Scientific Computing

Uncertainty, numerical conditioning, sensitivity.

Math 365

Introduction to Computational Mathematics

Conditioning

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

For example,

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

A very small number

was extremely sensitive to changes in ε.

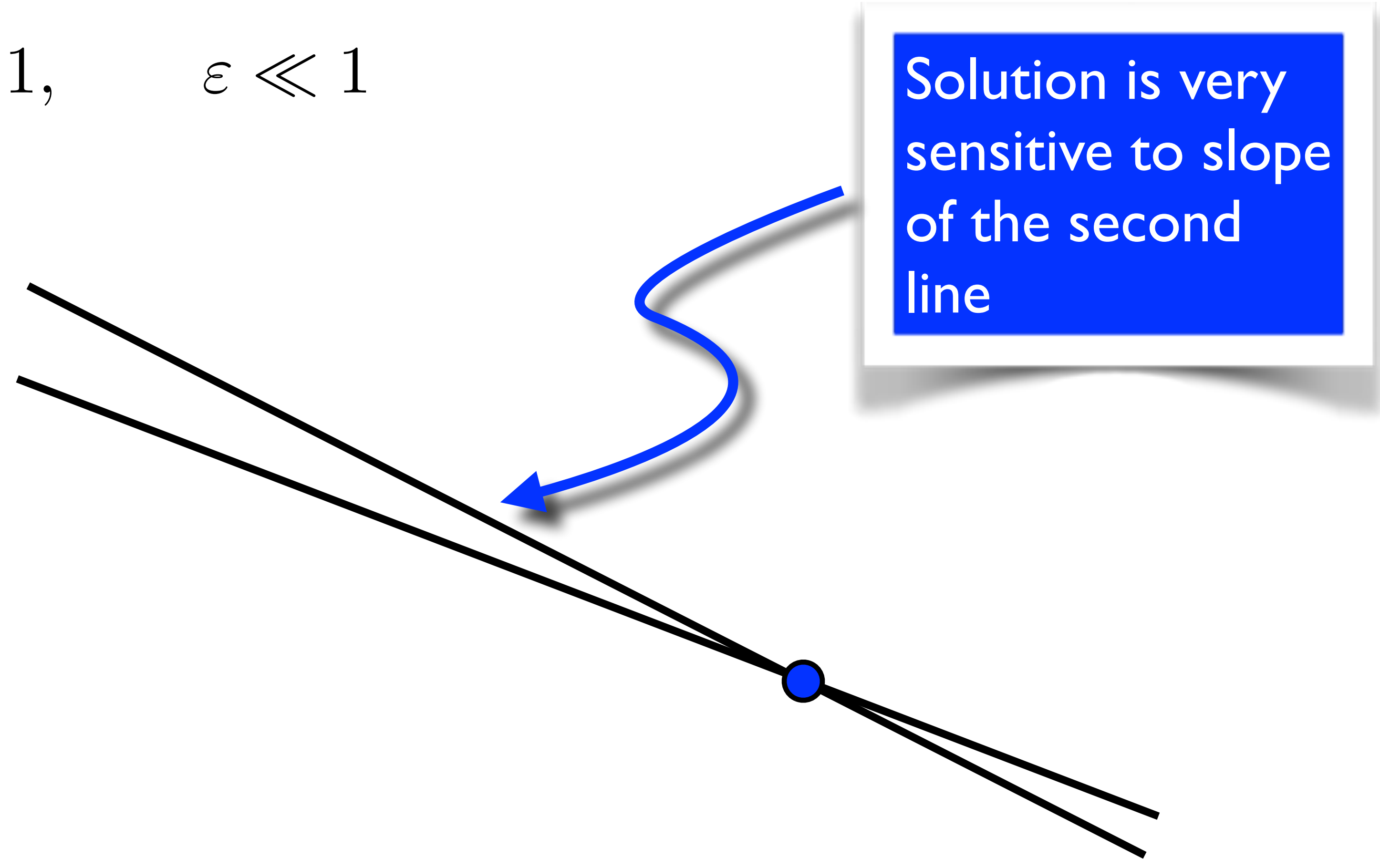
Could be a very big number!

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

Numerical conditioning

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

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



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

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

Big number!

using the inf-norm.

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.