

Integer Frank-Wolfe for Optimal Experiment Design

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Berlin Mathematics Research Center



Think scottish shortbread



Outline

1. A- and D-Optimal Experiment Design
2. Integer Frank-Wolfe: `Boscia.jl`
3. E-Optimal Design and Nesterov Smoothing
4. Summary

D-and A-Optimal Experiment Design

$$\begin{aligned} \min_{\mathbf{x}} \quad & -\log \det (A^T \text{diag}(\mathbf{x})A) \\ \text{s.t.} \quad & \sum_{i=1}^m x_i = N \\ & \mathbf{l} \leq \mathbf{x} \leq \mathbf{u} \\ & \mathbf{x} \in \mathbb{N}_0^m, \end{aligned} \tag{D}$$

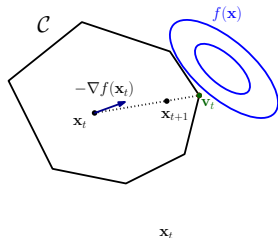
$$\begin{aligned} \min_{\mathbf{x}} \quad & \text{tr} ((A^T \text{diag}(\mathbf{x})A)^{-1}) \\ \text{s.t.} \quad & \sum_{i=1}^m x_i = N \\ & \mathbf{l} \leq \mathbf{x} \leq \mathbf{u} \\ & \mathbf{x} \in \mathbb{N}_0^m, \end{aligned} \tag{A}$$

Ponte, Fampa, and Lee 2025; Ahıpařaođlu 2021; Li et al. 2024

Ahıpařaođlu 2015; Sagnol and Pauwels 2019; Nikolov, Singh, and Tantıpongıpat 2022

where A encodes the experiments and $M(\mathbf{x}) = A^T \text{diag}(\mathbf{x})A$ is referred to as the *Information matrix*.

Integer Frank-Wolfe: Boscia.jl

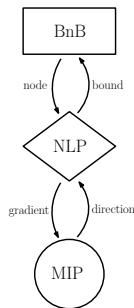


Frank and Wolfe 1956; Levitin and Polyak
1966; Braun et al. 2022

$$\begin{aligned} \min_{\mathbf{x}} \quad & f(\mathbf{x}) \\ \text{s.t. } \quad & \mathbf{x} \in \mathcal{X} \\ & \mathbf{x}_j \in \mathbb{Z} \quad \forall j \in J \end{aligned}$$

- f continuously differentiable, convex, L -smooth.
- $\mathcal{X}$ is a compact convex set, usually polyhedral.

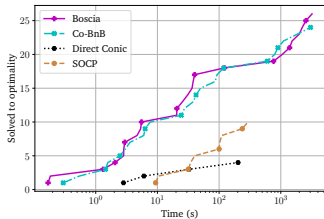
Hendrych et al. 2025



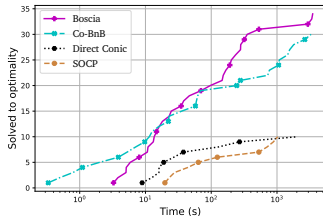
Schematic of the algorithm.

Experimental Results

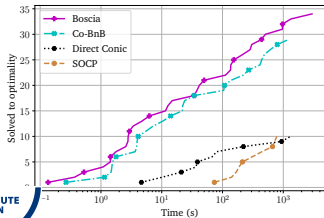
A-Optimal (Independent)



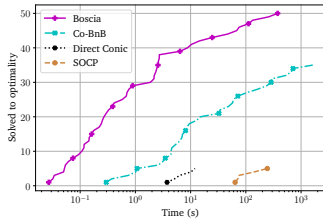
A-Optimal (Correlated)



D-Optimal (Independent)



D-Optimal (Correlated)



E-Optimal Experiment Design

$$\begin{aligned} \max_{\mathbf{x}} \quad & \lambda_{\min} (A^T \text{diag}(\mathbf{x})A) \\ \text{s.t.} \quad & \sum_{i=1}^m x_i = N \\ & \mathbf{l} \leq \mathbf{x} \leq \mathbf{u} \\ & \mathbf{x} \in \mathbb{N}_0^m, \end{aligned} \tag{E}$$

Brown, Laddha, and Singh 2024; Rendi, Vanderbei, and Wolkowicz 1995; Allen-Zhu et al. 2021

E-Criterion and smoothing

Issue

The subgradients of $\lambda_i(X)$ are the corresponding eigenvectors.
 $\Rightarrow$ the gradient $\nabla \lambda_i$ only exists if $\text{mult}(\lambda_i) = 1$.

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Solution - Smoothing

We use the smoothing introduced in Nesterov 2007.

$$\max \lambda_{\min}(X) \Leftrightarrow \min \lambda_{\max}(-X)$$

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$$\max \lambda_{\min}(X) \Leftrightarrow \min \lambda_{\max}(-X)$$

$$f_{\mu}(X) = -\mu \log \left(\sum_{i=1}^n e^{-\lambda_i(X)/\mu} \right) + \mu \log n \quad (1)$$

$$f_{\mu}(X) \geq f(X) \geq f_{\mu}(X) + \mu \log n \quad \forall X \in \mathbb{S}^n \quad (2)$$

Pruning, Dual Tightening and Approximate Gradient

Pruning

- Prune in the case of rank deficiency.
- Prune based on the maximal achievable eigenvalue.

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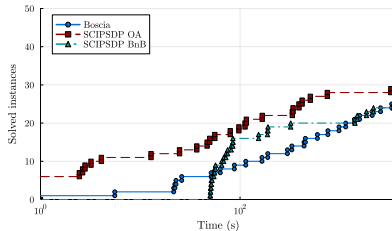
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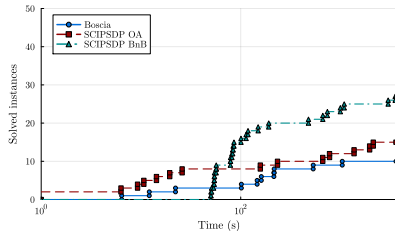
Approximate Gradient

- Drop the largest eigenvalues from the gradient inspired by d'Aspremont 2008.

Computational Results



correlated data



independent data

Another Application - Maximum Algebraic Connectivity

$$\begin{aligned} \max \quad & \lambda_2(L_{G(\mathbf{x})}) \\ \text{s.t. } & G(\mathbf{x}) \text{ satisfies graph some conditions} \end{aligned} \tag{3}$$

where $L_{G(\mathbf{x})}$ is the Laplacian of a subgraph of an undirected (weighted) graph G induced by $\mathbf{x}$.

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By Chan 2018 and Lamperski, Yang, and Prokopyev 2024, we have

$$\lambda_2(L) = \lambda_{\min}(L + \mathbb{1}\mathbb{1}^T)$$

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Somisetty, Nagarajan, and Darbha 2024 introduce a Maximum Algebraic Connectivity problem over spanning trees of a weighted graph.

Computational Results

Table: Performance comparison for ACST problem grouped by dimension. Geometric mean of the time is computed with a 1s shift. There are 12 instances in total.

Solver	Metric	45	66	105	300	all
Boscia	% sol.	100.0	0.0	0.0	0.0	14.3
	time (s)	500.8	3600.0	3600.3	3602.4	2716.4
	rel. gap	—	6.01e-01	2.01e+00	5.97e+00	6.84e+00
SCIPSDP (OA)	% sol.	0.0	0.0	0.0	0.0	0.0
	time (s)	3600.0	3600.0	3600.0	3600.0	3600.2
	rel. gap	—	—	5.53e+00	1.00e+20	7.47e+15
SCIPSDP (B&B)	% sol.	0.0	0.0	0.0	0.0	0.0
	time (s)	3600.0	3600.0	3600.0	3600.0	3600.0
	rel. gap	1.08e-01	7.24e-01	3.13e+00	2.09e+01	2.23e+04

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Summary

- B&B with Frank-Wolfe **scales better** when the SOCP and SDP formulations need to add a lot of additional variables and/or constraints
- The **SDP formulation** for maximizing the minimum eigenvalue **under simple budget constraints is tight** by the theory and the computational results support that.
- In case of harder combinatorial and/or linear constraints, **decoupling** them from the PSD constraints via smoothing shows the superior performance.

Summary

- B&B with Frank-Wolfe **scales better** when the SOCP and SDP formulations need to add a lot of additional variables and/or constraints
- The **SDP formulation** for maximizing the minimum eigenvalue **under simple budget constraints is tight** by the theory and the computational results support that.
- In case of harder combinatorial and/or linear constraints, **decoupling** them from the PSD constraints via smoothing shows the superior performance.
- Can we find tighter first-order approximations?

Thank you for your attention!

Convex mixed-integer optimization
with Frank–Wolfe methods



Solving the Optimal Experiment
Design Problem with Mixed-Integer
Convex Methods



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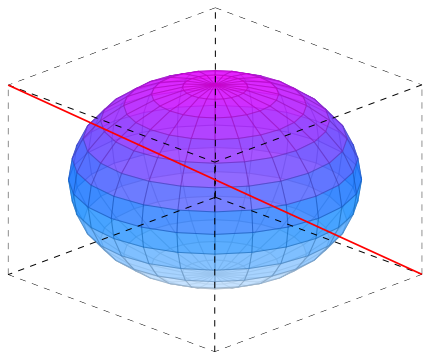
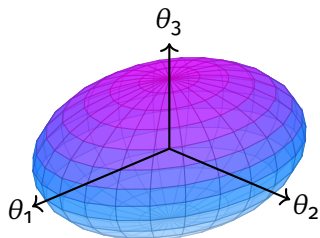
Set-up

- The ultimate goal is fitting a regression model.

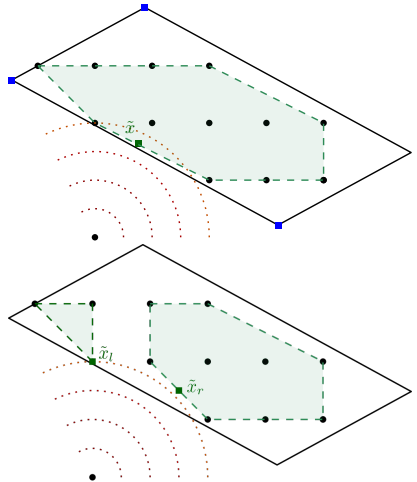
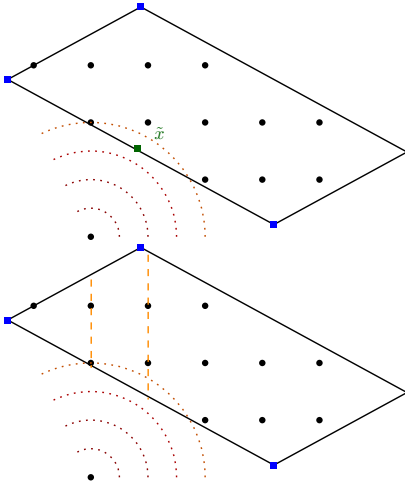
$$\min_{\theta \in \mathbb{R}^n} \|A\theta - \mathbf{y}\|_2^2$$

- $A = [-\mathbf{a}_i -]_{i=1}^m$ with $\mathbf{a}_i \in \mathbb{R}^n$ is the *Experiment Matrix*. Assumed to have full column rank.
- θ is the unknown set of parameters to be found.
- $\mathbf{y}$ is the **not-yet** measured response.
- **Issue:** Running all m experiments too costly and/or too time intensive.

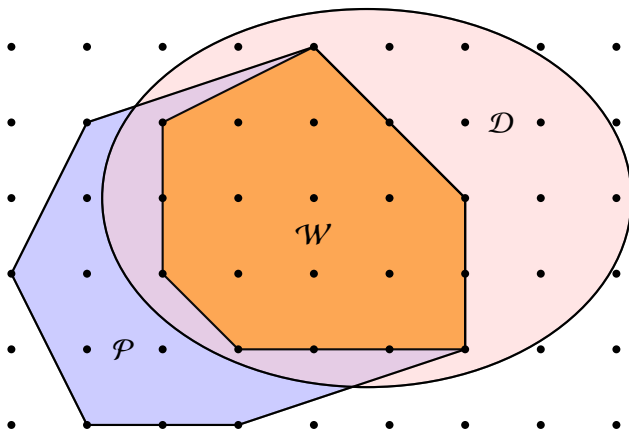
Graphical interpretation



Convex relaxation vs integer hull



Feasible region vs Domain



A schematic representation of the feasible region $\mathcal{P}$, the domain of the objective $\mathcal{D}$ and the convex hull of vertices that are both feasible and in the domain denoted as $\mathcal{W}$.

Generalized self-concordance

By Carderera, Besançon, and Pokutta 2021, we also have convergence if the objective is generalized self-concordant. Self-concordance was already proved for the $-\log \det(X)$ on $\mathbb{S}_{++}^n$.

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Theorem (GSC A-criterion hendrych2024optimal)

The function $g(X) = \text{tr}(X^{-p})$, with $p > 0$, is $\left(3, \frac{(p+2)\sqrt[p]{a^{2pn}}}{\sqrt{p(p+1)}}\right)$ -generalized self-concordant on $\text{dom}(g) = \{X \in \mathbb{S}_{++}^n \mid 0 \prec X \preccurlyeq aI\}$ where $a \in \mathbb{R}_{>0}$ bounds the maximum eigenvalue of X .

Other approaches

Co-BnB Ahipaşaoğlu 2021

- Branch-and-Bound with customized coordinate-descent-like algorithm for the node problems, exploits connection to Minimum Volume Enclosing Ellipsoid Problem.
- Developed for $m \gg n$.

Outer Approximation approaches

- Using the mixed-integer convex solver with conic certificates `Pajarito.jl` Coey, Kapelevich, and Vielma 2022a.
 1. **Direct Conic:** Natural formulation via `Hypatia.jl` Coey, Kapelevich, and Vielma 2022b.
 2. **SOCP:** as introduced in Sagnol 2011; Sagnol and Harman 2015.

Convergence results

Objective	Convergence	Linear Convergence
$f(\mathbf{x}) = -\log \det(X(\mathbf{x}))$	✓	✓*
$g(\mathbf{x}) = \text{tr}(X(\mathbf{x})^{-p})$	✓	Not guaranteed
$k(\mathbf{x}) = \log(\text{tr}(X(\mathbf{x})^{-p}))$	Conjecture	Not guaranteed

Table: Convergence of Frank-Wolfe on different objective functions.

*We adapted the proof from Zhao 2025 to the Blended Pairwise Conditional Gradient (BPCG).

Hendrych, D. and Besançon, M. and Pokutta, S. (2025). "Solving the Optimal Experiment Design Problem with Mixed-Integer Convex Methods." <https://arxiv.org/abs/2312.11200>

What do we need for convergence?

In short: Frank-Wolfe has to converge.

$$f(X) = -\log \det(X) \quad \text{and} \quad g(X) = \text{tr}(X^{-p}) \quad \text{and} \quad k(X) = \log \text{tr}(X^{-p})$$

We need:

- Convexity of the objective functions. ✓
- L -smoothness of the objective functions. → Issue with the domain.
- Generalized self-concordance of the objective functions.
- Strong convexity/Sharpness of the objective functions.

Hendrych, D. and Besançon, M. and Pokutta, S. (2025). "Solving the Optimal Experiment Design Problem with Mixed-integer Convex Methods." <https://arxiv.org/abs/2312.11200>

Theorem (L-smoothness for the Fusion Problems)

The functions $f_F(\mathbf{x}) = \log \det(X_C(\mathbf{x}))$, $g_F(\mathbf{x}) = \text{tr}(X_C(\mathbf{x})^{-p})$ and $k_F(\mathbf{x}) = \log(\text{tr}(X_C(\mathbf{x})^{-p}))$ are L-smooth on $x \in \mathbb{R}_{\geq 0}$.

L-smoothness

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Theorem (Local L-smoothness for the Optimal Problems)

The functions $f(X(\mathbf{x}))$, $g(X(\mathbf{x}))$ and $k(X(\mathbf{x}))$ are locally L-smooth on

$$\mathcal{L}_0 = \{\mathbf{x} \in \mathcal{D} \cap \mathcal{P} \mid (*) (\mathbf{x}) \leq (*) (\mathbf{x}_0)\}$$

where $()$ is a placeholder for each function and $x_0 \in \mathcal{D}$ an initial point.*

Sharpness

Theorem (Strong convexity)

The functions $f(X) = -\log \det(X)$ and $g(X) = \operatorname{tr}(X^{-p})$, $p > 0$, are strongly convex on $D := \{X \in \mathbb{S}_{++}^n \mid \lambda_{\max}(X) \leq \alpha\}$.

The function $k(X) = \log \operatorname{tr}(X^{-p})$, $p > 0$, is strongly convex on $D := \{X \in \mathbb{S}_{++}^n \mid \lambda_{\max}(X) \leq \alpha, \kappa(X) \leq \kappa\}$.

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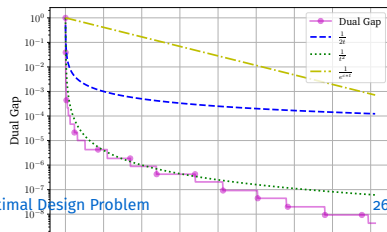
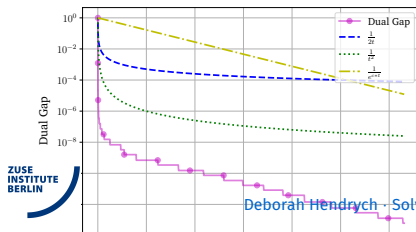
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Theorem

The compositions of f , g and k with the information matrix $X(\mathbf{x})$, respectively, are sharp **on $\mathcal{W}$** .

In general, the compositions do not have a unique minimizer.



A Custom Branch-and-Bound for OEDP under Matrix Means (Co-BnB)

Ahipaşaoğlu 2021

- Coordinate-Descent-like algorithm for the nodes.
- Developed for $m \gg n$.

$$\begin{aligned} \max_{\mathbf{w}} \quad & \log(\phi(X(\mathbf{w}))) \\ \text{s.t.} \quad & \sum_{i=1}^m w_i = 1 \\ & \mathbf{w} \in [0, 1]^m \\ & N\mathbf{w} \in \mathbb{Z}_{\geq 0}^m \end{aligned} \tag{M-OEDP}$$

- $\mathbf{w}$ can be interpreted as a probability distribution.
- Exploit connection to the Minimum Volume Enclosing Ellipsoid Problem (MVEP) for the termination criteria.

Direct Conic Formulation

coey2022conic; Coey, Kapelevich, and Vielma 2022a; Coey, Lubin, and Vielma 2020

- `Pajarito.jl` is a mixed-integer convex solver with conic certificates.
- `Hypatia.jl` is an interior point solver for conic optimization problems.
- D-Criterion:

$$\mathcal{K}_{\log \det} := \text{cl} \left\{ (u, v, W) \in \mathbb{R} \times \mathbb{R}_{>0} \times \mathbb{S}_{++}^n \mid u \leq v \log \det(W/v) \right\}$$

- A-Criterion: Dual of

$$\mathcal{K}_{\text{sepspec}} := \text{cl} \left\{ (u, v, w) \in \mathbb{R} \times \mathbb{R}_{>0} \times \text{int}(Q) \mid u \geq v \varphi(w/v) \right\}$$

- Q is the PSD cone and φ is the negative square root.
- The convex conjugate of the negative square root is the trace inverse.

Second-Order Conic Formulation (SOCP)

Sagnol 2011; Sagnol and Harman 2015

- In Sagnol 2011 the SOCP formulation for the continuous problem was introduced.
- The SOCP formulation of the exact formulation of OEDP was shown in Sagnol and Harman 2015.
- In theory, a nice result, but in practice, the problem size becomes much larger.
- For the A-Optimal Problem, we have $2m(n + 1)$ variables and $2(n + 1) + m$ constraints.
- For the D-Optimal Problem, we have $2m(1 + n) + n^2 + 1$ variables and $n(m + 1) + 3m + 4$ constraints.

SOCP A-Criterion

$$\begin{aligned} \min_{\substack{\mu \in \mathbb{R}^m \\ \mathbf{x} \in \mathbb{Z}^m \\ \forall i \in [m] \ Y_i \in \mathbb{R}^{1 \times n}}} \quad & \sum_{i=1}^m t_i \\ \text{s.t.} \quad & \sum_{i=1}^m A_i Z_i = I \\ & \forall i \in [m], \ \|Z_i\|_F^2 \leq t_i x_i \\ & \sum_{i=1}^m x_i = N \end{aligned} \quad (\text{A-SOCP})$$

SOCP D-Criterion

$$\min_{\substack{\mathbf{w} \in \mathbb{R}_{\geq 0}^m, \mathbf{x} \in \mathbb{Z}^m \\ J \in \mathbb{R}^{n \times n} \\ \forall i \in [m] \ Z_i \in \mathbb{R}^{1 \times n} \\ \forall i \in [m], j \in [n] \ t_{ij} \in \mathbb{R}_{\geq 0}}} \prod_{i=1}^m J_{ii}^{1/m}$$

$$\text{s.t. } \sum_{i=1}^m A_i Z_i = J$$

J lower triangle matrix

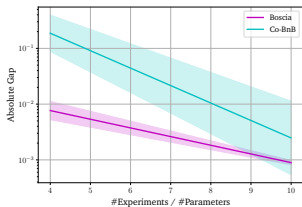
(D-SOCP)

$$\forall i \in [m], j \in [n] \ \|Z_i e_j\|_F^2 \leq t_{ij} w_i$$

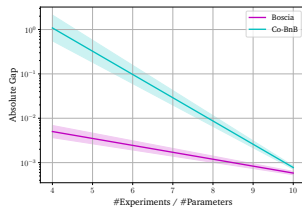
$$\forall j \in [n] \ \sum_{i=1}^m t_{ij} \leq J_{jj}$$

$$\mathbf{l} \leq \mathbf{x} \leq \mathbf{u} \text{ and } \sum_{i=1}^m w_i = 1$$

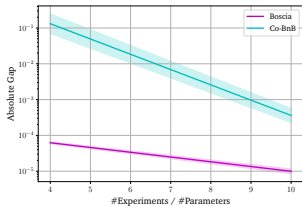
Effect of the conditioning of the problem



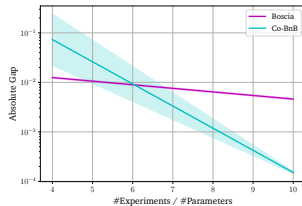
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