

ARTS retrieval options

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Optimal estimation, theory

A special case of Bayesian inference

- Generally:

- ▶ Forward model needed: $y = F(x, b)$

- ▶ Uncertainties can be represented with covariance matrices (S)

$$\hat{x} = \min_x \left((y - F(x, \hat{b}))^T S_e^{-1} (y - F(x, \hat{b})) + (x - x_a)^T S_a^{-1} (x - x_a) \right)$$

$$S_e = S_\varepsilon + K_b S_b K_b^T \quad \text{or just} \quad S_e = S_\varepsilon$$

- Solution for (local) linear forward model:

$$D_y = \left(K_x^T S_e^{-1} K_x + S_a^{-1} \right)^{-1} K_x^T S_e^{-1}$$

$$\hat{x} = x_a + D_y (y - F(x, \hat{b}))$$

$$A = D_y K_x$$

$$S = D_y S_e D_y^T + (A - I) S_x (A - I)^T$$

Bayesian inference with machine learning

See Pfreunds Schuh et al. (2018) for details

- Recipe:
 - ▶ Create a database of $\{x_i, y_i\}$ with x_i following prior distribution
 - ◇ This can be fully empirical with x_i taken from “ground truth”
 - ◇ Or by simulations: $y_i = F(x_i, b_i)$
 - ▶ Let neural network predict properties of the posterior
 - ◇ Such as quantiles if its CDF (QRNN)
- Advantages
 - ▶ No restrictions to Gaussian statistics or linearity of F
 - ▶ Retrievals fast when training done
- Disadvantages
 - ▶ Training can be computationally expensive
 - ▶ Limitations in the characterization. Not provided directly:
 - Error correlations between elements in x
 - The contribution from different sources to retrieval uncertainty
 - Averaging kernels
 - ▶ but seems possible to derive an ensemble mean characterization

Optimal estimation with ARTS

- The actual inversion can now be done inside ARTS
- Covariance matrices:
 - ▶ Methods to define diagonal and Markov-process covariance matrices
 - ▶ The common case of a block-diagonal structure can be used
- Minimization by linear, Gauss-Newton and Levenberg-Marquardt
- A conjugate gradient approach for large x
- Workspace methods for defining retrieval quantities:

retrievalAddAbsSpecies
retrievalAddCatalogParameter
retrievalAddCatalogParameters
retrievalAddFreqShift
retrievalAddFreqStretch
retrievalAddMagField
retrievalAddPointingZa

retrievalAddPolyfit
retrievalAddScatSpecies
retrievalAddSinefit
retrievalAddSpecialSpecies
retrievalAddSurfaceQuantity
retrievalAddTemperature
retrievalAddWind

- Transformations can be applied

Questions

- Anyone still using Qpack?
- How do you use ARTS' OEM?

- Missing retrieval variables?
- Anything else missing?