A path-following framework on fiber bundle for variational inequalities

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Abstract

Variational inequality (VI) is a fundamental mathematical framework for many classical problems. We present a path-following framework for finite-dimensional VIs with arbitrary continuous functions and compact convex domains. The approach first approximately reduces a general VI to a smooth VI on simplex. Its key innovation is to formulate the smooth VI on simplex on a fiber bundle called the fixed-point bundle. Exploiting this geometric structure, we systematically integrate starting point selection, path-following, and singularity avoidance. Without any assumptions such as monotonicity, the algorithm guarantees global linear convergence to nonsingular solutions. For singular solutions, it retains global linear reduction up to a fixed precision, after which convergence becomes sublinear as the required precision increases. In numerical experiments on 14400 randomly generated VIs of up to 800 dimensions, the algorithm succeeds in every instance, and iteration number increases only mildly with the dimension.

Keywords: variational inequality, interior point method, fiber bundle, path-following
MSCcodes: 49J40, 90C33, 90C51, 49M29

Contents

*Experiment codes and results are available at https://github.com/shb20tsinghua/FiberBundle_VI.

1 Introduction

1.1 Variational inequality problem

The theory of variational inequalities was established in the 1960s through the pioneering work of Fichera [1] and Stampacchia [2]. Initially applied primarily to mechanics, the versatility of this framework was soon recognized. Over time, variational inequalities have become a fundamental mathematical tool for numerous classical problems, including optimization [3], game theory [4], economics [5], traffic [6], contact mechanics [7], fluid flow [8], machine learning [9], and more [10].

Definition 1 (Variational inequality problem)**.** Let $K \subseteq \mathbb{R}^n$ be a nonempty compact convex set, and let $H : K \to \mathbb{R}^n$ be a continuous map. The variational inequality problem, denoted $\mathrm{VI}(H, K)$ is to find a point $x^* \in K$ such that

$$\langle H(x^*), x - x^* \rangle \geq 0$$

holds for all $x \in K$.

This paper focuses on the variational inequalities on finite-dimensional compact convex sets. A distinctive feature of this class of VIs is that the existence of their solutions are guaranteed by the Brouwer fixed-point theorem [11].

1.2 Related work

Existing methods for solving variational inequality problems can be broadly classified into several categories based on their underlying mathematical principles.

Projection method [12, 13] and proximal point method [14, 15] leverage the reformulation of variational inequalities as Brouwer fixed-point problems. These approaches iteratively project updated points onto the feasible set K while reducing the residual $\|x - \Pi_K(x - \rho H(x))\|$, where $\rho > 0$ is a step size parameter. The projection method performs updates of the form $x_{t+1} = \Pi_K(x_t - \rho_t H(x_t))$, while the proximal point method performs updates of the form $x_{t+1} = \Pi_K(x_t - (1/\rho_t) H(x_{t+1}))$, where the later is equivalent to solving a regularized variational inequality subproblem of $H(x) - \rho_k(x - x_t)$ to obtain x_{t+1}.

Reformulation-based methods transform variational inequality problems into optimization problems using merit functions [16, 17], such as the gap function $G(x) = \sup_{y \in K} \langle H(x), x - y \rangle$ or dual gap function $D(x) = \inf_{y \in K} \langle H(y), y - x \rangle$. Standard optimization techniques, including gradient descent, Newton methods, and sequential quadratic programming, are then applied to solve the resulting optimization problem.

Interior point methods [18, 19] reformulate variational inequality problems as complementarity problems and solve the perturbed KKT conditions to follow a central path parameterized by a barrier parameter.

Homotopy methods [20] employ continuous deformations to transform complex variational inequalities into simpler ones with known solutions. A typical homotopy $E(x,t) = (1-t)G(x)+tH(x)$ gradually deforms from a simple function $G(x)$ to the target function $H(x)$ as t varies from 0 to 1. Interior point methods can be viewed as a special case of homotopy methods.

Operator splitting methods apply when $H(x) = A(x)+B(x)$ decomposes into simpler components, allowing alternating solutions to subproblems involving $A(x)$ and $B(x)$. Notable examples include Douglas-Rachford splitting [21], forward-backward splitting [22], and the alternating direction method of multipliers (ADMM) [23].

Most existing methods provide convergence guarantees under monotonicity assumptions or weaker variants like pseudo-monotonicity or quasi-monotonicity. While later progress extend these classical paradigms to non-monotone cases, the resulting variants typically require additional assumptions to guarantee convergence.

Modern algorithms for variational inequality problems often incorporate machine learning techniques, such as adaptive methods, inertial methods, and stochastic methods, particularly for non-monotone and large-scale problems. Adaptive methods dynamically adjust step sizes based on local operator properties to improve convergence without monotonicity assumptions, where examples include adaptive proximal methods [24] and adaptive extragradient [25]. Inertial methods introduce momentum-like terms to accelerate convergence, as seen in inertial forward-backward [26] and inertial proximal methods [27]. Stochastic methods address large-scale and data-driven variational inequality problems, with variants like stochastic extragradient [28], stochastic mirror-prox [29], and variance-reduced methods [30] demonstrating robust convergence in high-dimensional settings.

However, no existing method applies to fully general cases with unconditional convergence guarantees. This paper proposes a globally convergent path-following algorithm for finite-dimensional variational inequality problem $\mathrm{VI}(H,K)$ with general compact convex set K and general continuous function H, requiring no assumptions to guarantee convergence. The resulting convergence to nonsingular solutions is linear, and to singular solutions, the algorithm retain linear reduction before reaching a fixed precision.

Our approach follows a predictor-corrector path-following framework [31] resembling the interior point framework [32], but introduces several key innovations: our algorithm follows a special central path that guarantees to lead to solutions of variational inequalities globally, and we formalize the path as a fiber bundle so that starting point selection, path-following, singularity avoidance can be systematically handled on the geometric structure.

1.3 Technical overview and main results

In section 2, we approximately reduce general finite-dimensional $\mathrm{VI}(H,K)$ with continuous functions and compact convex domains to variational inequalities in the form of $\mathrm{VI}(F,\Delta)$, where F is real analytic and Δ is a simplex. General compact convex sets are approximated using inner approximation of convex bodies, and general continuous functions on simplices are approximated using kernel averaging by Dirichlet distribution. Then, all the following developments are based on $\mathrm{VI}(F,\Delta)$.

In section 4, we derive three equivalent characterizations of $\mathrm{VI}(F,\Delta)$. The linear programming form provides an equation called unbiased KKT conditions combining the perturbed KKT conditions and a fixed-point condition, whose solution space leads to solutions of $\mathrm{VI}(F, \Delta)$. The Brouwer fixed-point form proves the existence theorem of solutions of $\mathrm{VI}(F, \Delta)$ by the Brouwer fixed-point theorem. The mixed complementarity problem form characterizes the solution space of the unbiased KKT conditions as a special central path. We use these three equivalent characterizations to study $\mathrm{VI}(F, \Delta)$ in the following developments.

In section 5, we formalize the solution space of the unbiased KKT conditions as a fiber bundle named as the fixed-point bundle. We introduce two sections of the fiber bundle, one characterizes the gap of $\mathrm{VI}(F, \Delta)$, the other characterizes the differential properties of the fixed-point bundle. Then, we analyze a few differential properties, including the differential equation and the manifold of singular points. The analytic curve on the fixed-point bundle proves the oddness theorem of solutions of $\mathrm{VI}(F, \Delta)$ by a parity arguement following from the Newton-Puiseux theorem. The geometric structure of the fixed-point bundle provides a systematic way for path-following and singularity avoidance. Our goal is to follow the analytic curve while avoiding the singular manifold along the fibers.

In section 6, we adopt the predictor-corrector framework as our path-following framework. Combining the analytic curve and singularity avoidance along the fibers, we obtain the path we follow on the fixed-point bundle. We show that there exists a compact neighborhood of the path containing only nonsingular points for the corrector to work. Then, we introduce a standard Newton corrector solving the fixed-point bundle equation, and use this corrector to prove the convergence result of the overall predictor-corrector path-following framework. Alternatively, we also introduce a gradient corrector optimizing the barrier mixed complementarity problem. These two correctors leads to two different regularized Newton correctors for practical use.

In the convergence rate proof, we show that the algorithm achieves global linear convergence to nonsingular solutions of $\mathrm{VI}(F, \Delta)$. For singular solutions, the algorithm retains global linear reduction before reaching a fixed precision, but the convergence reduces to sublinear as required precision increases.

In section 7, we provide the pseudocode of the predictor-corrector path-following algorithm in Algorithm 1 and the graph of the fixed-point bundle in Figure (1). In experiment, the algorithm converges to a solution on all 2000 randomly generated 100-dimensional $\mathrm{VI}(F, \Delta)$ instances.

2 Approximate reduction to smooth variational inequalities on simplices

2.1 Approximating compact convex sets via simplices

Any finite-dimensional compact convex set can be approximated by polytopes with arbitrary precision. For any $\epsilon > 0$, the open cover $K \subseteq \bigcup_{x \in K} O(x, \epsilon)$ of ϵ-balls admits a finite subcover $K \subseteq \bigcup_{i=1}^{k} O(x_i, \epsilon)$ by compactness. The convex hull $S = \mathrm{conv}(\{x_i | 1 \geq i \geq k\})$ then approximates K with Hausdorff distance

$$d_H(K, S) = \max \left\{ \sup_{x \in K} d(x, S), \sup_{s \in S} d(s, K) \right\} \leq \max(\epsilon, 0) = \epsilon.$$

This constitutes the Minkowski's theorem on inner approximation of the convex body K since $S \subseteq K$ [33]. However, the approximation accuracy $1/\epsilon$ is worst-case exponential to the number k of points [34].

Let $X = (x_1, \ldots, x_k)$ and represent any $x \in S$ as $x = X\sigma$ with $\sigma \in \Delta$. The variational inequality VI(H, K) is transformed into finding $\sigma^* \in \Delta$ such that for all $\sigma \in \Delta$,

$$\langle H(x^*), x - x^* \rangle = H^\top(X\sigma^*)(X\sigma - X\sigma^*) = \left\langle X^\top H(X\sigma^*), \sigma - \sigma^* \right\rangle \geq 0.$$

Thus, general variational inequalities can be approximated by corresponding problems on simplices.

2.2 Approximating continuous functions via analytic functions on simplices

General continuous functions can be approximated by smooth functions using kernel averaging. Our domain is simplex, we use Dirichlet distribution as the kernel to smooth continuous functions on simplices. The Dirichlet distribution Dir(α) is defined on simplex Δ, such that

$$\mathrm{Dir}(y; \alpha) = \frac{1}{B(\alpha)} \prod_{i=1}^{n} y_i^{\alpha_i - 1}, \quad \alpha > 0, \tag{2.1}$$

where $y \in \Delta$ is the variable, $\alpha > 0$ is a vector of concentration parameter, and $B(\alpha)$ is the Beta function. For the continuous function $F : \Delta \to \mathbb{R}^n$, the smoothed function $F_\epsilon : \Delta \to \mathbb{R}^n$ is given component-wise by

$$F_{\epsilon,i}(\sigma) = \mathbb{E}_{Y \sim \mathrm{Dir}(\sigma/\epsilon + c)} \left[F_i(Y) \right] = \int_\Delta F_i(y) \mathrm{Dir}(y; \sigma/\epsilon + c) \, dy. \tag{2.2}$$

For the i-th component, $F_{\epsilon,i}(\sigma)$ is the expectation of $F_i(Y)$ under Dirichlet distribution Dir$(\sigma/\epsilon + c)$ with concentration parameter $\sigma/\epsilon + c$, where $\epsilon > 0$ is a scalar for measuring approximation error, and $c > 0$ is a constant vector to ensure $\sigma/\epsilon + c > 0$ for all $\sigma \in \Delta$.

The smoothing in equation (2.2) can be viewed as a mollification-type approach [35], although the integral is not the classical convolution. However, the Dirichlet distribution Dir$(\sigma/\epsilon + c)$ is indeed a mollifier, such that it is nonnegative on the compact simplex, its mass integrates to 1, and its mass concentrates to σ as $\epsilon \to 0$. In standard mollification, the smoothed function converges uniformly to the original one. We state without proof that we also have uniform convergence such that

$$\lim_{\epsilon \to 0} \sup_{\sigma \in \Delta} \| F_\epsilon(\sigma) - F(\sigma) \| = 0.$$

For smoothness, $F_\epsilon(\sigma)$ is real analytic on Δ for every $\epsilon > 0$. A standard theorem on holomorphic (complex analytic) parameteric integrals in complex analysis can be used to show this [36]. Specifically, for a complex function $f(z, y)$ with $z \in Z$ and $y \in Y$, if $f(z, y)$ is holomorphic with respect to z, and $f(z, y)$ is uniformly integrable with respect to y (i.e., there exists a integrable function $g(y)$ such that $|f(z, y)| < g(y)$ for every $z \in Z$), then the parametric integral $h(z) = \int_Y f(z, y) \, dy$ is holomorphic on Z.

In our case, we need to study the complex parameteric function $F_i(y)\mathrm{Dir}(y; z/\epsilon + c)$ with $y \in \Delta$ and $z \in U_\sigma$, where $U_\sigma = \{z \in \mathbb{C}^n | \|z - \sigma\| \leq d\}$ is defined as the complex neighborhood of $\sigma \in \Delta$. In particular, we require that $\mathrm{Re}(z/\epsilon + c) \geq m > 0$ for every $z \in U_\sigma$. Such a pair of d and m exists for every $\sigma \in \Delta$ because $c > 0$. Then, we can show that $F_i(y)\mathrm{Dir}(y; z/\epsilon + c)$ is holomorphic in z and uniformly integrable in y.

For holomorphy, the Beta function $B(\alpha)$ is known to be holomorphic and nonzero on $\{\alpha \in \mathbb{C} | \mathrm{Re}(\alpha) > 0\}$, then $1/B(z/\epsilon + c)$ is holomorphic on U_σ since $\mathrm{Re}(z/\epsilon + c) \geq m > 0$. Then, $\prod_{i=1}^n y_i^{z_i/\epsilon + c_i - 1}$ is holomorphic in z for every $y > 0$ since it is an exponential function. Thus, $F_i(y)\mathrm{Dir}(y; z/\epsilon + c)$ is holomorphic in z on U_σ for every $y > 0$, while the set where $\min_i y_i = 0$ has measure zero and does not affect the integral.

For uniform integrability, $1/B(z/\epsilon + c)$ is continuous on the compact complex neighborhood U_σ, so it achieves an upper bound $|1/B(z/\epsilon + c)| < C_1$, and $F_i(y)$ is continuous on the compact simplex Δ, so it achieves an upper bound $|F_i(y)| < C_2$. Then, we have

$$|F_i(y)\mathrm{Dir}(y; z/\epsilon + c)| \leq C_1 C_2 \left| \prod_{i=1}^{n} y_i^{z_i/\epsilon + c_i - 1} \right| \leq C_1 C_2 \prod_{i=1}^{n} y_i^{\mathrm{Re}(z_i/\epsilon + c_i) - 1} \leq C_1 C_2 \prod_{i=1}^{n} y_i^{m-1},$$

where $\prod_{i=1}^{n} y_i^{m-1}$ is known to be integrable on Δ as the Dirichlet's multivariate beta integral. Thus, $F_i(y)\mathrm{Dir}(y; z/\epsilon + c)$ is uniformly integrable in y on Δ.

Therefore, by the standard holomorphic parameteric integral theorem, $F_{\epsilon,i}(z)$ is holomorphic on the complex neighborhood U_σ of every $\sigma \in \Delta$. It follows that $F_{\epsilon,i}(\sigma)$ is real analytic on $\sigma \in \Delta$. Then, the vector function $F_\epsilon(\sigma)$ is real analytic on $\sigma \in \Delta$ since each of its components is real analytic.

Next, we derive the derivative of $F_\epsilon(\sigma)$. For any distribution $\mathrm{D}(\alpha)$ and function $f(y)$, under some regularity conditions, there is a standard result

$$\frac{\partial}{\partial \alpha} \mathbb{E}_{Y \sim \mathrm{D}(\alpha)} \left[f(Y) \right] = \mathrm{Cov}_{Y \sim \mathrm{D}(\alpha)} \left[f(Y), S(Y; \alpha) \right], \tag{2.3}$$

which is derived from the following two identities, where $S(Y;\alpha) = \partial \log \mathrm{D}(Y;\alpha)/\partial\alpha$ is called the score function of distribution $\mathrm{D}(\alpha)$, and $\mathrm{Cov}_{Y\sim\mathrm{D}(\alpha)}$ is the covariance of the two random variables.

$$\frac{\partial}{\partial \alpha} \mathbb{E}_{Y \sim \mathrm{D}(\alpha)} \left[f(Y) \right] = \int_\Delta f(y) \frac{\partial}{\partial \alpha} \mathrm{D}(y;\alpha)\, dy = \int_\Delta f(y) \mathrm{D}(y;\alpha) S(y;\alpha)\, dy = \mathbb{E}_{Y \sim \mathrm{D}(\alpha)} \left[f(Y) S(Y;\alpha) \right]$$
$$\mathbb{E}_{Y \sim \mathrm{D}(\alpha)} \left[S(Y;\alpha) \right] = \int_\Delta S(y;\alpha) \mathrm{D}(y;\alpha)\, dy = \int_\Delta \frac{\partial}{\partial \alpha} \mathrm{D}(y;\alpha)\, dy = \frac{\partial}{\partial \alpha} 1 = 0$$

Then, the derivative $F'_\epsilon(\sigma)$ is derived as

$$\begin{aligned} \frac{\partial F_{\epsilon,i}(\sigma)}{\partial \sigma_j} &= \frac{\partial \alpha_j}{\partial \sigma_j} \frac{\partial}{\partial \alpha_j} \mathbb{E}_{Y \sim \mathrm{Dir}(\alpha)} \left[F_i(Y) \right] \\ &= \frac{1}{\epsilon} \mathrm{Cov}_{Y \sim \mathrm{Dir}(\alpha)} \left[F_i(Y), \frac{\partial}{\partial \alpha_j} (-\log B(\alpha) + \sum_{k=1}^{n} (\alpha_k - 1) \log Y_k) \right] \\ &= \frac{1}{\epsilon} \mathrm{Cov}_{Y \sim \mathrm{Dir}(\alpha)} \left[F_i(Y), \log Y_j \right]. \end{aligned} \tag{2.4}$$

3 Notation table

Next, we study variational inequality $\mathrm{VI}(F, \Delta)$ with smooth function and simplex domain, and below are the notations used in the following sections.

Symbol	**Meaning**
$\mathrm{VI}(F, \Delta)$	Variational inequality problem on simplex Δ with smooth function $F : \Delta \to \mathbb{R}^n$, where $n = \dim(\Delta)$
$a \circ b$, $A \circ b$, $b \circ A$	Hadamard (element-wise) product between vector a, vector b and matrix A, where $A \circ b = A\mathrm{diag}(b)$ and $b \circ A = \mathrm{diag}(b)A$
$\mathbf{1}$, $\mathbf{0}$, I	All-ones vector, all-zeros vector, identity matrix

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Symbol	Meaning
$\|a\|$, $\|A\|$	L^2 norm of vector a or matrix A, equals the Euclidean norm of a or the largest singular value of A
σ	Vector variable on simplex Δ, s.t. $\sigma \geq 0$ and $\mathbf{1}^\top \sigma = 1$
μ	Vector barrier parameter of the same dimension as σ, s.t. $\mu \geq 0$
$(\hat{\sigma}, r, v) = M(\sigma, \mu)$	Brouwer function such that the Brouwer fixed-point theorem applies to $\sigma \mapsto \hat{\sigma}$ on simplex Δ
UKKT	Simultaneous equation of perturbed KKT conditions and fixed-point condition $\hat{\sigma} = \sigma$
$G(\sigma, \mu) = 0$	Fixed-point bundle equation, equivalent to UKKT
E	Total space of fixed-point bundle, consists of (σ, μ)
$B(\sigma)$	Fiber of fixed-point bundle over σ, consists of μ
$\check{\mu}(\sigma)$, $\tilde{\mu}(\sigma)$	Sections of fixed-point bundle, map from σ to μ
$\mathrm{gap}(\sigma)$	Gap function of $\mathrm{VI}(F, \Delta)$, $\mathrm{gap}(\sigma) = \sup_{\sigma' \in \Delta} \langle F(\sigma), \sigma - \sigma' \rangle = \mathbf{1}^\top \check{\mu}(\sigma)$
θ	$\sigma = \mathrm{softmax}(\theta)$, where $\mathrm{softmax}(\theta) = \mathrm{softmax}(\theta + k\mathbf{1})$ for any scalar k
$\overline{d\theta}$	$\overline{d\theta} = (I - \mathbf{1}\sigma^\top) d\theta$, removes a scaled $\mathbf{1}$ so that $\sigma \overline{d\theta} = 0$
$J(\sigma)$	$\sigma \circ J(\sigma)$ is the Jacobian matrix of $\tilde{\mu}(\sigma)$
$J_G := J(\sigma) + (\mathbf{1}^\top \mu) I$	$\sigma \circ J_G$ is the Jacobian matrix of $G(\sigma, \mu) = 0$
S	Manifold of singular points of the fixed-point bundle, consists of real eigenvalues of $-J(\sigma)$
$\Gamma(\sigma_{\mathrm{init}})$	Analytic curve on the fixed-point bundle with starting point σ_{init}
$\tilde{\Gamma}$	Path on the fixed-point bundle that avoids singular points, consists of finitely many segments of different $\Gamma(\sigma_{\mathrm{init}})$
$\mathcal{N}_{\tilde{\Gamma}}$	Compact nonsingular neighborhood of $\tilde{\Gamma}$, where the algorithm works
$\tilde{G}(\sigma, \mu) = G(\sigma, \mu)/\sigma$	Affine scaled $G(\sigma, \mu)$, its Euclidean norm $\|\tilde{G}(\sigma, \mu)\| = \|G(\sigma, \mu)\|_{\mathrm{diag}(1/\sigma^2)}$ is the local norm induced by the Hessian of the log barrier $-\ln \sigma$ of $G(\sigma, \mu)$

4 Three equivalent characterizations

4.1 By linear programming problem

We begin by transforming $\mathrm{VI}(F, \Delta)$ into an optimization problem. Recall that $\mathrm{VI}(F, \Delta)$ seeks $\sigma^* \in \Delta$ such that $\langle F(\sigma^*), \sigma - \sigma^* \rangle \geq 0$ for all $\sigma \in \Delta$. This can be reformulated as the Brouwer fixed-point problem in the form of the parameterized linear programming (LP) (4.1), where $\hat{\sigma}$ is the optimization variable, σ is the parameter, and the goal is to find a fixed point such that $\hat{\sigma} = \sigma$.

$$\begin{aligned} \min_{\hat{\sigma}} \quad & \hat{\sigma}^\top F(\sigma) \\ \text{s.t.} \quad & \mathbf{1}^\top \hat{\sigma} = 1 \\ & \hat{\sigma} \geq 0 \end{aligned} \tag{4.1}$$

The Lagrangian function of LP (4.1) is

$$L = \hat{\sigma}^\top F(\sigma) + v(\mathbf{1}^\top \hat{\sigma} - 1) - r^\top \hat{\sigma} = \hat{\sigma}^\top (F(\sigma) + v\mathbf{1} - r) - v,$$

where $r \geq 0$ and v are Lagrangian multipliers. Then, the $\mu = 0$ case of equation (4.2a) plus $r \geq 0$ is the KKT conditions of LP (4.1), and the $\mu > 0$ case is the perturbed KKT conditions of LP (4.1) in interior point method. Since linear programming is a convex problem, $\hat{\sigma}$ is an optimal point if and only if $\hat{\sigma}$ satisfies KKT conditions (4.2a) and $r \geq 0$. Therefore, we equivalently study equation (4.2a) instead of LP (4.1). Specifically, $\sigma \in \Delta$ is a solution of VI(F, Δ) if and only if it is a fixed point of KKT conditions (4.2a) such that $\hat{\sigma} = \sigma$. We refer to the fixed-point equation as unbiased KKT conditions (UKKT) (4.2).

$$\begin{bmatrix} \hat{\sigma} \circ r - \mu \\ r - F(\sigma) - v\mathbf{1} \\ \mathbf{1}^\top \hat{\sigma} - 1 \end{bmatrix} = 0 \tag{4.2a}$$

$$\hat{\sigma} = \sigma \tag{4.2b}$$

4.2 By Brouwer fixed-point problem

Next, we study the $\mu > 0$ case of UKKT (4.2). Given $\mu > 0$, there is a correspondence from σ to $(\hat{\sigma}, r, v)$ satisfying perturbed KKT conditions (4.2a). Specifically, for every $\sigma \in \Delta$, there is a corresponding v satisfying $q(v) = 0$, where $q(v)$ and $dq(v)/dv$ is given by

$$q(v) = \mathbf{1}^\top \frac{\mu}{F(\sigma) + v\mathbf{1}} - 1, \quad \frac{dq(v)}{dv} = -\mathbf{1}^\top \frac{\mu}{(F(\sigma) + v\mathbf{1})^2}, \quad v \in (-\min_i F_i(\sigma), +\infty). \tag{4.3}$$

The derivative satisfies $dq(v)/dv < 0$. In addition, we have limiting behavior

$$\lim_{v \to (-\min_i F_i(\sigma))^-} q(v) = +\infty \quad \wedge \quad \lim_{v \to \infty} q(v) = -1.$$

Then, $q(v)$ monotonically decreases from $+\infty$ to -1 on the interval $(-\min_i F_i(\sigma), +\infty)$. Note also that $q(-\min_i F_i(\sigma) + \mathbf{1}^\top \mu) < 0$. Thus, there is a unique zero point of the bisection problem (4.4).

$$q(v) = \mathbf{1}^\top \frac{\mu}{F(\sigma) + v\mathbf{1}} - 1, \quad v \in [-\min_i F_i(\sigma), -\min_i F_i(\sigma) + \mathbf{1}^\top \mu]. \tag{4.4}$$

Therefore, for any $\mu > 0$ and $\sigma \in \Delta$, there is a unique $(\hat{\sigma}, r, v)$ satisfying perturbed KKT conditions (4.2a). We refer to this map as the Brouwer function $(\hat{\sigma}, r, v) = M(\sigma, \mu)$. Since perturbed KKT conditions (4.2a) is continuous, $(\hat{\sigma}, r, v) = M(\sigma, \mu)$ gives a continuous function mapping σ to $\hat{\sigma}$ on the simplex Δ. Then, Theorem 2 follows from the Brouwer fixed-point theorem, showing that there exist paths subject to UKKT (4.2) leading to the solutions of VI(F, Δ) as $\mu \to \mathbf{0}^+$.

Theorem 2 (Existence theorem)**.** *For any $\mu > 0$, there exists $\sigma \in \Delta$ satisfying UKKT* (4.2)*.*

4.3 By mixed complementarity problem

UKKT (4.2) is defined via the perturbed KKT conditions (4.2a) of linear programming (4.1) in the interior point method. Then, our framework must align with the interior point framework in certain ways. Here, we show that the path defined by UKKT (4.2) are actually a special central path of the mixed complementarity problem (MCP) in equation (4.5). In fact, existing research has built deep connections between complementarity problems, variational inequalities, and Brouwer fixed-point problems [37, 38, 39].

$$\begin{aligned} \min_{(\sigma, r, v)} \quad & \sigma^\top r - \mu^\top \ln \sigma - \mu^\top \ln r \\ \text{s.t.} \quad & r = F(\sigma) + v\mathbf{1} \\ & \mathbf{1}^\top \sigma = 1 \\ & (\sigma, r) \geq 0 \end{aligned} \tag{4.5}$$

The $\mu = 0$ case of equation (4.5) is the MCP directly derived by letting the complementarity pair $\sigma \circ r$ in UKKT (4.2) be the objective function, and the $\mu > 0$ case is the barrier problem of the MCP in interior point method. The Lagrangian function of MCP (4.5) is

$$L = \sigma^\top r + \bar{\lambda}^\top (r - F(\sigma) - v\mathbf{1}) + \tilde{\lambda}(\mathbf{1}^\top \sigma - 1) - \check{r}^\top \sigma - \breve{\sigma}^\top r,$$

where $\bar{\lambda}$, $\tilde{\lambda}$, $\breve{\sigma} \geq 0$, $\check{r} \geq 0$ are Lagrangian multipliers. Then, the perturbed KKT conditions of MCP (4.5) is

$$\begin{bmatrix} -\left(\partial F(\sigma)/\partial\sigma\right)^\top \bar{\lambda} + \tilde{\lambda}\mathbf{1} + r - \check{r} \\ \bar{\lambda} + \sigma - \breve{\sigma} \\ -\bar{\lambda}^\top \mathbf{1} \\ r \circ \breve{\sigma} - \mu \\ \sigma \circ \check{r} - \mu \\ r - F(\sigma) - v\mathbf{1} \\ \mathbf{1}^\top \sigma - 1 \end{bmatrix} = 0. \tag{4.6}$$

Comparing the above perturbed KKT conditions (4.6) with UKKT (4.2), it can be shown that for a solution $(\sigma, r, v, \bar{\lambda}, \tilde{\lambda}, \breve{\sigma}, \check{r})$ of perturbed KKT conditions (4.6), (σ, r, v) is a solution of UKKT (4.2) if and only if $\breve{\sigma} = \sigma$. Therefore, the path given by UKKT (4.2) is the specific central path of MCP (4.5) on which $\breve{\sigma} = \sigma$. Similar to the interior point method, we have Theorem 3 stating that the path leads to solutions of $\mathrm{VI}(F, \Delta)$ as μ tends to 0 from $\mu > 0$.

Theorem 3. *$\sigma^\star \in \Delta$ is a solution of $\mathrm{VI}(F, \Delta)$ if and only if $\sigma_t \to \sigma^\star$ as $\mu_t \to \mathbf{0}^+$ subject to UKKT (4.2).*

It is worth noting that $(\sigma, \mathbf{0})$ satisfying UKKT (4.2) is not always a solution of $\mathrm{VI}(F, \Delta)$, because $r \geq 0$ is additionally required for the $\mu = 0$ case. For $\sigma \in \Delta$, $r > 0$ if and only if $\mu > 0$. Therefore, $(\sigma^\star, \mathbf{0})$ satisfying UKKT (4.2) must be a limit point as μ approaches 0 from $\mu > 0$ to constitute a solution of $\mathrm{VI}(F, \Delta)$. This requiement aligns with the interior point method in which solutions are found as $\mu > 0$ tends to 0.

5 Fiber bundle as the solution space

5.1 The fixed-point bundle

We have established that UKKT (4.2) defines paths leading to solutions of $\mathrm{VI}(F, \Delta)$. In this section, we study the solution space of UKKT (4.2). First, we substitute $r = F(\sigma) + v\mathbf{1}$ into $\sigma \circ r = \mu$ to get $\sigma \circ F(\sigma) + v\sigma = \mu$. Then, equation (5.1) depicts the geometric structure of this solution space. For any $\sigma \in \Delta$, all the μ satisfying UKKT (4.2) forms a one-dimensional line spanned by $v \in \mathbb{R}$, denoted as $B(\sigma)$. The solution space consisting of (σ, μ) is the disjoint union of all these lines of μ over different $\sigma \in \Delta$, denoted as E. This geometric structure is called a fiber bundle, denoted as $(E, \Delta, \alpha : E \to \Delta)$, where E is the total space, Δ is the base space, $\alpha : E \to \Delta$ is the projection map, and $\alpha^{-1}(\sigma) = \{\sigma\} \times B(\sigma)$ is the fiber over σ. We refer to this fiber bundle as the fixed-point bundle, and conventionally, we also use the total space E to refer to the fiber bundle.

$$\begin{aligned} &E = \bigcup_{\sigma \in \Delta} \{\sigma\} \times B(\sigma) \\ &B(\sigma) = \{\sigma \circ F(\sigma) + v\sigma | v \in \mathbb{R}\} \\ &\alpha\left((\sigma, \mu)\right) = \sigma \end{aligned} \tag{5.1}$$

Using projection matrix $I - \sigma\mathbf{1}^\top$, we can totally eliminate v in UKKT (4.2). Then, the equation of this fiber bundle is $G(\sigma, \mu) = 0$ as defined in equation (5.2), and $G(\sigma, \mu) = 0$ is equivalent to UKKT (4.2). We also use $(\sigma, \mu) \in E$ to represent points that satisfies $G(\sigma, \mu) = 0$.

$$G(\sigma, \mu) = \left(I - \sigma\mathbf{1}^\top\right)(\sigma \circ F(\sigma) - \mu), \quad \sigma \in \Delta \tag{5.2}$$

The matrix $I - \sigma\mathbf{1}^\top$ is a projection. It projects along vector σ such that $(I - \sigma\mathbf{1}^\top)\sigma = 0$, and it projects onto the subspace orthogonal to vector $\mathbf{1}$ such that $\mathbf{1}^\top(I - \sigma\mathbf{1}^\top) = 0$. It is idempotent such that $(I - \sigma\mathbf{1}^\top)(I - \sigma\mathbf{1}^\top) = I - \sigma\mathbf{1}^\top$. The linear equation $(I - \sigma\mathbf{1}^\top)x = b$ has a solution when $\mathbf{1}^\top b = 0$, and the general solution is $x = b + k\sigma$ for $k \in \mathbb{R}$. And $I - \mathbf{1}\sigma^\top = (I - \sigma\mathbf{1}^\top)^\top$ is another projection matrix that has similar properties.

Next, we introduce two sections $\tilde{\mu}(\sigma)$ and $\check{\mu}(\sigma)$ of the fixed-point bundle as shown in equation (5.3). As sections of a fiber bundle, they map every σ to a point on the fiber $B(\sigma)$ over it. Note that $\mathbf{1}^\top\tilde{\mu}(\sigma) = 0$ and $\check{\mu}(\sigma) \geq 0$. $\tilde{\mu}(\sigma)$ is differentiable, thus it is utilized to analyze the differential property of the fixed-point bundle and the path-following algorithm in subsequent developments.

$$\begin{aligned}
\tilde{\mu}(\sigma) &= \sigma \circ \left(F(\sigma) - \left(\sigma^\top F(\sigma)\right)\mathbf{1}\right) = \left(I - \sigma\mathbf{1}^\top\right)(\sigma \circ F(\sigma)) \\
\check{\mu}(\sigma) &= \sigma \circ \left(F(\sigma) - \left(\min_i F_i(\sigma)\right)\mathbf{1}\right)
\end{aligned} \tag{5.3}$$

As for $\check{\mu}(\sigma)$, we have the following deduction.

$$\begin{aligned}
&\mathbf{1}^\top\check{\mu}(\sigma) = \sigma^\top F(\sigma) - \min_i F_i(\sigma) \\
=&\sigma^\top F(\sigma) - \min_i \left(\frac{G(\sigma, \mu) + \mu + (\sigma^\top F(\sigma) - \mathbf{1}^\top\mu)\sigma}{\sigma}\right)_i = \mathbf{1}^\top\mu - \min_i \left(\frac{G(\sigma, \mu) + \mu}{\sigma}\right)_i
\end{aligned}$$

A variational inequality is described by a gap function. For $\mathrm{VI}(F, \Delta)$, the gap function satisfies

$$\mathrm{gap}(\sigma) = \sup_{\sigma' \in \Delta} \left\langle F(\sigma), \sigma - \sigma' \right\rangle = \sigma^\top F(\sigma) - \min_i F_i(\sigma) \geq 0,$$

where $\mathrm{VI}(F, \Delta)$ requires solutions such that $\mathrm{gap}(\sigma^\star) = 0$. Then, we have Theorem 4. First, $\mathbf{1}^\top\check{\mu}(\sigma)$ assesses the convergence of the algorithm, and the solutions are the zero points of $\check{\mu}(\sigma)$. Second, if $|G(\sigma, \mu)| < \mu$ component-wise, then $\mathbf{1}^\top\check{\mu}(\sigma) < \mathbf{1}^\top\mu$. $G(\sigma, \mu)$ measures the proximity to the fixed-point bundle, and $\mathbf{1}^\top\mu$ measures the proximity of $\mu \to \mathbf{0}^+$, when they both have sufficient precision, $\mathbf{1}^\top\check{\mu}(\sigma)$ has sufficient precision. This transforms the precision approaching the path and the precision approaching the path endpoint to the precision to solving $\mathrm{VI}(F, \Delta)$.

Theorem 4. *The gap function of* $\mathrm{VI}(F, \Delta)$ *satisfies*

$$\mathrm{gap}(\sigma) = \mathbf{1}^\top\check{\mu}(\sigma) = \mathbf{1}^\top\mu - \min_i \left((G(\sigma, \mu) + \mu)/\sigma\right)_i. \tag{5.4}$$

It is worth noting that $\check{\mu}(\sigma)$ and $\tilde{\mu}(\sigma)$ do not have the same zero points. For example, all the vertices of the simplex are zero points of $\tilde{\mu}(\sigma)$, but not all of them are zero points of $\check{\mu}(\sigma)$ since they are not necessarily solutions of $\mathrm{VI}(F, \Delta)$. The reason is that we have the nonnegativity $F(\sigma) - (\min_i F_i(\sigma))\mathbf{1} \geq 0$, while $F(\sigma) - (\sigma^\top F(\sigma))\mathbf{1}$ does not have this nonnegativity. Thus, despite that $(\sigma, \check{\mu}(\sigma))$ and $(\sigma, \tilde{\mu}(\sigma))$ both satisfy UKKT (4.2), the corresponding r of $(\sigma, \check{\mu}(\sigma))$ satisfies $r \geq 0$, whereas the corresponding r of $(\sigma, \tilde{\mu}(\sigma))$ may have $r_i < 0$ for some index. That is why zero points of $\check{\mu}(\sigma)$ are equivalently solutions of $\mathrm{VI}(F, \Delta)$ while zero points of $\tilde{\mu}(\sigma)$ are not necessarily.

5.2 Differential properties

To maintain $\sigma \in \Delta$, we use the parameterization

$$\sigma = \text{softmax}(\theta) = \frac{\exp(\theta)}{\mathbf{1}^\top \exp(\theta)}. \tag{5.5}$$

The differential $d\sigma$ with respect to $d\theta$ is

$$d\sigma = \frac{\exp(\theta) \circ d\theta}{\mathbf{1}^\top \exp(\theta)} - \frac{\mathbf{1}^\top (\exp(\theta) \circ d\theta)}{(\mathbf{1}^\top \exp(\theta))^2} \exp(\theta) = \sigma \circ d\theta - (\sigma^\top d\theta)\sigma = \sigma \circ \left(I - \mathbf{1}\sigma^\top\right) d\theta. \tag{5.6}$$

Note that $\mathbf{1}^\top d\sigma = 0$ for any $d\theta$. Conversely, when $\mathbf{1}^\top d\sigma = 0$, the linear equation $d\sigma/\sigma = (I - \mathbf{1}\sigma^\top)d\theta$ admits the general solution $d\theta = d\sigma/\sigma + k\mathbf{1}$ with $k \in \mathbb{R}$. We denote $\overline{d\theta} := (I - \mathbf{1}\sigma^\top)d\theta$.

Next, we derive the differential $d\tilde{\mu}(\sigma)$ with respect to $\overline{d\theta}$. In the 2nd line, we use $\mathbf{1}^\top d\sigma = 0$. In the last line, we use $(I - \mathbf{1}\sigma^\top)\overline{d\theta} = \overline{d\theta}$.

$$\begin{aligned}
d\tilde{\mu}(\sigma) &= \left(I - \sigma\mathbf{1}^\top\right)\left(\sigma \circ \frac{\partial F(\sigma)}{\partial \sigma} + F(\sigma) \circ I\right) d\sigma - \mathbf{1}^\top (\sigma \circ F(\sigma))\, d\sigma \\
&= \left(I - \sigma\mathbf{1}^\top\right)\left(\sigma \circ \frac{\partial F(\sigma)}{\partial \sigma} + F(\sigma) \circ I\right) d\sigma - \mathbf{1}^\top (\sigma \circ F(\sigma))\, d\sigma + \left(\sigma^\top F(\sigma)\right) \sigma\mathbf{1}^\top d\sigma \\
&= \left(I - \sigma\mathbf{1}^\top\right)\left(\sigma \circ \frac{\partial F(\sigma)}{\partial \sigma} + F(\sigma) \circ I - (\sigma^\top F(\sigma))I\right) d\sigma \\
&= \sigma \circ \left(I - \mathbf{1}\sigma^\top\right)\left(\frac{\partial F(\sigma)}{\partial \sigma} \circ \sigma + \left(\left(I - \mathbf{1}\sigma^\top\right) F(\sigma)\right) \circ I\right) \frac{d\sigma}{\sigma} \\
&= \sigma \circ \left(I - \mathbf{1}\sigma^\top\right)\left(\frac{\partial F(\sigma)}{\partial \sigma} \circ \sigma + \left(\left(I - \mathbf{1}\sigma^\top\right) F(\sigma)\right) \circ I\right) \left(I - \mathbf{1}\sigma^\top\right) \overline{d\theta}
\end{aligned} \tag{5.7}$$

Here, we introduce the matrix $J(\sigma)$ in equation (5.8), where $k \in \mathbb{R}$ is an arbitrary scalar.

$$J(\sigma) := \left(I - \mathbf{1}\sigma^\top\right)\left(\frac{\partial F(\sigma)}{\partial \sigma} \circ \sigma + \left(\left(I - \mathbf{1}\sigma^\top\right) F(\sigma)\right) \circ I\right) \left(I - \mathbf{1}\sigma^\top\right) + k\mathbf{1}\sigma^\top \tag{5.8}$$

By $\sigma^\top \overline{d\theta} = 0$, we arrive at the following differential equation of $\tilde{\mu}(\sigma)$.

$$d\tilde{\mu}(\sigma) = \sigma \circ J(\sigma)\overline{d\theta} \tag{5.9}$$

The arbitrary scalar $k \in \mathbb{R}$ in $J(\sigma)$ is to adjust the eigenvalue corresponding to eigenvector $\mathbf{1}$. First, we consider $J(\sigma)$ with $k = 0$. It can be directly verified that $J(\sigma)$ always has a zero eigenvalue corresponding to eigenvector $\mathbf{1}$, and all other eigenvectors are orthogonal to σ since $\sigma^\top J(\sigma) = \mathbf{0}$. Then, with $k \neq 0$, we can further verify that all the eigenvectors remains the same as the $k = 0$ case, and the eigenvalues corresponding to the eigenvectors orthogonal to σ also remain unchanged, but the eigenvalue corresponding to eigenvector $\mathbf{1}$ changes from 0 to k. Thus, adding $k\mathbf{1}\sigma^\top$ removes the inherent zero eigenvalue of the $k = 0$ case of $J(\sigma)$. This is a trick preventing $J(\sigma)$ from being inherently singular for theoretical simplicity, however, we use $J(\sigma)$ with $k = 0$ in the algorithm for computational simplicity.

Next, we derive the differential equation of $G(\sigma, \mu) = 0$, i.e., the differential equation of the fixed-point bundle.

$$\begin{aligned}
G'_\theta(\sigma, \mu)d\theta &= -\, G'_\mu(\sigma, \mu)d\mu \\
\sigma \circ J(\sigma)\overline{d\theta} + (\mathbf{1}^\top \mu)\sigma \circ \overline{d\theta} &= \left(I - \sigma\mathbf{1}^\top\right) d\mu
\end{aligned} \tag{5.10}$$

Multiplying both sides with $1/\sigma$, we arrive at the differential equation of $G(\sigma,\mu)=0$ in equation (5.11). This differential equation provide the tangent step in θ with respect to the reduction $d\mu$ to follow the fixed-point bundle. We denote $J_G := J(\sigma) + (\mathbf{1}^\top\mu)I$.

$$\Big(J(\sigma) + (\mathbf{1}^\top\mu)I\Big)\,\overline{d\theta} = \Big(I - \mathbf{1}\sigma^\top\Big)\,(d\mu/\sigma) \tag{5.11}$$

The point (σ,μ) on the fixed-point bundle is called a singular point if $J(\sigma)+(\mathbf{1}^\top\mu)I$ is singular. Apparently, for any $\sigma\in\Delta$, there are at most $n-1$ singular points on the fiber $B(\sigma)$, corresponding to the eigenvalues of $-J(\sigma)$ except the arbitrary $-k$. Therefore, we can construct the singular manifold of the fixed-point bundle using the real eigenvalues of $J(\sigma)$. Denoting the real eigenvalues of $J(\sigma)$ except k as $\lambda_j^\perp(J(\sigma))\in\mathbb{R}$, we can formalize the set of all singular points of fixed-point bundle E as the singular manifold S in equation (5.12). Indeed, S is on E because for every $\sigma\in\Delta$, $\tilde{\mu}(\sigma)$ is a section of E and $-\lambda_j^\perp(J(\sigma))\sigma$ moves along the fiber over σ. And S consists of all the singular points of E because for every $\sigma\in\Delta$, $\mathbf{1}^\top(\tilde{\mu}(\sigma)-\lambda_j^\perp(J(\sigma))\sigma) = -\lambda_j^\perp(J(\sigma))$ includes all the values of $\mathbf{1}^\top\mu$ that can equal an eigenvalue of $-J(\sigma)$.

$$S = \Big\{(\sigma, \tilde{\mu}(\sigma) - \lambda_j^\perp\left(J(\sigma)\right)\sigma) | \lambda_j^\perp\left(J(\sigma)\right)\in\mathbb{R}, \sigma\in\Delta\Big\} \tag{5.12}$$

5.3 Analytic curves

We study the curve on the fixed-point bundle E defined by

$$\Gamma(\sigma_{\text{init}}) = \left\{(\sigma,\mu)\in E | \mu = \gamma\sigma_{\text{init}}, \gamma\in[0,+\infty)\right\}, \tag{5.13}$$

with designated $\sigma_{\text{init}}\in\Delta$. $\Gamma(\sigma_{\text{init}})$ is a one-dimensional curve parameterized by γ, where every $(\sigma,\mu)\in E$ on it satisfies $G(\sigma,\mu)=0$. When $F(\sigma)$ is real analytic, $G(\sigma,\mu)$ is real analytic. As the zero set of the analytic function $G(\sigma,\mu)=0$, $\Gamma(\sigma_{\text{init}})$ is called an analytic curve. By the following analysis, we can prove the parity arguement that leads to the oddness theorem stating that there are almost always an odd number of solutions of $\text{VI}(F,\Delta)$. The analysis is adopted from the proof of the oddness theorem of Nash equilibrium [40].

First, for any μ, there are at most finitely many solutions of $G(\sigma,\mu)=0$. Because Δ is a compact set, if there are infinitely many zero points, there must be a convergent zero point sequence. If an analytic function takes the value 0 on a convergent point sequence, the analytic function is constantly 0. Thus, there are always finitely many solutions of $G(\sigma,\mu)=0$ for any μ. Then, the analytic curve $\Gamma(\sigma_{\text{init}})$ consists of finitely many branches.

Second, since $G(\sigma,\mu)$ is analytic, the Newton-Puiseux theorem ensures that on every point of $\Gamma(\sigma_{\text{init}})$, the analytic curve can be expanded as a Puiseux series. In fact, the well-known implicit function theorem ensures a Taylor series expansion as a special Puiseux series expansion on nonsingular points, whereas the Newton-Puiseux theorem ensures a Puiseux series expansion on singular points. As a consequence, there is a unique analytic continuation beyond every point on $\Gamma(\sigma_{\text{init}})$, whether it is singular or nonsingular.

Third, since $\Gamma(\sigma_{\text{init}})$ has a unique analytic continuation beyond every point on it, the boundary of $\Gamma(\sigma_{\text{init}})$ can only be at where $\gamma\to 0^+$ and $\gamma\to+\infty$, and the branches of $\Gamma(\sigma_{\text{init}})$ connect them in pairs. The ending points at where $\gamma\to 0^+$ are equivalently the solutions of $\text{VI}(F,\Delta)$. The starting point at where $\gamma\to+\infty$ is a single point σ_{init}, since $\sigma\circ F(\sigma)+v\sigma = \gamma\sigma_{\text{init}}$. Therefore, the branches of analytic curve $\Gamma(\sigma_{\text{init}})$ connect the solutions of $\text{VI}(F,\Delta)$ and a single σ_{init} in pairs, which is called the parity arguement.

Finally, when all the solutions of $\text{VI}(F,\Delta)$ are nonsingular points, there is exactly one branch of $\Gamma(\sigma_{\text{init}})$ connecting to each solution due to the implicit function theorem. Thus, there are an odd number of solutions, which is the oddness theorem in Theorem 5. Note that the solutions of VI(F, Δ) are almost always all nonsingular.

Theorem 5 (Oddness theorem)**.** *If $F(\sigma)$ is analytic on the simplex Δ, and if $J(\sigma)$ is nonsingular on all the solutions, then there are an odd number of solutions.*

The above analysis reveals that there is an analytic curve branch connecting any designated starting point σ_{init} and a solution of VI(F, Δ). If we follow this path, we can achieve global convergence to solutions of VI(F, Δ). However, there can be singular points on the analytic curve, and path-following cannot go beyond a singular point, thus they must be avoided. On the fixed-point bundle, singularity avoidance is achievable simply by moving along the fiber $B(\sigma)$. Specifically, on a point (σ, μ) where $\mathbf{1}^\top \mu$ equals an eigenvalue of $-J(\sigma)$, we can simply jump to $(\sigma, \mu + \beta\sigma)$ with some β such that $\mu + \beta\sigma > 0$ and $\mathbf{1}^\top \mu + \beta$ is not an eigenvalue of $-J(\sigma)$. Then, $(\sigma, \mu + \beta\sigma)$ is not a singular point, and we can proceed to reduce $\mu + \beta\sigma$. This actually leads to a new analytic curve $\Gamma((\mu + \beta\sigma)/(\mathbf{1}^\top \mu + \beta))$ with different starting point.

6 Predictor-corrector path-following on the fixed-point bundle

We adopt the predictor-corrector framework to perform the path-following on the fixed-point bundle. Given a starting point on the path, the predictor-corrector path-following framework alternates between the predictor step and the corrector step. The predictor step moves a small step along the tangent direction of the path, and the corrector step is a subiteration that locally converges back onto the path.

6.1 The path and its nonsingular neighborhood

The path we follow is derived from the analytic curve $\Gamma(\sigma_{\text{init}})$ and singularity avoidance along the fiber, which can be formalized as $\tilde{\Gamma}$ in equation (6.1). The starting point $(\sigma_0, \gamma_0\mu_0) \in E$ is given by $\gamma_0\mu_0 = v_{\text{init}}\sigma_{\text{init}}$ with designated σ_{init} and a large enough v_{init}. Then, $\tilde{\Gamma}$ consists of segments of different analytic curve $\Gamma(\sigma_{\text{init}})$, which are connected in σ, but jump along the fibers in μ. $\tilde{\Gamma}$ eventually ends at the point where $\mathbf{1}^\top \mu = \zeta$. With $\zeta = 0$, the ending point of $\tilde{\Gamma}$ is $(\sigma^\star, \mathbf{0})$, where $\sigma^\star$ is a solution of VI(F, Δ).

$$
\begin{aligned}
\tilde{\Gamma} = \bigcup_{i=1}^{q} \left\{ (\sigma, \gamma\mu_i) \in E \middle| \mu_i = \gamma_{i-1}\mu_{i-1} + \beta_i\sigma_{i-1}, \gamma \in [\gamma_i, 1] \right\}, \\
\gamma_0\mu_0 = v_{\text{init}}\sigma_{\text{init}},\ \mu_i > 0,\ \gamma_q \mathbf{1}^\top \mu_q = \zeta
\end{aligned}
\tag{6.1}
$$

We wish to have $\tilde{\Gamma} \cap S = \varnothing$ for singularity avoidance, where S is the singular manifold. In fact, this can be done with only finite times of singularity avoidance. Because otherwise, there must be an accumulation point of the infinite sequence $(\sigma_i, \gamma_i\mu_i)$ in the bounded region $\Delta \times \{\mu | 0 \leq \mu \leq v_{\max}\}$. Then, infinitely many times of singularity avoidance near this accumulation point suggest that there exists an unavoidable singular point nearby. However, the only unavoidable singular point is $(\sigma^\star, \mathbf{0})$ when $J(\sigma^\star)$ is singular, because this is the only point where $\mathbf{1}^\top \mu$ must fix at 0. Thus, if $J(\sigma^\star)$ is nonsingular or $\mathbf{1}^\top \mu \geq \zeta > 0$, by contradiction, finitely many times of singularity avoidance suffices. Therefore, if $J(\sigma^\star)$ is nonsingular, we let $\tilde{\Gamma}$ end with $\zeta = 0$, and if $J(\sigma^\star)$ is singular, we let $\tilde{\Gamma}$ end with a fixed $\zeta > 0$. Then, we obtain a path $\tilde{\Gamma}$ such that $\tilde{\Gamma} \cap S = \varnothing$, and $\tilde{\Gamma}$ consists of finitely many segments of different $\Gamma(\sigma_{\text{init}})$.

In addition to $\tilde{\Gamma} \cap S = \varnothing$, we also need a neighborhood of $\tilde{\Gamma}$ that is disjoint to S, because the corrector is a subiteration that converges onto the path $\tilde{\Gamma}$ in its neighborhood. We can use compactness of both $\tilde{\Gamma}$ and S to establish the existence of such a neighborhood of $\tilde{\Gamma}$. $\tilde{\Gamma}$ is compact because the mapping from γ to each analytic curve segment is continuous on the compact interval in γ. S is compact because the mapping from σ to each eigenvalue of $J(\sigma)$ is continuous on the compact simplex Δ. Then, if two compact sets are disjoint, there must be a positive gap between them, which is in (σ, μ)-coordinate. We can further have a positive gap in $(\ln \sigma, \mu)$-coordinate because otherwise there would not be a positive gap in (σ, μ)-coordinate either, considering that the function softmax is continuous. Specifically, there exists

$$d = \frac{1}{2} \inf \left\{ \|(\ln \sigma_g, \mu_g) - (\ln \sigma_s, \mu_s)\| \,|(\sigma_g, \mu_g) \in \tilde{\Gamma}, (\sigma_s, \mu_s) \in S, \mu_g > 0, \mu_s > 0 \right\}$$

such that $d > 0$. Consequently, there exists a neighborhood with radius d of the path $\tilde{\Gamma}$ in $\ln \sigma$-coordinate that is disjoint to S. Since $\sigma_\mu > 0$ is needed to guarantee that $\ln \sigma_\mu$ is well-defined, we require $\mu > 0$, whereas the limit of the neighborhood near $\sigma^\star$ as $\mu \to \mathbf{0}^+$ can be included by taking closure. Therefore, we obtain the neighborhood $\mathcal{N}_{\tilde{\Gamma}}$ in equation (6.2).

$$\mathcal{N}_{\tilde{\Gamma}} = \text{Closure}\left(\left\{ (\text{softmax}(\theta), \mu) |\, \|\theta - \ln \sigma_\mu\| \leq d, (\sigma_\mu, \mu) \in \tilde{\Gamma}, \mu > 0 \right\} \right) \tag{6.2}$$

Closure operation does not break a positive gap, thus we obtain a compact path neighborhood $\mathcal{N}_{\tilde{\Gamma}}$ that satisfies $\mathcal{N}_{\tilde{\Gamma}} \cap S = \varnothing$. The $\ln \sigma$-coordinate aligns with our parameterization $\sigma = \text{softmax}(\theta)$, resulting in a neighborhood of σ_μ that always lies in the simplex even as σ_μ approaches the boundary. Note that $\|\theta - \ln \sigma_\mu\| \leq d$ is equivalently $\mathrm{e}^{-d} - 1 \leq (\sigma_\mu - \sigma)/\sigma \leq \mathrm{e}^{d} - 1$. In fact, the $\ln \sigma$-coordinate strongly resembles the local norm $\|V\|_{\text{diag}(1/\sigma^2)} = V^\top \text{diag}(1/\sigma^2) V$ in the interior point method, where $\text{diag}(1/\sigma^2)$ is the Hessian matrix of the log barrier $-\ln \sigma$. In the interior point method, the neighborhood defined by the Hessian-induced local norm is called the Dikin ellipsoid [41].

Finally, we bound two quantities on the compact nonsingular path neighborhood $\mathcal{N}_{\tilde{\Gamma}}$. First, the smallest singular value $s_{\min}(J(\sigma) + (\mathbf{1}^\top \mu) I)$ attains a lower bound $s_{\min}(J_G)$ because it is continuous on the compact set $\mathcal{N}_{\tilde{\Gamma}}$. If $J(\sigma^\star)$ is nonsingular, the bound $s_{\min}(J_G)$ is uniform over the entire path-following process till reaching $(\sigma^\star, \mathbf{0})$. However, if $J(\sigma^\star)$ is singular, the bound $s_{\min}(J_G)$ is uniform only over the part where $\mathbf{1}^\top \mu \geq \zeta > 0$. In addition, $s_{\min}(J_G)$ is dependent to ζ such that $s_{\min}(J_G) \to 0$ as $\zeta \to 0$. Thus, for a singular solution, our convergence result only holds for path-following that ends at $\mathbf{1}^\top \mu = \zeta$ with a fixed ζ.

The second quantity bounded on $\mathcal{N}_{\tilde{\Gamma}}$ is μ/σ, which is derived as

$$\mu/\sigma = (\sigma_\mu/\sigma) \circ r_\mu = (\sigma_\mu/\sigma) \circ (F(\sigma_\mu) + v_\mu \mathbf{1}).$$

The first term is the radio bounded by $\mathrm{e}^{-d} \leq \sigma_\mu/\sigma \leq \mathrm{e}^{d}$ on $\mathcal{N}_{\tilde{\Gamma}}$. In the second term, $F(\sigma_\mu)$ is bounded by continuity of $F(\sigma)$ on the compact simplex. v_μ is given by the bisection problem (4.4), which is continuous on the compact $\mathcal{N}_{\tilde{\Gamma}}$, because it is continuous on every $\sigma \in \Delta$ and $\mu > 0$, and the limit as $\mu \to \mathbf{0}^+$ exists and is $v \to -\min_i F_i(\sigma)$.

6.2 Corrector derived from perturbed KKT conditions

In the interior point method, perturbed KKT conditions and barrier problems are derived from the same original problem. However, our perturbed KKT conditions and barrier problem do not entirely align, so we can derive two different but deeply related correctors from them. We start with the Newton method solving fixed-point bundle equation $G(\sigma, \mu) = 0$, which is equivalently UKKT (4.2). The Newton equation of $G(\sigma, \mu) = 0$ is derived as follows, where $G'_\theta(\sigma, \mu) d\theta$ is previously obtained in differential equation (5.11).

$$
\begin{aligned}
G'_\theta(\sigma,\mu)d\theta &= -\,G(\sigma,\mu) \\
\sigma \circ \Big(J(\sigma) + (\mathbf{1}^\top\mu)I\Big)\,\overline{d\theta} &= -\,\Big(I - \sigma\mathbf{1}^\top\Big)\,(\sigma\circ F(\sigma) - \mu)
\end{aligned} \tag{6.3}
$$

Multiplying both sides with $1/\sigma$, we arrive at the Newton equation of $G(\sigma,\mu)=0$ in equation (6.4).

$$
\Big(J(\sigma) + (\mathbf{1}^\top\mu)I\Big)\,\overline{d\theta} = -\,\Big(I - \mathbf{1}\sigma^\top\Big)\,(F(\sigma) - \mu/\sigma) \tag{6.4}
$$

We denote the term appears in the right-hand side of Newton equation (6.4) as $\tilde{G}(\sigma,\mu) = G(\sigma,\mu)/\sigma$. $\tilde{G}(\sigma,\mu)$ is bounded on the neighborhood $\mathcal{N}_{\tilde{\Gamma}}$, because $I - \mathbf{1}\sigma^\top$ and $F(\sigma)$ are both bounded on the compact simplex by continuity, and μ/σ is bounded on $\mathcal{N}_{\tilde{\Gamma}}$ as we explained earlier. The first derivative of $\tilde{G}(\sigma,\mu)$ is derived as follows.

$$
\begin{aligned}
d\tilde{G}(\sigma,\mu) =& d\frac{G(\sigma,\mu)}{\sigma} = \frac{1}{\sigma}\circ\frac{\partial G(\sigma,\mu)}{\partial\sigma}\circ\sigma\circ\overline{d\theta} - G(\sigma,\mu)\circ(1/\sigma^2)\circ\sigma\circ\overline{d\theta} \\
=& \Big(J(\sigma) + (\mathbf{1}^\top\mu)I\Big)\,\overline{d\theta} - \tilde{G}(\sigma,\mu)\circ\overline{d\theta}
\end{aligned} \tag{6.5}
$$

The second derivative of $\tilde{G}(\sigma,\mu)$ has the following bound.

$$
\begin{aligned}
\left\|\tilde{G}''(\sigma,\mu)\right\| &= \left\|J'(\sigma) - \Big(\tilde{G}(\sigma,\mu)\circ I\Big)'\right\| \le \left\|J'(\sigma)\right\| + \left\|\tilde{G}'(\sigma,\mu)\right\| \\
&\le \left\|J'(\sigma)\right\| + \|J(\sigma)\| + \mathbf{1}^\top\mu + \left\|\tilde{G}(\sigma,\mu)\right\|
\end{aligned} \tag{6.6}
$$

We analyze the convergence rate of the predictor-corrector path-following framework with the standard Newton corrector in equation (6.4). Adapting the standard quadratic convergence proof of the standard Newton iteration, we have the following equation. The 1st line follows from Newton update $\theta_{k+1} = \theta_k + \overline{d\theta}$ in Newton equation (6.4). In the 2nd to the 4th lines, we use the fundamental theorem of calculus to substitute the residuals, where $\sigma_u = \sigma_k + u(\sigma_{k+1} - \sigma_k)$ and $\sigma_w = \sigma_u + w(\sigma_u - \sigma_k)$. L in the 5th line follows from the second derivative bound in the above equation, and we substitute $\theta_{k+1} - \theta_k$ with $\overline{d\theta}$.

$$
\begin{aligned}
&\left\|\tilde{G}(\sigma_{k+1},\mu)\right\| = \left\|\tilde{G}(\sigma_{k+1},\mu) - \tilde{G}(\sigma_k,\mu) - \Big(J(\sigma_k) + (\mathbf{1}^\top\mu)I\Big)\,(\theta_{k+1}-\theta_k)\right\| \\
=& \left\|\tilde{G}(\sigma_{k+1},\mu) - \tilde{G}(\sigma_k,\mu) - \Big(\tilde{G}'(\sigma_k,\mu) + \tilde{G}(\sigma_k,\mu)\circ I\Big)\,(\theta_{k+1}-\theta_k)\right\| \\
\le& \int_0^1 \left\|\tilde{G}'(\sigma_u,\mu) - \tilde{G}'(\sigma_k,\mu)\right\|\,\|\theta_{k+1}-\theta_k\|\;du + \left\|\tilde{G}(\sigma_k,\mu)\right\|\,\|\theta_{k+1}-\theta_k\| \\
\le& \int_0^1 \left\|\tilde{G}''(\sigma_w,\mu)\right\|\,u\,\|\theta_{k+1}-\theta_k\|^2\;du + \left\|\tilde{G}(\sigma_k,\mu)\right\|\,\|\theta_{k+1}-\theta_k\| \\
\le& \frac{1}{2}L\left\|\Big(J(\sigma_k) + (\mathbf{1}^\top\mu)I\Big)^{-1}\right\|^2\left\|\tilde{G}(\sigma_k,\mu)\right\|^2 \\
L :=& \sup_{\sigma\in\Delta}\left\|J'(\sigma)\right\| + 3\sup_{\sigma\in\Delta}\|J(\sigma)\| + 3\mathbf{1}^\top\mu + \sup_{\sigma\in\mathcal{N}_{\tilde{\Gamma}}}\left\|\tilde{G}(\sigma,\mu)\right\|
\end{aligned} \tag{6.7}
$$

In the above equation, $\|(J(\sigma_k) + (\mathbf{1}^\top\mu)I)^{-1}\|$ is uniformly bounded by $1/s_{\min}(J_G)$ on the neighborhood $\mathcal{N}_{\tilde{\Gamma}}$ as we explained earlier. L is also uniformly bounded, because the first two terms are bounded on the compact simplex by continuity, the third term is bounded on the compact neighborhood $\mathcal{N}_{\tilde{\Gamma}}$, and the last term is the infinitesimal itself that is bounded on $\mathcal{N}_{\tilde{\Gamma}}$. Therefore, standard Newton (6.4) achieves uniform quadratic convergence rate with a uniform Newton convergence region over all the corrector steps.

For the predictor step, the reduction $d\mu$ produces a difference $d\mu/\sigma$ in $\tilde{G}(\sigma, \mu)$. Then, the tangent step $d\sigma$ given by differential equation (5.11) is meant to further reduce the difference in $\tilde{G}(\sigma, \mu)$ to a second-order remainder. Thus, the difference in $\tilde{G}(\sigma, \mu)$ due to predictor step is bounded by $d\mu/\sigma$, where $d\mu = -\eta\mu$ with a step size $\eta \in (0, 1)$. Then, by the bound of μ/σ on $\mathcal{N}_{\tilde{\Gamma}}$, the difference in $\tilde{G}(\sigma, \mu)$ is uniformly bounded over all the predictor steps on $\mathcal{N}_{\tilde{\Gamma}}$ with a coefficient η. Thus, there exists a positive step size $\eta \in (0, 1)$ to keep $\tilde{G}(\sigma, \mu)$ in the Newton convergence region after every predictor step.

Therefore, we can draw the conclusion that the predictor-corrector algorithm achieves global linear convergence along the path $\tilde{\Gamma}$ to its ending point. Recall that if the solution $(\sigma^\star, \mathbf{0})$ is nonsingular, the ending point of $\tilde{\Gamma}$ is exactly $(\sigma^\star, \mathbf{0})$. However, if the solution $(\sigma^\star, \mathbf{0})$ is nonsingular, $\tilde{\Gamma}$ ends before $(\sigma^\star, \mathbf{0})$ at where $\mathbf{1}^\top \mu = \zeta$. In the singular solution case, the linear convergence rate to where $\mathbf{1}^\top \mu = \zeta$ is dependent to ζ and decreases to 1 as ζ tends to 0.

Standard Newton iteration is simple for theoretical analysis, however, its performance in practice is not ideal. Because the step length is affected by the smallest singular value $s_{\min}(J_G)$, such that the iteration appears to be unstable if $s_{\min}(J_G)$ is too small. A classic method addressing this issue is regularized Newton equation (6.8), derived from standard Newton equation (6.4) by multiplying both sides with $J_G^\top$ and adding the regularization term $\delta_H I$ with $\delta_H > 0$, so that the coefficient is positive semidefinite and controlled by δ_H. Indeed, the smallest singular value of the coefficient is now $s^2_{\min}(J_G) + \delta_H$, and the step length can be controlled with a mild δ_H. But the convergence reduces from quadratic convergence to linear convergence with rate $\delta_H/(s^2_{\min}(J_G) + \delta_H)$. Thus, regularization actually trades convergence speed for iteration stability.

$$\left(J_G^\top J_G + \delta_H I\right) \overline{d\theta} = -J_G^\top \tilde{G}(\sigma, \mu) \tag{6.8}$$

Note that regularized Newton equation (6.8) is approximately the regularized Gauss-Newton equation of the least square problem (6.9) with local norm induced by $\operatorname{diag}(1/\sigma^2)$. Since the local norm is induced by the Hessian matrix of the log barrier $-\ln \sigma$, problem (6.9) is actually a log barrier problem. Thus, the gradient descent with its inexact gradient $J_G^\top \tilde{G}(\sigma, \mu)$ works as a corrector solving $G(\sigma, \mu) = 0$ as well. Regularized Newton equation (6.8) mixes Newton steps and gradient steps, such that it reduces to standard Newton step (6.4) if $\delta_H = 0$, and it approximates gradient step $-(1/\delta_H) J_G^\top \tilde{G}(\sigma, \mu)$ if δ_H is large.

$$\min_\sigma \frac{1}{2} \left\| \tilde{G}(\sigma, \mu) \right\| = \min_\sigma \frac{1}{2} \left\| G(\sigma, \mu) \right\|_{\operatorname{diag}(1/\sigma^2)} \tag{6.9}$$

6.3 Corrector derived from barrier problem

Since the fixed-point bundle is also a special central path of the MCP (4.5), we can also derive a gradient from the barrier MCP (4.5) for corrector. First, we additionally require that (r, v) are subject to the Brouwer function $(\hat{\sigma}, r, v) = M(\sigma, \mu)$ in barrier MCP (4.5). Then, we can view σ as the only optimization variable, whereas (r, v) are intermediate variables, so the gradient is only with respect to $d\sigma$, and thus only with respect to $d\theta$. Additionally, this also enables us to use $\mathbf{1}^\top(\sigma - \hat{\sigma}) = 0$ to eliminate dv in the differential.

The gradient of barrier MCP (4.5) is derived as follows. In the 3rd line, we use $\mu/r = \hat{\sigma}$ and $\mathbf{1}^\top(\sigma - \hat{\sigma}) = 0$. In the 4th line, we use $(I - \sigma\mathbf{1}^\top)(\sigma - \hat{\sigma}) = (\sigma - \hat{\sigma})$. In the 4th line, we also use

$r = F(\sigma) + v\mathbf{1}$ and $\hat{\sigma}^\top F(\sigma) + v = \mathbf{1}^\top \mu$. In the 5th line, we use $\mathbf{1}^\top(\sigma - \hat{\sigma}) = 0$ in the first additive $J(\sigma)$ and use $(I - \mathbf{1}\sigma^\top)(I - \mathbf{1}\sigma^\top) = (I - \mathbf{1}\sigma^\top)$ in the second additive. In the 6th line, we use $\mathbf{1}^\top(\sigma - \hat{\sigma}) = 0$.

$$
\begin{aligned}
& d\left(\sigma^\top r - \mu^\top \ln \sigma - \mu^\top \ln r\right) = (\sigma - \mu/r)^\top dr + (r - \mu/\sigma)^\top d\sigma \\
=& (\sigma - \mu/r)^\top \left(\frac{\partial F(\sigma)}{\partial \sigma} \circ \sigma \circ \frac{d\sigma}{\sigma} + dv\mathbf{1}\right) + (\sigma - \mu/r)^\top \left(r \circ \frac{d\sigma}{\sigma}\right) \\
=& (\sigma - \hat{\sigma})^\top \left(\frac{\partial F(\sigma)}{\partial \sigma} \circ \sigma + r \circ I\right)\left(I - \mathbf{1}\sigma^\top\right) d\theta \\
=& (\sigma - \hat{\sigma})^\top \left(I - \mathbf{1}\sigma^\top\right)\left(\frac{\partial F(\sigma)}{\partial \sigma} \circ \sigma + \left(\left(I - \mathbf{1}\hat{\sigma}^\top\right) F(\sigma) + (\mathbf{1}^\top \mu)\mathbf{1}\right) \circ I\right)\left(I - \mathbf{1}\sigma^\top\right) d\theta \\
=& (\sigma - \hat{\sigma})^\top \left(J(\sigma) + \left(\mathbf{1}^\top \mu + (\sigma - \hat{\sigma})^\top F(\sigma)\right)\left(I - \mathbf{1}\sigma^\top\right)\right) d\theta \\
=& (\sigma - \hat{\sigma})^\top \left(J(\sigma) + \left(\mathbf{1}^\top \mu + (\sigma - \hat{\sigma})^\top F(\sigma)\right) I\right) d\theta
\end{aligned}
\tag{6.10}
$$

Ignoring the higher-order term $((\sigma-\hat{\sigma})^\top F(\sigma))(\sigma-\hat{\sigma})$, we arrive at the inexact gradient of MCP (4.5) in equation (6.11).

$$
\nabla_\theta \left(\sigma^\top r - \mu^\top \ln \sigma - \mu^\top \ln r\right) = \left(J(\sigma) + (\mathbf{1}^\top \mu) I\right)^\top (\sigma - \hat{\sigma}) \tag{6.11}
$$

Next, we can also derive a regularized Newton equation from standard Newton equation (6.4) with gradient $J_G^\top(\sigma - \hat{\sigma})$ on the right-hand side. We denote $v_g = \sigma^\top F(\sigma) - \mathbf{1}^\top \mu$ such that $\sigma \circ F(\sigma) + v_g \sigma - \mu = G(\sigma, \mu)$, and $(\hat{\sigma}, r, v_b) = M(\sigma, \mu)$ such that $\hat{\sigma} \circ (F(\sigma) + v_b \mathbf{1}) = \mu$. And we denote $v_{gb} = (v_g - v_b)/(\mathbf{1}^\top \mu + k)$. Then, the derivation is as follows, where the 3rd line follows from $J(\sigma)\mathbf{1} = k\mathbf{1}$.

$$
\begin{aligned}
\sigma \circ \left(J(\sigma) + (\mathbf{1}^\top \mu) I\right) \overline{d\theta} &= -\left(\sigma \circ F(\sigma) + v_g \sigma - \mu\right) \\
\sigma \circ \left(J(\sigma) + (\mathbf{1}^\top \mu) I\right) \overline{d\theta} + (v_g - v_b)\sigma &= -\left(\sigma \circ F(\sigma) + v_b \sigma - \mu\right) \\
\sigma \circ \left(J(\sigma) + (\mathbf{1}^\top \mu) I\right) \left(\overline{d\theta} + v_{gb}\mathbf{1}\right) &= -\left(\sigma \circ F(\sigma) + v_b \sigma - \mu\right) \\
\frac{\sigma}{r} \circ \left(J(\sigma) + (\mathbf{1}^\top \mu) I\right) \left(\overline{d\theta} + v_{gb}\mathbf{1}\right) &= -\left(\sigma - \hat{\sigma}\right) \\
\left(J(\sigma) + (\mathbf{1}^\top \mu) I\right)^\top \circ \frac{\sigma}{r} \circ \left(J(\sigma) + (\mathbf{1}^\top \mu) I\right) \left(\overline{d\theta} + v_{gb}\mathbf{1}\right) &= -\left(J(\sigma) + (\mathbf{1}^\top \mu) I\right)^\top (\sigma - \hat{\sigma})
\end{aligned}
\tag{6.12}
$$

Then, we arrive at the regularized Newton equation (6.13). Similar to regularized Newton equation (6.8), regularized Newton equation (6.13) mixes Newton steps and gradient steps, such that it reduces to standard Newton step (6.4) if $\delta_H = 0$, and it approximates gradient step $-(1/\delta_H)J_G^\top(\sigma - \hat{\sigma})$ if δ_H is large.

$$
\begin{aligned}
\left(J_G^\top \circ \frac{\sigma}{r} \circ J_G + \delta_H I\right) d\theta &= -\, J_G^\top (\sigma - \hat{\sigma}) \\
\overline{d\theta} &= \left(I - \mathbf{1}\sigma^\top\right) d\theta
\end{aligned}
\tag{6.13}
$$

Similar to regularized Newton equation (6.8), regularized Newton equation (6.13) also corresponds to a least square problem (6.14) with local norm. It can be verified that $J_G^\top(\sigma - \hat{\sigma})$ is the inexact gradient of this least square problem via similar derivation as that of $J_G^\top(\sigma - \hat{\sigma})$.

$$
\min_\sigma \|\sigma \circ r - \mu\|_{\mathrm{diag}(1/(\sigma \circ r))} = \min_\sigma (\sigma - \mu/r)^\top (r - \mu/\sigma) \tag{6.14}
$$

7 The unified framework

The predictor-corrector path-following algorithm on the fixed-point bundle is as Algorithm 1 shows. The algorithm follows the path $\tilde{\Gamma}$ in its neighborhood $\mathcal{N}_{\tilde{\Gamma}}$, from the starting point near $(\sigma_{\text{init}}, v_{\text{init}}\sigma_{\text{init}})$ for a sufficiently large v_{init} given any designated $\sigma_{\text{init}} \in \Delta$. The predictor step consists of three parts: avoiding singular points along the fibers, reducing μ, and updating σ along the tangent vector. The corrector step is a subiteration using either regularized Newton equation (6.8) or (6.13), in which obtaining $(\hat{\sigma}, r, v)$ involves solving bisection problem (4.4). The stopping criteria is $\mathbf{1}^\top \check{\mu}(\sigma) < \epsilon$, because $\mathbf{1}^\top \check{\mu}(\sigma)$ equals to the gap of $\text{VI}(F, \Delta)$. By Theorem 4, we have $\mathbf{1}^\top \check{\mu}(\sigma) < \epsilon$ when $\mathbf{1}^\top \mu < \epsilon$ and $G(\sigma, \mu) < \mu$ component-wise. Thus, if we truncate μ such that $\min_i \mu_i \geq \epsilon/(n+1)$, then $\|G(\sigma, \mu)\| < \epsilon/(n+1)$ suffices to imply $G(\sigma, \mu) < \mu$ component-wise, and μ can still decrease down below $\mathbf{1}^\top \mu < \epsilon$.

Algorithm 1 Path-following on the fixed-point bundle

Require: A smooth map $F : \Delta \to \mathbb{R}^n$ and its derivative $\partial F/\partial \sigma$, a designated starting point $\sigma_{\text{init}} \in \Delta$, and a desired precision $\epsilon > 0$

Set $(\sigma_0, \mu_0) = (\sigma_{\text{init}}, v_{\text{init}}\sigma_{\text{init}})$ for a sufficiently large v_{init}
repeat
  repeat
    Compute $(\hat{\sigma}_k, r_k, v_k) = M(\sigma_k, \mu_t)$ by solving bisection problem (4.4)
    Construct the matrix $J(\sigma_k)$ in equation (5.8)
    Solve regularized Newton equation (6.8) or (6.13) for $\overline{d\theta}_k$ with $\delta_H = \|G(\sigma_k, \mu_t)\|/n$
    Update $\sigma_{k+1} = \text{softmax}(\ln \sigma_k + \overline{d\theta}_k)$
  until $\|G(\sigma_k, \mu_t)\| < \epsilon/(n+1)$
  Set $\check{\mu}_t = \mu_t + \beta_t \sigma_k > 0$ such that $\mathbf{1}^\top \mu_t + \beta_t$ avoids the nonzero eigenvalues of $-J(\sigma_k)$
  Update and truncate $\mu_{t+1} = ((1 - \eta_t)\check{\mu}_t).\text{clip}(\min = \epsilon/(n+1))$ with a sufficiently small η_t
  Solve differential equation (5.11) for $\overline{d\theta}_t$ with $d\mu_t = \mu_{t+1} - \check{\mu}_t$
  Set $\sigma_0 = \text{softmax}(\ln \sigma_k + \overline{d\theta}_t)$
until $\mathbf{1}^\top \check{\mu}(\sigma_k) < \epsilon$
return σ_k as an approximate solution of $\text{VI}(F, \Delta)$

Comparing the two regularized Newton equations (6.8) and (6.13), despite that they are both equivalent to the standard Newton equation (6.4) when $\delta_H = 0$, they are different when $\delta_H \neq 0$. First, the former corresponds to a least square problem with local norm $\text{diag}(1/\sigma^2)$ that only penalizes σ approaching 0, whereas the latter corresponds to a least square problem with local norm $\text{diag}(1/(\sigma \circ r))$ that penalizes both σ approaching 0 and r approaching 0.

Second, the Hessian $J_G^\top J_G$ of regularized Newton (6.8) remains bounded as σ approaches 0, whereas the Hessian $J_G^\top \circ (\sigma/r) \circ J_G$ of regularized Newton (6.13) is more skewed. As σ approaches 0, some components of $J_G^\top \circ (\sigma/r) \circ J_G$ vanishes, but this is controlled by regularization parameter δ_H. As r approaches 0, some components of $J_G^\top \circ (\sigma/r) \circ J_G$ blows up, making step length to vanish in those components. Thus, regularized Newton (6.13) takes extra cautious steps as r approaches 0. This is a useful feature, because there is $\sigma \circ r = \mu$ along the path, and unlike σ approaching 0 but r is subject to a function, r approaching 0 can cause σ to blow up under iteration with fixed $\mu > 0$. Thus, regularized Newton equation (6.13) appears to be more stable approaching the boundary but overall slower than regularized Newton equation (6.8).

The algorithm is tested on randomly generated instances of $\text{VI}(F, \Delta)$ in different dimensions. Specifically, F is a neural network with a $[n, 50, n]$ architecture and tanh activation functions, initialized with random weights and biases. This neural network model is real analytic, and its

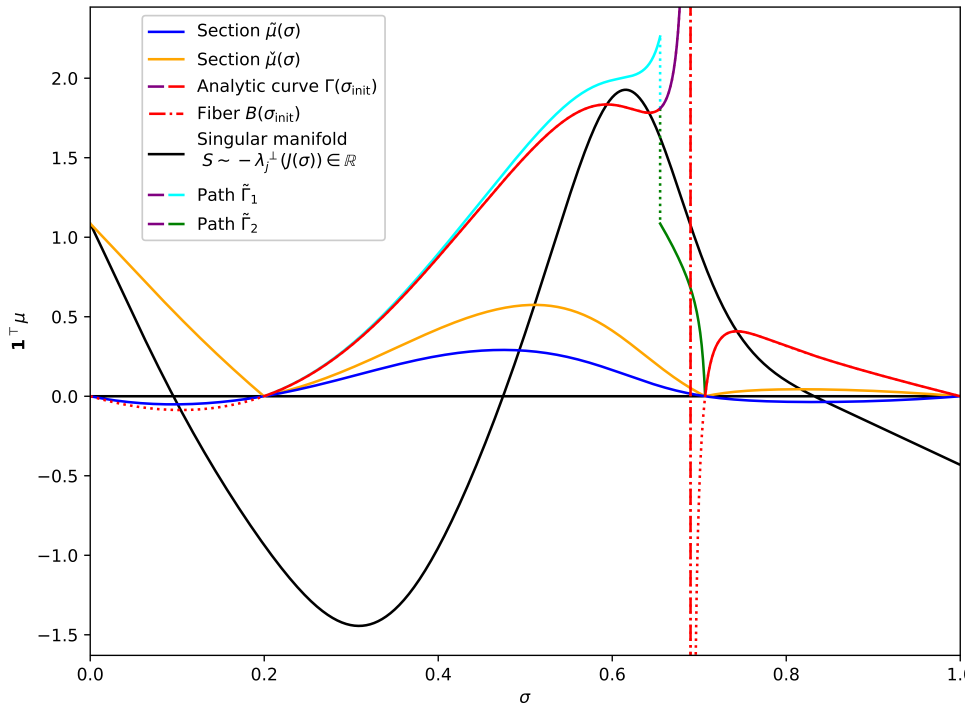

Figure 1: Graph of the fixed-point bundle. This graph shows the fixed-point bundle E of a 2-dimensional $\mathrm{VI}(F, \Delta)$. The horizontal axis in σ represents the simplex, and the vertical axis in $\mathbf{1}^\top \mu$ represents the fiber. Section $\tilde{\mu}(\sigma)$ is smooth and derives the matrix $J(\sigma)$ that measures the differential properties of E, whereas section $\check{\mu}(\sigma)$ is nonnegative and measures the gap of $\mathrm{VI}(F, \Delta)$. The analytic curve $\Gamma(\sigma_{\mathrm{init}})$ is the subcurve of $\{(\sigma, \gamma\sigma_{\mathrm{init}}) \in E | \gamma \in \mathbb{R}\}$ where $\mathbf{1}^\top \mu \geq 0$, setting aside the negative part represented by the red dashed curve. As $\mu \to \mathbf{0}^+$, σ tends to the zero points of $\check{\mu}(\sigma)$, which are equivalently solutions of $\mathrm{VI}(F, \Delta)$. Whereas as $\mu \to \mathbf{0}$, σ tends to the zero points of $\tilde{\mu}(\sigma)$, which are not always solutions of $\check{\mu}(\sigma)$. The analytic curve $\Gamma(\sigma_{\mathrm{init}})$ consists of several branches, one of the branches connects σ_{init} with one solution, and other branches connects the rest of the solutions in pairs, which is the parity arguement. The branch of $\Gamma(\sigma_{\mathrm{init}})$ that connects σ_{init} starts from a known point infinitely high on the fiber $B(\sigma_{\mathrm{init}})$, so we let path $\tilde{\Gamma}$ starts from σ_{init} and follows along $\Gamma(\sigma_{\mathrm{init}})$ as its first segment. However, $\Gamma(\sigma_{\mathrm{init}})$ may have singular points on it, and those are where it intersects with the singular manifold S. The singular manifold S is the manifold of real eigenvalues of $-J(\sigma)$. In this 2-dimensional case, S has a simple shape since $-J(\sigma)$ always has an eigenvalue $-k$ and another real eigenvalue, but S could have much more complex shapes in higher-dimensional cases where there could be complex eigenvalues. On a singular point of $\Gamma(\sigma_{\mathrm{init}})$, the direction that $\mathbf{1}^\top \mu$ moves reverses. As is shown, singular points are branch points of $\Gamma(\sigma_{\mathrm{init}})$ as $\mathbf{1}^\top \mu$ varies, and they are critical points of $\Gamma(\sigma_{\mathrm{init}})$ in variable σ. Singular points must be avoided because path-following cannot go beyond them, and this is done by moving μ along the fiber by adding $\beta\sigma$. There are two paths $\tilde{\Gamma}_1$ and $\tilde{\Gamma}_2$ in this graph, representing singularity avoidance with a positive β and a negative β. Singularity avoidance produces a segment of a different $\Gamma(\sigma_{\mathrm{init}})$ as the next segment of path $\tilde{\Gamma}$. At a suitable σ with a suitable β, the next segment no longer intersects with the singular manifold. Finally, after finitely many segments, $\tilde{\Gamma}$ leads to a solution of $\mathrm{VI}(F, \Delta)$.

Table 2: Iteration numbers solving $\mathrm{VI}(F, \Delta)$

Dimension	Regularized Newton (6.8)	Regularized Newton (6.13)
$[3, 50, 3]$	331 / 329	347 / 342
$[6, 50, 6]$	362 / 339	379 / 356
$[12, 50, 12]$	372 / 347	389 / 368
$[25, 50, 25]$	390 / 360	402 / 372
$[50, 50, 50]$	437 / 370	440 / 380
$[100, 50, 100]$	438 / 378	431 / 382
$[200, 50, 200]$	539 / 475	539 / 487
$[400, 50, 400]$[1]	655 / 528	640 / 546
$[800, 50, 800]$[1]	645 / 550	667 / 582

[1] Each entry in these two rows are based on 100 VI instances, while entries in the remaining rows are based on 1000 VI instances.

[2] Each entry is of the form mean / median over the iteration numbers solving instances.

[3] $[n, 50, n]$ is the architecture of the neural network modeling F.

derivative is computed via backpropagation [42]. The initial point σ_{init} is also randomly generated, and the required precision is set to 10^{-5}. We test the algorithm using both the two different regularized Newton correctors and record the number of iterations. For dimensions 3 to 200, we test 1000 instances, and for dimensions 400 and 800, we test 100 instances. The mean and median of the iteration numbers are reported in Table 7. It can be seen that the algorithm with regularized Newton corrector (6.13) is slower, but it is more stable since the mean and median iteration numbers are closer. Across all the 14400 test instances, the algorithm converges to a solution in every single instance, demonstrating its robustness in practice. Moreover, the increase in iteration number does not increase too drastically with the dimension, illustrating the scalability of the framework.

8 Conclusion

In this paper, we present a path-following framework on the fixed-point bundle for general finite-dimensional variational inequalities. First, we approximately reduce general variational inequality $\mathrm{VI}(H, K)$ to variational inequality $\mathrm{VI}(F, \Delta)$ with analytic function F and simplex domain Δ.

Then, we present three equivalent characterizations of $\mathrm{VI}(F, \Delta)$. The linear programming form produces UKKT (4.2), which leads to solutions of $\mathrm{VI}(F, \Delta)$ as $\mu \to \mathbf{0}^+$. The Brouwer fixed-point form is Brouwer function $(\hat{\sigma}, r, v) = M(\sigma, \mu)$ given by the bisection problem (4.4), such that Brouwer fixed-point theorem applies to it to guarantee the existence of solutions of $\mathrm{VI}(F, \Delta)$. The mixed complementarity problem form is MCP (4.5), such that the solution space of UKKT (4.2) is a special central path of it.

Next, we formalize the solution space of UKKT (4.2) as the fixed-point bundle E and equivalently transform UKKT (4.2) to the fixed-point bundle equation $G(\sigma, \mu) = 0$. We introduce two sections of the fixed-point bundle, $\check{\mu}(\sigma)$ measures the gap of $\mathrm{VI}(F, \Delta)$, and $\tilde{\mu}(\sigma)$ derives matrix $J(\sigma)$ that characterizes the differential properties of the fixed-point bundle. Through matrix $J(\sigma) + (\mathbf{1}^\top \mu) I$, we formalize the singular manifold S of the fixed-point bundle as the manifold of real eigenvalues of $-J(\sigma)$. By analyzing the analytic curve $\Gamma(\sigma_{\text{init}})$, we establish the parity arguement for $\mathrm{VI}(F, \Delta)$, which guarantees the oddness of the number of solutions of $\mathrm{VI}(F, \Delta)$.

Finally, we arrive at our predictor-corrector path-following framework on the fixed-point bundle. Combining the analytic curve $\Gamma(\sigma_{\text{init}})$ and singularity avoidance along the fibers, we formalize the path we follow as $\tilde{\Gamma}$, which consists of finitely many segments of different $\Gamma(\sigma_{\text{init}})$. We show that there exists a compact neighborhood $\mathcal{N}_{\tilde{\Gamma}}$ of $\tilde{\Gamma}$ satisfying $\mathcal{N}_{\tilde{\Gamma}} \cap S = \varnothing$ for the corrector to work. Then, we introduce standard Newton corrector (6.4) and prove the convergence result of the overall algorithm. Alternatively, we also introduce a gradient corrector (6.11). The standard Newton equation and the gradient equation lead to regularized Newton equation (6.8) and (6.13), which both work as a effective corrector for practical use.

The final convergence result is proved with the standard Newton corrector (6.4). The algorithm achieves global linear convergence to nonsingular solutions of $\text{VI}(F, \Delta)$. For singular solutions, the algorithm retains global linear reduction before reaching a fixed precision measured by $\mathbf{1}^\top \mu = \zeta > 0$, but the convergence rate reduces to 1 as ζ tends to 0.

In experiment, the algorithm is tested on 14400 randomly generated VIs of up to 800 dimensions using both the two regularized Newton correctors. It works in every single case, and iteration number increases only mildly with the dimension.

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