Multi-objective Bayesian Optimization of CO_2 Storage Inspired by Sleipner Project

Muhammad Amir Saeed, Jo Eidsvik and Antonio Candelieri

Department of Economics, Management and Statistics, University of Milano Bicocca, Italy

Department of Mathematical Sciences, Norwegian University of Science and Technology, Norway

Center of Geophysical Forecasting (CGF), Norwegian University of Science and Technology, Norway.

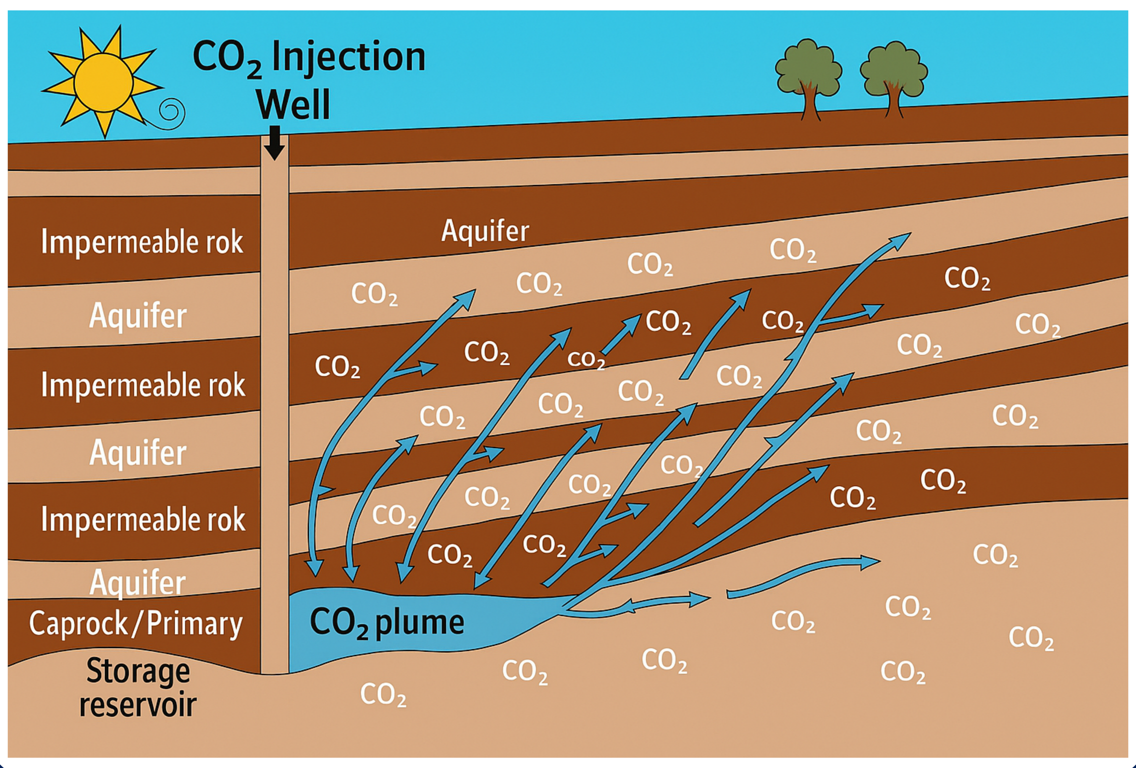
1. Abstract

We present a multi-objective Bayesian optimization framework to maximize CO_2 storage and minimize leakage during migration. The framework considers two conflicting objectives: maximizing CO_2 storage and minimizing leakage during migration via invasion percolation. Due to the presence of discrete inputs, we employ a multinomial logit model. Using the Pareto front, we compute the expected hypervolume improvement (EHVI) and evaluate other acquisition functions, including scalarized confidence bound (SCAL), Thompson sampling (TS), and expected preference improvement (EPI). The approaches are tested and compared on a 5-layer example and the 2019 Sleipner CO_2 storage project in the North Sea.

2. Problem Formulation

In geological CO_2 storage, operators must balance two conflicting goals:

- *Maximize* the net volume of CO_2 stored, and
- *Minimize* the cumulative CO_2 that leaks out of the formation.



3. Objective Functions

Objective 1: Maximize Total Stored CO_2
Focus solely on how much CO_2 ends up in the formation:

$$\boxed{f_1(X) = \sum_{i=1}^{N_{\text{stor}}} \int_0^T V_i(t)\,dt} = A\,\phi\,h_{\text{ref}}\,d \sum_{i=1}^{N_{\text{stor}}} (1-r)^{i-1} \int_0^T \frac{p_i(t)}{p_{\text{ref}}}\,dt.$$

Objective 2: Minimize Leakage of CO_2
Penalize any CO_2 that does not remain stored (i.e. the gap between injection and storage:

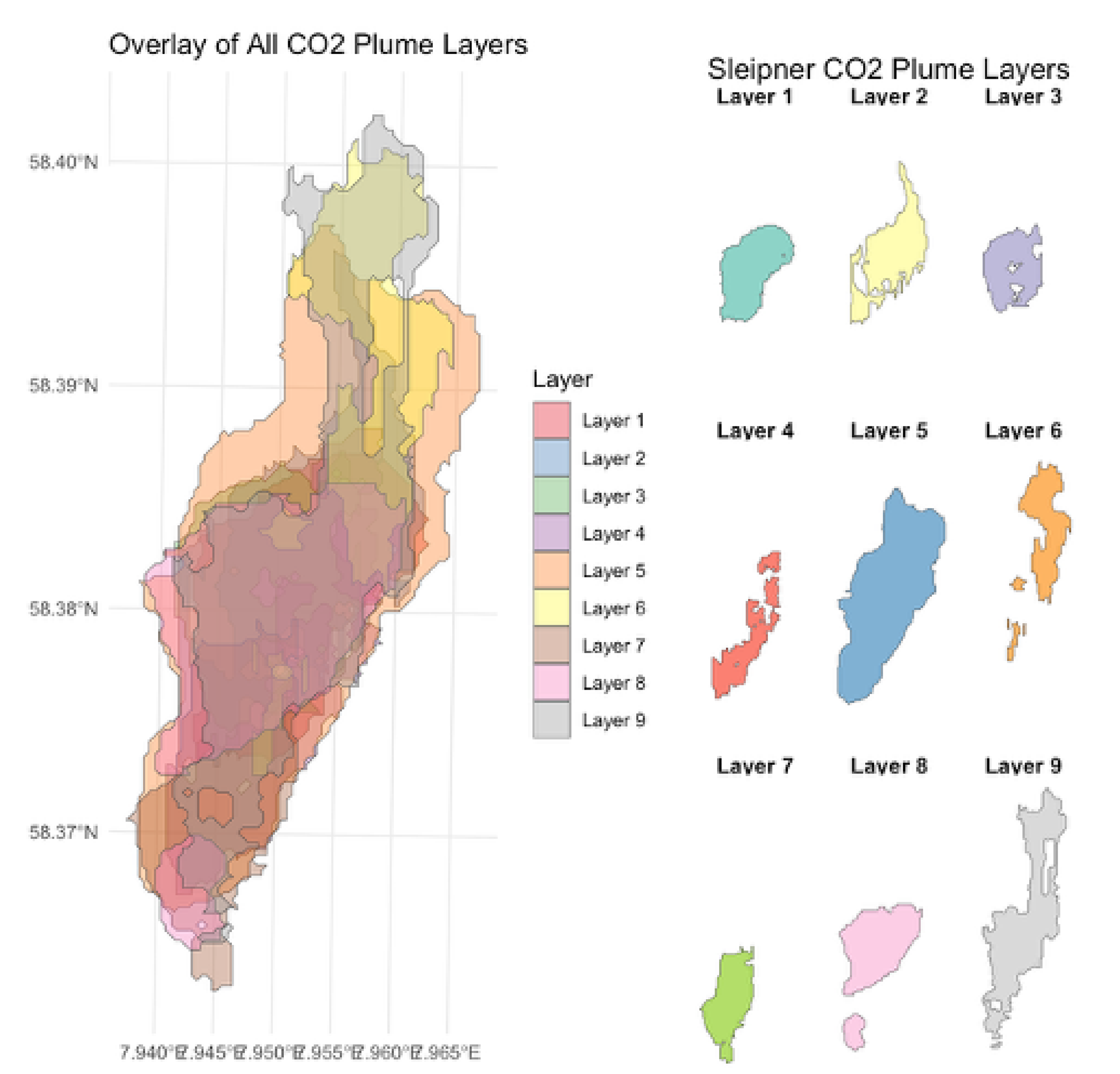
$$\boxed{f_2(X) = M_{\text{inj}} - \sum_{i=1}^{N_{\text{stor}}} \int_0^T V_i(t)\,dt}$$

Invasion Percolation Indicator:

$$\delta_{i\to i+1}(t) = \begin{cases} 1, & \underbrace{\Delta\rho\, g\, h_i(t)}_{P_c(t)} > \underbrace{\frac{2\,\gamma\,\cos\theta}{r_{c,i+1}(t)}}_{P_{\text{th}}(t)} \quad \text{and} \quad \underbrace{\frac{\mu\, q(t)}{\gamma}}_{\text{Ca}(t)} \le 10^{-4}, \\ 0, & \text{otherwise}, \end{cases}$$

$$f_2 = M_{\text{inj}} - f_1 = \int_0^T r_{\text{leak}}(t)\,\mathrm{d}t, \quad r_{\text{leak}}(t) = \sum_{i=1}^{N_{\text{stor}}} \delta_{i\to i+1}(t)\, V_i(t).$$

4. Sleipner 2019 Benchmark Model



5. Bayesian Optimization and Empirical Graphs

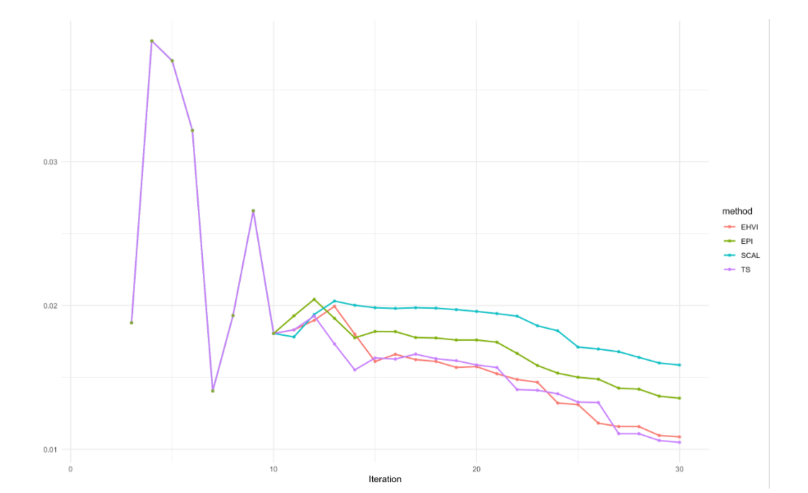
Bayesian Optimization Algorithm

Algorithm 1 Multi-Objective BO with Multinomial-Logit Surrogate

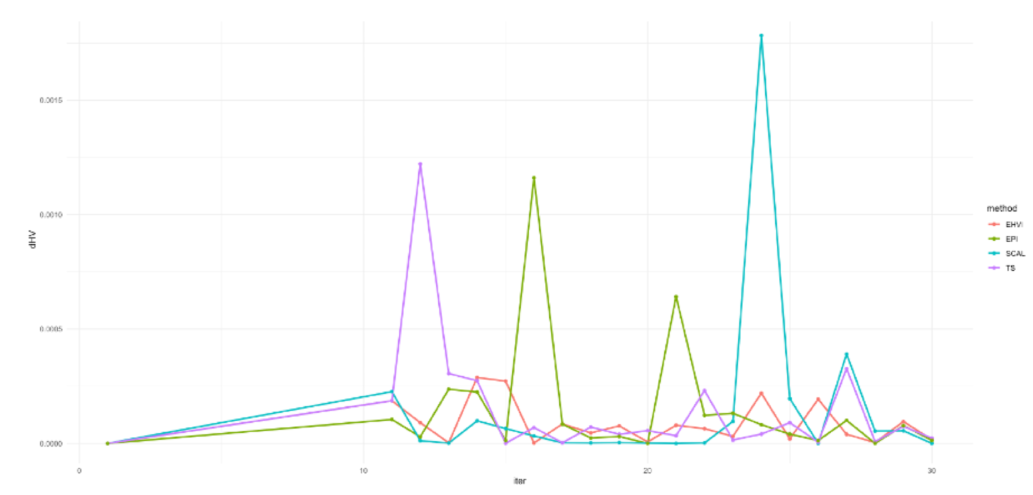
Require: Initial data $D = \{(x_i, f(x_i))\}_{i=1}^{n_{\text{init}}}$, budget N.

for $t = n_{\text{init}} + 1$ to N **do**
    Fit the multinomial surrogate on D.
    Generate candidate pool $\{x^{(j)}\}_{j=1}^{n_{\text{cand}}}$.
    Compute acquisition $\alpha(x^{(j)})$ via EHVI, TS, EPI or SCAL.
    Select $x^* = \arg\max_j \alpha(x^{(j)})$.
    Evaluate $f(x^*)$; augment $D \leftarrow D \cup \{(x^*, f(x^*))\}$.
    Update Pareto front $\mathcal{F}$.
end forreturn Final Pareto-optimal set from D.

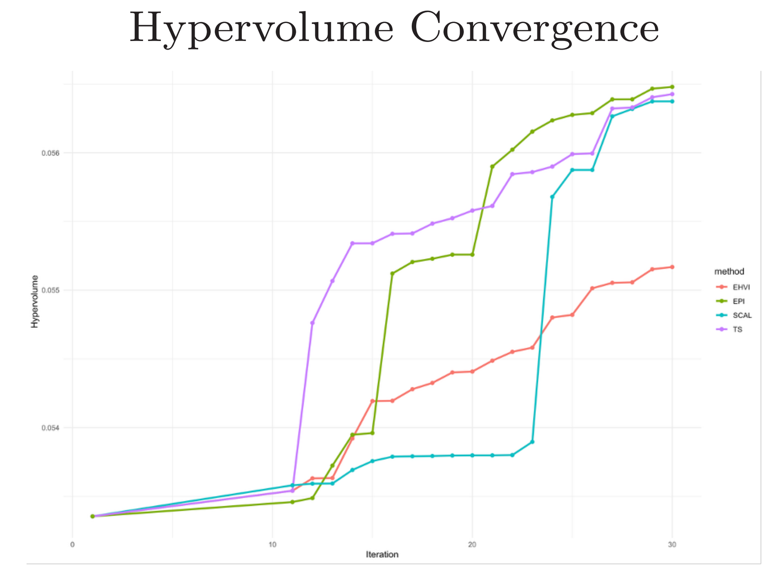
Diversity of Pareto front over iterations



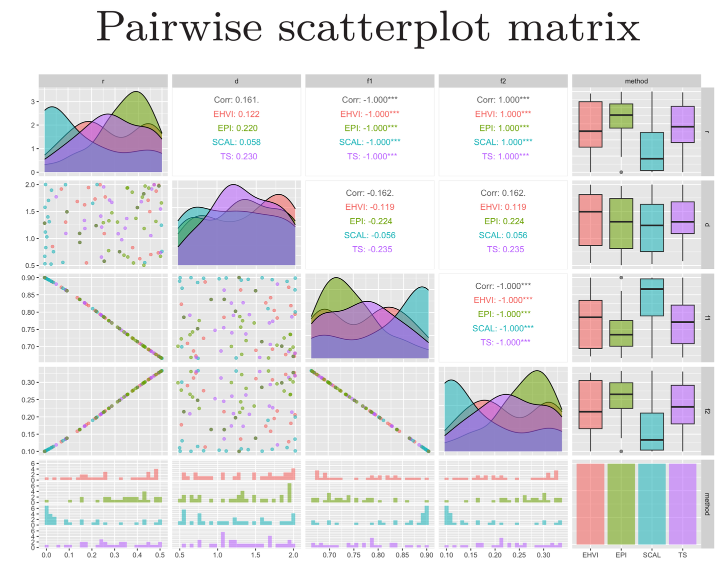
Hypervolume Increment per Iteration (ΔHV)



Hypervolume Convergence



Pairwise scatterplot matrix



6. Conclusions

We implemented a multi-objective Bayesian optimization framework to maximize CO_2 storage and minimize leakage, with formal mathematical formulations for the objectives. The BO algorithm employs acquisition functions such as EHVI, TS, EPI, and SCAL. It is tested on a simple 5-layer example with varying parameters and then applied to the 2019 Sleipner benchmark. The result shows the comparison of different acqusition functions and surrogate models.

7. References

References

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[2] Lu, X., Jordan, K. E., Wheeler, M. F., Pyzer-Knapp, E. O., & Benatan, M. (2022). Bayesian optimization for field-scale geological carbon storage. *Engineering*, 18, 96–104.

[3] Santi, A. C., Ringrose, P., Eidsvik, J., & Haugdahl, T. A. (2025). Invasion percolation Markov Chains–A probabilistic framework for assessing vertical CO_2 migration. *International Journal of Greenhouse Gas Control*, 142, 104338.