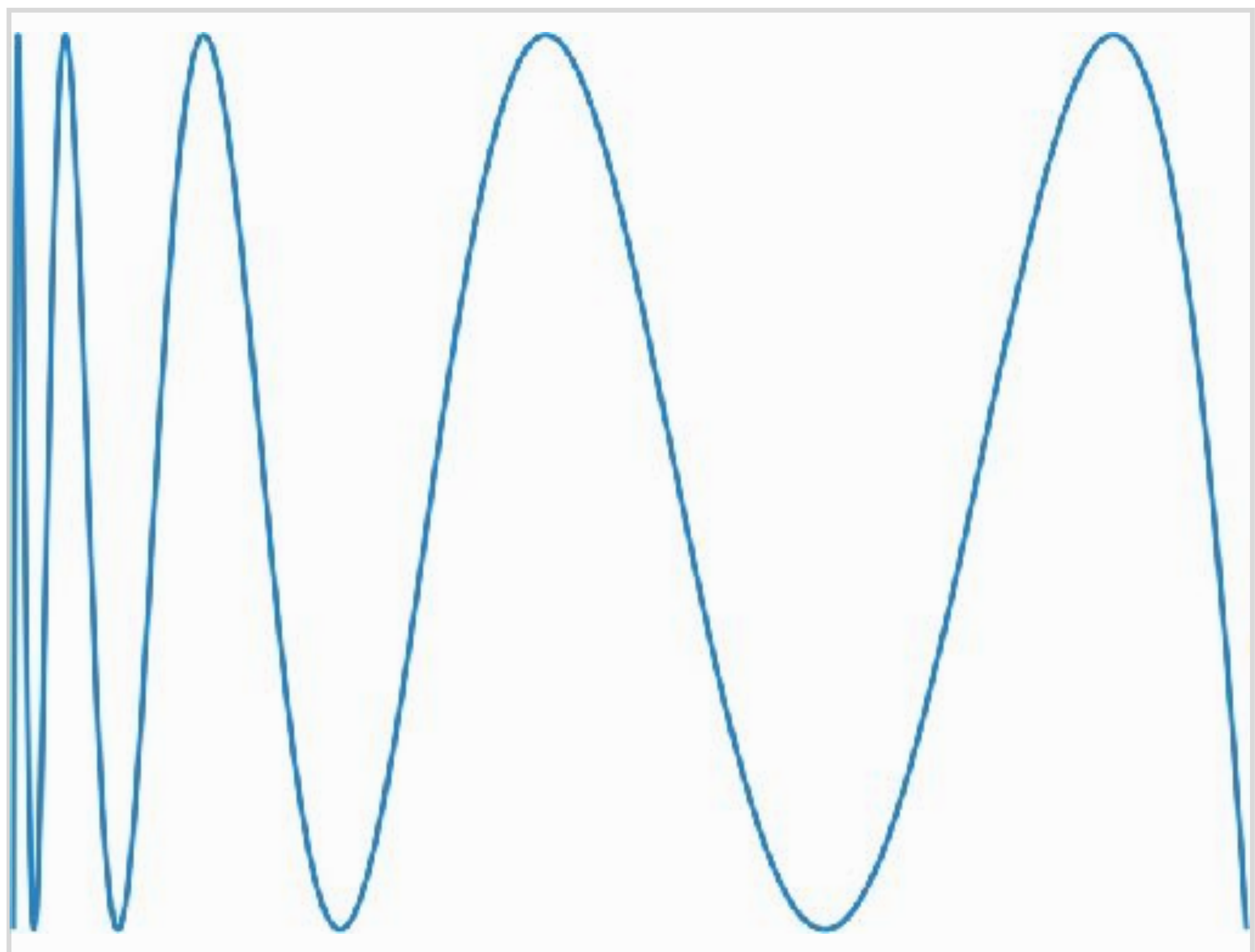
Connections in rational approximation, potential theory and numerical linear algebra



Rational approximation in numerical linear algebra

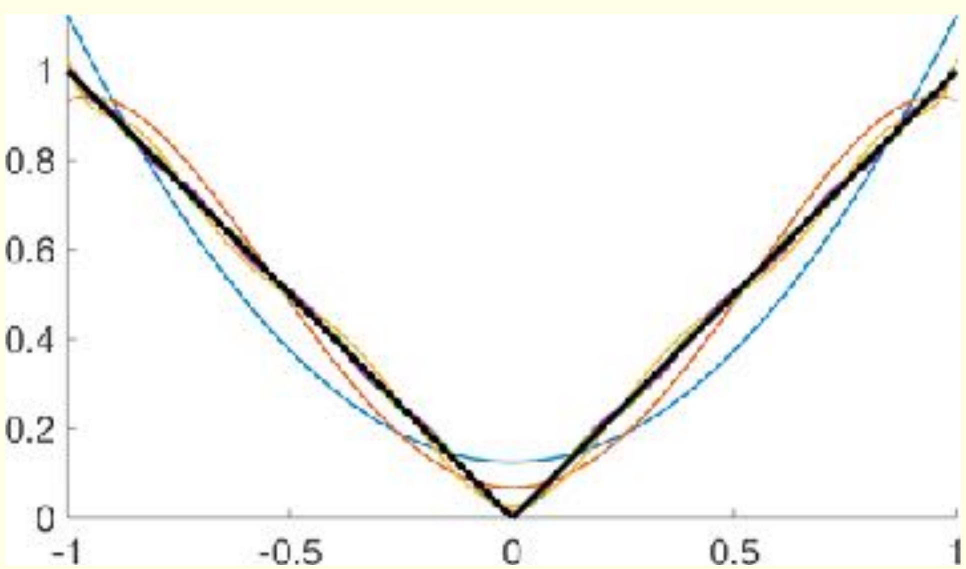
function approximation

$f(x) = |x| \qquad x \in [-1, 1]$

$f(x) = \sqrt{x} \qquad x \in [0, 1]$

$$\|f - p_n(x)\| = \mathcal{O}\left(\frac{1}{n}\right)$$

$$\|f - r_{n,n}(x)\| = \mathcal{O}(e^{-\sqrt{n}})$$



$$f(A) \approx r_{n,n}(A)$$

Sylvester matrix equation

$$AX - XB = F$$

ADI

Rational Krylov Subspace Method

Exponential sum approximations

Characteristic function approximations/filtering

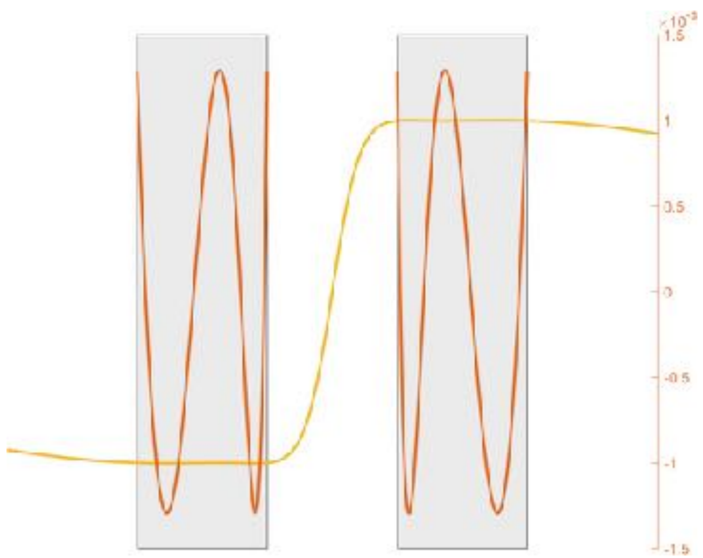
Quadrature formulas

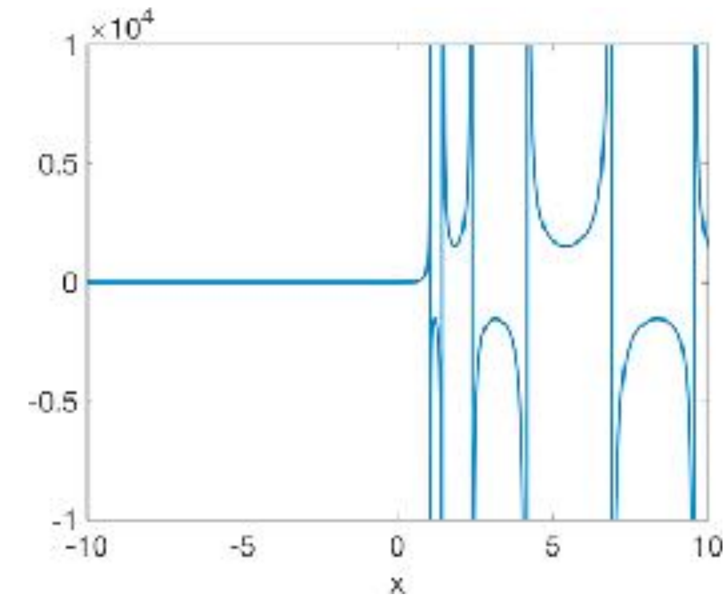
Polar decomposition

Many more...

(see Trefethen, Approx. Theory and Practice. Ch 23)

Two rational approximation problems and one electrostatics problem

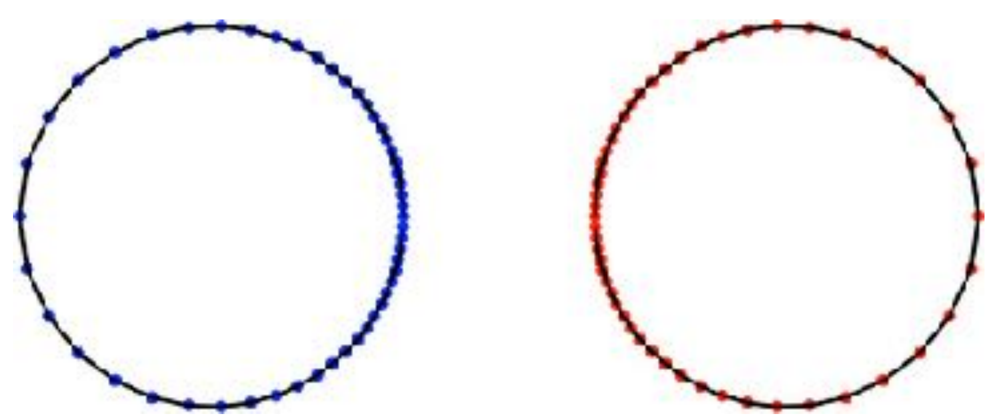




The polar decomposition

Solving the Sylvester matrix equation

The capacity of a condenser



Logarithmic potential and rational functions

$$p(z) = \prod_{j=0}^{n} (z - z_j)$$

$$\frac{-\log|p(z)|}{n+1} = \int \log \frac{1}{|z-t|} \mathrm{d}\nu_{n+1}(t)$$

$\nu_{n+1}(t)$ is the normalized discrete measure with mass 1 at each zero z_j

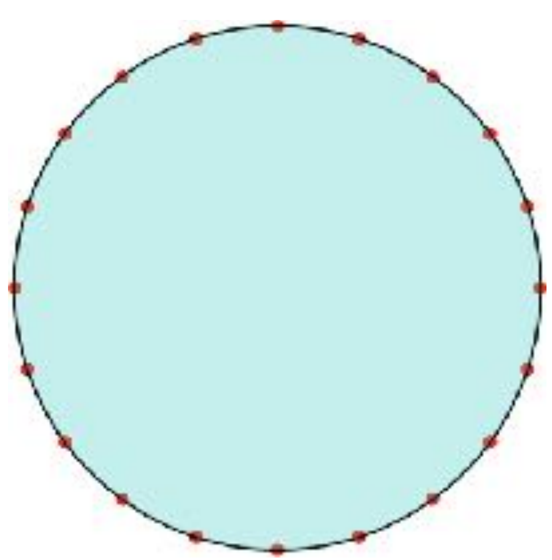
$$r(z) = \frac{p(z)}{q(z)}$$

$$\frac{-\log|r(z)|}{n+1} = \int \log \frac{1}{|z-t|} \mathrm{d}\mu_1(t) - \int \log \frac{1}{|z-t|} \mathrm{d}\mu_2(t)$$

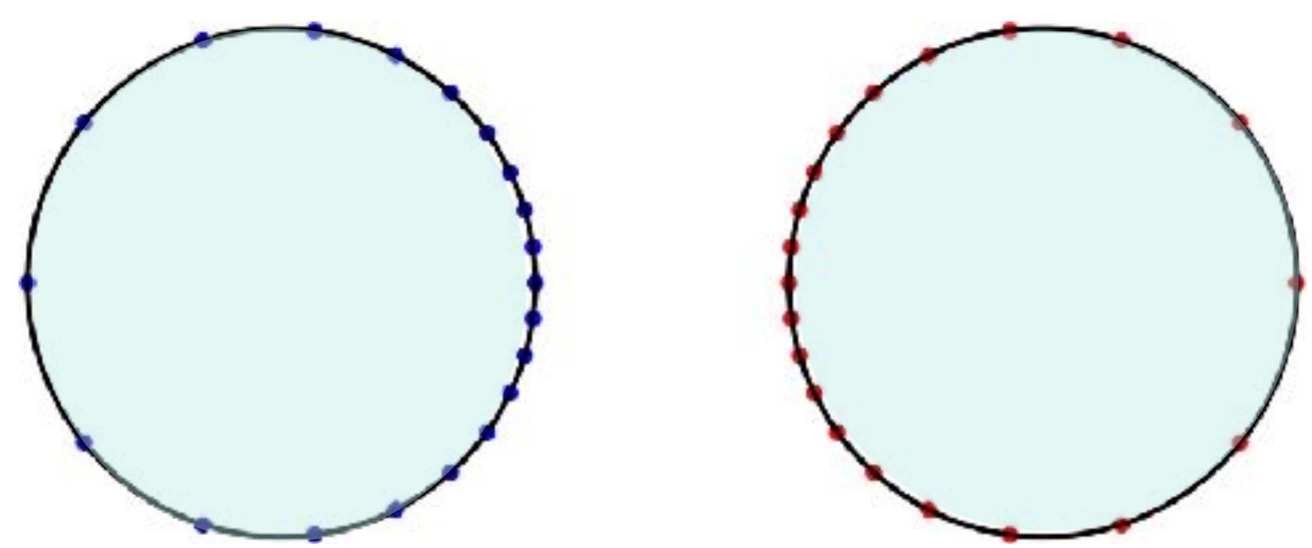
Signed measure: $\mu = \mu_1 - \mu_2$

$$\frac{-\log|r(z)|}{n+1} = \int \log \frac{1}{|z-t|} \mathrm{d}\mu(t)$$

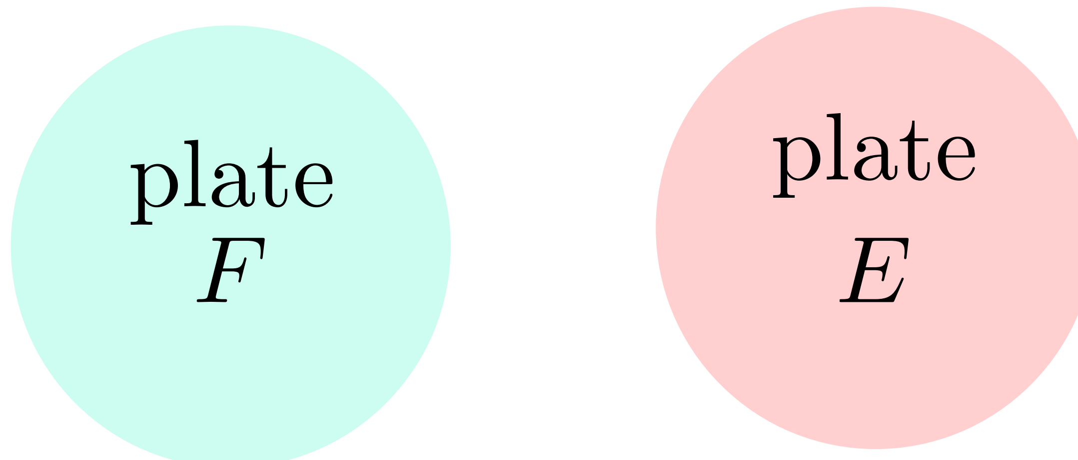
Polynomial



Rational function



the electrostatics problem



the condenser (E, F)

$$\mu = \mu_1 - \mu_2, \quad \mu_1, \mu_2 \in \mathcal{M}^+, \quad \operatorname{supp}(\mu_1) = E, \quad \operatorname{supp}(\mu_2) = F$$

$$U^\mu(z) = \int \log \frac{1}{|z-t|} \, \mathrm{d}\mu(t)$$ logarithmic potential

$$I(\mu) = \int \int \log \frac{1}{|z-t|} \, \mathrm{d}\mu(z) \mathrm{d}\mu(t)$$ logarithmic energy

$V(E, F) = \inf_\mu \{I(\mu)\}$

$\operatorname{cap}(E, F) = 1/V(E, F)$

condenser capacity

the electrostatics problem

Results from Saff, Totik, Ch. 8 "Logarithmic Potential with External Fields":

A unique signed measure $\mu^* = \mu_E^* - \mu_F^*$ exists such that $I(\mu^*) = V(E,F)$.

$U^{\mu^*} = c_1, \quad z \in E$ $\qquad\qquad V(E,F) = c_1 + c_2$

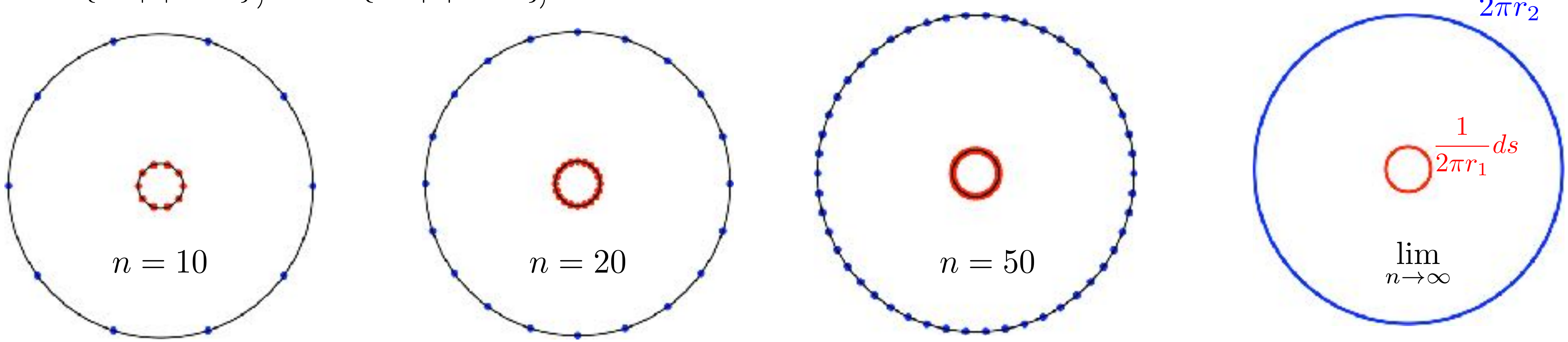
$U^{\mu^*} = c_2, \quad z \in F$ $\qquad\qquad V(E,F) = V(\partial E, \partial F)$

A sequence of normalized, discrete measures $\{\mu_n\}$ exist such that $\mu_n \to \mu^*$.

These measures are associated with the rational Fekete points $\{(z_k^{(E,n)}, z_k^{(F,n)}\}_{k=1}^n$.

<u>Example</u>

$E := \{z : |z| = r_1\}$, $F := \{z : |z| = r_2\}$, $\quad r_1 < r_2$



$$U^{\mu^*}(z) = \begin{cases} 0, & |z| > r_2, \\ \log(r_2/|z|), & r_1 \le |z| \le r_2, \\ \log(r_2/r_1), & |z| < r_1. \end{cases}$$

$$\mathrm{cap}(E,F) = 1/\log\frac{r_2}{r_1}$$

the electrostatics problem

Can we solve the electrostatics problem for $E = [a, b]$, $F = [-b, -a]$?

We consider the following result:

Let $r_n(z)$ be a rational function $p(z)/q(z)$, where $p, q \in \mathcal{P}^n$.

$$\lim_{n\to\infty} Z_n(E,F)^{1/n} = \exp\left(-1/\mathrm{cap}(E,F)\right), \text{ Then,}$$

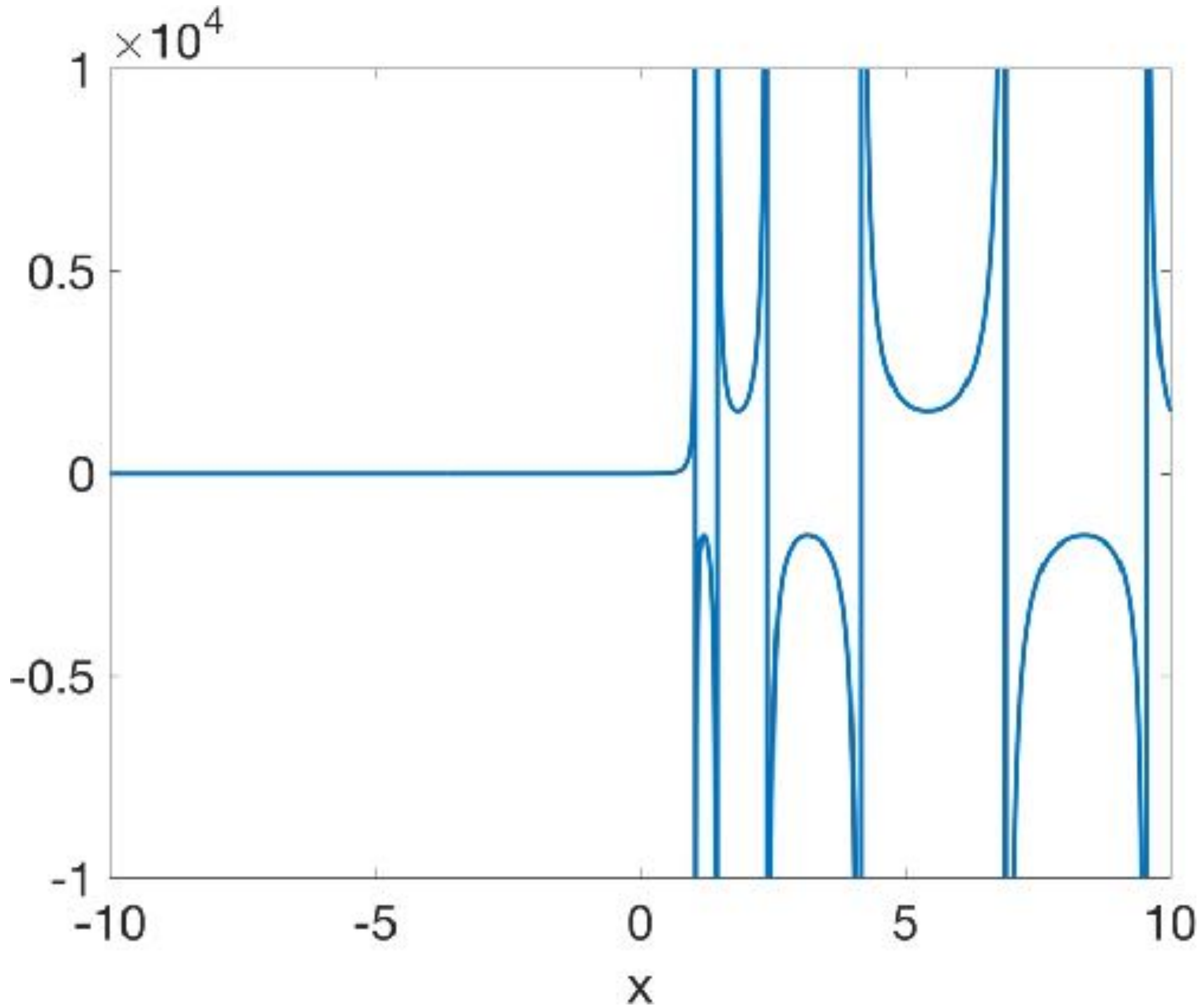
where $Z_k(E,F) = \inf\limits_{\deg(r)\leq n} \left\{ \frac{\sup_{z\in E} |r(z)|}{\inf_{z\in F} |r(z)|} \right\}.$

The condenser capacity appears in the limit of a rational approximation problem.

A rational approximation problem

$$Z_k(E,F) = \inf_{\deg(r)\le n} \left\{ \frac{\sup_{z\in E}|r(z)|}{\inf_{z\in F}|r(z)|} \right\}$$

Find the extremal rational function $r^*(x)$ that is as small as possible on a set E and satisfies $|r^*(z)| > 1$ on a set F.



(code from RKtoolbox for MATLAB) source : http://guettel.com/rktoolbox/examples/html/example_zolotarev.html (written by AT)

Solving the electrostatic problem with rational approximation

$$Z_k(E,F) = \inf_{\deg(r)\leq n} \left\{ \frac{\sup_{z\in E}|r(z)|}{\inf_{z\in F}|r(z)|} \right\}$$

Find the extremal rational function $r^*(x)$ that is as small as possible on a set E and satisfies $|r^*(z)| > 1$ on a set F.

For $E=[a,b]$, $F=[-b,-a]$, this problem is solved completely.

Yegor Ivanovich Zolotarev (1847-1879)

$$\rho^{-2n} \leq Z_n(E,F) \leq 4\rho^{-2n}, \text{ where } \rho = \exp\left(\frac{\pi^2}{2\mu_r(a/b)}\right) \leq \exp\left(\frac{\pi^2}{2\log(4b/a)}\right)$$

Since $\lim_{n\to\infty} Z_n(E,F)^{1/n} = \exp\left(-1/\mathrm{cap}(E,F)\right),$

$$\mathrm{cap}(E,F) = \frac{\mu_r(a/b)}{\pi^2}$$

An application in numerical linear algebra

Sylvester matrix equation

$$AX - XB = F$$

$$X = ZDY^*$$
$$F = MN^*$$

The ADI iteration:

1. Solve for $X^{(j+1/2)}$, where
$$(A - \beta_{j+1} I)\, X^{(j+1/2)} = X^{(j)}\, (B - \beta_{j+1} I) + F. \tag{1}$$

2. Solve for $X^{(j+1)}$, where
$$X^{(j+1)}\, (B - \alpha_{j+1} I) = (A - \alpha_{j+1} I)\, X^{(j+1/2)} - F. \tag{2}$$

Let $X^{(0)} = 0$. For k iterations, I need shift parameters $\{(\alpha_j, \beta_j)\}_{j=1}^{k}$.

$$X^{(k)} = Z^{(k)} D^{(k)} Y^{(k)^*}$$

An application in numerical linear algebra

$$AX - XB = F$$

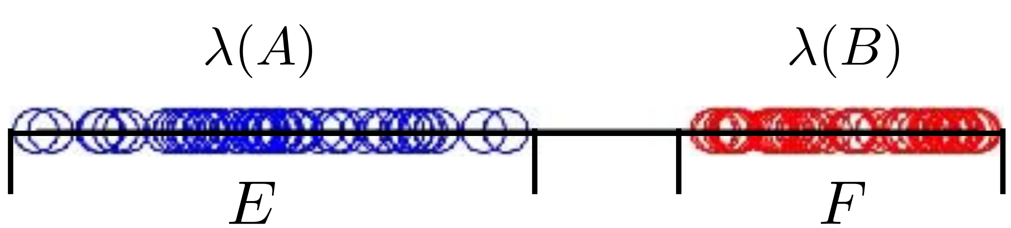
Let $X^{(0)} = 0$. For k iterations, I need shift parameters $\{(\alpha_j, \beta_j)\}_{j=1}^{k}$.

$$X^{(k)} = Z^{(k)} D^{(k)} {Y^{(k)}}^{*}$$

The ADI error equation:

$$X - X^{(k)} = r_k(A)(X - X_0) r_k(B)^{-1}, \qquad r_k(z) = \prod_{j=1}^{k} \frac{(z - \alpha_j)}{(z - \beta_j)}.$$

$$\|X - X^{(k)}\|_2 \le \|r_k(A)\|_2 \, \|r_k(B)^{-1}\|_2 \|X\|_2 \ \le \sup_{z \in \lambda(A)} |r_k(z)| \sup_{z \in \lambda(B)} \frac{1}{|r_k(z)|} \ = \frac{\sup_{z \in \lambda(A)} |r_k(z)|}{\inf_{z \in \lambda(B)} |r_k(z)|}$$

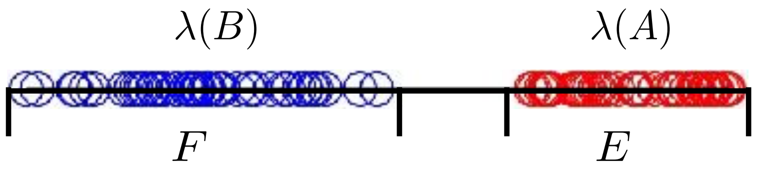


$$Z_k(E, F) = \inf_{\deg(r) \le k} \left\{ \frac{\sup_{z \in E} |r(z)|}{\inf_{z \in F} |r(z)|} \right\}$$

$$\|X - X^{(k)}\|_2 \le Z_k(E, F) \|X\|_2 \le 4 \exp\left(\frac{-2k}{\mathrm{cap}(E, F)} \right) \|X\|_2 \quad \le 4 \exp\left(\frac{\pi^2}{2 \log(4b/a)} \right)^{-2k} \|X\|_2$$

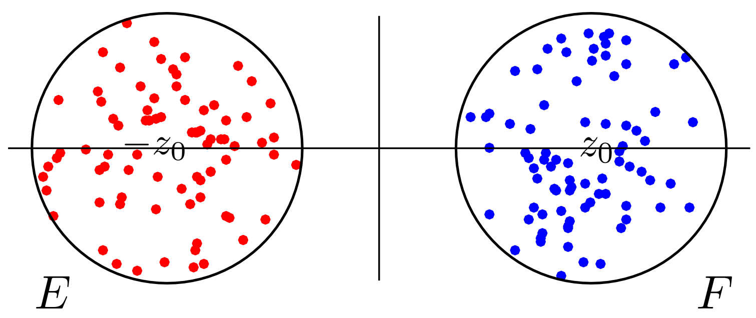
$$k = 2 \left\lceil \frac{1}{\pi^2} \log(4b/a) \log(4/\varepsilon) \right\rceil$$

An application in numerical linear algebra



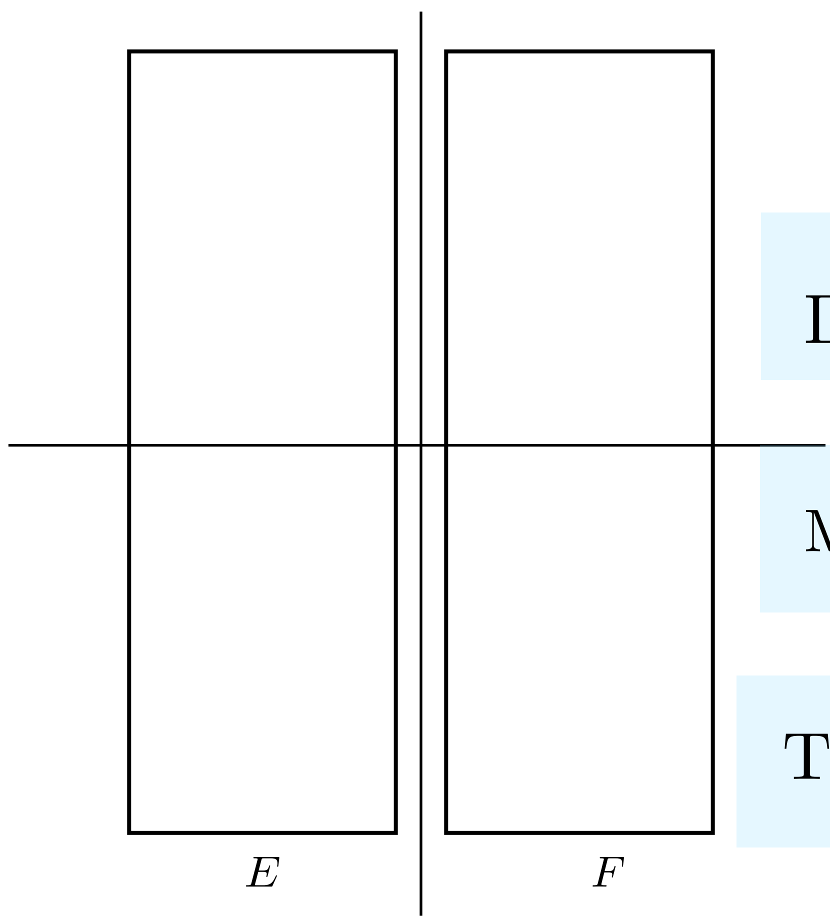
$$Z_k(E,F) \leq 4\exp\left(\frac{-2k}{\mathrm{cap}(E,F)}\right)$$

$r_k^*(z)$ computed via elliptic function



$$Z_k(E,F) = \exp\left(-k/\mathrm{cap}(E,F)\right)$$

$$r_k^*(z) = \left(\frac{z-\phi}{z+\phi}\right)^k, \quad \phi = \sqrt{z_0^2 - \eta^2}$$



$$Z_k(E,F) = ?$$

$$r_k^*(z) = ?$$

Develop a heuristic shift selection strategy.

Monitor ADI error.

The electrostatics problem can inform our shift selection.

An application in numerical linear algebra

From electrostatics, we know that

$$\lim_{n\to\infty} Z_n(E,F)^{1/n} = \exp\left(-1/\mathrm{cap}(E,F)\right),$$

But we also know much more!

$V(E,F) = I(\mu^*)$
$\mathrm{cap}(E,F) = 1/V(E,F)$

A sequence of normalized, discrete measures $\{\mu_n\}$ exist such that $\mu_n \to \mu^*$.

These measures are associated with the rational Fekete points $\{(z_k^{(E,n)}, z_k^{(F,n)}\}_{k=1}^n$.

These points define a rational Fekete polynomial, $\tilde{r}_n(z) = \dfrac{\prod_{k=1}^n z - z_k^{(E,n)}}{\prod_{=1}^n z - z_k^{(F,n)}}$,

$$\text{satisfying } \lim_{n\to\infty}\left(\frac{\sup_{z\in E}|\tilde{r}_n(z)|}{\inf_{z\in F}|\tilde{r}_n(z)|}\right)^{1/n} = \exp(-1/\mathrm{cap}(E,F))$$

Fekete points (rational functions) are said to be asymptotically optimal w.r.t. to the "Zolotarev problem".

The shift parameters $\{(z_k^{(E_n)}, z_k^{(F,n)}\}$ are a "good" suboptimal choice for ADI.

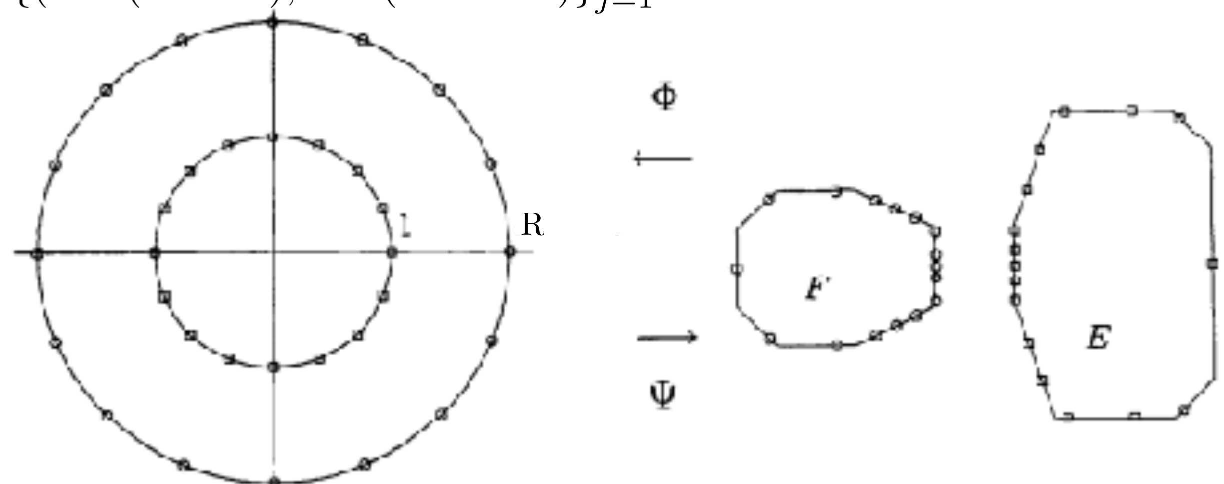
An application in numerical linear algebra

If $\tilde{r}_n(z) = \dfrac{\prod_{j=1}^n z-\alpha_j}{\prod_{j=1}^n z-\beta_j}$ and $\lim_{n\to\infty}\left(\dfrac{\sup_{z\in E}|\tilde{r}(z)|}{\inf_{z\in F}|\tilde{r}(z)|}\right)^{1/n} = \exp(-1/\mathrm{cap}(E,F))$, the shift parameter sets $S_n = \{(\alpha_j,\beta_j)\}_{j=1}^n$ are said to be asymptotically optimal.

Fekete points: generally hard to compute.

Walsh points: If $(E\cup F)^c = G$ is doubly-connected, then a conformal mapping Φ exists such that $\Phi : G \to D$, where $D(R) := \{z : 1 \le |z| \le R\}$, $R > 1$.

Construct conformal mapping $\Phi : (E\cup F)^c \to D$, $S_n = \{(\Phi^{-1}(e^{2\pi ij/n}), \Phi^{-1}(Re^{2\pi ij/n})\}_{j=1}^n$.



(from Starke, G, "Fejer-Walsh points for rational functions and their use in the ADI iterative method.")

Leja-Bagby points: Choose α_1 and β_1 in E, F, respectively. Setting $r_j(z) = \prod_{k=1}^j \dfrac{z-\alpha_k}{z-\beta_k}$,

$(\alpha_{j+1},\beta_{j+1})$ must satisfy $\max_{z\in E}|r_j(z)| = |r_{j+1}(\alpha_{j+1})|$ and $\min_{z\in F}|r_j(z)| = |r_{j+1}(\beta_{j+1})|$

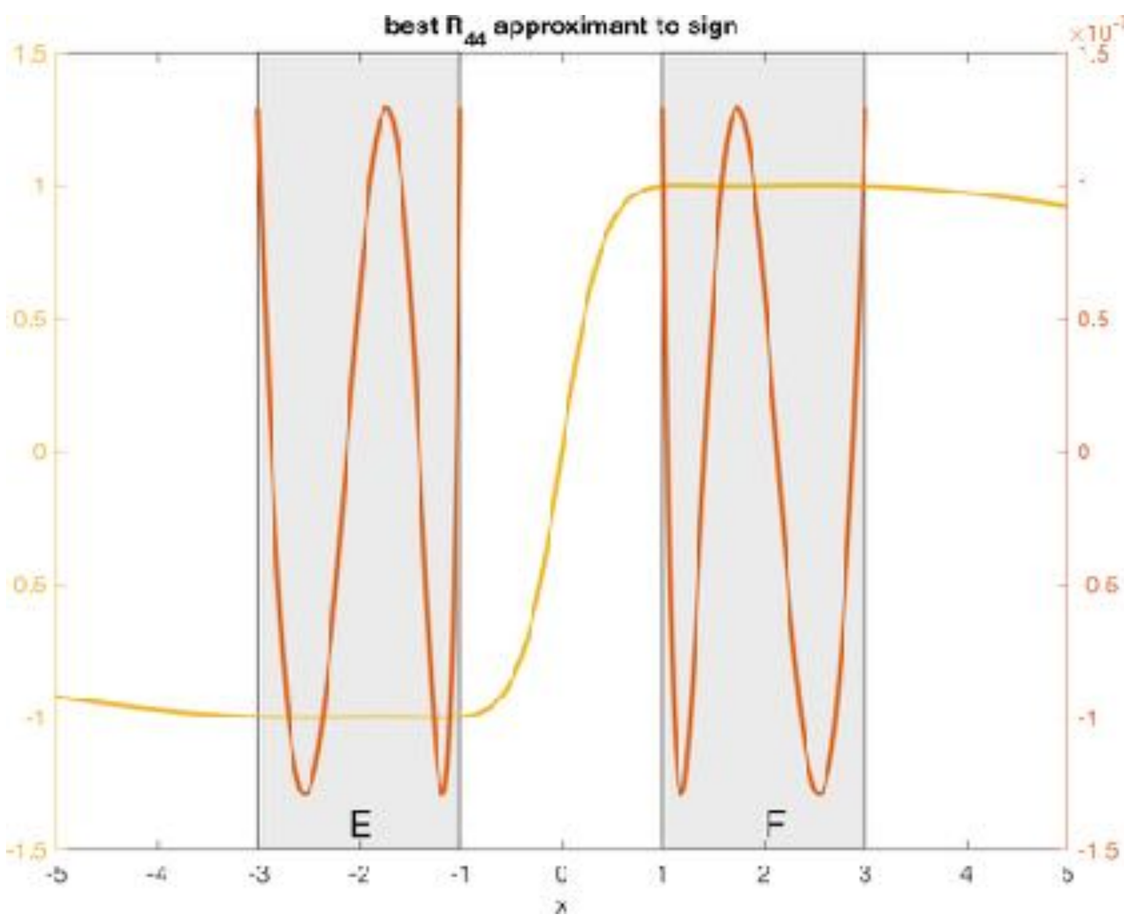
(A very involved proof of asymptotic optimality in T. Bagby, "On interpolation by rational functions.")

These results are also relevant to the Rational Krylov subspace projection method. (See Druskin, Knizhnerman, and Simoncini, "Analysis of the rational Krylov subspace and ADI methods for solving the Lyapunov equation.")

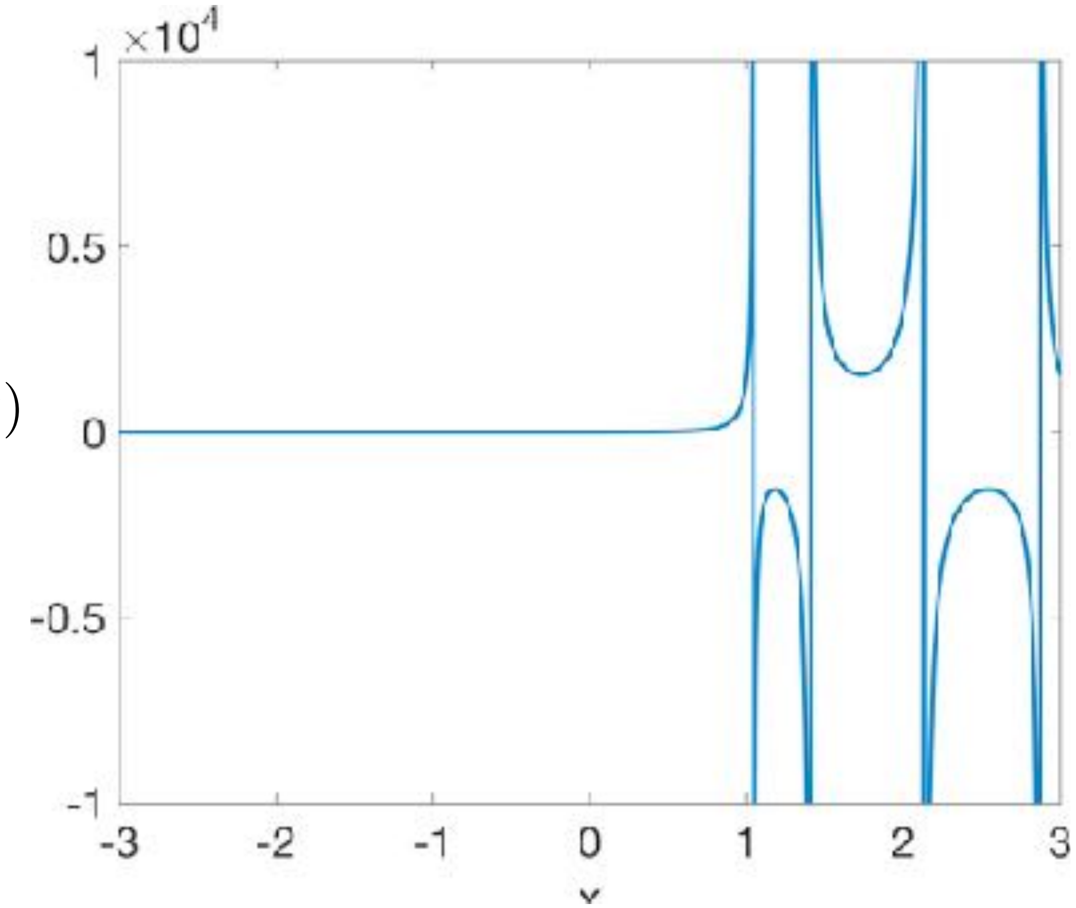
A second rational approximation problem

Given E and F, find $r_n^*(z)$ such that $\|r_n(z) - \text{sgn}(z)\|_{L^\infty(E \cup F)}$ is minimized,

$$\text{where} \quad \text{sgn}(z) = \begin{cases} 1, & z \in E, \\ -1, & z \in F. \end{cases}$$



$T(r_n^*(z)) = \tilde{r}_n(z)$



This problem is "equivalent" to the problem of finding $Z_k(E,F)$.

(See Saff and Totik (Ch. 8), Akhieser,, and Istace and Thiran)

Example: For $E = [a,b]$, $F = [-b,-a]$, $\quad \|r_n^*(z) - \text{sgn}(z)\|_{L^\infty(E \cup F)} = \dfrac{2\sqrt{Z_n(E,F)}}{1 + Z_n(E,F)}$

$$\|r_n^*(z) - \text{sgn}(z)\|_{L^\infty(E \cup F)} \le 4\exp(-n/\text{cap}(E,F))$$