High-Level Outline

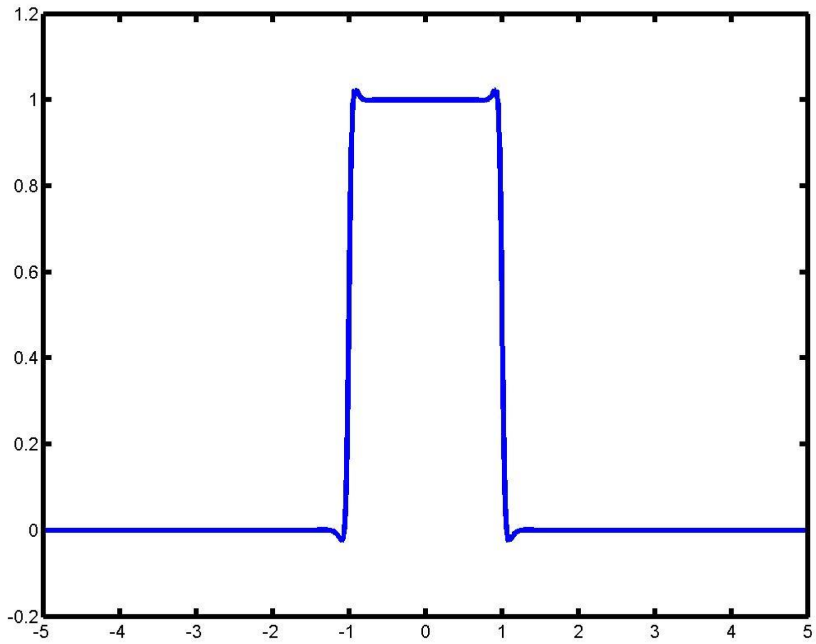
- FEAST as filtered subspace iteration, for Hermitian problems
- FEAST for non-Hermitian problems
- SS method as filtered Krylov subspace method
- Function approximation and computer arithmetic studies related to the filter

Some Function Approximation Connections

The filter function $\rho(\lambda)$ plays a crucial role in convergence, and convergence rate

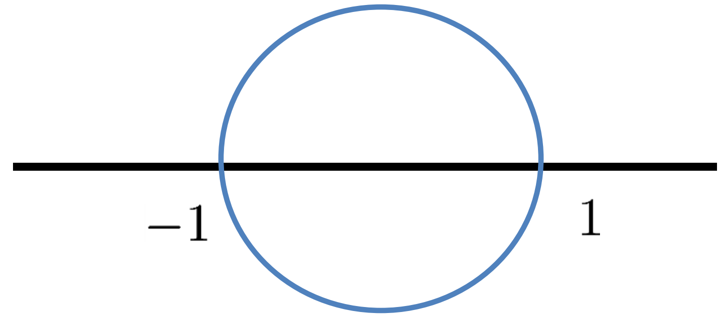
Consider reference case of $\mathcal{I} = [-1, 1]$.

We need $\rho(\lambda)$ big on $\mathcal{I}$
and small on all large $|\lambda|$



Let's examine the construction of a Gaussian based $\rho(\lambda)$ in detail

$$\pi(\mu) = \frac{1}{2\pi\iota} \oint \frac{1}{z-\mu} dz$$



parametrize: for $-1 \leq t \leq 3$

$$\phi(t) = e^{\iota \frac{\pi}{2}(1+t)}, \quad \phi'(t) = \iota \frac{\pi}{2} \phi(t)$$

$$\begin{aligned}
\pi(\mu) &= \frac{1}{2\pi\iota} \int_{-1}^{3} \frac{\phi'(t)}{\phi(t)-\mu} dt \\
&= \frac{1}{2\pi\iota} \int_{-1}^{1} \left[\frac{\phi'(t)}{\phi(t)-\mu} - \frac{\overline{\phi'(t)}}{\overline{\phi(t)}-\mu} \right] dt \\
&= \frac{1}{4} \int_{-1}^{1} \left[\frac{\phi(t)}{\phi(t)-\mu} - \frac{\overline{\phi(t)}}{\overline{\phi(t)}-\mu} \right] dt
\end{aligned}$$

For real μ

$$\pi(\mu) = \frac{1}{2} \int_{-1}^{1} \mathrm{Re} \left(\frac{\phi(t)}{\phi(t)-\mu} \right) dt$$

For Gauss-Legendra rule, (w_k, t_k), $k = 1, 2, \ldots, q$,

$$\begin{aligned}
\pi(\mu) \approx \rho(\mu) &= \frac{1}{2}\sum_{k=1}^{q} w_k \operatorname{Re}\left(\frac{\phi(t_k)}{\phi(t_k)-\mu}\right) \\
&= \frac{1}{2}\sum_{k=1}^{q} w_k \frac{1+\mu s_k}{1+2\mu s_k+\mu^2}, \qquad s_k = \sin(\pi t_k/2).
\end{aligned}$$

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Just by the generic form, can only conclude $\rho(\mu) = O(1/\mu)$,

and not clear at all if $|\mu\rho(\mu)|$ is small for large μ.

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Just by the generic form, can only conclude $\rho(\mu) = O(1/\mu)$,

and not clear at all if $|\mu\rho(\mu)|$ is small for large μ.

While for a finite interval $[-A, A]$ we can examine $\rho(\mu)$ numerically,

we NEED a better justification for $|\mu| > A$.

$$
\begin{aligned}
\pi(\mu) &= \frac{1}{2}\int_{-1}^{1} \mathrm{Re}\left(\frac{\phi(t)}{\phi(t)-\mu}\right) dt \\
&= \frac{1}{2}\int_{-1}^{1} f_\mu(t)dt, \qquad f_\mu(t) = \frac{1}{2}\,\frac{1+\mu\sin(\mu\,t/2)}{1+2\mu\,\sin(\mu\,t/2)+\mu^2}
\end{aligned}
$$

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Standard theory on Gaussian-Legendra quadrature says:

$$\left|\int_{-1}^{1} f_\mu(t)dt - \rho(\mu)\right| = \frac{2^{2q+1}(q!)^4}{(2q+1)((2q!))^2}\,\left|\frac{f_\mu^{(2q)}(t_0)}{(2q)!}\right|$$

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$$

But $\int_{-1}^{1} f_\mu(t)dt = 0$ for $|\mu| > 1$, and thus

$$
\left|\int_{-1}^{1} f_\mu(t)dt - \rho(\mu)\right| = |\rho(\mu)|, \qquad \text{for } |\mu| > 1
$$

Recap: for any $\mu > 1$,

$$|\rho(\mu)| = \frac{2^{2q+1}(q!)^4}{(2q+1)((2q!))^2} \left| \frac{f_\mu^{(2q)}(t_0)}{(2q)!} \right|, \qquad \text{for some } t_0 \in (-1,1)$$

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One can construct a function $\xi_q(\mu)$ such that

- $\xi_q(\mu) \geq \dfrac{2^{2q+1}(q!)^4}{(2q+1)((2q!))^2} \max\limits_{t\in[-1,1]} \left| \dfrac{f_\mu^{(2q)}(t)}{(2q)!} \right|$

- $\xi_q(\mu)$ is decreasing for $\mu > 1$

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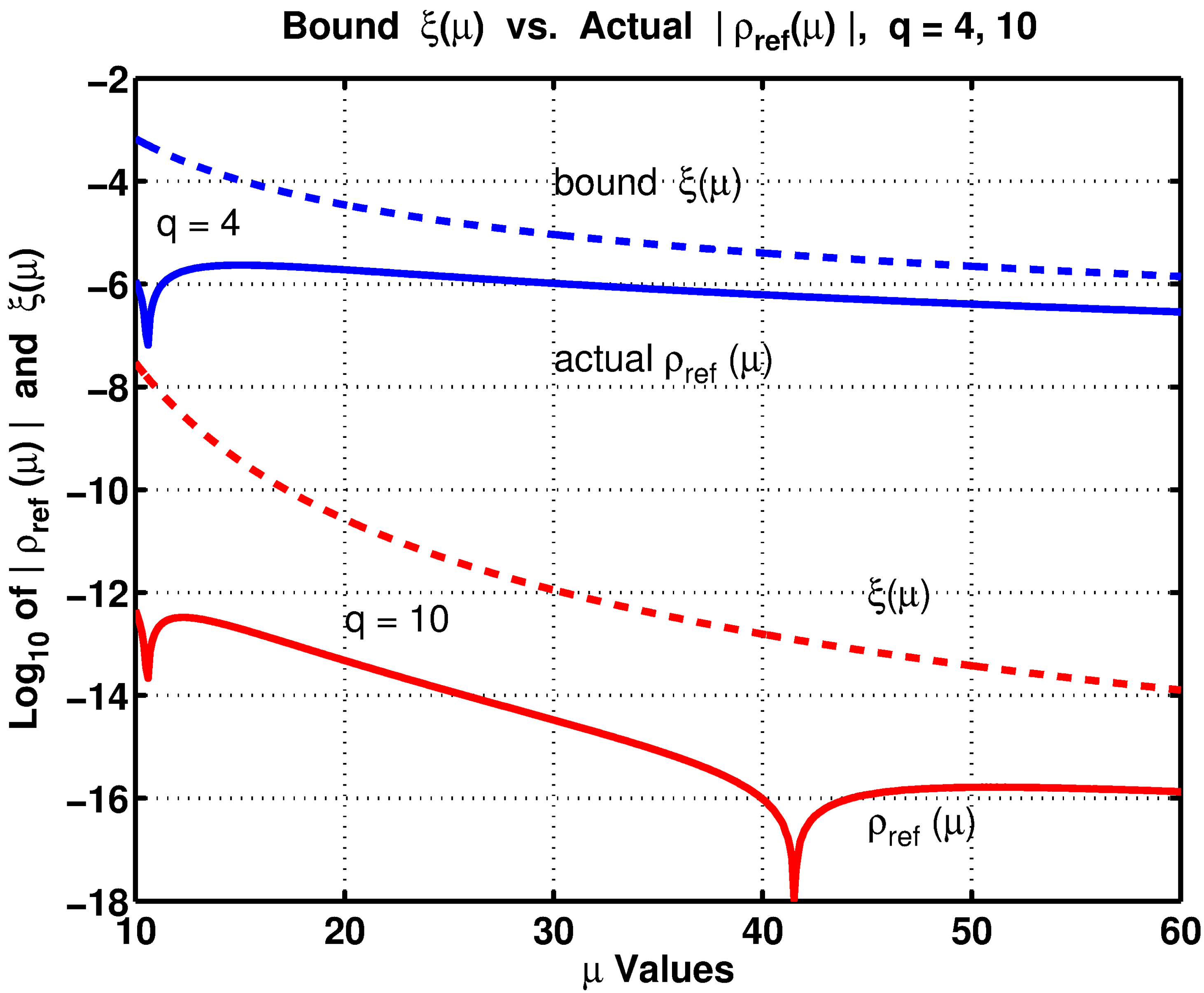
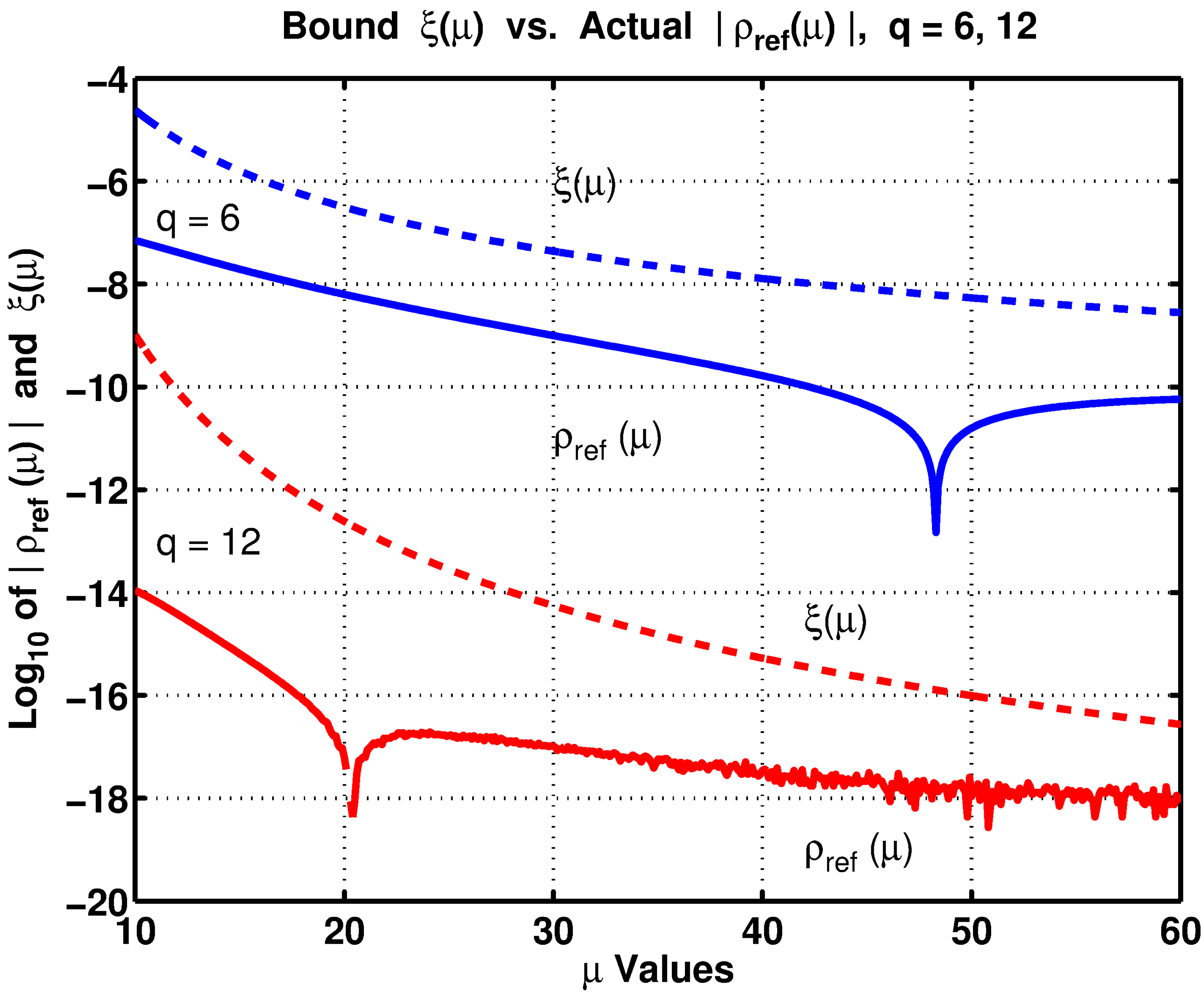
- $\xi_q(\mu)$ is decreasing for $\mu > 1$

Thus, evaluation $\xi_q(A)$ at a single point A gives a bound on $|\rho(\mu)|$ for all $\mu \geq A$.

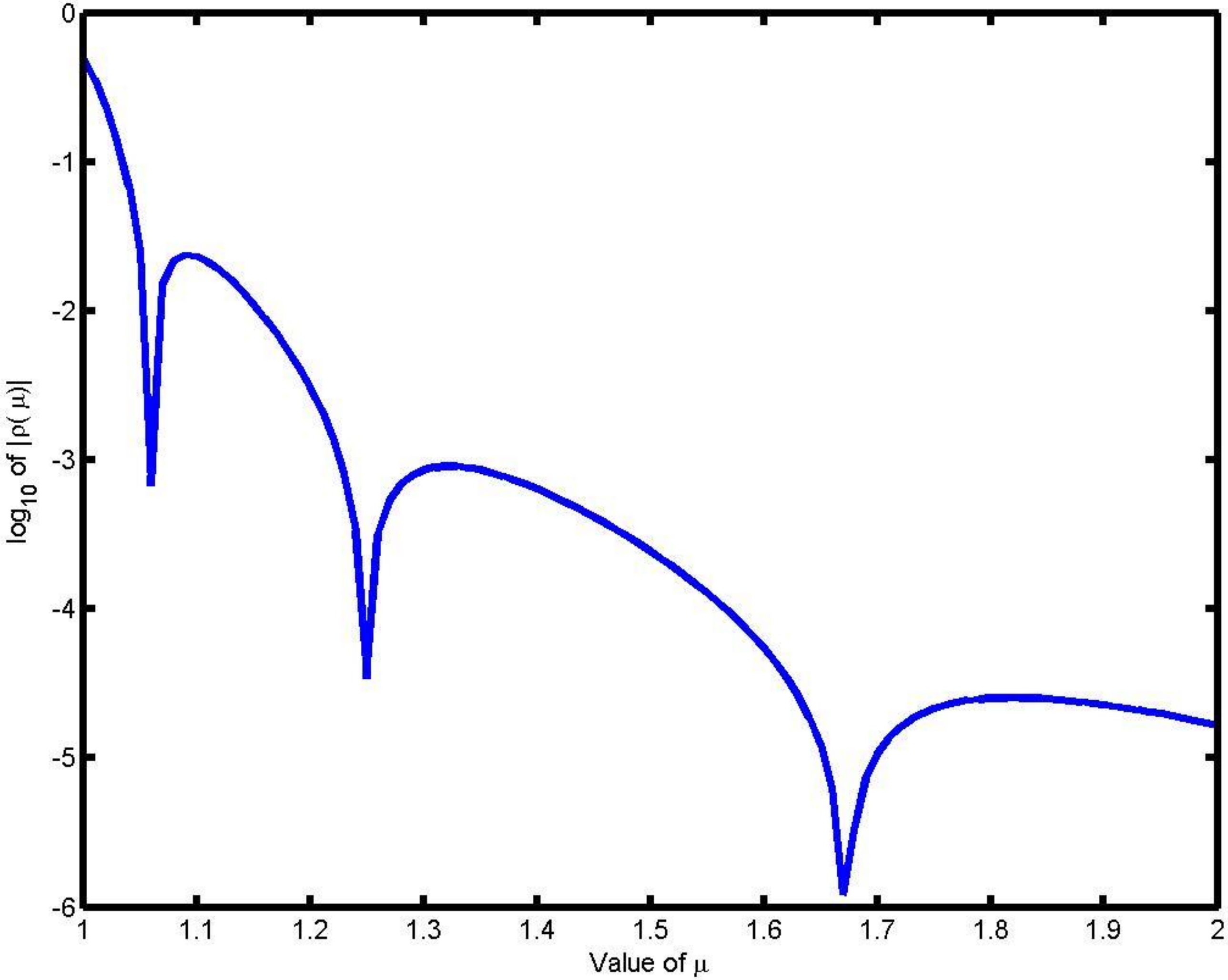


Bound ξ(μ) vs. Actual | ρref(μ) |, q = 4, 10
bound ξ(μ)
q = 4
actual ρref (μ)
ξ(μ)
q = 10
ρref (μ)
−2
−4
−6
−8
−10
−12
−14
−16
−18
10
20
30
40
50
60
μ Values
Log10 of | ρref (μ) | and ξ(μ)


Bound ξ(μ) vs. Actual | ρref(μ) |, q = 6, 12
Log10 of | ρref (μ) | and ξ(μ)
μ Values
q = 6
q = 12
ξ(μ)
ρref (μ)
ξ(μ)
ρref (μ)
−4
−6
−8
−10
−12
−14
−16
−18
−20
10
20
30
40
50
60

Formal-verification based method is an alternative (dormant work that can use help to revive).

$\rho(\mu)$ is a rational function, no poles. Can use FV to enumerate all local min/max.



0
-1
-2
-3
-4
-5
-6
1
1.1
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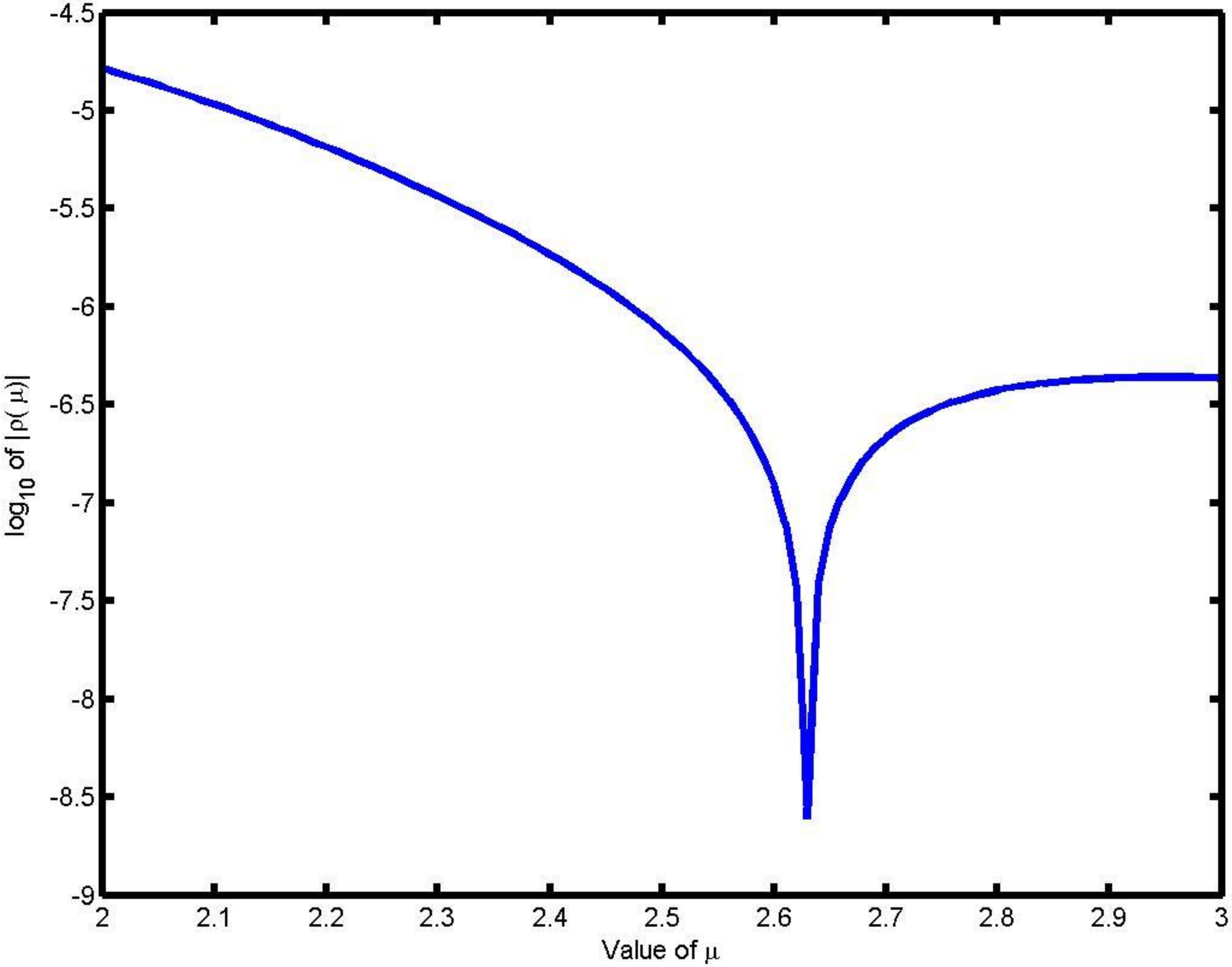
1.4
1.5
1.6
1.7
1.8
1.9
2
log10 of |ρ(μ)|
Value of μ



-4.5
-5
-5.5
-6
-6.5
-7
-7.5
-8
-8.5
-9
$\log_{10}$ of $|\rho(\mu)|$
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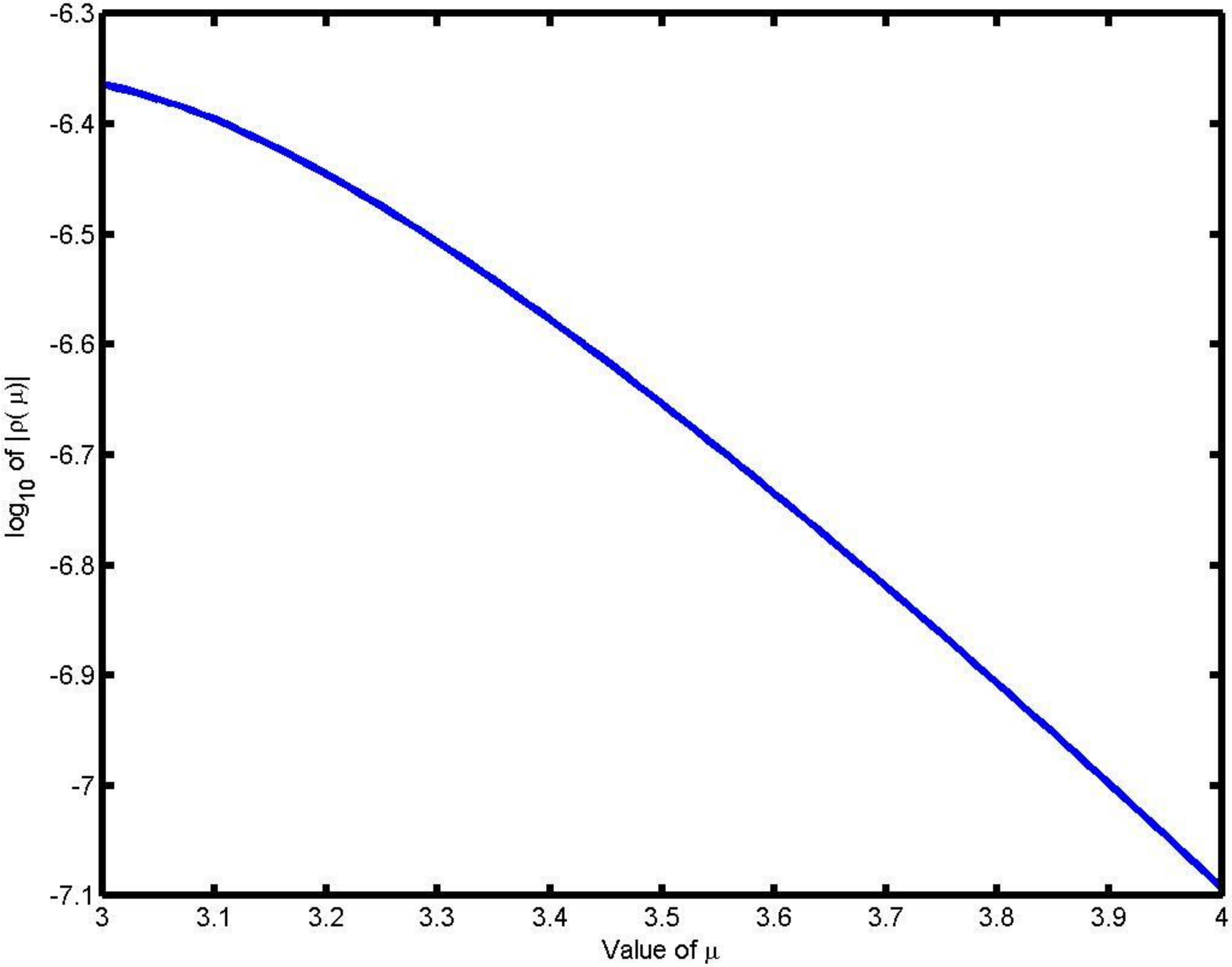
2.1
2.2
2.3
2.4
2.5
2.6
2.7
2.8
2.9
3
Value of μ


-6.3
-6.4
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-6.6
-6.7
-6.8
-6.9
-7
-7.1
log10 of |ρ(μ)|
3
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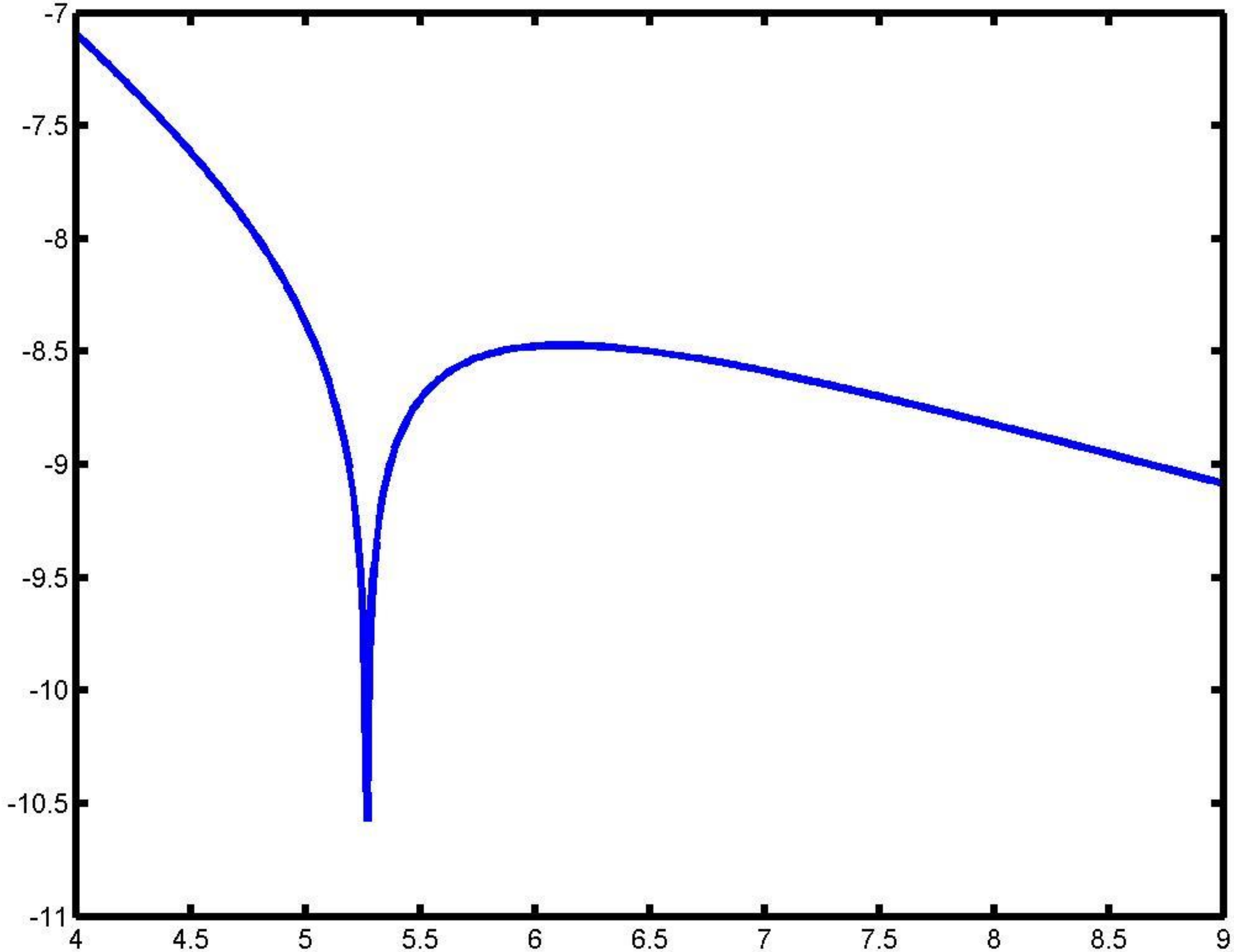
3.8
3.9
4
Value of μ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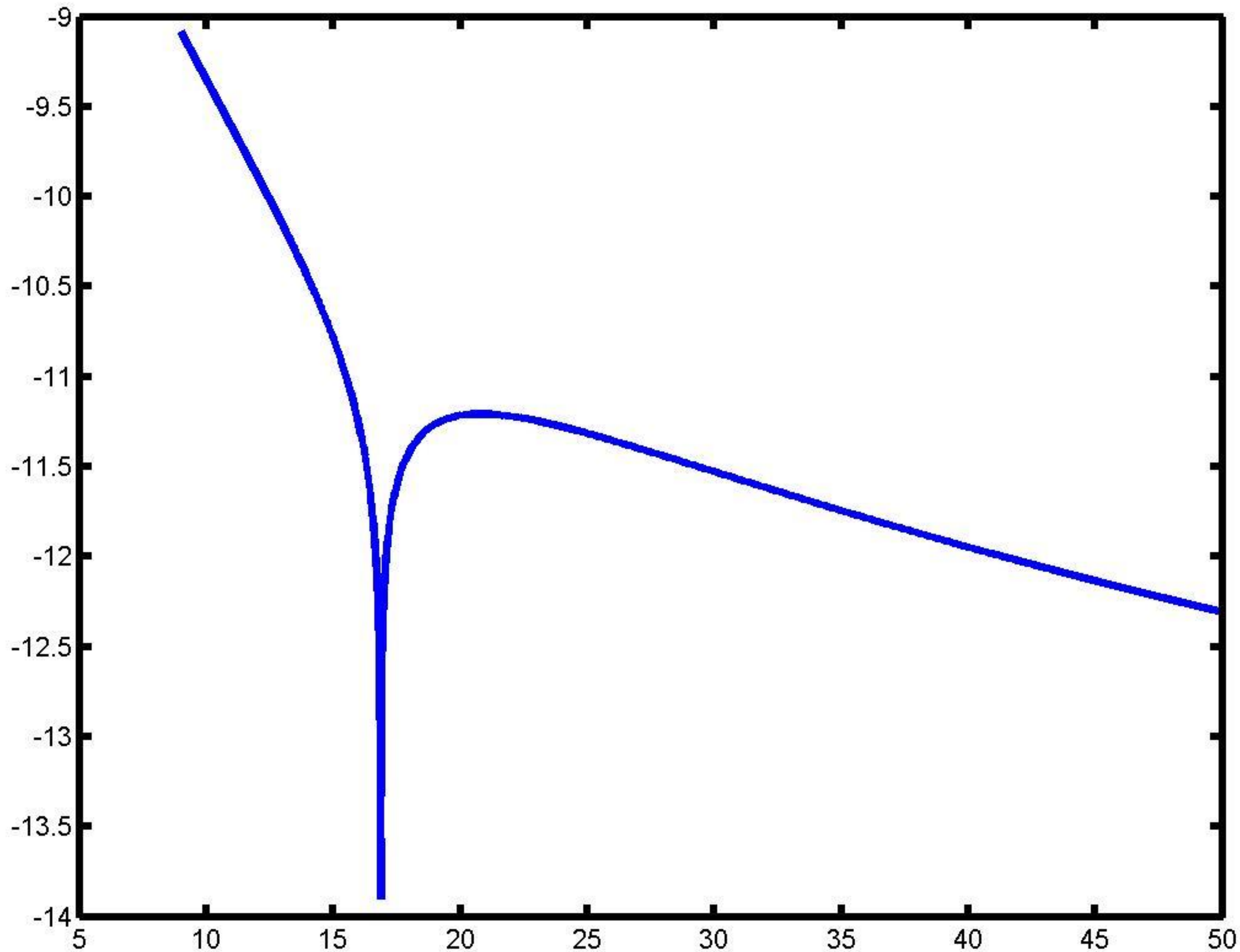
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Some Computer Arithmetic Connections

For Gauss-Legendra rule, (w_k, t_k), $k = 1, 2, \ldots, q$,

$$\pi(\mu) \approx \rho(\mu) = \frac{1}{2}\sum_{k=1}^{q} w_k \,\mathrm{Re}\left(\frac{\phi(t_k)}{\phi(t_k) - \mu}\right) \qquad s_k = \sin(\pi t_k/2).$$

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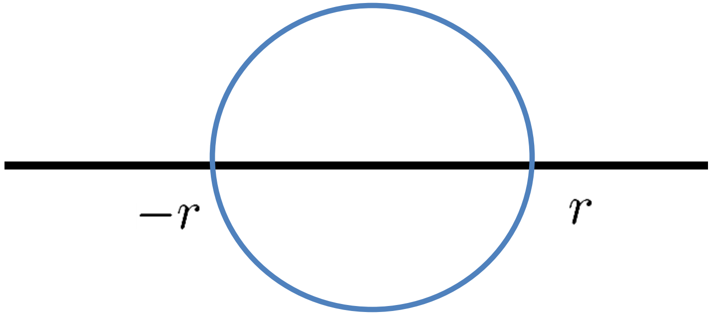

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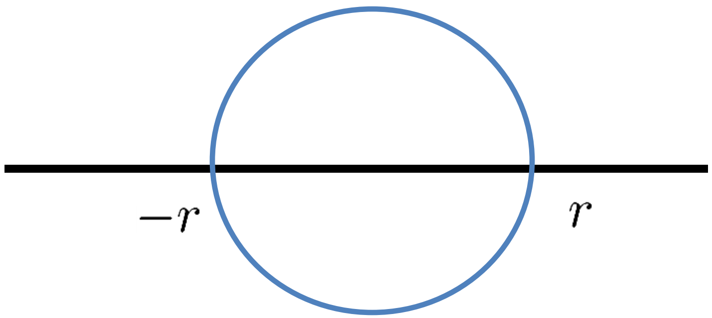
Let $(\lambda, \mathbf{x})$ be an eigenpair for A: $A\mathbf{x} = \lambda\mathbf{x}$

If computed exactly, $\rho(A)\mathbf{x} = \rho(\lambda)\mathbf{x}$



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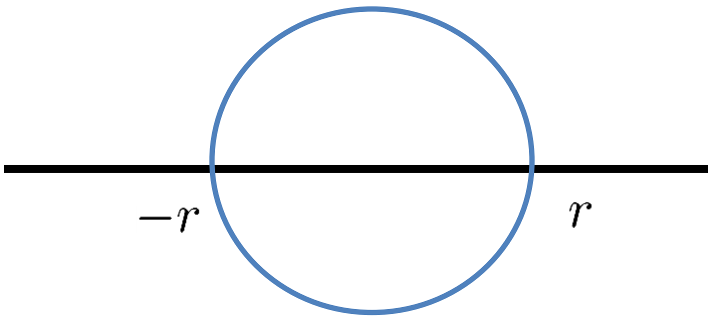

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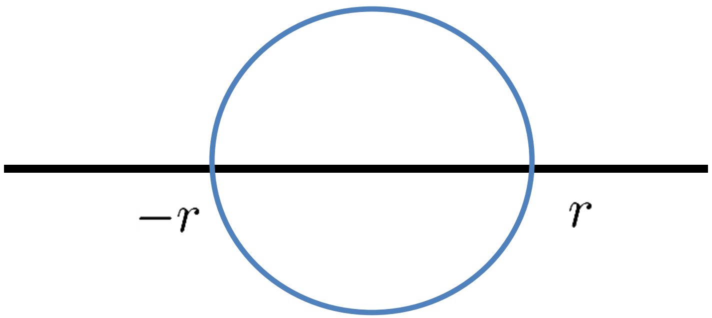

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$$\sum_{k=1}^{q} w_k \phi(t_k)\,\mathbf{x}_k \quad \text{vs} \quad \sum_{k=1}^{q} w_k \phi(t_k)\,\hat{\mathbf{x}}_k$$

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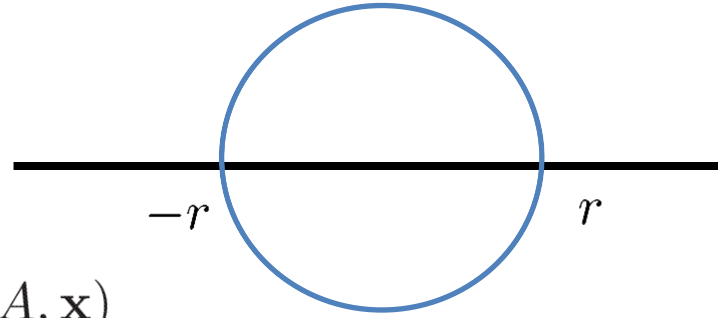

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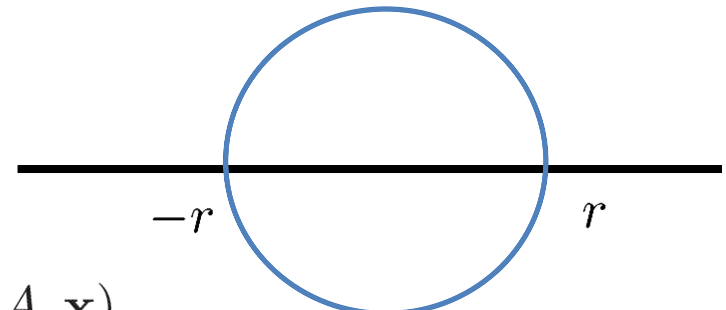

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$$\hat{\mathbf{x}}_k = \mathbf{x}_k + \Delta_k,$$

$$\|\Delta_k\| = O(u \, \kappa(A_k) \|\mathbf{x}_k\|), \quad A_k = \phi(t_k) I - A$$

$$\mathbf{x}_k = \mathbf{x} / (\phi(t_k) - \lambda)$$

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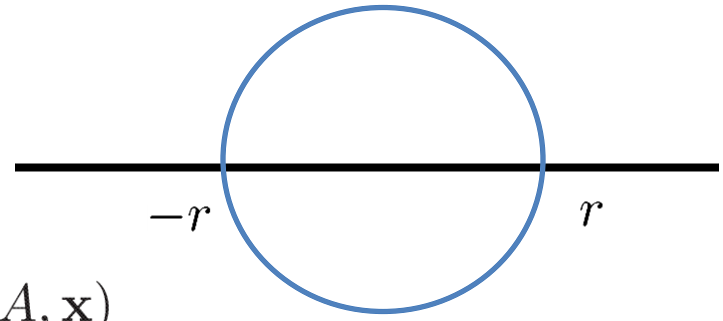

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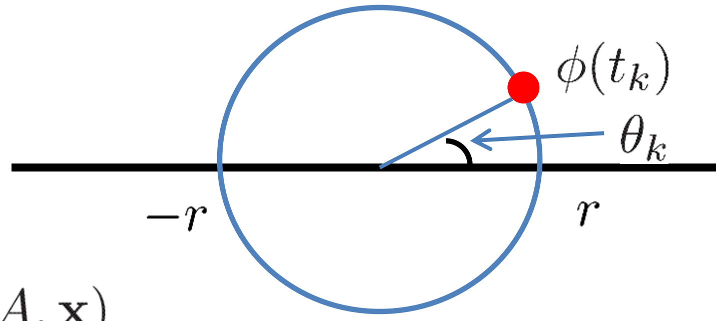

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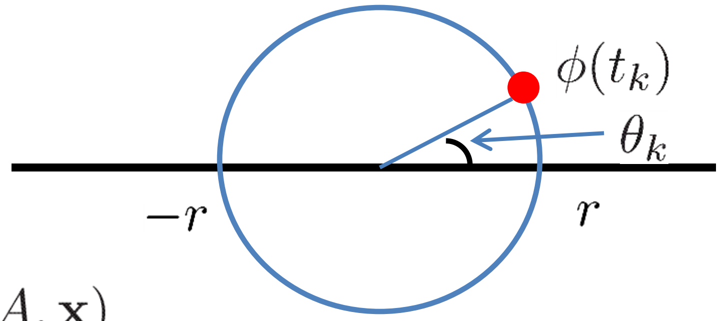
$$\|\Delta_k\| = O\left(\frac{u}{r^2 \sin^2(\theta_k)}\right)$$

$$\|\text{error}\| \le \sum_k r w_k \|\Delta_k\| = O\left(\frac{u}{r}\right) \sum_k \frac{w_k}{\sin^2(\theta_k)}$$

Some Computer Arithmetic Connections



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$$\|\Delta_k\| = O\left(\frac{u}{r^2 \sin^2(\theta_k)}\right)$$

Determined by quadrature rule.
For Gauss, 8-node, this is ≤ 60

$$\|\text{error}\| \leq \sum_k r w_k \|\Delta_k\| = O\left(\frac{u}{r}\right) \sum_k \frac{w_k}{\sin^2(\theta_k)}$$

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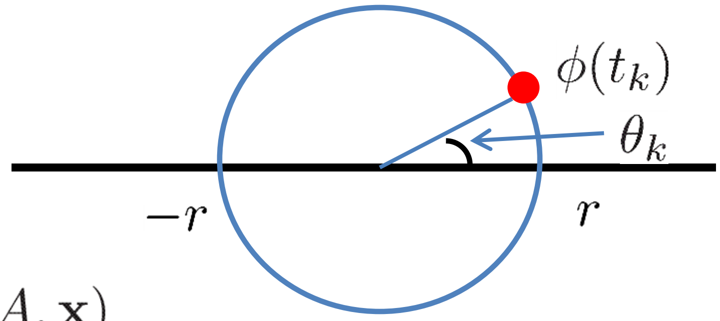

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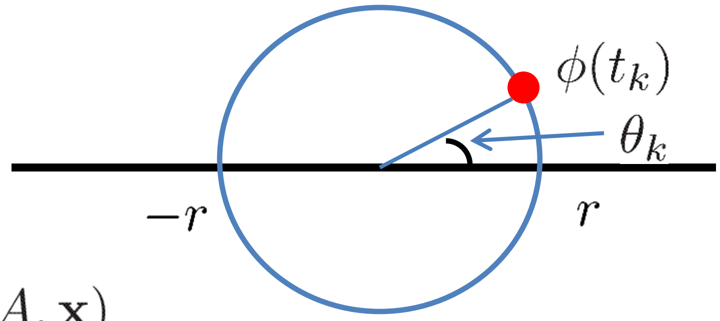
Iterative refinement (for higher accuracy) relies critically on accurate residual:

$$\text{residual vector} = \mathbf{x} - A_k \hat{\mathbf{x}}_k = \mathbf{x} - (\phi(t_k)\hat{\mathbf{x}}_k - A_k \hat{\mathbf{x}}_k)$$

Some Computer Arithmetic Connections

$$\sum_{k=1}^{q} w_k \phi(t_k)\, \mathbf{x}_k \quad \text{vs} \quad \sum_{k=1}^{q} w_k \phi(t_k)\, \hat{\mathbf{x}}_k$$



$$(\phi(t_k)I - A)\mathbf{x}_k = \mathbf{x}; \quad \hat{\mathbf{x}}_k = \text{Solve}(\phi(t_k)I - A, \mathbf{x})$$

$$\hat{\mathbf{x}}_k = \mathbf{x}_k + \Delta_k,$$

$$\|\text{error}\| \leq \sum_k r w_k \|\Delta_k\| = O\left(\frac{u}{r}\right) \sum_k \frac{w_k}{\sin^2(\theta_k)}$$

Iterative refinement (for higher accuracy) relies critically on accurate residual:

$$\text{residual vector} = \mathbf{x} - A_k\hat{\mathbf{x}}_k = \mathbf{x} - (\phi(t_k)\hat{\mathbf{x}}_k - A_k\hat{\mathbf{x}}_k)$$

Can use various computer arithmetic technique such as two-sum and error-free transformation (e.g. Rump's method)

Concluding Remarks

- Integral-based methods and approximate spectral projectors are very useful tools.
- They can be used in different contexts: subspace iterations, Krylov methods, spectrum estimation (not covered), and more.
- Sakurai and collaborators proposed SS method 2003; Polizzi proposed FEAST 2008.
- Tang/Polizzi published detail analysis on FEAST 2014.
- Intel Math Kernel Library has incorporated in it a FEAST-based eigensolver.
- Many problems need to be solved still; do jump in!
- Will include more references in posted material.