

Block Subset Selection based on Randomized QR with Column Pivoting

A Tensor \star_M Product Framework

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Motivation: Optimal Experiment Design

Goal: Find the best way to acquire more data, i.e. optimal experiment design (OED).

Definition (Fisher Information Matrix (FIM))

If there are m model parameters in experiment design c , with parameters $\boldsymbol{\theta} = (\theta_1 \ \theta_2 \ \cdots \ \theta_m)^\top$, and $f(X, \boldsymbol{\theta})$ is a probability density function, then the Fisher Information Matrix becomes

$$[\mathbf{F}(c, \boldsymbol{\theta})]_{i,j} = -\mathbb{E} \left[\left(\frac{\partial}{\partial \theta_i} \log f(X; \boldsymbol{\theta}) \right) \left(\frac{\partial}{\partial \theta_j} \log f(X; \boldsymbol{\theta}) \right) \mid \boldsymbol{\theta} \right] \quad (1)$$

If data is collected under design c with parameters $\boldsymbol{\theta}$, we want to solve

$$\max_{c \in \mathcal{S}} \phi(\mathbf{F}(c, \boldsymbol{\theta})) = \max_{c \in \mathcal{S}} \frac{1}{2} \log \det \mathbf{F}(c, \boldsymbol{\theta}) \quad (2)$$

over all designs in the design space, $\mathcal{S} \subset \mathcal{C}$.



(Block) Volume is important!

Definition (volume)

The *volume* of a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ is the product of the singular values:

$$\text{vol}(\mathbf{A}) = \prod_{j=1}^{\min(m,n)} \sigma_j(\mathbf{A}), \quad \text{and} \quad \text{if } m = n, \text{vol}(\mathbf{A}) = |\det(\mathbf{A})| \quad (3)$$

Under statistic assumptions,

$$\mathbf{F} = \begin{bmatrix} \mathbf{J}^\top & \mathbf{I} \\ & \mathbf{I} \end{bmatrix} = \mathbf{J}^\top \mathbf{J} + \mathbf{I} \quad \implies \quad \log \det \mathbf{F} = \log \det (\mathbf{J}^\top \mathbf{J} + \mathbf{I})$$

We **must** select a principal submatrix that respect block structure.



Block Column Pivoted Householder QR: Computing $\mathbf{AP} = \mathbf{QR}$

- 1: **function** col_block_pivoted_qr(\mathbf{A} , k)
- 2: $\mathbf{W} = \text{copy}(\mathbf{A})$ ▷ \mathbf{A} is $m \times (nb)$, require $k \leq \min\{m/b, n\}$
- 3: $\pi = (1, \dots, n)$
- 4: $i = 1$ ▷ i indicates the i^{th} column block
- 5: **while** $i \leq k$ **do** ▷ find and apply the pivot
- 6: $p = \text{find_pivot}(\mathbf{W}(:, i:n))$
- 7: $p = p + i - 1$
- 8: $\mathbf{W}(:, [i, p]) = \mathbf{W}(:, [p, i])$
- 9: $\pi([i, p]) = \pi([p, i])$ ▷ update \mathbf{W} and i
- 10: $[\mathbf{V}, \sim] = \text{qr}(\mathbf{W}(:, i), \text{"econ"})$
- 11: $\mathbf{W}(:, i) = \mathbf{V}$
- 12: $i = i + 1$
- 13: $\mathbf{W}(:, i:n) = (\mathbf{I}_m - \mathbf{V}\mathbf{V}^T)\mathbf{W}(:, i:n)$
- 14: **end while**
- 15: $\mathbf{Q} = \mathbf{W}(:, i:k)$
- 16: $\mathbf{R} = \mathbf{Q}^T \mathbf{A}(:, \pi)$
- 17: **return** ($\mathbf{Q}, \mathbf{R}, \pi$)



Connection between Volume, Singular Values, and Rank Revealers

Definition (Rank-revealer [1])

If there is a $\mu_{m,n,k} \in \text{poly}(m, n, k)$ such that for any $\mathbf{A} \in \mathbb{R}^{m \times n}$ and any $1 \leq k \leq \min(m, n)$, the *rank revealer* computes a rank $\leq k$ matrix \mathbf{A}_k such that

$$\frac{1}{\mu_{m,n,k}} \sigma_j(\mathbf{A}) \leq \sigma_j(\mathbf{A}_k) \leq \mu_{m,n,k} \sigma_j(\mathbf{A}), \quad 1 \leq j \leq k \quad (4)$$



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and

$$\frac{1}{\mu_{m,n,k}} \sigma_{k+j}(\mathbf{A}) \leq \sigma_j(\mathbf{A} - \mathbf{A}_k) \leq \mu_{m,n,k} \sigma_{k+j}(\mathbf{A}), \quad 1 \leq j \leq \min(m, n) - k \quad (5)$$



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Truncated SVD:

- rank-revealer:
 $\mu = 1 \odot$



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$$\mathcal{O}(mn \min(m, n)) \odot$$



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- practical: $\mathcal{O}(kmn) \odot$



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 $\mu = 2^k \sqrt{n-k} \odot$



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ν -Near local max vol QR [1]:

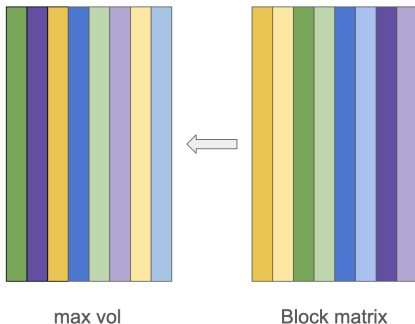
- rank-revealer:
 $\mu = \sqrt{1 + 5\nu^2 kn} \odot$



This ν -max vol framework is inadequate for our setting: a toy example

Let $\mathbf{A} = [\mathbf{A}_1 \ \mathbf{A}_2 \ \mathbf{A}_3 \ \mathbf{A}_4]$, where $\mathbf{A}_i \in \mathbb{R}^{m \times 2}$, $\|\mathbf{A}_i(:, 1)\| = 1$, $\|\mathbf{A}_i(:, 2)\| = \epsilon$, for all $i = 1, \dots, 4$.

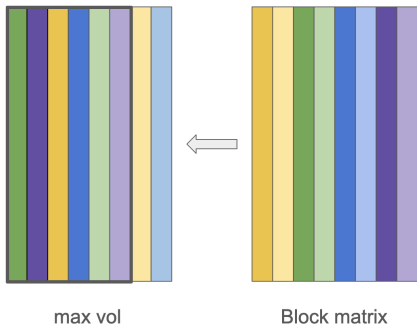
Goal: choose three blocks (six rows) such that we maximize $\text{vol}([\mathbf{A}_{\pi(1)} \ \mathbf{A}_{\pi(2)} \ \mathbf{A}_{\pi(3)}])$



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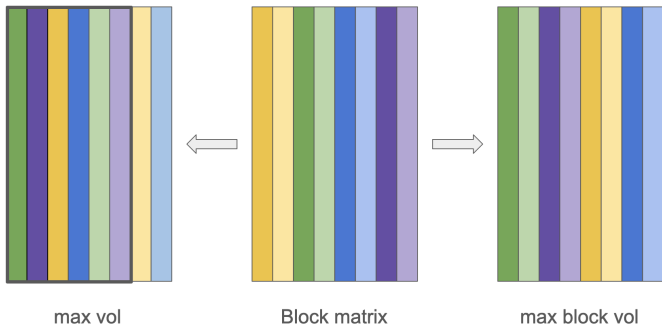
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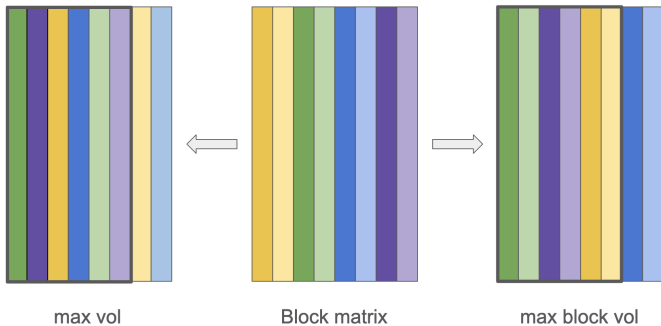
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Greedy OED as block pivoted QR

Let $b \geq 2$ be the block size. Define the helper function `expand` such that

$$\text{expand}([\]) = [\] \quad \text{and} \quad \text{expand}([i] + \mathcal{S}) = ib : (i + 1)b + \text{expand}(\mathcal{S})$$

Fact: If $[\sim, R_S] = \text{qr} \left(\begin{bmatrix} \mathbf{J}_C^\top \\ \mathbf{I}_{|C|b} \end{bmatrix} \left(:, \text{expand}(\mathcal{S}) \right) \right)$, then $\log \det(\mathbf{F}(c, \boldsymbol{\theta})) = \log \det(R_S)$

Idea: Define a suitable `block_pivoted_qr` function that we will call as

$$[\sim, R, \text{piv}] = \text{block_pivoted_qr} \left(b, \begin{bmatrix} \mathbf{J}_C^\top \\ \mathbf{I}_{|C|b} \end{bmatrix} \right),$$

and use $\mathcal{C}_{\text{ranked}} = \text{expand}^{-1}(\text{piv})$. Truncate $\mathcal{C}_{\text{ranked}}$ to get \mathcal{S} .



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The $\star_{\mathbf{M}}$ Product

Transform Domain

Let $\hat{\mathcal{T}} \in \mathbb{R}^{m \times n \times b}$ with i, j^{th} tube equal to the product of the i, j^{th} tube of tensor $\mathcal{T} \in \mathbb{R}^{m \times n \times b}$ with matrix $\mathbf{M} \in \mathbb{R}^{b \times b}$ by $\hat{\mathcal{T}} = \mathcal{T} \times_3 \mathbf{M}$,

$$(\mathcal{T} \times_3 \mathbf{M})(i, j, :) = \mathbf{M}\mathcal{T}(i, j, :).$$

Facewise-product

Here, the frontal facewise-product is defined in frontal slice k as

$$(\mathcal{T}_1 \Delta \mathcal{T}_2)(:, :, k) = \mathcal{T}_1(:, :, k) \mathcal{T}_2(:, :, k).$$

Definition ($\star_{\mathbf{M}}$ product [4, 5])

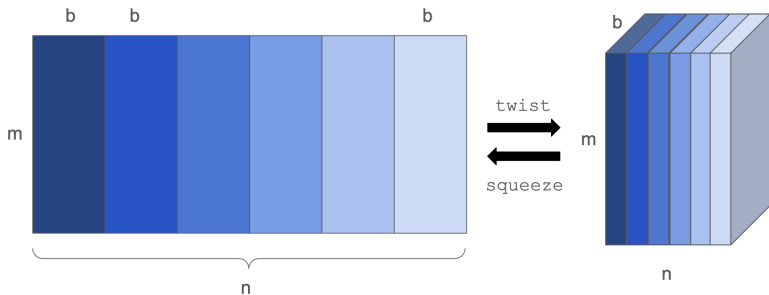
The $\star_{\mathbf{M}}$ product for invertible \mathbf{M} is defined as

$$\mathcal{A} \star_{\mathbf{M}} \mathcal{B} := ((\mathcal{A} \times_3 \mathbf{M}) \Delta (\mathcal{B} \times_3 \mathbf{M})) \times_3 \mathbf{M}^{-1}. \quad (6)$$

Block setting arises naturally in OED

We are concerned with blocks because

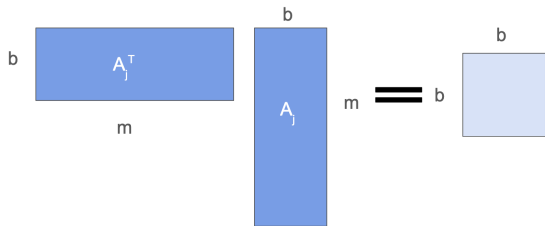
- m is the number of model parameters,
- b is the time series data, and
- n is the number of distinct experiments run.



Determine the “most important” prior experiment

Initialize the permutation $\pi = (1, \dots, n)$.

For each $1 \leq j \leq n$, compute $s_j = \log \det(\mathbf{A}_j^\top \mathbf{A}_j)$.



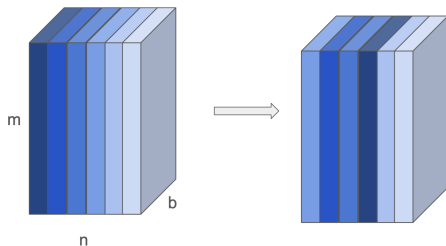
$$s_j = \log \det \left\{ \begin{array}{c} b \\ \square \\ b \end{array} \right\}$$

Then $k = \arg \max\{s_1, \dots, s_n\}$.

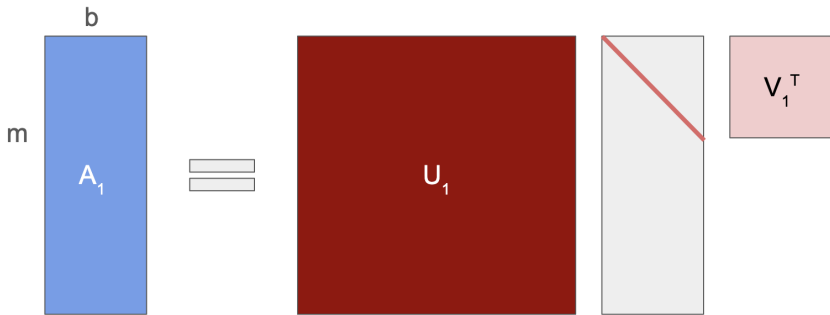
Permute the highest score'd experiment to the front.

Since $k = \arg \max\{s_1, \dots, s_n\}$, we let

- $\mathcal{A}(:, 1, :) \leftrightarrow \mathcal{A}(:, k, :)$ and
- $\pi(1) \leftrightarrow \pi(k)$



Obtain the right singular vectors of the best experiment



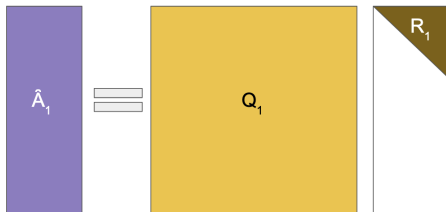
Update $\mathcal{A} \leftarrow \mathcal{A} \times_3 \mathbf{V}_1$



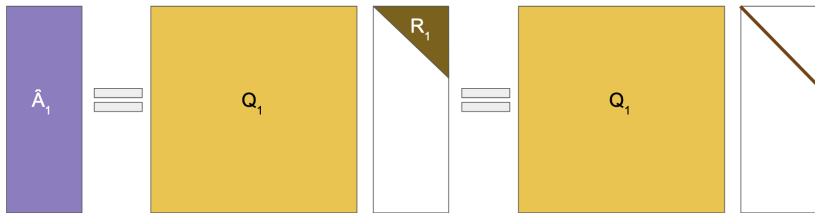
This is equivalent to lateral slice updates $\mathbf{A}_j \leftarrow \mathbf{A}_j \mathbf{V}_1^\top$



Compute the matrix QR on the transformed first lateral slice

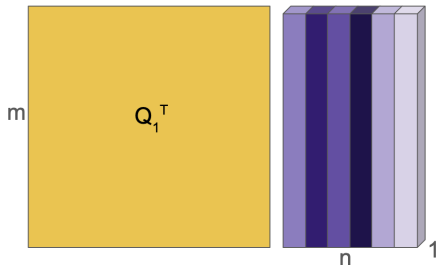


Compute the matrix QR on the transformed first lateral slice



Update the frontal slices

With access to \mathbf{Q}_1^T , we perform $\mathcal{A}(:, :, \ell) \leftarrow \mathbf{Q}_1^T \mathcal{A}(:, :, \ell)$ for all $\ell \in \{1, \dots, b\}$



This is equivalent to $\mathbf{A}_j \leftarrow \mathbf{Q}^T \mathbf{A}_j$



The \star_M product Decomposition

Let $\mathcal{A}^{(1)}$ denote the value of \mathcal{A} on *input* to the above procedure. By the end of the procedure we have a decomposition of the form

$$\mathcal{A}^{(1)} \star_{\mathbf{V}_1} \mathcal{P}^{(1)} = \mathcal{Q}^{(1)} \star_{\mathbf{V}_1} \mathcal{R}^{(1)}, \quad (7)$$

where $\mathcal{P}^{(1)}$, $\mathcal{Q}^{(1)}$, and $\mathcal{R}^{(1)}$ are defined implicitly; using π and \mathbf{V}_1 as they exist at step 3, and using \mathbf{Q}_1 from step 5, we have

$$[\mathcal{P}^{(1)} \times_3 \mathbf{V}_1](:, :, \ell) = \mathbf{I}_n(:, \pi) \quad (8)$$

$$[\mathcal{Q}^{(1)} \times_3 \mathbf{V}_1](:, :, \ell) = \mathbf{Q}_1 \quad (9)$$

$$[\mathcal{R}^{(1)} \times_3 \mathbf{V}_1](:, :, \ell) = \mathbf{Q}_1^\top [\mathcal{A}^{(1)} \times_3 \mathbf{V}_1](:, :, \ell) \mathbf{I}_n(:, \pi), \quad (10)$$

for each $\ell \in \{1, \dots, p\}$.



The \star_M Connection to Column Block Pivoted QR

```
1: function col_block_pivoted_qr(A, k)
2: W = copy(A)
3:  $\pi = (1, \dots, n)$ 
4: i = 1
5: while i ≤ k do
6:   p = find_pivot(W(:, i:n))
7:   p = p + i - 1
8:   W(:, [i, p]) = W(:, [p, i])
9:    $\pi$ ([i, p]) =  $\pi$ ([p, i])
10:  [V, ~] = qr(W(:, i), "econ")
11:  W(:, i) = V
12:  i = i + 1
13:  W(:, i:n) = (Im - VVT)W(:, i:n)
14: end while
15: Q = W(:, i:k)
16: R = QTA(:,  $\pi$ )
17: return (Q, R,  $\pi$ )
```

Consider the $m \times bn$ unfolding
 $\mathbf{A} := [\mathbf{A}_j]_{j=1}^n$ of \mathcal{A} .



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- Lines 8 and 9 are equivalent to right-multiplying \mathbf{A} by $\mathbf{I}_n(:, \pi) \otimes \mathbf{I}_b$.



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- Lines 8 and 9 are equivalent to right-multiplying \mathbf{A} by $\mathbf{I}_n(:, \pi) \otimes \mathbf{I}_b$.
- Line 13 is equivalent to right-multiplying \mathbf{A} by $\mathbf{I}_n \otimes \mathbf{V}_1^T$.



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Consider the $m \times bn$ unfolding $\mathbf{A} := [\mathbf{A}_j]_{j=1}^n$ of \mathcal{A} .

- Lines 8 and 9 are equivalent to right-multiplying \mathbf{A} by $\mathbf{I}_n(:, \pi) \otimes \mathbf{I}_b$.
- Step 4 is equivalent to right-multiplying \mathbf{A} by $\mathbf{I}_n \otimes \mathbf{V}_1^T$.
- Line 16 is equivalent to left-multiplying \mathbf{A} by \mathbf{Q}_1^T .



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15: Q = W(:, i:k)
16: R = QTA(:,  $\pi$ )
17: return (Q, R,  $\pi$ )

```

Consider the $m \times bn$ unfolding $\mathbf{A} := [\mathbf{A}_j]_{j=1}^n$ of \mathcal{A} .

- Lines 8 and 9 are equivalent to right-multiplying \mathbf{A} by $\mathbf{I}_n(:, \pi) \otimes \mathbf{I}_b$.
- Step 4 is equivalent to right-multiplying \mathbf{A} by $\mathbf{I}_n \otimes \mathbf{V}_1^T$.
- Line 16 is equivalent to left-multiplying \mathbf{A} by \mathbf{Q}_1^T .

We recurse on the $(m - b) \times (nb - b)$ submatrix $\mathbf{A}((b + 1):m, (b + 1):nb)$.



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Randomization can help!

The matrix $\mathbf{A} = \begin{bmatrix} \mathbf{J}_c^\top \\ \mathbf{I}_{|c|b} \end{bmatrix}$ is large!

Suppose we know \mathbf{J}_c has p columns, and we want to narrow down to k experiments.

For a tuning parameter $\gamma \in [1, 2]$, set $d = \lceil \gamma bk \rceil$. Our sketching matrix becomes

$$\mathbf{\Omega} = [\mathbf{\Omega}_1 \quad \mathbf{\Omega}_2,] \quad (11)$$

where $\mathbf{\Omega}_1 \in \mathbb{R}^{d \times p}$ and $\mathbf{\Omega}_2 \in \mathbb{R}^{d \times |c|b}$ are i.i.d. mean zero unit variance Gaussian entries. Instead of running the algorithm on \mathbf{A} , instead we can make pivot decisions on $\mathbf{\Omega A}$

$$\mathbf{\Omega A} = \mathbf{\Omega}_1 \mathbf{J}_c^\top + \mathbf{\Omega}_2$$

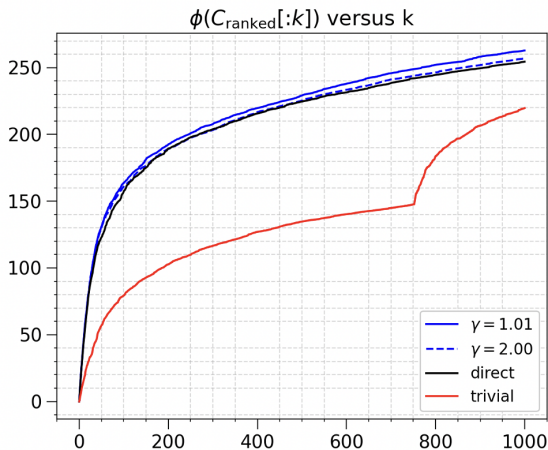


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Numerical Experiment: Choosing Quantum Gates Efficiently



Use randLAPACK's randomized block QRCP algorithm to make 1000 block pivot decisions.

Total time for block pivoted QR on sketch: **36 sec**

Total time for each input matrix:

- **SA** (direct): 48 minutes
- **$S\Omega_{2.00}A$** : 18 minutes
- **$S\Omega_{1.01}A$** : 7 minutes



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Open questions:

- max-volume pivoting is NP-hard, so what greedy heuristic should we use?
- can we quantify the suboptimality of the greedy method? sketched greedy method?



Questions?

Thank You!

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References

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