On stability of extrapolation of complex electromagnetic permittivity functions

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Joint work with Narek Hovesepyan

Herglotz-Nevanlinna Theory Applied to Passive Causal and Active Systems

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An EM wave in a dielectric

$\boldsymbol{E}(t)$ — applied field, $\boldsymbol{P}(t)$ — polarization field

Causal impulse response function

$$\boldsymbol{P}(t) = \int_{-\infty}^{+\infty} \chi(t-\tau)\boldsymbol{E}(\tau)d\tau, \qquad \chi(s) = 0 \text{ if } s < 0.$$

Complex susceptibility function

$$\widehat{\boldsymbol{P}}(\omega) = \chi(\omega)\widehat{\boldsymbol{E}}(\omega).$$

LTI, causal, real, passive, pasma limit

$$\chi(\omega) = \int_0^{\infty} \frac{d\sigma(\lambda)}{\lambda - \omega^2}, \quad \sigma \geq 0, \quad A = \int_0^{\infty} d\sigma(\lambda) < +\infty$$

Kramers-Kronig relations?

$$\chi'(\omega) = \frac{2}{\pi} P.V. \int_0^\infty \frac{s\chi''(s)}{s^2 - \omega^2} ds, \quad \chi''(\omega) = -\frac{2\omega}{\pi} P.V. \int_0^\infty \frac{\chi'(s)}{s^2 - \omega^2} ds$$

But $\lim_{\substack{\omega \to x \\ \mathfrak{Im}(\omega) > 0}} \int_0^\infty \frac{d\sigma(\lambda)}{\lambda - \omega^2}$ does not make sense pointwise!

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Implicit physics $\rightarrow$ more mathematical structure

$$\chi \in H^2(\mathbb{H}_+)$$

$$\sup_{\omega'' > 0} \int_{-\infty}^{\infty} |\chi(\omega' + i\omega'')|^2 d\omega' = \int_{-\infty}^{\infty} |\chi(\omega')|^2 d\omega' < +\infty.$$

Relaxation time

$$\exists \tau > 0 : \quad \begin{cases} |\chi(t)| \leq Ce^{-t/\tau}, & \text{if } t \geq 0 \\ \chi(t) = 0, & \text{if } t < 0 \end{cases}$$

$$\tau > 0 \;\Rightarrow\; \chi(\omega) \text{ is analytic in } \mathbb{H}_h = \{\omega \in \mathbb{C} : \omega'' > -h\}, \quad h = \frac{1}{\tau}$$

The space of admissible functions $\mathcal{K}_0^h$

- $f \in H^2(\mathbb{H}_h)$, $\mathbb{H}_h = \{\omega \in \mathbb{C} : \omega'' > -h\}$
- $\overline{f(\omega)} = f(-\overline{\omega})$
- $\mathfrak{Im}(f(\omega)) > 0$ if $\omega' > 0$ and $\omega'' > -h$
- $\exists A > 0$: $f(\omega) \sim -\dfrac{A}{\omega^2}$, $\omega \to \infty$

Least squares problem

$$\inf_{f \in \mathcal{K}_0^h} \int_0^1 |f(\omega) - f_{\mathrm{exp}}(\omega)|^2 d\omega$$

Theorem. The least squares problem has a unique solution in $\mathcal{K}^h$:

$$\mathcal{K}^h = \left\{ f(\omega) = \alpha + \int_0^\infty L(\omega, u + ih) d\mu(u) \right\},$$

$$\alpha \geq 0, \quad \int_0^\infty \frac{u d\mu(u)}{u^2 + 1} < \infty.$$

$$L(\omega, q) = \frac{1}{q + \omega} + \frac{1}{\overline{q} - \omega}, \quad q' > 0, \quad q'' > h$$

is called the Lorentzian.

From $\mathcal{K}_0^h$ to $\mathcal{K}_h$

$$f \in \mathcal{K}_0^h \quad \Longleftrightarrow \quad f(\omega) = \int_0^\infty L(\omega, u + ih) d\mu(u),$$

$$d\mu(u) = \mathfrak{Im}(f(u - ih))du \in L^2(0, +\infty) \cap L^1(0, +\infty)$$

Lemma. $\exists c, C > 0 : \ \forall f \in \mathcal{K}_0^h$

$$c\|f\|_{L^2(0,1)} \leq \|\mu\|_{\mathcal{M}} \leq C\|f\|_{L^2(0,1)}, \quad \|\mu\|_{\mathcal{M}} = \int_0^\infty \frac{u d\mu(u)}{u^2 + 1}.$$

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Proof of Theorem

Minimizing sequence $\mathcal{K}_0^h \ni f_n \rightharpoonup f$ in $L^2(0,1)$.

$$f_n(\omega) = \int_0^\infty \left\{ L(\omega, u+ih) - \frac{2u}{u^2+1} \right\} d\mu_n(u) + \int_0^\infty \frac{2ud\mu_n(u)}{u^2+1}$$

$$f_n(\omega) \rightharpoonup f(\omega) = \alpha + \int_0^\infty L(\omega, u+ih)d\mu(u) \quad \text{in } L^2(0,1)$$

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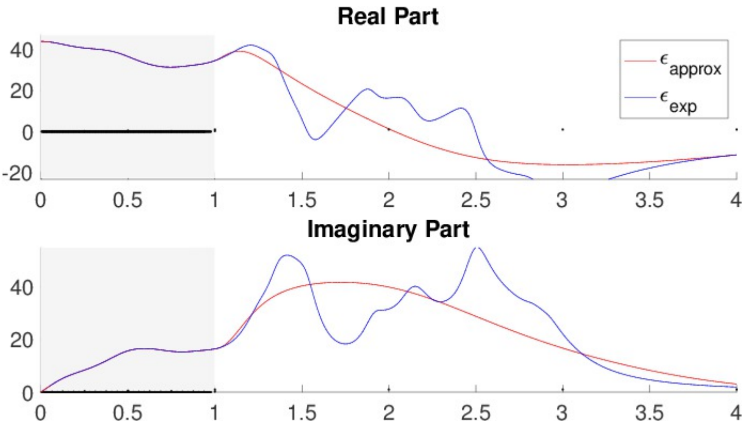

Is extrapolation an ill-posed problem?

$$U(\epsilon) = \left\{ (f,g) \in \mathcal{K}_0^h : \frac{\|f-g\|_{L^2(0,1)}}{\max(\|f\|,\|g\|)} \le \epsilon \right\}, \quad \|f\| = \|f\|_{H^2(\mathbb{H}_h)}$$

$$\Delta_\omega(\epsilon) = \sup_{(f,g)\in U(\epsilon)} \frac{|f(\omega)-g(\omega)|}{\max(\|f\|,\|g\|)}, \quad \omega > 1.$$

Can $\Delta_\omega(\epsilon)$ be large?

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What is going on here?

Recasting the problem

$$U(\epsilon) = \left\{ (f, g) \in \mathcal{K}_0^h : \frac{\|f - g\|_{L^2(0,1)}}{\max(\|f\|, \|g\|)} \leq \epsilon \right\}.$$

$$\Delta_\omega(\epsilon) = \sup_{(f,g)\in U(\epsilon)} \frac{|f(\omega) - g(\omega)|}{\max(\|f\|, \|g\|)},$$

$$\phi = f - g$$

$$U^*(\epsilon) = \left\{ \phi \in H^2(\mathbb{H}_h) : \frac{\|\phi\|_{L^2(0,1)}}{\|\phi\|} \leq \epsilon \right\}. \quad \Delta_\omega^*(\epsilon) = \sup_{\phi\in U^*(\epsilon)} \frac{|\phi(\omega)|}{\|\phi\|},$$

Theorem. $\displaystyle\lim_{\epsilon\to 0} \frac{\ln \Delta_\omega^*(\epsilon)}{\ln \epsilon} = \lim_{\epsilon\to 0} \frac{\ln \Delta_\omega(\epsilon)}{\ln \epsilon}$

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Passivity plays no additional regularizing role

Can a well-posed problem be ill-posed?

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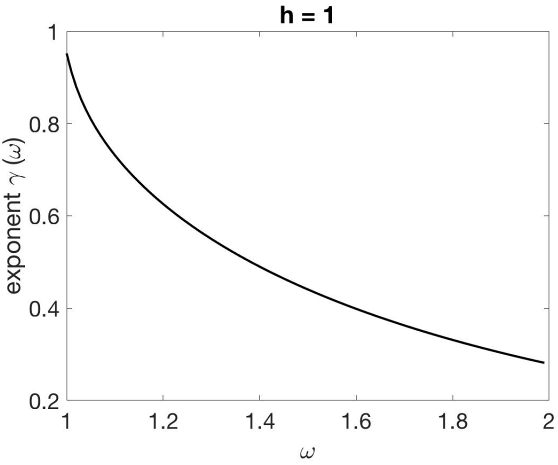
Theorem. $\Delta^*_\omega(\epsilon) \sim \epsilon^{\gamma(\omega)}$



The variational problem

$$\begin{cases} |\phi(\omega_0)| \to \max \\ \|\phi\|_{H^2} \leq 1 \\ \|\phi\|_{L^2(-1,1)} \leq \epsilon \\ \overline{\phi(\omega)} = \phi(-\overline{\omega}), \end{cases}$$

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Know how to solve

$$\begin{cases} |\phi(\omega_0)| \to \max \\ \|\phi\|_{H^2} \le 1 \\ \|\phi\|_{L^2(-1,1)} \le \epsilon \end{cases} \iff \begin{cases} \Re\mathfrak{e}(\phi(\omega_0)) \to \max \\ \|\phi\|_{H^2} \le 1 \\ \|\phi\|_{L^2(-1,1)} \le \epsilon \end{cases}$$

Making objective functional linear

$$|\phi(\omega)| = \max_{|\lambda|=1} \mathfrak{Re}(\lambda\phi(\omega)).$$

$$\begin{cases} \mathfrak{Re}(\lambda\phi(\omega_0)) \to \max \\ \|\phi\|_{H^2} \leq 1 \\ \|\phi\|_{L^2(-1,1)} \leq \epsilon \\ \overline{\phi(\omega)} = \phi(-\overline{\omega}), \end{cases}$$

The restriction operator $\mathcal{R} : H^2 \to L^2(-1,1)$, $\mathcal{K} = \mathcal{R}^*\mathcal{R}$

$$\|\phi\|^2_{L^2(-1,1)} = (\mathcal{K}\phi, \phi), \quad (\mathcal{K}\phi)(\omega) = \frac{1}{2\pi}\int_{-1}^{1} \frac{i\phi(x)dx}{\omega - x + 2ih}.$$

$K(\omega, z) = \dfrac{i}{2\pi(\omega - \overline{z} + 2ih)}$ is the reproducing kernel of $H^2(\mathbb{H}_h)$.

Eliminating symmetry constraint

$$(S\phi)(\omega) = \frac{\overline{\phi(-\overline{\omega})} + \phi(\omega)}{2}.$$

Key observations

1. $S\mathcal{K} = \mathcal{K}S$.
2. $\lambda\phi(\omega_0) = \lambda(\phi, K(\cdot, \omega_0)) = \lambda(S\phi, K(\cdot, \omega_0)) = (S\phi, \overline{\lambda}K(\cdot, \omega_0)) = (\phi, S(\overline{\lambda}K(\cdot, \omega_0))) = (\phi, p_\lambda)$

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Symmetry constraint is eliminated:

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$$(\phi, p_\lambda) = (S\phi, p_\lambda), \quad \|\phi\|^2 = \|S\phi\|^2 + \|(1-S)\phi\|^2 \ge \|S\phi\|^2,$$

$$(\mathcal{K}\phi,\phi) = (\mathcal{K}S\phi, S\phi) + (\mathcal{K}(1-S)\phi, (1-S)\phi) \ge (\mathcal{K}S\phi, S\phi).$$

The method of Lagrange multipliers

$$\max_{\phi}\{2\Re\mathfrak{e}(\phi, p_\lambda) - \mu(\phi,\phi) - \nu(\mathcal{K}\phi,\phi)\}$$

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$$p_\lambda = \mu\phi + \nu\mathcal{K}\phi \quad \Rightarrow \quad \phi = (\mu + \nu\mathcal{K})^{-1} p_\lambda .$$

$$\|(\mu + \nu\mathcal{K})^{-1} p_\lambda\|^2 = 1, \qquad (\mathcal{K}(\mu + \nu\mathcal{K})^{-1} p_\lambda, (\mu + \nu\mathcal{K})^{-1} p_\lambda) = \epsilon^2$$

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$$\Psi(\eta)\uparrow\uparrow, \quad \Psi(0+) = 0, \quad \Psi(\infty) = \frac{(\mathcal{K}p_\lambda, p_\lambda)}{\|p_\lambda\|^2} > 0.$$

$$\exists!\eta^*(\epsilon):\ \Psi(\eta^*(\epsilon)) = \epsilon^2, \qquad \eta^*(\epsilon) \sim \epsilon^2.$$

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Taking both roads at the fork

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Taking both roads at the fork

$$\phi = \min\left\{\frac{1}{\|u\|}, \frac{\epsilon}{\|u\|_{L^2(-1,1)}}\right\} u.$$

Then $\|\phi\| \le 1$, $\|\phi\|_{L^2(-1,1)} \le \epsilon$.

Main result

$$\Delta_z^*(\epsilon) \leq \frac{3}{2} \max_{|\lambda|=1} \min \left\{ \frac{|S(\lambda u)(\omega_0)|}{\|S(\lambda u)\|}, \frac{\epsilon |S(\lambda u)(\omega_0)|}{\|S(\lambda u)\|_{L^2(-1,1)}} \right\},$$

where u solves $\displaystyle\int_{-1}^{1} K(\omega, x)u(x)dx + \epsilon^2 u(\omega) = p_0(\omega)$

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Solution by diagonalization

$$\mathcal{K} e_n = \lambda_n e_n, \quad \|e_n\|_{L^2} = 1, \quad u_n = (u, e_n)_{L^2}, \quad \pi_n = (K(\cdot, \omega_0), e_n)_{L^2}$$

$$u_n = \frac{\pi_n}{\epsilon^2 + \lambda_n}, \quad u(\omega_0) = \sum_{n=1}^{\infty} u_n e_n(\omega_0) = \sum_{n=1}^{\infty} \frac{|\pi_n|^2}{\lambda_n(\epsilon^2 + \lambda_n)}.$$

$$e_n(\omega_0) = (e_n, \mathcal{K}(\cdot, \omega_0)) = \frac{1}{\lambda_n}(\mathcal{K} e_n, \mathcal{K}(\cdot, \omega_0)) = \frac{1}{\lambda_n}(e_n, \mathcal{K}(\cdot, \omega_0))_{L^2} = \frac{\overline{\pi_n}}{\lambda_n}.$$

Power law from exponential decay

$$\lambda_n \sim e^{-\alpha n}, \qquad |\pi_n|^2 = e^{-\beta b}, \quad \beta < \alpha < 2\beta.$$

$$u(\omega_0) \sim \sum_{n=1}^{\infty} \frac{e^{(\beta-\alpha)n}}{\epsilon^2 + e^{-\beta n}}.$$

$$f(\eta) = \sum_{n=0}^{\infty} \frac{a^n}{\eta + b^n}, \quad \eta \to 0^+, \qquad 0 < b < a < 1,$$

$$F(\eta) = \sum_{n\in\mathbb{Z}} \frac{a^n}{\eta + b^n} = f(\eta) + g(\eta), \qquad g(0) = \frac{b}{a-b}.$$

$$\frac{1}{\eta} = b^{-\frac{\ln \eta}{\ln b}} = b^{-p(\eta)}, \quad F(\eta) = \frac{a^{p(\eta)}}{\eta} \sum_{n\in\mathbb{Z}} \frac{a^{n-p(\eta)}}{1 + b^{n-p(\eta)}}$$

$$f(\eta) \sim F(\eta) = \eta^{\gamma} \sum_{n\in\mathbb{Z}} \frac{a^{n-\{p(\eta)\}}}{1 + b^{n-\{p(\eta)\}}} \sim \eta^{\gamma} \qquad \gamma = \frac{\ln a}{\ln b} - 1.$$

Exponential decay of eigenvalues of $\mathcal{K}$

$$(\mathcal{K}u)(x) = \frac{i}{2\pi}\int_{-1}^{1}\frac{u(y)dy}{x-y+2ih}$$

Displacement structure of the integral operator

$$M\mathcal{K} - \mathcal{K}M^* = \frac{i}{2\pi}1\otimes 1, \qquad (Mu)(x) = (x+ih)u(x).$$

Theorem(Beckermann-Townsend, 2017) If $\mathcal{K}$ has a displacement structure above then

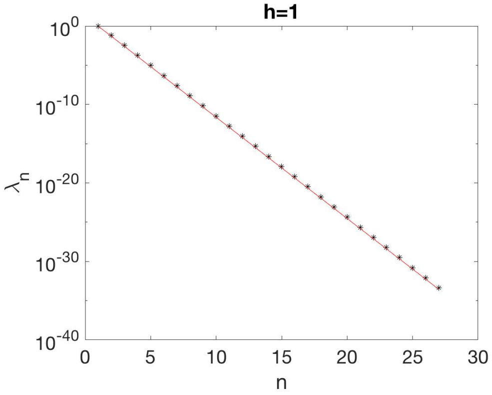
$$\lambda_n(\mathcal{K}) \leq Z_n(\sigma(M), \sigma(M^*))$$

$Z_n(A,B)$—nth Zolotarev (1877) number of disjoint closed set $\{A,B\}\subset\mathbb{C}$.
Theorem(Gonchar, 1969) If A and B are connected compact continua, then $Z_n(A,B)\sim\rho^{-n}$, where ρ is the Riemann invariant of $\mathbb{C}_\infty\setminus\{A\cup B\}$

Beckerman-Townsend upper bound for $\mathcal{K}$

$$\rho = e^{-2\pi K(1-m)/K(m)},$$

$$K(m)E(x(m)|m) - E(m)F(x(m)|m) = \frac{\pi}{2h}, \quad x(m) = \sqrt{\frac{K(m)-E(m)}{mK(m)}}.$$



Mechanism of flexibility: the annulus

$A_\rho = \{\rho < |z| < 1\}$, $\rho < r < 1$, $\Gamma_r = \{|z| = r\}$, $r < |z_0| < 1$.

$$\Delta(\epsilon) = \max_{\substack{\|\phi\|_{L^2(\Gamma_r)} \leq \epsilon \\ \|\phi\|_{H^2(A_\rho)} \leq 1}} |\phi(z_0)|$$

The maximizer is

$$M(z) = \epsilon^{2-\gamma(z_0)} \sum_{n=1}^{\infty} \frac{(z\overline{z_0})^n}{\epsilon^2 + r^{2n}}, \quad \gamma(z_0) = \frac{\ln|z_0|}{\ln r}.$$

The maximal relative error is $\Delta(\epsilon) \sim \epsilon^{\gamma(z_0)}$

Upper bound on $\gamma(\omega_0)$ for susceptibility

1. Map conformally $\mathbb{C}_\infty \setminus \{\Gamma \cup \Gamma^\#\}$ to the standard annulus $\mathbb{A}_\rho = \{\rho^{-1/2} < |z| < \rho^{1/2}\}$, where $\Gamma = [-1, 1]$, $\Gamma^\# = [-1, 1] - 2ih$–reflection of Γ with respect to $\partial\mathbb{H}_h$.

$$\Psi : \mathbb{C}_\infty \setminus \{\Gamma \cup \Gamma^\#\} \to \mathbb{A}_\rho$$

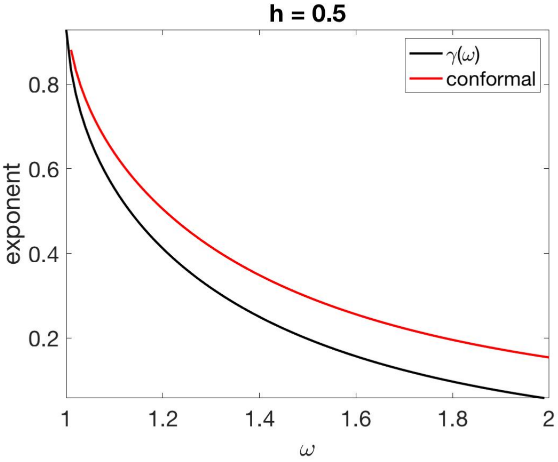
$$|\Psi([-1, 1])| = \rho^{-1/2}, \quad |\Psi(\mathbb{R} - ih)| = 1$$

2. Use "the mechanism" to build a test function

$$\phi(\omega) = \frac{\epsilon^{2-\tilde{\gamma}(\omega_0)}}{(\omega + 2ih)^2} \sum_{n=1}^{\infty} \frac{(\Psi(\omega)\overline{\Psi(\omega_0)})^n}{\epsilon^2 + \rho^n}, \quad \tilde{\gamma}(\omega_0) = \frac{\ln |\Psi(\omega_0)|}{\ln \sqrt{\rho}}$$

3. Our upper bound is $\gamma(\omega_0) \leq \tilde{\gamma}(\omega_0) = \dfrac{\ln |\Psi(\omega_0)|}{\ln \sqrt{\rho}}$.

Comparison between $\gamma(\omega)$ and $\tilde{\gamma}(\omega)$



If $h \geq 0.7$ there is no observable difference between $\gamma(\omega)$ and $\tilde{\gamma}(\omega)$.