# Simulation Based Identification of Piezoelectric Material Parameters

DFG Junior Research Group

*Inverse Problems in Piezoelectricity*

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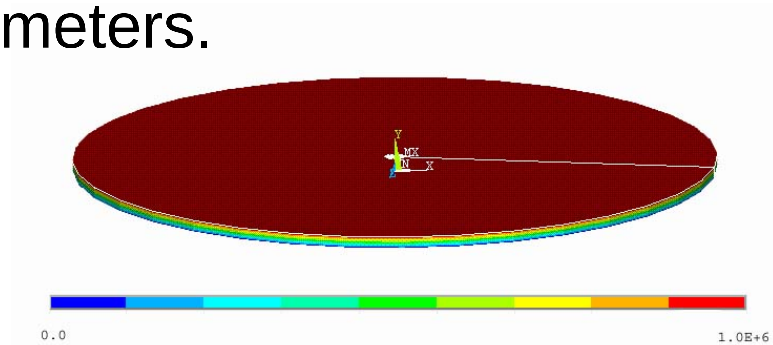
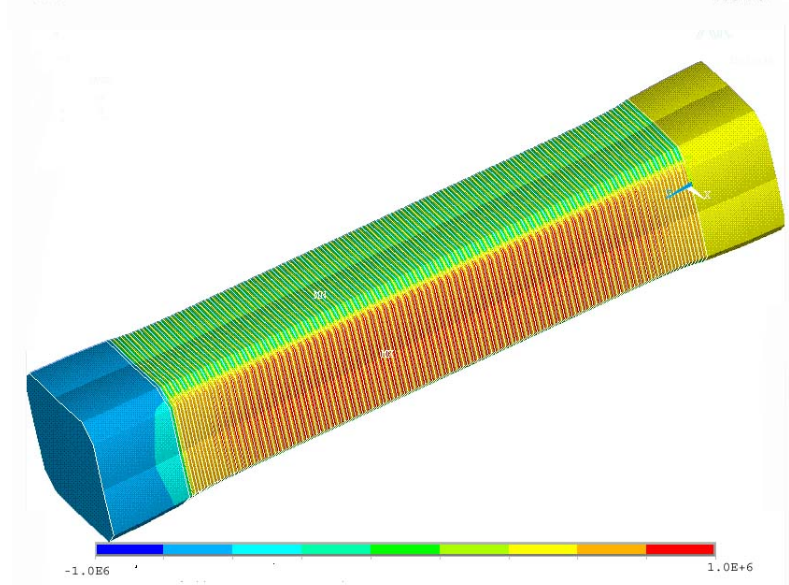
# Overview

- Piezoelectric PDEs and account for losses
- The linear forward problem
  - Well-posedness
  - Discretization
- The inverse problem
  - Simulation based identification principle
  - Ill-posedness
  - Regularization by inexact Newton methods
- Numerical results and optimal experiment design
- Summary and outlook

# Motivation

Good simulation results require exact knowledge of piezoelectric material parameters.



# Piezoelectric Effect

$$\vec{\sigma} = \mathbf{c}^E \vec{S} - \mathbf{e}^T \vec{E}$$
$$\vec{D} = \mathbf{e} \vec{S} + \varepsilon^S \vec{E}$$

| | | |
|---|---|---|
| $\vec{\sigma}$ | ... | mechanical stress |
| $\vec{S} = DIV \vec{u}$ | ... | mechanical strain |
| $\vec{E} = -grad \phi$ | ... | electric field |
| $\vec{D}$ | ... | dielectric displacement |
| $\vec{u}$ | ... | mechanical displacement |
| $\phi$ | ... | electric potential |

+ Newton's law: $\nabla \cdot \vec{\sigma} = \rho \frac{\partial^2 \vec{u}}{\partial t^2}$
+ Gauss' law: $\nabla \cdot \vec{D} = 0$

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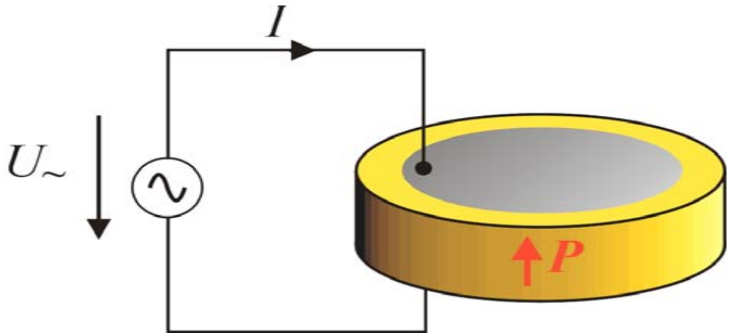
# Piezoelectric PDEs (transient)

$$\rho \frac{\partial^2 \vec{u}}{\partial t^2} - DIV\left( c^E DIV^T \vec{u} + e^T grad\phi \right) = 0 \in \Omega$$
$$-div\left( e DIV^T \vec{u} - \varepsilon^S grad\phi \right) = 0 \in \Omega$$




Boundary conditions:

$$N^T \sigma = 0 \quad \text{on} \partial\Omega$$
$$\phi = 0 \quad \text{on} \Gamma_g \text{...grounded electrode}$$
$$\phi = \phi^e \quad \text{on} \Gamma_e \text{...loaded electrode}$$
$$\vec{D} \cdot \vec{N} = 0 \quad \text{on} \partial\Omega \setminus (\Gamma_g \cup \Gamma_e)$$

# Piezoelectric Material Law

(6 mm crystal class)

$$
\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \\ D_1 \\ D_2 \\ D_3 \end{pmatrix}
=
\begin{pmatrix}
\mathbf{c}_{11}^E & \mathbf{c}_{12}^E & \mathbf{c}_{13}^E & \cdot & \cdot & \cdot & \cdot & \cdot & -\mathbf{e}_{13} \\
\mathbf{c}_{12}^E & \mathbf{c}_{11}^E & \mathbf{c}_{13}^E & \cdot & \cdot & \cdot & \cdot & \cdot & -\mathbf{e}_{13} \\
\mathbf{c}_{13}^E & \mathbf{c}_{13}^E & \mathbf{c}_{33}^E & \cdot & \cdot & \cdot & \cdot & \cdot & -\mathbf{e}_{33} \\
\cdot & \cdot & \cdot & \mathbf{c}_{44}^E & \cdot & \cdot & \cdot & -\mathbf{e}_{15} & \cdot \\
\cdot & \cdot & \cdot & \cdot & \mathbf{c}_{44}^E & \cdot & -\mathbf{e}_{15} & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \mathbf{c}_{66}^E & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & \mathbf{e}_{15} & \cdot & \varepsilon_{11}^S & \cdot & \cdot \\
\cdot & \cdot & \cdot & \mathbf{e}_{15} & \cdot & \cdot & \cdot & \varepsilon_{11}^S & \cdot \\
\mathbf{e}_{13} & \mathbf{e}_{13} & \mathbf{e}_{33} & \cdot & \cdot & \cdot & \cdot & \cdot & \varepsilon_{33}^S
\end{pmatrix}
\begin{pmatrix} S_1 \\ S_2 \\ S_3 \\ S_4 \\ S_5 \\ S_6 \\ E_1 \\ E_2 \\ E_3 \end{pmatrix}
$$

where $\mathbf{c}_{66}^E = \frac{1}{2}(\mathbf{c}_{11}^E + \mathbf{c}_{12}^E)$

elasticity [N/m²],

piezoelectric coupling [(C/m²)],

permittivity [F/m]

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# Complex Valued Material Parameters

The mathematical model describes additionally:

- Mechanical damping
- Imperfect piezoelectric energy conversion
- Dielectric dissipation

➢ More realistic model of piezoelectric transducer
➢ Usual Rayleigh damping is special case of complex – valued material parameters

# Forward Problem – Well Posedness

$$\int_\Omega \left(-\rho\omega^2 \vec{\tilde{u}}\vec{v} + (\mathbf{c}^E DIV^T \vec{\tilde{u}} + \mathbf{e}^T \text{grad}\hat{\phi}) DIV^T \vec{v}\right) dx = (\hat{f}_m, (\vec{v}, \psi))$$
$$\int_\Omega (\mathbf{e} DIV^T \vec{\tilde{u}} - \varepsilon^S \text{grad}\hat{\phi}) \text{grad}\psi \, dx = (\hat{f}_e, (\vec{v}, \psi))$$
$$\forall \vec{v} \in H_m(\Omega), \quad \forall \psi \in H_e(\Omega)$$

Quasistatic case : Sändig, Geis, Mishuris (2003)

Transient case: Nakamura, Akamatsu (2002); Miara (2001)

Harmonic case:

**Proposition:** Let

- $-Im(\mathbf{c}^E), -Im(\varepsilon^S)$ symm. pos. definite.
- $\lambda_{min}(-Im(\mathbf{c}^E)) \cdot \lambda_{min}(-Im(\varepsilon^S)) > \lambda_{max}(Re(\mathbf{e})^T Re(\mathbf{e}))$.

Then $\forall \omega \in \mathbf{R}$ a unique weak solution exists.

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# Forward Problem - Discretization

$$\begin{pmatrix} -\omega^2 \mathbf{M}_{uu} + \mathbf{K}_{uu} & \mathbf{K}_{u\phi} \\ \mathbf{K}_{u\phi}^T & -\mathbf{K}_{\phi\phi} \end{pmatrix} \begin{pmatrix} \vec{\hat{u}} \\ \hat{\varphi} \end{pmatrix} = \begin{pmatrix} \vec{\hat{f}}_m \\ \hat{f}_e \end{pmatrix}$$

$$(m_{uu})_{ij} = \int_\Omega \rho \underline{N}_i^{uT} \underline{N}_j^u \, d\Omega \quad \text{(mass matrix)}$$

$$(k_{uu})_{ij} = \int_\Omega (\underline{N}_i^{uT} DIV) \mathbf{c}^E (DIV^T \underline{N}_j^u) \, d\Omega \quad \text{(stiffness matrix)}$$

$$(k_{u\phi})_{ij} = \int_\Omega (\underline{N}_i^{uT} DIV) \mathbf{e} (\text{grad} N_j^\phi) \, d\Omega \quad \text{(piezo. coupling matrix)}$$

$$(k_{\phi\phi})_{ij} = \int_\Omega (\text{grad} N_i^\phi)^T \varepsilon^S (\text{grad} N_j^\phi) \, d\Omega \quad \text{(permittivity matrix)}$$

$N_i^u, N_i^\phi$ - nodal shape functions

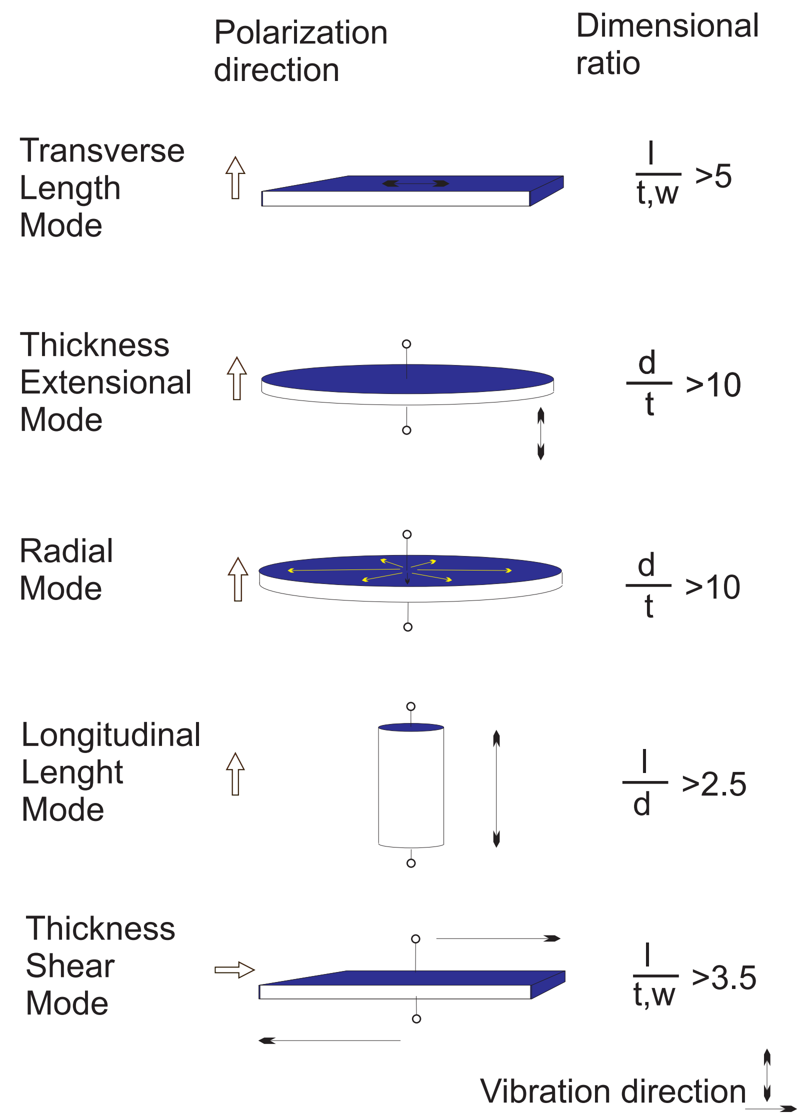
Properties of system matrix:

- Symmetric, not hermitian
- Indefinite spectrum

# Inverse Problem – State of the Art

- Analysis of vibrations of simple shaped transducers
- Explicit relations between material parameters and resonance frequencies

- Samples and measurements are costly
- Restricted to constant coefficients
- No identification out of more general geometries





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# Inverse Problem – Identification by Simulation of Piezoelectric PDEs

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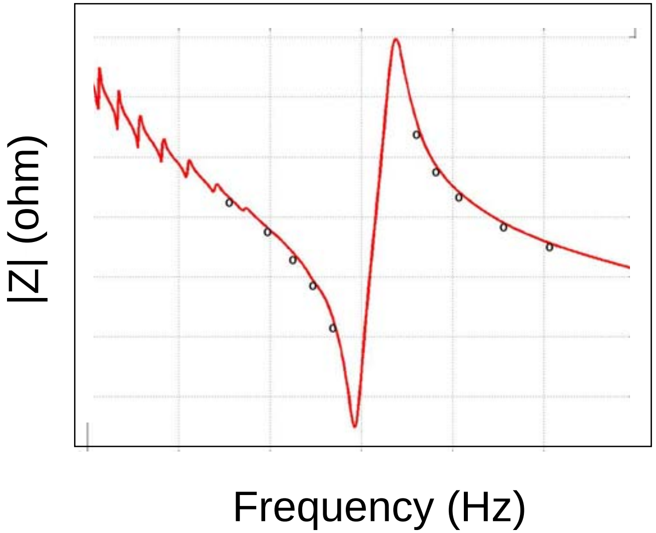


*Find material tensors* $\mathbf{c}^E$, $\mathbf{e}$, $\varepsilon^S$ *from impedance measurements for different frequencies* $\omega$

$$Z(\omega) = \frac{\widehat{\phi}^e(\omega)}{j\omega\widehat{q}^e(\omega)}$$

$$\widehat{q}^e = \int_{\Gamma_e} \vec{n}\left(\mathbf{e}DIV^T\vec{\widehat{u}} - \varepsilon^S \mathrm{grad}\widehat{\phi}\right) \mathbf{d}\Gamma_e$$

$Z$–impedance, $\phi^e$–impressed voltage, $\widehat{q}^e$–surface charge

- Nonlinear operator equation $\widehat{\mathbf{F}}(\mathbf{c}^E, \mathbf{e}, \varepsilon^S) = \widehat{q}^e_{meas}$
- Forward operator $\widehat{\mathbf{F}}$ involves set of PDE solution

# Inverse Problem – Ill Posedness

Since geometries of test samples are arbitrarily chosen

$$rank\left(F'(\mathbf{c}^E, e, \varepsilon^S)\right) \neq 10$$

Instabilities occur while solving the nonlinear operator equation due to

- Non convergence of generalized inverse of rank deficient matrices
- Low influence of certain parameters on solution of forward problem lead to small singular values

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# Inverse Problem – Solution/ Regularization by Inexact Newton Methods

Choose $\mathbf{p}^0 = (\mathbf{c}^E, \mathbf{e}, \varepsilon^S)^0$;
set $k = 0$;
while $\|\hat{y} - \hat{\mathbf{F}}(p^k)\| \geq \tau\delta$ do
    set $s_0^k = 0$;
    while $||\hat{y} - \hat{\mathbf{F}}(p^k) - \hat{\mathbf{F}}'(p^k)[s_n^k]|| \geq \eta_k ||\hat{y} - \hat{\mathbf{F}}(p^k)||$ do
        $s_n^k = \Phi\left(\hat{\mathbf{F}}'(p^k), \hat{y} - \hat{\mathbf{F}}(p^k), s_{n-1}^k\right)$;
        $n{+}{+}$;
    $\mathbf{p}^{k+1} = \mathbf{p}^k + s_n^k$;
    $k{+}{+}$;

$\delta$ - data noise, $\tau > 1$, $\eta_k$ - tolerance factor

Choices for $\Phi(\ldots)$:

Landweber's iteration, $\nu$-methods, CG

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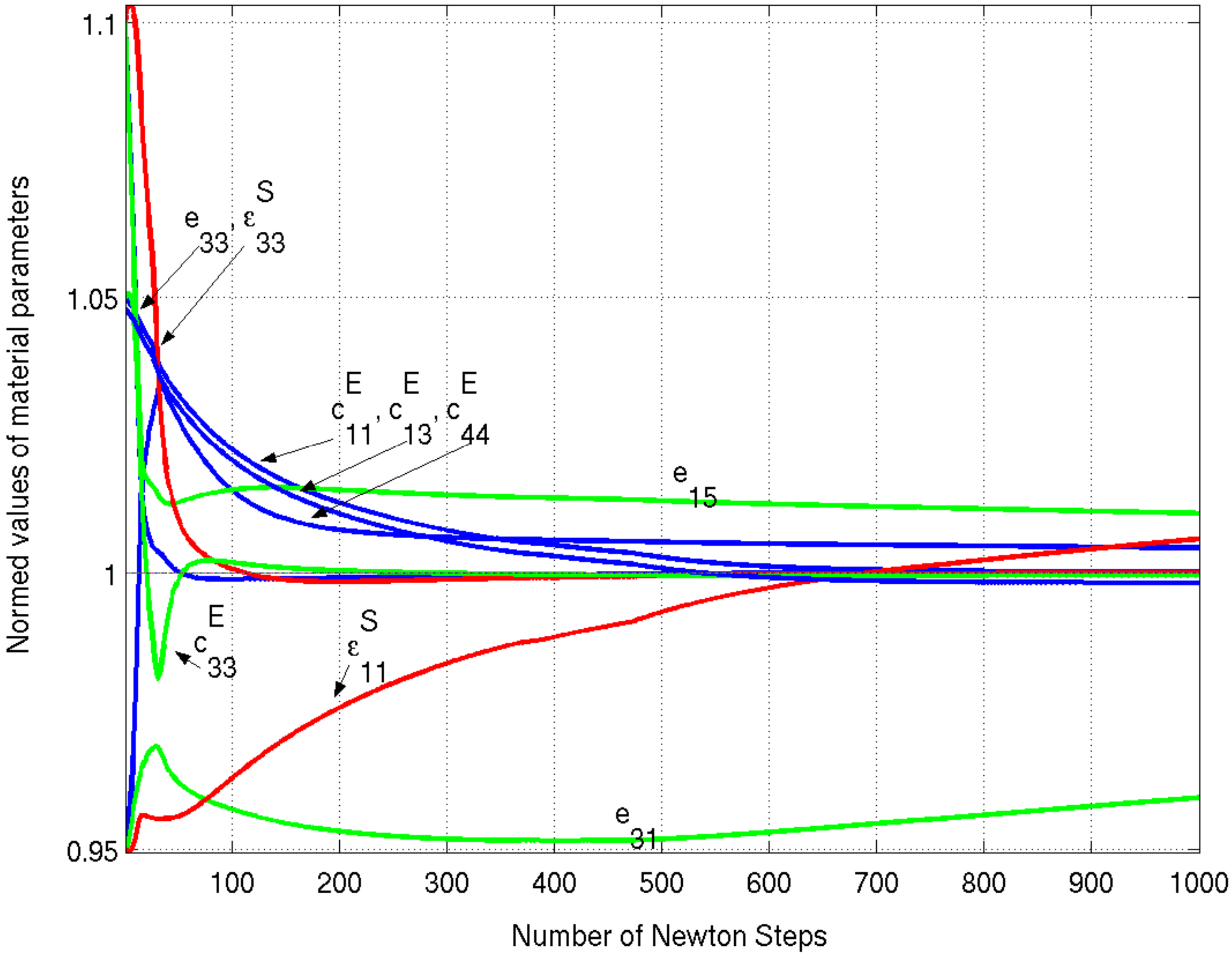
# Numerical Results – Simultaneous Reconstruction of all parameters

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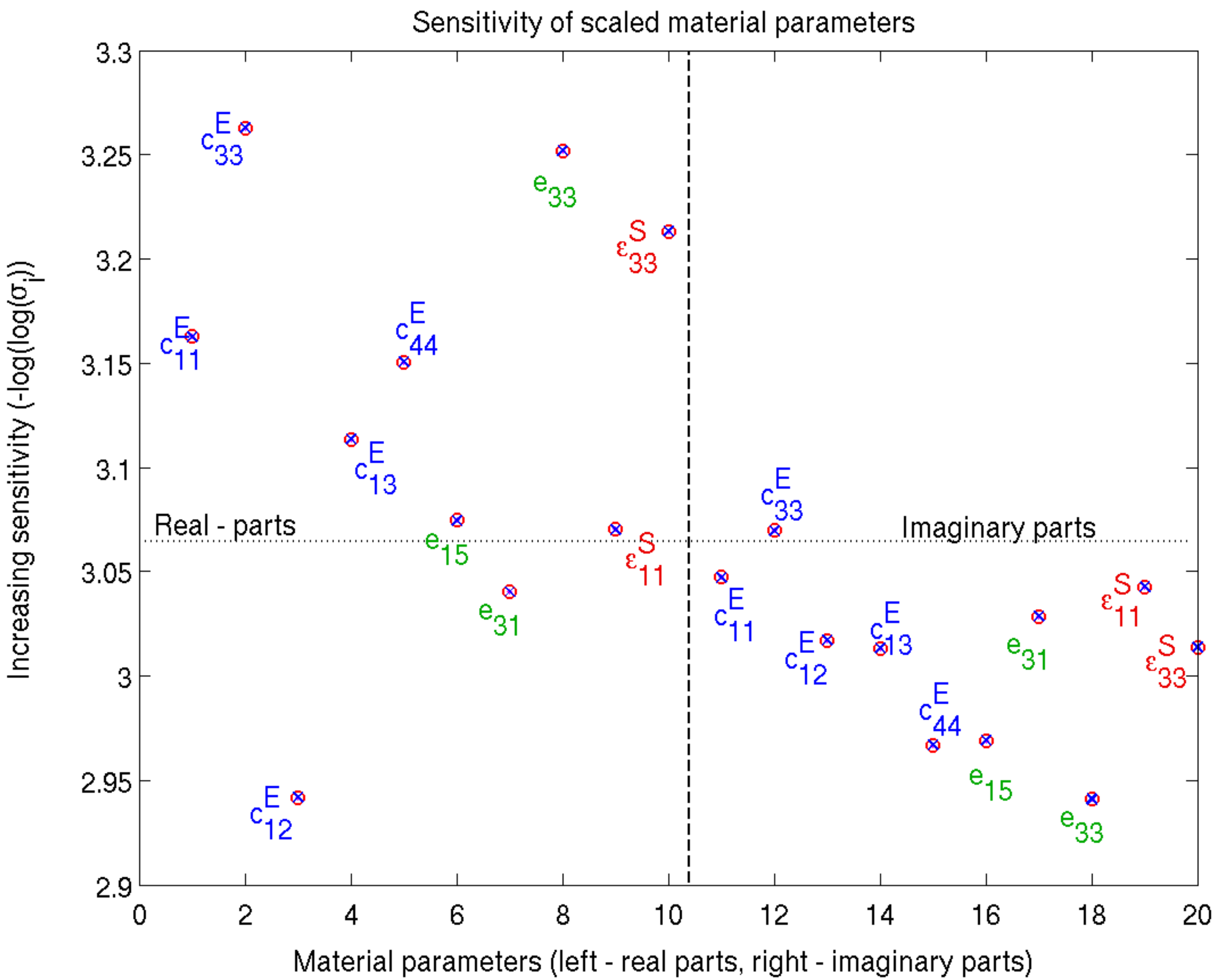
# Numerical Results - Sensitivity

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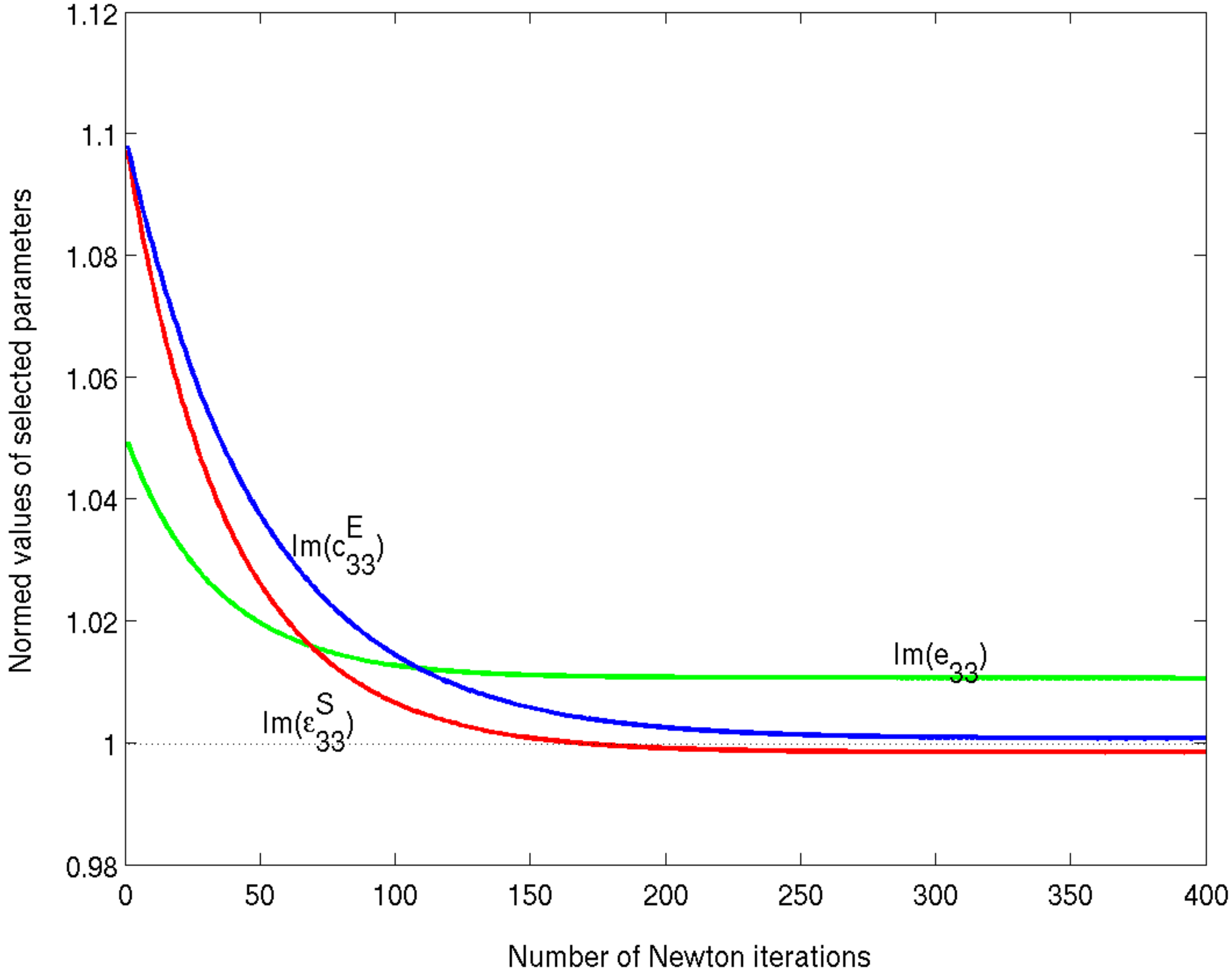
# Numerical Results - Complex Valued Parameter

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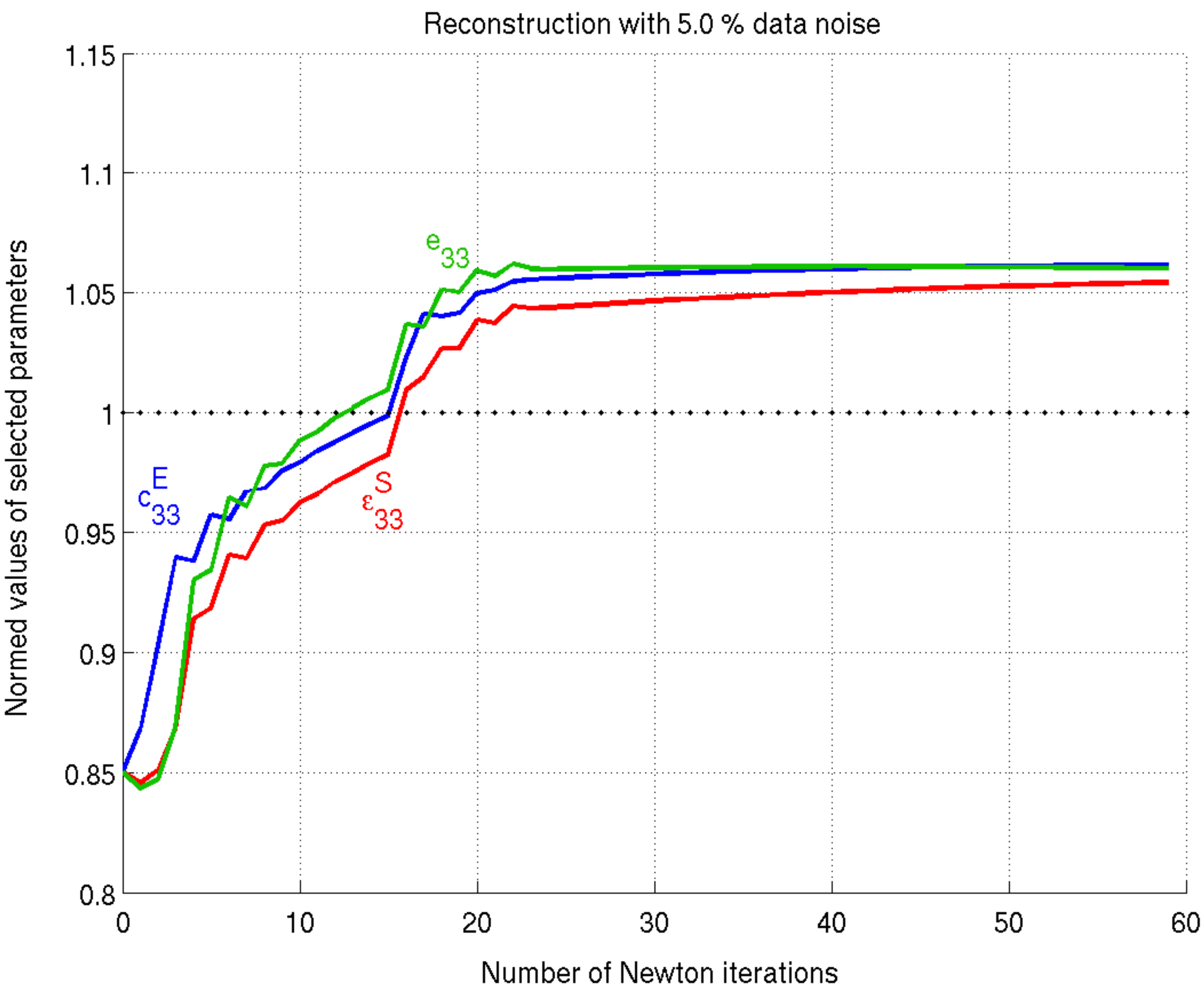
# Numerical Results - Noisy Data





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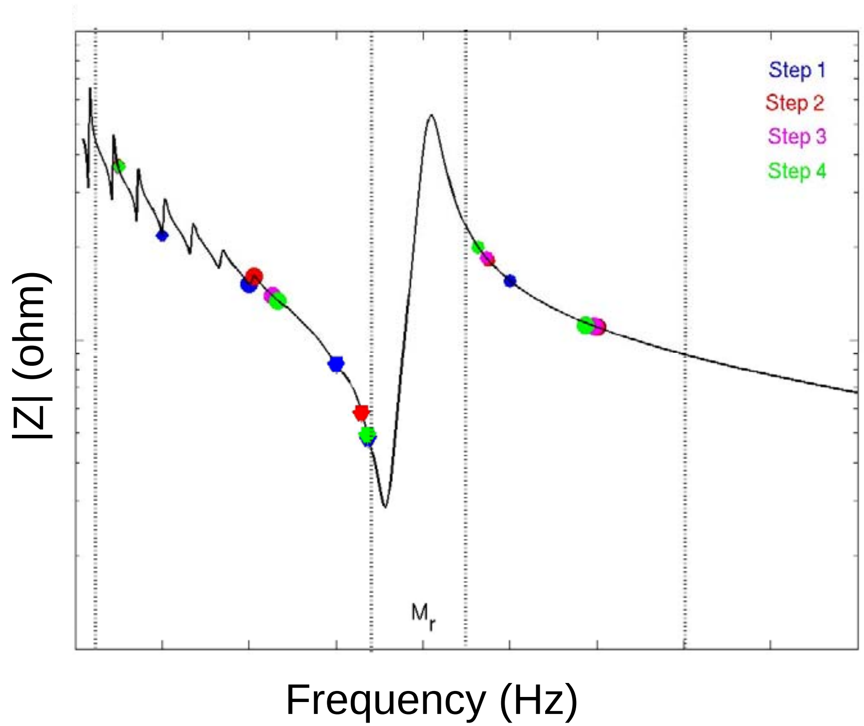
# Numerical Results - Improvement by Optimal Experiment Design I

Choose frequencies in $M_r$ in such a way that:

- Sensitivity of measurements is maximal
- Result of reconstruction is robust to data errors

$$\widehat{q}_i^{e,\delta} = \widehat{q}_i^e + \delta_i$$




$$\min_{\omega} \frac{1}{n_{par}} trace(Cov(p,\omega)), \text{ where } \delta_i \sim N(0, \sigma(\omega_i)^{-1})$$

$$Cov(p,\omega) = \left( \sum_{i=1}^{n_{freq}} \widehat{F}_p'(p,\omega_i)^H \sigma(\omega_i) \widehat{F}_p'(p,\omega_i) \right)^{-1}$$

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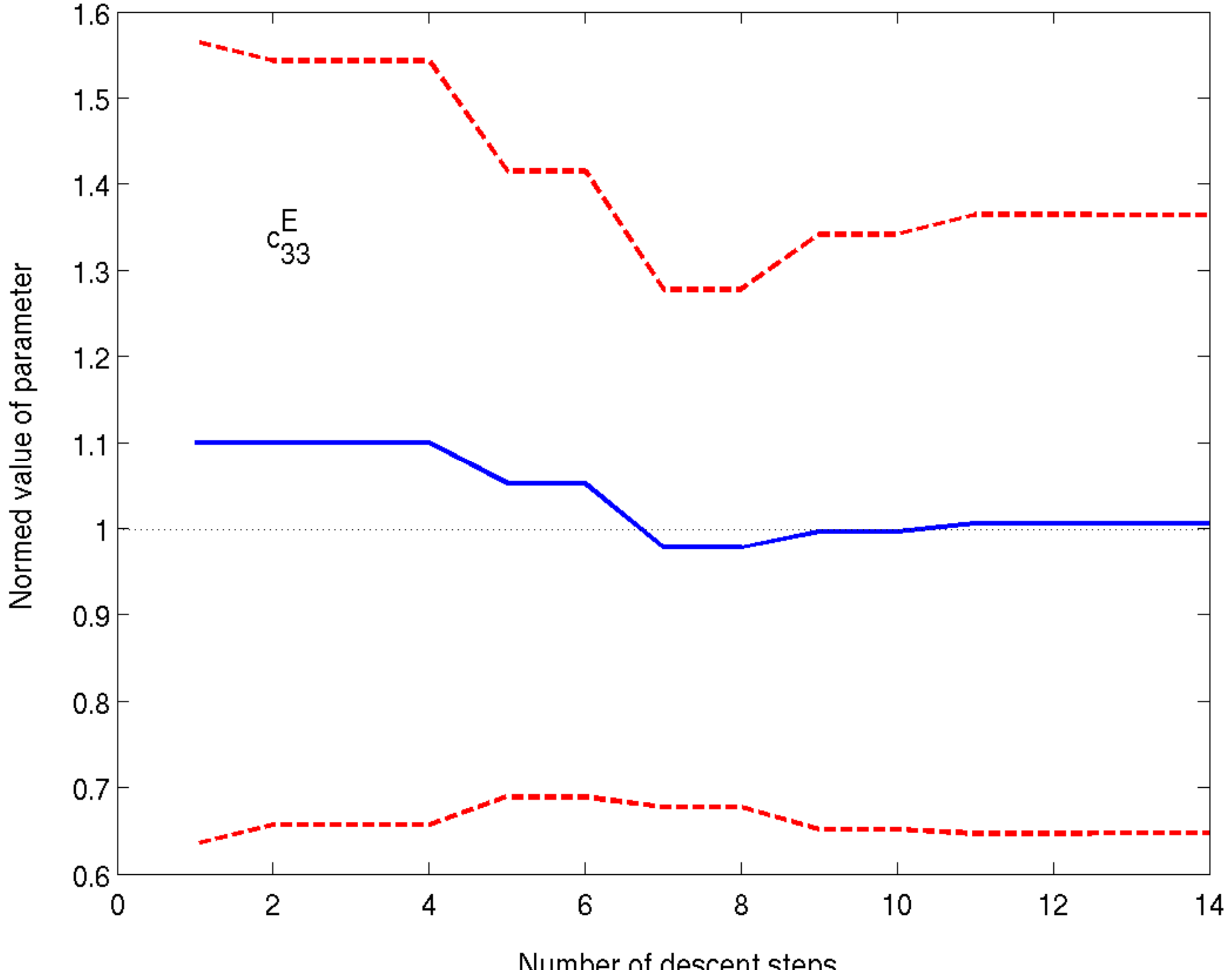
# Numerical Results - Improvement by Optimal Experiment Design I - Results

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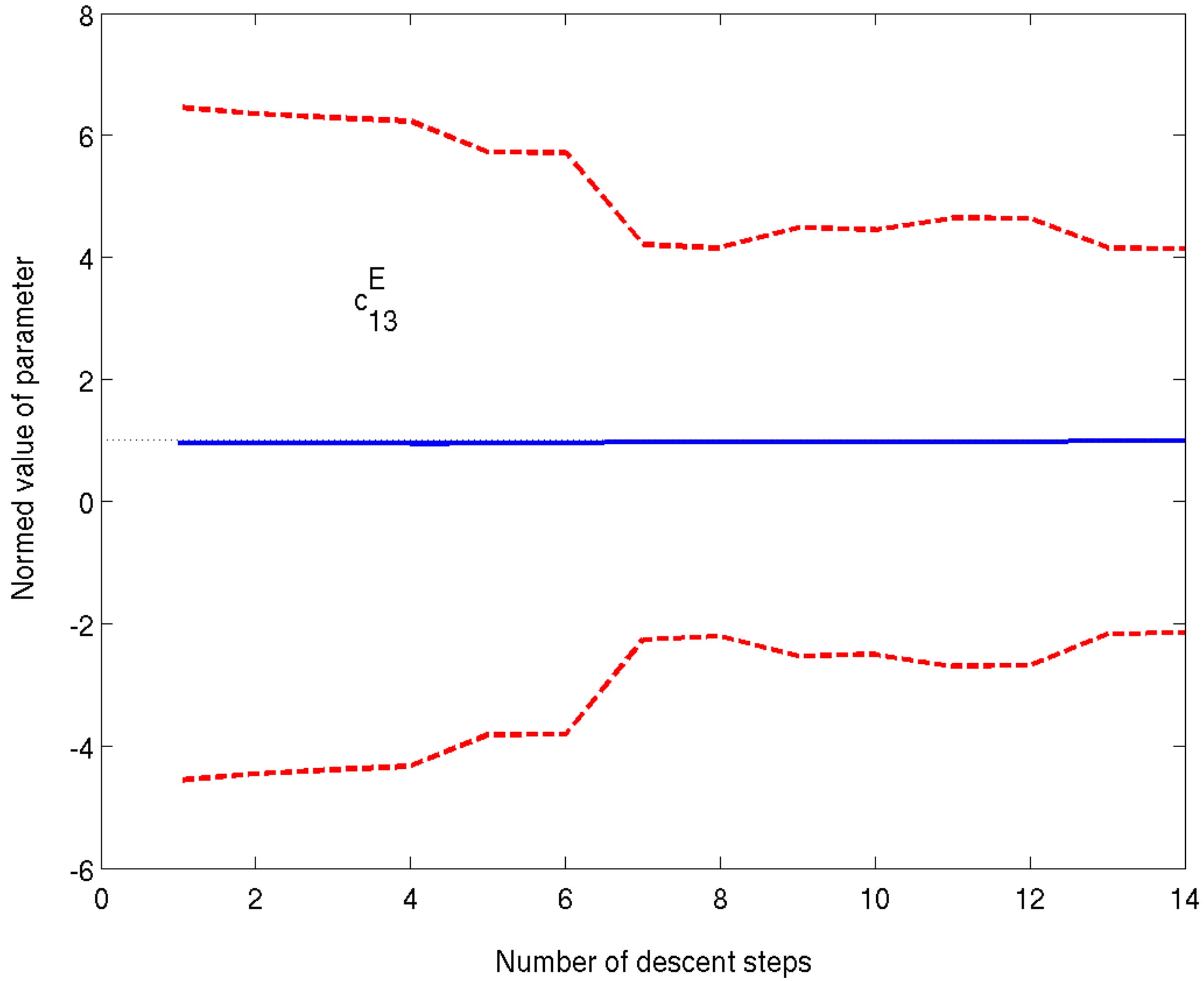



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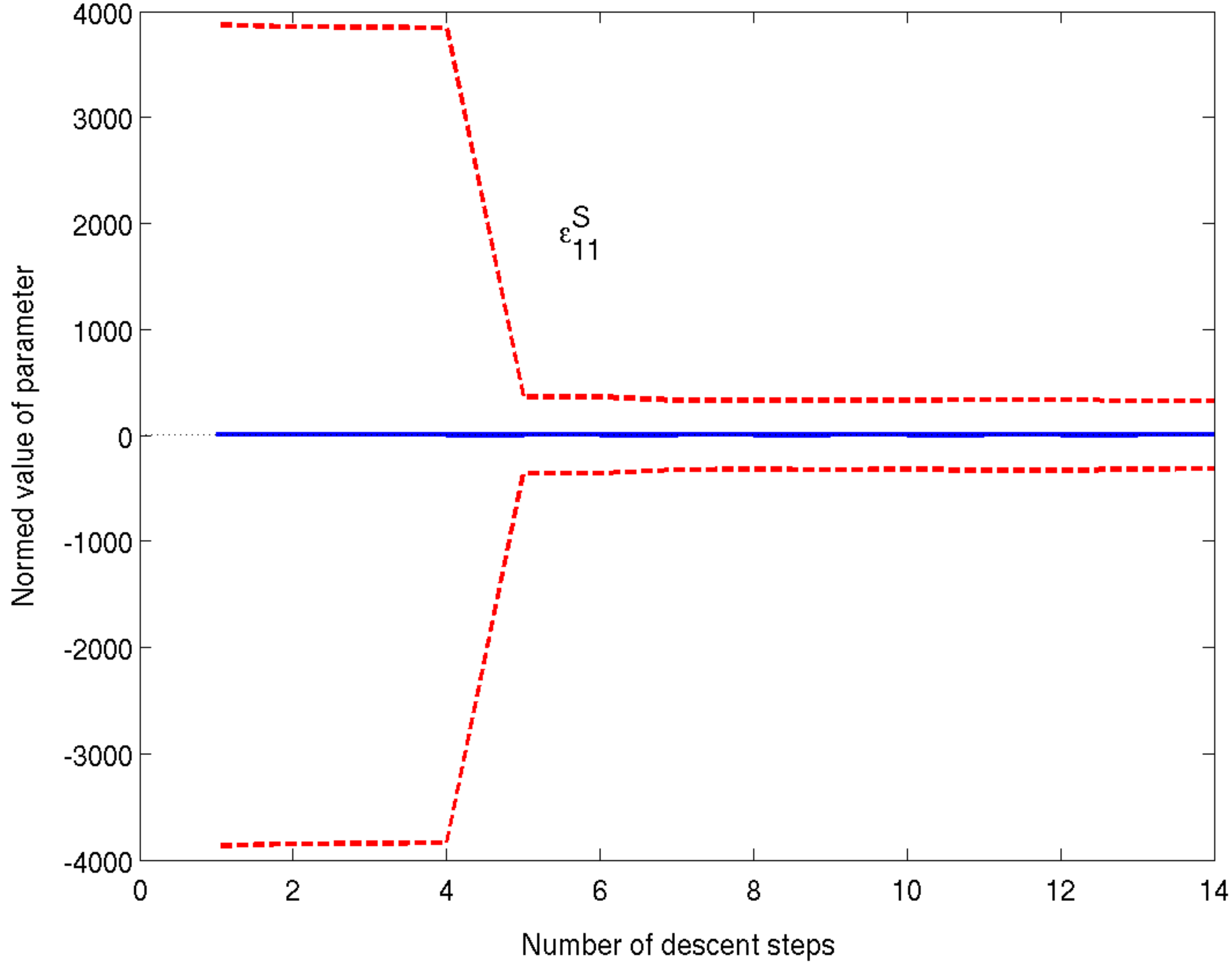
# Numerical Results - Improvement by Optimal Experiment Design I - Results

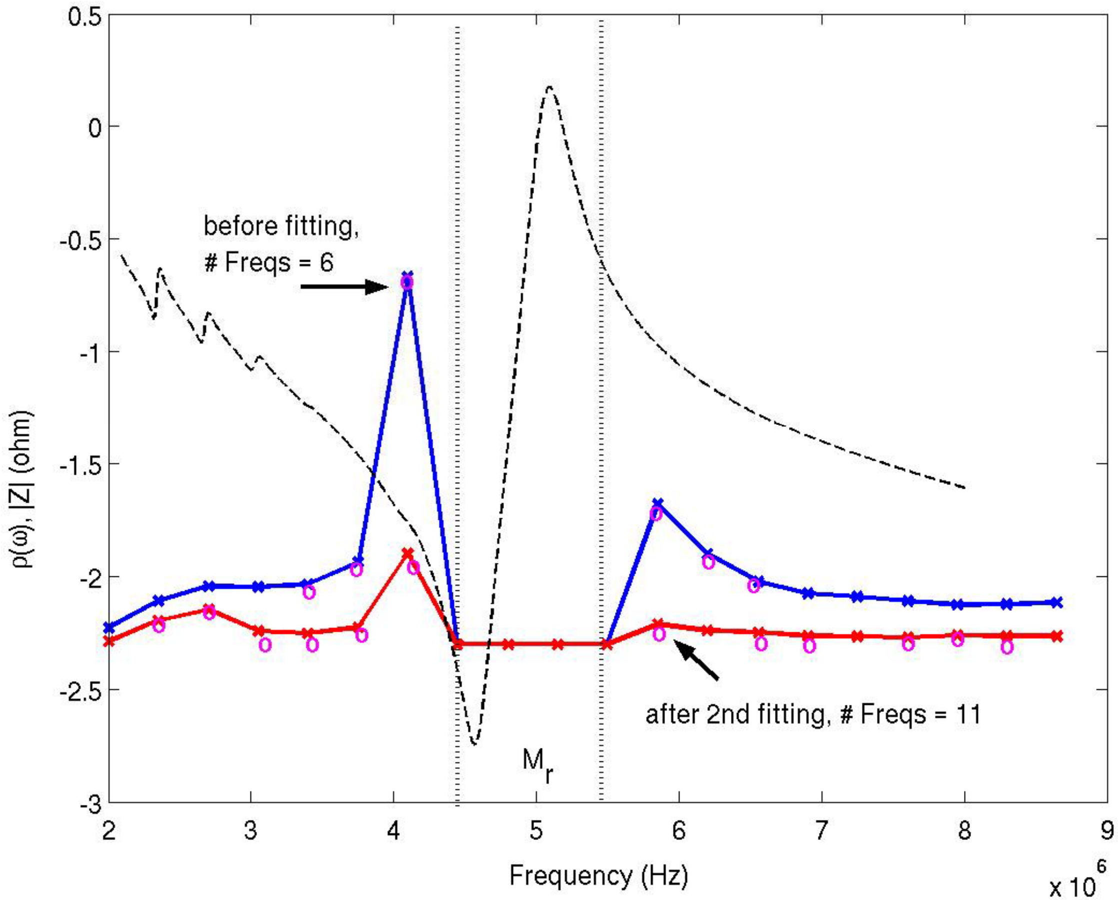


# Numerical Results - Improvement by Optimal Experiment Design II

Variable number of frequencies

- Measurements are weighted by density $\rho(\omega)$

- Select frequencies with large weights




$$\min_{0<\rho(\omega)\leq 1} \frac{1}{n_{par}} \left( \int_{\omega_0}^{\omega_f} \rho(\omega) \widehat{F}'(p,\omega)^H \sigma(\omega) \widehat{F}'(p,\omega) \right)^{-1}$$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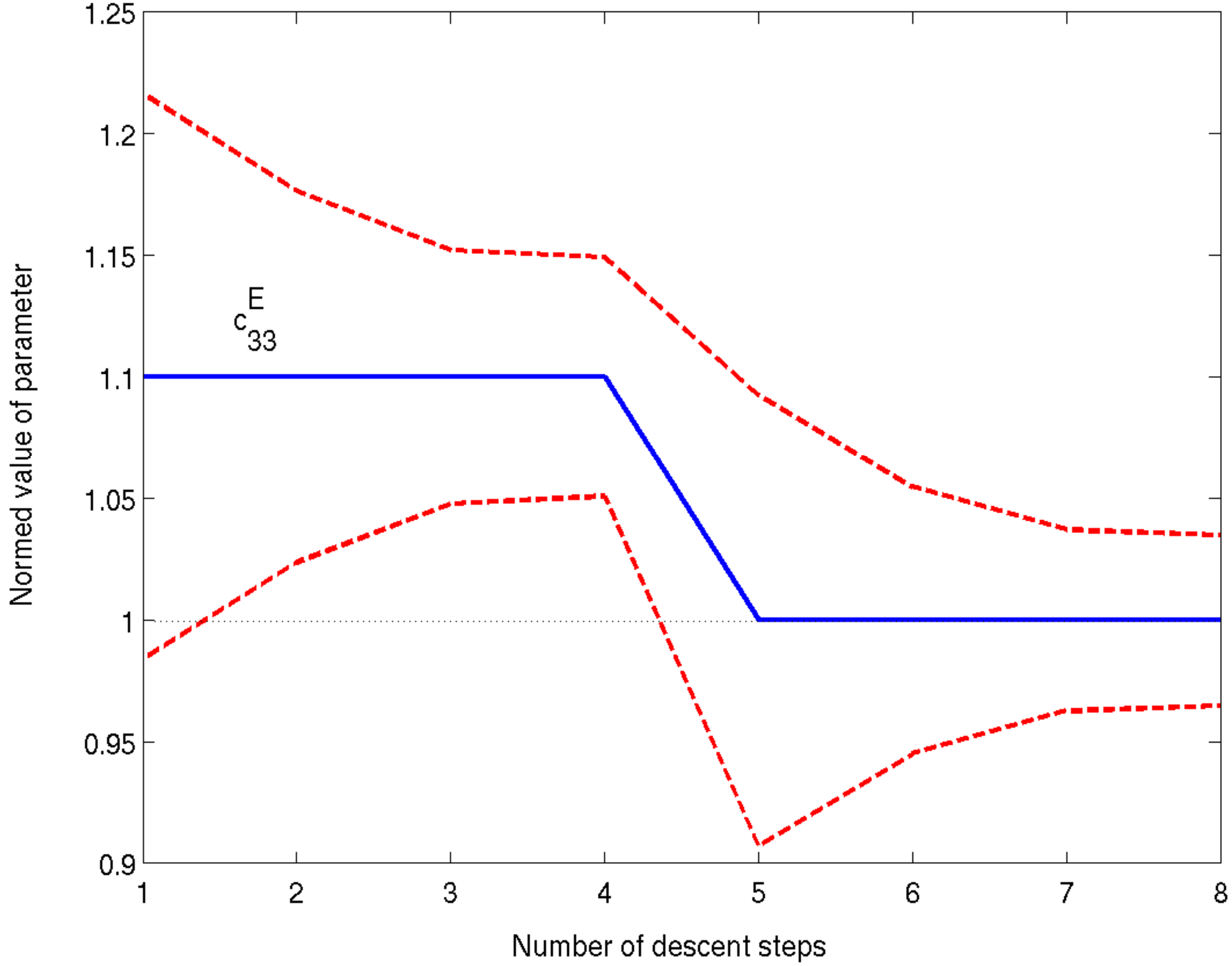
# Numerical Results - Optimal Experiment Design II - Results





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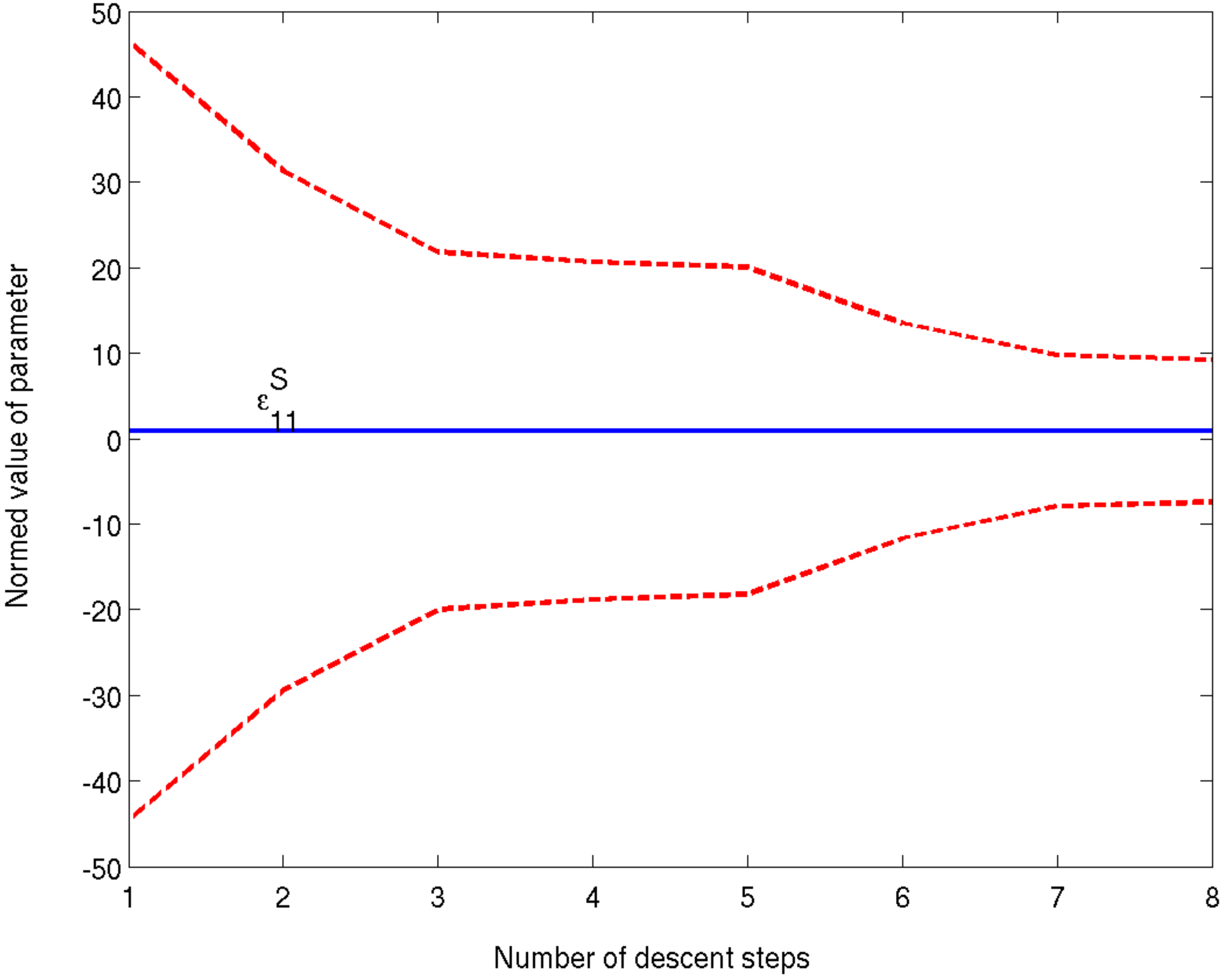
# Numerical Results - Optimal Experiment Design II - Results

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# Summary and Outlook

- Identification of piezoelectric material parameters by a simulation based inversion scheme
  - account for losses (complex valued parameters)
  - determine parameters in dependency of external heating, for different frequencies, …
  - sophisticated choice of measured data

- Consider nonlinear effects such as
  - high strains and electric field intensities
  - internal energy conversion, temperature dependency
  - hysteretic effects

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