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Variations of Optimal Designs

Week 11 – Advanced Topic 2

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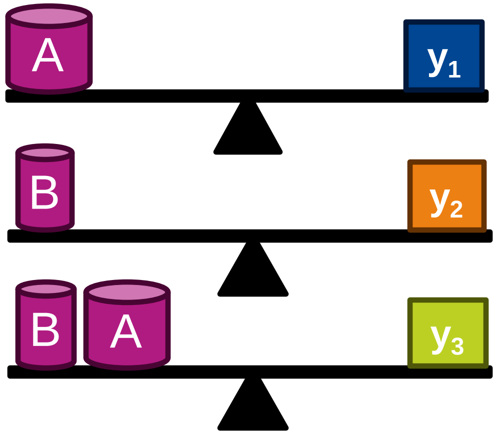
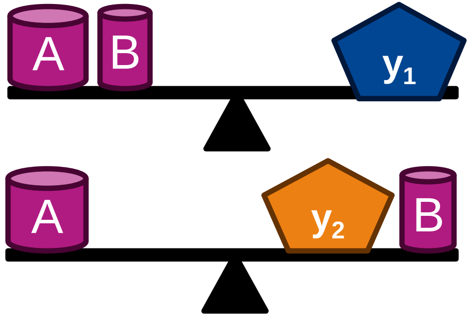
Optimal Experimental Design

- Optimization way in creating data with fewer trials / resources
- Statistical approach to select experimental points ➔ minimizing the number of experiments or trials



CLASSIC Design



OPTIMAL Design

Optimal Designs in DoE

What are Optimal Designs?:

Experimental setups tailored to specific objectives, providing the most informative data within given constraints (e.g. budget or time).

Why use Optimal Designs?:

Reduce costs, improve precision, and make experiments more efficient.

Optimal Designs in DoE

- The optimality of a design depends on the statistical **model** and is assessed with respect to a statistical **criterion**, which is related to the **variance-matrix** of the estimator.
- The inverse matrix of the variance-matrix is called the **information matrix**.
- Optimality-criteria are invariants of the information matrix.

Optimal Designs criteria

- **A**-optimality ("**average**" or **trace**)
  - It seeks to minimize the trace of the inverse of the information matrix. This criterion results in minimizing the average variance of the estimates of the regression coefficients.
  - When to use: average precision across all parameters is prioritized.
- **G**-optimality
  - It seeks to minimize the maximum entry in the diagonal of the projection matrix $X(X'X)^{-1}X'$. This results in minimizing the maximum variance of the predicted values.
  - When to use: for experiments where uniform predictive capability is important.

Optimal Designs criteria

- **D**-optimality
  - Aims at maximizing the determinant of the information matrix X'X of the design, leading to minimal parameter estimate variance.
  - When to use: For models requiring high precision in parameter estimation.
- **I**-optimality
  - Aims at minimizing the average prediction variance over the design space.
  - When to use: for applications that rely on accurate response predictions at any point within the design space.
- Other optimality criteria
  - C-optimality, E-optimality, S-optimality, T-optimality, etc.

The Fisher Information Matrix

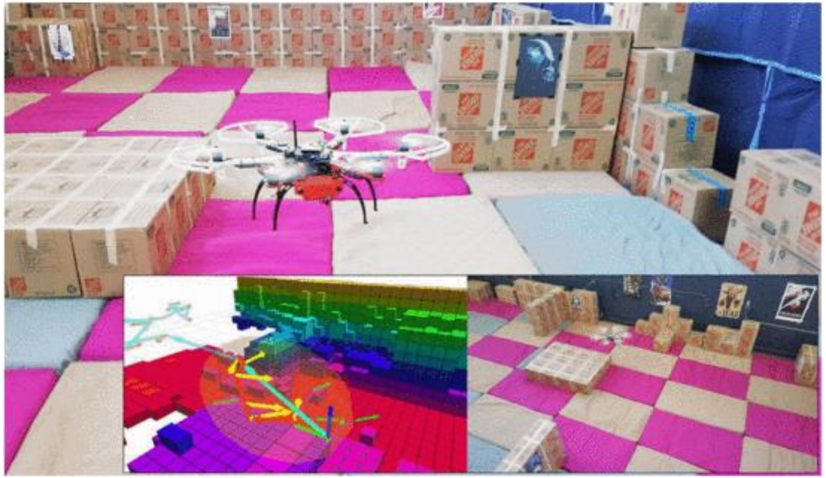
- The **Fisher Information Matrix (FIM)**: it captures how much information an experiment provides about the parameters of a model.
- The FIM is derived from the partial derivatives of the model's predicted responses with respect to the model parameters.
- Larger values in the FIM indicate the experimental setup provides more information about the parameters.
- In an experiment, the **covariance matrix** of the parameter estimates is proportional to the inverse of the FIM.

Applications and Examples

- Simultaneous Localization and Mapping (SLAM)
  - On the comparison of uncertainty criteria for active SLAM : https://ieeexplore.ieee.org/document/6224890
  - Uncertainty-aware receding horizon exploration and mapping using aerial robots: https://ieeexplore.ieee.org/document/7989531

  - Therefore, for two robot path policies σ_1^M and σ_2^M, D-opt is used to evaluate which of the two $(l_p+l_f)\times(l_p+l_f)$ covariance matrices $\Sigma_{p,f}(\sigma_1^M)$ and $\Sigma_{p,f}(\sigma_2^M)$ corresponds to more confident belief at the *end-vertex* of each path.

$$D_{opt}(\sigma^M) = \exp(\log([\det(\mathbf{\Sigma}_{p,f}(\sigma^M)]^{1/(l_p+l_f)}))$$

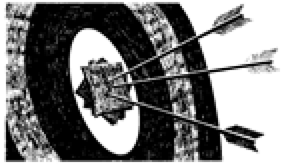


Applications and Examples

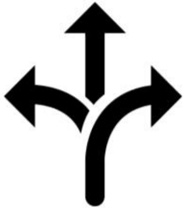
- **Visual 3-D reconstruction**
  - Active Visual Object Reconstruction using D-, E-, and T-Optimal Next Best Views: https://ieeexplore.ieee.org/abstract/document/4270361
  - "The reconstruction is based on a probabilistic state estimation with sensor actions. **The next best view is determined by a metric of the state estimation's uncertainty.** We compare three metrics: D-optimality, which is based on the entropy and corresponds to the (D)eterminant of the covariance matrix of a Gaussian distribution, E-optimality, and T-optimality, which are based on (E)igenvalues or on the (T)race of this matrix, respectively."

Advantages & Challenges

Less-resources for time-saving



Leads to better model predictions



Designed to specific needs

Requires the understanding of goal

Sometimes needs costly computation

Not always suitable / applicable

Conclusions

- **Classical designs** are easier to set up and compute, making them suitable for simpler, lower-dimensional experiments or when there's a predefined model structure.
- **Optimal designs** offer significant flexibility and statistical efficiency but require more computational effort and specialized software.
- Different types (D-, A-, G-, I-, and space-filling) ***respond to specific experimental needs***, such as parameter accuracy or prediction reliability.

Key:

- Understand the aims and resource restriction first, optimal experiment design may depend on them.

Thank you

References

- https://en.wikipedia.org/wiki/Optimal_experimental_design
- https://www.nature.com/articles/s41592-018-0083-2
- López-Fidalgo, J., 2023. Optimal Experimental Design. Lecture Notes in Statistics, 226.