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Measuring exploration: evaluation of modelling to generate alternatives methods in capacity expansion models

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Abstract

As decarbonisation agendas mature, macro-energy systems modelling studies have increasingly focused on enhanced decision support methods that move beyond least-cost modelling to improve consideration of additional objectives and tradeoffs. One candidate is modelling to generate alternatives (MGA), which systematically explores new objectives without explicit stakeholder elicitation. This paper provides comparative testing of four existing MGA methodologies and proposes a new Combination vector selection approach. We examine each existing method's runtime, parallelizability, new solution discovery efficiency, and spatial exploration in lower dimensional ($N \leqslant 100$) spaces, as well as spatial exploration for all methods in a three-zone, 8760 h capacity expansion model case. To measure convex hull volume expansion, this paper formalizes a computationally tractable high-dimensional volume estimation algorithm. We find random vector provides the broadest exploration of the near-optimal feasible region and variable Min/Max provides the most extreme results, while the two tie on computational speed. The new Combination method provides an advantageous mix of the two. Additional analysis is provided on MGA variable selection, in which we demonstrate MGA problems formulated over generation variables fail to retain cost-optimal dispatch and are thus not reflective of real operations of equivalent hypothetical capacity choices. As such, we recommend future studies utilize a parallelized combined vector approach over the set of capacity variables for best results in computational speed and spatial exploration while retaining optimal dispatch.

1. Introduction

Capacity expansion models optimize the strategic and operational decisions of the electricity system subject to technical, economic, and policy constraints to simulate the likely effects of novel technologies, investments, and policy interventions (Victoria *et al* 2020, Ricks *et al* 2022, van Ouwerkerk *et al* 2022). They are typically formulated as large-scale linear or mixed-integer linear programming problems with the explicit objective of minimizing cost (Cho *et al* 2022). And yet, real-world decisions are almost never made entirely on a least-cost basis. Nuanced objectives such as political feasibility, popularity, or energy security concerns inform decision-making, distributional outcomes shape stakeholder engagement in decision-making processes, and messy political processes mean optimality is never achieved regardless of objective choice (Trutnevyte 2016). Yet these multiple objectives and suboptimal or near-optimal real-world outcomes are typically omitted from explicit consideration in planning models.

Modelling to generate alternatives (MGA), a family of multi-objective optimization (MOO) techniques originally introduced by Brill (1979) and first applied to the energy systems modelling by DeCarolis *et al* (2011) and Trutnevyte *et al* (2011), (2012a), (2012b), offers a potential solution to three key limitations of current energy system models: structural uncertainty[4], non-modelled objectives/constraints, and the real-world never reaching true optimality. MGA assumes the option space of real-world decisions is contained by the technical requirements of the system along with a budget, defined as the maximum acceptable system cost (Trutenvyte *et al* 2012a). The methodology then aims to map the constrained feasible space, to give decision-makers a sense of the range of feasible, affordable options available. MGA distinguishes itself from traditional MOO in two ways. First, cost is explicitly constrained to a budget. Second, the objective set chosen is designed to approximate the shape of the near-optimal feasible space, rather than the Pareto frontier between pre-specified objectives (Guntara 2018). Given its potential utility, various algorithmic approaches to MGA have been applied to a variety of energy systems planning problems. Table 1 presents a listing of 17 papers that apply MGA in energy systems contexts. Please note that several papers that reference MGA, including Chen *et al* (2022), Prina *et al* (2023), Fioriti *et al* (2022), Dubois *et al* (2023) and Ihlemann *et al* (2022) have been excluded as they solely utilize MOO-type algorithms that seek to find Pareto fronts between explicitly defined alternative objectives rather than seeking to explore a budget constrained space (Gunantara 2018). Others, like Dubois (2023) and Fais *et al* (2016), appeared in the search but were not accessible to extract details about their implementation.

As table 1 illustrates, there has been a recent proliferation of different MGA algorithms applied to macro-energy system models. Yet prior to this work, there has been only minimal comparative testing of the performance of major MGA methods. This paper fills that gap by conducting the first systematic evaluation of four prevalent MGA methods, documenting the results, and providing usable recommendations for best practices when applying MGA methodologies to macro-energy system model applications.

We identified two prior comparative explorations of MGA method efficacy: Makowski *et al*'s paper on MGA algorithms in land use (2000), and Lombardi *et al*'s paper on computational trade-offs in MGA (Lombardi *et al* 2023). Both leave significant gaps in the literature addressed by this work. The Makowski *et al* study is applied to a small model with no exploration of dimensional scaling and each method is limited to finding 15–22 solutions, too few for modern applications. Lombardi *et al* (2023) apply a series of MGA methods to a contemporary macro-energy system model and generate 210 alternatives for each method. However, Lombardi *et al* (2023) do not test a variety of methods, particularly MAA and a parallelized random vector implementation, but rather a limited set of other weighting methods constructed for SPORES, a method combining variable Min/Max and HSJ. Furthermore, Lombardi *et al* (2023) provide only a few metrics on spatial exploration and do not analyse dimensional scaling and runtime. The limited evaluation of MGA methodologies in the macro-energy system context thus leaves significant uncertainty in the literature as to the performance of each method, including the portion of the near-optimal feasible space each method captures in large models and the computational scaling performance of each method.

This paper addresses this gap in the literature by quantitatively evaluating the procedure and performance of four families of MGA algorithms: (1) the Hop-Skip-Jump (HSJ) method first proposed by Chang *et al* (1983) and applied to macro-energy systems models by DeCarolis (2011); (2) Variable Max/Min first used by Trutnevyte *et al* (2012a); (3) random vector methods created by Berntsen and Trutnevyte (2017); and (4) Modelling All Alternatives (MAA) first described by Pedersen *et al* (2021b). The SPORES method is not examined here as it is a weighted combination of HSJ and variable Min/Max and, in our testing, behaved similarly to a parallelizable version of HSJ (Lombardi *et al* 2020). We provide a more in-depth discussion and testing results of SPORES in the SI. Efficient Random Generation is a specific class of random vectors, but only specifies random weights for a subset of capacity variables in each run, leaving the others weighted at 0 (Sasse and Trutnevyte 2023a). Thus, it should be relatively well represented by the random vector implementation included here. Sasse and Trutnevyte (2023a) combined MOO with MGA; we will focus on their MGA implementation here, which is well represented by random vector. Falcione (2022) applied a unique version of MOO which varies the weights of each variable in the specified objectives. As this is a variant with explicitly stated objectives, it is not considered here. Finally, the Distance algorithm is not included here due to the combination of its purely sequential nature and high computational intensity, as it requires the computation of Manhattan distance between each pair of points in the polyhedron. Furthermore, distance type methods have only been used in one paper that we found (Price and Keppo 2017).

We additionally address a gap in discussion of MGA variable choice. As demonstrated in table 1, there is no consensus on the impact of which decision variables are chosen to include in MGA objective functions (thus forming the exploration space). In capacity expansion modelling there are two primary options.

[4] Structural uncertainties involve uncertainty in the construction of the model itself. Models cannot fully represent the real world, and thus inherently make simplifying assumptions. While expert opinion, model validation, and inter-model comparisons can strengthen confidence surrounding the accuracy of modelled scenarios, structural uncertainty will always remain as to the true level of representativeness present in any given model.

Table 1. Energy system model MGA papers, applied methods, and applications.

Authors	Year	Method	Application	Zones	Variables explored	Time horizon
DeCarolis	(2011)	HSJ	Carbon mitigation	1	All variables	2050 wedge analysis
Trutnevyte *et al*	(2011)	Convex hull scenario generation	Small community case Study	1	All variables	2010–2035
Trutnevyte *et al*	(2012a)	Convex hull scenario generation	Small community case study	1	All variables	2010–2035
Trutnevyte *et al*	(2012b)	Variable Max	Small community case study	20, no links	Generation variables	Not specified
Trutnevyte	(2013)	Variable Max	Small community case study	20, no links	Generation variables	Not specified
Trutnevyte	(2014)	Variable Max	Small community case study	20, no links	Generation variables	Not specified
DeCarolis *et al*	(2016)	HSJ	Proof of concept	1	All variables	5 year blocks, 2015–2050
Li and Trutnevyte	(2017)	Variable Max	UK electricity sector transition	1	Capacity and generation decisions	2010–2050
Trutnevyte	(2016)	Variable Max	UK electricity sector backcasting	1	Capacity and generation decisions	1990–2014 with 5 year time steps
Berntsen and Trutnevyte	(2017)	Random vector	Energy supply scenario diversity	1	All variables	2035 and 2050
Price and Keppo	(2017)	Distance	Uncertainty exploration	16	Total energy variables	2005–2050 at 5 year intervals
Sasse and Trutnevyte	(2019)	Random vector	Distributional tradeoffs in renewables	2258, no links	Generation variables	2035
Nacken *et al*	(2019)	Variable Min/Max	Renewable energy system exploration	4	Capacity variables	2050
Jing *et al*	(2019)	HSJ and multi-objective optimization with epsilon constraints	Urban energy systems	9 buildings	Capacity and generation decisions	Not specified
Neumann and Brown	(2021)	Variable Max/Min	Energy supply scenario diversity	100	Capacity and generation variables	2018
Eshraghi	(2020)	Random vector	US energy system under uncertainty	1	Generation variables	2020–2050
Kumar	(2020)	Weighted multi-objective	Decarbonization planning	3	Generation variables	2013–2050
Lombardi *et al*	(2020)	SPORES	Renewables siting policy	6	Capacity variables	2050
Sasse and Trutnevyte	(2020)	Random vector	Energy system transition distribution in Europe	650 MGA nodes aggregated to 100 for analysis	Capacity variables	2035
Andre *et al*	(2021)	HSJ	Energy system in Belgium	1	All variables	2035
Moultak *et al*	(2021)	Variable Min/Max	Investment analysis	2	Capacity variables	2030–2060
Pedersen *et al*	(2021a)	MAA	Renewables siting, land use, equity, emissions	30	Aggregated capacity variables	2030
Pedersen *et al*	(2021b)	MAA	Renewables siting, land use, equity, emissions	30	Aggregated capacity variables	2030
Afolabi *et al*	(2022)	HSJ	Blue hydrogen in net zero electricity generation	6	Capacity variables	2020–2060
Falcione	(2022)	Weighted multi-objective optimization	Land Use and emissions in Italy	1	Capacity and generation variables	2050

(Continued.)

Table 1. (Continued.)

Lombardi *et al*	(2023)	SPORES	Energy system capacity exploration and methodological comparison	97	Capacity variables	Not specified
Pickering *et al*	(2022)	SPORES	Net zero options in Europe	98	Capacity variables	2018–2050
Patankar *et al*	(2022)	Random vector	Land use and capacity decisions in American West	6	Generation variables	2045
Dubois and Ernst	(2023)	Random vector	Resolution impact on feasible spaces	100, 200, 400	Capacity variables	2030
Luo *et al*	(2023)	Variable Min/Max	Decarbonization and public health	22	Capacity variables	2021–2050
Millinger *et al*	(2023)	Variable Min/Max	Biomass usage for emissions targets	37	Capacity and generation variables	2020–2050
Neumann and Brown	(2023)	Variable Max/Min	Investment decisions given price uncertainty	37 down-scaled to 128 regions	Capacity variables	2050
Sasse and Trutnevyte	(2023a)	Variable Max/Min	Regional interdependency in Europe's electricity system transition	8	Capacity variables	2035
Sasse and Trutnevyte	(2023b)	Multi-objective optimization and random vector	Examining regional inequity in European energy transition	296 MGA nodes aggregated to 128 for analysis	Generation and capacity variables	2035
Grochowicz *et al*	(2023)	MAA w/ Chebyshev ball	Finding capacity layouts for robust solutions to multiple weather year data	37	Aggregated capacity variables	2030
Sinha *et al*	(2024)	HSJ	Diverse decarbonisation pathways	9	All variables	2020–2050
Shi	(2023)	Random vector	Transmission expansion analysis in US	64	Generation variables	2050
Pedersen *et al*	(2023)	MAA	55% Decarbonization Scenarios for european electricity sector	33	Aggregated capacity variables	2030
Van der Weerd *et al*	(2023)	SPORES	Technology targets in Net Zero energy systems	98	Capacity variables	2030, 2050
Van Greevenbroek *et al*	(2023)	MAA w/ Chebyshev ball	Regional and integrated energy system design tradeoffs	60	Aggregated capacity variables	2050
Andreasen *et al*	(2024)	MAA	North Sea energy island planning	7	Aggregated capacity variables	2030
Esser *et al*	(2024)	Variations of HSJ	University energy system planning	1	Capacity and generation variables	2030, 2045
Mayer *et al*	(2024)	SPORES	Economic impacts of net zero energy systems	35	Capacity variables	2030, 2050
Schwaeppe *et al*	(2024)	Variable Min/Max	MGA scenario shadow price evaluation	128	Investment variables	2024

Capacity variables, which relate to the investment, retirement and sizing of generation capacities in each model region, and generation variables, which relate to the operational decisions in each time step (e.g. hour) for each generator. They can be included separately or combined. We thus compare the impacts of MGA runs varying capacity variables and generation variables on dispatch decisions.

1.1. Review of methods

MGA encompasses a variety of methods designed to explore the near-optimal feasible space of a constrained optimization model (DeCarolis 2011, Trutnevyte *et al* 2011). In the case of least-cost objective functions, MGA maps the feasible set of outcomes with tolerable costs (as specified by a budget constraint), which allows modellers and stakeholders to subselect modelled outcomes that satisfy a range of alternative objectives, including non-modelled but quantifiable outcomes, while emphasizing the degree of flexibility available in solution topographies (Berntsen and Trutnevyte 2017).

MGA methods consist of three primary steps, which may be accomplished in any number of ways. Visualized in figure 1, the steps are:

1. Solve the original optimization problem with a primary objective (e.g. minimize cost);
2. Transform the current objective into a new slack constraint added to the original feasible region;

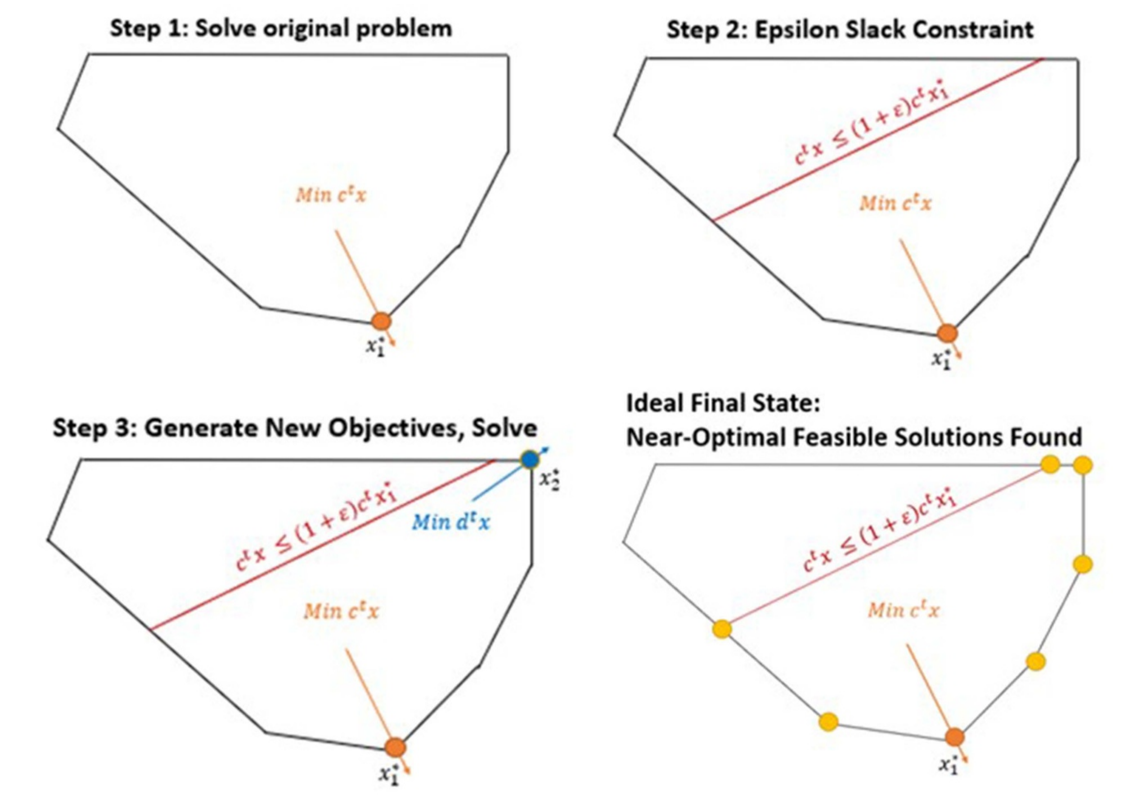

Figure 1. Modelling to generate alternatives procedure. Step 1: optimize for initial least-cost objective, step 2: impose epsilon-slack constraint, step 3: generate new objective weighting vector(s), here 'd', step 4: iterate until desired number of near-optimal feasible solutions found.

3. Generate a new objective and optimize to identify a new, near-optimal feasible solution within the budget slack constraint;
4. Repeat Step 3 many times to generate a range of candidate solutions until specified iterations are finished or convergence is reached.

The following sub-sections describe each of the four previously existing MGA algorithms assessed in this study.

1.1.1. HSJ

HSJ was formulated by Chang *et al* (1983) and applied to energy system models by DeCarolis (2011). HSJ is distinguished from other MGA methods by its objective formulation. Within this formulation the new objective is the minimization of the weighted sum of all decision variables with each weight determined by the number of solutions in which that variable has previously held a non-zero value (DeCarolis 2011). As such, each iteration aims to explore a vertex of the feasible space which contains as few previously relied upon decision variables as possible. While the HSJ method has been shown to successfully generate a diverse set of scenarios (DeCarolis 2011), HSJ inherently limits its exploratory power due to its restrictive objective formulation rules and its incompatibility with parallelization. By only including the minimization of positive weighted sums in its objective function and iteratively relying on results of prior solutions, HSJ tends to over explore the region of the space closest to the original objective, without deviating towards the rest of the polyhedron as noted by Eshraghi (2020). HSJ's strength is its focus on ensuring that it identifies edge cases that minimize each decision variable. By aiming to get only those solutions that expand edge cases for each optimization variable, it can begin to represent a fair breadth of the diversity of system configurations available while requiring relatively little raw computing power or sifting through a huge number of solutions, which can present challenges in cleaning and communicating findings.

1.1.2. Variable Min/Max

Variable Min/Max describes a family of MGA methods which rely on maximizing and minimizing a set of randomly or intentionally selected variables in each MGA iteration which was first introduced by Trutnevyte *et al* (2012a). Algorithmically speaking, when a set of MGA variables is presented, variable Min/Max assigns subsets of variables weights chosen from the set of integers $[1, 0, -1]$, indicating that that subset of variables should be minimized, maximized, or allowed to flex to accommodate other variables' optimization (Nacken *et al* 2019). Like the random vector methodology, variable Min/Max performs well on large problems due to its parallelizability and computationally inexpensive objective creation procedure. However, it exhibits the opposite characteristics as random vector with regards to dimensional inclusion and extreme points along axes: where random vector could explore all dimensions in relatively few iterations but fail to capture the most extreme points for specific variables, variable Min/Max tends to capture very extreme points for the variables included in each objective statement but will miss exploring dimensions that are not explicitly maximized or minimized in one or another objective statement. This problem can be blunted by ensuring all variables appear in at least one objective with a weight of 1 or -1. However, when many variables are maximized or minimized in the same objective, they typically pull against one another, resulting in less extreme values being found for each individual variable.

1.1.3. Random vector

Where the preceding two methods base their new optimization directions on the results of previous iterations, random vector MGA takes a different approach focused on generating the most diverse set of optimization vectors possible, ideally evenly sampling all regions of the *n*-dimensional polyhedron through the generation of a large quantity of random vectors corresponding to the number of iterations desired (Berntsen and Trutnevyte 2017). Random vector has three core strengths. First, it is computationally simple yet samples all directions, resulting in consistent exploration. Second, it is infinitely parallelizable, as separate iterations can be implemented on all processors without coordination without fearing replication. Third, in our testing, it consistently varies all MGA variables, ensuring some degree of flexibility is captured in any given run. The primary weakness of random vector is that it rarely points down an axis, or in the space spanned by only a subset of axes. Thus, while it consistently performs well by all metrics, the random vector methodology can struggle to find the maximum and minimum possible feasible values for specific variables.

1.1.4. MAA

MAA, shortened here to MAA, is a methodology designed on the principle of outward expansion (Pedersen *et al* 2021b). The method works by first finding a polyhedron of at least three initial exterior points, computing its convex hull, finding the face-normal vectors of the half-spaces that make up that convex hull, imposing each of them as the objective function of a cloned LP and maximizing the slack-constrained LP in those directions (Pedersen *et al* 2021b). The process is then repeated with the new set of exterior points. When MAA can compute all of the face normal vectors quickly (i.e. for problems with low MGA dimensionality) the consistent expansion in relatively separate directions allows it to find new exterior points on nearly every optimization.

MAA has two major limitations. First, in our testing, as problems increase in size past roughly 10 dimensions and 20 constraints and the numbers of solutions in the convex hull grows greater than 20, the Qhull algorithm slows down drastically, often failing entirely (Barber *et al* 1996). The same problem is noted by Pedersen *et al* (2021b). It is possible to reduce the dimensionality of capacity expansion models for MAA (or other MGA algorithms) by focusing on identifying variation in a limited number of decision variables, such as through clustering generation types across regions or only including certain metrics, such as generation capacity or overall transmission buildout in the MGA calculation as done by Pedersen *et al* (2021b), Grochowicz *et al* (2023) and Andreasen *et al* (2024). However, such simplification may lose much of the detailed value that MGA results offer in the process. Second, methods that maximize in directions chosen by some variation of face-normal vectors generate vectors that point between previously found extrema, thus generating a greater density of vectors in already heavily searched directions. While MAA attempts to minimize this difficulty by discarding vectors within a certain angle of one another (Pedersen *et al* 2021b), the sheer number of solutions present in even a 10-dimensional problem means that unique face-normal vectors could be generated almost ad-nauseum and find new solutions that do not violate the angular constraint but also do not contribute significant volume.

The rest of this paper is structured as follows: In sections 2.1 and 2.2, we detail the methodological contributions of this study, specifically the introduction of a combined random vector and variable Min/Max MGA objective selection method, and a method for estimating high-dimensional convex hull volumes. Section 2.3 discusses the testing regime carried out in this study, covering runtime and spatial exploration analysis in small randomized models and a capacity expansion model, as well as testing to isolate the effect of MGA variable choice on dispatch decisions. Section 3 covers the results of our testing across all problem sizes and both structures. Section 4 provides a discussion of the results and their impact, with 4.1 specifically covering the importance of the metrics we chose while reflecting on other possible metrics, 4.2 covering implementation recommendations based on our results, and 4.3 discussing convergence criteria in MGA algorithms. Section 5 concludes the paper and provides suggestions for future work.

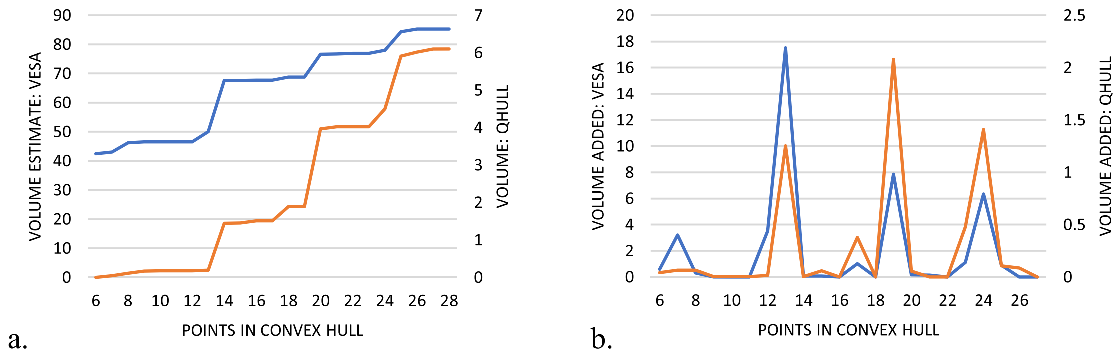

Figure 2. Results for comparative testing of QHull volume calculation (orange) and VESA volume estimate (blue) for 5-dimensional randomized convex hull. Points were added iteratively, with volume expanding with each point. (a). Convex hull volume estimate with each additional point calculated by each method, (b). Change in convex hull volume estimate with each additional point calculated by each method.

2. Methodology

We contribute two methodological innovations in this paper, a novel MGA vector selection methodology meant to hedge the strengths and weaknesses of variable Min/Max and random vector MGA, described in section 2.1, and a computationally tractable/scalable method for estimating the volume of high-dimensional convex hulls, described in section 2.2. Section 2.3 describes our testing regime, which includes runtime testing at small scales, volumetric testing at all scales, and testing on the set of MGA variables explored.

2.1. Combined variable Min/Max and random vector MGA

We introduce a new method that combines variable Min/Max and random vector MGA. The goal of the Combination (Combo) method is to complement the strengths of each method, providing both solid variable exploration from random vectors and solution extremity from variable Min/Max, as discussed in sections 1.1.3 and 1.1.4. As both methods pre-generate a list of vectors, then apply them to the set of MGA variables, they are highly compatible. The combined method proceeds identically to both variable Min/Max and random vector, except the generated set of MGA objective vectors, called *g* in the SI, includes both variable Min/Max vectors and random vectors, with the proportion of vectors utilizing each method adjustable. We used 75% variable Min/Max, 25% random vectors in this study.

2.2. Convex hull volume estimation

MGA work has largely avoided estimating the hypervolume it captures due to the computational difficulty involved. The only paper we identified in the macro-energy systems literature to do so is Pedersen *et al* (2021b), who use the QHull algorithm to provide volume calculations (Barber *et al* 1996). Unfortunately, due to the NP-hard computational complexity of evaluating high-dimensional convex hull volumes (Klimenko *et al* 2021), Pedersen *et al*'s (2021b) implementation is only practical if a small number (e.g. on the order of 10) decision variables or aggregated metrics are included in alternative MGA objective functions.

It is possible, however, to make similar volume metrics work for complex models, with a new procedure we have termed volume estimation by shadow addition, or VESA. We achieve this by first generating all combinatorial pairs of MGA variables. We then project all solutions onto each of these two-dimensional (2-D) subspaces and take the area of the resulting 2D convex hull of each pair, then sum them all to approximate the total volume. We use VESA in this work to estimate the volume of the convex hull each MGA algorithm generates.

It is important to note that VESA is intended to increase proportionately with the full convex hull, not precisely quantify the volume. To verify that VESA captures most volume additions, we generated a 5-dimensional randomized convex hull and found 28 points with random vector MGA using a slack of 100%. At each iteration, we evaluated the true volume using QHull and the VESA estimate of volume. The comparative results for the volume and the volume added with each iteration for both methods are shown in figure 2.

VESA is not a perfect estimation of volume and will not capture points that fall within the 'shadow' of the convex hull. An example of this case can be seen in figure 3. As demonstrated, however, the shadow is limited in volume and orientation. Thus, this error only occurs rarely with limited magnitude. Because this exception is small and infrequent, VESA is an appropriate metric to provide an ordinal ranking of volume exploration

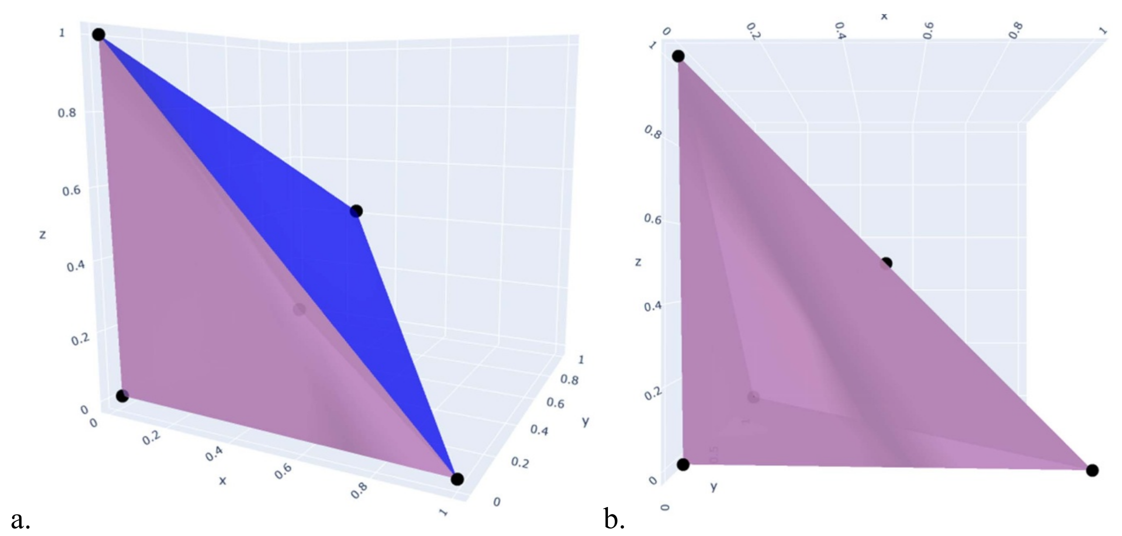

Figure 3. Example of a point addition to a three-dimensional shape that would not be captured by VESA. The initial shape is the pink tetrahedron formed by 4 points at (0,0,0), (1,0,0), (0,1,0), and (0,0,1). (a). A new point (0.5, 0.5, 0.5) is added which adds volume (shown in blue) to the convex hull. (b). VESA does not count any additional volume as all two-dimensional projections do not change in area. This case only occurs when a point is added within the blue region.

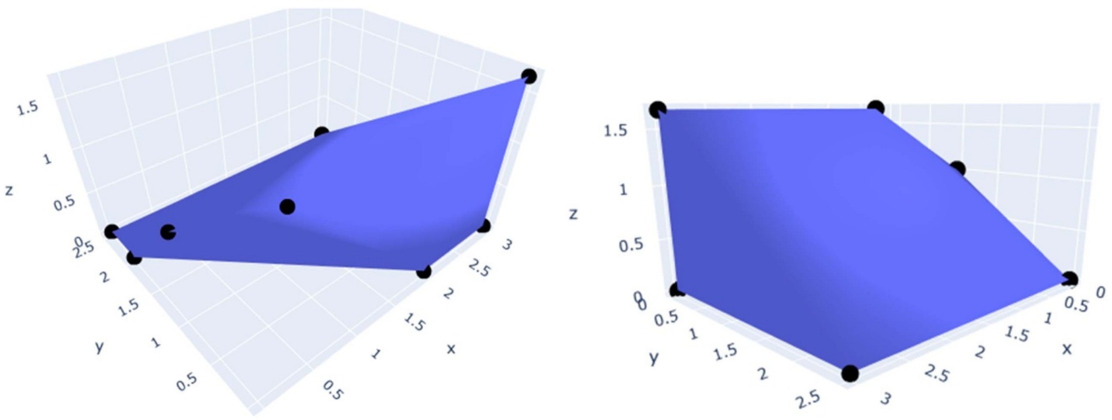

Figure 4. Three-dimensional test problem convex hull reference.

over many iterations by different algorithms (as used herein). It can also be employed as a convergence criterion to halt MGA algorithms once volume expansion with subsequent iterations becomes limited.

2.3. Testing regimes

To analyse the methods described in section 1.1, we utilized three different testbeds: a three-dimensional known, visualizable model, an N-dimensional randomized scalable LP generator, and a test scenario from the GenX electricity system model (Jenkins and Sepulveda 2017, Jenkins *et al* 2023).

The three-dimensional model, shown in equation (1), was designed and utilized to provide visual information as to the exploratory tendencies of each MGA method,

$$\begin{aligned}&\text{minimize } x_1 + 2x_2 + 2x_3\\ &\text{subject to : } x_1 + x_2 + x_3 \geqslant 2\\ &x_1 \leqslant 3\\ &2x_2 + 3x_3 \leqslant 5\\ &10 \geqslant x_1, x_2, x_3 \geqslant 0\end{aligned}\quad .$$

Equation 1. Initial 3-Dimensional LP.

As the three-dimensional space is small with relatively few vertices, we imposed a slack of 3, resulting in the shape visualized in figure 4. We used the Qhull algorithm to find the full convex hull of the

Table 2. Testing regime, all dimensions run 10x up until 100 dimensions, then 2x each.

System	Method	MGA dimensions	LP variables
Randomized LP MGA testbed	Hop-Skip-Jump	3, 5, 10, 20, 50, 100, 1000	3, 5, 10, 20, 50, 100
	Random	3, 5, 10, 20, 50, 100, 1000	3, 5, 10, 20, 50, 100
	Modelling All alternatives	3, 5, 10	3, 5, 10
	Variable Min/Max	3, 5, 10, 20, 50, 100, 1000	3, 5, 10, 20, 50, 100
GenX example System	Hop-Skip-Jump	18	∼1400 000
	Variable Min/Max	18	∼1400 000
	Random	18	∼1400 000
	Combo	18	∼1400 000

slack-constrained test problem for reference when verifying the implementation of each MGA method (Barber *et al* 1996).

While the three-dimensional test provides visual feedback as to how each method explores a space, it cannot provide adequate information about each method's performance in larger, higher-dimensional spaces akin to those important to MGA in energy modelling. To address this limitation, we developed an N-dimensional random LP generator with n variables and $2\,n$ constraints as shown in equation (2).

$$\begin{aligned} &\text{minimize} \sum_{j=1}^{n} c_j x_j \\ &\text{subject to} \sum_{j=1}^{n} A_{ij} x_j \geqslant b_i i = 1,\ldots,2n \\ &10 \geqslant x_j \geqslant 0, j = 1,\ldots,n \end{aligned}.$$

Equation 2. Random dimensional LP formulation.

We ran each MGA method on a series of random problems ranging from 3 to 1000 dimensions with a slack of 0.1 (10%). The full testing regime can be found in table 2. In addition to evaluating runtime and parallelizability, MGA methodologies are evaluated based upon how well they explore the near-optimal feasible space, defined as the area of the convex hull created by the original problem and cost constraint. Volume is estimated via VESA, as discussed in section 2.2.

To test spatial exploration in an electricity system model, trials were conducted within the GenX capacity expansion model, utilizing the three-zone ISONE example case in the GenX repository with 8760-hourly resolution for a single year (Jenkins *et al* 2023). All computation for this project was done on CPU nodes on the Della computer cluster at Princeton University. Please note that during the GenX testing, we selected a spatially aggregated version of the variable Min/Max algorithm as it tended to produce more extreme points, as discussed briefly in 1.1.2. Volume estimation is carried out through VESA for these problems as well.

Additionally comparative testing was carried out to demonstrate the difference between MGA using capacity variables and MGA using generation variables, typically formulated as annual sums of generation from each generator. We ran these tests on the same three-zone ISONE example case in GenX on the Della computer cluster at Princeton University. To isolate the impact on dispatch decisions of running MGA, we ran an initial MGA iteration on each variable set, then fixed the capacity decisions, changed the objective back to cost minimization, and re-optimized the model to compare least-cost operational results consistent with market-based economic dispatch (or social welfare maximizing system operations) and the results from MGA iterates.

3. Results

We evaluated each MGA algorithm for two primary characteristics: the speed at which the algorithm can be completed relative to problem scale, and the ability to approximate the convex hull of the full near-optimal feasible region of the problem. The following results indicate that the multithreaded random vector and variable Min/Max algorithms consistently perform the best on these criteria of all MGA methods for larger scale problems. Section 3.1 presents performance and spatial exploration findings in the small scale problems, while section 3.2 presents findings from the Capacity Expansion Model tests.

3.1. Small-scale problems

3.1.1. Computational performance: runtime

MGA subtypes are largely delineated based upon their respective objective vector creation methods with a wide variance in computational complexity between methods. To illustrate the differences, objective creation

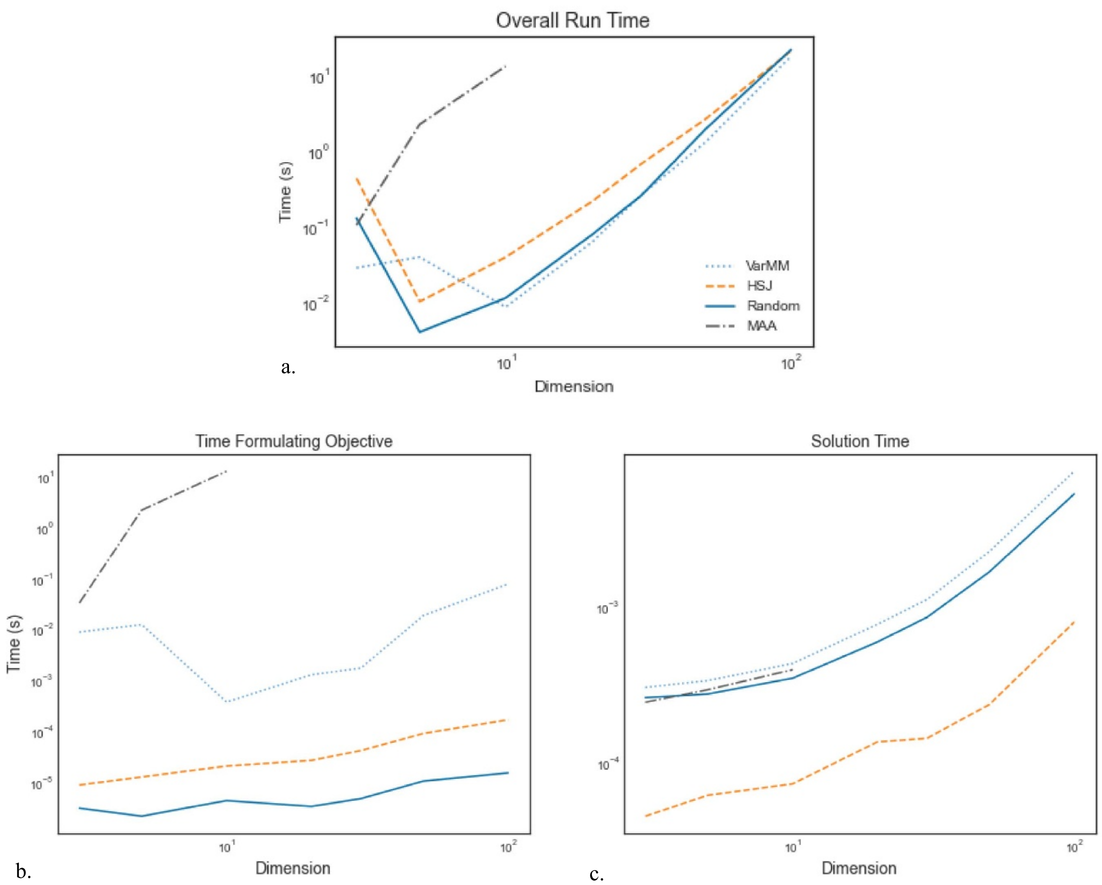

Figure 5. Key runtime metrics for variable Min/Max, HSJ, random vector, and MAA. Higher times indicate slower methodologies. (a). Average total runtime for one run of all MGA Methods in randomized testbed, including initialization, objective generation, solution times, and overhead. (b). Max objective formulation time for all MGA methods, (c). Average solution time for single iteration of all MGA methods in randomized testbed.

was timed for all methods using the Julia time_ns() implementation over the set of dimensions detailed in table 2. Each dimension and method ran 10 times, with MAA stopping at 10-dimensional problems, the maximum feasible dimensionality for QHull computations (Barber *et al* 1996, Pedersen *et al* 2021b). The 100-dimensional problems and 1000-dimensional problems were only run twice each due to runtime constraints. The results of this testing are presented in figure 5.

The results clearly divide MGA methods into two categories: those with complex, geometrically-based calculation for determining the next set of objective vectors, namely MAA, and those that rely on simple heuristics for the next set, HSJ, variable Min/Max, and the random vector method. Geometric methods tend to scale very poorly with dimension, due to the inability of convex hull algorithms to calculate high dimensional convex hulls, which is confirmed in this case by MAA devoting most of its runtime calculating objective vectors rather than solving the LPs in question. Considering the dimensional scale of electricity system models, only electricity system models which abstract away from the zonal structure typically used (e.g. those that consider only aggregate system-wide capacity outcomes), will be able to consider using MAA or similar methods. Including separate capacity decision variables for each zone within the MGA formulation, as seen in Lombardi *et al* (2023), is out of the question for these methods as it dramatically increases the dimensionality of the MGA space explored. This is usually desirable in macro energy applications, as two solutions with identical total buildout of a given resource will be disparate in other metrics if the distribution of those capacity changes is different (Lombardi *et al* 2023).

Among the simpler methods, variable Min/Max took more time to generate objective vector sets than HSJ and random vector as it often produces duplicate vectors which must be removed. In problems with many MGA dimensions, variable Min/Max requires a check to ensure that all variables of interest are maximized and minimized in one of the MGA iterations, otherwise those variables are frequently unexplored. In problems with few MGA dimensions, variable Min/Max requires checks for identical vectors since there are only three possible states for each weight, leading to higher likelihood of vector duplication. These additional checks take time and computational power relative to the HSJ and random vector methods.

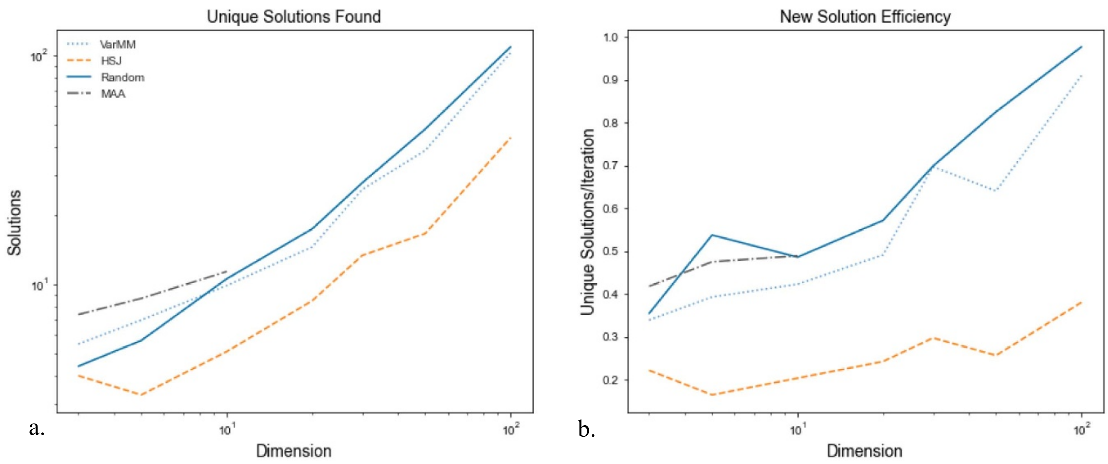

Figure 6. Unique solution exploration performance in N-dimensional random problem a. Average total number of unique solutions found by each method for a set number of iterations with increasing dimensions b. Average rate at which each method found unique solutions per optimization with increasing dimensions.

However, testing indicates that the computational time required for the variable Min–Max method to perform this check is relatively minor.

HSJ rivalled the multithreaded random vector and variable Min/Max methods in terms of runtime despite the latter group's ability to run eight models in parallel. Their convergence in times is largely due to the higher solve time the random vector and variable Min/Max methods experience with every iteration relative to HSJ. This difference can be attributed directly to the angular vector spread of the latter processes. By selecting points that lie on disparate sides of the polyhedron and rarely sampling similar directions sequentially, the random vector and variable Min/Max processes cannot readily warm start using previous iterations of the optimization solver as effectively as the less exploratory HSJ, resulting in longer solve times. When multithreaded, this issue is exacerbated, as each thread requires a separate instance of the model and solver, meaning that sequential warm starts cannot be carried over from run to run. However, as can be seen from the overall time graph, the speed gains associated with multithreading are enough to more than compensate for this issue and bring temporal performance comparable to HSJ to the random vector and variable Min/Max methods.

3.1.2. Spatial performance: unique solution set size and quality

MGA algorithm spatial performance is largely determined by two distinct metrics: (1) new solution efficiency, or the rate at which a new iteration of the model solution stage can be expected to find a unique solution; and (2) approximate convex hull volume, or an estimate of the extent to which the algorithm explores the near-optimal feasible region of the problem. Both metrics are used to estimate the performance of each method in the N-dimensional randomized LP testing up to 100 dimensions. Please note that the value of new solution efficiency decreases as the dimensionality and size of the space increases due to the exponential increase in the number of unique vertices present in the shape—several vectors separated by a hundredth of a radian may find unique solutions even though they may not contribute any significant additional volume to the convex hull. Accordingly, MGA runs on the larger-scale GenX test system are only evaluated by approximate convex hull volume (via VESA), rather than unique solutions produced.

The spatial results of the Randomized LP testing program, detailed in table 1, are reported in figures 6–8. Figure 6 relates both the total number of unique solutions each method was able to find in a set number of iterations and the efficiency with which each algorithm successfully found unique solutions (new solution efficiency). Figure 7 shows the portions of the 3-dimensional test convex hull discovered by each of the four methodologies discussed in this paper. Figure 8 illustrates the estimated convex hull volume found by each method for a given problem in 10, 100, and 1000 dimensions respectively.

Within smaller problems, where all methods were usable, MAA, variable Min/Max, and random vector consistently averaged more unique solutions identified and greater new solution efficiency than HSJ. MAA and random vector consistently had the highest new solution efficiency, likely due to the relatively precise geometric sampling method of finding face-normal vectors for MAA and the uniformity of sampling in random vector. Variable Min/Max also performed well but, for small problems, it was not quite as efficient as random vector and MAA. This is attributable to its tendency to search in lower variable subspaces, such as the x-y, y-z, or x-z plane in a 3-dimensional problem, which can risk missing points in which larger numbers

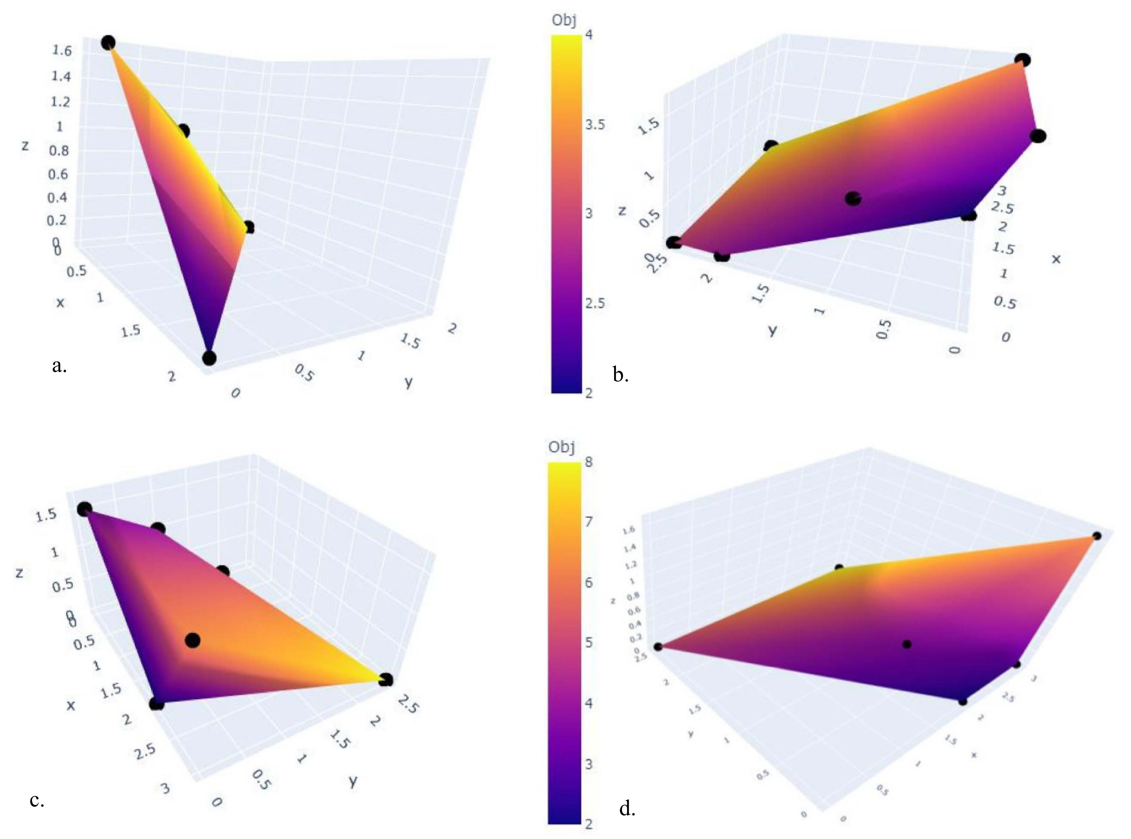

Figure 7. 3-dimensional example LP convex hulls found by each MGA method, illustrative of the characteristics of each methoda. Hop-skip-jump struggles to find much of the space, (b). Modelling all alternatives consistently finds all points in small spaces, (c). Randomized vector finds most points, but struggles with extreme points, (d). Variable Min/Max finds all extreme points but struggles to find ones between axes.

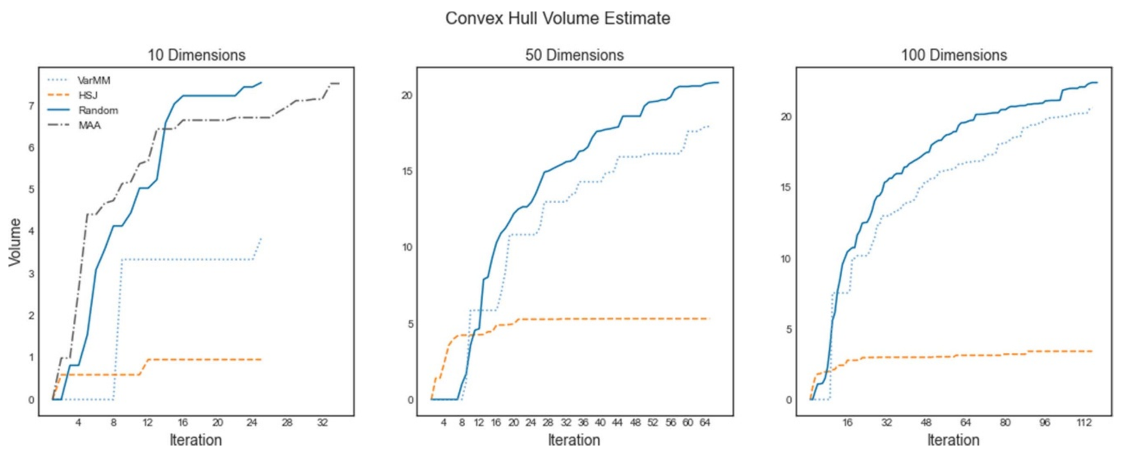

Figure 8. *N*-dimensional randomized LP convex hull volume estimates for an example run of each MGA method on the same randomized LP. Higher volumes are indicative of greater exploratory power. MAA is not included in the 50- and 100-dimension plots due to its dimensional limitations.

of dimensions are non-zero, a problem that is less noticable, though still existent, in larger dimensional problems.

Random vector and variable Min/Max methods regularly perform the best on spatial metrics, retrieving the greatest number of unique solutions with the greatest efficiency for test problems with dimensions between 10 and 100, the range in which MAA has become computationally intractable and the scale of the space has not grown to the size where functionally any angular change results in a new solution. Heuristic-type methods like random vector and variable Min/Max are not as consistent as MAA at finding new points in smaller spaces of dimension 10 or less due to the relatively large angular sweeps associated with each unique solution, which tend to reward geometrically-derived vectors rather than the random or semi-random sampling associated with the heuristic-type methods. Despite not being as efficent as MAA in small environments, random vector and variable Min/Max do perform more than adequately in these smaller environments, consistently outperforming HSJ.

While the random vector methods does uniformly and efficiently explore the space, which works well for randomly selected polytopes, the engineered world tends to design solutions to be present along certain axes, and we tend to care more about solutions that reside along certain axes or metrics: i.e. lowest carbon emissions, lowest cost, greatest renewable energy share, or least transmission expansion, etc. As it is completely randomized, the random vector method does not typically capture these extremes; even in a 3-dimensional space, for instance, the random generation of a [1, 0, 0] search vector is relatively unlikely. This notable weakness of the random vector method is clearly illustrated in figure 7, where the random vector method fails to capture the (3, 0, 0) point that MAA successfully captures. Conversely, variable Min/Max is designed to explore these 'down-axis' points extremely well, as it can only explore axes or lower-variable spaces, providing essentially the other side of the coin of random vector. This propensity is demonstrated in figure 7 as well, as variable Min/Max specifically captures all points that are down an axis or directly between two axes, but misses points that do not optimize an axis or sum of axes, like (0, 2, 0), which is obscured by (0, 2.5, 0) to the [0, 1, 0] search vector, or (0.33, 0, 1.66). As discussed in section 2.1 of this paper, these relative weaknesses of the random vector and variable Min/Max methods can be remedied by combining the two, resulting in a Combo method combining the variable-including robustness of the random vector iterations, with a set of variable Min/Maxing 'bracketing runs' which serve to find extreme points by following objectives aligned with certain axes or outcomes of interest that may not otherwise be optimized by the random vector algorithm.

We also consider spatial success for MGA methods in terms of their ability to identify solutions that describe a larger volume of the total near-optimal feasible region, shown in figure 8.

In cases with 10 or fewer dimensions, MAA and random vector tend to converge to the same general volume estimation at roughly the same rate, indicating that they have discovered most of the space. Variable Min/Max tends to struggle in smaller spaces due to its difficulty finding off-axis or off-plane points, resulting in substantial volume missed. However, it is still much better than HSJ, which does not perform well in volumetric terms in either these small dimensions or larger dimensions. MAA does tend to require many iterations to catch undersampled portions of the space, discussed further in the SI.

In higher dimensional cases, MGA method options are limited to random vector, variable Min/Max, and HSJ due to MAA's computational constraints. HSJ continues to struggle volumetrically in these larger problems, with its performance worsening especially in larger trials. In the 100-dimensional case trials, HSJ consistently failed to generate any meaningful volumes over 115 iterations. This is largely due to HSJ's inability to generate a broad diversity of objective vectors, tending to find solutions in the same general area of the polytope, as illustrated in figure 7 and discussed in section 1.1.1. By comparison, the volume found by the random vector and variable Min/Max algorithms typically require just 10 iterations or less to reach the maximum volume identified by HSJ, and these algorithms continued to increase the volume explored in subsequent iterations.

Random vector and variable Min/Max, on the other hand, tend to perform best in higher dimensional problems. While it always performs relatively well regardless of dimensionality, higher dimensional problems play to two of the strengths of these algorithms as they require more iterations and have a lower likelihood of coincident solutions. As the random vector algorithm functionally generates angularly uniformly distributed vectors, having a larger number of samples ensures a uniform distribution, while any angular perturbance will result in an entirely separate solution due to the sheer number of possible solutions present. In higher dimensional spaces, variable Min/Max typically generates a sufficiently large number of semi-random axis combination vectors that it also explores the space fairly well.

3.2. GenX three-zone ISO new england test system

While the previous testing has demonstrated clear differences in performance between MGA methods when applied to a randomly selected LP with standard structure, we have not yet demonstrated that similar findings hold when applied to case studies more typical of electricity system planning. Regardless of their specific parameters, linear capacity expansion models have a particular structure that is not at all spherical, as consistent constraints representing real-world phenomena make decision variables take values over several orders of magnitude. For instance, the energy transferred between two zones in a low hour may be on the order of a few MWhs, but the capacity of a nuclear power plant may be in the GWs, a difference of 5 orders of magnitude when represented in the model. When combined with relatively similar implementations across linear models for certain engineering requirements, like conservation of energy or estimation of transmission expansion cost, the overall structure of these models is often quite similar, resulting in relatively similarly shaped near-optimal feasible spaces, even if the specifics are different (Henry *et al* 2021). This section aims to test the consistency of our findings for typical electricity system capacity expansion problems, namely that the random vector and variable Min/Max methods outperform HSJ on larger problems, as well as to demonstrate the theorized strengths of the Combo method illustrated in section 2.1. We performed a series of test runs with random vector, variable Min/Max, Combo, and HSJ MGA in a well-documented Three Zone ISO New England test problem built into the repository of the open-source GenX electricity system model (Jenkins *et al* 2023). Note that as MAA is computationally constrained to only very low dimensional MGA implementations, it was not included in this set of tests.

3.2.1. Spatial exploration in capacity expansion models

The findings from this set of tests are presented in figures 9 and 10. Figure 9 illustrates, in real capacity, cost, and emissions terms, the difference in near-least-cost feasible space captured by four methods tested. Each subplot within the figure shows a specific pairwise tradeoff-space of feasible options, meant to demonstrate the level of flexibility and tradeoffs inherent between two resource types within a 10% budget slack. As the goal of MGA is to provide the best possible exploration of the near-optimal feasible space, the more area captured by a given method in each graph, the better it has performed, as more options and tradeoff relationships would be demonstrable to decisionmakers. Both consistency, as measured by finding volumes in all pairwise dimensions, and volume discovered are important in this context. Figure 10 collapses all these insights into one convex hull volume estimate using VESA.

In all tradeoff-spaces visualized in figure 8, random vector, variable Min/Max, and Combo significantly outperformed HSJ. Random vector shows great consistency across dimensions and trials, finding decent volume in all dimensions across all runs due to its inclusion of all MGA variables in each objective vector. Variable Min/Max regularly finds the most extreme points for the variables included in its objective statements but can miss out on variables that are not specifically included, like transmission as shown in the transmission/natural gas panel (7th row, 2nd column). Combo shows the desired characteristics of both methods, with improved consistency for variables not specifically included in objective vectors relative to variable Min/Max and improved extremity and diversity of points identified relative to random vector. The difference in how each methodology treats technologies not specifically included in the MGA procedure can be visualized by examining the subplots that include transmission. Transmission capacity expansion was intentionally not included in the set of MGA variables here but is obviously an important outcome of interest. Notably, while random vector and Combo capture significant range in the transmission capacity dimension, variable Min/Max fails entirely. As the MGA dimension increases in applied studies, this will be true of more and more dimensions or outcomes of interest not explicitly considered in the MGA objective function, with variable Min/Max thus missing important flexibility due to its hyper-focused nature. The random vector and Combo methodologies importantly mitigate this failing, albeit at the cost of some extremity of points explored as demonstrated in figure 10.

We do see new behaviour relative to the randomized LP testing emerge in the electricity system model context. Variable Min/Max, which had underperformed relative to random vector in volume metrics in the randomized LP testing, captures significantly more volume than the random vector method, as shown in figure 10. Random vector still performs better than HSJ, but its low volume relative to variable Min/Max does highlight how the specific optimization of limited technology combos results in more extreme points. The Combo method, as noted earlier, does explore more volume than random vector (though less than Min/Max), while preserving its consistency in dimensional exploration.

3.2.2. MGA variable choice and cost-optimal dispatch

Comparative testing of including capacity versus generation variables in MGA objective functions revealed that while least-cost dispatch is typically enforced by optimizing MGA objective functions over capacity variables, the same is not true of generation variables. When generation variables are explicitly included in the MGA objective function, these variables will be assigned alternative coefficients unrelated to the actual cost of generation. As a result, the optimizer will produce dispatch results that are not consistent with least-cost economic dispatch principles, resulting in unrealistic outcomes and unrealistic expectations for the performance of the proposed system in real operations. An example of this issue is demonstrated in figure 11. To our knowledge, this shortcoming of generation-based MGA has not been noted in previous literature.

In contrast, MGA using only capacity related decision variables in the objective function typically maintains cost-optimal dispatch due to the combination of two factors. First, it does not explicitly change operational objective coefficients, which would immediately change dispatch, as demonstrated for generation variables. Second, MGA objectives over capacity decisions typically result in solutions where the budget constraint is binding due to MGA weight vectors generally being sufficiently different in angle from the least-cost vector. When MGA objectives with capacity variables are tight to the budget, they minimize

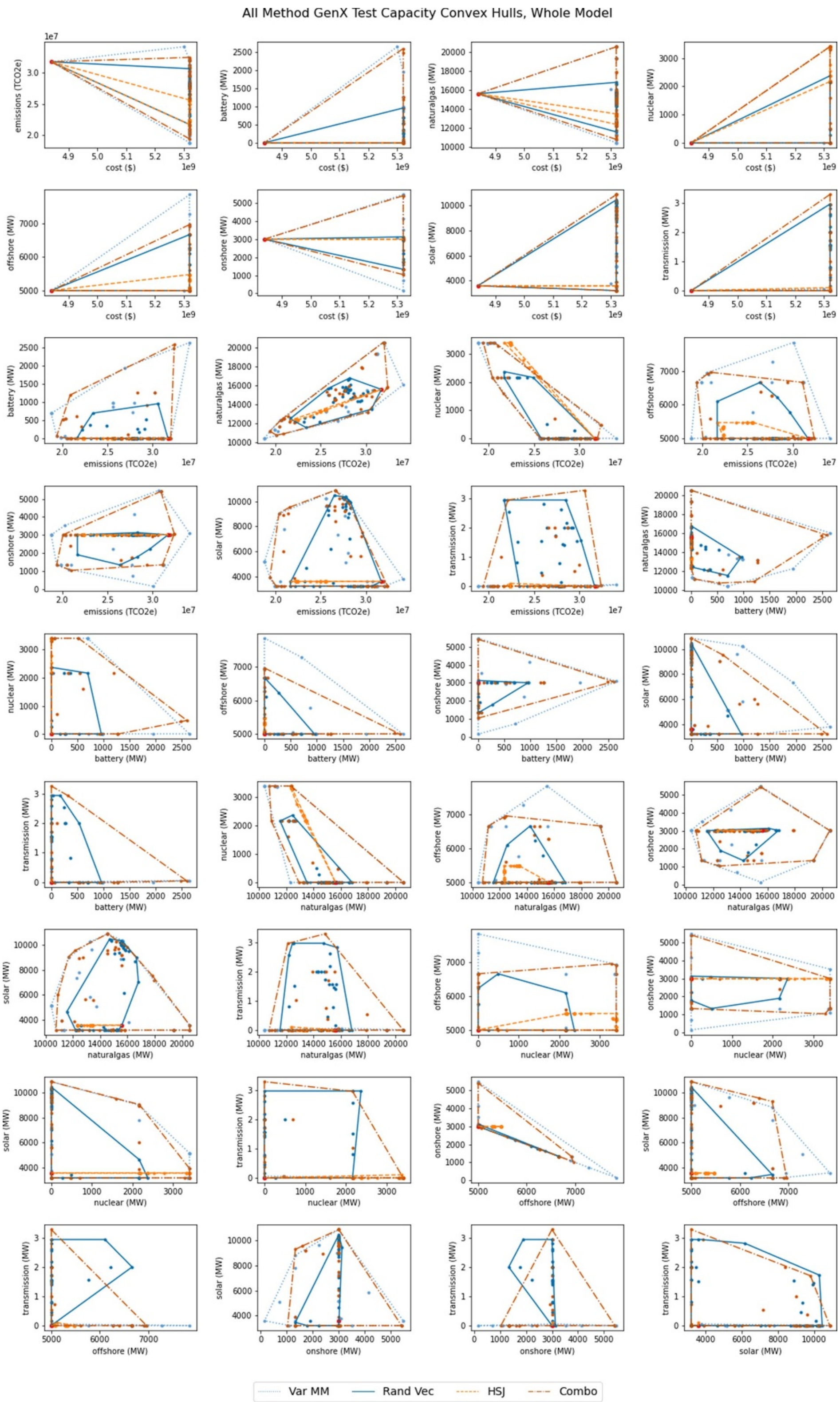

Figure 9. Comparison of pairwise convex hulls of capacity groupings by technology, cost, and emissions outcomes for the GenX ISONE three zone test system captured by all MGA methods with a 10% budget slack. Optimal solution in red. Greater area in each panel is desirable, as is capturing diversity in all metrics.

operational cost, as encoded in the budget constraint, to enable larger variation in capacity variables, and thus capacity-related objective costs. In theory, it is possible for MGA run on capacity variables to not maintain cost-optimal dispatch if the objective does not produce an optimal capacity mix where the budget constraint is binding. However, the MGA objective weight vector of such a run would need nearly identical weight proportions on capacity as the original least-cost solution, which is highly unlikely given MGA

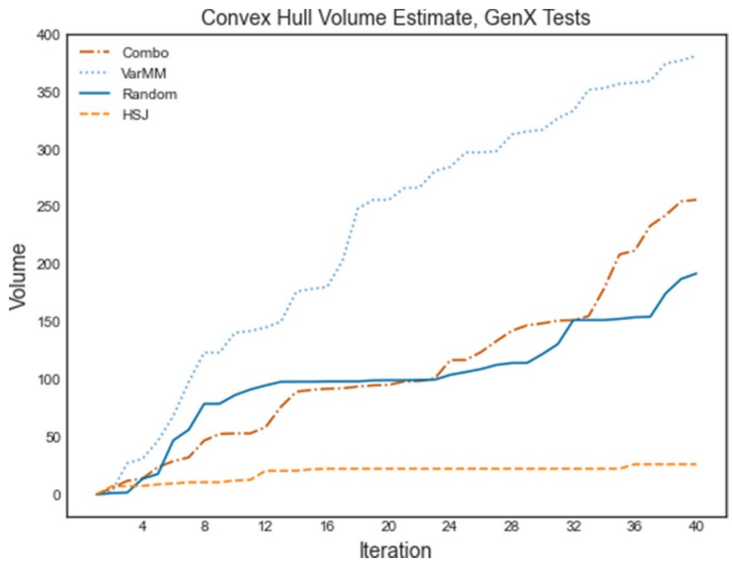

Figure 10. Comparison of the convex hull volume estimate created through VESA for each MGA method on the GenX ISONE three zone test system at every MGA iteration. Greater volume is better.

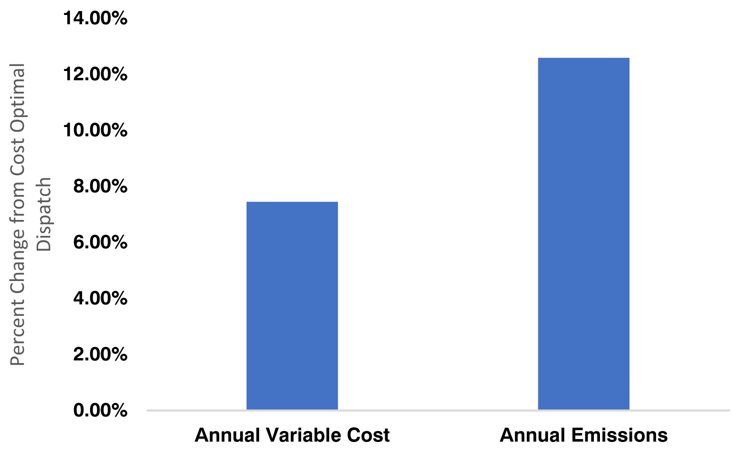

Figure 11. Example percent error from cost-optimal dispatch with fixed capacities in annual variable cost and annual emissions for MGA run using annual generation variables in GenX three-zone ISONE test system. MGA using capacity variables matches cost-optimal dispatch.

objective vector selection. Accordingly, we have not observed this occurrence for any MGA-type objective vectors in practice. In an example test run of 40 solutions with random vector, with the binding status of the budget recorded, all iterates were tight to the budget.

4. Discussion

The discussion is structured as follows: section 4.1 discusses our choice of metrics, section 4.2 highlights the implications of our findings on suggested usage of MGA, and section 4.3 discusses the topic of convergence metrics in MGA algorithms.

4.1. On metric choice

We chose to focus on computational performance and spatial exploration in this paper. Computational performance and parallelizability is vital because it allows for the compilation of more solutions, which results in greater volume. Spatial exploration, in turn, is vital for accurate policy support. Consider, for instance, the tradeoff plot between solar PV and offshore wind generation capacity in figure 8. With HSJ, any decision-maker provided this modelling would conclude that while offshore wind has some capacity flexibility (as it can be built out to 5000–5500 MW), the system seems to *require* 3500 MW of solar PV capacity. However, with the improved visibility provided by, for instance, the Combo method, we can see that such a conclusion would be badly misinformed: there remains, in fact, substantial flexibility in both offshore wind capacity development and solar buildout within the 10% budget slack, with offshore wind capacities ranging from roughly 5000–7000 MW and solar capacities from about 3200 to 11 000 MW, with combinations of capacities with high offshore wind and high solar or low offshore wind and low solar simultaneously achievable within the near-optimal feasible space. The volume captured by more spatially exploratory methods thus translates to increased visibility of real options.

This paper's findings are directly contingent on the choice of indicators. While spatial exploration and computational runtime are important indicators of the success of an MGA method, we recognize these are not the exclusive metrics of success. Specifically, the generation of interior solutions can be desirable to represent the messiness of real-world politics (Trutnevyte 2016). On this metric, methods that may not perform as well in this paper may shine, like MAA which includes an interior sampling methodology as a second step. Further analysis could be carried out in the future on comparative testing of other metrics of success in MGA.

4.2. Implications on suggested usage

4.2.1. Method selection and tradeoffs

These findings carry several major implications for future MGA analyses. First and foremost, the random vector and variable Min/Max methods are superior to other MGA methods from both a runtime and spatial perspective, and they can be easily combined to access both of their relative benefits (as in the Combo method presented in section 2.1). Between their computational ease, simplicity of implementation, and parallelizability, these methods offer the lowest additional computational and coding burden of any of the MGA methods examined here. Random vector, variable Min/Max, or Combo should work similarly well for any linear capacity expansion model and could easily be extended to mixed integer problems with no modification, albeit while incurring significantly longer solution time per iteration required to solve a MILP. Additionally, due to the low computational difficulty associated with calculating its objective vectors, the dimensionality of the MGA space can increase almost arbitrarily. However, more variables would mean more iterations for the VESA metric for spatial exploration to converge to a consistent value, due to the increased number of vertices in high dimensional spaces.

Random vector and variable Min/Max performed well in all tests carried out for this study but can be parallelized further with the delegation of more computational resources. Increasing the quantity of iterates calculated will further improve the solution sets discovered by each of these two methods. As random vector is random, any parallel set of runs can be superimposed to discover new solutions, unlike deterministic methods like HSJ. Thus, in the same wall-clock runtime, the number of solutions that random vector could discover is theoretically limited only by access to computational resources. In low-dimensional problems, the same is not true of variable Min/Max. Due to the limited number of possible states for each MGA variable, the combinatoric likelihood that an objective vector is repeated across parallel processes increases as the number of iterates increases and the number of MGA variables decreases, making it important to check for duplicate vectors when superimposing multiple sets of separately generated variable Min/Max objectives or solutions to avoid wasting computational resources.

MGA algorithms can be complemented with the idea of 'bracketing runs', a preset list of objective functions like those used in MOO determined to be of particular interest to the research question or to intended audiences including, for example, maximum solar capacity, minimum transmission capacity, or lowest carbon emissions.

Modelling All Alternatives showed some promise in spatial metrics on the small problems for which it can successfully compute objective sets. As such, it could be used in models with very few MGA dimensions. However, MAA's dimensional limitations are not trivial, and do meaningfully restrict its utility.

Generally, HSJ should not be used for capacity expansion models. For HSJ, its lack of exploratory power makes generating useful and generalizable takeaways from identified solutions difficult if not impossible, and the prospects for increasing the method's exploratory power seem limited due to its lack of parallelizability.

4.2.2. MGA variable choice and cost-optimal dispatch

The findings presented in section 3.2.2 indicate that using MGA objective vectors with capacity variables results in least-cost dispatch while using generation variables does not. Maintaining economic dispatch is extremely important for capacity expansion models as their operational constraints are meant to represent the way generation decisions are made in competitive markets (e.g. by deregulated utilities) or in social welfare-maximizing centrally-planned dispatch (Marzbani and Abdelfatah 2024). As a result, MGA run over generation variables finds dispatch regimes different from that which would appear in real-world regimes, creating unrealistic operational decisions for the set of capacities found. This finding affects all metrics which are dependent on operations variables including but not limited to carbon emissions, utilization rates for thermal plants, operational costs, and local air pollution. In contrast, one can still produce a wide range of generation-related outcomes by applying MGA to capacity decision variables (which will indirectly drive variation in generation outcomes) while being assured that such decisions are consistent with least-cost dispatch or competitive market principles.

4.3. Convergence criteria for MGA algorithms

Stopping criteria and convergence metrics for MGA algorithms have not been discussed extensively in existing literature. Most papers utilizing MGA tend to document the number of iterations completed and rely upon ex-post methods to select a small subset of maximally diverse options from amongst the identified solutions (Berntsen and Trutnevyte 2017, Price and Keppo 2017, Esser *et al* 2024). However, without assurance that these approaches generate sufficient iterates to approximate the full near-optimal feasible region, it is unclear whether the 'maximally diverse' set of options is truly represented. In a departure from prior papers, Pedersen *et al* (2021b) use volume calculations from QHull as a convergence criterion by calculating the volume of the convex hull formed by all identified solutions at each iteration and terminating when the per-iteration change falls below a threshold (Barber *et al* 1996). While the computational performance of the QHull algorithm makes Pedersen *et al*'s (2021b) implementation impractical for MGA formulations with a large number of objective values, this approach gives as close as possible to a guarantee that the full space of the near-optimal feasible region has been explored. As there are pseudo-infinite vertices in high-dimensional convex hulls, like those created by macro-energy systems models, true convergence of the discovered convex hull with the true shape of the near-optimal feasible region is impossible (Klimenko *et al* 2021), but convergence of the convex hull volume to a stable value after multiple iterations likely indicates a close approximation.

Since, by definition of convexity, convex hulls cannot shrink in volume with the addition of a point, the computationally-efficient VESA metric proposed in this paper will catalogue most volume additions to the convex hull. The change in VESA over a set of iterations can compared to a convergence threshold, allowing for a consistent and computationally tractable termination criteria which provides some reassurance that the method has found most of the accessible volume.

The primary drawback with the use of volume estimation methods as a convergence criterion is that methodological deficiencies may lead to the appearance of convergence without fully exploring the space. This difficulty is most present with HSJ, which has very limited exploratory efficiency. It is not uncommon for HSJ iteration volume estimates to converge to relatively small but stable values compared to the volume found by other methods in the same space, implying that HSJ is getting stuck in a region without a way to escape and diversify its vector selection. A volume-based convergence metric will not change that and will only give a false sense that the algorithm has captured the majority of the space, when instead it has only found all of the solutions the method is capable of finding—two distinct concepts. This also implies that it is important that the exploratory performance of any new MGA methods proposed in the future are tested in a similarly rigorous manner as employed in this paper, so that users can understand whether convergence of a volume-based estimate to a stable value is truly a valid stopping criteria or not.

5. Conclusion

Modelling to Generate Alternatives is a powerful methodology to generate a wide range of near-optimal feasible solutions for energy system planning problems, with many possible applications to enhance decision support. This paper has shown, however, that the vector selection methodology used to explore the near-optimal feasible space has profound implications for the utility of any MGA application. While geometrically calculated methods like Modelling All Alternatives provide reasonable spatial exploration in tests, it is restricted by computational difficulties to relatively small-scale problems exploring variation in no more than a dozen decision variables (or groupings of variables), limiting its practical applicability in macro-energy system modelling, where higher dimensional MGA is often desirable depending on the research question. HSJ MGA, on the other hand, performs well in a computational run-time sense, but has extremely limited exploratory power, limiting the insights it can deliver, and potentially giving a false (overly constrained) sense of the tradeoffs available within a given circumstance and cost slack. The best traditional methods, per the testing conducted here, are the random vector and variable Min/Max methods, which performed well in both volumetric expansion and runtime in both a contrived testbed setting and in actual macro-energy systems modelling. However, each of these methods presents the opposite side of a tradeoff: random vector offers great guarantees that all dimensions will be explored, whether they are included in the MGA objective function explicitly or not, but struggles to find each variable's most extreme values, while variable Min/Max ensures that the dimensions that are specifically included in the MGA objective function are explored close to their extremes but may not optimize every dimension. Notably, as demonstrated here, these methods can be improved via their combination into a new Combined method, capturing the strengths of each while mitigating their relative weaknesses.

We also introduce a novel method of estimating the volume of the near-optimal feasible region explored by various MGA methods in high-dimensional spaces: Volume Estimation by Shadow Addition, or VESA. This metric is a computationally efficient alternative to calculating the full N-dimensional convex hull. VESA can be used to evaluate the relative performance of different methods (as employed herein) as well as employed as a convergence criterion to terminate MGA algorithms.

Finally, we demonstrate that MGA problems, as traditionally formulated, do not maintain economic dispatch when operational decision variables are included in the MGA objective function, resulting in unrealistic dispatch decisions. This erodes the decision-support value of MGA findings when operational decisions are included in the MGA search vector (objective function). In the context of macro-energy systems planning (or capacity expansion) models, we consequently recommend limiting the application of MGA to explore variation in capacity related decision variables.

Data availability statement

The data that support the findings of this study are openly available at the following URL/DOI: https://doi.org/10.5281/zenodo.11088682 (Lau *et al* 2024). All code can be found at: https://github.com/ml6802/MGAExploration.git.

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