Highly Accurate Computation of the Generalized Dirichlet-Neumann Map

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Highly Oscillatory Problems: Computation, Theory and Application

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27 February 2007

Overview: The Fokas Method

Laplace Equation: With $z = x + iy$, $q_z = \frac{1}{2}(q_x - iq_y)$, and $q_{\bar{z}} = \frac{1}{2}(q_x + iq_y)$:

$$q_{z\bar{z}} = 0 \qquad \text{on domain } D \tag{*}$$

Global Relation: For any $k \in \mathbb{C}$, the 1-form $W = e^{-ikz} q_z \, dz$ is closed: $dW = 0$ by (*), so its integral around any closed contour in D vanishes. Choose ∂D:

$$\int_{\partial D} e^{-ikz} q_z \, dz = 0, \qquad \forall k \in \mathbb{C}$$

Theorem: The global relation is necessary and sufficient for the solution of (*)

Generalized Dirichlet-Neumann Map:

- Specify one component of q_z on the boundary
- Solve the global relation for the other component

Question: How to solve the global relation?

Outline

Numerical Solution of the Global Relation

- Formulation
- Discretization
- Numerical results
- Improvements

Spectral Collocation Projections

- Formulation
- Sine collocation projection
- Convergence

Conclusions

Collaborators

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Y. Saridakis, A. G. Sifalakis (Technical University of Crete)

References

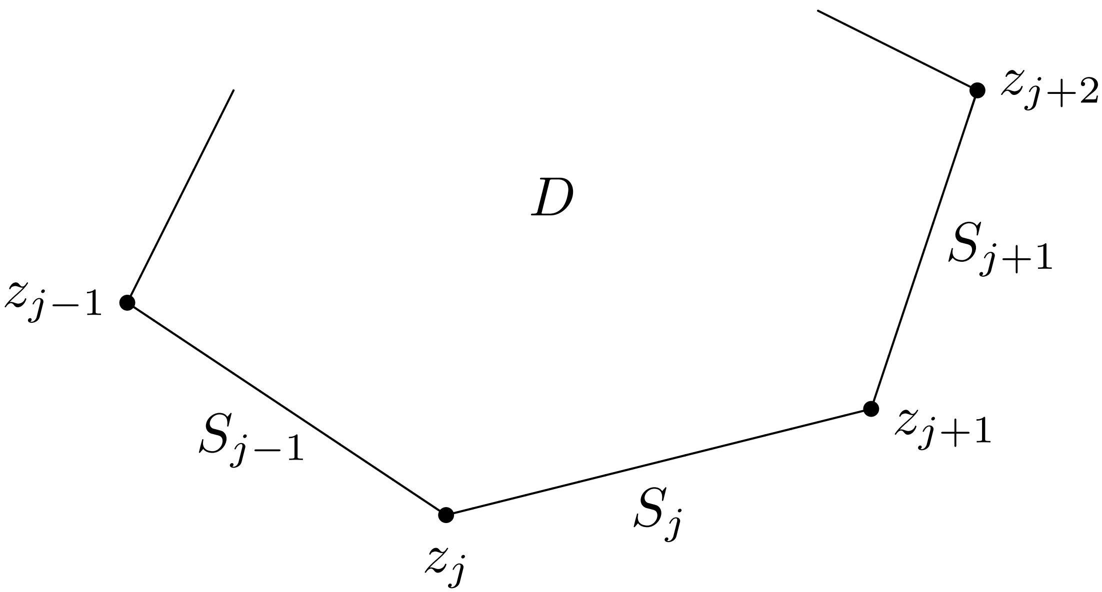
Fokas, 2001: Two-dimensional linear PDEs in a convex polygon, *Proc. R. Soc. London*, **A 457**, 371–393.

[FFX] Fulton, Fokas, and Xenophontos, 2004: An analytical method for linear elliptic PDEs and its numerical implementation. *J. Comp. Appl. Math.* **167**, 465–483.

[SFFS] Sifalakis, Fokas, Fulton, and Saridakis, 2007: The generalized Dirichlet-Neumann Map for linear elliptic PDEs and its numerical implementation. Submitted.

Problem Formulation

Domain: Bounded convex polygon with interior D (with vertices z_j and sides S_j, $j = 1, \ldots, n$, indexed modulo n):



Global Relation:

$$\sum_{j=1}^{n} \underbrace{\int_{S_j} e^{-ikz} q_z \, dz}_{\rho_j(k)} = 0, \qquad \forall k \in \mathbb{C}$$

Theorem [FFX]

For each $j = 1, \ldots, n$ let $r^{(j)} \in H^{\frac{1}{2}+\epsilon}(S_j)$ for some $\epsilon > 0$, assume that $r^{(j)}(z_{j+1}) = r^{(j+1)}(z_{j+1})$, and define $\rho_j(k)$ by the line integral

$$\rho_j(k) = \int_{S_j} e^{-ikz} r^{(j)}(z)\, dz, \quad \forall k \in \mathbb{C}$$

along that side. Assume that the functions ρ_j satisfy the global relation

$$\sum_{j=1}^{n} \rho_j(k) = 0, \quad \forall k \in \mathbb{C}$$

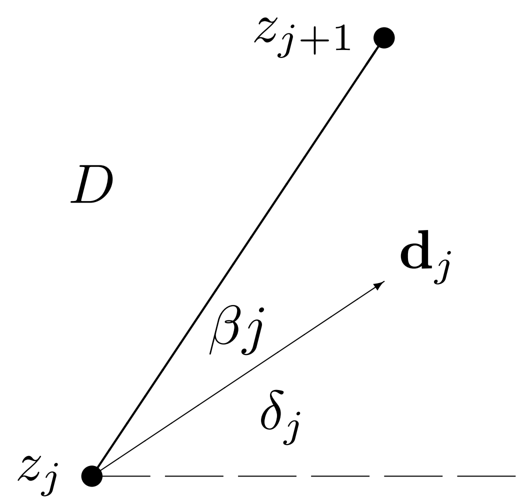
and define the ray $\ell_j = \{k \in \mathbb{C} : \arg(k) = -\arg(z_{j+1} - z_j)\}$. Then the function

$$r(z) := \frac{1}{2\pi} \sum_{j=1}^{n} \int_{\ell_j} e^{ikz} \rho_j(k)\, dk$$

and its antiderivative $q(z)$ are continuous on $D \cup S$ and analytic on D, $\mathrm{Re}(q)$ satisfies the Laplace equation on D, and on each side S_j $(j = 1, \ldots, n)$, $q_z = r = r^{(j)}$.

Boundary Conditions

On each side $S_j = (z_j, z_{j+1})$:



- Specify the derivative in some direction $\mathbf{d}_j$:

$$g^{(j)} = q_x \cos \delta_j + q_y \sin \delta_j \qquad \text{(known)}$$

- Seek the corresponding component:

$$f^{(j)} = q_x \sin \delta_j - q_y \cos \delta_j \qquad \text{(unknown)}$$

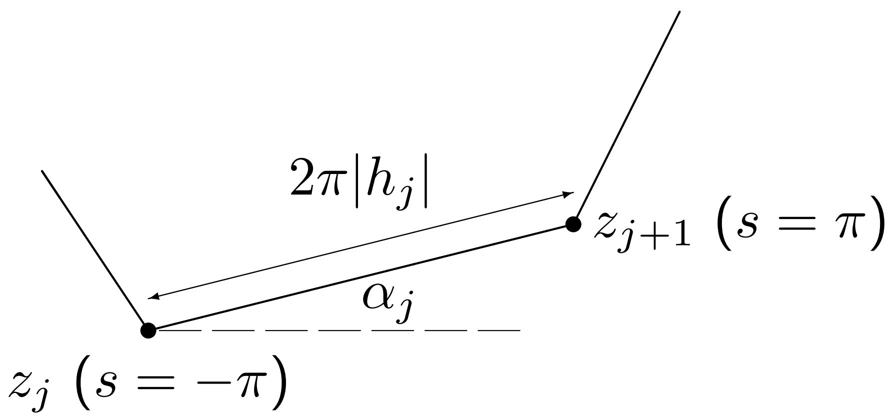
Then

$$q_z^{(j)} = \frac{1}{2} e^{-i\delta_j} \left(g^{(j)} + i f^{(j)} \right)$$

Special cases:

- $\beta_j = 0$: Dirichlet
- $\beta_j = \frac{\pi}{2}$: Neumann

Parameterization (I)



On each side $S_j = (z_j, z_{j+1})$ parameterize:

$$z = \frac{(\pi - s)\, z_j + (\pi + s)\, z_{j+1}}{2\pi} = m_j + h_j s,$$

where

$$m_j = \frac{z_j + z_{j+1}}{2}, \qquad h_j = \frac{z_j - z_{j+1}}{2\pi} = |h_j| e^{i\alpha_j}$$

with $\alpha_j = \beta_j + \delta_j$.

Parameterization (II)

On each side $S_j = (z_j, z_{j+1})$:

$$\rho_j(k) = \frac{h_j}{2} e^{-i\delta_j} e^{-ikm_j} \int_{-\pi}^{\pi} e^{ikh_j s} \left[g^{(j)}(s) + i f^{(j)}(s) \right] \, ds$$

For any function $\psi \in C[-\pi, \pi]$ define the Fourier transform

$$\widehat{\psi}(k) := \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-iks} \psi(s) \, ds.$$

Then

$$\rho_j(k) = \pi h_j e^{-i\delta_j} e^{-ikm_j} \left[\widehat{g}^{(j)}(kh_j) + i \widehat{f}^{(j)}(kh_j) \right]$$

so the global relation becomes

$$\sum_{j=1}^{n} h_j e^{-i\delta_j} e^{-ikm_j} \widehat{f}^{(j)}(kh_j) = i \underbrace{\sum_{j=1}^{n} \left[\widehat{g}^{(j)} \right]}_{\text{same form}}, \qquad \forall k \in \mathbb{C}$$

The Choice of k (I)

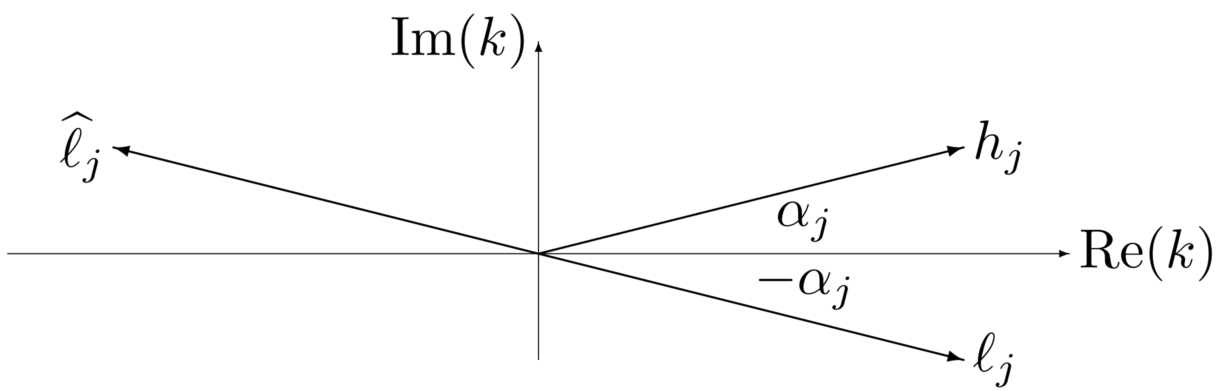
For the solution q_z we need $\rho_j(k)$ on the ray $\ell_j = \{k \in \mathbb{C} : \arg(k) = -\alpha_j = -\arg(h_j)\}$.
Compare with the integrand in $\rho_j(k)$:

$$e^{ikh_js} \text{ is bounded as } |k| \to \infty$$

for $s \in [-\pi, \pi]$ if and only if kh_j is real. There are two choices:

1. $k \in \ell_j$: then $|e^{-ikm_j}| < 1$ so the $f^{(j)}$ are *weakly coupled* by the global relation.

2. $k \in \widehat{\ell}_j$: then $|e^{-ikm_j}| > 1$ so the $f^{(j)}$ are *strongly coupled* by the global relation.



The Choice of k (II)

Conclusion: With $kh_j = -l \in \mathbb{R}$:

- Use $l > 0$ ($k \in \widehat{\ell}_j$) to solve the global relation for $\widehat{f}^{(j)}(kh_j) = \widehat{f}^{(j)}(-l)$
- Use $l < 0$ ($k \in \ell_j$) to evaluate the solution q_z

Observe: For $l \in \mathbb{Z}$ the numbers $\widehat{f}^{(j)}(l)$ are the coefficients in the Fourier series

$$f^{(j)}(s) = \sum_{l=-\infty}^{\infty} \widehat{f}^{(j)}(l) e^{ils}$$

Global relation:

$$\sum_{j=1}^{n} \tau_{p,j} \sigma_{p,j}^{l} \widehat{f}^{(j)}(-lh_j/h_p) = i \sum_{j=1}^{n} \left[\widehat{g}^{(j)} \right] \qquad (l \in \mathbb{R}^+)$$

for $p = 1, \ldots, n$, where $\sigma_{p,j} := e^{i(m_j - m_p)/h_p}$ and $\tau_{p,j} := (h_j/h_p) e^{-i(\delta_j - \delta_p)}$

Observe: For $p \neq j$, $|\sigma_{p,j}| < |\sigma_{p,p}| = 1$: off-diagonal terms are exponentially small

Continuity Conditions

Idea:

- For $k = 0$ the equations are degenerate (same equation from each side)
- Use continuity of q_z at vertices to determine endpoint values of each $f^{(j)}$
- Subtract a known linear piece $f_*^{(j)}$ on each side:

$$f^{(j)} = f_*^{(j)} + F^{(j)},$$

where $F^{(j)}(-\pi) = F^{(j)}(\pi) = 0$

Resulting Global Relation:

$$\boxed{\sum_{j=1}^{n} \tau_{p,j} \sigma_{p,j}^{l} \widehat{F}^{(j)}(-lh_j/h_p) = i \sum_{j=1}^{n} \left[\widehat{G}^{(j)} + \widehat{H}^{(j)} \right] \qquad (l \in \mathbb{R}^+)}$$

for $p = 1, \ldots, n$, where $H^{(j)}(s) = g_*^{(j)}(s) + i f_*^{(j)}(s)$.

Discretization

Approximation Subspace: Choose a basis $\{\varphi_r(s)\}_{r=1}^{N}$ for a subspace of $C_0[-\pi,\pi]$ (with dimension N even) and approximate

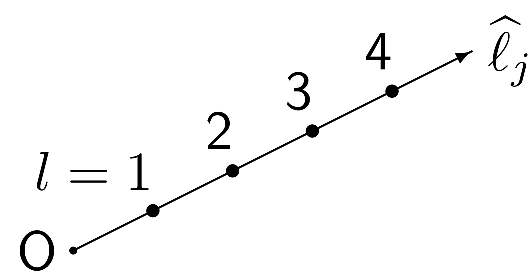
$$F_N^{(j)}(s) = \sum_{r=1}^{N} c_r^{(j)} \varphi_r(s), \qquad G_N^{(j)}(s) = \sum_{r=1}^{N} d_r^{(j)} \varphi_r(s)$$

Spectral Collocation Projection: Force the global relation to hold at $k = -l/h_p$ for $l = 1, \ldots, M = N/2$ and $p = 1, \ldots, n$:

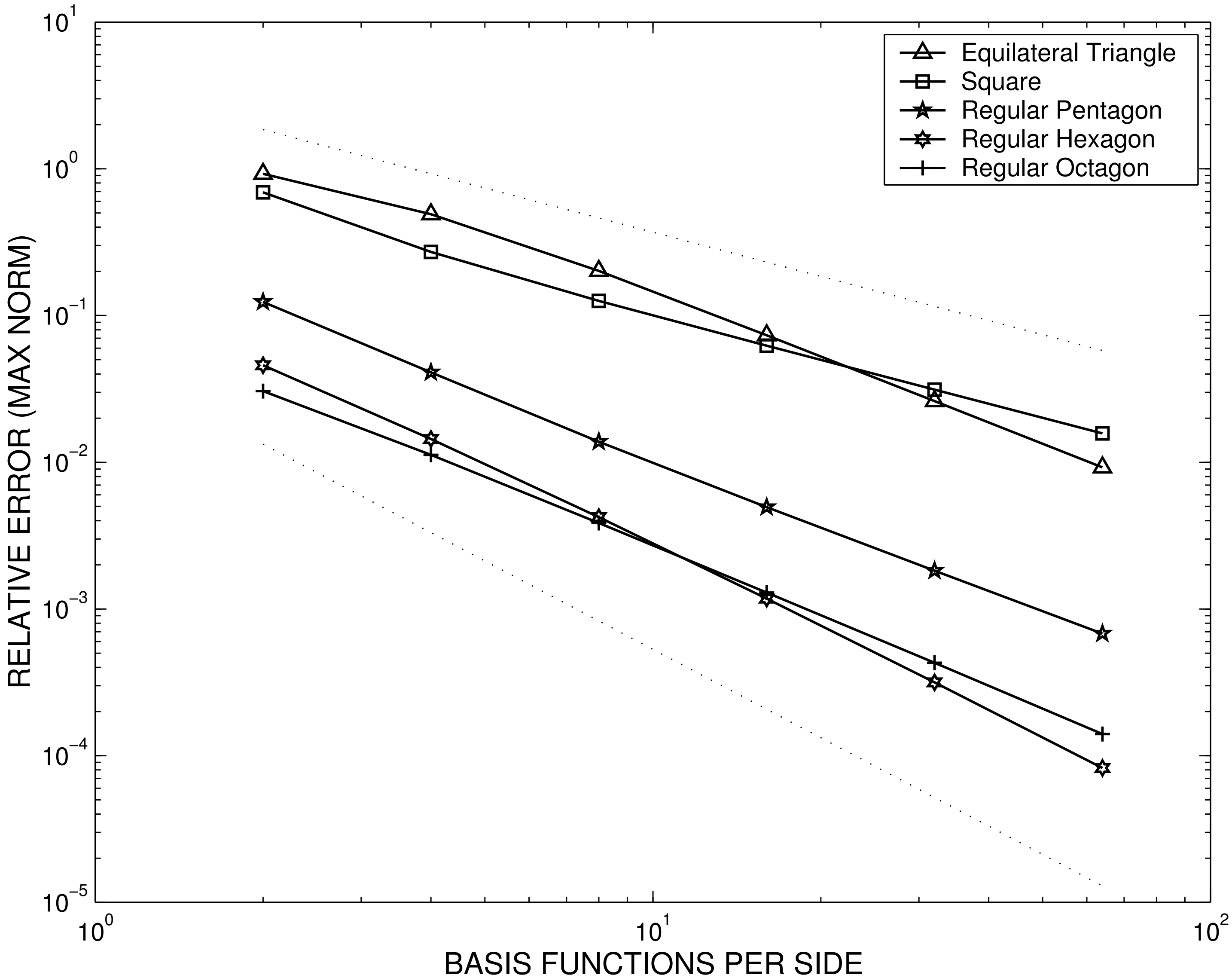
$$\boxed{\sum_{j=1}^{n} \tau_{p,j} \sigma_{p,j}^{l} \sum_{r=1}^{N} c_r^{(j)} \widehat{\varphi}_r(-l h_j / h_p) = i \sum_{j=1}^{n} \left[d_r^{(j)} \right]}$$

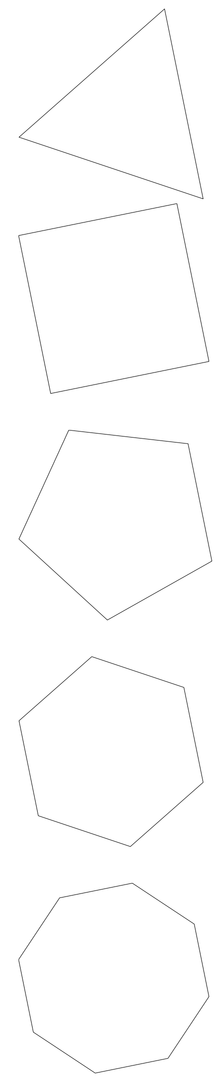
"The count":

- nN unknowns (real)
- nM equations (complex)

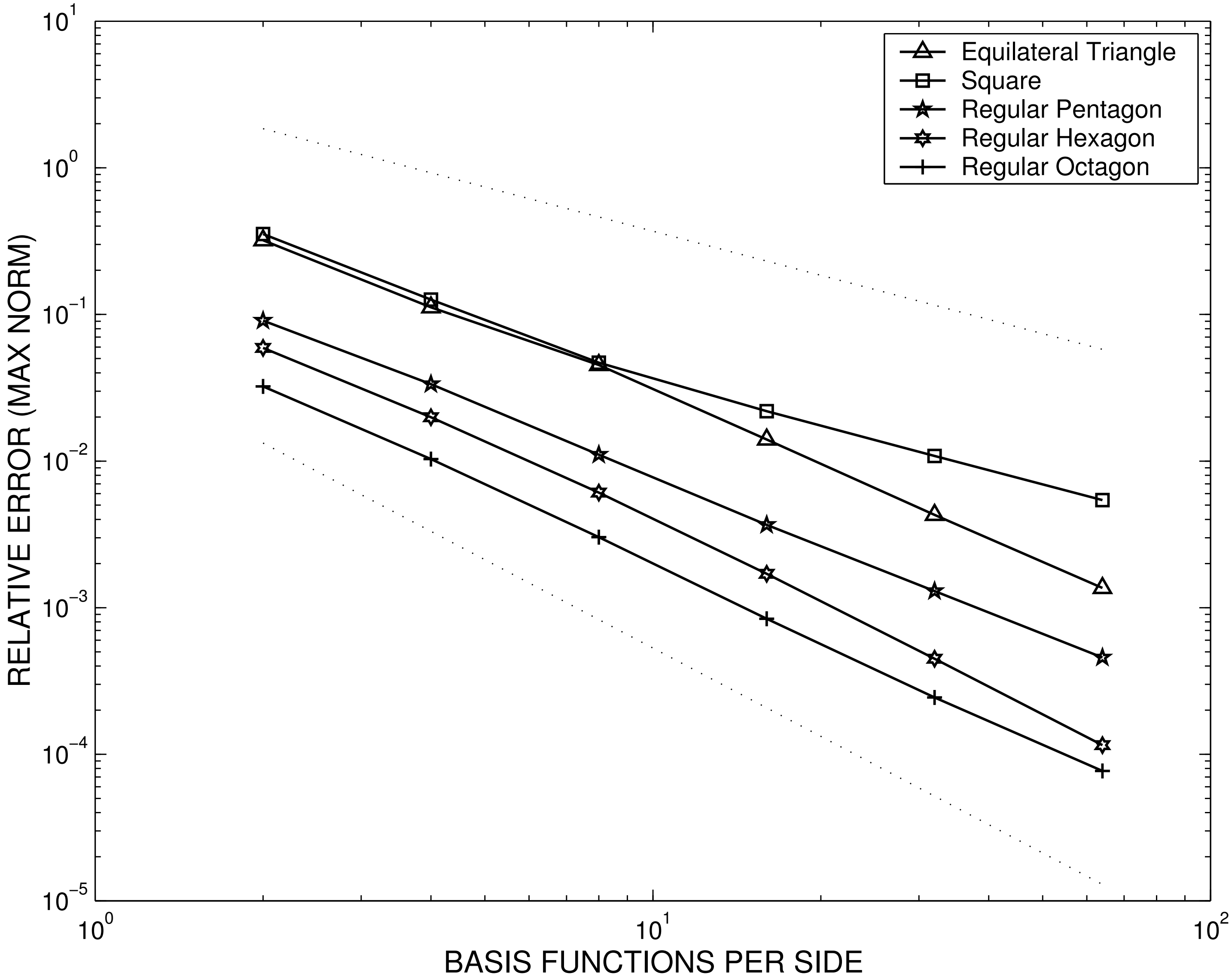


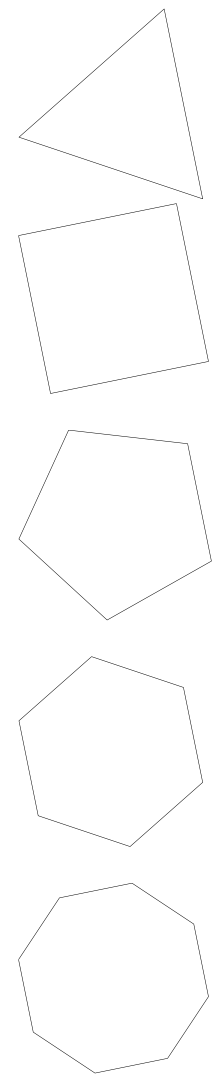
Regular Polygons–Dirichlet BCs



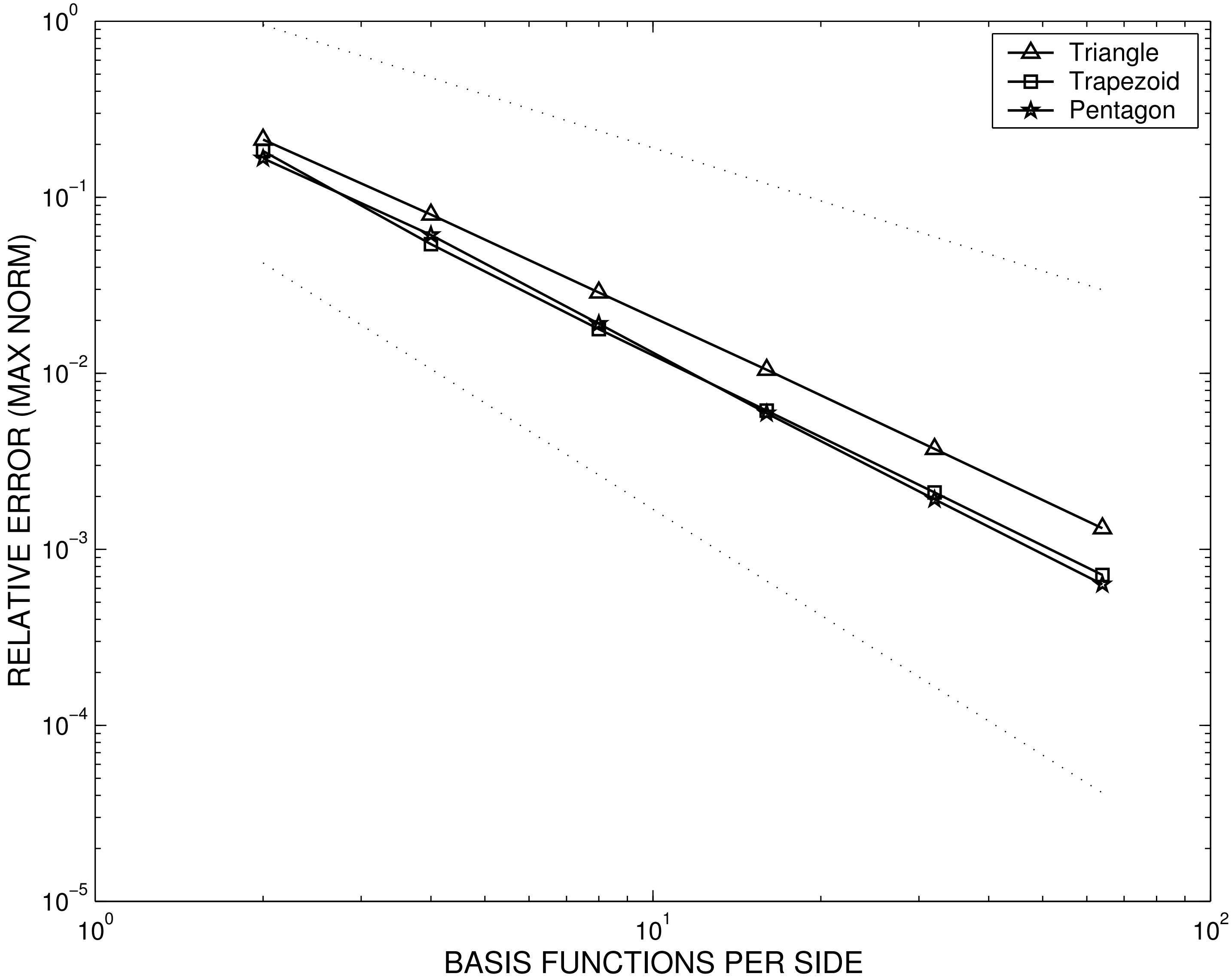


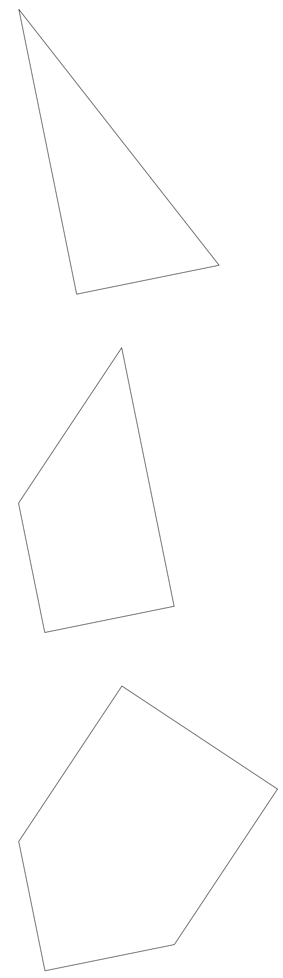
Regular Polygons–Neumann BCs





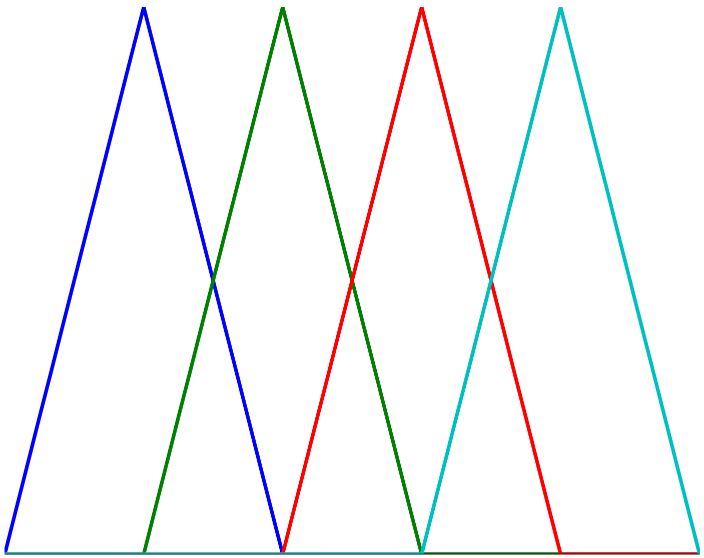
General Polygons–Mixed BCs





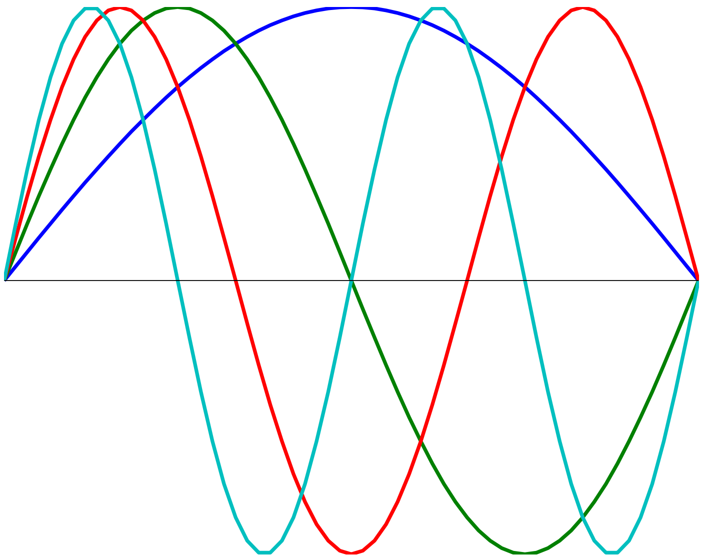
Choice of Basis

Hat functions



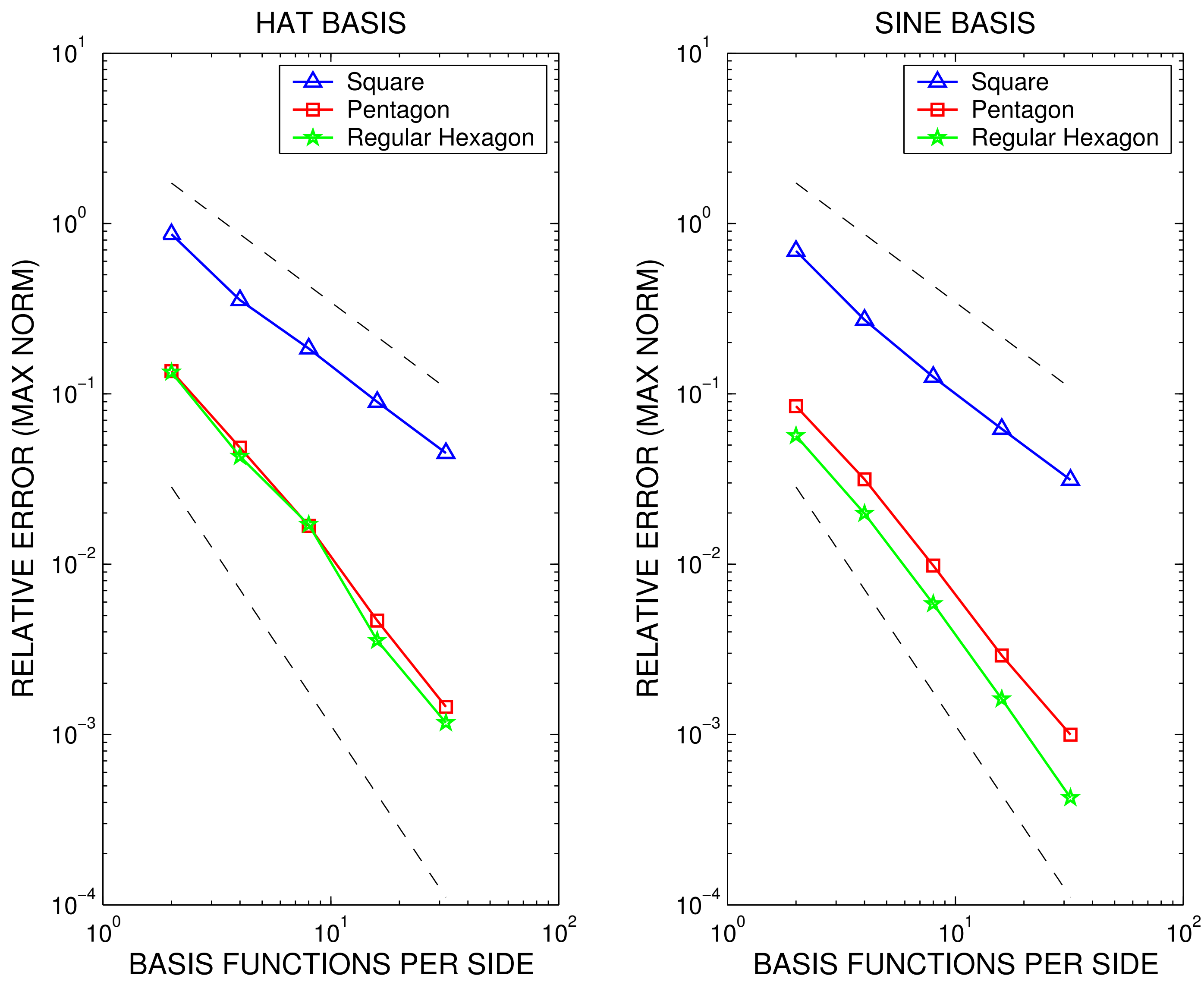
(piecewise linear)

Sine functions

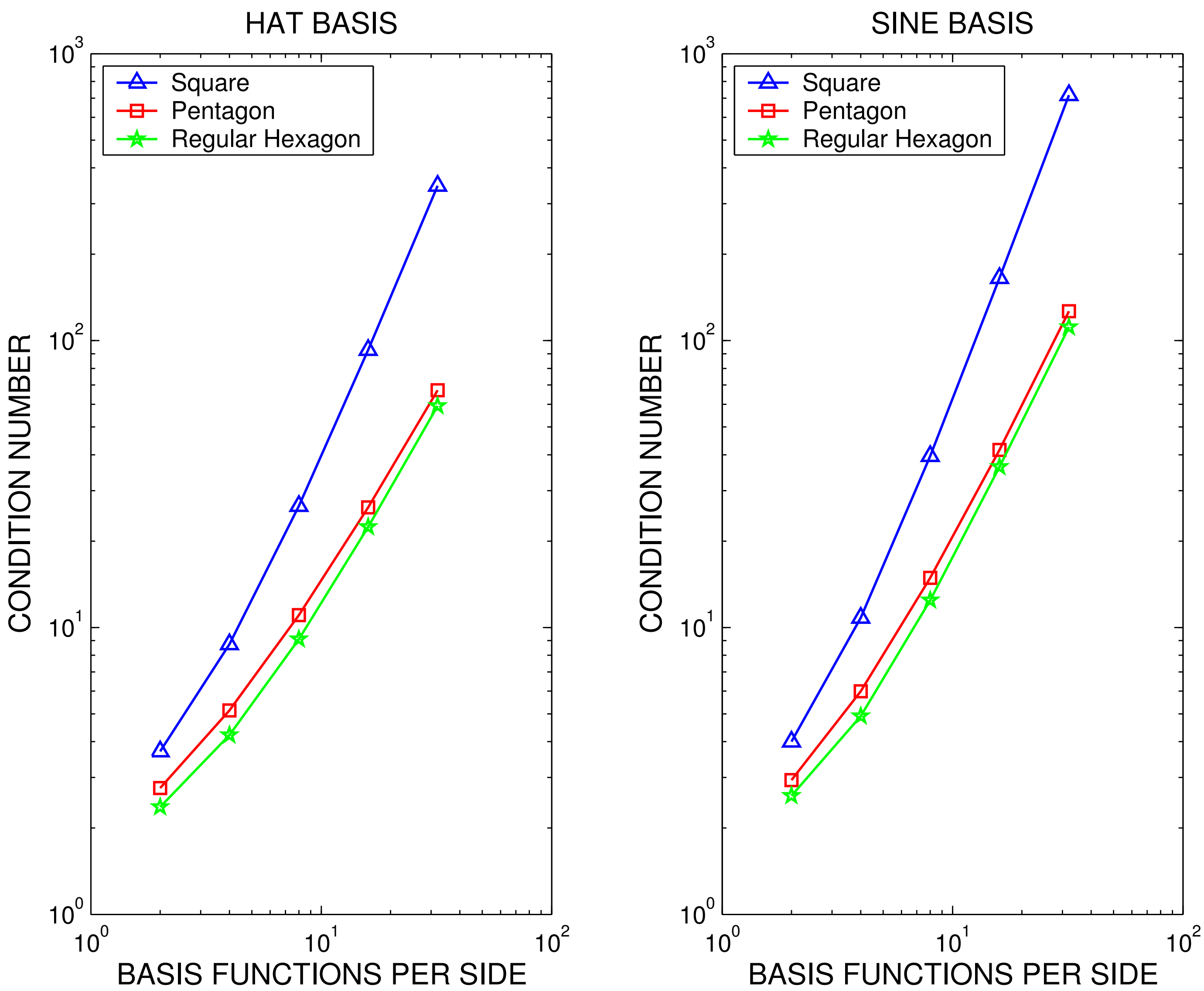


$$\varphi_r(s) = \sin\left[r\left(\frac{s+\pi}{2}\right)\right]$$

Effect of Basis: Errors



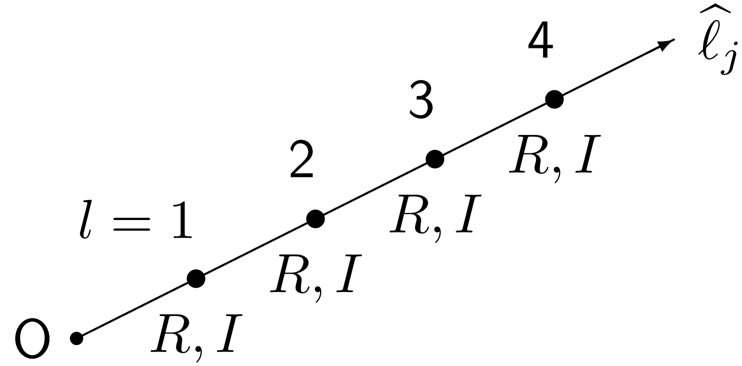
Effect of Basis: Condition Number



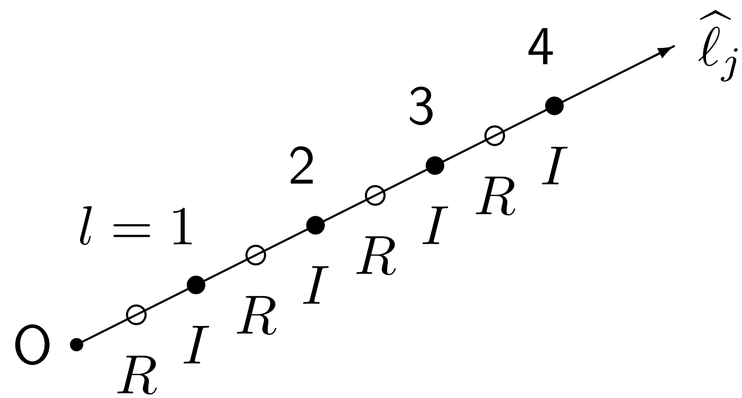
SFFS Improvements (I): Collocation Points

Recall: Must choose k on the ray $\widehat{\ell_j}$ ($-kh_j = l \in \mathbb{R}^+$)—but which points to use?

- FFX method: real and imaginary parts of equation at integer l

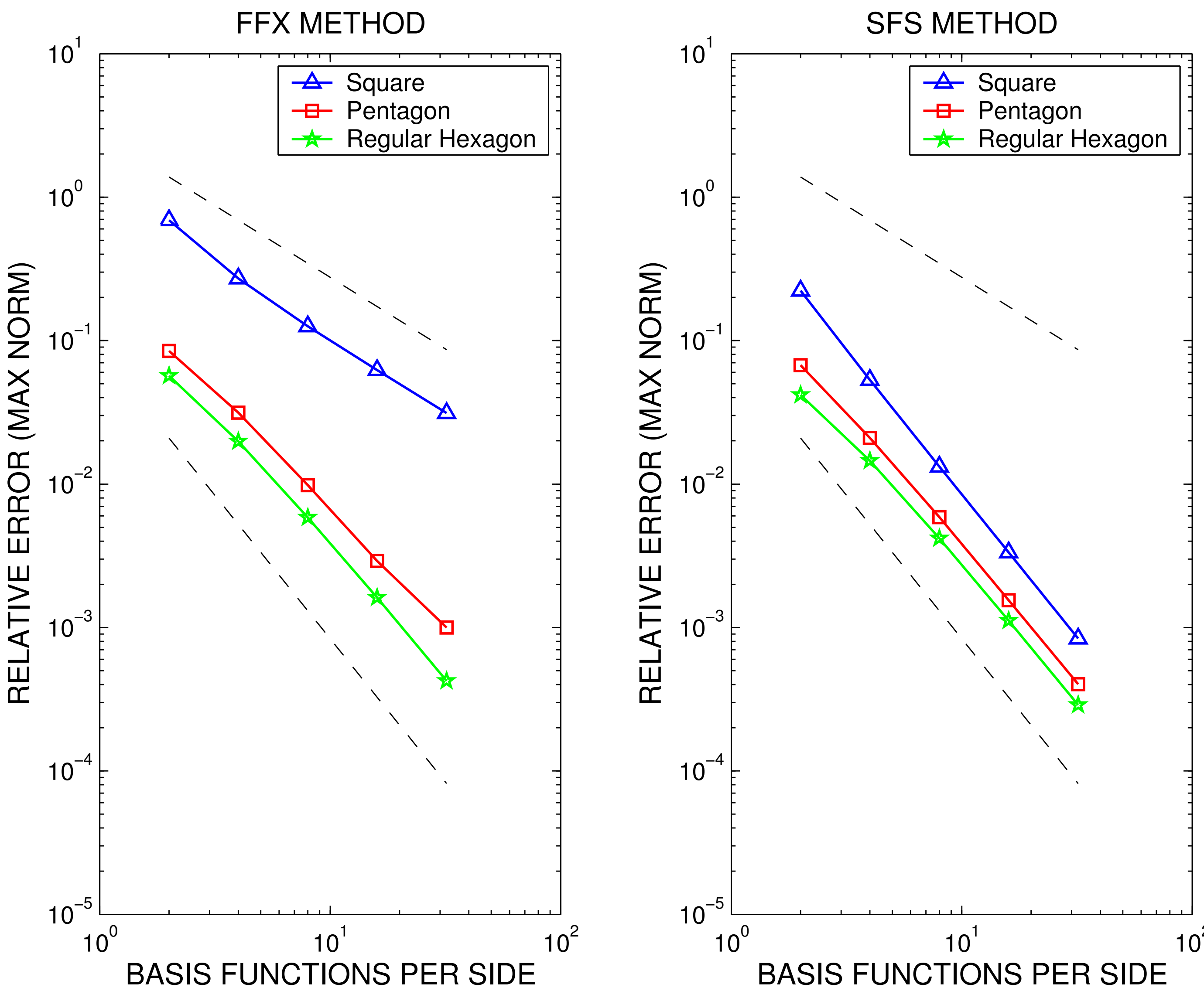


- SFFS method: real parts at half-integer l, imaginary parts at integer l

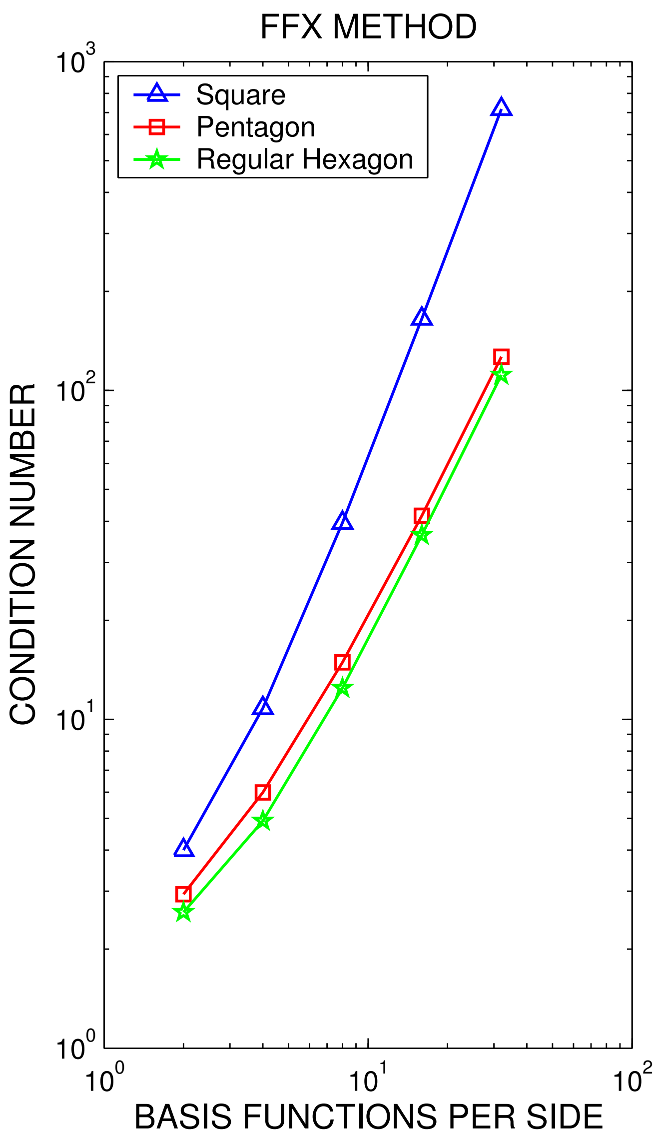


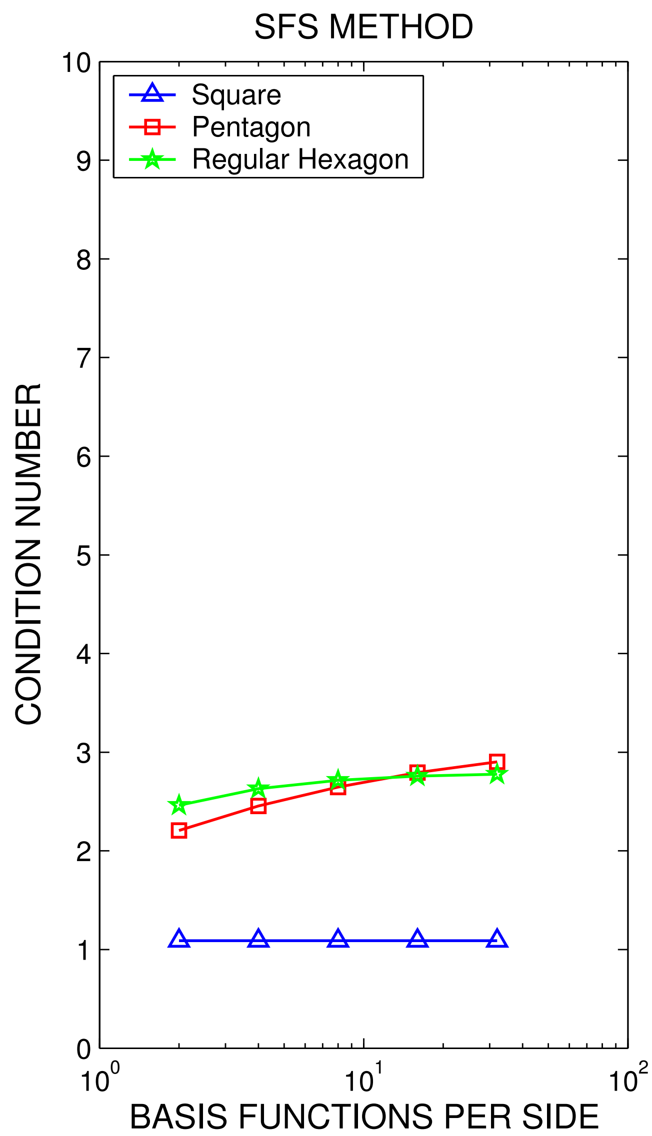
Note: Both methods give diagonal blocks on the main diagonal

Effect of Collocation Points: Errors

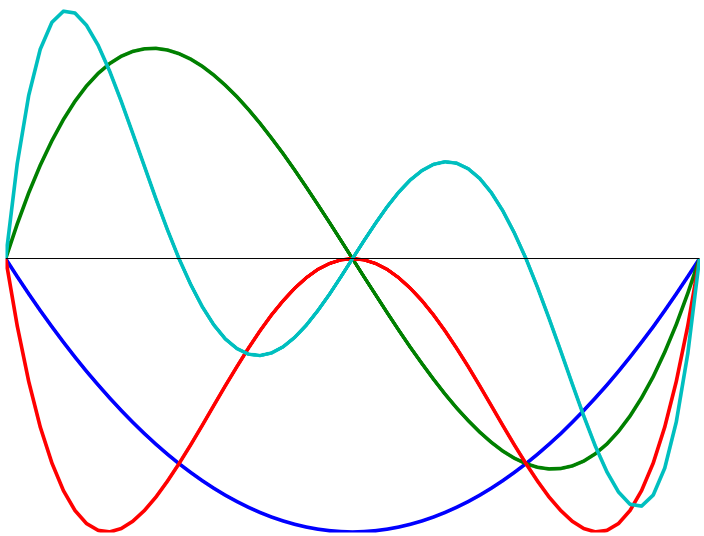


Effect of Collocation Points: Condition Number



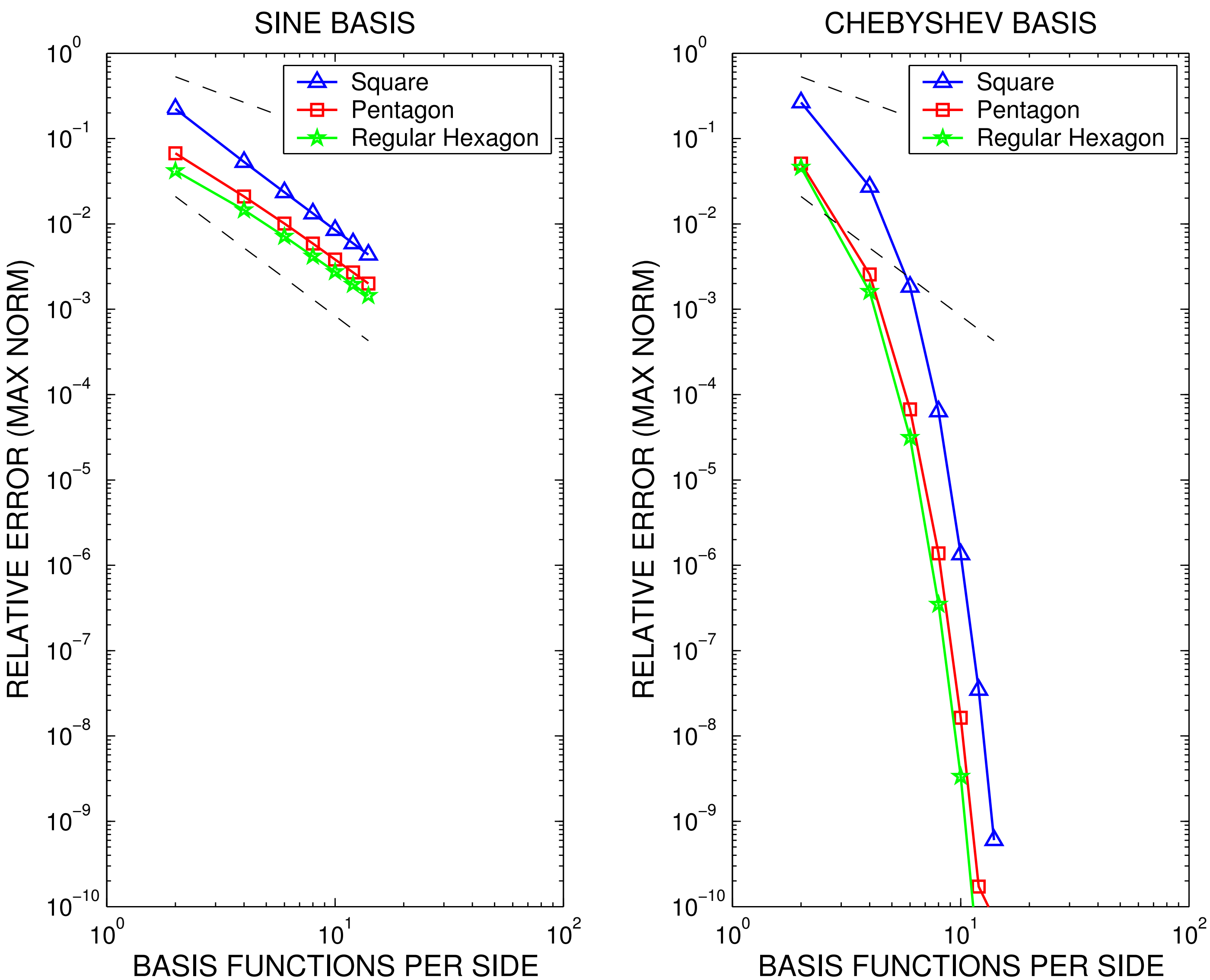


SFFS Improvements (II): Chebyshev Basis

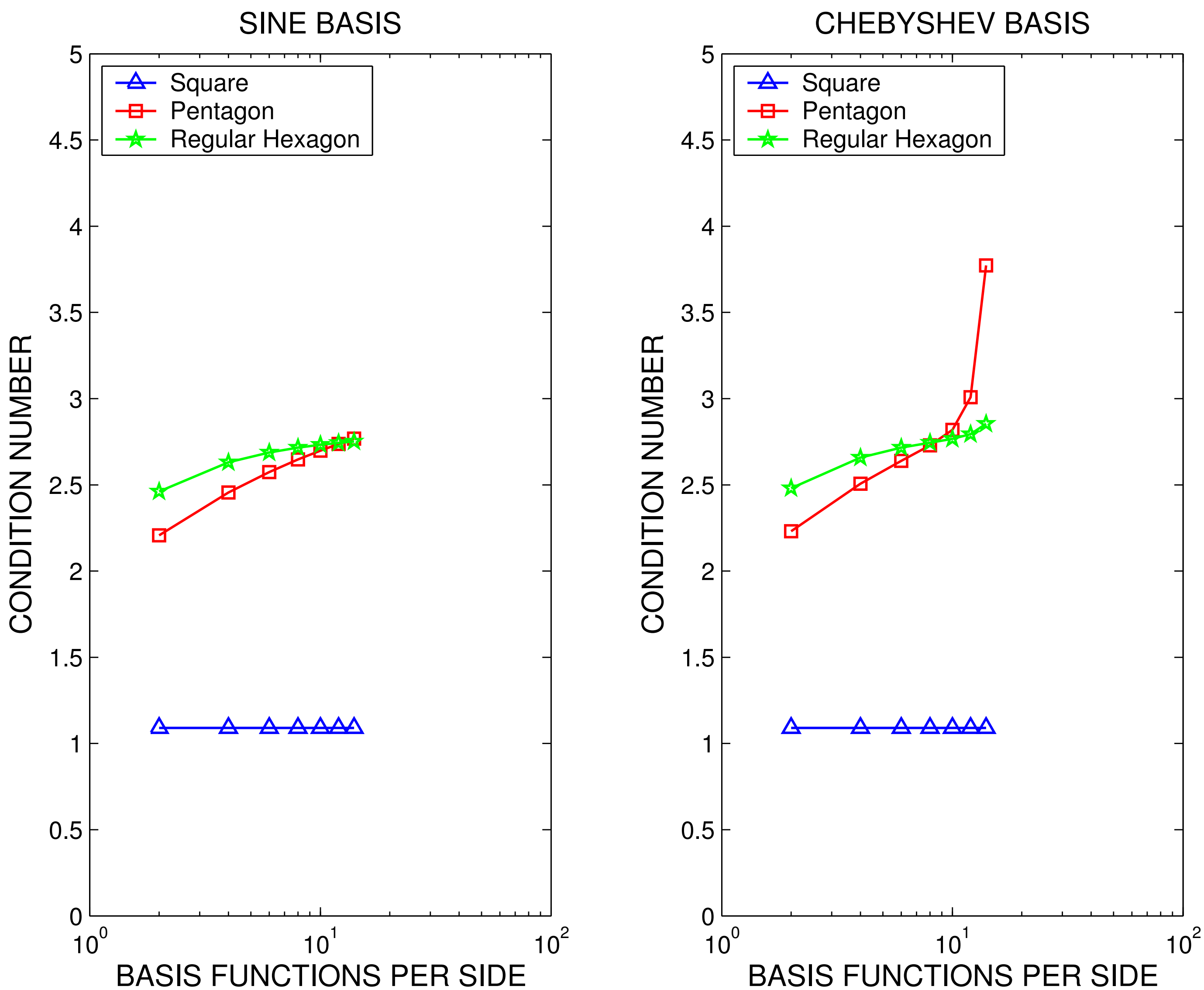


$$\varphi_r(s) = \begin{cases} T_{r+1}\left(\dfrac{s}{\pi}\right) - T_0\left(\dfrac{s}{\pi}\right), & r \text{ odd} \\ T_{r+1}\left(\dfrac{s}{\pi}\right) - T_1\left(\dfrac{s}{\pi}\right), & r \text{ even} \end{cases}$$

Effect of Chebyshev Basis: Errors



Effect of Chebyshev Basis: Condition Number



Spectral Collocation Projections

Collocation Point Values: Let $V = L^2[-\pi,\pi]$ and $k_1,\ldots,k_N \in \mathbb{C}$. Define $\mathcal{C}_N \colon V \to \mathbb{R}^N$ by

$$\mathcal{C}_N(f) = \left[R_1\big(\widehat{f}(k_1)\big),\ldots,R_N\big(\widehat{f}(k_N)\big)\right]^T$$

Spectral Collocation Projection: Let V_N be an N-dimensional subspace of V. Define $\mathcal{P}_N \colon V \to V_N$ as the map which for each $f \in V$ returns $f_N = \mathcal{P}_N f \in V_N$ satisfying the spectral collocation equations

$$\mathcal{C}_N(f_N) = \mathcal{C}_N(f)$$

Note: $\mathcal{P}_N$ is a projection onto V_N iff

$$\forall g \in V_N,\ \mathcal{C}_N(g) = 0 \text{ iff } g = 0$$

Example: Sine Collocation Projection

Notation: Map $s \in [-\pi, \pi]$ to $t \in [0, \pi]$ and use the Fourier sine transform

$$\widetilde{f}(k) := \frac{2}{\pi} \int_0^\pi \sin(kt) f(t)\, dt \qquad (k \in \mathbb{C})$$

Fourier sine series:

$$f(t) = \sum_{l=1}^{\infty} \widetilde{f}_l \sin(lt), \qquad \widetilde{f}_l = \widetilde{f}(l), \quad l \in \mathbb{Z}^+$$

Projection: Define $\mathcal{C}_N(f) = \left[\widetilde{f}_1, \ldots, \widetilde{f}_N\right]^T$ so $f_N = \mathcal{P}_N f$ satisfies

$$\widetilde{f}_N(l) = \widetilde{f}_l, \qquad l = 1, \ldots, N$$

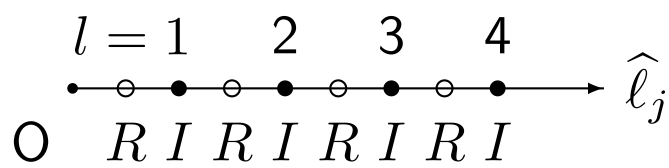
Connection with Fokas Method

Fourier vs. Sine Transforms:

$$\widetilde{f}(l) = \begin{cases} 2(-1)^{(l-1)/2}\,\mathrm{Re}[\widehat{f}(-l/2)], & l \text{ odd}, \\ 2(-1)^{l/2}\,\mathrm{Im}[\widehat{f}(-l/2)], & l \text{ even}. \end{cases}$$

Therefore: **sine collocation projection = collocation at SFFS points**

SFFS points:



Also:

$$f(t) = \sum_{l=1}^{\infty} \widetilde{f}_l \sin(lt) = \sum_{m=1}^{\infty} \left\{ \widehat{f}_m^{C'} \cos\left[(m - \tfrac{1}{2})s\right] + \widehat{f}_m^{S} \sin(ms) \right\}$$

$$= \sum_{m=1}^{\infty} \left\{ \widehat{f}_m^{C'}\,\mathrm{Re}\left[e^{i(m-1/2)s}\right] + \widehat{f}_m^{S}\,\mathrm{Im}\left[e^{ims}\right] \right\}$$

Convergence of Spectral Collocation Projection

Lemma 1. *Let* $\mathcal{P}_N : V \to V_N$ *be a spectral collocation projection, let* $\| \, \|_V$ *denote any norm on* V*, and assume that* $\mathcal{P}_N$ *is bounded in the corresponding operator norm. Then for any* $f \in V$*,*

$$\|f - \mathcal{P}_N f\|_V \leq \left(1 + \|\mathcal{P}_N\|_V\right) \min_{g \in V_N} \|f - g\|_V$$

Lemma 2. *Suppose there exist positive constants* c_1*,* c_2 *such that*

$$\|\mathcal{C}_N f\|_2 \leq c_1 \|f\|_V \quad (\forall f \in V)$$

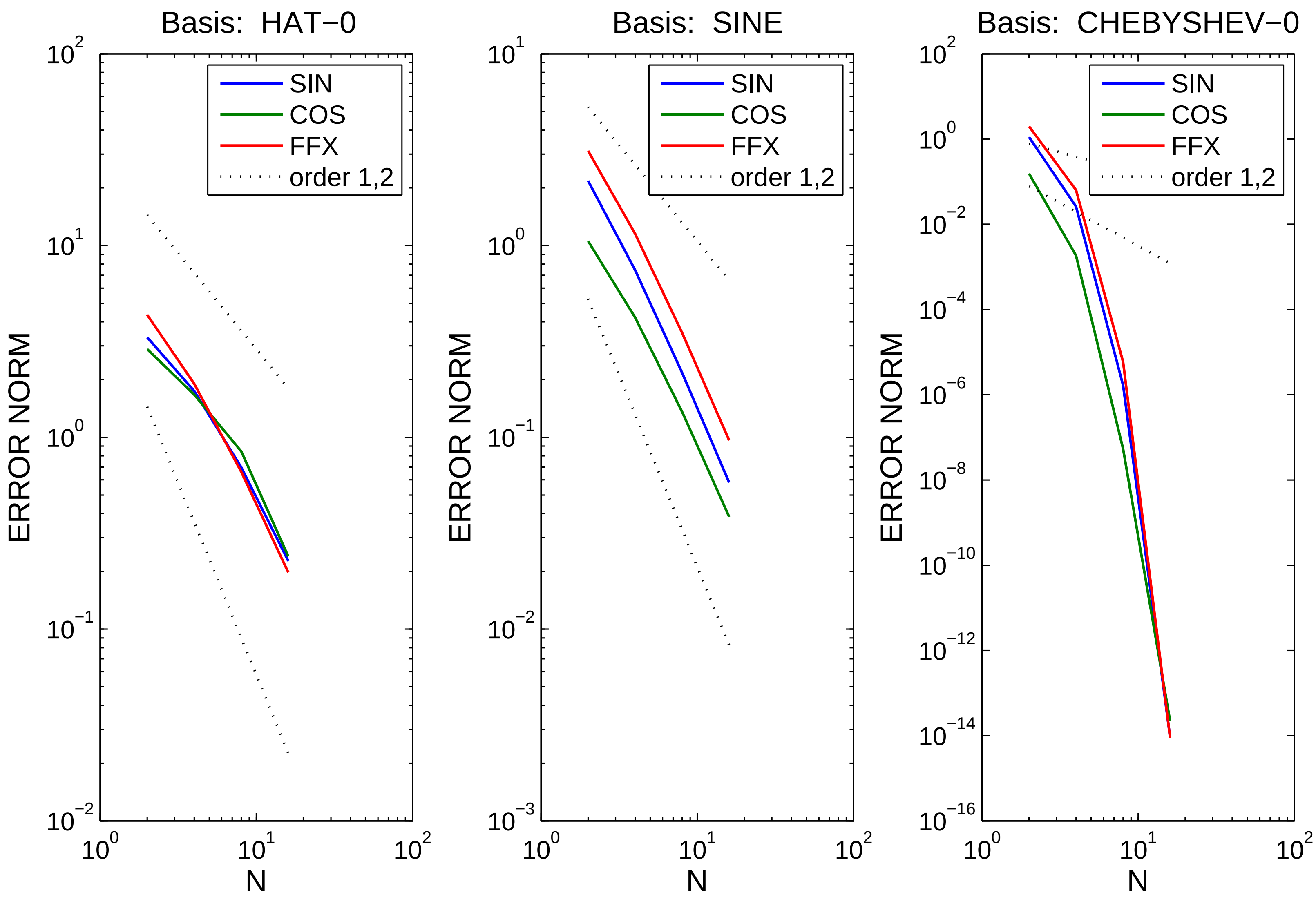
and

$$\|\mathcal{C}_N g\|_2 \geq c_2 \|g\|_V \quad (\forall g \in V_N).$$

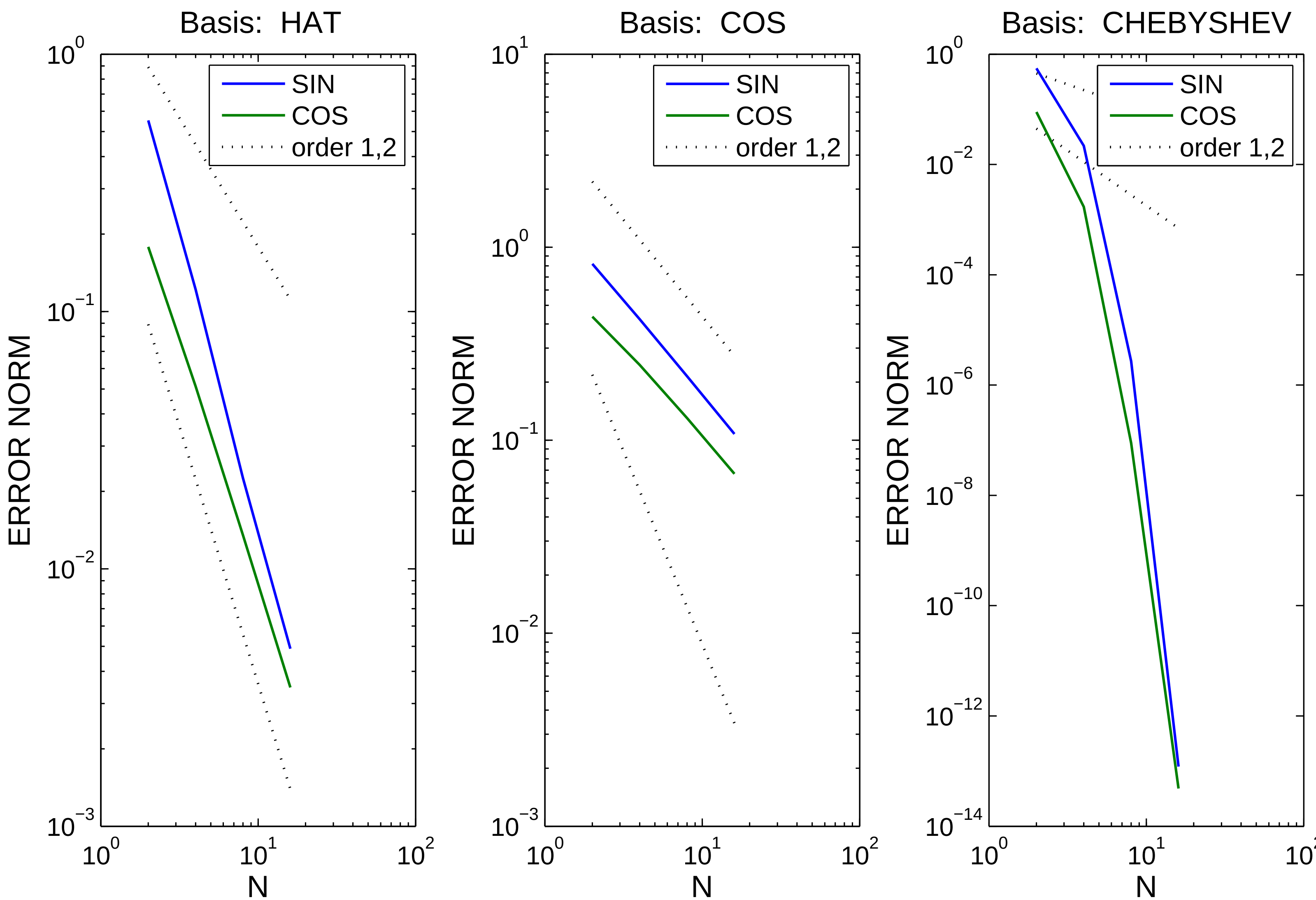
Then $\|\mathcal{P}_N\|_V \leq c_1/c_2$*.*

Result: If c_1 and c_2 are independent of N then the projection converges at the rate determined solely by the approximation properties of the subspace V_N.

Convergence: Zero Endpoint Values



Convergence: Nonzero Endpoint Values



Summary

Keys to the method:

- Global relation is necessary and sufficient
- Solve by collocation at complex k on the appropriate rays

Performance:

- Collocation at sine points gives convergence at rate governed by subspace
- With subspace of polynomials the convergence appears to be exponential

Analysis:

- Spectral collocation projection well understood
- Convergence of method?

Future work:

- Vertex singularities
- Modified Helmholtz
- Biharmonic . . .