Lecture 1 INF-MAT 4350 2008: Cubic Splines and Tridiagonal Systems

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Plan for the day

- Notation
- Piecewise Linear Interpolation (C^0)
- Cubic Hermite Interpolation (C^1)
- Cubic Spline Interpolation (C^2)
- The equations for C^2
- The spline matrices for different boundary conditions
- Non-singularity of the spline matrices
- LU-factorization of a tridiagonal matrix
- Strictly diagonally dominant matrices
- Existence of LU-factorization for the spline matrices

Notation

- The set of natural numbers, integers, rational numbers, real numbers, and complex numbers are denoted by $\mathbb{N}, \mathbb{Z}, \mathbb{Q}, \mathbb{R}, \mathbb{C}$, respectively.
- $\mathbb{R}^n(\mathbb{C}^n)$ is the set of n-tuples of real(complex) numbers which we will represent as column vectors. Thus $\mathbf{x} \in \mathbb{R}^n$ means

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix},$$

where $x_i \in \mathbb{R}$ for $i = 1, \ldots, n$. Row vectors are normally identified using the transpose operation. Thus if $\mathbf{x} \in \mathbb{R}^n$ then $\mathbf{x}$ is a column vector and $\mathbf{x}^T$ is a row vector.

Notation2

- $\mathbb{R}^{m,n}(\mathbb{C}^{m,n})$ is the set of $m \times n$ matrices with real(complex) entries represented as

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}.$$

  The entry in the ith row and jth column of a matrix $\mathbf{A}$ will be denoted by $a_{i,j}$, a_{ij}, $\mathbf{A}(i,j)$ or $(\mathbf{A})_{i,j}$.

The Interpolation Problem

- Given a non-negative integer m,
- $m + 2$ x-values $\mathbf{x} = [x_0, \ldots, x_{m+1}]$ with $x_i = a + ih$ and $h = (b - a)/(m + 1)$.
- $m + 2$ real y-values $\mathbf{y} = [y_0, \ldots, y_{m+1}]$.
- Find a function $p : [a, b] \to \mathbb{R}$ such that $p(x_j) = y_j, \quad \text{for } j = 0, \ldots, m + 1.$
- p can be a polynomial or a piecewise polynomial of low degree.

Piecewise Linear Interpolation (C^0)

- The piecewise linear function $p : [a, b] \to \mathbb{R}$ given by

$$p(x) = p_i(x) = y_i(1 - t) + y_{i+1}t,\ t = \frac{x - x_i}{h},\ x \in [x_i, x_{i+1}],$$

  satisfies $p(x_i) = y_i$ for $i = 0, \ldots, m + 1$.
- $p \in C[a, b]$ since $p_{i-1}(x_i) = p_i(x_i) = y_i$ at the knots.
- By the chain rule $\frac{dp_i}{dx} = \frac{dp_i}{dt}\frac{dt}{dx} = \frac{1}{h}\frac{dp_i}{dt}$
- $p'(x_i) = \delta_i := (y_{i+1} - y_i)/h$.
- Normally $\delta_{i-1} \neq \delta_i$ and the derivative has breaks at the break-points (x_i, y_i).

Cubic Hermite Interpolation (C^1)

- Given in addition $m+2$ derivative values $\mathbf{s} = [s_0, \ldots, s_{m+1}]$.

- Theorem

Let $p : [a, b] \to \mathbb{R}$ be the piecewise cubic function given for $i = 0, \ldots, m$ and $x \in [x_i, x_{i+1}]$ by

$$p(x) = p_i(x) = c_0(1-t)^3 + c_1 3t(1-t)^2 + c_2 3t^2(1-t) + c_3 t^3, \; t = \frac{x - x_i}{h}. \tag{1}$$

where

$$c_0 = y_i, \quad c_1 = y_i + \frac{h}{3}s_i, \quad c_2 = y_{i+1} - \frac{h}{3}s_{i+1}, \quad c_3 = y_{i+1}. \tag{2}$$

Then $p(x_j) = y_j, \; p'(x_j) = p_j, \; \text{for } j = 0, \ldots, m+1.$

Example

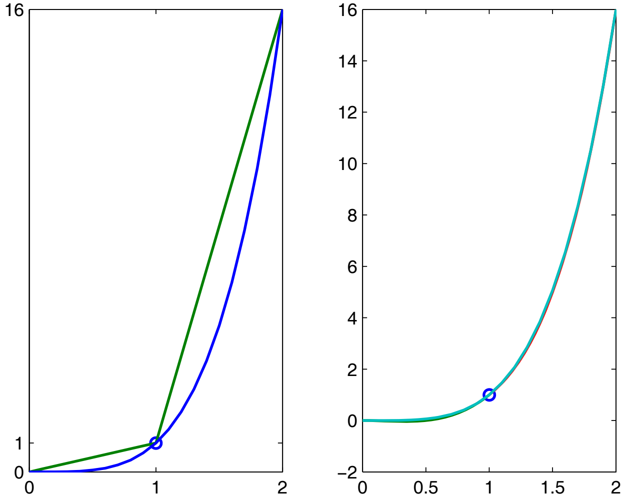

Figure: *A piecewise linear interpolant to* $f(x) = x^4$ *(left) and a cubic Hermite interpolant (right).*

The C^2 equation

- The cubic Hermite interpolant p is continuous and has a continuous derivative for all $x \in [a, b]$, i. e., $p \in C^1[a, b]$.
- Suppose that instead of specifying the derivative values $\mathbf{s}$ we determine them so that the interpolant p has a continuous second derivative i. e., $p \in C^2[a, b]$.
- The continuity requirement $p''_{i-1}(x_i) = p''_i(x_i)$ for the 2. derivative leads to
- $$s_{i-1} + 4s_i + s_{i+1} = 3\frac{y_{i+1} - y_{i-1}}{h} =: \beta_i, \quad i = 1, \dots, m,$$

Boundary Conditions

- $s_{i-1} + 4s_i + s_{i+1} = \beta_i$, $i = 1, \ldots, m$
- m equations with $m+2$ unknowns $s_0, \ldots, s_{m+1}$
- need two boundary conditions
- Clamped (1. derivative) s_0 and s_{m+1} given
- The second derivative $p''(x_0) = q_0$ and $p''(x_{m+1}) = q_{m+1}$
- Natural $q_0 = q_{m+1} = 0$.
- Not-a-knot $p_0 = p_1$ and $p_{m-1} = p_m$.

Figure: *A physical spline with ducks*

The Clamped System

- $s_{i-1} + 4s_i + s_{i+1} = \beta_i$, $i = 1, \ldots, m$
- $$\begin{bmatrix} 4 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 1 & 4 \end{bmatrix} \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_{m-1} \\ s_m \end{bmatrix} = \begin{bmatrix} \beta_1 - s_0 \\ \beta_2 \\ \vdots \\ \beta_{m-1} \\ \beta_m - s_{m+1} \end{bmatrix}.$$
- tridiagonal $m \times m$ system $\mathbf{N}_1 \mathbf{s} = \mathbf{b}$.
- strictly diagonally dominant

The 2. derivative system

- $$\begin{bmatrix} 2 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 1 & 2 \end{bmatrix} \begin{bmatrix} s_0 \\ s_1 \\ \vdots \\ s_m \\ s_{m+1} \end{bmatrix} = \begin{bmatrix} \nu_0 \\ \beta_1 \\ \vdots \\ \beta_m \\ \nu_{m+1} \end{bmatrix},$$
- $\nu_0 = 3\delta_0 - hq_0/2, \quad \nu_{m+1} = 3\delta_m + hq_{m+1}/2.$
- tridiagonal $(m+2) \times (m+2)$ system $\mathbf{N}_2\mathbf{s} = \mathbf{b}$.
- strictly diagonally dominant

The not-a-knot system

- $$\begin{bmatrix} 1 & 2 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 2 & 1 \end{bmatrix} \begin{bmatrix} s_0 \\ s_1 \\ \vdots \\ s_m \\ s_{m+1} \end{bmatrix} = \begin{bmatrix} \gamma_0 \\ \beta_1 \\ \vdots \\ \beta_m \\ \gamma_{m+1} \end{bmatrix},$$
- $\gamma_0 = \frac{5}{2}\delta_0 + \frac{1}{2}\delta_1, \quad \gamma_{m+1} = \frac{1}{2}\delta_{m-1} + \frac{5}{2}\delta_m.$
- tridiagonal $(m+2) \times (m+2)$ system $\mathbf{N}_3\mathbf{s} = \mathbf{b}$.
- not strictly diagonally dominant

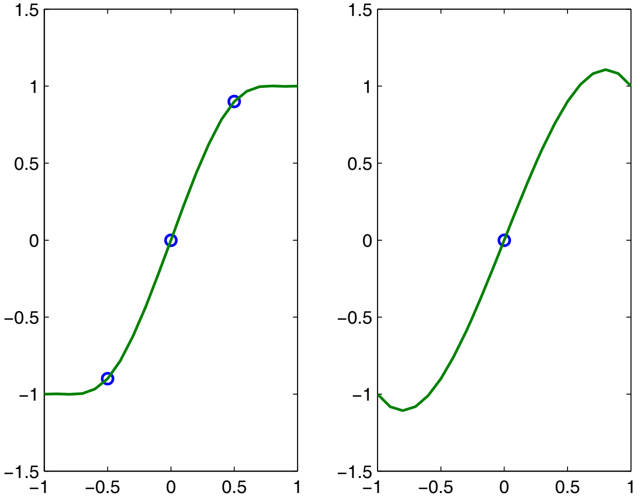

Figure: Cubic spline interpolation. Clamped (left) and not-a-knot (right). The break points are marked with circles

The tridiagonal matrix

- $$\mathbf{A} = \begin{bmatrix} d_1 & c_1 & & & \\ a_2 & d_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1} & d_{n-1} & c_{n-1} \\ & & & a_n & d_n \end{bmatrix}$$
- Non-singular?
- Gaussian elimination (LU-factorization) without row interchanges well defined?

Non-singular matrix

Definition

A square matrix $\mathbf{A}$ is said to be **non-singular** if the only solution of the homogenous system $\mathbf{Ax} = \mathbf{0}$ is $\mathbf{x} = \mathbf{0}$. The matrix is **singular** if it is not non-singular.

- Suppose $\mathbf{A}$ is non-singular.
- The linear system $\mathbf{Ax} = \mathbf{b}$ has a unique solution $\mathbf{x}$ for any $\mathbf{b}$
- $\mathbf{A}$ has an inverse
- If $\mathbf{A} = \mathbf{BC}$ then $\mathbf{B}$ and $\mathbf{C}$ are non-singular.

Lemma

Suppose $\mathbf{A}$ *is the block matrix*

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{22} & \mathbf{0} \\ \mathbf{0} & \mathbf{A}_{32} & \mathbf{A}_{33} \end{bmatrix},$$

where each diagonal block $\mathbf{A}_{ii}$ *is square and non-singular. Then* $\mathbf{A}$ *is non-singular.*

- **Proof** Let $\mathbf{A}\mathbf{x} = \mathbf{0}$ and let $\mathbf{x} = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3]^T$ be partitioned conformally with $\mathbf{A}$.
- $$\mathbf{A}\mathbf{x} = \begin{bmatrix} \mathbf{A}_{11}\mathbf{x}_1 + \mathbf{A}_{12}\mathbf{x}_2 \\ \mathbf{A}_{22}\mathbf{x}_2 \\ \mathbf{A}_{32}\mathbf{x}_2 + \mathbf{A}_{33}\mathbf{x}_3 \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{bmatrix}.$$
- $\mathbf{x}_2 = \mathbf{0}$ since $\mathbf{A}_{22}\mathbf{x}_2 = \mathbf{0}$ and $\mathbf{A}_{22}$ is non-singular.
- $\mathbf{x}_1 = \mathbf{0}$ and $\mathbf{x}_3 = \mathbf{0}$ since $\mathbf{A}_{11}\mathbf{x}_1 = \mathbf{0}$, $\mathbf{A}_{33}\mathbf{x}_3 = \mathbf{0}$ and these matrices are non-singular.
- Thus $\mathbf{x} = \mathbf{0}$ and $\mathbf{A}$ is non-singular.

Strict diagonal dominance

- A matrix $\mathbf{A} \in \mathbb{C}^{n,n}$ is said to be **strictly diagonally dominant** if $\sigma_i := |a_{ii}| - \sum_{j \neq i} |a_{ij}| > 0$ for $i = 1, \ldots, n$.
- The clamped- and 2. derivative spline matrices are strictly diagonally dominant, the not-a-knot is not.

- Lemma
  A strictly diagonally dominant matrix $\mathbf{A} \in \mathbb{C}^{n,n}$ is non-singular.
  - **Proof**
  - Let $\mathbf{x}$ be any solution of $\mathbf{Ax} = \mathbf{b} = \mathbf{0}$
  - let i be such that $|x_i| = \max_j |x_j|$.
  - $0 = |a_{ii} x_i + \sum_{j \neq i} a_{ij} x_j| \geq |a_{ii} x_i| - \sum_{j \neq i} |a_{ij} x_j| \geq |x_i| \sigma_i$.
  - Since $\sigma_i > 0$ it follows that $|x_i| = 0$. But then $\mathbf{x} = \mathbf{0}$ and $\mathbf{A}$ is non-singular.

Non-singularity of the spline matrices

- Theorem
  The three spline matrices $\mathbf{N}_1$, $\mathbf{N}_2$, *and* $\mathbf{N}_3$ *are non-singular.*
  - **Proof** The matrices $\mathbf{N}_1$ and $\mathbf{N}_2$ are strictly diagonally dominant and therefore non-singular.
  - Transform $\mathbf{N}_3$ to block form with strictly diagonally dominant diagonal blocks. Consider $m = 3$.
  - $$\mathbf{B} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \ \mathbf{A} := \mathbf{B}\mathbf{N}_3 = \left[\begin{array}{c|ccc|c} 1 & 2 & 0 & 0 & 0 \\ \hline 0 & 2 & 1 & 0 & 0 \\ 0 & 1 & 2 & 0 & \\ 0 & 0 & 1 & 2 & 0 \\ \hline 0 & 0 & 0 & 2 & 1 \end{array}\right].$$
  - $\mathbf{A}$ is non-singular by Lemma and therefore $\mathbf{N}_3$ is non-singular.

Given a linear system $\mathbf{Ax} = \mathbf{b}$, where $\mathbf{A} = \text{tridiag}(a_i, d_i, c_i) \in \mathbb{R}^{n,n}$ is non-singular and tridiagonal. We try to construct triangular matrices $\mathbf{L}$ and $\mathbf{R}$ such that the product $\mathbf{A} = \mathbf{LR}$ has the form

$$\begin{bmatrix} d_1 & c_1 & & & \\ a_2 & d_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1} & d_{n-1} & c_{n-1} \\ & & & a_n & d_n \end{bmatrix} = \begin{bmatrix} 1 & & & \\ l_2 & 1 & & \\ & \ddots & \ddots & \\ & & l_n & 1 \end{bmatrix} \begin{bmatrix} r_1 & c_1 & & \\ & \ddots & \ddots & \\ & & r_{n-1} & c_{n-1} \\ & & & r_n \end{bmatrix}. \tag{3}$$

Note that $\mathbf{L}$ has ones on the diagonal, and that we can use the same c_i entries on the super-diagonals of $\mathbf{A}$ and $\mathbf{R}$.

LU for $n = 3$

$$\begin{bmatrix} d_1 & c_1 & 0 \\ a_2 & d_2 & c_2 \\ 0 & a_3 & d_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ l_2 & 1 & 0 \\ 0 & l_3 & 1 \end{bmatrix} \begin{bmatrix} r_1 & c_1 & 0 \\ 0 & r_2 & c_2 \\ 0 & 0 & r_3 \end{bmatrix}$$

- Given a_i, d_i, c_i. Find l_i, r_i. Compare (i, j) entries on both sides
- $(1,1): \; d_1 = r_1 \;\Rightarrow\; r_1 = d_1$
- $(2,1): \; a_2 = l_2 r_1 \;\Rightarrow\; l_2 = a_2/r_1$
- $(2,2): \; d_2 = l_2 c_1 + r_2 \;\Rightarrow\; r_2 = d_2 - l_2 c_1$
- $(2,3): \; a_3 = l_3 r_2 \;\Rightarrow\; l_3 = a_3/r_2$
- $(3,3): \; d_3 = l_3 c_2 + r_3 \;\Rightarrow\; r_3 = d_3 - l_3 c_2$
- In general

$$r_1 = d_1, \quad l_k = \frac{a_k}{r_{k-1}}, \quad r_k = d_k - l_k c_{k-1}, \quad k = 2, 3, \ldots, n.$$

Use LU to solve $\mathbf{Ax} = \mathbf{b}$

- $\mathbf{Ax} = \mathbf{L}(\mathbf{Rx}) = \mathbf{b}$
- $\mathbf{Ly} = \mathbf{b}$
- $\mathbf{Rx} = \mathbf{y}$
- $$\begin{bmatrix} 1 & 0 & 0 \\ l_2 & 1 & 0 \\ 0 & l_3 & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$
- $y_1 = b_1,\ y_2 = b_2 - l_2 y_1,\ y_3 = b_3 - l_3 y_2$ (Forward substitution)
- $$\begin{bmatrix} r_1 & c_1 & 0 \\ 0 & r_2 & c_2 \\ 0 & 0 & r_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$$
- $x_3 = y_3/r_3,\ x_2 = (y_2 - c_2 x_3)/r_2,\ x_1 = (y_1 - c_1 x_2)/r_1$ (Backward substitution)

The Algorithm

- $\mathbf{A} = \mathbf{LR}$ (LU-factorization)
- $\mathbf{Ly} = \mathbf{b}$ (forward substitution)
- $\mathbf{Rx} = \mathbf{y}$ (backward substituion)
- $$r_1 = d_1, \quad l_k = \frac{a_k}{r_{k-1}}, \quad r_k = d_k - l_k c_{k-1}, \quad k = 2, 3, \ldots, n.$$
- $y_1 = b_1, \qquad y_k = b_k - l_k y_{k-1}, \qquad k = 2, 3, \ldots, n,$
- $x_n = y_n / r_n, \quad x_k = (y_k - c_k x_{k+1}) / r_k, \quad k = n-1, \ldots, 2, 1.$
- This process is well defined if $r_k \neq 0$ for all k
- The number of arithmetic operations (flops) is $8n - 7 = O(n)$.

Enough that $r_k \neq 0$ for $k \leq n-1$

- If $\mathbf{A}$ is non-singular and $r_k \neq 0$ for $k \leq n-1$ then also $r_n \neq 0$.
- For the LU-factorization exists and is unique if $r_i \neq 0$ for $i = 0, 1, \ldots, n-1$.
- Since $\mathbf{A}$ is non-singular the matrices $\mathbf{L}$ and $\mathbf{R}$ are non-singular.
- We show next time that a triangular matrix is non-singular if and only if all diagonal entries are non-zero. It follows that r_n is non-zero.

$r_j \neq 0$ for $j \leq n-1$?

Theorem

Suppose $\mathbf{A}$ *is strictly diagonally dominant and tridiagonal. Then* $\mathbf{A}$ *has a unique LU-factorization.*

- Recall
  $r_1 = d_1, \quad l_k = \frac{a_k}{r_{k-1}}, \quad r_k = d_k - l_k c_{k-1}, \quad k = 2, 3, \dots, n.$
- We show that $|r_k| > |c_k|$ for $k = 1, 2, \dots, n$.
- Using induction on k suppose for some $k \leq n$ that $|r_{k-1}| > |c_{k-1}|$. This holds for $k = 2$.
- $|r_k| = |d_k - l_k c_{k-1}| = |d_k - \frac{a_k c_{k-1}}{r_{k-1}}| \geq |d_k| - \frac{|a_k||c_{k-1}|}{|r_{k-1}|} > |d_k| - |a_k| > |c_k|$.
- The uniqueness follows since any LU-factorization must satisfy the above equations.

Existence of LU for not-a-knot

$$\mathbf{N}_k = \begin{bmatrix} 1 & 2 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 2 & 1 \end{bmatrix} = \begin{bmatrix} d_1 & c_1 & & & \\ a_2 & d_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n-1} & d_{n-1} & c_{n-1} \\ & & & a_n & d_n \end{bmatrix}$$

- $r_1 = d_1, \quad l_k = \frac{a_k}{r_{k-1}}, \quad r_k = d_k - l_k c_{k-1}, \quad k = 2, 3, \ldots, n.$
- We need to show that $r_k \neq 0$ for $k = 1, \ldots, n-1$.
- $r_1 = d_1 = 1,\ l_2 = \frac{a_2}{r_1} = 1,\ r_2 = d_2 - l_2 c_1 = 2.$
- Thus $|r_2| > 1 = |c_2|$.
- Suppose $|r_{k-1}| > |c_{k-1}|$ for some k with $3 \leq k \leq n-1$.
- Since $|d_k| > |a_k| + |c_k|$ the same calculation as for strict diagonally dominance shows that $|r_k| > |c_k|$. Since $r_1 \neq 0$ we have shown that $r_k \neq 0$ for $k = 1, \ldots, n-1$.

Summary

- Studied linear systems arising from cubic spline interpolation
- Each leads to a tridiagonal matrix
- Introduced the concepts of strict diagonal dominance
- studied non-singularity
- existence of LU-factorization for tridiagonal systems
- LU-factorization in $O(n)$ flops.