Supplementary Information.

Declarations

- Funding: This work was supported in part through a research seed grant, “Systems Analytics for Small Farms Animal Waste Resource Recovery” awarded by Abdul Latif Jameel Water and Food Systems Lab (J-WAFS) at the Massachusetts Institute of Technology (MIT).
- Conflict of interest/Competing interests: None
- Ethics approval: N/A
- Consent to participate: N/A
- Consent for publication: N/A
- Availability of data and materials: The data needed to reproduce all results are available in .csv format at the following GitHub repository: https://github.com/schmedeman/Biogas-networks-in-Brazil
- Code availability: The code supporting this study consists of scripts written in Python, and is available at: https://github.com/schmedeman/Biogas-networks-in-Brazil
- Authors’ contributions: A.S., J.C.P.L., F.S.M., and O.W. planned the research project. P.S., K.R., C.J., and C.H.T. developed the model and coded the computation algorithms. P.S. and K.R. obtained numerical results and drafted the paper. J.C.P.L. and F.S.M. obtained data and provided feedback and validation throughout the analytical development. A.S. and O.W. reviewed and edited the paper, supervised the project, and acquired the funding.

Appendix A Supplementary Information: Sustainable regional biogas networks in Southern Brazil

A.1 Supplementary Results

Table A1 Data summary for case study locations.

			Livestock (thousands)			Wet Manure (kg/day)			Biogas Yield
Regions	Area	Muni.	Bovines	Pigs	Poultry	Min	Max	Total	(m^3/day)
1. Cianorte micro	4,874	11	227	12	23,871	137,000	4,239,000	10,625,000	1,064,830
2. Toledo micro	5,307	11	251	2,524	22,828	569,000	6,775,000	18,378,000	1,635,294
3. Toledo meso	13,440	26	526	3,372	53,202	61,000	6,775,000	34,193,000	3,184,704
4. Castro meso	26,544	16	659	896	14,693	27,000	4,226,000	18,165,000	1,079,187

Region 1: Cianorte Microregion

The Cianorte microregion comprises 11 municipalities totaling 4,874 km^2 and reports 227k bovines, 12k pigs, and 23,871k chickens. This livestock mixture generates a wet manure supply of 10.62 million kg per day with an average biogas yield of 0.0952 m^3 per kg of manure, and average methane yield of 0.0553 m^3 per kg manure.

The optimal (i.e., biomethane) architecture for the Cianorte microregion is estimated to generate profits of US$84.24 million from 240.24 million m^3 of biomethane while offsetting 3.54 billion kg of CO_2e greenhouse gas annually. The most profitable electricity design achieves a profit of US$43.10 million from selling 863.79 GWh of electricity and offsets 3.43 billion kg CO_2e GHG annually.

Region 2: Toledo Microregion

The Toledo microregion comprises 11 municipalities totaling 5,307 km^2 and reports 251k bovines, 2,524k pigs, and 22,828k chickens. This livestock mixture generates a wet manure supply of 18.38 million kg per day with an average biogas yield of 0.0795 m^3 per kg of manure, and average methane yield of 0.0462 m^3 per kg manure.

The optimal (i.e., biomethane) architecture for the Toledo microregion is estimated to generate profits of US$128.24 million from 368.76 million m^3 of biomethane while offsetting 5.40 billion kg of CO_2e greenhouse gas annually. The most profitable electricity design achieves a profit of US$63.58 million from selling 1,353.76 GWh of electricity and offsets 5.25 billion kg CO_2e GHG annually.

Region 3: Toledo Mesoregion—Arroio Fundo Basin and the Paraná River

The Toledo mesoregion comprises 26 municipalities totaling 13,440 km^2 and reports 526k bovines, 3,372k pigs, and 53,202k chickens. This livestock mixture generates a wet manure supply of 34.19 million kg per day with an average biogas yield of 0.0838 m^3 per kg of manure, and average methane yield of 0.0487 m^3 per kg manure.

The optimal (i.e., biomethane) architecture for the Toledo mesoregion is estimated to generate profits of US$249.72 million from 718.22 million m^3 of biomethane while offsetting 10.55 billion kg of CO_2e greenhouse gas annually. The most profitable electricity design achieves a profit of US$198.86 million from selling 2,632.88 GWh of electricity and offsets 9.93 billion kg CO_2e GHG annually.

Region 4: Castro Mesoregion—Centro Oriental Paranaense

The Castro mesoregion comprises 26 municipalities totaling 26,544 km^2 and reports 659k bovines, 896k pigs, and 14,693k chickens. This livestock mixture generates a wet manure supply of 18.16 million kg per day with an average biogas yield of 0.0519 m^3 per kg of manure, and average methane yield of 0.0303 m^3 per kg manure.

The optimal (i.e., biomethane) architecture for the Castro mesoregion is estimated to generate profits of US$72.39 million from 244.29 million m^3 of biomethane while offsetting 3.45 billion kg of CO_2e greenhouse gas annually. The most profitable electricity design achieves a profit of US$27.35 million from selling 887.74 GWh of electricity and offsets 3,196.95 billion kg CO_2e GHG annually.

Table A2 Summary of main results. Here, we report the profit and GHG offset of the best network architectures for the four regions. The biomethane design is optimal for all regions. For electricity designs, the objective weighting factor (λ) is used to trade off between the two objectives. When $\lambda = 1$ profit is maximized without regard to the environmental impact, and the opposite is true when $\lambda = 0$. Profits are reported in US$.

Design Scenarios	Profit ($M/yr)	GHG Offset (M kg CO_2e/yr)
Cianorte Microregion		
Biomethane (all values of λ)	84.24	3,544.85
Electricity $\lambda = 1$ (max profit)	43.10	3,427.45
Electricity $\lambda = 0.75$	43.10	3,427.45
Electricity $\lambda = 0.5$	43.10	3,427.45
Electricity $\lambda = 0.25$	42.47	3,439.22
Electricity $\lambda = 0$ (max GHG)	24.36	3,544.85
Toledo Microregion		
Biomethane (all values of λ)	128.24	5,397.10
Electricity $\lambda = 1$ (max profit)	63.58	5,245.34
Electricity $\lambda = 0.75$	63.58	5,245.34
Electricity $\lambda = 0.5$	63.56	5,245.36
Electricity $\lambda = 0.25$	62.77	5,245.37
Electricity $\lambda = 0$ (max GHG)	38.48	5,397.10
Toledo Mesoregion		
Biomethane (all values of λ)	249.72	10,545.91
Electricity $\lambda = 1$ (max profit)	198.86	9,932.45
Electricity $\lambda = 0.75$	197.63	9,944.93
Electricity $\lambda = 0.5$	122.61	10,140.40
Electricity $\lambda = 0.25$	114.24	10,273.15
Electricity $\lambda = 0$ (max GHG)	74.62	10,545.91
Castro Mesoregion		
Biomethane (all values of λ)	72.39	3,447.69
Electricity $\lambda = 1$ (max profit)	27.35	3,196.95
Electricity $\lambda = 0.75$	27.35	3,196.95
Electricity $\lambda = 0.5$	25.34	3,291.66
Electricity $\lambda = 0.25$	12.23	3,447.69
Electricity $\lambda = 0$ (max GHG)	12.23	3,447.69

A.2 Supplementary Methods

Fig. A1 provides a top level structural overview of the simulation model, depicting the various modules and their relational connectivity to each other.

Transportation Module

The Transportation module uses the manure process rate per municipality (in kg/day) from the design vector as an input. It also takes the calculated supply of manure (in kg/day) available in each municipality and a MxM matrix of distances (km) between municipalities, where M is the number of municipalities. This module performs a pseudo-optimization whereby the specified manure process rate per municipality (or manure demand) is satisfied first by the municipality's manure supply, starting with the municipality with the largest supply. If the municipality's manure supply is not enough to satisfy

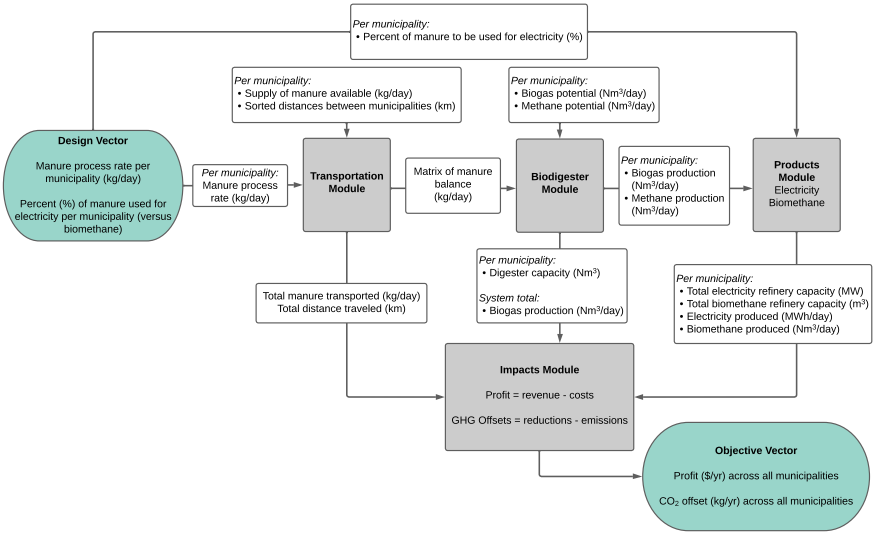

Fig. A1 Simulation model block diagram. Manure collected from farms is converted into biogas through anaerobic digestion. Biogas is used to produce electricity or upgraded to biomethane. Farms benefit from digestate (used as fertilizer) and revenues.

the specified processing rate, the algorithm will try to satisfy the demand with manure supplied from the municipalities that are geographically the closest (i.e., minimum distance between centroids of the municipalities). After which, the algorithm will repeat these steps with the next municipality in order of supply. This process repeats until demand is satisfied or supply is depleted. This module outputs a MxM matrix with manure movements between municipalities in kg/day, a scalar quantity representing the total distance (km) traveled, a scalar quantity representing the total amount of manure transported (kg/-day) across all municipalities, and a scalar quantity representing a dot product of the mass of manure transported and the distance (kg-km/day).

Digester Module

The Digester module takes in the MxM matrix output from the Transportation module as an input. It also takes the calculated potential for biogas (Nm^3/day, where Nm^3 refers to normal m^3) and the calculated potential for pure methane (Nm^3/day) as parameters determined by the manure supply in each municipality and specific empirical conversion factors between manure, biogas, and pure methane as a function of which animal produces the manure. Using these inputs, the Digester module calculates and outputs a $Mx1$ vector with the final amount of biogas (Nm^3/day) generated and a $Mx1$ vector with the quality of the biogas (percentage of methane) generated in each municipality. The Digester module also approximates the size of the anaerobic digester (AD) in each municipality required to process the amount of manure in the municipality and the total amount of biogas generated across all municipalities.

Products Module

The products module has three inputs: (i) the volume of biogas generated in each municipality (Nm^3/day) (ii) the biogas quality by methane content (%), and (iii) the percentage of manure to be used for electricity production (%). The first two inputs are received from the Digester module, and the third is received from the design vector since it is a decision variable. Using these inputs, the Products module computes the total amount of electricity and biomethane generated by municipality, using the electricity percentage decision variable to determine how the total amount of biogas (or methane) in each municipality is utilized. This module determines the size and efficiency of the production facilities based on the volume of biogas. The Products module returns the following values per each municipality: (i) the amount of electricity produced per municipality (MWh/day), the amount of biomethane produced (Nm^3/day) per municipality, the size of the electricity generation facility (MW), and the size of the biomethane refining facility (m^3).

Impacts Module

The Impacts module receives inputs from the Transportation, Digester, and Products modules and outputs the model's objective vectors. This module calculates the financial revenues and costs for the profit objective (J_1) as well as GHG avoidance and emissions in in CO_2 equivalent for the GHG offset objective (J_2). Revenues consist of the sum of the revenues from the sales of biomethane and electricity produced and offset payments if included, given input biomethane, electricity, and PES parameters. Costs consist of the sum of expenses from transportation (given a transportation cost parameter) and annualized costs of anaerobic digesters, electricity generation facilities, and biomethane refining facilities. GHG avoidance is calculated from the methane content in the total amount of biogas produced from manure (which directly offsets methane emissions to the atmosphere), while GHG emissions are calculated from the manure transportation involved.

Table A3 reports the modeling parameters. When possible, parameters specific to the region of focus (i.e., Paraná, Brazil) are used. Currencies are reported in US$ with a conversion rate of 5.24 Brazilian Reals (R$) to US$1, which is current as of February, 2023.

Table A3 Modeling parameters.

Parameter	Description	Value	Units	Reference
K^{Manure}	Manure density	1000	kg/m^3	[1]
E^{Col}	Manure collection CO_2 emissions	0.0084	kg/kg	[2]
E^{Stor}	Manure storage CO_2 emissions	0.05	kg/kg	[2]
K^{Truck}	Truck volume	40	m^3	[3]
E^{Trans}	Transportation CO_2 emissions	0.458	kg/km	[3]
C^{Trans}	Transportation cost	0.03438	US$/km-$m^3$	Provided by CIBiogás (F.S.M.)
K^{ADret}	AD hydraulic retention time	17	days	[4]
$size^{ref}$	AD investment reference capacity	8.5	m^3	Provided by CIBiogás (F.S.M.)
$C^{AD,ref}$	AD investment reference cost	17,273	US$	Provided by CIBiogás (F.S.M.)
K^{AD}	AD O&M cost percent of investment	13	%	[5]
K^{scale}	AD economies of scale factor	0.85		Calculated, see Model Validation
$K^{MethToPwr}$	Pure methane ideal power conversion	0.0105	MWh/m^3	[6]
$K^{Elec,1}$	Electrical efficiency, motogenerator	35	%	[7]
$K^{Elec,2}$	Electrical efficiency, Aeroderivative	38	%	[8]
$K^{Elec,3}$	Electrical efficiency, OCGT	45	%	[9]
$K^{Elec,4}$	Electrical efficiency, CCGT	64	%	[9]
$C^{Elec,1}$	Elec. gen. cost per MW, motogenerator	1,426,550	US$	[7]
$C^{Elec,2}$	Elec. gen. cost per MW, aeroderivative	1,232,000	US$	[10]
$C^{Elec,3}$	Elec. gen. cost per MW, OCGT	895,826	US$	[11]
$C^{Elec,4}$	Elec. gen. cost per MW, CCGT	980,944	US$	[11]
R^{Elec}	Electricity revenue per MWh	66.84	US$	[12]
K^{Elec}	Annual electric O&M cost percent	3	%	[13]
$C^{Bio,inv}$	Biomethane facility cost m^3 per hr	172	US$	Provided by CIBiogás (F.S.M.)
$C^{Bio,O\&M}$	Biomethane O&M cost per m^3	0.149	US$	Provided by CIBiogás (F.S.M.)
$K^{BioMeth}$	Biomethane CH_4 content	94	%	[14]
R^{Bio}	Biomethane revenue per m^3	0.59	US$	[15]
K^{Cap}	Capital recovery factor (30 year)	6.1	%	[16]
K^{CO_2}	CH_4 to CO_2e conversion factor	25		[17]
$K^{MethVol}$	Methane kg/m^3 at NTP	0.668		

Table A4 summarizes the parameters used for manure to biogas conversion according to livestock type. Parameters for the manure, biogas, and methane yields of each animal type is provided by from [18] and [19]. Information on bovine manure supply is from [20] and we applied a ratio of 60:40 beef bovines to dairy bovines for Brazil, in accordance with [21]. Data on the yield of biogas from poultry manure is from [22]. The methane content of biogas from poultry manure is from [23]. Since the yield of biogas is different for broilers and layers, it is assumed that 90% of poultry is broilers according to [24].

Table A4 Livestock-specific manure rates and yields.

Animal type	$\frac{\text{kg manure}}{\text{animal per day}}$	$\frac{\text{m}^3\text{ biogas}}{\text{kg manure}}$	$\frac{\text{m}^3\text{ biogas}}{\text{animal per day}}$	%CH_4
Bovine	17.20	0.0236	0.406	59.2
Pig	3.04	0.079	0.24	58.0
Poultry	0.28	0.1451	0.014	58.0

The first objective, profit (J_1), is the regional-level difference between the annual revenues and costs. Annual revenues are from the (assumed) sale of electricity and biomethane. Annual costs are the sum of the annuities paid on the initial capital expenditures for facilities, O&M, and transportation costs.

$$\begin{aligned}\text{Profit } (J_1) = &\text{ electricity revenue } (Rev^{Elec}) \\ &+ \text{biomethane revenue } (Rev^{Bio}) \\ &- \text{annualized capital costs } (C^{Cap}) \\ &- \text{O\&M } (C^{\text{O\&M}}) \\ &- \text{transportation costs } (C^{TransTotal})\end{aligned} \tag{A1}$$

$$Rev^{Elec} = \sum_{m \in \mathcal{M}} \left(R^{Elec} * X_m * Y_m * A_m * K^{MethToPwr} * K_m^{Elec,i} \right) \tag{A2}$$

Where A_m is the municipality-specific methane yield based on the livestock mixture and $K_m^{Elec,i}$ is the efficiency factor associated with the electricity generator as a function of the amount of biogas directed towards electricity production in municipality m.

$$Rev^{Bio} = \sum_{m \in \mathcal{M}} \left(R^{Bio} * X_m * (1 - Y_m) * A_m * \frac{1}{K^{BioMeth}} \right) \tag{A3}$$

The pure methane production of each municipality is calculated by $X_m * (1 - Y_m) * A_m$ and is divided by the assumed pure methane content of biomethane $K^{BioMeth}$ to arrive at the total amount of biomethane produced in each municipality.

$$C^{Cap} = K^{Cap} * \sum_{m \in \mathcal{M}} \left(C_m^{AD,inv} + C_m^{Elec,inv} + C_m^{Bio,inv} \right) \tag{A4}$$

Where K^{Cap} represents the capital recovery factor used to annualize the initial capital expenditures for the production facilities.

$$C_m^{AD,inv} = C^{AD,ref} * \left(\frac{size_m^{AD,inv}}{size^{AD,ref}} \right)^{K^{scale}} \tag{A5}$$

$$C_m^{Elec,inv} = C^{Elec,i_m} * X_m * Y_m * K^{Elec,i_m} \tag{A6}$$

$$C_m^{Bio,inv} = C^{Bio,inv} * X_m * (1 - Y_m) * A_m * \frac{1}{K^{BioMeth}} \tag{A7}$$

For anaerobic digesters and electricity generators, the facility O&M is calculated as a percent of the initial capital expenditure. For biomethane facilities, O&M is calculated as a function of the facility throughput.

$$C^{\text{O\&M}} = \sum_{m \in \mathcal{M}} \left(C_m^{AD,\text{O\&M}} + C_m^{Elec,\text{O\&M}} + C_m^{Bio,\text{O\&M}} \right) \tag{A8}$$

$$C_m^{AD,\text{O\&M}} = K^{AD} * C_m^{AD,inv} \tag{A9}$$

$$C_m^{Elec,\text{O\&M}} = K^{Elec} * C_m^{Elec,i} \tag{A10}$$

$$C_m^{\text{Bio,O\&M}} = 365 * C^{Bio,O\&M} * X_m * (1 - Y_m) * A_m * \frac{1}{K^{BioMeth}} \tag{A11}$$

The transportation cost is calculated as:

$$C^{TransTotal} = 365 * T^{ManureDist} * \frac{C^{Trans}}{K^{Manure}} \tag{A12}$$

Where $T^{ManureDist}$ represents a dot product of the mass of manure in kg and the distance it was transported in km.

The second objective, GHG offset (J_2), is the regional-level difference between the annual emissions avoided and produced by the system.

$$\begin{aligned} \text{GHG offset } (J_2) = \; & \text{avoided emissions } (E^{Avoid}) \\ & - \text{collection emissions } (E^{ColTotal}) \\ & - \text{transportation emissions } (E^{TransTotal}) \end{aligned} \tag{A13}$$

Emission avoidance is calculated from the methane content of the biogas production.

$$E^{Avoid} = \sum_{m \in \mathcal{M}} \left(X_m * A_m * K^{MethVol} * K^{CO_2} * 365 \right) \tag{A14}$$

The system produces emissions from the collection and transportation of manure. Collection emissions include on-farm transportation and the release of methane during collection. Storage emissions includes methane released from the manure while awaiting municipality-level collection.

$$E^{ColTotal} = \sum_{m \in \mathcal{M}} \left(X_m * 365 * (E^{Col} + E^{Stor}) \right) \tag{A15}$$

Transportation emissions are the sum of the emissions of the trucks used to transport the manure and methane released from the manure during transportation, where T^{Manure} is the total mass of manure transported in kg.

$$E^{TransTotal} = \sum_{m \in \mathcal{M}} \left(\frac{T^{ManureDist}}{K^{Manure}} * \frac{E^{Trans}}{K^{Truck}} + T^{Manure} * E^{Stor} \right) * 365 \tag{A16}$$

Model Validation

To validate the simulation model, we conducted expert interviews, reviewed literature, and benchmarked against existing biogas facilities. J.L.P. and F.S.M. provided current values specific to southern Brazil for estimates for biomethane prices, electricity prices, anaerobic digester manure processing rates, and capital costs.

To determine the power law exponent to use to calculate economies of scale, we used figures from the Raizen-Geo Energetica project [25, 26] and the Caieiras thermal power biogas plant [27, 28]). Although these projects generate biogas from sources other than manure (vinasse and landfill gas respectively), the mass flowrates processed by these projects are on the same order of magnitude as the lower end of our system (9.2 million kg/day and 8 million kg/day respectively versus our lower end of 10.6 million kg/day). Using these projects as references, we calculated a power law exponent of 0.85, as shown in Equation A17.

$$\text{cost}_2 = \text{cost}_1 * (\frac{\text{size}_2}{\text{size}_1})^{0.85} \tag{A17}$$

We validated the power law exponent using IEA Bioenergy Task 37 ([29]) case study data for anaerobic digesters (Lemvig Biogas [30], Sonderjysk [31], Solrod [32], Ringkobing [33], and Bording [34]) in Denmark:

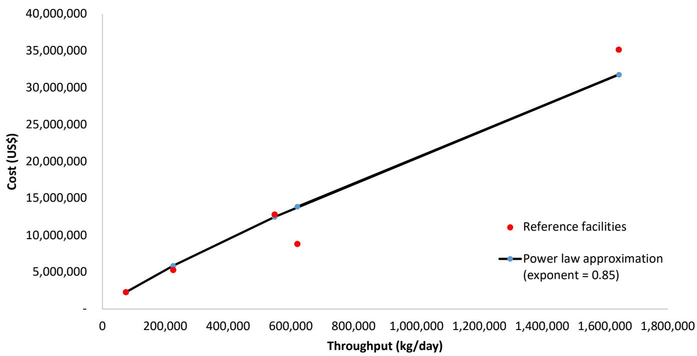

Fig. A2 Anaerobic digester economies of scale factor. The economies of scale factor (0.85) was estimated using a collection of case studies by [29]. [29]

Note that we could only benchmark the power law exponent (0.85) up to 1.7 million kg/day manure, but the regions in this study have wet manure supplies ranging from 10.62 million kg per day to 34.19 million kg per day. We assume that this parameter is still valid in the extended range.

With the power law exponent determined by data on the Raizen-Geo Energetica and Caieiras thermal power biogas plant projects and validated by IEA Bioenergy Task 37 case study data on plants in Denmark, we were able to produce reasonable estimates for the cost of anaerobic digesters and biomethane

Table A5 Comparison of order of magnitude profitability of Solrød and the proposed system in Cianorte

Biogas Plant	Manure throughput (kg / day)	Profitability ($ / kg feed)
Solrød, Denmark	550,000	0.025
Proposed system	8,900,000	0.023

facilities in Brazil. In Table A5, we compare the throughput and specific profitability (in US$ earned by the system per kilogram of manure processed by the system) of the Solrød plant in Denmark with our model's estimate of the throughput and specific profitability of a proposed electricity-only manure processing system in Cianorte. Although Solrød processes more than 10 times less than the manure that our system proposes to handle, this validation provides confidence that our model solutions are accurate from an order of magnitude perspective.

Solution Algorithm Pseudocode

Algorithm 1 Simulated annealing algorithm to solve the biogas network design problem

– Input: municipality biogas yields and distances; design vector X; system energy E; initial and minimum system temperature T; difference in system energy between two design vectors Δ

while $T > T_{min}$ stopping criterion is not met **do**
    Select a random $X_{i'}$
    Evaluate $E(X_i)$ using the biogas simulation model
    Perturb X_i to obtain a neighboring design vector (X_{i+1})
    Evaluate $E(X_{i+1})$ using the biogas simulation model
    if $E(X_{i+1}) < E(X_i)$ **then**
        $E(X_{i+1})$ is the new current solution
    end if
    if $E(X_{i+1}) >= E(X_i)$ **then**
        Accept $E(X_{i+1})$ as the new current solution with a probability $e^{(-\Delta/T)}$ were $\Delta = E(X_{i+1}) - E(X_i)$
    end if
    Reduce the T according to the cooling schedule $T_{j+1} = T_j - \Delta T$
end while
Terminate the algorithm

For each region and value of λ, we conduct two passes over the algorithm. We employ exponential cooling with an initial temperature (T_0) of 10,000 and a cool-down factor of 0.999, producing 12,201 iterations in the cooling schedule.

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