RECENT ADVANCES IN POSITIVE SEMIDEFINITE MATRIX APPROXIMATION

Cameron Musco (Microsoft Research)

Simons Workshop on RandNLA & Applications

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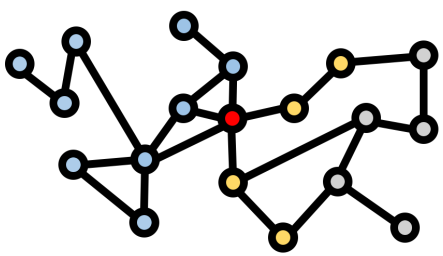
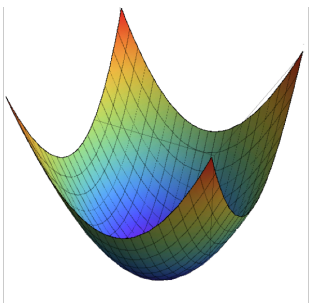
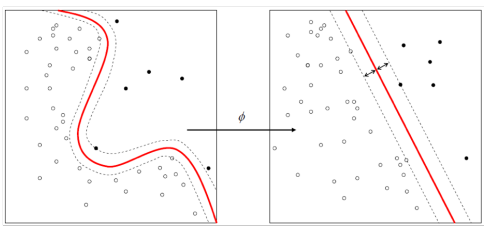
- Include graph Laplacians, Gram matrices and kernel matrices, covariance matrices, Hessians for convex functions, etc.







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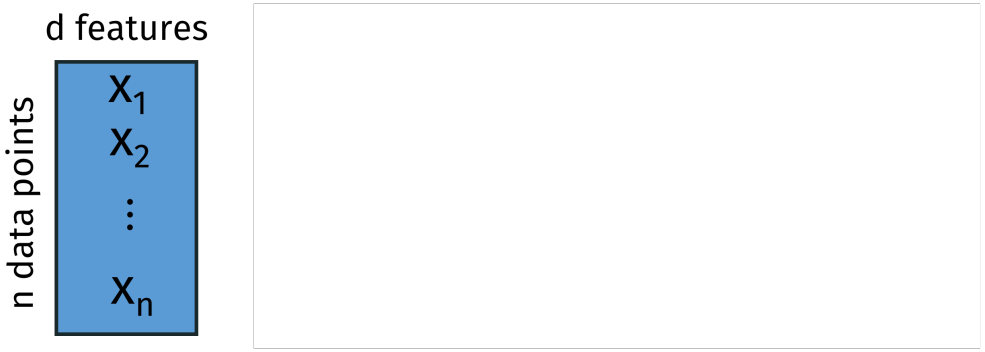

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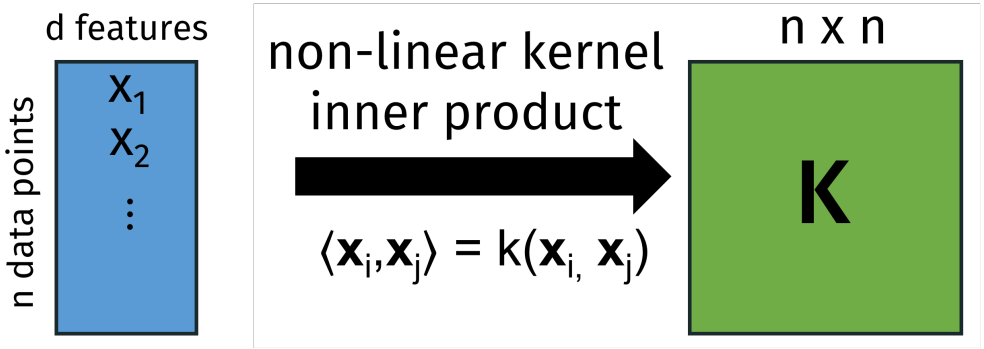

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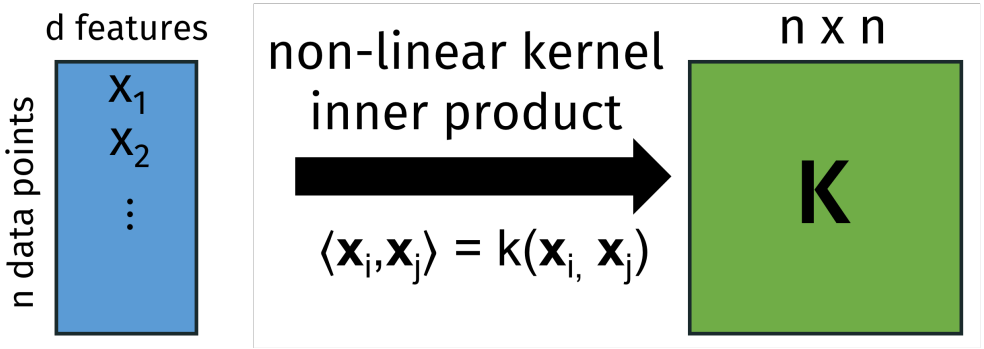

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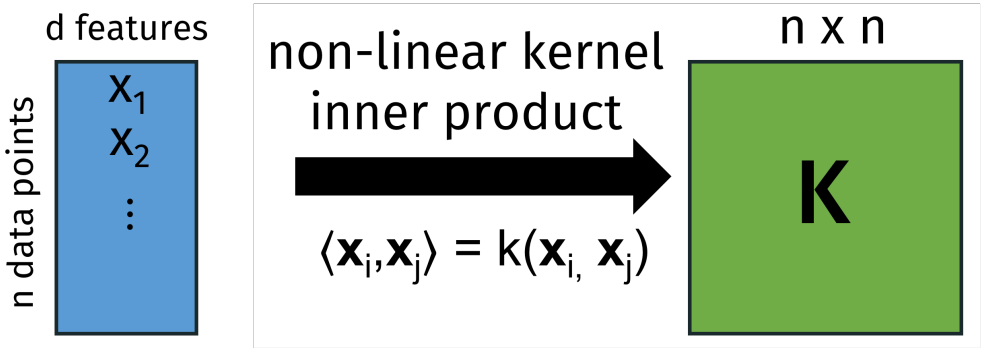

- Even writing down $\mathbf{K}$ or performing a single iteration of an iterative solver takes $\Omega(n^2)$ time.
- For $n = 100,000$, $\mathbf{K}$ has 10 billion entries. Takes 80 GB of storage if each is a `double`.

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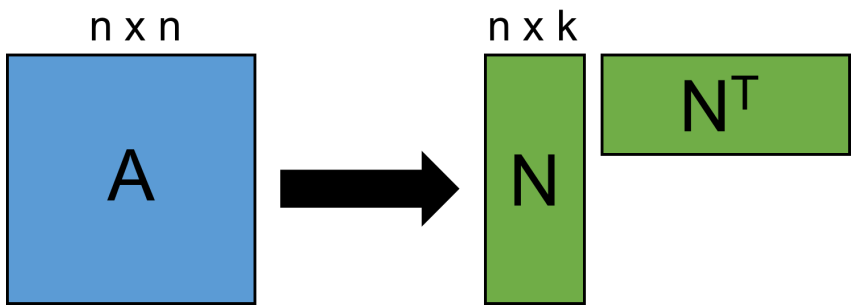
- E.g., exploit low-rank structure.



PSD MATRIX APPROXIMATION

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  - Incomplete Cholesky factorization (Fine & Scheinberg '02, Bach & Jordan '02).
  - Entrywise sampling (Achlioptas, McSherry, & Schölkopf '01).
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- A variety of approximation bounds, some under assumptions. Nothing as strong as e.g., $\|\mathbf{A} - \mathbf{N}\mathbf{N}^T\|_F^2 \leq (1+\epsilon)\|\mathbf{A} - \mathbf{A}_k\|_F^2$.

Our Goal: Give strong worst case approximation bounds for sublinear time (i.e., $o(n^2)$) methods. Build a new toolkit for PSD matrix algebra in the process.

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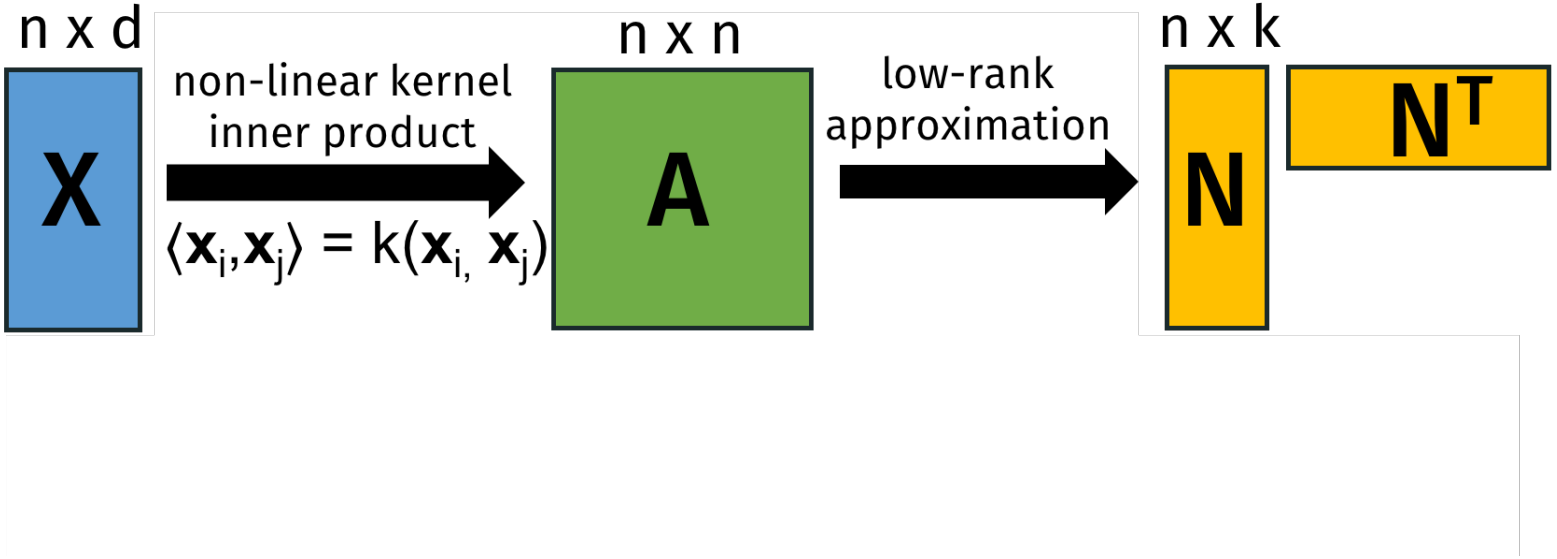

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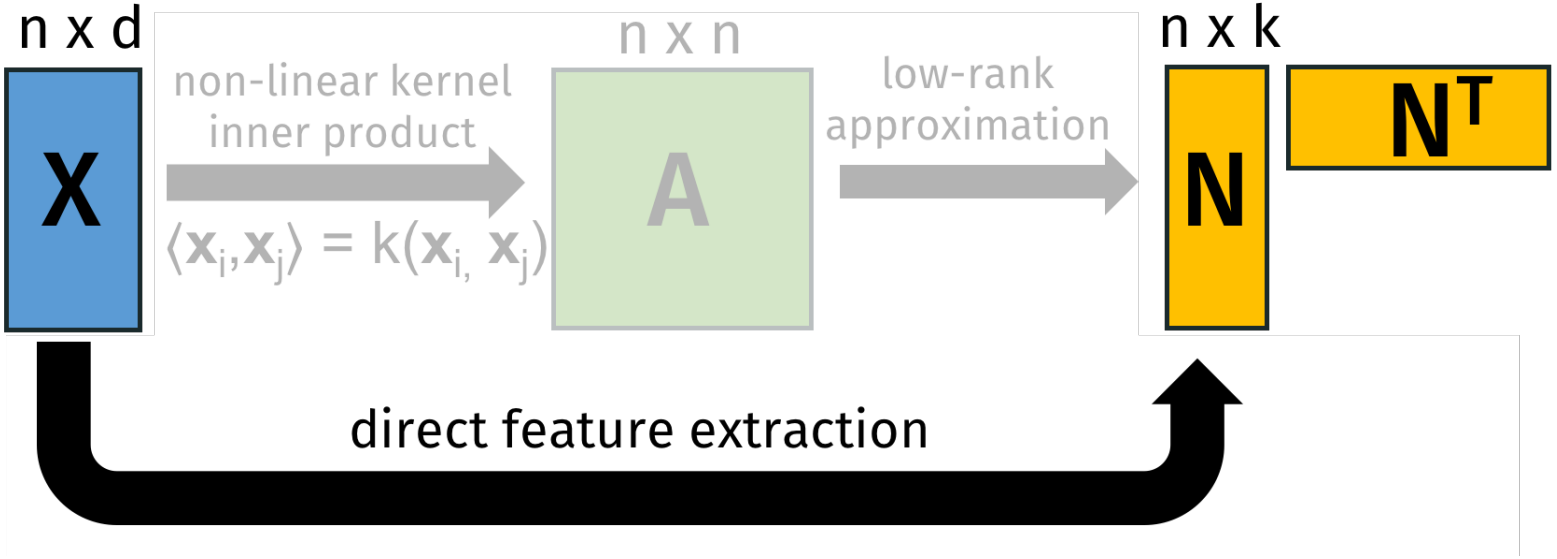

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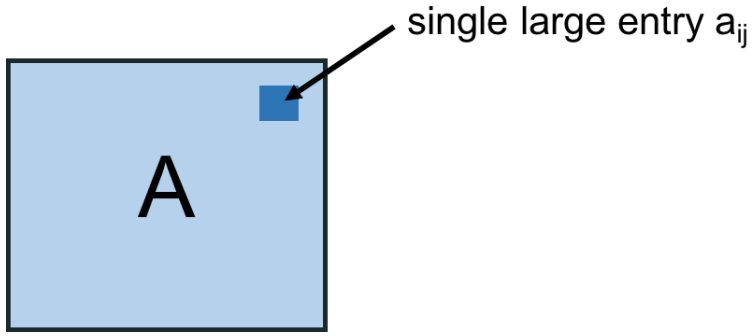

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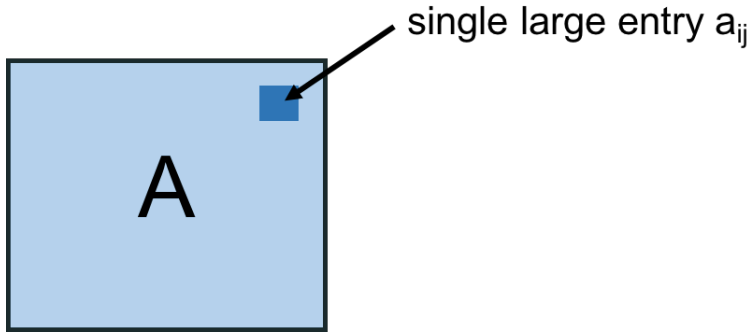

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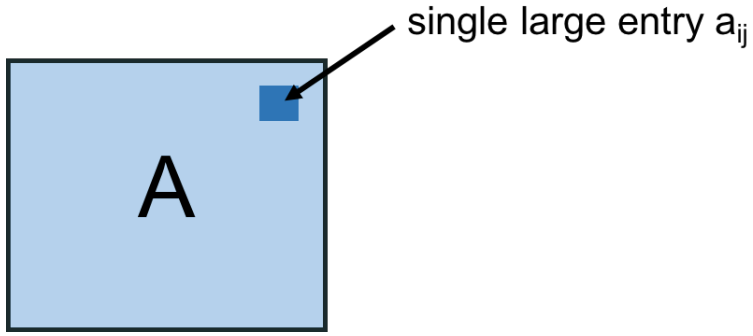


- Rules out, e.g., for any $\Delta < 1$, approximation of the form:

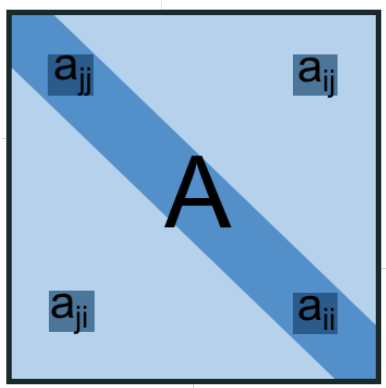
$$\|\mathbf{A} - \mathbf{N}\mathbf{N}^T\|_F \leq \Delta \|\mathbf{A}\|_F^2.$$

WHAT ABOUT FOR PSD MATRICES?

Observation: For PSD $\mathbf{A}$, we have for any entry $\mathbf{a}_{ij}$:

$$\mathbf{a}_{ij} \leq \max(\mathbf{a}_{ii}, \mathbf{a}_{jj})$$

since otherwise $(\mathbf{e}_i - \mathbf{e}_j)^T \mathbf{A}(\mathbf{e}_i - \mathbf{e}_j) < 0$.



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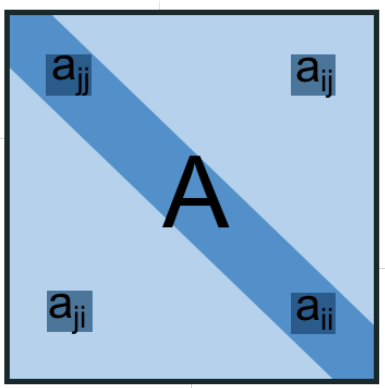
- So we can find any 'hidden' heavy entry by looking at its corresponding diagonal entries.



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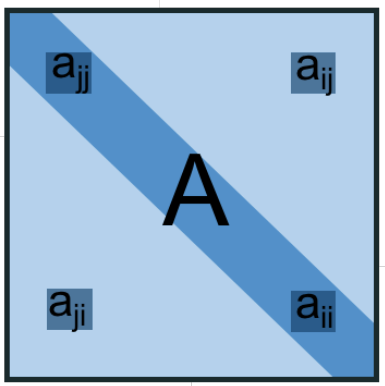

Question: How can we use additional structure arising from PSD-ness to achieve non-trivial approximation in sublinear time?

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Very Simple Fact: Every PSD matrix $\mathbf{A} \in R^{n \times n}$ can be written as $\mathbf{B}^T\mathbf{B}$ for some $\mathbf{B} \in \mathbb{R}^{n \times n}$.

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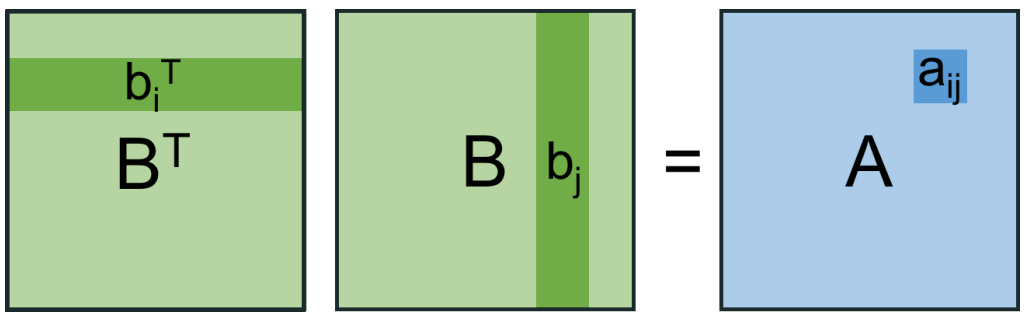
- Letting $\mathbf{b}_1, ..., \mathbf{b}_n$ be the columns of $\mathbf{B}$, the entries of $\mathbf{A}$ contain every pairwise dot product $\mathbf{a}_{ij} = \mathbf{b}_i^T\mathbf{b}_j$.



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Another View: $\mathbf{A}$ contains a lot of information about the column span of $\mathbf{B}$ in a very compressed form – with every pairwise dot product stored as $\mathbf{a}_{ij}$.

FACTOR MATRIX LOW-RANK APPROXIMATION

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- E.g. an optimal low-rank approximation for B gives an optimal low-rank approximation for $\mathsf{A} = \mathsf{B}^T\mathsf{B}$.

Low-rank approximation via adaptive sampling

Theorem (Deshpande, Vempala '06)

For any $\mathsf{B} \in \mathbb{R}^{n \times n}$, *there exists a subset of* $\tilde{O}(k^2/\epsilon)$ *columns whose span contains* $\mathsf{Z} \in \mathbb{R}^{n \times k}$ *satisfying:*

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Adaptive Sampling

Initially, start with an empty column subset $\mathcal{S} := \{\}$.

For $t = 1, \ldots, \tilde{O}(k^2/\epsilon)$

Let $\mathbf{P}_{\mathcal{S}}$ be the projection onto the columns in $\mathcal{S}$.

Add $\mathbf{b}_i$ to $\mathcal{S}$ with probability $\frac{\|\mathbf{b}_i - \mathbf{P}_{\mathcal{S}}\mathbf{b}_i\|^2}{\sum_{i=1}^{n}\|\mathbf{b}_i - \mathbf{P}_{\mathcal{S}}\mathbf{b}_i\|^2}$.

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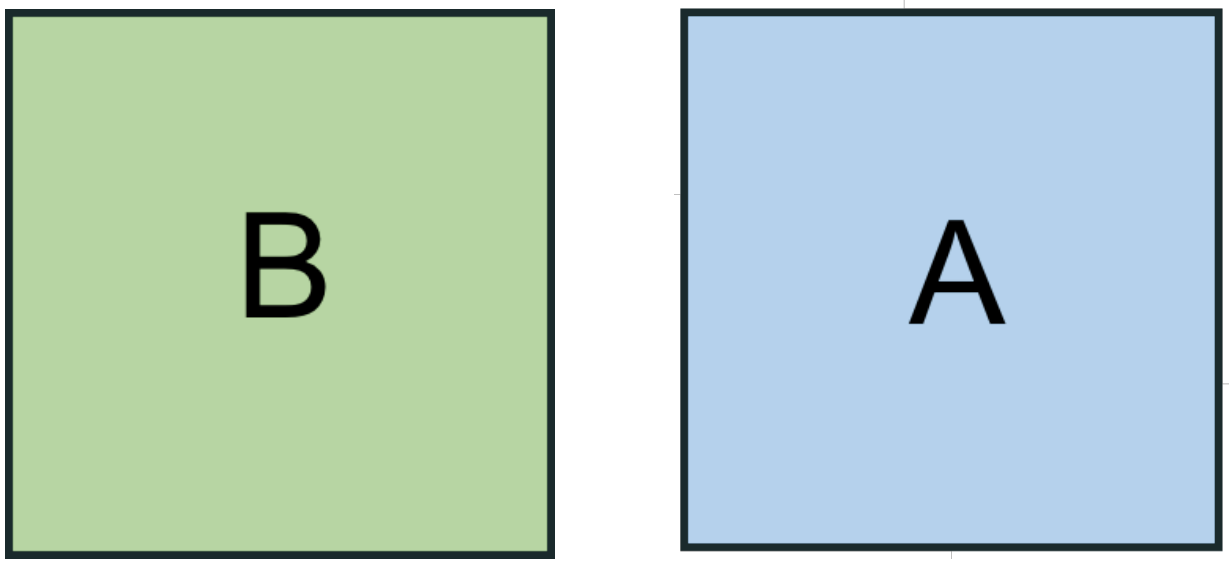

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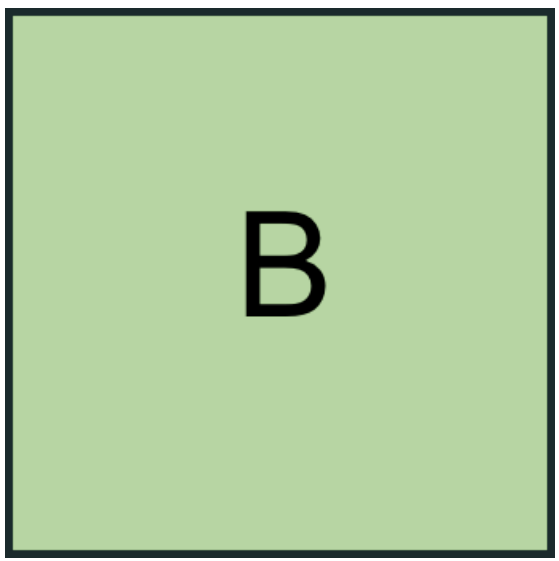

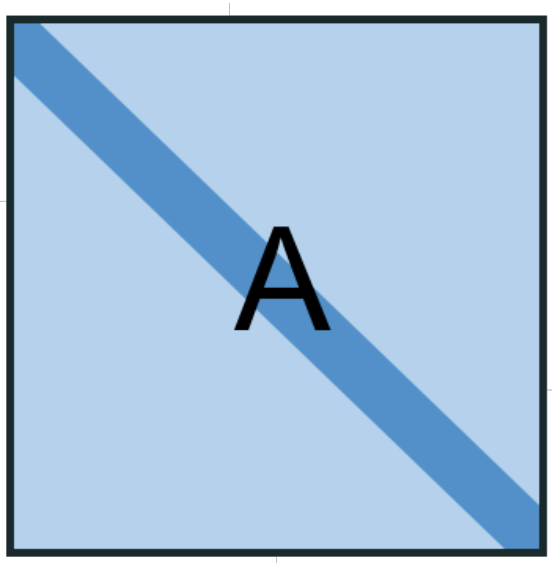

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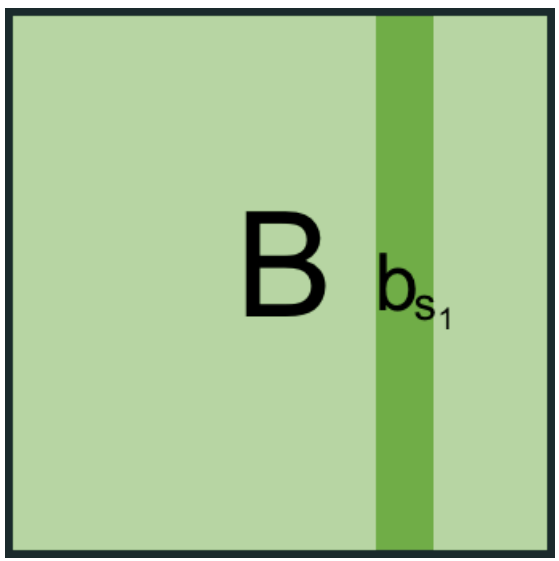

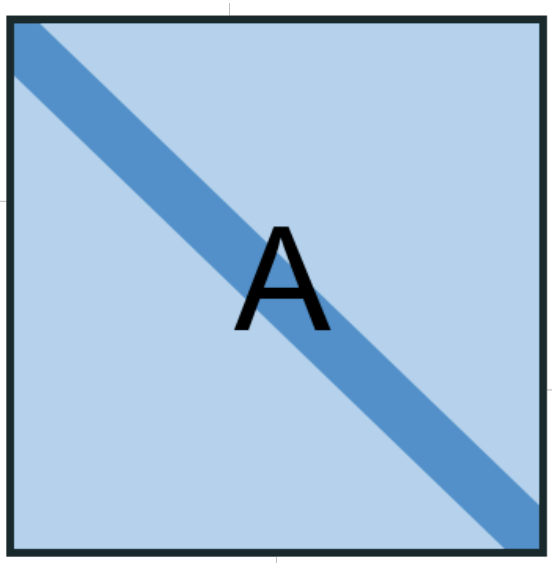

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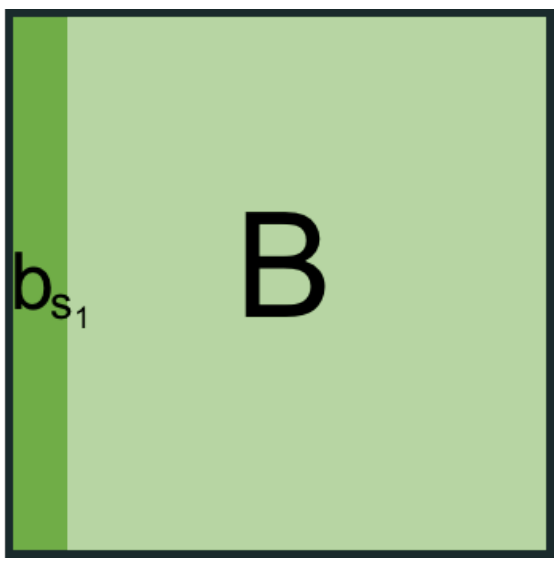

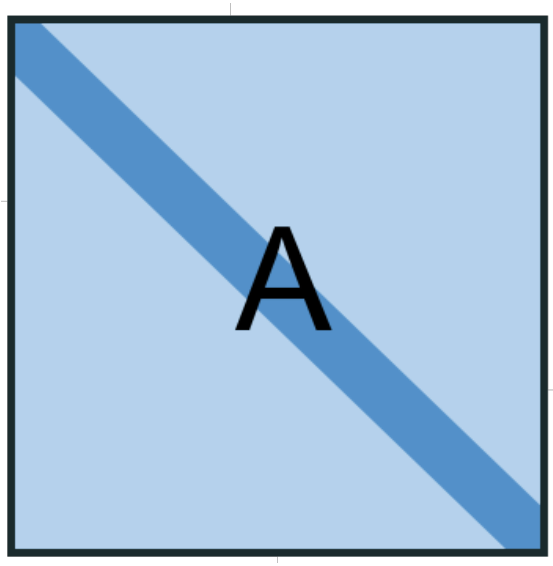

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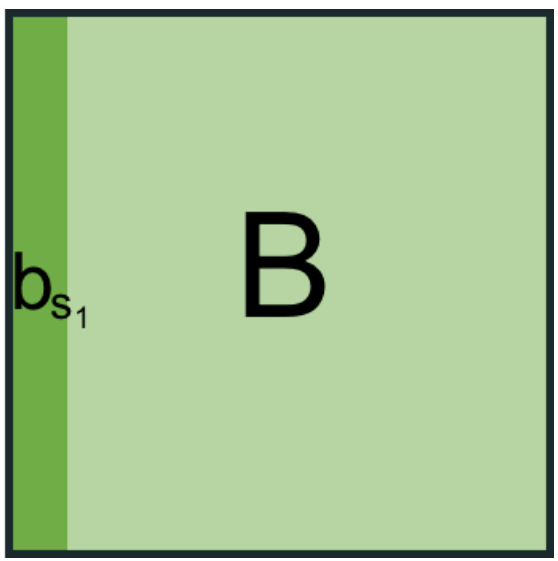

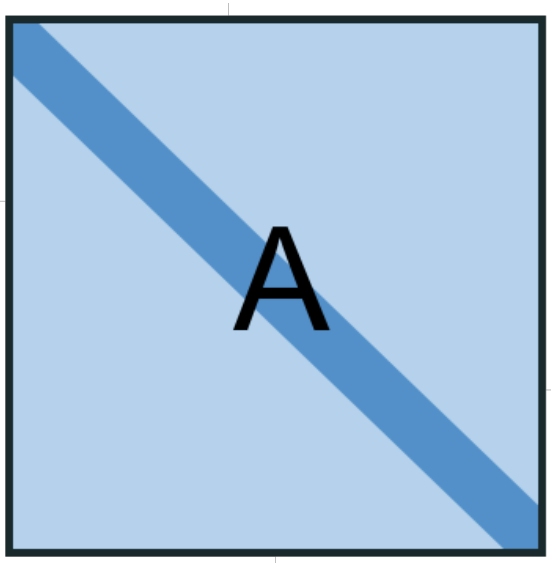

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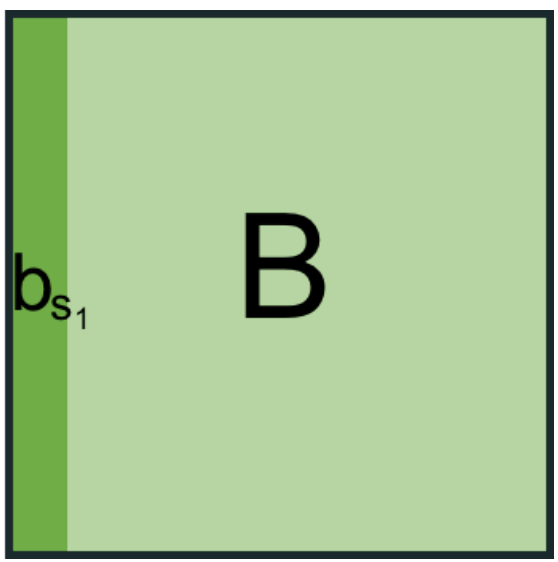

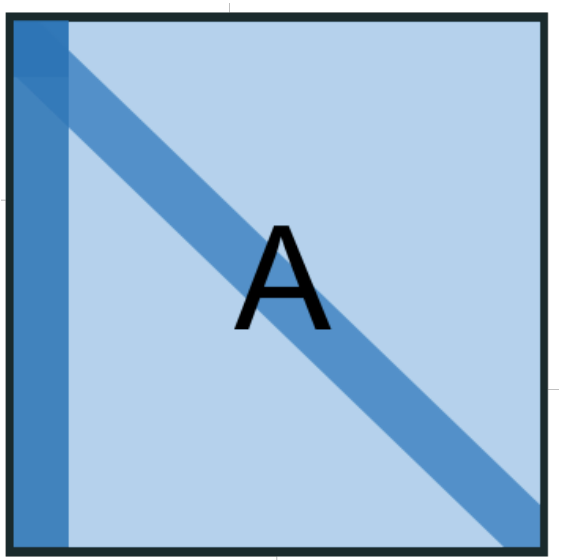

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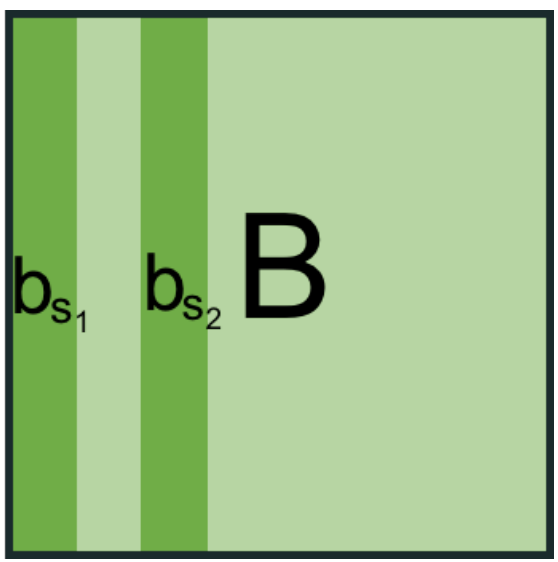

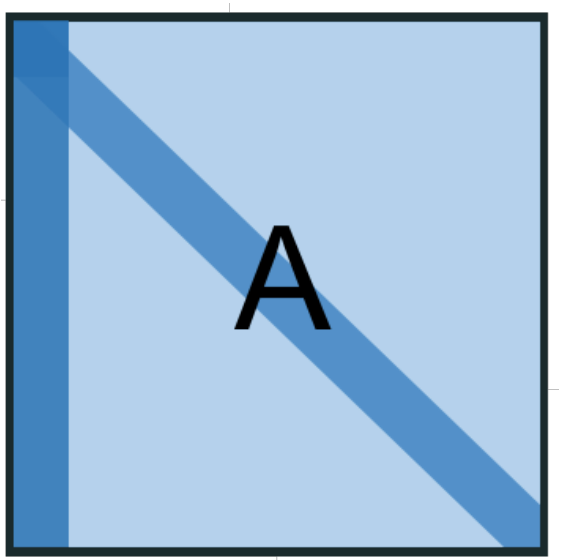

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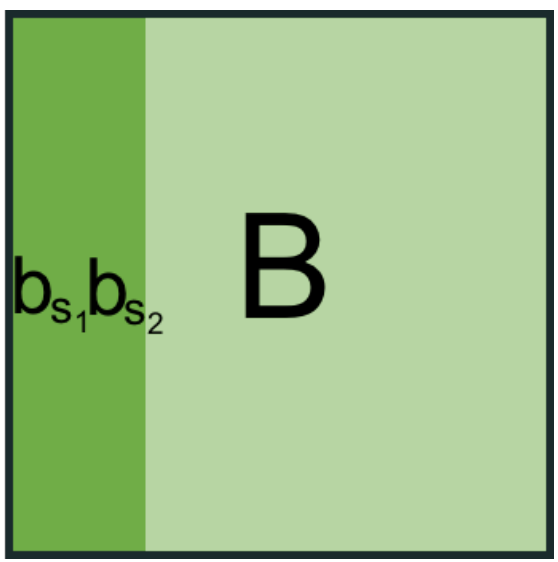

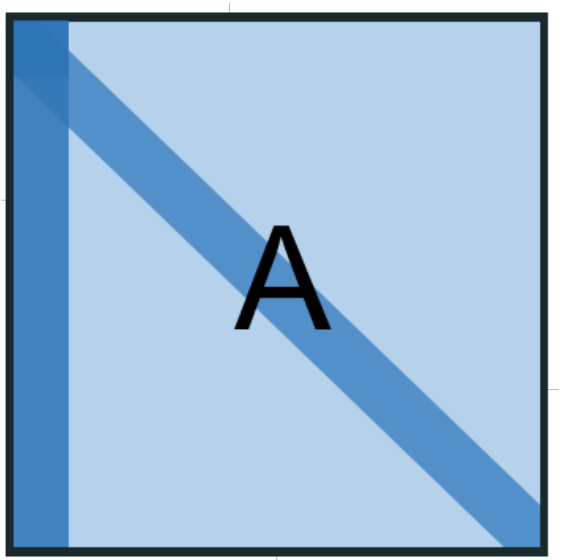

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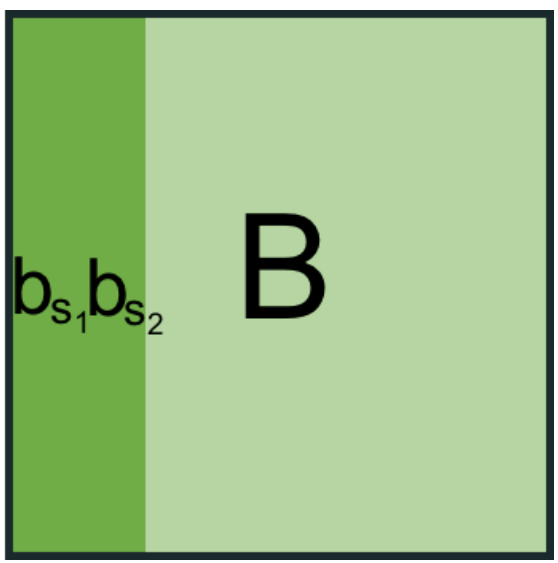

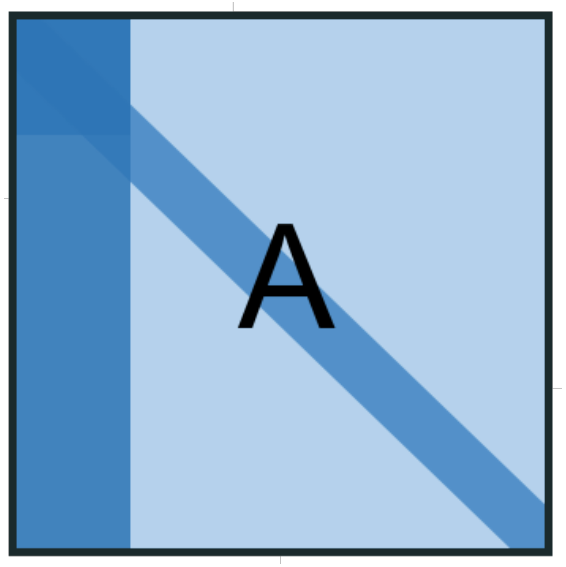

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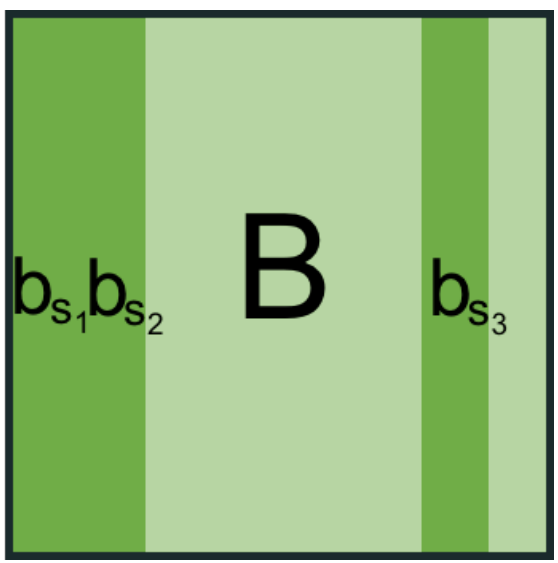

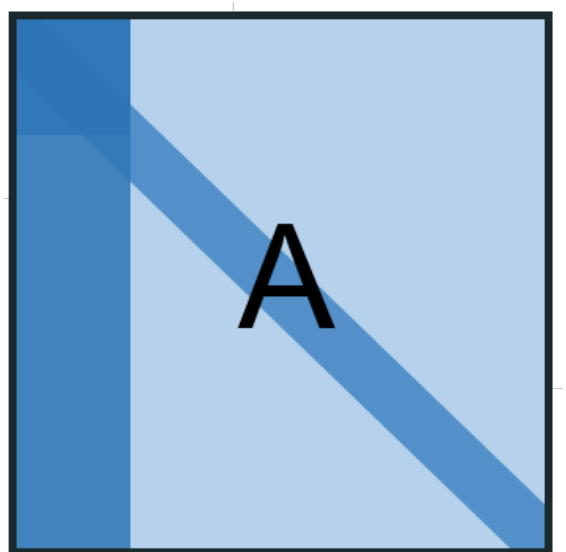

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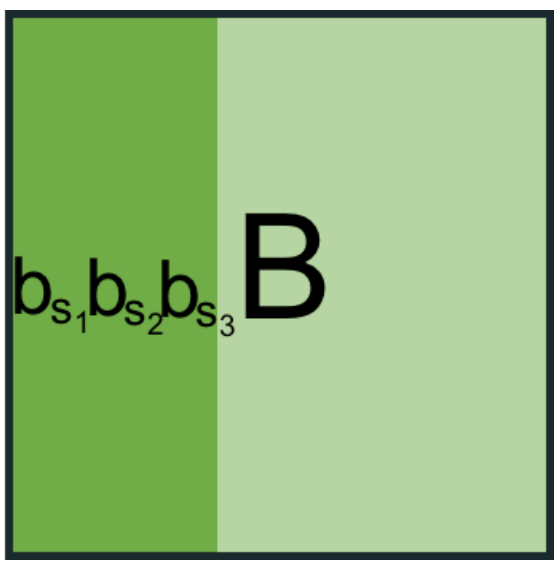

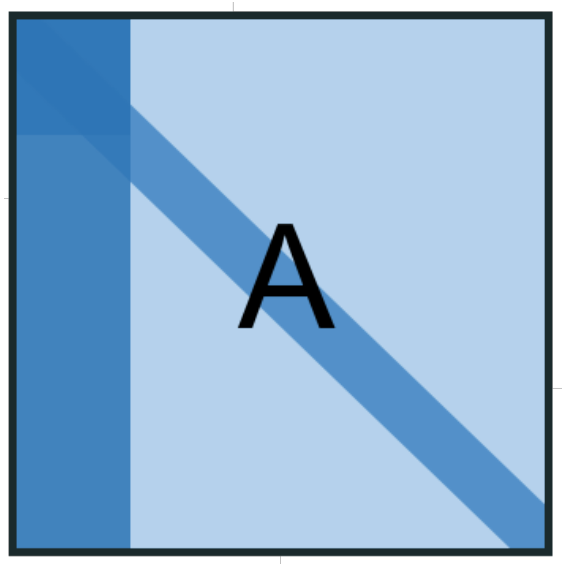

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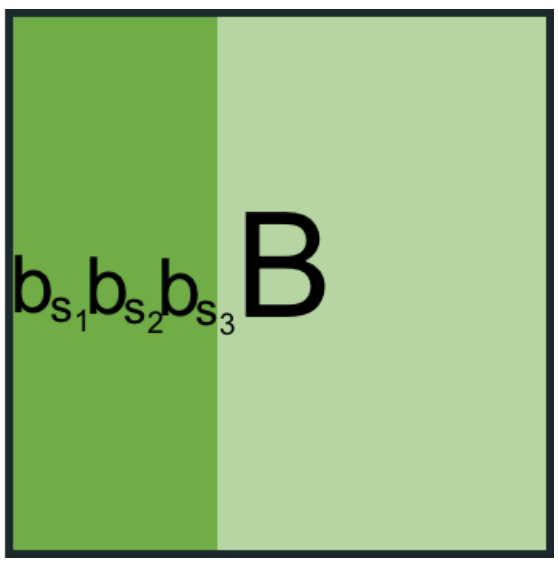

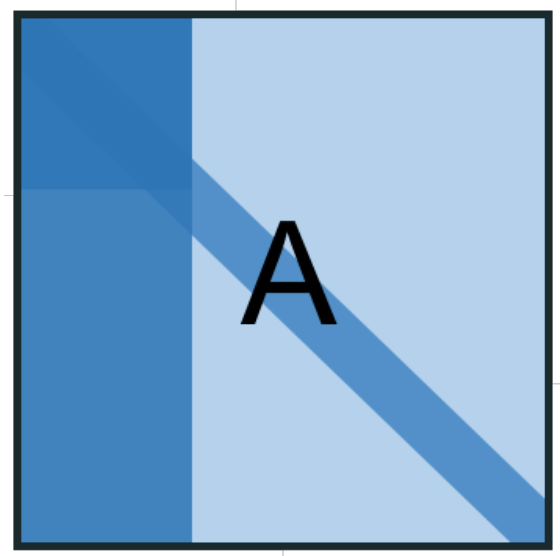

Theorem (Factor Matrix Low-Rank Approximation)

There is an algorithm using $\tilde{O}(nk^2/\epsilon)$ accesses to $\mathbf{A} = \mathbf{B}^T\mathbf{B}$ that computes $\mathbf{Z} \in \mathbb{R}^{n\times k}$ satisfying with probability 99/100:

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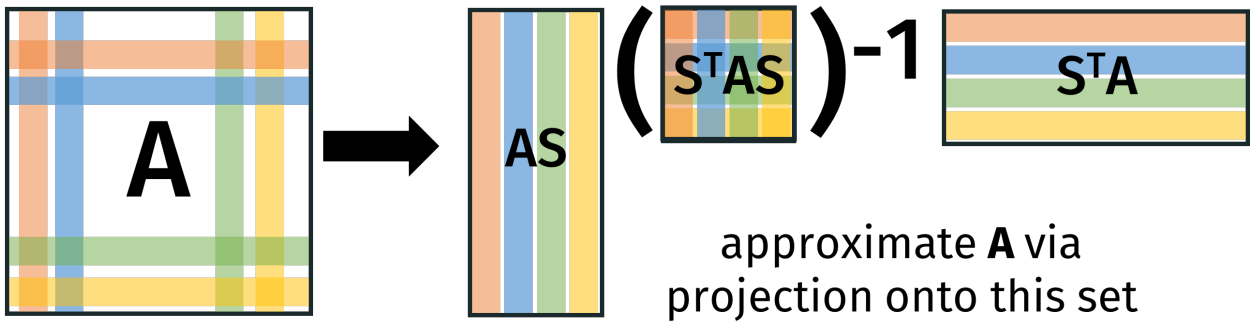
- How does this translate to low-rank approximation of $\mathbf{A}$?
- Nyström algorithm computes $\mathbf{N}$ with $\mathbf{N}\mathbf{N}^T \preceq \mathbf{A} \preceq \mathbf{N}\mathbf{N}^T + \lambda\mathbf{I}$, with essentially optimal tradeoff between rank and λ.

NYSTRÖM ALGORITHM



select k ‘landmark’ indices

approximate **A** via projection onto this set

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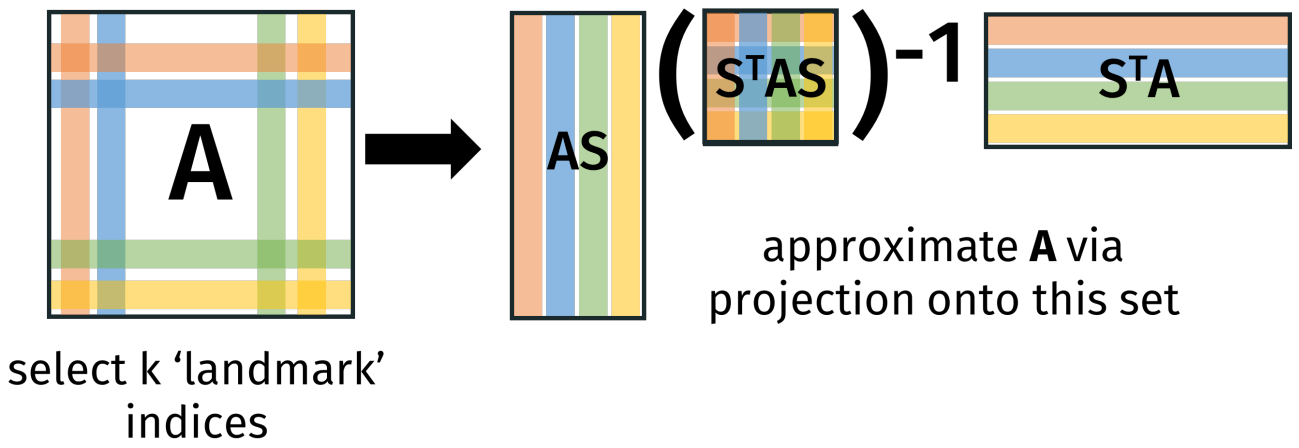

- If we think of **A** as a kernel matrix, this corresponds to performing column subset selection in kernel space.

LIMITATIONS OF COLUMN SAMPLING

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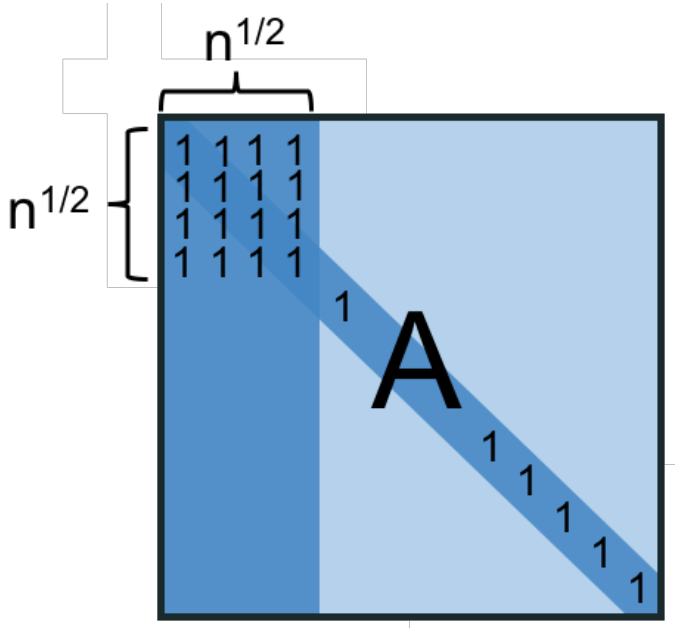

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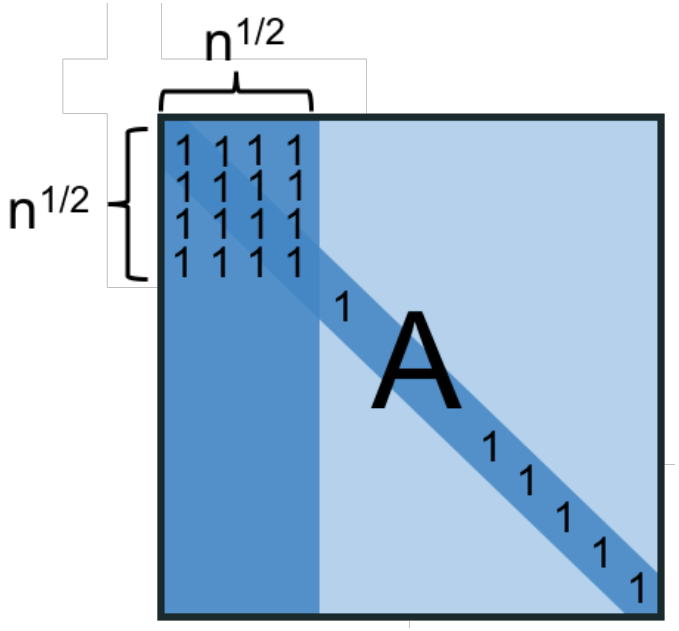

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- Sample $\mathbf{AS}$ is a projection-cost-preserving sketch for $\mathbf{A}$ [Cohen et al '15,'17]. For any rank-k projection $\mathbf{P}$

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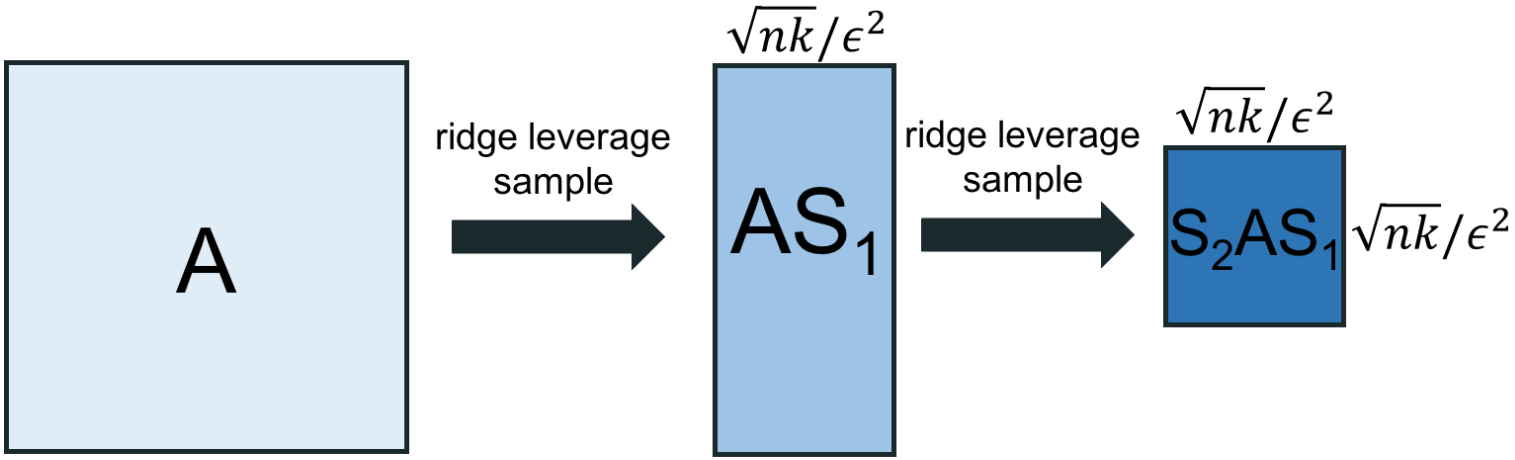

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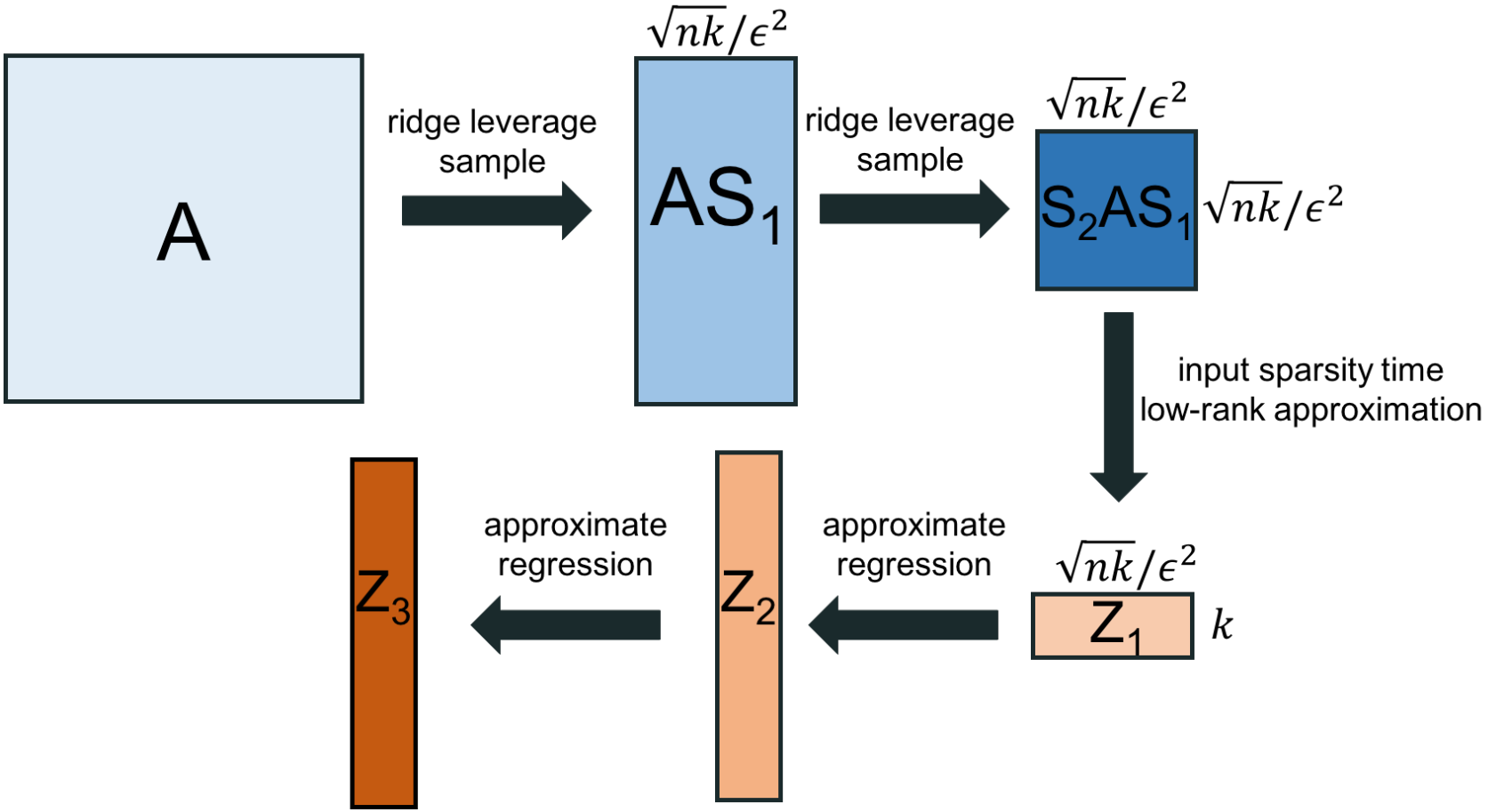

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There is an algorithm that, given PSD $\mathbf{A}$*, accesses* $\tilde{O}\left(\frac{nk}{\epsilon^{2.5}}\right)$ *entries of* $\mathbf{A}$ *and outputs* $\mathbf{N}, \mathbf{M} \in \mathbb{R}^{n \times k}$ *satisfying with probability* 99/100*:*

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- Are there other natural classes of matrices that admit sublinear time low-rank approximation?
  - E.g. distance matrices [Bakshi, Woodruff '17]
- Can we do even better for PSD matrices with additional structure? E.g. kernel matrices.

EXPLOITING ADDITIONAL STRUCTURE

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- Obtaining $O(\text{nnz}(\mathbf{X}))$ time is open when approximation can be in terms of $\|\mathbf{A} - \mathbf{A}_k\|_*$ or for computing $\mathbf{N}\mathbf{N}^T$ satisfying

$$(1-\epsilon)\mathbf{N}\mathbf{N}^T \preceq \mathbf{A} \preceq (1+\epsilon)\mathbf{N}\mathbf{N}^T + \lambda\mathbf{I}.$$

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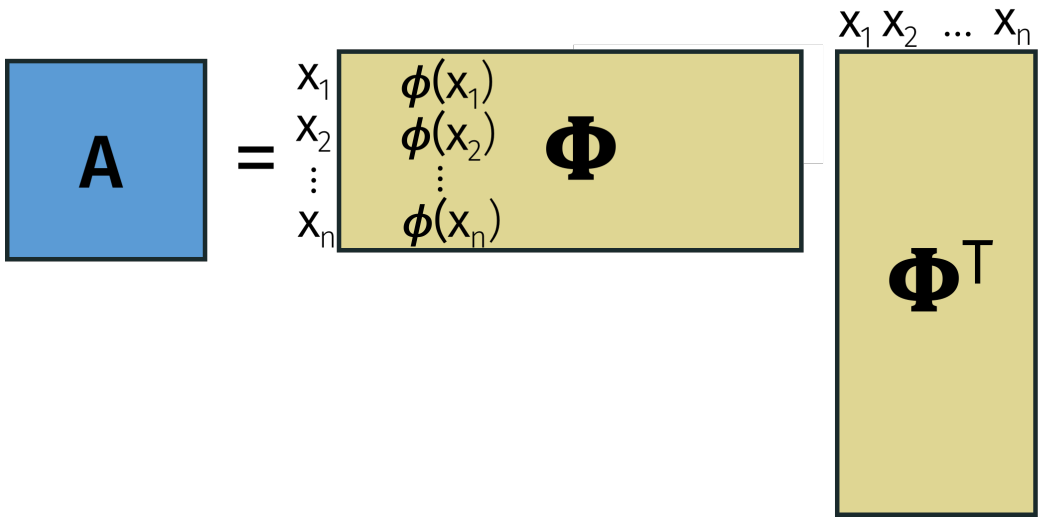

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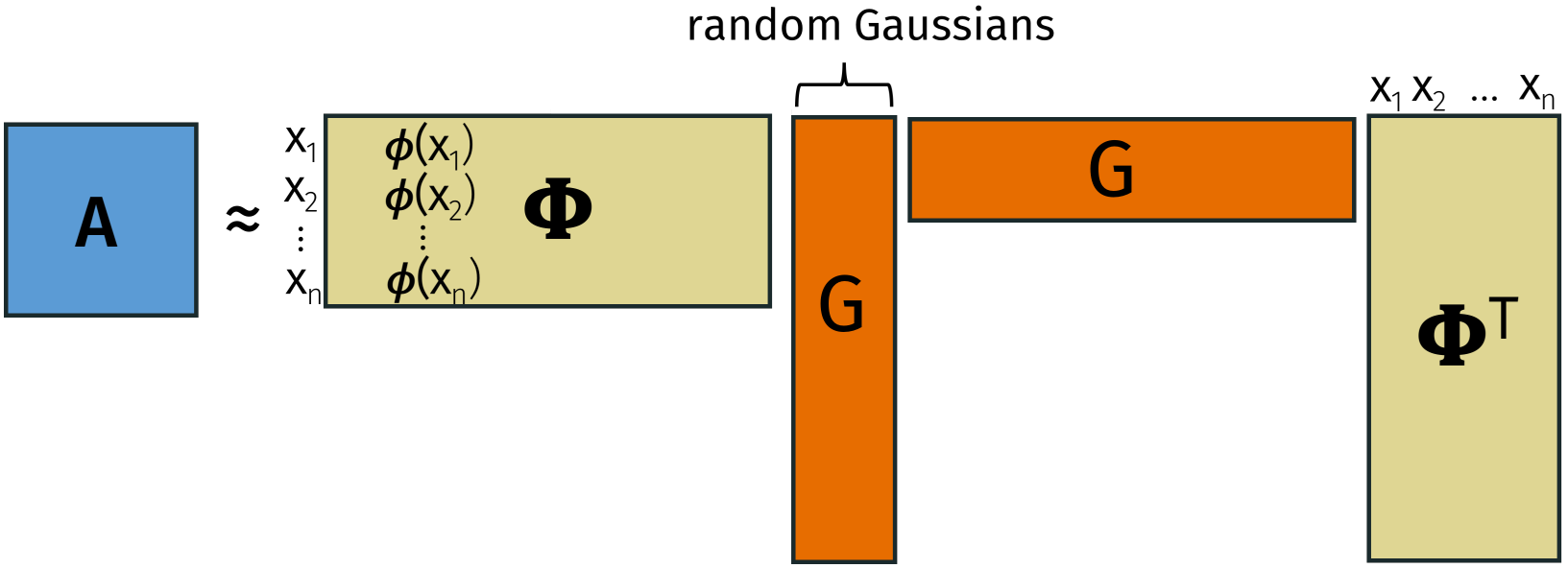

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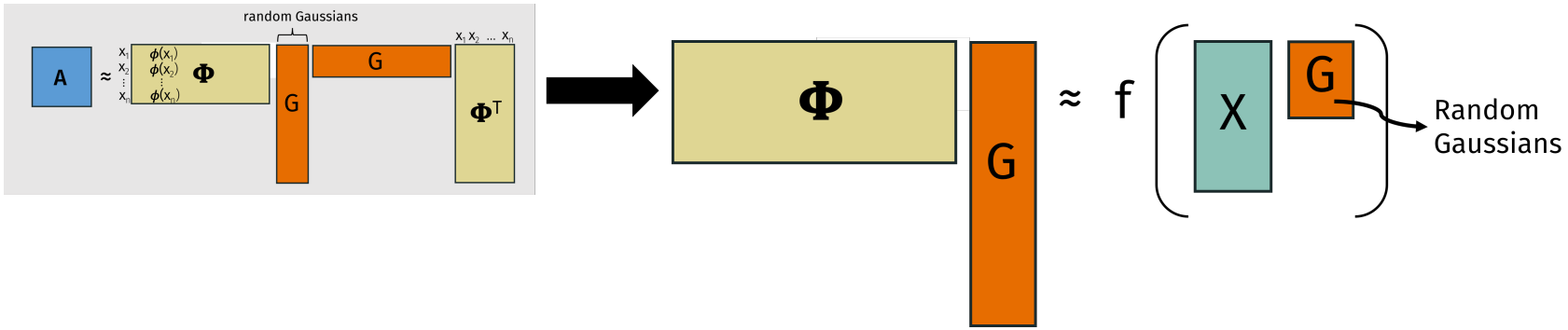

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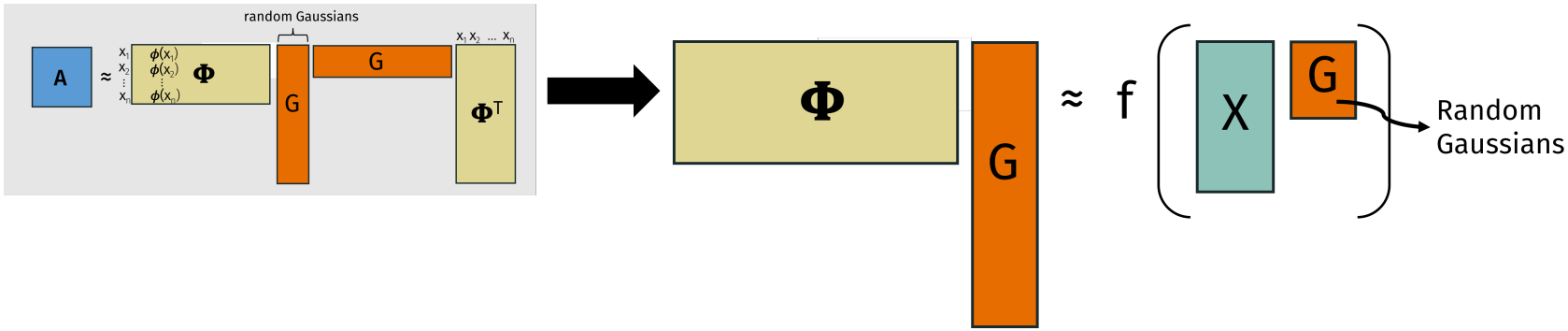

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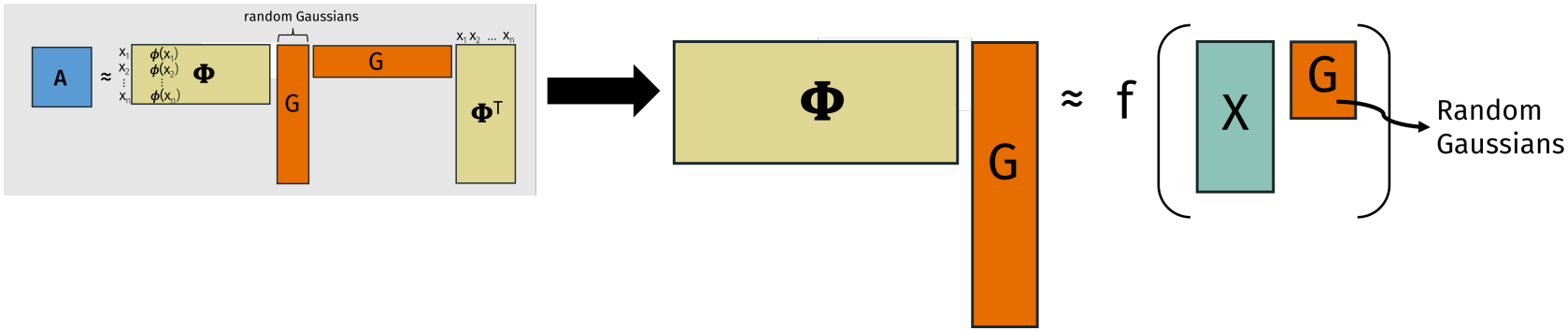

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- Further progress possible with better understanding of *fourier leverage scores*.

Thanks! Questions?

Remembering Michael Cohen (1992-2017)

Michael B. Cohen

"Michael was more than just inclusive: he actively engaged with everyone around him, on any topic, and generously shared his knowledge and observations with others. He loved teaching, and it was a joy to watch him do it."

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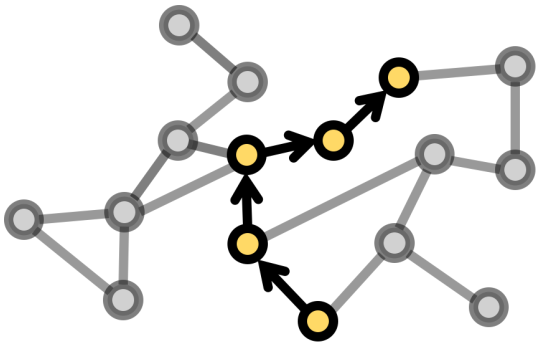

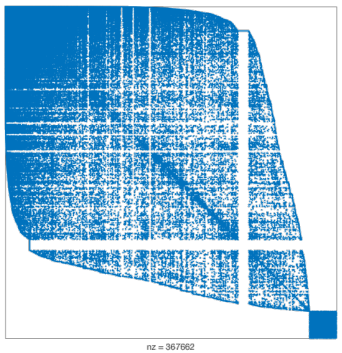

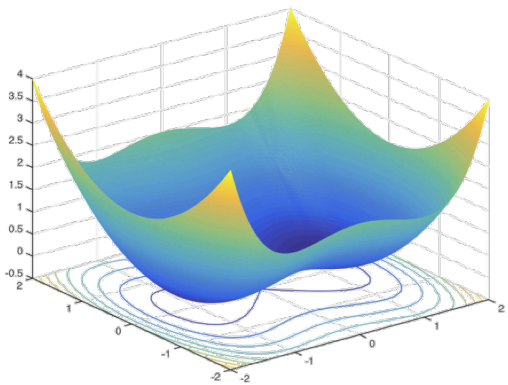

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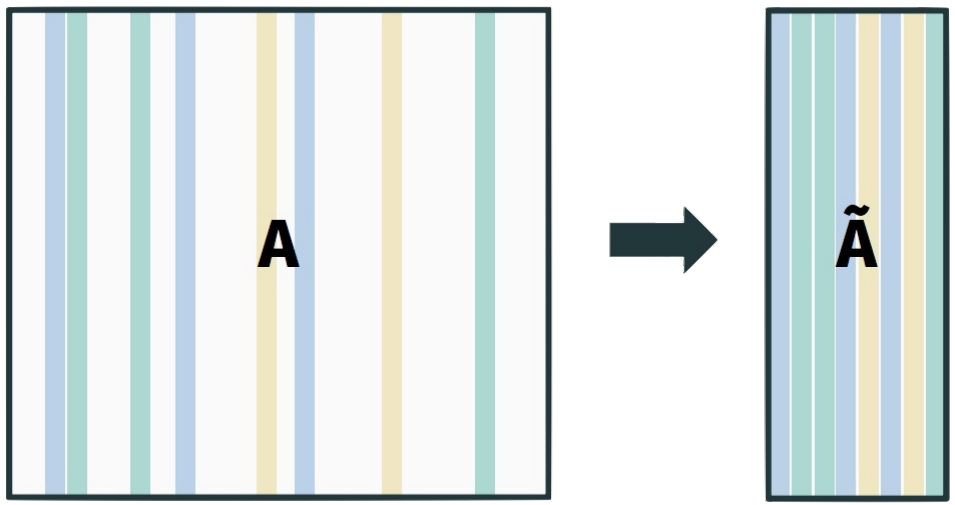

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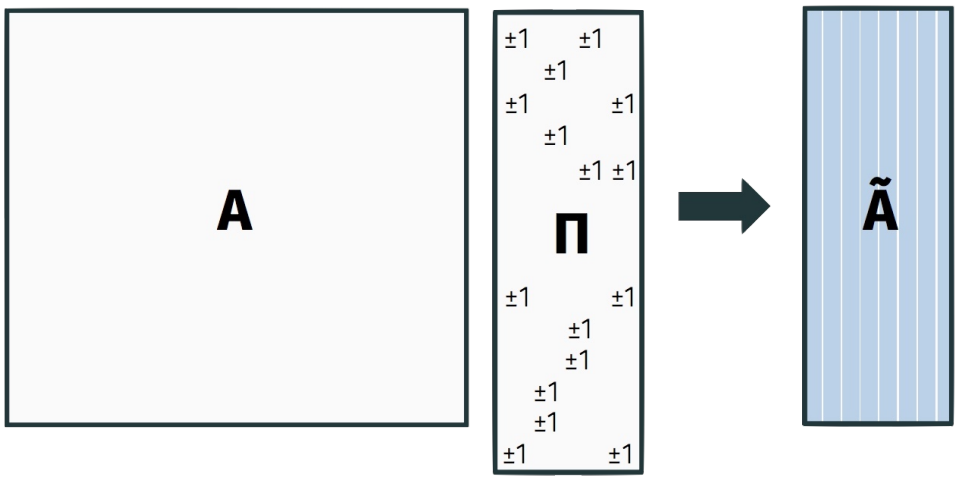

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Moment of Silence