Scientific Computing

Uncertainty, numerical conditioning, sensitivity.

Wednesday, March 6th

Math 365

Week #7

Uncertainty

When attempting to solve problems in science in engineering, we have to worry about how sources of uncertainty are reflected in the solution we are trying to compute.

Sources of uncertainty include *observational uncertainty* (e.g we are not able to measure things perfectly), uncertainty in *physical model parameters* (which may also be difficult to determine), *uncertainty in our model* (do we understand all of the physical processes involved? What we are neglecting?).

Model conditioning

The conditioning of a model characterizes how small changes to the input values (the right hand side) is reflected in the solution.

Perfect conditioning is when the small changes in the input are exactly reflected in the output.

Poorly conditioned problems are when small changes in the input may result in large changes in output.

Conditioning

A model may be *poorly conditioned* if it is very sensitive to data inputs.

For example, we saw last time :

$$x + 2y = 1$$
$$(2+\varepsilon)x + 4y = 1, \qquad \varepsilon \ll 1$$

A very small number

was extremely sensitive to changes in ε.

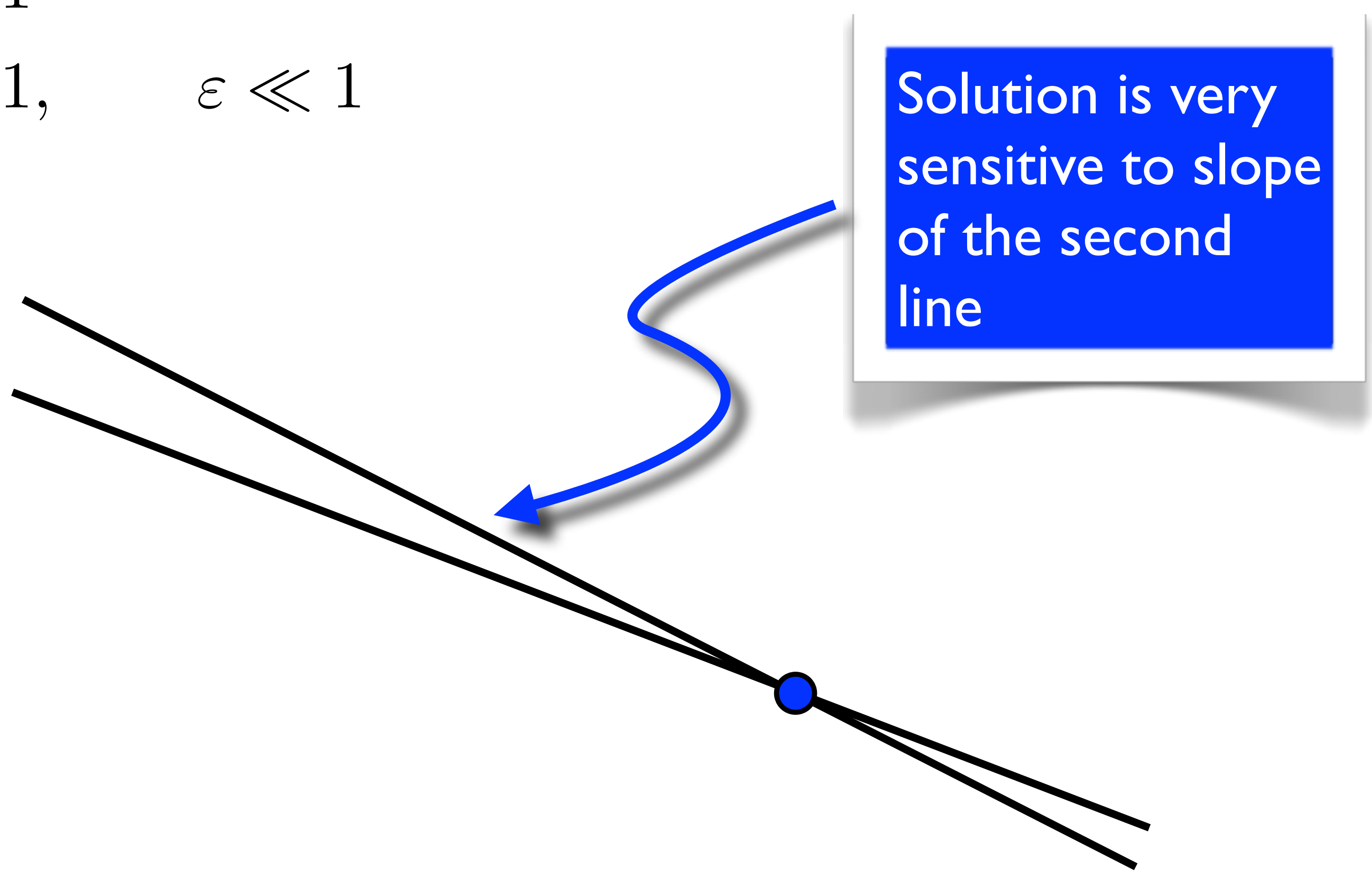
Could be a very big number!

$$x = -\frac{1}{\varepsilon}, \qquad y = \frac{1}{2}\left(1 + \frac{1}{\varepsilon}\right)$$

Numerical conditioning

The problem is that our model is poorly conditioned.
In this case, our system is nearly singular.

$$
\begin{aligned}
x + 2y &= 1 \\
(2+\varepsilon)x + 4y &= 1, \qquad \varepsilon \ll 1
\end{aligned}
$$



Numerical conditioning

What about changes to the right hand side?

$$x + 2y = 1$$
$$(2+\varepsilon)x + 4y = 1 + \sigma$$

$$x = -\frac{1-\sigma}{\varepsilon} \qquad y = \frac{1}{2}\left(1 - \frac{1-\sigma}{\varepsilon}\right)$$

For $\sigma \neq 1$, the solution will still be very sensitive to ε, but not nearly as much to σ.
What happens if $\sigma = 1$? In this case, the solution is completely independent of ε. (The solution is on the y-intercept, a point which doesn't change because of the slope.)

Numerical conditioning

What to do?

- Change the model - think carefully about what we are trying to do, or
- We may just have a poorly conditioned problem, in which case we have to be careful about the numerical method we choose.

In any case, we need to be aware of the source of the ill-conditioning, and deal with it appropriately.

Condition number

If we have a model described by a linear system of equations, we can use the *condition number* to determine if model is well-conditioned or not.

The condition number of a matrix A is defined as

$$\kappa = \| A \| \| A^{-1} \|$$

where $\| A \|$ is a matrix *norm*. Depending on the norm chosen, this could be the large entry in the matrix, or the average values of the entries in the matrix.

Matrix norms

Examples of matrix norms for $A \in \mathcal{R}^{m \times n}$:

$$\| A \|_1 = \max_{1 \le j \le n} \sum_{i=1}^{m} |a_{ij}|, \quad \text{the largest column sum}$$

$$\| A \|_\infty = \max_{1 \le i \le m} \sum_{j=1}^{n} |a_{ij}|, \quad \text{the largest row sum}$$

Regardless of which norm we choose, the condition number will still show the same behavior.

Condition number

The condition number of our matrix is given by

$$\left\| \begin{bmatrix} 1 & 2 \\ 2+\varepsilon & 4 \end{bmatrix} \right\| \cdot \left\| \frac{1}{\varepsilon} \begin{bmatrix} -2 & 1 \\ 1+\frac{\varepsilon}{2} & -\frac{1}{2} \end{bmatrix} \right\| = \frac{6}{\varepsilon} + 1$$

using the inf-norm.

Big number!

The identity matrix (and any scalar multiple of the identity matrix) has perfect conditioning, i.e. $\kappa = 1$.

A singular matrix has an infinite condition number.

Condition number

Why do we care about the condition number?

The solution error is proportional to the condition number.

Let $\hat{x}$ be the numerical solution to the linear system $Ax = b$. Note : $\hat{x} \neq x$. Define the residual to be

$$r = A\hat{x} - b$$

Fact : Gaussian elimination produces a small residual.

Does this mean our numerical solution is accurate?

Depends on the condition number of the system!

Condition number

The error in the solution is proportional to the condition number. Let u be the unit round off error. Then

$$\frac{\| \hat{x} - x \|}{\| x \|} \approx \mathbf{u}\kappa(A)$$

The error in our solution is only as good as the conditioning of the problem!

Condition number of a function

We can also talk about the conditioning of a function.

$$\kappa(f(x)) = \frac{|x||f'(x)|}{|f(x)|}$$

The function $f(x) = x$ has perfect conditioning, whereas the function $f(x) = 1/(1-x)$ is poorly conditioned near $x = 1$.

$$\kappa(f(x)) = \frac{|x|}{|1-x|}$$

Near 1, the function is extremely sensitive to small changes in x.