Robust Design in Game Theory: Bayesian Optimization Approach to Minimax Problems with Equilibrium Constraints

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Modern engineering systems have become increasingly complex due to the integration of human actors and advanced artificial intelligence, both of which can be interpreted as intelligent agents. Game theory is a mathematical framework that provides an explanatory model for systems constituted of those intelligent agents. It postulates that the apparent behavior of a system is an equilibrium resulting from each agent within the system individually optimizing their own objectives. Thus, designing an intelligent system is to identify a configuration such that its equilibrium is desirable with respect to some external criteria. However, equilibria are often not unique and form sets that lack topological properties on which optimization heavily relies on, e.g., convexity, connectedness, or even compactness in some cases. The unsureness nature, i.e., uncertainty, of equilibria also appeals for another common design criterion: robustness. In this context, a robust design should reach worst-case optimality to avoid sensitivity to the eventual outcome among all possible equilibria.

In this dissertation, I incorporate both the game theoretical aspect and the robustness requirement of system design using the formulation of minimax problems with equilibrium constraints. The complexity of the problem structure and the non-uniqueness of potential equilibria require a new solution strategy different from traditional gradient based methods. I propose a Bayesian approach which infers the probabilistic belief of the optimality of a design given sampled objective function values. Due to the anisotropic natural of systems of independent agents, I then revisit the original Kushner's Wiener process prior instead of radial basis kernel prior despite their popularity for other global optimization applications. I also derive theoretical results on sample maxima and their locations, develop an effective method to decompose the search space into independent regions, and design necessary adaptations to take into account the equilibrium constraints and minimax objective. Finally, I discuss a few applications of the proposed design framework.

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1.0 Introduction

Human-in-the-loop systems and artificial intelligent systems have increasing applications in engineering. The dynamics of individual components in these systems may not be directly understood or engineered, but their interactions often follow basic principles put forward by the game theory. Game theory is a mathematical framework which provides an explanatory model for systems constituted of multiple intelligent agents. It postulates that the apparent behavior of a system is an equilibrium resulting from each agent within the system individually optimizing their own objectives. In this dissertation, I investigate optimal design problems in this game theoretical framework, which aims at finding the values of game parameters which fulfill desired criteria.

In the rest of the first chapter, I give a brief history regarding the subjects of interest. A motivating example is then given to illustrate the problems this dissertation attempts to solve. The contributions of this dissertation is summarized. In the second chapter, I discuss some theoretical aspects in optimization, especially the topological properties. The mathematical formulation of the main focus of this dissertation is given and the basic properties are discussed. In the third chapter, mathematical programming methods based on Bayesian optimization are developed to effectively solve the design problems. In the fourth chapter, I show more concrete applications related to the proposed framework of game design.

1.1 Background

Modern game theory was established by John von Neumann with his 1928 paper [34], in which he proved the existence of mixed-strategy equilibria in two-person zero-sum finite games using Brouwer's fixed-point theorem. John Nash [23] proposed a solution concept to games with multiple players, generalizing the work of von Neumann. Game theory at-

tracted considerable development since 1950s and found phenomenal achievements especially in mathematical economics. Nobel Memorial Prize in Economic Sciences was rewarded to game theorists in numerous years.

Way before the modern game theory was conceived, in the 17th century mathematicians started to study a different aspect of games. In the letter exchange between Blaise Pascal and Pierre Fermat, they discussed the problem of division of the stakes, consisting in designing a game of chance which is fair to the players. To define fairness, they established the concept of expected values. Their foundational discussion is now considered as the birth of the probability theory [30]. In the 18th century, Thomas Bayes and Pierre-Simon Laplace proved a powerful theorem for data analysis, known as Bayes' theorem today. This theorem was developed into Bayesian inference, which revolutionized the study of probability and statistics. Today, Bayesian methods empowers numerous algorithms in machine learning for classification and regression.

Game theory has benefit from recent rapid development of machine learning. Reinforcement learning is a branch of machine learning inspired by the mathematical theory of optimal control and the biological function of dopamine in nervous system. Using the concept of reward, reinforcement learning can solve complex problems in game theory [26]. On the other hand, game theoretical framework also inspired powerful machine learning algorithm such as generative adversarial networks [13]. Inverse reinforcement learning consists in recovering the unknown reward structure guiding the behavior of an agent from the external observation of the agent's behavior. It is an active and fruitful field of research [1, 25] and gave rise to generalizations to multi-agent system [14, 24].

The existing literature on the design problems in game theory [5, 2, 36] almost exclusively focuses on local solutions using gradient-based methods. The existence of multiple equilibria, a significant feature of games, is often overlooked. This dissertation tries to fill up this gap by providing a global point of view with the introduction of the concept of robustness and a Bayesian solution approach.

1.2 Example

To illustrate the type of engineering problems interested in this dissertation, I propose the following example.

Example 1. In a country with the geography $\mathcal{X} = [0,1]^2$, let there be N cities located respectively at $(x_i, y_i) \in \mathcal{X}$, each having a potential air traffic market of size z_i, and M airline hubs located respectively at $(u_j, v_j) \in \mathcal{X}$, each having the control over their service radius r_j for a cost $g(r_j^2) = g_0 \exp(\alpha r_j^2)$ where $\alpha \geq 0$. If a city falls in the service area of multiple hubs, then the air traffic market of that city is equally shared among those hubs. Suppose all the hubs aim at maximizing their profits and their service radii reach a Nash equilibrium, which solves the following optimization problems.

$$
\begin{aligned}
(r_j^*, s_j^*) \in \arg\max_{r_j, s_j} \left(-g(r_j^2) + \sum_{i=1}^{N} \frac{z_i s_{ij}}{\sum_{k=1}^{M} s_{ik} + (1 - s_{ij})} \right) & \qquad \forall j \\
\text{s.t. } s_{ij}(r_j^2 - d_{ij}^2) \geq 0 & \qquad \forall i, j \\
0 \leq s_{ij} \leq 1 & \qquad \forall i, j \\
0 \leq r_j \leq 1 & \qquad \forall j
\end{aligned}
$$

The constant $d_{ij}^2 = (x_i - u_j)^2 + (y_i - v_j)^2$ is the squared distance between city i and airport j, the variable s_{ij} represents whether city i is served by airport j. A best response (r_j^*, s_j^*) of airport j always satisfies $r_j^* \in \{d_{ij}\}, s_{ij}^* \in \{0, 1\}$. As a result, the action space of each player is effectively finite with cardinality N, the equilibria of the game can be obtained through iterated elimination of strictly dominated strategies. As we will be interested in the variables M and α, denote the set of equilibria by $\Phi(M, \alpha)$.

Now the government is planning an infrastructure project that will entirely determine the cost parameter α. Suppose the government wants to avoid a game of multiple equilibria, which causes market uncertainty. Then the parameter α needs to solve the following problem.

$$
\begin{aligned}
\min_{\alpha} \max_{s, s'} \sum_{ij} |s_{ij} - s'_{ij}| \\
\text{s.t. } (r, s) \in \Phi(M, \alpha) \\
(r', s') \in \Phi(M, \alpha)
\end{aligned}
$$

Suppose, in a different scenario, the government wants to maximize the total air traffic coverage and at the same time to hedge against a potential recession that only M' hubs will survive. The hedging objective is to reduce the worst-case loss of previously established coverage during the recession. Then this problem can be formulated as follows.

$$\begin{aligned} \max_{\alpha} \min_{s,s'} \quad & \left(\frac{1}{M} \sum_{ij} s_{ij} - \mu \sum_{ij} (s_{ij} - s'_{ij})^+ \right) \\ \text{s.t. } & (r, s) \in \Phi(M, \alpha) \\ & (r', s') \in \Phi(M', \alpha) \end{aligned} \tag{1.1}$$

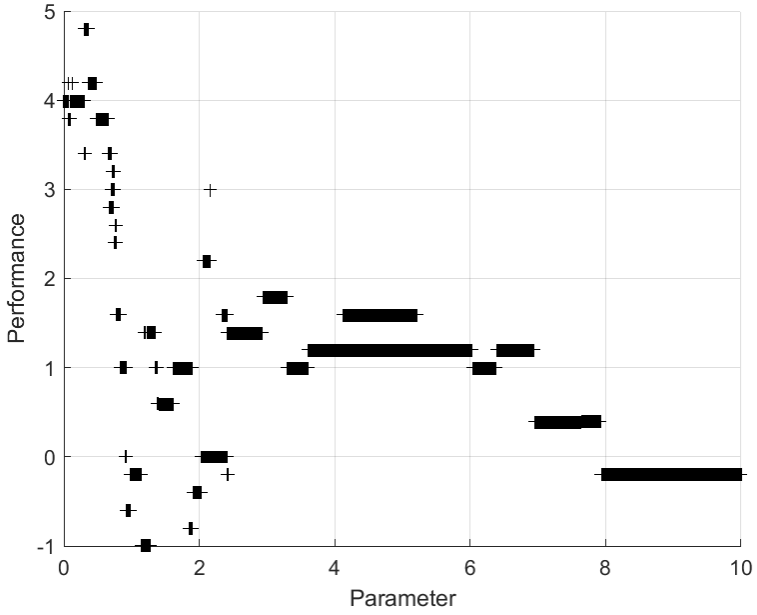

Figure 1: Performance (1.1) of the equilibria given the parameter α. Multiple points with the same abscissa result from different Nash equilibria attained at that value of α. The optimal worst-case performance is reached at any value of α in $[0.300, 0.303]$ or in $[0.325, 0.356]$. $(N = 20, M = 5, M' = 3, g_0 = 2, \mu = 0.4)$

The design problems I illustrate here are examples of MPEC (mathematical programming with equilibrium constraints). Specifically, they look for optimal designs which relate two or more versions of a game by posing optimization problems with their Nash equilibria as the constraints. At the same time, the upper level of these problems are minimax problems. Due to the possibility of multiple equilibria in a game, a robust design should take into consideration the worst-case scenario and aims at achieving optimality in this case.

1.3 Contributions

This dissertation examines minimax problems with equilibrium constraints and proposes a solution based on Bayesian optimization. Although minimax problems and equilibrium constraints have been long studied as separate subjects, they have received little attention as a combined problem due to the complexity. In this dissertation, I highlight with examples the importance of this formulation in designing multi-agent systems. Instead of the traditional optimization techniques focused on gradient-based methods, a novel solution methodology is proposed to treat this type of problems. I make a few adaptations of the existing Bayesian optimization specifically to incorporate equilibrium constraints and minimax objective. Among others, I show the Wiener process prior proposed by Kushner does not provide a uniform prior on the maximizers and I propose a simple method to obtain a uniform prior. I propose a generalization of the Wiener process to higher dimensions for the purpose of finding game equilibria. This generalization is different from traditional high dimensional Bayesian optimization which prefers the isotropy of search space. The lack of isotropy in my generalization is justified by the anisotropic nature of systems of independent agents. I show how this generalization decomposes the search space into independent regions given sampled objective function values. Theoretical results on sample maxima can be applied on each of the regions, and be combined to obtain the probabilistic belief of the optimality of a design. This novel solution approach can also be generalized and applied to related problems such as other multilevel optimization problems.

2.0 Theoretical Models of Optimization and Games

In this section, I first review some standard optimization problems and state compactness results of their solutions. Then I continue the same discussion for games. These are the theoretical basis upon which we can further build design problems.

Optimization theory makes use heavily of the theory of correspondences. A correspondence from the set X to the set Y is a function from the set X to the power set 2^Y. It can also be characterized by a binary relation between X and Y, or equivalently the graph of the relation. The use of correspondences instead of functions reflect the key property of optimization that a problem can have zero, one, or multiple optimizers.

Optimization problems are characterized by the mathematical structures they are endowed with, notably their topological property. In consequence, different notions of continuity of correspondences [6] play a major role in providing topological properties to the optimizers of a problem.

2.1 Single-Agent Optimization

The input-output relation of complex systems demonstrates the property of agency. Such systems are called agents. Optimization problems are a mathematical model of agents.

Definition 1 (Optimization problem)**.** An optimization problem $\mathcal{P}$ constitutes of a set X called the state space, a set Y called the action space, a function $f : X \times Y \to \mathbb{R}$ called the payoff function, and a correspondence $C : X \rightrightarrows Y$ called the constraint. The correspondence $F : X \rightrightarrows Y$ given by $F(x) = \arg\max\{f(x, y) \mid y \in C(x)\}$ is called the solution. A selector of F is called a strategy.

The following proposition gives conditions which guarantee the existence of a strategy to $\mathcal{P}$.

Proposition 1. *If Y is a topological space, f is upper semicontinuous in y, and C has nonempty and compact values, then $\mathcal{P}$ admits a nonempty and compact set of strategies.*

Proof. By [6, Theorem 2.43], $F(x)$ are nonempty and compact. Hence, the set of strategies is nonempty by the axiom of choice and compact by Tychonoff's theorem. □

An additional property of agents, which may affect their outputs, is the information available to them. The information structure of an agent is modeled by a σ-algebra on X so that a strategy is compatible with the information structure if and only if it is measurable. The following proposition gives additional conditions which guarantee the existence of a measurable strategy.

Proposition 2. *If X is a measurable space, Y is a separable metrizable space, f is measurable in x and continuous in y, and C is measurable and has nonempty and compact values, then $\mathcal{P}$ admits a nonempty and compact set of measurable strategies.*

Proof. By [6, Theorem 18.19], F admits a measurable selector. As Y is metrizable, the space of measurable functions from X to Y is closed. By Proposition 1, the set of selectors is compact. The set of measurable selectors, being the intersection of a closed subset and a compact subset within the Hausdorff space Y^X equipped with the product topology, is compact. □

When X is a measure space and Y is a Banach space, we can discuss the compactness of the set of strategies in $L^p(X, Y)$.

Proposition 3. *Suppose X is a perfect probability space and Y is a bounded subset of a Banach space. The set of measurable strategies is nonempty and compact in $L^p(X, Y)$.*

Proof. Let $N : Y \to \mathbb{R}$ be the norm on Y. Consider the map $\varphi_1 : Y^X \to \mathbb{R}^X$ given by $f \mapsto N \circ f$. First prove that φ_1 is continuous with respect to the product topologies. The set of all subsets $V := \{g : X \to \mathbb{R} \mid g(x_0) \in U\}$, where $x_0 \in X$ and $U \subseteq \mathbb{R}$ is an open set, is a subbase of the product topology on $\mathbb{R}^X$. The preimage of V by φ_1 is $\{f : X \to Y \mid N(f(x_0)) \in U\} = \{f : X \to Y \mid f(x_0) \in N^{-1}(U)\}$. As the norm N is continuous, $N^{-1}(U)$ is open in Y and $\varphi_1^{-1}(V)$ is open in the product topology of Y^X.

Let K be the compact set of measurable strategies $X \to Y$. As φ_1 is continuous, the image $\varphi_1(K)$ is compact in $\mathbb{R}^X$. By [12], pointwise compactness implies L^0-compactness. By the Vitali convergence theorem, L^0-compactness implies L^p-compactness given uniformly integrability. Therefore, $\varphi_1(K)$ is nonempty and compact in $L^p(X, \mathbb{R})$.

The boundedness of Y ensures $K \subseteq L^p(X, Y)$. Consider the map $\varphi_2 : K \to L^p(X, \mathbb{R})$ given by $f \mapsto N \circ f$. Prove that φ_2 is continuous with respect to the L^p-norms. Let $\varepsilon > 0$ and $\delta = \varepsilon > 0$, then whenever $\|f_n - f\| = \int_X (N \circ (f_n - f))^p d\mu < \delta$, by the triangle inequality, $\|N \circ f_n - N \circ f\| = \int_X |N \circ f_n - N \circ f|^p d\mu \leq \int_X (N \circ (f_n - f))^p d\mu < \delta = \varepsilon$. As a continuous map from a compact space to a Hausdorff space, φ_2 is proper. Therefore K is compact in $L^p(X, Y)$.

□

An agent has partial information when the state space is (X, Σ) but f is not Σ-measurable in x. Expected utility theory postulates that, provided with a belief structure modeled by a probability space $(X, \mathcal{F}, \mu)$ on X such that $\sigma(f) \subseteq \mathcal{F}$ and $\Sigma \subseteq \mathcal{F}$, the agent follows a strategy given in the following proposition.

Proposition 4. *Let $Y \subseteq \mathbb{R}^d$ be a Euclidean domain. Suppose C is Σ-measurable and has nonempty and compact values. Let $f_y : X \to \mathbb{R}$ be the $\mathcal{F}$-measurable function $x \mapsto f(x, y)$. If $y \mapsto f_y$ is an α-Hölder continuous function $Y \to L^p(X, \mathcal{F}, \mu)$ where $p \geq 1$ and $\alpha p > d$, then there is a conditional expectation of f_y with respect to Σ, denoted by g_y, such that the correspondence $G : X \rightrightarrows Y$ given by $G(x) = \arg\max\{g_y(x) \mid y \in C(x)\}$ admits a Σ-measurable selector. The set of all such Σ-measurable selectors is compact in the quotient topology under almost-sureness.*

Proof. Let h_y be a conditional expectation of f_y with respect to Σ. By the conditional Jensen's inequality [37], $y \mapsto h_y$ is an α-Hölder continuous function $Y \to L^p(X, \Sigma, \mu|_\Sigma)$. By the Kolmogorov continuity theorem [22, Theorem 2.1], $y \mapsto h_y$ admits a Σ-measurable continuous modification $y \mapsto g_y$. By Proposition 2, G admits a nonempty and compact set of Σ-measurable selectors.

Two conditional expectations only differ on a null set, so any strategies associated to them only differ on a null set. On the other hand, if a Σ-measurable function $\psi : X \to Y$

differs from a strategy associated to g_y on a null set N, then let $h_y(x) = g_y(x)$ for all $x \notin N$, let $h_y(x) = 0$ for all $x \in N$ and $y \neq \psi(x)$, and let $h_y(x) = 1$ for all $x \in N$ and $y = \psi(x)$, so that h_y is a conditional expectation of f_y and $\psi(x) \in \arg\max\{h_x(x) \mid y \in C(x)\}$, i.e. ψ is also a strategy given by a conditional expectation. Therefore, in the quotient space, the set of all Σ-measurable strategies associated to any conditional expectations is identified with the compact set of Σ-measurable strategies associated to a single conditional expectations g_y. □

Remark 1. A generalization of the Kolomogorov continuity theorem to dyadically separable metric spaces is given by [27].

2.2 Multi-Agent Games

Non-cooperative games are a mathematical model of systems constituted of multiple agents, in which the behavior of the agents are commonly modeled with Nash equilibria.

Definition 2 (Normal-form game)**.** A normal-form game $\mathcal{G}$ constitutes of a set A whose elements are called agents, a set X called the state space, and, for each agent $a \in A$, a set Y_a called the action space, a correspondence $C_a : X \times Y \rightrightarrows Y_a$ called the constraint, and a function $f_a : X \times Y \to \mathbb{R}$ called the payoff function, where $Y := \prod_{a \in A} Y_a$.

For each agent $a \in A$, an optimization problem $\mathcal{P}_a$ is associated to $\mathcal{G}$, of which the state space is $X \times Y$, the action space is Y_a, the constraint is C_a, and the payoff function is $\psi_a := f_a \circ (\mathrm{id}_X \times r_a)$, where the substitution function $r_a : Y \times Y_a \to Y$ is given by $\mathrm{proj}_a(r_a(y, \hat{y}_a)) = \hat{y}_a$ and $\mathrm{proj}_b(r_a(y, \hat{y}_a)) = \mathrm{proj}_b(y)$ for all $b \in A \setminus \{a\}$. Let $F_a : X \times Y \rightrightarrows Y_a$ be the solution to $\mathcal{P}_a$.

Let $\Psi_x : Y \rightrightarrows Y$ be the correspondence given by $\Psi_x(y) = \prod_{a \in A} F_a(x, y)$. Denote the set of fixed point of Ψ_x by Φ_x. The correspondence $\Phi : X \rightrightarrows Y$ given by $\Phi(x) = \Phi_x$ is called the solution to $\mathcal{G}$. A selector of Φ is called a Nash equilibrium of $\mathcal{G}$.

Proposition 5. *Let Y_a be nonempty compact convex subsets of locally convex Hausdorff spaces. Suppose C_a are continuous and have nonempty, compact, and convex values. Suppose*

f_a is continuous in y and quasiconcave in y_a. Then $\mathcal{G}$ has a nonempty and compact set of Nash equilibria. In addition, Φ is upper hemicontinuous if X is Hausdorff.

Proof. By the maximum theorem [33, Theorem 9.17], F_a is upper hemicontinuous with nonempty, compact, and convex values. By Kakutani fixed point theorem, Φ_x is nonempty and compact. The upper hemicontinuity of Φ is given in [11, Proposition 3.5]. □

Games with non-trivial information structure are defined in [35] and [9].

Definition 3 (Extensive-form game)**.** The state space $(X, \mathcal{X})$ is a measurable space. The action space $(Y_a, \mathcal{Y}_a)$ of each agent $a \in A$ is a measurable space. The information structure Σ_a of each agent a is a sub-σ-algebra of $\Sigma := \mathcal{X} \otimes \left(\bigotimes_{a\in A} \mathcal{Y}_a\right)$. The strategy of each agent is a $(\Sigma_a, \mathcal{Y}_a)$-measurable function. A player is a subset of agents $p \subseteq A$ such that the set of players is a partition of the set of agents. Each player has a $(\Sigma, \mathcal{B}_{\mathbb{R}})$-measurable payoff function f_p and a belief μ_p on $(X, \mathcal{X})$. The best response of player p is the correspondence F_p which maps a strategy profile $\lambda := (\lambda_a)_{a\in A}$ to the set of optimal strategies $\lambda_p^* := (\lambda_a^*)_{a\in p}$ which solve

$$\max_{\eta, \lambda_p^*} \int_X (f_p \circ \eta) d\mu_p \tag{2.1}$$

$$\text{s.t. } \lambda_a \circ \eta = \text{proj}_a \circ \eta \qquad \forall a \notin p \tag{2.2}$$

$$\lambda_a^* \circ \eta = \text{proj}_a \circ \eta \qquad \forall a \in p \tag{2.3}$$

$$\lambda_a^* : X \times Y \to Y_a \text{ is } \Sigma_a\text{-measurable} \qquad \forall a \in p \tag{2.4}$$

$$\eta : X \to X \times Y \text{ is } \Sigma\text{-measurable.} \tag{2.5}$$

A Bayesian Nash equilibrium of the game is a fixed point of the correspondence $\lambda \mapsto \prod_p F_p(\lambda)$ together with the function $\eta : X \to X \times Y$ it uniquely determines.

Proposition 5 is a special case where all the players have no information exchange with any other players. But in general, the Kakutani fixed point theorem can be inapplicable due to the lack of convexity in the constraints (2.2) and (2.3). Thus it is necessary to acknowledge that the set of equilibria of an extensive-form game may be empty or non-compact in further discussions.

2.3 Parametrized Game Optimization

Let $\mathcal{G}$ be a game defined in Definition 2 where X and Y are compact Hausdorff spaces and $\Phi : X \rightrightarrows Y$ be its solution. Consider X as the action space of an additional agent whose payoff function is denoted by $\varphi : X \times Y \to \mathbb{R}$. Define the worst-case value function $v : X \to \mathbb{R}$ by $v(x) = \inf\{\varphi(x, y) \mid y \in \Phi(x)\}$ and consider the constrained minimax problem.

$$\sup_{x \in X} \inf_{y \in \Phi(x)} \varphi(x, y). \tag{2.6}$$

Assume Φ has nonempty and compact values. Some sufficient conditions regarding whether the infimum or the supremum is attainable are stated as follows.

- If X is a finite set, then the supremum is attainable. If Y is a finite set, then the infimum is attainable. If φ takes discrete values, then both the infimum and the supremum are attainable.
- If Φ is upper hemicontinuous and φ is lower semicontinuous, then the infimum is attainable [6, Lemma 17.30].
- If Φ is lower hemicontinuous and φ is upper semicontinuous, then the supremum is attainable [19, Theorem 9.2.1].

However, the solution to a game is not lower hemicontinuous in general. If the supremum is not attainable, the agent has to select a suboptimal solution in the nonempty set $V_\varepsilon := \{x \in X \mid v(x) \geq \sup v - \varepsilon\}$ for a small threshold ε.

Similarly for games with non-trivial information structures, let Φ' be the set of η that constitutes an equilibrium and consider

$$\sup_{x \in X} \inf_{\eta \in \Phi'} \varphi(\eta(x)). \tag{2.7}$$

This formulation transforms the coupled constraint $(x, y) \in \operatorname{Gr} \Phi$ into separate constraints $x \in X, \eta \in \Phi'$ at the price of considering functions $\eta : X \to Y$ instead of points $y \in Y$. From the game theoretical point of view, the minimax problem (2.7) is a two-player zero-sum Stackelberg game. However, the minimax theorem cannot be applied here without Φ' being nonempty, compact, and convex.

2.4 Gradient-Based Methods

Problem (2.6) is a special minimax problem with an equilibrium constraint $y \in \Phi(x)$. The lower level MPEC problem can be solved by replacing the equilibrium constraints with the KKT (Karush–Kuhn–Tucker) conditions. Suppose there are finite number of agents and each agent's action space is a sublevel set of a convex function within an affine Euclidean subspace, i.e., $Y_a = g_a^{-1}(\mathbb{R}_-^{p_a}) \cap h_a^{-1}(\{0\}^{q_a})$ where $g_a : \mathbb{R}^{n_a} \to \mathbb{R}^{p_a}$ is convex and $h_a : y_a \mapsto A_a y_a + b_a$ is affine. For all $j = 1, \cdots, p_a$, assume $g_{aj}(y_a^*) < 0$ for some $y_a^* \in h_a^{-1}(\{0\}^{q_a})$ in the affine subspace and $\lim_{t\to\infty} g_{aj}(ty_a) = +\infty$ for all $y_a \neq 0$, so that g_a satisfy Slater's condition and Y_a are nonempty and bounded. Let $f_{x,a}(y, y_a) := f_a(x, r_a(y, y_a))$. The constraint $y \in \Phi(x)$ can be written as

$$\forall a : \begin{cases} y_a \in \arg\max\limits_{y_a'} & f_{x,a}(y, y_a') \\ \text{s.t.} & g_a(y_a') \geq 0 \\ & h_a(y_a') = 0. \end{cases}$$

Assume the smoothness of f_a and g_a, then a relaxation to the above constraint is stated by the KKT conditions

$$\begin{aligned} L_{al}(x, y, \mu, \lambda) &= 0 && \forall l = 1 \cdots, n_a \\ G_{ak}(y, \mu) &= 0 && \forall k = 1, \cdots, p_a \\ h_{aj}(y_a) &= 0 && \forall j = 1 \cdots, q_a \\ & && \forall a = 1, \cdots, |A| \end{aligned}$$

where

$$\begin{aligned} L_a(x, y, \mu, \lambda) &= f_{x,a}(y) + \sum_{k=1}^{p_a} \mu_{ak} g_{ak}(y_a) + \sum_{j=1}^{q_a} \lambda_{aj} h_{aj}(y_a) \\ L_{al}(x, y, \mu, \lambda) &= \frac{\partial L_a}{\partial y_{al}}(x, y, \mu, \lambda) \\ G_{ak}(y, \mu) &= \sqrt{\mu_{ak}^2 + g_{ak}(y_a)^2} - \mu_{ak} - g_{ak}(y_a). \end{aligned}$$

The complementarity condition is formulated with the Fischer-Burmeister merit function [21], to translate the disjunction $g_{ak}(y_a) \geq \mu_{ak} = 0$ or $\mu_{ak} \geq g_{ak}(y_a) = 0$. It has numerical advantages over the inner product formulation $\mu_a^{\mathrm{T}} g_a(y_a) = 0$ [16, 17].

Having the above KKT conditions as the constraints in (2.6), the constrainted minimax problem

$$\sup_{x \in X} \inf_{\substack{y \in Y \\ \mu, \lambda}} \{\varphi(x, y) \mid \forall l, k, j, a : L_{al}(x, y, \mu, \lambda) = G_{ak}(y, \mu) = h_{aj}(y) = 0\}$$

can be solved with further KKT conditions or with appropriate relaxations [31].

3.0 Bayesian Approach to Parametrized Games

Gradient-based methods suffer from a few limitations in our application. First, the functions involved need to have (sub-)gradients. Second, two levels of optimization together with an equilibrium constraint results in a large set of KKT equations, high order of derivatives, and accumulated relaxations or approximations. Third and most importantly, the equilibria of a game can have non-connected components, all of which need to be considered in a design process. This cannot be achieved effectively through a local method. In this chapter, I propose the application of the Bayesian optimization method to solve parametrized game problems.

The Bayesian optimization method was first proposed by Kushner [20], and has found many applications in machine learning [32]. Two main ingredients of a typical Bayesian optimization method are a Gaussian process prior and an acquisition function. The Gaussian process prior models how samples inform the belief and the acquisition function models how the belief guides sampling in return. In recent literature, the most popular prior is the squared exponential kernel, the most popular acquisition function is the expected improvement. In this dissertation, I use the Wiener process prior originally proposed by Kushner. It has the advantage of having an analytical expression of the probability of reaching maximum. So the acquisition function used in this dissertation is based on optimality instead of improvement.

3.1 Single-Variable Bayesian Optimization

A fundamental assumption of games with perfect information is that the payoff functions are common knowledge. From the theoretical point of view, knowing the function and knowing all the values of the function are equivalent. But from the computational point of view, they are distinct. A function f is known in the sense that there is a known algorithm which outputs the function value $f(t)$ when a variable t is provided as input. In other words,

before the input is provided and the output is probed, the value of the function is *a priori* unknown, although the function is assumed known. This uncertainty justifies a Bayesian approach to optimization, as first proposed in [20].

For simplicity, suppose f is a real-valued continuous function defined on the unit interval $[0,1]$. Let $(t_i)_{1\le i\le n}$ be a strictly monotonically increasing sequence [1] on $[0,1]$ and F_n a random process on $[0,1]$ such that the distribution of $F_n(t)$ describes the Bayesian belief of $f(t)$ after all the function values $(f(t_i))_{1\le i\le n}$ are obtained.

A simple way to construct F_n is to use Wiener processes. The standard Wiener process $(W(t))_{t\ge 0}$ can be defined as the zero-mean Gaussian process on $\mathbb{R}_+$ characterized by the covariance function $\mathbb{E}[W(t)W(s)] = \min\{t,s\}$. It can also be characterised by its properties.

P1: Starting at the origin: $W(0) = 0$,

P2: Continuous path: $W(t)$ is continuous in t,

P3: Markovian increments: $W(s) - W(t)$ is independent of $(W(\tau))_{\tau\le\min\{t,s\}}$.

P4: Stationary Gaussian increments: $W(s) - W(t)$ is Gaussian $\mathcal{N}(0, |s-t|)$.

Stationarity in **P4** reflects a homogeneous uncertainty of the function values at all points. The Markov property in **P3** requires the uncertainty of the function to propagate without memory. The distribution of increments is assumed Gaussian, but we will discuss later whether any modification may be needed. **P2** reflects the continuity of f as desired. In fact, the support of the Wiener measure is the set of all continuous functions starting from the origin [28, Corollary 3.31]. **P1** provides the Wiener process a deterministic endpoint. This is somehow undesired in our application because the function values at the endpoints are also *a priori* unknown. To obtain a deterministic value of the function, we must sample it. So instead of postulating a prior belief F_0, we begin by establishing F_1 as

$$F_1(t) = f(t_1) + W^1(t) - W^1(t_1) = \begin{cases} f(t_1) + W^2(t_1 - t), & t \in [0, t_1] \\ f(t_1) + W^1(t - t_1), & t \in [t_1, 1]. \end{cases}$$

where W^1 and W^2 are two independent Wiener processes. More generally, the process of sampling simply breaks down the process F_i into one forward Wiener process, one backward

[1] Sampling needs not to be performed in increasing order. The monotonocity is assumed only to simplify notation. Sampling at repeating locations are simply redundant, as we assume the observation is noiseless.

Wiener process, and $(n-1)$ Brownian bridges in-between. In particular, the marginal distribution of $F_n(t)$ is a Gaussian with the mean and the variance

$$t \in [0, t_1] : \begin{cases} \mu(t) = f(t_1) \\ \sigma^2(t) = t_1 - t \end{cases} \tag{3.1}$$

$$t \in [t_i, t_{i+1}] : \begin{cases} \mu(t) = (f(t_{i+1})(t - t_i) + f(t_i)(t_{i+1} - t))/(t_{i+1} - t_i) \\ \sigma^2(t) = (t_{i+1} - t)(t - t_i)/(t_{i+1} - t_i) \end{cases} \tag{3.2}$$

$$t \in [t_n, 1] : \begin{cases} \mu(t) = f(t_n) \\ \sigma^2(t) = t - t_n. \end{cases} \tag{3.3}$$

Now consider the maximum of F_n and where it is reached. Let $\bar{W}(t) := \max_{s\in[0,t]} W(s)$ and $\bar{F}_n := \max_{s\in[0,1]} F_n(s)$. For $n = 1$, the cumulative distribution function of the maximum $\bar{F}_1$ is given by

$$\begin{aligned} \mathbb{P}(\bar{F}_1 \le f(t_1) + \varepsilon) &= \mathbb{P}(\bar{W}(t_1) \le \varepsilon)\mathbb{P}(\bar{W}(1 - t_1) \le \varepsilon) \\ &= \operatorname{erf}\left(\frac{\varepsilon}{\sqrt{2t_1}}\right) \operatorname{erf}\left(\frac{\varepsilon}{\sqrt{2(1-t_1)}}\right) \\ &= \frac{2}{\pi}\frac{1}{\sqrt{t_1(1-t_1)}}\varepsilon^2 + o(\varepsilon^2). \end{aligned}$$

Figure 2 plots this probability as a function of t_1 for small ε and shows that a function value sampled close to the boundary has a higher chance to be close to the function maximum. This imbalance is a direct result of the property of Gaussian increments in **P4**. If this imbalance is unwanted, we can model F_n with deterministically time-changed Wiener processes instead. Let

$$F_1(t) = \begin{cases} f(t_1) + W^1(\phi(t_1 - t)) - W^1(\phi(0)), & t \in [0, t_1] \\ f(t_1) + W^2(\phi(t - t_1)) - W^2(\phi(0)), & t \in [t_1, 1]. \end{cases}$$

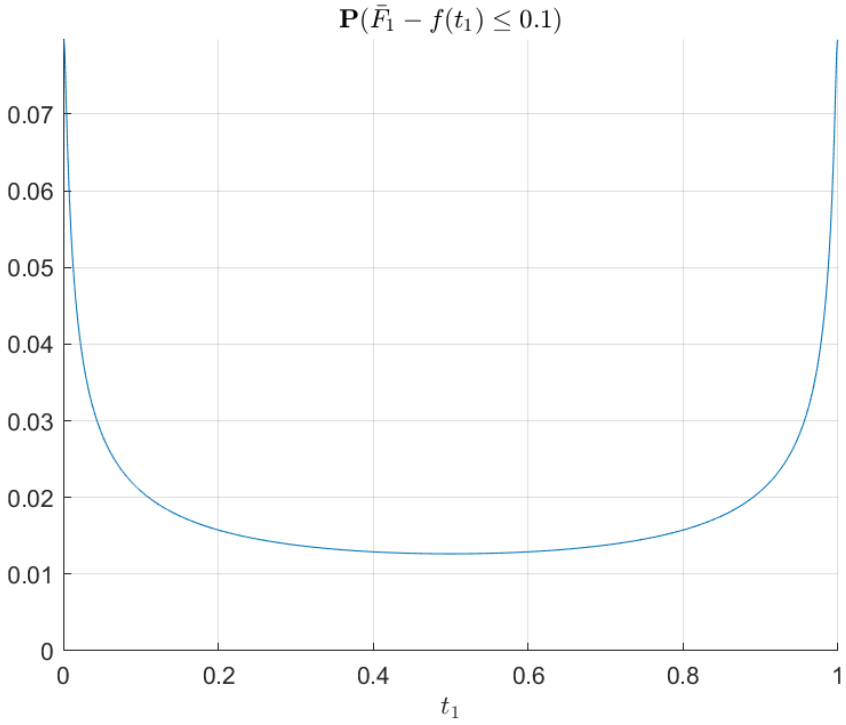

Figure 2: Probability of the first sampled function value being close to the function maximum as a function of the sample location.

then the probability is given by

$$\begin{aligned}\mathbb{P}(\bar{F}_1 \le f(t_1)+\varepsilon) &= \mathbb{P}(\bar{W}(\phi(t_1)) \le \varepsilon)\mathbb{P}(\bar{W}(\phi(1-t_1)) \le \varepsilon) \\ &= \operatorname{erf}\left(\frac{\varepsilon}{\sqrt{2(\phi(t)-\phi(0))}}\right)\operatorname{erf}\left(\frac{\varepsilon}{\sqrt{2(\phi(1-t)-\phi(0))}}\right) \\ &= \frac{2}{\pi}\frac{1}{\sqrt{(\phi(t)-\phi(0)))(\phi(1-t)-\phi(0)))}}\varepsilon^2 + o(\varepsilon^2).\end{aligned}$$

When $\phi(t) = t/(1-t)$, this probability is independent of t for small ε. This time change balances out the effect in Figure 2 by hyperbolically stretching out the uncertainty of the function values when t gets away from t_1.

Our objective is to locate the function maximum given F_n, so we want to calculate the distribution of $\bar{F}_{n+1}$ as a function of $t_{n+1} \in [0,1]$ for the next sample. Let $(x_i)_{0\le i\le n+2}$ be the monotonically increasing sequence of all the elements in $\{0,1,t_{n+1}\} \cup \{t_i\}_{1\le i\le n}$ [2]. For $i = 1, \cdots, n$, let B_i be the Brownian bridge over $[x_i, x_{i+1}]$ where $B_i(x_i) = f(x_i)$ and $B_i(x_{i+1}) = f(x_{i+1})$. Let $\bar{B}_i = \max_{x\in[x_i,x_{i+1}]} B_i(x)$ be their respective maxima. At the two extremities, let $B_0(x) = W(x_1 - x) + f(x_1)$ and $B_{n+1}(x) = W(x - x_{n+1}) + f(x_{n+1})$. Their maxima are respectively $\bar{B}_0 = \bar{W}(x_1) + f(x_1)$ and $\bar{B}_{n+1} = \bar{W}(1 - x_{n+1}) + f(x_{n+1})$. The cumulative distribution functions of maxima are given by

$$\mathbb{P}(\bar{B}_0 \le m) = \operatorname{erf}\left(\frac{m - f(x_1)}{\sqrt{2x_1}}\right) \tag{3.4}$$

$$\mathbb{P}(\bar{B}_i \le m) = 1 - \exp\left(-2\frac{(m-f(x_i))(m-f(x_{i+1}))}{(x_{i+1}-x_i)}\right) \tag{3.5}$$

$$\mathbb{P}(\bar{B}_{n+1} \le m) = \operatorname{erf}\left(\frac{m - f(x_{n+1})}{\sqrt{2(1-x_{n+1})}}\right) \tag{3.6}$$

$$\mathbb{P}(\bar{F}_{n+1} \le m) = \prod_{i=0}^{n+1} \mathbb{P}(\bar{B}_i \le m). \tag{3.7}$$

The above expressions make use of the function value in the next sample $f(t_{n+1})$, what we really want is to use only the information from the first n samples to examine whether

[2] Assuming no repeating elements among them.

$F_n(t_{n+1})$ is close to $\bar{F}_n$ without knowing the value of $f(t_{n+1})$. To this end, we simply apply the law of total probability to the $\bar{F}_{n+1}$ and we obtain

$$\mathbb{P}(\bar{F}_n \leq F_n(t_{n+1}) + \varepsilon) = \int_{\bar{m}}^{\infty} \mathbb{P}(\bar{F}_{n+1} \leq m + \varepsilon | f(t_{n+1}) = m) \phi_{F_n(t_{n+1})}(m) dm. \tag{3.8}$$

where $\bar{m} = \max_{1 \leq i \leq n} f(x_i) - \varepsilon$ and $\phi_{F_n(t_{n+1})}$ is the Gaussian probability distribution function of $F_n(t_{n+1})$. We observe that when $\bar{m} \gg f(x_i)$ and $\bar{m} \gg f(x_{i+1})$, we have $\mathbb{P}(\bar{B}_i \leq m) \approx 1$ and $\phi_{F_n(t_{n+1})} \approx 0$ for $t_{n+1} \in [t_i, t_{i+1}]$. This reflects the intuition that the function maximum is most likely to be reached in the intervals whose endpoints are close to the sample maximum. If we use this approximation very generously in calculating (3.7), then $\mathbb{P}(\bar{F}_{n+1} \leq m) = 1$ if $m > \bar{m}$ and $\mathbb{P}(\bar{F}_{n+1} \leq m) = 0$ if $m < \bar{m}$. Instead of points close to the maximum, we simply look for points greater than the sample maximum. This is the traditional acquisition function used in Bayesian optimization [4, §2.3].

The integral (3.8) can be written as

$$\sum_{I \subseteq \{1, \cdots, n\}} (-1)^{|I|} \int_{\bar{m}}^{\infty} dm \operatorname{erf}\left(\frac{m + \varepsilon - f(x_1)}{\sqrt{2x_1}}\right) \operatorname{erf}\left(\frac{m + \varepsilon - f(x_{n+1})}{\sqrt{2(1 - x_{n+1})}}\right)$$
$$\exp\left(-\frac{(m - \mu(t_{n+1}))^2}{2\sigma^2(t_{n+1})} - 2\sum_{i \in I} \frac{(m + \varepsilon - f(x_i))(m + \varepsilon - f(x_{i+1}))}{(x_{i+1} - x_i)}\right).$$

Each integral takes the form

$$\int_{\bar{m}}^{\infty} \operatorname{erf}(a_1(m - b_1)) \operatorname{erf}(a_2(m - b_2)) \exp\left(-a_0(m - b_0))^2\right) dm. \tag{3.9}$$

The error functions can be expanded into integrals and (3.9) becomes a Gaussian integral over a polytope

$$\frac{1}{\alpha} \iiint_{\mathcal{S}} \exp(-(s_1^2 + s_2^2 + s_3^2)) ds_1 ds_2 ds_3$$

where $\mathcal{S} = \{(s_1, s_2, s_3) \in \mathbb{R}^m \mid 0 \leq s_1 \leq a_1' s_3 - b_1', 0 \leq s_2 \leq a_2' s_3 - b_2', s_3 \geq \bar{m}'\}$. This integral can be numerically evaluated with Monte Carlo integration or other approximation methods [7, 18].

3.2 Multi-Variable Bayesian Optimization

In game theory, the Nash equilibrium is defined through the concept of best responses. Each player does not have the intent to optimize their payoff function over the entire space of strategy profiles, but instead, they optimize their payoff function along their own action space while assuming other players' actions are kept fixed. In this section, we still assume the action space of each player is one-dimensional, but we extend the Bayesian optimization approach to include all the players of a game.

3.2.1 A Generalization of the Wiener process

Unknown values of a function with several real variables can be modeled with random fields, which generalize stochastic processes. Traditionally, the generalization is carried out isotropically with respect to the variables, because most applications of Bayesian optimization seek global optima of a function. However, as we are interested in equilibria of games, we only need optimality along one variable with all the other variables kept fixed, so we can generalize the Wiener process in an anisotropic fashion by requiring the generalized Wiener process to be a Wiener process in each of its variables.

Definition 4 (Generalized Wiener Process on $\mathbb{R}^m_+$)**.** A function $\psi : \mathbb{R}^m_+ \to L^0(\Omega, \mathbb{R})$ is a generalized Wiener process if, for any $y \in \mathbb{R}^m_+$ and any $k \in \{1, \cdots, m\}$, the function $(\psi_{y,k} - \psi_{y,k}(0))/\sigma$ is a standard Wiener process for some $\sigma > 0$, where $\psi_{y,k} : \mathbb{R}_+ \to L^0(\Omega, \mathbb{R})$ is the function given by $\psi_{y,k}(x) = \psi(y_1, \cdots, y_{k-1}, x, y_{k+1}, \cdots, y_m)$.

The simplest generalization of the Wiener process can be given as the follows.

Proposition 6. *Let $\psi : \mathbb{R}^m_+ \to L^0(\Omega, \mathbb{R})$ be a zero-mean Gaussian process given by the covariance matrix*

$$\mathbb{E}[\psi(y)\psi(y')] = \sum_{j=1}^{m} \min\{y_j, y'_j\}. \tag{3.10}$$

Then ψ is a generalized Wiener process.

Proof. By definition, $\psi_{y,k}$ is also a zero-mean Gaussian process and $\mathbb{E}[\psi_{y,k}(x)\psi_{y,k}(x')] = \|y\|_1 - y_k + \min\{x, x'\}$. Hence $\mathbb{E}[(\psi_{y,k}(x) - \psi_{y,k}(0))(\psi_{y,k}(x') - \psi_{y,k}(0))] = \min\{x, x'\}$. □

The process defined above can be written as a sum of m independent Wiener processes along each coordinate of its variables $\psi(y) = \sum_{j=1}^{m} W_j(y_j)$. However, this process has a fundamental flaw, that is the values of ψ at certain locations are perfectly correlated.

Proposition 7. *The two-dimensional generalized Wiener process ψ defined in Proposition* 6 *satisfies $\psi(1,1) = \psi(1,0) + \psi(0,1)$.*

Proof. By 3.10, we have $\mathbb{E}[\psi(1,1)\psi(1,1)] = \mathbb{E}[(\psi(1,0) + \psi(0,1))(\psi(1,0) + \psi(0,1))] = \mathbb{E}[\psi(1,1)(\psi(1,0) + \psi(0,1))] = 2$. Therefore $\psi(1,1) = \psi(1,0) + \psi(0,1)$. □

A quadratic term can be added to (3.10) to fix this problem.

Proposition 8. *Let $\lambda > 0$. Let $\psi : \mathbb{R}_+^m \to L^0(\Omega, \mathbb{R})$ be a zero-mean Gaussian process given by the covariance matrix*

$$\mathbb{E}[\psi(y)\psi(y')] = \sum_{j=1}^{m} \min\{y_j, y'_j\} + \frac{\lambda}{2} \sum_{j \neq l} \min\{y_j, y'_j\} \min\{y_l, y'_l\}. \tag{3.11}$$

Then ψ is a generalized Wiener process without linear correlation.

Proof. By definition, $\psi_{y,k}$ is also a zero-mean Gaussian process and $\mathbb{E}[\psi_{y,k}(x)\psi_{y,k}(x')] = (1-\lambda y_k)(\|y\|_1 - y_k) + (\lambda/2)(\|yy^{\mathrm{T}}\|_{1,1} - y^{\mathrm{T}}y) + (1+\lambda\|y\|_1 - \lambda y_k)\min\{x, x'\}$. Hence $\mathbb{E}[(\psi_{y,k}(x) - \psi_{y,k}(0))(\psi_{y,k}(x') - \psi_{y,k}(0))] = (1 + \lambda\|y\|_1 - \lambda y_k)\min\{x, x'\}$.

The Cauchy-Schwarz inequality states $\mathbb{E}[\psi(y)(a\psi(y') + b\psi(y''))]^2 \leq \mathbb{E}[\psi(y)^2]\mathbb{E}[(a\psi(y') + b\psi(y''))^2]$. Without loss of generality, assume $a > 0$ and $b > 0$. Expand all the terms in the inequality and write them in terms of $u_j = \min\{y_j, y'_j\}$, $v_j = \min\{y_j, y''_j\}$, and $w_j = \min\{y'_j, y''_j\}$. We obtain that the equality holds if and only if $u = y = y'$ and $v = y = y''$. □

Another direction of generalization is to extend the domain of the process from the positive quadrant to the entire Euclidean space.

Definition 5 (Generalized Wiener Process on $\mathbb{R}^m$)**.** A function $\psi : \mathbb{R}^m \to L^0(\Omega, \mathbb{R})$ is a generalized Wiener process if, for any binary vector $s \in \{-1, +1\}^m$, the function $y \mapsto \psi(s_1 y_1, \cdots, s_m y_m)$ restricted on $\mathbb{R}_+^m$ is a generalized Wiener process.

A straightforward generalization is given as follows.

Proposition 9. *For any pair of points $y \in \mathbb{R}^m$ and $y' \in \mathbb{R}^m$, if $y_i y'_i \geq 0$ then let $z_i = |y_i|$ and $z'_i = |y'_i|$, if $y_i y'_i \leq 0$ then let $z_i = z'_i = 0$. Let ψ be a generalized Wiener process on $\mathbb{R}^m_+$. Then the zero-mean Gaussian process ψ' on $\mathbb{R}^m$ given by the covariance matrix $\mathbb{E}[\psi'(y)\psi'(y')] = \mathbb{E}[\psi(z)\psi(z')]$ is a generalized Wiener process. In addition, for any $y \in \mathbb{R}^m$ and any $k \in \{1, \cdots, m\}$, the functions defined on $\mathbb{R}_+$ by $x \mapsto (\psi'_{y,k}(x) - \psi'_{y,k}(0))/\sigma$ and $x \mapsto (\psi'_{y,k}(-x) - \psi'_{y,k}(0))/\sigma$ are two independent standard Wiener processes for some $\sigma > 0$, where $\psi'_{y,k} : \mathbb{R} \to L^0(\Omega, \mathbb{R})$ is the function given by $\psi'_{y,k}(x) = \psi'(y_1, \cdots, y_{k-1}, x, y_{k+1}, \cdots, y_m)$.*

Proof. Let $s \in \{-1, +1\}^m$, $y \in \mathbb{R}^m_+$, and $y' \in \mathbb{R}^m_+$, then $\mathbb{E}[\psi'(sy)\psi'(sy')] = \mathbb{E}[\psi(y)\psi(y')]$, so ψ' is a generalized Wiener process on $\mathbb{R}^m$.

If $x \geq 0$ and $x' \geq 0$, then $\mathbb{E}[\psi'_{y,k}(x)\psi'_{y,k}(x')]$ is an affine function in $\min\{x, x'\}$. If $x \geq 0$ and $x' \geq 0$, then $\mathbb{E}[\psi'_{y,k}(x)\psi'_{y,k}(x')]$ is an affine function in $\min\{-x, -x'\}$. This provides two Wiener processes as constructed in the proposition. If $xx' \leq 0$, then $\mathbb{E}[\psi'_{y,k}(x)\psi'_{y,k}(x')] = \mathbb{E}[\psi'_{y,k}(0)\psi'_{y,k}(0)]$. Therefore, these two Wiener processes are independent. □

3.2.2 Bayesian Inference

The Bayesian inference for Gaussian processes follows a simple procedure. Let $(f_i)_i$ be a sequence of known function values at the respective points y_i and $(f'_j)_j$ a sequence of unknown function values at the respective points y'_j. By definition, (f, f') is a multivariate Gaussian with the mean vector (m, m') where $m_i = \mu(y_i)$ and $m'_j = \mu(y'_j)$ and the covariance matrix

$$\begin{pmatrix} R & U^{\mathrm{T}} \\ U & W \end{pmatrix}$$

where $R_{ik} = \Sigma(y_i, y_k)$, $W_{jl} = \Sigma(y'_j, y'_l)$, and $U_{ji} = \Sigma(y_i, y'_j)$. Let

$$\begin{pmatrix} P & M^{\mathrm{T}} \\ M & Q \end{pmatrix} = \begin{pmatrix} R & U^{\mathrm{T}} \\ U & W \end{pmatrix}^{-1}$$

be the precision matrix. Bayes's theorem states that the conditional distribution $\phi(f'|f) \propto \phi(f, f')$ is again a multivariate Gaussian and $\ln \phi(f'|f) = -\frac{1}{2}(f')^{\mathrm{T}} Q f' + (f')^{\mathrm{T}}(Qm' - M(f -$

$m)) + A$ for some constant A. Hence, the mean vector of $\phi(f'|f)$ is given by $m' - Q^{-1}M(f - m) = m' + UR^{-1}(f - m)$ and the covariance matrix of $\phi(f'|f)$ is given by $Q^{-1} = W - UR^{-1}U^{\mathrm{T}}$.

To establish the prior using a generalized Wiener process, we need to define an origin. It has to be a point where the function has a known deterministic value or at least a known probability distribution. Given a sequence of known function values $(f_i)_i$ at the respective points y_i, we can pick an arbitrary i and let y_i be the origin. However, it is important to make sure that the inference result does not depend on the index i we choose.

Proposition 10. *Let ψ be the generalized Wiener process constructed in Proposition 9 from Proposition 6. Bayesian inference performed based on this prior does not depend on the choosing of the origin.*

Proof. Let y_1 be the origin, $f = (f_2)$, and $f' = (f_1')$, then the inferred mean of f' is given by

$$f_1 + \frac{\Sigma(y_2 - y_1, y_1' - y_1)}{\Sigma(y_2 - y_1, y_2 - y_1)}(f_2 - f_1).$$

Let y_2 be the origin, $f = (f_1)$, and $f' = (f_1')$, then the inferred mean of f' is given by

$$f_2 + \frac{\Sigma(y_1 - y_2, y_1' - y_2)}{\Sigma(y_1 - y_2, y_1 - y_2)}(f_1 - f_2).$$

The inferred means are identical if and only if

$$\frac{\Sigma(y_2 - y_1, y_1' - y_1)}{\Sigma(y_2 - y_1, y_2 - y_1)} + \frac{\Sigma(y_1 - y_2, y_1' - y_2)}{\Sigma(y_1 - y_2, y_1 - y_2)} = 1.$$

Processes constructed in Proposition 9 satisfy $\Sigma(-x, -x') = \Sigma(x, x')$. So the inferred means are identical if and only if

$$\Sigma(y_1 - y_2, y_1 - y_1') + \Sigma(y_1 - y_2, y_1' - y_2) = \Sigma(y_1 - y_2, y_1 - y_2). \tag{3.12}$$

Consider the jth component $\Sigma(y_{1j} - y_{2j}, y_{1j} - y_{1j}') + \Sigma(y_{1j} - y_{2j}, y_{1j}' - y_{2j}) - \Sigma(y_{1j} - y_{2j}, y_{1j} - y_{2j})$. Without loss of generality, assume $y_{2j} \geq y_{1j}$.

- Suppose $y_{2j} \geq y_{1j} \geq y_{1j}'$, then $\Sigma(y_{1j} - y_{2j}, y_{1j} - y_{1j}') + \Sigma(y_{1j} - y_{2j}, y_{1j}' - y_{2j}) - \Sigma(y_{1j} - y_{2j}, y_{1j} - y_{2j}) = 0 + (y_{2j} - y_{1j}) - (y_{2j} - y_{1j}) = 0$.
- Suppose $y_{2j} \geq y_{1j}' \geq y_{1j}$, then $\Sigma(y_{1j} - y_{2j}, y_{1j} - y_{1j}') + \Sigma(y_{1j} - y_{2j}, y_{1j}' - y_{2j}) - \Sigma(y_{1j} - y_{2j}, y_{1j} - y_{2j}) = (y_{1j}' - y_{1j}) + (y_{2j} - y_{1j}') - (y_{2j} - y_{1j}) = 0$.

- Suppose $y'_{1j} \geq y_{2j} \geq y_{1j}$, then $\Sigma(y_{1j} - y_{2j}, y_{1j} - y'_{1j}) + \Sigma(y_{1j} - y_{2j}, y'_{1j} - y_{2j}) - \Sigma(y_{1j} - y_{2j}, y_{1j} - y_{2j}) = (y_{2j} - y_{1j}) + 0 - (y_{2j} - y_{1j}) = 0$.

Therefore, (3.12) holds. As a result of (3.12), the inferred variances of f' are also identical regardless of which origin is chosen. □

The quadratic terms in (3.11) fail (3.12). To restore the symmetry among y_i, we add the respective quadratic terms for each i into (3.11)

$$\mathbb{E}[\psi(z)\psi(z')] = \sum_{j=1}^{m} \min\{z_j, z'_j\} + \frac{\lambda}{2} \sum_{i=1}^{n} \sum_{j \neq l} \min\{z_j - y_{ij}, z'_j - y_{ij}\} \min\{z_l - y_{ij}, z'_l - y_{ij}\}.$$

Unlike traditional Bayesian inference, each observation of the function values adds uncertainty onto the prior.

3.2.3 Bayesian Optimization

The generalizations proposed in §3.2.1 allow us to make use of the properties of the standard Wiener process and Brownian bridge by restricting the multivariate process along any of its variables. More specifically, the mean of $\psi_{z,k}(x)$ is piecewise affine in x and the variance of $\psi_{z,k}(x)$ is piecewise quadratic in x. These pieces are connected at the kth coordinates of the points where the function values are known. Let $r_{z,k}(x) = (z_1, \cdots, z_{k-1}, x, z_{k+1}, z_m)$. Suppose we want to calculate the probability that a point $C = r_{z,k}(x_C)$ reaches the path maximum within a tolerance ε along the affine line $\{y \in \mathbb{R}^m \mid \forall i \neq k : y_i = z_i\}$. Then we only need to perform Bayesian inference at point C, the connecting points $r_{z,k}(y_{ik})$, and the boundary points $r_{z,k}(0)$ and $r_{z,k}(1)$. Let $(x_0, \cdots, x_{n+1})$ be the strictly increasing sequence of the elements of $\{0, 1, y_{ik} \mid 1 \leq i \leq n\}$. Let μ_f and Σ_f be the mean vector and the covariance matrix of the function values $f := (f_0, f_1, \cdots, f_n, f_{n+1}, f_C)$ corresponding to the points $(x_0, \cdots, x_{n+1}, x_C)$. Then the probability $\mathbb{P}(F(C) \geq \bar{F}_z - \varepsilon)$ is given by the law of total probability

$$\mathbb{P}(F(C) \geq \bar{F}_z - \varepsilon) = \int \mathbb{P}(F(C) \geq \bar{F}_z - \varepsilon | F(x) = f) \phi_{F(x)}(f) df \tag{3.13}$$

$$= \int_{\mathcal{S}} \mathcal{G}(f - \mu_f, \Sigma_f) \prod_{i=0}^{n+1} \left(1 - \exp\left(-2 \frac{(f_C + \varepsilon - f_{i+1})(f_C + \varepsilon - f_i)}{x_{i+1} - x_i}\right)\right) df \tag{3.14}$$

where $\mathcal{S} := \{f \in \mathbb{R}^{n+3} \mid \forall i = 0, \cdots, n+1 : f_C \geq f_i - \varepsilon\}$. This integral can again be expressed as a sum of Gaussian integrals over polytopes.

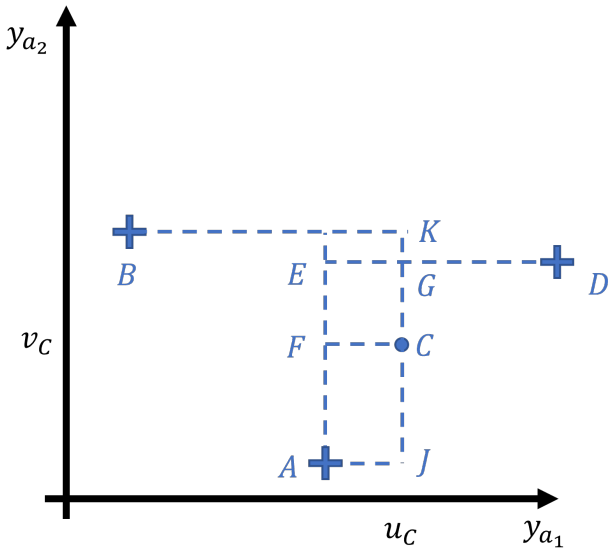

Figure 3: Example problem. Given the function values $f(A)$, $f(B)$, and $f(D)$, we want to calculate the probability that $F(C)$ reaches the path maximum $\max\{F(C) \mid u_C \text{ fixed}\}$. The connecting points where the Bayesian inference is performed is K, G, J, and C.

Example 2. Consider the problem illustrated in Fig 3. We want to find out the probability that the action v_C of player a_2 is a best response to the action u_C of player a_1 within a tolerance level ε after knowing the a_2's payoff function values at three strategy profiles A, B, and D. The conditional distribution of $F(C)$ is given by the Gaussian

$$\phi(f_C | f_A, f_B, f_D) \propto \phi(f_B, f_D, f_C | f_A).$$

The mean and the variance of this Gaussian are piecewisely affine or quadratic, as plotted in Fig 4. On each segment, we recognise either expression from (3.1) - (3.3).

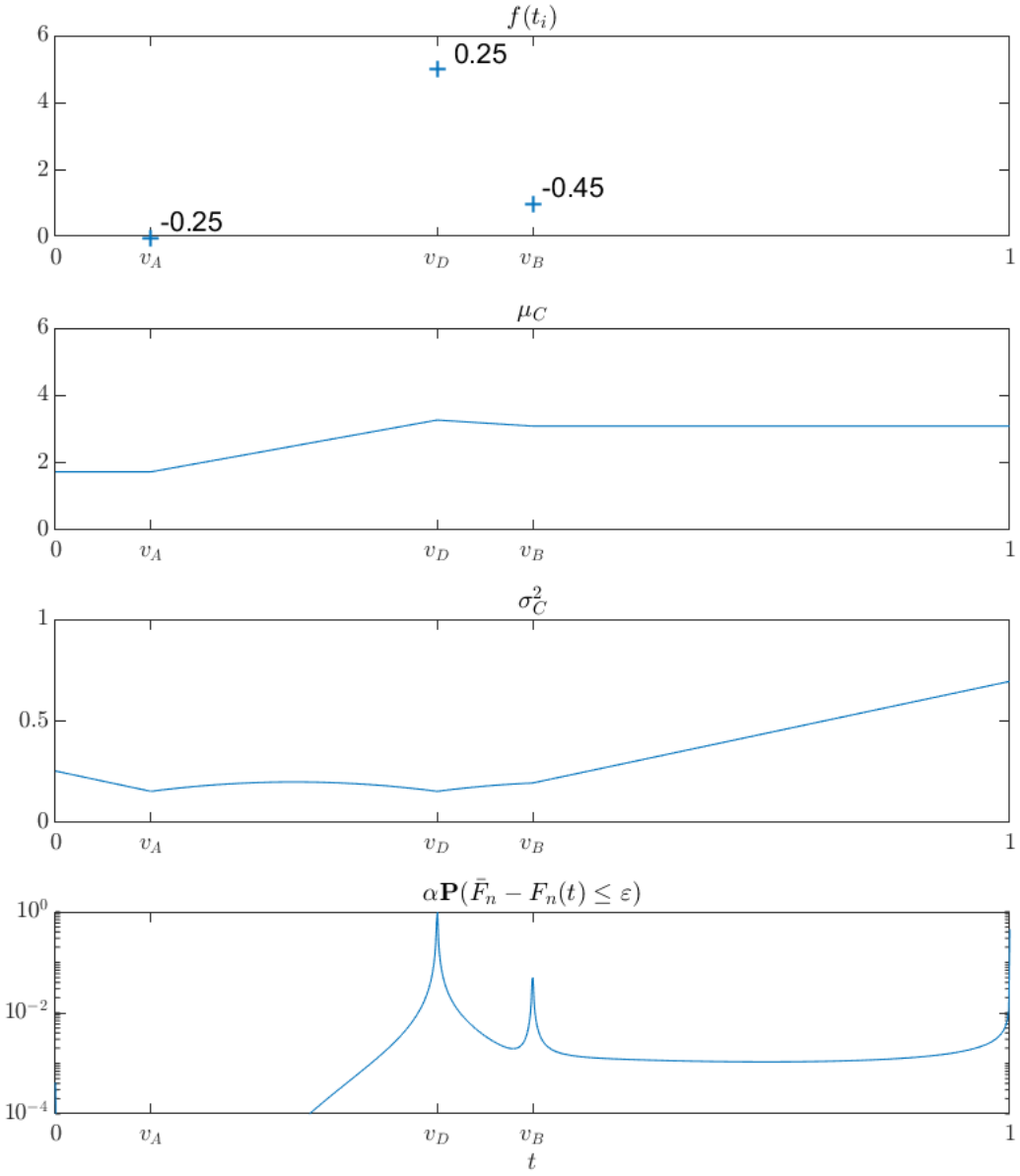

Figure 4: Numerical results of Fig 3 as function of the coordinate along the search dimension. (a) The first plot shows the function values at the sample points. The numbers printed next to the points represents the position of the respective sample points relative to the search dimension. (b, c) The mean and the variance of the probabilistic belief of the function values along the search dimension. (d) The probability that the path maximum is attained within a small threshold along the search dimension.

3.3 Bayesian Optimization for Parametrized Games

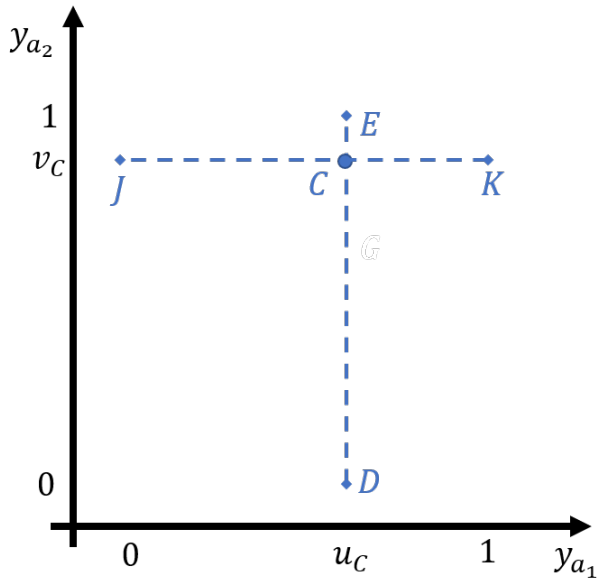

Figure 5: A strategy profile C of a two-player game within the action spaces.

The point C in Fig 5 is a Nash equilibrium of the two-player game as if $\bar{F}_{a_2}(\overline{DE}) \leq F_{a_2}(C)$ and $\bar{F}_{a_1}(\overline{DE}) \leq F_{a_1}(C)$. The probability that C reaches a Nash equilibrium within a small threshold is

$$\mathbb{P}(\bar{F}_{a_2}(\overline{DE}) \leq F_{a_2}(C) + \varepsilon \text{ and } \bar{F}_{a_1}(\overline{JK}) \leq F_{a_1}(C) + \varepsilon) \tag{3.15}$$

As increments along y_{a_1} and y_{a_2} are mutually independent given $F(C)$, the above probability (3.15) can be written as

$$\int \mathbb{P}(\bar{F}_{a_2}(\overline{DE}) \leq m_2 + \varepsilon)\mathbb{P}(\bar{F}_{a_1}(\overline{JK}) \leq m_1 + \varepsilon)\phi_{F(C)}(m_1, m_2)dm.$$

We can generalize (3.15) for finite players and write out the explicit probabilities using (3.14), then (3.15) becomes

$$\int_{\mathcal{S}} \mathcal{G}(f-\mu_f,\Sigma_f)\prod_{a\in A}\prod_{i=0}^{n+1}\left(1-\exp\left(-2\frac{(f_{a,C}+\varepsilon-f_{a,i+1})(f_{a,C}+\varepsilon-f_{a,i})}{x_{a,i+1}-x_{a,i}}\right)\right)df$$

where $\mathcal{S}=\prod_{a\in A}\mathcal{S}_a=\{f\in\mathbb{R}^{(n+3)|A|}\mid f_{a,C}\geq f_{a,i}-\varepsilon\}$.

The minimax problem without equilibrium constraints

$$\sup_{x\in X}\inf_{y\in Y}\varphi(x,y)$$

is a two-player zero-sum game, the probability of a point (x,y) reaching minimax is given by

$$\int \mathbb{P}(\underline{\varphi}(x)\geq m-\varepsilon)\mathbb{P}(\bar{\varphi}(y)\leq m+\varepsilon)\phi_{\varphi(x,y)}(m)dm \tag{3.16}$$

where $\bar{\varphi}(y)=\max_{x\in X}\varphi(x,y)$ and $\underline{\varphi}(x)=\min_{y\in Y}\varphi(x,y)$. The minimization over y is a high dimensional global optimization. However, coordinate descent given as follows only produces a local minimum.

$$\int_{\mathcal{S}} \mathcal{G}(\varphi-\mu_\varphi,\Sigma_\varphi)\prod_{i=0}^{n+1}\left(1-\exp\left(-2\frac{(\varphi_C+\varepsilon-\varphi_{i+1})(\varphi_C+\varepsilon-\varphi_i)}{x_{i+1}-x_i}\right)\right)$$
$$\prod_{a\in A}\left(1-\exp\left(-2\frac{(\varphi_C-\varepsilon-\varphi_{i+1})(\varphi_{a,C}-\varepsilon-\varphi_i)}{y_{a,i+1}-y_{a,i}}\right)\right)d\varphi.$$

So it is necessary to compare the values reached at the probable local minima. To do so, we can perform Bayesian inference for all the probable local minima.

Given the equilibrium constraint $y\in\Phi(x)$, we first question whether (x,y) is feasible, if so, then it has a chance greater than (3.16) of being a solution, because some of its competitors may be eliminated for being unfeasible. Suppose the increment $\varphi(x',y)-\varphi(x,y)$ is a Gaussian with mean μ and variance σ^2. The chance of this increment being positive is

$$\frac{1}{2}\left(1+\operatorname{erf}\left(\frac{\mu}{\sqrt{2\sigma^2}}\right)\right).$$

Take into consideration of the equilibrium constraint $y\in\Phi(x)$, and let q be the probability of (x',y) being a game equilibrium. The point (x',y) eliminates (x,y) as a minimax solution

if the increment $\varphi(x', y) - \varphi(x, y)$ is positive and (x', y) is a game equilibrium. Suppose the values of φ and F_a are independent, then this occurs at the probability of

$$\frac{1}{2}q\left(1 + \text{erf}\left(\frac{\mu}{\sqrt{2\sigma^2}}\right)\right).$$

We want to transform this multiplicative effect on the probability into an additive effect on the Gaussian. Define the effective mean of the Gaussian increment $\varphi(x', y) - \varphi(x, y)$ as $\mu' := \mu - \delta$ where the correction term δ satisfy

$$\frac{1}{2}\left(1 + \text{erf}\left(\frac{\mu - \delta}{\sqrt{2\sigma^2}}\right)\right) = \frac{1}{2}q\left(1 + \text{erf}\left(\frac{\mu}{\sqrt{2\sigma^2}}\right)\right).$$

The values of δ and μ' as a function of q and μ are shown in Fig 6.

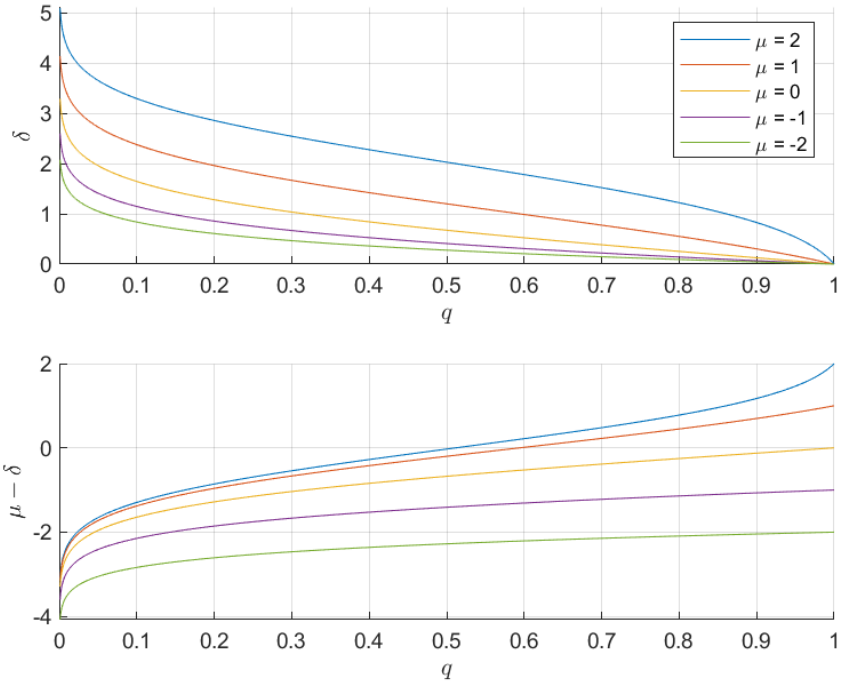

Figure 6: δ and μ' as a function of q and μ. Both functions have a vertical asymptote at $q = 0$.

There are two adverse consequences of this method. First, the modified process reaches $-\infty$ at some points. These are the sampled points strictly dominated by other sampled points. From a probabilistic point of view, we are not interested in these isolated points, but their neighboring points may have mean of very large magnitude and cause numerical instability. To avoid this, we can let the effective mean be $\max\{\mu', \theta\}$ instead for some threshold $\theta < 0$. We can see from Fig 6 that we do not need to set θ very small to avoid a noticeable false increase in q. Second, the effective mean μ' may not be piecewise linear in x' although the original mean μ is. To circumvent this problem, we can make use of linear interpolation to divide the whole segment into smaller pieces, then the formulae (3.4) - (3.6) are again applicable on each segment.

Finally, the probability that (x, y) solves the general problem

$$\sup_{x \in X} \inf_{y \in \Phi(x)} \varphi(x, y). \tag{3.17}$$

is given by

$$\int \mathbb{P}(\bar{\varphi}(y) \geq m_0 - \varepsilon) \left(\prod_{a \in A} \mathbb{P}(\underline{\varphi}(x, y_{-a}) \leq m_0 + \varepsilon) \mathbb{P}(\bar{F}_a(x, y_{-a}) \geq m_a - \varepsilon) \right) \phi_{x,y}(m) dm \tag{3.18}$$

where $m := (m_0, m_a)_{a \in A}$ and $\phi_{x,y}(m)$ is the joint distribution of $\varphi(x, y) = m_0$ and $F_a(x, y) = m_a$. We assume x and y_a are all one-dimensional, but this can be generalized into high dimensional variables by optimizing over each of their coordinates and compare the function values of their local optima. Each probability factor is calculated with (3.7) using (3.4) - (3.6) on separate segments. These functions are obtained by solving Gaussian inference problems. These functions for φ are adjusted and linearly interpolated by δ according to Fig 6, where q is calculated as

$$\int \prod_{a \in A} \mathbb{P}(\bar{F}_a(x, y_{-a}) \geq m_a - \varepsilon) \phi_{x,y}(m) dm. \tag{3.19}$$

To conclude, the remarkable feature of the Bayesian optimization is its flexibility in dealing with complex structures such as multilevel optimization and equilibrium constraints, because it can use simple rules of probabilities to translate the logical problem behind the complex formulation.

4.0 Applications and Related Problems

The mathematical problem of minimax programming with equilibrium constraints

$$\sup_{x \in X} \inf_{y \in \Phi(x)} \varphi(x, y). \tag{4.1}$$

admits many specific applications, which will be discussed in this chapter.

4.1 Centralization and Decentralization

Real world applications often face different levels of centralization in a system. This can be a design problem in the organization of governments, in the control of currencies and transactions, or in smart grid or IoT (Internet of things) protocols. Centralized systems are often characterized as efficient yet prone to risk and error, and decentralized systems the opposite.

The game $F_a(x, y)$ describes the behavior of a decentralized system. The objective function $\varphi(x, y)$ in (4.1) describes the behavior of a centralized system. By establishing the equilibrium as the constraint in (4.1), we make sure that both systems achieve the same outcome y when they reach optimality and equilibrium respectively. Suppose φ is independent of x, then (4.1) describes the following problem: given a centralized system that optimizes φ, we want to design a decentralized system (by choosing a value of x), so that its worst-case outcome has the same characteristics as the centralized system: optimizing φ as much as possible. On the other hand, suppose F_a is independent of x, then (4.1) describes the following problem: given a decentralized system F_a, we want to design a centralized system (by choosing a value of x) that is optimal when it operates under the worst-case outcome of the decentralized system.

More generally, we can put two games of different levels of decentralization as the constraints. This is the case of the example proposed in introduction.

$$\begin{aligned} \sup_{x \in X} \inf_{\substack{y_1 \in Y_1 \\ y_2 \in Y_2}} \ & \varphi(x, y_1, y_2) \\ \text{s.t. } & y_1 \in \Phi_1(x) \\ & y_2 \in \Phi_2(x) \end{aligned}$$

One game may have M players while the other may have M' players. Having two games in the constraints does not change the nature of the problem, because we can consider two games as a single game of two groups of players where each group of player have no impact on the payoff of the players in the other group.

4.2 Linear-Quadratic Games

Linear-quadratic games are the most basic type of dynamical games with nice properties and well studied solutions. When there is only one agent, the game is simply a control problem. Consider the two-variable centralized control problem

$$\begin{aligned} \max_{x, u_1, u_2} \ & \int (x^{\mathrm{T}} Q x + u_1^{\mathrm{T}} R_1 u_1 + u_2^{\mathrm{T}} R_2 u_2) dt \\ \text{s.t. } & \dot{x} = Ax + B_1 u_1 + B_2 u_2 \end{aligned}$$

and the two-player decentralized game problem with the same dynamics

$$\begin{aligned} \max_{x, u_1} \ & \int (x^{\mathrm{T}} Q_1 x + u_1^{\mathrm{T}} R_{11} u_1 + u_2^{\mathrm{T}} R_{12} u_2) dt \\ \text{s.t. } & \dot{x} = Ax + B_1 u_1 + B_2 u_2 \\ \max_{x, u_2} \ & \int (x^{\mathrm{T}} Q_2 x + u_1^{\mathrm{T}} R_{21} u_1 + u_2^{\mathrm{T}} R_{22} u_2) dt \\ \text{s.t. } & \dot{x} = Ax + B_1 u_1 + B_2 u_2. \end{aligned}$$

Suppose these two problems admit the same linear feedback $u_i = K_i x$ as solution, then they are related by the following system of equations

$$\begin{aligned} A_c =& A - B_1 K_1 - B_2 K_2 && (4.2)\\ 0 =& B_i^{\mathrm{T}} P - R_i K_i && (4.3)\\ 0 =& B_i^{\mathrm{T}} P - R_{ii} K_i && (4.4)\\ 0 =& Q + P A_c + A_c^{\mathrm{T}} P + K_1^{\mathrm{T}} R_1 K_1 + K_2^{\mathrm{T}} R_2 K_2 && (4.5)\\ 0 =& Q_1 + P_1 A_c + A_c^{\mathrm{T}} P_1 + K_1^{\mathrm{T}} R_{11} K_1 + K_2^{\mathrm{T}} R_{12} K_2 && (4.6)\\ 0 =& Q_2 + P_2 A_c + A_c^{\mathrm{T}} P_2 + K_2^{\mathrm{T}} R_{22} K_2 + K_1^{\mathrm{T}} R_{21} K_1. && (4.7) \end{aligned}$$

Here, Eqs (4.2), (4.3), and (4.5) solve the centralized control, while Eqs (4.2), (4.4), (4.6), and (4.7) solve the decentralized game.

Assume the system dynamics (A, B_1, B_2) are known, the conversion from control to game is to solve for (Q_i, R_{ij}) given (P, Q, R_i), and vice versa for conversion from game to control. For either direction of the conversion we perform, K_i and A_c can always be expressed by known quantities by solving the original problem, then the decision variables are reduced to (P, Q, R_i) or (P_i, Q_i, R_{ij}), in which the remaining constraints (4.3), (4.5) or (4.4), (4.6), (4.7) are a linear system.

Assume that both players have the same control space. Denote the dimension of the state space by n_x and the dimension of the control space by n_u. When the centralized control is converted to the decentralized control, there are $2n_x(n_x+1) + 2n_u(n_u+1)$ scalar unknowns and $2n_x n_u + n_x(n_x+1)$ scalar equations. As expected, this system is always under-determined. When the decentralized control is converted to the centralized control, there are $n_x(n_x+1)+n_u(n_u+1)$ scalar unknowns and $2n_x n_u + n_x(n_x+1)/2$ scalar equations. Note that there is no guarantee whether this system is under-determined or over-determined. When the system is over-determined, the core of these two players is empty. They cannot achieve a unifying goal following their own agenda.

4.3 Inverse Game

The problem of inverse game is closely related to the problem of game design. The inverse problem of dynamic games is a natural extension of the single-agent IRL (inverse reinforcement learning) problem. Our focus here is the static games instead.

Let $(\hat{y}_i)_{1\leq i\leq n}$ be n sample points in Y. The inverse game problem looks for a value of the parameter $x \in X$ such that all the sample points are equilibria of the game, i.e.

$$f_a(x, \hat{y}_i) \geq f_a(x, r_a(\hat{y}_i, y_{ai}))$$

for all $i \in \mathbb{N}$ such that $1 \leq i \leq n$, for all $a \in A$, and for all $y_{ai} \in Y_a$.

Suppose A is finite. A solution to the inverse game problem is a solution to the minimax problem

$$\min_{x\in X} \max_{y\in Y^n} \sum_{ai} (f_a(x, r_a(\hat{y}_i, y_{ai})) - f_a(x, \hat{y}_i)).$$

A solution to the minimax problem is a solution to the inverse game problem if the minimax has a value of zero. Otherwise, it suggests all the samples cannot be equilibria of a feasible game simultaneously.

Suppose Y is compact and f_a are twice continuously differentiable, uniformly bounded, and uniformly equicontinuous in x. The minimax problem can be approximated by the smooth minimization when $\sigma \to 0$ [10]

$$\min_{x\in X} \prod_{a,i} \int_{Y_a} \exp\left(\frac{1}{2\sigma^2}(f_a(x, r_a(\hat{y}_i, y_{ai})) - f_a(x, \hat{y}_i))\right) dy_{ai}.$$

Instead of matching the payoffs, the inverse game problem can also match the actions through an SIP (semi-infinite programming)

$$\begin{aligned} &\min_{x,y} \ \|\hat{y} - y\|^2 \\ &\text{s.t. } \forall y' : f_a(x, y_{ai}) \geq f_a(x, r_a(y_i, y'_{ai})) \end{aligned}$$

or through an equivalent MPEC

$$\min_{x,y} \|\hat{y} - y\|^2 \tag{4.8}$$

$$\text{s.t. } y_{ai} \in \arg\max_{y'_{ai}} f_a(x, r_a(y_i, y'_{ai})). \tag{4.9}$$

In addition, any occurrence of y in the constraints can be replaced by $\hat{y}$.

Problem (4.8) is structurally similar to (4.1). They are both bilevel optimizations with an MPEC as the inner optimization. On the other hand, we can formulate (4.1) using a relaxation based on (4.8).

$$\max_{x} \min_{\hat{y},y} \lambda\|\hat{y} - y\|^2 + \varphi(x, y)$$

$$y_a \in \arg\max_{y'_a \in Y_a} f_{x,a}(\hat{y}, y'_a)$$

This relaxation transform the equilibrium constraint in (4.1) into optimality constraint by decoupling the actions and the responses.

4.4 Inverse Bimatrix Game

Bimatrix games are one of the easiest and most researched types of games in modern game theory. A bimatrix game consists of two players with finite action spaces. To study the equilibrium of a bimatrix game, we suppose the players have the ability to randomize their actions over the entire action spaces with any desired probabilities, and their goals are to maximize their respective expected payoffs. These probability distributions are called mixed strategies and the Nash equilibrium of mixed strategies with respect to the expected payoffs are called mixed strategy Nash equilibrium.

Definition 6. A bimatrix game consists of a pair of matrices $(C_A, C_B) \in \mathcal{M}(m, n)^2$. A pair of discrete probability distributions $(p_A, p_B) \in \Delta^{m-1} \times \Delta^{n-1}$ is a mixed strategy Nash equilibrium to the bi-matrix game if

$$p_A \in \arg\max_{q_A \in \Delta^{m-1}} q_A^{\mathrm{T}} C_A p_B$$

$$p_B \in \arg\max_{q_B \in \Delta^{n-1}} p_A^{\mathrm{T}} C_B q_B.$$

Theorem 1 (Nash)**.** *Every bimatrix game has a mixed strategy Nash equilibrium.*

The equilibrium condition can also be written as

$$e_i^{\mathrm{T}} C_A p_B \geq e_j^{\mathrm{T}} C_A p_B \tag{4.10}$$

$$p_A^{\mathrm{T}} C_B e_k \geq p_A^{\mathrm{T}} C_B e_l \tag{4.11}$$

for all $i \in \operatorname{supp} p_A$, $k \in \operatorname{supp} p_B$, $j \in \{1, \cdots, m\}$, and $l \in \{1, \cdots, n\}$. Inequality (4.10) states that all the row vectors of C_A belong to one of the two half-spaces separated by a hyperplane orthogonal to p_B and the row vectors indexed by $\operatorname{supp} p_A$ belong to that hyperplane.

To study the payoff matrices, we need to understand how much information they actually provide.

Definition 7. Two matrices $(C_A, C'_A) \in \mathcal{M}(m,n)^2$ are equivalent if for any matrix $C_B \in \mathcal{M}(m,n)$ and any pair of distributions $(p_A, p_B) \in \Delta^{m-1} \times \Delta^{n-1}$: (p_A, p_B) is an equilibrium to (C_A, C_B) if and only if it is also an equilibrium to (C'_A, C_B).

The equivalence defines the quotient topology. For instance, when $m = 2$ and $n = 1$, the best response is uniquely determined by $\operatorname{sign}((C_A)_{21} - (C_A)_{11})$. An equivalent condition of equivalence between C_A and C'_A is that they satisfy (4.10) simultaneously for any p_B. Consider C_A as the polytope in $\mathbb{R}^n$ with m vertices being the m row vectors of C_A, then C_A is uniquely determined upto equivalence by all the facets whose outward-pointing normal vector is nonnegative. Translations and uniform positive scalings are equivalence. So we can limit C_A in a unit cube.

It is more common that an external agent is able to observe an outcome (i, k) than the equilibrium (p_A, p_B), so it is necessary to first estimate the probability distributions from a few outcomes. However, if a game admits multiple equilibria, then different outcomes may come from different distributions. If there may or may not be other equilibria other than (p_A, p_B), without additional information, it is reasonable to postulate that all the possible equilibria altogether bring an additional uniform probability to all the outcomes, as if the actual outcome was drawn with the probability $(p'_A, p'_B) := r(\frac{1}{m}, \frac{1}{n}) + (1-r)(p_A, p_B)$ for some

$r \in (0,1)$. This provides a method to infer the equilibrium (p_A, p_B) from an outcome count $c(i,k)$ using the Dirichlet distribution with a modification

$$f(p_A, p_B) \propto \prod_{i=1}^{m}\prod_{k=1}^{n}(((1-r)p_A(i) + r/m)((1-r)p_B(k) + r/n))^{\alpha(i,k)+c(i,k)-1}$$

where $\alpha(i,k) > 0$ is the concentration parameter of the Dirichlet distribution. It can be used to reflect preferred outcomes such as focal points [29].

The MLE of the equilibrium is the mode of the Dirichlet distribution.

$$p_A(i) = \frac{1}{1-r}\left(\frac{\sum_k c'(i,k)}{\sum_{ik} c'(i,k)} - \frac{r}{m}\right)$$
$$p_B(k) = \frac{1}{1-r}\left(\frac{\sum_i c'(i,k)}{\sum_{ik} c'(i,k)} - \frac{r}{n}\right)$$

where $c'(i,k) = \alpha(i,k) + c(i,k) - 1$. The positivity of probabilities requires r to be small. If one of the payoff matrix C_B is known, the equilibrium condition can be incorporated into the MLE.

$$\begin{aligned} &\max_{p_A, p_B} f(p_A, p_B) \\ \text{s.t. } &\textstyle\sum_i p_A = 1, \sum_k p_B = 1, p_A \geq 0, p_B \geq 0 \\ &p_A^{\mathrm{T}} C_B e_k \geq p_A^{\mathrm{T}} C_B e_l \text{ or } p_B^{\mathrm{T}} e_k = 0. \end{aligned}$$

To more accurately infer the payoff matrix of a player A, they need to play games against different adversaries B, so that each adversary provides a different constraint.

4.5 Neural Network Representation

In our model, the payoff functions and the design objectives are parametrized by the design variable x. The universal approximation theorem suggests that a neural network can approximate any continuous function on a compact Euclidean set to a given degree of precision with a finite set of parameters. So even when the underlying functions are completely left for design, we can using neural networks to represent them.

Represent the payoff functions in the game by a single-layer artificial neural network using the universal approximation theorem. Let $x := (v, w) \in \mathbb{R}^M := \mathbb{R}^{W\times K} \times \mathbb{R}^{W\times(1+N)}$ be the parameters of the artificial neural network $\bar{f} : \mathbb{R}^M \times \mathbb{R}^N \to \mathbb{R}^K$ given by $\bar{f}_k(x, \bar{y}) = \sum_{j=1}^{W} v_{jk}\sigma(\sum_{i=1}^{N} w_{ji}\bar{y}_i + w_{j0})$ where σ is a smooth discriminatory function [8]. Let $r_k : \mathbb{R}^N \times \mathbb{R}^{n_k} \to \mathbb{R}^N$ be the kth substitution function and $f_k : \mathbb{R}^N \times \mathbb{R}^{n_k} \to \mathbb{R}$ the kth player's payoff function given by $f_{x,k}(\bar{y}, y_k) := \bar{f}_k(x, r_k(\bar{y}, y_k))$.

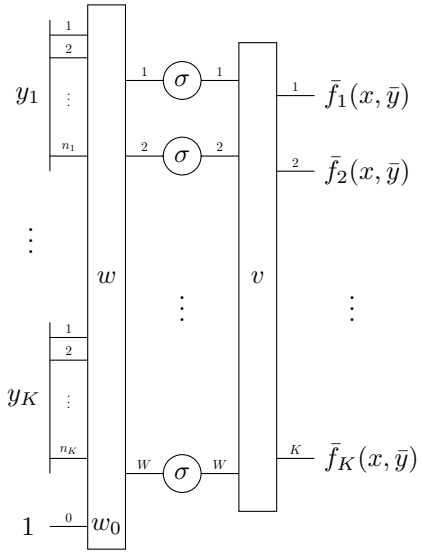

Figure 7: Structure of the single-layer artificial neural network representing the payoff functions. The numbers above lines are indices of the corresponding variables.

The downside of representing the objective functions with neural networks is that the function they represent may be too arbitrary. It is hard to ensure the existence of an equilibrium because the weights do not provide much information about the function properties.

One solution is to limit the functions to be designed within the set of convex functions, which guarantees the existence of a solution under mild conditions. Convexity may also be a desired property of the function to be designed.

A fully input-convex neural network [3] is a recurrent neural network whose output z_k is a convex function of the input y through k layers of activation

$$\forall i = 0, \cdots, k-1 : \qquad z_{i+1} = \sigma_i(U_i z_i + V_i y + b_i)$$

where U_i are matrices of nonnegative components and σ_i are nondecreasing convex functions.

Because of the recurrent nature of the fully input-convex neural network, the backpropagation of gradient can be numerically challenging. The Bayesian approach can have an advantage in finding the optimal weights in this type of networks.

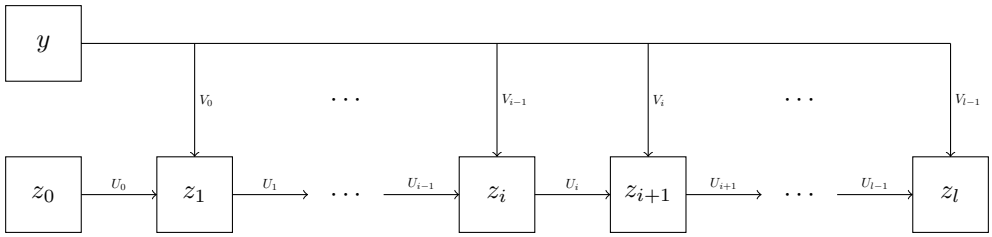

Figure 8: Structure of a fully input-convex neural network.

4.6 Partial Information

The design problems we study in this dissertation focus on the explicit parameters in the payoff functions. There are also many other degrees of freedom in games that control the players' behavior. Player's reaction to uncertainties is one major factor. This is traditionally captured by the expected utility or other risk measure functionals. In this section, I propose the multi-objective optimization approach to games with partial information [15]. As a result, the design parameter may appear not only in the payoff functions, but also in the game constraints.

The information structure of a game with partial information is modeled mathematically by a σ-algebra on the state space for each agent. The simplest σ-algebras are those generated by finite partitions of the state space, called the information partitions. As a result, measurable functions have constant value on each element of the partition, so a strategy of agent a can be characterized by a function $u_a : P_a \to U_a$ or a vector $u_a \in U_a^{|P_a|}$ where U_a is their action space and P_a is their information partition.

Instead of the exact value of the state, the players in a game with partial information only know the sets in their respective information partitions to which the state belongs $x \in E_a \in P_a$. A greedy player would like to find a strategy $u_a(E_a)$ optimal in all the possible states $x \in E_a$. This is however a multi-objective optimization problem. In general, multi-objective optimization problems have no solution which simultaneously optimizes all the objectives. Instead, we study all the non-dominated solutions in multi-objective optimization problems. In games with partial information, we can study all the equilibria constituted of non-dominated responses. By combining the weighted sum method and the ϵ-constraint method in multi-objective optimization, I propose the following definition.

Definition 8. In a two-player normal-form game with partial information, a pure strategy profile (u_A^*, u_B^*) is an equilibrium of ε_X-constrained F_X-optimal strategies if $\forall E_A \in P_A, \forall E_B \in P_B$:

$$u_A^*(E_A) \in \arg\max_{u_A \in U_A} F_A[J_A(\cdot, u_A, u_B^*(\cdot))] \tag{4.12-A}$$
$$\text{s.t.} J_A(\cdot, u_A, u_B^*(\cdot)) \geq \varepsilon_A \text{ on } E_A$$
$$u_B^*(E_B) \in \arg\max_{u_B \in U_B} F_B[J_B(\cdot, u_A^*(\cdot), u_B)] \tag{4.12-B}$$
$$\text{s.t.} J_B(\cdot, u_A^*(\cdot), u_B) \geq \varepsilon_B \text{ on } E_B$$

where ε_X is a real function on E_X and F_X is a non-trivial positive continuous linear functional of functions on E_X.

I proved in [15] the conditions under which these equilibria exist and are equivalent to non-dominated responses in multi-objective optimization. Bayesian Nash equilibria are special cases where F_X are probability measures and ε_X are lower bounds. But in general, Definition 8 also offers solutions that are not attainable as Bayesian Nash equilibria. The

parameters ε_X are very critical to the properties of these equilibria. Large values of ε_X can make both players' payoffs meet desired thresholds but may also lead to infeasibility instead. Posing a minimax problem subject to the equilibrium constraints (4.12) with ε_X as the upper level optimization variable allows us to find an equilibrium with the best performance among all of those constituted of non-dominated responses.

5.0 Conclusion and Future Research Directions

Minimax problems with equilibrium constraints are a fundamental subject in engineering design worthy of great attention from both theoretical and numerical research. They translate the robustness of a design against the uncertainty due to the possible presence of a multitude of equilibria in a game. A significant contribution of this dissertation is to shed light on the importance and the complexity of this type of problems. I wish to continue on this line of work by applying this design principle to real engineering or economic applications.

The Bayesian approach proposed in this dissertation is a novel strategy to solve MPEC and multilevel programming. Its ability to solve these problems comes from the simple rules of probabilities which translate the logical problem behind the complex formulations. It also provides a global point of view which allows a robust optimal design within the parameter space. Other numerical programming methods with a global characteristics can also be considered in the future as a solution methodology to enrich the toolbox for this type of problems.

Bayesian optimization itself is an area of active research, especially for its applications in machine learning. This dissertation shows the power of Bayesian optimization in dealing with minimax problems with equilibrium constraints. With proper examination, the same methodology can be applied to other game theoretical problems, which I would also like to investigate in the future. The Bayesian approach proposed in this dissertation also requires further works to consolidation its theoretical soundness and improve numerical efficacy.

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