Investigation of Market Mechanisms for Distribution Level Energy Management

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Except where otherwise indicated, this thesis is my own original work.

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Abstract

Electricity systems are facing the pressure to change in response to the effects of new technology, particularly the proliferation of renewable technologies (such as solar PV systems and wind generation) leading to the retirement of traditional generation technologies that provide stabilising inertia. These changes create an imperative to consider potential future market structures to facilitate the participation of distributed energy resources (DERs; such as EVs and batteries) in grid operation. However, this gives rise to general questions surrounding the ethics of market structures and how they could be fairly applied in future electricity systems. Particularly the most basic question "how *should* electricity be valued and traded" is fundamentally a moral question without any easy answer. We give a survey of philosophical attitudes around such a question, before presenting a series of ways that these intuitions have been cast into mathematics, including: the Vickrey-Clarke-Groves mechanism, Locational Marginal Pricing, the Shapley Value, and Nash bargaining solution concepts.

We compared these different methods, and attempted a new synthesis that brought together the best features of each of them; called the 'Generalised Neyman and Kohlberg Value' or the GNK-value for short. The GNK value was developed as a novel bargaining solution concept for many player non-cooperative transferable utility generalised games, and thus it was intrinsically flexible in its application to various aspects of powersystems. We demonstrated the features of the GNK-value against the other mathematical solutions in the context of trading the immediate consumption/generation of power on small sized networks under linear-DC approximation, before extending the computation to larger networks. The GNK value proved to be difficult to compute for large networks but was shown to be approximable for larger networks with a series of sampling techniques and a proxy method. The GNK value was ethically compared to other mechanisms with the unfortunate discovery that it allowed for participants to be left worse-off for participating, violating the ethical notion of 'euvoluntary exchange' and 'individual rationality'; but was offered as an interesting innovation in the space of transferable utility generalised games notwithstanding.

For sampling the GNK value, there was a range of new and different techniques developed for stratified random sampling which iteratively minimise newly derived concentration inequalities on the error of the sampling. These techniques were developed to assist in the computation of the GNK value to larger networks, and they were evaluated in the context of sampling synthetic data, and in computation of the Shapley Value of cooperative game theory. These new sampling techniques were demonstrated to be comparable to the more orthodox Neyman sampling method despite not having access to stratum variances.

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Nomenclature

Anacronyms

- AC – Alternating Current
- AEMO – Australian Energy Market Operator
- ARENA – Australian Renewable Energy Agency
- DC – Direct Current
- DER – distributed energy resource
- DR – demand response
- EBB – Empirical Bernstein Bound
- EEBB – Unioned Engineered EBB sampling method
- EV – electric vehicle
- FCAS – Frequency Control Ancillary Services
- FTR – Financial Transmission Rights
- GHG – greenhouse gasses
- GNK – Generalized Neyman and Kohlberg Value
- IIA – Independence of irrelevant alternatives axiom
- ISO – Independant System Operator
- KKT – Karush–Kuhn–Tucker conditions
- LBP – linear bilevel program
- LMP – Locational Marginal Pricing
- M-GNK – modified GNK value
- NEL – Australia's National electricity law
- NEM – Australia's National Electricity Market
- NEO – Australia's National Electricity Objective

- NTU – non-transferable utility game
- OPF – Optimal Power Flow problem
- P2P – peer-to-peer electricity trading
- PEEF – pareto-efficient envy-free allocation
- PV – solar photovoltaic system
- RHS – right hand side
- SEBB – Stratified Empirical Bernstein Bound
- SEBM – Stratified Empirical Bernstein Method
- SEBM* – Stratified empirical Bernstein method with variance assistance
- SEBM-W – Stratified empirical Bernstein method with replacement
- SECB – Stratified Empirical Chebyshev Bound
- TU – transferable utility game
- UC – Unit Commitment problem
- VCG – Vickrey-Clarke-Groves mechanism
- VPP – virtual power plant

Symbols

Chapter 2

- I indicator function
- $u_i(\cdot)$ utility of player i
- π_i resource bundle of player i

Chapter 3

- X set of physical outcomes
- n number of agents
- v_i valuation over physical outcomes for player i
- x^* socially optimal physical outcome
- $d_i(v)$ VCG payment for player i, given valuation set v

- u_i utility of player i
- C_{-i} a pivot rule in groves mechanism
- $D(x)$ demand curve in marginal pricing game
- $S(x)$ supply curve in marginal pricing game
- $U_d(x)$ buyers total utility in marginal pricing game
- $U_s(x)$ sellers total utility in marginal pricing game
- $L(a, b, \lambda)$ lagrangian function, for amount bought a and amount sold b, with lagrange multiplier λ
- N is set of players 1 to n
- $v : S \subseteq N \to \mathbb{R}$ is a characteristic function
- $C(v)$ the Core of a cooperative game with characteristic function v
- $C_\epsilon(v)$ the strong epsilon Core of a cooperative game with characteristic function v
- $\hat{v}_{i,k}$ average marginal contribution of player i across coalitions of size k in a cooperative game with characteristic function v
- $\varphi_i(\langle N, v\rangle)$ the Shapley Value for player i, for a coaltional game with player set N and characteristic function v
- $\pi(N)$ the permutations of join orderings of the player set N
- $Pre^i(O)$ as the set of predecessors of player i's addition in that ordering $O \in \pi(N)$
- F is a set of potential outcomes
- $P = \{p_1, p_2, \ldots\}$ is set of players
- $u_{p\in P}(f)$ for $f \in F$ is utility of outcome f for player p
- d is the disagreement outcome
- $\text{nash}(F, d)$ is the nash bargaining solution
- S_i strategy set for player i
- $p_1(s_1, s_2)$ and $p_2(s_1, s_2)$ for $s_1 \in S_1$ and $s_2 \in S_2$ is payoffs for players 1 and 2 for playing strategies s_1 adn s_2
- B set of cooperative strategies
- d_i demand of player i
- t_i threat of player i

Chapter 4

- N is a finite set of n players
- $v : 2^N \to \mathbb{R}$ is characteristic function
- $\mathbb{D}$ the set of all games of threats
- $\varphi_i(\langle N, v\rangle)$ the GNK value for player i of player set N for characteristic function v
- $A \subseteq \prod_{i \in N} A^i$ is a set of all possible joint strategies, where A^i denotes the set of strategies available to player $i \in N$
- $u_i(a)$ is player i's payoff/utility when joint strategy $a \in A$ is executed
- $v_o(S)$ Neymann & Kohlberg's original value function
- $v_m(S)$ von Neumann and Morgenstern's historic value function
- B set of busses in a network
- p_i power consumption/generation at bus i
- θ_i phase angle at bus i
- $C \subseteq B \times B$ set of lines in network
- $b_{i,j}$ susceptance of the line between busses i and j
- $p_{i,j}$ power flow from bus i to j
- h_j and g_k (for indices j, k) are shorthand for equality and inequality constraints in DC OPF
- $u_i(p_i)$ utility for players at bus i for power consumption at bus i, p_i
- $\mathcal{KKT}[\cdot]$ set of KKT points to the optimisation problem
- λ_k is kth lagrange multiplier
- Z_k activation binary variable for kth complementary slackness constraint
- $\mathbb{KKT}(\cdot)$ set of KKT points for optimisation problem under binary relaxation of complementary slackness constraint
- d_i VCG payment to player i
- $v_{shap}(S)$ characteristic function for Shapley Value formulation of network

Chapter 6

- N_i the size of strata i
- n_i/m_i the number of samples taken from strata i
- σ_i^2 the variance of data in strata i
- μ the mean of the population
- $\hat{\mu}$ the estimate of the population mean using stratified sampling
- a the data lower bound
- b the data upper bound
- D the data bound width $= b - a$
- $\mathbb{E}[\cdot]$ the expecation operator
- $\hat{\sigma}^2$ the sample variance estimator
- $\hat{\sigma}_0^2$ the average of sample squares
- X a random variable
- $X_1, \ldots, X_n$ random samples of X
- $Y_1, \ldots, Y_n$ random samples of X drawn without replacement
- D_i data bound width of strata i
- $\hat{\sigma}_i^2$ the sample variance of strata i
- $X_{i,j}$ the jth random sample taken from strata i
- H_1^n the RHS of Bennett's inequality, Theorem 9
- H_2^n the RHS of our sample squares bound, Theorem 7
- H_3^n the RHS of a variance bound 10
- h placeholder function in Theorem 11
- f placeholder functions in Theorems 11 and 3
- z placeholder function in Theorem 11
- κ placeholder real variable
- s placeholder real variable
- t placeholder real variable

- x placeholder real variable
- y placeholder real variable
- q placeholder real variable
- α placeholder parameter/variable
- β placeholder parameter/variable
- γ placeholder parameter/variable
- $x_1, x_2 \ldots$ population of finite data points
- Ω_m^n parameters from Theorem 10
- Ψ_m^n parameters from Theorem 10
- $\bar{\Omega}_m^n$ parameters from Theorem 11
- $\bar{\Psi}_m^n$ parameters from Theorem 11
- χ_{i,m_i} the sample mean of strata i, after taking m_i samples
- $\hat{\sigma}_i^2$ the biased sample variance estimator of statum i
- $\hat{\hat{\sigma}}_i^2$ the unbiased sample variance estimator of statum i
- τ_i the weight of data in stratum i
- θ_i temporary variable for stratum i
- Γ the gamma function
- $\phi(x)_{\{\alpha,\beta\}}$ the probabiliyt density function for Beta distributed data
- $v(S)$ characetistic function for coalition S
- w_i the weight of player i in coatlitional game
- e^{Ma} the error in Maleki's method from section 6.6
- e^{sim} the error in Castro's simple sampling method from section 6.6
- e^{Ca} the error in Castro's Neyman sampling method from section 6.6
- e^{SEBM} the error in our SEBM sampling method in section 6.6
- $\mu_{i,j}$ is the jth component of the mean vector from the ith stratum
- $D_{i,j}$ is the data bound width of the jth vector component of the ith stratum
- $\sigma_{i,j}^2$ the variance of the jth vector component of the ith stratum

- $X_{i,k,j}$ is the jth component, of the kth vector from stratum i
- $\chi_{i,m_i,j}$ being the jth component of the average of m_i sampled vectors from the ith stratum
- $\hat{\hat{\sigma}}^2_{i,j} = \frac{i}{m_i-1}\sum_{k=1}^{m_i}(X_{i,k,j} - \chi_{i,m_i,j})^2$ be the unbiased sample variance of the first m_i of these random variables in the jth component of the ith stratum.
- α_j placeholder parameter/variable with index j
- β_j placeholder parameter/variable with index j
- γ_j placeholder parameter/variable with index j

Chapter 1

Introduction

The Australian electricity grid is facing structural changes in response to the pressures of new technology. And the way in which the grid should change to meet these new pressures is cause for reflection on the morally ambiguous question at the heart of electrical transactions on the grid - how *should* electricity be valued and traded?

Or, to ask our research question with more granularity: when the possible powerflows on an electricity network are valued and influenced by participants differently, what is a reasonable electrical outcome for the network and what monetary transactions *should* occur between the participants?

Existing electrical power systems in many countries implicitly embody a historic answer to this essential question, however electrical power systems have a history of evolution over time, particularly with the introduction of new technologies and new demands, and this trend continues today as new technology is driving a need for additional changes. This technological drive for additional changes is felt by various electricity systems across the world, however here we focus on the Australian case as an instance.

1.1 The changing nature of supply, and the introduction of demand elasticity

One of most notable technological changes occurring in electricity networks around the world is the development and continued proliferation of renewable energy technologies. For instance, between the fiscal years 2008/2009 - 2018/2019 the Australian Government [2018] reported that the volume of renewable electricity generated on Australia's National Electricity Market (NEM) increased from 18,645 GWh to 44,292 GWh, an increase of approximately 10% per year, increasing the proportion of renewable energy in the network from 7.5% to 17% over the same period. This increase was primarily achieved by the deployment of wind and solar generation, with 90% of solar generation currently being created by small-scale solar photovoltaic (PV) systems, with Australian Energy Market Operator [2018a] projecting that solar PV generation will triple by the year 2030.

In contrast, there is an increasing number number of coal fired power stations being retired from the grid, with Burke et al. [2019] reporting that almost a third of

Australia's coal-fired power stations closed between 2012 and 2017, and Australian Energy Market Operator [2018a] reporting an extra 12 coal fired power plants are expected to be retired over the next 30 years.

The Australian Energy Market Operator (AEMO) operates multiple markets, but particularly the day-ahead and spot-markets operate on marginal-pricing principles where the most expensive generator that is dispatched to meet demand sets the price which is paid for all dispatched electricity. In this context the witnessed changes in supply (specifically the retirement of coal fired power and its replacement by variable renewable electricity generation) have created a situation whereby it is increasingly more likely that more expensive generators are setting the marginal price. This dynamic is identified as being a part of the reason that the average price of electricity for consumers between 2008 and 2018 increased by 35% [Australian Competition and Consumer Commission, 2018].

This is an example of a technological change creating an emerging problem for existing electricity networks. The problem is made clear specifically as the stability and efficiency of the grid in providing affordable electricity for customer needs are core components of Australia's National Electricity Objective (NEO)[1].

One option to avert this problem is the prospect of a 'Demand Response' programs, whereby consumers (large and potentially small) are contracted and paid to reduce their consumption in times of peak demand to avoid dispatch of the more expensive generators which would subsequently set the marginal price, thus making electricity less expensive for everybody. Demand response programs are one example of participatory scheme designed to interact with consumers to bring greater regularity to electricity grid, and the offering and accepting of such contracts naturally constitutes a new and prospective market structure. In line with the potential for such a participatory system, there are presently (at time of writing) 12 different Australian Renewable Energy Agency (ARENA) funded Demand response pilot programs across the country (totalling over 100 million dollars of grant money). Additionally the Australian Energy Market Commission [2020] is actively drafting rule changes to formally recognise organisations that provide Demand Response services to the grid, as being electricity market participants directly equivalent to wholesale generators.

The effect of these demand-response programs is to attempt to bring the market price down by creating mechanisms where the demand of electricity effectively becomes more elastic, and one of the more direct way of doing this is to produce a market structure to implement demand-responsive consumption against generation, or a 'two sided market'. The idea of a two-sided market is something that is something that recognised by Australian Energy Market Commission [2020] as an enduring solution for the Australian electricity grid, and is currently being investigated by the COAG energy council [2020]. This is one example of a potential future market

[1] the NEO is part of Australia's National electricity law (NEL) "to promote efficient investment in, and efficient operation and use of, electricity services for the long term interests of consumers of electricity with respect to: price, quality, safety and reliability and security of supply of electricity; and the reliability, safety and security of the national electricity system."

system which may become necessary in response to present technology changes; but it is not the only one.

With the consideration of demand response programs, the question is how the time-limited curtailment of consumption of electricity be traded and valued?
And this reflects the broader question: "how should electricity be valued and traded?"

1.2 Increasingly variable supply, and the potential of battery storage

The increasing number of solar PV systems connected to the Australian grid is changing the characteristic demand profile on the network and its variability; and this has the potential to create issues surrounding grid frequency and stability.

Solar PV systems are often behind-the-meter and have the effect that they change the amount of electricity that consumers require throughout the day from the grid. This effect is particularly manifest in the middle of the day where the abundance of solar energy offsets household electricity requirements and create the ever increasingly severe decrease in grid demand (the infamous 'duck-curve') which is identified to be one source of potential future difficulty. Not only does solar PV change the average demand profile on the network but it also recognised as a source of variability; because solar output is linked to weather there is the ready potential for large swings of localised solar power output, which is recognised by Australian Energy Market Operator [2018a] as potentially creating stability issues related to frequency and voltage control. These demand side changes are compounded by supply side changes such as the retirement of traditional generators which provide stabilising inertia, and continued uptake of industrial wind and solar generation capacity.

One of the primary ways in which sudden changes in supply/demand is manifest on the grid is by frequency drift. In order to keep synchrony, the frequency of the grid needs to be closely monitored and kept on a single frequency and this is an essential stability requirement for the operation of the grid. When there is an increase in supply or a decrease in demand, there is an excess of power on the network which causes a decrease on the electromagnetic drag on traditional generation rotors, causing them to speed up, leading to a increase in their frequency of rotation and frequency of the power they generate. Conversely a decrease in supply, or increase in demand, will cause a decrease in frequency. With the rate at which these frequency increase/decrease occurs being related the inertia of generators.

However the decrease in traditional generation technologies which carry generation inertia is expected to cause the system frequency to be more sensitive to supply/demand variability, at the same time that variability is set to increase due to the increase in renewable generation technologies. There are multiple prospective ways of ameliorating this emerging problem (as discussed by Hartmann et al. [2019]) such as to attempt to build artificial inertia into renewable generators, and another is to requisition generation capacity specifically to maintain system frequency.

Presently there exist a range of electricity markets within the Australian system, including a day-ahead market, a spot-market and several capacity markets specifically for the stabilisation of grid frequency. Some of these ancillary service markets are the Frequency Control Ancillary Services (FCAS) markets, and there exist six of them, particularly for bidding for the contracts to deposit and/or withdraw power from the electricity system where needed, at an upper, middle and lower timeframe for the response (6 second, 60 seconds, 5 minute respectively). In light of the technological changes that are being realised it is anticipated that these frequency response markets will become increasingly important to maintain grid stability [Riesz et al., 2015].

However, a limitation of some traditional generating technologies that operate with large synchronous rotors, is that they are unable to respond quickly to assist in the maintaining of system frequency, and therefore unable to support grid frequency or bid into FCAS markets due to their ramp-rate limitations and costs. [Gonzalez-Salazar et al., 2018] And while there does exist some technology for rapid response gas generators (as discussed by Gonzalez-Salazar et al. [2018]) the more promising renewable technology for this purpose is battery technologies, which have characteristically fast response times. While there does presently exist some large institutionally owned grid connected batteries, a large number of batteries currently connected to the grid are residential small scale batteries often connected to solar PV systems. Additionally it is the expected by Australian Energy Market Operator [2019] that there will be an increase in the adoption of electric vehicles (EVs) with grid connected batteries, with predictions ranging upto 4.5 million EVs on Australian roads by 2040. In this way there is an expected potential for batteries and electric vehicles to be a source of future grid stability.

However there does not currently exist any unified national infrastructure to facilitate these distributed energy resources (DERs) such as EVs and small batteries participating in Australian grid stability. As presently, network participants are payed for the power they consume/generate largely behind their own meter, inducing them to utilise their DERs to optimise their own energy consumption. One current avenue being explored to create such infrastructure is the creation of virtual power plants (VPPs) as large scale aggregators of DER power capabilities, and these projects are currently being developed and are the subject of experimentation [Australian Energy Market Operator, 2018b]. In this way, VPPs are another example of market structure that potentially could emerge in response to current technological trends.

With the consideration of the various ways of trading, valuing and integrating storage in providing diachronic arbitrage of electrical energy to offset frequency deviations, the question is how the storage and time-sensitive rapid injection/consumption of electricity be traded and valued? Because an answer to this should be a consequence of an answer to the broader and more general question: "how should electricity be valued and traded?"

1.3 DERs and the potential for a prosumer era

Another change that is happening, is that increasingly not only are consumers generating their own electricity via solar panels, but they are also expected to be increasingly storing that energy as well; leading to an increasing level of consumer energy independence and the potential attractiveness of going 'off-grid'. However, there may be future role for electricity consumers not only to participate in network support and have access to market structures; but also ideas that might induce consumers to create more social benefits, such as directly sharing their electricity with each other. Particularly, there is an idea that the grid might be able to support consumers selling their excess power and storage capacity to each other, as a peer-to-peer electricity trading (P2P) system.

There are many different visions of what the structure the future electricity system might have, and what features it might have to support trading between producer-consumers, or so-called 'prosumers', such as considered out by Parag and Sovacool [2016]. These future visions describe ideas about how prosumers might trade directly or indirectly between themself and the wider grid; such as perhaps between P2P trading and/or aggregation into many larger virtual power plants (VPPs) or via localised community storage Morstyn et al. [2018].

However the vision of incorporating prosumers into the national electricity market poses a range of gains and challenges, particularly with regards to the voltage and frequency management on distribution networks. Bell and Gill [2018] enumerates some of the challenges, such as: providing grid stability by securing timely reactive and real power supply to stabilise voltages and frequency, grid robustness such as blackout protection and islanding, improving system efficiency by minimising long-distance transmission costs, and facilitating the advent of a green electricity network, by fairly and equitably managing the interaction between prosumer's devices while preserving their privacy, in a scalable way while minimising the complexity of the management of such devices.

With the consideration of the various ways of facilitating the fair trading of energy between heterogeneous devices on distribution networks between consumers, the question is how to integrate these various factors in a flexible and equitable way.
And this reflects the broader question: "how should electricity be valued and traded?"

1.4 A summary of the future of the Australian grid

The way that electricity is being produced and consumed is expected to change in the future, from a system which supports the supply of energy from a few big generation companies to many small consumers, to being a system in which prosumers potentially exchange energy with each other. And there is an increasing interest in the design of new market systems that are appropriate for the future electricity grid.

The technological changes witnessed are seen as potentially leading to future problems associated with frequency and grid stability, in which batteries and other distributed energy resources (DERs) are seen as being important; and new market structures are being considered to provide a platform for them to participate in grid operations.

In this context, there are many potentially important engineering considerations in the operation of powergrids which may bear importance for the exchange of energy between such prosumers - such as voltage rises and line limits, real and reactive power compensation, phase connections, network topologies etc, and it is hoped that a properly designed system might be extensible to be able to accommodate these technical considerations where applicable.

Potential future markets are subject to many requirements, outside of simply delivering a reliable and cheap electricity service to consumers, and sometimes they are even directly quoted as subject to ethical design considerations, such as implementing a “Level playing field” where:

"all competitors, irrespective of their size or financial strength, get equal opportunity to compete. It is not enough if all players play by the same rules. The rules must accommodate the needs of all, whether small or large, so the market is free of impediments to smaller players." Australian Energy Market Operator [2018a]

Ethical criteria such as this, as well as wider political and social implications bear on this discussion. Thus our investigation is to explore and evaluate the research question of what kinds of market structures should be implemented in the new world.
By these considerations we can attempt a new answer to the broader and more general question: “how should electricity be valued and traded?”

1.5 Research and problem approach

The fundamental research question is ‘how *should* electricity be valued and traded?’, which is general and multifaceted question without an easy or established answer (from previous sections 1.1-1.4)

The research question is easily identified as having a moral and ethical quality, and thus in Chapter 2 we survey some of the relevant philosophy associated with the ethics of *Distributive Justice*. Distributive Justice is a branch of moral philosophy associated with the distribution of goods and services in society, about which electricity and electrical services are naturally considered as an example. In this context the philosophy considers different ideas that people have about distribution in relation to more general moral principles, particularly such as various descriptions of ‘Equality’, ‘Deservedness’, ‘Reward’, ‘Efficiency’, etc. It is unfortunately seen that these broad and blurry ethical ideals conflict between themselves and do not logically imply specific market structures or analytic criteria.

However there do exist various mathematical solutions and structures which have been developed as mathematical formulations of these different ethical perspectives, particularly we review a range of different structures and show how they attempt to describe different broader ethical ideas in Chapter 3. These existing solutions form a part of the background of our research, and also provide inspiration and contrast for further developments. For instance, we review the details about the Vickrey-Clarke-Groves (VCG) mechanism, showing that it embodies an idea about compensation for contribution, and identify how it has been proposed as a mechanism for dictating payments between participants on electricity networks. Other mechanisms which we consider include Locational Marginal Pricing (LMP), cooperative game theory solutions such as the Shapley Value, and descriptions of idealised bargaining such as Nash bargaining solution concepts. These mechanisms were investigated specifically because of their abstract and general applicability, and hence they could (in theory) account all the practical factors and possible confluences of electrical system details to ascribe value to disparate electrical devices on a future smart-grid.

Each of these mechanisms embody specific ideas about ethics, and they are identified as having features and shortcomings. Because of this we attempted to take the best features of these mechanisms and synthesise a genuinely novel solution for the pricing of electrical resources on electricity networks. We developed a novel solution concept which we called the *Generalized Neyman and Kohlberg Value* or the *GNK value* in Chapter 4.

We identified that Nash bargaining was a particularly interesting mechanism which was able to provide a unique and direct answer to the question of how electricity should be traded between two participants that could directly consider all possible ways that the electrical participants could interact and influence each other. Our new solution, the GNK value, was designed as a generalisation of Nash bargaining to larger numbers of players (more than two), additionally it was made to be even more extensible as it was designed to work in the space of generalised games and so able to account for arbitrary constraints on mutual player interactions. The GNK value embodies the cooperative game theory axioms (and the marginalism) of the Shapley Value, and contrasts against the more immediate marginalism of VCG and LMP. We developed and applied the GNK value against VCG and LMP in the context of randomly generated electricity networks, to witness and discuss the differences between them.

The GNK value is rooted in bargaining perspective and rewards participants for the advantage they might have in an idealised competition with others. It was hoped that an idealised bargaining solution like this would mirror the kinds of arrangements that people with divergent interests would freely come to anyway, and hence would ascribe reasonable economic value to electrical resources in the most natural way; however this process ultimately yielded a disappointing result, as the net result failed specific ethical criteria. The specific major ethical issue witnessed in the GNK value was that it does not respect the ethical criterion called 'individual rationality' - the desirable quality that every participant is ascribed non-negative net utility. Particularly if zero utility is interpreted as the utility of a non-participant, then individual rationality property implies that every participant is made better-off by participating.

The GNK value extends from the Shapley Value axioms, and so it inherits the NP-hard computational burden associated with the Shapley Value. However through investigation into sampling techniques and in utilising a particular proxy we were able to extend the GNK value from being intractable for $\sim$ 14 bus sized nodal networks, to being readily computable to about $80 - 100$ sized nodal networks with a standard desktop computer. This was identified as a computational accomplishment particularly because if the GNK value were to be calculated exactly for a 100 sized nodal network it would involve 2^{100} power flow optimisations. This computational accomplishment was done through a process of considering the different ways that the GNK value value could be sampled, and we developed our own sampling technique called the Stratified Empirical Bernstein Method (SEBM).

The SEBM was derived as a online method of choosing samples in the context of stratified sampling, where the orthodox method of choosing samples (called Neyman sampling) necessarily takes two unique stages to complete. The development of the SEBM method was conducted in the context of evaluating other methods for sample selection in Chapter 6, and the performance of multiple methods were evaluated on sampling synthetic data sets. All of the stratified sampling methods were identified as being applicable for sampling the Shapley Value and GNK value, and the performance of these sampling methods for such a task was evaluated. The SEBM method was identified as being computationally expensive but well performing, and the method was extended into a multidimensional form.

1.5.1 Contributions

Within the research program, the primary contributions made are:

- We developed the GNK value as an extension of Nash bargaining to many players in the context of generalised actions spaces.
- We developed, applied, and ethically evaluated the GNK value against LMP and VCG in the context of ~ 100 node synthetic electricity networks.
- We developed new concentration inequalities in the context of stratified sampling, leading to new methods of stratified sample selection, and consequently evaluated the effectiveness of these methods for synthetic data sets and in approximation of the Shapley Value.

The contributions in this thesis are also partially given in the following works:

"The Generalized N&K Value: An Axiomatic Mechanism for Electricity Trading" by Mark Burgess, Archie Chapman and Paul Scott
International Conference on Autonomous Agents and Multiagent Systems (AAMAS) 2018
(accessible: ifaamas.org/Proceedings/aamas2018/pdfs/p1883.pdf)

"An Engineered Empirical Bernstein Bound" by Mark Burgess, Archie Chapman and Paul Scott
European Conference on Machine Learning (ECML-PKDD) 2019
(accessible: ecmlpkdd2019.org/downloads/paper/435.pdf)

"Approximating the Shapley Value Using Stratified Empirical Bernstein Sampling"
by Mark Burgess and Archie Chapman
International Joint Conference on Artificial Intelligence (IJCAI-2021)
(accessible: https://www.ijcai.org/proceedings/2021/0011.pdf)

Particularly, we would like to make note some specific contributions: that Archie Chapman provided the idea of using Empirical Bernstein Bounds to derive novel method of sampling the Shapley Value. That Paul Scott encouraged the use of complementary slackness conditions in solving the KKT conditions to allow the solving the bilevel optimisations in GNK value on electricity network examples. I would like to claim for myself specific contributions of developing the mathematics for Stratified Empirical Bernstein Method & Method, and the idea behind extending Neyman & Kohlberg's value formulation into generalised games, and for developing software and techniques for scaling the GNK computation. Additionally both Paul Scott and Arhcie Chapman is directly credited with providing direction, guidance in the production of this research and its publications.

1.6 Thesis outline

The thesis is arranged into the following chapters:

1. in Chapter 2, we give a series of brief philosophical points to provide ethical background for the underlying question of 'how *should* electrical energy be traded?'. In this section, we refer to the diversity of conceptions about social Equality, the different ways in which systems can be considered better/worse apart from equality (particularly by notions of Efficiency), and by ethical rules and guidance in proportion to various norms and reference points.

2. in Chapter 3, we provide a presentation of some of the core ideas and background of already developed and/or applied solutions to electricity networks, particularly each of these ideas mathematically embody different ideas about distributive ethics. The particular ideas we briefly present, are the Vickrey-Clarke-Groves (VCG) mechanism, the Locational Marginal Pricing (LMP) method, cooperative game theory solutions such as the Shapley Value and The Core, and the approach of bargaining solution concepts such as Nash bargaining.

3. in Chapter 4, we develop and explore a new solution concept called the GNK value, that is derived from Shapley Value axioms and relates directly to Nash bargaining, and we compare it against LMP and VCG results in the context of simulated electricity networks. Particularly the advantages and disadvantages of the new approach are discussed and related back to the ethical qualities established in Chapter 2. The particular difficulty of computing this new GNK value is addressed and overcome by utilising sampling techniques in the presence of a proxy.

4. in Chapter 6, we investigate a range of stratified sampling techniques which

were developed for computing the new GNK value. this investigation covered different techniques of conducting stratified sampling by minimising concentration inequalities, and a new technique was resolved called the stratified empirical Bernstein method (SEBM).

Chapter 2

Some background philosophy on Distributive Justice

In considering the question of what electricity market structure *should* be implemented, it is essential to at least acknowledge that there exists a wide range of moral and practical factors that bear on the question.

In this chapter we briefly consider some of the moral considerations that frame the question, however in doing so we must make clear that the deliberate brevity of this chapter is not to suggest that these moral considerations are not important and worthy of much greater treatment. But that we are not philosophers, and hence we intend only to acknowledge the moral situation with some of its depth.

The moral and ethical side of our question is associated with a branch of moral philosophy called *Distributive Justice*, which seeks to ask and make headway on the question of how different kinds of resources (such as money/power/goods/etc) should be distributed in society; and this is a broader question.

We begin by acknowledging the ambiguous nature of moral knowledge, and the approach that we take notwithstanding, before addressing some different categories of moral intuitions surrounding the nature of distributive justice. Particularly we give brief surveys about ideas of: formal equality, social equality, efficiency, proportionality, and envy-freeness.

- in section 2.1 we introduce the context of our approach to discussing these philosophical topics
- in section 2.2 we introduce a series of moral factors that may bear relevance to a solution, particularly:
  - in subsection 2.2.1 we introduce and talk about the different ideas about moral equality before considering two specific formulations
  - in subsection 2.2.2 we consider the notion of formal equality, that of identical or equal treatment
  - in subsection 2.2.3 we consider the articulation of equality with respect to social freedoms in a broad sense

  - in subsection 2.2.4 we contrast against the ideas of equality by considering differing ideas about utilitarian efficiency
  - in subsection 2.2.5 we consider the ideas of fairness by proportionality with respect to various possible normative reference points
  - in subsection 2.2.6 we consider the idea of justice defined by envy-freeness in society
  - in subsection 2.2.7 we briefly consider some philosophical considerations of import regarding climate change and other environmental priorities
- in section 2.3 we conclude and summarise the discussion before introducing the next chapter where these ideas are rendered in mathematics.

2.1 A philosophical prelude

We begin by noting there is a long history of philosophical scepticism about the nature of moral knowledge and judgements, and Distributive Justice is not exceptional in this regard.

An example historical argument is Hume's 'Guillotine' [Hume, 1739][1] which is often read as stating that: no material facts about how the physical world *is*, by-themself, could ever seem to logically imply any claim about how the world (or its material components) *should* be.

Another historic argument is G.E. Moore's open-question argument [Moore, 1903][2], which argues that for anything which defines what is morally good, then a question-about or statement-of that equivalence would only be tautology.

Such arguments are probably best used as discussion-starters today, however, talking about the ontological nature and the basis of moral knowledge is not our focus. Instead, our focus tends towards discussion around the moral views that people are likely to have upon reflection; and we give an extremely brief survey some of the attitudes expressed in literature.

What is quite evident, is that different people have different conceptions of how the world should be, and not all of these conceptions are compatible with each other. That any particular ethical system is likely to be rooted in a specific focus (as encoded

[1] "For as this ought, or ought not, expresses some new relation or affirmation, it is necessary that it should be observed and explained; and at the same time that a reason should be given, for what seems altogether inconceivable, how this new relation can be a deduction from others, which are entirely different from it. But as authors do not commonly use this precaution, I shall presume to recommend it to the readers; and am persuaded, that this small attention would subvert all the vulgar systems of morality, and let us see, that the distinction of vice and virtue is not founded merely on the relations of objects, nor is perceived by reason." T3.1.1

[2] "Moreover any one can easily convince himself by inspection that the predicate of this proposition - 'good' - is positively different from the notion of 'desiring to desire' which enters into its subject: 'That we should desire to desire A is good' is not merely equivalent to 'That A should be good is good.' ... clearly that we have two different notions before our minds."Ch1:13
"If I am asked 'What is good?' my answer is that good is good, and that is the end of the matter. Or if I am asked 'How is good to be defined?' my answer is that it cannot be defined, and that is all I have to say about it." Ch 1:6

by principles, maxims, cultural narrative, language etc) and will yield outcomes that may be disagreeable to some people and agreeable to others.

We attempt to give a brief survey to address what we believe are often some of the elements that feature in people's moral thinking, and attempt to develop a novel synthesis about electricity systems, which bears some relevance to these moral considerations.

While we must acknowledge the moral ambiguity inherent in the question of electricity allocation, we contend that this does not mean that any answer is simply *as good* as any other. But only that we believe that the suitability of our answer is not something we can totally demonstrate, in principle.

Let us begin.

2.2 Introducing moral factors about distributive justice

The choice of centralised market structures and processes can be seen as a choice between methods of allocating resources between multiple parties in a system based on the parties interaction within it. In this context the choice of the market structures and also the resultant likely distribution of resources can be viewed as being morally/socially desirable or undesirable based on a number of factors. What constitutes a desirable distribution of resources?

Throughout time there have been an array of philosophers who have discussed ideas surrounding the moral distribution of resources and capital; and one of the major ideas surrounding the ethics of distribution is *Equality*.

2.2.1 Moral equality

> "A common characteristic of virtually all the approaches to the ethics of social arrangements that have stood the test of time is to want equality of *something*... They are all 'egalitarians' in some essential way ... To see the battle as one between those 'in favour of' and those 'against' equality (as the problem is often posed in the literature) is to miss something central to the subject."[Sen, 1992, Chapter 1]

> "for all men have some natural inclination to justice ... what is equal appears just, and is so; but not to all; only among those who are equals: and what is unequal appears just, and is so; but not to all, only amongst those who are unequals;
> which circumstance some people neglect, and therefore judge ill; the reason for which is, they judge for themselves, and every one almost is the worst judge in his own cause." [Aristotle, Politics, chapter III.9]

People tend to believe that they are, should be, or be treated, 'equal' in some sense, And this broad conception has changed throughout time and place in history. [Capaldi, 2002]. From at least as far back as Aristotle[3], notions and concepts about

[3] see section quote

equality have come from across culture and peoples, and between Spiritual [4] and the Materialist [5] thought. Throughout the ages the way in which equality in society has been constructed and implemented has varied dramatically.

There is something appealing about the idea of Equality between people. From the aesthetic perspective equality is an ideal with a simple structure. From a humanitarian perspective equality is associated with relief from envy and want. From the social perspective it is associated with community and solidarity.

On a practical level, the divergences between people's ideas of equality can be seen as regarding what things should-be equal (when, where and for whom); and also what should be done about inequalities as they may exist.

The question: "Equality of what?" can have many answers, some of which are commonly held and seldom controversial today, such as might be gleamed from the United Nation's declaration of Human Rights: Equality before the Law, Democratic Equality to vote, equal freedoms to marry and to live, etc. However more controversial answers tend to have broader social and political scope, such as: Equality of Opportunity, and Equality of Welfare and/or Economic Equality.

For some, equality is a contestable notion, or an ideal for the direction of efforts in narrow and specific contexts, but for others equality is an attainable and far-reaching goal with multifaceted implications across social spheres, as reflected by works of Walzer [2008]; Miller and Walzer [1995]; Baker [1992].

There are many ways in which equality of specific things have been argued; particularly, a person can advocate for an equality in a given context *directly* or alternatively as a means to some other end, ie. *instrumentally*. So, What amounts to an equal allocation can also instrumentally satisfy other values, for instance, Miller [1998] gives some broad examples of reasons for equalities in society: for aesthetic and pro-social reasons, because it can be a sufficiently practical and simple social contract, or because it might be politically inevitable etc. Alternatively, there have been arguments *directly* for the equality of specific things, particularly from (or in light of) more abstract concepts such the notion that people have *equal moral worth* or *moral equality* - see discussions in Steinhoff [2015].

Though it is difficult to define[6], the notion that people have equal moral worth is sometimes seen not to logically imply any very specific kind of equality of measure.

> "The distinction between "equal treatment" and "treatment as equals" expresses this difference between offering people the same treatment, and

[4] across multiple religions, eg. in Islam "No Arab is superior to a non-Arab, no coloured person to a white person, or a white person to a coloured person except by Taqwa (piety)." [Ahmad and At-Tirmithi], and in Christianity, St Paul's Galatians 3:28 "There is neither Jew nor Gentile, neither slave nor free, nor is there male and female, for you are all one in Christ Jesus" (NIV)

[5] Such as in Engel's Anti-Dühring Part 1 Chapter 10 "The idea that all men, as men, have something in common, and that to that extent they are equal, is of course primeval. But the modern demand for equality is something entirely different from that; this consists rather in deducing from that common quality of being human, from that equality of men as men, a claim to equal political social status for all human beings"

[6] for instance, Discussion about *who* has equal moral worth (or alternatively *how/why* they do) seems to occasionally to turn into a discussion about the moral rights of animals, Steinhoff [2015]

> acting in accordance with the fact that they are moral equals. Equal status does not constrain us to a set of identical actions regardless of our differences." [Nathan, 2015]

The question about what things should be equal (rights, freedoms, duties, responsibilities etc, and for whom and when) can be seen as forming a large component of the various moral systems. It is also sometimes seen that moral equality simply cannot be a logical premise for these questions.

> "The idea of moral equality, while fundamental, is too abstract to serve as a premise from which we deduce a theory of justice. What we have in political argument is not a single premise and then competing deductions, but rather a single concept and then competing conceptions or interpretations of it. Each theory of justice is not *deduced from* the ideal of equality, but rather *aspires to* it, and each theory can be judged by how well it succeeds in that aspiration." [Kymlicka, 2002]

Thus it is perhaps better to take a more descriptive process to analysing equality, rather than a deductive one. So for instance, expecting any particular person to give a precisely defined answer to the question "Equality of what?" may be asking too much; as even the phrases which people use in everyday life are seldom given exact specifications[7], let alone concepts pertaining to the spectra of possible societies. In this way, the space of various contemporary political philosophies which faithfully attempt to construct and interpret some reasonable form of equality between persons has been described as belonging to an 'egalitarian plateau' [Brown, 2007].[8] Or conversely, while a specific ethical equality may not be agreed upon, perhaps there may be a more broadly accepted notion of what an 'inequality' looks like, particularly as it is sometimes blurred with the concept of a 'social injustice'.[9]

And in this way, the concept of Equality is seen as a vague notion that can be inclusive-of and also contrasted-against other views; such as those that emphasise the priority of resources to the poor, or such as emphasise alleviation of insufficiency among the poor; broadly termed "prioritarianism" and "sufficientarianism" respectively, such as by Arneson [2013][10]

Although the concept of equality is the subject of wider analysis, we will focus on two specific interpretations of equality which we feel can be made relevant to mechanisms for electricity allocation.

[7]Degrees of vagueness are well witnessed in everyday sentences, "There are a gathering of people near that tree", such as argued in the classic Sorties paradox [Frances, 2018]

[8]The phrase is originally attributed to Dworkin and subsequently adopted by others.

[9]There is some debate as to when/where/how an inequality also becomes an injustice. It is possible to believe that an inequality constitutes an injustice directly, or perhaps that an inequality is proof (or perhaps only potential evidence) of a injustice in procedure or treatment. see Parfit's concept of Telic vs. Deontic Egalitarianism. [Parfit, 1997]

[10]for good measure we might also consider Rawls [2005]'s Theory of Justice as a specific kind of (layered) priority principle.

2.2.2 Formal equality

One of the most common interpretation of equality is that people should be subject to systems that treat them in a manner that is *impartial*. The minimal idea is that an impartial system should not afford arbitrary or unjustified special treatment toward any particular individual/s. Hence that systems should operate by rules which are blind to particular identity and sensitive only to morally relevant characteristics.

Straightforward examples of this doctrine are embedded in anti-discrimination legislation, and Mason and Press [2006] gives some examples. A person's religion for instance, is not generally a morally relevant characteristic for employability decisions, except in some example cases, such as in the performance of religious positions (eg. a Priest), or where a person's religious practice (such as wearing religious clothing, eg. a turban) may directly affect performance (such as on the construction site, requiring a hard-hat). Many more examples exist, but what is notable is that where and when morally relevant characteristics arise is not always easy.

At a more general level, the idea of moral impartiality has been clarified by various thought experiments and also stated with moral maxims. Particularly famous devices include Rawl's "Original Position", Kant's categorical imperatives, or various positions defined by hypothetical ideal sympathy and/or perfect detachment — Smith [2018]; Gauthier [1986]; Firth [1952]. Additionally the idea of impartiality is perhaps somewhat mathematically expressible, in that people who are (in all the relevant ways) equal should be treated equally; and this has been called *formal equality* as in [Nathan, 2015].

Although formal equality is occasionally seen as being an important part of a fair system, it is also sometimes seen to be insufficient to capture broader notions of equality and justice.

> "In its majestic equality, the law forbids rich and poor alike to sleep under bridges, beg in the streets and steal loaves of bread."
> –Anatole France, Le Lys Rouge [The Red Lily] (1894), ch. 7

Indeed, by imagination many kinds treatment or processes could be rationalised as being issued by impartial principles which are universally applied. Furthermore, not all kinds of desirable impartiality are mutually compatible, or perfectly achievable in practical settings, such as discussed by Hutchinson and Mitchell [2019].

Notwithstanding, formal equality can be seen as a basic doctrine that ascribes value to the incorporating degrees (and/or kinds) of impartiality into the design of social processes from the outset.

In all developments in this thesis, the principle of formal equality - that individuals are treated equally but-for specific factors - is assumed.

2.2.3 Equalities of social freedoms

> "I want to emphasise what is, on my view, the most important object of egalitarian distribution, and that is *power*. Of course power is not something which can be parcelled up and shared out like a commodity but

> we can properly talk of 'the distribution of power' and this is, more than anything, the determinant of whether a community is authentically cooperative." [Norman, 1998]

There are different and interrelated ways of how to conceive of wider social equality, and one historic way of framing social equality is in terms of power. For some people, the ideal of equality encodes the hope of a society free of abusive power relations that perpetuate social injustices.

One of the more historically notable instances of this framing is featured in Marxist thought, which focuses on abusive economic power relations between social classes. This frame also shows up historically in feminist thought (eg. Cudd [2006]) where the inequalities of power between men & women are considered as a form of oppressive dominance & submission.[11]

But what is notable is that neither Marxist nor feminist writers always viewed power itself, negatively. For instance, Marx opposed private property (as capitalistic ownership) but seems to have had a more complex attitude toward property relations generally.[12] Additionally some feminists (such as Allen [1998]) occasionally consider power in the positive (or potentially neutral) language of *empowerment*.

One feature of power that is associated with abuse, is the exercise of 'power over' other people, or 'power to' do things which impinge upon other's rights. But dissecting when and where an exercise of power constitutes an abusive or morally objectionable act may not be easy. Particularly the 'power to' do something is straightforwardly an example of a freedom, and one well known dichotomy exists between *positive* and *negative* freedoms[13] particularly in the discussion of doing or allowing harm. But even more broadly, freedoms can be considered (such as by Gerald C. MacCallum [1967]) as triadic relationships: a freedom *of* a person, *from* particular preventing conditions, *to* do certain things.

However different freedoms are not equally valued (or compatible), and some are esteemed by individuals and societies more than others. Some would place an importance on political freedoms (to openly discuss, vote, and run for office) or economic freedoms (to work, to buy, sell and lease property), etc. But particularly, the having and actualising of freedoms associated with the meeting of needs; such as basic needs (of shelter, food, etc - as at the bottom of Maslow's hierarchy) as well as

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[11] eg. MacKinnon writes "difference is the velvet glove on the iron fist of domination. The problem is not that differences are not valued; the problem is that they are defined by power"MacKinnon [1989].

[12] "the theory of the Communists may be summed up in the single sentence: Abolition of private property ... Do you mean the property of the petty artisan and of the small peasant, a form of property that preceded the bourgeois form? There is no need to abolish that"Engels and Marx [1848]
"Property thus originally means no more than a human being's relation to his natural conditions of production as belonging to him, as his, as presupposed along with his own being; relations to them as natural presuppositions of his self, which only form, so to speak, his extended body."[Marx, 1857, Notebook V]

[13] While vague, a negative freedom is associated with an absence of external obstacles to conducting the specific action, and a positive freedom is associated with the possibility (or actuality) of doing the act in accordance with one's will and purposes. The positive/negative dichotomy is also associated with what is or is not effort-full. [Mossel, 2009]

higher needs (such as social belonging and self-actualisation); can be considered as defining of human wellbeing, and perhaps even a constituent of the state of having 'Freedom' - the moral and political ideal.

Unfortunately most of these (and other) wider conceptions of societal Equality are beyond the scope of what we can earnestly engineer directly. But what we can do is to reflect and evaluate the influence that any proposed system might have on the freedoms of individuals and the wellbeing of society - and this is a task we attempt in later section 5.4.

2.2.4 Efficiency and utility maximisation

> "It is the greatest happiness of the greatest number that is the measure of right and wrong." [Jeremy Bentham, 1776]

> "Essentially, Utilitarianism sees persons as locations of their respective utilities ... Persons do not count as individuals in this any more than individual petrol tanks do in the analysis of the national consumption of petrolium." [Sen and Williams, 1982]

It is occasionally thought that what is morally good for society should have some relationship with what is good for the individuals of society; and there is a question about how to characterise that relationship. Historically what is morally good for individuals has been associated with such things as happiness [Burns, 2005] or subjective welfare [Dworkin, 1981a], access to resources (such as electrical power) [Dworkin, 1981b], and/or opportunity for welfare [Christiano, 1991].

In more immediate and material contexts, what is good for an individual may be more straightforward such as: access to sufficient food and medicine, monetary yields, opportunities for educational attainment, probability of survival etc.[14] But for whatever measures are considered to be relevant, the question of how these quantities should combine to bear on the broader moral judgement about what is good for society, has a variety of answers. It is useful to illustrate the question by introducing the concept of utility as a quantification of what is good for individuals.

The concept of utility has changed over time[15] but minimally it is conceived as a measure of the strength of the preference (or value) that a specific person does (or alternatively should, rationally, pragmatically and/or morally) attach to different possible outcomes. The concept can be seen to extend from the consideration that such preferences should be transitive and comparable between people: If a person prefers A to B, and also B to C, then they ought to also prefer A to C. Additionally, if a person/s can prefer A 'more' than another person/people prefer B - then it remains a task of invention to associate numbers to the strength of these preferences over outcomes. Utility or value is relatively abstract concept that is sometimes difficult

[14] many thought experiments invoke lifeboat/classroom/triage/trolley-problem circumstances, where what is good for specific individuals is unambiguous

[15] historically and notably held by famous utilitarians such as John Stuart Mill [1863] and Jeremy Bentham (see section quote), who defined it in terms of happiness or pleasure/pain [Bentham, 1823]

to elicit or measure in practice (measurement via monetary equivalence is seen to have potential issues), and numbers that are associated with utility are not objective but inherently defined by being relative to each other, hence equivalent under affine transformations.

In anycase, for these definitions, the sum of utility is straightforwardly one of many examples of a *collective utility function*, a function that aggregates the utility of individuals and hence is a possible target for moral decision making - a topic more widely discussed by Holtug [2015]. As another example, some people's egalitarian intuitions might be satisfied by moral decision making that affords equal utility for all individuals - and in some contexts this may be appropriate, even though it might not maximise the sum of utility. This outcome could be constructed as an alternative collective utility function.

What is to be realised is that maximising one collective utility function does not necessarily maximise the other. Particularly this is made clear in the famous 'levelling-down objection', which loosely stated, is the objection that a person implementing a strict Egalitarian distribution of utility would potentially prefer a world in which every single person had less, if it were more equal; as considered by Parfit [1997]; Temkin [2003].

These considerations frame some possible articulations of the broader contrast between the values of Equality and 'Efficiency'; where the specific concept of efficiency considered in the levelling-down objection is *Pareto optimality*. In this context outcome is Pareto optimal if there does not exist another outcome which is weakly better for every person and strongly better for atleast one. Pareto optimality is one commonly discussed and formalised efficiency condition, and is a property which we satisfy in our subsequent developments. Particularly, as it is the case that maximising the sum of utility is Pareto optimal and forms an axiom in our treatment (as it is given by our efficiency axiom (4.2) in chapter 4).

As a total theory of ethics, Utilitarianism has a substantial history in moral thought and many criticisms have been made of it throughout the years. Particular objections can be drawn about whether the moral conditions and preferences between people can actually be compared, and thus measured/quantified, and then faithfully rendered into a kind of calculus for moral decision making. Indeed the feeling about utilitarianism is that it has the potential to be dehumanising (see section quote about petrol tanks), and specific arguments attempt to bring forth this objection - eg. that utilitarians should prefer be plugged into pleasure machines Nozick [1974] or should lie and betray each other Kymlicka [2002] etc. However, as stated previously, in more immediate and material contexts the moral conditions and preferences between people are potentially more straightforward and comparable (such as the costs and supply of electricity between homes), and ultimately *some* kind of calculus must be either explicitly drawn or implicitly acted upon to make systematic decisions in a particular sphere anyway.

However, of general note, is that in various realistic situations the difference between sensible outcomes which are better or best for more people, and what is more equal for them, can be the subject of dispute (such as in the medical field [Reidpath et al., 2012; Culyer, 2015], the provision of welfare [Headey et al., 2000], and economics [Andersen and Maibom, 2019]). Notwithstanding the philosophical distinction (and potential conflict) between the various articulations of efficiency between people and equality among them, can remain.

2.2.5 Fairness by proportionality to some reference point

There are various ways in which what is considered fair is determined in relation to what is normative, and/or related to the various counterfactual events that could happen. One of the more basic and famous examples of this relationship is given by Mill's harm principle:

> "That the only purpose for which power can be rightfully exercised over any member of a civilised community, against his will, is to prevent harm to others." [John Stuart Mill, 1859, Chapter 1]

Insofar as the harm principle is accepted, there subsequently remains a question about defining where and when harm occurs. Among its features, harm is often considered to be negative and defined with respect to a more normative (and potentially counterfactual) 'unharmed' state. However in more complicated cases, it is not always clear what the more normative 'unharmed' state should be (eg. who is harmed by whom).

But also reversely, there are also various conceptions of justice which involve compensation for providing benefit to others. For instance, in Business ethics there is a viewpoint (such as held by Sternberg [2000]) where an employee's just wage should be in proportion to their contribution to the value and productivity of the firm. In this context, the contribution may by measured by profit relative to their absence and/or by the replacement cost of contracting equivalent work (potentially depending on which ever is more pertinent). Particularly, the idea that people should be rewarded in proportion to their contribution to the social good above their absence individually, is most directly rendered by the Vickrey-Clarke-Groves (VCG) mechanism - see section 3.1.

We note that this relation to a reference points may be somewhat associated with the ideas of deservedness, compensation, reward and/or proportionality; however these relation is not necessarily exact. For instance, the idea of compensation is most often associated with damages or injury to others, but less commonly associated detracting gain that occurs to them (eg. beating someone in competition), the notion of reward is often associated specifically with incentivising particular pro-social behaviours among individuals, and to some extent the same is true of the validity of deservedness claims. Furthermore in considering the notion of proportionality, the one primary question which occurs, is 'proportionality with respect to what?' - ie. what should the reference point be?

However, thinking in terms of proportionality may be slightly misleading as example of a normative reference point is also found in Business ethics. Particularly there is a viewpoint (such as held by Boatright [2010]) where a business transaction (such as pay for an employee's work) is considered justified if it was attained by a process of truly-free negotiation between the parties, such as to make all parties better off than they would be otherwise. This 'truly-free' exchange (sometimes called *euvolentary exchange* by Guzmán and Munger [2019]) is particularly defined by the fact that all parties could have realistically elected to walk away from the negotiation. The event that would be triggered if the parties did not successfully negotiate is sometimes called the 'disagreement event', the existence of which is the normative reference point that determines the morality of the transaction. Some of these ideas are mathematically rendered by various bargaining solution concepts, such as Nash bargaining - see section 3.4.

In these cases we can see instances where the morality of an event is defined by normative reference points. And this dynamic can extend even to groups of individuals, as we might consider ways that groups of individuals might be exploited even if their individual interactions are truly-free.

> "This is the main aim of John Roemer's work on [Marxist] exploitation. ... If we view the different groups in the economy as players in a game whose rules are defined by existing property-relations then a group is exploited if its members would do better if they stopped playing the game, and withdrew their per capita share of external resources and started playing their own game." [Kymlicka, 2002]

And this idea of allocation exceeding what any group could achieve if they withdrew to cooperate among themselves, is most directly articulated and formalised by the *Core* solution concept of cooperative game theory - see section 3.3.

Similarly, another solution concept in cooperative game theory is the *Shapley Value* (see section 3.3.2), which can be summarised as allocating compensation in proportion to each individuals contribution (in expectation) to group welfare above their absence, under uncertainty about the presence of other group members.

The consideration that the relevant normative reference point occurs under uncertainty (or in expectation), is featured in other formulations. For instance, if we expect that euvolentary market exchanges would normally occur at a certain market price, then we may consider that the moral trading of goods would occur at this market price. One famous example of this idea is featured in John Locke's short essay 'Venditio' [Locke and Wootton, 2003] where it is argued that a fair price for something is simply its normal market price at its location. (see section 3.2 for elaboration)

In all these cases, the morality of a situation is defined with respect to various reference points, which of these reference points are most relevant (and to what extent) may depend on a range of practical and moral factors.

It is also worth noting that these decisions about normative reference points can be defined by social policies and embodied in moral codes and standards; and in this thesis, we consider development of a novel synthesis that extends from a specific reference point – see Chapter 4.

2.2.6 The concept of envy-freeness

> "... an allocation is equitable if and only if each person in the society prefers his consumption bundle to the consumption bundle of every other person in the society." [Foley, 1966, Chapter 4]

Although it will be of lesser relevance to the developments in this thesis, it would be remiss of us to neglect a discussion of the concept of envy-freeness as a significant concept in the discussion of distributive justice. As introduced by Foley [1966] and stated in this section's quote, an allocation is 'envy-free' iff every person prefers their allocation of resources which they receive to that received by everyone else. There has been significant research examining the contexts in which envy-free allocations of resource bundles exist and can be computed, and the development of similar/-substitute qualities where they cannot.

The first and most notable notable quality of the envy-freeness condition is that it has a genuinely straightforward ethical appeal, particularly the transparent envy-free allocation of resources could be expected to minimise a certain kind of social discontent defined by interpersonal comparisons. Additionally, the minimising of social discontent may overlap and/or motivate other ethical measures, for instance, an equal or egalitarian allocation may also be envy-free and/or efficient.

However, the envy-free criterion my not necessarily select a unique outcome or indeed necessarily any outcome at all, and even insofar as envy-free allocations are known to exist, they may be time-prohibitive to compute. Envy free allocations may exist or not depending on many conditions, such as whether the resources are divisible and/or indivisible. The case of indivisible goods envy-free allocations may not exist (consider a single item and two agents) [Manurangsi and Suksompong, 2019], and even when such allocations do exist they may be NP-hard to compute, as even the case of identical valuations of indivisible goods between two agents is directly equivalent to the classic NP-hard PARTITION problem. [Nguyen and Rothe, 2014] However even in the continuous case, although Pareto-efficient and envy-free are guaranteed to exist in some circumstances [Weller, 1985; Cole and Tao, 2021], they may be prohibitive to compute, see for instance the problem of envy free cake cutting for discontinuous slices and for arbitrary number of players was solved by Aziz and Mackenzie [2016] requiring as many as $n^{n^{n^{n^{n^{n}}}}}$ operations. There are also situations with mixed divisible and indivisible goods which are not necessarily more simple.[Bei et al., 2021] In recourse to these problems, some alternative measures have been adopted and investigated, such as the various conceptions of envy-minimisation, in these conceptions some aggregate envy criteria are possible [Benade et al., 2018; Lipton et al., 2004; Nguyen and Rothe, 2014], for instance if $u_i(\pi_j)$ is the utility player i would receive from receiving player j's resource bundle, and if I is the indicator function then:

- the number of envious individuals, $\sum_i I[\sum_j I[u_i(\pi_j) > u_i(\pi_i)] > 0]$
- the number of envy-relations, $\sum_{i,j\neq i} I[u_i(\pi_j) > u_i(\pi_i)]$

- the maximum envy-difference $\max_{i,j}\{\max\{0, u_i(\pi_j) - u_i(\pi_i)\}\}$
- the maximum envy-ratio defined by how much a player values the allocation of another over their own $\max_{i,j}\{1, \frac{u_i(\pi_j)}{u_i(\pi_i)}\}$

Since allocating nothing to every player (if possible) is straightforwardly envy-free, there is a secondary question about what efficiency measure should also be optimised in this context. Examples include: egalitarian social welfare (ie. maximising the utility of the worst-off agent) or utilitarian social welfare (ie. maximising the sum of all agents' utilities) or satisfying Pareto efficiency, or Nash social welfare (see also Section 3.4) [Nguyen and Rothe, 2014].

The notion of envy-freeness relies on comparisons between agents and the bundles of resources which they could gain, however there is some flexibility about how the agents and bundle comparisons are defined. For instance, a similar and more expansive notions of envy-freeness such as applied to groups ('group envy freeness') are even more restrictive and difficult to compute; Group envy freeness was first introduced by Berliant et al. [1992] for equally sized groups, and for heterogeneously sized groups by Conitzer et al. [2019]. Or conversely, there are other paths to more relaxed envy-free conditions, such as include constructions where there is envy-freeness only between specific pairs of individuals, such as specified on a group or graph structure (see Flammini et al. [2019]) sometimes called 'social/local/network envy-freeness'. Another more relaxed notion is that of envy-freeness prior to a random assignment, or envy-freeness in expectation ie. 'ex-ante' envy-freeness - contrasing 'ex-post' envy-freeness.

We will consider the application and implications of the concept of envy-freeness in the context of electricity markets in Section 3.5.

2.2.7 Broader environmental considerations

Additional to the topics thus far considered in this chapter, there is a broader context and special considerations regarding environmentalism and how it intersects with energy systems and policy. Environmental considerations focus on the externalities of decisions and interactions on third parties, particularly of importance in the energy context, is the production and emission of greenhouse gasses (GHG) into the atmosphere causing anthropogenic climate change, which is expected to cause harm to human life and property in the coming decades.[IPCC, 2022]

The emission of GHG causing harm to the environment and damage to the lives of others, is an example of an externality in the context of the electricity system, and there is the question of how and-or if such externalities should be accounted for in an electricity context.

There is, for instance, the question about how (and how much) the wellbeing of future generations be accounted and considered relative to the wellbeing of those presently living. [Meyer, 2021] Or how should international effort and compensation costs be divided between nation states today. [Gardiner, 2004] However more specific energy considerations exist, particularly if electricity market structures are the best place for such externalities to be accounted for. Particularly, a uniform tax or trading system on GHG pollution across industries and sectors would be more consistent with handling the externality holistically. Contrastingly, there are some who have considered that the policies of 'resource neutrality' evident in energy systems may also an issue. [Outka, 2021]

As an example, Australia's National Energy Objective (NEO) is part of Australia's National electricity law (NEL) is an example of a resource neutral policy in that it does not prioritise particular forms of generation or consumption over others, as stated: "to promote efficient investment in, and efficient operation and use of, electricity services for the long term interests of consumers of electricity with respect to: price, quality, safety and reliability and security of supply of electricity; and the reliability, safety and security of the national electricity system."

At issue is that the long-term interests of consumers may be broader than simply reliable and cheap electricity, and that such policy directives have the potential to focus attention on mitigating shorter term risks to energy reliability (such as may be produced by the integration of renewables) rather than focus on the actual interests of people in the longer term (such as energy consequences, as may be brought about by GHG driven climate change and its political ramifications).

The question is to what extent should electricity market systems prioritise, by design, renewable generation over GHG emitting technologies. By considering this question, we see that ideally a comprehensive answer to the question of how electricity should be valued and traded (our research question) would hopefully be adaptive and tunable to such politically relevant priorities. As considered in the introductory chapter, Sections 1.1-1.4, we outlay the circumstance that existing renewable integration has potential to create issues with electricity affordability and reliable access. From this, rethinking electricity market systems to ameliorate these issues is certainly consistent with resource-neutral energy directives, however it is also of interest to consider systems which prioritise renewable generation (and compensation for renewable generation) atleast as much as on a neutral basis. Furthermore, considering the design systems to support renewable generation without sacrificing other qualities (such as reliability and safety, etc) is of interest anyway, particularly as the intermittency of renewable generation is a primary objection against action on climate change anyway. [Shrader-Frechette, 2017]

There is much that could be further said about Climate Change and energy policy that is genuinely worth saying and beyond our current scope of investigation. This is true, as our focus is on the more abstract and generative question about how electricity should be valued and traded, on a broad level, as might flexibly incorporate these and other relevant political factors.

2.3 A summary on our philosophy of distributive justice

There is wide range of perspectives on distributive justice which we can only begin to survey in this chapter. And there are many other positions that we could address, including conceptions of fairness as issuing from envy-freeness, ideas of fairness defined by equal share of social surplus, and all the various ways these viewpoints can intersect.

Moral considerations are at the heart of the question of how electricity and monetary payments should be distributed. Unfortunately questions such as these do not have analytically demonstrable answers, but we can make judgements by considering the various flavours of moral ideas which people might assert. Particularly we summarise some of the various conceptions of Equality, Formal Equality, and Equality concerned with social freedoms. Additionally we frame some of the concepts of Efficiency particularly as it is contrast against Equality. And highlight the ways in which morality can be defined in relation to various normative reference points, with consideration of the concept of envy minimisation.

We focus particularly on these factors as our further developments relate directly to them. Ultimately our solution obeys formal equality principles, maximises efficiency, and is formalised by reference to normative reference points defined by idealised competition – see chapter 4.

Chapter 3

Existing solutions

In the previous chapter we discussed some of the philosophy surrounding distributive justice, and in this chapter we discuss some of the various ways those ideas have been made quantitatively precise.

In this chapter we consider some of the relevant formulations of the ways in which moral ideas about distribution have been mathemetised, primarily because our later developments extends from them and also ultimately contrasts against them.

We consider the following formulations:

- in section 3.1, we consider the Vickrey-Clarke-Groves (VCG) mechanism,
- in section 3.2, we consider Locational Marginal Pricing (LMP),
- in section 3.3, we consider the Core and the Shapley Value,
- in section 3.4, we consider Nash's bargaining solution concepts.
- in section 3.5, we consider mathematical considerations associated with the concept of envy-freeness.

These different approaches stem from different moral considerations and have specific context and unique properties; we will introduce and discuss each of them in turn. In the next chapter 4 we attempt a new synthesis which brings many of these conceptual elements together.
Let us begin with the VCG mechanism.

3.1 VCG

In section 2.2.5 we briefly presented the idea that people might be rewarded in proportion to their contribution to social welfare, above their absence, individually. While this idea may be simple, its mathematisation has some surprising features. The most direct mathemetisation of this idea is the Vickrey-Clarke-Groves (VCG) mechanism with Clark pivot.

The VCG mechanism (with Clark pivot) is an allocation process where each player is payed 'transferable utility' (or money) equal to the impact that their presence has upon others (ie. their externality) in the decision process which selects an outcome that maximises the sum of utility. Let us explain with some mathematics:

3.1.1 The minimal VCG process - with Clark pivot

If we frame the VCG process as a bidding process of n agents over a possible set of outcomes X. We assume that every agent i has a valuation (or utility) v_i for any outcome in X:

$$v_i \ : \ X \rightarrow \mathbb{R}_{\geq 0}$$

The VCG bidding process asks every agent i for their valuations and calculates the outcome that maximises the sum of the reported valuations:

$$x^* = \underset{x \in X}{\operatorname{argmax}} \sum_{i=1}^{n} v_i(x)$$

This outcome is implemented and the process pays each agent i the utility value d_i (which may be positive or negative):

$$d_i(v) = \sum_{j \neq i} v_j(x^*) - \max_{x' \in X} \sum_{j \neq i} v_j(x') \tag{3.1}$$

This value d_i is the value that the player's presence adds to the utility of others minus the sum of the other player's utility which would have been obtained in the player's absence - ie. the player's externality. In this equation the sum of other player's utility which would have been obtained in the player's absence $\max_{x' \in X} \sum_{j \neq i} v_j(x')$ is a special term called the 'Clark pivot', and in section 3.1.3.1 we discuss alternatives to this term.

Example. Consider a set of outcomes $X = \{A, B, C\}$ and three agents with valuations

$$\begin{array}{ccc} v_1(A) = 2 & v_2(A) = 4.5 & v_3(A) = 2 \\ v_1(B) = 4 & v_2(B) = 2 & v_3(B) = 1 \\ v_1(C) = 3 & v_2(C) = 1 & v_3(C) = 5 \end{array}$$

In this context $x^* = C$ is implemented (as $\sum_{i=1}^{n} v_i(C) = 9$ is the largest)
And: $d_1 = 6 - 6.5 = -0.5 \qquad d_2 = 8 - 8 = 0 \qquad d_3 = 4 - 6.5 = -2.5$

3.1.2 Discussion about VCG

The VCG mechanism with Clark pivot might be seen as an straightforward way of assigning an outcome and allocating ethical payments; if a player's presence adds to the utility of others then they are positively compensated, and if a player's influence detracts from the utility of others then they are penalised in proportion. Since the set of possible outcomes X are arbitrary it is possible to consider the application of the VCG mechanism in a wide variety of contexts. However VCG has some particular advantages and disadvantages. The first and most notable property is that

VCG mechanisms have been demonstrated by Roberts [1979]; Lavi et al. [2008] to be *truthful* or *incentive compatible*, in the sense that that no single player can positively gain by misreporting their valuations in the event that all other players are truthfully reporting their valuations, and in the event that the utility of the agents is *quasilinear*. An agent's utility is quasilinear if their utility is equal to their valuation of the outcome plus any transfers they receive, and hence their utility u_i has form:

$$u_i = d_i(v) + v_i$$

In this way if VCG's incentive compatibility induces the players not to bid strategically then it can reduce a potential overhead of their participation, and potentially eliminates a source of instability in the resulting system.

Another interesting property is called *individual rationality*, in that no agent (assuming quasilinear utility) will ever be left with a net negative utility. Particularly if the utility of zero is regarded as the utility of non-participation, then individually rational means that everybody is left being better-off (or atleast not worse-off) by participating than they would be otherwise. Hence individual rationality is a possible articulation of ethical euvolentary negotiation (see chapter 2.2.5).

It is also worth noting that VCG mechanisms are also *efficient* in the sense that the process actualises the utilitarian socially optimal solution $x^*(v) \in X$.

However, more negative features of VCG exist, one primary drawback of this mechanism is that it is not *budget balanced*, in that it is possible that the amount of utility that is transferred between the players might not sum to zero. Because of this an implementation of VCG might require regular budget injection to maintain and/or produce a budget surplus, hence sapping money from between the participants (see example). As VCG may produce a budget surplus it is thus easy to note that the maximum amount of utility is not being given to the participants, and hence VCG is not efficient in the sense of maximising utility for the participants (see section 2.2.4).

Although VCG has a very positive property by being incentive compatible, it has some additional drawbacks and criticisms as noted by various authors [Shoham and Leyton-Brown, 2009; Rothkopf, 2007], particularly:

- The fact that VCG's truthfull equilibrium is a weak-equilibrium, and a player can misreport their valuations to harm others
- If generating or submitting a valuation in a VCG mechanism incurs some cost, over not participating, then it is no longer individually rational
- If the externalities and social optima x^* are not solved exactly, but only approximately, then this will destroy the truthfulness property of VCG.
- If any players are budget-constrained (eg. they cannot afford to pay their true valuations for particular outcomes), then the truthfulness property is destroyed.
- If VCG mechanism does succeed in incentivising players to submit their true valuations, this is potentially has privacy and information disclosure issues.

- VCG is not completely immune from the possibility of cheating: by groups of players, by players submitting multiple bids under many names, or players who know that strategies in a series of VCG auctions may not be incentive compatible. etc.
- VCG may (depending on context) also have higher computational complexity than other mechanisms.

Though some of these drawbacks and criticisms can be ameliorated, the VCG mechanism is widely discussed as potential mechanism in various real-world contexts, as we consider in section 3.1.4.

As VCG has positive and negative features, it is possible to ask if there are similar mechanisms which avoid some of the negative features. But it is unfortunate, that some of these properties (incentive compatible, individually rational, budget balanced, and efficiency) are known to be impossible to combine in the general case (where there are a plurality of outcomes and the valuations are unrestricted), and these impossibility theorems are a feature in the study of *Mechanism Design*.

3.1.3 Mechanism Design, is there a better VCG?

The VCG mechanism is a cornerstone example in the field of Mechanism Design, and there exist many good sources giving extended discussions on the field - such as Vohra [2011]. But generally, Mechanism Design conducts the analysis of systems which select social outcomes based upon the result of strategic interactions of multiple parties with divergent interests.

One of the features of Mechanism Design that the VCG mechanism illustrates, is the potential for considering and apprehending the way in which a system is likely to behave between rational individually strategising agents. This possibility extends beyond VCG, as it has been discovered that any system which is implemented between strategising agents can be altered such as to make it incentive compatible for them; this is called the revelation principle - see Gibbard [1973] [Vohra, 2011, Chapter 2.3]. The revelation principle has various formulations, but generally, for any system there will some Nash equilibria in the interaction between the agents, and consequently an incentive compatible mechanism can be constructed by asking the agents for their true valuations and then implementing the corresponding Nash equilibria directly. Unfortunately, it is sometimes the case that the Nash equilibria between strategising agents may not coincide with what is socially optimal for them; and the general difficulty of designing systems where the socially optimal outcome is always a Nash equilibrium is rendered in some of the famous impossibility theorems in Mechanism Design.

Some of the primary historic impossibility proofs in Mechanism Design concern voting and social choice systems, and notably include Arrow's impossibility theorem, and the Gibbard-Satterthwaite theorem. But the difficulty does not necessarily recede even if monetary compensations between parties are included into consideration, such as per the Myerson-Satterthwaite theorem. Another impossibility theorem was also proven by Green and Laffont [1979] to the effect of proving that there is no easy alternative to VCG - a mechanism which is incentive compatible, has unrestricted player preferences, has individual rationality, and implements a socially optimal outcome, in the case of quasilinear utilities.

In the evolving field of Mechanism Design there are several avenues of mitigating some of the impossibilities.

One of the main problems in applying VCG to electricity networks is the fact that it is not budget-balanced, and this raises a question of where the budget surplus/deficit should be channelled to/from. Particularly if the money should be directed back to the participants in the electricity network, then it would destroy the incentive compatibility that was part of the scheme in the first place. This is a direct consequence of the impossibility result of Green and Laffont [1979] and hence we are constrained to consider mechanisms which are suboptimal in relation to these qualities (budget balance, incentive compatibility, individually rational, and efficiency). However it is also shown by Yi and Li [2016] that there are no mechanisms which allow bounded deviations from the efficiency, incentive compatibility and budget-balance.

Thus a search for a better alternative than VCG needs to outright sacrifice or substitute some of these desirable properties.

Although we cannot go into too much detail about the field of Mechanism Design in this chapter (and the different kinds of impossibility theorems and kinds of incentive compatibility), we can highlight some interesting options.

3.1.3.1 Redistribution in Groves mechanisms

One potential avenue of averting the impossibility result is to discard the assumption that the player's valuation over outcomes are unrestricted, and recognise that some of the budget surplus/deficit can be redistributed without destroying the incentive compatibility property.

To frame this approach, we must make a technical distinction between a Groves mechanism and its particular instance - in the VCG mechanism. A Groves mechanism is exactly the same as the VCG mechanism except instead of paying players per equation 3.1, instead it pays them per:

$$d_i(v) = \sum_{j \neq i} v_j(x^*) - C_{-i} \tag{3.2}$$

where C_{-i} is some function that is independent of i's reported preferences. In this context it is notable that the VCG mechanism is a special case of a Groves mechanism [Groves, 1973] where $C_{-i} = \max_{x' \in X} \sum_{j \neq i} v_j(x')$. Groves mechanisms are a class of mechanisms which include VCG, and are categorically incentive compatible.

The challenge therefore is to derive optimal functions C_{-i} which minimise the budget surplus/deficit while maintaining individual rationality in the context of restricted player valuations. For this purpose there has been significant discussion about deriving these C_{-i} functions, also known as 'VCG redistribution' rules.

One of the first to propose such a rule was Cavallo [2006], who showed that much of the VCG surplus can be redistributed in a process of allocating a single physical object exclusively to one party (called 'All-Or-Nothing' games), where it can be naturally assumed that any party has a utility of zero if they do not receive the physical object. This redistribution was possible primarily because there exists a simple constraint on player valuations - ie. not receiving the object has utility of zero. Similarly in other situations where there are restrictions on the players' valuation over the outcomes, there is the potential for deriving different VCG redistribution rules.

However there are some difficulties with this approach, particularly it is known that even with VCG redistribution rules there will almost always be some remaining budget surplus, and even then the process of deriving optimal redistribution rules can be a difficult task — even to the point where neural networks have been employed to approximate such functions (see Manisha et al. [2018]).

3.1.3.2 Sacrificing efficiency with budget sinks

Another avenue of averting the impossibility result is to sacrifice efficiency of outcome selection. One of the simplest such schemes is given by Boi Faltings [2004, 2011] who proceeds about the process of designing a non-Pareto optimal VCG mechanism by splitting the population into two groups. In this scheme, the VCG outcome from the first group is selected irrespective of the preferences in the second group and where the second group (the 'sink') receives the budget surplus from the VCG mechanism applied to the first group. This mechanism constitutes a budget balanced VCG-type mechanism which can be made more regular (suggested by Guo et al. [2011]) by randomly selecting an individual as the 'sink', and splitting the budget surplus between the parties evenly without knowledge of who will be selected.

This kind of method of developing non-Pareto optimal VCG mechanisms has been the subject of investigation by Nath and Sandholm [2019], and the process is proven to necessarily need a 'sink', although this such a sink can be randomly selected. Notwithstanding it is expected that such a mechanism of randomly assigning a sacrificial 'sink' could potentially be ethically dangerous; potentially falling afoul of Formal Equality ideas (see section 2.2.2) as one member (or group of members) would be randomly singled out to equalise the budget surplus/deficit.

3.1.4 Applications of VCG to electricity systems

VCG has properties that make it attractive from from a theoretical standpoint, particularly its incentive compatability property brings the promise of alleviating the cost and potential system instability inherent between strategising agents that can be manifest in cases of market collapse. Additionally it has a straightforward ethical interpretation, that is, as a policy of compensation for externality. These advantages have led VCG to be often discussed, but its weaknesses have led to its being reportedly seldom implemented in practice, including in the context of electricity networks [Ausubel and Milgrom, 2006; Fabra et al., 2002].

In these discussions the primary difference between proposals of VCG application is the context of the events&bids to which it is applied. Thus VCG has been considered as a mechanism for allocating physical and monetary outcomes in various contexts within electricity networks by various authors:

- VCG-like schemes have been considered as means of extracting truthfull preferences and allocating costings for demand across electric vehicle charging stations [Ligao et al., 2020]

- VCG has been considered as a mechanism to determine compensation and induce truthfull information about consumer's inconvenience functions to demand response aggregators in demand response (DR) programs [Nekouei et al., 2015]

- VCG has been contrasted with other auction mechanisms in auctions for demand curtailment contracts under network uncertainty [Heinrich et al., 2021]

- VCG has been considered as a possible auction mechanism for renewable energy aggregators to purchase and reward variable renewable energy generators for providing and truthfully reporting the distribution of their energy supply [Tang and Jain, 2011]

- VCG has been considered as a mechanism for allocating wholesale dispatch of electricity generation and consumption across a network:

  - such as between multiple network nodes with AC/DC links [Wang et al., 2020; Tang and Jain, 2013],
  - between multiple auctions for the supply of timely generation and ancillary services in a network [Greve and Pollitt, 2016; Wang et al., 2022; Sessa et al., 2017]
  - as a means of allocating power and payments between generators and storage providers (such as EV owners) across stretches of time [Satchidanandan and Dahleh, 2021; Valogianni, 2015; Xu and Low, 2017]
  - and/or all these at once [Seklos et al., 2020]

In this way there are many possible context of VCG's application, however there are also some interesting innovations on VCG in the electricity context, such as: VCG qualities can be improved is by considering mechanisms where VCG (or approximately VCG) payments are also in the Core (see Section 3.3.1) thus offering increased robustness properties against coalition strategising [Sessa et al., 2017; Karaca, 2020; Karaca and Kamgarpour, 2017]. Additionally there is specific VCG redistribution mechanisms discussed in the electricity context, particularly: such as using deep-learning to derive VCG redistribution rules in the context of EV bidding into a local energy market, as considered by Qian et al. [2022], or as a means of redistribution to minimise budget imbalance, such as described by Exizidis et al. [2019].

3.1.5 Summary and discussion of VCG

The VCG mechanism frames a elegant ethical schema for distributive payments and is directly applicable to electricity systems. Although it is incentive compatible, the primary practical draw-back to such a system is that it is not budget-balanced. Unfortunately there is no easily implementable system that is like VCG which is incentive compatible and budget-balanced without forcing participants to potentially trade at a loss.

Notwithstanding it is a possible scheme for the trading of electricity and electric resources, and in the following chapter we will compare the allocations of power/-money in randomly generated networks under VCG against other schemes.

One of the most central features about VCG, is that it is one of the most direct expressions of marginal payments - in that each participant is payed the marginal difference their presence causes to the well-being of the other participants in a utility maximising process. This marginal difference consideration is shared by two other solutions of this chapter, particularly Locational Marginal Pricing (LMP) (section 3.2) and Shapley Value (section 3.3.2).

One of the most notable qualities of VCG is that when it is scaled up to large numbers of participants (and no specific participants are particularly influential) then VCG often limits to another solution concept called Locational Marginal Pricing, which often is budget balanced — see Nath and Sandholm [2019]; Tanaka et al. [2018].

3.2 Locational marginal pricing

In Section 2.2.5 we briefly considered the notion that the morality of a transaction could be framed with respect to the normal market prices. There is potentially no greater framework for describing nominal market pricing in economic thought more influential than the concept of the *margin* or more specifically *marginal pricing*.

The idea that normal market trading should have any relation to moral trading was seen in John Locke's short essay Venditio where it is argued that a fair price for something is simply its normal market price at its location.[1] John Locke argues for this thesis, by considering that negotiating above market price for a good would be unethical primarily because any transaction would be taking advantage of ignorance or special circumstances of the buyer. Conversely, negotiating below market price for a good would only incentivise reselling and allow others to profit at the original seller's loss, or alternatively, that selling below market price only to those who are needy is certainly a charity and hence cannot be required by justice. By these considerations, justice only requires offering no more than the same nominal market price for everybody.

While John Locke's arguments may or may not be convincing, it is useful to consider the transactions and pricing that would occur under idealised or norma-

[1] "... the market price at the place where he sells. Whosoever keeps to that in whatever he sells I think is free from cheat, extortion and oppression, ..." [Locke and Wootton, 2003]

tive euvoluntary trading as these prices might be considered moral in-themself (by Locke's argument), or provide a back-drop for the framing of more moral trading. In section 3.4 we consider mathematical schemas used to describe idealised normative bargaining between small numbers of participants, but in this section we describe some economic theory that has been used to describe normalised trading between large numbers of market participants.

Historic economic thought lends consideration to the idea that market prices can be described by combinations of factors, not limited to, supply and demand functions, market uncertainty, production costings and transport tariffs etc. and the combination of these may be related to the pricing and subsequent trading of the goods. However, the way in which these factors have been seen to influence (or define) economic value has changed over time.

3.2.1 A brief summary on the history of value

In the history of economic thought, there was some general idea that the economic value of something (and hence its normal market price) should, in some way, be related to its usefulness in fulfilling human needs (however fickle or not) as things which are utterly useless seldom fetch any price. But, above this, there was a difficulty explaining how it was that things which were most useful to satisfying needs often had little economic value, and things which were more useless were sometimes most economically valuable. This apparent contradiction is known as the water-diamond paradox, best put by Adam Smith:

> "The word VALUE, it is to be observed, has two different meanings, ... The things which have the greatest value in use have frequently little or no value in exchange; ... Nothing is more useful than water; but it will purchase scarce any thing; ... A diamond, on the contrary, has scarce any value in use; but a very great quantity of other goods may frequently be had in exchange for it." [Adam Smith, 1776]

In answer to this, there was promoted the idea that economic value reflects labor, as water is easy to procure but diamond is not so. This 'labor theory of value' was held by many authors (including Adam Smith[2], David Riccardo[3], and many others) but most notably by Karl Marx:

> "It suffices to say that if supply and demand equilibrate each other, the market prices of commodities will correspond with their natural prices, that is to say with their values, as determined by the respective quantities of labour required for their production" [Marx et al., 1965, Chapter 2]

[2] "The real price of every thing, what every thing really costs to the man who wants to acquire it, is the toil and trouble of acquiring it."Adam Smith [1776]

[3] "The value of a commodity, or the quantity of any other commodity for which it will exchange, depends on the relative quantity of labour which is necessary for its production..."[Riccardo, 1817, Section 1, Chapter 1]

And this idea, that the quantity of labour should (in some way) define market prices at market equilibrium, was subject to analysis and verification. But ultimately the question of how to transform volumes of labour into competitive market prices became a difficult problem known as the 'Transformation Problem'.

However, the various utilitarians of the 19th century viewed utility not only as a direction of moral efforts, but as a fundamental drive of human behaviour[4], including market behaviours such as price setting; and ultimately, this perspective yielded a new explanation for economic value.

The utilitarian perspective sought to explain market dynamics in terms of people's efforts to maximise their own utility (or more practically, profit), and in this context stable (and hence normal) market prices were associated with the equilibrium of those efforts. This perspective yielded a link between market dynamics with the concept of the margin - or 'marginalism'.

Although the concept of the margin was evidenced in some writings in the earlier half of the 19th century (such as in the works of Jules Dupuit and Hermann Heinrich Gossen), it took to the end of the century for the idea to become more thoroughly developed - see Stigler [1950]. Although there was much discussion about the relationship between the labour theory of value and marginalism at the end of the 19th century (such as reported by Steedman [2003]) ultimately marginalism was adopted mainstream in the so-called 'marginal revolution', which has been identified (such as by Screpanti and Zamagni [1995]) as defining the beginning of neoclassical economics.

The marginalist revolution saw that economic prices were not just equal to the summation of normal production costs[5] (ultimately depending on the value of labor), but instead depended on the cost of production of the most marginal unit produced to meet demand.

3.2.2 A sketch of marginalism

The idea of marginalism is best illustrated with a graph, in Figure 3.1 there is an illustration of a hypothetical market for a particular economic good, with many suppliers and many buyers. In the figure we have the plotted the 'Supply curve', identifying how many units of the good could be sustainably supplied to the market if the units sold for a particular price. And we also have the 'Demand curve', identifying how many units of the good would natrually be sold depending on the price which the goods sold at. So for instance, at \$30 sale price per good, the market would be able to reliably support the production of ~ 7 goods, and the demand would be ~ 23, identifying a situation of unmet demand.

[4]for instance see Bentham: "Nature has placed mankind under the governance of two sovereign masters, pain and pleasure. It is for them alone to point out what we ought to do, as well as to determine what we shall do."Bentham [1823]

[5]Such as promoted by Riccardo, "The real and ultimate regulator of the relative value of any two commodities, is the cost of their production, and neither the respective quantities which may be produced, nor the competition amongst the purchasers."Riccardo [1817]

In this way, if the market is functioning ideally, then there is only one sensible outcome: that the goods should be sold in the number (and therefore at the price), that is at the intersection of the supply and demand curves - ie. the marginal price point. For if there were more goods produced, then those excess units would be unsold hence their production would be unprofitable, and if there were less goods produced, then there would be unmet demand which would spur more production. The graph shown might be indicative of a market for a finite resource (where increasing supply costs more), and where there is decreasing demand with increasing price.

Different sellers may choose different prices in a realistic market, however in this idealised situation where everybody is selling at the marginal price point, if any small individual seller tried to deviate from this price then it would be a disadvantageous for them. For instance, If a seller tried to set a higher price than the marginal price then it would result in a failure to sell, or if a seller set a lower price then it would only result in less profit. In this way, the marginal price point identifies an equilibrium of peoples utility (or profit) maximising efforts.

This kind of marginal analysis is a short sketch of the analysis and treatment in modern microeconomic texts (such as Vohra [2020]). This marginalist analysis is also widely regarded to resolve the water-diamond paradox, in that water is cheap because its marginal unit is cheap to produce.

Over time the marginalist synthesis was developed more comprehensively in the presence of many discussions and criticisms. Particular criticisms attack the academic assertion that market participants are psychologically driven by rational utility maximisation (such as Stigler [1950])[6], and the more pragmatic assertion that markets are approximately ideal and tend towards the stability of equilibrium (such as Keen [2011])[7].

Notwithstanding, one of the most notable features of this neoclassical analysis is that the equilibrium marginal price point also maximises the sum of utility of those that participate in the market. This can be seen from Figure 3.1 where all the buyers who value the goods the most are provided from all the sellers who can supply those goods at lowest cost up until the marginal point where no further trade is viable.

This point of utility maximisation is seen in Neoclassical analysis more generally, where market equilibrium prices (at and/or between markets) occur at the point of the maximisation of the sum of utility. Indeed, the process of mathematically deriving these marginal prices developed into a kind of calculus, where the marginal prices fall out as Lagrange multipliers in the process of maximising the sum of utility.

To see this, consider the curves in figure 3.1 where the Demand function is $D(x) = \frac{40}{1+(x/40)^2}$ and the Supply function is $S(x) = 20(x/40)^2$.

[6] individual traders may be partially driven by irrationality such as fear, ignorance, gambling

[7] as might be most directly witnessed in markets where is inherent uncertainty, notably in speculative markets such as stocks, housing and crypto-currency

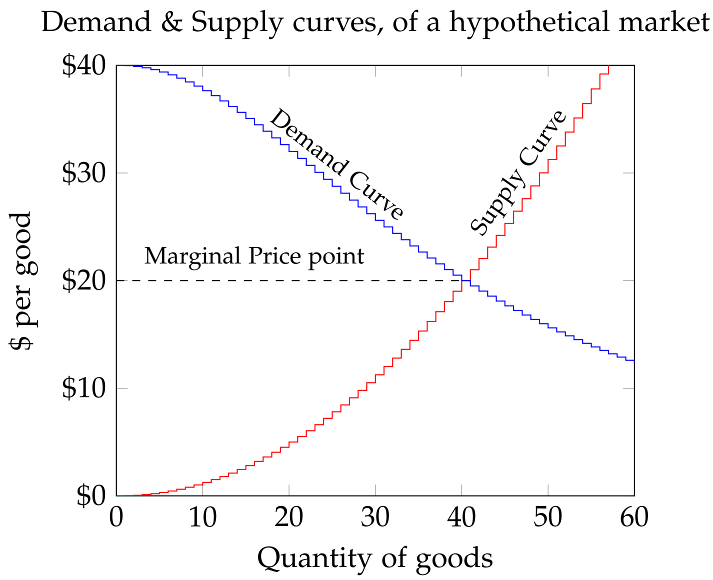


Figure 3.1: The Demand and Supply curves of a hypothetical market.

From these functions[8] we construct the utility of the buyers and sellers as:

$$U_d(x) = \int_0^x \frac{40}{1+(z/40)^2} dz \qquad \text{and} \qquad U_s(x) = -\int_0^x 20\left(\frac{z}{40}\right)^2 dz$$

In this context $U_d(x)$ represents the sum of utilities of the buyers for x goods sold to them[9] and $U_s(x)$ represents the sum of costs suffered by the sellers for x goods produced by them[10].

If the amount of the goods bought is a and the amount supplied is b then we can construct the utility function as $U(a,b) = U_d(a) + U_s(b)$ and to maximise this subject to the conservation constraint $a = b$, we use lagrange's method of multipliers, and form lagrangian: $L(a,b,\lambda) = U_d(a) + U_s(b) + \lambda(b-a)$

$$\frac{\partial L}{\partial a} = \frac{40}{1+(a/40)^2} - \lambda = 0 \qquad \text{thus:} \qquad a = 40\sqrt{40/\lambda - 1}$$

$$\frac{\partial L}{\partial b} = -20\left(\frac{b}{40}\right)^2 + \lambda = 0 \qquad \text{thus:} \qquad b = 40\sqrt{\lambda/20}$$

[8]We could, more directly, observe that by solving $S(x) = D(x)$ we get $x = 40$.

[9]The equation is an integration because, if x is zero, then the utility of the buyers is zero because there are no goods transacted, if x is 1 we might imagine that the good goes to the buyer who values it the most and whose utility is given the maximum leftmost point on the demand curve, if x is 2 then the utility of the buyers is the sum utility of the one who values it the most and the second most, if x is 3 then it is the sum of utilities of the 3 most buyers, etc.

[10]The equation is an integration because, if x is zero, then there are no goods produced and no costs to the sellers, if x is 1 then we might imagine that the good was produced by the cheapest seller, who's cost is given by the leftmost point on the supply curve, if x is 2 then the utiltiy is the sum of costs of the two chepest sellers, etc.

substituting into the constraint $a = b$ gives $\lambda = 20$ and thus $a = b = 40$
In this way the Lagrange multiplier on the conservation constraint gives the marginal price of the good - which is also called the 'shadow price'.

The general development of the mathematics is slightly beyond our scope here, but the general process is:

1. Formulate the utility function from all the market participants, including all variables

2. Form an optimisation problem for utility maximisation with appropriate conservation constraints

3. Solve the optimisation problem, and record the Lagrange multipliers of the conservation constraints as shadow prices.

This process, of using calculus to determine nominal prices has been proposed in the electricity space - such as by Scott and Thiébaux [2015]; Tang and Jain [2013]; Parhizi et al. [2017]; Tang and Jain [2015]. Particularly as the process of maximising utility on an electricity grid is a well known problem called the 'Optimal Power Flow' problem (OPF), where the power conservation constraint at each bus of the network, identifies the marginal price of electrical power on that bus. This particular scheme is called 'Locational Marginal Pricing' (LMP); and we will investigate and compare against it against other solutions in section 4.4.

Particularly, we note that LMP has been implemented for real-time-pricing of transmission power in some existing electricity systems - such as reported by Wang et al. [2015]; Holmberg and Lazarczyk [2012]. And that although LMP is like VCG in that it is ultimately not budget balanced, unlike VCG there are specifically identifiable cases where budget imbalance occurs, particularly in the context of network *congestion* - see Tang and Jain [2013].

3.2.3 Applications of Locational Marginal Pricing to electricity systems

In the historical context of power systems, one of contested and contrasted options in electricity market structure was Discriminatory/Pay-As-Bid-Pricing and Uniform/Marginal Pricing.[Wolfram, 1999; Ren and Galiana, 2004; Haghighat et al., 2012; Griffin and Puller, 2009; Necoechea-Porras et al., 2021; Fabra et al., 2002] In the electricity market context, generator companies 'bid' into a system an offer consisting of what amount of power/s they can supply and at what amount they expect to be paid for the respective dispatch. This can occur in a day-ahead market structure, where a central and Independent System Operator (ISO) collects bids and accepts them to meet anticipated demand the following day. The primary question between Pay-As-Bid and Marginal Pricing is if the generator companies who's bids are accepted should simply be paid their monetary bid amount, or should directly be paid the cost of the marginal unit of power dispatched.

While it may initially seem as if Pay-As-Bid pricing would be most reasonable, it is demonstrated that strategic equilibrium in the bidding of generator companies should ideally yield the respective Marginal Pricing values anyway (as already indicated in section 3.2.2 and demonstrated in Klemperer [1999]). In this way, the question between Pay-As-Bid and Marginal Pricing is if the market operator should shortcut the strategising of generator companies, and thus afford the marginal prices directly.

This discussion between Pay-As-Bid-Pricing and Marginal Pricing was mostly discussed throughout the deregulation process of electricity networks that occurred in many countries throughout the 80's to the 2000's [Joskow, 2008], and was also reconsidered in the aftermath of the California electricity crisis. [Kahn et al., 2001a,b] However, in real terms, Marginal Pricing of some sort is more the commonly implemented rule, as opposed to Pay-As-Bid, and a centralised Marginal Pricing rule is a direct precursor to a locationally variant Marginal Pricing rule - that is, Locational Marginal Pricing (LMP).

However with the implementation of LMP, there are additional factors that may need to be addressed in practical settings, such as:

- LMP schemes can be considered to various levels of refinement, such as between zonal and nodal levels [Wang et al., 2015; Holmberg and Lazarczyk, 2012] where the degree of refinement and the boarders between zones potentially have practical and social consequences, and influence computational difficulty in the calculation.

- LMP is inherently built upon an electrical network optimisation scheme which potentially includes various elements of complexity. For instance, LMP prices can be built upon a DC approximation model of electricity flow (it computationally the more simple), but in principle various AC models (and their relaxations) are possible candidates. [Wang and Hijazi, 2018]

- LMP method does not directly incorporate or account for discontinuous variables. This factor is most notable in the Unit Commitment (UC) stage of generators scheduling to meet demand, as generator state cannot always be continuous (such as on/off state). For these discontinuous parameters, LMP prices can be supplemented by side payment methods to support the dispatch of power. There exists discussions about different schemes to calculate and organise these side-payments. [Eldridge et al., 2020; Johnson et al., 1997]

- Locational Marginal Prices vary over time and between zones/nodes of the network which are subject to congestion and whereby congestion rents are extracted. These congestion rents need to be redistributed and secondary markets may be implemented for these as a consequence, notably Financial Transmission Rights (FTR) auction processes. Financial Transmission Rights are financial instruments which ISOs offers to generator companies to hedge against LMP volatility [Zakeri and Downward, 2010], these FTRs then alter the pricing landscape in electricity network context which then has potential secondary effects. [Wu and Zheng, 2022]

- LMP is static for a single timeframe and is not completely incentive compatible, and these factors yield real world strategising in electricity markets [Hu et al., 2005; Dungey et al., 2018], and this is most notably true around the mechanism of revising bids or 'rebidding', over a finite time horizon [Scott and Thiébaux, 2019].

- LMP is tacitly based on full and static information, and although there is some attempt to integrate uncertainty into the marginal price mechanism itself Fang et al. [2021]; Mieth and Dvorkin [2020], there is a broader discussion about different ways to accommodate uncertainty from historical data into the design and operation of electricity systems generally [Riaz et al., 2022]. In-practice the value of short-term demand/supply uncertainty and imbalance is not reflected in Locational Marginal Prices, but can be addressed via secondary ancillary support markets - such as providing frequency stability.[Ela et al., 2016]

These considerations extend primarily from there being factors (discontinuous, diachronic, probabilistic, etc.) that are outside of the Marginal Pricing calculus that cannot (or are not often, or easily) incorporated, thus adding to the complexity of LMP in real-world markets. Notwithstanding these considerations, LMP has particular advantages such as its ability to be computed and its linkage to economically relevant rationale, that means that it is actually implemented over other schemes in practice [Holmberg and Lazarczyk, 2012], and serves us as a benchmark to compare other schemes against.

3.2.4 Summary and discussion of Locational Marginal Pricing

Locational Marginal Pricing is a historic example of an economic framework of integrating market conditions (supply and demand information) to give equilibrium price points. It can be seen to provide a description of normal trading value, and thence (perhaps) moral trading value.

Locational Marginal Pricing and VCG provide some of the most direct expressions of Marginalism as a concept, and (as considered in section 3.1.5) one can limit to the other for large markets. Particularly VCG rewards participants with economic incentives equal to their direct impact on group wellbeing above their absence, whereas Locational Marginal Pricing can be seen as providing participants with economic incentives in proportion to their presence's marginal (or incremental) impact on group wellbeing.

With VCG it is directly considered what the notion of absence means, particularly the direct difference the presence of a participant makes is in relation to the affect the participant's utility brings upon the social utility maximum. However the notion of absence under LMP may be less clear; the marginal prices are the rate of incremental utility value of additional goods at the respective location, which in turn is the incremental rate that each participant's presence brings at that location.

In the following chapter 4, LMP and VCG are implemented and the differences between the two can be witnessed.

Both LMP and VCG root their concept of value in the idea of marginal contribution implicitly with respect to some notion of absence. However, in other contexts it may not be clear what this means, in section 3.4 we outlay some solutions concepts which which embrace this ambiguity.

However before we move to section 3.4, we notice that both LMP and VCG only treat every player individually, but neglect any consideration of possible groups of players and their influence. And so, in the next section 3.3 we consider solution concepts which explicitly consider groups and their marginal contributions.

3.3 Cooperative game theory

In section 2.2.5 we considered the idea that groups of people could be afforded what they could achieve 'by themself'. And this idea is most directly articulated by the *Core* of cooperative game theory. In that same section we also mentioned the idea that people could be rewarded for their contribution under uncertainty about the presence of other group members, and that this idea was most directly articulated by the *Shapley Value* of cooperative game theory.

Both of these ideas directly or implicitly consider possible groups and how much value each group has 'by itself', and this is directly the ground of cooperative game theory.

The basic elements of a classic cooperative game are that there is a set of players or individuals $N = \{1, 2, \ldots n\}$ and a function $v : S \subseteq N \to \mathbb{R}$ with $v(\emptyset) = 0$ called the *characteristic function*. The characteristic function identifies in some sense the 'worth' or 'value' of any group of players (a 'coalition') which might be interpreted in terms of utility or monetary value. In this context, one aim of cooperative game theory is to develop schemes (or 'solution concepts') which split the wealth achieved if everybody cooperated (that is $v(N)$) between all the players.

Fundamentally, this kind of analysis hinges on there being a clearly defined concept and determination of the value of each possible group (ie. the characteristic function), however it is not always the case that there is such a clearly defined notion. Consider the words of Lloyd Shapley about the characteristic function:

> "The idea is to capture in a single numerical index the potential <u>worth</u> of each coalition of players...
>
> With the characteristic function in hand, all questions of tactics, information, physical transactions, etc., are left behind. The characteristic function is primarily a device for dividing the difficulties – for eliminating as many distractions as possible in preparation for the confrontation with the indeterminacy of what we have called the "n-person problem". Engrossed with this problem, many authors writing after von Neumann and Morgenstern have begun by basing their solution concepts on the characteristic function above, with no initial concern for the concrete rules of the game, in strategic or extensive form.

> Unfortunately, not all games admit a clean separation between strategic and coalitional questions, and for those that do not the characteristic function approach must be modified or abandoned."
> [Shapley and Shubik, 1973]

In this light, there exist situations where the 'worth' of a coalition may be ambiguous such as where there are strategic considerations between possible coalitions, and there is no uniquely defined value that members of a coalition could/would achieve. However, some situations do cleanly admit a definable 'worth' for groups of individuals, for instance, the Characteristic function may identify the amount of money that members of a coalition could, and unambiguously would, achieve by working for themself irrespective of the actions of those not belonging to the coalition.

In these cases, if everybody works together to achieve some maximal sum of money there are a set of possible ways the money can be divided between everybody. One of the most natural divisions is that every subgroup should be given at least more than they could feasibly achieve by working for by themself as a group. And this is an allocation most naturally described by the *Core*.

3.3.1 The Core

The Core is an example solution concept for cooperative games, in that for any set of players $N = \{1, 2, \ldots n\}$ and any characteristic function $v : S \subseteq N \to \mathbb{R}$ with $v(\emptyset) = 0$, the Core is a set of possible payoff allocations to each of the players $C(v)$ in which each subgroup is given at least the value of the characteristic function for that subgroup:

$$C(v) = \left\{ x \in \mathbb{R}^n : \sum_{i \in N} x_i = v(N); \sum_{i \in S} x_i \geq v(S), \forall S \subseteq N \right\}$$

The Core is the set of possible allocations such that for any group of individuals, the sum allocated to the group is greater than what the group could achieve by working by themself. The allocations in the Core might be seen to have a kind of stability property - in that no coalition would have an incentive to leave the grand coalition. One major drawback about the Core is that it does not determine a unique outcome, but potentially a range of outcomes or potentially none at all, depending on the cooperative game.

Indeed the Core may be empty, and in this case no solution can have the same kind of desirable stability, however there are alternative allocations that minimise this shortcoming. Most notably, the *least-Core* solution concept.

The least-Core solution concept is a particular instance of the *strong* ϵ *Core* which is very similar to the Core, and is defined as follows:

$$C_\epsilon(v) = \left\{ x \in \mathbb{R}^n : \sum_{i \in N} x_i = v(N); \sum_{i \in S} x_i \geq v(S) - \epsilon, \forall S \in N \right\}$$

The strong ϵ core is the set of allocations in which each coalition is allocated atleast their value minus some constant ϵ. The strong ϵ Core can be defined for positive and negative ϵ values, it will certainly be non-empty for very large and positive ϵ values and certainly be empty for very negative ϵ values. In this way we can consider the limiting case between these two, the smallest value of ϵ in which the strong ϵ Core is non-empty — and this is the least-core, see Maschler et al. [1979]. The least-core is therefore always non-empty and may even identify a singular solution point, which that can be said to identify the point of minimum 'dissatisfaction' between the groups.

The Core is an intuitive solution concept in the context where the characteristic function identifies the 'worth' of individuals and groups 'by-themself' and the dynamics are driven by this isolation mechanic. However in other cases the 'worth' identified by the characteristic function may be in the context of cooperation with the others. And in this context the Core is not the only solution concept worth considering.

3.3.2 The Shapley Value

The *Shapley Value* is another specific and well known solution concept in cooperative game theory. Particularly the Shapley Value allocates to each individual the average contribution they would add across the possible coalitions to which they could join.

Particularly, for any coalition S which does not include a player i, then player i's marginal contribution is $v(S \cup \{i\}) - v(S)$. If we average such contributions for coalitions of size k:

$$\hat{v}_{i,k} = \frac{1}{\binom{n-1}{k}} \sum_{S \subseteq N \setminus \{i\}, |S|=k} (v(S \cup \{i\}) - v(S)) \tag{3.3}$$

Then we have the average marginal contribution of player i to coalitions of size k, and if we average this over coalitions of different size, we get the Shapley Value:

$$\varphi_i(\langle N, v \rangle) = \frac{1}{n} \sum_{k=0}^{n-1} \hat{v}_{i,k} \tag{3.4}$$

Or more directly as:

$$\varphi_i(\langle N, v \rangle) = \sum_{S \subset N, i \notin S} \frac{(n - |S| - 1)!\, |S|!}{n!} (v(S \cup \{i\}) - v(S)) \tag{3.5}$$

The Shapley Value is an averaging over a players marginal contributions, which is thus a unique allocation for any cooperative game.

The Shapley Value for a player can also be formulated as being the expected marginal contribution across all join ordering processes. So for instance, if we let $\pi(N)$ denote the set of all ordered permutations of the player set N and if we denote $Pre^i(O)$ as the set of predecessors of player i's addition in that ordering $O \in \pi(N)$.

Then the Shapley Value can be expressed as the average marginal contribution across orderings, see Weber [1988]:

$$\varphi_i(\langle N, v\rangle) = \frac{1}{n!} \sum_{O \in \pi(N)} v(Pre^i(O) \cup \{i\}) - v(Pre^i(O)) \tag{3.6}$$

In this way the Shapley Value for a player can be directly expressed as the average marginal contribution across possible join order processes.

The Shapley Value has perhaps some moral intuition behind it - rewarding each person in proportion to what they would add across any ordering that the coalition could form. But more than that, the Shapley Value has been derived from different sets of quite intuitive axioms. For instance:

- **Efficiency**: That the total dividend is broken up, $\sum_i \varphi(\langle N, v\rangle)_i = v(N)$
- **Symmetry**: If two players i and j are substitutes and contribute the same to all coalitions, such that if $v(S \cup i) = v(S \cup j) \quad \forall S \subseteq N \setminus \{i, j\}$, then $\varphi(\langle N, v\rangle)_i = \varphi(\langle N, v\rangle)_j$
- **Dummy Player**: A player i is a dummy player if the amount that i contributes to any coalition is the amount that i is able to achieve alone (i.e. $v(S \cup \{i\}) - v(S) = v(\{i\}) \;\; \forall S \subseteq N \setminus \{i\}$) then $\varphi(\langle N, v\rangle)_i = v(\{i\})$
- **Additivity**: That for any two games, the imputation for the two together is the sum of the imputations in each, for any v_1 and v_2, $\varphi(\langle N, v_1 + v_2\rangle) = \varphi(\langle N, v_1\rangle) + \varphi(\langle N, v_2\rangle)$

These axioms might seem pretty reasonable and they lead uniquely to the Shapley Value allocation - per Shapley [1953]; additionally there are other possible sets of axioms which also lead to the Shapley Value aswell. These axioms (particularly Efficiency and Symmetry axioms) relate directly to morally relevant points raised in the philosophy chapter 2 (Efficiency and formal equality conditions respectively).

In considering the Shapley Value, there is the additional question of when the Shapley Value is in the Core - and thus has that particular stability that would disincentivise any subgroup from leaving. One example case where the Shapley Value is always in the Core is the case of Convex cooperative games, see [Chakravarty et al., 2014, Chapter 6]: A cooperative game is *convex* if the value that two coalitions together has is greater than the value of their parts minus the value of their intersection, ie. iff:

$$\forall S, T \subset N \quad v(S \cup T) \geq v(S) + v(T) - v(S \cap T) \tag{3.7}$$

Which is potentially a common condition in which each coalition is informally 'greater than the sum of its parts'. We consider an example:

Example. Consider player set $N = \{1, 2, 3\}$ with characteristic function:
$v(S) = (\prod_{i \in S} i) - 1$ (ie. the multiplication of their player numbers minus one).[11]

[11] We are assuming that the product over an empty set is one.

Solve for the Shapley Value, and show that it is efficient and also in the core.

Solution. To calculate the Shapley Value for player C, we consider the marginal contributions it can make to other coalitions:
$v(\{C\}) - v(\emptyset) = 2 - 0 = 2, \quad v(\{C,A\}) - v(\{A\}) = 2 - 0 = 2$
$v(\{C,B\}) - v(\{B\}) = 5 - 1 = 4, \quad v(\{C,A,B\}) - v(\{A,B\}) = 5 - 1 = 4$
Thus the Shapley Value for player C is: $\varphi_C = \frac{1}{3}\left(2 + \frac{1}{2}(2+4) + 4\right) = 3$, and contiuing for the other players gives: $\varphi_A = 0, \quad \varphi_B = 2$
The Shapley Value is efficient as: $\varphi_A + \varphi_B + \varphi_C = 5 = v(\{A,B,C\})$
and also in the Core, as it is true that:
$\varphi_A + \varphi_B = 2 \geq v(\{A,B\}) = 1$
$\varphi_A + \varphi_C = 3 \geq v(\{A,C\}) = 2$
$\varphi_B + \varphi_C = 5 \geq v(\{B,C\}) = 5$
It is also simple enough to verify that the cooperative game is convex.

3.3.3 Summary and applications to electricity systems

Cooperative game theory concepts centre on the consideration of groups and how reward or surplus utility should be divided among members, and particularly the Shapley Value is most famous.

Indeed the Shapley Value has been considered as a potential mechanism for pricing in the various facets of electricity system operation. Such as:

- Credits in demand response participation [O'Brien et al., 2015; Khalid et al., 2019; Wang et al., 2019]
- Compensation for the aggregation of power [Perez-Diaz et al., 2018; Baeyens et al., 2013]
- Allocating transmission costs and losses [Tan and Lie, 2002; Sharma and Abhyankar, 2017]
- Dividing profits for retailers and [Acuña et al., 2018; Wang et al., 2019]
- Allocating surplus and savings in microgrids [Wu et al., 2017; Lo Prete and Hobbs, 2016]
- Sharing costs in distribution and embedded networks [Chapman et al., 2017; Chiş and Koivunen, 2019; Bremer and Sonnenschein, 2013; Lee et al., 2014; Han et al., 2019; Azuatalam et al., 2019]

In each of these cases, the primary difference is the context of application and the specific way in which the characteristic function is constructed.

The Shapley Value has notable strengths and weaknesses, particularly the simplicity of its axioms have obvious appeal, and similar to LMP and VCG it is a more expansive marginalist approach (as it is expressible the an average over a larger range of marginal contributions by equations 3.4 or 3.6). However a primary drawback of the Shapley Value in practice is the difficulty of computing it as calculating all of the marginal contributions of all players to the $2^n - 1$ possible coalitions is identified as being rapidly difficult to scale to sizes of participants on realistic networks. This drawback has attracted attention and attempts at remediation, such as employing techniques of sample-bassed approximations (see citations in Section 6.6) or approaches that employ techniques like player clustering Han et al. [2019].

Shapley Value approaches may or may-not suffer other disadvantages depending on context, such as being incentive incompatable, privacy preserving, or having envy-freeness, however the primary weakness of the Shapley Value approach is that it only applies when there is a coherent conception of a characteristic function. That is, (as identified in the quote by Lloyd Shapley at the beginning of this section 3.3) cooperative game theory is most applicable when the 'worth' or 'value' of a coalition is unambiguous, and when specific strategic considerations between the coalitions are unimportant (or are otherwise accounted for). Unfortunately in a meshed electricity network with a confluence of electricity details and a range of strategies available to each of the participants, such a notion of 'worth' may not be very obvious. Thus in the next section 3.4 we consider some solution concepts which apply in circumstances where it is not easy to describe the 'worth' or 'value' of a coalition of players; where strategic considerations between them are important and it is not easy to make sense of a characteristic function. Particularly, we describe bargaining solution concepts.

3.4 Bargaining solution concepts

In our discussion of Locational Marginal Pricing in section 3.2, we considered one way of describing normalised pricing in large markets. However in this section we consider some of the various ways of describing normalised pricing among a small number of market participants where their individual strategic options are relevant.

Particularly, we consider the situation where there are a small numbers of market participants negotiating over a set of possible outcomes. In this context we consider the question about what the likely outcome of an idealised bargaining process would be.

We begin with one of the most historic classes of bargaining solution concepts, particularly Nash bargaining with endogenous disagreement outcome.

3.4.1 Nash bargaining with exogenous disagreement point

A bargaining solution concept applies in a situation where there are a number of parties (or agents, or market participants) and a space of possible outcomes which those agents can reach by bargaining and which each of them may value differently. In this context, a bargaining solution concept identifies an outcome, which may be interpreted as one which the agents 'will' (or 'should') reach. Perhaps the most famous bargaining solution concept is called the Nash-bargaining solution concept.

Nash bargaining was introduced by John Nash [Nash, 1950] as an axiomatic approach to predict the normal result of idealised bargaining over potential outcomes. It is defined over a set of potential outcomes F where each of the players

$P = \{p_1, p_2, \dots\}$ value the outcomes differently with utilities $u_{p\in P}(f)$ for $f \in F$. Additionally there is a privileged outcome called the 'disagreement' outcome d which represents the event of the negotiation between the players breaking down, and which any player can unilaterally implement.

Nash identified that in this case there is a unique solution satisfying some very intuitive axioms:

- *Invariant to affine transformations*: that the solution should not change if the utilities of any of the players are scaled (by some positive factor) or offset, ie that they are invariant under the set of affine transformations
- *Pareto optimality*: That there will not exist another solution point that is weakly better than the solution for all players, and strongly better for atleast one player.
- *Independence of irrelevant alternatives* (IIA): If any subset of potential outcomes does not feature the solution point or the disagreement point, then it could be removed from consideration without affecting the solution.
- *Symmetry*: The solution is invariant with regards to the ordering of the players.

Nash identified that this solution maximises the product of utilities above the utility of the disagreement point:

$$\mathrm{nash}(F, d) = \underset{(f \geq d) \in F}{\mathrm{argmax}} \prod_{p \in P} (u_p(f) - u_p(d)) \tag{3.8}$$

In many cases of physical bargaining (which might involve alternating offers etc.) the 'disagreement outcome' is seen (such as by Nash [1953]) to be often naturally dictated by the context of the bargaining process - such as the event of quitting in the context of a wage-negotiation or of walking-away from a potential sale - and can be seen as the point of 'threat' from which the bargaining process proceeds.

There has been much work since Nash published his famous paper [Nash, 1950] investigating other and/or similar solution concepts, and these bargaining solutions (such as Kalai and Smorodinsky [1975]; Balakrishnan et al. [2011]; Anbarci et al. [2002]) often relate to different axioms (most often rejecting axiom IIA) and privilege different points in the bargaining process.

One objection to the Nash bargaining solution is that it may not be considered natural or a reliable description of real-world bargaining. Although there does exist evolutionary models suggesting that Nash bargaining might naturally emerge in some social dynamics (such as modelled by Cho and Matsui [2013]), there also exists experimental work by Kroll et al. [2014] finding that real behaviour between humans exhibits ambiguity even in the case when the disagreement point is naturally given by the setting.

However in other cases (such as in an electricity network) a singular disagreement outcome may not be very clearly given by the context to begin with. And so for a Nash bargaining solution concept to be applied, a disagreement outcome must be chosen from the set of possible outcomes, which leads to the question of how this should be done.

3.4.2 Nash bargaining with endogenous disagreement point

In John Nash's paper "*Two-person cooperative games*" [Nash, 1953], He explicitly addresses the consideration of the agents choosing a disagreement point between themselves in a prior stage in the bargaining process.

Particularly he considers a game specifically between two players, who reach a cooperative outcome in a series of stages of negotiations. He considers that each of the players has a space of mixed strategies S_i in a normal form game, and for each possible pair of mixed strategies that the players might execute, each receives an immediate payoff $p_1(s_1, s_2)$ and $p_2(s_1, s_2)$ respectively ($s_1 \in S_1$, $s_2 \in S_2$). He also considers that there is a set B of possible payoffs for the players if they cooperate, which may be bigger than the set of payoffs in the normal form game.
ie. $\forall s_1 \in S_1, s_2 \in S_2 \quad (p_1(s_1, s_2), p_2(s_1, s_2)) \in B$

Nash then considers a specific negotiation process:

1. Each player i chooses a mixed strategy $t_i \in S_i$ that will be used if the two cannot come to an agreement - this is the threat.

2. The players inform each other of their threats.

3. Each player i decides upon a 'demand' d_i which is an amount of utility which they will not accept less than, without triggering the chosen threat.

4. If there is a point (u_1, u_2) in B such that $u_1 \geq d_1$, and $u_2 \geq d_2$ (ie. if there is a possible way the demands can be mutually satisifed), then the pay-off to each player i is d_i. Otherwise, the pay-off to each player i is given by the result of their threats, $p_i(t_l, t_2)$.

This process encodes a process that includes two choices for the players, first, they must choose a 'threat' strategy t_i which they will be forced to execute if they cannot reach further agreement, and secondly they need to choose a 'demand' d_i of the utility which they would like to receive from the negotiation. If it so happens that it is possible for the players to have their demands mutually met then they receive the utility associated with their demand, otherwise they receive the utility given by the actualisation of their threats.

Nash identifies that a natural choice of compatible demands in the second part of the game occurs at the maximising of the Nash product (Equation 3.8) above a disagreement point determined by the execution of threat strategies (as elucidated in the previous section 3.4.1) Nash then identifies that in light of this result for the second part of the game there exists a unique set of optimal choice of threats t_i for the two players in the first part of the game; which is a Nash equilibrium of them with respect to the subsequent maximisation of the Nash product.

Nash also identifies this result via axioms:

1. For each game (S_1, S_2, B) there is a unique solution $(v_1, v_2) \in B$
2. If (u_1, u_2) is in B and $u_1 \geq v_1$ and $u_2 \geq v_2$ then $(u_1, u_2) = (v_1, v_2)$
3. That order preserving linear transformation of utilities do not change the solution. ie. for games with all utilities scaled (ie $u_1' = a_1 u_1 + b_1, u_2' = a_2 u_2 + b_2$ for $a_1, a_2 \geq 0$) result in solution (v_1', v_2') where $v_1' = a_1 v_1 + b_1$ and $v_2' = a_2 v_2 + b_2$.
4. The solution does not depend on which player is player 'one', ie. all functions are symmetrical
5. If points from B are removed except (v_1, v_2) and the points $(p_1(s_1, s_2), p_2(s_1, s_2))$ for all strategies $s_1 \in S_1, s_2 \in S_2$ then the new game yields the same solution.
6. A restriction of strategies for a player cannot increase his/her resulting payoffs, ie. for $S_1' \subset S_1$ then $v_1(S_1', S_2, B) \leq v_1(S_1, S_2, B)$
7. There exists single (unmixed) strategies such that player one's value wont increase, ie. there exists s_1, s_2 such that $v_1(s_1, s_2, B) \leq v_1(S_1, S_2, B)$

These axioms are very similar to, but perhaps a little less obvious than Nash's game with exogenous disagreement point (as given in the previous subsection 3.4.1). Let us consider an example game for the calculation of Nash bargaining with endogenous disagreement point:

Example. Consider the matrix representation of the strategic normal-form game between two players (a row player and column player respectively):

$$\begin{bmatrix} 2,1 & -1,-2 \\ -2,-1 & 1,2 \end{bmatrix} \tag{3.9}$$

What is the Nash bargaining solution for this game, if the set of possible payoffs is only that which can be attained by mixed strategies?

Solution. We consider the space of possible payoffs between the players in the game for mixed strategies (see shaded region in figure 3.2) and note that if the pure strategy payoff $(-1, -2)$ within the shaded region was chosen as the threat point by the players (highlighted by a black point; corresponding to the payoff in game row 1 & column 2), then the subsequent payoff to the players would be $(2, 1)$, since it is the point within the shaded region that maximises the product of utilities above $(-1, -2)$ (per equation 3.8). We also observe that the $(-1, -2)$ is a Nash equilibrium as a choice of threat point, as if the column player chose the alternate column 1 instead, then the threat point would be $(2, 1)$ which would effect the same outcome, and if the row player chose the alternate row 2 then the threat point would be $(1, 2)$ which would be worse for the row player. In this way it is seen that $(2, 1)$ is the Nash bargaining solution for this game.

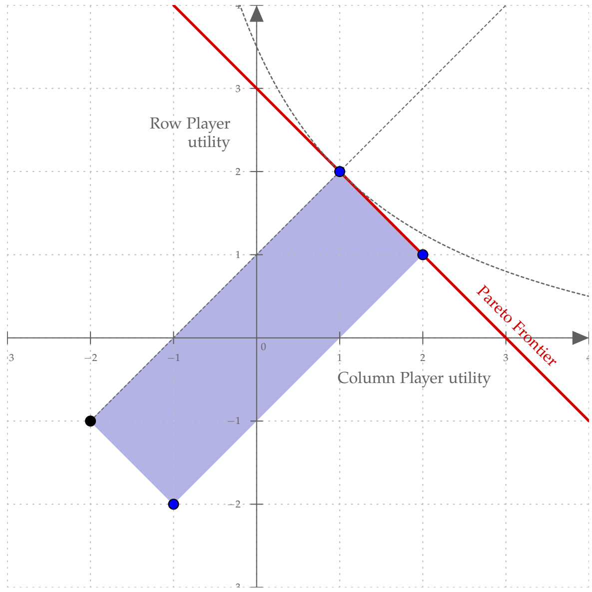


Figure 3.2: The potential outcomes for the TU example game (Equation 3.9), shown in blue, with a red Pareto frontier for transferrable utility, and nash product maximisation over a black threat point.

This illustrative example comes directly from the papers of Kohlberg and Neyman [2017, 2015], where it is explained that Nash's solution concept has a particularly simple form in games where utility is transferable (TU) (as has been identified multiple times Kohlberg and Neyman [2017]; Shapley [1984]; Kohlberg and Neyman [2015]).[12] The approach involves converting the normal form game (3.9) into a zero sum game by calculating the player advantage in payoffs, and our example zero sum game matrix is given by (3.10). If d is the minimax value of the zero sum game, and if s is the maximum sum of utility achievable in the normal form game, then the Nash bargaining solution is $(\frac{1}{2}s + \frac{1}{2}d, \frac{1}{2}s - \frac{1}{2}d)$.

$$\begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} \tag{3.10}$$

Solution (TU approach)**.** From (3.9) we see that the maximum sum of utility achievable between the players $s = 3$. Then we compute the minimax value of the zero sum game (3.10), $d = 1$ Which indicates that the row player has a greater threat power. The Nash bargaining solution between the two players gives them utility as $(\frac{1}{2}s + \frac{1}{2}d, \frac{1}{2}s - \frac{1}{2}d) = (2, 1)$

It may seem to be a bit difficult to see how these two approaches are related at first glance. However, it can be realised that in the context of selecting a threat point (for a TU game), all that matters is the player's payoff advantage over their opponent. This fact can be seen by inspection of Figure 3.2, where maximising the

[12] It also coincides with the 'coco-value' in the case of complete information [Kalai and Kalai, 2013, 2010].

Nash product over a threat point places the final payoff point directly above and to the right (on the Pareto frontier) at a 45 degree angle. In this context, the threat point only matters to the players insofar as it serves to moves the resulting payoff point along the Pareto frontier. The Pareto frontier defines the sum of player payoffs to be distributed, and hence the threat point only defines the difference of how much is distributed to one player over another - ie. their payoff advantage. We also note that for these bargaining solution concepts, that there is a way in which an 'individual rationality' property can be guaranteed, specifically, if both players have the ability to unilatterally implement zero utility for themself, then any disagreement point must be in the first quadrant, guaranteeing non-negative final utility for both parties.

3.4.3 Discussion of Nash bargaining concepts

In this section we considered some bargaining solution concepts, particularly Nash's bargaining solution concept which gives an outcome that implicitly incorporates all the possible influences which the players can bear upon each other. The solution concept for games of transferable utility (TU) depend primarily on the minimax of payoff advantages between the players. In this way payoff advantage is considered as a measure of the strength of a player's bargaining position.

Nash's bargaining solution was principally suited for 2 players, however some extensions of it to many players have been developed. In the following Chapter 4 we develop these extensions of Nash's bargaining solution concept into a scheme applicable to electricity networks called the GNK value.

However, the contemplation of Nash bargaining solutions leads to the question of whether 'threat' strategies should (or would) naturally play a role in the division of resources - such as in an electricity system.

Nash bargaining solutions are a primary example of a solution concept that explicitly considers the direct selection of possible 'threat' strategies for the players, and how these might bear on the result of cooperative negotiations. This consideration contrasts against the LMP, VCG and Shapley Value concepts where the implicit reference point for each player may be interpreted as an articulation of their absence from cooperation - which may also be interpreted as a 'threat'. However, unlike these other concepts, Nash bargaining with endogenous disagreement point removes any ambiguity and explicitly selects the point that would correspond to a failure of cooperation.

The moral ideas surrounding proportionality (per section 2.2.5) suggest that monetary compensation should be defined in relation to reference point/s, and Nash bargaining is one example solution concept that explicitly selects such a reference point; the question therefore is whether this selection process is the right one.

Nash bargaining attempt to mathematically identify outcomes that are a cooperative result underpinned by perfect competition under equilibrium, and hence can potentially serve as a description of normalised and idealised trading; In more realistic contexts, the selection of moral reference points may be influenced by a range of moral or practical factors, and we can ask, when an equilibrium of 'threat' strategies would bear practical relevance. Particularly it is identified by Nash that the role of threats in negotiations depends on a dynamic about their ability to be plausibly enforced.

> "A common device in negotiation is the threat ... If one considers the process of making a threat, one sees that its elements are as follows: A threatens B by convincing B that if B does not act in compliance with A's demands, then A will follow a certain policy T. Supposing A and B to be rational beings, it is essential for the success of the threat that A be compelled to carry out his threat T if B fails to comply. Otherwise it will have little meaning. For, in general, to execute the threat will not be something A would want to do, just of itself." [Nash, 1953]

In this light, it is pertinent to consider where threats do and do not play a role in real-world negotiations (such as discussed in Anbarci et al. [2002]) and subsequently to consider whether or not threat dynamics could or should be manifest in electricity systems. In the following Chapter 4 we explore this question by developing a direct extension of Nash's bargaining solution concept into a scheme applicable to electricity networks called the GNK value, and apply it to electricity systems to witness its features.

3.5 Envy-Free systems

In Section 2.2.6 we introduced the concept of envy-freeness at a conceptual level; envy-freeness is a general condition of allocation where every person prefers their own bundle of allocated resources to that allocated to everyone else. However there are multiple questions in-practice in allocating resources in an envy-free manner, and one of the primary questions is what the bundles of resources are.

In the most simple case, that of the simple divisible homogeneous good that is valued monotonically by all players, the only envy-free allocation is an equal allocation of the good between all participants, which is not neurally an outcome that maximises utilitarian efficiency, but potentially straightforward to implement and has an obvious egalitarian appeal. Feige and Tennenholtz [2014] Adding transferable utility transactions to the bundles allows envy-free allocation of equal utilities to all participants.

For practical purposes, the bundles of resources can include more interesting elements, for instance, in the context of the supply of homogeneous Electricity to consumers, adding uncertainty over the supply creates more complex case, where *ex-ante* envy-freeness can be considered.Bürmann et al. [2020] Or as another example the authors of Tushar et al. [2017] consider envy free allocations in the context of selling homogeneous electricity surplus, together with a convex pressure to sell parameter α per player. Another electricity example application of envy-free concepts is in the allocation and evaluation of load-shedding algorithms Oluwasuji et al. [2019] where maximum envy difference is considered as a target for minimisation and a metric of evaluating performance. In these contexts optimising for envy-freeness can impart utilitarian social cost, the so called 'price of envy-freeness' Bertsimas et al. [2011].

In these these and other electricity contexts, the envy-freeness condition can act as a constraint on possible allocations reducing them to a set of consistent possibilities, Then there is a secondary question about which of these is most appropriate to be implemented. Such as (per previous examples) may be Pareto efficient, utility maximising, or maximising the wellbeing of the worst off; particularly, there is an extant body of literature examining Pareto-efficient envy-free allocation (PEEF) Weller [1985]; Cole and Tao [2021]; Varian [1974],

Another dimension of envy-free allocation in practice, is the degree to which the respective envy-free allocation is truthful or *incentive compatible* for the participants. The consideration of true strategy-proof envy-freeness was first considered in the context of cake-cutting Chen et al. [2013], but further investigation has established several restricted impossibility proofs surrounding the concept under various conditions Bei et al. [2017]; Aziz and Ye [2014]; Kurokawa et al. [2013] A secondary question is thus, how likely are envy-free allocation mechanisms likely to perform under strategising agents, and then specifically in such conditions as may be present in electricity contexts.

Another dimension is which specific conception of envy-freeness is most appropriate in practice. So for instance, should allocation optimise envy-relations between all consumers or between local consumers (such as graph envy-free conditions - see Section 2.2.6), or how should envy-relations be considered between resource bundles and consumer which by happenstance cannot feasibly consume them, should measures be envy-free or only envy-minimising and if-so at what cost to social or utilitarian efficiency. In this way there is a range of social possibilities in designing envy-free systems in practice.

Unfortunately, at this stage, there is no well established singular way of trading resources such as electrical energy that is envy-free, quite as much as envy-freeness is a desirable property sometimes witness in various mechanisms that are sometimes discussed in an electricity context. An implementation of the envy-free condition in electricity systems may or may not have other advantages and drawbacks, such as incentive compatibility, budget-balance, Pareto-efficiency, and may or may not be computable and scalable to the sizes of realistic networks (particularly as computation difficulty is potential drawback, as identified in section 2.2.6).

3.6 Comparison & summary

In this chapter we have explored five different ways in which ethical ideas about distribution can be mathematised, and each of them have different features and encode different moral perspectives.

Specifically we have introduced and illustrated the Vickrey-Clarke-Groves (VCG) mechanism, Locational Marginal Pricing (LMP), the Shapley Value, and Nash bargaining solution concepts, and envy-free applications. Each of the ideas embody different rules and respect different moral reference points.

And as identified by the philosophy of the previous chapter, none of these solutions are simply right or wrong per sei; but each have their features and limitations, and hence have arenas where they are potentially more suitable than others. We note that the approaches discussed in this chapter can encode different ways of valuing resources in their context. Because these different approaches are defined in a generalised context and thus can apply to many different contexts within electricity network systems. Additionally, because of these approaches beging defined in a generalised context, each of them can be adaptable to any relevent set of quirks or facets of the system to which they are applied, and thus sensitive to any confluence of elctrical system considerations. The broad issues facing real-world electricity systems (such as detailed in Chapter 1) may or may not be reduced or exacurbated by any of approaches applied to particular electrical system subproblem. However in the next chapter we attempt to create a entirely new approach to the valuation of resources such as may be relevent to electricity systems.

One particularly interesting feature of the Nash-bargaining solution is that it considers the minimax payoff advantage as a measure of competitive strength between participants, and it allocates utility accordingly. However the Nash bargaining solution is limited to two players, as for three (or more) players there may not exist a unique zero-sum minimax value. In the following chapter 4 we construct an extension of Nash bargaining solution called the GNK value, that is built around Shapley Value axioms; and compare it to LMP and VCG in the context of the immediate generation/consumption of electrical power on electricity networks.

Chapter 4

The GNK value: A new solution

In the previous chapter we introduced several different solution concepts, each stemming from different ethical principles and perspectives. In this chapter we detail a new approach that combines some of the features of the solution concepts outlaid in the previous chapter. The primary motivation for this new solution, is to attempt to distil the intuition behind the Nash bargaining solution concepts (per section 3.4) into a description of total allocation that is suitable for arbitrary number of players - rather than just two. Our solution extends the work of others to the space of generalised non-cooperative games, which are then suitable for application in various electrical network contexts.

Our solution relates to many of the concepts of the previous chapter: where we have a fundamentally coalitional scheme (per Coalitional Game Theory), that rewards based upon disagreement points (Bargaining Theory), which is partially informed by how much individual's participation influences the group's wellbeing (reminiscent of VCG), and attempts to describe normative trading between large numbers of participants (Marginalism).

We call our new solution concept the *Generalized Neyman and Kohlberg Value* or *GNK value* for short, and is computed and directly compared against other solutions concepts of the previous chapter in the context of electricity allocation. By this comparison it is seen that the different solution concepts give different outcomes, and we discuss these differences in light of our ethical considerations (from Chapter 2).

The material from this chapter extends from work which was originally submitted to AAMAS, and was accepted as an extended abstract:

"The Generalized N&K Value: An Axiomatic Mechanism for Electricity Trading"
International Conference on Autonomous Agents and Multiagent Systems
(AAMAS) 2018 (accessible: ifaamas.org/Proceedings/aamas2018/pdfs/p1883.pdf)

This chapter consists of the following parts:

- In sections 4.1 and 4.2, we introduce and define the GNK value, relating it to historical roots and similar solution concepts.

- In section 4.3, we consider how the GNK value can be computed to derive financial and electrical outcomes on a DC electricity network, against LMP and VCG.

- In section 4.4, we point-by-point discuss the features GNK, LMP and VCG as they are expressed in the context of an example electricity network.

We identify that the GNK value is difficult to compute for large numbers of players, and so in the next chapter 5 we address and consider the GNK value at scale against ethical criteria.

4.1 Introduction to the GNK value

How should we model ideal competition? In the two player case, existing bargaining solutions (such as Nash's) seem rather difficult to surpass as they describe a singular and axiomatic outcome that is both cooperatively Pareto optimal and also accounts for anti-cooperative strategising.

In the context of Nash bargaining with endogenous disagreement point (per section 3.4.2), the disagreement point was interpreted as a unique point defined by a minimax equilibrium in the payoff-advantage of strategies. However there exists a problem extending this scheme directly to three or more players, as there may not exist a unique minimax equilibrium in payoff-advantages for strategies in a game of more than two players. The question then is how to logically and consistently extend Nash's bargaining solution with endogenous disagreement point to an arbitrary number of players.

While it may be possible to arbitrarily choose one of those possible minimax equilibria in a 3+ person game as the disagreement point, instead we consider all the possible divisions of players between two groups and then consider all the two-player minimax payoff advantages between them. We then integrate this information via Shapley Value axioms to form a unique outcome, that does not depend on any arbitrary choice. In this way our new solution allocates outcomes in proportion to the aggregate leverage that all the individuals - and groups of individuals - could hypothetically posses in bargaining for outcomes they desire. In the following sections of this chapter (sections 4.2 to 4.3) we give all the details of this process.

The fundamental idea behind our approach was first detailed by Harsanyi [1963]. So far as we know, Harsanyi's solution concepts have never been applied to electricity networks, as there exists a particular problem in doing so, particularly that Harsanyi's solution concepts apply to non-cooperative games but cannot apply to generalised non-cooperative games. The details of this problem and our novel remedy are given in following section 4.2.2.

But briefly, in electricity network contexts the mutual interactions of participants can be limited by the physical constraint of the network, for instance: network participants cannot simply draw or push power to/from the network without restraint, as doing so would lead to damage to the network. And these limitations on the space of possible mutual actions is best modelled by a generalised non-cooperative game, and unfortunately in the context of such a generalised game there is no unique minimax point between two players. Our principle and novel development in this chapter is the provision of a remedy, such that Harsanyi's solution can then be applied. The remedy is to take the expected outcome on a coin-flip on who chooses actions first in the minimax strategies - and as we shall see - this turns out to be a unique value that satisfies all required properties, and thus leads to a coherent outcome.

The resulting outcome we call the *Generalized Neyman and Kohlberg Value* or the *GNK value* for short, as Harsanyi's solution was also axiomatically derived by Kohlberg and Neyman [2017, 2018]. This solution concept is shown to apply for all transferable utility (TU) generalised non-cooperative games, and directly equivalent to the Nash bargaining with endogenous disagreement point under transferable utility (TU) between two players (such as per section 3.4.1, as in the example in that section).

The GNK value is thus flexible enough to extend to many contexts, but we focus particularly on the specific case of allocating monetary payments over Optimal Power Flow (OPF) instances under the DC approximation - as we will explain.

Let us derive the GNK value (in section 4.2) before giving details of its application to DC networks (in section 4.3), discussing it (section 4.4) and scaling it (section 5).

4.2 Deriving the GNK value

We begin by presenting the axiomatic foundations of the GNK value, in a similar manner as Kohlberg and Neyman [2017]'s exposition. We begin by defining the GNK value to be the integration of *threat* values between possible coalitions; defined via Shapley Value axioms. We then describe the *threat* or *advantage* of a coalition $v(S)$ in the context of a *generalized non-cooperative game* (which is our key point of novelty in the solution concept). And then we clarify how the GNK value relates to other prominent solution concepts in non-cooperative games.

4.2.1 Axiomatic foundations and the *Value*

We begin by considering Kohlberg and Neyman [2018]'s *coalitional game of threats*, which is a coalitional game defined by a pair $\langle N, v\rangle$ in which:

- $N = \{1, \ldots, n\}$ is a finite set of *players* or *agents*, and
- $v : 2^N \to \mathbb{R}$ is a *characteristic function* with

$$v(S) = -v(N \setminus S) \quad \forall S \subseteq N. \tag{4.1}$$

The intuition for (4.1) is that the characteristic function of this game is a measure of the strength of the bargaining position (the 'threat' or 'advantage') that a coalition, S, has over its complement, $N \setminus S$. This contrasts with classical cooperative game theory games, where the characteristic function $v(\emptyset) = 0$ and equation 4.1 does not generally hold (see section 3.3).

Neyman and Kohlberg's key result was to prove that if $\mathbb{D}$ is the set of all such games, then there exists a unique mapping $\varphi : \mathbb{D} \to \mathbb{R}^n$ that satisfies the following four axioms:

- **Efficiency**: $\sum_i \varphi(\langle N, v\rangle)_i = v(N)$ (4.2)
- **Symmetry**: If two players i and j are substitutes, such that if $v(S \cup i) = v(S \cup j) \ \ \forall S \subseteq N \setminus \{i, j\}$, then $\varphi(\langle N, v\rangle)_i = \varphi(\langle N, v\rangle)_j$
- **Null Player**: If a player i is a null player (i.e. $v(S \cup i) = v(S) \ \ \forall S \subseteq N$) then $\varphi(\langle N, v\rangle)_i = 0$
- **Additivity**: for any v_1 and v_2, $\varphi(\langle N, v_1 + v_2\rangle) = \varphi(\langle N, v_1\rangle) + \varphi(\langle N, v_2\rangle)$

Letting agent i's element of φ be denoted by φ_i, this mapping is:

$$\varphi_i(\langle N, v\rangle) = \frac{1}{n}\sum_{k=1}^{n} v_{i,k} = \frac{1}{n}\sum_{k=1}^{n} \frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S \\ |S|=k}} v(S) \tag{4.3}$$

Where $v_{i,k}$ is the average value of $v(S)$ for all coalitions of size k that include i. This mapping gives a distribution of the total surplus $v(N)$ among the players, and Kohlberg and Neyman [2018] appropriately call this unique mapping the 'Shapley Value' of the game of threats as it mirrors the classic *Shapley Value* of cooperative game theory.

Indeed Kohlberg and Neyman [2018] have shown that for any game of threats $\langle N, v\rangle$ there is a classic cooperative game $\langle N, v'\rangle$ where the two Shapley Values are the same. It is possible to map a game of threats v to a cooperative game v' via relation:

$$v'(S) = \frac{1}{2}v(S) + \frac{1}{2}v(N) \tag{4.4}$$

A central question in Kohlberg and Neyman [2018]'s coalitional game of threats, is what the 'threat' of a coalition of players $v(S)$ should be (such as on an electricity network), and one way of considering this is in relation to the actions that the coalition could exert and their consequences (positive and negative) over other players; such as may be described in non-cooperative game theory.

4.2.2 Defining threats in games with general action spaces

In this subsection we define the characteristic function $v(S)$, in the context of a *generalized non-cooperative game*. A generalised non-cooperative game is a game where the strategies available to one player may be restricted by the strategy choice of others. Such games were introduced by Debreu [1952] and the problem of finding equilibria in such games has been a topic of further research [Facchinei and Kanzow, 2007; Fischer et al., 2014].

In more detail, a generalised non-cooperative game consists of a triplet $G = \langle N, A, u\rangle$ in which:

- $N = \{1, \ldots, n\}$ is a finite set of players,
- $A \subseteq \prod_{i\in N} A^i$ is a set of all possible joint strategies, where A^i denotes the set of strategies available to player $i \in N$, and A is a subset of their product space

- $\{u_i(a) : A \to \mathbb{R}\}_{i \in N}$ is a set of functions of each player's payoff/utility when joint strategy $a \in A$ is executed.

In this context, we wish to describe the payoff 'threat' or 'advantage' $v(S)$ of a coalition $S \subseteq N$ (letting $A^S = \prod_{i \in S} A^i$), taking into account the constraints that apply to the joint action space. A key contribution in our research is the following construction of the coalitional game of threat's characteristic function. Denoting $(x, y) \in A$ as a partition of a joint action between two coalitions S and $N \setminus S$, the characteristic function for the game of threats with generalised action spaces is given by:

$$\begin{aligned} v(S) =& \frac{1}{2} \min_{\substack{y \in A^{N \setminus S} \\ \text{s.t.} \exists x, (x,y) \in A}} \max_{\substack{x \in A^S \\ \text{s.t.} (x,y) \in A}} \left(\sum_{i \in S} u_i(x, y) - \sum_{i \in N \setminus S} u_i(x, y) \right) \\ &+ \frac{1}{2} \max_{\substack{x \in A^S \\ \text{s.t.} \exists y, (x,y) \in A}} \min_{\substack{y \in A^{N \setminus S} \\ \text{s.t.} (x,y) \in A}} \left(\sum_{i \in S} u_i(x, y) - \sum_{i \in N \setminus S} u_i(x, y) \right) \end{aligned} \tag{4.5}$$

The requisite condition $v(S) = -v(N \setminus S)$, as given in (4.1), is immediately satisfied irrespective of the structure of strategy space A, insofar as the max and min terms are defined. Thus, (4.5) is a feasible representation of the competitive advantage (or threat) that a coalition has over its complement in a generalised strategy space. With the characteristic function (4.5), the formulation of φ (per (4.3)) defines the GNK value. This is a novel extension of existing work to the space of generalised games (see Section 4.2.4).

4.2.3 Understanding the GNK value

In the characteristic function (4.5), the inner term:

$$\sum_{i \in S} u_i(x, y) - \sum_{i \in N \setminus S} u_i(x, y)$$

is the sum of payoffs that the coalition S receives, minus the sum of payoffs that the complement $N \setminus S$ receives, under the joint strategy $(x, y) \in A$, we call this the *payoff advantage* to S.

The first line of $v(S)$ in (4.5) is half the payoff advantage achieved if, the players in S collectively choose their strategies to maximise the payoff advantage knowing that the players in $N \setminus S$ will subsequently choose their strategies to minimise it - and thus this dynamic constitutes a bilevel optimisation problem. Then the second line of (4.5) is an additional half of the payoff advantage achieved if the ordering of choice were reversed, with $N \setminus S$ choosing first. In this way, (4.5) can be interpreted as the expectation of Nash equilibrium payoff advantage of S over its complement under a fair coin-toss of who chooses their strategies first.

In this formulation $v(N) = \max_{a \in A}(\sum_{i \in N} u_i(a))$ is the maximum achievable sum of payoffs that the players can achieve, and the GNK value φ, splits all of this amount between the players (by the efficiency axiom). The allocation of utility that the

GNK value allocates can be realised by having the players execute the strategies that achieve this maximal sum, and then enacting appropriate utility transfers between the players. In this way the GNK value can be seen as a method of allocating a Pareto optimal outcome and budget-balanced payments between players, to attain utility proportional to their competitive advantages.

4.2.4 Relation to other solution concepts

The GNK value is closely related to several other solution concepts, and even equivalent to them under certain conditions.

Most immediately, the GNK value is identical to Kohlberg and Neyman [2017]'s Value when the strategy space A represents a mixed strategy game that is not generalised; that is when the strategy space, A, is an unconstrained combination of strategies for all agents (ie. $A = \prod_{i \in N} A^i$). To see this, we observe that the two halves of (4.5) are equal in the absence of joint action constraints (via direct application of von Neumann's minimax theorem[1]), and hence the characteristic value reduces to that used in Neyman and Kohlberg's original definition:

$$v_o(S) = \max_{x \in A^S} \min_{y \in A^{N \setminus S}} \left(\sum_{i \in S} u_i(x, y) - \sum_{i \in N \setminus S} u_i(x, y) \right). \tag{4.6}$$

That is, Neyman and Kohlberg's Value is the formulation of φ (per (4.3)) with $v_o(S)$ (per (4.6)). Unfortunately Neyman and Kohlberg's Value cannot be directly applied to generalised games because the required condition $v_o(S) = -v_o(N \setminus S)$ can fail to hold in that case.

Neyman and Kohlberg's Value (and the GNK value) are also directly conceptually related to Harsanyi [1963]'s solution in this context, while in the 2-player context, it is identical to Kalai and Kalai [2013, 2010]'s *coco-value* in the context of complete information and also identical to Nash [1953]'s bargaining solution in the context of transferable utility (see Kohlberg and Neyman [2017], or section 3.4.2). It also shares a conceptual similarity with Aumann [1961]'s α and β core solution concepts, and von Neumann and Morgenstern [1944]'s historic formulation :

$$v_m(S) = \max_{x \in A^S} \min_{y \in A^{N \setminus S}} \sum_{i \in S} u_i(x, y). \tag{4.7}$$

In this way the GNK value can be seen as a conceptual continuation of historic solution concepts, and can be judged according to how well it derives outcomes in application contexts.

As a simple example demonstration, it is possible to see how the GNK value is identical to Nash bargaining in the context of transferable utility games (such as in the example matrix game 3.9 of section 3.4.2), we calculate all the terms $v(S)$ for coalitions of players 1 and 2, particularly:

[1] see Lemma 1 of Kohlberg and Neyman [2017]

$$
\begin{aligned}
v(\{1,2\}) &= \max\max \begin{bmatrix} 3 & -3 \\ -3 & 3 \end{bmatrix} = 3 \\
v(\{1\}) &= \frac{1}{2}\min\max \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} + \frac{1}{2}\max\min \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} = 1 \\
v(\{2\}) &= \frac{1}{2}\min\max \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix} + \frac{1}{2}\max\min \begin{bmatrix} 1 & 1 \\ -1 & -1 \end{bmatrix} = -1 \\
v(\emptyset) &= -\max\max \begin{bmatrix} 3 & -3 \\ -3 & 3 \end{bmatrix} = -3
\end{aligned}
$$

From this:

$$
\begin{aligned}
\varphi_1(\langle N, v\rangle) &= \frac{1}{2}(v(\{1,2\}) + v(\{1\})) = \frac{1}{2}(3+1) = 2 \\
\varphi_2(\langle N, v\rangle) &= \frac{1}{2}(v(\{1,2\}) + v(\{2\})) = \frac{1}{2}(3-1) = 1
\end{aligned}
$$

Which matches exactly the result in section 3.4.2. In section 3.4.2 we considered that the minimax in the payoff advantage matrix (ie. d in that section) was the nash equilibrium point of threat in bargaining between the players in choosing a subsequent point on the Pareto frontier (see Figure 3.2) that divides the maximum possible sum revenue (ie s in that section). The GNK value also directly encodes this same logic as $v(\{1\}) = -v(\{2\})$ is the minimax in the payoff advantage between the player (in this ungeneralised game), and $v(\{1,2\})$ is the maximum sum revenue which is split. This result is the same as we would get by the *coco-value*, and working with Neyman and Kohlberg's value (equation 4.6).

In the following section we describe the setup for an application and evaluation of the GNK value in the context of DC-approximated electrical networks.

4.3 GNK value computation on DC powerflows

Because of its flexibility the GNK value has the potential to be used in a large range of different contexts, however in this section we focus solely on the development of a simple case — the pricing of the immediate consumption and generation of power on a meshed network under DC approximation, where all participants have linear utilities over their own power. Although this construction simplifies away some key technical problems in power networks, it allows us to clarify the analysis of the GNK value and its features.

In this section, we consider the DC network model, discuss how to calculate the GNK value as well as LMP and VCG for it, before in the next section 4.4 we discuss the features of these mechanisms with an example.

4.3.1 Network model

We begin by setting out the elements of an electricity network under DC approximation:

- A set of buses B with, for all $i \in B$:
  - Power consumption at each bus p_i, and
  - A bus voltage phase-angle θ_i,
- Lines $C \subseteq B \times B$, with, for all $(i,j) \in C$:
  - Line susceptance $b_{i,j}$, and
  - Power flow $p_{i,j}$ (power from bus i to j), with $p_{i,j} = -p_{j,i}$.

In this context, the DC approximated powerflow constraints (per Wang and Hijazi [2018]) are expressed as follows:

$$\begin{aligned} &\text{DC-powerflow} \\ \text{Variables:}\quad & p_{i\in B},\ \theta_{i\in B},\ p_{(i,j)\in C} \\ \text{constraints:}\quad & p_i^l \le p_i \le p_i^u \\ & p_{i,j}^l \le p_{i,j} \le p_{i,j}^u \\ & p_j = \sum_{(i,j)\in C} p_{i,j} \\ & p_{i,j} = -b_{i,j}(\theta_i - \theta_j) \end{aligned} \tag{4.8}$$

where p_i^l, p_i^u, $p_{i,j}^l$, $p_{i,j}^u$ are the upper and lower bounds on power consumption/generation and line limits, respectively.

We can eliminate redundant variables, such as θ_i and $p_{i,j}$, and to ease presentation, and use the abstract functions h_j and g_k (for indices j,k) to represent the remaining linear functions:

$$\begin{aligned} &\text{DC-powerflow} \\ \text{Variables:}\quad & p_{i\in B} \\ \text{constraints:}\quad & h_j(p_1, p_2, \dots) = 0 \quad \forall j \\ & g_k(p_1, p_2, \dots) \le 0 \quad \forall k \end{aligned} \tag{4.9}$$

In this DC powerflow network the participants on each bus are treated as players in a game. For simplicity, we have one player per bus (i.e. $N = B$), and the power consumption of that bus is the respective player's strategy space (i.e. $A_i = [p_i^l, p_i^u]$). Then the DC constraints define the space of jointly executable strategies — forming the generalised strategy space A.

We further assume that there is a linear utility (or payoff) associated with the power consumption of each player, denoted $u_i(p_i)$ for player i, which makes all the components of a generalised game.[2] We now consider how to calculate the GNK value against LMP and VCG for such a generalised game.

4.3.2 Computing the GNK value

The GNK value is difficult to solve because of the bilevel structure of (4.5) which must be computed for each of the possible coalitions of network participants. Even though we have modelled our example network with a set of linear utility functions and linear constraints (as given in section 4.3.1), equation (4.5) is still quite difficult to solve as it constitutes a linear bilevel program (LBP) which are a class of problems known by to be NP-hard. [Sinha et al., 2018; Ben-Ayed and Blair, 1990]

There exist a range of techniques which can be used to solve LBPs, such as summarised by Sinha et al. [2018]; Dempe [2018]. Some of the many methods include: vertex enumeration processes [Bialas and Karwan, 1984; Shi et al., 2005a; Liu and Spencer, 1995]; penalty method schemes [Kleinert and Schmidt, 2019; Önal, 1993; Dempe, 1987]; cutting plane approaches [Marcotte, 1998]; branch-and-bound/cut methods [Shi et al., 2005b; Hansen et al., 1992; Audet et al., 2007]; and approximating algorithms [Pineda et al., 2018; He et al., 2014; Wang et al., 2007].

One well known way of addressing LBPs involves converting the inner optimisation constraints into KKT conditions (introduced by Kuhn and Tucker [1951]), and then converting the complementarity conditions into disjunctive constraints with binary variables - see Fortuny-Amat and McCarl [1981]; Pineda et al. [2018]. In this way, a bilevel program is converted into a mixed integer linear program, which is then directly amenable to standard optimisation software. This method was chosen, and the SCIP Optimisation Suite was employed to compute the GNK value for an example network as described in the next section 4.4.

KKT conditions are a well known set of algebraic tests which imply that the function under consideration is locally optimal (maximal or alternatively minimal) with respect to its variables under a set of constraint functions (with some regularity assumptions on those functions). KKT are well documented, and extend the method of Lagrange multipliers.

Specifically for maximising an objective function $f(\mathbf{x})$ subject to multiple constraints:

$$g_k(\mathbf{x}) \leq 0 \tag{4.10}$$

$$h_j(\mathbf{x}) = 0 \tag{4.11}$$

Then $\mathbf{x}*$ is a local maximum if the following KKT conditions are true:

$$\nabla f(\mathbf{x}*) - \sum_k \lambda_k \nabla g_k(\mathbf{x}*) - \sum_j \mu_k \nabla h_k(\mathbf{x}*) = 0 \tag{4.12}$$

[2] the Linear utility assumption simplifies the mathematics, as it makes the objective function linear, intuitively consumers should value consuming more power more, and generators cost producing more power more with some gradient.

and equations 4.10 and 4.11 hold for $\mathbf{x}*$, and for all i that $\lambda_i \geq 0$ and $\lambda_i g_i(\mathbf{x}*) = 0$.

By KKT conditions, we can convert the DC powerflow constraints given by equations 4.9 into a set of equations for maximising an objective function $f(p_{i\in B})$:

$$\forall i \;\; \frac{\partial f}{\partial p_i}(p_{i\in B}) = \sum_j \mu_j \frac{\partial h_j}{\partial p_i}(p_{i\in B}) + \sum_k \lambda_k \frac{\partial g_k}{\partial p_i}(p_{i\in B}) \tag{4.13}$$

$$\forall j \;\; h_j(p_{i\in B}) = 0 \tag{4.14}$$

$$\forall k \;\; g_k(p_{i\in B}) \leq 0 \tag{4.15}$$

$$\forall k \;\; \lambda_k \geq 0 \tag{4.16}$$

$$\forall k \;\; \lambda_k g_k(p_{i\in B}) = 0 \tag{4.17}$$

Hence the reformulation of our LBPs in equation 4.5 involves transforming the inner maximisation/minimisation constraints into KKT conditions. The sets of variable values which satisfy the KKT conditions are called KKT points, if we denote the set of values of an maximised objective function $f(p_{i\in B})$ at the KKT points as $\mathcal{KKT}(f(p_{i\in B}))$. Then reformulation of the inner part of (4.5) to involve KKT conditions is as follows:

$$\begin{aligned} v(S) =& \frac{1}{2} \max_{\substack{p_i \\ i\in S}} \min \left[-\mathcal{KKT}\left(-\sum_{i\in S} u_i(x,y) + \sum_{i\in N\setminus S} u_i(x,y) \right) \right] + \\ & \frac{1}{2} \min_{\substack{p_i \\ i\notin S}} \max \left[\mathcal{KKT}\left(\sum_{i\in S} u_i(x,y) - \sum_{i\in N\setminus S} u_i(x,y) \right) \right] \end{aligned} \tag{4.18}$$

By reformulating the inner maximisations/minimisations of (4.5) in this way we replaced the inner minimisations/maximisations in the space $(x,y) \in A$ with minimisations/maximisations over KKT points in the same space.

As the constraints under DC-approximation are linear and hence define a convex polygon, and as the functions $u_i(p_i)$ are linear (per the assumption of linear utility in section 4.3.1), then there will only be a single maximum/minimum value of these inner minimisations/maximisations - which will be the global maximum/minimum value.[3] In this way the inner maximisation (minimisation) over the KKT points can be ignored.

It was also realised that a binary reformulation of the complementary slackness conditions (equation 4.17) would increase computational efficiency, and so we transformed these complementarity constraints into disjunctive binary constraints.

Specifically, for each complementary slackness condition $\lambda_k g_k(p_{i\in B}) = 0$ we in-

[3] as linear optimisation problem has a unique solution, although there may be multiple points which attain this maximum/minimum value

troduced a binary variable Z_k to indicate whether λ_k or $g_k(p_{i\in B})$ was zero and then introduced large numbers $\bar{\lambda}_k$ and $\underline{g_k}$ such as to make the complementary slackness condition equivalent to: $(1-Z_k)\bar{\lambda}_k \geq \lambda_k \geq 0$ and $\underline{g_k} Z_k \leq g_k(p_{i\in B}) \leq 0$. Where $\bar{\lambda}_k$ and $\underline{g_k}$ are the estimated upper and lower bounds on the KKT multipliers and constraint functions respectively.

the resulting KKT conditions for maximising and objective function $f(p_{i\in B})$ under this complementary slackness conditions are as follows:

$$\forall i \;\; \frac{\partial f}{\partial p_i}(p_{i\in B}) = \sum_j \mu_j \frac{\partial h_j}{\partial p_i}(p_{i\in B}) + \sum_k \lambda_k \frac{\partial g_k}{\partial p_i}(p_{i\in B}) \tag{4.19}$$

$$\forall j \;\; h_j(p_{i\in B}) = 0 \tag{4.20}$$

$$\forall k \;\; g_k(p_{i\in B}) \leq 0 \tag{4.21}$$

$$\forall k \;\; (1-Z_k)\bar{\lambda}_k \geq \lambda_k \geq 0 \tag{4.22}$$

$$\forall k \;\; \underline{g_k} Z_k \leq g_k(p_{i\in B}) \leq 0 \tag{4.23}$$

if we denote the set of values of an maximised objective function $f(p_{i\in B})$ that satisfy these new KKT conditions $\mathbb{KKT}(f(p_{i\in B}))$. Then reformulation of the inner part of (4.5) to involve KKT conditions is as follows:

The resulting reformulation is as follows:

$$\begin{aligned} v(S) =& \frac{1}{2} \max_{\substack{p_i \\ i\in S}} \left[-\mathbb{KKT}\left(-\sum_{i\in S} u_i(x,y) + \sum_{i\in N\setminus S} u_i(x,y) \right) \right] + \\ & \frac{1}{2} \min_{\substack{p_i \\ i\notin S}} \left[\mathbb{KKT}\left(\sum_{i\in S} u_i(x,y) - \sum_{i\in N\setminus S} u_i(x,y) \right) \right] \end{aligned} \tag{4.24}$$

This reformulation renders the LBP into a mixed integer program which is directly amenable for calculation by optimisation solvers, and the SCIP optimisation suite was used in our case.

4.3.3 Computing the LMP transfers

Computing the Locational Marginal Price (LMP) transfers for DC electricity networks is a process described in various literature - such as by Scott and Thiébaux [2015]; Tang and Jain [2013].

Particularly we consider optimising the sum of utility: $\sum_{i\in B} u_i(p_i)$ subject to the DC powerflow constraints in equations 4.8. In this context the power conservation constraints on each bus are the constraints $p_j = \sum_{(i,j)\in C} p_{i,j}$, and the lagrange multipliers associated with these constraints are the marginal prices for power on each of the respective busses. This process is an application of the more general marginal price calculation procedure discussed previously in section 3.2.2. We utilised the SCIP optimisation suite[4].

4.3.4 Computing the VCG imputations

From section 3.1 the VCG payment that a participant makes is the difference between the sum of other's utility at the social optimum point x^*, and the utility that others would have if the participant were not present and the optimisation were only over the remaining participants, as seen in equation 3.1.

In this way the socially optimum value x^* needs to be computed, and then additionally an additional optimisation problem for each player - where we assume that the excluded participant has power zero $p_i = 0$. Thus in our context, equation 3.1 becomes:

$$d_i = \underset{\sum_j u_j(p_j)}{\operatorname{argmax}} \sum_{j \neq i} u_j(p_j) - \underset{\sum_{j \neq i} u_j(p_j), p_i = 0}{\operatorname{argmax}} \sum_{j \neq i} u_j(p_j) \tag{4.25}$$

The first term in this equation is the sum of utilities at the point which maximises the sum of utilities minus the player i. The second term in this equation is the sum of other's utilities (ie. excluding player i) at the point which maximises the sum of other's utilities in the context that the players power is zero. The first part of the equation is common to all player's contributions d_i, but the second negative part is unique for each. In this way, if there are n participants, there are $n+1$ comparable OPF optimisation problems which need to be solved to calculate VCG payments. The SCIP optimisation suite was used solving these optimisation problems.

4.3.5 Computing the Shapley Value imputations

From section 3.3.2 the Shapley Value utility imputations that a participant receives is the average marginal contribution that it adds to a characteristic function under ambiguity of the join ordering. In this way we need to consider a characteristic function in the context of DC networks:

$$v_{shap}(S) = \max \sum_j u_j(p_j) \quad \text{s.t. } \forall i \notin S \;\; p_i = 0$$

This characteristic function describes the utility that a coalition could achieve by themselves, absent any consumption/generation from those not in the coalition - it is one possible way of creating a characteristic function for DC networks.

The utilities under the Shapley Value (by efficiency axiom) sum to give the value of the grand coalition $v_{shap}(N)$ which occurs at the optimal operating point x^*. Thus the Shapley Value can be implementing by enacting electrical outcomes described by x^* and conducting budget balanced utility transfers between participants. To calculate the Shapley Value imputations, the maximal sum of utilities under OPF for all the possible $2^n - 1$ coalitions need computed, and the SCIP optimisation suite was used for these calculations.

[4]development reported by Maher et al. [2017]

Busses:	$B = \{1,2,3,4,5\}$
Lines:	$C = \{(1,2),(1,3),$ $(1,4),(3,5)\}$
Susceptances:	$b_{1,2} = -1$ $b_{1,3} = -1$ $b_{1,4} = -1$ $b_{3,5} = -1$
Line Limits:	$p^l_{1,2} = -70$ $p^u_{1,2} = 70$ $p^l_{1,3} = -140$ $p^u_{1,3} = 140$ $p^l_{1,4} = -70$ $p^u_{1,4} = 70$ $p^l_{3,5} = -70$ $p^u_{3,5} = 70$
Power Limits:	$p^l_1 = \text{free}$ $p^u_1 = 0$ $p^l_2 = 0$ $p^u_2 = 100$ $p^l_3 = 0$ $p^u_3 = 100$ $p^l_4 = 0$ $p^u_4 = 100$ $p^l_5 = 0$ $p^u_5 = 100$
Utilities:	$u_1(p_1) = 0.2p_1$ $u_2(p_2) = 1.9p_2$ $u_3(p_3) = 1.8p_3$ $u_4(p_4) = 1.7p_4$ $u_5(p_5) = 1.6p_5$

Table 4.1: Paramters for the example 5-bus system. Note p^l_1 is left free to allow for a parameter search over it, for analysis of the GNK and LMP values.

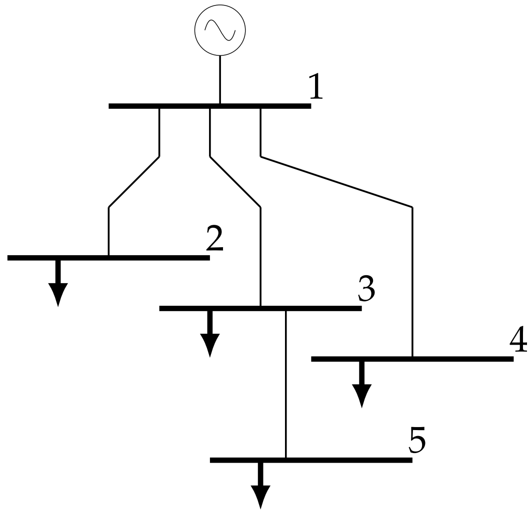
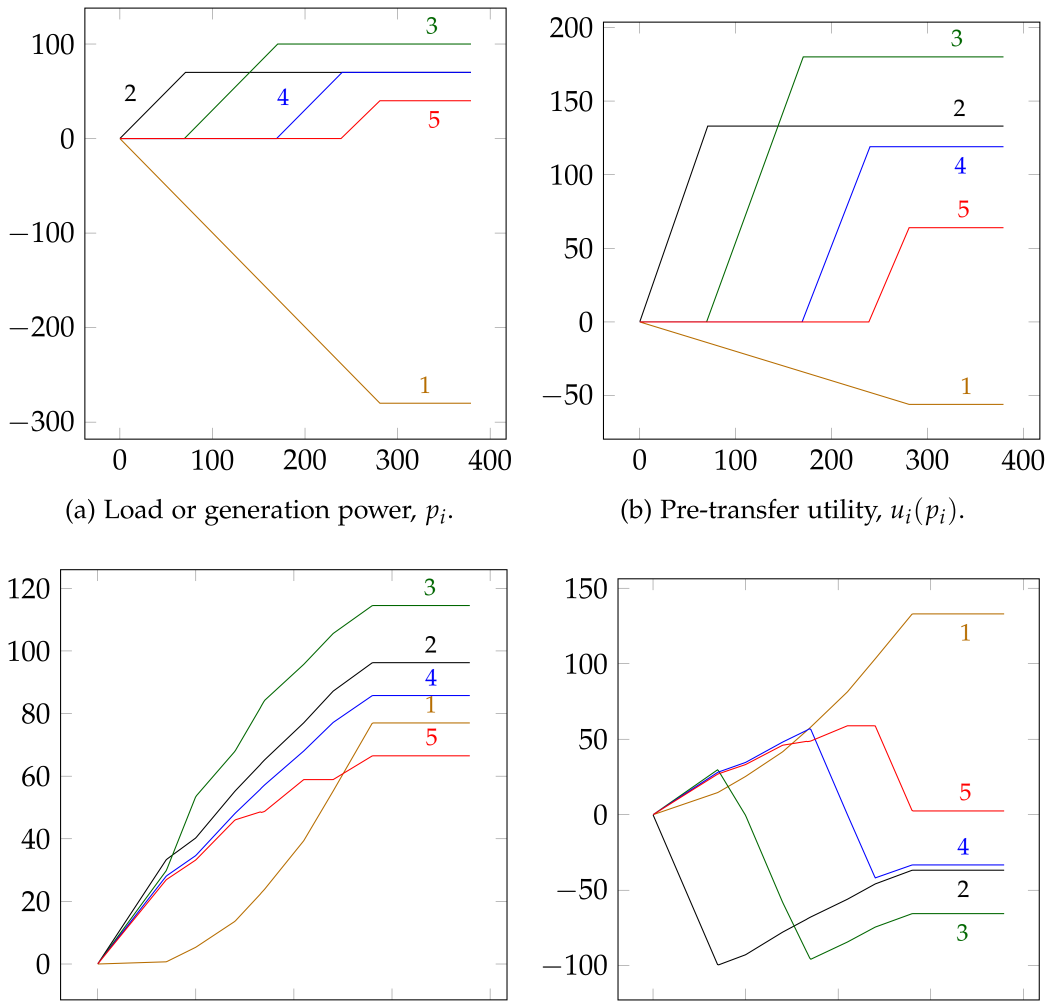


Figure 4.1: Line diagram for the example 5-bus electricity system.

4.4 Some features of GNK, in context of an example

In the previous section 4.3 we detailed a procedure to calculate the financial payments and dispatched powers under the GNK value as well as LMP, VCG and Shapley Value, so that now we can compute and compare them with an example. In this section we are thus able to witness and discuss the characteristics of the GNK value, in the context of an example 5-bus network shown in Figure 4.1, with parameters given in Table 4.1. In this example we calculate and subsequently consider the features of the GNK value against LMP, VCG and Shapley Value against parameter p^l_1 (the generator capacity in the network). The results of these calculations of the financial payments are plotted against p^l_1 in Figures 4.2d, 4.3b, 4.3d and 4.4b for GNK, LMP, VCG and Shapley Value respectively. Which in addition to the utilities derived from power consumption/generation (Figure 4.2b) form the post payment utility imputations as Figures 4.2c, 4.3a, 4.3c and 4.4a.

In Figure 4.2a, increasing the generator capacity from 0 shows that power is initially consumed entirely by the consumer at bus 2, who uses all p^l_1kW of power and values it at a rate of 1.9 units of utility. This continues until the power constraint on line (1,2) binds, at 70kW. Then the consumer at bus 3 begins to be supplied with power, who values it at a rate of 1.8 units of utility until its consumption is max-



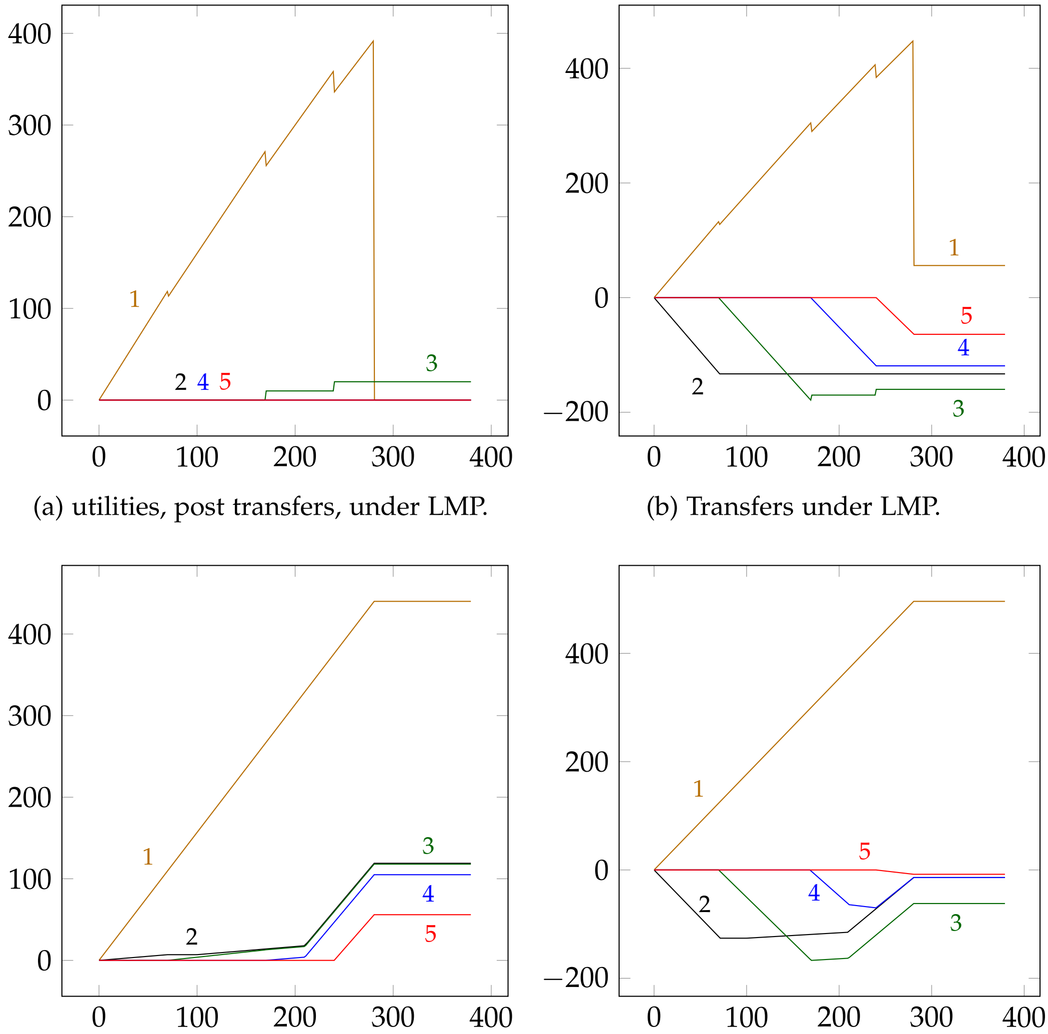
(a) Load or generation power, p_i.

(b) Pre-transfer utility, $u_i(p_i)$.

(c) Utilities, post transfers, under the GNK value, $\varphi(\langle N, v\rangle)_i$.

(d) Transfers under the GNK value, $\varphi_i(\langle N, v\rangle) - u_i(p_i)$.

Figure 4.2: For the Power levels (figure 4.2a), and utilities or costs for power (figure 4.2b), the GNK value and transfers under the GNK value. All x-axes are the system generation capacity, $-p_1^l$



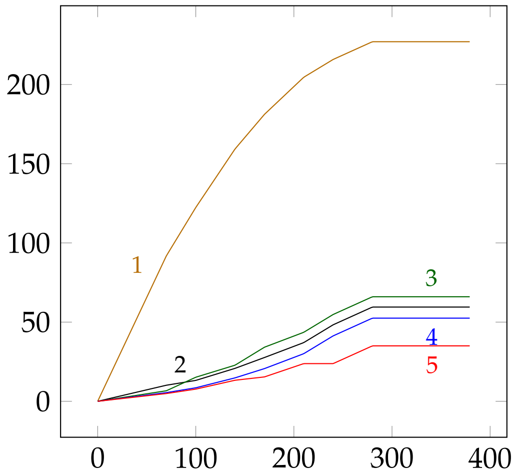
(a) utilities, post transfers, under LMP.

(b) Transfers under LMP.

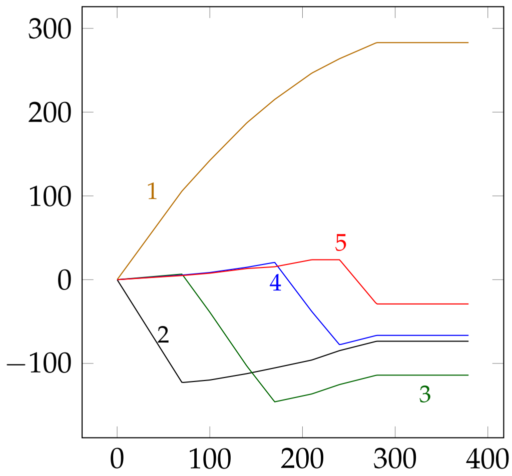
(c) utilities, post transfers, under VCG.

(d) Transfers under VCG.

Figure 4.3: The utilities and transfers under LMP, as well as the utilities and transfers under VCG for the example network. All x-axes are the system generation capacity, $-p_1^l$



(a) utilities, post transfers, under Shapley Value.



(b) Transfers under Shapley Value.

Figure 4.4: The utilities and transfers under Shapley Value for the example network. All x-axes are the system generation capacity, $-p_1^l$

imised at 100kW. This dynamic is then repeated for the agent with the next-highest marginal utility for power (given by the utility function coefficients in Table 4.1), until the respective line constraints are also met.

In the interval of the first 70 units of generator capacity (ie. $p_1^l \in [0, -70]$), the LMP price for this power, for both the generator at bus 1 and the consumer at bus 2, is given by its marginal value 1.9 (as the line constraint is not active). This corresponds to the slope of the black line in Figure 4.3b (or 4.2b) over this interval. More generally, the full set of the LMP transfers plotted in Figure 4.3b are given by the Lagrange multiplier for power conservation in the OPF optimisation multiplied by the power consumed at that bus, and that as the generation capacity increases the marginal price of power changes, and the gradients of the lines change in discrete steps as the utility functions in the example network are linear.

Additionally, the VCG payments are plotted against p_1^l in Figures 4.3d and resulting utilities in Figure 4.3c. The VCG payments are similar to the LMP payments, except that instead of payment proportional to the marginal unit of electricity, each player is compensated at his/her marginal cost of their participation. VCG takes into account the marginal effect that each of the player's participation has upon each other at the social optimum

In contrast VCG and LMP, the GNK value takes into account the full bargaining position of each agent and also every possible coalition of agents when determining transfers, which are based on the utilities (or costs, in the case of the generator) of all agents in the system, and not just the marginal value of participation or electrical supply. The GNK value is plotted against p_1^l for our example in Figure 4.2c, and the resulting transfers (GNK value less utility) are plotted in Figure 4.2d.

In contrast to VCG, LMP and GNK, the Shapley Value exhibits character traits that are similar to LMP and VCG, particularly as the Shapley value is composed of many more marginal contributions than those ones inherent to VCG, which is in turn proportional to the marginalism inherent in LMP. Furthermore it has a superficial similarity to the GNK value as they both extend from the same axioms - either exhibited in section 4.2.1, or by conversion to Shapley value by equation 4.4 thus having exactly the same axioms as in section 3.3.2. The Shapley Value results are plotted against p_1^l for our example in Figure 4.4a, and the resulting transfers (GNK value less utility) are plotted in Figure 4.4b.

From these graphs we can witness some of the qualities of the GNK value against LMP and VCG and the Shapley Value:

The GNK value, VCG and Shapley Value imputations are continuous in the parameters of the network

The GNK value has some evident continuity properties, as can be seen from equation 4.5, in which the minimax characteristic function, $v(S)$, always changes continuously with the utility functions u. This continuity property is proven in the Appendix A, together with some associated monotonicity properties. This continuity is similarly witnessed in VCG imputations, but notably not in the context of LMP payments.

It is seen that LMP features discontinuous changes in financial transfers and this can clearly be seen from the jagged edges in Figure 4.3b, where the payments received by generator 1 drop sharply with increasing generator capacity. This happens because the change in generator capacity is changing the parameters of the network itself and its feasibility region, which yields discontinuous changes in network operating point, and thus marginal prices. This dynamic under LMP might be seen to lead to a somewhat perverse incentive to produce less power than what is socially optimal, and in contrast, the utilities under the GNK value (Figure 4.2c), VCG (Figure 4.3c) and Shapley Value (Figure 4.4a) which feature no such drops or discontinuities. In a power systems context under LMP, these discontinuities are known to occur precisely in the event of network *congestion* which is one known cause of the volatility experienced in electricity markets - see Hadsell and Shawky [2006]. In contrast, the post-payment utilities under the GNK value and VCG are always continuous with network parameters.

The GNK and Shapley Value payments are always budget balanced

The transactions under VCG are not necessarily budget-balanced and can yield a surplus or deficit, and transactions under LMP can yield a budget surplus (they are weakly budget balanced Wu et al. [1996][Fact 4]), whereas payments under the GNK value and Shapley Value are strongly budget-balanced and result in no surplus or deficit. This is an outcome of the GNK value's axiomatic derivation, as given by equation (4.2), which is reflective of the Shapley Value axioms, per section 3.3.2. Under LMP, each participant is credited or debited at the effective rate of supply for their location but there is no guarantees that the total payments should add to zero. This can be seen by inspecting the region $x > 300$ in Figure 4.3b, where generator 1 is credited \$56 while the consumers are debited at \$133.0, \$160.0, \$119.0, and \$64.0 respectively, leading to a budget surplus of \$420. The surplus of \$420 comes particularly from the existence of congestion in the example network which is well known to introduce so-called 'congestion-rents'. Additionally VCG payments are known not to be budget balanced generally and may yield a surplus or deficit depending on various conditions, as considered in section 3.1.

The GNK value (but not VCG or LMP) can offset those that do not receive or generate power

The GNK value can allocate payments between parties such that the consumers that receive power compensate those that are excluded from receiving it. This can be seen from Figures 4.2a and 4.2c particularly in the region where $x < 50$. In this region there is only sufficient power to supply consumer 2 (who has the highest utility for that power) whereas consumers 3, 4 and 5 who would otherwise be in a position to receive that power are compensated such as to be barely worse off (as can be seen from 4.2c).

For instance at $x = 50$, generator 1 produces 50kW which is consumed entirely by consumer 2; the utilities of the participants before transfers are: $-10, 95, 0, 0, 0$ respectively (which can be seen from Figure 4.2b). However under the GNK value, consumer 2 must pay both the generator and also the other consumers for its right-of-way to consumption.

The utilities after the transfers of the participants are: $0.5, 23.83, 21.33, 20.08, 19.25$ respectively (which can be seen from Figure 4.2c). In a power systems context, this is likely to be seen as a desirable quality as it may correspond to people's intuitions about the fair allocation of resources. For example, distribution network feeders that have a high penetration of PV systems have been identified by Carvalho et al. [2008] to experience voltage rise problems at times of high-supply/low-demand, particularly at the feeder extremities. In these settings, the inverters of PV owners at the bottom are unable to inject their power into the network and also typically get no compensation for essentially a forced curtailment of their electricity generation.

In this context under LMP, curtailed generators that dont inject their power get no reward, and under VCG curtailed generators will only be allocated utility if their presence or absence would make a difference to the network operating point, which is not assured. Under Shapley Value, it is witnessed that there is some rather small offset for those that do not receive power, though this is mostly determined by marginal coalitional considerations that exclude most other consumers.

The GNK value is not incentive compatible

Unlike VCG, the GNK value, LMP and Shapley Value are not *incentive compatible* in the sense that is often referred-to in Mechanism Design (see Section 3.1). Specifically, the payments between parties are potentially subject to strategic manipulation if the agents are freely able to report their utility. In the GNK value this can be seen in (4.5), or more easily in its reduced form, (4.6), where the payoff advantage of a coalition $v(S)$ is based on its reported utilities in minimax strategies which may not be actualised; the same consideration holds for the Shapley Value. Because of this consideration, misreporting the utilities of these unactualised events may change the $v(S)$ and hence the GNK value itself. Additionally, LMP is known not to be incentive compatible, and there is further work to understand exactly how consequential this would likely be - such as by Scott and Thiébaux [2019]. In section 5.4.5 we continue discussion about this point.

The GNK value and Shapley Value are computationally difficult

The GNK value is more difficult than the Shapley Value, which is more difficult than VCG, which is more difficult than LMP, to compute. This can be seen via (4.3) where calculating the GNK value exactly requires calculating $v(S)$ for all the $2^n - 1$ possible coalitions S, and each calculation of $v(s)$ is an NP-hard bilevel optimisation problem. The Shapley Value also requires calculating $v_{shape}(S)$ for all the $2^n - 1$ possible coalitions S, but the calculation of $v_{shape}(S)$ is not necessarily NP-hard problem, as DC OPF problem can be a linear optimisation. Conversely VCG calculation for n agents requires $n + 1$ OPF optimisations (which are potentially linear in the DC case) per equation 4.25, where as LMP calculation requires exactly one OPF optimisation (as identified in section 4.3.3).

The computational difficulty of the GNK value is reflected in a later Figure 5.2 where it is seen that even using sampling to approximate the GNK value to sufficient accuracy is witnessed to be a double-exponentially complex process.

4.5 Summary

In this Chapter we have introduced the GNK value from its axioms and we have considered its conceptual inheritance from other solution concepts. In order to apply the GNK value to the pricing of immediate power generation and consumption in small DC networks we formally introduced the elements of the DC network and have detailed a computation methodology for the GNK value in that context. We then compared the GNK against LMP, VCG and Shapley Value on a small example network to examine their features, particularly we identified that the GNK value has some nice budget-balance and continuity properties, however we also realised that the GNK is not incentive compatable and that it is difficult to calculate for larger electricity networks.

In the next chapter we consider the ways in which the computational difficultly of calculating the GNK value on larger networks can be ameliorated. The two primary techniques to ameliorate this difficulty are principally by sampling, and also by the adoption of a proxy for the inner optimisations. We discuss these to directions in the next chapter 5 before actually applying these techniques for an application of GNK to larger network in section 5.3 where we discuss in section 5.4.

Chapter 5

Evaluating the GNK value at scale

In the previous chapter we introduced the GNK value and detailed a procedure to calculate it for the context of small DC networks. However it was quickly identified to be quite difficult to calculate for larger networks with many players. In this chapter we address this weakness by outlaying two specific ways to remedy this problem. Firstly, we consider possible sampling processes to approximate the summation of the many terms inherent to the GNK value (particularly the summation over all exponentially many coalitions in equation 4.3). Secondly, we consider a proxy inplace of the minimax optimisations at the heart of the GNK value (per equation 4.5).

Using these two remedies it is seen that it is possible to calculate the GNK value on networks upto size of about 100 nodes within 10 minutes of runtime on a desktop PC. Because of this freedom, we are able to compare the features of GNK against LMP and VCG on networks of this size, and we do so with an example, before making a more thorough discussion of the GNK value against the ethical considerations identified in chapter 2.

This chapter is composed of the following sections:

- In section 5.1 we describe and employ sampling techniques to reduce the number of minimax optimisations that need to be conducted to approximate the GNK value to sufficient accuracy.

- In section 5.2 we introduce a polynomial-time computable proxy inplace of the minimax optimisations in the characteristic function (4.5) of the GNK value.

- In section 5.3 we calculate the GNK value against LMP and VCG for a larger DC network, and discuss some features

- in section 5.4 we conclude our discussion of the GNK value by comparing it against ethical criteria identified in chapter 2.

After this chapter we delve into the details of the sampling techniques that were developed and tested throughout this research, particularly the SEBM method in Section 6.4, which was evaluated as a method to sample the GNK value (alongside others) in Section 5.1.

5.1 Sampling techniques

To compute the GNK value to a required accuracy, not all of the minimax optimisations $v(S)$ need to be performed (per equation 4.5), as sampling techniques may be used to approximate the sum. We consider two different approaches for bias free sampling of the GNK value:

1. By the inspection of equation 4.3, we see that the GNK value of any player i is an average over $v_{i,k}$, and that by randomly sampling coalitions of size k which include i we can sample for estimations of each $v_{i,k}$.

2. By utilizing equation 4.4 we convert the problem into a standard cooperative game, where we can then compute the GNK value via the many existing sampling techniques developed for approximating the Shapley Value.

The first of these two is an uncomplicated approach consisting of randomly generating coalitions $S \subset N$, and then approximating $v_{i,k}$ by averaging the appropriate $v(S)$, which are then averaged to approximate the GNK value φ via equation 4.3. We denote this method 'Simple'.

The second of these two approaches is more complicated, since it involves converting the problem into a cooperative game and then a selecting a technique to sample the Shapley Value. Some of the possible techniques include: Neyman Sampling ('Neyman') [Castro et al., 2017; Neyman, 1938], sampling to minimize a Hoeffding-type inequality ('Hoeffding') [Maleki et al., 2013], as well as a random stratified join-order sampling method ('Join') [Castro et al., 2017], and unstratified random join-order sampling 'ApproShapley' ('Appro') [Castro et al., 2009]. We consider these alongside our own developed method, the Stratified Finite Empirical Bernstein Sampling method ('SEBM') (as developed in Section 6.4 of Chapter 6).

We compare the performance of these sampling approaches in section 5.1.2, but first we will summarise some of the differences between the Shapley Value sampling techniques first.

5.1.1 Differences in sampling approaches

All the Shapley Value sampling technique sample over marginal contributions in slightly different ways; but primarily, they differ in whether they employ stratified sampling or not.

Stratified sampling is a well established statistical methodology to estimate a mean value of a population, by breaking it into subpopulations and sampling them independently to create an estimate of the means of each of the subpopulations to be weighted as an estimate for the whole population - for an introduction to it please consult Section 6.1. In this context, if a technique uses stratified sampling to approximate the shapley Value, then it samples the subpopulations of marginal contributions by player i to coalitions of size k, and from these they estimate of the mean of these subpopulations $\hat{v}_{i,k}$ (ie. approximating the terms of (3.3) and then using (3.4)), and

Method	Stratified	Join-Order	Sampling Choice
Appro	No	Yes	random
Join	Yes	Yes	random
Hoeffding	Yes	No	Hoeffding-type inequality
Neyman	Yes	No	by variance of the strata
SEBM	Yes	No	speciality inequality

Table 5.1: Different Shapley Value sampling methods and their features

these estimates are weighted to form an estimation of the Shapley Value itself. Conversely, for those techniques which do not employ stratified sampling, then they directly approximate the Shapley Value via equation (3.6).

Secondarily the techniques differ in whether or not they sample by a join-order process or not. Sampling over marginal contributions involves calculating the difference between $v(S)$ and $v(S \cup \{i\})$ for various players i and coalitions S, and one particularly easy way of doing this is to start with the empty coalition $\emptyset$ and generate a permutation of players that sequentially join the coalition and each make a marginal contribution in turn, in this way $n+1$ evaluations of $v(S)$ can be used to calculate n marginal contributions. Conversely, if they do not use a join-order process, then the methods randomly select coalitions S and player i and calculate the marginal contribution $v(S \cup \{i\}) - v(S)$, thus taking two evaluations of $v(S)$ for one marginal contribution sample point.

Between the methods, as shown in Table 5.1: Appro randomly samples in join orders without stratification, Join randomly samples in join orders with stratification, Hoeffding samples with stratification and without join orders, to minimise a sum of Hoeffding-type concentration inequalities on each of the estimates $\hat{v}_{i,k}$, Neyman samples with stratification without join orders to the sample each $\hat{v}_{i,k}$ proportional to the sample variance of the marginal contributions which make up each, and SEBM samples with stratification without join orders to sample $\hat{v}_{i,k}$ in order to maximally reduce a complicated concentration inequality on the resultant estimated Shapley Value itself.

The full details about each of the methods can be found in their respective source documents [Castro et al., 2017; Maleki et al., 2013; Castro et al., 2009] (and Chapter 6). We note that the methods that use join order sampling exploit the specific marginal nature of the Shapley Value, and hence are not compared against other methods of stratified sampling in Section 6.5. The performance of using these different methods is evaluated in the next section 5.1.2.

5.1.2 Sampling the GNK value at scale

To analyse the performance of approximating the GNK with different sampling techniques we calculated the average absolute error in the approximated GNK value for randomly generated electricity networks. We used a known process of generating pseudo random meshed networks of buses and lines reminiscent of real electricity networks. The particular algorithm is called the 'Simple minimum-distance graph' method as expounded by Hines et al. [2010] and is given as Algorithm 1.

Algorithm 1 Simple minimum-distance graph algorithm

Require: number of nodes N, number of links m
Require: natural numbers n_i, such that $\forall\ i\ n_i \leq i$ and also $\sum_{i=1}^{N} n_i = m$
  $M = \emptyset$ is set of nodes
  for $a = 1 : N$ **do**
    Randomly generate planar coordinates for node index a, (x_a, y_a) with uniform distribution
    $M_a = \emptyset$ is set of links for node index a
    for $k = 1 : n_a$ **do**
      select a novel $b \in M$ to minimise the Euclidean distance to node index a:
        $\min_b \quad (x_a - x_b)^2 + (y_a - y_b)^2 \quad \text{s.t} \quad (a, b) \notin M_a$
      Add the link a-to-b:
        $M_a = M_a \cup \{(a, b)\}$
        $M_b = M_b \cup \{(b, a)\}$
    end for
    Add the node a:
      $M = M \cup \{(x_a, y_a)\}$,
  end for
  Output M and M_a

Using this algorithm we considered networks which were randomly generated to have 10 nodes with 12 lines between them, which was sufficiently small enough for it to be possible to solve the GNK value exactly. In each of these randomly generated networks, each line had randomly generated line limits (uniformly between 20 and 300kW) and each node was randomly assigned to be either a generator or consumer of electricity (probability of being a consumer begin 80%) with a randomly generated linear utility function (uniformly between 0.1 and 2.1 $ per kW) with randomly generated consumption/generation limits (uniformly between 10 and 200kW).[1]

By computing the exact GNK value for these networks we were then able to compute the average absolute error achieved by each of the different sampling methods for different sample budgets. For a given budget, all the algorithms called for the computation of different numbers of the bilevel optimisations $v(S)$ (per equation 4.5). And by plotting the average absolute error achieved against the number of unique optimisations called, we can see the performance of the sampling methods as shown in Figure 5.1.

From this graph it is seen that the methods which utilised stratification (HOEFFDING, NEYMAN, SEBM and JOIN) generally performed better than those that did not use stratification (particularly SIMPLE and APPRO). And particularly that the JOIN method, which utilises stratification and join-order sampling is quite effective over a range of situations.

[1] All sourcecode for these experiments found at: https://github.com/Markopolo141/Thesis_code

On this graph, the sampling methods which utilised stratification were warm-started with a budget of 200 samples (two from each strata), as methods like NEYMAN required atleast two samples per stratum minimum (totalling 200) for a bias-free estimate of the variances which they run on. Conversely SIMPLE and APPRO were able to be run with a smaller sample budget. It is noted that the methods HOEFFDING, NEYMAN, SEBM and JOIN perform exactly the same at 200 samples, as they each have two samples per stratum and no extra budget for any difference in logic to operate on. It was also recognised that because of our 10 bus networks, there are only 1024 unique optimisations $v(S)$ that can be called, and hence the x-axis stops at 1024. Each of the methods were run multiple times with increasing sample budget allowances, up until a point where the computation time became prohibitive, particularly some of the methods which used sampling without replacement would only call a stochastic number of unique optimisations, and hence it became time-prohibitive to sample to perfect accuracy utilising them.

5.1.3 Selection of sampling method

From the Figure 5.1 we witnessed that JOIN was seen to be reasonably effective and it was chosen for all further analysis. The reason for this superiority is the additional power of sampling with stratification and by join-orders. As already stated, by using join orders, it is possible to calculate n marginal contributions using $n + 1$ evaluations of $v(S)$ as opposed to taking two evaluations of $v(S)$ for one marginal contribution sample point. This simple factor outweighed the advantage of the extra sophistication associated with SEBM and NEYMAN methods, which did not use join-order sampling - even though SEBM was seen to be more performant for larger sample budgets. We note that the SEBM method is developed in Section 6.4 of subsequent Chapter 6.

Another advantage that was witnessed in utilising the JOIN method was that it didn't have the computational overhead of using the formulas present in the SEBM method, and additionally the join-order sampling allowed each new optimisation that was called to be warm-started by the previous one as each new addition to the coalition would yield an optimisation similar to the previous one. These factors made JOIN appear as a simpler and more effective method for our purposes.

To evaluate the performance of the JOIN method in approximating the GNK value for larger networks, we generated random networks of different sizes (with parameters given in section 5.1.2) and estimated the GNK value using 8 simultaneous estimations, and timed how long it took for the average magnitude of error between these estimations to reach an one percent of each other. A scatter plot of the run-time performance of JOIN in approximating the GNK value for variously sized random networks by this process was generated and the results are shown in Figure 5.2.

From this figure it is witnessed that the GNK value appears to be doubly exponentially complex to approximate by sampling and quickly becomes intractable for networks consisting of more than 16 busses. This double-exponential complexity was somewhat expected as solving the GNK value exactly is identified as a calcu-

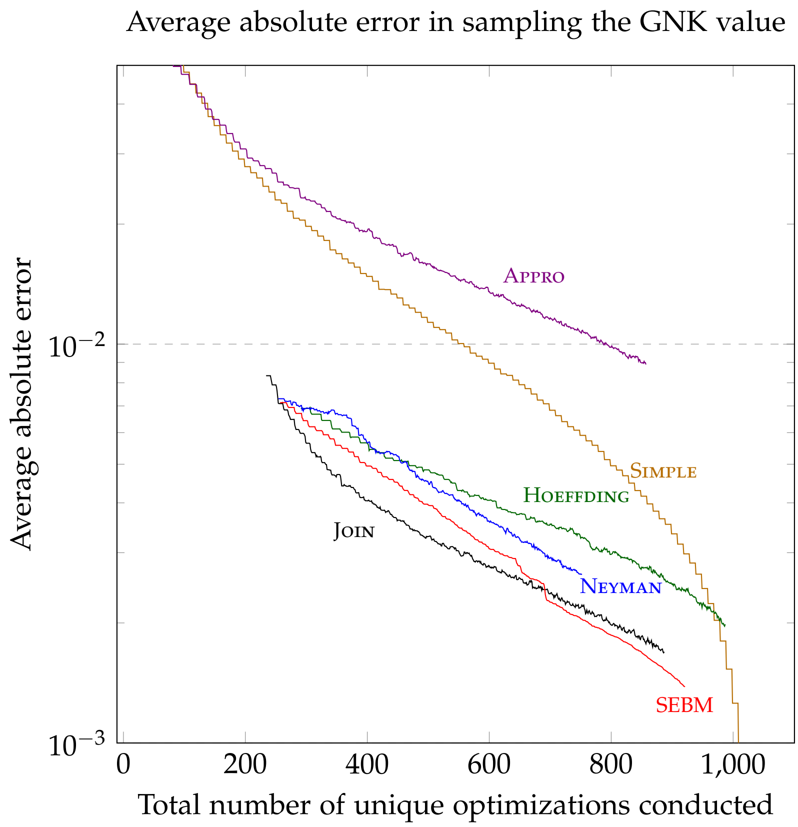


Figure 5.1: The average absolute error in the sample approximated GNK value for different sampling methods across randomly generated 10-bus networks.

lation that involves exponentially many (per equation 4.3) NP-hard computations (per equation 4.5). In light of this realisation we sought to make simplifications to the GNK value's inner optimisations (equation 4.5) to ease this intractability. Specifically we considered a polynomial-time computable proxy inplace of the minimax optimisations in the characteristic function (4.5) of the GNK value.

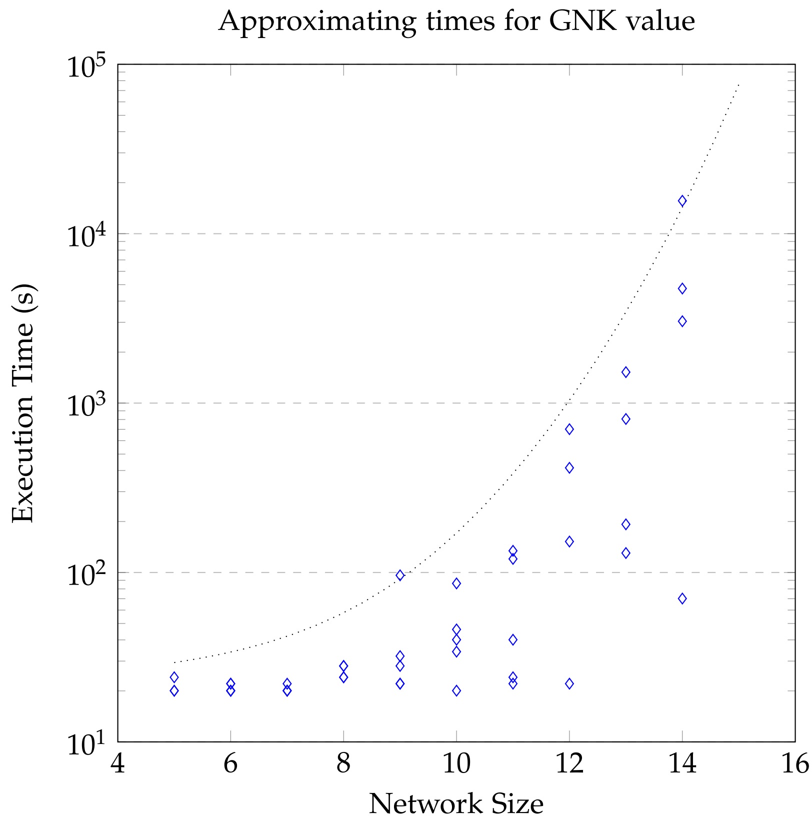


Figure 5.2: Execution times in approximating the GNK value on a selection of randomly generated example networks of different sizes, to 0.01 average magnitude of the error (relative to the magnitude of the estimated GNK value), between 8 independent estimations using JOIN method, with 20 seconds of validation time. The dashed curve $20 + \exp(\exp(n/6.2))$ indicates double exponential complexity

5.2 Sampling a modified GNK value (M-GNK) at scale

Given the intractable nature of the GNK value for large networks, we considered a proxy inplace of the minimax optimisations of the characteristic function that define the GNK value (equation 4.5). Particularly we considered a relaxation:

$$
\begin{aligned}
v(S) = &+\frac{1}{2}\left(\sum_{i\in S} u_i(p_i) - \sum_{i\in N\setminus S} u_i(p_i)\right)\\
&\qquad\qquad \text{s.t}\left[\{p_i\}_{i\in N} = \operatorname*{argmax}_{p\in A}\left(\sum_{i\in S} u_i(p_i) + \sum_{i\in N\setminus S} \epsilon u_i(p_i)\right)\right]\\
&-\frac{1}{2}\left(\sum_{i\in N\setminus S} u_i(p_i) - \sum_{i\in S} u_i(p_i)\right)\\
&\qquad\qquad \text{s.t}\left[\{p_i\}_{i\in N} = \operatorname*{argmax}_{p\in A}\left(\sum_{i\in N\setminus S} u_i(p_i) + \sum_{i\in S} \epsilon u_i(p_i)\right)\right]
\end{aligned}
\tag{5.1}
$$

Where ϵ is a sufficiently small positive value, and where all the DC power constraints noted to apply in both argmax.[2]

Rather than equation (4.5), this equation (5.1) encapsulates the expected payoff advantage of the coalition under a 50:50 coinflip of who goes first, where in each case the leader chooses the powerflows that strictly prioritise their own utility and then the follower's utility is maximised secondarily, we call this proxy GNK value the 'M-GNK value'.[3] This expression encodes much of the same dynamic as the original expression (equation 4.5) but avoids much of the adversarial strategic counter-considerations that make the original expression NP-hard, as the leader is unwilling to sacrifice their utility to harm the follower's utility and vice versa.

This proxy replaces the two-part NP-hard bilevel problems of equation 4.5, into two-part single-level linear programming problems. This transformation makes the M-GNK value much easier to compute at scale, but potentially at the cost of being a less perfect description of idealised minimax bargaining - even though no axioms (from section 4.2.1) would be lost. Thus, the use of this proxy might potentially see the introduction of artefacts - we discuss the similarity and the resulting numerical differences between the original GNK and M-GNK in section 5.4.5.

Some of the runtime statistics of sampling this M-GNK value with Join sampling for randomly generated network sizes (with parameters, and generated by the algorithm of section 5.1.2) are shown in Figure 5.3. From the figure it is seen that it is readily possible to calculate to about one percent accuracy this M-GNK value in

[2] using such an ϵ forces the optimiser to optimise one factor in the objective function strictly over the other, if the ϵ is too large in its context then the optimiser will likely do this imperfectly, and if the ϵ is too small then rounding issues can potentially occur in optimiser software, ϵ should be chosen to be as small as not to induce rounding issues in the solver

[3] This dynamic is evident for sufficiently small ϵ in the formula, but the same dynamic could also be achieved more directly by a two stage optimisation process.

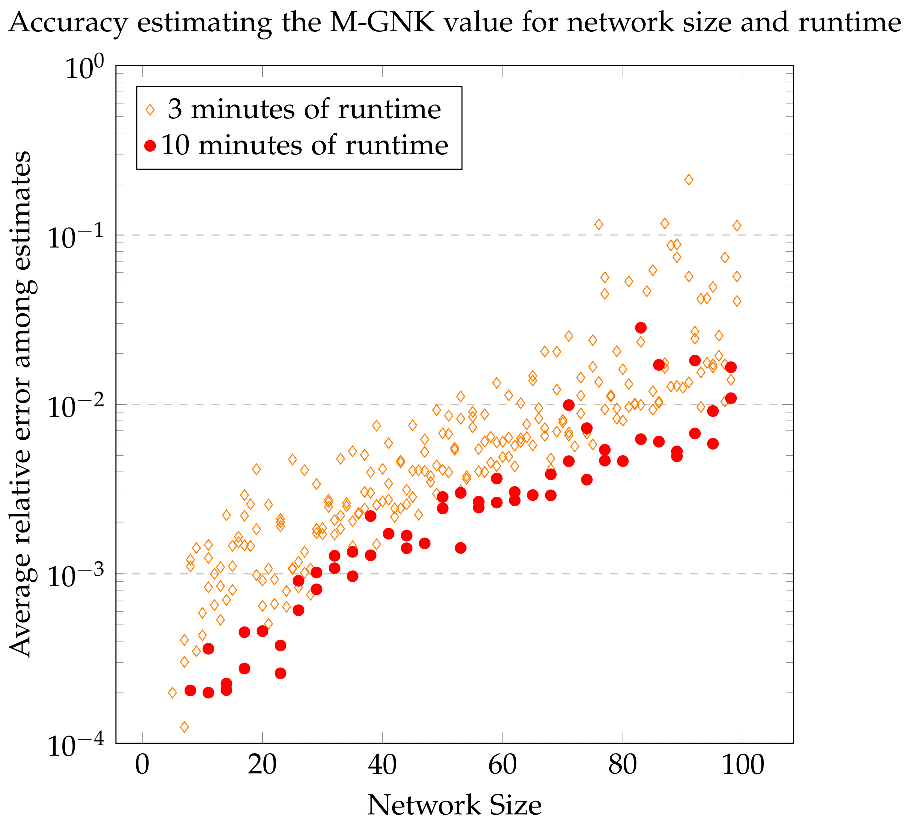


Figure 5.3: Average magnitude of error relative to the magnitude of the estimated M-GNK value between 8 independent simultaneous estimations on randomly generated networks of different sizes, for 3 and 10 minutes runtime on a desktop computer.

three minutes of runtime for networks of up to the size of about 50 nodes, and with ten minutes of runtime up to about 80 nodes.[4]

Using this ability to calculate the M-GNK value for larger networks, we can now consider the features of the M-GNK value in comparison with LMP and VCG for larger networks.

5.3 Results and evaluation of the GNK value at scale

In this section we consider and discuss some of the behaviour exhibited by the M-GNK value against VCG, LMP and Shapley Value for randomly generated larger networks. Particularly in Figures 5.4, and 5.5-5.8 we show the results of these techniques applied to an example 90 bus network (generated by algorithm 1), consisting of a 50-50 split of small consumers and small generators of electricity. In in this randomly generated networks (given by algorithm in section 5.1.2), there was no

[4] All calculations were performed on an Dell Optiplex 9020, with Intel i7 quad core 3.6GHz processor, and all source-code available at:
github.com/Markopolo141/The_Generalized_N-K_Value

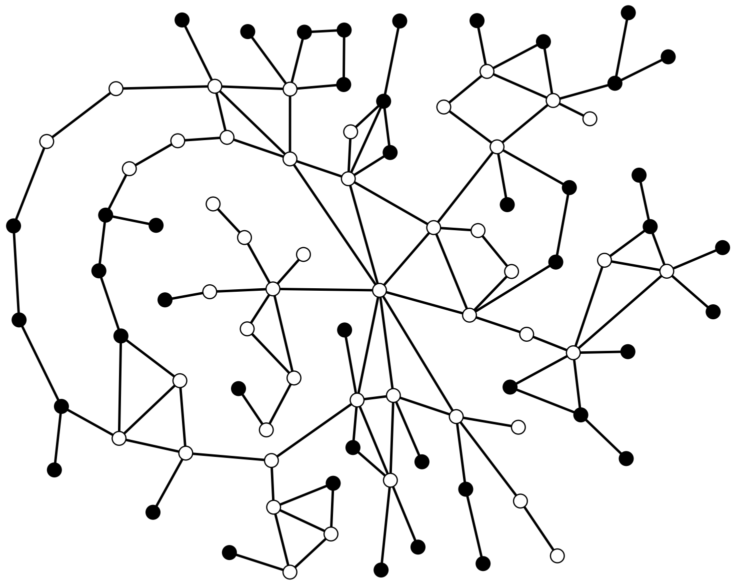


Figure 5.4: Node-line diagram for the example randomly generated 90-bus system, showing a 50-50 mix of small generators (black) and consumers (white)

constriction on power line limits, and each node has a randomly generated linear utility function (uniformly between 0.1 and 2.1 $ per kW) with randomly generated consumption/generation limits (uniformly between 1 and 15kW). For this randomly generated network we were able to calculate the GNK value, as well as LMP and VCG, and from these calculations we were able to see some of the distinct features of these techniques when applied to a large number of players.[5]

The most immediate result is that LMP and VCG are nearly identical (Figures 5.5 and 5.6) while it is noticed that the Shapley Value exhibits a very similar but slightly offset shape (see axes of Figure 5.8) and the GNK is distinctly different (5.7). The similarity between VCG and LMP can be explained by a variety of means, but a most informal explanation is that both LMP and VCG implement the same electrical outcome, and allocate payments in proportional to marginal differences about the socially optimal point. The confluence between VCG and LMP is not only witnessed by us, but also has been noted in a more general settings where there are many small participants [Nath and Sandholm, 2019; Tanaka et al., 2018] (see section 3.1.5).The similarity between the Shapley Value and LMP/VCG can be considered as an indication that the final marginal contribution in forming the grand coalition is most significant, whereas most other marginal contributions balance out between the players.

In Figures 5.5, 5.6 and 5.8 we see that there are no negative utility imputations, but that positive utility is allocated to those generators who are able to provide power the cheapest, and those consumers who value power the greatest (high x-value &

[5] All sourcecode for these experiments found at: https://github.com/Markopolo141/Thesis_code

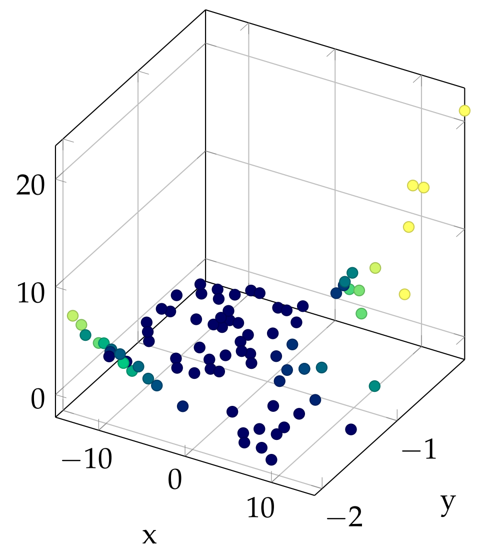


Figure 5.5: Post payment utility under LMP (z-axis & colour, in $) against generation/consumption capacity (x, positive being generation, in kW) with generation/consumption utility (y, in $/kW)

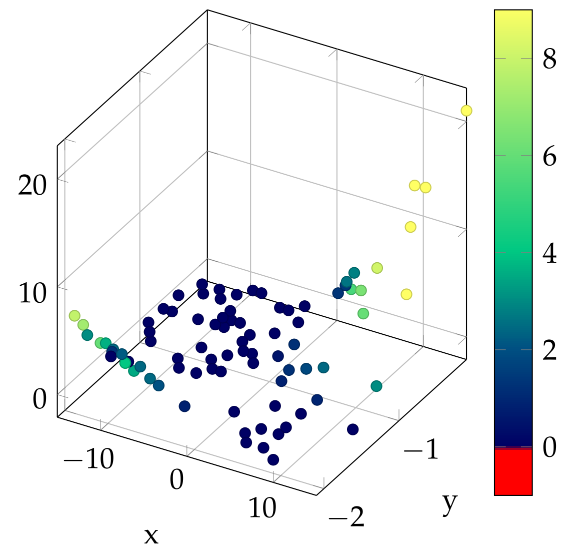


Figure 5.6: Post payment utility under VCG (z-axis & colour, in $) against generation/consumption capacity (x, positive being generation, in kW) with generation/consumption utility (y, in $/kW)

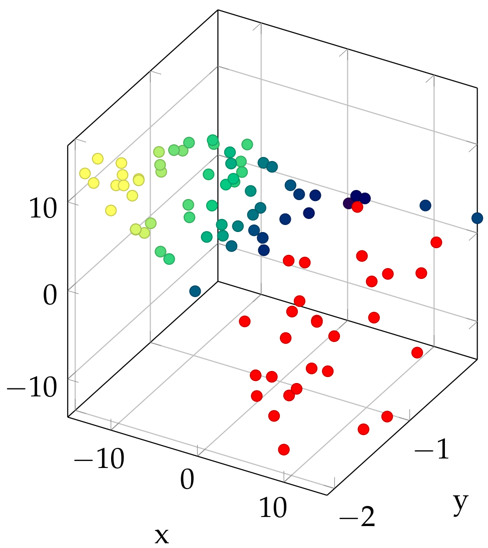


Figure 5.7: Post payment utility under proxy GNK (z-axis & colour, in $) against generation/consumption capacity (x, positive being generation, in kW) with generation/consumption utility (y, in $/kW)

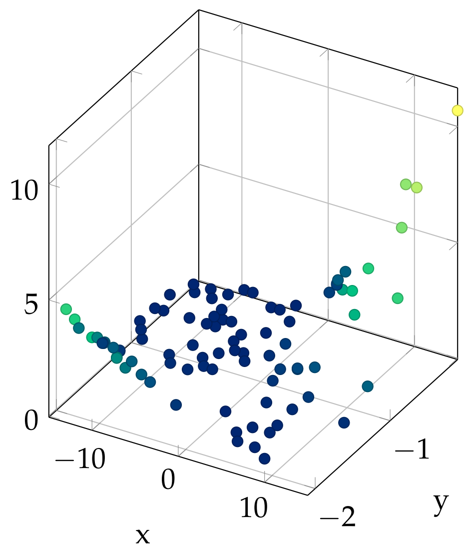


Figure 5.8: Post payment utility under Shapley Value (z-axis & colour, in $) against generation/consumption capacity (x, positive being generation, in kW) with generation/consumption utility (y, in $/kW)

low y-value, and low x-value & high y-value respectively). This is because the LMP creates prices for power such that the cheapest generators are scheduled to create power which is consumed by the most desiring consumers up until a marginal point where any further dispatch/consumption would be unmotivated, and because VCG schemes allocate non-negative utilities by their axiomatic construction (per axiom of individual rationality). From these graphs we straightforwardly identify those consumers/generators which generate/receive power as they are rewarded with positive utility.

Conversely we notice in Figure 5.7 a completely different result for the M-GNK value, particularly that the M-GNK imputes utility to those consumers who do not receive power (as already noted in section 4.4), but furthermore, it allocates negative net utility to all but the cheapest generators, even those who generate power at the socially optimal point (as identified by the previous paragraph as those generators who have positive imputation under LMP, in Figure 5.5), and this dynamic is not particularly easy to explain.

One primary explanation, lies in considering the average additional playoff advantage to a coalition of a high-cost generator. Particularly, if we consider the taking of a 50-50 coin flip about whether the coalition or its complement chooses their strategies first, and if the coalition goes first, then the generator will be idle (bringing no benefit to the coalition), whereas if the complement goes first, then it potentially will get dispatched (hence causing a loss to the coalition) because the complement will choose to consume power and power-constraints must be obeyed, giving them a greater pay off advantage. Hence the high-cost generator only brings negative payoff-advantage which is reflected in the M-GNK value.

Or more succinctly, the way in which the generators get allocated negative utility is that they are targets of being forced to generate at their own deficit since power-conservation constraints must be obeyed, and this dynamic becomes a negotiating lever, in the selection of threat points. This consideration works reversely for consumers, who can only consume at a positive utility to them, thus they are at a bargaining advantage which is then reflected in the positive utility they are rewarded with under M-GNK.

This behaviour in the context of large networks was somewhat unexpected; and we summarise the consequences in the following section 5.4.

5.4 Discussion and conclusion

To consider the social and ethical value of the GNK value we must loop back to consider some of the topics explored in Chapter 2. Particularly we briefly considered some moral elements about the distribution of resources, including Equality, Efficiency, and the various normative reference points which may be pertinent. We will consider the GNK in light of each of these in turn.

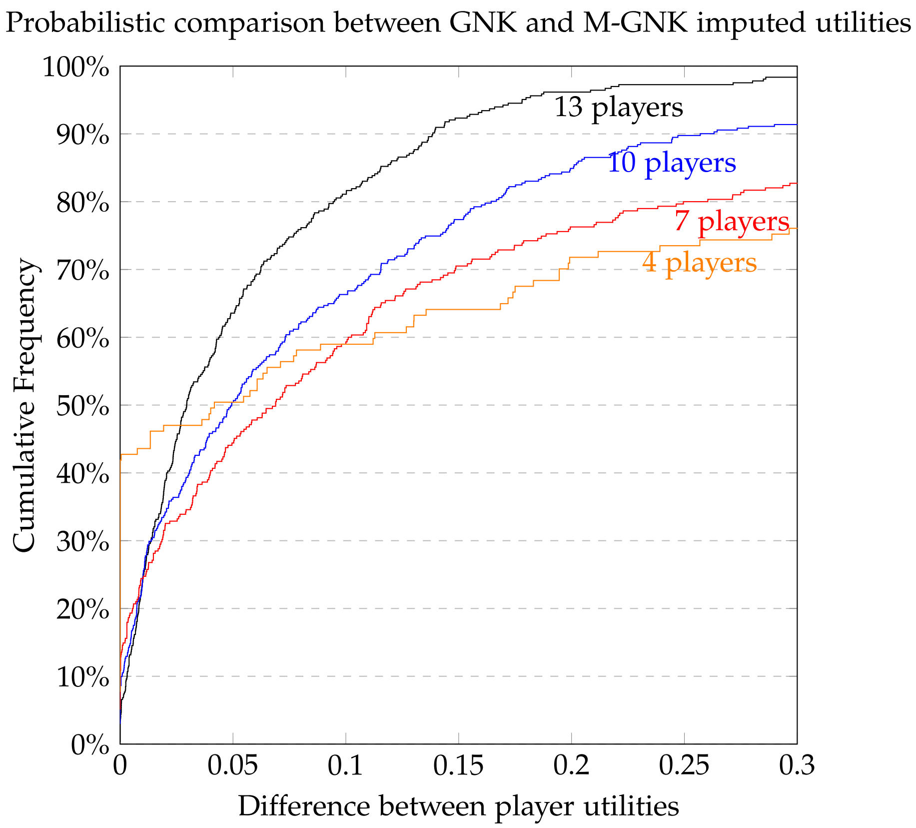


Figure 5.9: The cummulative frequency of a player obtaining an imputed M-GNK utility within a certain proportion with the GNK solution, for randomly generated network instances for each network size (4 to 13 players). The error is the proportionate utility difference, normalised by total player utlity.

5.4.1 Efficiency

It is easy to realise that the GNK value is axiomatically efficient, specifically in terms of maximising the sum of utility, by axiom (equation 4.2); and as it is efficient in this regard it is also therefore Pareto optimal. The way this efficiency is implemented is that the GNK designates the electrical outcome which maximises the sum of utility, and issues budget-balanced utility transfers between the players. Neither LMP or VCG has a similar efficiency claim, as both allocate payments between network participants are not necessarily budget balanced. However in order to consider whether this axiomatic efficiency is actually a good thing we need to consider it in terms of what is socially good.

While there are different and potentially competing philosophical notions of what social 'efficiency' should mean, the maximisation of the sum of utility is a very classical notion. The implementation of the GNK value assumes that utility is transferable, and the easiest way of comprehending this is in terms of utility as measured by money. And hence, in this context the maximisation of utility might be seen as corresponding to the maximisation of the monetary value of outcomes.

However it is worth noting that this might not be socially desirable, as there may be some sense in thinking that maximising utility via monetary measurement could potentially be prone to social problems, specifically as there exists some agreement of the diminishing value for money itself, in that the rich are made only a little better off by an amount of money, that would be more appreciated by the poor.

The GNK value allocates the utilitarian outcome, however it is not necessarily required that utility be measured in money (even though this is the easiest interpretation). It is also possible to note that there exist non-transferable-utility (NTU) modifications - such as also considered by Kohlberg and Neyman [2015] - which could be modified to yield a NTU GNK value. Such solution concepts could be utilised where utility is not directly transferable and which could incorporate non-linear utilities over possible monetary transactions, potentially resulting in more egalitarian outcomes.

The potential for modifying the GNK value for application in NTU settings in order to account for different efficiency measures is a topic of potential future investigation.

5.4.2 Formal-equality

All the techniques considered (GNK, VCG and LMP, etc.) satisfy formal-equality, as they only treat different participants differently in relation to specific morally relevant characteristics — particularly their utility preferences, and how their presence and actions can affect the utility of others. In the electricity context, this involves the utility of electricity and capacity to deliver/generate electricity at their location in relation to the utility of that electricity for others.

However, whetherornot these qualify as morally warranted bases for differential treatment is the subject of a wider discussion, particularly as differential treatment gives rise to differential incentives. For instance, the idea of people being afforded different effective prices for electricity depending on the location of their electrical influence may be regarded as being ethically unfair to some people (especially perhaps between close neighbours whose grid connections are electrically different), however a negation of this also destroy any incentive for people to install additional generation capacity in electrically advantageous locations.

Differential treatment can be seen as the mirror image of differential incentives, and a comprehensive reflection of the incentives that would be given under LMP against VCG and GNK are beyond the scope of our consideration. However we can speculate that there exists a primary difference between VCG and LMP (which give similar results) and GNK, in that LMP and VCG incentivise behaviour that could affect the network operating point; particularly affecting only those generators/consumers which would (or do) generate or consume power at the network operating point. Wherease GNK is more comprehensive in its consideration, as it affords utility for every possible way that the network could degenerate into adversarial competition; thus we might speculate that the GNK value (or something similar to it) might incentives robustness in the network.

5.4.3 Heterogeneity of normative points

The essential feature of the GNK value is that it is an extension of bargaining solution concepts to multiple players over the restricted strategy space of a generalised non-cooperative games. The GNK value inherits the assumption from Nash bargaining that the minimax of the zero-sum game is the point which is/should-be the disagreement point between any two coalitions for the system, and that all coalitions are equally weighted - however this construction can be questioned.

Firstly, the GNK can be seen to assign equal weight for every possible coalition that could form, irrespective of the likelihood that such coalitions would actually form in competition. It may be possible to construct a weighted GNK value to account for differential likelihoods of different coalitions forming, but that is a remaining further consideration.

Secondly, the minimax of the zero-sum game identifies a point of maximum strategising to gain payoff advantage specifically over the opponent, irrespective of the absolute payoff to the player. And in this way minimax of the zero-sum game identifies a point of maximally engaged competition between the players. Against this consideration, it is good to note, that while the GNK (and Nash bargaining solution concepts) can be viewed as a description of perfect competition between individuals, it can also directly account for the possibility that that groups (or subgroups) of players may be altruistic; in that altruism may be accounted for by a player's utility function including terms associated with positive utility for others.

However this might not be sufficient, and the GNK value contrasts against other similar solutions over non-cooperative games (as briefly mentioned in section 4.2.4) such von Neumann and Morgenstern's solution (per equation 4.7), where the characteristic function is identified as minimax payoff, not minimax payoff advantage. In this way von Neumann and Morgenstern's characteristic function can be considered as descriptive of a point of less totally engaged competition between coalitions - which might be more appropriate or pertinent for electricity networks. Von Neumann and Morgenstern's characteristic function is not the only alternative way that the characteristic function could be constructed, but unfortunately these alternative constructions would not necessarily yield Nash bargaining solution in the two player case.

5.4.4 Wider equality

In the development of this research it was hoped that the GNK value would ultimately be witnessed to have a similar individual rationality property as VCG. Particularly that no participant should be allocated less than zero utility, which might be interpreted as being what they would get if they did not participate in the mechanism. The ethical importance of individual rationality cannot easily be overstated, particularly as a primary notion of ethical exchange is the concept of 'euvoluntary' exchange (see section 2.2.5) which is (at least) where every party is not left worse-off for participating.

However, it is evident that GNK seems to violate this property, as it is possible for participants to be allocated with less utility than zero. We would expect that this particular absence of a guarantee for participants would be a major hindrance to GNK's application in electricity systems; hence an ethical failing.

In the designing of the GNK value it was hoped that individual rationality would be a property which would be present for larger networks, particularly as it was suspected in section 3.4.2 that if it was possible for players to unilaterally implement an outcome which guaranteed them a utility of zero, then they would be guaranteed a non-negative net utility. However in our GNK application to electricity networks, the enforcement of the power conservation constraints (per equation 4.8) seems to have disallowed this eventuality.

For instance, under GNK value in the context of our generalised game modelling DC networks, the power conservation constraint causes the incorporation of unrealistic bargaining manoeuvres, such as participants extortionately threatening to oversupply others. It is very possible that alterations to the GNK value, and similar types of Shapley Value structures over non-cooperative game solutions could be made to amend this issue.

It may be possible, for instance, to reconsider the electrical interaction between participants, perhaps by allowing player's action space to be selection of voltage level at their location, rather than directly their power input/output; however in this context power line limits would be manifest as non-linear constraints on the optimisation problem, subsequently making computation more difficult. Alternatively, it might also be possible to implement blackout costs to participants to curtail the possibility of unrealistic bargaining manoeuvres in the GNK value logic.

In these cases, it might be possible to give participants actions to guarantee themself a disagreement point which affords them a zero utility, and hence potentially restore individual rationality to the resultant GNK value; however these investigations are a topic for future research.

At a broader level of consideration, it is interesting how perfect competition may or may not coincide with what is equal and ethical. The question of when and where these coincide, and particularly if they might coincide in the context of electricity networks, was part of the motivation of this research. Unfortunately our investigations demonstrated that the most direct application of the GNK value would be expected to fail wider social equality considerations.

5.4.5 Future work and possible extensions

One primary question is how much the behaviour exhibited in Figure 5.7 is entirely the result of us using a modified characteristic function, per the M-GNK value (equation 5.1), over the more original characteristic function of the GNK value (equation 4.5). In order to investigate this question, the error of using this modification across randomly generated networks was calculated and shown in Figure 5.9. This graph shows the cumulative probability of the difference in payments between the GNK and M-GNK - and shows for instance, that 60% of participants could expect to receive within 10% what they would have between GNK and M-GNK values, and that this similarity increases for larger network sizes.

From this graph it is noticed that the GNK and M-GNK values feature similarity which seems to increase with the size of the network under consideration — although for computational reasons, it is increasingly difficult to confirm for networks with a size greater than 13 nodes. This limited observation coincides with expectations that the possible strategic counter-considerations that are discarded by using equation 5.1 over equation 4.5 become less relevant in the context of larger networks; but such a claim warrants further investigation. But further investigation on the degree of similarity and/or difference between GNK and M-GNK is warranted.

Another observation, is that while the GNK remains soluble for networks of less than 13 nodes and the M-GNK value remains soluble for up to 80 node networks (to about 1% accuracy, as per Figure 5.3), however these numbers might still be regarded as being too small for real-world electrical network modelling. Larger networks are expected to be tractable for the M-GNK value with more computing power and/or execution time, however further methodological improvements may be necessary to make the GNK value (or anything similar to it) capable of bearing on larger and real world networks. Some possible avenues of investigation include employing further approximations such as player clustering (such as implemented by Han et al. [2019]), or transforming the problem into a non-atomic form, similar to non-atomic Shapley Value.

Another outstanding question, is what the likely outcome would be, under GNK, in the context of strategising network participants. So, while VCG has some explicit consideration of the strategising of individual agents, and LMP is identified to be largely identical to it in the context of large numbers of small players, the consequences of agents strategising under GNK is not considered here. As the GNK is not incentive incompatible and also quite complex, this issue constitutes both a major consideration and a difficult question. While there does exist some work on similar (but more complex) solution concepts like GNK that are incentive compatible (such as presented by Myerson [1980]; Salamanca [2019]) their investigation and evaluation in the context of electricity networks remain a topic for further investigation.

The GNK value and similar measures are by the generality of their construction potentially applicable to more than the contexts in which we have applied them in these chapters, and many of the issues of real electricity markets raised in Chapter 1, may be alleviated by measures such as these. The actual details of their application in those spaces, is potentially valuable future work.

5.4.6 Conclusion

Throughout this research program we have undertaken an investigation into the space of possible mechanisms for valuing electricity. Most particularly, we investigated the space of possible mechanisms which can be bring into account all the possible confluences of electrical system details, as well as all the possible leverages and counter considerations which could play in an idealised negotiation between all parties about such an electricity system. A mechanism which considered the unrestricted span of possible considerations and counterconsiderations between electrical system participants and the system, was seen to be an important quality as it is understood that the future smart grid will encompass a host of differing electrical situations with a range of smart devices, and the way in which the value of these devices and the electricity they consume/generate will be determined is in need of an answer.

The original research question was:

How *should* electricity be valued and traded?

We have identified (in Chapter 2) that such a question is not easy to answer and has strong ethical undertones, making a comprehensively demonstrable answer impossible in principle, but an object of important investigation notwithstanding. To investigate, we covered some existing solution concepts (in Chapter 3) such as Nash's axiomatic bargaining, Cooperative game theory topics such as the core and Shapley Value, the VCG mechanism from mechanism design and marginal pricing theory. And from this investigation we attempted to take the best features of these concepts and synthesise a genuinely novel solution for the pricing of electrical resources on electricity networks, in Chapter 4, which we then evaluated at scale in this chapter.

Our new GNK solution is essentially rooted in bargaining perspective, rewarding participants for the advantage they might have in competition with all others, and it was hoped that an idealised bargaining solution like this, would yield the kinds of arrangements that people with divergent interests would freely and naturally negotiate towards. In this way, we hoped it would ascribe economic value to electricity resources in the most natural way; however this process ultimately yielded a disappointing result.

The GNK value extended from the Shapley Value axioms, and as such it inherits the NP-hard computational difficulty associated with the Shapley Value. However, through investigation into sampling techniques and in utilising a particular proxy for the minimax-optimisations, we were able to extend the GNK value from being intractable for ~ 14 bus nodal networks to being computable for about $80 - 100$ bus nodal networks, for a desktop computer. This was seen as an accomplishment, particularly as if the GNK value were calculated exactly for a 100 sized nodal network it would involve $\sim 2^{100}$ optimisation terms.

Through the process of considering the different ways that the GNK value could be sampled we developed some of our own complicated techniques which proved to be competitive against existing methods for sampling the Shapley Value and hence the GNK value. This novel method extended from a consideration of of possible concentration inequality which which could be developed specifically for stratified sampling. We developed novel and tailored concentration inequalities for stratified sampling, and this formed the basis of our new method. The development of this new concentration inequality (SEBB) and sampling methodology (SEBM) is detailed in the next chapter. In the next chapter we delve into the details of the sampling techniques that were developed and tested throughout this research, particularly the SEBM method in Section 6.4, which was evaluated as a method to sample the GNK value (alongside others) in Section 5.1.

Chapter 6

Stratified sampling

In the previous chapter we introduced the GNK value and recognised that it could be approximated by a stratified sampling process (section 5.1). Accordingly, in this chapter we investigate the different possible rules for choosing samples from strata in the context of stratified sampling.

We review the orthodox solution to the problem which is called Neyman allocation, and show how it is equivalent to minimising a concentration inequality called Chebyshev's ineqality. We then turn our attention to two different approaches to developing novel concentration inequalities for stratified sampling, whose minimisation yields new stratified sampling methods. These new sampling methodologies are then tested for their performance in the context of synthetic sample data sets, and in the context of sampling the Shapley Value of cooperative games.

The structure of this Chapter is as follows:

1. In section 6.1, we give a review of relevant background information and techniques, particularly addressing the recent innovation of Empirical Bernstein Bounds (EBBs).

2. In section 6.2, of this chapter we show how EBBs can be bound together to create concentration inequalities appropriate for Stratified Sampling and give an algorithm for choosing samples to minimise these bounds.

3. In section 6.3 of this chapter we derive a unique and stronger EBB, for the purposes of evaluation in the context of stratified sampling.

4. In section 6.4, we provide multi-part derivations of complicated concentration inequalities specifically tailored for the purposes of stratified sampling, and give an algorithm for choosing samples to minimise these inequalities.

5. In section 6.5, we give the performance results of various methods of stratified sampling in the context of synthetic data sets, and in the application of approximating the Shapley Value.

6. In section 6.7 we give discussion to the derivations and results,

7. in section 6.8 and talk briefly about future work about a multidimensional stratified sampling EBB, and conclude.

The work and development from the second and third section most directly reflects published material: "An Engineered Empirical Bernstein Bound",
European Conference on Machine Learning (ECML-PKDD) 2019
(accessible: ecmlpkdd2019.org/downloads/paper/435.pdf)
The work and development from the fourth and fifth section most directly reflect published material: "Approximating the Shapley Value Using Stratified Empirical Bernstein Sampling", IJCAI 2021
(accessible: ijcai.org/proceedings/2021/0011.pdf)

6.1 Introduction and background

Stratified sampling is a well known example of a process of selecting samples to most accurately estimate an average over weighted sample averages. Particularly stratified random sampling is a process of estimating the average over a population by breaking a population into mutually-exclusive subgroups and sampling them randomly. Such stratified sampling has been identified to lead to improved reliability in estimation over simple random sampling of the population by Neyman [1938]; Wright [2012] particularly when:

- The population is divisible into strata, in which there is less variance in each stratum than across them all
- When the size of the strata are known or reasonably estimated
- When sampling selectively from each strata is possible

The concept of stratified random sampling is easily illustrated, for instance, to poll the population of a country's support for a particular government policy, it is possible to sample the different demographic regions within the country. For instance, if regions A,B and C contain 10%, 40% and 50% of a population, and sampling of these regions reliably show support levels of 2%, 70% and 30%, respectively, then it is possible to discern that 43.2% of the total population supports the policy.

Our primary investigative question of this chapter is this: when we have a population decomposed into strata of known sizes which we can selectively sample from, how do we choose samples from the strata to get the most accuracy in the final population estimate?

For instance, if we sample primarily from a single stratum, we would likely have a very good estimate of the average for that one stratum, but no accuracy in estimate for the others, leading to a weak estimate of the population average. Conversely, if we choose to take the same number of samples from all the strata, some of the strata might be far smaller or have far less variance than others, resulting in those strata being oversampled.

This question has been considered before, and the most direct historical answer to the question is called *Neyman allocation* or *sampling* [Neyman, 1938]. The principle of Neyman sampling is that it seeks the minimise the weighted variance of the population estimate assuming knowledge of the variances of the strata, and it can most directly be interpreted as a process of minimising Chebyschev's inequality.

6.1.1 Neyman allocation

Neyman allocation identifies that in order to minimise the variance in the final estimate of the population, that sampling should be directly in proportion to the stratum variances multiplied by their sizes. We present Neyman allocation rule with its proof to illustrate the connection with allocation rule with a concentration inequality:

Theorem 1 (Neyman allocation)**.** *For m strata, of sizes N_i, with variance σ_i^2. For a sample budget n, and there is a choice how much to sample from each strata n_i, in which sampling is done with replacement (ie. all samples are independent and identically distributed) Then the selection of n_i which minimises the variance of our population estimate μ is:*

$$n_i = \frac{nN_i\sigma_i}{\sum_j N_j\sigma_j}$$

Proof. For any independant random variables X and Y (and for any $a, b \in \mathbb{R}$), $\text{Var}(aX + bY) = a^2\text{Var}(X) + b^2\text{Var}(Y)$.
So, if $X_{i,j}$ are the random variable of the jth sample from the ith stratum, then:

$$\hat{\mu} = \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k} \frac{1}{n_i} \sum_{j=1}^{n_i} X_{i,j} \qquad \text{and hence} \qquad \text{Var}(\hat{\mu}) = \frac{1}{\left(\sum_k N_k\right)^2} \sum_{i=1}^{m} \frac{N_i^2}{n_i}\sigma_i^2 \tag{6.1}$$

To minimise the variance of our estimate $\text{Var}(\mu)$ by selecting n_i subject to the constraint that $\sum_{i=1}^m n_i = n$, we form the Lagrangian (with Lagrange multiplier λ):

$$L = \text{Var}(\hat{\mu}) + \lambda\left(\sum_{i=1}^{m} n_i - n\right) = \sum_{i=1}^{m}\left(\frac{N_i^2\sigma_i^2}{n_i\left(\sum_k N_k\right)^2} + \lambda\left(n_i - \frac{n}{m}\right)\right)$$

Hence for any i solving for $\frac{\partial L}{\partial n_i} = 0$ leads to: $n_i = \frac{N_i\sigma_i}{\lambda\sum_k N_k}$ and using $\sum_{i=1}^m n_i = n$, to eliminate λ gives the result □

This allocation rule begs the question of why we would specifically want to minimise the variance of our population mean estimate. And the primary reason is that that the variance of an estimate bounds the probability of error in the estimate, and this can be seen most directly by Chebyshev's inequality.

Theorem 2 (Chebyshev's inequality)**.** *for any random variable — in this case $\hat{\mu}$ is a random variable — with variance $Var(\hat{\mu})$ then the error of $\hat{\mu}$ from its mean is probability bounded:*

$$\mathbb{P}\left(|\hat{\mu} - \mu| \geq k\sqrt{Var(\hat{\mu})}\right) \leq \frac{1}{k^2}$$

Thus if μ is the true population mean, then the error in our stratified estimate of the population mean $\hat{\mu}$ is probability bounded by the variance of it. So, for instance, Chebyshev's inequality guarantees that there will always be less than a 25% chance that the error in our estimate of the population mean will be more than twice the square root of its variance. In this context, Chebyshev's is an example of a *concentration inequality*, as it provides probability bounds on the concentration of the estimate around its mean value.

An additional and perhaps more intuitive angle by which Neyman allocation may be seen to be appropriate, is that if sufficiently large numbers of samples have been taken then the sample means of the strata will tend to be Gaussian distributed by the Central Limit Theorem. In this context the strata means have a distribution that is entirely characterised by their mean and variance, and hence so too therefore is the population mean. In this context the variance of the sampled population mean is the only parameter controlling the error, and minimising it directly translates into improved accuracy.

One primary limitation of using Neyman allocation, is that is presupposes knowledge of the variances of the strata, which usually aren't available beforehand or in practice. One relatively easy way of going around this problem is to go through a process to estimate the variances of the strata, perhaps as a prior step, and then using this knowledge with Neyman allocation to choose further samples. And while this idea certainly works, it leaves open the question about how much sampling should be done to estimate the strata variances against how much sampling should be left to sample by those estimated variances.

Neyman allocation is an orthodox sampling rule which directly extends from minimising a specific concentration inequality that unfortunately depends on known variances. It is therefore suitable to ask if there are alternative concentration inequalities which do not depend on known variances, which can be minimised to form novel sampling rules for stratified sampling.

6.1.2 Concentration inequalities and Chernoff bounds

In order to consider what alternative concentration inequalities exist, we need to turn to the space of concentration inequalities generally.

Neyman allocation implicitly minimises Chebyshev's inequality, but Chebyshev's inequality is one example of many concentration inequalities. Concentration inequalities are applied in a range of data science contexts for a variety of prediction, machine learning and hypothesis testing tasks, including: change detection [Kifer et al., 2004; Bhaduri et al., 2017] and classification [Rehman et al., 2012] in data streams; outlier analysis in large databases [Aggarwal, 2015]; online optimisation [Flaxman et al., 2005; Agarwal et al., 2010]; online prediction and learning problems [Mnih et al., 2008; Thomas et al., 2015; Maurer and Pontil, 2009], and in settings with bandit feedback [Auer et al., 2003; Audibert and Bubeck, 2009; Tran-Thanh et al., 2012].

There are many famous concentration inequalities such as Chebyshev's inequality [Bienaymé, 1853], Bernstein's inequalities [Bernstein, 1924], Hoeffding's inequalities [Hoeffding, 1963] and Bennett's inequalities [Bennett, 1962]. New analysis has yielded a wider range of concentration inequalities and methods of generating them. In particular, various innovations concern the concentration of more-general functions of random variables, such as the Efron-Stein [Efron and Stein, 1981] and entropy methods [Boucheron et al., 2003].

Recently, concentration inequalities have been developed which do not rely on variance information, but incorporate uncertainty about variance information via the sample variance, these bounds are sometimes called *Empirical Bernstein Bounds* (EBB). These concentration inequalities describe the likely difference of a sample mean from the population mean in terms of the *sample* variance, some of the first EBBs given in literature are:

Theorem 3 (Maurer and Pontil [2009])**.** *Let X be a real-valued random variable that is bounded $a \leq X \leq b$, with $D = b - a$. Then for $x_1, x_2, \dots, x_n$ independent samples of X the mean $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and sample variance $\hat{\sigma}^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})^2$ are probability bounded by t for any $t > 0$:*

$$\mathbb{P}\left(\mu - \hat{\mu} \geq \sqrt{\frac{2\hat{\sigma}^2 \log(2/t)}{n}} + \frac{7D\log(2/t)}{3(n-1)}\right) \leq t \tag{6.2}$$

Theorem 4 (Audibert et al. [2007])**.** *In exactly the same context as in Theorem 3*

$$\mathbb{P}\left(\mu - \hat{\mu} \geq \sqrt{\frac{2\hat{\sigma}^2 \log(3/t)}{2n}} + \frac{3D\log(3/t)}{2n}\right) \leq t. \tag{6.3}$$

The derivation of these EBBs are of interest, because they illustrate how it is possible to derive concentration inequalities which involve variance information but do not depend directly on the variance itself, and which might be extended to develop alternative methods of stratified sampling. Unfortunately these EBBs cannot directly be used to minimise the error in the aggregated population estimate, as the aggregated population estimate does not itself have a sample variance. But in later section 6.2.1 we will show how these types of inequalities can be modified and subsequently minimised to create new methods of sample selection in stratified random sampling.

In section 6.3 we will also show how it is possible to derive stronger EBBs, thus we introduce some of the components used in the process of deriving EBBs.

6.1.3 Components of concentration inequality derivations

One of the more famous concentration inequalities is *Hoeffding's Inequality* which is one of a class of concentration inequalities called *Chernoff bounds*.

Lemma 1 (Chernoff Bound)**.** *If $\hat{\mu}$ is sample mean of n independent and identically distributed samples of random variable X then for any $s > 0$ and t:*

$$\mathbb{P}(\hat{\mu} \geq t) \leq \mathbb{E}\left[\exp(sX)\right]^n \exp(-snt)$$

Proof of Chernoff Bound - Lemma 1.

$$\mathbb{P}(\hat{\mu} \geq t) = \mathbb{P}\left(\exp\left(s\sum_{i=1}^{n} x_i\right) \geq \exp(snt)\right)$$

$$\leq \mathbb{E}\left[\exp\left(s\sum_{i=1}^{n} x_i\right)\right]\exp(-snt) \leq \mathbb{E}\left[\exp\left(sX\right)\right]^n \exp(-snt)$$

using Markov's inequality and the i.i.d of the samples, respectively. □

Here we have given the general form of Chernoff bounds for the sample mean of random variable, parameterised by a choice of $s > 0$ and t. Using this kind of lemma, many well-known examples of Chernoff bounds follow from the derivation of upper bounds for $\mathbb{E}\left[\exp(sX)\right]$, also known as the *moment generating function*.

For any upper bound $\mathbb{E}[\exp(sX)] \leq g(s)$ then $\mathbb{P}(\hat{\mu} > t) \leq g^n(s)\exp(-snt)$ is an upper bound for the deviation of the sample mean, which can then be subsequently minimised with s, forming a concentration inequality; in this way a Chernoff concentration inequality can be deduced from a bound on the moment-generating-function. Hoeffding's inequality [Hoeffding, 1963] is an illustrative example of this process of deriving a Chernoff bound (which we will do in many times in this chapter), and we give a short refactored proof of this process:

Theorem 5 (Hoeffding's inequality for mean zero). *Let X be a real-valued random variable that is bounded $a \leq X \leq b$, with a mean μ of zero. Then for $D = b - a$ and any $t > 0$, the mean $\hat{\mu}$ of n independent samples of X is probability bounded by:*

$$\mathbb{P}(\hat{\mu} \geq t) \leq \exp\left(\frac{-2nt^2}{D^2}\right) \tag{6.4}$$

Proof. If X has a probability density function $f(x)$, then we can linearise $\exp(sx)$ as:

$$\mathbb{E}[\exp(sX)] = \int_a^b f(x)\exp(sx)dx \leq \int_a^b f(x)\left(\frac{x-a}{b-a}\exp(sb) + \frac{b-x}{b-a}\exp(sa)\right)dx \tag{6.5}$$

Using the fact that the mean $\mu = \int_a^b f(x)xdx = 0$ thus:

$$\mathbb{E}[\exp(sX)] \leq \frac{1}{sb - sa}\left(sb\exp(sa) - sa\exp(sb)\right) \tag{6.6}$$

Given the fact that for any $\kappa > 0, \gamma < 0$:

$$\frac{\kappa\exp(\gamma) - \gamma\exp(\kappa)}{\kappa - \gamma} \leq \exp\left(\frac{1}{8}(\kappa-\gamma)^2\right) \tag{6.7}$$

thus:

$$\mathbb{E}[\exp(sX)] \leq \exp\left(\frac{1}{8}s^2(b-a)^2\right) \tag{6.8}$$

Applying our Chernoff bound lemma 1 we get:

$$\mathbb{P}(\hat{\mu} \geq t) \leq \exp\left(\frac{1}{8}s^2(b-a)^2 n - snt\right)$$

And minimising with respect to s yields the required result. □

The most limiting feature of the derivation is the requirement that the mean is zero however this is immaterial and is used to simplify the derivation, as any statistic can be shifted such that its expectation value becomes zero, hence:

Theorem 6 (Hoeffding's inequality)**.** *Let X be a real-valued random variable that is bounded $a \leq X \leq b$. Then for $D = b - a$ and any $t > 0$, the mean $\hat{\mu}$ of n independent samples of X is probability bounded by:*

$$\mathbb{P}(\hat{\mu} - \mu \geq t) \leq \exp\left(\frac{-2nt^2}{D^2}\right) \tag{6.9}$$

Alternatively by rearranging:

$$\mathbb{P}\left(\hat{\mu} - \mu \geq \sqrt{\frac{D^2 \log(1/t)}{2n}}\right) \leq t \tag{6.10}$$

In this way Hoeffding's inequality is a rather friendly result that states that the concentration of sample mean is probability bounded by a Gaussian function, and this might be seen as an intuitive corollary of the Central Limit Theorem. We provide the derivation of Hoeffding's inequality to illustrate the technique of deriving Chernoff bounds. Additionally we will utilise Equation 6.8 in further derivations - also called Hoeffding's Lemma:

Lemma 2 (Hoeffding's Lemma)**.** *Let X be a real-valued random variable that is bounded $a \leq X \leq b$, with a mean μ of zero, then for $D = b - a$ and any $s > 0$:*

$$\mathbb{E}[\exp(sX)] \leq \exp\left(\frac{1}{8}s^2 D^2\right)$$

This process of deriving and minimising a bound for the moment-generating-function will be used repeatedly to create novel concentration inequalities in sections 6.2 and 6.4.

6.1.3.1 A further note Chernoff bounds, sampling with or without replacement

In many cases, the derivation of concentration inequalities assume that the values that the samples take are independently from each other. This most naturally corresponds to the schema of sampling *with* replacement, rather than sampling *without* replacement. However Chernoff probability bounds that assume independence of the samples are also suitable to the case of sampling without replacement, this is due to a result shown by Hoeffding [1963]:

Lemma 3 (Hoeffding's reduction)**.** *let $X = (x_1, \ldots, x_n)$ be a finite population of n real points, let $X_1, \ldots, X_n$ denote random samples without replacement from X and $Y_1, \ldots, Y_n$ denote random samples with replacement from X. If $f : \mathbb{R} \to \mathbb{R}$ is continuous and convex, then:*

$$\mathbb{E}\left[f\left(\sum_{i=1}^{n} X_i\right)\right] \leq \mathbb{E}\left[f\left(\sum_{i=1}^{n} Y_i\right)\right]$$

Using the continuous and convex function $f(x) = \exp(sx)$ it can be seen via the construction of Chernoff bounds (Theorem 1) that this result implies that all Chernoff bounds developed for sampling with replacement also hold for sampling without replacement.

6.1.4 Other general probability lemmas

There are further lemmas that are necessary for the further derivations for this chapter. The first lemma is an often-used and rather weak result used to fuse simple statements of probability (provided with proof for completeness of information):

Lemma 4 (Probability Union)**.** *For any random variables a, b and c:*

$$\mathbb{P}(a > c) \ \leq \ \mathbb{P}(a > b) + \mathbb{P}(b > c)$$

Proof of Probability Union - Lemma 4. For events A and B

$$\mathbb{P}(A \cup B) \leq \mathbb{P}(A) + \mathbb{P}(B)$$

hence for events $a > b$ and $b > c$:

$$\mathbb{P}((a > b) \cup (b > c)) \leq \mathbb{P}(a > b) + \mathbb{P}(b > c)$$

If $a > c$, then $(a > b) \cup (b > c)$ is true irrespective of b, so:

$$\mathbb{P}(a > c) \leq \mathbb{P}((a > b) \cup (b > c))$$

□

This relationship is a well known and useful tool for settings where the probability relationship between a and c is unknown but the relationship between a and some b, and also between that b and c is known. Although this relationship is quite useful, it is known to be a very weak relationship, as it holds with equality (ie. $\mathbb{P}(a > c) = \mathbb{P}(a > b) + \mathbb{P}(b > c)$) only if $\mathbb{P}((a > b) \cap (b > c)) = 0$.

Note also, that the same proof method for probability union also works straightforwardly for various substitutions of the $\geq$ symbol for the $>$ in the inner inequalities, with the exception that: $\mathbb{P}(a \geq c) \ \leq \ \mathbb{P}(a > b) + \mathbb{P}(b > c)$ may be false.[1]

[1] ie. In the context of lemma 4 the following inequalities can be proven by much the same logic $\mathbb{P}(a > c) \leq \mathbb{P}(a \geq c) \leq \mathbb{P}(a \geq b) + \mathbb{P}(b > c)$ and $\mathbb{P}(a > c) \leq \mathbb{P}(a \geq c) \leq \mathbb{P}(a \geq b) + \mathbb{P}(b \geq c)$, however care must be taken because $\mathbb{P}(a \geq c) \leq \mathbb{P}(a > b) + \mathbb{P}(b > c)$ may not be true

A second Lemma is a straightforward and commonly known result of algebra that relates the sample squares about the mean and the mean squared, to the sample variance (provided with proof for completeness of information).

Lemma 5 (Variance Decomposition)**.** *For n samples x_i, sample mean $\hat{\mu} = \frac{1}{n}\sum_i x_i$, sample variance $\hat{\sigma}^2 = \frac{1}{n-1}\sum_i (x_i - \hat{\mu})^2$, and average of sample squares $\hat{\sigma}_0^2 = \frac{1}{n}\sum_i x_i^2$, the following relationship holds:*

$$\hat{\sigma}_0^2 = \hat{\mu}^2 + \frac{n-1}{n}\hat{\sigma}^2$$

Proof of Variance Decomposition - Lemma 5. By expanding $\hat{\sigma}^2$ into parts:

$$\hat{\sigma}^2 = \frac{1}{n-1}\sum_i \left(x_i - \frac{1}{n}\sum_j x_j \right)^2 = \frac{1}{n-1}\left(\sum_i x_i^2 - \frac{1}{n}\sum_{i,j} x_i x_j \right) = \frac{n}{n-1}\left(\hat{\sigma}_0^2 - \hat{\mu}^2 \right)$$

□

This lemma will prove to be important to us, as we will use it as a means of constructing probability bounds on the error of the sample variance $\hat{\sigma}^2$ in terms of the error of the mean squared $\hat{\mu}^2$ and error of the average sample squares $\hat{\sigma}_0^2$. Once constructed, integrating these probability bounds then allows us to eliminate the variance σ^2 from our equations, which is an essential part of deriving our new EBBs (such as per equations 6.18 and 6.27).

6.2 Stratified sampling by union of unstratified probability bounds

The minimisation of existing EBBs (such as Theorems 3 and 4) cannot be directly be used as a method of choosing samples in stratified sampling, since the aggregated population mean estimate does not itself have a sample variance but only the strata have means and sample variances. Such EBBs can be applied as a bound for the mean of an individual stratum but such an EBB cannot bind the aggregation of the mean estimates of all the strata.

In this section, we show that these EBBs can be combined by probability unions to create a bound for the error of the stratified mean estimate, which can then be minimised to create new stratified sampling methodologies. The combined probability bound will not depend on the variance of the strata, but only depend on the sample variances of the strata. And thus the resulting sampling methodologies will implicitly be sensitive to the variances of the strata but not requiring foreknowledge of them - unlike Neyman sampling.

6.2.1 Stratified sampling via EBBs and sequential unions

To create a bound on the error in stratified sampling from EBBs, it is necessary to use probability unions to bind the EBBs together. We derive the following two theorems

7 and 8 that give derivations on the error, and the absolute error, of the stratified mean estimator.

Theorem 7. *If we have m strata of sizes N_i. If we have taken n_i samples $X_{i,1}, X_{i,2}, \ldots, X_{i,n_i}$ from each stratum, resulting in a stratum sample mean $\hat{\mu}_i = \frac{1}{n_i}\sum_{j=1}^{n_i} X_{i,j}$ and stratum sample variance $\hat{\sigma}_i^2 = \frac{1}{n_i}\sum_{j=1}^{n_i}(X_{i,j} - \hat{\mu}_i)^2$. If the error in the sample mean of a stratum is bounded by an Empirical Bernstein Bound: $\mathbb{P}(\hat{\mu}_i - \mu_i \geq Z(n_i, D_i, \hat{\sigma}_i^2, t)) \leq t$*
Then the error in our stratified estimation of the population mean itself is probability bounded:

$$\mathbb{P}\left(\hat{\mu} - \mu \geq \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k} Z(n_i, D_i, \hat{\sigma}_i^2, t/m)\right) \leq t$$

Proof. We begin by considering that the stratified mean estimate is given by:

$$\hat{\mu} = \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k}\hat{\mu}_i \qquad \text{and thus:} \qquad \hat{\mu} - \mu = \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k}(\hat{\mu}_i - \mu_i)$$

Thence because we can scale (by positive factor) the inside of the EBB inequality (for any $j \in \{1, \ldots, m\}$):

$$\mathbb{P}\left(\frac{N_j}{\sum_k N_k}(\hat{\mu}_j - \mu_j) \geq \frac{N_j}{\sum_k N_k} Z(n_j, D_j, \hat{\sigma}_j^2, t)\right) \leq t \tag{6.11}$$

adding identical terms to both sides of the inner inequality gives:

$$\mathbb{P}\left(\sum_{i=1}^{m} \frac{N_i}{\sum_k N_k}(\hat{\mu}_i - \mu_i) \geq \frac{N_j}{\sum_k N_k} Z(n_j, D_j, \hat{\sigma}_j^2, t) + \sum_{\substack{i=1 \\ i\neq j}}^{m} \frac{N_i}{\sum_k N_k}(\hat{\mu}_i - \mu_i)\right) \leq t \tag{6.12}$$

now since equation 6.11 also holds for any $l \in \{1, \ldots, m\}$ other j then:

$$\mathbb{P}\left(\frac{N_l}{\sum_k N_k}(\hat{\mu}_l - \mu_l) \geq \frac{N_l}{\sum_k N_k} Z(n_l, D_l, \hat{\sigma}_l^2, t)\right) \leq t$$

hence by adding terms to both sides of the inner inequality:

$$\mathbb{P}\left(\begin{array}{c} \frac{N_j}{\sum_k N_k} Z(n_j, D_j, \hat{\sigma}_j^2, t) \\ + \sum_{\substack{i=1 \\ i\neq j}}^{m} \frac{N_i}{\sum_k N_k}(\hat{\mu}_i - \mu_i) \end{array} \geq \begin{array}{c} \frac{N_j}{\sum_k N_k} Z(n_j, D_j, \hat{\sigma}_j^2, t) + \\ \frac{N_l}{\sum_k N_k} Z(n_l, D_l, \hat{\sigma}_l^2, t) + \\ \sum_{\substack{i=1 \\ i\neq j \\ i\neq l}}^{m} \frac{N_i}{\sum_k N_k}(\hat{\mu}_i - \mu_i) \end{array}\right) \leq t \tag{6.13}$$

Applying probability union (lemma 4) to equations 6.12 and 6.13 gives:

$$\mathbb{P}\left(\hat{\mu}-\mu \geq \begin{array}{c} \frac{N_j}{\sum_k N_k} Z(n_j, D_j, \hat{\sigma}_j^2, t) + \\ \frac{N_l}{\sum_k N_k} Z(n_l, D_l, \hat{\sigma}_l^2, t) + \\ \sum_{\substack{i=1\\ i\neq j\\ i\neq l}}^{m} \frac{N_i}{\sum_k N_k}(\hat{\mu}_i - \mu_i) \end{array}\right) \leq 2t$$

We can repeat this process of taking equation 6.11 for a new index $q \neq j \neq l$, adding appropriate terms to the inner inequality and using probability union lemma 4, gives:

$$\mathbb{P}\left(\hat{\mu}-\mu \geq \begin{array}{c} \frac{N_q}{\sum_k N_k} Z(n_q, D_q, \hat{\sigma}_q^2, t) + \\ \frac{N_j}{\sum_k N_k} Z(n_j, D_j, \hat{\sigma}_j^2, t) + \\ \frac{N_l}{\sum_k N_k} Z(n_l, D_l, \hat{\sigma}_l^2, t) + \\ \sum_{\substack{i=1\\ i\neq j\\ i\neq l\\ i\neq q}}^{m} \frac{N_i}{\sum_k N_k}(\hat{\mu}_i - \mu_i) \end{array}\right) \leq 3t$$

and so on, and ultimately gives:

$$\mathbb{P}\left(\hat{\mu}-\mu \geq \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k} Z(n_i, D_i, \hat{\sigma}_i^2, t)\right) \leq mt$$

And scaling t gives result. □

The result of this novel proof is an inequality bounding the error of the stratified mean estimate by the number of samples and the width and sample variance of each of the strata. If instead of the error, we are concerned about the absolute error of the stratified estimate $|\hat{\mu}-\mu|$ then by a similar procedure (inspired by the utilisation of the triangle inequality in the proofs of Maleki et al. [2013]) we can derive a similar probability bound:

Theorem 8. *In the same context of the statement of theorem 7 the absolute error of the stratified estimation is probability bounded:*

$$\mathbb{P}\left(|\hat{\mu}-\mu| \geq \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k} Z(n_i, D_i, \hat{\sigma}_i^2, t/2m)\right) \leq t$$

Proof. If $\mathbb{P}(\hat{\mu}_i - \mu_i \geq Z(n_i, D_i, \hat{\sigma}_i^2, t)) \leq t$ then $\mathbb{P}(|\hat{\mu}_i - \mu_i| \geq Z(n_i, D_i, \hat{\sigma}_i^2, t)) \leq 2t$. Then by repeated application of probability unions (similar to that process used in the proof of theorem 7) we get:

$$\mathbb{P}\left(\sum_{i=1}^{m} \frac{N_i}{\sum_k N_k}|\hat{\mu}_i - \mu_i| \geq \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k} Z(n_i, D_i, \hat{\sigma}_i^2, t)\right) \leq 2mt \tag{6.14}$$

Now, via the triangle inequality:

$$\hat{\mu} - \mu = \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k}(\hat{\mu}_i - \mu_i) \qquad \text{implies} \qquad |\hat{\mu} - \mu| \leq \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k}|\hat{\mu}_i - \mu_i|$$

then $\mathbb{P}(|\hat{\mu} - \mu| > \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k}|\hat{\mu}_i - \mu_i|) \leq 0$ and by probability union with (6.14):

$$\mathbb{P}\left(|\hat{\mu} - \mu| \geq \sum_{i=1}^{m} \frac{N_i}{\sum_k N_k} Z(n_i, D_i, \hat{\sigma}_i^2, t)\right) \leq 2mt$$

And the result follows by scaling t. □

These two theorems make clear that sampling to minimise either the error or the absolute error, essentially amounts to minimising the same target. It is possible to apply these theorems with a choice of EBB to create a bound for the stratified mean error, which can then be minimised by choosing appropriate sample numbers.

This method is made clear in pseudocode in technically-novel algorithm 2. Where a scan is conducted over the possible strata in lines 4-10, and the improvement that would be offered by taking an additional sample from the stratum's respective EBB is calculated. The strata that gives the most reduction of its EBB for a prospective additional sample is chosen to have an additional sample taken, and its sample variance is recalculated in lines 11-13; this process repeats until the sample budget is exhausted.

Algorithm 2 Stratified Error bound reduction algorithm by unionised EBBs - by Theorem 8

Require: probability t, number of strata N, initial sample numbers m_i, initial stratum sample variances $\hat{\sigma}_i^2$, widths D_i, maximum sample budget B, for an EBB per the following form: $\mathbb{P}(\hat{\mu}_i - \mu_i \geq Z(m_i, D_i, \hat{\sigma}_i^2, t)) \leq t$

1: **while** $\sum_k m_k < B$ **do**
2: $\quad$ $\mathit{beststrata} \leftarrow -1$
3: $\quad$ $\mathit{bestimprovement} \leftarrow 0$
4: $\quad$ **for** $i = 1$ to N **do**
5: $\quad\quad$ $\mathit{improvement} \leftarrow \frac{n_i}{\sum_k n_k}\left(Z(m_i, D_i, \hat{\sigma}_i^2, t) - Z(m_i + 1, D_i, \hat{\sigma}_i^2, t)\right)$
6: $\quad\quad$ **if** $\mathit{improvement} > \mathit{bestimprovement}$ **then**
7: $\quad\quad\quad$ $\mathit{beststrata} \leftarrow i$
8: $\quad\quad\quad$ $\mathit{bestimprovement} \leftarrow \mathit{improvement}$
9: $\quad\quad$ **end if**
10: $\quad$ **end for**
11: $\quad$ take an extra sample from strata: *beststrata*
12: $\quad$ $m_{beststrata} \leftarrow m_{beststrata} + 1$
13: $\quad$ recalculate $\hat{\sigma}^2_{beststrata}$
14: **end while**

The numerical performance of this process in the context of stratified sampling is shown in section 6.5. In the next section we derive and numerically generate a stronger EBB for application in the context of these theorems for stratified sampling.

6.3 The derivation of a stronger EBB

There are various EBBs which place variance-sensitive bounds on the mean, and it remains an outstanding task is to see how much these EBBs can be improved; we take inspiration from the work of Maurer and Pontil [2009] to develop a new and stronger EBB. However, due to its analytic intractability, we complete the derivation by discussing how to numerically determine the bound.

In this section, we derive two Chernoff bounds, for the sample mean and the mean of sample squares, (Theorem 7 and Lemma 10, respectively). These are fused using a probability union (Theorem 4) and variance decomposition (Theorem 5) to derive a bound for the sample variance. This bound is then used to derive our new EBB, as presented in Theorem 11.

Within this section there are multiple parts:

1. subsection 6.3.1 presents and provides a derivation of Bennett's inequality
2. subsection 6.3.2 presents and derives a Chernoff bound on the error of the sample squares
3. subsection 6.3.3 shows how these two can be used to create a bound on the sample variance
4. subsection 6.3.4 shows how a bound on the sample variance and a bound on the mean can be used to derive an EBB
5. subsection 6.3.5 we give details on the numerical determination of a new EBB using all appropriate elements, and present a numerically fitted symbolic envelope over the numerical determinations.

6.3.1 A presentation of Bennett's inequality

Our first part of the derivation of our new EBB is a Chernoff bound on the sample mean called *Bennett's inequality*. This bound is not new and was derived by Hoeffding [1963] and Bennett [1962] and has subsequently been a subject of discussion and many further developments; it is known to be quite strong [Bentkus and Juškevičius, 2008; Pinelis, 2014; Talagrand, 1995]; We derive and present a refactored summary proof of Bennett's inequality as the theorem 9, whose proof involves the use of an intermediate theorem 6. We present it here in a way conducive to the manipulation we will subsequently perform with it (modifying it into proof of Theorem 8).

Theorem 9 (Bennett's inequality). *Let X be a real-valued random variable with a mean of zero and variance σ^2, that is bounded $a \leq X \leq b$. Then for $t > 0$, the mean $\hat{\mu}$ of n samples of X is probability bounded by:*

$$\mathbb{P}(\hat{\mu} \geq t) \leq H_1^n\left(\frac{\sigma^2}{b^2}, \frac{t}{b}\right), \tag{6.15}$$

where:

$$H_1^n\left(\frac{\sigma^2}{b^2},\frac{t}{b}\right)=\left(\left(\frac{\frac{\sigma^2}{b^2}}{\frac{\sigma^2}{b^2}+\frac{t}{b}}\right)^{\frac{\sigma^2}{b^2}+\frac{t}{b}}\left(1-\frac{t}{b}\right)^{\frac{t}{b}-1}\right)^{\frac{n}{\frac{\sigma^2}{b^2}+1}}$$

Proof. As random variable X is bounded $a \leq X \leq b$, for any $s > 0$, by Lemma 6, there exist parameters α, β, γ such that, $\alpha s^2 X^2 + \beta s X + \gamma \geq \exp(sX)$ is always satisfied, hence for these we have:

$$\mathbb{E}\left[\exp(sX)\right] \leq \mathbb{E}[\alpha s^2 X^2 + \beta s X + \gamma] \leq \alpha s^2\,\mathbb{E}[X^2] + \gamma \leq \alpha s^2 \sigma^2 + \gamma$$

$$\leq (\sigma^2 \exp(sb) + b^2 \exp(-s\sigma^2/b))(\sigma^2 + b^2)^{-1}$$

Hence by application of lemma 1:

$$\mathbb{P}(\hat{\mu} \geq t) \;\leq\; (\sigma^2 \exp(sb) + b^2 \exp(-s\sigma^2/b))^n((\sigma^2 + b^2)\exp(st))^{-n}$$

minimising with respect to s completes the proof, minimum s occurs at:

$$s = \frac{b}{\sigma^2 + b^2}\log\left(\frac{b(\sigma^2 + tb)}{\sigma^2(b - t)}\right)$$

□

Lemma 6 (Parabola Fitting). *For $b > 0$, $a < b$ and $z > 0$, there exists an α, β, γ such that: $\alpha x^2 + \beta x + \gamma \geq \exp(x)$ for all $a \leq x \leq b$, and:*

$$z\alpha + \gamma = (z\exp(b) + b^2\exp(-z/b))(z + b^2)^{-1}$$

Proof. A example parabola $\alpha x^2 + \beta x + \gamma$ which that satisfies these requirements tangentially touches the exponential curve at one point (at $x = f < b$) and intersects it at another (at $x = b$), as illustrated in Figure 6.1. Thus the parabola's intersection at $x = b$ and its tangential intersection at $x = f$ can be written in matrix algebra:

$$\begin{bmatrix}\alpha\\ \beta\\ \gamma\end{bmatrix} = \begin{bmatrix} b^2 & b & 1\\ f^2 & f & 1\\ 2f & 1 & 0\end{bmatrix}^{-1}\begin{bmatrix}\exp(b)\\ \exp(f)\\ \exp(f)\end{bmatrix}$$

This gives our parabola parameters α, β, γ, in terms of f and b, hence:

$$z\alpha + \gamma = (((z + fb - b)(f - b - 1) - b)e^f + (f^2 + z)e^b)(b - f)^{-2}$$

Minimizing with respect to f occurs at $f = \frac{-z}{b}$ and gives the result. □

The derivation of Bennett's inequality is separated into two parts as the above Lemma 6 will also be reused to derive a weaker but more mathematically manipulatable inequality later (as Lemma 8).

The essential difference between Bennett's inequality and Hoeffding's inequality is the fitting of a parabola instead of a linear term over the exponential function. And this second order parabolic term makes Bennett's inequality sensitive to the variance of the distribution whereas Hoeffding's inequality is not. Bennett's inequality provides a probability bound for the difference of the sample mean from the true mean given the variance, however the true variance is not often known in practice.

6.3.2 A Chernoff bound on the sample squares

As already stated, the variance is often unknown in practice, but can only be estimated via the sample variance statistic. In order to derive a bound for the error between the sample variance and the variance we derived a concentration inequality for the sample squares to use in conjunction with the variance decomposition Lemma 5. The following novel concentration inequality was derived:

Lemma 7 (Sample square bound). *Let X be a real-valued random variable with a mean of zero and variance σ^2, that is bounded $a \le X \le b$, if $d = \max(b, -a)$ then for $y > 0$, the mean of sample squares $\hat{\sigma}_0^2 = \frac{1}{n}\sum_i x_i^2$ is probability bounded:*

$$\mathbb{P}(\sigma^2 - \hat{\sigma}_0^2 > y) \le H_2^n\left(\frac{\sigma^2}{d^2}, \frac{y}{d^2}\right), \tag{6.16}$$

where:

$$H_2^n\left(\frac{\sigma^2}{d^2}, \frac{y}{d^2}\right) = \left(\left(\frac{1-\frac{\sigma^2}{d^2}}{1+\frac{y}{d^2}-\frac{\sigma^2}{d^2}}\right)^{1+\frac{y}{d^2}-\frac{\sigma^2}{d^2}}\left(\frac{\frac{\sigma^2}{d^2}}{\frac{\sigma^2}{d^2}-\frac{y}{d^2}}\right)^{\frac{\sigma^2}{d^2}-\frac{y}{d^2}}\right)^n$$

Proof. There exist parameters α, γ such for all $a \le X \le b$ that $\alpha X^2 + \gamma \ge \exp(-qX^2)$ whence:

$$\mathbb{E}[\exp(-qX^2)] \le \mathbb{E}[\alpha x^2 + \gamma] \le \alpha\sigma^2 + \gamma$$

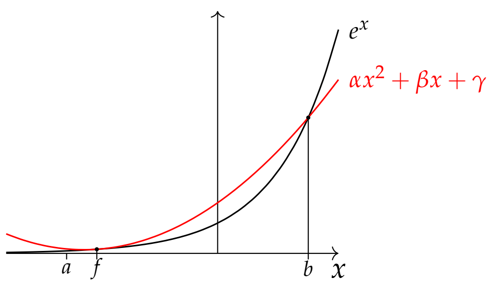


Figure 6.1: A parabola parametarised by touching and intercepting points f, b above an exponential curve for all $a \le x \le b$

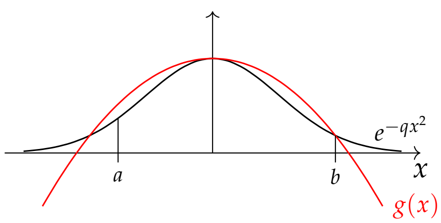


Figure 6.2: $g(x) = (e^{-qd^2} - 1)d^{-2}x^2 + 1$ over function $f(x) = e^{-qx^2}$ for all $a \le x \le b$ where $d = \max(b, -a)$

With $d = \max(b, -a)$, we choose (see Fig 6.2) $\alpha = (\exp(-qd^2) - 1)d^{-2}$ and $\gamma = 1$ Then applying lemma 1 to the mean of the negated sample squares gives:

$$\mathbb{P}(-\hat{\sigma}_0^2 \geq t) \leq \left(\frac{\sigma^2}{d^2}\exp(-qd^2) + 1 - \frac{\sigma^2}{d^2}\right)^n \exp(-qnt)$$

Substituting t for $y - \sigma^2$ and minimising with q completes the proof, minimum q occurs at:

$$q = \frac{1}{d^2}\log\left(\frac{\sigma^2(-\sigma^2 + d^2 + y)}{(\sigma^2 - d^2)(y - \sigma^2)}\right)$$

□

Note that the application of this inequality (and thence the domain of function H_2^n) are only sensibly considered in certain settings, such as when: (i) it is defined for $a < 0 < b$ (because otherwise the mean could not be zero), and (ii) $\sigma^2 \leq -ab \leq (b-a)^2/4$ by Popoviciu's inequality[2] (as it is not possible for the variance to be larger given the width of the data bounds).

6.3.3 A new bound on the sample variance

By Theorem 9 and Lemma 7 we have a probability bound on the mean squared and a probability bound on the sample squares, and from these it is possible to create novel a bound on the sample variance using lemma 5, as follows:

Theorem 10 (Sample Variance Bound). *For a random variable that is bounded $a \leq X \leq b$ with variance σ^2 and a mean of zero, if $d = \max(b, -a)$ then for $w > 0$, the sample variance $\hat{\sigma}^2$ of n samples is probability bounded by:*

$$\mathbb{P}(\sigma^2 - \hat{\sigma}^2 > w) \leq H_3^n(a, b, w, \sigma^2), \tag{6.17}$$

where:

$$H_3^n(a,b,w,\sigma^2) = \min_{\phi\in[0,1]}\left\{\begin{array}{c} H_1^n\left(\frac{\sigma^2}{b^2}, \frac{\sqrt{\phi(\frac{n-1}{n}w + \frac{1}{n}\sigma^2)}}{b}\right) \\ +H_1^n\left(\frac{\sigma^2}{a^2}, \frac{-\sqrt{\phi(\frac{n-1}{n}w + \frac{1}{n}\sigma^2)}}{a}\right) \\ +H_2^n\left(\frac{\sigma^2}{d^2}, \frac{(1-\phi)(\frac{n-1}{n}w + \frac{1}{n}\sigma^2)}{d^2}\right) \end{array}\right\}$$

Proof. By Lemmas 7 and 5:

$$\mathbb{P}\left(\sigma^2 - \hat{\sigma}^2 > \frac{n}{n-1}\left(\hat{\mu}^2 + y - \frac{1}{n}\sigma^2\right)\right) \leq H_2^n\left(\frac{\sigma^2}{d^2}, \frac{y}{d^2}\right) \tag{6.18}$$

[2] see Sharma et al. [2010]

By inspection of equation 6.15 we can convert to a double-sided version:

$$\mathbb{P}(\hat{\mu}^2 \geq r^2) = \mathbb{P}(\hat{\mu} \geq r) + \mathbb{P}(\hat{\mu} \leq -r) \leq H_1^n\left(\frac{\sigma^2}{b^2}, \frac{r}{b}\right) + H_1^n\left(\frac{\sigma^2}{a^2}, \frac{-r}{a}\right) \tag{6.19}$$

Also, by manipulating the inner inequality of this equation:

$$\mathbb{P}\left(\frac{n}{n-1}\left(\hat{\mu}^2 + y - \frac{1}{n}\sigma^2\right) \geq \frac{n}{n-1}\left(r^2 + y - \frac{1}{n}\sigma^2\right)\right) \leq H_1^n\left(\frac{\sigma^2}{b^2}, \frac{r}{b}\right) + H_1^n\left(\frac{\sigma^2}{a^2}, \frac{-r}{a}\right) \tag{6.20}$$

Applying lemma 4 to the equations 6.20 and 6.18 gives:

$$\mathbb{P}\left(\sigma^2 - \hat{\sigma}^2 > \frac{n}{n-1}\left(r^2 + y - \frac{1}{n}\sigma^2\right)\right) \leq H_2^n\left(\frac{\sigma^2}{d^2}, \frac{y}{d^2}\right) + H_1^n\left(\frac{\sigma^2}{b^2}, \frac{r}{b}\right) + H_1^n\left(\frac{\sigma^2}{a^2}, \frac{-r}{a}\right)$$

For a choice of parameter $w = \frac{n}{n-1}\left(r^2 + y - \frac{1}{n}\sigma^2\right)$ there is a range of possible $r, y > 0$ which we can parameterise by value ϕ, such that $0 \leq \phi \leq 1$:

$$y(\phi) = (1-\phi)\left(\frac{n-1}{n}w + \frac{1}{n}\sigma^2\right) \quad \text{and} \quad r(\phi)^2 = \phi\left(\frac{n-1}{n}w + \frac{1}{n}\sigma^2\right)$$

Thus:

$$\mathbb{P}\left(\sigma^2 - \hat{\sigma}^2 > w\right) \leq H_2^n\left(\frac{\sigma^2}{d^2}, \frac{y(\phi)}{d^2}\right) + H_1^n\left(\frac{\sigma^2}{b^2}, \frac{r(\phi)}{b}\right) + H_1^n\left(\frac{\sigma^2}{a^2}, \frac{-r(\phi)}{a}\right)$$

The result of this proof follows by taking the minimum over ϕ. □

The use of this Theorem 10 (and thus implicitly the domain of function H_3^n) is subject to the same restrictions as Lemma 7 (and its domain as H_2^n); specifically that it is defined for $a < 0$ and $b > 0$ and for $\sigma^2 \leq -ab$; as otherwise the configuration is senseless.

6.3.4 Generalised EBB creation process

Theorem 9 presents a bound for the sample mean given the variance, and Theorem 10 presents a probability bound for the error of the sample variance from the variance. The task remaining is to create a new EBB by binding these two together. To combine these two theorems to create a bound for the sample mean given the sample variance, we give a theorem that is representative of a slightly improved derivation process than that followed by Maurer and Pontil [2009], where they use this process to create their EBB.

Before beginning this theorem, we need to introduce some notation to ease presentation. For a function f with ordered inputs, we denote the inverse of f with respect to its ith input (counting from one) as $f^{-(i)}$, assuming it exists. We summarily denote probability bounds on the differences of the sample mean from the mean, and the sample variance from the variance, by $\mathbb{P}(\hat{\mu} - \mu > t) \leq h(\sigma^2, t)$ and

$\mathbb{P}(\sigma^2 - \hat{\sigma}^2 > w) \leq f(\sigma^2, w)$, respectively. And note that functions h and f may have additional arguments not limited to σ^2 and t, and σ^2 and w, respectively; but that these are not considered in the theorem and proof for brevity.

Theorem 11 (Essential EBB). *For probability bounds $\mathbb{P}(\hat{\mu} - \mu > t) \leq h(\sigma^2, t)$ and $\mathbb{P}(\sigma^2 - \hat{\sigma}^2 > w) \leq f(\sigma^2, w)$, if $f^{-(2)}$ and $h^{-(2)}$ both exist, and also if $h^{-(2)}$ is monotonically increasing in its first argument, so that we can define:*

$$z(\sigma^2, w) = \sigma^2 - f^{-(2)}\left(\sigma^2, w\right)$$

If $z^{-(1)}$ exists and is monotonic increasing in its first argument, then for any $x \in [0, y]$, the following relationship holds:

$$\mathbb{P}\left(\hat{\mu} - \mu > h^{-(2)}\left(z^{-(1)}\left(\hat{\sigma}^2, y - x\right), x\right)\right) \leq y$$

Proof. Substituting w for $f^{-(2)}(\sigma^2, w)$ gives:

$$\begin{aligned}
w &\geq \mathbb{P}\left(\sigma^2 - \hat{\sigma}^2 > f^{-(2)}\left(\sigma^2, w\right)\right) \\
&\geq \mathbb{P}\left(z\left(\sigma^2, w\right) > \hat{\sigma}^2\right) \\
&\geq \mathbb{P}\left(\sigma^2 > z^{-(1)}\left(\hat{\sigma}^2, w\right)\right) \\
&\geq \mathbb{P}\left(h^{-2}\left(\sigma^2, t\right) > h^{-(2)}\left(z^{-(1)}\left(\hat{\sigma}^2, w\right), t\right)\right)
\end{aligned}$$

Substituting t for $h^{-(2)}(\sigma^2, t)$ gives:

$$\mathbb{P}\left(\hat{\mu} - \mu > h^{-(2)}\left(\sigma^2, t\right)\right) \leq t.$$

Applying probability union (lemma 4) gives:

$$\mathbb{P}\left(\hat{\mu} - \mu > h^{-(2)}\left(z^{-(1)}\left(\hat{\sigma}^2, w\right), t\right)\right) \leq t + w.$$

Letting $y = t + w$ and $x = y - w$ completes the proof. □

The result of this Theorem is an Empricial Bernstein Bound. And our novel EBB is completed by substituting $h(\sigma^2, t) = H_1^n\left(\sigma^2/b^2, t/b\right)$ (from Theorem 9) and $f(\sigma^2, w) = H_3^n\left(a, b, w, \sigma^2\right)$ (from Theorem 10) into Theorem 11. In this process care was taken in applying this theorem that all the assumptions hold, the necessary inverses exist, and that the domains of the functions were propagated through the analysis.

6.3.5 Numerical determination

The Empirical Bernstein Bound described in the previous subsection 6.3.4 consists of inversions and compositions of functions H_1 and H_3 from theorems 9 and 10, is identified to be challenging to analytically determine but much more possible to numerically determine. Calculating this EBB numericaly consisted of three primary parts:

1. Computating function $f(\sigma^2, w) = H_3^n(a, b, y, \sigma^2)$
2. Verifying the assumptions of Theorem 11 hold for $h(\sigma^2, t) = H_1$ and $f(\sigma^2, w) = H_3$
3. Calculating the subsequent result of Theorem 11

First, the function $f(\sigma^2, w) = H_3^n(a, b, w, \sigma^2)$ (per Theorem 10) was identified as the solution to an optimisation problem that solves for the minima of an objective function subject to constraint $\phi \in [0, 1]$. Despite its complexity, solutions of this sort can be found quickly using a single variable parameter sweep.

Second, it was necessary to verify the assumptions that $h^{-(2)}$, $f^{-(2)}$ and $z^{-(1)}$ exist and that $z^{-(1)}$ and $f^{-(2)}$ are monotonically increasing in their first argument. It was easy to note that $h(\sigma^2, t) = H_1^n\left(\sigma^2/b^2, t/b\right)$ is a closed-form function that is monotonically decreasing from 1 to 0 on the second argument, so $h^{-(2)}$ exists and is monotonically increasing in its first argument. However the remaining of these assumptions are more difficult to verify. For any function, the values that the function takes can be plotted as an array of points and the values that the inverse of that function takes can be determined by conducting coordinate swapping on those points. The values of $f(\sigma^2, w) = H_3^n(a, b, w, \sigma^2)$ were computed and were seen to be monotonically decreasing in its second argument confirming that $f^{-(2)}$ exists. The function $z(\sigma^2, w) = \sigma^2 - f^{-(2)}\left(\sigma^2, w\right)$ is then a manipulation on the coordinate swapped points of $f(\sigma^2, w) = H_3^n(a, b, w, \sigma^2)$. By coordinate swapping again, $z^{-(1)}$ was seen to be a regular function monotonically increasing on its first argument, hence satisfying assumptions.

Third, to numerically calculate the result of Theorem 11 the functions $h^{-(2)}$ and $z^{-(1)}$ were numerically evaluated by direct parameter searches and then composed as: $h^{-(2)}(z^{-(1)}(\hat{\sigma}^2, y - x), x)$ - which was the inner part of the expression of the new EBB parameterised by x explicitly and also a, b implicitly. However we typically don't know the values of a and b, but instead know the mean is somewhere within a finite interval of width $D = b - a$, in this context was taken the worst case values of a and b consistent with a given D, and then the best $x \in [0, y]$ was taken subject to all other bounds.

Throughout this three stage process the new EBB was numerically determined by a series of coordinate manipulations and mundane parameter searches.[3] For the ease of this application of our EBB, we hand-tuned an envelope of our EBB's probability 0.5 bound, where the process of creating such an expression involved plotting the numerical data, and manually fitting a symbolic expression above the data:

$$\mathbb{P}\left(\mu - \hat{\mu} \geq \frac{D}{\sqrt{n}} \min\left[\sqrt{2\log 2}, \left(\begin{array}{c} \frac{3}{5}\sqrt{\min\left[1, \frac{\hat{\sigma}^2}{D^2} + \frac{25}{n}\right]} \\ + \ln\left(\max\left[1, n\left(1 - \frac{\hat{\sigma}^2}{D^2}\right)\right]\right)^{-4} \end{array}\right)\right]\right) \lessapprox 0.5 \tag{6.21}$$

[3]sourcecode available at:
https://github.com/Markopolo141/Engineered-Empirical-Bernstein-Bound

The strength of this new EBB against existing EBBs are discussed in section 6.7, and the performance of this new EBB in the context of stratified sampling is reported in section 6.5. We now turn away from the subject matter of the unionisation of EBBs for stratified sampling (in the previous section 6.2) and the creation of a new EBB for this purpose in this section, to the creation of a completely novel bound directly tailored for stratified sampling.

6.4 Stratified sampling by a stratified probability bound

In the previous section we considered different possible EBBs as a way of bounding the error in the context of stratified random sampling, and for this purpose developed a new EBB. This process of using EBBs involved binding EBBs applied to different strata together using union bounds to create a bound on the stratified sample mean error (via Theorem 7).

What is worth noting is that this process of binding EBBs together by probability unions is expected to result in a rather weak bound and that this weakness is expected to increase with larger numbers of strata as there are more probability unions needed to bind it together. It is noted that the triangle equality $|A + B| \leq |A| + |B|$, is only an equality in the event that the elements A and B are of the same sign, and in the context of theorems 7 and 8 the bound for the error is developed by effectively assuming all the errors of the estimates of the strata are additive - which is the worst case. Whereas by assumption, the errors in the strata estimates are independent of each other and hence a overestimation in one stratum estimate is likely to be somewhat countered by an underestimation in another. By using this knowledge stronger bounds can be created, and in this section we do just that. We have created an empirical (ie. depending on sample variances) concentration inequality specifically for stratified random sampling.

The resulting concentration inequality gives an analytic bound on the error of the stratified mean and explicitly considers the sample variances, data widths, sample numbers, and any additional weights on the strata; and includes factors specifically for strata sampled with and/or without replacement.

We proceed with the derivation of this new bound and method in a series of stages:

1. in subsection 6.4.1 we outlay some lemmas which are the building blocks of further derivations in this section, these are new upper bounds are for the moment generating function of samples and sample squares, as well as the sample means depending on whether sampling is done with or without replacement.

2. in subsection 6.4.2 we use these elements to begin the derivation of the new bound, called the Stratified Empirical Bernstein Bound (SEBB)

3. in subsection 6.4.3 we additionally derive a variant of the SEBB which uses Chebyshev's inequality

4. in subsection 6.4.4 we describe the algorithm of choosing samples in stratified sampling to minimise the new SEBB bound.

After these subsections, in the next section 6.5 we consider the numerical performance of minimising these new bounds in the context of stratified sampling. Let us begin with the elements in these new derivations. We note in this section, all proofs and demonstrations are our own, and are novel, except where otherwise explicitly noted.

6.4.1 Some new bounds on the moment generating function

To begin the derivation of our new concentration inequality for stratified random sampling, we build upon some of the results of the previous sections. Specifically we utilise three upper bounds for various moment generating functions. The first of which has already been given in the previous section, and is Hoeffding's lemma - Lemma 2. The other two are given here, and are bounds strongly related to Theorems 9 and 7 respectively.

The first of these other two upper bounds is very much like Hoeffding's Lemma, except it involves additional information about the variance of the random variable.

Lemma 8. *For a random variable X that is bounded on an interval $a \leq X \leq b$ with $D = b - a$ and variance σ^2, and any $s > 0$:*

$$\mathbb{E}\left[\exp(s(X - \mathbb{E}[x]))\right] \leq \exp\left(\left(\frac{D^2}{17} + \frac{\sigma^2}{2}\right)s^2\right)$$

Proof. We assume without loss of generality that X is centred to have a mean of zero. Then we construct an upper bound for $\mathbb{E}\left[\exp(sX)\right]$ in terms of D by a parabola over $\exp(sX)$ for the permitted values of X in the same way as in the proof of Theorem 9. By Lemma 6 there exists an α, β, γ such that $\alpha s^2 X^2 + \beta s X + \gamma \geq \exp(sX)$, and for all $a \leq X \leq b$, hence:

$$E\left[\exp(sX)\right] \leq \mathbb{E}[\alpha s^2 X^2 + \beta s X + \gamma] = \alpha s^2\, \mathbb{E}[X^2] + \gamma = \alpha s^2 \sigma^2 + \gamma$$

Where it follows that:

$$E\left[\exp(sX)\right] \leq \left(\frac{\sigma^2}{b^2}\exp\left(s\left(b + \frac{\sigma^2}{b}\right)\right) + 1\right)\exp\left(-\frac{s\sigma^2}{b}\right)\left(\frac{\sigma^2}{b^2} + 1\right)^{-1}.$$

This relationship is exactly as in Theorem 9, now we do something slightly different - the expression in (6.22) is monotonically increasing with b, and $D > b$, therefore substituting D for b gives:

$$\log(E\left[\exp(sX)\right]) \leq \log\left(\frac{\sigma^2}{D^2}\exp\left(s\left(D + \frac{\sigma^2}{D}\right)\right) + 1\right) - \frac{s\sigma^2}{D} - \log\left(\frac{\sigma^2}{D^2} + 1\right) \quad (6.22)$$

Because it is true that for any $\kappa, x \geq 0$, that:

$$\log(\kappa \exp(x) + 1) \leq \log(\kappa + 1) + \frac{x\kappa}{\kappa + 1} + x^2 \frac{\frac{1}{17} + \frac{\kappa}{2}}{(\kappa + 1)^2} \tag{6.23}$$

Thus letting $\kappa = \frac{\sigma^2}{D^2}$ and $x = s(D + \sigma^2/D)$ if follows that:

$$\log(E\left[\exp(sX)\right]) \leq \left(\frac{D^2}{17} + \frac{\sigma^2}{2}\right) s^2 \tag{6.24}$$

□

We note that this process of fitting a parabola over the exponential function is exactly the same process as used to derive Bennett's inequality (Theorem 9), but that we derive a weakened result from that same approach.

The next lemma that we present, is similar to the former, however this time we consider the random variable X^2 instead of X, and present a weakened bound on the moment generating function of it via a similar process as was used to derive Theorem 7:

Lemma 9. *Let X be a random variable of finite support on an interval $a \leq X \leq b$, with $D = b - a$ and variance $\sigma^2 = \mathbb{E}[(X - \mathbb{E}[x])^2] = \mathbb{E}[X^2] - \mathbb{E}[X]^2$. Then for any $q > 0$:*

$$\mathbb{E}[\exp(q(\sigma^2 - (X - \mathbb{E}[X])^2))] \leq \exp\left(\frac{1}{2}\sigma^2 q^2 D^2\right)$$

Proof. We assume without loss of generality (and for ease of presentation) that X is centred to have a mean of zero. We construct an upper bound for $\mathbb{E}\left[\exp(-qX^2)\right]$ in terms of D by a parabola over $\exp(-qX^2)$ for the permitted values of X.

For an α, γ such that $\alpha X^2 + \gamma \geq \exp(-qX^2)$ then:

$$\mathbb{E}[\exp(-qX^2)] \leq \alpha\sigma^2 + \gamma.$$

If $d = \max(b, -a)$ we can choose $\gamma = 1$ and $\alpha = (\exp(-qd^2) - 1)d^{-2}$ (see figure 6.2), Thus:

$$\begin{aligned}\mathbb{E}[\exp(-qX^2)] &\leq \frac{\sigma^2}{d^2}\exp(-qd^2) - \frac{\sigma^2}{d^2} + 1 \leq \frac{\sigma^2}{D^2}\exp(-qD^2) - \frac{\sigma^2}{D^2} + 1 \\ &\leq \exp\left(\log\left(\frac{\sigma^2}{D^2}\exp(-qD^2) - \frac{\sigma^2}{D^2} + 1\right)\right)\end{aligned}$$

Given that for any $0 \leq \kappa \leq 0.5$ and $x \leq 0$ that:

$$\log\left(\kappa \exp(x) - \kappa + 1\right) \leq \kappa x + \frac{1}{2}\kappa(1 - \kappa)x^2$$

Letting $\kappa = \frac{\sigma^2}{D^2}$ and $x = -qD^2$, which is valid by Popoviciu's inequality (see Sharma et al. [2010]) $\sigma^2 \leq D^2/4$, then:

$$\mathbb{E}[\exp(-qX^2)] \leq \exp\left(\frac{1}{2}\sigma^2 q^2 (D^2 - \sigma^2) - \sigma^2 q\right) \leq \exp\left(\frac{1}{2}\sigma^2 q^2 D^2 - \sigma^2 q\right)$$

and the result follows by multiplying by $\exp(q\sigma^2)$. □

The inequalities above, Lemmas 8 and 9, as well as Lemma 2, are used in the derivation of our stratified sampling concentration inequality in Section 6.4.2. One of the primary reasons for utilising these weakened bounds on the moment generating function is that they make the subsequent mathematics far more tractable. However in order to use these moment generating functions we need to explicitly describe the difference between the moment generating functions of individual random variables (which these are) and the moment generating function of the sample mean of them.

6.4.1.1 Some bounds on the moment generating function of sample means

In order to use the previous bounds on the moment generating function we need a relationship between the moment generating function of a random variable, and the moment generating function of the average of samples of that random variable. To do this we state two further inequalities, where the first one (Lemma 10) is most appropriate for sampling average is taken with replacement, and the second (Lemma 11) can optionally be used in the context that the sampling average is without replacement - and may (or may not) give a tighter result.

We first state a lemma that is essentially is a formalisation of the process we are familiar with in the last section (see Lemma 1):

Lemma 10 (Replacement Bound)**.** *Let X be a random variable that is bounded $a \leq X \leq b$ with a mean of zero, with $D = b - a$ and variance σ^2. Let $\chi_m = \frac{1}{m}\sum_{i=1}^m X_i$ be the average of m independently drawn (with replacement) samples of this random variable. If there exists an $\alpha, \beta \geq 0$ such that for any $s > 0$ that $\mathbb{E}[\exp(sX)] \leq \exp((\alpha D^2 + \beta\sigma^2)s^2)$ then:*

$$\mathbb{E}[\exp(s\chi_m)] \leq \exp(\alpha s^2 D^2 \tfrac{1}{m} + \beta s^2 \sigma^2 \tfrac{1}{m}) = \exp((\alpha D^2 \Omega_m^n + \beta\sigma^2 \Psi_m^n)s^2)$$

where $\Omega_m^n = \Psi_m^n = \frac{1}{m}$

Proof. By the independence of samples, we have:

$$\mathbb{E}[\exp(s\chi_m)] = \mathbb{E}\left[\exp\left(\frac{s}{m}\sum_{i=1}^m X_i\right)\right] = \prod_{i=1}^m \mathbb{E}\left[\exp\left(\frac{s}{m}X\right)\right]$$

Thus:

$$\mathbb{E}[\exp(s\chi_m)] \leq \exp\left(\frac{s^2}{m^2}\sum_{i=1}^m \left(\alpha D^2 + \beta\sigma^2\right)\right)$$ □

For the case of sampling without replacement, there is an alternative result that can be directly substituted, given in Lemma 11, below, which can be tighter in certain cases. Before this, particular note must be made that the inequality above, Lemma 10 can be used in the context of either sampling with or without replacement. In contrast, Lemma 11 can only be used when sampling without replacement. This distinction was shown to be true by Hoeffding [1963], and is rooted in an already presented Lemma 3.

We now state Lemma 11, an inequality regarding the moment generating function of the average of samples taken specifically *without replacement*. When the sampling takes place without replacement the inequality of Lemma 10 can potentially be tightened to take advantage of the finite size of the population. This inequality extends an important martingale inequality from Bardenet and Maillard [2015]:

Lemma 11 (Martingale Bound)**.** *For finite data $x_1, x_2, \dots x_n$ that is bounded $a \le x_i \le b$, and has a mean of zero and variance $\sigma^2 = \frac{1}{n}\sum_{i=1}^n x_i^2$, denote $X_1, X_2, \dots, X_n$ the random variables corresponding to the data sequentially drawn randomly without replacement, and χ_m the average of the first m of them. If for any random variable Z with a mean of zero such that $a \le Z \le b$ and $D = b - a$, with variance σ_Z^2 that there exists an $\alpha, \beta \ge 0$ such that for any $s > 0$ that $\mathbb{E}[\exp(sZ)] \le \exp((\alpha D^2 + \beta\sigma_Z^2)s^2)$ then:*

$$\begin{aligned}\mathbb{E}[\exp(s\chi_m)] &\le \exp\left(\alpha s^2 D^2 \sum_{k=m}^{n-1} \frac{1}{k^2} + \beta s^2 \sigma^2 \sum_{k=m}^{n-1} \frac{n}{k^2(k+1)}\right) \\ &\le \exp((\alpha D^2 \bar{\Omega}_m^n + \beta\sigma^2 \bar{\Psi}_m^n)s^2)\end{aligned}$$

where $\bar{\Omega}_m^n = \sum_{k=m}^{n-1} \frac{1}{k^2} \approx \frac{(m+1)(1-m/n)}{m^2}$ and $\bar{\Psi}_m^n = \sum_{k=m}^{n-1} \frac{n}{k^2(k+1)} \approx \frac{n+1-m}{m^2}$.

Proof. Observe that:

$$\begin{aligned}\chi_m &= \frac{1}{m}\sum_{i=1}^m X_i = \chi_{m+1} + \frac{1}{m}(\chi_{m+1} - X_{m+1}) \\ &= (\chi_m - \chi_{m+1}) + (\chi_{m+1} - \chi_{m+2}) + \cdots + (\chi_{n-1} - \chi_n) \\ &= \frac{1}{m}(\chi_{m+1} - X_{m+1}) + \frac{1}{m+1}(\chi_{m+2} - X_{m+2}) + \cdots + \frac{1}{n-1}(\chi_n - X_n).\end{aligned}$$

Then because:

$$\exp(s\chi_m) = \prod_{k=m}^{n-1} \exp\left(\frac{s}{k}(\chi_{k+1} - X_{k+1})\right),$$

we also have that:

$$\mathbb{E}[\exp(s\chi_m)] = \mathbb{E}\left[\prod_{k=m}^{n-1} \mathbb{E}\left[\exp\left(\frac{s}{k}(\chi_{k+1} - X_{k+1})\right) |\chi_{k+1} \dots \chi_n\right]\right]$$

by repeated application of the Law of total expectation. Since:

$$\mathbb{E}[X_{k+1}|\chi_{k+1} \dots \chi_n] = \chi_{k+1},$$

then $\chi_{k+1} - X_{k+1}$ is a random variable with a mean of zero bounded within width

D, and it also has a variance given by:

$$\sigma_{k+1}^2 = \frac{n\sigma^2 - \sum_{j=k+1}^{n} X_j^2}{n-(n-k-1)} - \chi_k^2 \leq \frac{n\sigma^2}{k+1} \tag{6.25}$$

by application of Lemma 5. Therefore:

$$\mathbb{E}[\exp(s\chi_m)] \leq \exp\left(\sum_{k=m}^{n-1}\left(\alpha D^2 + \beta\frac{n\sigma^2}{k+1}\right)\frac{s^2}{k^2}\right) \qquad \square$$

This martingale result relates the moment generating function bound of the average of finite variables relative to their mean, to the moment generating function bounds of the differences of the incremental averages relative to their mean. We note that this result could potentially be made much stronger by working around the use of Equation (6.25), but this comes at a cost of increased mathematical complexity.

Since Lemmas 11 and 10 share a common form, and because of Hoeffding's reduction (Lemma 3), all the derivations that follow that invoke Lemma 10 have direct analogues using Lemma 11 for the context of sampling without replacement. Note, however, that the bound without replacement (Lemma 11) may or may not be tighter than the bound with replacement (Lemma 10). However, the process of substituting one for the other can be done judiciously on a case-by-case basis to create the tightest possible bound. All the numerical results in Section 6.5 (that are relevant to sampling without replacement) have been produced with this judicious choice conducted.

6.4.2 The Stratified finite Empirical Bernstein Bound (SEBB)

In this section we derive a novel probability bound for the error of the stratified random sampling estimate, and use it to define a sequential stratified sampling algorithm. Before this, we begin by precisely defining the context of our derivations, to which our bound applies.

Definition 1 (Problem context)**.**

- *Let a population consist of n number of strata,*
- *where n_i is the total number of data points in the ith stratum.*
- *All values in a stratum are bound within a finite support of width D_i.*
- *the mean of the ith stratum is μ_i, and its variance σ_i^2.*
- *the random variables corresponding to the samples drawn from the i stratum are: $X_{i,1}, X_{i,2}, \dots, X_{i,n_i}$*
- *for each stratum m_i samples are taken*
- *forming the sample mean of each stratum: $\chi_{i,m_i} = \frac{1}{m_i}\sum_{j=1}^{m_i} X_{i,j}$*

- *the biased sample variance of each stratum:* $\hat{\sigma}_i^2 = \frac{1}{m_i}\sum_j^{m_i}(X_{i,j} - \chi_{i,m_i})^2$
- *the unbiased sample variance of each stratum:* $\hat{\hat{\sigma}}_i^2 = m_i\hat{\sigma}_i^2/(m_i - 1)$
- *we consider the average of the means of the strata as weighted by constant positive factors* $\{\tau_i\}_{i\in\{1,\dots,n\}}$
- *And throughout the derivation we also use temporary arbitrary positive variables* $\{\theta_i\}_{i\in\{1,\dots,n\}}$

The bound is now developed in four theorems, which build on each other in sequence:

1. in subsubsection 6.4.2.1 Theorem 12 develops a concentration inequality for the error in the stratified population mean estimate $\sum_{i=1}^n \tau_i\chi_{i,m_i}$ in the context of the knowledge of stratum variances.
2. in subsubsection 6.4.2.2 Theorem 13 is a concentration inequality of the difference between the stratum variances and sample variances in the context the sum of knowledge of the squared stratum mean errors.
3. in subsubsection 6.4.2.3 Theorem 14 is an inequality directly that binds the sum of sample squared stratum mean errors.
4. in subsubsection 6.4.2.4 Theorem 15 combines the three previous theorems together using two union bounds to create a concentration inequality for the error in the stratified population mean estimate given the sample variances.

6.4.2.1 A bound on the sample mean assuming variances

In a similar way to what was done in the previous section, to derive an Empirical Bernstein Bound we begin with a derivation of a probability bound on the error of the sample mean of a random variable in terms of the random variable's variance. In the previous section the bound in question was the venerable Bennett's inequality (Theorem 9) however in this section we consider a more relaxed and similar version of it which is more easy for us to manipulate, and in this case the random variable in question is the weighted mean $\sum_{i=1}^n \tau_i\chi_{i,m_i}$.

This is probability bound on the absolute error of the weighted stratified sample means about the weighted strata means, which we call a variance-assisted SEBB (stratified empirical Bernstein bound).

Theorem 12 (Variance-assisted SEBB)**.** *Assuming the context given in Definition 1, and let* $\Omega_{m_i}^{n_i}$ *and* $\Psi_{m_i}^{n_i}$ *be given as in Lemma 10, then:*

$$\mathbb{P}\left(\left|\sum_{i=1}^n \tau_i(\chi_{i,m_i} - \mu_i)\right| \geq \sqrt{4\log(2/t)\sum_{i=1}^n\left(\frac{1}{17}D_i^2\Omega_{m_i}^{n_i} + \frac{1}{2}\sigma_i^2\Psi_{m_i}^{n_i}\right)\tau_i^2}\right) \leq t \tag{6.26}$$

Proof. In a similar way as Lemma 1 we consider a bound for the weighted mean by the moment generating function of the stratum means:

$$\begin{aligned}\mathbb{P}\left(\sum_{i=1}^{n}\tau_i\chi_{i,m_i}-\sum_{i=1}^{n}\tau_i\mu_i\geq t\right)&\leq\mathbb{E}\left[\exp\left(\sum_{i=1}^{n}\tau_i s\left(\chi_{i,m_i}-\mu_i\right)\right)\right]\exp(-st)\\&=\prod_{i=1}^{n}\mathbb{E}\left[\exp\left(\tau_i s\left(\chi_{i,m_i}-\mu_i\right)\right)\right]\exp(-st)\end{aligned}$$

This involves the assumption that the sampling -between- the strata is independent. This form is sufficient for Lemma 10 with Lemma 8 to apply, resulting in a double-sided tail bound:

$$\mathbb{P}\left(\left|\sum_{i=1}^{n}\tau_i(\chi_{i,m_i}-\mu_i)\right|\geq t\right)\leq 2\exp\left(\sum_{i=1}^{n}\left(\frac{1}{17}D_i^2\Omega_{m_i}^{n_i}+\frac{1}{2}\sigma_i^2\Psi_{m_i}^{n_i}\right)\tau_i^2 s^2-st\right)$$

Minimizing with respect to s and rearranging gives result. □

This particular bound assumes knowledge of the variances of the strata, and will be used as a tool for selecting samples primarily for comparison with other sampling methods (such as Neyman sampling) in Section 6.5.

It is a concentration inequality for the weighted stratum means, leading to the more general question of what the weights should be. In most cases, the weights τ_i can be considered as the probability weights $\tau_i = n_i/(\sum_{j=1}^n n_j)$ of standard stratified sampling. In this context this probability bound can be used as-is for a measure of uncertainty in stratified random sampling if the true variances (or alternatively, upper bounds on the true variances) of the strata are known. However the weights may be assigned differently - and we will investigate such a case for the Shapley Value in section 6.5.

The bound depends on a weighted sum of strata variances $\sum_{i=1}^n \sigma_i^2\Psi_{m_i}^{n_i}\tau_i^2$, and in most situations these values aren't known. Hence to use this inequality we need to consider the probable error between the weighted sum of strata variances and the weighted sum of strata sample variances.

6.4.2.2 A bound on the sample variance in terms of sample error squares

To create a bound on the error between the strata variances and the strata sample variances we develop a probability bound for the error estimate of the sum of variances (as weighted by arbitrary θ_i) in terms of the sample square errors (which will also consequently be bounded), as follows:

Theorem 13. *Assuming the context given in Definition 1. Then with $\Psi_{m_i}^{n_i}$ per Lemma 10:*

$$\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\sigma_i^2-\hat{\sigma}_i^2-(\mu_i-\chi_{i,m_i})^2)\geq\sqrt{2\log(1/y)\sum_{i=1}^{n}\sigma_i^2\theta_i^2D_i^2\Psi_{m_i}^{n_i}}\right)\leq y \tag{6.27}$$

Proof. To create a probability bound for the sum of variances (weighted by arbitrary positive θ_i), we consider the average square of samples about the strata means. Applying Lemma 1 gives:

$$\begin{aligned}
&\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\sigma_i^2 - \frac{1}{m_i}\sum_{j=1}^{m_i}(X_{i,j}-\mu_i)^2) \geq y\right)\\
&\leq \mathbb{E}\left[\exp\left(\sum_{i=1}^{n}s\theta_i\left(\sigma^2 - \frac{1}{m_i}\sum_{j=1}^{m_i}(X_{i,j}-\mu_i)^2\right)\right)\right]\exp(-sy)\\
&\leq \exp(-sy)\prod_{i=1}^{n}\mathbb{E}\left[\exp\left(\frac{s\theta_i}{m_i}\sum_{j=1}^{m_i}(\sigma^2-(X_{i,j}-\mu_i)^2)\right)\right]
\end{aligned}$$

And this reason is by the assumption of the independence of the sampling -between-the strata. This resulting form is sufficient for Lemma 10 with Lemma 9 to apply, giving:

$$\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\sigma_i^2 - \frac{1}{m_i}\sum_{j=1}^{m_i}(X_{i,j}-\mu_i)^2) \geq y\right) \leq \exp\left(\frac{1}{2}\sum_{i=1}^{n}\sigma_i^2\theta_i^2 s^2 D_i^2 \Psi_{m_i}^{n_i} - sy\right)$$

Minimizing with respect to s, rearranging, and applying Lemma 5 gives result. □

This inequality gives the probability bound between the arbitrarily (by θ_i) weighted variances of the strata and also the same weighted (biased estimator) sample variances. However it also additionally involves the weighted square error of the sample means as a complicating factor. Although the weighted square error of the sample means may go to zero quickly as additional samples are taken, we nonetheless need to develop another probability bound to incorporate the specific consideration of it.

6.4.2.3 A bound on weighted sample error squares

In the previous Theorem 13 the weighted sum of sample squares was a complicating factor which we seek to bound and incorporate. The following probability inequality bounds the weighted square error of the sample means directly:

Theorem 14. *Assuming the context given in Definition 1. Then with $\Omega_{m_i}^{n_i}$ as in Lemma 10:*

$$\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\mu_i - \chi_{i,m_i})^2 \geq \frac{\log(2n/r)}{2}\sum_{i=1}^{n}\theta_i D_i^2 \Omega_{m_i}^{n_i}\right) \leq r \tag{6.28}$$

Proof. We consider the weighted square error of the sample means, and by probability complimentarity we know:

$$\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\mu_i - \chi_{i,m_i})^2 \geq r\right) = 1 - \mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\mu_i - \chi_{i,m_i})^2 < r\right)$$

As the probability that sum of any random variables is less than r is obviously greater than the probability that those random variables individual are all less than specific values that sum to r hence, for r_i such that $\sum r_i = r$:

$$\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\mu_i - \chi_{i,m_i})^2 \geq r\right) \leq 1 - \prod_{i=1}^{n}\mathbb{P}\left(\theta_i(\mu_i - \chi_{i,m_i})^2 < r_i\right)$$

hence by probability complimentarities again:

$$\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\mu_i - \chi_{i,m_i})^2 \geq r\right) \leq$$
$$1 - \prod_{i=1}^{n}\left(1 - \mathbb{P}\left(\mu_i - \chi_{i,m_i} \geq \sqrt{\frac{r_i}{\theta_i}}\right) - \mathbb{P}\left(\chi_{i,m_i} - \mu_i \geq \sqrt{\frac{r_i}{\theta_i}}\right)\right)$$

And this is exactly the form which we want, in terms of the products of the error in each of the strata sample means. Thus we can apply Lemma 1 together with Lemmas 10 and 2, which gives:

$$\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\mu_i - \chi_{i,m_i})^2 \geq r\right) \leq 1 - \prod_{i=1}^{n}\left(1 - 2\exp\left(-\frac{2r_i}{\theta_i D_i^2 \Omega_{m_i}^{n_i}}\right)\right)$$

Next, choosing r_i to minimise the right hand side of this expression gives:

$$r_i = \frac{r\theta_i D_i^2 \Omega_{m_i}^{n_i}}{\sum_j \theta_j D_j^2 \Omega_{m_j}^{n_j}}$$

In this context, we therefore deduce that:

$$\mathbb{P}\left(\sum_{i=1}^{n}\theta_i(\mu_i - \chi_{i,m_i})^2 \geq r\right) \leq 1 - \prod_{i=1}^{n}\left(1 - 2\exp\left(\frac{-2r}{\sum_j \theta_j D_j^2 \Omega_{m_j}^{n_j}}\right)\right)$$

Using the fact that $\log(1-(1-\exp(x))^n) \leq x + \log(n)$ for any negative x, and rearranging, gives the required result. □

This theorem directly bounds the weighted square errors of the sample means independently of any other specifically unknown factors.

6.4.2.4 The centerpiece of the SEBB

In the previous three theorems we have a bound on the stratified mean estimate in terms of the variances, a bound on the variances in terms of the sample variances by the sample square errors, and a bound on the sample square errors. In the next step we combine all the inequalities of Equations (6.26), (6.27) and (6.28) from Theorems 12, 13 and 14 together, to complete our derivation of a probability bound for the error in stratified sampling in terms of stratum sample variances - our SEBB.

Theorem 15 (Stratified Empirical Bernstein Bound (SEBB)). *Assuming the context given in Definition 1. Then with $\Omega^{n_i}_{m_i}, \Psi^{n_i}_{m_i}$ per Lemma 10:*

$$\mathbb{P}\left(\left|\sum_{i=1}^{n}\tau_i(\chi_{i,m_i}-\mu_i)\right| \geq \sqrt{\log(6/p)\left(\alpha+\left(\sqrt{\beta}+\sqrt{\gamma}\right)^2\right)}\right) \leq p \tag{6.29}$$

where:

$$\begin{aligned}
\alpha =& \sum_{i=1}^{n}\frac{4}{17}\Omega^{n_i}_{m_i}D_i^2\tau_i^2\\
\beta =& \log(3/p)\left(\max_i \tau_i^2{\Psi^{n_i}_{m_i}}^2 D_i^2\right)\\
\gamma =& 2\sum_{i=1}^{n}\tau_i^2\Psi^{n_i}_{m_i}(m_i-1)\hat{\sigma}_i^2/m_i + \log(6n/p)\sum_i \tau_i^2 D_i^2\Omega^{n_i}_{m_i}\Psi^{n_i}_{m_i}\\
&+\log(3/p)\left(\max_i \tau_i^2{\Psi^{n_i}_{m_i}}^2 D_i^2\right).
\end{aligned}$$

Proof. By widening the bound of Equation (6.27) we get:

$$\mathbb{P}\left(\begin{matrix}\sum_{i=1}^n\theta_i\sigma_i^2 - \sum_{i=1}^n\theta_i(\hat{\sigma}_i^2+(\mu_i-\chi_{i,m_i})^2) \geq \\ \sqrt{2\log(1/y)(\max_i\theta_i D_i^2\Psi^{n_i}_{m_i})\sum_{i=1}^n\theta_i\sigma_i^2}\end{matrix}\right) \leq y.$$

Completing the square gives for $\sqrt{\sum_{i=1}^n\theta_i\sigma_i^2}$ gives:

$$\mathbb{P}\left(\sqrt{\sum_{i=1}^{n}\theta_i\sigma_i^2} \geq \begin{matrix}\sqrt{\begin{matrix}\sum_{i=1}^n\theta_i(\hat{\sigma}_i^2+(\mu_i-\chi_{i,m_i})^2)\\ +\frac{\log(1/y)}{2}\left(\max_i\theta_i D_i^2\Psi^{n_i}_{m_i}\right)\end{matrix}}\\ +\sqrt{\frac{\log(1/y)}{2}\left(\max_i\theta_i D_i^2\Psi^{n_i}_{m_i}\right)}\end{matrix}\right) \leq y.$$

Combining with Equation (6.28) with a union bound (Lemma 4) gives:

$$\mathbb{P}\left(\sqrt{\sum_{i=1}^{n}\theta_i\sigma_i^2} \geq \begin{matrix}\sqrt{\begin{matrix}\sum_{i=1}^n\theta_i\hat{\sigma}_i^2+\frac{\log(2n/r)}{2}\sum_i\theta_i D_i^2\Omega^{n_i}_{m_i}\\ +\frac{\log(1/y)}{2}\left(\max_i\theta_i D_i^2\Psi^{n_i}_{m_i}\right)\end{matrix}}\\ +\sqrt{\frac{\log(1/y)}{2}\left(\max_i\theta_i D_i^2\Psi^{n_i}_{m_i}\right)}\end{matrix}\right) \leq y+r, \tag{6.30}$$

which is a bound for the weighted sum variances in terms of the sample variances. Letting $\theta_i = \frac{1}{2}\tau_i^2\Psi^{n_i}_{m_i}$ and combining with (6.26) with a union bound (Lemma 4), and then assigning $r=t=y=p/3$ and rewriting in terms of unbiased sample variance, gives the result. □

This completes the derivation of the SEBB. In Equation (6.29) of Theorem 15, we have a concentration inequality for the sum of weighted strata sample mean errors relative to the sample variances. In this context, the weights τ_i are flexible but would naturally be probability weights proportional to strata size, $\tau_i = n_i/(\sum_{j=1}^n n_j)$, in which case the inequality provides a concentration of measure in stratified random sampling.

6.4.3 A Stratified Empirical Chebyshev Bound (SECB)

It is also possible to consider another strongly related bound on the error in stratified sampling. Since the last Theorem 15 ultimately builds upon Theorem 12 which was the embodiment of a simplification of Bennett's inequality per Lemma 8. And since we will ultimately compare performance of these bounds against Neyman sampling which is conceptually built upon the minimisation of Chebyshev's inequality (Theorem 2) we will also consider and compare against a empirical Chebyshev's inequality for stratified sampling.

Theorem 16 (Stratified Empirical Chebyshev Bound (SECB))**.** *Assuming the context given in Definition 1. Then with $\Omega^{n_i}_{m_i}, \Psi^{n_i}_{m_i}$ per Lemma 10:*

$$\mathbb{P}\left(\left|\sum_{i=1}^{n}\tau_i(\chi_{i,m_i}-\mu_i)\right| \geq \sqrt{\frac{3}{p}}\left(\sqrt{\alpha+\beta}+\sqrt{\beta}\right)\right) \leq p \tag{6.31}$$

where:

$$\begin{aligned}\alpha =& \sum_{i=1}^{n}\tau_i^2\Psi^{n_i}_{m_i}(m_i-1)\hat{\hat{\sigma}}_i^2/m_i + \frac{\log(6n/p)}{2}\sum_i \tau_i^2\Psi^{n_i}_{m_i}D_i^2\Omega^{n_i}_{m_i}\\ \beta =& \frac{\log(3/p)}{2}\left(\max_i \tau_i^2 D_i^2 {\Psi^{n_i}_{m_i}}^2\right)\end{aligned}$$

Proof. We can use Chebyshev's inequality (Theorem 2) for the strata sample estimator giving:

$$\mathbb{P}\left(\left|\sum_{i=1}^{n}\tau_i(\chi_{i,m_i}-\mu_i)\right| \geq \frac{1}{\sqrt{k}}\sqrt{\mathrm{Var}\left(\sum_{i=1}^{n}\tau_i\chi_{i,m_i}\right)}\right) \leq k$$

Which is a probability bound for the error of the stratum mean estimator in terms of its variance. Whereby we can assume the independence of the sampling between the strata and sampling with replacement, giving the decomposition of the variance of the estimator (in a similar process to Equation 6.1), giving:

$$\mathrm{Var}\left(\sum_{i=1}^{n}\tau_i\chi_{i,m_i}\right) = \sum_{i=1}^{n}\tau_i^2\mathrm{Var}(\chi_{i,m_i}) = \sum_{i=1}^{n}\frac{\tau_i^2\sigma_i^2}{m_i}$$

Hence:

$$\mathbb{P}\left(\left|\sum_{i=1}^{n}\tau_i(\chi_{i,m_i}-\mu_i)\right| \geq \frac{1}{\sqrt{k}}\sqrt{\sum_{i=1}^{n}\Psi^{n_i}_{m_i}\tau_i^2\sigma_i^2}\right) \leq k$$

Which is a Chebyshev type inequality for the error of the stratum mean estimator in terms of a sum of the stratum variances - and is very analogous to Equation 6.26 of

Theorem 12. And since equation 6.30 (from the previous proof) is a general bound for an arbitrary sum of the stratum variances we can combine with it (in the case of setting $\theta_i = \tau_i^2 \Psi_{m_i}^{n_i}$) by a union bound (Lemma 4), giving:

$$\mathbb{P}\left(\left|\sum_{i=1}^{n} \tau_i(\chi_{i,m_i} - \mu_i)\right| \geq \frac{1}{\sqrt{k}}\left(\begin{array}{c}\sqrt{\begin{array}{c}\sum_{i=1}^{n} \tau_i^2 \Psi_{m_i}^{n_i} \hat{\sigma}_i^2 + \frac{\log(2n/r)}{2} \sum_i \tau_i^2 \Psi_{m_i}^{n_i} D_i^2 \Omega_{m_i}^{n_i} \\ + \frac{\log(1/y)}{2}\left(\max_i \tau_i^2 D_i^2 \Psi_{m_i}^{n_i\,2}\right)\end{array}} \\ + \sqrt{\frac{\log(1/y)}{2}\left(\max_i \tau_i^2 D_i^2 \Psi_{m_i}^{n_i\,2}\right)}\end{array}\right)\right) \leq y + r + k$$

And setting $r = k = y = p/3$ and rewriting in terms of unbiased sample variance, gives the result. □

We will now turn to how minimising these bounds on the stratified sample mean estimate (theorems 15 and 16) can be used as a method of choosing samples in the context of stratified sampling. And afterwards, in the next section 6.5 we will compare how all these methods work in actually sampling stratified data.

6.4.4 Sequential sampling using the stratified empirical bernstein method (SEBM)

In this section, we developed a concentration inequality to bound the error of the sampling mean estimate in stratified random sampling, called the SEBB - as per Theorem 15. The process of selecting additional samples to minimise this probability bound on the error is introduced in this section. And we call it the *stratified empirical Bernstein method* (SEBM).

The fundamental principle of the SEBM, is that it is an online method of choosing additional samples which repeatedly scans through possible stratum for optimum sample choice, and the strata which would result in the most reduction of the SEBB bound is then recommended for additional sampling. The pseudo-code for this process of sampling, is given as Algorithm 3.

Specifically, Algorithm 3 is a repetitive process involving a scan through the possible strata and then the selection of one stratum to sample from. The process of scanning involves calculating the confidence bound width (SEBB) that would result if an additional sample were to be taken from that stratum without changing its sample variance (line numbers 5-17 in Algorithm 3). The stratum that yields the smallest confidence bound width in the context of an additional sample is then selected (line 18-21) and sampled (line 24), the sample variance of that stratum is updated (line 26); this process repeats until the maximum sample budget is reached (per the outer loop, line 1). In this way the process attempts to iteratively minimise the SEBB in expectation with each additional sample taken; and hence lead to potentially greater accuracy in stratified sampling as a result.

The primary assumption that exists in this method's selection calculus is that it assumes that the sample variance of the strata would likely remain unchanged for the taking of the additional sample from any strata. While this technically isn't true, the unbiased sample variance is expected to be almost as likely to increase as it is likely to decrease from the taking of an additional sample. Plus developing an even more complicated probability bound that explicitly takes account of the likely change in error of the stratified mean estimate due to the expected change in the sample variance is beyond the scope of our investigation.

This SEBM method (Algorithm 3) requires the sample variances of all the strata to be calculated. And accordingly, Algorithm 3 must be initialised with at least two samples from each stratum so that sample variance can be calculated for it to be able to function.

We also note that Algorithm 3 describes a process specific to the sampling without replacement of all strata, and involves the calculation of the SEBB with the tightest possible use cases of Lemmas 11 and 10. In particular, for any stratum i that is sampled without replacement, any specific bound with an associated $\Omega_{m_i}^{n_i}$ and $\Psi_{m_i}^{n_i}$ may be substituted for $\bar{\Omega}_{m_i}^{n_i}$ and $\bar{\Psi}_{m_i}^{n_i}$ to potentially tighten the bound, and this corresponds to choice of Lemma 11 or Lemma 10 in the bound's derivation. Since the SEBB is a composition of such bounds with such choices throughout, there is a structure of valid pairs of substitutions Ω, Ψ for $\bar{\Omega}, \bar{\Psi}$ in the optimal calculation of the SEBB, which is shown in the steps 8-15 of Algorithm 3. The equivalent algorithm for sampling with replacement simply is the same algorithm altered by replacing all use of $\bar{\Omega}, \bar{\Psi}$ with Ω, Ψ respectively.

Similarly it is elementary to modify the terms of Algorithn 3 to be amenable to be minimising SECB bound (Theorem 16).

In the next section 6.5 we will compare how algorithms 2 and 3 work in actually sampling stratified data.

Algorithm 3 Stratified Empirical Bernstein Method (SEBM) algorithm, with replacement

Require: probability p, strata number N, stratum sizes n_i, initial sample numbers m_i, initial stratum sample variances $\hat{\hat{\sigma}}_i^2$, weights τ_i, widths D_i, maximum sample budget B

while $\sum_i m_i < B$ **do**
  $beststrata \leftarrow -1$
  $lowestbound \leftarrow \infty$
  for $k = 0$ to N **do**
    $m_k \leftarrow m_k + 1$
    $a \leftarrow [0,0]$, $b \leftarrow [0,0]$, $c \leftarrow [0,0]$, $d \leftarrow [0,0]$
    for $i = 0$ to N **do**
      $a_0 \leftarrow a_0 + \log(6N/p) D_i^2 \bar{\Psi}_{m_i}^{n_i} \min(\bar{\Omega}_{m_i}^{n_i}, \Omega_{m_i}^{n_i}) \tau^2$
      $a_1 \leftarrow a_1 + \log(6N/p) D_i^2 \Psi_{m_i}^{n_i} \min(\bar{\Omega}_{m_i}^{n_i}, \Omega_{m_i}^{n_i}) \tau^2$
      $b_0 \leftarrow \max(b_0, \log(3/p) D_i^2 \bar{\Psi}_{m_i}^{n_i} \min(\bar{\Psi}_{m_i}^{n_i}, \Psi_{m_i}^{n_i}) \tau^2)$
      $b_1 \leftarrow \max(b_1, \log(3/p) D_i^2 \Psi_{m_i}^{n_i} \min(\bar{\Psi}_{m_i}^{n_i}, \Psi_{m_i}^{n_i}) \tau^2)$
      $c_0 \leftarrow c_0 + 2\bar{\Psi}_{m_i}^{n_i}((m_i - 1)\hat{\hat{\sigma}}_i^2 / m_i) \tau^2$
      $c_1 \leftarrow c_1 + 2\Psi_{m_i}^{n_i}((m_i - 1)\hat{\hat{\sigma}}_i^2 / m_i) \tau^2$
      $d_0 \leftarrow d_0 + \frac{4}{17} D_i^2 \bar{\Omega}_{m_i}^{n_i} \tau^2$
      $d_1 \leftarrow d_1 + \frac{4}{17} D_i^2 \Omega_{m_i}^{n_i} \tau^2$
    end for
    $boundwidth \leftarrow \sqrt{\log(6/p) \min_j (d_j + (\sqrt{c_j + a_j + b_j} + \sqrt{b_j})^2)}$
    if $boundwidth < lowestbound$ **then**
      $beststrata \leftarrow k$
      $lowestbound \leftarrow boundwidth$
    end if
    $m_k \leftarrow m_k - 1$
  end for
  take an extra sample from strata: *beststrata*
  $m_{beststrata} \leftarrow m_{beststrata} + 1$
  recalculate $\hat{\hat{\sigma}}_{beststrata}^2$
end while

6.5 Results and evaluation of methods

In this section, different schemes of sampling in the context of Stratified sampling are compared in the context of synthetic data, primarily in the context of Beta-distributed data, and also in a more specific Bernoulli-uniform data set. In the next subsection 6.6 we consider the effectiveness of these different methods of sampling specifically to approximate the Shapley Value in the context of various cooperative games. The results and analysis of these methods are discussed in the following discussion section 6.7.[4]

6.5.1 Benchmarks algorithms

We outline a range of benchmark algorithms used to evaluate the performance of various methods in the context of synthetic data sets. Then Section 6.5.2 describes two synthetic data sets and reports on the resulting distribution of errors under our benchmarks algorithms.

In the numerical evaluations for synthetic data, we compare the following sampling methods:

- SEBM (Stratified empirical Bernstein method, without replacement): our SEBM method (per Algorithm 3) of iteratively choosing samples from strata to minimise the SEBB, given in Equation (6.29). An initial sample of two data points from each strata is used to initialise the sample variances of each, with additional samples made to maximally minimise the inequality at each step. All samples are drawn *without* replacement.

- SEBM-W (Stratified empirical Bernstein method with replacement): as above, with the exception that all samples are drawn *with* replacement, and consequently the inequality does not utilise the martingale inequality given in Lemma 11.

- Simple (Simple random sampling, without replacement): simple random sampling from the population irrespective of strata *without* replacement.

- Simple-W (Simple random sampling with replacement): simple random sampling from the population irrespective of strata *with* replacement.

- Ney (Neyman sampling, without replacement): the method of maximally choosing samples *without* replacement from strata proportional to the strata variance (via Theorem 1).

- Ney-W (Neyman sampling with replacement): the method of choosing samples *with* replacement proportional to the strata variance (via Theorem 1).

[4]Sourcecode for all the experiments in this paper are available at:
https://github.com/Markopolo141/Stratified_Empirical_Bernstein_Sampling

- SEBM* (Stratified empirical Bernstein method with variance assistance): the method of iteratively choosing samples *without* replacement from strata to minimise Equation (6.26), utilizing martingale Lemma 11.

- SEBM*-W (Stratified empirical Bernstein method with variance assistance): the method of iteratively choosing samples *with* replacement from strata to minimise Equation (6.26).

- SECM (Stratified empirical Chernoff method): the method of iteratively choosing samples from strata *without* replacement to minimize the SECB, given in Equation (6.31). An initial sample of two data points from each strata is used to initialise the sample variances of each, with additional samples made to maximally minimize the inequality at each step. All samples are drawn *without* replacement.

- Hoeffding (Unionised EBBs with Hoeffding's inequality): The method of sampling *with* replacement to minimise probability bound of Theorem 8 applied with Hoeffding's inequality (Theorem 6)

- Audibert (Unionised EBBs with Audibert et.al's EBB): The method of sampling *with* replacement to minimise probability bound of Theorem 8 applied with Audibert et.al's EBB (Theorem 4)

- Maurer (Unionised EBBs with Maurer & Pontil's EBB): The method of sampling *with* replacement to minimise probability bound of Theorem 8 applied with Maurer & Pontil's EBB (Theorem 3)

- EEBB (Unionised EBBs with our Engineered EBB): The method of sampling to *with* replacement to minimise the probability bound of Theorem 8 applied with our fitted EBB (Equation 6.21)

- Random (stratified sampling with random samples from strata): The process of stratified sampling *with* replacement, choosing random numbers of samples from each of the strata.

We consider that the three methods (Ney,Ney-W and SEBM*) are built apon the assumption of known variances for the strata, which are supplied to them, so that they may serve as a comparrison with the performance which would be possible for various methods which such information. Additionally we note that for all other methods (where appropriate) we selected for minimising a 50% confidence interval (i.e. constant $p = 0.5$ and $t = 0.5$).

The differences between these methods provide comparisons of different algorithmic factors, such as the dynamics of sampling: with and without replacement; with stratification and without; between our method and Neyman sampling, and; with and without perfect knowledge of stratum variances. For these methods, we consider the effectiveness of sampling Beta distributed data and for a case of uniform-and-Bernoulli data.

6.5.2 Synthetic data

The most immediate way to compare the effectiveness of our method(s) is to generate sets of synthetic data, and then numerically examine the distribution of errors generated by the different methods of choosing samples. In this section, we describe two types of synthetic data sets used in this evaluation, namely:

1. Beta distributed stratum data, which are intended reflect possible real-world data, and

2. a particular form of uniform and Bernoulli distributed stratum data, where our sampling method (SEBM) was expected to perform poorly.

6.5.2.1 Beta-distributed data

The first pool of synthetic data have between 5 and 21 strata, with the number of strata drawn with uniform probability, and each strata sub-population has sizes ranging from 10 to 201, also drawn uniformly. The data values in each strata are drawn from Beta distributions, with classic probability density function:

$$\phi(x)_{\{\alpha,\beta\}} = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

with α and β parameters drawn uniformly between 0 and 4 for each stratum, and Γ is the gamma function.

Figures 6.3 and 6.4 compare the distribution of absolute errors achieved by each of the sampling methods over 5000 rounds of these data sets. Each panel presents the results that the methods achieve for a given budget of samples, expressed as a multiple of the number of strata (noting that data sets where the sampling budget exceeded the volume of data were excluded). From the plots in Figures 6.3 and 6.4, we can see that our sampling technique (SEBM and SEBM-W) performs comparably to Neyman sampling (Ney and Ney-W) despite not having access to knowledge of stratum variances. Also, there is a notable similarity between SEBM* and SEBM. As expected, sampling without replacement always performs better than sampling with replacement for the same method, and this difference is magnified as the number of samples grows large in comparison to the population size. Finally, simple random sampling almost always performs worst, because it fails to take advantage of any variance information. These results and their interpretation are discussed and detailed in Section 6.7 along with results from the other test cases discussed below.

6.5.2.2 A uniform and Bernoulli distribution

We also to examine data distributions in which our sampling method (SEBM) performs poorly, particularly compared to Neyman sampling (Ney). For this purpose, a data-set with two strata is generated, with each stratum containing 1000 points. The data in the first stratum is uniform continuous data in range $[0,1]$, while the

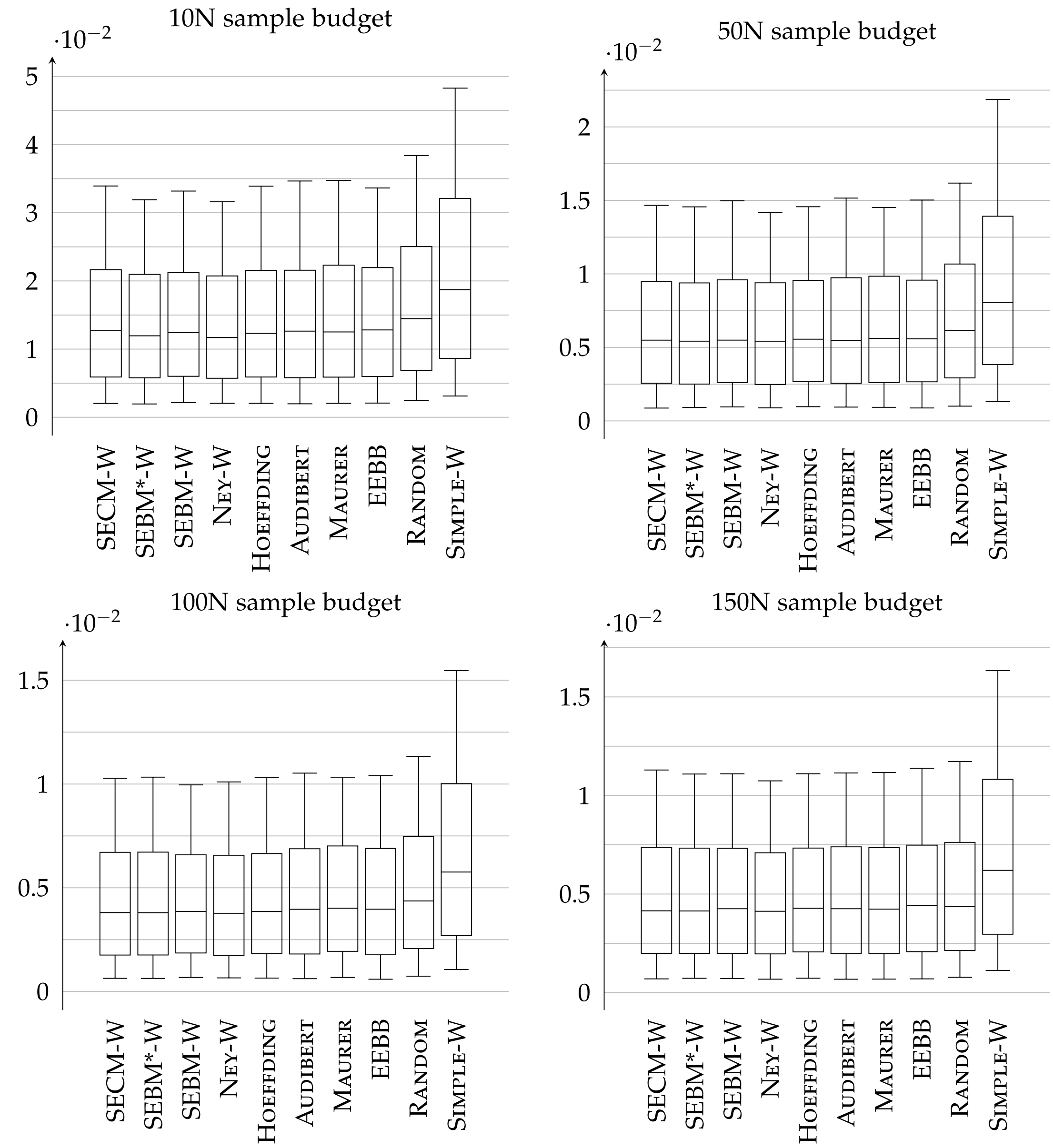


Figure 6.3: The distribution of numerical absolute errors across 5000 rounds of Beta-distributed data, for different methods of stratified sampling *with* replacement, for a sample budget of $10N$, $50N$, $100N$ and $150N$ samples where N number of strata. Whiskers show the 9th and 91st percentiles.

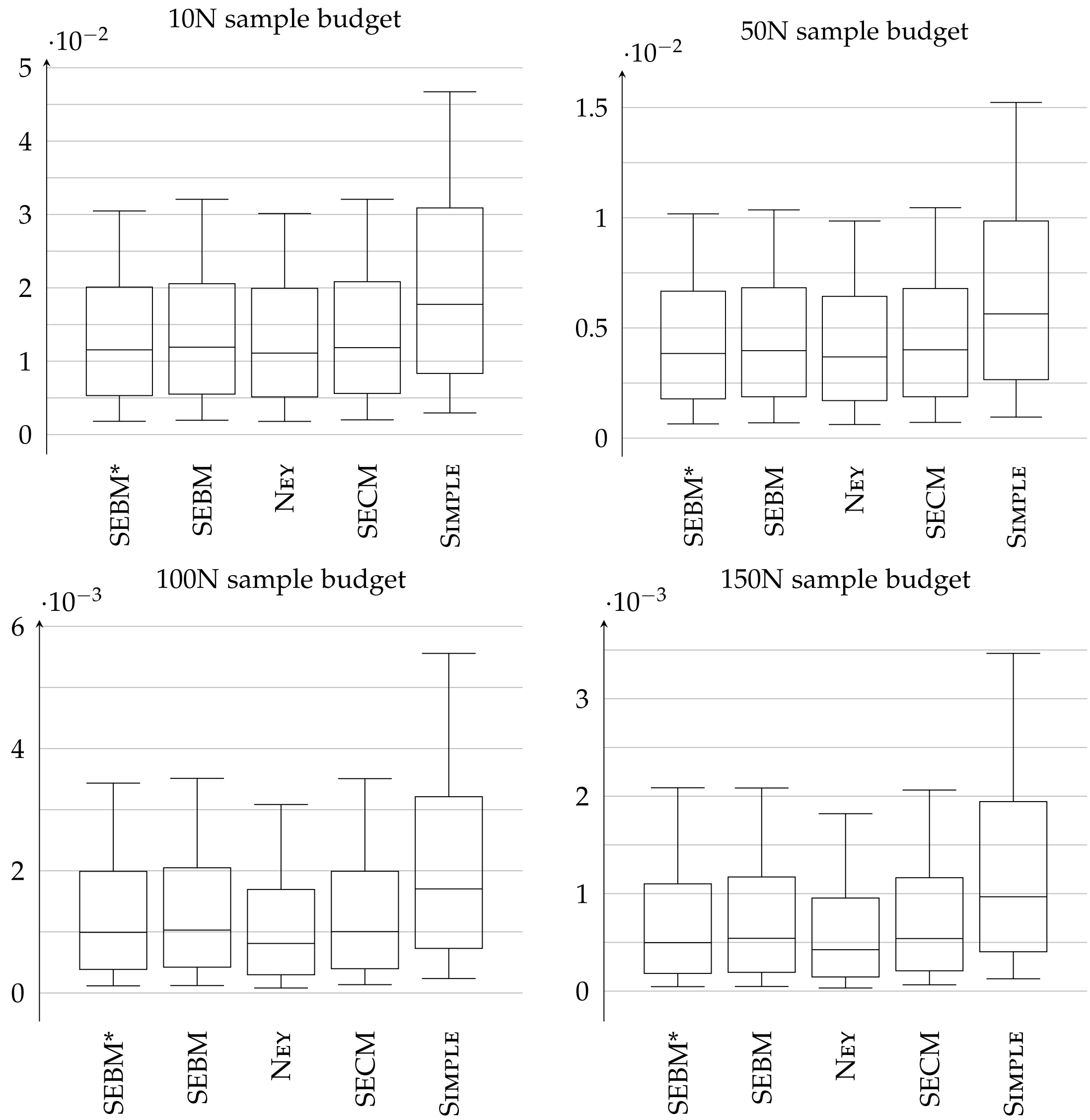


Figure 6.4: The distribution of numerical absolute errors across 5000 rounds of Beta-distributed data, for different methods of stratified sampling *without* replacement, for a sample budget of $10N$, $50N$, $100N$ and $150N$ samples where N number of strata. Whiskers show the 9th and 91st percentiles.

data in the second is Bernoulli distributed, with all zeros except for a specified small number a of data points, with value 1. For this problem, we conduct stratified random sampling with a budget of 300 samples, comparing the SEBM*, SEBM and Ney methods. The average error returned by the methods across 20,000 realisations of this problem, plotted against the number of successes a, are shown as a graph in Figure 6.6. This figure demonstrates that SEBM and SEBM* perform poorly when a is small. This under-performance is not simply a result of the SEBM method over-sampling in a process of learning the stratum variances (which was the intended demonstration), but the under-performance was present in SEBM* as well. The reasons for this under-performance are discussed in in more detail in Section 6.7.2. But before this discussion, we also considered the approximation of the Shapley Value as an example application of our stratified sampling method.

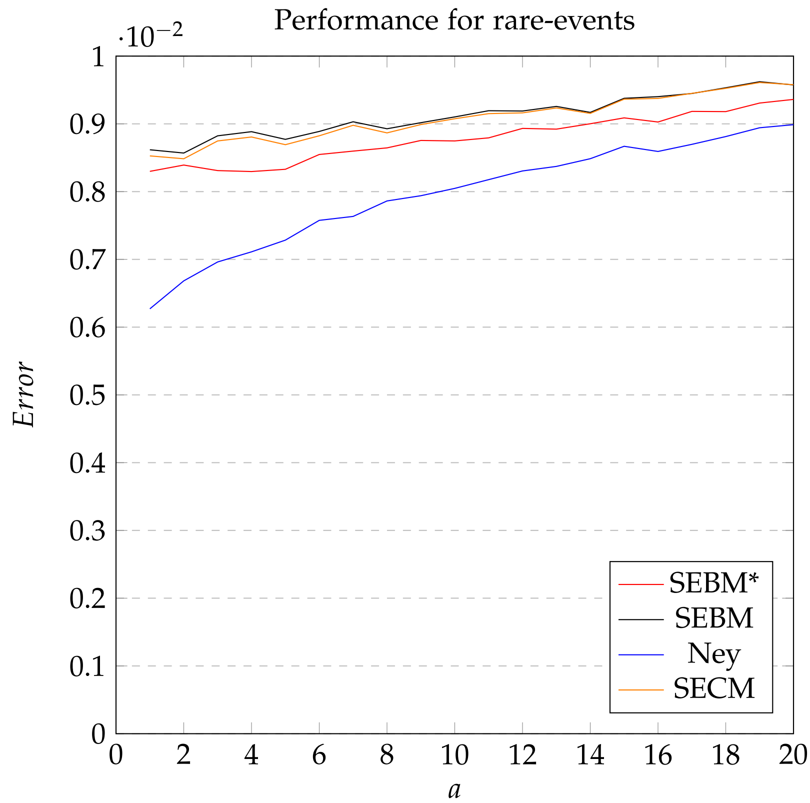


Figure 6.5: Average error of three stratified random sampling methods for the uniform-Bernoulli data sets of Section 6.5.2.2, plotted against success parameter a, across 20,000 rounds.

6.6 Shapley Value approximation

The Shapley Value is a cornerstone measure in cooperative game theory (introduced in section 3.3.2). It is an axiomatic approach to allocating a divisible reward or cost between participants where there is a clearly defined notion of how much surplus or profit a coalition of participants could achieve by themselves. It has many applications, including analysing the power of voting blocks in weighted voting games [Bachrach et al., 2009], in cost and surplus division problems [Aziz et al., 2016; Chapman et al., 2017], and as a measure of network centrality [Michalak et al., 2013]. But primarily, is useful to us as a method of allocating financial payments in electricity network contexts (see section 4.2.1).

Though the Shapley Value is conceptually simple, its use is hampered by the fact that its total expression involves exponentially many evaluations of the characteristic function (there are $n \times 2^{n-1}$ possible marginal contributions between n players). However, since the Shapley Value is expressible as an average over averages by Equation (3.4), it is possible to approximate these inner averages via sampling techniques, and then these averages are naturally stratified by coalition size, forming an instance of stratified sampling. For a given inner average in the Shapley Value expression, we approximate such an average by randomly selecting marginal contributions, calculating the sample average. Thus the question then becomes how many samples should we compute for each strata to attain the best estimate of the Shapley Value.

In previously published literature, other techniques have been used to allocate samples in this context of Shapley Value sampling approximation, particularly simple sampling [Castro et al., 2009], Neyman allocation [Castro et al., 2017; O'Brien et al., 2015], and allocation to minimise Hoeffding's inequality [Maleki et al., 2013].

We assess the benefits of using our bound by comparing its performance to the approaches above in the context of some example cooperative games, with results analysed in Section 6.7. The example games are described below:

Example Game 1 (Airport Game)**.** *An $n = 15$ player game with characteristic function:*

$$v(S) = \max_{i \in S} w_i$$

where $w = \{w_1, \ldots, w_{15}\} = \{1, 1, 2, 2, 2, 3, 4, 5, 5, 5, 7, 8, 8, 8, 10\}$. The maximum marginal contribution is 10, so we assign $D_i = 10$ for all i.

Example Game 2 (Voting Game)**.** *An $n = 15$ player game with characteristic function:*

$$v(S) = \begin{cases} 1, & \text{if} \quad \sum_{i \in S} w_i > \sum_{j \in N} w_j / 2 \\ 0, & \text{otherwise} \end{cases}$$

where $w = \{w_1, \ldots, w_{15}\} = \{1, 3, 3, 6, 12, 16, 17, 19, 19, 19, 21, 22, 23, 24, 29\}$. The maximum marginal contribution is 1, so we assign $D_i = 1$ for all i.

Example Game 3 (Simple Reward Division)**.** *An $n = 15$ player game with characteristic function:*

$$v(S) = \frac{1}{2} \left(\sum_{i \in S} \frac{w_i}{100} \right)^2$$

where $w = \{w_1, \ldots, w_{15}\} = \{45, 41, 27, 26, 25, 21, 13, 13, 12, 12, 11, 11, 10, 10, 10\}$
The maximum marginal contribution is 1.19025*, so we assign* $D_i = 1.19025$ *for all* i*.*

Example Game 4 (Complex Reward Division)**.** *An* $n = 15$ *player game with characteristic function:*

$$v(S) = \left(\sum_{i \in S} \frac{w_i}{50}\right)^2 - \left\lfloor \left(\sum_{i \in S} \frac{w_i}{50}\right)^2 \right\rfloor$$

where $w = \{w_1, \ldots, w_{15}\} = \{45, 41, 27, 26, 25, 21, 13, 13, 12, 12, 11, 11, 10, 10, 10\}$
In this game, we assign $D_i = 2$ *for all* i*.*

For each game, we compute the exact Shapley Value, and then the average absolute errors in the approximated Shapley Value for a given budget m of marginal-contribution samples across multiple computational runs. The results are shown in Table 6.5, where the average absolute error in the Shapley Value is computed by sampling with Maleki's method [Maleki et al., 2013] is denoted e^{Ma}, e^{sim} is Castro's stratified simple sampling method [Castro et al., 2009], e^{Ca} is Castro's Neyman sampling method [Castro et al., 2017], and e^{SEBM} is the error associated with our method, SEBM. The results in Table 6.5 show that our method performs well across the benchmarks. A discussion of all of the results is considered in the next section.

6.7 Discussion

This section contains discussion of all the parts of this chapter, particularly the nature of the techniques employed, the nature of the mechanisms discovered and the experimental effectiveness of them in the context of synthetic data.

- in subsection 6.7.1 we discuss the nature and effectiveness of our derived EBB from section 6.3.
- in subsection 6.7.2 we discuss the performance of our new SEBM method, in the context of synthetic data
- in subsection 6.7.3 we discuss the performance of our SEBM method in the context of sampling the Shapley Value.
- in subsection 6.8 we give indication of future work regarding the extension of SEBB to multidimensional data, and conclude.

6.7.1 The effectiveness of our new EBB

In section 6.3 we went through the process of deriving an EBB using complex components, thus yielding a requirement for its numerical determination. The resulting numerical EBB was then fitted with a symbolic envelope for ease of use - per equation 6.21.

Table 6.1: Airport Game Average Errors

m/n^2	10	50	100	500	1000
e^{Ma}	298.4	133.1	99.64	41.96	29.26
e^{sim}	357.8	146.1	106.2	44.55	36.33
e^{Ca}	325.7	115.8	75.85	31.01	22.12
e^{SEBM}	**259.2**	**73.8**	**54.76**	**7.71**	**1.30**

Table 6.2: Voting Game Average Errors

m/n^2	10	50	100	500	1000
e^{Ma}	131.0	57.78	41.52	18.66	13.18
e^{sim}	145.7	59.72	40.31	17.56	12.84
e^{Ca}	142.1	**47.35**	**31.05**	14.08	9.800
e^{SEBM}	**122.8**	47.44	33.18	**8.55**	**1.995**

Table 6.3: Simple Reward Division Game average errors

m/n^2	10	50	100	500	1000
e^{Ma}	25.68	11.62	7.792	3.481	2.290
e^{sim}	22.10	9.045	6.218	2.642	1.938
e^{Ca}	22.37	8.925	6.692	2.727	1.940
e^{SEBM}	**19.25**	**7.044**	**5.158**	**1.183**	**0.2817**

Table 6.4: Complex Reward Division Game average errors

m/n^2	10	50	100	500	1000
e^{Ma}	276.1	118.9	87.00	40.15	27.44
e^{sim}	251.4	108.0	78.63	34.64	26.82
e^{Ca}	290.5	116.5	81.82	35.70	26.50
e^{SEBM}	**214.2**	**78.47**	**54.10**	**12.45**	**2.711**

Table 6.5: Average absolute errors in the Shapley Value calculation across all players in the four cooperative games (units in 10^{-4}), for the different sampling schemes with different sampling budgets m per number of strata (with $n^2 = 15^2$ for all). lowest error results are boldened.

It is interesting to compare the strength of the new EBB against other EBBs, particularly we considered that most of the elements in our new EBB were improvements upon the process used in the derivation of Maurer and Pontil's EBB.

And so we compared our EBB directly with Maurer and Pontil [2009]'s EBB given by theorem 3 as:

$$\mathbb{P}\left(\mu - \hat{\mu} \geq \sqrt{\frac{2\hat{\sigma}^2 \log(2/t)}{n}} + \frac{7D\log(2/t)}{3(n-1)}\right) \leq t$$

We felt that it would only be fair to compare our EBB to Maurer and Pontil's EBB if they had applied Popoviciu's inequality as an appropriate domain restriction and carried it through their derivation, as we did to our own EBB. Specifically, this is the domain where:

$$\frac{1}{2} > \frac{\sqrt{\hat{\sigma}^2}}{D} + \sqrt{\frac{2\log(2/t)}{n-1}}$$

We plotted the improvement our EBB offers in this domain, as shown in Figure 6.6.

In this plot, a probability 0.5 bound is shown to shrink by approximately one third. And we observed that our refinement of Maurer and Pontil's EBB was uniformly tighter across a large range of values.

While this may be an interesting result, we also sought to put this in perspective with what could ideally be achieved. And so we conducted a comparison about the further improvement over our EBB that might be achieved with perfect information about the variance; specifically that, Bennett's inequality is used assuming $\hat{\sigma}^2 = \sigma^2$. The improvement that Bennett's inequality (with perfect variance information) has over our EBB is plotted in Figure 6.7, which shows that when the variance is small, uncertainty about the variance is the most detrimental to an EBB, such as ours. However, it is witnessed that loosely going from our EBB to perfect variance information shrinks the bound by about another third. In this way (although the results are loose) we can witness that our EBB provides approximately a half-way mark from existing state-of-the-art EBBs to an impossible ideal of having perfect variance information.

The purpose of developing a stronger EBB was to see if it could be used to improve the selection of samples in the context of stratified sampling (particularly of the Shapley Value) over other EBBs. It was expected that the better and more tight the EBBs used, the more likely it would be that iteratively choosing samples to minimise such a bound would produce better sample choices and thus yield better estimate of the population mean.

And while it is evident that the EBB we produced was tighter than Maurer and Pontil's EBB, the actual resulting performance difference in selecting samples (as seen between EEBB and Maurer in Table 6.3) is surprisingly marginal; so marginal in fact, it was comparable to the performance of using unioned Hoeffding bounds - the Hoeffding method. We continue discussion of this surprising result in the context of all the other methods in the next section 6.7.2.

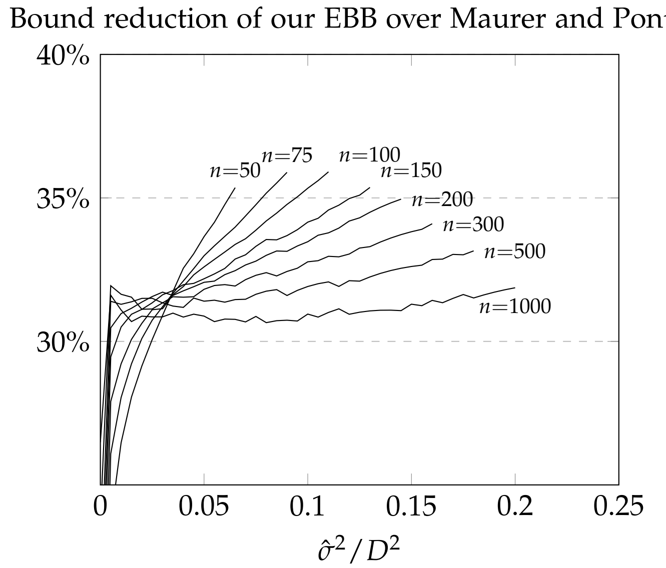


Figure 6.6: The percent reduction of the 0.5 probability bound, that going from Maurer and Pontil's EBB to our EBB would achieve, for various n, in the domain valid for their EBB.

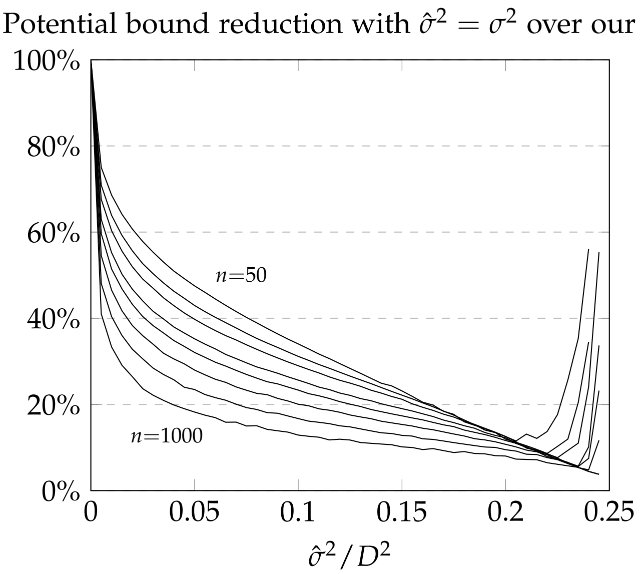


Figure 6.7: The percent reduction in the 0.5 probability bound that going from our EBB to using Bennett's inequality (perfect variance information, $\hat{\sigma}^2 = \sigma^2$) achieves, for $n = 50, 75, 100, 150, 200, 300, 500, 1000$.

6.7.2 Discussion of stratified sampling results

The results for our different sampling methods are shown across Figures 6.3,6.4 and 6.6, with the main observation that most of the techniques performed well and similar to Neyman sampling, and that our sampling technique (including SEBM (or SEBM-W) and SECM) performed competitively to Neyman sampling (Ney or Ney-W) despite not having access to knowledge of strata variances.

It is also observed that Neyman sampling was ultimately the most accurate, for reasons that were hinted in section 6.1.1. Particularly that if sufficient samples have been taken then the sample means of the strata will tend to approximately be Gaussian distributed by the Central Limit Theorem. In this context the strata means have a distribution that is entirely characterised by their mean and variance, and hence so too is the population mean estimate. Thus the variance of the sampled population mean is the only parameter determining its error, and minimising it directly translates into improved accuracy. The fact that the variances of the strata are the only parameters determining the error in the stratified sampling process is most directly exploited by Neyman allocation but is more obscured in SEBM* allocation methodology (as it is based only on a simplification of Bennett's inequality), thus leading to slightly worse results, particularly in Figure 6.6.

However this mode of explanation is perhaps the underlying reason for the similarity in performance of many of the other methods as well, particularly that after sufficiently many samples have been taken the sample means of all of the strata become Gaussian distributed and the performance of the methods then depend primarily on how effectively they estimate the variances of the strata and then allocate accordingly. Perhaps in our Beta synthetic data there was not sufficient spread of data variances for it to make significant difference how effectively this variance estimation and allocation was done.

Conversely the Bernoulli-uniform synthetic data was specifically designed to create a significant spread in variance between the strata. And the results (plotted in 6.6) reveal the design to amplify the detriment in stratified sampling that uncertainty about the variances would yield. In this context Neyman sampling is very efficient as it samples based on perfect variance information, and reversely our method SEBM performs worse as it extends from minimising only a simplification of Bennett's inequality under uncertainty of the variance - this is most evident in figure 6.6. Because of this uncertainty about the variance, the more infrequent the Bernoulli outlier, the more likely that the methods without variance information would over-sample the Bernoulli stratum - which they did. The relative inefficiency of the SECM method is also interesting, particularly as it sought to minimise Chebyshev's inequality for the stratified sampling, and under perfect variance information would be identical to Neyman sampling. The implication in this context is that the inefficiency of utilising these methods primarily extends from uncertainty about the variances of the strata and how to integrate it.

From between Figures 6.3 and 6.4 we observe that sampling without replacement always performs better than sampling with replacement for the same method, and this improvement is magnified as the number of samples grows large relative to the size of the population. At the same time, simple Random sampling almost always performs worst, because it fails to take advantage of any variance information, and Simple sampling performs even worse as it fails to take into account data stratification, these results are as expected. Therefore from the Figures 6.3 and 6.4 we see that the primary increase in performance comes from employing stratified sampling over simple sampling, sampling without replacement over sampling with replacement, and then using some method that is more intelligent than randomly selecting samples (ie. Random method) and preferably using stratum variance information to get close to the ideal of Neyman sampling.

Aside from comparing the different performances of these bounds as a target for minimisation by selective sampling, it also was seen to be productive to consider them on their own - simply as bounds on the stratified mean error. Particularly we can see a range of different strengths of the bounds in Figure 6.8.

In Figure 6.8 we have plotted the bound widths of the various probability bounds of this paper in the context of the Beta-distributed data we considered in section 6.5.2.1 achieved after a sample budget $n = 50N$ samples allocated using Ney-W method. In this graph we considered the following bounds for the error:

- Ney-B The bound attained using knowledge of the variances of the strata using Chebyshev's inequality (Theorem 2) in conjunction with the additivity of variance rule (Equation 6.1)

- SEBB* The bound of Theorem 12 with variance knowledge of the variances, also using sampling without replacement sharpening (Theorem 11) where optimal.

- SEBB*-W The bound of Theorem 12 with variance knowledge of the variances, not using sampling without replacement sharpening (Theorem 11).

- SECB The bound of Theorem 16, which utilises Chebyshev's inequality together with our probability bound on error deviation.

- SEBB The bound of Theorem 15, using sampling without replacement sharpening (Theorem 11) where optimal.

- SEBB-W The bound of Theorem 15, not sampling without replacement sharpening (Theorem 11).

- Hoeffding-B The bound attained by Hoeffding's inequality (Theorem 6) for the strata, unioned together (via Theorem 8) to create a bound on the stratified sampling error.

- Audibert-B The bound attained by Audibert et.al's EBB inequality (Theorem 4) for the strata, unioned together (via Theorem 8) to create a bound on the stratified sampling error.

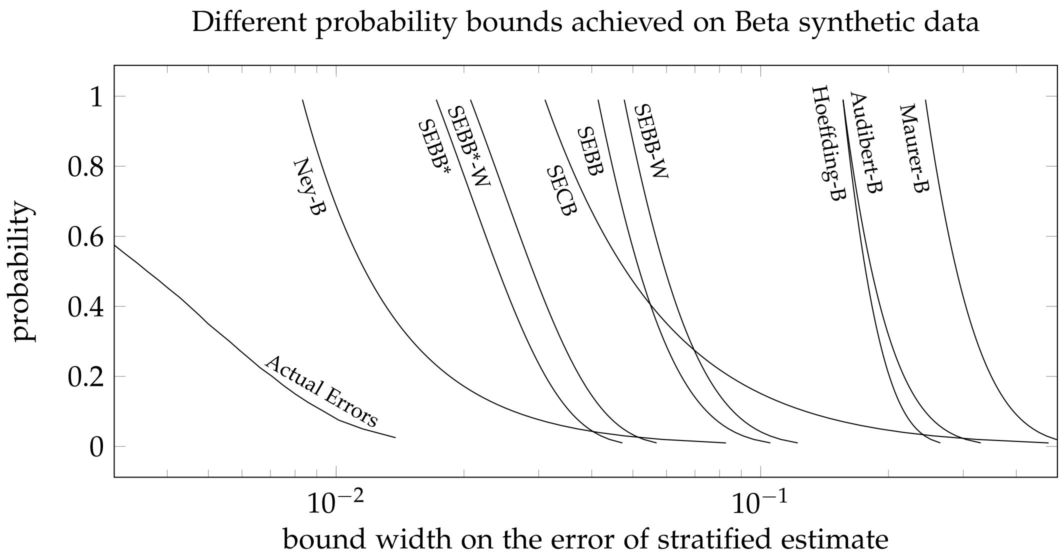


Figure 6.8: Different probability bound widths for the Beta-distributed data (per section 6.5.2.1) at the point of sample budget $n = 50N$ for Ney sampling method (see section 6.7 for descriptions of the bounds) against the actual distribution of errors on the data

- Maurer-B The bound attained by Maurer and Pontil's EBB inequality (Theorem 3) for the strata, unioned together (via Theorem 8) to create a bound on the stratified sampling error.

Particularly we see from Figure 6.8 that tightest bounds are given by those methods which are rooted in perfect variance information, and the widest bounds are given by those methods which utilise probability unions to bind EBBs together (via Theorem 8). What is most notable is the dissimilarity between the widths of the bounds and their effectiveness as a target for sampling minimisation; as choosing samples to minimise a probability bound is sensitive to the shape of the bound, not its magnitude. Also comparing this Figure 6.8, with Figures 6.3,6.4 we can see that the width of the bounds are much wider than the magnitudes of the error which are actually achieved; and this is quite expected, as analytic concentration inequalities function as conservative confidence intervals on the error of sampling.

6.7.3 Discussion of Shapley Value results

In considering the comparison of approaches to approximating the Shapley Value, our sampling method (SEBM, with error e^{SEBM}) shows improved performance on almost all accounts, as shown in Table 6.5. This was particularly the case in the context of large sample budgets, as our method sampled without replacement, while the other methods sampled with replacement. And we also note that our method's performance could potentially be further improved by selecting more refined D_i values in the context of our example games.

We attribute our methods success in estimating the Shapley Value primarily to the design decisions used in the creation of those other methods. Particularly we note that Castro's Neyman sampling method (with error e^{Ca}) deploys about half the samples learning about the variance and the other half using a Neyman style allocation. The choice of allocating half the samples was identified as a default by Castro with the acknowledgement that the proportion should be treated as a tunable parameter depending on the particular context of the cooperative game. However, to make a fair comparison did not tune any such parameters for any of the methods.

In the process of generating these results one of the major effects that was witnessed in our sampling method (SEBM) was the computational overhead of iteratively minimising (one sample at a time) our inequality (equation 6.29) in the context of our simple example games. Although we acknowledged and expected a computational overhead, we designed our method with the intention of using it to approximate the GNK value (per section 5.1), where each additional sample requires running an optimisation problem, and in this context a computational overhead about which sample to choose was deemed less relevant.

One primary limitation of our method(s) is that it rests on assumption of known data widths D_i (and in the case of sampling-without-replacement, also on strata sizes N_i), which may not be exactly known in practice. One way to overcome this may be to use our method with a reliable overestimate these parameters (by expert opinion or otherwise) and such estimation may itself open consideration of other probability bounds and/or sampling methods. Conversely, it might also be advisable to run our method with an underestimate of the data widths, as in-practice the sampling process is fundamentally sensitive to the shape of the inequality and not necessarily its magnitude or accuracy as a bound.

6.8 Conclusion and Future Work: applications of a multidimensional extension

It was noticed that our SEBB can be extended to multidimensional data by a simple modification. Specifically, instead of considering data that is single-valued, we consider data points that are vectors.

Formally, for n strata of finite data points which are all vectors of size M, let n_i be the number of data points in the ith stratum. Let the data in the ith stratum have a mean vector values μ_i (with $\mu_{i,j}$ for the jth component of the vector), which are value bounded within a finite width $D_{i,j}$, and have vector value variances $\sigma^2_{i,j}$. Given this, let $X_{i,1}, X_{i,2}, \ldots, X_{i,n_i}$ (where $X_{i,k,j}$ is the jth component, of the kth vector from stratum i) be vector random variables corresponding to those data values randomly and sequentially drawn (with or without) replacement. Denote the average of the first m_i of these random variables from the ith stratum by $\chi_{i,m_i} = \frac{1}{m_i}\sum_{k=1}^{m_i} X_{i,k}$ (with $\chi_{i,m_i,j}$ being the jth component of that vector average). Let $\hat{\hat{\sigma}}^2_{i,j} = \frac{i}{m_i-1}\sum_{k=1}^{m_i}(X_{i,k,j} - \chi_{i,m_i,j})^2$ be the unbiased sample variance of the first m_i of these random variables in the jth component. As before, we assume weights τ_i for each stratum.

In this context we have the following theorem:

Theorem 17 (Vector SEBM bound). *In the context above, then with $\Omega^{n_i}_{m_i}, \Psi^{n_i}_{m_i}$ per Lemma 10:*

$$\mathbb{P}\left(\begin{array}{l}\sum_{j=1}^{M}\left(\sum_{i=1}^{n}\tau_i(\chi_{i,m_i,j}-\mu_{i,j})\right)^2 \geq \\ \qquad \log(6/p)\sum_{j=1}^{M}\left(\alpha^{n_i}_{m_i,j}+\left(\sqrt{\beta^{n_i}_{m_i,j}}+\sqrt{\gamma^{n_i}_{m_i,j}}\right)^2\right)\end{array}\right) \leq Mp \tag{6.32}$$

where:

$$\begin{aligned}
\alpha_j =& \sum_{i=1}^{n}\frac{4}{17}\Omega^{n_i}_{m_i}D^2_{i,j}\tau_i^2 \\
\beta_j =& \log(3/p)\left(\max_i \tau_i^2{\Psi^{n_i}_{m_i}}^2 D^2_{i,j}\right) \\
\gamma_j =& 2\sum_{i=1}^{n}\tau_i^2\Psi^{n_i}_{m_i}(m_i-1)\hat{\hat{\sigma}}^2_{i,j}/m_i+\log(6n/p)\sum_i \tau_i^2 D^2_{i,j}\Omega^{n_i}_{m_i}\Psi^{n_i}_{m_i} \\
&+\log(3/p)\left(\max_i \tau_i^2{\Psi^{n_i}_{m_i}}^2 D^2_{i,j}\right)
\end{aligned}$$

Proof. Squaring (6.29) and applying it specifically to the jth component of all the vectors gives:

$$\mathbb{P}\left(\frac{\left(\sum_{i=1}^{n}\tau_i(\chi_{i,m_i}-\mu_i)\right)^2}{\log(6/p)} \geq \alpha_j+\left(\sqrt{\beta_j}+\sqrt{\gamma_j}\right)^2\right) \leq p$$

Taking a series of union bounds (Lemma 4) over j gives result. □

The left hand side of the inequality in (6.32) is the square Euclidean distance between our weighted stratified sample vector estimate $\sum_{i=1}^{n}\tau_i\chi_{i,m_i}$ and the true mean stratified vector $\sum_{i=1}^{n}\tau_i\mu_i$. In this context, an example sampling process might consist of sampling to maximally minimise the right hand side of the inequality (similar to our SEBM process, described in Section 6.4.4). This formulation can be applied to more involved computational tasks that involve approximating averages over large sets of data with multiple features or auxiliary variables.

Potentially the application of our multi-dimensional extension of the SEBB to a range of tasks (such as neural network minibatch smart sampling) could be quite rewarding.

6.8.1 Conclusion

Stratified sampling is a well known example of a statistical process of estimating a population mean by breaking it into strata, and then sampling the mean of each of the strata. Our primary investigative question of this chapter was how best to choose samples from the strata to get most accuracy in the final population estimate. To do this investigation we considered different means of estimating the error in the final population estimate - these took the form of analytically derived concentration inequalities. These concentration inequalities were developed and then the process of sampling to minimise them formed a sampling methodology, which was evaluated.

In the first part of this chapter, Section 6.1, we introduced the problem of stratified sampling, and a few statistical lemmas. Afterwards we considered different possible EBBs as a way of bounding the error in the context of stratified random sampling, and for this purpose developed a new EBB, in Sections 6.2 and 6.3. This process of using EBBs involved binding EBBs applied to different strata together using union bounds to create a bound on the stratified sample mean error (via Theorems 7 or 8).

From this investigation we learned that it was possible to create stronger bounds for stratified sampling (which dont use as many union bounds as there are strata), which in the next part of this chapter we developed, in Section 6.4. These sampling methodologies were then evaluated on synthetic data sets in Section 6.5, and discussed in Section 6.7.

There are potential future improvements to our concentration inequality and resulting sampling method (SEBB & SEBM - developed in Section 6.4), such as potentially:

- Investigating ways to minimise the computational overhead of the method.
- Possibly modify the method to take advantage of join order process in Shapley Value sampling.
- Or to use more complicated algebra, and less simplification to further tighten the concentration inequality.

Notwithstanding, our concentration inequality (SEBB) gives an analytic bound on the error of the stratified mean and explicitly considers the sample variances, data widths, sample numbers, and any additional weights on the strata; and includes factors specifically for strata sampled with and/or without replacement. It is complex and tailored specifically to stratified sampling, and performs well in the sampling of synthetic data sets.

The relevance of this new method of doing stratified sampling, has wider relevance, but also relevance to sampling the Shapley Value (or solution concepts similar to it such as the GNK value, as in Section 5.1) in electricity network contexts.

Appendix A

Some continuity and monotonicity properties of the GNK value

From inspection of equations 4.5 and 4.3 it defined that the GNK value is a summation over maximum of minimum terms and it should be rather evident that there is present some nice continuity properties:

Theorem 18 (GNK continuous with utilities)**.** *For utility functions $u_i(x, y)$ if we consider any bounded perturbations $\epsilon\Delta_i(x, y)$ then the GNK value is continuous with ϵ.*

Proof. To demonstrate that the GNK value is continuous with change in utility functions we consider that for all $(x, y) \in A$ we consider any set of utility perturbing functions $\Delta_i(x, y)$ with a magnitude $\max_{(x,y)\in A, i\in N} |\Delta_i(x, y)| = d$. For any coalition S, if we consider that advantage $v(S)$ with the original utility functions as $v_u(S)$ and with the perturbed utility function multiplied by a parameter ϵ as $v_{u+\epsilon\Delta}(S)$ then we can realise that:

$$-n\epsilon d \leq v_u(S) - v_{u+\epsilon\Delta}(S) \leq n\epsilon d$$

Therefore for any individual $i \in N$ the average over the advantage terms $v(S)$ for coalitions which include i of size k is similarly bounded.

$$-n\epsilon d \leq \frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S\\ |S|=k}} v_u(S) - \frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S\\ |S|=k}} v_{u+\epsilon\Delta}(S) \leq n\epsilon d$$

Therefore the average of these terms over sizes $k = 1 \ldots n$ is also bounded.

$$-n\epsilon d \leq \frac{1}{n} \sum_{k=1}^{n} \frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S\\ |S|=k}} v_u(S) - \frac{1}{n} \sum_{k=1}^{n} \frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S\\ |S|=k}} v_{u+\epsilon\Delta}(S) \leq n\epsilon d$$

Which is the difference in the GNK value for an individual i between the perturbed and unperturbed utility function. Thus for any prospective utility perturbation Δ with a magnitude d there is a δ $(= n\epsilon d)$ such that there exists a perturbation factor ϵ, such that if the utility functions are ϵ perturbed then the GNK value is δ bounded. □

This continuity property for utilities is potentially nice in that participants in a system under GNK, can be be assured that regardless of their bids, that small difference in their utility bids will not yield large differences in their utility payoff, this adds regularity and predictability to the system. Conversely for a potential operator of such a hypothetical GNK system, that this continuity property may add to the predictability of the system.

The GNK also has elementary monotonicity properties that are partially inherited from its relation to the Shapley Value.

Theorem 19 (GNK is monotonic). *If we consider advantage functions v and v' and the GNK value with those advantage function φ_i^v and $\varphi_i^{v'}$. Then for any individual $i \in N$, if all coalitions S such that $i \in S$ it is true that $v'(S) \geq v(S)$ then $\varphi_i^{v'} \geq \varphi_i^v$.*

Proof.

$$\varphi_i^v = \frac{1}{n}\sum_{k=1}^{n}\frac{1}{\binom{n-1}{k-1}}\sum_{\substack{S:i\in S\\|S|=k}} v(S) \leq \frac{1}{n}\sum_{k=1}^{n}\frac{1}{\binom{n-1}{k-1}}\sum_{\substack{S:i\in S\\|S|=k}} v'(S) = \varphi_i^{v'}$$

□

This monotonicity property ensures that individuals which have uniformly higher payoff advantages are afforded more utility under the GNK, which is a basic regularity reminiscent of the logic of the GNK value itself. Particularly, as the GNK value is an articulation of a bargaining solution concept, then individuals who have greater leverage in negotiation will (or should) have an outcome more favourable to them. Conversely, we could imagine the potential absurdity of a system opposite were true, in that individuals with greater leverage in bargaining would be afforded less.

In considering this monotonicity property, we can ask what changes in strategies and/or utility functions and network constraints yield this kind of monotonicity condition. The most direct case is shift invariance, which is inherited from Nash bargaining roots Nash [1953] and directly stated as an axiom in the case of the 'coco' value Kalai and Kalai [2013].

Theorem 20 (GNK is shift invariant). *For any two utility profiles $u_i^1(x,y)$ and $u_i^2(x,y)$, and GNK defined by these utility profiles φ_i^1 and φ_i^2. Then for any individual $i \in N$, if $u_i^2(x,y) = u_i^1(x,y) + c$ for some constant c, and for all $j \neq i$ that $u_i^2(x,y) = u_i^1(x,y)$, then $\varphi_i^2 = \varphi_i^1 + c$*

Proof. If we consider advantage functions v_1 and v_2 defined by utility functions $u_i^1(x,y)$ and $u_i^2(x,y)$ then for any coalition S including individual i:

$$\begin{aligned}
v_2(S) =& \frac{1}{2}\min_{\substack{y\in A^{N\setminus S}\\ \text{s.t.}(x,y)\in A}}\left[\max_{\substack{x\in A^S\\ \text{s.t.}\exists y,(x,y)\in A}}\left(\sum_{i\in S} u_i^1(x,y) + c - \sum_{i\in N\setminus S} u_i^2(x,y)\right)\right] \\
&+ \frac{1}{2}\max_{\substack{x\in A^S\\ \text{s.t.}(x,y)\in A}}\left[\min_{\substack{y\in A^{N\setminus S}\\ \text{s.t.}\exists x,(x,y)\in A}}\left(\sum_{i\in S} u_i^1(x,y) + c - \sum_{i\in N\setminus S} u_i^2(x,y)\right)\right] \\
&= v_1(S) + c
\end{aligned}$$

The above step simply brings the additive constant out the front of the max and min terms. Therefore for every coalition S which includes individual i of size k, $v_2(S) = v_1(S) + c$, therefore the average of these values over such coalitions has a similar relation.

$$\frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S\\|S|=k}} v_2(S) = \frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S\\|S|=k}} v_1(S) + c$$

therefore the average of these averages over sizes of coalitions $k = 1\dots n$ is again similar:

$$\frac{1}{n}\sum_{k=1}^{n} \frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S\\|S|=k}} v_2(S) = \frac{1}{n}\sum_{k=1}^{n} \frac{1}{\binom{n-1}{k-1}} \sum_{\substack{S:i\in S\\|S|=k}} v_2(S) + c$$

which is to say that $\varphi_i^2 = \varphi_i^2 + c$. □

Shift invariance is important but not particularly interesting property. It more-or-less identifies that a participant who affords a higher utility should be rewarded with a GNK value which is that same degree higher. This Shift invariance relation is essentially consistent with the idea that utility functions are invariant to affine transformation, more particularly translation. If a participant modifies his/her utility function by an offset, this GNK value will afford that individual with exactly the same physical outcomes and utility transfers to give them a net utility that is that same extent offset. This shift invariance property is good sanity check on a minimally sufficient bargaining solution concept.

So instead we also consider a very similar monotonicity property with regards to any utility perturbation that non-decreases a player's utility.

Theorem 21 (GNK is monotonic with increasing player utility). *For any two utility profiles $u_i^1(x,y)$ and $u_i^2(x,y)$, and GNK values defined by these utility profiles: φ_i^1 and φ_i^2. Then for any individual $i \in N$, if $u_i^2(x,y) = u_i^1(x,y) + f(x,y)$ for some non-negative function f, and for all $j \neq i$ that $u_j^2(x,y) = u_j^1(x,y)$, then $\varphi_i^2 \geq \varphi_i^1$*

Proof. If we consider advantage functions v_1 and v_2 defined by utility functions $u_i^1(x,y)$ and $u_i^2(x,y)$ then for any coalition S including individual i:

$$\begin{aligned}
v_2(S) =& \frac{1}{2} \min_{\substack{y\in A^{N\setminus S}\\ \text{s.t.}(x,y)\in A}} \left[\max_{\substack{x\in A^S\\ \text{s.t.}\exists y,(x,y)\in A}} \left(\sum_{i\in S} u_i^1(x,y) + f(x,y) - \sum_{i\in N\setminus S} u_i^2(x,y) \right) \right] \\
&+ \frac{1}{2} \max_{\substack{x\in A^S\\ \text{s.t.}(x,y)\in A}} \left[\min_{\substack{y\in A^{N\setminus S}\\ \text{s.t.}\exists x,(x,y)\in A}} \left(\sum_{i\in S} u_i^1(x,y) + f(x,y) - \sum_{i\in N\setminus S} u_i^2(x,y) \right) \right] \\
&= v_1(S) + c
\end{aligned}$$

If we pull out the inner maximisation and minimisation for the perturbed and unperturbed problems respectively, ie:

$$g_1(y) = \max_{\substack{x \in A^S \\ \text{s.t.}\exists y,(x,y)\in A}} \left(\sum_{i\in S} u_i^1(x,y) + f(x,y) - \sum_{i\in N\setminus S} u_i^2(x,y) \right)$$

$$g_2(y) = \max_{\substack{x \in A^S \\ \text{s.t.}\exists y,(x,y)\in A}} \left(\sum_{i\in S} u_i^1(x,y) - \sum_{i\in N\setminus S} u_i^2(x,y) \right)$$

$$h_1(x) = \min_{\substack{y \in A^{N\setminus S} \\ \text{s.t.}\exists x,(x,y)\in A}} \left(\sum_{i\in S} u_i^1(x,y) + f(x,y) - \sum_{i\in N\setminus S} u_i^2(x,y) \right)$$

$$h_2(x) = \min_{\substack{y \in A^{N\setminus S} \\ \text{s.t.}\exists x,(x,y)\in A}} \left(\sum_{i\in S} u_i^1(x,y) - \sum_{i\in N\setminus S} u_i^2(x,y) \right)$$

Now since $f(x,y)$ is non-negative therefore $g_1(y) \geq g_2(y)$ and $h_1(x) \geq h_2(x)$ irrespective of x and y. therefore

$$\min_{\substack{y \in A^{N\setminus S} \\ \text{s.t.}(x,y)\in A}} g_1(y) \geq \min_{\substack{y \in A^{N\setminus S} \\ \text{s.t.}(x,y)\in A}} g_2(y)$$

$$\max_{\substack{x \in A^S \\ \text{s.t.}(x,y)\in A}} h_1(x) \geq \max_{\substack{x \in A^S \\ \text{s.t.}(x,y)\in A}} h_2(x)$$

and

$$v_2(S) \geq v_1(S)$$

And the result that $\varphi_i^2 \geq \varphi_i^1$ follows by monotonicity (theorem 19). □

This monotonicity property in Theorem 21 most directly encodes the idea that the GNK value is monotone with player utilities, particularly if a players utility by some arbitrary non-negative function then their GNK value should also. it is more general in its application than the shift invariance established by Theorem 20. and is most directly relevant to the logic of the GNK value, that players with a greater payoff advantage will be afforded more utility, and thus if a players utility increases in some way, so too should the GNK value. Contrastingly we could imagine a system where the opposite is true, in that if a player has a higher utility for a specific outcome that the system would afford them less, would be less intuitive.

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