Flexible Regularized Estimating Equations: Some New Perspectives

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Abstract

In this note, we make some observations about the equivalences between regularized estimating equations, fixed-point problems and variational inequalities. A summary of our findings is given below.

- A regularized estimating equation is equivalent to a fixed-point problem, specified by the proximal operator of the corresponding penalty.
- A regularized estimating equation is equivalent to a generalized variational inequality.
- Both equivalences extend to any estimating equations and any penalty functions.

To our knowledge, these observations have never been presented in the literature before. We hope our new findings can lead to further research in both computational and theoretical aspects of the regularized estimating equations.

1 Introduction

Suppose \( U(\beta) = (U_1(\beta), \ldots, U_p(\beta))^\top \) is an estimating function for \( \beta = (\beta_1, \ldots, \beta_p)^\top \) based on a random sample of size \( n \), where \( U(\cdot) : \mathbb{R}^p \to \mathbb{R}^p \) is a vector-valued function. For example, in maximum likelihood estimation, \( U(\beta) \) is the negative score function. In general, \( U(\beta) \) may not necessarily correspond to the negative gradient of an objective function, such as a likelihood. Consider the standard estimating equation

\[
U(\beta) = 0. \quad (1)
\]

Assume that the solution of (1) exists, which is denoted by \( \hat{\beta} \). Note that for any \( \tau > 0 \),

\[
U(\hat{\beta}) = 0 \iff \hat{\beta} = \hat{\beta} - \tau U(\hat{\beta}).
\]
This motivates us to rewrite (1) as a fixed-point problem:

\[ \hat{\beta} \in \mathbb{R}^p \text{ such that } \hat{\beta} = f(\hat{\beta}), \text{ with } f(\hat{\beta}) \equiv \beta - \tau \mathbf{U}(\beta). \]  

(2)

We can also show that (1) is equivalent to the following variational inequality problem:

\[ \text{find } \hat{\beta} \in \mathbb{R}^p \text{ such that } \mathbf{U}(\hat{\beta})^\top (\beta - \hat{\beta}) \geq 0, \text{ for all } \beta \in \mathbb{R}^p. \]  

(3)

This is because if \( \mathbf{U}(\hat{\beta}) = 0 \), then inequality (3) holds with equality for all \( \beta \). Conversely, if \( \hat{\beta} \) satisfies (3), we can choose \( \beta = \hat{\beta} - \mathbf{U}(\hat{\beta}) \), which implies that \( -\mathbf{U}(\hat{\beta})^\top \mathbf{U}(\hat{\beta}) \geq 0 \) and therefore \( \mathbf{U}(\hat{\beta}) = 0 \).

These results may have very little practical relevance, but it raises an interesting question, that is, whether the equivalences between estimating equations, fixed-point problems and variational inequalities carry over to the regularization setting?

## 2 Regularized estimating equations

In this section, we extend the results to the more interesting regularization cases. Existing literature on regularized estimating equations (Fu, 2003; Johnson et al., 2008) typically considers the following formulation:

\[ \mathbf{U}(\beta) + q_\lambda(\|\beta\|) \odot \text{sgn}(\beta) = 0, \]  

(4)

where \( \text{sgn}(\beta) = (\text{sgn}(\beta_1), \ldots, \text{sgn}(\beta_p))^\top \) and \( q_\lambda(\|\beta\|) = (q_\lambda(|\beta_1|), \ldots, q_\lambda(|\beta_p|))^\top \) with \( q_\lambda(\cdot) \) being a continuous function. Here \( \odot \) denotes the component-wise product. The tuning parameter \( \lambda > 0 \) determines the amount of regularization. Johnson et al. (2008) mainly considered the case where \( q_\lambda(|\beta_j|) = \frac{dp_\lambda(t)}{dt} |_{t=|\beta_j|} \equiv p'_\lambda(|\beta_j|) \) is the derivative of some penalty function \( p_\lambda(\cdot) \) evaluated at \( |\beta_j| \) for \( j = 1, \ldots, p \). Some example penalties include (a) the lasso penalty (Tibshirani, 1996), \( p_\lambda(|t|) = \lambda |t| \); (b) the elastic net penalty (Zou and Hastie, 2005), \( p_\lambda(|t|) = \lambda_1 |t| + \lambda_2 |t|^2 \); and (c) the SCAD penalty (Fan and Li, 2001), defined by

\[ p'_\lambda(|t|) = \lambda \left\{ I(|t| < \lambda) + \frac{(a\lambda - |t|)_-}{(a-1)\lambda} I(|t| \geq \lambda) \right\}, \]

for \( a > 2 \).

Note that formulation (4) only works for penalties with element-wise separability and cannot be directly applied to many other commonly-used penalties, such as the group lasso (Yuan and Lin, 2006) and the sparse group lasso (Simon et al., 2013). In this article, we consider the regularized estimating equation in a slightly more general form:

\[ 0 \in \mathbf{U}(\beta) + \lambda \partial \Omega(\beta), \]  

(5)

where \( \Omega(\cdot) : \mathbb{R}^p \rightarrow \mathbb{R} \) is a general convex penalty and \( \partial \Omega(\beta) \) denotes the set of all subgradients of \( \Omega(\cdot) \) at \( \beta \). A subgradient of \( \Omega(\cdot) \) at \( \beta \in \mathbb{R}^p \) is defined as any vector \( g \in \mathbb{R}^p \) such that

\[ \Omega(\beta') \geq \Omega(\beta) + g^\top (\beta' - \beta) \quad \text{for all } \beta'. \]

Note that \( \partial \Omega(\beta) \) is a closed and convex set. Several examples of formulation (5) follow.
Ridge. If $\Omega(\cdot)$ is a convex and differentiable function, then $\partial \Omega(\beta) = \{ \nabla \Omega(\beta) \}$, i.e., the gradient of $\Omega(\beta)$ at $\beta$ is its only subgradient. Therefore, for the ridge penalty $\Omega(\beta) = \|\beta\|_2^2$, the sub-differential set contains only the regular gradient $\partial \Omega(\beta)/\partial \beta = 2\beta$ and thus (5) reduces to the regular estimating equation $U(\beta) + 2\lambda \beta = 0$.

Lasso. If $\Omega(\cdot)$ is the lasso penalty $\Omega(\beta) = \|\beta\|_1$, then $\beta$ must satisfy the equation

$$U(\beta) + \lambda v = 0,$$

where $v \in \partial \|\beta\|_1$ is a subgradient of $\|\beta\|_1$, evaluated at $\beta$. The $j$th element of $v$ is

$$v_j = \begin{cases} \text{sgn}(\beta_j), & \text{if } \beta_j \neq 0, \\ \in [-1, 1], & \text{if } \beta_j = 0, \end{cases}$$

for $j = 1, \ldots, p$. The estimating equation (6) yield the following equivalent conditions

$$\begin{cases} U_j(\beta) + \lambda \text{sgn}(\beta_j) = 0, & \text{if } \beta_j \neq 0, \\ |U_j(\beta)| \leq \lambda, & \text{if } \beta_j = 0. \end{cases}$$

Note that the first condition in (8) for $\beta_j \neq 0$ coincides with the original formulation (4) by Johnson et al. (2008) with $q_{\lambda}(\|\beta_j\|) = \lambda$, but (4) did not explicitly handle the scenario $\beta_j = 0$. When $U(\beta) = -X^T(y - X\beta)$ is the negative gradient of the least squares objective $L(\beta) = \frac{1}{2}\|y - X\beta\|^2$, (8) corresponds to the KKT conditions of the lasso regularized least squares problem.

Group lasso. Suppose the $p$ predictors are divided into several non-overlapping groups. Let $G = \{g_1, \ldots, g_{|G|}\}$ be a partition of the index set $\{1, \ldots, p\}$. Each group $g_j$ is a subset of the index set $G$, with no overlaps with other groups, $g_j \cap g_k = \emptyset$ for $k \neq j$. Let $|G|$ be the number of groups and let $m_g$ be the size of group $g$. The union of all $|G|$ groups covers the entire index set such that $\bigcup_{j=1}^{|G|} g_j = G$. For the coefficient vector $\beta = (\beta_1, \ldots, \beta_p)\top$, we let $\beta_g$ denote the sub-vector of $\beta$ whose indices are within $g$. Yuan and Lin (2006) proposed the group lasso regularization $\Omega(\beta) = \sum_{g \in G} \sqrt{m_g} \|\beta_g\|_2$. For ease of notation, we omit the weights $\sqrt{m_g}$ in the penalty term. The corresponding regularized estimating equation is

$$0 \in U(\beta) + \lambda \partial \left( \sum_{g \in G} \|\beta_g\|_2 \right).$$

Denote by $[x]_g$ the sub-vector of $x$ for group $g$. The solution to (9) satisfies the following equation, for each group $g$:

$$[U(\beta)]_g + \lambda u_g = 0,$$

where $u_g$ is the subgradient of $\|\beta_g\|_2$ evaluated at $\beta_g$ with

$$u_g = \begin{cases} \beta_g/\|\beta_g\|_2, & \text{if } \beta_g \neq 0, \\ \in \{x : \|x\|_2 \leq 1\}, & \text{if } \beta_g = 0. \end{cases}$$

The subgradient equation (9) yields the following equivalent conditions

$$\begin{cases} [U(\beta)]_g + \lambda \frac{\beta_g}{\|\beta_g\|_2} = 0, & \text{if } \beta_g \neq 0, \\ \|U(\beta)\|_2 \leq \lambda, & \text{if } \beta_g = 0. \end{cases}$$
Sparse group lasso. As an important extension of the group lasso, Simon et al. (2013) proposed the sparse group lasso which allows both group-wise and within-group sparsity. The penalty is a convex combination of the lasso and group-lasso penalties, \( \Omega(\beta) = \sum_{g \in G} (1 - \alpha)\|\beta_g\|_2 + \alpha\|\beta\|_1 \), where \( \alpha \in [0, 1] \). For each group \( g \), the corresponding regularized estimating equation is

\[
[U(\beta)]_g + \lambda(1 - \alpha)u_g + \lambda v_g = 0,
\]

where \( u_g \) is a subgradient as defined in (10) and \( v_g \) is the sub-vector of a subgradient \( v \) as defined in (7).

3 Fixed-point formulation

In this section, we provide a connection between regularized estimating equations and fixed-point problems. Assume that the solution of (5) exists, which is denoted by \( \hat{\beta} \). Then we have the following equivalent conditions for \( \tau > 0 \):

\[
0 \in U(\hat{\beta}) + \lambda \partial \Omega(\hat{\beta}) \\
\iff 0 \in \hat{\beta} - (\hat{\beta} - \tau U(\hat{\beta})) + \tau \lambda \partial \Omega(\hat{\beta}) \\
\iff 0 \in \frac{1}{2} \nabla_\beta \|\beta - (\hat{\beta} - \tau U(\hat{\beta}))\|_2^2 \bigg|_{\beta = \hat{\beta}} + \tau \lambda \partial_\beta \Omega(z) \bigg|_{\beta = \hat{\beta}},
\]

where the differentiation \( \nabla_\beta \) and subdifferential \( \partial_\beta \) are with respect to \( \beta \). If \( \Omega(\beta) \) is a convex penalty, the last line of (12) characterizes the necessary and sufficient condition for \( \hat{\beta} \) to be a minimizer of the penalized quadratic function:

\[
\hat{\beta} = \arg\min_\beta \frac{1}{2}\|\beta - (\hat{\beta} - \tau U(\hat{\beta}))\|_2^2 + \tau \lambda \Omega(\beta).
\]

Let \( \text{prox}_\Omega : \mathbb{R}^p \to \mathbb{R}^p \) be the proximal operator (Parikh and Boyd, 2014) of the convex penalty function \( \Omega \),

\[
\text{prox}_\Omega(v) = \arg\min_z \frac{1}{2}\|z - v\|_2^2 + \Omega(z).
\]

Since the regularized quadratic function on the right-hand side of (14) is strongly convex, it has a unique minimizer for every \( v \in \mathbb{R}^p \). Now we can rewrite (13) as a fixed-point problem:

\[
\text{find } \hat{\beta} \in \mathbb{R}^p \text{ such that } \hat{\beta} = f(\hat{\beta}), \text{ with } f(\beta) \equiv \text{prox}_{\tau \lambda \Omega}(\beta - \tau U(\beta)).
\]

Therefore \( \hat{\beta} \) is a solution to (5) if and only if \( \hat{\beta} \) is a solution to (15). Note that if \( \lambda = 0 \), the operator \( \text{prox}_{\tau \lambda \Omega}(v) \) reduces to \( v \), thus (15) simplifies to (2).

Evaluating the proximal operator of a function requires solving a small strongly convex optimization problem (14). In many cases, these problems often have closed form solutions or can be solved very efficiently using specialized algorithms. We present several examples below.

Lasso. When the penalty is lasso, the \( j \)-th element of the proximal operator is

\[
[\text{prox}_{\tau \lambda \|\cdot\|_1}(v)]_j = \text{sgn}(v_j)(|v_j| - \tau \lambda)_+ \equiv S_{\tau \lambda}(v_j),
\]

which is the soft-thresholding rule.
**Group lasso.** The group lasso penalty has a closed form proximal operator (Parikh and Boyd, 2014): for group $g$,

$$\left[ \text{prox}_{\tau \lambda \Omega}(v) \right]_g = \left( 1 - \frac{\tau \lambda}{\|z_g\|_2} \right) v_g,$$

where $[x]_g$ is the sub-vector corresponding to group $g$ of $x$.

**Sparse group lasso.** The sparse group lasso also has a closed form proximal operator (Simon et al., 2013): for group $g$,

$$\left[ \text{prox}_{\tau \lambda \Omega}(v) \right]_g = \text{arg min}_{z_g} \frac{1}{2} \|z_g - v_g\|_2^2 + \tau \lambda \left( (1 - \alpha)\|z_g\|_2 + \alpha ||z_g||_1 \right)$$

$$= \left[ \left( 1 - \frac{(1 - \alpha)\tau \lambda}{\|S_{\alpha \tau \lambda}(v_g)\|_2} \right) S_{\alpha \tau \lambda}(v_g) \right]_g,$$

where $S_{\alpha \tau \lambda}(v_g) \equiv (S_{\alpha \tau \lambda}([v_{g1}], \ldots, S_{\alpha \tau \lambda}([v_{gm}]))^T$ with $S_{\alpha \tau \lambda}(x) = \text{sgn}(x)(|x| - \alpha \tau \lambda)_+.$

### 4 Variational inequality formulation

After establishing the equivalences between regularized estimating equations and fixed-point problems, we also show a connection between regularized estimating equations and generalized variational inequalities. This is not surprising since equivalences between fixed-point problems and variational inequalities are well known (see, e.g., Malitsky, 2019).

Following (5), a solution $\hat{\beta}$ should satisfy $-U(\hat{\beta})/\lambda \in \partial \Omega(\hat{\beta})$. This implies that $-U(\hat{\beta})/\lambda$ is a subgradient of $\Omega$ at $\hat{\beta}$. Thus, by the definition of a subgradient,

$$\Omega(\beta) \geq \Omega(\hat{\beta}) - U(\hat{\beta})^T (\beta - \hat{\beta})/\lambda \tag{16}$$

for any $\beta$. It follows that (16) can be rewritten as a variational inequality problem:

$$\text{find } \hat{\beta} \in \mathbb{R}^p \text{ such that } U(\hat{\beta})^T (\beta - \hat{\beta}) + \lambda (\Omega(\beta) - \Omega(\hat{\beta})) \geq 0, \text{ for all } \beta \in \mathbb{R}^p. \tag{17}$$

Note that if $\lambda = 0$, (17) reduces to (3). Unlike formulations (5) and (15), which require either specification of the subgradient or evaluation of the proximal operator for $\Omega$, formulation (17) only needs us to specify $U(\beta)$ and $\Omega(\beta)$.

### 5 Extensions to constrained forms

Alternative to the Lagrangian form (5), one may also consider the constrained form of the regularized estimating equations

$$U(\beta) = 0, \text{ such that } \beta \in \mathcal{C}, \tag{18}$$

where $\mathcal{C}$ is a convex set. For example, $\mathcal{C}$ can be a normed ball $\{\beta : \Phi(\beta) \leq r\}$ with the norm function $\Phi(\cdot)$ and radius $r > 0$. One can set $\Phi(\beta)$ to be $\|\beta\|_1$ for the lasso constraint, and
$\sum_{g \in G} \|\beta_g\|_2$ for the group lasso constraint, etc. Intriguingly, \((\ref{eq:18})\) can still be viewed as an instance of \((\ref{eq:5})\). Let $I_C(\beta) : \mathbb{R}^p \rightarrow \mathbb{R}$ be an indicator function

$$I_C(\beta) = \begin{cases} 0 & \text{if } \beta \in C \\ \infty & \text{if } \beta \notin C. \end{cases}$$

Assume the solution of \((\ref{eq:18})\) exists, then \((\ref{eq:18})\) is equivalent to \((\ref{eq:5})\) with $\Omega(\beta) = I_C(\beta)$ and $\lambda = 1$. Let $\hat{\beta}$ be the solution of \((\ref{eq:18})\), the fixed-point formulation thus apply

\[
\begin{align*}
0 & \in \mathbf{U}(\hat{\beta}) + \partial I_C(\hat{\beta}) \\
\iff & \quad \hat{\beta} = \text{prox}_{\tau I_C}(\hat{\beta} - \tau \mathbf{U}(\hat{\beta})) \\
\iff & \quad \hat{\beta} = \arg\min_{\beta \in C} \frac{1}{2} \|\beta - (\hat{\beta} - \tau \mathbf{U}(\hat{\beta}))\|_2^2 \\
\iff & \quad \hat{\beta} = P_C(\hat{\beta} - \tau \mathbf{U}(\hat{\beta})), \quad (\ref{eq:19})
\end{align*}
\]

where the projection operator onto $C$ is defined as

$$P_C(y) = \arg\min_{x \in C} \frac{1}{2} \|x - y\|_2^2.$$  

From \((\ref{eq:19})\) we can see that the proximal operator associated with the constraint $I_C(\hat{\beta})$ becomes the projection on the convex set $C$, which shows that \((\ref{eq:18})\) can be rewritten as the fixed-point problem

find $\hat{\beta} \in \mathbb{R}^p$ such that $\hat{\beta} = f(\hat{\beta})$, with $f(\beta) \equiv P_C(\beta - \tau \mathbf{U}(\beta))$.

On the other hand, \((\ref{eq:18})\) can also be represented as the variational inequality problem

find $\hat{\beta} \in \mathbb{R}^p$ such that $\mathbf{U}(\hat{\beta})^\top (\beta - \hat{\beta}) \geq 0$, for all $\beta \in C$.

To see this, let $\mathcal{N}_C(\beta)$ be the normal cone of $C$ at $\beta$,

$$\mathcal{N}_C(\beta) = \{ g \in \mathbb{R}^p : g^\top (\beta' - \beta) \leq 0 \quad \text{for all } \beta' \in C \}.$$  

For $\beta \in C$, we know that $\partial I_C(\beta) = \mathcal{N}_C(\beta)$, this gives

\[
\begin{align*}
0 & \in \mathbf{U}(\hat{\beta}) + \partial I_C(\hat{\beta}) = \mathbf{U}(\hat{\beta}) + \mathcal{N}_C(\hat{\beta}) \\
\iff & \quad -\mathbf{U}(\hat{\beta}) \in \mathcal{N}_C(\hat{\beta}) \\
\iff & \quad \mathbf{U}(\hat{\beta})^\top (\beta' - \hat{\beta}) \geq 0 \quad \text{for all } \beta' \in C,
\end{align*}
\]

as desired.

### 6 Computation

Formulations \((\ref{eq:15})\) and \((\ref{eq:17})\) reveal interesting connections between regularized estimating equations, fixed-point problems and variational inequalities. To solve large-scale regularized estimating equations, it might be worth pursuing computation from \((\ref{eq:15})\) and \((\ref{eq:17})\). While fast computational algorithms are less developed for \((\ref{eq:4})\), there are many efficient solvers for fixed-point problems and variational inequalities. In this regard, we apply some efficient and scalable solvers to \((\ref{eq:15})\) and \((\ref{eq:17})\), and examine their performance against existing algorithms for regularized estimating equations.
6.1 Existing approaches

To solve (4), many existing works (e.g., Johnson et al., 2008) adopted the local quadratic approximation (LQA) approach proposed by Fan and Li (2001). Specifically, they considered a local quadratic approximation to the penalty function

\[ p_\lambda(\beta_j) \approx p_\lambda(\tilde{\beta}_j) + \frac{1}{2} \left( \frac{p_\lambda'(|\tilde{\beta}_j|)}{|\tilde{\beta}_j|} \right) (\beta_j^2 - \tilde{\beta}_j^2) \]

around an iterate \( \tilde{\beta}_j \). This yields the following approximation to the subgradient of \( p_\lambda(\beta_j) \) when \( \tilde{\beta}_j \neq 0 \):

\[ \frac{\partial}{\partial \beta_j} p_\lambda(\beta_j) = p_\lambda'(|\beta_j|) \text{sgn}(\beta_j) \approx \frac{p_\lambda'(|\tilde{\beta}_j|)}{|\tilde{\beta}_j|} \beta_j. \] (20)

By this local quadratic approximation, the Newton–Raphson algorithm was used to solve the following equation

\[ Q_\beta(\beta) := U(\beta) + \Lambda_\lambda(\tilde{\beta}) \odot \beta = 0, \] (21)

where \( \Lambda_\lambda(\tilde{\beta}) = \text{diag}\{p_\lambda'(|\tilde{\beta}_1|)/|\tilde{\beta}_1|, \ldots, p_\lambda'(|\tilde{\beta}_p|)/|\tilde{\beta}_p|\} \). Let \( \beta^{(k)} = (\beta_1^{(k)}, \ldots, \beta_p^{(k)})^T \) be the k-th iterate of \( \beta \). The algorithm finds the next update \( \beta^{(k+1)} \) using

\[ \beta^{(k+1)} = \beta^{(k)} - \left[ \frac{\partial Q_{\beta^{(k)}}(\beta^{(k)})}{\partial \beta^{(k)^T}} \right]^{-1} Q_{\beta^{(k)}}(\beta^{(k)}) \]

\[ = \beta^{(k)} - \left[ \frac{\partial U(\beta^{(k)})}{\partial \beta^{(k)^T}} + \Lambda_\lambda(\beta^{(k)}) \right]^{-1} Q_{\beta^{(k)}}(\beta^{(k)}). \] (22)

Note that once a component \( \beta_j^{(k)} \) becomes zero during the iteration, the term \( p_\lambda'(|\beta_j^{(k)}|)/|\beta_j^{(k)}| \) in \( \Lambda_\lambda(\beta^{(k)}) \) becomes illy defined. To continue the iteration, the algorithm would have to stop updating those zero components and simply set their final estimates to zero, and then work only with the nonzero components of \( \beta \). This treatment, however, creates a potential problem, that is, once a component becomes zero, it is permanently deleted and will never again receive updates. To fix this, Hunter and Li (2005) replaced \( (p_\lambda'(|\tilde{\beta}_j|)/|\tilde{\beta}_j|) \beta_j \) in (20) with \( (p_\lambda'(|\tilde{\beta}_j|)/(|\tilde{\beta}_j| + \epsilon)) \beta_j \) for some \( \epsilon > 0 \). This leads to a modified \( \Lambda_\lambda(\tilde{\beta}) = \text{diag}\{p_\lambda'(|\tilde{\beta}_1|)/(|\tilde{\beta}_1| + \epsilon), \ldots, p_\lambda'(|\tilde{\beta}_p|)/(|\tilde{\beta}_p| + \epsilon)\} \) in (21) and (22).

The algorithms by Fan and Li (2001) and Hunter and Li (2005) suffer from some significant drawbacks: (a) they cannot easily handle more complex penalty functions, such as the group and sparse group lassos; (b) the Newton–Raphson update in (22) involves the inversion of the \( p \times p \) matrix \( \partial U(\beta^{(k)})/\partial \beta^{(k)^T} + \Lambda_\lambda(\beta^{(k)}) \), so if \( p \gg n \), the computational cost of (22) becomes \( \mathcal{O}(p^3) \), which renders the algorithm extremely impractical for high-dimensional data, when, e.g., \( p = 100,000 \); (c) the update in (22) does not directly produce a sparse solution, so one needs to manually truncate the \( \tilde{\beta}_j \)’s to zero when \( |\tilde{\beta}_j| < c \) for some threshold \( c \), but there is no theoretical guideline on how to choose the value of \( c \), and in practice it is just set to an arbitrarily small number; and (d) the convergence properties of the algorithm in (22) were studied only for the maximum penalized likelihood (Hunter and Li, 2005), but have never been established for the regularized estimating equations.
6.2 Computation for the fixed-point formulation

Suppose \( f : \mathbb{R}^p \rightarrow \mathbb{R}^p \) has Lipschitz constant \( L > 0 \) such that

\[
\| f(\beta) - f(\beta') \|_2 \leq L \| \beta - \beta' \|_2, \quad \text{for all } \beta, \beta' \in \mathbb{R}^p.
\]  

When \( L = 1 \), \( f \) is referred to as a nonexpansive mapping and its set of fixed points \( \mathcal{P} = \{ \beta : f(\beta) = \beta \} \) is closed and convex (can be empty or contain many points; see Ryu and Boyd, 2016). Instead, if \( L < 1 \), \( f \) is called a contraction and has exactly one fixed point (Ryu and Boyd, 2016, page 6).

A very straightforward algorithm for solving (15) is the fixed-point iteration (Picard, 1890; Lindelöf, 1894; Banach, 1922), also called the Picard iteration:

\[
\beta^{(k+1)} = f(\beta^{(k)}), \quad k = 0, 1, 2, \ldots ,
\]  

with an initial value \( \beta^{(0)} \). One can show that if \( f \) is a contraction with Lipschitz constant \( L < 1 \), the fixed-point iteration described in Algorithm 1 can converge to the unique fixed-point \( \hat{\beta} \) of \( f \) with a geometric rate (p15, Ryu and Boyd, 2016):

\[
\| \beta^{(k)} - \hat{\beta} \| \leq L^k \| \beta^{(0)} - \hat{\beta} \|.
\]

However, if \( f \) is only nonexpansive, the fixed-point iteration (24) may not converge to the set of fixed-points \( \mathcal{P} \). Alternatively, we can use the Krasnosel'skiĭ–Mann iteration (KM, Mann, 1953; Krasnosel’skiĭ, 1955):

\[
\beta^{(k+1)} = (1 - \rho)\beta^{(k)} + \rho f(\beta^{(k)}), \quad k = 0, 1, 2, \ldots ,
\]

with \( \rho \in (0, 1) \). Assume the set of fixed-points \( \mathcal{P} \) is nonempty. Then the KM iteration detailed in Algorithm 2 will yield updates \( \beta^{(k)} \rightarrow \hat{\beta} \) for some \( \hat{\beta} \in \mathcal{P} \), that satisfy Fejér monotonicity

\[
\inf_{\beta \in \mathcal{P}} \| \beta^{(k)} - \hat{\beta} \| \rightarrow 0.
\]

Moreover, the points yielded by the KM iteration satisfies the fixed-point condition (15) arbitrarily closely,

\[
\| f(\beta^{(k)}) - \beta^{(k)} \|_2 \rightarrow 0,
\]

with rate \( O(1/k) \). Specifically, we have

\[
\min_{j=0,\ldots,k} \| f(\beta^{(j)}) - \beta^{(j)} \|_2^2 \leq \frac{\| \beta^{(0)} - \hat{\beta} \|}{(k+1)(1-\rho)}.
\]

Choosing \( \rho = 1/2 \) can maximize \( \rho(1-\rho) \), and therefore minimizes the righthand side of the inequality (26). This suggests a possible choice \( \rho = 1/2 \), which gives the simple iteration

\[
\beta^{(k+1)} = (1/2)\beta^{(k)} + (1/2)f(\beta^{(k)}), \quad k = 0, 1, 2, \ldots .
\]
Algorithm 1: fixed-point iteration.

**Input:** Regularization parameter $\lambda > 0$, function $U$, $\tau > 0$
1. Initialize $\beta^{(0)}$;
2. for $k = 1, 2, \ldots$ do
3. \[ \beta^{(k+1)} = \text{prox}_{\tau\lambda\Omega}(\beta^{(k)} - \tau U(\beta^{(k)})); \]
4. end

Algorithm 2: Krasnosel’skii iteration.

**Input:** Regularization parameter $\lambda > 0$, function $U$, $\rho \in (0, 1)$, $\tau > 0$
1. Initialize $\beta^{(0)}$;
2. for $k = 1, 2, \ldots$ do
3. \[ \beta^{(k+1)} = (1 - \rho)\beta^{(k)} + \rho \text{prox}_{\tau\lambda\Omega}(\beta^{(k)} - \tau U(\beta^{(k)})); \]
4. end

6.3 Computation for variational inequality formulation

We can solve the variational inequality (17) using the Golden Ratio Algorithm (GRA) proposed by Malitsky (2019). At each iteration, the algorithm only requires the evaluation of $U$ and $\text{prox}_{\lambda\Omega}$. Algorithm 3 provides the computational details of this method with a fixed stepsize.

Algorithm 3: Golden ratio algorithm with a fixed step size.

**Input:** Lipschitz constant $L$, function $U$.
1. Initialize $\beta^{(1)}$ and $\bar{\beta}^{(0)}$, golden ratio $\phi = \sqrt{5}+1$, fixed step size $t \in (0, \frac{\phi}{2L}]$;
2. for $k = 1, 2, \ldots$ do
3. Compute $\bar{\beta}^{(k)} = \frac{(\phi-1)\beta^{(k)} + \bar{\beta}^{(k-1)}}{\phi}$;
4. \[ \beta^{(k+1)} = \text{prox}_{\lambda\Omega}(\bar{\beta}^{(k)} - t U(\bar{\beta}^{(k)})); \]
5. end

Followed from Theorem 1 of Malitsky (2019), we know that if $U$ in (17) is monotone, i.e.
\[ \langle U(\beta) - U(\beta'), \beta - \beta' \rangle \geq 0, \quad \text{for all } \beta, \beta' \in \mathbb{R}^p, \]
and is $L$-Lipschitz continuous, i.e.
\[ \| U(\beta) - U(\beta') \|_2 \leq L \| \beta - \beta' \|_2, \quad \text{for all } \beta, \beta' \in \mathbb{R}^p, \]
then with arbitrary initialization $\beta^{(1)}$, $\bar{\beta}^{(0)} \in \mathbb{R}^p$ and a fixed stepsize $t \in (0, \frac{\phi}{2L}]$, the sequences $(\beta^{(k)})$ and $(\bar{\beta}^{(k)})$ generated by Algorithm 3 converge to the solution of (17) with rate $O(1/k)$.

Algorithm 3 uses a fixed stepsize $t \in (0, \frac{\phi}{2L}]$, which requires the knowledge of the Lipschitz constant $L$. If the value of $L$ is not available, one can adopt an adaptive stepsize version of the GRA algorithm for solving (17) (see details in Algorithm 4). This approach does not require a line-search. The adaptive GRA computes the stepsizes in each iteration by approximating
an inverse local Lipschitz constant of $U$, which has the same computational cost as the fixed stepsize version. Malitsky (2019) showed that, even when $U$ is only locally Lipschitz (that is, on every bounded set $S \subset \mathbb{R}^p$, for each $\beta_0 \in S$, there is a constant $L_0 > 0$ and a $\delta_0 > 0$ such that $\|\beta - \beta_0\|_2 < \delta_0$ implies $\|U(\beta) - U(\beta_0)\|_2 \leq L_0 \|\beta - \beta_0\|_2$), with arbitrary initialization $\beta^{(1)}$ and $\beta^{(0)} \in \mathbb{R}^p$, the updating sequences $(\beta^{(k)})$ and $(\tilde{\beta}^{(k)})$ generated by Algorithm 4 can converge to a solution of (17) with rate $O(1/k)$.

### Algorithm 4: Adaptive golden ratio algorithm.

**Input:** golden ratio $\bar{t} > 0$, $\phi = \frac{\sqrt{5} + 1}{2}$, $\varphi \in (1, \phi]$, $\rho = \frac{1}{\varphi} + \frac{1}{\varphi^2}$, function $U$.

1. Initialize $\beta^{(0)}$ and $\beta^{(1)} = \beta^{(0)}$, stepsize $t_0 = \frac{\|\beta^{(1)} - \beta^{(0)}\|}{\|U(\beta^{(1)}) - U(\beta^{(0)})\|}$, $\theta_0 = 1$;
2. for $k = 1, 2, \ldots$ do
3.   Find the step size
4.     $t_k = \min \left\{ \rho t_{k-1}, \frac{\varphi \theta_{k-1}}{4 \ell_{k-1} \|U(\beta^{(1)}) - U(\beta^{(0)})\|^2}, \bar{t} \right\}$.
5.     Update
6.     $\tilde{\beta}^{(k)} = \frac{(\varphi - 1)\beta^{(k)} + \tilde{\beta}^{(k-1)}}{\varphi}$, $\beta^{(k+1)} = \text{prox}_{t_k \lambda \Omega}(\tilde{\beta}^{(k)} - t_k U(\tilde{\beta}^{(k)}))$.
7.     Update $\theta_k = \frac{t_k}{t_{k-1}} \varphi$.
8. end
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