

Cooperative equilibria in the finite iterated prisoner’s dilemma

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Nash equilibria are defined using uncorrelated behavioural or mixed joint probability distributions effectively assuming that players of bounded rationality must discard information to locate equilibria. We propose instead that rational players will use all the information available in correlated distributions to constrain payoff function topologies and gradients to generate novel “constrained” equilibria, each one a backwards induction pathway optimizing payoffs in the constrained space. In the finite iterated prisoner’s dilemma, we locate constrained equilibria maximizing payoffs via cooperation additional to the unconstrained (Nash) equilibrium maximizing payoffs via defection. Our approach clarifies the usual assumptions hidden in backwards induction.

I. INTRODUCTION

Payoff maximization in the single stage Prisoner’s Dilemma (PD) locates a unique Nash equilibrium point, mutual defection, which garners players a non-Pareto efficient outcome. Finite repetition of this single stage game defines the finite Iterated Prisoner’s Dilemma (IPD) which is apparently solved by inductively propagating the single stage Nash equilibrium of mutual defection backwards through every stage of the game to establish “All Defect” as the unique Nash equilibrium path. This single rational play strategy prevents players from cooperating to achieve higher payoffs. Nevertheless, in experimental tests (see [1–4]), people often cooperate to garner a greater payoff indicating either that modelling in game theory is somehow incomplete or that people behave irrationally. Many different proposals have been made along these two lines including suggestions to modify definitions of rationality and to bound rationality [5–9], to take account of incomplete information [10–13] and uncertainty in the number of repeat stages [14], to bound the complexity of implementable strategies [15–17], to account for communication and coordination costs [18], to incorporate reputation and experimentation effects [19] or secondary utility functions as in benevolence theory [20] or in moral discussions [21], to include adaptive learning [22] or fuzzy logic [23], or more directly, to employ comprehensive constructions of normal form strategy tables [24–26]. Interestingly, quantum correlations can be introduced to resolve the prisoner’s dilemma [27].

As noted above, these proposals generally modify the definition of either the IPD or of player rationality to explain deviations from the single unique Nash equilibrium pathway. By contrast, in this paper we assume Common Knowledge of Rationality (CKR) for all players and no modification of the IPD game definition. Then we generalize the analysis of the IPD to regimes where the fixed point theorems underlying existing equilibria do not apply. In providing an existence proof for mixed strategy equilibria, Nash and Kuhn made the overly restrictive as-

sumption that each player’s mixed or behavioural strategy choice probability distributions were continuous and uncorrelated and so strictly independent [28, 29]. This assumption allowed the analytic continuation of game payoff functions over a convex probability polytope enabling the use of fixed point theorems to locate mixed strategy equilibria [28]. The subsequent widespread use of this existence proof as a definition of “Nash equilibria” requires rational players to locate equilibria by discarding information inherent in correlations, in effect, an assumption of “bounded” rationality. For multi-stage games, this same assumption that players of bounded rationality (employing myopic agents)³ must discard information by adopting uncorrelated play allowed Kuhn to define subgame equilibria and subgame decompositions [29]. While this assumption is always valid for single stage games with an empty history set, in multistage games the joint strategy choice probability distributions of all players can be more generally correlated through being conditioned on game history sets, with these correlations invalidating the *a priori* assumption of uncorrelated mixed or behavioural strategies. Hence, we propose that players of unbounded rationality, in contrast to those of “bounded” rationality, will make use of all available information by exploiting correlated mixed or behavioural joint strategy choice probability distributions to optimize payoffs.

In this paper, by considering broader classes of correlated joint probability distributions, we significantly generalize the analysis of the IPD at the cost of a greater analytic complexity stemming for instance, from the non-applicability of fixed point theorems. It may be questioned whether this cost is a price worth paying. However, we have seen little in the literature considering regimes where these *a priori* assumptions are invalid, though these regimes might provide the mathematical arena to model broader classes of experimental game behaviours. Especially so given that well established techniques for manipulating conditioned and correlated joint probability distributions exist.

Previous efforts to model correlated strategy choices have attempted this task discursively—see for instance the descriptive derivations of strategy function equilibria in differential games [30] and trigger function equilibria in supergames where players encourage adherence to a cooperation pathway using deviations to “trigger” credible punishments [31–35]. These previous treatments have

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strongly insisted that players prespecify an outcome for absolutely every possible (and impossible) situation that might arise in a supergame—for justifying quotations, see note [36]. As a result, current supergame analysis must either assume that all mixed or behavioural strategy choice variables are independent and optimized via a Nash procedure, or that all variables are fully specified by strategy functions which are themselves independently selected and again optimized via a Nash procedure.

This paper fills in the missing middle ground here, and considers correlated mixed or behavioural joint probability distributions conditioned by sets of strategy functions which specify only some fraction of the possible variables (defining a dependent set) while leaving the remaining variables unspecified (an independent set) to be optimized by standard Nash techniques. (Here, the dependent variables are described by correlated probability distributions conditioned on game history sets.) As such, we introduce no additional properties to the IPD and our use of strategy functions and Nash optimization techniques are entirely standard. Optimizing functions over a set of independent variables given a set of constrained dependent variables is the subject matter of constrained optimization theory as in Lagrange multipliers [39, 40], variational calculus [41–43], and dynamic programming [44]. Each adopted constraint set generalizes the *a priori* assumption made by Nash and Kuhn that each player’s mixed or behavioural strategy choice probability distributions are uncorrelated and separable. In fact, Nash and Kuhn’s multistage analysis corresponds to the special case where the constraint set is empty, and Nash equilibria are defined only for empty constraint sets. Hence, in our generalized analysis (as in any constrained optimization procedure), we must first take account of applied constraint sets prior to locating “constrained equilibria” in the constrained probability space. (We note that games with mixed strategies constrained to lie within convex hyperpolyhedron by linear inequalities and equations have been considered in Refs. [45, 46].)

To avoid any confusion about our generalization, we first review the original Nash equilibrium definitions in the next section (II), and then generalize these definitions to define constrained equilibria applicable to non-empty constraint sets in the section following (III). In section IV, we derive constrained equilibria in the IPD, and observe the different player behaviours arising from adopted constraints. Further, we apply the Nash equilibria definitions on the constrained equilibrium space to specify global equilibria. Finally we discuss the role of the backwards induction argument as it is applied to finite supergames in section V.

II. REVIEW OF NASH EQUILIBRIA

Throughout this paper, we consider supergames formed by finitely iterating a single stage game over $1 \leq n \leq N$ stages where each stage is played between two non-communicating rational players denoted P_x and P_y . In the n^{th} stage, players P_x and P_y choose their respective stage strategies, denoted x_n and y_n , from the same strategy set S , that is $x_n, y_n \in S$, where $S = \{s_1, \dots, s_s\}$ and s is the total number of strategies, or alternatively, $S = \{s | s \in \mathbb{R}, s_1 \leq s \leq s_s\}$ when strategy choice is con-

tinuous. Game history sets H_n known to both players in stage $(n + 1)$ record occurring events with $H_0 = \emptyset$, and $H_n = \{x_1, \dots, x_n, y_1, \dots, y_n\}$. The payoffs Π_x and Π_y for players P_x and P_y are each specified as mappings (or functions) from the set of all chosen strategies $H_N = \{x_1, \dots, x_N, y_1, \dots, y_N\}$ to the real line [47, 48] via

$$\Pi_z = \Pi_z(x_1, \dots, x_N, y_1, \dots, y_N), \quad z \in \{x, y\}. \quad (1)$$

We consider supergames where these mappings are defined as summations of the respective n^{th} stage player payoffs $\pi_x(x_n, y_n) \geq 0$ and $\pi_y(x_n, y_n) \geq 0$ assumed non-negative without loss of generality, giving

$$\Pi_z = \sum_{n=1}^N \pi_z(x_n, y_n), \quad z \in \{x, y\}, \quad (2)$$

nominally functions of $2N$ variables $\{x_1, \dots, x_N\}$ and $\{y_1, \dots, y_N\}$. The goal of each player is to maximize their respective total payoff functions Π_x and Π_y .

Strategy choices are defined as a functional mapping from the game history sets H_n to the strategy set S , which specify after each history the specific strategy choices x_n and y_n to be selected [47, 48]. Thus, following standard definitions [47]:

A pure strategy $[x_n]$ of player $[P_x]$ is a function

$$x_n : H_{n-1} \rightarrow S = \{s_1, s_2, \dots\}. \quad (3)$$

In Ref. [28], Nash defined mixed strategy equilibria in terms of expected value payoff functions. The most general possible expected payoff functions are

$$\langle \Pi_z \rangle = \sum_{x_1 \dots x_N, y_1 \dots y_N = s_1}^{s_s} P(x_1, \dots, x_N, y_1, \dots, y_N) \times \Pi_z(x_1, \dots, x_N, y_1, \dots, y_N) \quad (4)$$

for $z \in \{x, y\}$, and where the probability that player P_x (P_y) chooses strategy choice $x_n \in S$ ($y_n \in S$) in stage n for $1 \leq n \leq N$ is $P(x_1, \dots, x_N, y_1, \dots, y_N)$. Here, the average is calculated over an ensemble of trials representing every possible circumstance and outcome. In particular, the total ensemble consists of an infinite number of subensembles, one for every possible joint probability distribution, each one of which contains an infinite number of trial outcomes. This is in accord with von Neumann and Morgenstern’s definition of a strategy as “a complete plan: a plan which specifies what choices [a player] will make in every possible situation, for every possible actual information which [that player] may possess at that moment” [49]. We emphasize that a player’s complete strategy list is not synonymous with a mere listing of all the possible choices determining every pathway through the complete game tree despite this common usage in Ref. [49]—such a listing is missing information. A full listing of every possible situation which might occur will contain a successive listing of all the many possible joint strategy choice probability distributions which might be adopted by the players as well as subsidiary information about all the possible pathways through the associated game tree generated under those adopted distributions. If the

information about the joint probability distributions is absent, this is equivalent to making a default assumption that all pathways are equally weighted (as conversely, differing joint probability distributions weight pathways differently). In actuality, discarding information about adopted joint probability distributions is equivalent to an assumption of bounded rationality, and the necessity of such restrictions has never been demonstrated. In particular, von Neumann and Morgenstern specifically asserted that they were using a method of “indirect proof” to imagine the form of a successful theory and to test the consequences for problems and contradictions [49]. Naturally, such contradictions were never found as restricting the solution space to a valid subensemble ensures the absence of contradictions though at the expense of incomplete results. In this paper we do not make this unjustified assumption. As usual then, using $P(A \text{ and } B) = P(A)P(B|A)$ we have

$$P(x_1, \dots, x_N, y_1, \dots, y_N) = P_{1x}(x_1)P_{1y}(y_1) \times P(x_2, \dots, y_2, \dots | H_1), \quad (5)$$

and the iterated identity

$$P(x_n, \dots, x_N, y_n, \dots, y_N | H_{n-1}) = P_{nx}(x_n | H_{n-1}) \times P_{ny}(y_n | H_{n-1})P(x_{n+1}, \dots, y_{n+1}, \dots | H_n), \quad (6)$$

successively applied for all n . Here, same stage choices x_n and y_n are independent events conditioned on the history set H_{n-1} and so potentially correlated. We also elect here to maintain the time ordering of conditioning events, though this is not necessary—probability distributions can be pre- or post-conditioned, so two events A and B occurring at two different times have joint probability $P(A \text{ and } B) = P(A)P(B|A) = P(B)P(A|B)$. So also, a player in their pregame analysis can condition events in one stage n on either earlier or later stage events as desired. The most general possible expected payoff functions are then

$$\begin{aligned} \langle \Pi_z \rangle &= \sum_{\substack{s_1 \leq x_n, y_n \leq s_s \\ H_{n-1}}} P(H_{n-1})P(x_n, y_n | H_{n-1})\Pi_z(x_1, \dots) \\ &= \sum_{\substack{x_1 \dots x_N \\ y_1 \dots y_N}} P_{1x}(x_1)P_{1y}(y_1) \times \dots \times P_{Nx}(x_N | H_{N-1}) \\ &\quad \times P_{Ny}(y_N | H_{N-1})\Pi_z(x_1, \dots, x_N, y_1, \dots, y_N) \\ &= \sum_{n=1}^N \sum_{\substack{x_1 \dots x_n \\ y_1 \dots y_n}} P_{1x}(x_1)P_{1y}(y_1) \times \dots \\ &\quad \times P_{nx}(x_n | H_{n-1})P_{ny}(y_n | H_{n-1})\pi_z(x_n, y_n), \quad (7) \end{aligned}$$

for $z \in \{x, y\}$. Each of the conditioned distributions $P_{nz}(z_n | H_{n-1})$ can be written as a list of potentially correlated behavioural strategy distributions

$$P_{nz}(z_n | H_{n-1}) = \begin{cases} P_{nz, H'_{n-1}}(z_n), & \text{if } H_{n-1} = H'_{n-1} \\ P_{nz, H''_{n-1}}(z_n), & \text{if } H_{n-1} = H''_{n-1} \\ \vdots & \vdots \end{cases} \quad (8)$$

with up to $2^{2(n-1)}$ entries, one for each possible history set H_{n-1} . The individual distributions $P_{nz, H_{n-1}}(z_n)$ and

$P_{n'z', H_{n'-1}}(z'_{n'})$ can still be correlated as when, for instance, a single “dice” is used to determine both outcomes. (For completeness, note [50] lists the definitions of correlated variables in terms of their covariance, variance and means.) Such correlations further imply that these distributions are not necessarily continuous. These potentially correlated behavioural strategy distributions allow writing the most general expected payoff functions as

$$\langle \Pi_z \rangle = \sum_{\substack{x_1 \dots x_N \\ y_1 \dots y_N}} P_{1x}(x_1)P_{1y}(y_1) \times \dots \times P_{Nx, H_{N-1}}(x_N) \times P_{Ny, H_{N-1}}(y_N)\Pi_z(x_1, \dots, x_N, y_1, \dots, y_N). \quad (9)$$

Here, all possible contingent histories have been taken into account weighted by their respective conditioned probabilities. Players can now seek to optimize their payoffs by applying any relevant optimization technique to these general expected payoff functions. Of course, if the functions are correlated and discontinuous then fixed point theorems cannot be used to locate optima, and also, if the variables are correlated it is absolutely necessary to resolve the correlations as imposed constraints prior to applying any optimization procedure. That is, if correlations exist, any optimization procedure such as backwards induction must take those correlations into account as imposed constraints before seeking to derive an optimal pathway.

Given these most general expected value payoff functions, we now revisit the definition of Nash equilibria as developed by Nash [28] and as explicated by Kuhn [29]. When introducing behavioral strategies Kuhn “explicitly assumed that the choices of alternatives at different history sets are made independently. Thus it might be reasonable to call them ‘uncorrelated’ or ‘locally randomized’ strategies.” [29]. Such uncorrelated behavioral strategies capture the myopic viewpoint of non-communicating agents possessing “a local perspective [which] decentralizes the strategy decision of player i into a number of local decisions.” [51]. In this, the agent-normal game form, myopic agents at each history set determine paths through the game tree using probability distributions which are uncorrelated and independent. This assumption allowed Kuhn to prove the equivalence of uncorrelated behavioural strategies and the uncorrelated mixed strategies introduced by Nash in games of perfect recall [29]. This equivalence was established by recognizing that player P_x (P_y) could index all their possible pure strategies by parameter α (β) with the probability of playing that strategy being $P_x(\alpha)$ ($P_y(\beta)$) given by an appropriate product of the uncorrelated behavioural strategies $P_{nx, H_{n-1}}(x_n)$ ($P_{ny, H_{n-1}}(y_n)$). This then allowed writing the non-general expected payoff functions as

$$\langle \Pi_z \rangle = \sum_{\alpha, \beta} P_x(\alpha)P_y(\beta)\Pi_z(\alpha, \beta) \quad (10)$$

for $z \in \{x, y\}$ where here, the summation is over an appropriately limited set of α and β values. Nash considered the mixed strategies $P_x(\alpha)$ and $P_y(\beta)$ as “a collection of non-negative numbers which have unit sum and are in one to one correspondence with his pure strategies.” so the expected payoff functions were linear in

the mixed strategies for each player allowing optimization over a “convex subset of a real vector space” via fixed point theorems [28]. This definition follows that of von Neumann and Morgenstern [49] in establishing a one to one correspondence between a player’s pure and mixed strategies which are subject to appropriate normalization constraints but to no other constraints such as might result from using fully general joint strategy choice probability distributions. Of course, these restrictive assumptions limit the ensemble over which payoff averages are calculated, and in the full ensemble correlated behavioural strategies can break the one-to-one correspondence between the mixed strategies and the full set of uncorrelated pure strategies, can render expected payoff functions discontinuous, and can invalidate the use of fixed point theorems as an optimization technique.

The assumption that players employ uncorrelated mixed or behavioural strategy choices then allows the definition of Nash equilibria in terms of the probabilities $\bar{p} \equiv \{P_x(\alpha), \forall \alpha\}$ and $\bar{q} \equiv \{P_y(\beta), \forall \beta\}$. Following Nash [28],

If and only if each player’s mixed or behavioural strategy choices are uncorrelated and independent, then a 2-tuple (\bar{p}^*, \bar{q}^*) of unconditioned probability distributions forms a mixed strategy equilibrium point if and only if for all players,

$$\begin{aligned} \langle \Pi_x(\bar{p}^*, \bar{q}^*) \rangle &= \max_{\bar{p}} [\langle \Pi_x(\bar{p}, \bar{q}^*) \rangle] \\ \langle \Pi_y(\bar{p}^*, \bar{q}^*) \rangle &= \max_{\bar{q}} [\langle \Pi_y(\bar{p}^*, \bar{q}) \rangle]. \end{aligned} \quad (11)$$

Thus an equilibrium point is a 2-tuple (\bar{p}^*, \bar{q}^*) such that each player’s pure strategy maximizes their payoff if the strategies of the others are held fixed. Thus each player’s strategy is optimal against those of the others [28].

We note here that Nash proved an existence theorem in Ref. [28] and not a uniqueness theorem, and it is well known that when the restrictive assumptions are not made then mixed strategy equilibria do not necessarily exist [37, 38, 52–56].

Pure strategy Nash equilibria can be defined by further specializing the strategy choice probability distributions to be either zero or one, $P_x(\alpha), P_y(\beta) \in \{0, 1\}$ for all values of α and β , so one or another pure strategy is independently chosen by each player with certainty. Then pure strategy Nash equilibria can be defined following Nash [28]:

If and only if each player’s pure strategy choices are uncorrelated and independent, then a 2-tuple (α^*, β^*) is a pure strategy equilibrium point if and only if for all players,

$$\begin{aligned} \Pi_x(\alpha^*, \beta^*) &= \max_{\alpha} [\Pi_x(\alpha, \beta^*)] \\ \Pi_y(\alpha^*, \beta^*) &= \max_{\beta} [\Pi_y(\alpha^*, \beta)]. \end{aligned} \quad (12)$$

Another situation where the Nash definition can be applied is when all variables are fully specified by strategy functions which are themselves independently selected. In this case, strategy choices are conditioned on earlier

events and so possibly correlated in any stage despite being chosen independently by each player [30–34]. However strategy functions introduced in these approaches are very limited in the sense that any implemented strategy function set must fully specify an outcome for every stage and every possible situation which might arise in a game. (For justifying quotations see [36].) Because players P_x and P_y independently choose sets of N strategy functions denoted $\mathcal{A}_x = \{x_n : H_{n-1} \rightarrow S, 1 \leq n \leq N\}$ and similarly for \mathcal{A}_y to generate payoffs $\Pi_z(\mathcal{A}_x, \mathcal{A}_y)$ for $z = \{x, y\}$, it is possible to define strategy function Nash equilibria [28, 30]:

If and only if all $2N$ strategy choice variables are functionally specified, a 2-tuple strategy profile $\phi = \{\mathcal{A}_x^*, \mathcal{A}_y^*\}$ is a strategy function Nash equilibria if and only if for all players,

$$\begin{aligned} \Pi_x(\mathcal{A}_x^*, \mathcal{A}_y^*) &= \max_{\mathcal{A}_x} [\Pi_x(\mathcal{A}_x, \mathcal{A}_y^*)] \\ \Pi_y(\mathcal{A}_x^*, \mathcal{A}_y^*) &= \max_{\mathcal{A}_y} [\Pi_y(\mathcal{A}_x^*, \mathcal{A}_y)]. \end{aligned} \quad (13)$$

Essentially equivalent definitions underly trigger function equilibria [30–34].

Based on the equilibria definitions above, supergame analysis must either assume that all variables are independent and optimized via a Nash procedure, or that all variables are fully specified by strategy functions. To treat more general strategy functions, it is necessary to extend the Nash equilibrium concept to regimes where fixed point theorems are inapplicable. The next section does this by defining new constrained equilibria.

III. CONSTRAINED EQUILIBRIA

In this section we define constrained equilibria through allowing the use of correlated multivariate probability distributions to optimize expected payoffs.

We note firstly that neither Nash nor Kuhn provided any rationale requiring rational players to restrict the size of the ensemble used to calculate payoff averages by only employing uncorrelated mixed or behavioural probability distributions. Likely, this assumption was made in the context of an existence proof to simplify analysis as the fully general treatment of correlated multivariate probability distributions is difficult. However, adopting correlated distributions can often greatly simplify analysis. Consider that when events A and B are perfectly correlated, the joint probability of both events reduces to $P(A \text{ and } B) = P(A)P(B|A) = P(A)$, so one variable entirely disappears reducing the dimensionality of the problem space and simplifying the problem. (This dimensionality reduction is a normal result whenever constraints are applied in optimization problems.)

In fact, any assumption that players must adopt the restricted ensemble available under uncorrelated play is equivalent to a claim that players must discard information and so amounts to an assumption of bounded rationality. (For completeness, note [57] details the mutual information content of correlated joint probability distributions.) How might rational players exploit the information in correlated distributions? A minimum necessary condition for the existence of an equilibrium point

is that opponents must be unable to improve their payoffs by altering their strategy choices, so essentially, opponent's payoff function "gradients" must be negative at equilibrium points. Now, rational players can exploit correlations to constrain the payoff function space topology so as to alter the possible directions in which payoff functions can change. As "gradients" can only be taken along allowed directions, such constraints alter the payoff function "gradients" at any point. Thus, it is possible for rational players to choose correlations to alter payoff function "gradients" to generate novel equilibria at novel points. In this paper, we assume that rational players will make use of all available information including that implicit in correlated joint probability distributions.

In this paper, constrained equilibria are defined for pairs of sets of strategy functions $\{\{X_n\}, \{Y_n\}\}$. For the pure strategy case, these strategy functions Z_n may be represented as

$$\begin{aligned} x_n &= X_n(x_1, \dots, x_{n-1}, y_1, \dots, y_{n-1}) \\ y_n &= Y_n(x_1, \dots, x_{n-1}, y_1, \dots, y_{n-1}). \end{aligned} \quad (14)$$

Here x_n and y_n might be independent variables or dependent on some or all of the variables $x_1, \dots, x_{n-1}, y_1, \dots, y_{n-1}$. For the pure strategy case, neither these variables nor the strategy functions are probabilistic. In terms of conditioned probability distributions, these constraints take the form

$$\begin{aligned} P_{nx}(x_n|H_{n-1}) &= \delta_{x_n, X_n(H_{n-1})} \\ P_{ny}(y_n|H_{n-1}) &= \delta_{y_n, Y_n(H_{n-1})}, \end{aligned} \quad (15)$$

where $\delta_{a,b}$ is one if $a = b$ and zero otherwise. (Of course, more general distributions could be considered.) These functional notations, though widely used to represent payoff functions, have not been widely employed for strategy functions. We note that it has been used in the derivation of best reply (strategy) functions [34, 38], Stackelberg duopolies [38], a two-stage prisoner's dilemma [58], correlation in randomized strategies [56], and differential games [30], while a number of texts describe strategies as "functions" without actually introducing a function notation [37, 46–48].

Suppose player P_x (or P_y) chooses a set of strategy functions, which we might conveniently call their algorithm denoted as $\mathcal{A}_x = \{X_m, \dots, X_k\}$ (or $\mathcal{A}_y = \{Y_n, \dots, Y_j\}$), to constrain some (or none) of their strategy choice variables creating a set of dependent variables and a remaining set of independent variables. For notational convenience, we relabel the independent variable sets for P_x and P_y as respectively $\bar{\alpha} = \{u_1, \dots, u_{\hat{x}}\} \in S^{\times \hat{x}}$ and $\bar{\beta} = \{v_1, \dots, v_{\hat{y}}\} \in S^{\times \hat{y}}$ where $0 < \hat{x} + \hat{y} \leq 2N$. We assume here that at least one variable remains independent as otherwise, the optimization becomes trivial. Immediately then, the payoff functions for the players become composite with reduced dimensionality (and changed properties) given by

$$\Pi_z \rightarrow \Pi_z(\bar{\alpha}, \bar{\beta}), \quad z \in \{x, y\}. \quad (16)$$

Here, no dependent variables, such as $x_2 = X_2(x_1, y_1)$ say, appear in the composite payoff functions.

With the representation of strategy functions in terms of the independent variables, the Nash equilibrium definition can be applied to the space of independent variables to define pure strategy constrained equilibria via:

Given a particular constraint set \mathcal{A}_x and \mathcal{A}_y , a 2-tuple $(\bar{\alpha}^*, \bar{\beta}^*)$ is a pure strategy constrained equilibria if and only if for all players,

$$\begin{aligned} \Pi_x(\bar{\alpha}^*, \bar{\beta}^*) &= \max_{\bar{\alpha}}[\Pi_x(\bar{\alpha}, \bar{\beta}^*)] \\ \Pi_y(\bar{\alpha}^*, \bar{\beta}^*) &= \max_{\bar{\beta}}[\Pi_y(\bar{\alpha}^*, \bar{\beta})]. \end{aligned} \quad (17)$$

We now generalize this definition to mixed strategy constrained equilibria. In this case, strategies at any stage can be probabilistic, so the strategy functions of Eqs. (14) and (15) applied at stage n map each history set H_{n-1} to a probability distribution. The set of these probabilistic strategy functions $P_{nz}(z_n|H_{n-1})$ forms an algorithm \mathcal{A}_z . For a pair of algorithms $\{\mathcal{A}_x, \mathcal{A}_y\}$, the expected total payoffs given as Eq. (4) can be rewritten in terms of independent probability distributions $\{\bar{p}, \bar{q}\}$ only, where $\bar{p} = \{p_1, \dots\}$ specifies the probability that any allowed value of $\bar{\alpha}$ is implemented, while $\bar{q} = \{q_1, \dots\}$ specifies the probability that any allowed value of $\bar{\beta}$ is implemented. Here we used the same relabelling as in the pure strategy case above. Then, we can define mixed strategy constrained equilibria as:

Given a particular constraint set \mathcal{A}_x and \mathcal{A}_y , a 2-tuple (\bar{p}^*, \bar{q}^*) is a mixed strategy constrained equilibria if and only if for all players,

$$\begin{aligned} \langle \Pi_x(\bar{p}^*, \bar{q}^*) \rangle &= \max_{\bar{p}}[\langle \Pi_x(\bar{p}, \bar{q}^*) \rangle] \\ \langle \Pi_y(\bar{p}^*, \bar{q}^*) \rangle &= \max_{\bar{q}}[\langle \Pi_y(\bar{p}^*, \bar{q}) \rangle]. \end{aligned} \quad (18)$$

As is usual in optimization theory, every alternate strategy function set $\{\mathcal{A}_x, \mathcal{A}_y\}$ imposes constraints on either the space of possible pure strategy choice variables or the space of possible mixed strategy probability distributions. Geometrically, these constraints take a cross-section onto some subspace wherein all constraints are satisfied, and in which the composite payoff functions exhibit changed continuity properties and altered maxima. The composite payoff functions of reduced dimensionality define pruned extensive form game trees involving only independent variables—variational optimization techniques can only ever be applied to independent variables. Consequently, subgame decompositions, and Nash equilibria can be applied to extensive form game trees only after these have been pruned of dependent variables. As is usual in constrained optimization problems, different constraint sets generate novel trees defining novel equilibria. In the next section we demonstrate how these new equilibria emerge in the IPD analysis. A question which might arise here is how to determine the best equilibrium among these new equilibria. As is well known in game theory, in general, there is no simple way to choose between many alternate Nash equilibria [26, 37, 38, 59]. However, through the example of an IPD in the next section, we will show a way to address this issue using standard Nash techniques.

IV. CONSTRAINED EQUILIBRIA IN THE FINITE ITERATED PRISONER'S DILEMMA

In this section we determine constrained equilibria in the finite IPD and demonstrate that cooperation can

naturally emerge as a consequence of constraints. In this supergame, each player has two possible single stage strategy choices $S = \{C, D\}$ for Cooperate and Defect respectively with stage payoffs $\pi_x(x_n, y_n) \geq 0$ and $\pi_y(x_n, y_n) \geq 0$ determined by the payoff matrix

$$P_x \begin{array}{c|cc} & \begin{array}{c} P_y \\ C \quad D \end{array} \\ \hline \begin{array}{c} C \\ D \end{array} & \begin{array}{cc} (2, 2) & (0, 3) \\ (3, 0) & (1, 1) \end{array} \end{array} \quad (19)$$

This payoff matrix defines single stage payoff functions

$$\begin{aligned} \pi_x(x_n, y_n) &= 2 + x_n - 2y_n \\ \pi_y(x_n, y_n) &= 2 - 2x_n + y_n, \end{aligned} \quad (20)$$

where z_n represents the strategy choice for player P_z such that 0 represents cooperation and 1 represents defection. Total game payoffs of a finite IPD of the length N are then

$$\begin{aligned} \Pi_x(x_1 \dots x_N, y_1 \dots y_N) &= \sum_{n=1}^N (2 + x_n - 2y_n) \\ \Pi_y(x_1 \dots x_N, y_1 \dots y_N) &= \sum_{n=1}^N (2 - 2x_n + y_n). \end{aligned} \quad (21)$$

Following Eq. 7, the expected payoff functions for players P_x and P_y are then

$$\begin{aligned} \langle \Pi_x \rangle &= 2N + \sum_{n=1}^N \sum_{\substack{x_1 \dots x_n \\ y_1 \dots y_n}} P_{1x}(x_1) P_{1y}(y_1) \times \dots \\ &\quad \times P_{nx, H_{n-1}}(x_n) P_{ny, H_{n-1}}(y_n) (x_n - 2y_n), \\ \langle \Pi_y \rangle &= 2N + \sum_{n=1}^N \sum_{\substack{x_1 \dots x_n \\ y_1 \dots y_n}} P_{1x}(x_1) P_{1y}(y_1) \times \dots \\ &\quad \times P_{nx, H_{n-1}}(x_n) P_{ny, H_{n-1}}(y_n) (-2x_n + y_n). \end{aligned} \quad (22)$$

We now derive the unconstrained Nash equilibrium for the IPD after applying the assumption of bounded rationality so all probability distributions are uncorrelated. We first note that the total rate of change of the expected payoff function with respect to the changing probability distributions is

$$\frac{d\langle \Pi_z \rangle}{d[P_{nz, H_{n-1}}(1)]} = \frac{\partial \langle \Pi_z \rangle}{\partial [P_{nz, H_{n-1}}(1)]} - \frac{\partial \langle \Pi_z \rangle}{\partial [P_{nz, H_{n-1}}(0)]} \quad (23)$$

due to the normalization constraint $P_{nz, H_{n-1}}(0) = 1 - P_{nz, H_{n-1}}(1)$. The shorthand notation $H_n = \{H_{n-1}, x_n, y_n\}$ and some algebra allows writing the optimization conditions for player P_x as the set of simultaneous equations

$$\begin{aligned} \frac{d\langle \Pi_x \rangle}{d[P_{1x}(1)]} &= \dots, \\ &\vdots \\ \frac{d\langle \Pi_x \rangle}{d[P_{(N-1)x, H_{N-2}}(1)]} &= 1 + \\ &\sum_{\substack{x_1 \dots x_{N-2} \\ y_1 \dots y_{N-2}}} P_{1x}(x_1) \dots P_{(N-2)y, H_{N-3}}(y_{N-2}) \times \end{aligned}$$

$$\begin{aligned} &\sum_{y_{N-1}} P_{(N-1)y, H_{N-2}}(y_{N-1}) \sum_{x_N y_N} (x_N - 2y_N) \times \\ &[P_{Nx, \{H_{N-2}, 1, y_{N-1}\}}(x_N) P_{Ny, \{H_{N-2}, 1, y_{N-1}\}}(y_N) - \\ &P_{Nx, \{H_{N-2}, 0, y_{N-1}\}}(x_N) P_{Ny, \{H_{N-2}, 0, y_{N-1}\}}(y_N)], \\ &\frac{d\langle \Pi_x \rangle}{d[P_{Nx, H_{N-1}}(1)]} = 1. \end{aligned} \quad (24)$$

The equivalent simultaneous optimization conditions for player P_y are

$$\begin{aligned} \frac{d\langle \Pi_y \rangle}{d[P_{1y}(1)]} &= \dots, \\ &\vdots \\ \frac{d\langle \Pi_y \rangle}{d[P_{(N-1)y, H_{N-2}}(1)]} &= 1 + \\ &\sum_{\substack{x_1 \dots x_{N-2} \\ y_1 \dots y_{N-2}}} P_{1x}(x_1) \dots P_{(N-2)y, H_{N-3}}(y_{N-2}) \times \\ &\sum_{x_{N-1} y_N} P_{(N-1)x, H_{N-2}}(x_{N-1}) \sum_{x_N y_N} (y_N - 2x_N) \times \\ &[P_{Nx, \{H_{N-2}, x_{N-1}, 1\}}(x_N) P_{Ny, \{H_{N-2}, x_{N-1}, 1\}}(y_N) - \\ &P_{Nx, \{H_{N-2}, x_{N-1}, 0\}}(x_N) P_{Ny, \{H_{N-2}, x_{N-1}, 0\}}(y_N)], \\ &\frac{d\langle \Pi_y \rangle}{d[P_{Ny, H_{N-1}}(1)]} = 1. \end{aligned} \quad (25)$$

Subsequently each player, denoted P_z , solves their respective sets of simultaneous equations to maximize their payoff by setting $P_{Nz, H_{N-1}} = 1$ for all history sets H_{N-1} , and by setting $P_{(N-1)z, H_{N-2}} = 1$ for all history sets H_{N-2} , and so on. The final result is that both players defect at every stage giving the optima as $(x_n, y_n) = (1, 1) \equiv (D, D)$ for all n . At this point, payoffs are $(\langle \Pi_x \rangle, \langle \Pi_y \rangle) = (N, N)$.

Now, we generate constrained equilibria using correlated distributions in the most general expected payoff functions of Eq. (7). As a first step, we consider player P_x adopts Markovian-like (MKV) strategy functions dependent only on the results of the previous stage via

$$x_n = X_n(y_{n-1}) = y_{n-1}, \quad (26)$$

for $2 \leq n \leq N$. We assume P_y adopts an empty constraint set so all $P_{ny, H_{n-1}}(y_n)$ distributions are independent. The imposed constraints are equivalent to the correlated probability distributions $P_{nx}(x_n | H_{n-1}) = \delta_{x_n, y_{n-1}}$, so the most general expected payoff functions become

$$\begin{aligned} \langle \Pi_z \rangle &= \sum_{x_1, y_1, \dots, y_N} P_{1x}(x_1) P_{1y}(y_1) P_{2y}(y_2 | H_1) \times \dots \\ &\quad \times P_{Ny}(y_N | H_{N-1}) \Pi_z(x_1, y_1, \dots, y_N) \end{aligned} \quad (27)$$

for $z \in \{x, y\}$, with generated payoffs

$$\begin{aligned} \Pi_x(x_1, y_1, \dots, y_N) &= 2N + x_1 - \sum_{n=1}^{N-1} y_n - 2y_N \\ \Pi_y(x_1, y_1, \dots, y_N) &= 2N - 2x_1 - \sum_{n=1}^{N-1} y_n + y_N. \end{aligned} \quad (28)$$

The expected payoff functions for players P_x and P_y are then

$$\begin{aligned} \langle \Pi_x \rangle &= 2N + \sum_{x_1} P_{1x}(x_1)x_1 + \\ &\quad - \sum_{n=1}^{N-1} \sum_{y_1 \dots y_n} P_{1y}(y_1) \dots P_{ny, H_{n-1}}(y_n)y_n + \\ &\quad - 2 \sum_{y_1 \dots y_N} P_{1y}(y_1) \dots P_{Ny, H_{N-1}}(y_N)y_N, \\ \langle \Pi_y \rangle &= 2N - 2 \sum_{x_1} P_{1x}(x_1)x_1 + \quad (29) \\ &\quad - \sum_{n=1}^{N-1} \sum_{y_1 \dots y_n} P_{1y}(y_1) \dots P_{ny, H_{n-1}}(y_n)y_n + \\ &\quad \sum_{y_1 \dots y_N} P_{1y}(y_1) \dots P_{Ny, H_{N-1}}(y_N)y_N. \end{aligned}$$

The generated constrained equilibria are now calculated by applying the assumption of bounded rationality so all remaining distributions are uncorrelated. Immediately then, player P_x optimizes their expected payoff via satisfying the condition

$$\frac{d\langle \Pi_x \rangle}{d[P_{1x}(1)]} = 1. \quad (30)$$

Consequently, player P_x optimizes their first and final stage payoff by setting $P_{1x}(1) = 1$ and so defects in this first stage. The shorthand notation $H_n = \{H_{n-1}, y_n\}$ for $n \geq 1$ and some algebra allows writing the optimization conditions for player P_y as the set of simultaneous equations

$$\begin{aligned} \frac{d\langle \Pi_y \rangle}{d[P_{1y}(1)]} &= \dots, \\ &\vdots \\ \frac{d\langle \Pi_y \rangle}{d[P_{(N-1)y, H_{N-2}}(1)]} &= -1 + \\ &\quad + \sum_{y_1 \dots y_{N-2}} P_{1y}(y_1) \dots P_{(N-2)y, H_{N-3}}(y_{N-2}) \times \\ &\quad \sum_{y_N} y_N [P_{Ny, \{H_{N-2}, 1\}}(y_N) - P_{Ny, \{H_{N-2}, 0\}}(y_N)], \\ \frac{d\langle \Pi_y \rangle}{d[P_{Ny, H_{N-1}}(1)]} &= 1. \quad (31) \end{aligned}$$

Hence, player P_y optimizes their payoff by setting $P_{Ny, H_{N-1}}(1) = 1$ for every history set H_{N-1} , and by setting $P_{(N-1)y, H_{N-2}}(1) = 0$ for every history set H_{N-2} , and eventually by setting $P_{ny, H_{n-1}}(1) = 0$ for $1 \leq n \leq (N-1)$. These conditions locate the constrained equilibria at the point $(x_1, y_1, \dots, y_N) = (1, 0, \dots, 0, 1)$ generating the play sequence

$$(x_n, y_n) = (D, C)(C, C) \dots (C, C)(C, D) \quad (32)$$

to give expected payoffs $(\langle \Pi_x \rangle, \langle \Pi_y \rangle) = (2N-1, 2N-1)$. Here, player P_x defects in the first stage as their opponent cannot respond without decreasing their payoff, while P_y can defect in the last stage when P_x can no longer respond.

Next we treat another combination of constraints assuming the Markovian strategy algorithms for both players as

$$\begin{aligned} x_n &= y_{n-1} \\ y_n &= x_{n-1}, \quad (33) \end{aligned}$$

for $2 \leq n \leq N$, equivalent to the conditioned probability distributions $P_{nx}(x_n|H_{n-1}) = \delta_{x_n, y_{n-1}}$ and $P_{ny}(y_n|H_{n-1}) = \delta_{y_n, x_{n-1}}$. These constraint sets project the most general expected payoff functions to

$$\langle \Pi_z \rangle = \sum_{x_1, y_1} P_{1x}(x_1)P_{1y}(y_1)\Pi_z(x_1, y_1) \quad (34)$$

for $z \in \{x, y\}$, where for a given play sequence (x_1, y_1) , the payoffs are

$$\begin{aligned} \Pi_x &= \begin{cases} 2N - \frac{N}{2}x_1 - \frac{N}{2}y_1, & N \text{ even} \\ 2N - \frac{N-3}{2}x_1 - \frac{N+3}{2}y_1, & N \text{ odd} \end{cases} \\ \Pi_y &= \begin{cases} 2N - \frac{N}{2}x_1 - \frac{N}{2}y_1, & N \text{ even} \\ 2N - \frac{N+3}{2}x_1 - \frac{N-3}{2}y_1, & N \text{ odd.} \end{cases} \quad (35) \end{aligned}$$

The N stage supergame has now been exactly reduced to a single stage game with variables x_1 and y_1 with payoff matrices, for N even of

$$P_x \begin{array}{c|cc} & \begin{matrix} P_y \\ C \quad D \end{matrix} \\ \hline \begin{matrix} C \\ D \end{matrix} & \begin{matrix} (2N, 2N) & (\frac{3}{2}N, \frac{3}{2}N) \\ (\frac{3}{2}N, \frac{3}{2}N) & (N, N) \end{matrix} \end{array} \quad (36)$$

and for odd N of

$$P_x \begin{array}{c|cc} & \begin{matrix} P_y \\ C \quad D \end{matrix} \\ \hline \begin{matrix} C \\ D \end{matrix} & \begin{matrix} (2N, 2N) & \frac{3}{2}[N-1, N+1] \\ \frac{3}{2}[N+1, N-1] & (N, N) \end{matrix} \end{array} \quad (37)$$

Here, the constraining strategy functions have changed the off-diagonal elements of the effective payoff matrix to modify equilibria. As usual, the generated constrained equilibria are now calculated by applying the assumption of bounded rationality so all remaining distributions are uncorrelated. The expected payoff functions are then

$$\begin{aligned} \langle \Pi_x \rangle &= \begin{cases} 2N - \frac{N}{2}P_{1x}(1) - \frac{N}{2}P_{1y}(1), & N \text{ even} \\ 2N - \frac{N-3}{2}P_{1x}(1) - \frac{N+3}{2}P_{1y}(1), & N \text{ odd} \end{cases} \\ \langle \Pi_y \rangle &= \begin{cases} 2N - \frac{N}{2}P_{1x}(1) - \frac{N}{2}P_{1y}(1), & N \text{ even} \\ 2N - \frac{N+3}{2}P_{1x}(1) - \frac{N-3}{2}P_{1y}(1), & N \text{ odd.} \end{cases} \quad (38) \end{aligned}$$

As usual, the constrained equilibria are located via

$$\begin{aligned} \frac{\partial \langle \Pi_x \rangle}{\partial [P_{1x}(1)]} &= \begin{cases} -\frac{N}{2}, & N \text{ even} \\ -\frac{1}{2}(N-3), & N \text{ odd} \end{cases} \\ \frac{\partial \langle \Pi_y \rangle}{\partial [P_{1y}(1)]} &= \begin{cases} -\frac{N}{2}, & N \text{ even} \\ -\frac{1}{2}(N-3), & N \text{ odd.} \end{cases} \quad (39) \end{aligned}$$

$(\langle \Pi_x \rangle, \langle \Pi_y \rangle)$	$j = 0$	1	2	3	4	\dots	$N - 2$	$N - 1$
$k = 0$	\ddot{N}, \ddot{N}	$\ddot{N}^{-2}, \ddot{N}^{+1}$	=	=	=	\dots	$\ddot{N}^{-2}, \ddot{N}^{+1/-2}$	$\ddot{N}^{-1}, \ddot{N}^{-1}$
1	$\ddot{N}^{+1}, \ddot{N}^{-2}$	$\ddot{N}^{-1}, \ddot{N}^{-1}$	\ddot{N}^{-3}, \ddot{N}	=	=	\dots	$\ddot{N}^{-3}, \ddot{N}^{+0/-3}$	$\ddot{N}^{-2}, \ddot{N}^{-2}$
2	"	\ddot{N}, \ddot{N}^{-3}	$\ddot{N}^{-2}, \ddot{N}^{-2}$	$\ddot{N}^{-4}, \ddot{N}^{-1}$	=	\dots	$\ddot{N}^{-4}, \ddot{N}^{-1/-4}$	$\ddot{N}^{-3}, \ddot{N}^{-3}$
3	"	"	$\ddot{N}^{-1}, \ddot{N}^{-4}$	$\ddot{N}^{-3}, \ddot{N}^{-3}$	$\ddot{N}^{-5}, \ddot{N}^{-2}$	\dots	$\ddot{N}^{-5}, \ddot{N}^{-2/-5}$	$\ddot{N}^{-4}, \ddot{N}^{-4}$
4	"	"	"	$\ddot{N}^{-2}, \ddot{N}^{-5}$	$\ddot{N}^{-4}, \ddot{N}^{-4}$	\dots	$\ddot{N}^{-6}, \ddot{N}^{-3/-6}$	$\ddot{N}^{-5}, \ddot{N}^{-5}$
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots	\dots	\vdots	\vdots
$N - 4$	"	"	"	"	$\ddot{N}^{-3}, \ddot{N}^{-6}$	\dots	$\ddot{N}^{+2}, \ddot{N}^{+5/+2}$	$\ddot{N}^{+3}, \ddot{N}^{+3}$
$N - 3$	$\ddot{N}^{+1/-2}, \ddot{N}^{-2}$	$\ddot{N}^{+0/-3}, \ddot{N}^{-3}$	$\ddot{N}^{-1/-4}, \ddot{N}^{-4}$	$\ddot{N}^{-2/-5}, \ddot{N}^{-5}$	$\ddot{N}^{-3/-6}, \ddot{N}^{-6}$	\dots	$\ddot{N}^{+1}, \ddot{N}^{+4/+1}$	$\ddot{N}^{+2}, \ddot{N}^{+2}$
$N - 2$	"	"	"	"	"	\dots	$\ddot{N}^{+2}, \ddot{N}^{+2}$	$\ddot{N}^{+1}, \ddot{N}^{+1}$
$N - 1$	$\ddot{N}^{-1}, \ddot{N}^{-1}$	$\ddot{N}^{-2}, \ddot{N}^{-2}$	$\ddot{N}^{-3}, \ddot{N}^{-3}$	$\ddot{N}^{-4}, \ddot{N}^{-4}$	$\ddot{N}^{-5}, \ddot{N}^{-5}$	\dots	$\ddot{N}^{+1}, \ddot{N}^{+1}$	\ddot{N}, \ddot{N}

TABLE I: A partial listing of constrained equilibria for the IPD when player P_x implements a Markovian strategy algorithm MKV- k I, while player P_y implements an MKV- j I algorithm. Here, every shown payoff pair is a constrained equilibrium point making selection of a single best payoff maximization strategy difficult. For brevity, we restrict consideration to large $N > 8$ say, and write $\ddot{N}^{\pm k} = (N \pm k)$ and $\ddot{N}^{\pm k} = (2N \pm k)$. Fractional indices ($+k/-j$) indicate alternate equilibria with payoff increments of $+k$ and $-j$ respectively. Ditto signs (" \ddot{N} ") and equal signs (" $=$ ") copy values downwards and to the right respectively.

These conditions select the equilibrium points $P_{1x}(1) = 0$ and $P_{1y}(1) = 0$ or $(x_1, y_1) = (0, 0) \equiv (C, C)$ for either N even or for N odd and greater than 3, while for $N = 1$ the equilibria is $P_{1x}(1) = 1$ and $P_{1y}(1) = 1$ or $(x_1, y_1) = (1, 1) \equiv (D, D)$. When $N = 3$ these conditions are satisfied for any values of (x_1, y_1) requiring examination of actual payoffs motivating the selection $(x_1, y_1) = (0, 0) \equiv (C, C)$. The generated sequences of play are

N	(x_1, y_1)	$(\langle \Pi_x \rangle, \langle \Pi_y \rangle)$
1	(1, 1)	(DD) (1, 1)
$N \geq 2$	(0, 0)	(CC) ... (CC) (2N, 2N)

(40)

The sheer number of possible strategy functions which might be adopted make it necessary to consider more general functional classes. To this end, we consider that each player adopts a mixed Markovian-Independent strategy, denoted MKV- k I, where the MKV strategy is chosen from the first to $(N - k)$ -th stages while k I indicates that IND strategies are adopted for the last k stages. For player P_x then, an MKV- k I strategy sets

$$x_n = \begin{cases} y_{n-1} & 2 \leq n \leq N - k \\ x_1, x_{N-k+1}, \dots, x_N \text{ independent.} \end{cases} \quad (41)$$

Similar strategy functions denoted MKV- j I are implemented by P_y . These constraints are equivalent to the correlated probability distributions $P_{nx}(x_n|H_{n-1}) = \delta_{x_n, y_{n-1}}$ for $2 \leq n \leq N - k$ and $P_{ny}(y_n|H_{n-1}) = \delta_{y_n, x_{n-1}}$ for $2 \leq n \leq N - j$.

The general MKV- k I strategy subsumes a number of other strategy functions of interest. For instance, setting $k = N - 1$ or $k = N$ makes all variables independent (IND), so MKV- $(N - 1)$ I=MKV-NI=IND. More interestingly, this strategies subsumes certain deterministic strategies. To see this, suppose that players consider a deterministic strategy choice D in the last stage, and so implement the strategy MKV-1D. More generally, players may also consider strategies MKV- k D forcing the choice D in the last k stages. However, it is not difficult to see that this class of deterministic strategies is weakly dominated by the class of MKV- k I. For the same k , MKV- k I

guarantees an equal or larger payoff than achievable using MKV- k D against any strategy algorithm of the opponent. In particular, the motivation to defect at the last stage for a larger payoff is taken into account in the strategy class MKV- k I. Exactly similar considerations establish that MKV- k I strategies weakly dominate Tit-For-Tat strategies which specify cooperation in the first stage.

Although the class of strategies MKV- k I is small in comparison to the set of all possible strategies, it contains enough complexity to demonstrate novel equilibria in the IPD. We consider player P_x to implement strategy function MKV- k I, while player P_y implements MKV- j I, so the most general expected payoff functions become

$$\langle \Pi_z \rangle = \sum_{\substack{x_1, x_{N-k+1}, \dots, x_N \\ y_1, y_{N-j+1}, \dots, y_N}} P_{1x}(x_1)P_{1y}(y_1) \times \dots \times P_{Ny, H_{N-1}}(y_N)\Pi_z \quad (42)$$

for $z \in \{x, y\}$, where the payoffs for a given play sequence $(x_1, x_{N-k+1}, \dots, x_N, y_1, y_{N-j+1}, \dots, y_N)$ are

$$\Pi_z = 2N + \sum_{n=1}^N A_{zn}x_n + \sum_{n=1}^N B_{zn}y_n \quad (43)$$

with variables A_{zn} and B_{zn} as specified in Appendix A. The assumption of bounded rationality and that all remaining distributions are uncorrelated now allows calculating the respective constrained equilibria with the optimized payoffs as shown in Table I for all combinations of k and j .

Every listed payoff pair in Table I is an actual constrained equilibrium point optimizing payoffs given imposed constraints. As noted previously, there is no generally accepted method to choose between alternate Nash equilibria. However, strategy algorithms are independently selectable by each player, so we can think that these strategy algorithms and constrained equilibria create a new game defined by Table I. In this game on the constrained equilibrium space, each strategy algorithm becomes a strategy choice, and each equilibrium point becomes a pair of payoffs. In the case where each pair of strategy algorithms defines unique equilibrium payoffs, it is obvious that this table can be considered as a

game matrix. Hence standard Nash techniques can be applied to determine global equilibria among the located constrained equilibria. However, we note that in general we have to take care to deal with multiple equilibria generated by a pair of strategy algorithms. By applying the Nash equilibrium definition to Table I, we obtain global equilibria at (k, j) for either $k = 0$ and $3 \leq j \leq (N - 2)$, or $j = 0$ and $3 \leq k \leq (N - 2)$.

These global equilibria can be considered rational for the IPD in this restricted class of strategies, and there is no established way to select a particular one among these. The more important feature given from this analysis is that cooperation naturally arises from these equilibria. The pathways produced by these equilibria are dominated by cooperation apart from some different choices at the last stage. This cooperative behaviour is caused by the imposition of strategy function constraints.

V. CORRELATED PLAY AND THE LAST STAGE OF THE IPD

In the previous sections, we have emphasized the importance of correlated play in supergame analysis and the assumption of independent mixed or behavioural strategy choice variables required by the Nash equilibrium definition. Although experiments on the IPD (and other games) have shown significantly different behaviours from that predicted by the Nash analysis, there has been little motivation to revise this assumption and extend the Nash definition of equilibrium to a fully correlated analysis. Many alternate approaches have been proposed, and the field has developed in the direction of explaining why people do not behave as rationally as they could. In the IPD this explanatory emphasis resulted largely because of the typical use of the backwards induction (BI) argument. However, the results obtained by our general correlated analysis differ from the predictions of the typical BI argument, implying misuse of the BI optimizing technique in application to the IPD analysis. In this section we clarify the confusion introduced by the typical BI argument in the IPD analysis.

As noted, BI is based on dynamic programming techniques, and like any variational optimization technique, it is applied only to uncorrelated independent variables. That is, any correlations or constraints must be resolved before optimization commences. Necessarily then, BI must derive the same solution as the Nash analysis under the same assumed constraint set. As typically used, the BI argument in the IPD is commonly used to justify the assumption of independent variables underlying the Nash equilibrium solution. As is well known, the rationale commences with the last stage of a finite supergame. In the typical BI argument, the last stage has a special role, and the rest of the argument follows in exactly the way by iteration. In particular, the usual claim is that BI requires that the last stage of an IPD is to be considered an independent stage. It is argued that, although there are many reasons for players to cooperate, such as the presence of any of long range considerations [20], reputation effects [60], off-equilibrium pathway signals [61], or punishments and rewards [59], at the last stage none of these are present. Hence, it is claimed, the last stage is an independent stage, i.e. a single PD. Once we have

accepted the last stage as a single PD, then under CKR, BI automatically derives the unique Nash path. In this sense, BI is a complement of the Nash analysis to establish the Nash unique solution of the IPD. This argument would succeed with the addition of a proof that these, and only these effects permitted correlated play. Unfortunately, this is not the case.

The significant difference introduced by allowing rational players to adopt correlated play whenever that turns out to be payoff maximizing, is that they will consider the IPD as a whole, which they are able to do as unbounded rational agents. The correlated analysis in the previous sections has shown that the first step of the BI argument about the last stage is not necessarily optimal. In addition, CKR by itself specifies nothing about whether the last stage of an IPD is or is not equivalent to a single stage game. However, under CKR, players of unbounded rationality must take account of the payoffs available under correlated play. In general then, the typical usage of a BI argument to justify a Nash pathway as being optimal is not correct under CKR and correlated strategies are required for an optimal solution. For the typical BI argument to justify the Nash pathway as uniquely optimal, it is necessary that the game analysis, and hence CKR, is restricted to a particular kind of correlation, namely the assumption of independent variables. Even though there are apparently no overt motivations for players to cooperate in the last stage, it is not optimal and hence not rational for players to even consider “what should we do if we are at the last stage?”.

VI. CONCLUSION

This paper defines novel constrained equilibria in the middle ground between current definitions which require that supergame strategy choices be either all independent or all fully specified by strategy functions. We employ standard conditioned history expansions of the joint correlated probability distributions describing expected payoff functions which specify only some (or no) strategy choice variables (a dependent set) in terms of other variables (an independent set). We then apply standard optimization procedures such as Nash equilibria procedures or backwards induction to the composite payoff functions defined over the remaining independent variables to locate novel constrained equilibria. The methods developed in this paper ensure that there is no conflict between game theoretic optimization techniques and more general variational optimization procedures. We derive novel constrained equilibria in the finite iterated prisoner’s dilemma showing in particular, that backwards induction establishes that it can be payoff maximizing to cooperate in the finite IPD including in the last stage of this game. These results contrast with existing claims that payoff maximization requires defection in this last stage, but these results all depend on the *a priori* assumption that choice variables are uncorrelated. We conclude by discussing the validity of typical arguments proving that ALL DEFECT is the privileged optimal pathway in the IPD.

This paper derived novel constrained equilibria using general Markovian-like strategy functions, and a broader analysis of the many possible unknown contingent strate-

gies requires a functional representation for algorithms. A mathematical functional analysis would allow us to consider multiple algorithms using a functional metric to measure the ability of different algorithms to determine supergame outcomes. However, the utility of such a functional analysis remains an open question and will be dealt with in later work.

Game theory was originally proposed to provide a simple analytic environment for economic and social interactions and the analysis of this paper has broader application to this wider sphere. For instance, constrained equilibria eliminates the first-mover advantage in iterated bargaining games and explains experimental observations of more equitable play. In such applications however, the lack of a systematic way to select a particular equilib-

rium among others becomes a more serious and important problem. This issue and the broader application to economics, social games and evolutionary games will be addressed in later work.

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APPENDIX A: CONSTRAINED EQUILIBRIA IN THE IPD

Suppose player P_x adopts an MKV- k I strategy and player P_y adopts an MKV- j I strategy function leaving independent variables $(x_1, x_{N-k+1}, \dots, x_N)$ and $(y_1, y_{N-j+1}, \dots, y_N)$, where we also assume $N \geq 3$.

For $1 \leq k \leq (N-1)$ and $j = 0$, the independent variables are $(x_1, x_{N-k+1}, \dots, x_N)$ and y_1 , and payoffs are

$$\begin{aligned} \Pi_x &= \begin{cases} 2N + \frac{k-N}{2}x_1 + \frac{k-4-N}{2}y_1 - \sum_{n=N-k+1}^{N-1} x_n + x_N, & (N-k) \text{ even} \\ 2N + \frac{k-1-N}{2}x_1 + \frac{k-3-N}{2}y_1 - \sum_{n=N-k+1}^{N-1} x_n + x_N, & (N-k) \text{ odd.} \end{cases} \\ \Pi_y &= \begin{cases} 2N + \frac{k-N}{2}x_1 + \frac{2+k-N}{2}y_1 - \sum_{n=N-k+1}^{N-1} x_n - 2x_N, & (N-k) \text{ even} \\ 2N + \frac{k-1-N}{2}x_1 + \frac{3+k-N}{2}y_1 - \sum_{n=N-k+1}^{N-1} x_n - 2x_N, & (N-k) \text{ odd.} \end{cases} \end{aligned} \quad (\text{A1})$$

For $1 \leq k \leq (N-1)$ and $j = (N-1)$, the independent variables are $(x_1, x_{N-k+1}, \dots, x_N)$ and (y_1, \dots, y_N) , and payoffs are

$$\begin{aligned} \Pi_x &= 2N + x_1 + \sum_{n=N-k+1}^N x_n - \sum_{n=1}^{N-k-1} y_n - 2 \sum_{n=N-k}^N y_n, \\ \Pi_y &= 2N - 2x_1 - 2 \sum_{n=N-k+1}^N x_n - \sum_{n=1}^{N-k-1} y_n + \sum_{n=N-k}^N y_n. \end{aligned} \quad (\text{A2})$$

For $1 \leq k = j \leq (N-1)$, the independent variables are $(x_1, x_{N-k+1}, \dots, x_N)$ and $(y_1, y_{N-k+1}, \dots, y_N)$, and payoffs are

$$\begin{aligned} \Pi_x &= \begin{cases} 2N + \frac{k-N}{2}x_1 + \frac{k-N}{2}y_1 + \sum_{n=N-k+1}^N x_n - 2 \sum_{n=N-k+1}^N y_n, & (N-k) \text{ even} \\ 2N + \frac{3+k-N}{2}x_1 + \frac{k-3-N}{2}y_1 + \sum_{n=N-k+1}^N x_n - 2 \sum_{n=N-k+1}^N y_n, & (N-k) \text{ odd} \end{cases} \\ \Pi_y &= \begin{cases} 2N + \frac{k-N}{2}x_1 + \frac{k-N}{2}y_1 - 2 \sum_{n=N-k+1}^N x_n + \sum_{n=N-k+1}^N y_n, & (N-k) \text{ even} \\ 2N + \frac{k-3-N}{2}x_1 + \frac{3+k-N}{2}y_1 - 2 \sum_{n=N-k+1}^N x_n + \sum_{n=N-k+1}^N y_n, & (N-k) \text{ odd.} \end{cases} \end{aligned} \quad (\text{A3})$$

For $1 \leq k \leq (N-1)$ and $1 \leq j \leq (N-1)$ with $k > j$, the independent variables are $(x_1, x_{N-k+1}, \dots, x_N)$ and $(y_1, y_{N-j+1}, \dots, y_N)$, and payoffs are

$$\begin{aligned} \Pi_x &= \begin{cases} 2N + \frac{k-N}{2}x_1 + \frac{k-4-N}{2}y_1 - \sum_{n=N-k+1}^{N-j-1} x_n + \sum_{n=N-j}^N x_n - 2 \sum_{n=N-j+1}^N y_n, & (N-k) \text{ even} \\ 2N + \frac{k-1-N}{2}x_1 + \frac{k-3-N}{2}y_1 - \sum_{n=N-k+1}^{N-j-1} x_n + \sum_{n=N-j}^N x_n - 2 \sum_{n=N-j+1}^N y_n, & (N-k) \text{ odd} \end{cases} \\ \Pi_y &= \begin{cases} 2N + \frac{k-N}{2}x_1 + \frac{2+k-N}{2}y_1 - \sum_{n=N-k+1}^{N-j-1} x_n - 2 \sum_{n=N-j}^N x_n + \sum_{n=N-j+1}^N y_n, & (N-k) \text{ even} \\ 2N + \frac{k-1-N}{2}x_1 + \frac{3+k-N}{2}y_1 - \sum_{n=N-k+1}^{N-j-1} x_n - 2 \sum_{n=N-j}^N x_n + \sum_{n=N-j+1}^N y_n, & (N-k) \text{ odd.} \end{cases} \end{aligned} \quad (\text{A4})$$

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- [36] Contingent strategy functions have specified every possible strategy choice. For instance, Ref. [37] specifies a contingent strategy as
- “a function that assigns an action in [the action set] to every nonterminal history” and “a strategy specifies the action chosen by a player for every history after which it is his turn to move, even for histories that, if the strategy is followed, are never reached.” (emphasis in original).
- When defining strategies in terms of automata, it was also noted that the automata implements a function
- “that assigns an action to every state” attainable during the game [37].
- Ref. [38] notes that
- “a pure strategy for player i is simply a contingent plan of how to play in each stage k for [every] possible history h^k ” so “stage-0 actions are $a^0 = s^0(h^0)$, the stage-1 actions are $a^1 = s^1(a^0)$, stage-2 actions are $a^2 = s^2(a^0, a^1)$, and so on.”
- Similarly, Ref. [30] states that
- “A strategy is a function that tells the player how to select one of his feasible actions whenever he must make a move, for all possible events that may have occurred so far.”
- Ref. [35] noted “As usual, a strategy for [player] i in [game] Γ is just a mapping from [all of] i 's vertices in Γ to actions.”, while finally, to define grim trigger strategies, Ref. [34] noted that “player i chooses s_i^* in period 0” and continues to do so as long as all players cooperate, while any deviation causes player i to switch to other prespecified non-cooperative choices.

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- $$\text{cor}(z, z') = \frac{\text{cov}(z, z')}{\sigma_z \sigma_{z'}},$$
- defined in terms of the covariance
- $$\text{cov}(z, z') = \langle zz' \rangle - \langle z \rangle \langle z' \rangle,$$
- the variance $\sigma_z^2 = \text{cov}(z, z)$, and mean $\langle z \rangle$ [63].
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