Numerical Analysis and Computing

Lecture Notes #1 — First Meeting

Peter Blomgren,
⟨blomgren.peter@gmail.com⟩

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://terminus.sdsu.edu/

Fall 2014

Outline

Academic Life — MSc

- KTH MSc. Engineering Physics, Royal Institute of Technology (KTH), Stockholm, Sweden. Thesis Advisers: Michael Benedicks, Department of Mathematics KTH, and Erik Aurell, Stockholm University, Department of Mathematics. Thesis Topic: *"A Renormalization Technique for Families with Flat Maxima."*

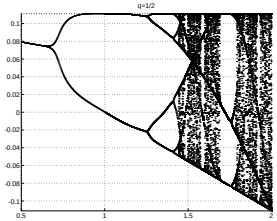


Figure: Bifurcation diagram for the family $f_{a,\frac{1}{2}}$ [Blomgren-1994]

Academic Life — PhD

- UCLA PhD. UCLA Department of Mathematics. Adviser: Tony F. Chan. PDE-Based Methods for Image Processing. Thesis title: *"Total Variation Methods for Restoration of Vector Valued Images."*

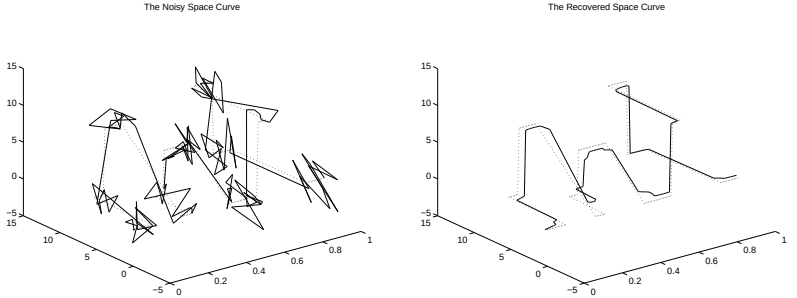


Figure: The noisy (SNR = 4.62 dB), and recovered space curves. Notice how the edges are recovered. [Blomgren-1998]

- Research Associate. Stanford University, Department of Mathematics. Main Focus: Time Reversal and Imaging in Random Media (with George Papanicolaou, *et. al.*)

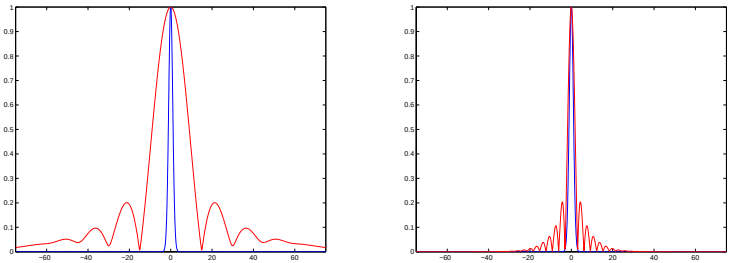


Figure: Comparison of the theoretical formula for a medium with $L = 600\,m$, $a_e = 195\,m$, $\gamma = 2.12 \times 10^{-5}\,m^{-1}$. [LEFT] shows a homogeneous medium, $\gamma = 0$, with $a = 40\,m$ TRM (in red / wide Fresnel zone), and a random medium with $\gamma = 2.12 \times 10^{-5}$ (in blue). [RIGHT] shows $\gamma = 0$, with $a = a_e = 195\,m$ (in red), and $\gamma = 2.12 \times 10^{-5}$, with $a = 40\,m$ (in blue). The match confirms the validity of [the theory]. [BLOMGREN-PAPANICOLAOU-ZHAO-2002]

- SDSU Professor, San Diego State University, Department of Mathematics and Statistics. Projects: Computational Combustion, Biomedical Imaging (Mitochondrial Structures, Heartcell Contractility, Skin/Prostate Cancer Classification).

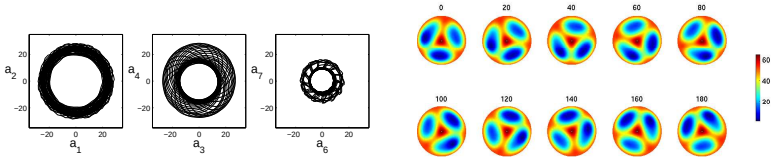


Figure: [LEFT] Phase-space projections produced by the time coefficients of the POD decomposition of the rotating pattern shown in [RIGHT]. [BLOMGREN-GASNER-PALACIOS-2005]

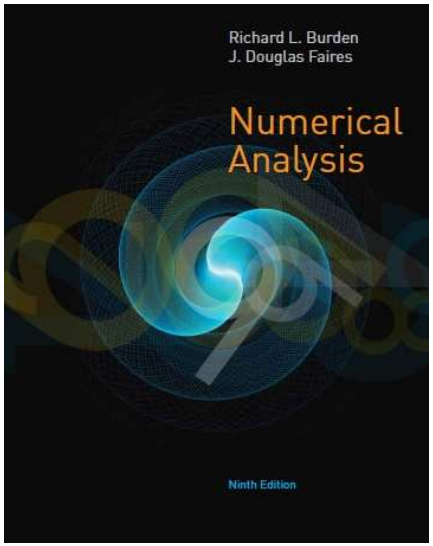
Contact Information

Office	GMCS-587
Email	**blomgren.peter@gmail.com**
Web	**http://terminus.sdsu.edu/SDSU/Math541_f2014/**
Phone	(USE EMAIL)
Office Hours	TuTh: 3:30pm – 5:00pm, and by appointment

Fun Times... ⇒ Endurance Sports

- Triathlons:
  - (10) Ironman distance (2.4 + 112 + 26.2) — 11:48:57
  - (15) Half Ironman distance — 5:14:20
- Running
  - (1) Trail Double-marathon (52 miles) — 10:59:00
  - (4) Trail 50-mile races — 9:08:46
  - (6) Trail 50k (31 mile) races — 5:20:57
  - (12) Road Marathons — 3:26:19 (7:52/mi)
  - (18) Road/Trail Half Marathons — 1:36:25 (7:21/mi)

Basic Information: The Book Class Conceptualized out of 7th (5th?) Edition



Title:
"Numerical Analysis,"
9th Edition (older OK)

Authors:
Richard L. Burden &
J. Douglas Faires

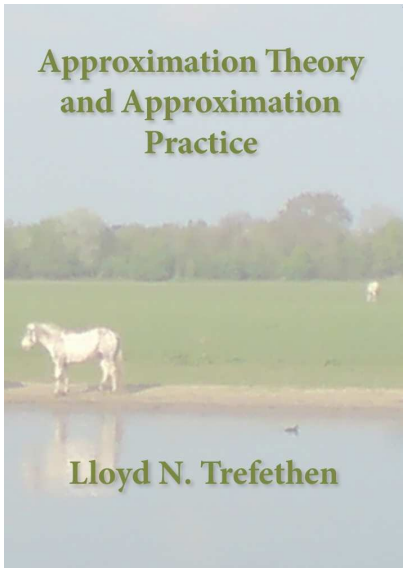
Publisher:
Brooks/Cole
CENGAGE Learning

ISBN-10:
0-534-73351-9

Basic Information: Syllabus

Chapter	Title
1	Mathematical Preliminaries
2	Solutions of Equations in One Variable
3	Interpolation and Polynomial Approximation
4	Numerical Differentiation and Integration
6	Direct Methods for Solving Linear Systems
8	Approximation Theory
Math 542: Numerical Solutions of Differential Equations	
5	Initial-Value Problems for ODEs
11	Boundary Value Problems for ODEs
Math 543: Numerical Matrix Analysis	
7	Iterative Techniques in Matrix Algebra
9	Approximating Eigenvalues
Math 693a: Advanced Numerical Analysis (Numerical Optimization)	
10	Numerical Solution of Nonlinear Systems of Equations
Math 693b: Advanced Numerical Analysis (Numerics for PDEs)	
12	Numerical Solution of PDEs

Recent (and Growing) Influence on the Class



Title:
"Approximation Theory and Approximation Practice,"

Author:
Lloyd N. Trefethen

Publisher:
SIAM

ISBN:
978-1-611972-39-9

Basic Information: Grading

Homework*	25%
Midterm #1$^+$	25%
Midterm #2$^+$	25%
Final$^\times$	25%

* There will be ≈8 homework assignments; they will be posted and submitted thru `http://webwork.sdsu.edu/`

$^+$ The midterms(s) may be take-home (target date(s): week #6, week #11.)

$^\times$ Scheduled time: Tuesday, Dec 16, 1:00pm – 3:00pm. (Details to be determined.)

Homework ∼ Webwork

"WeBWorK is a web-based interactive system designed to make homework in mathematics and the sciences more effective and efficient."

- Info resource `http://webwork.maa.org/wiki/Category:Students`
- Homeworks will "open" (on `http://webwork.sdsu.edu/`), on the first day material relevant to the HW is covered in class.
- Homeworks will "close" (be due), no less than 8 days after the last material relevant to the HW is covered in class.
- Your **Lastname** is your LoginID, and **RedID** is your initial password.
  - If your **Lastname** is not unique, then your loginID is **Lastname**+**Firstname-initial**.

Homework ∼ Webwork

- Most HW problems involve both a theoretical, and implementation (programming) part — Matlab is the recommended and supported environment, but feel free to program in 6510 assembler, Java, Fortran, C/C++, M$-D$^{\flat}$...
- You will enter specific results from your code into Webwork.
- Some assignments may require additional hardcopy submissions; read the webwork instructions.
- Start Assignments EARLY.
- Sometimes "interesting" things happen in Webwork (which does computations using Perl), which make Webwork computations different from Matlab computations.

Expectations and Procedures, I

- Most class attendance is "OPTIONAL" — Homework and announcements will be posted on the class web page. If/when you attend class:
  - Please be on time.
  - Please pay attention.
  - Please turn off mobile phones.

  - Please be courteous to other students and the instructor.
  - Abide by university statutes, and all applicable local, state, and federal laws.

Expectations and Procedures, II

- Please, turn in assignments on time. (The instructor reserves the right not to accept late assignments.)
- The instructor will make special arrangements for students with documented learning disabilities and will `try` to make accommodations for other unforeseen circumstances, *e.g.* illness, personal/family crises, etc. in a way that is fair to all students enrolled in the class. **Please contact the instructor EARLY regarding special circumstances.**
- Students are expected **and encouraged** to ask questions in class!
- Students are expected **and encouraged** to to make use of office hours! If you cannot make it to the scheduled office hours: contact the instructor to schedule an appointment!

Expectations and Procedures, III

- Missed midterm exams: Don't miss exams! The instructor reserves the right to schedule make-up exams, make such exams oral presentation, and/or base the grade solely on other work (including the final exam).
- Missed final exam: Don't miss the final! Contact the instructor ASAP or a grade of `WU` or `F` will be assigned.
- **Academic honesty**: submit your own work — but feel free to discuss homework with other students in the class! It's OK to ask "Uncle Google" and "Aunt Wiki" for help and ideas, but process the information and make it your own, AND cite any and all sources you use.

Honesty Pledges, I

- The following **Honesty Pledge** must be included in all programs you submit (as part of homework and/or projects):
  - I, (your name), pledge that this program is completely my own work, and that I did not take, borrow or steal code from any other person, and that I did not allow any other person to use, have, borrow or steal portions of my code. I understand that if I violate this honesty pledge, I am subject to disciplinary action pursuant to the appropriate sections of the San Diego State University Policies.
- Work missing the honesty pledge **may not be graded!**

Honesty Pledges, II

- Larger reports must contain the following text:
  - I, (your name), pledge that this report is completely my own work, and that I did not take, borrow or steal any portions from any other person. Any and all references I used are clearly cited in the text. I understand that if I violate this honesty pledge, I am subject to disciplinary action pursuant to the appropriate sections of the San Diego State University Policies. `Your signature`.
- Work missing the honesty pledge `may not be graded!`

Computer Resources

- Access to a (somewhat) current release of Matlab is highly recommended.
- The GMCS-422/428 labs will be available.
- You can also use the Rohan Sun Enterprise system or another capable system.
- How to open a ROHAN account: **http://www-rohan.sdsu.edu/raccts.shtml**
- You may also want to consider buying the student version of Matlab: **http://www.mathworks.com/**
- SDSU students can download a copy of matlab from **http://www-rohan.sdsu.edu/∼download/matlab.html**

`Math 254`, or `Math 342A`

`254` ⇒ **Introduction to Linear Algebra**

- Matrix Algebra, Gaussian elimination, determinants, vector spaces, linear transformations, orthogonality, eigenvalues and eigenvectors.

`342A` ⇒ **Methods of Applied Mathematics, I**

- Vector analysis, divergence and Stokes' theorem, integral theorems. Matrix analysis, eigenvalues and eigenvectors, diagonalization. Introduction to ODEs. Computer software for matrix applications, solving, and graphing differential equations.

`CS 106`, `CS 107` or `CS 205`

`106` ⇒ **Intro to Programming: FORTRAN**

- Problem solving using a computer, design of algorithms.

`107` ⇒ **Intro to Programming: JAVA**

- Programming methodology and problem solving. Basic concepts of computer systems, algorithm design and development, data types, program structures.

`205` ⇒ **Intro to Programming and Visualization**

- Problem solving skills for science, computing/software tools of computational science, computer communications, programming and visualization.

- Numerical tools for problem solving:

⇒ `powertool`	Newton's Method for $f(x) = 0$.
⇒ `powertool`	Least squares approximation.
⇒ `powertool`	The Fast Fourier Transform (FFT).
⇒ `tool`	Polynomial Interpolation.
⇒ `tool`	Numerical differentiation and integration.
⇒ `foundation`	Taylor's Theorem.
⇒ `foundation`	Weierstrass' Theorem.

`Q:` Why are numerical methods needed?

`A:` To accurately approximate the solutions of problems that cannot be solved exactly.

`Q:` What kind of applications can benefit from numerical studies?

`A:` Engineering, physics, chemistry, computer, biological and social sciences.

Image processing / computer vision, computer graphics (rendering, animation), climate modeling, weather predictions, "virtual" crash-testing of cars, medical imaging (CT = Computed Tomography), AIDS research (virus decay vs. medication), financial math...

Computing: Historical Perspective...

The Apollo Guidance Computer (1969)	
Word Length	15 bits plus parity
Fixed Memory Registers	36,864 Words
Erasable Memory Registers	2,048 Words
Number of Normal Instructions	34
Number of Involuntary Instructions	10
Number of Interface Circuits	227
Memory Cycle time	11.7 μs (85 kHz)
Addition Time	23.4 μs
Multiplication Time	46.8 μs
Number of Logic Gates	5,600 (2,800 packages)
Volume	0.97 cubic feet
Weight	70 pounds
Power Consumption	55 watts

Counting Work: Ancient, Old, and Somewhat Recent Measures

We need some measure of how fast, or slow, an algorithm is... (independent of the computational architecture)

In the **old-old days** multiplications (and divisions) where a lot slower additions (and subtractions) $T_{*,/} \gg T_{+,-}$; so one would count the number of multiplications (see *e.g.* the timings for the Apollo guidance computer.)

Then chip designers figured out how to make multiplications faster, so $T_{*,/} \approx T_{+,-}$, so in the **old days** one would count all operations.

Yesterday, processors where so fast that **memory accesses** dominated the processing time; in particular **cache-misses**, so we end up with a completely different model...

Counting Work: The Memory Access Latency Model

If we have three cache-levels (L1, L2, and L3), some average hit-rate (and hence miss-rate) for each level and the time it takes to access that cache-level (the hit-cycle-time), then we end up with a measure for the average memory access latency per memory access

$$\begin{aligned} T \sim\ & (\texttt{L1\_hit\_rate} * \texttt{L1\_hit\_cycle\_time}) \\ & + (\texttt{L1\_miss\_L2\_hit\_rate} * \texttt{L2\_hit\_cycle\_time}) \\ & + (\texttt{L2\_miss\_L3\_hit\_rate} * \texttt{L3\_hit\_cycle\_time}) \\ & + (\texttt{L3\_miss\_rate} * \texttt{[S]DRAM\_latency}) \end{aligned}$$

If this does not scare you, please get a Ph.D. in algorithm design on the compiler / silicon level !!!

Meanwhile, the rest of us will count **"flops"**, *i.e.* floating-point operations (multiplications and additions)!

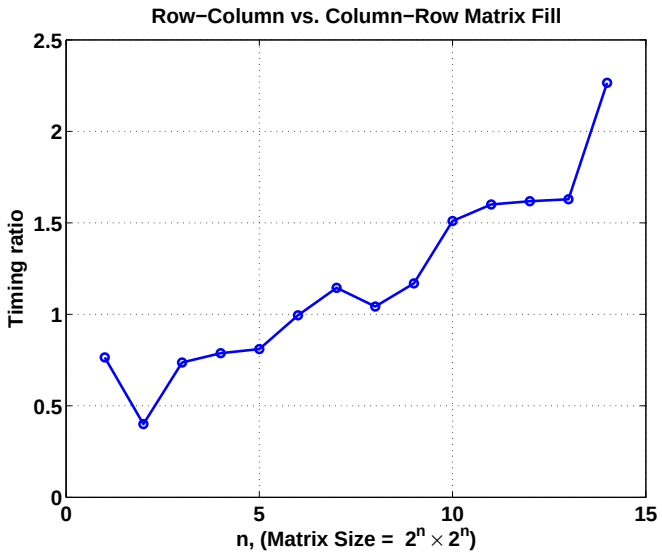
Performance Impact of Accessing Memory (Matrix) Matlab Code

```
for pow=1:14
  n=2^pow;

  clear A
  A = zeros(n,n);
  a0 = clock;
  for c=1:n
    for r=1:n
      A(r,c) = 1/(1+r+c);
    end
  end
  a1 = clock;

  clear B
  B = zeros(n,n);
  b0 = clock;
  for r=1:n
    for c=1:n
      B(r,c) = 1/(1+r+c);
    end
  end
  b1 = clock;

  a_time = [a_time etime(a1,a0)];
  b_time = [b_time etime(b1,b0)];
end
plot((1:14),b_time./a_time,'o-')
ax = axis;
axis([0 15 ax(3:4)])
grid on
xlabel('n, (Matrix Size = 2^n × 2^n)')
ylabel('Timing ratio')
title('Row-Column vs.  Column-Row Matrix Fill')
```



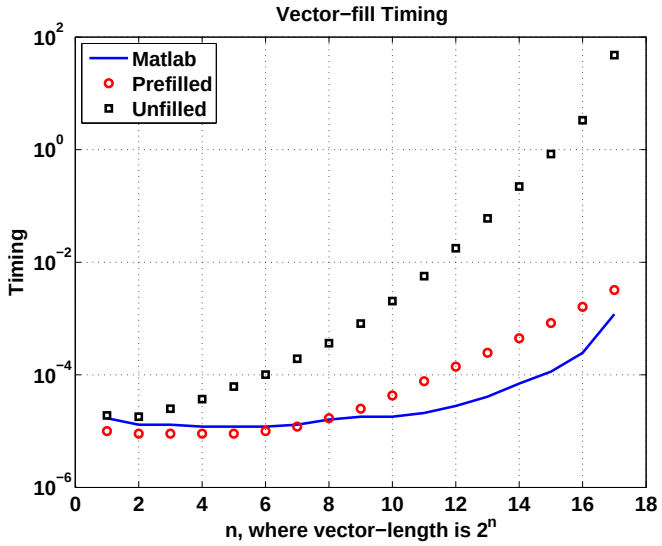

```
matlab_time = []; prefill_time = []; loop_time = [];
for pow=1:17
  n=2^pow;

  % Matlab
  clear test_vec
  a0 = clock;
  test_vec = 1:n;
  a1 = clock;

  % Pre-allocated
  clear test_vec
  test_vec=zeros(1,n);
  b0 = clock;
  for k=1:n
    test_vec(k) = k;
  end
  b1 = clock;

  % Un-allocated
  clear test_vec
  c0 = clock;
  for k=1:n
    test_vec(k) = k;
  end
  c1 = clock;

  matlab_time = [matlab_time etime(a1,a0)];
  prefill_time = [prefill_time etime(b1,b0)];
  loop_time = [loop_time etime(c1,c0)];
end
semilogy(1:max_pow,matlab_time,'b-', 1:max_pow,prefill_time,'ro',
    1:max_pow,loop_time,'ks')
legend('Matlab','Prefilled','Unfilled','Location','NorthWest')
xlabel('n, where vector-length is 2^n')
ylabel('Timing')
title('Vector-fill Timing')
grid on
ax = axis;
axis([0 max_pow+1 ax(3:4)])
```

Our Universe...

Clearly, the question **"How fast is [any given] algorithm?"** has many answers.

For starters, we will keep things simple, and think about old "flops" measurements.

However, it is good to be aware that other aspects of the computer architecture have great impact on the overall performance.

Note that the results in the previous example(s) are mathematically equivalent, but in the vector-fill example the worst/best-timing-ratio for the vector of size 2^{17} is $\sim 10^4$.

Links

- http://terminus.sdsu.edu/SDSU/Math541_f2014/
  - The Class website
- http://webwork.sdsu.edu/
  - Webwork server, for homework.
- http://webwork.maa.org/wiki/Category:Students
  - Some information about Webwork
- http://www-rohan.sdsu.edu/raccts.shtml
  - "Obtaining a ROHAN Computer Account"
- http://www.mathworks.com/
  - Mathworks, the makers of Matlab
- http://www-rohan.sdsu.edu/~download/matlab.html
  - On-campus matlab download.