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A Comparison of the Rate of Convergence, Efficiency and Condition Number of Chebyshev and Legendre Polynomial Series with Prolate Spheroidal, Kosloff/Tal-Ezer and Theta-Mapped Fourier Basis Sets

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Pseudospectral Methods: Good & Bad

Good:

- Geometric Converge: $E(N) \propto \exp(-qN)$ ["Infinite Order", "Exponential", "Spectral"]
- With domain decomposition, ("spectral elements"), parallelizes well

Bad:

- "Stiffness": CFL limit is $O(1/N^2)$ vs. $O(1/N)$ for equispaced finite difference.
- Highly Non-Uniform Resolution:
  Linear-Density-in-Interior,
  Quadratic-Density-in-Boundary Layers
- Highly Non-Uniform Grid in each element.

THEMES:

- All five spectral basis sets here are
  cosines-with-change-of-coordinate

$$u(f[t]) = \sum_{j=1}^{\infty} a_j \cos(jt[x])$$

only the mapping $t(x)$ is different.

- Non-Chebyshev mappings can
  improve grid uniformity which implies
  Much longer stable timestep

$$O\left(\sqrt{N}\right)$$

Better accuracy

[asymptotically $(\pi/2)$ per dimension]

- Multiple non-Chebyshev choices:
  Kosloff/Tal-Ezer basis, prolate spheroidal,

  theta-mapped cosines [NEW]

Mapped-Cosine Basis Functions

Ancient identity:

$$T_n(x) \equiv \cos(nt[x]), \qquad t(x) \equiv \arccos(x) \quad (1)$$

Legendre polynomials are mapped cosines too:

$$P_n(x) \sim \{\mathrm{sign}(x)\}^n \; \frac{\sqrt{\arccos(|x|)}}{\left(1 - x^2\right)^{1/4}} \times \; J_0\left(\left[n + \frac{1}{2}\right] \arccos(|x|)\right) + O\left(\frac{0.062}{n^{3/2}}\right) \quad (2)$$

Except near $x = \pm 1$, this simplifies to

$$P_n(x) \sim \frac{\{\mathrm{sign}(x)\}^n}{\left(1 - x^2\right)^{-1/4}} \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt{n + 1/2}} \times \cos\left(\left[n + \frac{1}{2}\right] \arccos(|x|) - \frac{\pi}{4}\right)$$

Query: Is the Mapping $t = \arccos(x)$ Optimum?

Three Mapped-Cosine Species That are Better Than Chebyshev/Legendre:

1. **Kosloff/Tal-Ezer Basis**
2. **Prolate Spheroidal Functions**
3. **Theta-Mapped Cosines**

Advantages

- Nearly-Uniform Grid Improves Resolution by $\pi/2 \approx 1.57$ *per dimension*
- Timestep Lengthened by Order-of-Magnitude

Limits on Mapped Cosine Functions

Theorem 1 (Mapping Constraints) *Let*

$$u(f[t]) = \sum_{j=1}^{\infty} a_j \cos(jt[x]) \qquad (3)$$

Infinite order convergence requires

1. *All odd derivatives of $f(\tau)$ are zero at both $\tau = 0$ and $\tau = \pi$*
2. *$f(\tau)$ is symmetric with respect to both $\tau = 0$ and $\tau = \pi$*
3. *$f(\tau)$ is periodic with period 2π.*
4. *The inverse function, $\tau = f^{-1}(x)$, has branch points at $x = \pm 1$; if $d^2 f/d\tau^2 \neq 0$ at $\tau = 0, \pi$, then the branch points are square roots.*

Implications:

1. Grid cannot be completely uniform.
2. dt/dx must rise to vertical at $x = \pm\pi$.

Quasi-uniform, better-than-Chebyshev grid

IS POSSIBLE

Resolution of Mapped Cosines

- Evenly-spaced t-grid $\Rightarrow$ non-uniform x-grid.
- Larger $dt/dx \Rightarrow$ smaller δx
- Higher minimum resolution (by $\pi/2$) than Chebyshev.

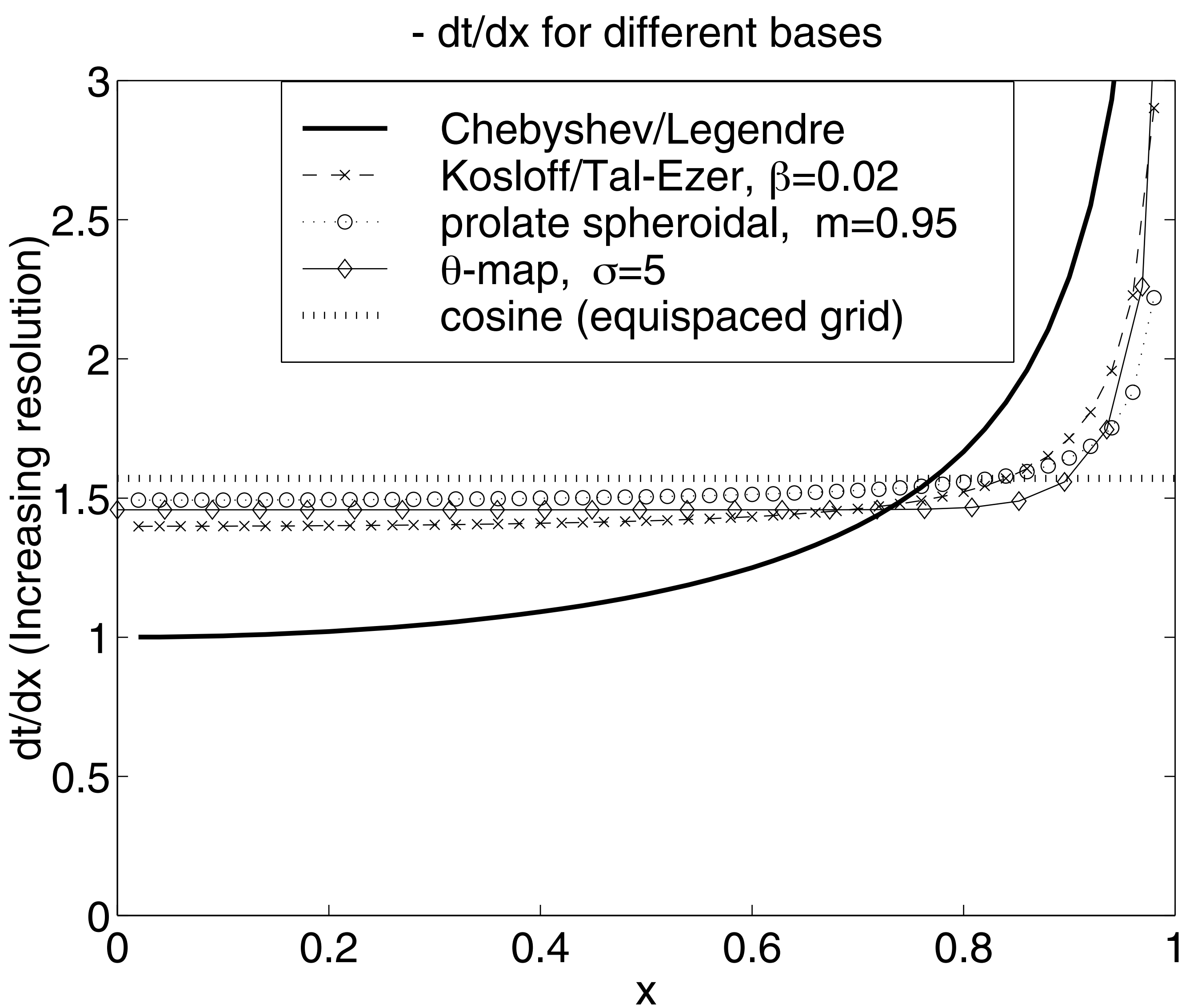

Figure 1: The slopes, $d\tau/dx$, for six different basis sets.

Kosloff/Tal-Ezer Basis

$$\phi_n^{KT}(x;\beta) \equiv \cos(n\, t^{KT}(x))$$

$$t^{KT} = \arccos\left\{ \frac{\sin \arcsin(1-\beta)x}{1-\beta} \right\} \qquad (4)$$

$$\frac{dt^{KT}}{dx} \approx -\frac{\pi}{2} \qquad \forall |x| < 1 - O(\sqrt{\beta}), \qquad \beta << 1$$

i. e., maximum gridpoint separation $(\pi/2)$ smaller than Chebyshev

Table 1: Theory and Applications of Kosloff/Tal-Ezer Mapping

References	Comments
Kosloff&Tal-Ezer (1993)	Introduction and numerical experiments
Tal-Ezer(1994)	Theory; optimization of map parameter
Carcione(1994a)	Compares standard Chebyshev grid with Kosloff/Tal-Ezer grid
Renaut&Frohlich(1996)	2D wave equations, one-way wave equation at boundary
Carcione(1996)	wave problems
Godon(1997b)	Chebyshev-Fourier polar coordinate model, stellar accretion disk
Renaut(1997)	Wave equations with absorbing boundaries
Don&Solomonoff(1997)	Accuracy enhancement and timestep improvement, especially for higher derivatives
Renaut&Su(1997)	3rd order PDE; mapping was not as efficient as standard grid for $N < 16$
Don&Gottlieb(1998)	Shock waves, reactive flow
Mead&Renaut(1999)	Analysis of Runge-Kutta time-integration
Hesthaven, Dinesen & Lynov(1999)	Diffractive optical elements; chose $\beta = 1 - \cos(1/2)$ to double timestep versus standard grid
Abril-Raymundo & García-Archilla(2000)	Theory and experiment for convergence of the mapping
Zhan&Ng	cardial modelling in 2D

Kosloff/Tal-Ezer Basis: Virtues & Vices

Virtues

If $\beta \sim \text{constant}/N^2$:

1. Nearly-uniform grid; $\pi/2$ better than Chebyshev/Legendre
2. CFL limit $O(1/N)$, same as finite difference.

Vices

1. Mapping is *singular*;
   branch point moves to $x \in [-1, 1]$ as $\beta \to 0$
2. $\beta \sim O(1/N^2)$ destroys spectral accuracy

Kosloff/Tal-Ezer: Error in Series of $u(x) \equiv x$

- Geometric convergence is saved only if β is *indpendent* of N (bottom curve)
- CFL limit is still $O(1/N^2)$, but may gain a factor of two.

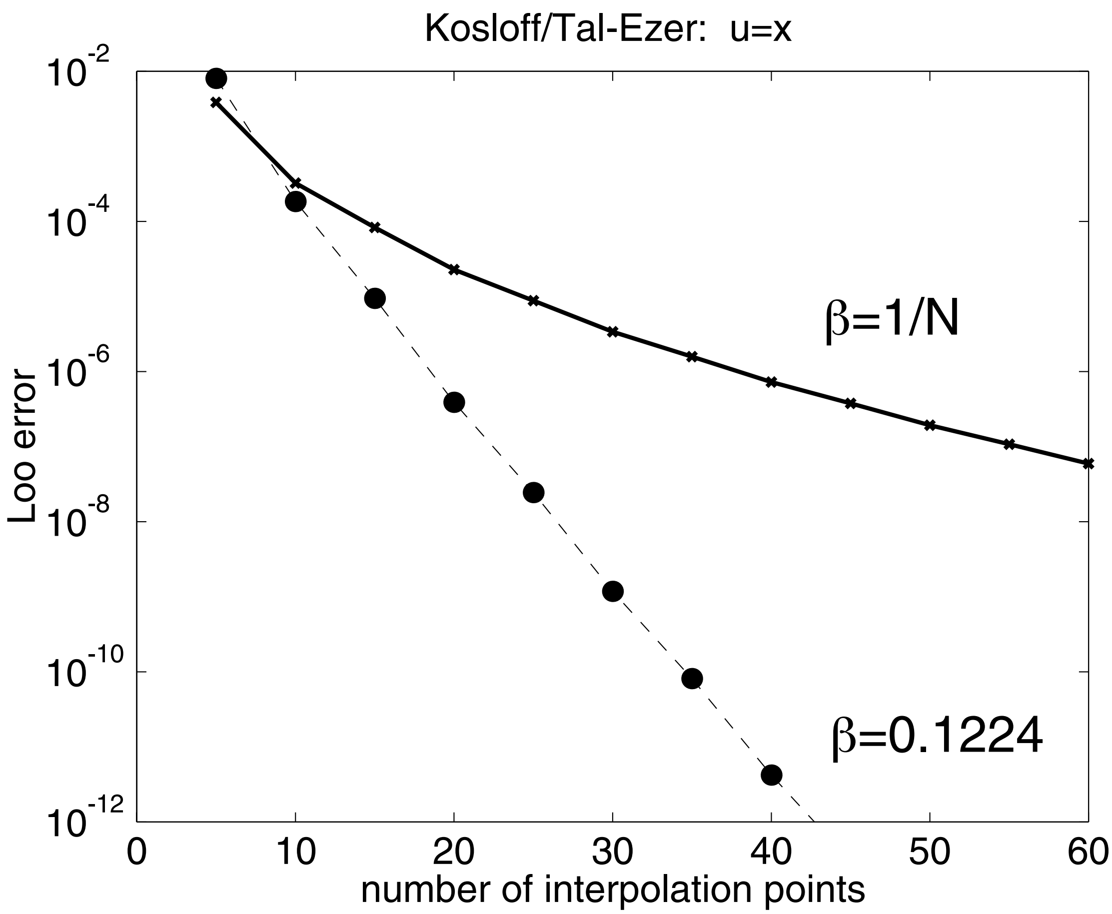

Figure 2: The error in the approximation of the linear function, $u(x) \equiv x$, by a Fourier cosine series using the Kosloff/Tal-Ezer mapping. When $\beta = 0.1224$, the choice of Hesthaven, Dinesen and Lynov(1999), the timestep limit is increased only by a factor of two, but the approximation still converges geometricaly. When $\beta = 1/N$, the timestep limit for a first order hyperbolic problem shrinks only as $O(1/N^{3/2})$ versus the more severe Chebyshev/Legendre/Hesthaven *et al.* limit of $O(1/N^2)$. However, the usual rate of geometric convergence with N has been slowed to a subgeometric rate (upper curve) with an error falling as $\exp(-\text{constant} N^{1/2})$.

Prolate Spheroidal Functions of Zeroth Order

"Prolate Spheroidal Wave Functions are likely to be a better tool for the design of spectral and pseudo-spectral techniques than the orthogonal polynomials and related functions"
— Xiao, Rokhlin & Yarvin(2001), pg. 837.

- Defined as solutions $\psi_n(x, c)$ of
$$(1 - x^2)\psi_{xx} - 2x\psi_x + \left\{\chi - c^2x^2\right\}\psi = 0$$
n is the mode number, χ_n is eigenvalue and c is a constant,the "bandwidth" parameter.
- $\psi_n(x; c = 0) = P_n(x)$
- Complete asymptotic expansions are messy
- Relevant asymptotic expansion is simple.

Prolate Spheroidal Functions

"Transition bandwidth parameter"

$$\boxed{c_*(n) \equiv \frac{\pi}{2}\,(n + 1/2)}$$

Prolate functions span $x \in [-1, 1]$ only if

$$c \leq c_*(n)$$

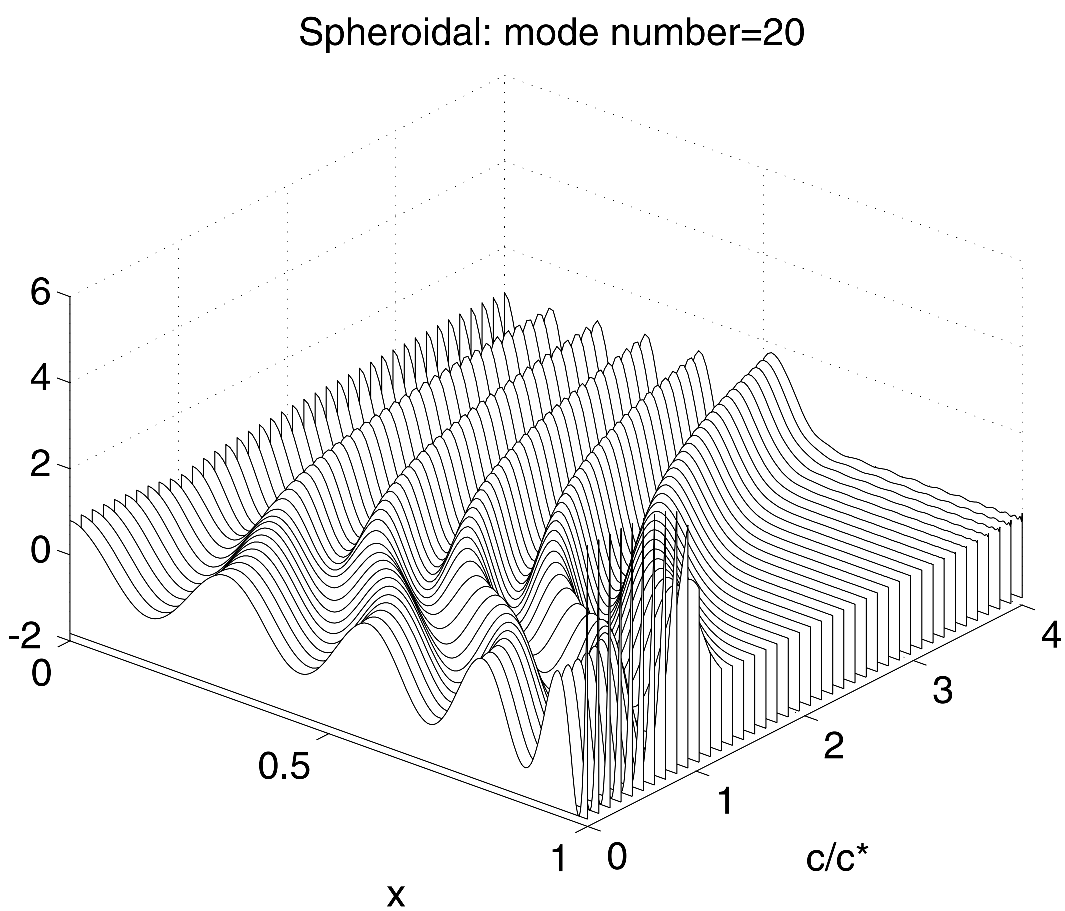

Figure 3: $\psi_{20}(x; c)$ in the $x - c$ plane.

Prolate Spheroidal Asymptotics

$$\psi_n(x;c) \sim \frac{\sqrt{\mathcal{E}(x;m)}}{(1-x^2)^{1/4}(1-mx^2)^{1/4}} \times J_0\left(\frac{c}{\sqrt{m}}\mathcal{E}(x;m)\right)$$

$$\mathcal{E}(x;m) \equiv \int_x^1 dt \frac{\sqrt{1-mt^2}}{\sqrt{1-t^2}}; \qquad m \equiv c^2/\chi_n$$

When $|x| < 1 - O(1/\sqrt{c})$,

$$\psi_n(x;c) \sim \sqrt{\frac{2}{\pi}} \frac{m^{1/4}}{\sqrt{\chi_n}} \frac{1}{(1-x^2)^{1/4}(1-mx^2)^{1/4}} \times \cos\left(\frac{c}{\sqrt{m}}\mathcal{E} - \pi/4\right)$$

If $c = c_*(n)$, then

$$\psi_n(x;c=c_*(n)) \sim \sqrt{\frac{2}{\pi}} \frac{1}{c} \frac{1}{(1-x^2)^{1/2}} \times \cos\left(\frac{\pi}{2}n(1-x)\right) \quad (5)$$

Prolate Spheroidal Basis: Virtues & Vices

Virtues

1. Nearly-uniform grid; $\pi/2$ better than Chebyshev/Legendre
2. CFL limit $O(1/N^{3/2})$
3. Orthogonal with unit weight, like Legendre

Vices

1. Complicated to precompute function values & grid points

   Symmetric tridiagonal Legendre-Galerkin

   Newton-Ralphson iteration for grid
2. Poorly-developed theory

Theta-Mapped Cosines

$$\phi_n^\theta(x;\sigma) \equiv \cos(n\, t^\theta(x))$$

$$t^\theta = \Xi^{-1}(x;\sigma) \tag{6}$$

$$\Xi(t;\sigma) \equiv \sum_{m=-\infty}^{\infty} (-1)^m\, V(t-\pi m) \Big/ \sum_{m=-\infty}^{\infty} (-1)^m\, V(\pi m)$$

where

$$V = \frac{\pi}{2} t\, \mathrm{erf}(\sigma t) + \frac{\sqrt{\pi}}{2\sigma} \exp(-\sigma^2 t^2) \tag{7}$$

- Ξ is 2d integral of Jacobian θ-function.
- $\Xi(t,0) \equiv \cos(t)$; basis $\Rightarrow T_n(x)$
- Unlike Kosloff/Tal-Ezer basis,
  θ-map is free of singularities

$$\frac{dt^{\theta}}{dx} \approx -\frac{\pi}{2} \qquad \forall |x| < 1 - O(1/\sigma), \qquad \sigma >> 1$$

i. e., maximum grid point separation $(\pi/2)$ smaller than Chebyshev

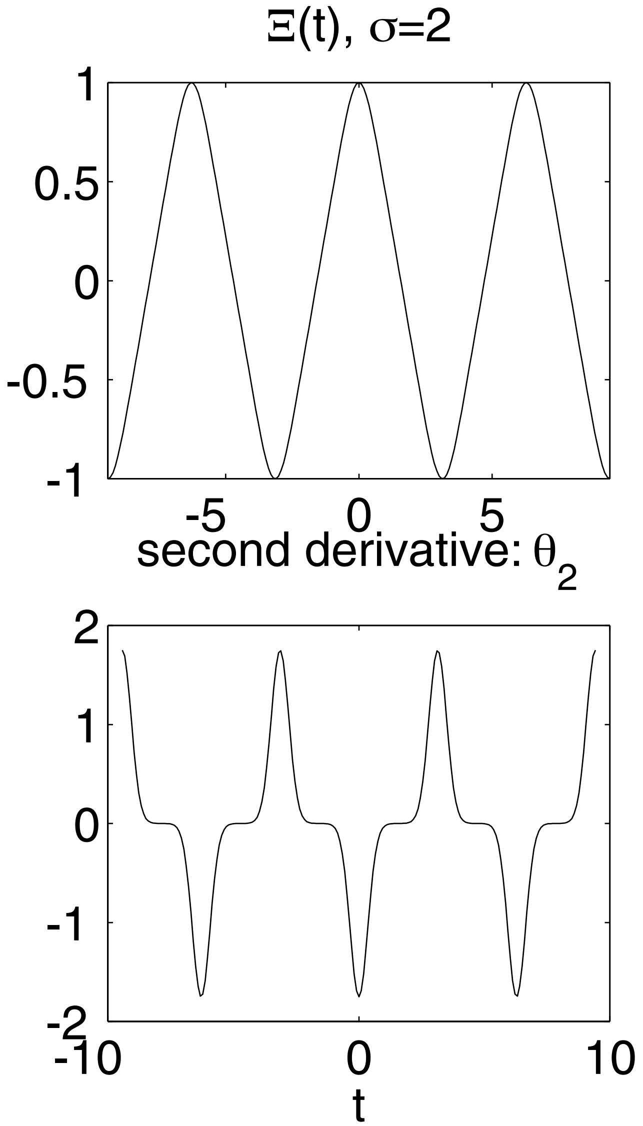

Figure 4: Illustrated over three periods to explicitly show the periodicity of the map.

Theta-Mapped Cosines

Minor disadvantage:

lack of explicit inverse $t(x)$

Easy to compute numerically by bisection

Table 2: Inverse of Theta-Map: $t(x)$

```
 function t=finverse_thetamap(x,sigma);
  itermax=50;     epsilon = 1.E-12;   t1=0;  t2=pi;
   ff=Theta Map(t1,sigma) - x;
    fmiddle=ThetaMap(t2,sigma) - x;
  if ff < 0,  t=t1;  deltax=t2-t1;
  else     t=t2;  deltax=t1-t2;       end \% if
   for j=1:itermax
  deltax=deltax*0.5; tmiddle=t + deltax;
        fmiddle= ThetaMap(tmiddle,sigma) - x;
      if(fmiddle <= 0), t=tmiddle;  end \% if
   if ((abs(deltax) < epsilon) | (fmiddle == 0)),
break; end % if !
 end \% j loop
```

Theta-Mapped Cosines: Comparisons with Chebyshev Polynomials

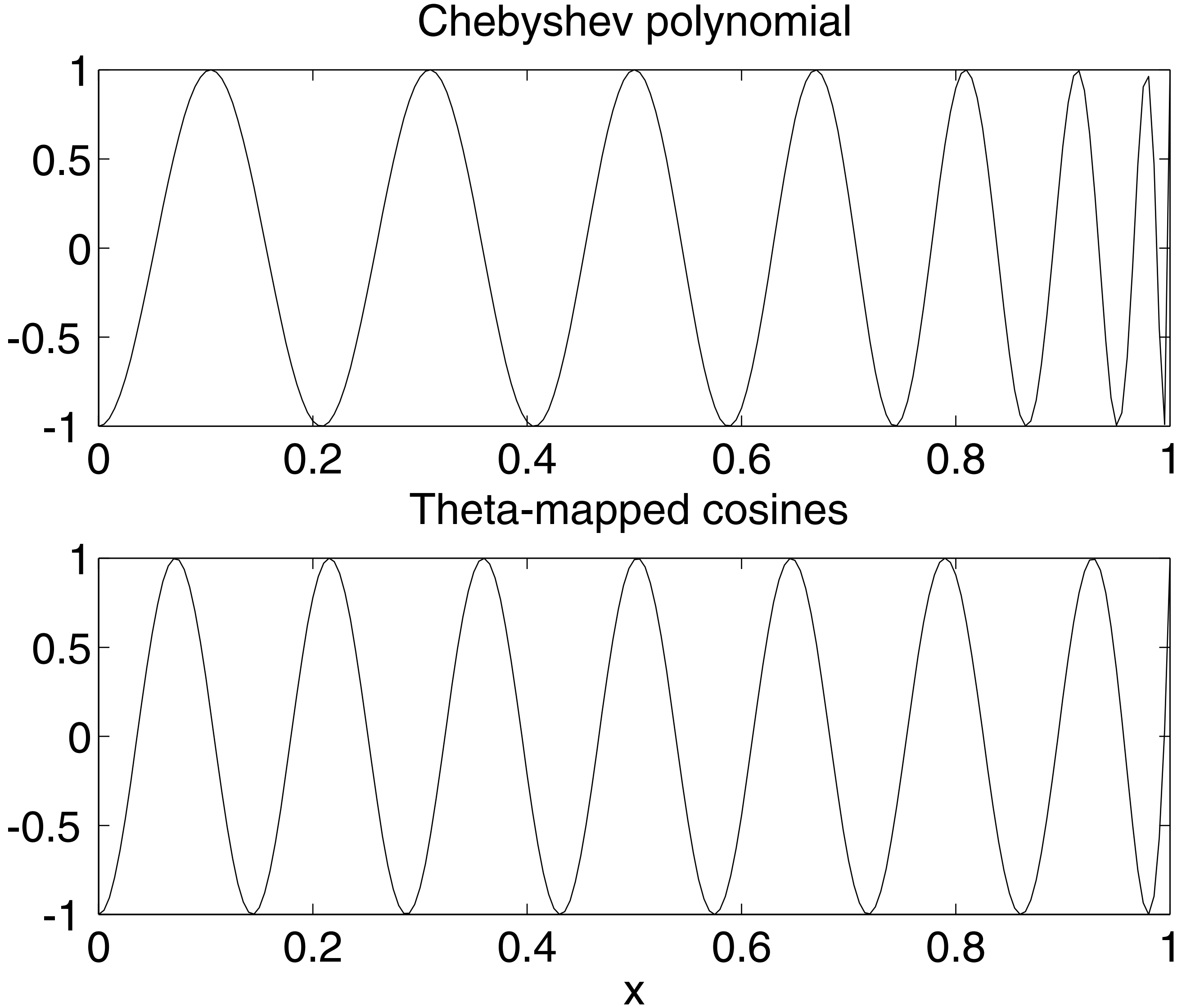

Figure 5: $N = 30$. For the θ-mapping, $\sigma = 5$

Theta-Mapped Cosines: Comparisons with Chebyshev Grid

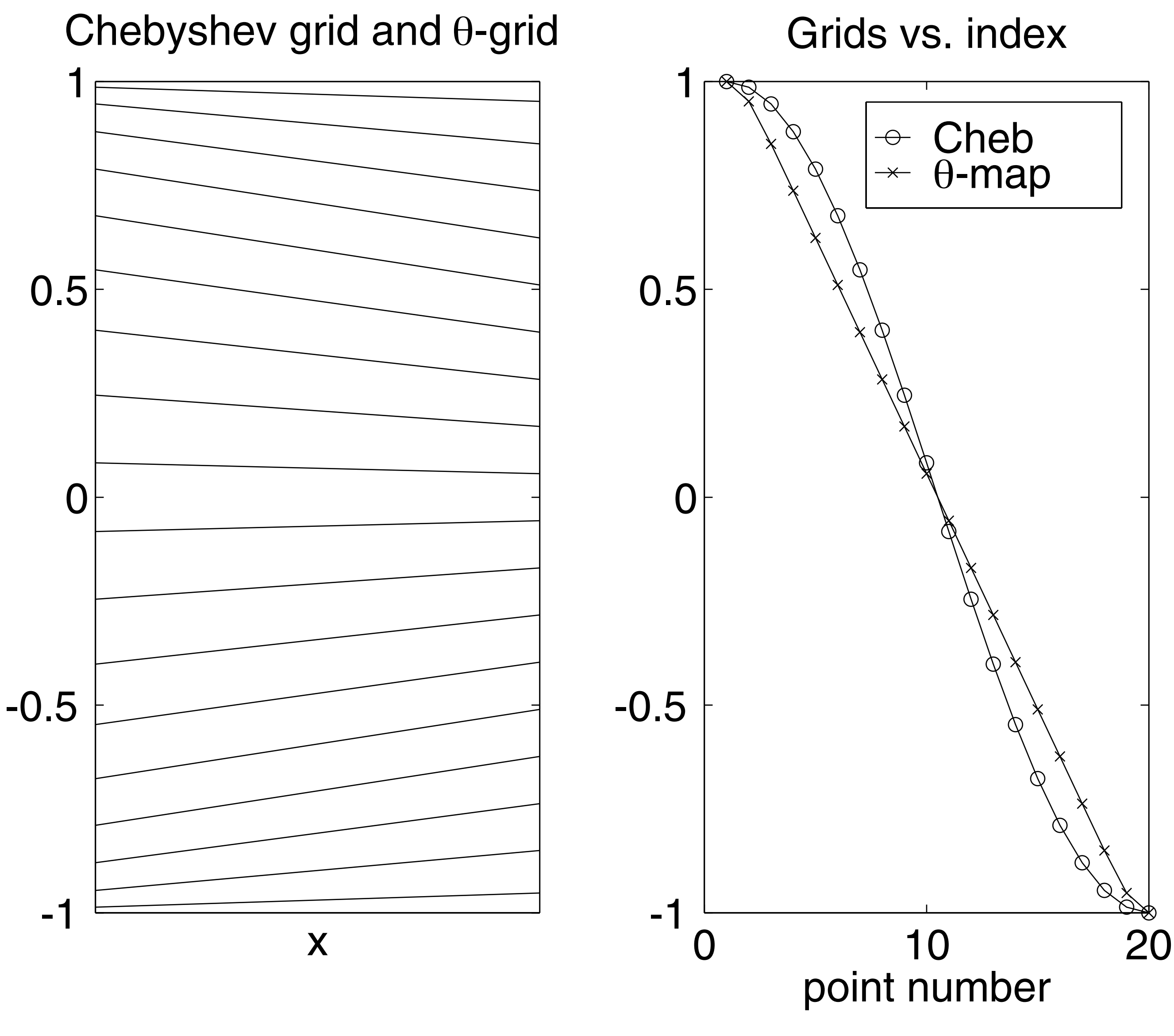

Figure 6: Left panel: Chebyshev grid on left, θ-grid on right.

Theta-Mapped Cosines: Error for $u(x) \equiv x$

- Geometric convergence requires $\sigma \sim O(\sqrt{N})$
- Minimum grid spacing is then $O(N^{3/2})$
- $\sigma \sim O(N) \Rightarrow$ uniform grid,
  but exponential convergence is destroyed

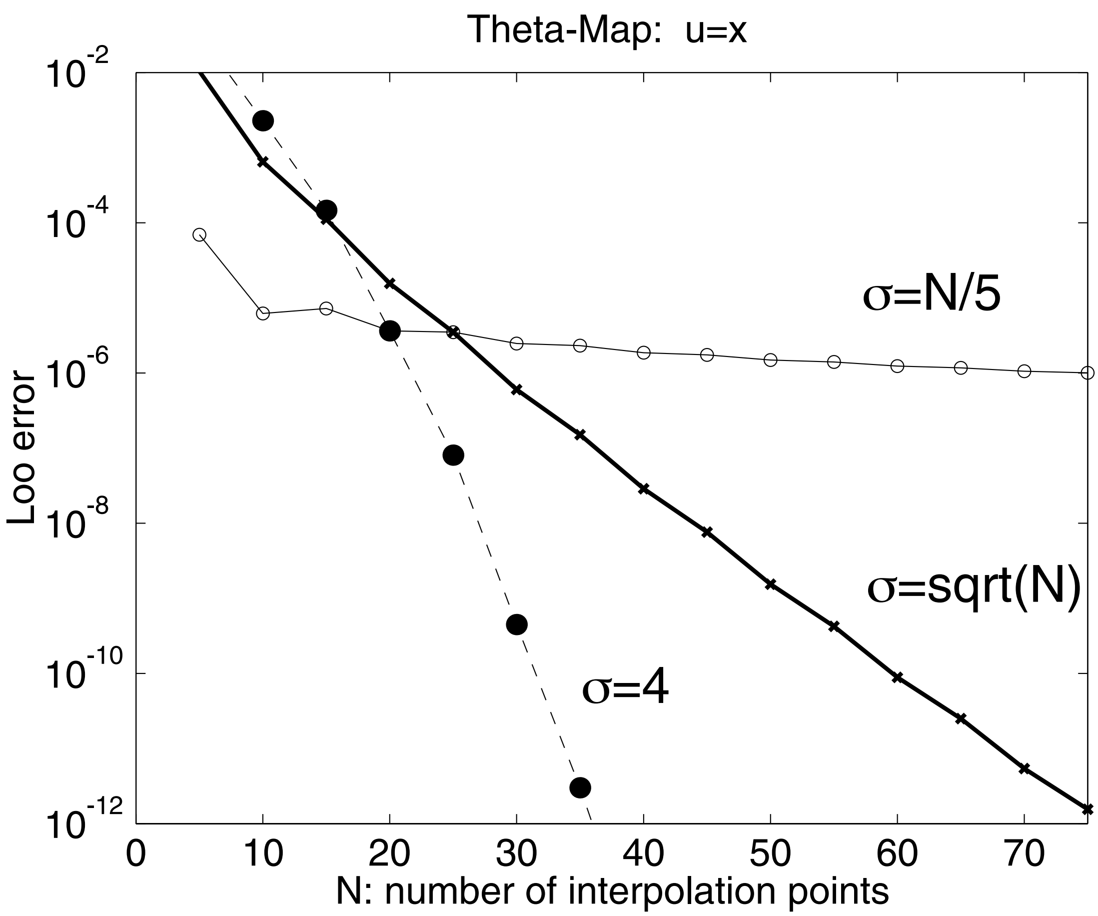

Figure 7:

θ-Mapped Cosines: Derivative Condition Numbers

- Chebyshev:

$$\max\left(\left|eig\left(\vec{\vec{\delta}}_2\right)\right|\right) \sim 0.045\, N^4 \qquad (8)$$

- θ-map with $\sigma = \sqrt{N}$:

$$\max\left(\left|eig\left(\vec{\vec{\delta}}_2\right)\right|\right) \sim 0.100\, N^3 \qquad (9)$$

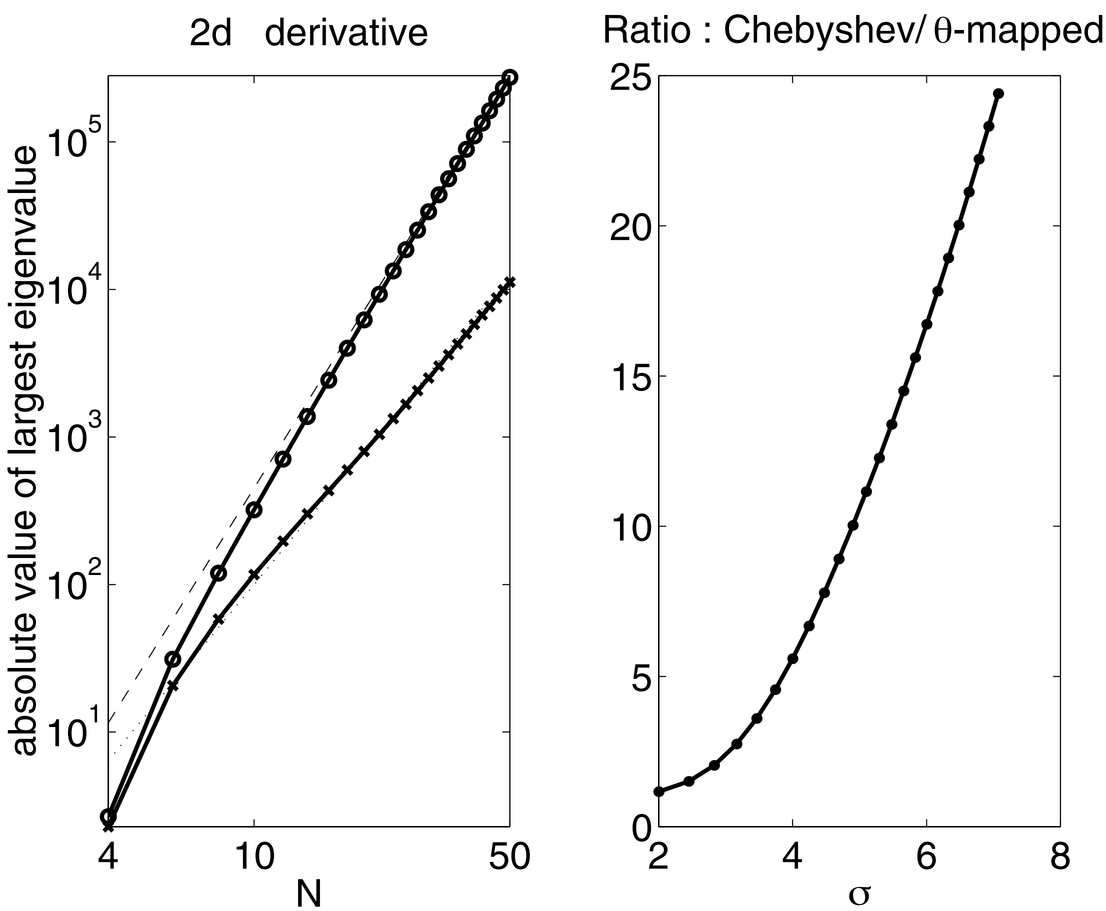

Figure 8: The guidelines (dashed) are the asymptotic forms.

Theta-Mapped Cosines: Error for $u(x) \equiv \cos(kx)$

- Chebyshev needs *minimum* of $N = k$ pts.
  Map reduces this to $N = (2/\pi)k$
  [asymptotically as $N \to \infty$]
- For well-resolved oscillations
  Map dramatically reduces error

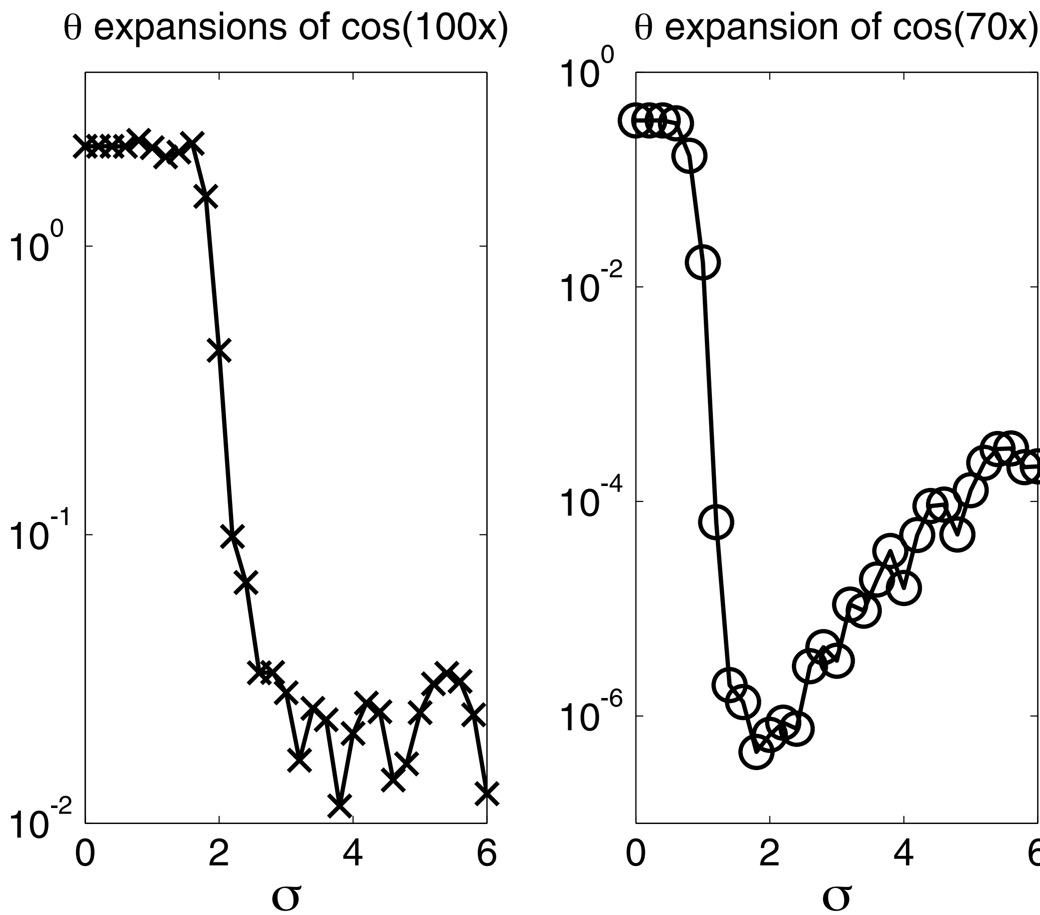

Figure 9: $N = 100$ point expansions of $\cos(100x)$ and $\cos(70x)$.

Theta-Mapped Cosines: Error for $u(x) \equiv \cos(kx)$

- $\sigma = 0$ [left axis] is Chebyshev polynomials
- Error grows monotonically with k for fixed σ.
- As $N \to \infty$, error contours bunch up
- As $N \to \infty$, contours asymptote to $\pi/2$ from below.

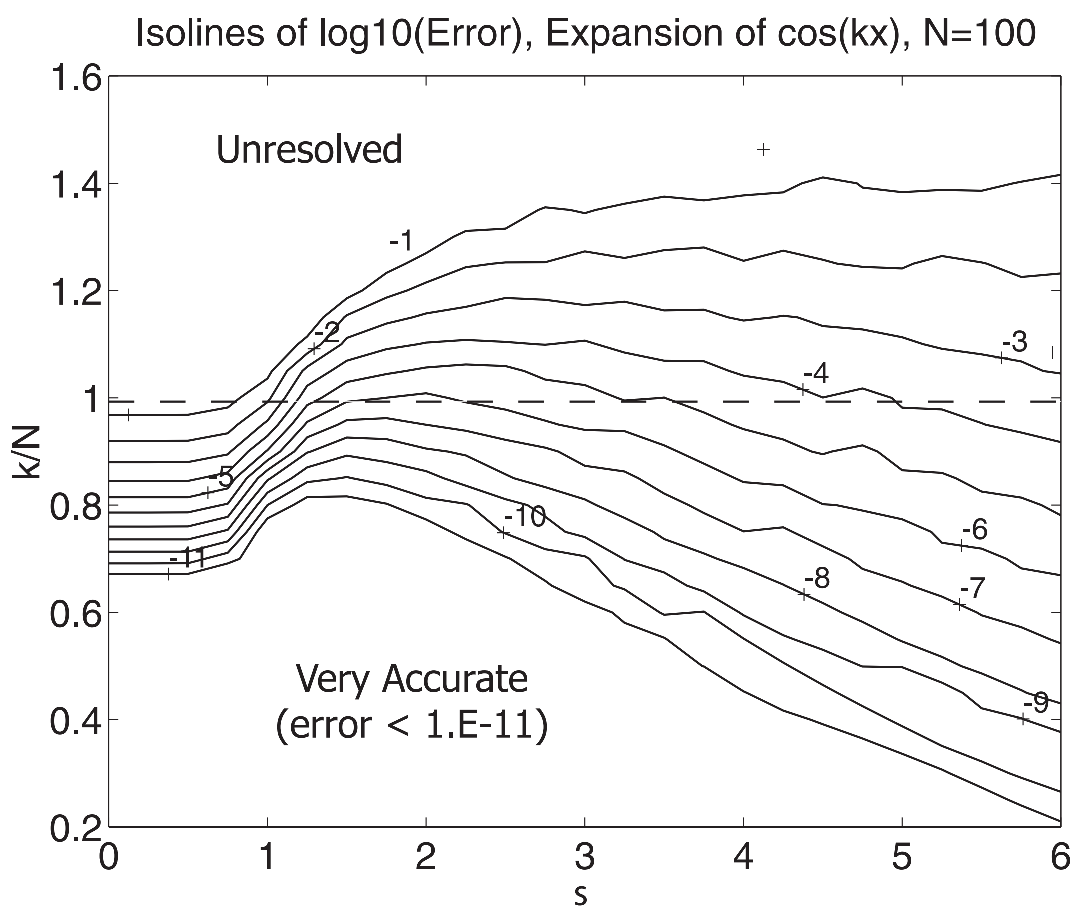

Figure 10: $N = 100$ expansions of $\cos(kx)$ for various k with the θ-map with various σ. Dashed line is the asymptotic Chebyshev limit for the highest resolved wavenumber.

Theta-Mapped Cosines: Error for $u(x) \equiv \cos(kx)$

For a given error, σ was chosen to push the error contour as high in k as possible; the maximum k for that error is then plotted.

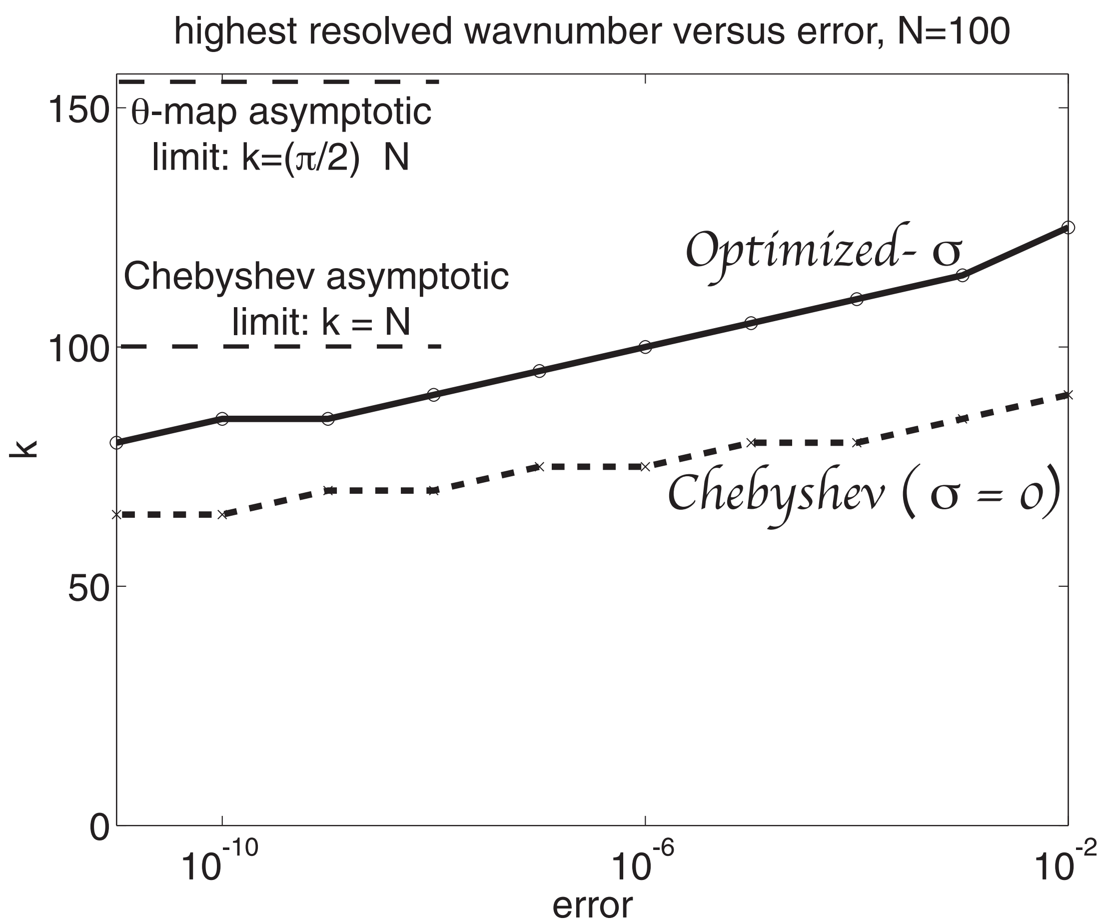

Figure 11: Number of resolved wavenumbers when σ has its optimum value, the value that pushes that particular error contour highest in k.

Optimizing Parameters

- No comprehensive theory as yet
- Theta-mapped theory harder than unbounded
  domain via steepest descent analysis
- Prolate theory *really* hard because
  prolate $\Rightarrow$ Legendre for *fixed* c;
- Empirical, problem-dependent experimentation
  is best strategy for now
- Experimentation cost-effective for
  community models

Spectral Elements

- Prolate orthogonal with UNIT WEIGHT
  $\Rightarrow$ trivial to replace Legendre
- Needs only grid, weights, derivatives-at-grid
- grid & weights: Newton-Ralphson iteration
  functions/derivatives: Symmetric
  tridiagonal Legendre-Galerkin
- Theta-mapped cosines are *almost* orthogonal
  easy to Gram-Schmidt orthogonalize
- Best basis for multi-domains?

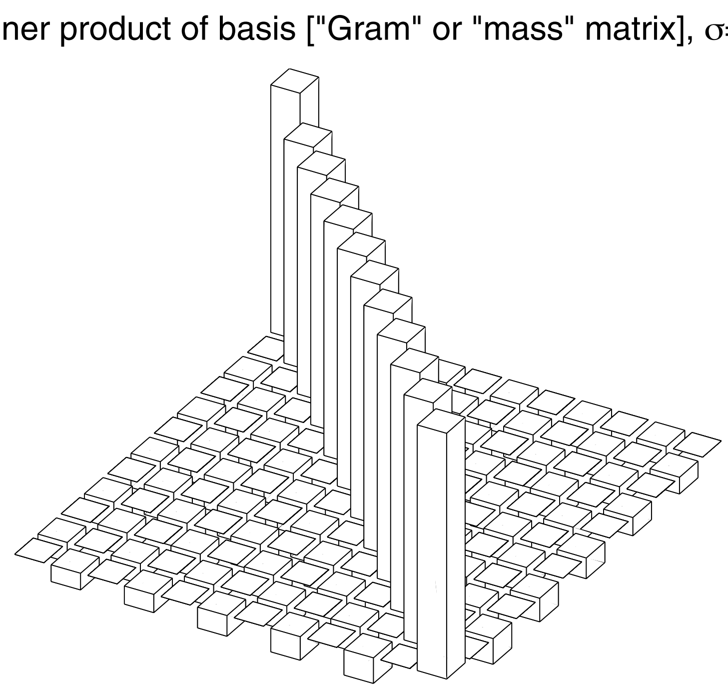

Figure 12:

Virtues of Cosine-Mapped Functions

1. Better resolution by $\pi/2$
2. More uniform grid
3. Much larger CFL timestep limit

Vices

1. All contain a free parameter
2. No theory for choosing parameter
3. More complicated to program than Chebyshev

Additional Conclusions

- Kosloff/Tal-Ezer inferior because of map singularity
- Prolate are orthogonal with unit weight easy to drop into spectral elements
- θ-map is best for single-domain (simplest!)

Future Problems

- *theory for optimizing* σ *or* c
- Empirical guidelines for σ or c
- Practical experience with "prolate elements", "theta elements", etc., on hard problems