Noise propagation on the Golub-Kahan iterative bidiagonalization process

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Outline

$Ax = b$

- We want to solve the problem:

$$Ax = b, \quad A \in \mathbb{R}^{n \times n}, \quad b = b^{exact} + b^{noise}.$$

- b^{noise} is a white noise vector with unknown noise level δ_{noise}.
- Information on how the noise propagates can be used to develop a stopping criteria for hybrid methods (iterate and regularize).
- The Golub-Kahan iterative bidiagonalization process provides a way to analyze how the noise spreads into the core problem.

Golub-Kahan Iterative Bidiagonalization process

- Given $w_0 = 0$, $s_1 = b/\beta_1$, where $\beta_1 = \|b\| \neq 0$:

$$\begin{aligned} \alpha_j w_j &= A^T s_j - \beta_j w_{j-1}, & \|w_j\| &= 1, \\ \beta_{j+1} s_{j+1} &= A w_j - \alpha_j s_j, & \|s_{j+1}\| &= 1 \end{aligned}$$

  until $\alpha_j = 0$ or $\beta_{j+1} = 0$, or we reach the dimensionality of the problem.
- The vectors s_k and w_k are orthonormal.

Matrix form

- Let $S_k = [s_1, \ldots, s_k]$ and $W_k = [w_1, \ldots, w_k]$, then:

$$A^T S_k = W_k L_k^T, \quad AW_k = [S_k, s_{k+1}] L_{k+},$$

where

$$L_k = \begin{bmatrix} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_k & \alpha_k \end{bmatrix}, \quad L_{k+} = \begin{bmatrix} L_k \\ \beta_{k+1} e_k^T \end{bmatrix}$$

- This bidiagonal decomposition can be used to calculate the SVD of A in a stable way. $A = S_k L_k W_k^T = S_k U \Sigma V^T W_k^T$ $= U_k \Sigma V_k^T$, with U_k and V_k unitary.

Lanczos tridiagonalization of AA^T

- Using the starting vector $s_1 = b/\beta_1$, $\beta_1 = \|b\|$, yields in k steps:
$$AA^T S_k = S_k T_k + \alpha_k \beta_{k+1} s_{k+1} e_k^T,$$
and
$$T_k = L_k L_k^T = \begin{bmatrix} \alpha_1^2 & \alpha_1\beta_2 & & \\ \alpha_1\beta_2 & \alpha_2^2+\beta_2^2 & \ddots & \\ & \ddots & \ddots & \alpha_{k-1}\beta_k \\ & & \alpha_{k-1}\beta_k & \alpha_k^2+\beta_k^2 \end{bmatrix}$$
- The matrix L_k from the GKIB is a Cholesky factor of the matrix T_k.

The core problem

- Consider $x_k = W_k y_k$ as an approximation for the solution of $Ax_k \approx b$.
- Looking to the residual:

$$r_k = b - AW_k y_k = S_{k+1}(\beta_1 e_1 - L_{k+} y_k)$$
$$= S_k(\beta_1 e_1 - L_k y_k) - (\beta_{k+1} e_k^T y_k) s_{k+1},$$

we get two subproblems:

1. $L_k y_k = \beta_1 e_1$, for r_k orthogonal to S_k (CGME);
2. $y_k = \min_y \|L_{k+} y - \beta_1 e_1\|$, if we minimize r_k (LSQR or CGLS).

Summarizing

- The bidiagonalization concentrates the useful information of the main problem on its bidiagonal block.
- In presence of noise, those subproblems might be polluted by the noise.
- An investigation on how the noise propagates might aid on solving the ill-posed problem. (When to stop the iteration procedure).
- We will use two main approaches: one looks to the behavior of the high frequencies of the vectors s_k and the other its normalized cumulative periodogram.

- The test problem utilized for the numerical experiments was `shaw(400)`, which satisfy the *discrete Picard condition* on average.
- We used the following noise levels $\delta_{noise} = 10^{-14}, 10^{-8}, 10^{-4}$. Where

$$\delta_{noise} = \frac{\|b^{noise}\|}{\|b^{exact}\|}.$$

Picard plot

- u_j are the left singular vectors of A.

Spectral coefficients

Left singular vectors

Analizing the spectral coefficients

- Using the SVD of A and the Lanczos tridiagonalization of AA^T:

$$\Sigma^2(U^T S_k) = (U^T S_k)(L_k L_k^T) + \alpha_k \beta_{k+1}(U^T s_{k+1})e_k^T.$$

- Setting $k = 1$ we can see how the noise spreads to s_2 (looking to the last column):

$$\alpha_1 \beta_2 (U^T s_2) = (\Sigma^2 - \alpha_1^2 I) U^T s_1$$

- The matrix acts like a filter on the lower frequencies

$$\frac{\sigma_i}{\alpha_1 \beta_2} - \frac{\alpha_1}{\beta_2}$$

- α_1 / β_2 is likely to be larger than 1.

Generalizing

Normalized Cumulative Periodogram (NCP)

- Definition:

$$\mathbf{c}_j = |dft(\mathbf{y})_j|^2, \quad z_j = \frac{\sum_{i=1}^{j} \mathbf{c}_i}{\sum_{i=1}^{q} \mathbf{c}_i}, \quad j = 1, \ldots, q.$$

- Kolmogorov-Smirnonoff at 5% significance level: the NCP curve must lie between the limits $\pm 1.35 q^{-1/2}$ of the straight line (diagonal).
- There are other kind of measures for testing if a distribution is white-noise like, e.g., *total deviation*.

NCP plot

White-noise measures

Comparing the methods to find k_{noise}

problem	`shaw(400)`			
δ_{noise}	10^{-14}	10^{-8}	10^{-4}	10^{-2}
k_{noise} (GKIB)	17	11	7	3
k_{noise} (NCP)	27	26	8	23
$\tilde{\delta}_{noise}$ (GKIB)	$5.9E-15$	$1.2E-8$	$5.3E-5$	$1.6E-2$
$\tilde{\delta}_{noise}$ (NCP)	$1.5E-15$	$8.1E-9$	$3.7E-4$	$3.6E-3$

- $\tilde{\delta}_{noise}$ indicates the estimated noise level.

Resolution matrix of the GKIB process

- $R^\sharp = W_k(L_k^T L_k)^{-1} L_k^T S_k^T A$.
- Show the resolution matrix in Matlab.