LECTURE NOTES FOR MTH 371, WINTER 2022 "LARGE SCALE DATA ALGORITHMS"

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1. Homework # 5: Due March 9

Problem 1.1 (Preconditioned conjugate gradient (PCG) method)**.**

(i) *Implement the PCG algorithm (see below) which takes as input a $n \times n$ s.p.d. matrix A (or a function that computes its actions), a preconditioner B that is either given as a s.p.d. matrix, or as a function that takes as input $\mathbf{r}$ and returns $\overline{\mathbf{r}} = B^{-1}\mathbf{r}$ which is the solution of $B\overline{\mathbf{r}} = \mathbf{r}$. Examples for B are the ℓ_1-smoother, the symmetric Gauss-Seidel, and a two-level algorithm. The complete set of input parameters for the PCG algorithm are given in the algorithm below.*

(ii) *Run the PCG algorithm for three preconditioners: (i) B being the diagonal of A, (ii) B being the symmetric Gauss-Seidel algorithm, (iii) B being defined by a symmetrized two-level algorithm (see below).*

Algorithm 1.1 (Preconditioned Conjugate Gradient (PCG) Method)**.**

Given an s.p.d. matrix A (via its actions), r.h.s. $\mathbf{b}$, initial iterate $\mathbf{x}$ (zero or a random vector), tolerance ϵ $(= 10^{-6})$and a maximal number of iterations, $\max\_iter$ $(= 1000)$*. For a given s.p.d. preconditioner B, which computes $B^{-1}\mathbf{r}$ for any given vector $\mathbf{r}$, we perform:*

- *Initiate: compute initial residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$, the preconditioneed residual $\overline{\mathbf{r}} = B^{-1}\mathbf{r}$, the squared norm $\delta_0 = \mathbf{r}^T B^{-1}\mathbf{r} = \|\mathbf{r}\|^2_{B^{-1}} = \mathbf{r}^T\overline{\mathbf{r}}$, $\delta = \delta_0$, and let $\mathbf{p} = \overline{\mathbf{r}}$ be the initial search vector.*
- *Loop: for iter $= 1, 2, \ldots,$* $\max\_iter$ *compute*
  - $\mathbf{g} = A\mathbf{p}$.
  - $\alpha = \frac{\mathbf{r}^T B^{-1}\mathbf{r}}{\mathbf{p}^T A\mathbf{p}} = \frac{\delta}{\mathbf{p}^T\mathbf{g}}$.
  - *Update iterate $\mathbf{x} := \mathbf{x} + \alpha\mathbf{p}$.*
  - *Update residual $\mathbf{r} = \mathbf{r} - \alpha A\mathbf{p} = \mathbf{r} - \alpha\mathbf{g}$.*
  - *New preconditioned residual: $\overline{\mathbf{r}} = B^{-1}\mathbf{r}$.*
  - *Let $\delta_{old} = \delta$.*
  - *Compute $\delta = \mathbf{r}^T B^{-1}\mathbf{r} = \mathbf{r}^T\overline{\mathbf{r}}$.*
  - *Check for convergence: If $(\delta < \epsilon^2\delta_0)$ exit due to achieved convergence tolerance.*
  - *Compute next search direction:*
    - *Compute $\beta = \frac{\mathbf{r}^T B^{-1}\mathbf{r}}{\mathbf{r}^T_{old} B^{-1}\mathbf{r}_{old}} = \frac{\delta}{\delta_{old}}$.*
    - *Next search direction is: $\mathbf{p} = \overline{\mathbf{r}} + \beta\mathbf{p}$.*
- *End of Loop on iter.*

Algorithm 1.2 (Symmetric two-level algorithm)**.**

*Let A be a $n \times n$ s.p.d. matrix. Given a convergent method based on a matrix M (either ℓ_1–smoother or the forward Gauss-Seidel) and consider M^T as well (it will be either the ℓ_1-smoother, i.e., $M^T = M$, or the backward Gauss-Seidel, if M is the forward Gauss-Seidel). We also need the matrix P corresponding to a set of aggregates, i.e., the relation "*vertex_aggregate*" constructed for the sparsity graph of the sparse matrix A for example by the Luby's algorithm. We also need the coarse matrix $A_c = P^T AP$. The two-level algorithm requires function that solves equations with A_c (use the LDL^T or LU factorization of the s.p.d. matrix A_c).*

The symmetric two-level algorithm takes as input a vector $\mathbf{r}$ and provides on output $\overline{\mathbf{r}} = B^{-1}\mathbf{r}$, which is defined by the following steps;

- *Solve for $\mathbf{y}$, $M\mathbf{y} = \mathbf{r}$.*
- *Compute coarse r.h.s. $\mathbf{r}_c = P^T(\mathbf{r} - A\mathbf{y})$.*
- *Solve the coarse problem for $\mathbf{y}_c$, $A_c\mathbf{y}_c = \mathbf{r}_c$ (use LDL^T or LU facorization of A_c).*
- *Update $\mathbf{y} = \mathbf{y} + P\mathbf{y}_c$.*
- *Solve for correction $\mathbf{z}$, $M^T\mathbf{z} = \mathbf{r} - A\mathbf{y}$.*
- *Update $\mathbf{y} := \mathbf{y} + \mathbf{z}$.*
- *$\overline{\mathbf{r}} = \mathbf{y}$.*

The above mapping $B^{-1}: \mathbf{r} \mapsto \overline{\mathbf{r}}$ is referred to as the two-level preconditioner, and B is sometimes denoted B_{TL}.

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