



Comparison of Low-Rank Update Techniques for \mathcal{H} -Arithmetic

R. Kriemann
MPI MIS Leipzig

SIAM CSE21



Update Handling

Eager Update Evaluation

Updates are computed as soon as possible and immediately applied to leaf blocks.

For low-rank matrices this induces a truncation. For structured matrices *multiple* truncations may result.

$$\begin{array}{|c|c|c|}\hline \textcolor{blue}{\blacksquare} & \textcolor{blue}{\blacksquare} & \textcolor{blue}{\blacksquare} \\ \hline \textcolor{blue}{\blacksquare} & \textcolor{blue}{\blacksquare} & \textcolor{red}{\blacksquare} \\ \hline \end{array} + = \begin{array}{|c|c|c|}\hline \textcolor{blue}{\blacksquare} & \textcolor{blue}{\blacksquare} & \textcolor{red}{\blacksquare} \\ \hline \textcolor{blue}{\blacksquare} & \textcolor{blue}{\blacksquare} & \textcolor{red}{\blacksquare} \\ \hline \end{array} \cdot \begin{array}{|c|}\hline \textcolor{red}{\blacksquare} \\ \hline \end{array} + \cdots$$

$$\begin{array}{|c|}\hline \textcolor{blue}{\blacksquare} \\ \hline \end{array} + = \begin{array}{|c|}\hline \textcolor{red}{\blacksquare} \\ \hline \end{array} \cdot \begin{array}{|c|}\hline \textcolor{red}{\blacksquare} \\ \hline \end{array} + \cdots$$

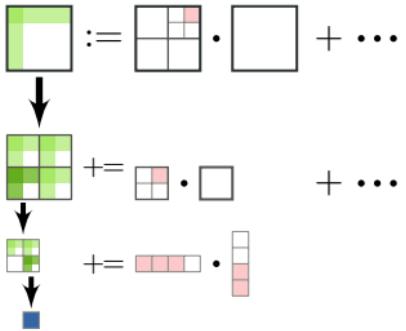
$$\begin{array}{|c|}\hline \textcolor{blue}{\blacksquare} \\ \hline \end{array} + = \begin{array}{|c|c|c|}\hline \textcolor{red}{\blacksquare} & \textcolor{red}{\blacksquare} & \textcolor{red}{\blacksquare} \\ \hline \end{array} \cdot \begin{array}{|c|}\hline \textcolor{red}{\blacksquare} \\ \hline \end{array}$$

```

function HMUL(in: A, B, inout: C)
  if A, B, C are structured then
    for i = 0, ..., n do
      for j = 0, ..., m do
        for k = 0, ..., ℓ do
          hmul(Aik, Bkj, Cij);
  else
    T := A · B;
    if C is low-rank then
      C := truncate(C + T);
    else if C is structured then
      for all sub-blocks Cij of C do
        Cij := truncate(Cij + Tij);
    else
      C := C + T;
```

Accumulated Updates

Updates are computed and collected *per level* and *shifted down* to sub blocks.



Reduced number of low-rank truncations.

Start for $C := C + A \cdot B$:

`hmul(C, {A, B}, 0);`

```

function HMUL(inout:  $C$ , in:  $\mathcal{U}_C, \mathcal{U}_C$ )
    // Compute non-recursive updates
    for all  $A^k, B^k \in \mathcal{U}_C$  do
        if  $A^k$  or  $B^k$  is not structured then
             $\mathcal{U}_C := \text{truncate}(\mathcal{U}_C + A^k \cdot B^k)$ ;
             $\mathcal{U}_C := \mathcal{U}_C \setminus \{(A^k, B^k)\}$ ;
        if  $C$  is structured then
            // Push down recursive updates
            for  $i = 0, \dots, n$  do
                for  $j = 0, \dots, m$  do
                     $\mathcal{U}_{C_{ij}} = \emptyset$ ;
                    for all  $(A^k, B^k) \in \mathcal{U}_C$  do
                        for  $\ell = 0, \dots, r$  do
                             $\mathcal{U}_{C_{ij}} := \mathcal{U}_{C_{ij}} \cup \{(A_{i\ell}^k, B_{\ell,j}^k)\}$ ;
                    hmul( $C_{ij}$ ,  $\mathcal{U}_C|_{t_i, s_j}$ ,  $\mathcal{U}_{C_{ij}})$ ;
            else
                // Apply all accumulated updates
                 $C := \text{truncate}(C + \mathcal{U}_C)$ ;

```

Lazy Update Evaluation

Updates are handled *implicitly* until leaves are reached, i.e., low-rank (and dense) blocks are (virtually) sub-divided.

■ $= \text{[low-rank]} + \text{[low-rank]} + \text{[dense]} + \dots$

```

function HMUL(inout:  $C_{t \times s}$ , in:  $\mathcal{U}$ )
  if  $C_{t \times s}$  is structured then
    // Push down updates
    for  $t_i \in \mathcal{S}(t)$  do
      for  $s_j \in \mathcal{S}(s)$  do
         $\mathcal{U}' = \emptyset;$ 
        for all  $(A_{t \times r}^k, B_{r \times s}^k) \in \mathcal{U}$  do
           $\mathcal{U}' = \mathcal{U}' \cup \{(A^k|_{t_i \times r}, B^k|_{r \times s_j})\};$ 
        hmul( $C_{t_i \times s_j}$ ,  $\mathcal{U}'$ );
    else
      // Apply all updates
       $C := \text{truncate}(C + \sum_k A^k \cdot B^k);$ 
  
```

All updates are applied *simultaneously*.

Number of updates in $\mathcal{O}(\log n)$.

J. Dölz, H. Harbrecht, M.D. Multerer: "On the Best Approximation of the Hierarchical Matrix Product", SIAM J. Matrix Anal. Appl., 40(1), 147–174 (2019)

Lowrank Approximation

Lowrank Approximation

Singular Value Decomposition (SVD)

Rank Revealing QR (RRQR)

Randomized LR/SVD (RandLR/SVD)

Cross Approximation (ACA)

Lánczos Bidiagonalization (Lanzcos)

Computes **best approximation**.

Runtime complexity is $\mathcal{O}(n \cdot k^2 + k^3)$ for input rank k and block size n .

```
function SVD(in: U, V, ε, out: W, X)
    [QU, RU] := qr(U);
    [QV, RV] := qr(V);
    [Us, Ss, Vs] := svd( RU · RVH );
    k := rank(Ss, ε);
    W := QU · Us(:, 1 : k) · Ss(1 : k, 1 : k);
    X := QV · Vs(:, 1 : k);
```

Lowrank Approximation

Singular Value Decomposition (SVD)

Rank Revealing QR (RRQR)

Randomized LR/SVD (RandLR/SVD)

Cross Approximation (ACA)

Lánczos Bidiagonalization (Lanzcos)

Based on reordering the remaining columns during QR.

Approximation rank and error control defined by matrices $R(i : k, i : k)$.

```
function RRQR(in:  $U, V, \varepsilon$ , out:  $W, X$ )
     $k := \text{rank}(U);$ 
     $[Q_V, R_V] = \text{qr}(V);$ 
     $[Q, R, P] = \text{qrp}(U \cdot R_V^H);$ 
    for  $i = 1, \dots, k$  do
         $S(i) := \|R(i : k, i : k)\|_F;$ 
         $k' := \text{rank}(S, \varepsilon);$ 
         $W := Q(:, 1 : k');$ 
         $X := Q_V \cdot P \cdot R(1 : k', :)^H;$ 
```

Lowrank Approximation

Singular Value Decomposition (SVD)

Approximate column basis of operator.

Only **operator evaluation** required.

Rank Revealing QR (RRQR)

Randomized LR/SVD (RandLR/SVD)

Cross Approximation (ACA)

Lánczos Bidiagonalization (Lanczos)

function RANDLR(**in:** M, ε , **out:** W, X)

$W := \text{ColumnBasis}(M, \varepsilon);$
 $X := M^H \cdot W;$

function RANDSVD(**in:** M, ε , **out:** W, X)

$B := \text{ColumnBasis}(M, \varepsilon);$
 $[Q, R] := \text{qr}(M^H \cdot B);$
 $[U_s, S_s, V_s] := \text{svd}(R);$
 $k := \text{rank}(S_s, \varepsilon);$
 $W := B \cdot V_s(:, 1:k) S(1:k, 1:k);$
 $X := M^H \cdot B \cdot U_s(:, 1:k);$

Lowrank Approximation

Singular Value Decomposition (SVD)

Rank Revealing QR (RRQR)

Randomized LR/SVD (RandLR/SVD)

Cross Approximation (ACA)

Lánczos Bidiagonalization (Lanzcos)

Successively selects pairs of rows/columns for rank-1 updates.

Only *requested coefficients* needed.

Different pivot search strategies available.

```
function ACA(in: M, ε, out: W, X)
    c₁ = 1;
    for i = 1, … do
        wᵢ := column(M, cᵢ) – W · X(cᵢ, :)';
        rᵢ := maxidx(wᵢ); wᵢ := wᵢ / wᵢ(rᵢ);
        xᵢ := row(M, rᵢ)' – X · W(rᵢ, :)';
        W := [W, wᵢ]; X := [X, xᵢ];
        if ‖wᵢ · xᵢ'‖_F ≤ ε ‖W · X^H‖_F then
            break;
        cᵢ₊₁ := maxidx(xᵢ);
```

Lowrank Approximation

Singular Value Decomposition (SVD)

Rank Revealing QR (RRQR)

Randomized LR/SVD (RandLR/SVD)

Cross Approximation (ACA)

Lánczos Bidiagonalization (Lanzcos)

For $M \in \mathbb{C}^{n \times m}$, iteratively computes bases W_k and X_k of

$$\mathcal{K}(MM^H, w_1) = \text{span} \left\{ (MM^H)^i w_1 : 0 \leq i \leq k \right\}$$

$$\mathcal{K}(M^H M, x_1) = \text{span} \left\{ (M^H M)^i x_1 : 0 \leq i \leq k \right\}$$

with random w_1 , $x_1 = M^H w_1 / \|M^H w_1\|$
such that

$$M \approx W_k B_k X_k^H$$

and bidiagonal B_k .

Also only **operator evaluation** required.

Model Problems

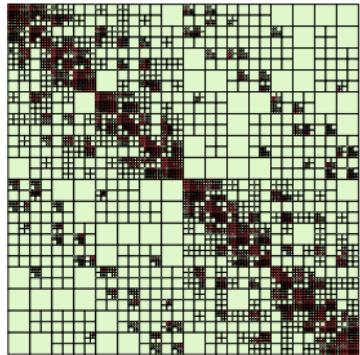
Model Problems

Laplace SLP

Defined by

$$\int_{\Gamma} \frac{1}{\|x - y\|_2} u(y) dy = f(x), \quad x \in \Gamma$$

with $\Gamma = \{x \in \mathbb{R}^3 : \|x\|_2 = 1\}$.



Matrix condition: 500, ..., 5000.

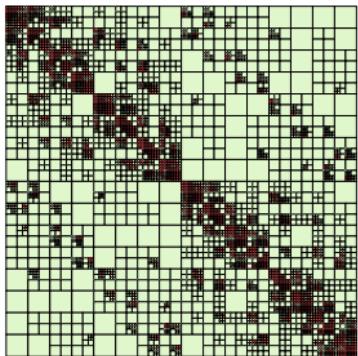
Model Problems

Laplace SLP

Defined by

$$\int_{\Gamma} \frac{1}{\|x - y\|_2} u(y) dy = f(x), \quad x \in \Gamma$$

with $\Gamma = \{x \in \mathbb{R}^3 : \|x\|_2 = 1\}$.



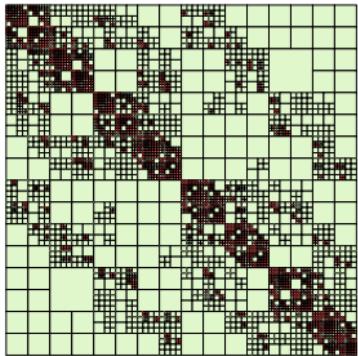
Matrix condition: 500, ..., 5000.

Matérn Covariance

Defined by

$$C(x, y; \theta) = \frac{\sigma^2}{2^{\nu-1}\Gamma(\nu)} \left(\frac{\|x - y\|}{\ell} \right)^{\nu} K_{\nu} \left(\frac{\|x - y\|}{\ell} \right)$$

with parameters $\theta = (\sigma, \ell, \nu)$ and random positions in $[0, 1]^3$.

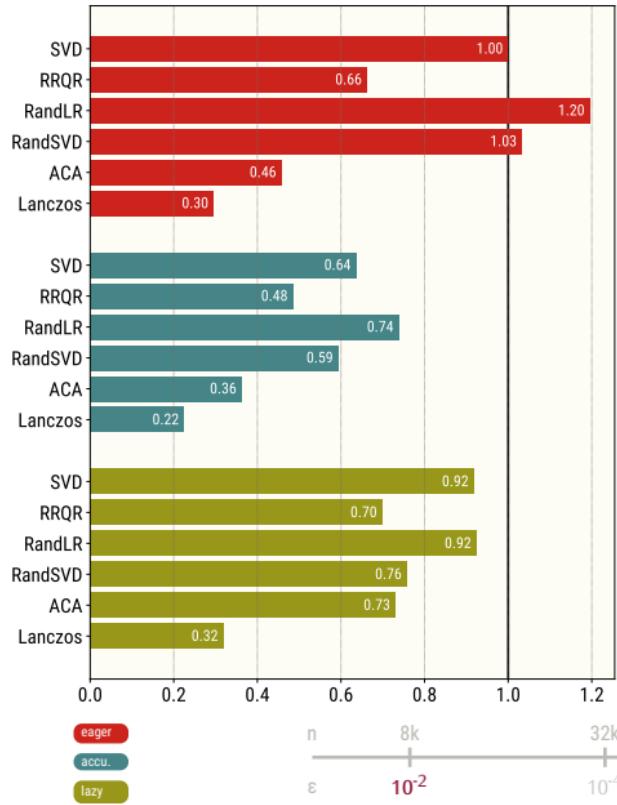


Matrix condition: $10^6, \dots, 10^8$.

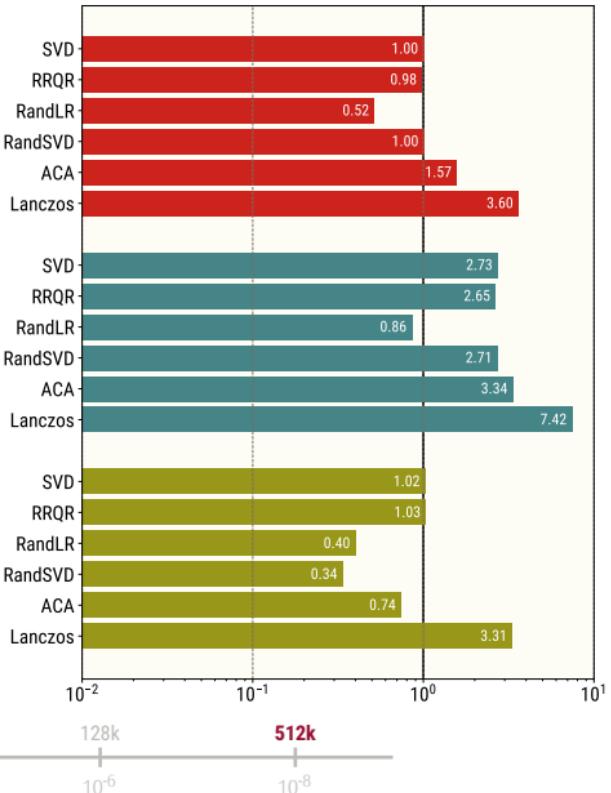
Results

Laplace SLP: H-LU

Runtime

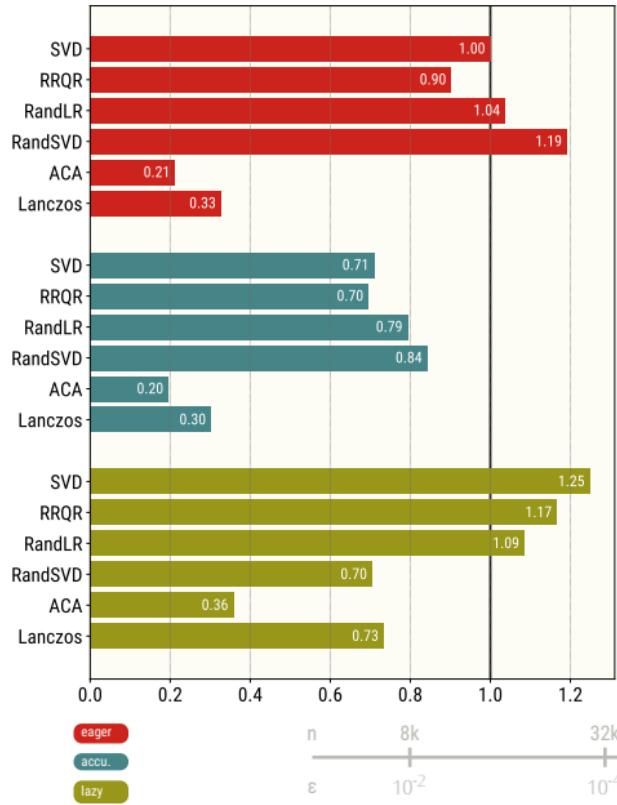


Error

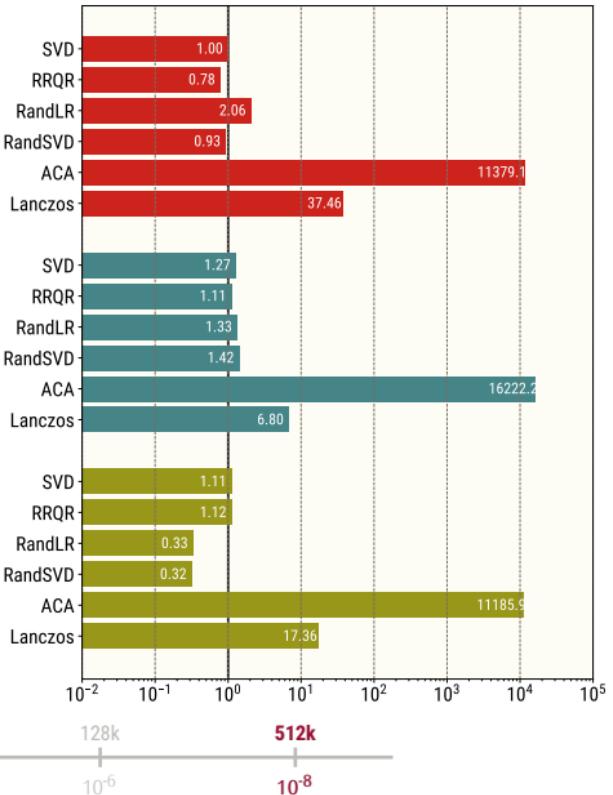


Laplace SLP: H-LU

Runtime

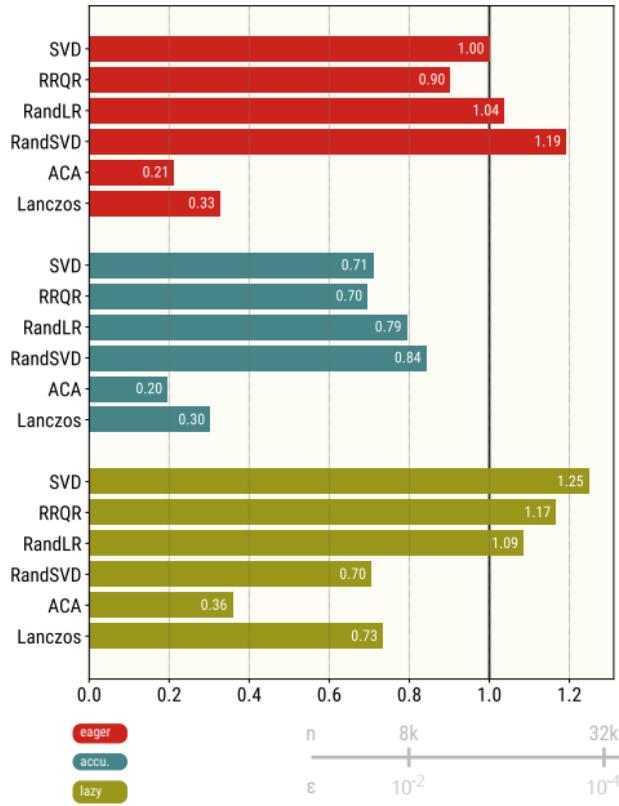


Error

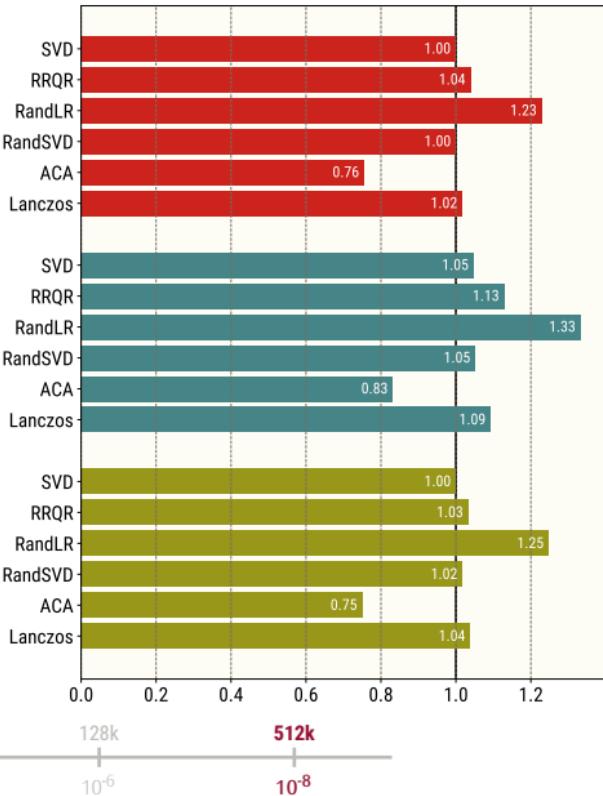


Laplace SLP: H-LU

Runtime

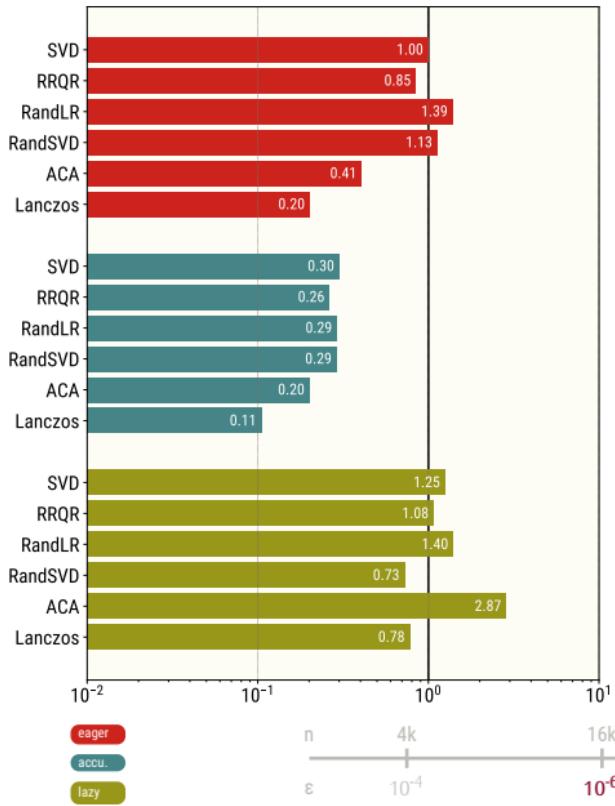


Memory

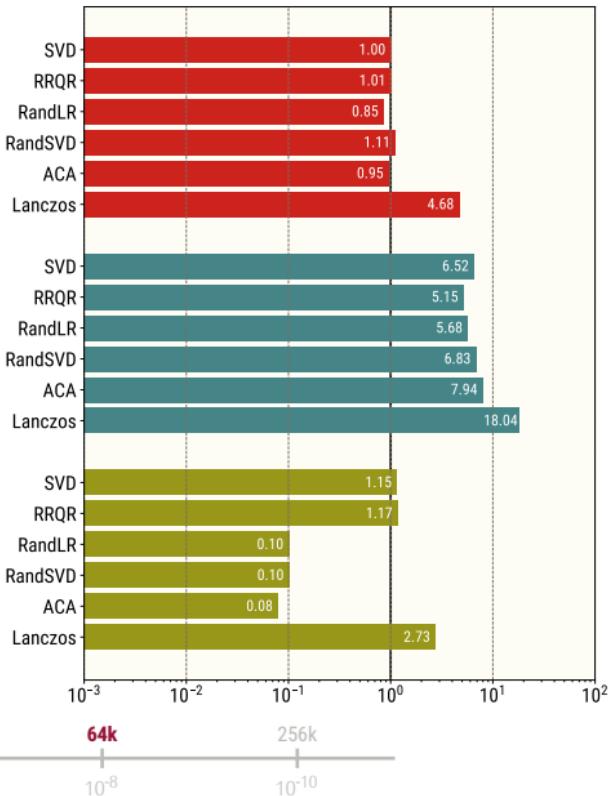


Matérn Covariance: H-LU

Runtime

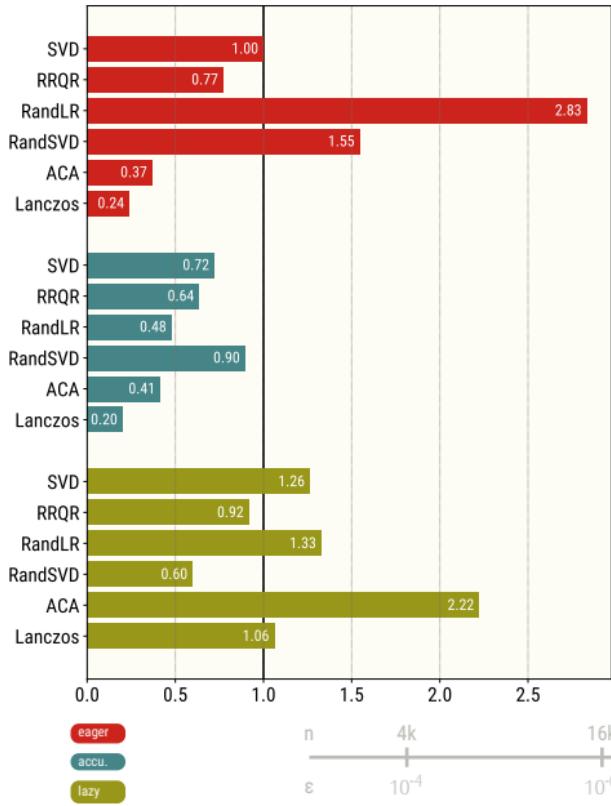


Error

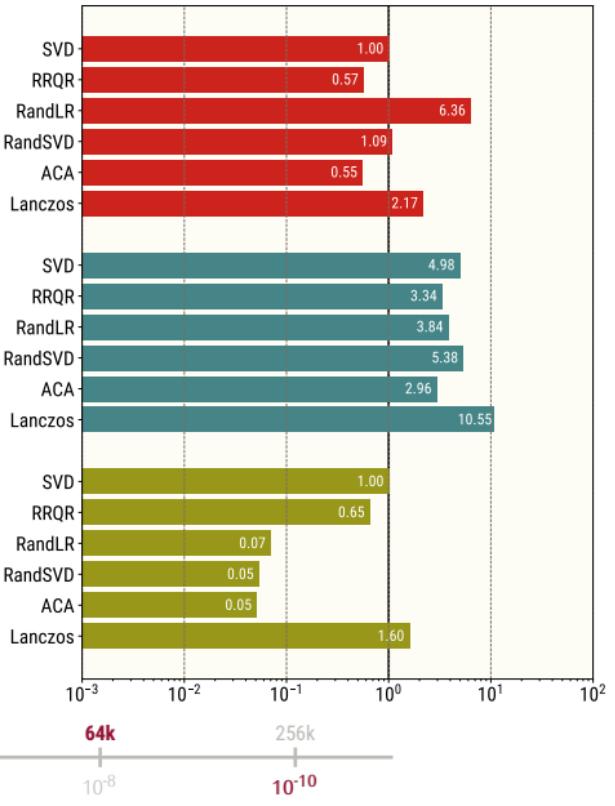


Matérn Covariance: H-LU

Runtime

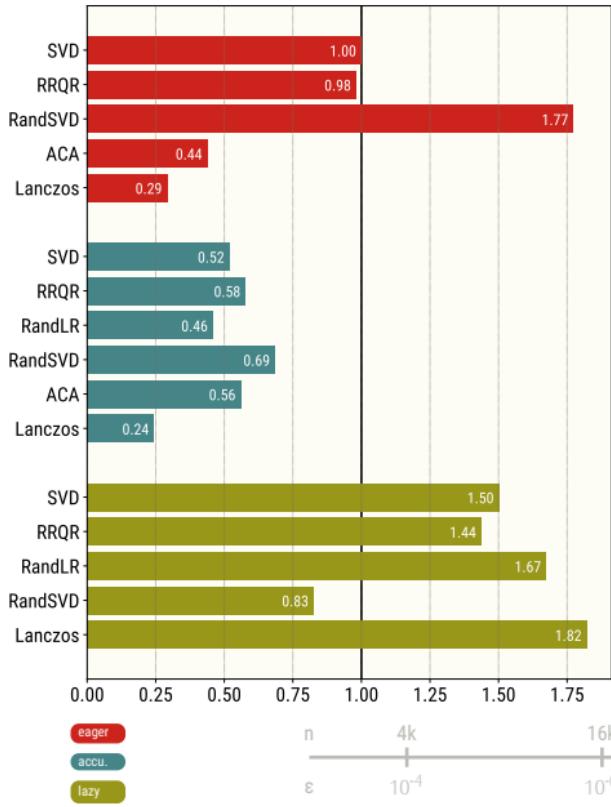


Error

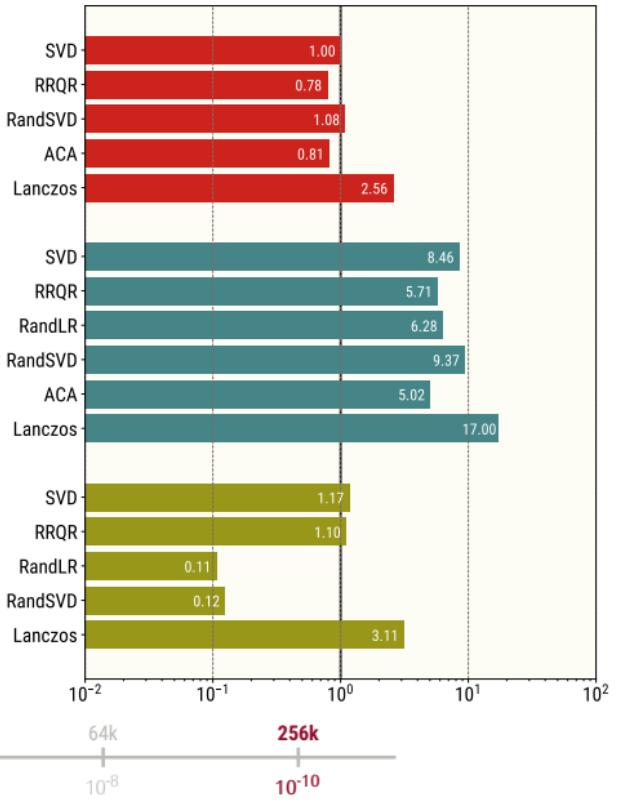


Matérn Covariance: H-LU

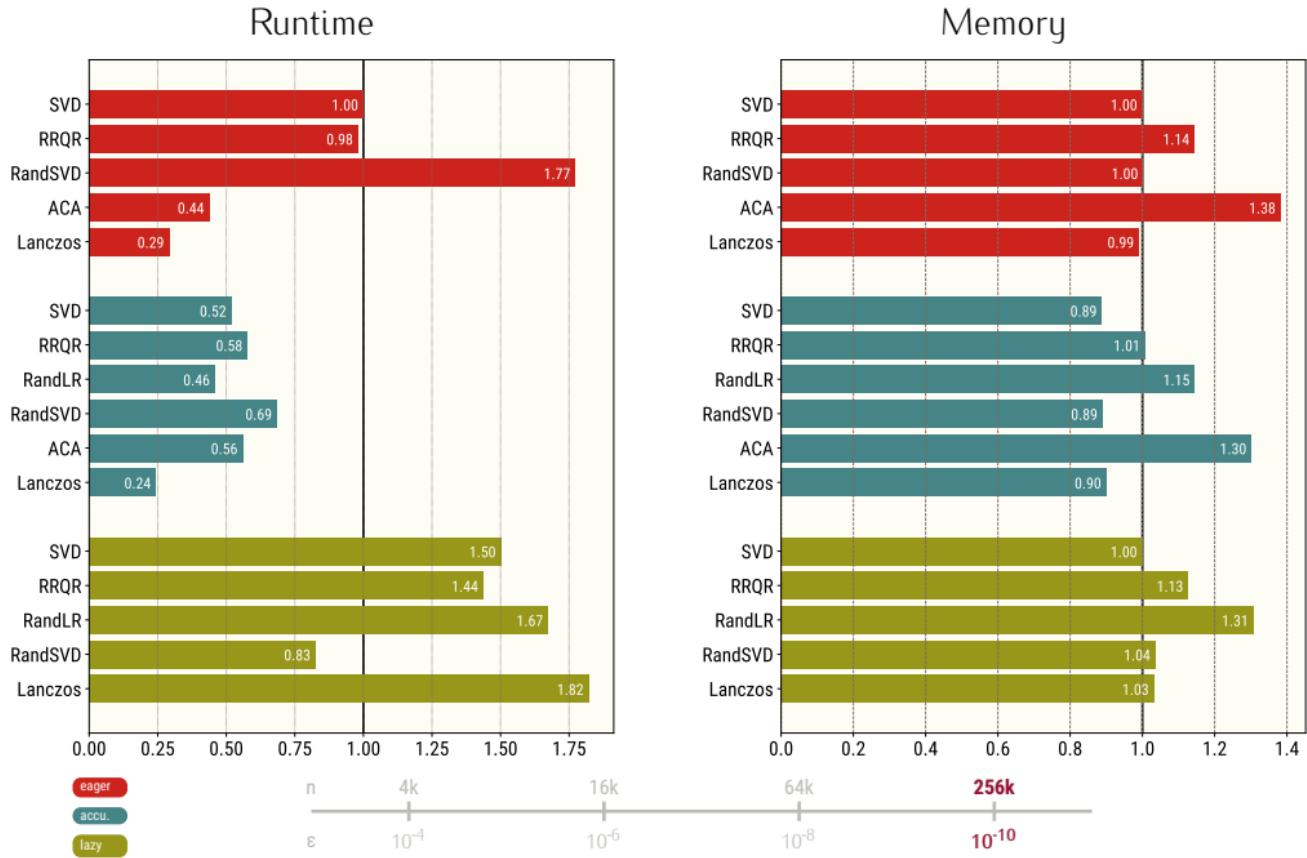
Runtime



Error



Matérn Covariance: H-LU



Conclusion

Based on the presented results:

- RRQR is a safe, faster replacement for SVD,
- accumulator arithmetic is faster but less accurate,
- ACA may shine or fail,
- Lanczos is fast but has accuracy issues,
- randomized methods *efficiently* exploit lazy arithmetic with *high* accuracy.

Conclusion

Based on the presented results:

- RRQR is a safe, faster replacement for SVD,
- accumulator arithmetic is faster but less accurate,
- ACA may shine or fail,
- Lanczos is fast but has accuracy issues,
- randomized methods *efficiently* exploit lazy arithmetic with *high* accuracy.

More comparisons available at

libhlr.org/programs/approx

Conclusion

Based on the presented results:

- RRQR is a safe, faster replacement for SVD,
- accumulator arithmetic is faster but less accurate,
- ACA may shine or fail,
- Lanczos is fast but has accuracy issues,
- randomized methods *efficiently* exploit lazy arithmetic with *high* accuracy.

More comparisons available at

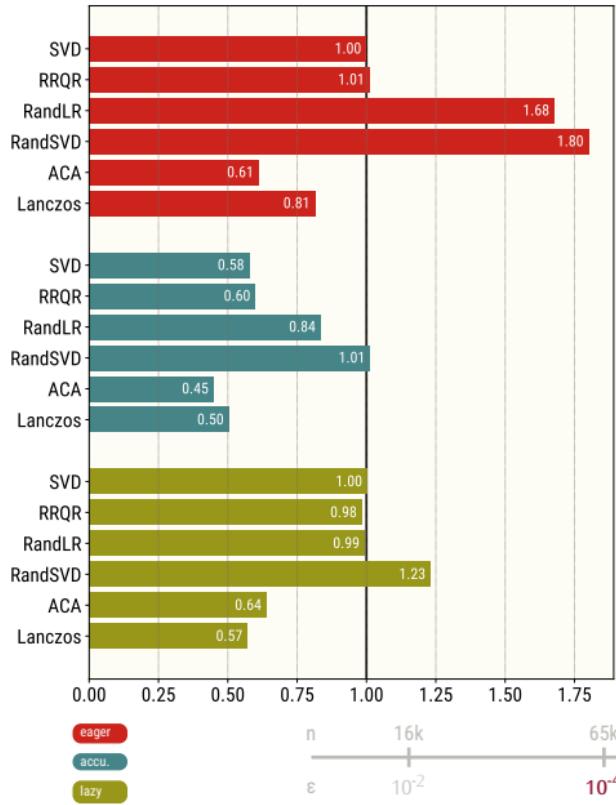
libhlr.org/programs/approx

Next:

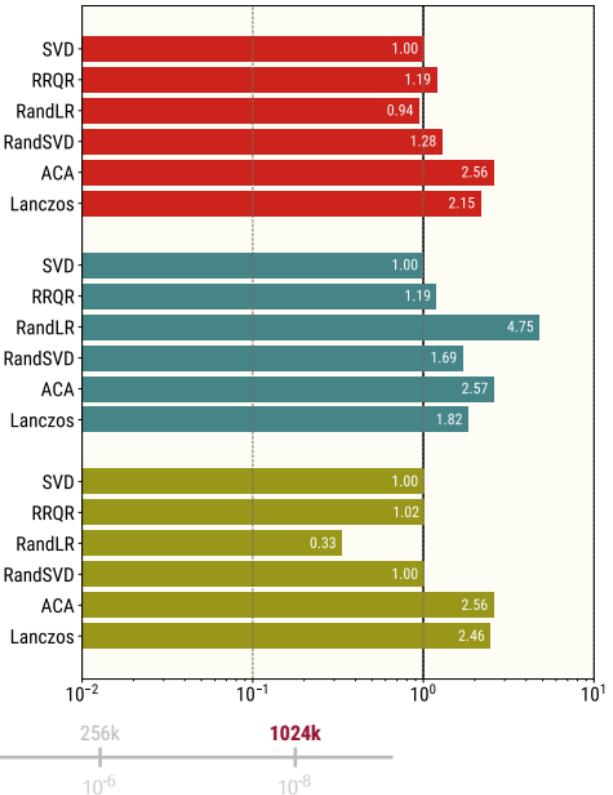
different *H²-arithmetic* with different approximation techniques

LogKernel / HODLR: H-LU

Runtime

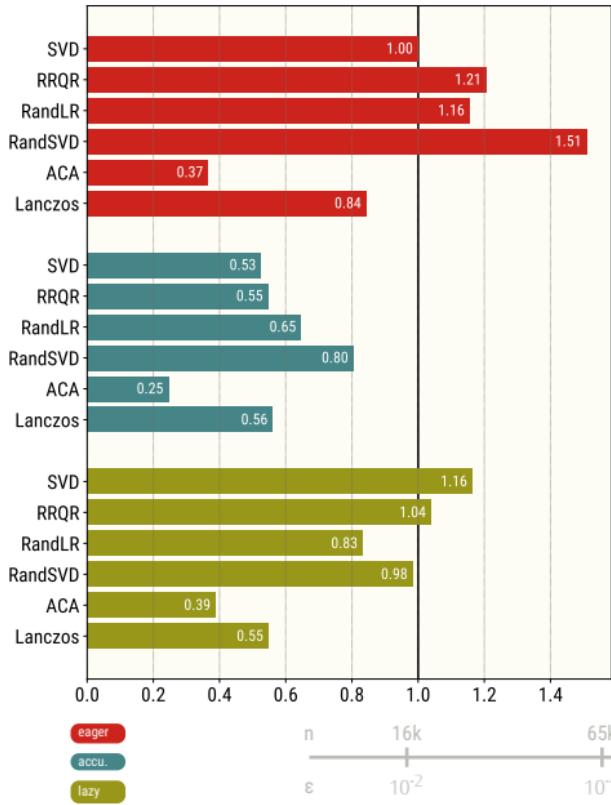


Error

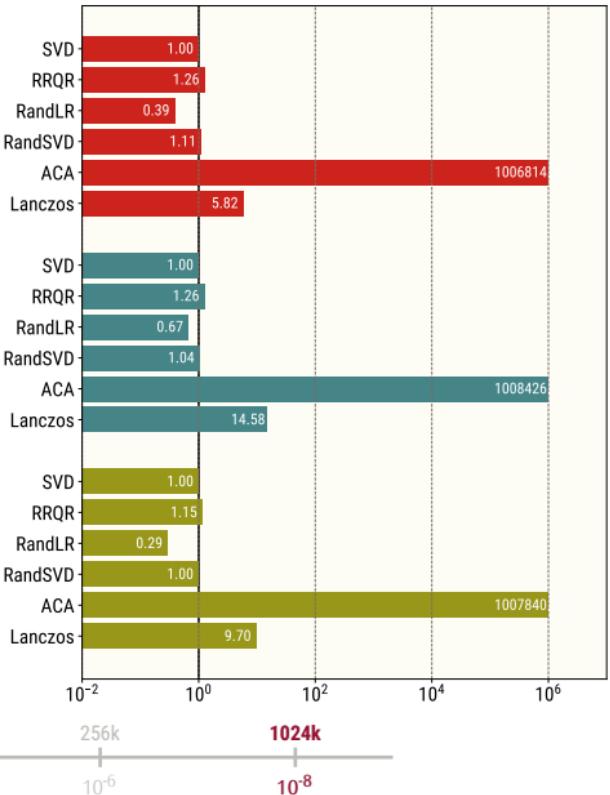


LogKernel / HODLR: H-LU

Runtime

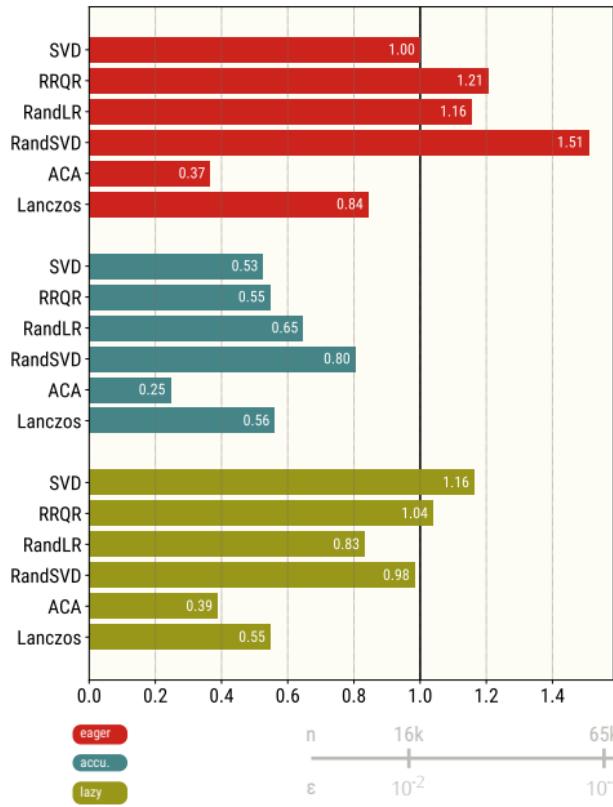


Error

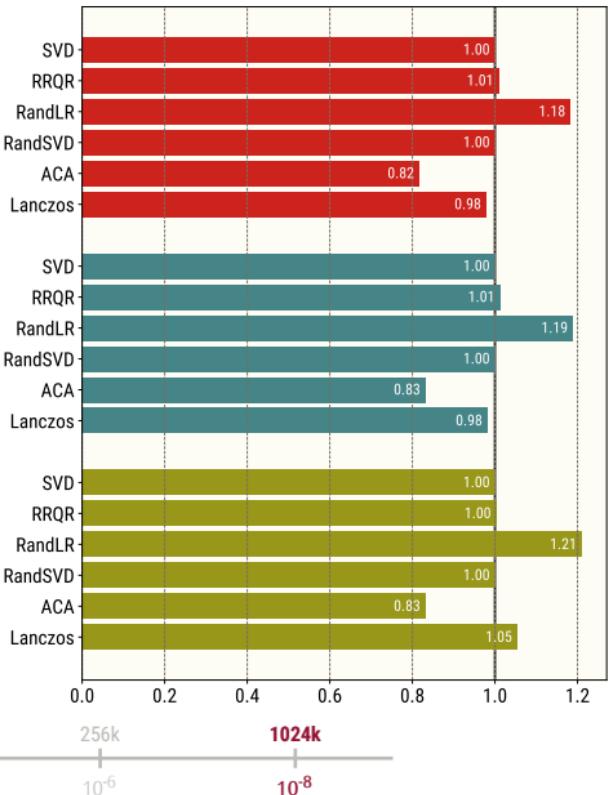


LogKernel / HODLR: H-LU

Runtime

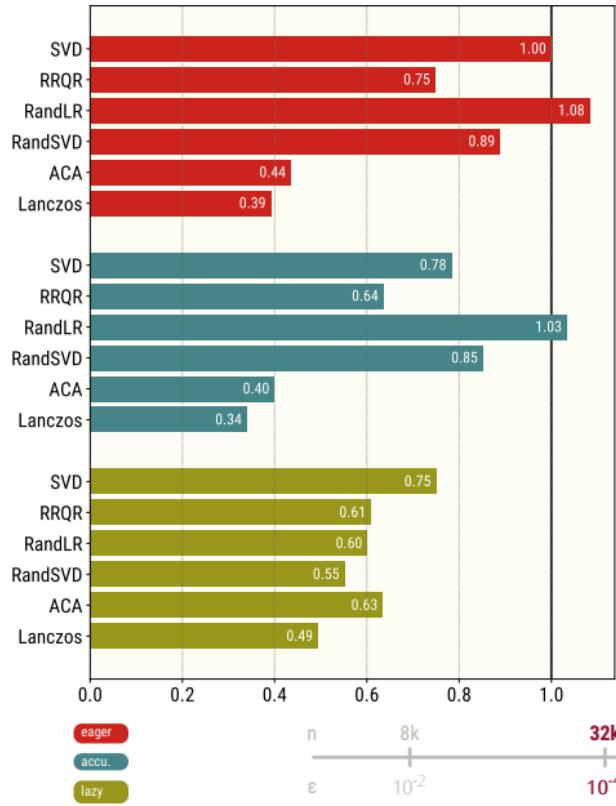


Memory

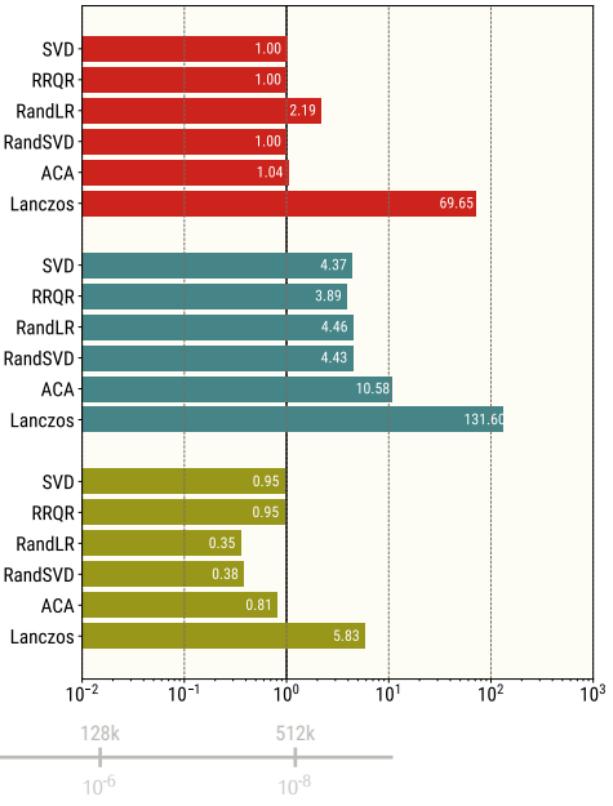


LaplaceSLP / TLR: H-LU

Runtime

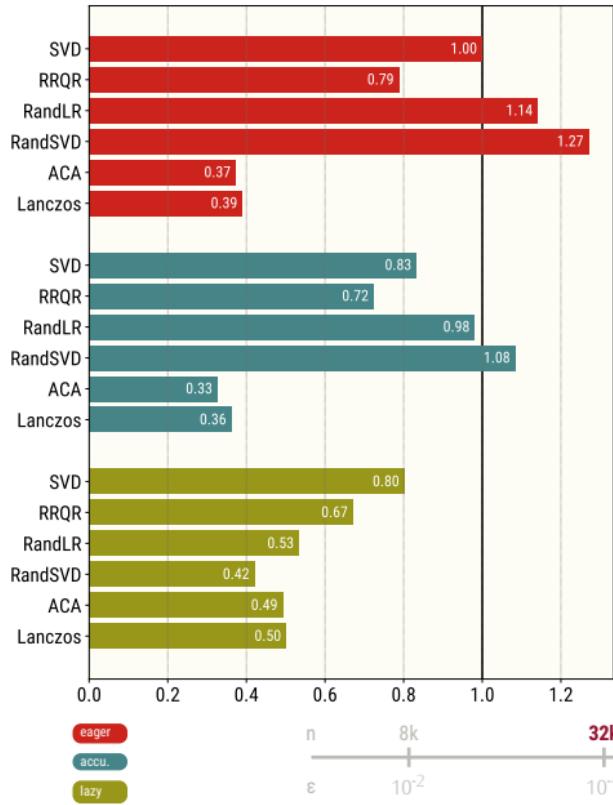


Error

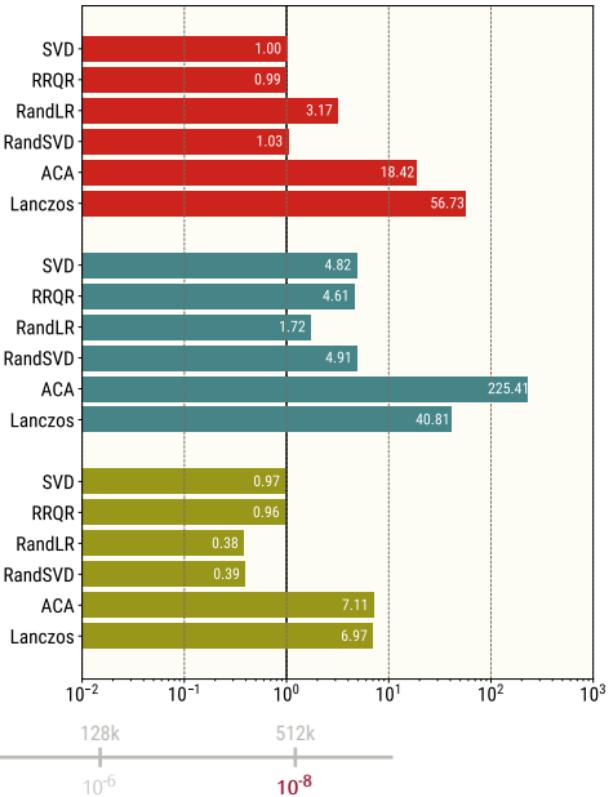


LaplaceSLP / TLR: H-LU

Runtime

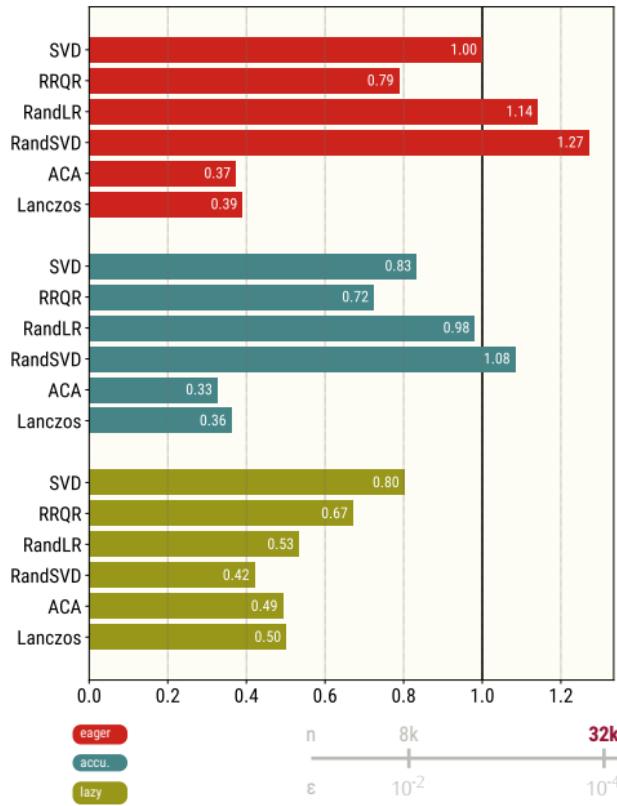


Error



LaplaceSLP / TLR: H-LU

Runtime



Memory

