## MSPAI Probing Variants

Basic formulation for general matrices $C_0, B_0 \in \mathbb{R}^{n\times n}$, probing vectors $e \in \mathbb{R}^{n\times k}$, and weight $\rho \geq 0$ in order to obtain MSPAI $M \in \mathbb{R}^{n\times n}$:

$$\min_M \left\| \begin{pmatrix} C_0 \\ \rho e^T C_0 \end{pmatrix} M - \begin{pmatrix} B_0 \\ \rho e^T B_0 \end{pmatrix} \right\|_F^2 \quad \Longrightarrow \quad \begin{array}{rcl} C_0 M & \approx & B_0 \\ e^T C_0 M & \approx & e^T B_0 \end{array},$$

which is equivalent to $\min_M \|W(C_0 M - B_0)\|_F^2$ with weight matrix $W = \begin{pmatrix} I \\ \rho e^T \end{pmatrix}$.

### Sparse Approximate Inverse Probing

$$\min_M \left\| \begin{pmatrix} A \\ \rho e^T A \end{pmatrix} M - \begin{pmatrix} I \\ \rho e^T \end{pmatrix} \right\|_F^2 \quad \Longrightarrow \quad \begin{array}{rcl} M & \approx & A^{-1} \\ e^T A M & \approx & e^T \end{array}.$$

If $A$ is not given explicitly, set $C_0 = \tilde{A}$, where $\tilde{A}$ is some sparse approximation to $A$, but still compute $e^T A$ exactly. For given approximate inverse factorization $UAL \approx I$ or $UL \approx A^{-1}$:

$$\min_{\tilde{L}} \left\| \begin{pmatrix} UA \\ \rho e^T UA \end{pmatrix} \tilde{L} - \begin{pmatrix} I \\ \rho e^T \end{pmatrix} \right\|_F^2 \quad \Longrightarrow \quad \begin{array}{rcl} UA\tilde{L} & \approx & I \\ e^T UA\tilde{L} & \approx & e^T \end{array}.$$

Obtain the corresponding probed upper triangular factor $\tilde{U}$ through transposition.

### Explicit Probing

$$\min_M \left\| \begin{pmatrix} I \\ \rho e^T \end{pmatrix} M - \begin{pmatrix} A \\ \rho e^T A \end{pmatrix} \right\|_F^2 \quad \Longrightarrow \quad \begin{array}{rcl} M & \approx & A \\ e^T M & \approx & e^T A \end{array}.$$

Again, for implicitly given $A$ substitute $B_0$ by some sparse approximation $\tilde{A}$, but provide $e^T A$ exactly. In case of given explicit factorization $LU \approx A$:

$$\min_{\tilde{U}} \left\| \begin{pmatrix} L \\ \rho e^T L \end{pmatrix} \tilde{U} - \begin{pmatrix} A \\ \rho e^T A \end{pmatrix} \right\|_F^2 \quad \Longrightarrow \quad \begin{array}{rcl} L\tilde{U} & \approx & A \\ e^T L\tilde{U} & \approx & e^T A \end{array}.$$

Transposition yields probed lower triangular factor $\tilde{L}$.

### Schur Complement Probing

MSPAI probing for block matrix $H = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$:

$$\min_{M_B, M_D} \left\| \begin{pmatrix} A & B \\ C & D \\ 0 & \rho e^T S_D \end{pmatrix} \begin{pmatrix} M_B \\ M_D \end{pmatrix} - \begin{pmatrix} 0 \\ I \\ \rho e^T \end{pmatrix} \right\|_F^2 \quad \Longrightarrow \quad \begin{array}{rcl} M_D & \approx & S_D^{-1} \\ e^T M_D & \approx & e^T \end{array},$$

where $S_D^{-1}$ denotes the lower right block of $H^{-1}$.

**Box 3.1:** Employment of MSPAI probing for different applications, where $A$ in general denotes the coefficient matrix in $Ax = b$ and $I$ the unity matrix with the respective dimension.