Variable projection for nonsmooth models

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Abstract
Variable projection solves structured optimization problems by completely minimizing over a subset of the variables while iterating over the remaining variables. Over the last 30 years, the technique has been widely used, with empirical and theoretical results demonstrating both greater efficacy and greater stability compared to competing approaches. Classic examples have exploited closed form projections and smoothness of the objective function. We extend the approach to problems that include nonsmooth terms, and where the projection subproblems can only be solved inexactly by iterative methods. We propose an inexact algorithm for solving such problems and analyze its computational complexity. Finally, we show how the theory can be used to design methods for selected problems occurring frequently in machine-learning and high-dimensional inference.

1 Introduction
In this paper we consider finite-dimensional optimization problems of the form

\[ \min_{x,\theta} f(x, \theta) + r_1(x) + r_2(\theta), \]

(1)

where \( f \) smoothly couples \((x, \theta)\) but may be non-convex, while \( r_1 \) and \( r_2 \) may be constraints or regularizers. We are particularly interested in the case where \( f(x, \cdot) + r_2 \) is (strongly) convex in \( \theta \), so that fast solvers are available for optimizing over \( \theta \) for fixed \( x \).

These problems arise any time nonsmooth regularization or constraints are used to regularize solutions to certain difficult non-linear inverse problems or regression problems. We give two motivating examples below.

**Exponential fitting** Consider the non-linear exponential fitting problem

\[ \min_{x,\theta} \|A(x)\theta - y\|^2, \]

where the entries of \( A(x) \) are exponential functions of \( x \), while \( \theta \) recovers the linear combinations of interest. Including constraints or sparse regularization on \( \theta \), or bounds on the exponential terms \( x \) immediately gives rise to a problem of form \([1]\).

**DE-constrained optimization problems** Consider a relaxed form of a PDE- or ODE-constrained optimization problem

\[ \min_{x,\theta} \|R\theta - y\|^2 + \lambda\|A(x)\theta - q\|^2, \]

(2)

where \( A(x)\theta = q \) represents the DE, \( x \) are the parameters of interest and \( q \) represents a source term or initial condition, \( R \) is a linear map that yields observations \( y \). Simple regularization of the solution \( \theta \) or DE parameters \( x \) recovers \([1]\).

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The development of specialized algorithms for (1) goes back to the classic Variable Projection (VP) technique for separable non-linear least-squares problems of the form:

$$\min_{x,\theta} \| A(x)\theta - y \|^2_2,$$

where the matrix-valued map $A: \mathbb{R}^n \to \mathbb{R}^{m \times k}$ is smooth and the matrix $A(x)$ has full rank for each $x$. Early work on the topic, notably by Golub and Pereyra (1973) has found numerous applications in chemistry, mechanical systems, neural networks, and telecommunications. See the surveys of Golub and Pereyra (2003) and Osborne (2007), and references therein.

The VP approach is based on eliminating the variable $\theta$, as for each fixed $x$ we have

$$\theta(x) = A(x)^\dagger y,$$

where $A(x)^\dagger$ denotes the pseudo-inverse of $A(x)$. We can thus express (3) as

$$\min_x \| (A(x)A(x)^\dagger - I)y \|^2_2,$$

which is a non-linear least-squares problem. Note that $A(x)A(x)^\dagger - I$ is an orthogonal projection of $y$ onto the null-space of $A(x)^T$; hence the name variable projection.

It was shown by Golub and Pereyra (1973) that the Jacobian of $A(x)A(x)^\dagger$ contains only partial derivatives of $A(x)$ w.r.t. $x$ and does not include derivatives of $\theta(x)$ w.r.t. $x$. Ruhe and Wedin (1980) showed that when the Gauss-Newton method for (3) converges superlinearly, so do certain Gauss-Newton variants for (4).

Numerical practice shows that the latter schemes actually outperform the former on the account of a better conditioning of the reduced problem.

The underlying principle of the VP method is much broader than the class of separable non-linear least squares problems. For example, Bell and Burke (2008), Aravkin and van Leeuwen (2012) consider the class of problems

$$\min_{x,\theta} f(x, \theta),$$

where $f: \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$ is a $C^2$-smooth function; the classic VP problem (3) is a special case of (5). Although we generally do not have a closed-form expression for $\theta(x)$, we define it as

$$\theta(x) = \arg\min_x f(x, \theta),$$

and express (5) using the projected function

$$\overline{f}(x) := f(x, \theta(x)).$$

Projection in the broader context of (5) refers to epigraphical projection [Rockafellar and Wets (1998)], or partial minimization of $\theta$.

Under mild conditions, $\overline{f}(x)$ is $C^2$ – smooth as well and its gradient is given by

$$\nabla \overline{f}(x) = \nabla_x f(x, \theta(x)),$$

i.e., it is the gradient of $f$ w.r.t. $x$, evaluated at $\theta$. [Bell and Burke (2008)]. Again, we do not need to compute any sensitivities of $\theta(x)$ w.r.t. $x$. This is seen by formally computing the subdifferential of $\overline{f}$ using the chain-rule:

$$\partial_x \overline{f} = \partial_x f(x, \theta(x)) + \partial_\theta f(x, \theta(x)) \cdot \partial_\theta \theta(x).$$

Since $\theta(x)$ is a minimizer of $f(x, \theta)$ it satisfies $\partial_\theta f(x, \theta(x)) = 0$ and the second term vanishes. It turns out that the Hessian of $\overline{f}$ is the Schur complement of $\partial_\theta^2 f$ of the full Hessian of $f$ [Ruhe and Wedin (1980)]. It follows that a local minimizer, $x^*$, of $\overline{f}$ together with $\theta(x^*)$ constitute a local minimizer of $f$. The expression for the derivative furthermore suggests that we can approximate the gradient of $\overline{f}$ when $\theta(x)$ is known only approximately by ignoring the second term.
We may extend this approach to solve problems of the form (1) by including $r_2$ in the computation of $\vartheta(x)$ and using an appropriate algorithm to minimize $\bar{f} + r_1$. We can then view the entire approach as prox-gradient descent on the projected function $\bar{f}$:

$$x^+ = \operatorname{prox}(x - \alpha \nabla \bar{f}(x))$$

where $\alpha$ is an appropriate step. The gradient $\nabla \bar{f}$ is computed using partial minimization, as shown in Algorithm 1.

Algorithm 1 Prototype algorithm for solving (1)

Input: Initial iteration, $x$, estimate of the Lipschitz constant, $L$, of $\bar{f}$

while not converged do

$\vartheta := \operatorname{argmin}_{\theta} f(x, \theta) + r_2(\theta)$

$x := \operatorname{prox}_{(1/L)r_1}(x - (1/L)\nabla_x f(x, \vartheta))$

The goal of this paper is to extend the variable projection technique to problems of the form (5) with nonsmooth regularization terms, which arise in high-dimensional statistics, signal processing, and many machine learning problems; sparse regularization and simple constraints are frequently used in this setting.

Contributions Our contributions are as follows:

1. Using results from variational analysis to establish conditions under which $\bar{f}$ is smooth and its gradient can be evaluated by (7);
2. Proposing a simple smoothing technique for cases (1) where $\bar{f}$ is nonsmooth;
3. Proposing an inexact Algorithm 1 based on inexact evaluations of $\vartheta(x)$.

In Section 2 we develop derivative formulas for the value function (6) and design an inexact version of Algorithm 1. In Section 3 we present a few case studies. Conclusions complete the paper.

2 Derivative Formulas and Inexact VP

In this section, we present derivative formulas and develop the approaches briefly described in the introduction.

2.1 Derivatives and Partial Minimization

[Rockafellar and Wets(1998)] Theorem 10.58 establishes strict differentiability of projected functions, along with derivative formulas.

Theorem 1 (Derivative of the projected function). Consider a function $f : \mathbb{R}^n \times \mathbb{R}^k \to \mathbb{R}$ satisfying the following properties

1. $f$ is continuous;

2. for any $\alpha \in \mathbb{R}$ and any compact set $X \subset \mathbb{R}^n$, the union of sublevel sets $\bigcup_{x \in X} \{\theta : f(x, \theta) \leq \alpha\}$ is bounded.

3. the gradient $\nabla_x f(x, \theta)$ exists for all $(x, \theta)$ and depends continuously on $(x, \theta)$.

Denote the projected function and the minimizing set as

$$\bar{f}(x) := \inf_{\theta} f(x, \theta) \quad \text{and} \quad \Theta(x) := \operatorname{argmin}_{\theta} f(x, \theta).$$

Then $\bar{f}$ is strictly differentiable at any point $x$ for which the set of minimizers $\{\nabla_x f(x, \theta) : \theta \in \Theta(x)\}$ is a singleton, and in this case we have $\nabla \bar{f}(x) = \nabla_x f(x, \vartheta(x))$ holds.
Then the function

\[ f(x, \theta) = \theta_1(x + 1)^2 + \theta_2(x - 1)^2 + \delta_{\hat{\Delta}_1}(\theta), \]  

where \( \hat{\Delta}_1 = \{ \theta \in [0,1]^2 : \theta_1 + \theta_2 = 1 \} \) is the capped simplex and \( \delta_C(\cdot) \) denotes the indicator function of the set \( C \) (i.e., \( \delta_C(\theta) = 0 \) if \( \theta \in C \) and \( \delta_C(\theta) = \infty \) otherwise). At \( x = 0 \), any \( \theta \in \hat{\Delta}_1 \) is a minimizer and so the set \( \Theta(0) \) is not a singleton. The minimizers can be made unique, however, by adding a small quadratic:

\[ f_\beta(x, \theta) = f(x, \theta) + (\beta/2)\|\theta\|^2. \]  

The resulting projected function \( \bar{f}_\beta \) is smooth as can be seen in Figure 1. However, the smoothing is also a modification to the original problem. As \( \beta \downarrow 0 \), we approach the original (nonsmooth) model.

The quadratic plays a key role in variable projection, and its presence covers cases where Theorem 1 does not apply; particularly when \( \theta \) is constrained, as in (13). The next theorem is adapted from \( \text{Rockafellar and Wets}(1998) \) [Theorem 2.26] and complements Theorem 1.

**Theorem 2** (Moreau). Let \( g : \mathbb{R}^m \to \mathbb{R} \) be any closed convex function, and let \( B \in \mathbb{R}^{n \times m} \) be any linear map. Define 

\[ f(z, \theta) := \frac{\eta}{2} \|z - \theta\|^2 + g(\theta). \]

Then the function \( \bar{f} : \mathbb{R}^n \to \mathbb{R} \)

\[ \bar{f}(z) := \min_{\theta} f(z, \theta) \]

is \( C^1 \) with \( \nabla \bar{f}(z) = \eta(z - \bar{\theta}) \) for the unique \( \bar{\theta} \in \Theta(x) \), and \( \text{lip}(\nabla \bar{f}(z)) \leq \eta. \)

Theorem 2 is useful since the assumptions on \( g \) are weak. In particular \( g \) could be the indicator function of a convex set, encoding equality and inequality constraints. In (8), we take \( g(\theta) = \delta_{\hat{\Delta}_1}(\theta) \), and rewrite \( f_\beta(x, \theta) \) in (10) as

\[ f_\beta(x, \theta) = g(\theta) + \frac{\beta}{2} \|\theta + \left[\frac{(x + 1)^2/\beta}{(x - 1)^2/\beta}\right]\|^2 - \frac{1}{2\beta} \left\|\left[\frac{(x + 1)^2}{(x - 1)^2}\right]\right\|^2. \]

The smoothness of \( \bar{f}_\beta(x) \) and its gradient formula follow immediately by introducing the composition

\[ z(x) = \left[\frac{(x + 1)^2}{(x - 1)^2}\right]^T \]

and applying Theorem 2 together with the standard chain rule. A similar argument gives a general result for a broad range of exponential fitting problems that include nonsmooth regularizers and/or constraints.

**Corollary 1** (Exponential fitting). Consider the function

\[ f(x, \theta) = \frac{1}{2} \|A(x)\theta - y\|^2 + g(\theta), \]

where

\[ A(x) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \frac{\eta}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \]

The smoothness of \( \bar{f}_\beta(x) \) and its gradient formula follow immediately by introducing the composition

\[ z(x) = \left[\frac{(x + 1)^2}{(x - 1)^2}\right]^T \]

and applying Theorem 2 together with the standard chain rule. A similar argument gives a general result for a broad range of exponential fitting problems that include nonsmooth regularizers and/or constraints.
where \( g \) is any closed convex function and either \( A(x) \) is a full-rank \( C^1 \) map, with \( A(x)^T A(x) \) invertible for every \( x \), or \( g \) is strongly convex, then

\[
\overline{f}(x) = \min_\theta f(x, \theta)
\]

is \( C^1 \) with gradient given by

\[
\nabla \overline{f}(x) = J(x)(A(x)\overline{\theta} - y), \quad J(x) = \partial_x(A(x)\theta)
\]

for the unique \( \overline{\theta} \in \Theta(x) \).

**Proof:** For \( x \) fixed, set \( A \equiv A(x) \). Since \( A^T A \) is invertible, we can compute the Cholesky decomposition

\[
A^T A = LL^T.
\]

Now, using the substitution \( z = L^T \theta \) and completing the square, we can rewrite (11) as

\[
f(x, z) = \frac{1}{2} \|z - L^{-1}A^T y\|^2 + g(L^{-T}z) - \frac{1}{2} \|L^{-1}A^T y\|^2.
\]

The conclusion follows immediately by Theorem 2. If \( A \) is not invertible but \( g(\theta) \) is strongly convex, i.e. can be written as \( \tilde{g}(\theta) + \alpha \|\theta\|^2 \) for \( \alpha > 0 \), repeat the proof with \( LL^T = (A^T A + \alpha I) \).

**Corollary 2** (DE-Constrained Optimization with Nonsmooth Loss). Consider the modified problem (2):

\[
f(x, \theta) = g(R\theta - y) + \lambda \|A(x)^{-1}q - \theta\|^2,
\]

where \( g \) is any closed convex function. Then

\[
\overline{f}(x) = \min_\theta f(x, \theta)
\]

is \( C^1 \) with gradient given by

\[
\nabla \overline{f}(x) = \lambda J(x)(A(x)q - \overline{\theta}), \quad J(x) = \partial_x(A(x)^{-1}q).
\]

for the unique \( \overline{\theta} \in \Theta(x) \).

Corollary 2 shows that ODE-constrained optimization with sharp data fit loss, such as the \( \ell_1 \)-norm, are still smooth in the underlying \( x \) parameter.

### 2.2 Inexact Gradients

In many applications, we do not have a closed-form expression for \( \overline{\theta} \) and it must be computed with an iterative scheme. To make the algorithms efficient, it is desirable to stop the inner computation early, giving an inexact gradient of the projected function.

Given an approximation, \( \overline{\theta}_\epsilon \) of \( \overline{\theta} \), we may approximate \( \overline{f} \) and its gradient as

\[
\overline{f}_\epsilon(x) = f(x, \overline{\theta}_\epsilon),
\]

\[
\nabla \overline{f}_\epsilon(x) = \nabla_x f(x, \overline{\theta}_\epsilon).
\]

The errors can bounded as

\[
|\overline{f}_\epsilon(x) - \overline{f}(x)| \leq L_\theta(x)\|\overline{\theta}_\epsilon(x) - \overline{\theta}(x)\|,
\]

\[
||\nabla \overline{f}_\epsilon(x) - \nabla \overline{f}(x)|| \leq L_{x\theta}(x)\|\overline{\theta}_\epsilon(x) - \overline{\theta}(x)\|,
\]

where \( L_\theta(x) \) is the Lipschitz constant of \( f(x, \cdot) \) and \( L_{x\theta} \) is the Lipschitz constant of \( \nabla_x f(x, \cdot) \).

Once (15) and (16) are established, we can minimize \( \overline{f} \) with inexact gradients, replacing the basic iteration (8) by

\[
x^+ = \text{prox}_{\alpha \nabla \overline{f}(x)}(x - \alpha \nabla \overline{f}_\epsilon(x)),
\]
Table 1: Complexity in terms of the total number of iterations (inner × outer) needed to reach an outer tolerance of $\tau = 1/p$ for various combinations of inner and outer algorithms.

| inner / outer | linear $\rho^t$ | sublinear $t^{-2}$ | sublinear $t^{-1}$ |
|---------------|------------------|---------------------|---------------------|
| linear $\rho^t$ | $(\log p)^2$ | $\sqrt{p} \log p$ | $p \log p$ |
| sublinear $t^{-1}$ | $\sqrt{p}$ | $p$ | $p \sqrt{p}$ |
| sublinear $t^{-2}$ | $p$ | $p \sqrt{p}$ | $p^2$ |

with details given in Algorithm 2 [Devolder et al.(2014)Devolder, Glineur and Nesterov]. Devolder et al. looks at smooth optimization with an inexact oracle, while [Schmidt et al.(2011)Schmidt, Roux and Bach] develops inexact proximal gradient methods.

When $f(x, \cdot)$ is strongly convex, it allows for a linearly convergent algorithm and we can compute $\theta_\epsilon$ in $O(\log \epsilon^{-1})$ iterations. When $\tilde{f}$ is strongly convex as well, an inexact gradient method will converge linearly when decreasing the tolerance exponentially with the iteration, e.g., $\epsilon_t = \gamma^t$ with $\gamma < 1$ [?, prop. 4]schmidt2011convergence.

Algorithm 2 Algorithm for (1) with inexact inner solves

Input: Initial iteration, $x$, estimate of the Lipschitz constant, $L$, of $\tilde{f}$, initial tolerance, $\epsilon$ and rate $\gamma$.

while not converged do
    $\theta_\epsilon := \arg\min_{\theta} f(x, \theta) + r_2(\theta)$
    $x := \text{prox}_{\frac{1}{L} f(x, \theta_\epsilon)} (x - \frac{1}{L} \nabla f(x, \theta_\epsilon))$
    $\epsilon := \gamma \epsilon$

A total of $T$ outer iterations of Algorithm 2 then has an asymptotic complexity of

$$\sum_{t=1}^{T} \log(\epsilon_t^{-1}) = \sum_{t=1}^{T} t \log(\gamma^{-1}) = O(T^2).$$

Aiming for an overall tolerance of $\tau$, then takes $O(\log 1/\tau)$ outer iterations, which has an asymptotic complexity of $O\left((\log 1/\tau)^2\right)$.

If the outer algorithm has a slower convergence rate, we can decrease the tolerance $\epsilon$ at a slower rate as well [Schmidt et al.(2011)Schmidt, Roux and Bach]. The overall complexity of various combinations of inner/outer convergence rates is listed in Table 1.

3 Case studies

3.1 Exponential data-fitting

We begin with the general class of exponential data-fitting problems – one of the prime applications of variable projection [Pereyra and Scherer(2012)]. The general formulation of these problems assumes a model of the form

$$y_i = \sum_{j=1}^{k} \theta_j \exp(-\phi_{ij}(x)),$$

where $\theta \in \mathbb{R}^k$ are unknown weights, $y \in \mathbb{R}^m$ are the measurements, and $\phi_{ij}$ are given functions that depend on an unknown parameter $x \in \mathbb{R}^n$. Some examples of this class are given in table 2.

In many applications it is natural to include a regularization term and formulate the problem as

$$f(x, \theta) = \|A(x)\theta - y\|_2^2 + \lambda r(\theta).$$

For example, [Cornelio et al.(2012)Cornelio, Piccolomini and Nagy] Shearer and Gilbert(2013) consider positivity constraints $\theta \geq 0$, in which case $r$ is the indicator function of the positive cone. Another natural
Table 2: Some examples of exponential data-fitting in applications.

| problem          | known       | unknown      | $\phi_{ij}$ |
|------------------|-------------|--------------|-------------|
| pharmaco-kinetic | $t_j$       | decay $x_i t_j$ |             |
| signal classification | $h_j$ | directions $x_i$ | $x_i h_j$ |
| radial basis functions | $c_j$ | centers $x_i$ and scales $\alpha_i$ | $\alpha_i^2 \|x_i - c_j\|^2$ |

regularization is $r(\cdot) = \|\cdot\|_1$ which enforces sparsity of $\theta$. This is useful in cases where the system is over-parametrized and we are looking for a fit of the data with as few components as possible. The differentiability of the resulting projected functions is guaranteed by Corollary 2.

3.2 Trimmed Robust Formulations in Machine Learning

Many formulations in high-dimensional regression, machine learning, and statistical inference can be formulated as minimization problems

$$\min_x \sum_{i=1}^n f_i(x) + r(x),$$

where the training set comprises $n$ examples, $f_i$ is the error or negative log-likelihood corresponding to the $i$th training point, and $r(x)$ is a smooth regularizer.

All of these approaches can be made robust to perturbations of input data (for example, incorrect features, gross outliers, or flipped labels) using a trimming approach. The idea, first proposed by [Rousseeuw(1984)] in the context of least squares fitting, is to minimize the $\ell \leq n$ best residuals. The general trimmed approach, formulated and studied by [Yang et al.(2016)Yang, Lozano and Aravkin], considers the equivalent formulation

$$\min_{x, \theta} \sum_{i=1}^n \theta_i f_i(x) + r(x), \quad \theta \in \hat{\Delta}_\ell,$$

$$\hat{\Delta}_\ell := \{\theta \in [0,1]^n : 1^T \theta = \ell\}.$$

The set $\hat{\Delta}_\ell$ is known as the capped simplex, and admits and efficient projection [Aravkin and Davis(2016)]. Jointly solving for $(x, \theta)$ detects the $\ell$ inliers as the model $x$ is fit. Indeed, the reader can check that the solution in $\theta$ for fixed $x$ selects the smallest $\ell$ terms $f_i$. The problem therefore looks like a good candidate for VP, but the projected function $\bar{f}(x)$ is highly nonsmooth, as was illustrated in Fig. 1.

However, the smoothed formulation

$$\min_{x, \theta} f_\beta(x, \theta) := \delta_{\hat{\Delta}_\ell}(\theta) + \sum_{i=1}^n \theta_i f_i(x) + r(x) + \frac{\beta}{2} \|\theta\|^2,$$

(18)

does lead to a differentiable $\bar{f}_\beta(x)$ with

$$\nabla \bar{f}_\beta(x) = \sum_{i=1}^n \bar{\theta}_i \nabla f_i(x) + \nabla r(x) + \beta \bar{\theta}.$$

This allows for efficient implementations for large-scale applications using, e.g., a Quasi-Newton method. The extension to (convex) nonsmooth $r$ is straight-forward.
3.3 Multiple Kernel Learning

Kernel methods are a powerful technique in classification and prediction [Schölkopf and Smola(2002), Smola and Schölkopf(2004)]. In such problems we are given a set of $k$ samples $a_i \in \mathbb{R}^m$ and corresponding labels $y_i \in \mathbb{R}$ and the goal is to classify new samples. To do so, we search for a function $g(a) = \langle z, \Phi(a) \rangle : \mathbb{R}^m \rightarrow \mathbb{R}$, with $\Phi$ a given map from $\mathbb{R}^m$ to a specified (possibly infinite-dimensional) function class $H$ (Reproducing Kernel Hilbert Space [Saitoh(1988), Schölkopf et al.(2001) Schölkopf, Herbrich and Smola]), such that $\langle z, \Phi(a_i) \rangle \approx y_i$. We can then use $z$ to classify new samples. This problem can be formalized as follows

$$
\min_{z \in H, \alpha \in \mathbb{R}} \frac{1}{2} \|z\|_H^2 + C \sum_{i=1}^{k} (1 - y_i (\langle z, \Phi(a_i) \rangle + \alpha))_+,
$$

with $r_+ = \max(r, 0)$. The dual to this problem is a finite dimensional Quadratic Program (QP):

$$
\min_{x \in [0, C]^k} \frac{1}{2} \|x\|_K^2 - 1^T z \quad \text{s.t.} \quad x^T y = 0,
$$

(19)

where $K$ is the Kernel matrix given by $K_{ij} := y_i y_j \langle \Phi(a_i), \Phi(a_j) \rangle$. Once the dual is solved, $z$ is recovered via

$$
z = \sum_{i=1}^{k} x_i y_i \Phi(a_i),
$$

with several strategies available to recover $\alpha$, see e.g. [Smola and Schölkopf(2004)].

The choice of kernel is an art-form; there are many options available, and different kernels perform better on different problems. To develop a disciplined approach in this setting, multiple kernel learning (MKL) has been proposed. Given $n$ kernels functions $\Phi_i$ with corresponding kernels $K_i$, we consider the weighted linear combination

$$
K(\theta) = \sum_{i=1}^{n} \theta_i K_i.
$$

A natural question is to find the best weights $\theta$ [Rakotomamonjy et al.(2007) Rakotomamonjy, Bach, Canu and Grandvalet]. Requiring $\theta$ to be in the unit simplex yields the problem

$$
\min_{\theta \in \Delta_1, x \in [0, C]^k} \frac{1}{2} \|x\|_K^2 - 1^T z, \quad x^T y = 0.
$$

(20)

This problem was solved in [Rakotomamonjy et al.(2007) Rakotomamonjy, Bach, Canu and Grandvalet] by using variable projection, with the outer problem in $\theta$ solved by prox-gradient. The downside of the approach is that each iteration requires solving a QP.

To make the scheme more efficient, we switch which variable is projected out. Analogously to the trimmed regression case, consider

$$
\min_{x \in [0, C]^k} \overline{f}(x) - 1^T x \quad \text{s.t.} \quad x^T y = 0,
$$

(21)

where

$$
\overline{f}(x) = \min_{\theta \in \Delta_1} \frac{1}{2} \sum_{i} \theta_i \langle K_i x, x \rangle + \frac{\beta}{2} \|\theta\|^2.
$$

This problem has closed-form solution, since the objective is linear in $\theta$:

$$
\overline{\theta} = \text{proj}_{\Delta_1}(-r/\beta), \quad r_i = \|x\|_{K_i}^2.
$$

We have used the same smoothing modification as for trimmed regression to smooth $\overline{f}$. 



### 3.4 Total least squares

Total least squares \cite{Golub1980} gives another rich class of problems for the variable projection technique, with numerous applications \cite{Markovsky2007}. Consider a regression problem where the operator $A$ may have errors; the optimization model to account for this is given by

$$
\min_{x,A} f(x,A) := \frac{1}{2} \|Ax - b\|^2 + \frac{\lambda}{2} \|A - A_0\|^2_2.
$$

The optimization is over both $A$ and $x$. We can project out either variable, but for large scale systems, elimination of $A$ is especially appealing, as the minimizer of the implicit function is a simple rank-1 modification:

$$
\overline{A}(x) = A_0 + \frac{1}{\lambda + \|x\|^2}(b - A_0)x^T.
$$

When $\overline{A}$ is available through matrix vector products, we can quickly compute such products with $\overline{A}(x)$ using (22). Theorem 1 guarantees differentiability of the projected function $f(x)$ in this case. For $\overline{A}$ as in (22), we have

$$
\nabla f(x) = \overline{A}^T(\overline{A}x - b).
$$

### 4 Conclusions

Variable projection has been successfully used in a variety of contexts; the popularity of the approach is largely due to its superior numerical performance when compared to joint optimization schemes. In this paper, we considered a range of nonsmooth applications, illustrating the use of variable projection for sparse deconvolution and direction of arrivals estimation. We showed that differentiability of the value function can be understood using basic variational analysis, and the value function is not differentiable for important cases, including robust formulations and multiple kernel learning. To circumvent this difficulty, we proposed a novel smoothing technique for the inner problem that preserves feasibility and structure of the solution set, while guaranteeing differentiability of the projected function.

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