High Dimensional Nonparametric Regresssion via Additive Kernel Ridge Models

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Abstract

We describe additive kernel ridge regression (Add-KRR), a generalisation of the kernel ridge method for nonparametric regression. Nonparametric regression is exponentially difficult in high dimensions. It is difficult to make progress without making strong assumptions about the function. A common assumption in high dimensional regression models is to assume that the function is additive. In this work, we leverage this assumption, but considerably generalise existing additive models. We propose a convex optimisation objective for our problem. We compare several algorithms to optimise this objective on synthetic datasets. We also demonstrate that Add-KRR significantly outperforms other popular algorithms for nonparametric regression on moderate dimensional problems.

1 Introduction

Nonparametric regression in high dimensions is an inherently difficult problem with known lower bounds depending exponentially in dimension [5]. Nonparametric methods typically work well only under at most $4-6$ dimensions. In this project we intend to make progress in this problem by treating the *estimate* of the function as an additive function of lower dimensional components.

Using additive models is fairly standard in high dimensional regression literature [6, 7, 11]. However, we wish to consider additive models which are more expressive than previous work. When the true underlying function f exhibits additive structure, using an additive model for estimation is understandably reasonable. However, even when f is not additive, using an additive model has its advantages. It is a well understoon notion in Statistics that when we only have a few samples, using a simpler model to fit our data may give us a better tradeoff for variance against bias. This is because additive functions are *statistically simpler* than more general (non-additive) functions. Typically, in most nonparametric regression methods using kernels such as the Nadaraya-Watson (NW) estimator and Kernel Ridge Regression (KRR), the bias-variance tradeoff is managed via the bandwidth of the kernel. However, this is only one way to manage the tradeoff. In this work we demonstrate that using an additive model provides another "knob" to control this tradeoff and provides significant gains in high dimensional regression.

Our methods are based on KRR, where we choose to model the low-order interaction implicitly using kernels acting on subsets of the coordinates (groups). We minimize the squared-error loss with a squared RKHS norm penalty to enforce smoothness and a mixed $\ell_{1,2}$-norm (group lasso style) penalty to enforce a sparse collection of functions. This leads to a convex objective function where the number of parameters is the product of the number of samples and the number of basis functions.

Our work extends Sparse Additive Models (SpAM) [11] to multidimensional nonparametric basis functions. Our proposed method also extends recent work on Generalized Additive Models plus Interactions [8]. However, in this work the interaction model was assumed to follow a specific

functional form, leading to an optimization method tailored to their interaction model. Our research is also related to existing work on using linear combinations of kernels for kernel learning, called multiple kernel learning [4].

Optimization for our proposed method is complicated by the non-smooth $\ell_{1,2}$-norm regularization penalty. Algorithms for group lasso have addressed this problem through a variety of approaches. Proximal gradient [1] has cheap iterations and relatively fast convergence if combined with acceleration. An block coordinate descent method has also been developed [10]. Further, the general Coordinate Gradient Descent method [13] can also be specialized to $\ell_{1,2}$-penalized problems [3, 9]. Recent work [16] on the group fused lasso has sidestepped the $\ell_{1,2}$-norm penalty, transforming it to a smooth objective with non-negativity constraint. Finally, safe screening rules for the group lasso have been developed [15] which quickly eliminate many of the all-0 groups. For Sparse Additive Models, parameters are typically optimized via the backfitting algorithm [11], a special case of (block) coordinate descent with group sizes of 1.

2 Problem Set up & Algorithm

2.1 Problem Statement & Notation

Let $f : \mathcal{X} \to \mathbb{R}$ be the function of interest. Here $\mathcal{X} \ni x = [x_1, \ldots, x_D] \in \mathbb{R}^D$ and $\mathcal{X} \subset \mathbb{R}^D$. We have data $(X_i, Y_i)_1^n$ and wish to obtain an estimate $\hat{f}$ of f. In this work, we seek an additive approximation to the function. That is, $\hat{f}$ can be expressed as,

$$\hat{f}(x) = \hat{f}^{(1)}(x^{(1)}) + \hat{f}^{(2)}(x^{(2)}) + \cdots + \hat{f}^{(M)}(x^{(M)}), \tag{1}$$

where $x^{(j)} \in \mathcal{X}^{(j)} \subset \mathbb{R}^{d_j}$ and $\hat{f}^{(j)} : \mathcal{X}^{(j)} \to \mathbb{R}$. We shall refer to the $\mathcal{X}^{(j)}$'s as *groups* and the collection of all groups $\bigcup_{j=1}^{M} \mathcal{X}^{(j)}$ as the *decomposition*. We are particularly interested in the case where D is very large and the group dimensionality is bounded– i.e. $d_j \leq d \ll D$.

The work in Hastie and Tibshirani [6] treats $\hat{f}$ as a sum of one dimensional components. The decomposition here corresponds to $x^{(j)} = x_j$, $d_j = d = 1$ $\forall j$ and $M = D$. In this project, we would like to be more expressive than this model. We will consider decompositions for which $d > 1$ and more importantly allows for overlap between the groups. For e.g. $\hat{f}(x_1, x_2, x_3) = \hat{f}^{(1)}(x_1) + \hat{f}^{(2)}(x_1, x_2) + \hat{f}^{(3)}(x_2, x_3)$. Ravikumar et al. [11] treat $\hat{f}$ as a sparse combination of one dimensional functions. While this is seemingly restrictive than [6], the sparse approximation may provide favourable bias-variance tradeoffs in high dimensions. Drawing inspiration from this, we will consider models where M is very large and seek a sparse collection of groups to approximate the function - i.e. $\hat{f}^{(j)} = \mathbf{0}$ for several j.

2.2 Additive Kernel Ridge Regression

We begin with a brief review on Kernel Ridge Regression. One of several ways to formulate a nonparametric regression problem is to minimise an objective of the form $J(f) = \sum_{i=1}^{n} \ell(f(X_i), Y_i) + \lambda P(f)$ over a nonparametric class of functions $\mathcal{F}$. Here ℓ is a loss function and P is a term that penalises the complexity of the function f. Several nonparametric regression problems such as smoothing splines, natural splines and Kernel Ridge Regression can be written this way. Central to KRR is a positive semidefinite kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ [12]. Then, $\mathcal{F}$ is taken to be the reproducing kernel Hilbert space (RKHS) $\mathcal{H}_k$ corresponding to k, P to be the squared RKHS norm of f and ℓ the squared error loss. Accordingly, KRR is characterised via,

$$\hat{f} = \operatorname*{argmin}_{f \in \mathcal{H}_k} \sum_{i=1}^{n} (Y_i - f(X_i))^2 + \lambda \|f\|_{\mathcal{H}_k}^2$$

However, as mentioned previously KRR suffers from the curse of dimensionality. To obtain an additive approximation using a given decomposition $\bigcup_j \mathcal{X}^{(j)}$, we consider kernels $k^{(j)} : \mathcal{X}^{(j)} \times \mathcal{X}^{(j)} \to \mathbb{R}$ acting on each group and their associated RKHSs $\mathcal{H}_{k^{(j)}}$. Further, since we will set M to be large and seek a sparse collection of functions in our additive model we introduce an additional

penalty term for nonzero $f^{(j)}$. Putting it all together, our additive Kernel Ridge Regressin (Add-KRR) is characterised via the following problem where we jointly optimise over $f^{(1)}, \ldots, f^{(M)}$,

$$\left(f^{(1)}, f^{(2)}, \ldots, f^{(M)}\right) = \underset{f^{(j)} \in \mathcal{H}_{k^{(j)}}, j=1,\ldots,M}{\operatorname{argmin}} F\left(\{f^{(j)}\}_{j=1}^{M}\right) \quad \text{where,} \tag{2}$$

$$F\left(\{f^{(j)}\}_{j=1}^{M}\right) = \frac{1}{2}\sum_{i=1}^{n}\left(Y_i - \sum_{j=1}^{M} f^{(j)}(x^{(j)})\right)^2 + \frac{\lambda_1}{2}\sum_{j=1}^{M}\|f^{(j)}\|^2_{\mathcal{H}_{k^{(j)}}} + \lambda_2 \sum_{j=1}^{M} \mathbb{1}(f^{(j)} \neq \mathbf{0})$$

Our estimate for f is then $\hat{f}(\cdot) = \sum_j \hat{f}^{(j)}(\cdot)$.

Via an argument that uses the representer theorem it is straightforward to show that $f^{(j)}$ will be in the linear span of the reprodcing kernel maps of the training points ${X^{(j)}}_1^n$ – i.e. $f^{(j)}(\cdot) = \sum_j \alpha^{(j)}{}_i k^{(j)}(\cdot, X_i^{(j)})$. Then, the j^{th} term inside the summations of the second and third terms of equation (2) can be written as ${\alpha^{(j)}}^\top K^{(j)} \alpha^{(j)}$ and $\mathbb{1}(\alpha^{(j)} \neq 0)$. Here $K^{(j)} \in \mathbb{R}^{n \times n}$ $\forall j$ such that ${K^{(j)}}_{rc} = k^{(j)}(X_r, X_c)$. Since the latter term is nonconvex we relax it via a group lasso type penalty. After simplifying the first term, our optimisation objective can be written as, $\boldsymbol{\alpha} = \operatorname{argmin}_{\boldsymbol{\alpha} \in \mathbb{R}^{nM}} F(\boldsymbol{\alpha})$ where,

$$F(\boldsymbol{\alpha}) = \frac{1}{2}\|Y - \sum_{j=1}^{m} K^{(j)}\alpha^{(j)}\|_2^2 + \frac{\lambda_1}{2}\sum_{j=1}^{M} {\alpha^{(j)}}^\top K^{(j)} \alpha^{(j)} + \lambda_2 \sum_{j=1}^{M} \|\alpha^{(j)}\|_2. \tag{3}$$

Here $\alpha^{(j)} \in \mathbb{R}^n$ $\forall j$, $\boldsymbol{\alpha} = [{\alpha^{(1)}}^\top, \ldots, {\alpha^{(M)}}^\top]^\top \in \mathbb{R}^{nM}$. Given the solution to the above, our estimate is obtained via $\hat{f}(\cdot) = \sum_{j=1}^{M}\sum_{i=1}^{n} \alpha^{(j)}{}_i k^{(j)}(\cdot, X_i^{(j)})$. Equation (3) will the (convex) optimisation problem in our algorithm. We call this algorithm Additive Kernel Ridge Regression and abbreviate it Add-KRR.

2.3 Practical Considerations

All that is left to do to complete the specification of our algorithm is to describe the allocation of coordinates into different groups and the kernel used for each such group. For the former, we tried 3 different strategies, all of which require the specification of a group size parameter d. The first sets $M = \binom{D}{d}$ and uses all combinations of size d groups. The second sets $M = \sum_{k=1}^{d}\binom{D}{k}$ and uses all combinations of up to size d. In the third we also specify M and then randomly generate M groups of size d. All three performed equally well so we only consider the third option as M does not grow combinatorially with D and d.

As is the case in most kernel methods, the choice of the kernel is important for good empirical performance. For each $k^{(j)}$ we use an RBF kernel, with scale σ_j and bandwidth h_j.

$$k^{(j)}(x_s^{(j)}, x_t^{(j)}) = \sigma_j \exp\left(\frac{\|x_s^{(j)} - x_t^{(j)}\|_2^2}{2h_j^2}\right)$$

Here σ_j captures the variation in the output and h_j captures the variation in the input. In KRR, these parameters along with the penalty coefficient λ are chosen via cross validation. However, this is infeasible in our setting as M is potentially very large. In our case we set $h_j = 1.5\|\text{std}({X^{(j)}}_1^n)\|_2 n^{\frac{-1}{4+d_j}}$. Here $\text{std}({X^{(j)}}_1^n)$ is the vector of standard deviations of the training dataset on the coordinates belonging to group j. This choice of bandwidth is motivated by the Silverman bandwidth and several kernel methods which choose a bandidth on the order $O(n^{\frac{-1}{2\beta+p}})$ where β is the smoothness of the function [14] and p is the dimensionality. We set $\sigma_j = \text{std}(Y)/\sqrt{M}$ to capture the per group variance. The performance of the algorithm was usually insensitive to the choices of h_j and σ_j provided they were roughly in the correct range. The penalty coefficients λ_1 and λ_2 are chosen via cross validation.

3 Optimisation Methods

Subgradient Method

Because our objective function is non-smooth, the simplest method is to solve it via the subgradient method. We implemented subgradient method with decreasing step sizes for our experiments. While subgradients can be computed cheaply in $O(nM)$, we observed poor convergence on our problem.

Proximal Gradient Method

Note that we can write the objective (3) as $F(\boldsymbol{\alpha}) = G(\boldsymbol{\alpha}) + \Psi(\boldsymbol{\alpha})$ where G is smooth and Ψ is not. Ψ is the popular group lasso penalty. Via the Moreau decomposition, and using the fact that the argument in the prox operator is separable, the prox operator can be shown to be,

$$[\text{prox}_{\Psi,t}(\boldsymbol{\alpha})]^{(j)} = \text{prox}_{\Psi,t}(\alpha^{(j)}) = \begin{cases} \alpha^{(j)} - t\frac{\alpha}{\|\alpha^{(j)}\|_2} & \text{if } \|\alpha^{(j)}\| < t \\ \mathbf{0} & \text{otherwise} \end{cases}$$

Obtaining the prox operator takes $O(nM)$ time and has cost comparable to computing the gradient of $G(\boldsymbol{\alpha})$. We use the above to implement proximal gradient method as described in the class notes. We use backtracking to determine the step size and experimented both with and without acceleration.

Exact Block Coordinate Descent via Newton trust region

We can optimize the objective function over group $\alpha^{(j)}$ with all other groups $\alpha^{(i)}, i \neq j$ fixed. The objective is then

$$\arg\min_{\alpha^{(j)}} \frac{1}{2}{\alpha^{(j)}}^T A_j \alpha^{(j)} + b_j^T \alpha^{(j)} + \lambda_2 \|\alpha^{(j)}\|_2$$

where $A_j = {K^{(j)}}^T K^{(j)} + \frac{\lambda_1}{2} K^{(j)}$ and $b_j = -{K^{(j)}}^T (y - \sum_{i \neq j} K^{(i)} \alpha^{(i)}$. This problem can be efficiently solved [10] by converting it to a one-dimensional trust-region problem. When $\|b_j\|_2 \leq \lambda_2$, we have $\alpha^{(j)} = 0$. Otherwise, there exists t_j such that $\alpha^{(j)}$ is the solution of the following problem

$$\arg\min_{\alpha^{(j)}} \frac{1}{2}{\alpha^{(j)}}^T A_j \alpha^{(j)} + b_j^T \alpha^{(j)}, \text{ such that } \|\alpha^{(j)}\|_2 \leq t_j.$$

If t_j is known we have $\alpha^{(j)} = t_j * \left(-(t_j A_j + \lambda_2 I_n)^{-1} b_j\right)$ Because in this case $\|\alpha^{(j)}\|_2 = t_j$, we have $\|(t_j A_j + \lambda_2 I_n)^{-1} b_j\|_2 = 1$. As described in Qin et al. [10], we can use Newton's method to solve this equation efficiently using the eigendecomposition of A_j, which is constant and needs to be computed only once. However, this method does not scale well with n, since we still need to solve an $n \times n$ linear system after t_j is computed. Thus, updating all blocks costs $O(n^3 M)$.

Block Coordinate Gradient Descent

Because $\Psi(\boldsymbol{\alpha})$, our $\ell_{1,2}$ group lasso penalty, is non-smooth yet block-separable, we can apply the Coordinate Gradient Descent method [13]. For each block of $\alpha^{(j)}$, we solve

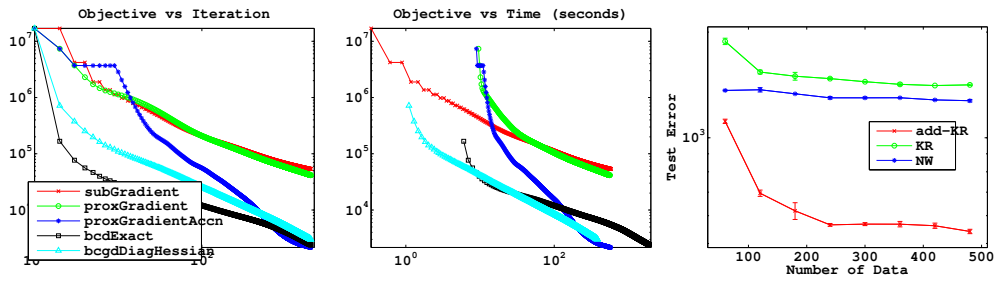
$$\arg\min_{d_j} \frac{1}{2} d_j^T H_j d_j + \nabla_j G(\boldsymbol{\alpha})^T d_j + \lambda_2 \|\alpha^{(j)} + d_j\|_2$$

where $H_j \approx \nabla^2_{jj} G(\boldsymbol{\alpha}) = {K^{(j)}}^T K^{(j)} + \frac{\lambda_1}{2} K^{(j)}$ and $\nabla_j G(\boldsymbol{\alpha}) = -{K^{(j)}}^T (y - \sum_{i \neq j} K^{(i)} \alpha^{(i)})$. As suggested Tseng and Yun [13], we use a diagonal matrix to approximate the true block Hessian. We set $H_j = \max(\text{diag}(\nabla^2_{jj} G(\boldsymbol{\alpha})))I_n := h_j I_n$, so that a closed-form solution exists for d_j:

$$d_j = \frac{1}{h_j}\left(\lambda_2 \frac{\nabla_j G(\boldsymbol{\alpha}) - h_j \alpha^{(j)}}{\|\nabla_j G(\boldsymbol{\alpha}) - h_j \alpha^{(j)}\|_2}\right).$$

We use backtracking to determine the step size, then update $\alpha^{(j)} \leftarrow \alpha^{(j)} + t d_j$.

Because the Hessian is constant, each block update costs $O(n)$ and updating all blocks costs $O(nM)$. Alternatively, as suggested in Friedman et al. [3], rather than using the diagonal Hessian approximation, we could approximately solve each block subproblem via coordinate descent.



(a) (b) (c)

Figure 1:Figures (a) and (b) plot the objective value vs iteration and cpu time respectively. Accelerated proximal gradient descent (blue curve) seems to perform best. Figure (c) plots the test set error for Add-KRR , KRR and NW on a synthetic problem. Add-KRR outperforms both methods.

4 Experiments

We experimentally evaluate two criteria: the performance of the different optimisation algorithms to minimise (3), and the performance of Add-KRR and other nonparametric regression methods.

Experimental set up : For our synthetic experiments, we take $\mathcal{X} = [-1, 1]^D$. We constructed a function of 3 modes by taking the logarithm of 3 Gaussian bumps whose centres are randomly chosen from $\mathcal{X}$. We uniformly randomly sample 500 points each for training and testing from $\mathcal{X}$ and uses the true function values as the labels. In the examples we consider below we take $D = 20$, $d = 4$ and $M = 50$. Therefore, our optimisation problem had $50 \times 500 = 25,000$ parameters.

Comparison of Optimisation Algorithms : We compared the five methods specified above on the synthetic example outlined above. Figures 1(a) and (b) shows the improvement in the objective over iterations and time respectively over 2000 iterations. subGradient and proxGradient exhibit slow convergence but proxGradientAccn , bcdExact and bcdDiagHessian perform quite well. proxGradientAccn does marginally better than the rest. Even for different values of D, d, M we found that the latter three methods did better but their relative performances varied slightly. In our experiments below we use proxGradientAccn .

Comparison with other Regression Algorithms : We use the same experimental set up as explained above to compare Add-KRR against the KRR and NW methods. To choose the kernel bandwidth for NW we used 5-fold cross validation. Due to time constraints, parameter selection for Add-KRR and KRR was very coarse – we tried only 5 different choices for (λ_1, λ_2) and used 2-fold cross validation. Despite this, Add-KRR significantly ourperforms both KRR and NW on the synthetic problem. The results are depicted in Figure 1(c). These results are quite encouraging as they attest well to our intuitions about favourable bias variance tradeoffs when using (statistically simpler) additive models for high dimensional regression.

Parkinson's Speech Dataset : We compared Add-KRR, KRR and NW on the above dataset from the UCI repository. We used 21 of the given features to predict the median pitch of the speaker. The dataset had 1040 instances, and we split them up equally for training and testing. For Add-KRR we used $M = 50$, $d = 4$. The test set errors for Add-KRR, KRR and NW were respectively 482.31, 1071.80 and 1072.88. As before, Add-KRR outperforms other alternatives.

5 Conclusion

Our initial results using the proposed method is fairly promising. Going forward we wish to perform comparisons with other nonparametric regression methods such as Gaussian process regression, locally polynomial regression and other additive models [2, 6, 11] on other synthetic and real datasets.

Because we hope to apply the proposed method to high-dimensional problems, we are especially interested in making the proposed method scalable for large M. A safe screening method [15] was recently developed for the group lasso problem. We hope to adapt this method to our problem, which could potentially lead to large speedup since for high-dimensional problems only a small fraction of the M groups will be chosen as non-zero.

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