to the linear term.) In block
coordinate descent, we cycle through the $\beta_j$'s and for the $j$th block, solve the subproblem

$$\min_{\beta_j} \frac{1}{2N} \| r_j - Q_j \beta_j \|_2^2 + \lambda \alpha \| \beta_j \|_2 + \lambda (1 - \alpha) \| \beta_{j-1} \|_2, \tag{9}$$

where $r_j = y - \sum_{k \neq j} Q_k \beta_k$ is the $j$th partial residual.

For general $Q_j$, this update would require an iterative approach, but since $Q_j$ is an orthogonal matrix, we can equivalently minimize

$$\text{Algorithm 2 SPLAM via BCD (for quadratic loss $L$ and $Q_j \in \mathbb{R}^{n \times M}$ orthonormal)}$$

1: $\beta_0 \leftarrow 0$
2: while not converge do
3: for $j = 1$ to $p$ do
4: $g_j \leftarrow Q_j^T r_j$, where $r_j = y - \sum_{k \neq j} Q_k \beta_k$
5: $\hat{y}_2 \leftarrow \Pi_{j, \lambda(1-\alpha)}(g_{j-1})$
6: $\hat{y}_1 \leftarrow \Pi_{j, \lambda \alpha}(g_j - [0, \hat{y}_2^T]^T)$
7: $\beta_j \leftarrow g_j - \hat{y}_1 - [0, \hat{y}_2^T]^T$

$$\min_{\beta_j} \frac{1}{2N} \| Q_j^T r_j - \beta_j \|_2^2 + \lambda \alpha \| \beta_j \|_2 + \lambda (1 - \alpha) \| \beta_{j-1} \|_2, \tag{10}$$

which we recognize as the optimization problem from BCGD, in which we apply the proximal operator to $Q_j^T r_j$ instead of to $\beta_j - t_j \nabla_{\beta_j} L(\beta)$. Thus, by using BCD instead of BCGD we obviate the need to select a step size, making the optimization much more efficient.

To get the orthonormal basis, $Q_j$, we begin with a basis $X_j$ and then perform a QR decomposition for each block $j$ using the Gram–Schmidt process to preserve the linear basis in the first column of each block. Algorithm 2 summarizes our BCD algorithm.

### 4. STATISTICAL THEORY

In this section, we seek a deeper understanding of the regimes in which SPLAM works well. In Section 4.1, we prove an upper bound on SPLAM’s prediction error in the regression setting. This establishes SPLAM as a reliable method even when $p \gg N$ and gives insight into the factors that influence its prediction performance. In Section 4.2, we consider an asymptotic regime that highlights SPLAM’s potential statistical advantage over SpAM.

#### 4.1 ORACLE INEQUALITY

Oracle inequalities have been proved for the hierarchical group lasso (see, e.g., Chatterjee et al. 2012) that could be applied to SPLAM. These results follow from the unified framework of Negahban et al. (2012), which gives both oracle inequalities and recovery guarantees for a wide class of estimators based on decomposable regularizers. However, such results (and others of its kind) make potentially strong (and unverifiable) assumptions on the design matrix (e.g., the restricted isometry property, Candès and Tao 2007; the compatibility condition, Bühlmann and van de Geer 2011; van de Geer 2007; small coherence, Candès and Plan 2009, etc. See van de Geer and Bühlmann 2009). Since SPLAM’s
design matrix consists of derived features, such assumptions become even more difficult to interpret. There is, however, a different class of oracle inequalities, known as “slow rates,” that make no assumptions on the design matrix (Dalalyan, Hebiri, and Lederer 2014). In addition, despite their name, these inequalities have been shown in some cases to give faster rates of convergence than the more standard “fast rates” (Dalalyan, Hebiri, and Lederer 2014). They are particularly useful in situations where the various assumptions made by the fast rate bounds are known not to apply or would be particularly difficult to interpret.

We derive in this section slow rate bounds for SPLAM, thereby giving us an understanding of its statistical performance under no conditions on $X$. To the best of our knowledge, these are the first such slow rate bounds derived for the hierarchical group lasso.

Suppose

$$y_i = f^0(x_i) + e_i \text{ for } i = 1, \ldots, N,$$

where $x_i \in \mathbb{R}^p$ is a vector of features, $e_i \sim N(0, \sigma^2 I_N)$ is a random vector of noise, and $f^0$ is the underlying function. Let $\hat{\beta} \in \arg \min_{\beta \in \mathbb{R}^{pM}} \left\{ \frac{1}{2N} \| y - \sum_j X_j \beta_j \|_2^2 + \lambda \Omega^{\text{SPLAM}}(\beta) \right\}$ denote a solution of SPLAM in which we have orthogonalized each feature’s design matrix, that is, $\frac{1}{N}X_j^T X_j = I_M$ and let $\hat{f} = \sum_j X_j \hat{\beta}_j \in \mathbb{R}^N$ denote the set of fitted values at these $N$ points. The following theorem provides a slow rate for SPLAM’s prediction error. In an abuse of notation, we let $f^0$ denote the vector with $i$th element given by $f^0(x_i)$.

**Theorem 1.** If we take $\lambda \geq 2(1+2\sqrt{6})\sigma \sqrt{\log p/N}$ and $\alpha = (1+\sqrt{6})/(1+2\sqrt{6})$, then

$$\frac{1}{N} \| \hat{f} - f^0 \|^2 \leq \min_{\beta \in \mathbb{R}^{pM}} \left\{ \frac{1}{N} \| f^0 - \sum_{j=1}^p X_j \beta_j \|^2 + 3\lambda \Omega^{\text{SPLAM}}(\beta) \right\}$$

holds with probability at least $1 - 4/p$ as long as $\log p \geq M/8$.

**Proof.** See supplementary materials.

The above theorem makes no assumptions about the underlying function $f^0$, and shows that SPLAM works well if there exists $\beta$ for which $\sum_j X_j \beta_j$ is not too far from $f^0$ and $\Omega^{\text{SPLAM}}(\beta)$ is small. In the special case that $f^0 = \sum_j X_j \beta^0_j$ for some sparse vectors $\beta^0_1, \ldots, \beta^0_p$, the result takes a simpler form. We describe the sparsity of $\beta^0 \in \mathbb{R}^{pM}$ in two senses: first, in terms of whether a feature is at all relevant, $\mathcal{S}_0 = \{ j : \beta^0_j \neq 0 \}$, and, second, in terms of whether the feature is nonlinear, $\mathcal{N}_0 = \{ j : \beta^0_{j, -1} \neq 0 \}$. We also define the set of linear features, $\mathcal{L}_0 = \mathcal{S}_0 \setminus \mathcal{N}_0$. Under this stronger assumption on $f^0$, the statement simplifies greatly, revealing the roles that $\mathcal{L}_0$ and $\mathcal{N}_0$ play in the performance of the estimator.

**Corollary 1.** Suppose $f^0 = \sum_j X_j \beta^0_j$ with $\mathcal{L}_0$ and $\mathcal{N}_0$ defined as above. If we take $\lambda \geq 2(1+2\sqrt{6})\sigma \sqrt{\log p/N}$ and $\alpha = (1+\sqrt{6})/(1+2\sqrt{6})$, then

$$\frac{1}{N} \| \hat{f} - f^0 \|^2 \leq 3\lambda \left[ \alpha \sum_{j \in \mathcal{L}_0} | \beta^0_j | + \sum_{j \in \mathcal{N}_0} \| \beta^0_j \|_2 \right]$$

holds with probability at least $1 - 4/p$ as long as $\log p \geq M/8$. 

Proof. See supplementary materials. □

The above corollary implies that for suitably chosen \( \lambda \), SPLAM’s prediction error converges to 0 in probability as \( N \to \infty \) even if we let \( p \) grow like \( e^{\gamma N} \) with \( \gamma < 1 \) (assuming the sets \( \mathcal{L}_0 \) and \( \mathcal{N}_0 \) and the coefficients of features in this set remain fixed). It also shows that our error grows linearly in the number of both linear and nonlinear features in the true model. An interesting implication of the theorem is that \( \alpha \approx 0.58 \) is a theoretically justifiable choice (although better performance may be achievable by tuning \( \alpha \)).

When all features are linear (\( \mathcal{N}_0 = \emptyset \)), this result reduces to the traditional slow rate bound for the lasso (up to constants) (Rigollet and Tsybakov 2011). Such bounds have been improved for the lasso by careful incorporation of the design matrix (Hebiri and Lederer 2013), and we speculate that similar improvement could be developed here.

### 4.2 A Comparison to SPAM When All Features Are Linear

We have seen in the previous section that SPLAM is consistent in prediction error in the presence of both linear and nonlinear features even when \( p \gg N \). Since SpAM is a special case of SPLAM (with \( \alpha = 1 \)), similar bounds follow easily. A natural question then is whether there is any statistical reason to prefer SPLAM over SpAM (aside from the easier interpretation of a GPLAM over a GAM when many features are linear). Intuitively, it seems that when many features are truly linear, SpAM incurs variance for estimating nonlinear terms without a useful reduction in bias; on the other hand, for SPLAM this would not happen, assuming a sufficiently large parameter for the nonlinear-specific penalty. We make this intuition more precise by considering a scenario in which SPLAM is consistent whereas SpAM is not, implying that there is indeed a statistical advantage to using SPLAM.

Suppose that all \( p \) features are linear with equal coefficients, that is, \( \beta_0^j = b e_1 \in \mathbb{R}^M \), and consider an asymptotic regime in which \( p \) is fixed and \( N = pM \) with \( M, N \to \infty \) (note, Theorem 1 does not apply since here \( M > 8 \log p \)). We assume that all features are orthogonal, that is, \( \frac{1}{N} X^T X = I_N \), so that SpAM has a simple closed-form expression:

\[
\hat{\beta}_{\text{SpAM}}^j = \left( 1 - \frac{\lambda}{\| \frac{1}{N} X_j^T y \|_2} \right) + \frac{1}{N} X_j^T y.
\]

A several-line argument in the supplementary material establishes that

\[
\lim_{N,M \to \infty} \frac{1}{N} \| X \hat{\beta}_{\text{SpAM}} - X \beta_0 \|_2^2 \geq \frac{b^2}{1/b^2 + p/\sigma^2} > 0.
\]

Thus, in the asymptotic regime in which one allows the number of basis vectors to grow linearly with \( N \), one finds that the prediction error is bounded away from zero (regardless of the choice of \( \lambda \)). Interestingly, this lower bound matches (up to constants) the upper bound for the group lasso in Theorem 8.1 of Bühlmann and van de Geer (2011).

By contrast, consider SPLAM with \( \lambda \alpha = 0 \) and \( \lambda (1 - \alpha) = \infty \) (e.g., take \( \alpha \to 0 \) and \( \lambda = \alpha^{-1/2} \)). With this choice of parameters, it is apparent that \( \hat{\beta}_{\text{SPLAM}}^j = X_j^T y \cdot e_1 \) is simply the least-square solution on the correct set of variables and

\[
\lim_{N,M \to \infty} \frac{1}{N} \| X \hat{\beta}_{\text{SPLAM}} - X \beta_0 \|_2^2 \to 0.
\]
While assuming that the number of basis functions, $M$, is growing linearly in $N$ is of course particularly unfavorable to SpAM (indeed, Ravikumar et al. 2009 noted that $M$ growing like $N^{1/5}$ is a standard choice), it does serve to support the intuition regarding the statistical cost of incorrectly assuming nonlinearity. Indeed, in Section 5.1 (Figure 2) we show that there is a wide range of scenarios in which SPLAM does in fact have better performance than SpAM.

5. EMPIRICAL STUDY

In this section, we report experimental results for SPLAM. For all our experiments, we use cubic splines with 10 knots for basis expansion: $b(x_j) = [x_j, x_j^2, x_j^3, (x_j - x_{j1}^*)^3, \ldots, (x_j - x_{j10}^*)^3]$ (i.e., $M = 13$), where $(\cdot)^+$ represents the nonnegative part and the knot $x_{j1}^*$ is chosen from quantiles in the sample. We choose the best parameters on a held-out validation set and report model performance on a test set. The code is available at https://github.com/yinlou/mltk.

5.1 SYNTHETIC PROBLEM

To illustrate the use of SPLAM, we generate $N = 2000$ points from the model $y = 2\sin(2x_1) + x_2^2 + \exp(-x_3) + x_4 - 3x_5 + 2.5x_6 + 10x_7 + 2x_8 - 7x_9 + 5x_{10} + \epsilon$, where $\epsilon \sim \mathcal{N}(0, 1)$. In this experiment, we create an additional 90 random features (so $p = 100$). The first three nonlinear features are generated uniformly in $[-2.5, 2.5]$, and all other features are uniformly in $[0, 1]$.

We plot estimated components in Figure 1. Figure 1(a)–1(c) visualize the nonlinear components in SPLAM for $f_1$, $f_2$, and $f_3$, respectively. We can see that the estimated shape of the component function is very close to the true functions. On this sample, SPLAM perfectly recovers which features are linear and nonlinear while SpAM treats all selected features as nonlinear. For coefficients on linear components in SPLAM, the relative error is less than 0.1%. For comparison, we visualize $f_5$ in SpAM in red in Figure 1(d). The ground truth linear function is plotted in black. We can see that the component itself is not exactly linear and that it overfits to the noise.
In this section, we perform a large-scale simulation to gain deeper insights into the lasso (Tibshirani 1996), SPLAM, and SpAM (Ravikumar et al. 2009). We consider the models with $p = 100$ features: $y = \sum_{j \in L} x_j + \sum_{j \in N} \sin(x_j) + \epsilon$, where $\epsilon \sim N(0, 1)$, $L \cap N = \emptyset$. We use two parameters $\gamma$ and $\delta$ to control the cardinality of $L$ and $N$, respectively, that is, $|L| = \gamma p$ and $|N| = \delta p$. We choose $\gamma = 0, 0.1, \ldots, 1.0$ and $\delta = 0.0, 0.1, \ldots, 1.0$ ($\gamma + \delta \leq 1$), and for each $(\gamma, \delta)$ pair, we generate 10 different models. For each of those models, we generate $N_{\text{train}}$ points for training, $N_{\text{valid}}$ points for validation, and $N_{\text{test}}$ points for testing. We consider three different settings of simulations, $(N_{\text{train}}, N_{\text{valid}}, N_{\text{test}}) = (200, 100, 100), (500, 100, 100), (1000, 200, 200)$.

For SPLAM, we consider $\alpha \in \{0.05, 0.1, \ldots, 0.95, 1\}$. For all of the three methods, we consider the full regularization path with 100 $\lambda$‘s spaced evenly on a log scale. In our experiments, this range is sufficient to find the optimal model structure. Best model parameters are chosen using the validation set, and model accuracy is evaluated as the average RMSE of 10 models on test sets. For all successive experiments, we use the same method to choose parameters.

Figure 2 shows the results for the simulations. For each $(\gamma, \delta)$ pair, we plot which model wins on average. It is clear that for pure linear ($\delta = 0$) and pure additive ($\gamma = 0$), SPLAM has no advantage over the lasso or SpAM.

When $N_{\text{train}} = 200$, both SpAM and SPLAM overfit significantly when there are a lot of nonlinear components, since a large number of nonlinear components lead to a large parameter space and this small amount of data is not enough for reliable estimates. The lasso wins over the other methods on most of the cases by trading off variance for bias. SPLAM outperforms the lasso in regimes with a mixture of small nonlinear components and a reasonable number of linear components. When we increase the number of data points in the training set ($N_{\text{train}} = 500$), more reliable estimates can be obtained so SpAM wins back from the lasso on cases where we only have nonlinear components (the lasso, having only linear features, is incapable of estimating the nonlinear effects present in the data). Interestingly, the lasso is still the best when there are a lot of nonlinear components since in this regime the data cannot support the large number of parameters for reliable estimation. SPLAM, however, is the winner in most settings since it can better model the mixture of linear and nonlinear effects when there are enough data. Not surprisingly, when there are enough data ($N_{\text{train}} = 1000$), SPLAM dominates all cases in which both linear and nonlinear components are present. This is because the lasso is unable to model nonlinear effects and because SpAM has higher variance than SPLAM without being less biased.

### 5.3 Real Problems

In this section, we report experimental results on several real classification problems. We choose datasets with different dimensions and sizes. Table 1 summarizes the characteristics of the datasets and presents the predictive performance of the lasso, SPLAM, and SpAM with means and standard deviations on five trials. Best parameters are chosen on a held-out validation set on each trial. We note that SPLAM outperforms the lasso and SpAM on most of the trials. We also list the number of selected nonlinear features and total number of selected features in Table 1. In our experiments, features are forced to be linear
Table 1. Size (total number of points) and dimension of datasets and performance of methods. For each method, we report the mean error (standard deviation in parentheses) and how many of the selected features are nonlinear, written as $|\hat{N}|/(|\hat{N}| + |\hat{L}|)$. Bold indicates the method with the lowest mean error.

| Dataset       | Size  | Test  | $p$  | Lasso   | SPLAM   | SpAM   |
|---------------|-------|-------|------|---------|---------|--------|
| Spambase      | 4601  | 920   | 57   | 7.38 (0.87) | 0/52    | 6.57 (0.91) | 38/41 |
| Gisette       | 6000  | 1200  | 5000 | 2.43 (0.54) | 0/717   | 2.18 (0.59) | 10/733 |
| RCV1          | 697,641 | 418,584 | 47,236 | 2.71 (0.02) | 0/7652 | 2.67 (0.01) | 4/5293 |
| Pantheon      | 62,849 | 37,709 | 10,000 | 9.34 (0.12) | 0/1859 | 9.22 (0.16) | 27/1853 |

if they have fewer than 10 unique values. This is the case with SpAM on Gisette and RCV1 dataset.

Email Classification. We first consider a classification problem for detecting spam emails (Spambase) (Hastie, Tibshirani, and Friedman 2009). The features include statistics of particular words or letters in an email. We see from Table 1 that by allowing features to act nonlinearly, the error of SpAM decreases substantially compared to the lasso. However, by explicitly setting some of the variables to stay linear, SPLAM further outperforms SpAM.

Handwritten Digit Recognition. We use the “Gisette” dataset constructed from NIPS 2003 feature selection challenge (http://www.nipsfsc.ecs.soton.ac.uk/). The problem is to separate the highly confusible digits “4” and “9.” Features in this dataset contain pixels that are necessary to distinguish “4” from “9,” but higher order features from those pixels as well as random noise features are also added. Since the dimension of this dataset is significantly larger than the previous dataset while the size of the dataset remains similar, we expect SpAM to overfit as shown in Table 1. In our experiments, the best SpAM model that we can get is always worse than the lasso on each cross-validation set while our SPLAM outperforms the lasso on most cross-validation sets. Our SPLAM selects about 733 features, with about 10 of them being nonlinear and the rest being linear, while the lasso selects 717 features. This confirms that by allowing a small number of features to act nonlinearly, we can further improve the classification performance, and yet by setting most of the features as linear, we effectively control the complexity and avoid overfitting.

Text Categorization. Text categorization is an important task for many natural language processing applications. We use Reuters Corpus Volume I (RCV1) that involves binary classification (Lewis et al. 2004). From Table 1 we see that SPLAM outperforms the others. This suggests that in high dimensions, there is extra accuracy that can be obtained over the lasso if some features are allowed to be nonlinearly transformed. However, if all features are allowed to be nonlinearly transformed, such as in SpAM, the model will overfit and a suboptimal model is obtained. On average SPLAM selects 5293 features with 4 of them being nonlinear, and the lasso selects 7652 features. Figure 3 visualizes some components in SPLAM, SpAM, and the lasso. Each feature in this dataset relates to the (normalized) frequency of some word in a document. In general, we find that SPLAM strikes a compromise between the lasso and SpAM fits, using nonlinearity only sparingly. Figure 3(a) shows a feature that is identified as nonlinear by both SPLAM and SpAM. Notice that both SPLAM and SpAM find a model with similar shape. In Figure 3(b), we show a feature that appears to be nearly linear in SPLAM. In this case, SpAM oscillates in a way that might suggest that it is overfitting to the noise; by contrast, SPLAM’s fit is mostly linear, only exhibiting nonlinear effects when the input gets large. Notice SPLAM and the
Figure 3. Estimated component functions on RCV1 dataset.

The lasso almost agree with each other when the feature value is small. Finally, in Figure 3(c) we show a feature that is linear in both SPLAM and the lasso. SPLAM’s estimation of the slope is very similar to that of the lasso. By contrast, SpAM treats this as a nonlinear effect. In light of SPLAM’s better misclassification rate in this dataset, one might suppose that SpAM’s more pronounced deviations from linearity are in fact cases of overfitting to noise. Likewise, SPLAM’s better misclassification rate compared to the lasso suggests that the latter may be failing to model some of the nonlinear effects.

Image Matching. Many new computer vision applications are using large-scale datasets of places derived from the many billions of photos on the Web. Image matching is a central procedure to those applications that test whether two images are geometrically consistent (Lou, Snavely, and Gehrke 2012). Since image matching is an expensive procedure, image pairs are usually prefiltered with a lightweight classification procedure to estimate whether two images are likely to pass the geometric verification. In this study, we use the “Pantheon” dataset in Lou, Snavely, and Gehrke (2012). Each image is represented using a bag-of-visual-words model with a vocabulary of 10,000 visual words. From Table 1, we again observe that by carefully controlling the complexity of the model, SPLAM has better predictive performance than the other two models. On average the lasso selects 1859 features while SPLAM selects 1853 features with only 27 of them being nonlinear.

6. CONCLUSION

In this article, we introduce the sparse partially linear additive model that performs two model-selection tasks within a single convex hierarchical sparse regularization problem. This formulation permits an efficient optimization algorithm, making the GPLAM framework practical in machine learning settings. We develop an oracle inequality of SPLAM that makes no assumptions on the design matrix, and we study SPLAM’s advantage over SpAM when many of the features in the model are linear. Our thorough experiments demonstrate that SPLAM can effectively and accurately find relevant components with proper complexity and is very competitive for additive modeling. In particular, on large-scale, high-dimensional datasets, SPLAM improves accuracy over the popular linear model by allowing a small set of features to have a nonlinear effect.
SUPPLEMENTARY MATERIALS

In the supplementary materials, we include proofs of the theoretical results in this article, discuss practical issues regarding implementation of SPLAM, and present timing experiments for several algorithms.

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