Stability and residual

The easiest way to prove backward stability is using residuals.

Suppose we have solved a linear system with Matlab:

```
>> A = randn(4, 4); b = randn(4, 1);
>> x = A \ y;
>> A*x - y
ans =
          0
 -1.3878e-17
          0
  2.2204e-16
```

Does a small residual $A\widetilde{\mathbf{x}} - \mathbf{y} = \widetilde{\mathbf{r}}$ mean that we have an accurate solution?

Residual and backward stability

Small residual implies backward stability (and vice versa).

For linear systems: if $A\tilde{\mathbf{x}} - \mathbf{y} = \widetilde{\mathbf{r}}$, then $\tilde{\mathbf{x}}$ is the exact solution of

$$A\tilde{x} = \underbrace{\mathbf{y} + \widetilde{\mathbf{r}}}_{:=\hat{\mathbf{y}}}.$$

Conversely, if $\tilde{\mathbf{x}}$ solves $(A + \delta_A)\tilde{\mathbf{x}} = \mathbf{y} + \delta_{\mathbf{y}}$, then

$$\|A\tilde{\mathbf{x}} - \mathbf{y}\| = \|\delta_{\mathbf{y}} - \delta_A\tilde{\mathbf{x}}\| \leq \|\delta_{\mathbf{y}}\| + \|\delta_A\|\|\tilde{\mathbf{x}}\| \leq O(\mathrm{u})(\|\mathbf{y}\| + \|A\|\|\mathbf{x}\|).$$

(The quantities $\|A\|\|\mathbf{x}\|$ and $\|\mathbf{y}\| = \|A\mathbf{x}\|$ are typically similar in magnitude.)

This idea works also for other problems: e.g., $\tilde{Q}\tilde{R} - A = \delta_A \iff \tilde{Q}\tilde{R}$ is an exact factorization of $\tilde{Q}\tilde{R} = A + \delta_A$.

A posteriori stability test for linear systems

Theorem (residual bound)

Let $A \in \mathbb{R}^{m \times m}, \mathbf{y} \in \mathbb{R}^m$, and $\mathbf{x}$ be the solution of $A\mathbf{x} = \mathbf{y}$.
For a given $\widetilde{\mathbf{x}}$, define $\widetilde{\mathbf{r}} = A\widetilde{\mathbf{x}} - \mathbf{y}$. Then,

$$\frac{\|\widetilde{\mathbf{x}} - \mathbf{x}\|}{\|\mathbf{x}\|} \leq \kappa(A) \frac{\|\widetilde{\mathbf{r}}\|}{\|\mathbf{y}\|}.$$

Proof: $\widetilde{\mathbf{x}}$ is the exact solution of the perturbed system

$$A\widetilde{\mathbf{x}} = \mathbf{y} + \widetilde{\mathbf{r}}.$$

Then we can use the condition number bound: a relative perturbation of size $\frac{\|\widetilde{\mathbf{r}}\|}{\|\mathbf{y}\|}$ is amplified by $\kappa(A)$.

(Note that on a computer the computed value of $\widetilde{\mathbf{r}} = A\widetilde{\mathbf{x}} - \mathbf{y}$ might be inaccurate, too, but we can still trust its order of magnitude, because the error in the product is typically not larger than $\widetilde{\mathbf{r}}$.)

Residual of least squares problems

Now for least squares problems: $\min\|A\mathbf{x}-\mathbf{y}\|$, with computed solution $\widetilde{\mathbf{x}}$.

Can one expect $\widetilde{\mathbf{r}} = A\widetilde{\mathbf{x}} - \mathbf{y}$ to be small? No: for the exact solution $\mathbf{x}$, $\mathbf{r} = A\mathbf{x} - \mathbf{y}$ is not zero; it is the distance between $\mathbf{y}$ and $\operatorname{im}(A)$, which can be as large as $\|\mathbf{y}\|$.

What's small then? Optimization says: the gradient.

$$f(\mathbf{x}) = \frac{1}{2}\|A\mathbf{x}-\mathbf{y}\|^2; \quad \nabla f(\widetilde{\mathbf{x}}) = A^T A\widetilde{\mathbf{x}} - A^T\mathbf{y} = A^T\widetilde{\mathbf{r}}.$$

Can we turn this into a bound? If we apply the residual bound to the normal equations $A^TA\mathbf{x} = A^T\mathbf{y}$, we get

$$\frac{\|\widetilde{\mathbf{x}}-\mathbf{x}\|}{\|\mathbf{x}\|} \leq \kappa(A^TA)\frac{\|A^T\widetilde{\mathbf{r}}\|}{\|A^T\mathbf{y}\|}.$$

however, $\kappa(A^TA) = \kappa(A)^2$ may be much larger than the condition number of the problem. Can we do better?

Augmented system

Trick: convert the LS problem into a bigger square linear system:

Augmented system

$\mathbf{x}$ solves the LS problem $\min \|A\mathbf{x} - \mathbf{y}\|$ if and only if

$$\begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} -\mathbf{r} \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix}.$$

Indeed, expanding we get $-\mathbf{r} = \mathbf{y} - A\mathbf{x}$, $\mathbf{0} = -A^T\mathbf{r} = A^T(A\mathbf{x} - \mathbf{y})$.

Interesting connection: this is (essentially) the KKT system of the constrained problem $\min_{\mathbf{r}=A\mathbf{x}-\mathbf{y}} \frac{1}{2}\|\mathbf{r}\|^2$.

(You will see other KKT systems with this block structure with prof. Frangioni.)

Augmented system bound

Augmented system bound

For any $\tilde{\mathbf{x}}$, set $\widetilde{\mathbf{r}} = A\tilde{\mathbf{x}} - \mathbf{y}$. Then,

$$\frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|}{\left\| \begin{bmatrix} -\mathbf{r} \\ \mathbf{x} \end{bmatrix} \right\|} \leq \kappa \left(\begin{bmatrix} I & A^T \\ A & 0 \end{bmatrix} \right) \frac{\|A^T \widetilde{\mathbf{r}}\|}{\|\mathbf{y}\|}.$$

Proof: apply the residual bound to the extended linear system, and note that

$$\|\tilde{\mathbf{x}} - \mathbf{x}\| \leq \left\| \begin{bmatrix} -\tilde{\mathbf{r}} \\ \tilde{\mathbf{x}} \end{bmatrix} - \begin{bmatrix} -\mathbf{r} \\ \mathbf{x} \end{bmatrix} . \right\|$$

since the LHS is a block of the RHS.

Problem: $\|\mathbf{r}\|$ can be much larger than $\|\mathbf{x}\|$, and when this happens our bound becomes useless.

Scaling the augmented system

Even if we prove that $\left\| \begin{bmatrix} -\tilde{\mathbf{r}} \\ \tilde{\mathbf{x}} \end{bmatrix} - \begin{bmatrix} -\mathbf{r} \\ \mathbf{x} \end{bmatrix} \right\| = O(\mathrm{u}) \left\| \begin{bmatrix} -\mathbf{r} \\ \mathbf{x} \end{bmatrix} \right\|$, this does not imply that $\|\tilde{\mathbf{x}} - \mathbf{x}\| = O(\mathrm{u})\|\mathbf{x}\|$, because the two blocks can have very different magnitudes, e.g., $\|\mathbf{r}\| \approx 1$, $\|\mathbf{x}\| \approx 10^{-16}$.

Solution: switch to a scaled version of the augmented system.

Augmented system

$\mathbf{x}$ solves the LS problem $\min\|A\mathbf{x} - \mathbf{y}\|$ if and only if

$$\begin{bmatrix} \alpha I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} -\frac{1}{\alpha}\mathbf{r} \\ \mathbf{x} \end{bmatrix} = \begin{bmatrix} \mathbf{y} \\ \mathbf{0} \end{bmatrix}.$$

Choosing a suitable value of α can improve the bound.

A residual test for least squares problem

Augmented system bound

For any $\tilde{\mathbf{x}}$, set $\widetilde{\mathbf{r}} = A\tilde{\mathbf{x}} - \mathbf{y}$. Then, for each $\alpha > 0$,

$$\frac{\|\tilde{\mathbf{x}} - \mathbf{x}\|}{\left\| \begin{bmatrix} -\frac{1}{\alpha}\mathbf{r} \\ \mathbf{x} \end{bmatrix} \right\|} \leq \kappa \left(\begin{bmatrix} \alpha I & A^T \\ A & 0 \end{bmatrix} \right) \frac{\|\frac{1}{\alpha} A^T \widetilde{\mathbf{r}}\|}{\|\mathbf{y}\|}.$$

Residuals as an *a posteriori* stability test

- If I obtain (no matter how!) a solution $\tilde{\mathbf{x}}$ for which the residual $\frac{\|\mathbf{r}\|}{\|\mathbf{y}\|}$ is of the order of machine precision, then I have solved my problem as accurately as possible.
- Even if residuals (relative!) reach $O(\mathrm{u})$ (which will happen with a good algorithm) errors on $\tilde{x}$ are $\kappa_{problem} O(\mathrm{u})$.

  We have shown this result for both linear systems and least squares problems.

This is called an *a posteriori* bound: we show stability *after* computing the solution.

For some algorithms, we can prove backward stability a priori: even without checking the residual, we can be sure that they provide an error that can be seen as perturbations $\|\Delta A\|/\|A\| = O(\mathrm{u})$.

Solving least squares problems with QR is one of these algorithms; we will see it in the next set of slides.

Book references Trefethen–Bau, Chapter 20. This includes a more complicated expression for the exact backward error (Theorem 20.5).