Adjoint-State Fréchet Derivatives and Gauss–Newton Hessian for Full-Wave Maxwell Inversion

1 Forward Problem

We consider the frequency-domain Maxwell equation:

$$\nabla \times (\mu^{-1} \nabla \times \boldsymbol{E}) - i\omega\sigma\boldsymbol{E} - \omega^2 \varepsilon \boldsymbol{E} = \boldsymbol{f}. \tag{1}$$

Define operator:

$$\mathcal{A}(m)\boldsymbol{E} = \boldsymbol{f}, \quad m = (\sigma, \varepsilon, \mu).$$

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2 Misfit Functional

$$J(m) = \frac{1}{2} \sum_r \|\boldsymbol{P}_r \boldsymbol{E} - \boldsymbol{d}_r\|^2. \tag{2}$$

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3 First-Order Linearization

Let

$$m \to m + \delta m, \quad \boldsymbol{E} \to \boldsymbol{E} + \delta \boldsymbol{E}.$$

Linearizing:

$$\mathcal{A}(m)\delta\boldsymbol{E} = -D_m \mathcal{A}[\delta m]\boldsymbol{E}.$$

Thus,

$$\delta \boldsymbol{E} = -\mathcal{A}^{-1} D_m \mathcal{A}[\delta m]\boldsymbol{E}. \tag{3}$$

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4 Jacobian Operator

Define the parameter-to-data map:

$$\boldsymbol{F}(m) = \boldsymbol{P}\boldsymbol{E}(m).$$

Linearization:

$$D\boldsymbol{F}[\delta m] = \boldsymbol{P}\delta\boldsymbol{E} = -\boldsymbol{P}\mathcal{A}^{-1}D_m\mathcal{A}[\delta m]\boldsymbol{E}.$$

Define Jacobian operator:

$$\mathcal{J} = -\boldsymbol{P}\mathcal{A}^{-1}D_m\mathcal{A}.$$

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5 Gauss–Newton Hessian

The Gauss–Newton approximation neglects second-order derivatives of $\boldsymbol{E}$.

$$H_{GN} = \mathcal{J}^*\mathcal{J}.$$

Substitute expression:

$$H_{GN} = (D_m\mathcal{A})^*(\mathcal{A}^{-1})^*\boldsymbol{P}^*\boldsymbol{P}\mathcal{A}^{-1}D_m\mathcal{A}.$$

If residual is small:

$$\boldsymbol{P}^*\boldsymbol{P} \approx \text{data weighting}.$$

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6 Explicit Kernel Representation

We insert the explicit Fréchet derivatives.

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6.1 Derivative w.r.t. σ

$$D_\sigma\mathcal{A}[\delta\sigma]\boldsymbol{E} = i\omega\delta\sigma\boldsymbol{E}.$$

Thus Jacobian action:

$$\delta d = -i\omega\boldsymbol{P}\mathcal{A}^{-1}(\delta\sigma\boldsymbol{E}).$$

Hence Hessian kernel:

$$H_{\sigma\sigma}(x, x') = \omega^2\Re\left[\boldsymbol{E}(x)\cdot\boldsymbol{\Lambda}(x')\right], \tag{4}$$

where $\boldsymbol{\Lambda}$ solves adjoint problem.

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6.2 Derivative w.r.t. ε

$$D_\varepsilon \mathcal{A} = \omega^2 \delta\varepsilon \boldsymbol{E}.$$

Thus,

$$H_{\varepsilon\varepsilon} \sim \omega^4 (\boldsymbol{E} \cdot \boldsymbol{\Lambda}). \tag{5}$$

High-frequency amplification factor:

$$H_{\varepsilon\varepsilon} \propto \omega^4.$$

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6.3 Derivative w.r.t. μ

$$D_\mu \mathcal{A} = -\nabla \times (\mu^{-2} \delta\mu \nabla \times \boldsymbol{E}).$$

After adjoint manipulation:

$$H_{\mu\mu} \sim \mu^{-4} (\nabla \times \boldsymbol{E}) \cdot (\nabla \times \boldsymbol{\Lambda}). \tag{6}$$

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7 Block Hessian Structure

Let

$$m = \begin{pmatrix} \sigma \\ \varepsilon \\ \mu \end{pmatrix}.$$

Then Gauss–Newton Hessian has block form:

$$H_{GN} = \begin{pmatrix} H_{\sigma\sigma} & H_{\sigma\varepsilon} & H_{\sigma\mu} \\ H_{\varepsilon\sigma} & H_{\varepsilon\varepsilon} & H_{\varepsilon\mu} \\ H_{\mu\sigma} & H_{\mu\varepsilon} & H_{\mu\mu} \end{pmatrix}.$$

Cross terms arise from mixed Jacobians.
Example:

$$H_{\sigma\varepsilon} \sim \omega^3 (\boldsymbol{E} \cdot \boldsymbol{\Lambda}).$$

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8 Multi-Frequency Joint Inversion

For frequencies $\{\omega_k\}_{k=1}^K$:

$$J(m) = \sum_{k=1}^{K} J^{(k)}(m).$$

Total Gauss–Newton Hessian:

$$H_{GN} = \sum_{k=1}^{K} H_{GN}^{(k)}.$$

Each block scales as:

$$H_{\sigma\sigma}^{(k)} \sim \omega_k^2, \quad H_{\varepsilon\varepsilon}^{(k)} \sim \omega_k^4, \quad H_{\mu\mu}^{(k)} \sim O(1).$$

Thus multi-frequency stacking improves conditioning:

$$H_{total} = \sum_k \mathcal{J}_k^* \mathcal{J}_k.$$

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9 Compact Operator Form

$$H_{GN} = \sum_k (D_m \mathcal{A}_k)^* (\mathcal{A}_k^{-1})^* W_k \mathcal{A}_k^{-1} D_m \mathcal{A}_k.$$

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10 Key Observations

- ε Hessian scales as ω^4.
- σ Hessian scales as ω^2.
- Multi-frequency inversion yields block-sum structure.
- Cross-talk between σ and ε grows with frequency.
- Helmholtz operator causes indefiniteness in Hessian.