Optimal Diagonal Preconditioner: Theory and Practice

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Today’s Talk

I. The Optimal Diagonal Preconditioner via Semidefinite Programming

II. Towards Practical Approximate Optimal Diagonal Preconditioner
Optimal Diagonal Preconditioner [QGHYZ 20]

Given matrix \( M = X^TX > 0 \), iterative methods are applied to solve

\[
Mx = b
\]

- Convergence of iterative methods depends on the condition number \( \kappa(M) \)
- Good performance needs preconditioning and we solve \( P^{-1/2}MP^{-1/2}x' = b \)
  A good preconditioner reduces \( \kappa(P^{-1/2}MP^{-1/2}) \)
- Diagonal \( P = D \) is called diagonal preconditioner
  Most popular in practice: Jacobi, Ruiz, ADAM,…

More generally, we wish to find \( D \) (or \( E \)) such that \( \kappa(DXE) \) is minimized?

Is it possible to find optimal \( D^* \) and \( E^* \)? \( \text{SDP works!} \)
Optimal Diagonal Preconditioner

\[
\begin{align*}
\min_{D \text{ diagonal}, D \geq 0} & \kappa(DMD) \\
\text{subject to} & \quad I \leq DMD \leq \kappa I
\end{align*}
\]

\[
\begin{align*}
\min_{D, \kappa} & \quad \kappa \\
\text{subject to} & \quad \kappa X^TDX \geq I
\end{align*}
\]

\[
\begin{align*}
\text{subject to} & \quad X^TDX \geq \tau \\
\text{subject to} & \quad I \geq X^TDX
\end{align*}
\]

• Finding the optimal diagonal preconditioner is an SDP
• Two SDP blocks and sparse coefficient matrices
• Trivial dual interior-feasible solution
• An ideal formulation for dual SDP methods \( D = \sum d_i e_i e_i^T \)

What about two-sided?
Extension: Optimal preconditioner with arbitrary sparsity pattern

SDP can be generalized to tackle preconditioners with arbitrary sparsity pattern

Given sparsity pattern \( S \), find \( P \in S \) such that \( \kappa(P^{-1}M) \) minimized

Given sparsity pattern \( S \), find \( P^{-1} \in S \) such that \( \kappa(P^{-1}M) \) minimized

- Both problems are SDP-representable
- Providing benchmark for non-diagonal preconditioners
  e.g., tridiagonal, sparse approximate inverse...
Two-Sided Preconditioner

\[
\min_{D_1 \succeq 0, D_2 \succeq 0} \kappa(D_1 X D_2)
\]

- Common in practice and popular heuristics exist
  e.g. Ruiz-scaling, matrix equilibration & balancing
- Not directly solvable using SDP
- Can be solved by iteratively fixing \(D_1 \) (\(D_2\)) and optimizing the other side
  Solving a sequence of SDPs
- Benchmark to answer questions:
  How far can diagonal preconditioners go?
  How good are those Heuristics?
Computational results: How far can optimal preconditioner go?

Distribution of condition number improvement on SuiteSparse matrix collection

- A median of 2.2 factor of improvement for optimal right preconditioner
- 2.5 factor of improvement for optimal left preconditioner
- 3.6 factor of improvement for optimal two-sided preconditioner
Computational results: How good are the heuristic preconditioners

We use the optimal preconditioner to evaluate two heuristic preconditioners: one-sided Jacobi and two-sided Ruiz

- A median factor of 1.5 improvement over Jacobi
- A median factor of 2.1 improvement over Ruiz
- For some matrices the improvement reaches >100
  heuristics are often good, but sometimes harmful
Computational results: Randomized preconditioner

- Many matrices result from statistical datasets
- $M = X^TX$ estimates the covariance matrix
- It suffices to use a few samples to approximate

![Graphs showing condition numbers and norms for different values of $m/M$.]

How few? As few as $O(\log(\text{sample}))$!

Experiment over regression datasets shows that

- It generally takes 1% to 5% of the samples to approximate well
- Scales well with dimension and saves much time for matrix-matrix multiplication
Takeaways

• Finding optimal (non)diagonal preconditioner can be modeled by SDP
• Optimal preconditioner exhibits nice empirical performance for real-life matrices
• Providing a benchmark for evaluating heuristic preconditioners
• Good for solving systems with fixed left-hand-side matrices

The theory of optimal preconditioner is attractive, but

• For an \( n \times n \) matrix, we need to solve a dual SDP of \( n + 1 \) variables
• Interior point method solves a \( (n + 1) \times (n + 1) \) dense linear system in a iteration
• Not scalable to matrices of size 5000

Finding the optimal preconditioner seems impractical in a real-time fashion

What about an approximately optimal preconditioner?
Today’s Talk

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Approximately optimal preconditioner is acceptable

- Condition number optimization is different from common convex optimization problems
- Performance of algorithms moderately depends on condition number, e.g., $O(\kappa \log(1/\varepsilon))$
- An error of condition number up to moderate $\varepsilon$ does not affect performance
- We can be aggressive in the trade-off between accuracy and scalability

Our approach:

Step 1: we show that dimension of SDP can be reduced

Step 2: we show that the SDP can be solved via LP with cutting-planes
Step 1: Optimal combination of existing preconditioners

- The bottleneck of optimal diagonal preconditioner comes from \( n + 1 \) SDP variables
- Each “1” from \( n \) corresponds to a column of the identity matrix
  as if we are combining \( n \) bases in the space of diagonal preconditioner.

Focusing on the whole space is expensive. How about a subspace?

- Pick \( k \) “base” preconditioners \( D_1, \ldots, D_k \) that work well in practice
  e.g. Jacobi, Ruiz, Sparse approximate inverse ...
- Restrict preconditioner to lie in the subspace spanned by these bases
- Reducing the SDP to \( k + 1 \) variables
- Get the optimal combination of the basic preconditioners
  No worse than the best of them
Computational results: optimal combination of preconditioners

- Choosing three basis preconditioners: Jacobi, Ruiz and Identity
- Able to deal with sparse matrices of size up to 20000
- 2.5 factor of improvement beyond Jacobi
- 2.8 factor of improvement beyond Ruiz
- 1.2 factor of improvement beyond best among Jacobi/Ruiz/None

We are much more scalable now. But solving an SDP is still not ideal. Can we go further?

Yes! We can even be “SDP-free”
Step 2: Semi-infinite linear programming and cutting plane method

We are faced with a dual SDP

- with very few dual variables
  in practice 3 to 10 base preconditioners are needed
- with most constraint matrices diagonal

Recall that an SDP conic constraint $S \succeq 0$ can be represented by infinite linear constraints

$$ C - A^* y \succeq 0 \iff \langle a, (C - A^* y)a \rangle \geq 0, \text{ for all } a \in \mathbb{R}^n \iff \langle A(aa^T), y \rangle \leq a^T Ca $$

- the SDP can be written as an LP with infinite number of constraints and few variables
- we can employ a cutting plane/constraint generation approach to solve the LP
- similar to the interior point cutting plane method for semi-infinite programming
Cutting plane method for optimal preconditioner

To implement the cutting plane approach

- we initialize with a set of linear constraints
- solve the LP and obtain the LP solution
  the LP has very few variables
- call the separation oracle
  compute the minimum eigenvalue of the dual slack (efficiently computable using Lanczos iteration)

\[ \lambda_{\min}(C - \mathcal{A}^*y) < -\varepsilon, \text{ then there exists } \langle d, (C - \mathcal{A}^*y)d \rangle < 0 \]

  cutting plane \( \langle \mathcal{A}(dd^T), y \rangle \leq d^T Cd \) is added to the problem

- iterate till convergence

- We solve a sequence of low-dimension LPs rather than the original SDP
- LPs can be efficiently warm-started using dual simplex

How well does the cutting plane approach work in practice?
Computational results: LP + cutting plane

How does the method work in practice?

- For moderate number (<30) of base preconditioners, only 5~20 LPs are needed to reach good accuracy
- The separation oracle runs very fast when the matrix is sparse
- Dual simplex solves the LPs efficiently
- A 10000 by 10000 sparse matrix needs <5 seconds scalable to very large matrices

x-axis: number of LP iterations
y-axis: up: violation of SDP conic constraint
low: relative optimality in condition number
**Summary**

- Finding the optimal (non)diagonal preconditioner can be modeled by SDP: another SDP application
- The optimal diagonal preconditioner serves as a benchmark and has desirable empirical performances compared to heuristic approaches

We further show that

- Finding the optimal combination of few heuristic diagonal preconditioners can be modeled by SDP, and it improves scalability of the SDP approach without compromising much performances
- The SDP from optimal combination of preconditioners can be efficiently solved using Semi-infinite optimization + LP dual simplex + cutting plane method,…

*Finding approximate optimal diagonal preconditioners may be scalable?*