Approximating Dispersive Mechanisms Using the Debye Model with Distributions of Dielectric Parameters

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1. **Background**
   - Maxwell's Equations
   - The One Dimensional Problem
   - Dielectric Parameters of Interest
2. **Cole-Cole and Debye Models**
   - Cole-Cole and Debye Models
   - Distributions
3. **Inverse Problems**
   - Frequency-domain Inverse Problem
   - Time-domain Inverse Problem

Maxwell's Equations

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} = \nabla \times \mathbf{H} \qquad \text{(Ampere)}$$
$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \qquad \text{(Faraday)}$$
$$\nabla \cdot \mathbf{D} = \rho \qquad \text{(Poisson)}$$
$$\nabla \cdot \mathbf{B} = 0 \qquad \text{(Gauss)}$$

$\mathbf{E} =$ Electric field vector

$\mathbf{H} =$ Magnetic field vector

$\rho =$ Electric charge density

$\mathbf{D} =$ Electric displacement

$\mathbf{B} =$ Magnetic flux density

$\mathbf{J} =$ Current density

We impose homogeneous initial conditions and boundary conditions.

Constitutive Laws

Maxwell's equations are completed by constitutive laws that describe the response of the medium to the electromagnetic field.

$$\boxed{\begin{aligned} \mathbf{D} &= \epsilon \mathbf{E} + \mathbf{P} \\ \mathbf{B} &= \mu \mathbf{H} + \mathbf{M} \\ \mathbf{J} &= \sigma \mathbf{E} + \mathbf{J}_s \end{aligned}}$$

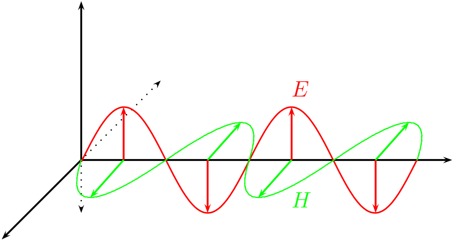
$\mathbf{P} =$	Polarization	$\epsilon =$	Electric permittivity
$\mathbf{M} =$	Magnetization	$\mu =$	Magnetic permeability
$\mathbf{J}_s =$	Source Current	$\sigma =$	Electric Conductivity

Maxwell's Equations in One Space Dimension

- Assume that the electric field is polarized to oscillate only in the y direction, propagates in x direction, and everything is uniform in z direction.

Equations involving E_y and H_z.

$$\epsilon \frac{\partial E_y}{\partial t} = -\frac{\partial H_z}{\partial x} - \sigma E_y - \frac{d\mathbf{P}}{dt}$$
$$\mu \frac{\partial H_z}{\partial t} = -\frac{\partial E_y}{\partial x}$$



- If $\sigma = 0$ and $\mathbf{P} = 0$, then $E = E_y$ satisfies the 1D wave equation with $c = 1/\sqrt{\epsilon\mu}$

$$\frac{\partial^2 E(x,t)}{\partial t^2} = c^2 \frac{\partial^2 E(x,t)}{\partial x^2}$$

Constitutive Relations

- Recall

$$\mathbf{D} = \epsilon \mathbf{E} + \mathbf{P}$$

where $\mathbf{P}$ is the dielectric polarization.

- We can generally define $\mathbf{P}$ in terms of a convolution

$$\mathbf{P}(t, \mathbf{x}) = g \star \mathbf{E}(t, \mathbf{x}) = \int_0^t g(t-s, \mathbf{x}; \nu) \mathbf{E}(s, \mathbf{x}) ds,$$

where g is a general dielectric response function (DRF), and ν is some parameter set.

DRF Examples

- Debye model

$$g(t,\mathbf{x}) = \epsilon_0(\epsilon_s - \epsilon_\infty)/\tau \;\; e^{-t/\tau}$$
$$(\text{or } \tau\dot{\mathbf{P}} + \mathbf{P} = \epsilon_0(\epsilon_s - \epsilon_\infty)\mathbf{E})$$

- Lorentz model

$$g(t,\mathbf{x}) = \epsilon_0\omega_p^2/\nu_0 \;\; e^{-t/2\tau} sin(\nu_0 t)$$
$$(\text{or } \ddot{\mathbf{P}} + \frac{1}{\tau}\dot{\mathbf{P}} + \omega_0^2\mathbf{P} = \epsilon_0\omega_p^2\mathbf{E})$$

Frequency Domain

- Converting to frequency domain via Fourier transforms

$$\hat{\mathbf{D}} = \epsilon(\omega)\hat{\mathbf{E}}$$

- Debye model

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + i\omega\tau} + \frac{\sigma}{i\omega\epsilon_0}$$

- Cole-Cole model

$$\epsilon(\omega) = \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + (i\omega\tau)^{1-\alpha}} + \frac{\sigma}{i\omega\epsilon_0}$$

Multi-pole models

In general there are multiple mechanisms at various scales that account for polarization. To attempt to account for several of these over a range of frequencies, researchers tend to use multi-pole models:

- Multi-pole Debye model:

$$\epsilon(\omega)_D = \epsilon_\infty + \sum_{m=1}^{n} \frac{\Delta\epsilon_m}{1 + i\omega\tau_m} + \frac{\sigma}{i\omega\epsilon_0}$$

- Multi-pole Cole-Cole model:

$$\epsilon(\omega)_{CC} = \epsilon_\infty + \sum_{m=1}^{n} \frac{\Delta\epsilon_m}{1 + (i\omega\tau_m)^{(1-\alpha_m)}} + \frac{\sigma}{i\omega\epsilon_0}$$

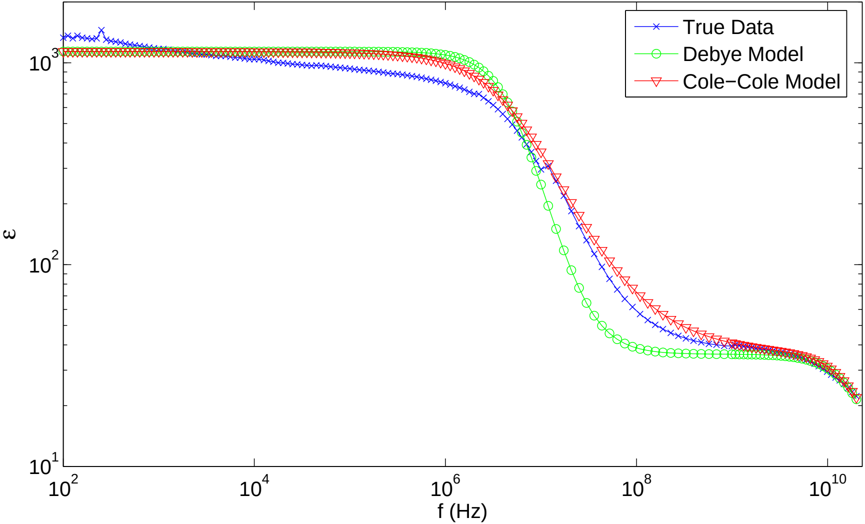


Figure: Real part of $\epsilon(\omega)$, ϵ, or the permittivity.

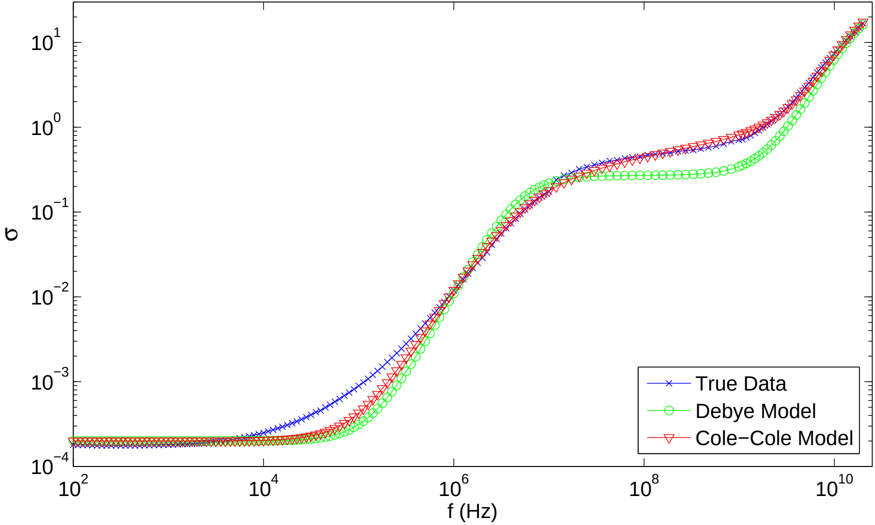


Figure: "Imaginary part" of $\epsilon(\omega)$, σ, or the conductivity.

Distributions of Parameters

To account for the possible effect of multiple parameter sets ν, consider

$$h(t, \mathbf{x}; F) = \int_{\mathcal{N}} g(t, \mathbf{x}; \nu) dF(\nu),$$

where $\mathcal{N}$ is some admissible set and $F \in \mathfrak{P}(\mathcal{N})$.
Then the polarization becomes:

$$\mathbf{P}(t, \mathbf{x}) = \int_0^t h(t - s, \mathbf{x}) \mathbf{E}(s, \mathbf{x}) ds.$$

Motivation: match data even better than multi-pole Cole-Cole, and more efficient to simulate.

Two Approaches

We will consider the problem of determining the distribution of dielectric parameters which describe a material by using the following as data:

- Complex permittivity (frequency-domain)
- Electric field (time-domain)

Inverse Problem for F

- Given data $\{\hat{\epsilon}\}_j$ we seek to determine a probability measure F^*, such that

$$F^* = \min_{F \in \mathfrak{P}(\mathcal{N})} \mathcal{J}(F),$$

where, for example,

$$\mathcal{J}(F) = \sum_j \left[\epsilon(\omega_j; F) - \hat{\epsilon}_j\right]^2 .$$

- As $\epsilon(\omega)$ is complex, we define $e = [\Re(\epsilon(\omega_j)), \Re(\epsilon(\omega_j) i\omega_j \epsilon_0)]$ and minimize the ℓ_2-norm of the relative error between $e(F)$ and $\hat{e}$.
- Given a trial distribution F_k we compute $\epsilon(\omega_j; F_k)$ and test $\mathcal{J}(F_k)$, then update F_{k+1} as necessary.

Monte Carlo Simulations

- To compute $\epsilon(\omega; F_k)$ we perform N Monte Carlo (MC) simulations.
- Each MC simulation consists of drawing trial values of one or more of the following according to the definition of the distribution F: ϵ_{∞_ℓ}, $\Delta\epsilon_\ell$, τ_ℓ, σ_ℓ
- We then compute

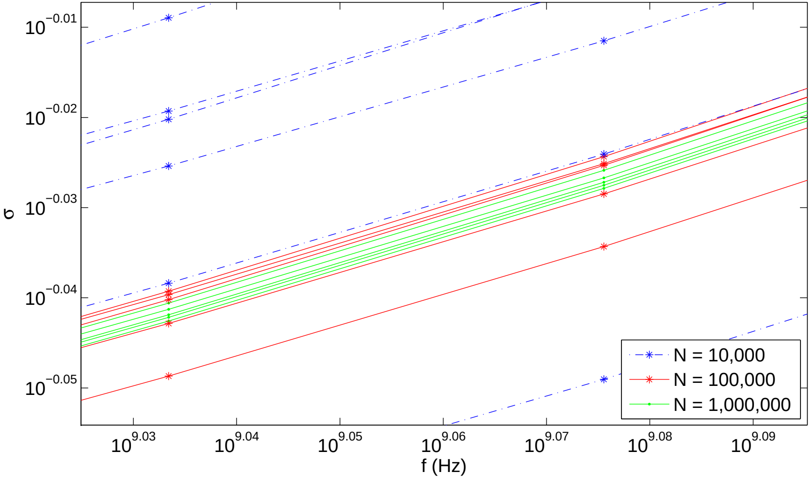
$$\epsilon(\omega)_\ell = \epsilon_{\infty_\ell} + \frac{\Delta\epsilon_\ell}{1 + (i\omega\tau_\ell)} + \frac{\sigma_\ell}{i\omega\epsilon_0}$$

- The term $\epsilon(\omega; F)$ is simply computed as the sample mean of the $\epsilon(\omega; F)_\ell$,

$$\epsilon(\omega)_{DD} = \frac{1}{N}\sum_{\ell=1}^{N} \epsilon(\omega)_\ell.$$

Convergence of MC

We need to select N (the number of MC simulations in the computation of $\epsilon(\omega)_{DD}$) sufficiently large so as to reduce variability.



Multi-pole Example

- Consider

$$\epsilon(\omega)_\ell = \epsilon_\infty + \sum_{m=1}^{n} \frac{\Delta\epsilon_{m_\ell}}{1 + (i\omega\tau_{m_\ell})} + \frac{\sigma}{i\omega\epsilon_0}$$

- For each pole m, we randomly sample each $\Delta\epsilon_{m_\ell}$ and τ_{m_ℓ} where

$$\tau_{m_\ell} \sim \mathcal{U}\left[(1-a_m)\tau_m, (1+b_m)\tau_m\right],$$

and

$$\Delta\epsilon_{m_\ell} \sim \mathcal{U}\left[(1-c_m)\Delta\epsilon_m, (1+d_m)\Delta\epsilon_m\right]$$

for some given "reference values" of τ_m and $\Delta\epsilon_m$.

- Thus, F is determined by a_m, b_m, c_m and d_m, i.e., they are the values of interest in our inverse problem.

Dry Skin Problem

- We use complex permittivity measurements from [GLG96] describing dry skin as data.
- We use the estimates from [GLG96] for $\epsilon_\infty, \sigma, \tau_m$ and $\Delta\epsilon_m$ as our "reference values".
- The constraints on the distribution parameters were

$$\begin{array}{rr} a_1 \in [0,1] & b_1 \in [0,1] \\ a_2 \in [.5,1.5] & b_2 \in [1,2] \\ c_1 \in [0,1] & d_1 \in [0,1] \\ c_2 \in [0,1] & d_2 \in [0,1] \end{array}$$

- The results from DIRECT (global constrained optimization) were

$$\begin{array}{ll} a_1 = 0.1337 & b_1 = 0.6646 \\ a_2 = 1.0000 & b_2 = 1.7840 \\ c_1 = 0.4630 & d_1 = 0.5000 \\ c_2 = 0.5988 & d_2 = 0.4630 \end{array}$$

$$J = 12.1945$$

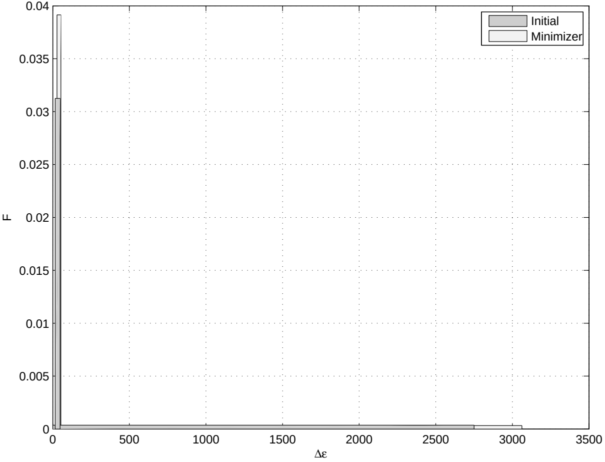


Figure: Uniform distributions for $\Delta\epsilon$ values in multi-pole Debye model for dry skin.

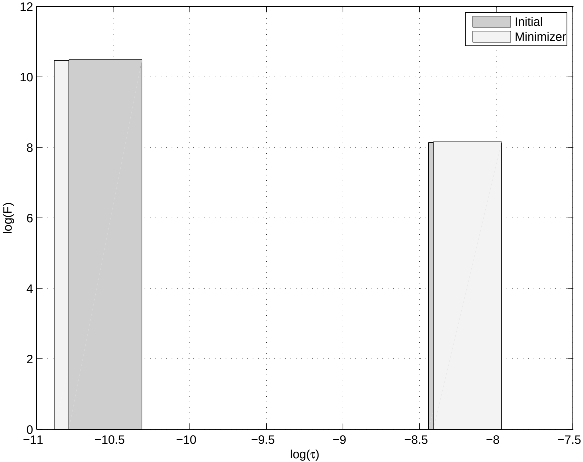


Figure: Uniform distributions for τ values in multi-pole Debye model for dry skin.

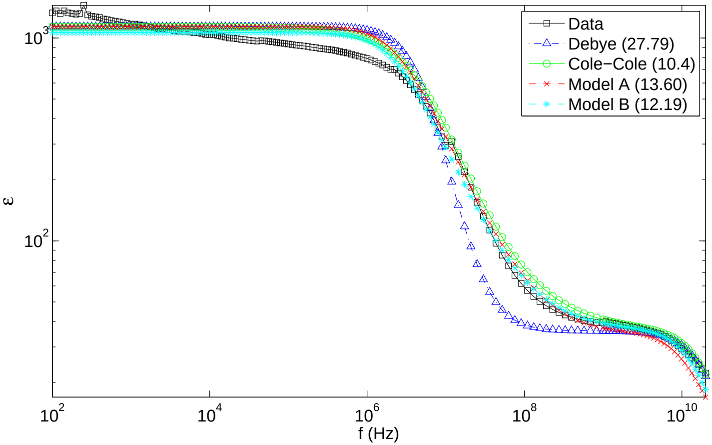


Figure: Real part of $\epsilon(\omega)$, σ, or the permittivity. Model A refers to the Debye model with distributions only on τ. Model B refers to the Debye model with distributions on both τ and $\Delta\epsilon$. Note: $U_{156} = 18.0443$, $\chi^2(4) : \alpha = \{.05, .01, .001\} \implies \tau = \{9.49, 13.28, 18.47\}$

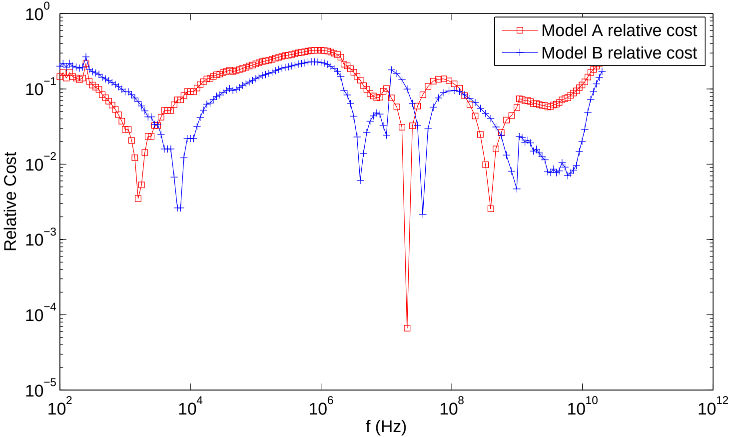


Figure: The relative costs between Model A and the true data and between Model B and the true data. Model A refers to the Debye model with distributions only on τ. Model B refers to the Debye model with distributions on both τ and $\Delta\epsilon$.

Comments on Optimization

- Levenberg-Marquardt failed to find a local minimum.
- In addition, programs such as `fminsearch` and `fmincon` (`fminsearch` subject to a set of constraints) were also tried.
- This difficulty was mentioned in [GLG96].
- The randomness of the inverse problem implies that it is ill-posed; gradient-based algorithms will often choose a non-descent direction.
- Methods for implementation of such local minimum searches is an area which should be explored further.

To compare the time-domain response of each model of dry skin (Debye, Cole-Cole, and Distributed Debey), we simulate a broad-band pulse through the materials.

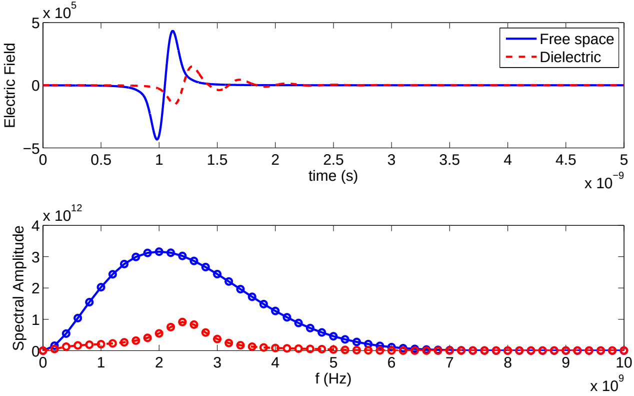


Figure: The top plot shows the value of the electric field at a fixed point in space as time varies. The bottom shows the FFT of the two signals.

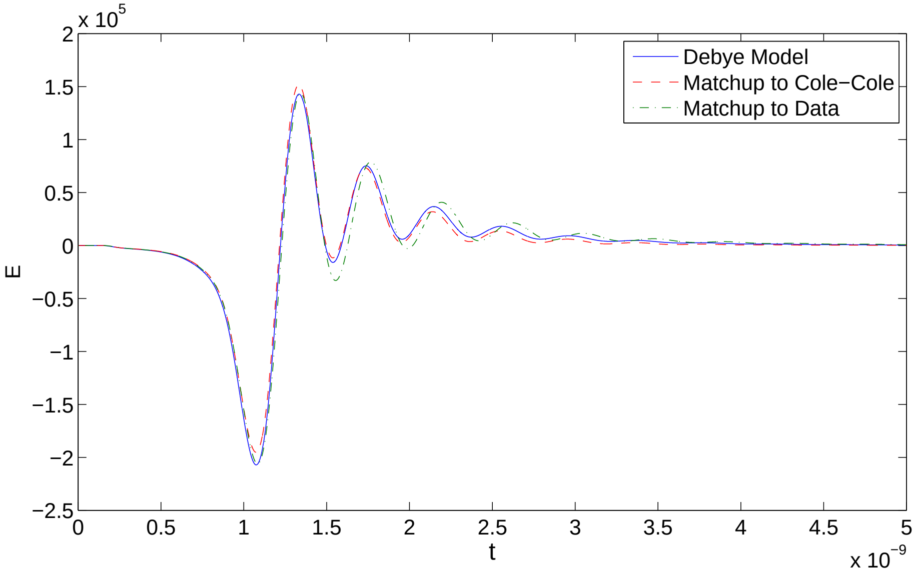


Figure: Forward simulations with different distributions of dielectric parameters.

Inverse Problem for F

- Given data $\{\hat{E}\}_j$ we seek to determine a probability measure F^*, such that

$$F^* = \min_{F \in \mathfrak{P}(\mathcal{N})} \mathcal{J}(F),$$

where, for example,

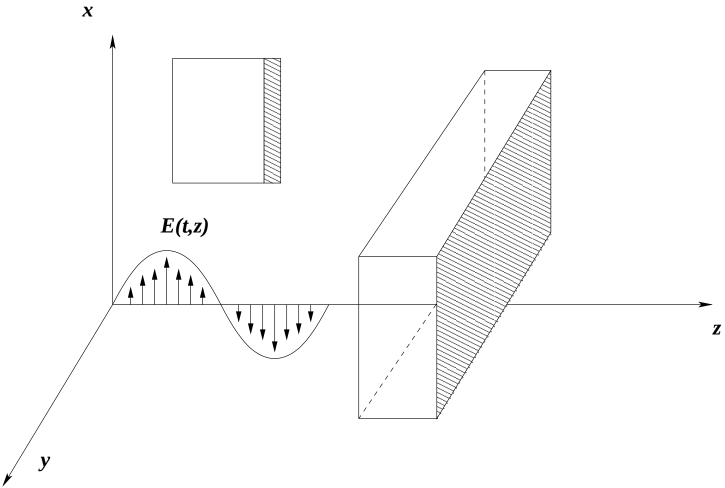
$$\mathcal{J}(F) = \sum_j \left(E(0, t_j; F) - \hat{E}_j \right)^2 .$$

- Given a trial distribution F_k we compute $\epsilon(\omega_j; F_k)$ and test $\mathcal{J}(F_k)$, then update F_{k+1} as necessary.
- Need a (fast) (numerical) method for computing $E(x, t; F)$.

Stability of Inverse Problem

- Continuity of $F \to (E, \dot{E}) \implies$ continuity of $F \to \mathcal{J}(F)$
- Compactness of $\mathcal{N} \implies$ compactness of $\mathfrak{P}(\mathcal{N})$ with respect to the Prohorov metric
- Therefore, a minimum of $\mathcal{J}(F)$ over $\mathfrak{P}(\mathcal{N})$ exists

1D Example



$$J_s(t,z) = \delta_0(z)\sin(\omega t) I_{[0,t_f]}(t)$$

Numerical Discretization

$$\epsilon \frac{\partial E}{\partial t} = -\frac{\partial H}{\partial x} - \sigma E - \frac{dP}{dt}$$
$$\mu \frac{\partial H}{\partial t} = -\frac{\partial E}{\partial x}$$
$$P(t,x) = \int_{\mathcal{N}} \int_0^t g(t-s,\mathbf{x};\nu)E(s,x)ds\, dF(\nu).$$

- Second order FEM in space
  - piecewise linear splines
- Second order FD in time
  - Crank-Nicholson (P)
  - Central differences (E)
  - $e_n \longrightarrow p_n \longrightarrow e_{n+1} \longrightarrow p_{n+1} \longrightarrow \cdots$
- Use quadrature (trapezoidal) for distribution

Discrete Distribution Example

- Mixture of two Debye materials with τ_1 and τ_2
- Total polarization a weighted average

$$P = \alpha_1 P_1(\tau_1) + \alpha_2 P_2(\tau_2)$$

- Corresponds to the discrete probability distribution

$$dF(\tau) = [\alpha_1 \delta(\tau_1) + \alpha_2 \delta(\tau_2)]\, d\tau$$

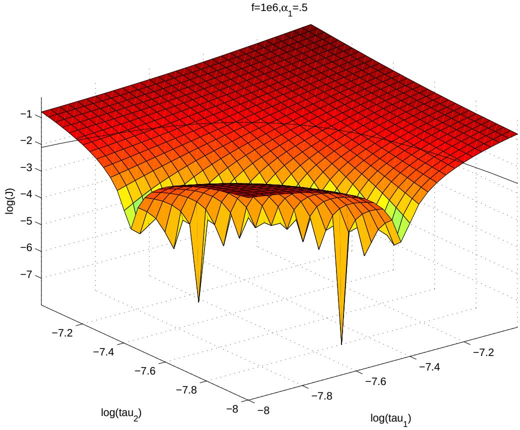
Discrete Distribution Inverse Problem

- Assume the proportions α_1 and $\alpha_2 = 1 - \alpha_1$ are known.
- Define the following least squares optimization problem:

$$\min_{(\tau_1,\tau_2)} \mathcal{J} = \min_{(\tau_1,\tau_2)} \sum_j \left| E(t_j, 0; (\tau_1, \tau_2)) - \hat{E}_j \right|^2 ,$$

where $\hat{E}_j$ is *synthetic* data generated using (τ_1^*, τ_2^*) in our simulation routine.

Discrete Distribution J using $10^6 Hz$



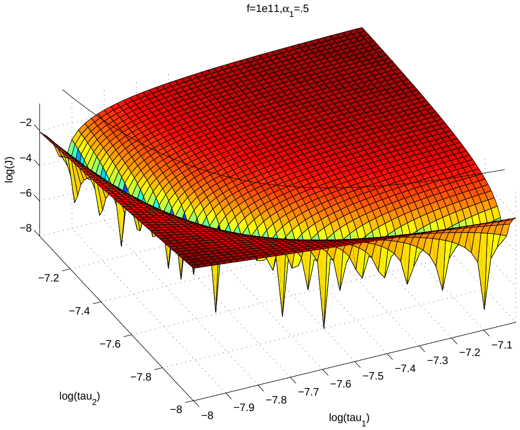
The solid line above the surface represents the curve of constant $\tilde{\tau} := \alpha_1\tau_1 + (1-\alpha_1)\tau_2$. Note: $\omega\tilde{\tau} \approx .15 < 1$.

Inverse Problem Results $10^6 Hz$

	τ_1	τ_2	$\tilde{\tau}$
Initial	3.95000e-8	1.26400e-8	2.60700e-8
LM	3.19001e-8	1.55032e-8	2.37016e-8
Final	3.16039e-8	1.55744e-8	2.37016e-8
Exact	3.16000e-8	1.58000e-8	2.37000e-8

- Levenberg-Marquardt converges to curve of constant $\tilde{\tau}$
- Traversing curve results in accurate final estimates

Discrete Distribution J using $10^{11}\,Hz$



The solid line above the surface represents the curve of constant $\tilde{\lambda} := \frac{1}{c\tilde{\tau}} = \frac{\alpha_1}{c\tau_1} + \frac{\alpha_2}{c\tau_2}$. Note: $\omega\tilde{\tau} \approx 15000 > 1$.

Inverse Problem Results $10^{11} Hz$

	τ_1	τ_2	$\tilde{\lambda}$
Initial	3.95000e-8	1.26400e-8	0.174167
LM	4.08413e-8	1.41942e-8	0.158333
Final	3.16038e-8	1.57991e-8	0.158333
Exact	3.16000e-8	1.58000e-8	0.158333

- Levenberg-Marquardt converges to curve of constant $\tilde{\lambda}$
- Traversing curve results in accurate final estimates

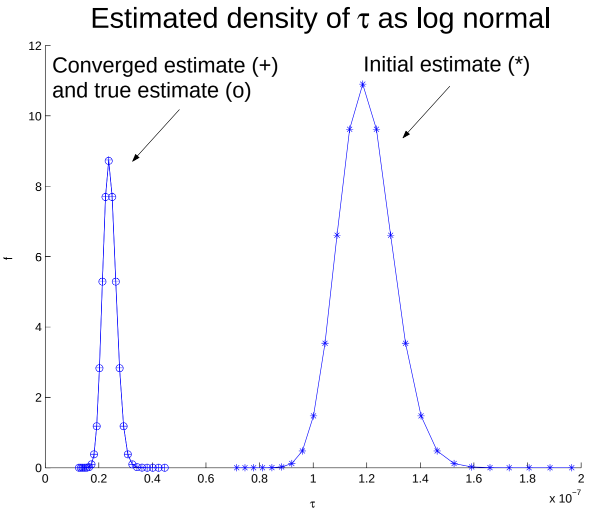
Log-Normal Distribution of τ

- Gaussian distribution of $\log(\tau)$ with mean μ and with standard deviation σ:

$$dF(\tau;\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma^2}}\frac{1}{\ln 10}\frac{1}{\tau}\exp\left(-\frac{(\log\tau-\mu)^2}{2\sigma^2}\right)d\tau,$$

- Corresponding inverse problem:

$$\min_{q=(\mu,\sigma)}\sum_j\left|E(t_j,0;(\mu,\sigma))-\hat{E}_j\right|^2.$$



Shown are the initial density function, the minimizing density function and the true density function (the latter two being practically identical).

Bi-gaussian Distribution of $\log \tau$

- Bi-gaussian distribution with means μ_1 and μ_2 and with standard deviations σ_1 and σ_2:

$$dF(\tau) = \alpha_1 d\hat{F}(\tau; \mu_1, \sigma_1) + (1 - \alpha_1) d\hat{F}(\tau; \mu_2, \sigma_2),$$

where

$$d\hat{F}(\tau; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \frac{1}{\ln 10} \frac{1}{\tau} \exp\left(-\frac{(\log \tau - \mu)^2}{2\sigma^2}\right) d\tau,$$

- Corresponding inverse problem:

$$\min_{q=(\mu_1,\sigma_1,\mu_2,\sigma_2)} \sum_j \left| |E(t_j, 0; q)| - |\hat{E}_j| \right|^2.$$

Bi-gaussian Results with $10^6 Hz$

case	μ_1	σ_1	μ_2	σ_2	$\tilde{\tau}$
Initial	1.58001e-7	0.036606	3.16002e-9	0.0571969	8.1201e-8
μ_1,μ_2	4.27129e-8	0.036606	4.24844e-9	0.0571969	2.36499e-8
Final	3.09079e-8	0.0136811	1.63897e-8	0.0663628	2.37978e-8
Exact	3.16000e-8	0.0457575	1.58000e-8	0.0457575	2.37957e-8

- Levenberg-Marquardt converges to curve of constant $\tilde{\tau}$
- Traversing curve results in accurate final estimates

Note: for this continuous distribution,

$$\tilde{\tau} = \int_{\mathcal{T}} \tau dF(\tau).$$

Bi-gaussian Results with $10^{11} Hz$

case	μ_1	σ_1	μ_2	σ_2	$\tilde{\lambda}$
Initial	1.58001e-7	0.036606	3.16002e-9	0.0571969	0.538786
μ_1,μ_2	1.58001e-7	0.036606	1.12595e-8	0.0571969	0.158863
Final	3.23914e-8	0.0366059	1.56020e-8	0.0571968	0.158863
Exact	3.16000e-8	0.0457575	1.58000e-8	0.0457575	0.158863

- Levenberg-Marquardt converges to curve of constant $\tilde{\lambda}$
- Traversing curve results in accurate final estimates

Note: for this continuous distribution,

$$\tilde{\lambda} = \int_{\mathcal{T}} \frac{1}{c\tau} dF(\tau).$$

Comments on Time-domain Inverse Problems

- We have shown well-posedness of the problem for determining distributions of dielectric parameters
- Our estimation methods worked well for discrete distributions
- Our estimation methods worked well for the continuous uniform distribution and gaussian distributions
- We are currently only able to determine the means in the bi-gaussian distributions, the data is relatively insensitive to the standard deviations

Homogenization

- A good fit when $\tilde{\lambda}$ (or $\tilde{\tau}$) is constant suggests using a single τ, even for the bi-gaussian case
- This modeling approach concludes that the "effective" parameter should be $\tilde{\tau}$ if $\omega\tau < 1$, else $1/c\tilde{\lambda}$
- We have also considered a traditional homogenization method based on "periodic unfolding" (See [BBC+06] for details)
- This approach allows us to use information about the periodic structure, i.e., hexagonal cells.

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