Golub-Kahan iterative bidiagonalization and stopping criteria in ill-posed problems

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Outline

1. Problem formulation
2. Regularization by Golub-Kahan bidiagonalization
3. How to identify the noise
4. Summary and future work

1. Problem formulation

Consider an ill-posed linear system

$$Ax \approx b, \qquad A \in \mathbb{R}^{n \times m}, \qquad b \in \mathbb{R}^n,$$

with a noise contaminated right-hand side

$$b = b^{exact} + b^{noise} \neq 0 \in \mathbb{R}^n, \quad \| b^{exact} \| \gg \| b^{noise} \|.$$

Possible difficulties:

- the noise component b^{noise} is unknown;
- the rank of A is not well defined (singular values of A decay gradually to zero);
- the solution is sensitive on small perturbations in data.

Denote $l = \text{rank}(A)$. Consider the singular value decomposition

$$A = \tilde{U}\,\tilde{\Sigma}\,\tilde{V}^T = \sum_{i=1}^{l} \tilde{u}_i \tilde{\sigma}_i \tilde{v}_i^T \,,$$

$$\tilde{U} = [\tilde{u}_1, \ldots, \tilde{u}_l], \quad \tilde{V} = [\tilde{v}_1, \ldots, \tilde{v}_l], \quad \tilde{\Sigma} = \text{diag}(\tilde{\sigma}_1, \ldots, \tilde{\sigma}_l)\,.$$

The least squares method (LS) minimizes $\|b - Ax\|$ and

$$\begin{aligned} x^{LS} &= \sum_{i=1}^{l} \frac{\tilde{u}_i^T b}{\tilde{\sigma}_i} \tilde{v}_i \\ &= \sum_{i=1}^{l} \frac{\tilde{u}_i^T b^{exact}}{\tilde{\sigma}_i} \tilde{v}_i + \sum_{i=1}^{l} \frac{\tilde{u}_i^T b^{noise}}{\tilde{\sigma}_i} \tilde{v}_i \,. \end{aligned}$$

Thus components of the solution corresponding to small singular values may be dominated by errors in b, the solution is meaningless.

Regularization methods are used to suppress the effect of errors in the data and extract the essential information about the system, e.g.,

- truncated SVD, truncated total least squares, Tikhonov regularization, see [Hansen, O'Leary – 97], [Fierro, Golub, Hansen, O'Leary – 97], [Hansen - 98], [Golub, Hansen, O'Leary - 99], [Sima, Van Huffel, Golub - 04], [Kilmer, Hansen, Espanol - 06], ...
- methods based on iterative Golub-Kahan bidiagonalization as LSQR, hybrid methods, see [Paige, Saunders – 82], [Bjorck – 96], [Hansen – 97], [Hanke – 01], ...

2. Regularization by Golub-Kahan bidiagonalization

Consider Golub-Kahan bidiagonalization (GK) of A in the form

$$
\begin{aligned}
& w_0 = 0\,, \quad s_1 = b\,/\,\beta_1\,, \quad \text{where} \quad \beta_1 = \|b\|_2\,, \\
& \text{for} \quad j = 1, 2, 3, \ldots \\
& \quad \alpha_j\, w_j = A^T s_j - \beta_j\, w_{j-1}\,, \qquad \|w_j\| = 1\,, \\
& \quad \beta_{j+1}\, s_{j+1} = A\, w_j - \alpha_j\, s_j\,, \quad \|s_{j+1}\| = 1\,, \\
& \text{end}\,.
\end{aligned}
$$

Denote $S_k = [u_1, \ldots, s_k]$, $W_k = [w_1, \ldots, w_k]$ resulting matrices with orthonormal columns and

$$
L_k = \left[\begin{array}{cccc} \alpha_1 & & & \\ \beta_2 & \alpha_2 & & \\ & \ddots & \ddots & \\ & & \beta_k & \alpha_k \end{array} \right], \qquad L_{k+} = \left[\begin{array}{c} L_k \\ e_k^T \beta_{k+1} \end{array} \right].
$$

Regularization methods based on GK compute the solution in two steps. First the problem is projected on the Krylov subspace using k steps of bidiagonalization, i.e.

$$A\,W_k \;=\; S_{k+1}\,L_{k+}\,.$$

Then an inner regularization is applied to the projected problem

$$A\,x \approx b \;\longrightarrow\; L_{k+}\,y \approx \beta_1\,e_1\,.$$

When to stop the bidiagonalization?

Core reduction:

From the core theory [Paige, Strakoš – 06] it follows that there exists a fundamental decomposition

$$P^T \, [\, b \,|\, A\, Q \,] = \left[\begin{array}{c||c|c} b_1 & A_{11} & 0 \\ \hline 0 & 0 & A_{22} \end{array} \right] , \qquad P^T = P^{-1} \, , \qquad Q^T = Q^{-1} \, ,$$

yielding a subproblem

$$A_{11} \, x_1 \; \approx \; b_1 \, ,$$

which contains all necessary and sufficient information to solve the original problem,

$$x = Q \left[\begin{array}{c} x_1 \\ 0 \end{array} \right] .$$

Computation of the core problem:

If the GK bidiagonalization of A with $u_1 \equiv b/\beta_1$, $\beta_1 \equiv \|b\|$ stops with

- $\beta_{p+1} = 0$ or $p = n$, then $S_p^T\,[b, AW_p] \;=\; [\beta_1 e_1, L_p] \;\equiv\; [b_1, A_{11}]$ and

$$L_p\, y \;=\; \beta_1\, e_1$$

  is the core problem;

- $\alpha_{p+1} = 0$ or $p = m$, then $S_{p+1}^T\,[b, AW_p] \;=\; [\beta_1 e_1, L_{p+}] \;\equiv\; [b_1, A_{11}]$ and

$$L_{p+}\, y \;\approx\; \beta_1\, e_1$$

  is the core problem.

In exact arithmetic

GK stops with $\beta_{p+1} = 0$ or $\alpha_{p+1} = 0$. Then the bidiagonal problem

$$L_p\, y = \beta_1\, e_1 \quad \text{or} \quad L_{p+}\, y \approx \beta_1\, e_1$$

contains all necessary and sufficient information to solve the original problem.

In floating-point arithmetic

we have to stop GK by using some stopping criteria. We can view the stopping as a perturbation of the bidiagonal matrix

$$\beta_{k+1} \longrightarrow \tilde{\beta}_{k+1} = 0 \quad \text{or} \quad \alpha_{k+1} \longrightarrow \tilde{\alpha}_{k+1} = 0\,,$$

which yields the modified matrix $\tilde{L}_k$ or $\tilde{L}_{k+}$, respectively.

How to define the stopping criteria for GK if the ill-posed problem with a noisy right-hand side is considered?

3. How to identify the noise

GK starts with the normalized noisy right-hand side $s_1 = b\,/\,\|b\|$, thus vectors s_j has to contain some information about the noise.

Our idea is: **An information about the noise level can be obtained by Fourier analysis of the vectors s_j generated by GK.**

We used two different Fourier basis:

• basis of the left singular vectors $\tilde{u}_j$ of A (basis useful for the theoretical analysis but not in practical computations);

• trigonometric basis (well applicable in practical computations, e.g., the fast Fourier transform algorithm – FFT).

An example:

Consider the problem SHAW(400) from [Hansen, RTools] with a noisy right-hand side (the noise was artificially added)

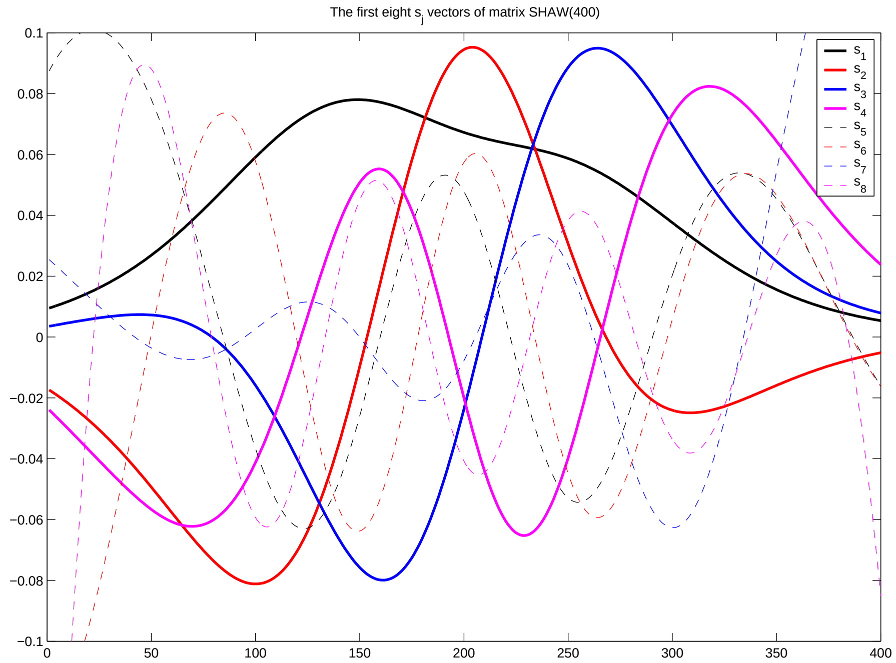
$$46.6225 = \| b^{exact} \| \gg \| b^{noise} \| = 10^{-12} .$$

We study the noise-contaminated vectors s_j in the noise-free basis $\tilde{U} = [\tilde{u}_1, \ldots, \tilde{u}_n]$ and in the frequency domain,

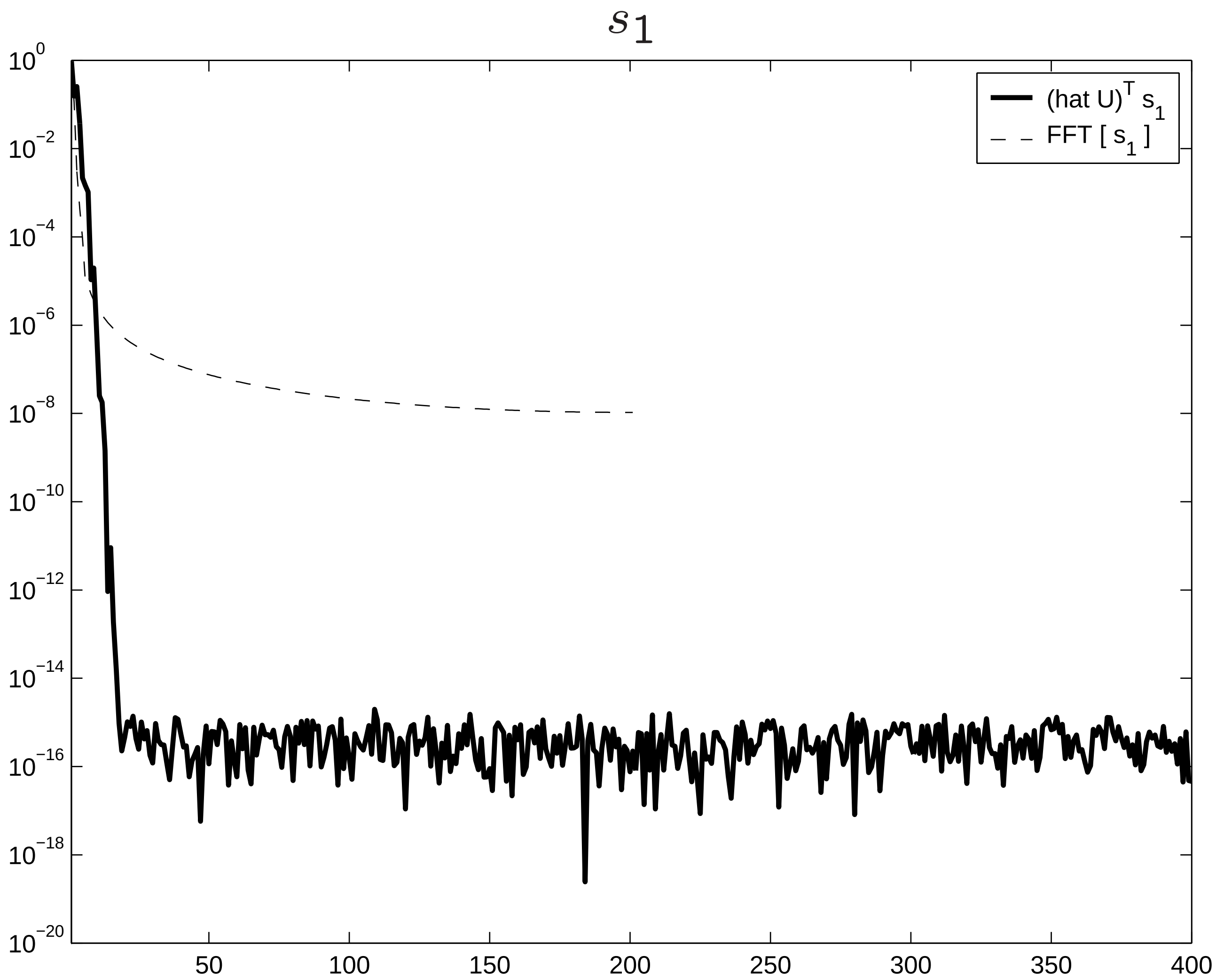
$$(\tilde{U}^T s_j) \quad \text{and} \quad F [s_j] , \qquad j = 1, 2, \ldots ,$$

where F denotes the FFT operator.

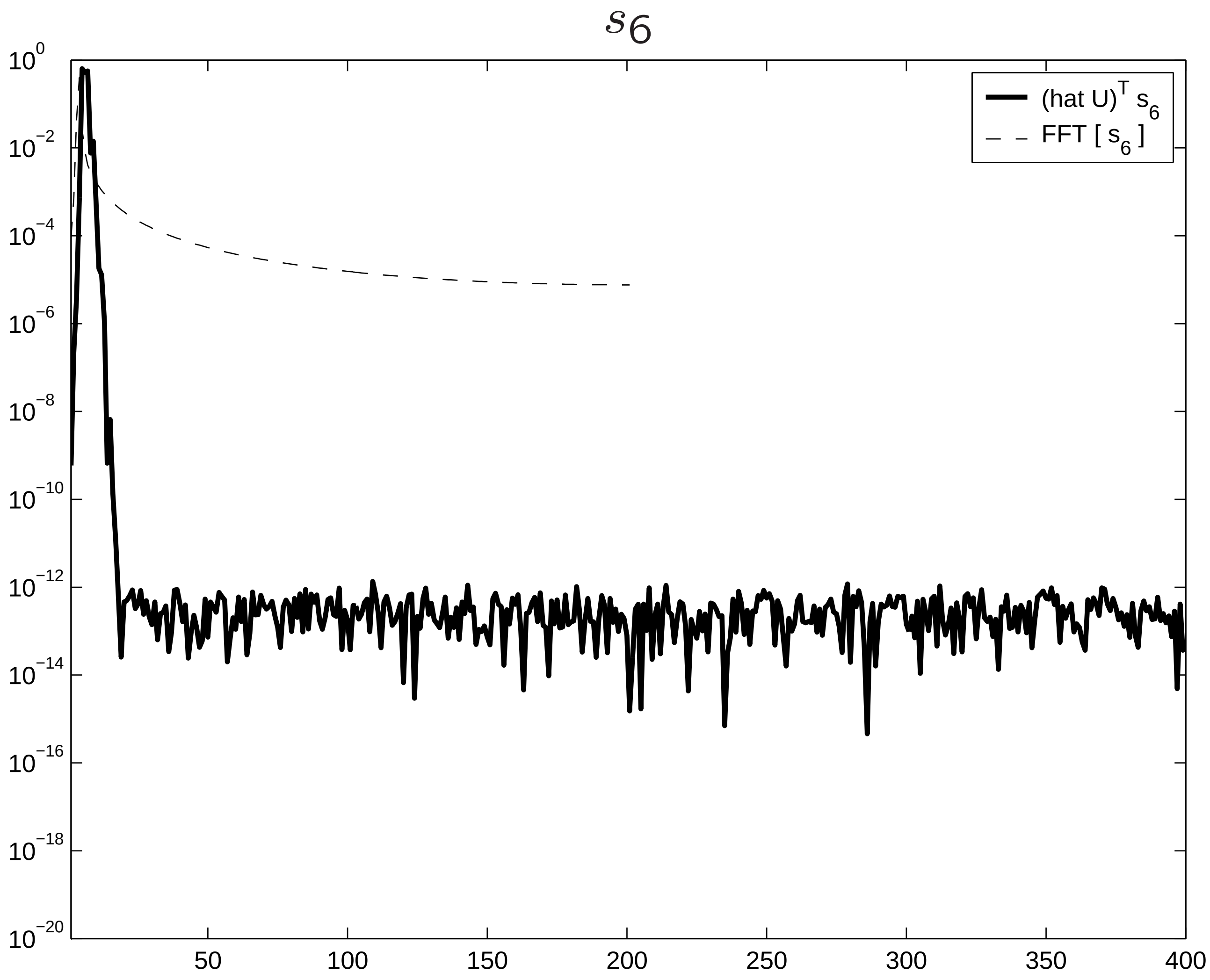
The vector s_1 is **dominated by low frequencies**, thus it has dominant projection in the direction of the left singular vector $\tilde{u}_1$ and possibly several next vectors. Analogously s_2, s_3, ...



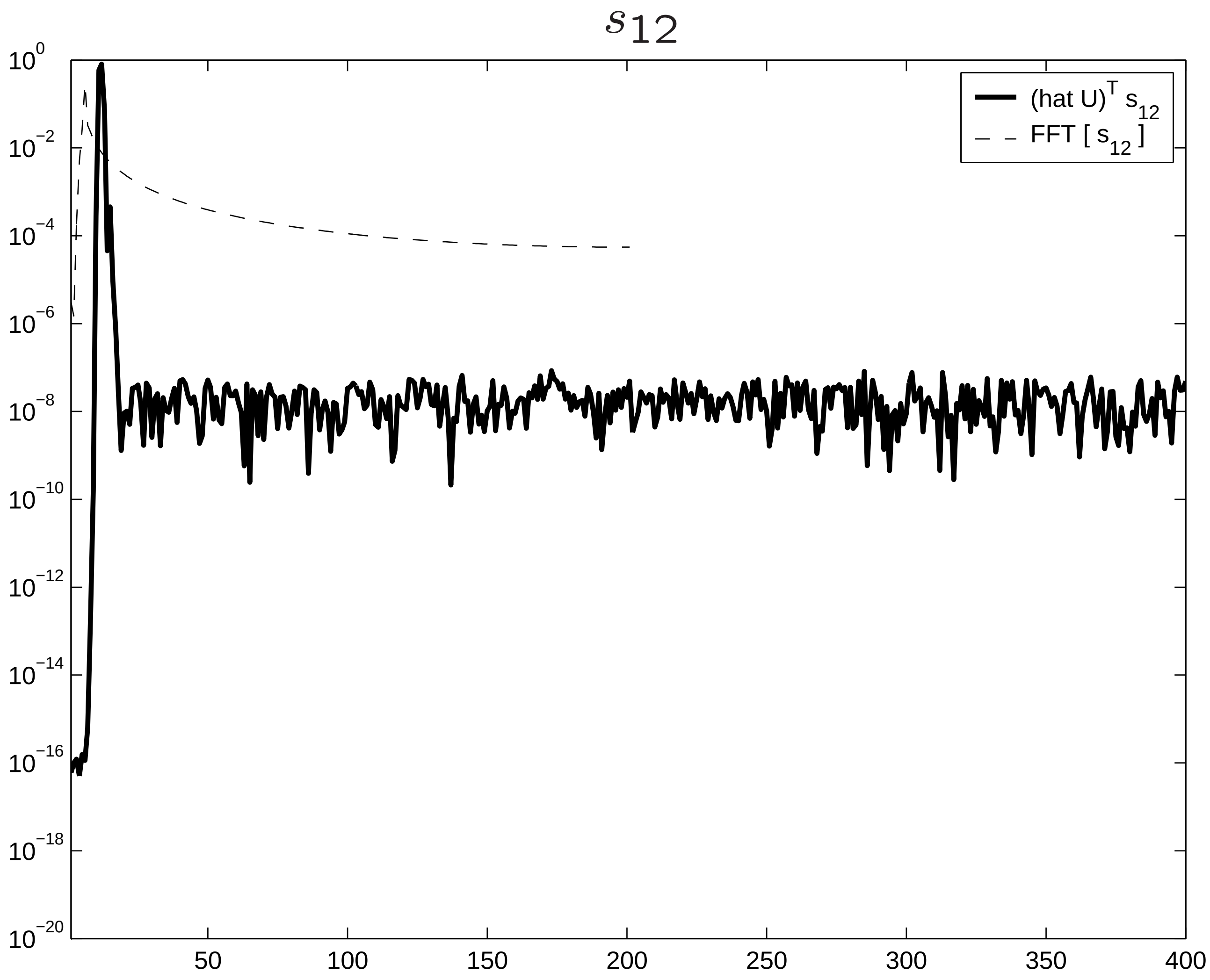
For some index $j = k$ the low frequencies information is projected out from s_k by orthogonalization against the previous vectors s_j, $j = 1, 2, 3, \dots, k-1$, and the noise is revealed.



s_1
(hat U)^T s_1
FFT [s_1]
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
10^-12
10^-14
10^-16
10^-18
10^-20
50
100
150
200
250
300
350
400

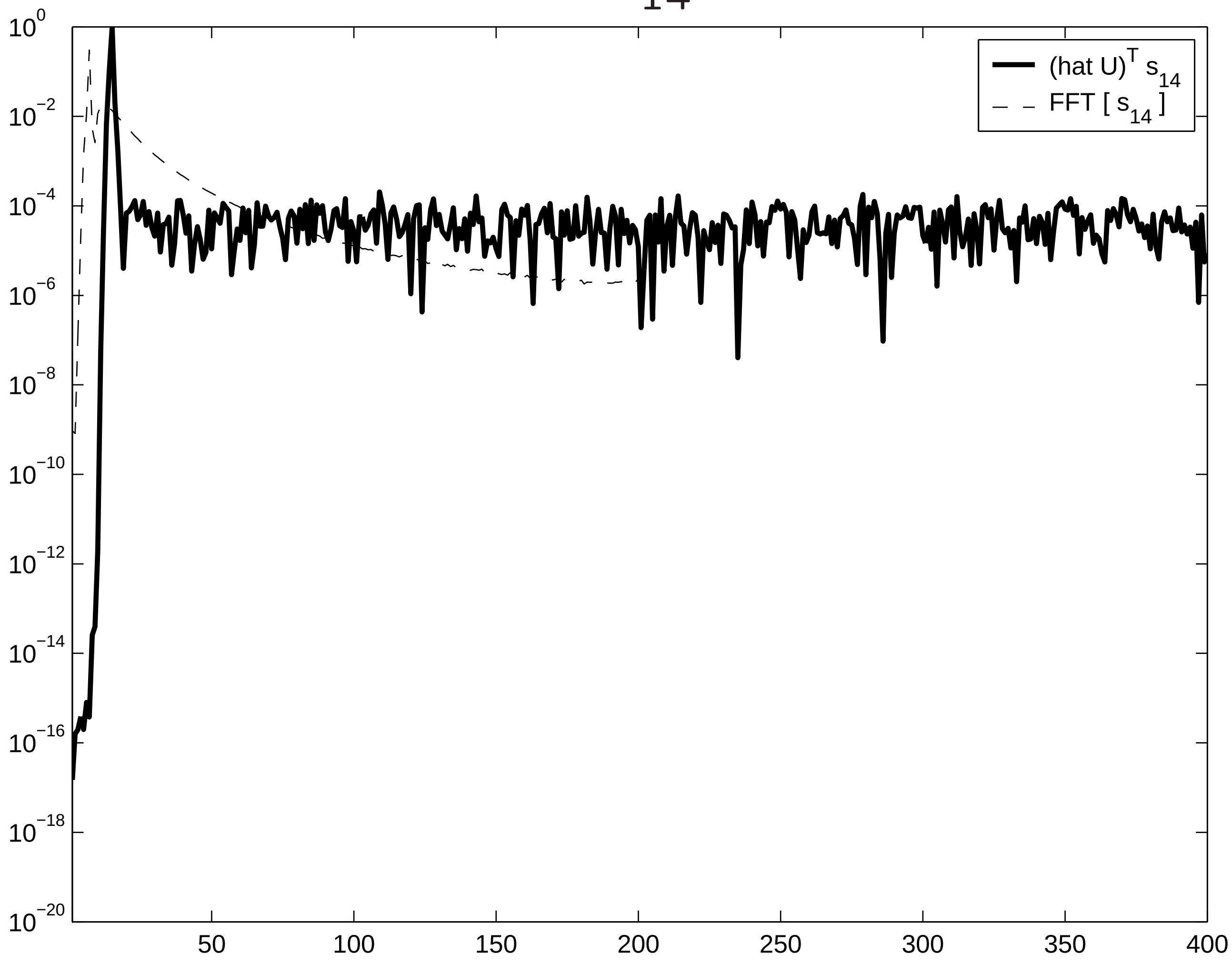


s_6
(hat U)^T s_6
FFT [s_6]
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
10^{-20}
50
100
150
200
250
300
350
400

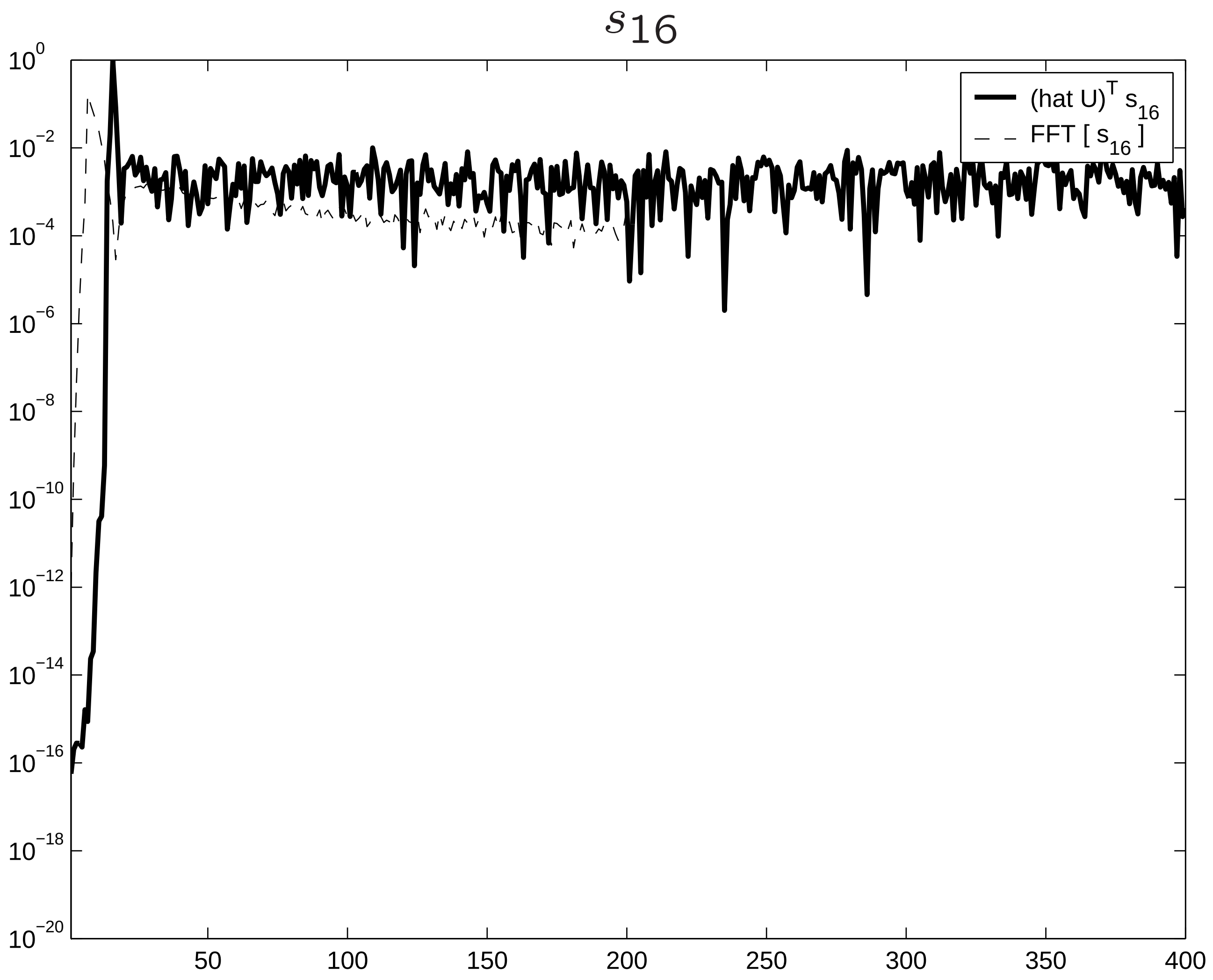


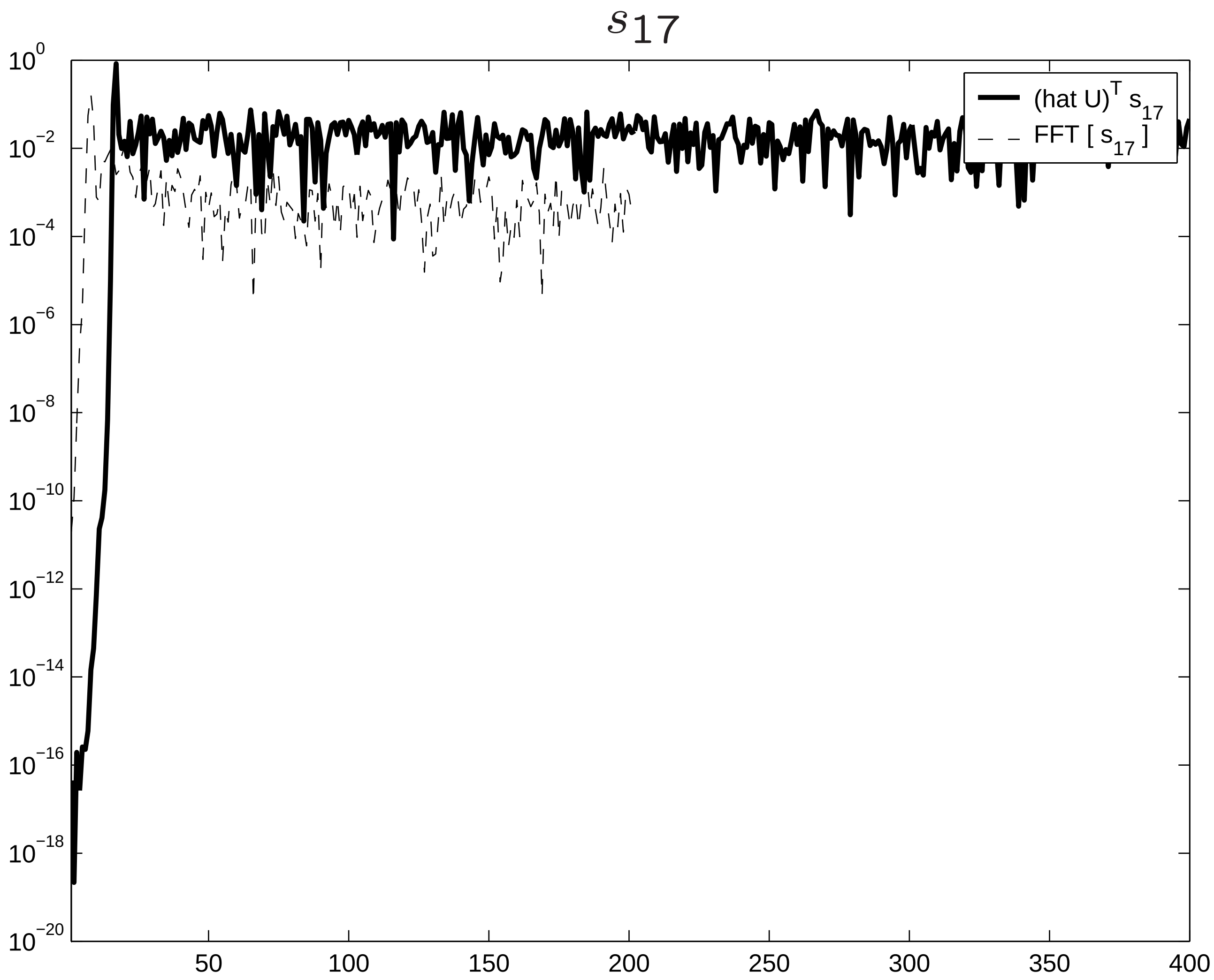
s_{12}
(hat U)^T s$_{12}$
FFT [s$_{12}$]
10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
10^{-20}
50
100
150
200
250
300
350
400

s_{14}

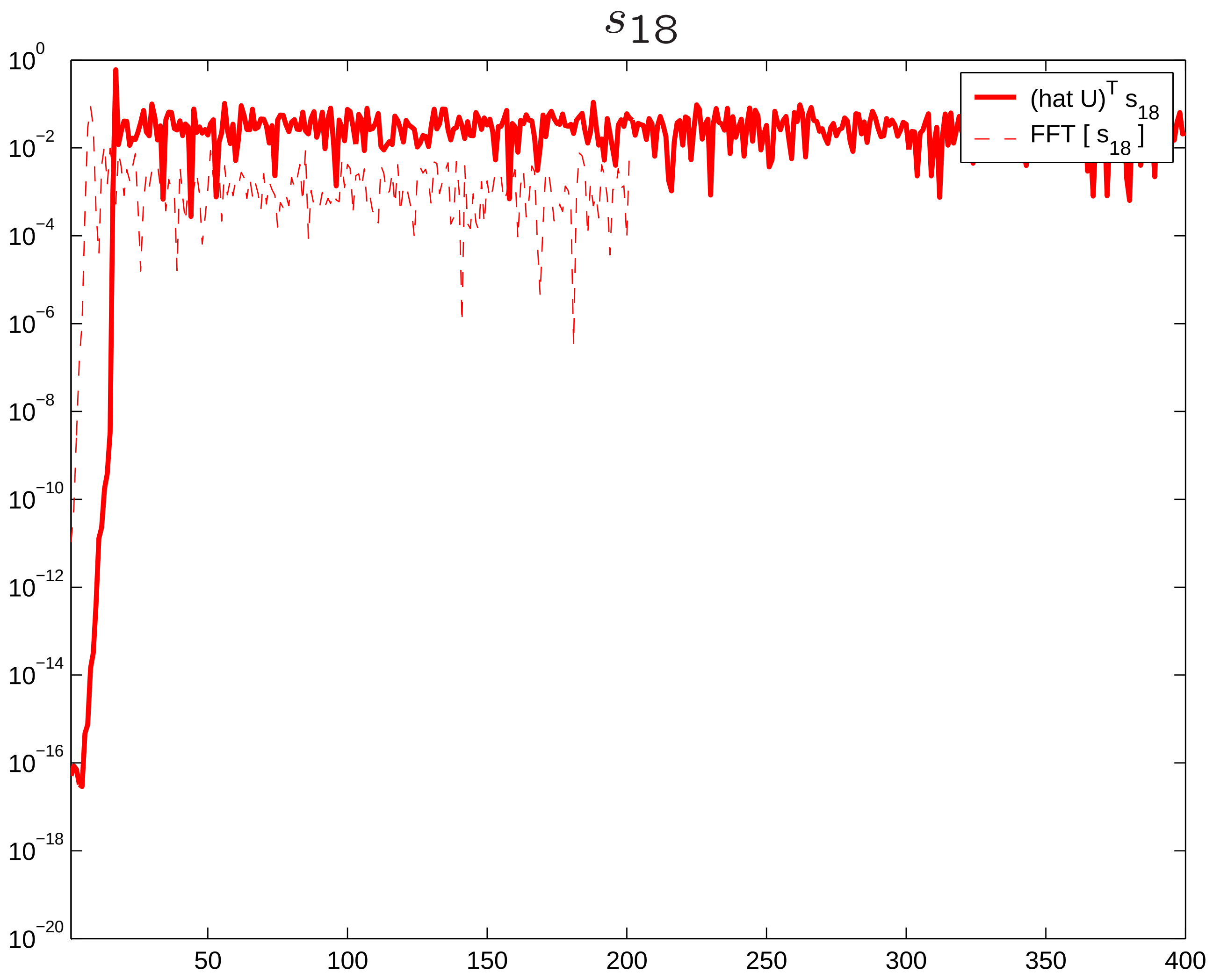


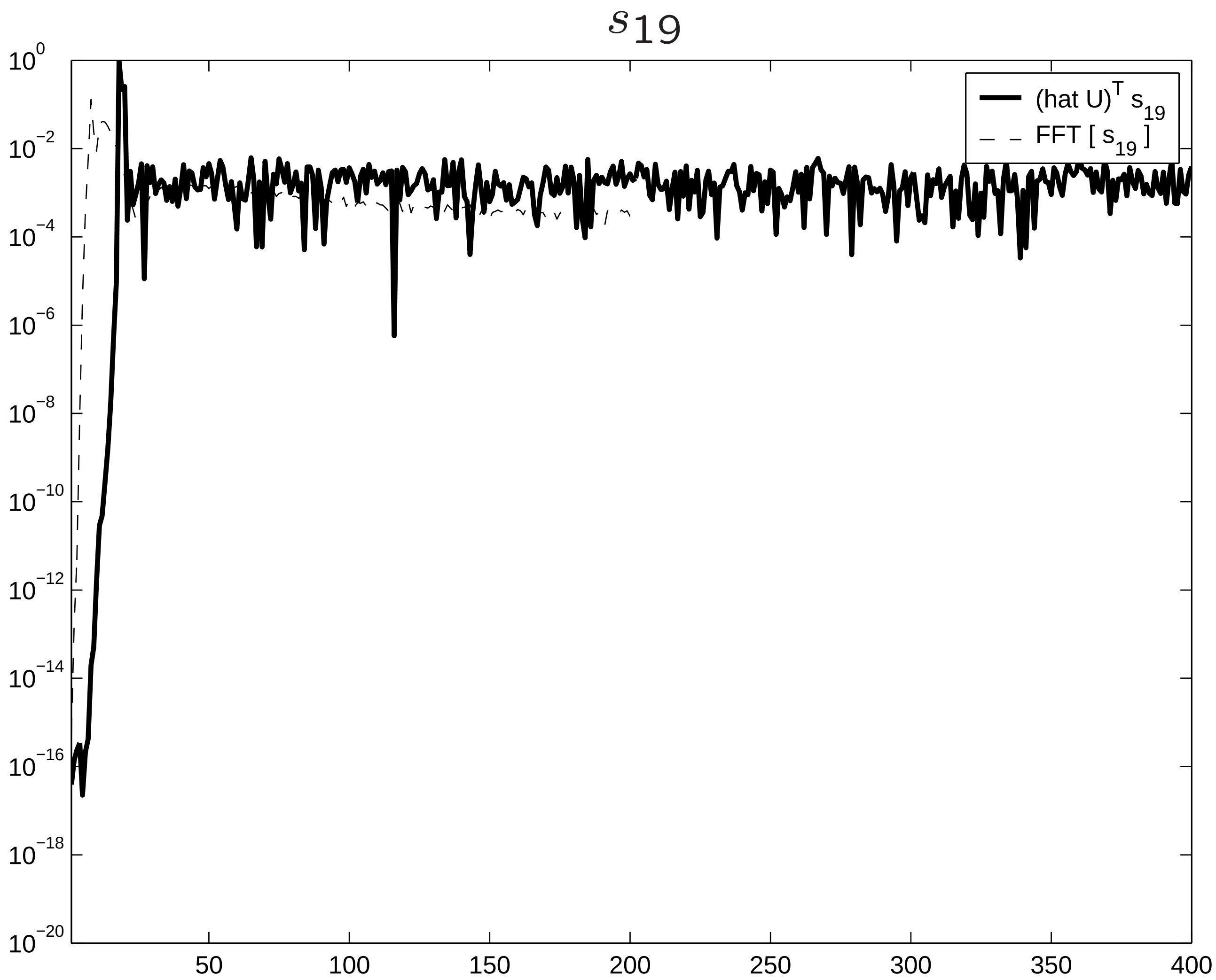
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−14
10^−16
10^−18
10^−20
50
100
150
200
250
300
350
400
(hat U)^T s_14
FFT [s_14]


s_{16}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
10^{-20}
50
100
150
200
250
300
350
400
$(\text{hat U})^T s_{16}$
FFT [s_{16}]



s_{17}
(hat U)^T s_17
FFT [s_17]
10^0
10^-2
10^-4
10^-6
10^-8
10^-10
10^-12
10^-14
10^-16
10^-18
10^-20
50
100
150
200
250
300
350
400


s_{18}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
10^{-20}
50
100
150
200
250
300
350
400
(hat U)^T s_{18}
FFT [s_{18}]


s_{19}
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
10^{-16}
10^{-18}
10^{-20}
50
100
150
200
250
300
350
400
(hat U)^T s_{19}
FFT [s_{19}]

Vector s_{18} is fully dominated by noise –

the noise level is revealed.

Now we get explicit information when the noise begins to cover useful information in the data. The solution of the original problem $A\,x \approx b$ computed through the bidiagonal problem

$$L_{j+}\,y \approx \beta_1\,e_1\,,$$

for $j > k = 18$ can be significantly polluted by the noise.

(In the 19th step, the noise is partially projected out because vectors s_j has to be mutually orthonormal.)

4. Summary and future work

Information about the noise can be obtained directly from the Golub-Kahan bidiagonalization.

Opened questions:

- How to implement this idea as a stopping criterion in hybrid methods?
- Relationship to common stopping criteria in hybrid methods?

Thank you for your attention!

References

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