



Validating uncertainty estimates

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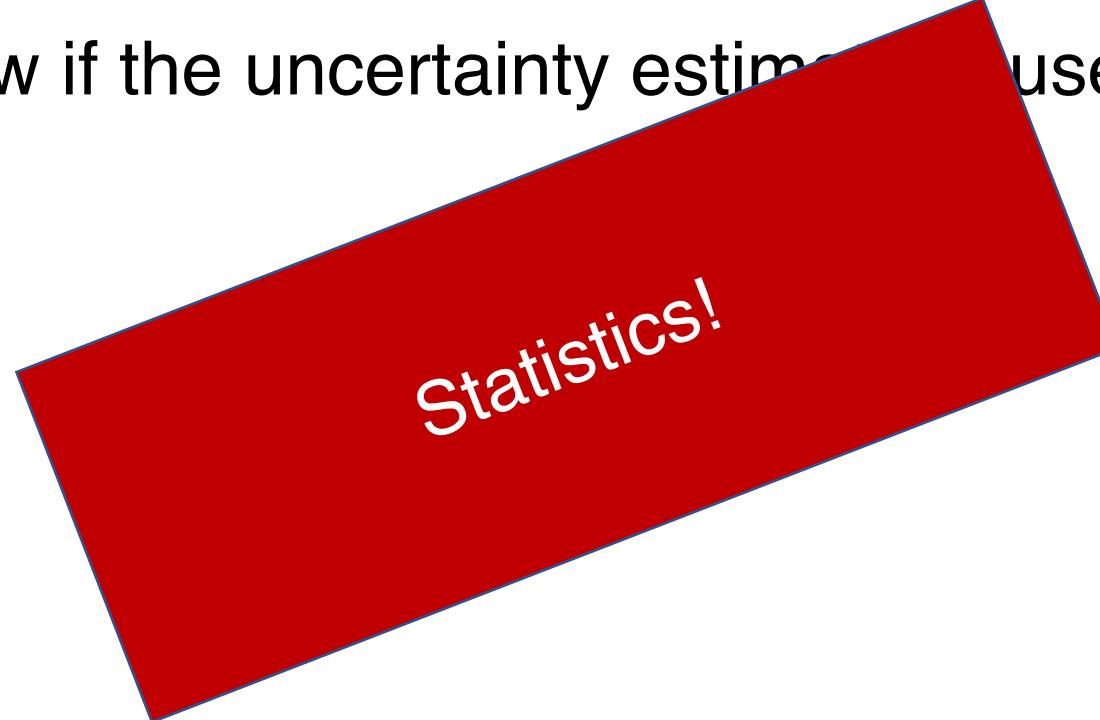
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So your retrieval has an uncertainty estimate...

- How do we know if the uncertainty estimate is useful or realistic?



Statistics!

Reminder: uncertainty and error are different

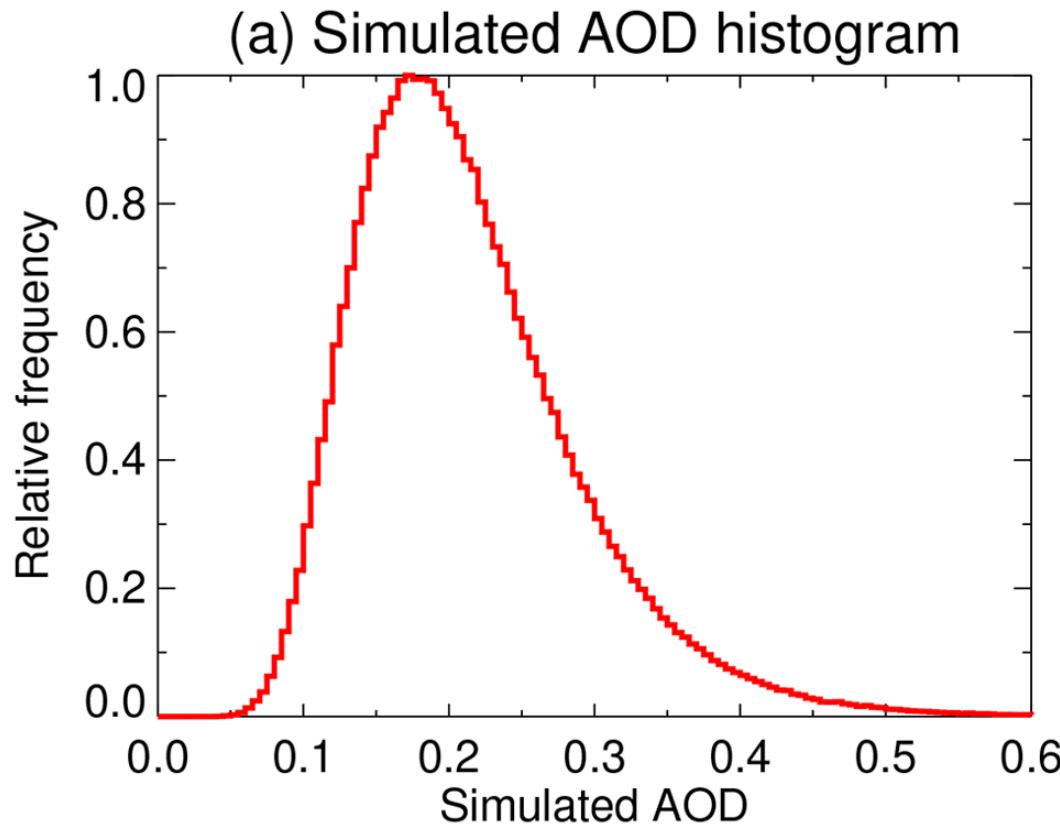
- Uncertainty is an *expected level of dispersion*
 - Typically one standard deviation (1σ , ~68% of the time as good as X)
- Error is an observed quantity
 - A *draw from the distribution* of possible errors given the uncertainty level



You expect 3.5
You get 1, 2, 3, 4, 5, or 6

Uncertainty distributions and error distributions

- Suppose AOD uncertainty is $\pm(0.05+15\%)$. Then:



Sayer *et al.*, AMT (2020)

Solution: compare distributions of observed errors to expected discrepancy (ED)

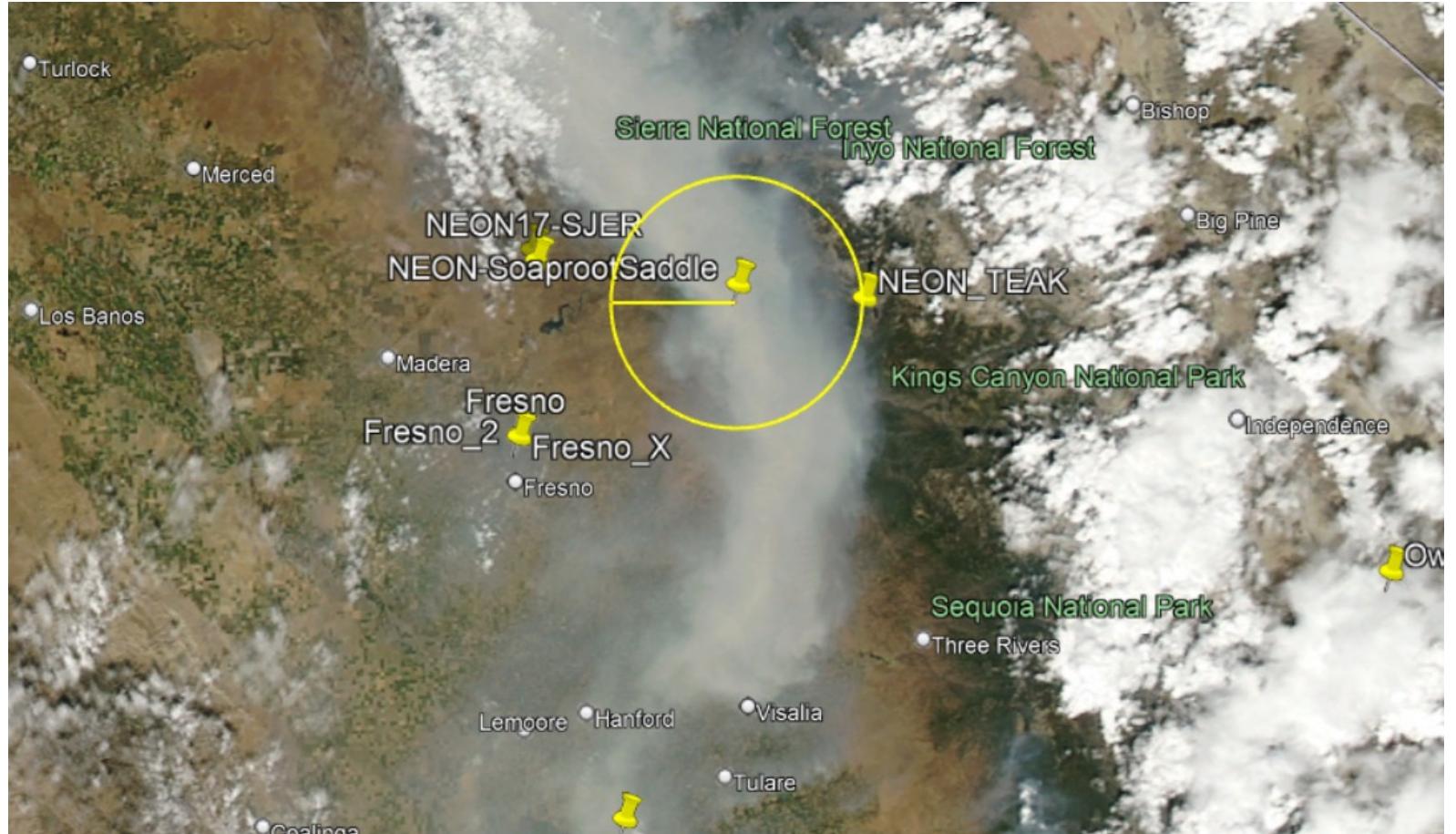
- Observed error = (truth – retrieval)
- Expected discrepancy contains contributions from:
 - Retrieval uncertainty σ_{sat}
 - Reference uncertainty σ_{ref}
 - Spatiotemporal variability inherent in the comparison σ_{var}
- If assumed independent, then:

The diagram shows the formula for Expected Discrepancy (ED) as a light blue horizontal bar containing the equation $ED = \sqrt{(\sigma_{\text{sat}}^2 + \sigma_{\text{ref}}^2 + \sigma_{\text{var}}^2)}$. Three red circles, each containing one term of the equation, are overlaid on the bar. Red lines point from text labels above the circles to each circle: the left circle is labeled "Propagated or simulated", the middle circle is labeled "Documented and small (hopefully)", and the right circle is labeled "Can be a real pain to generalise".

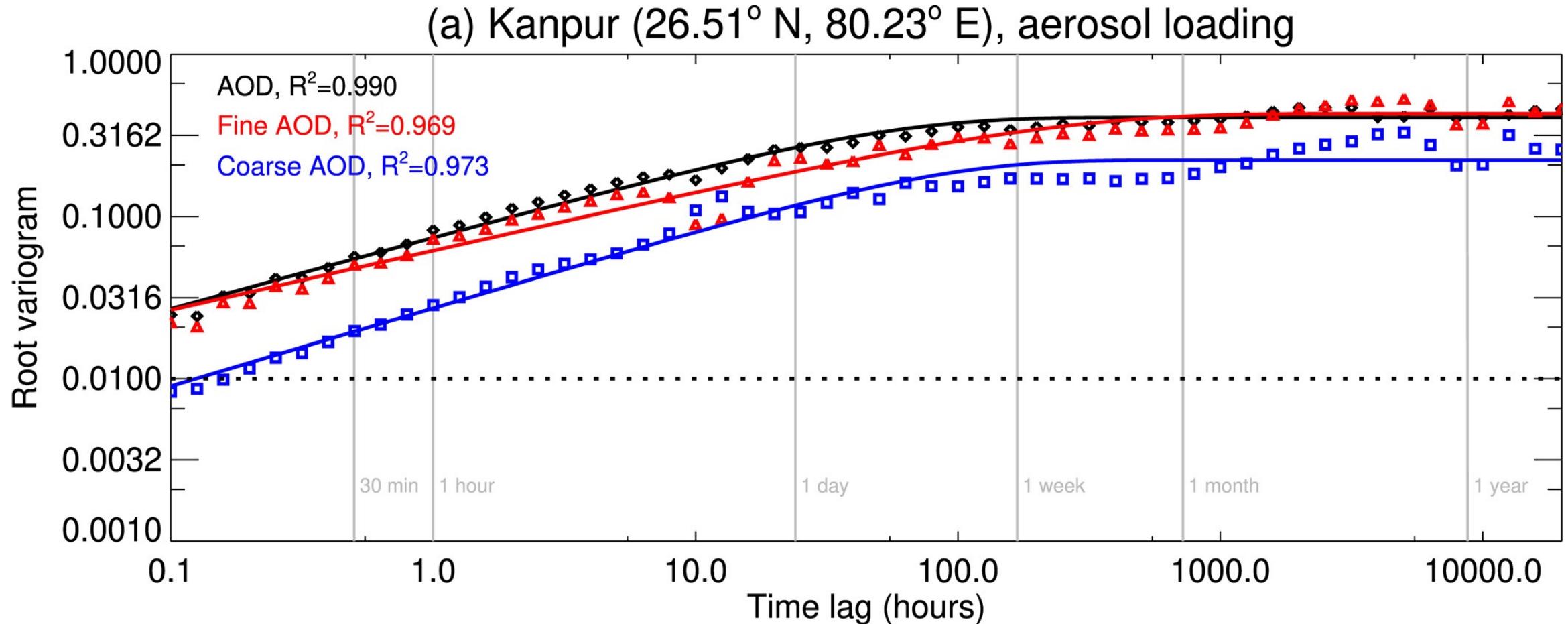
$$ED = \sqrt{(\sigma_{\text{sat}}^2 + \sigma_{\text{ref}}^2 + \sigma_{\text{var}}^2)}$$

Spatial and temporal variations can both be important

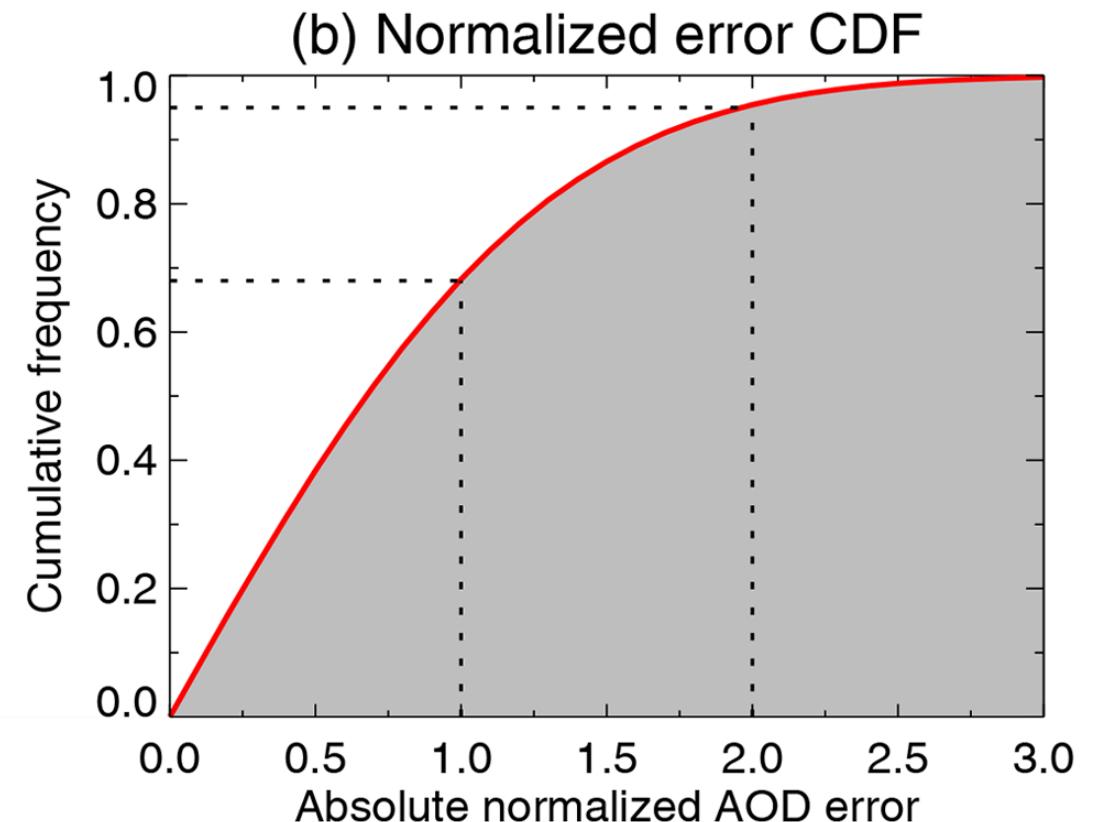
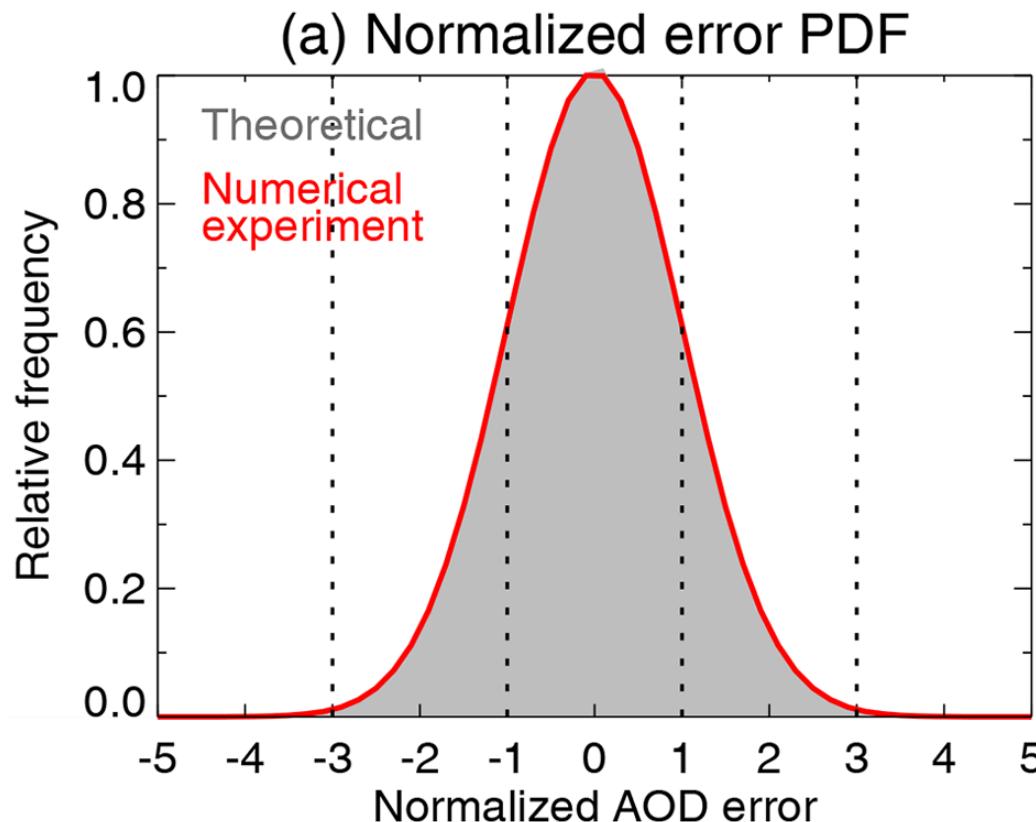
- Look at *spatial statistics* of satellite data in the area, *temporal statistics* of the ground data
- Generalise based on a model
- Use *robust statistics* (e.g., median not mean)
- Shrink area aggregated or comparison window



Spatial and temporal variations can both be important



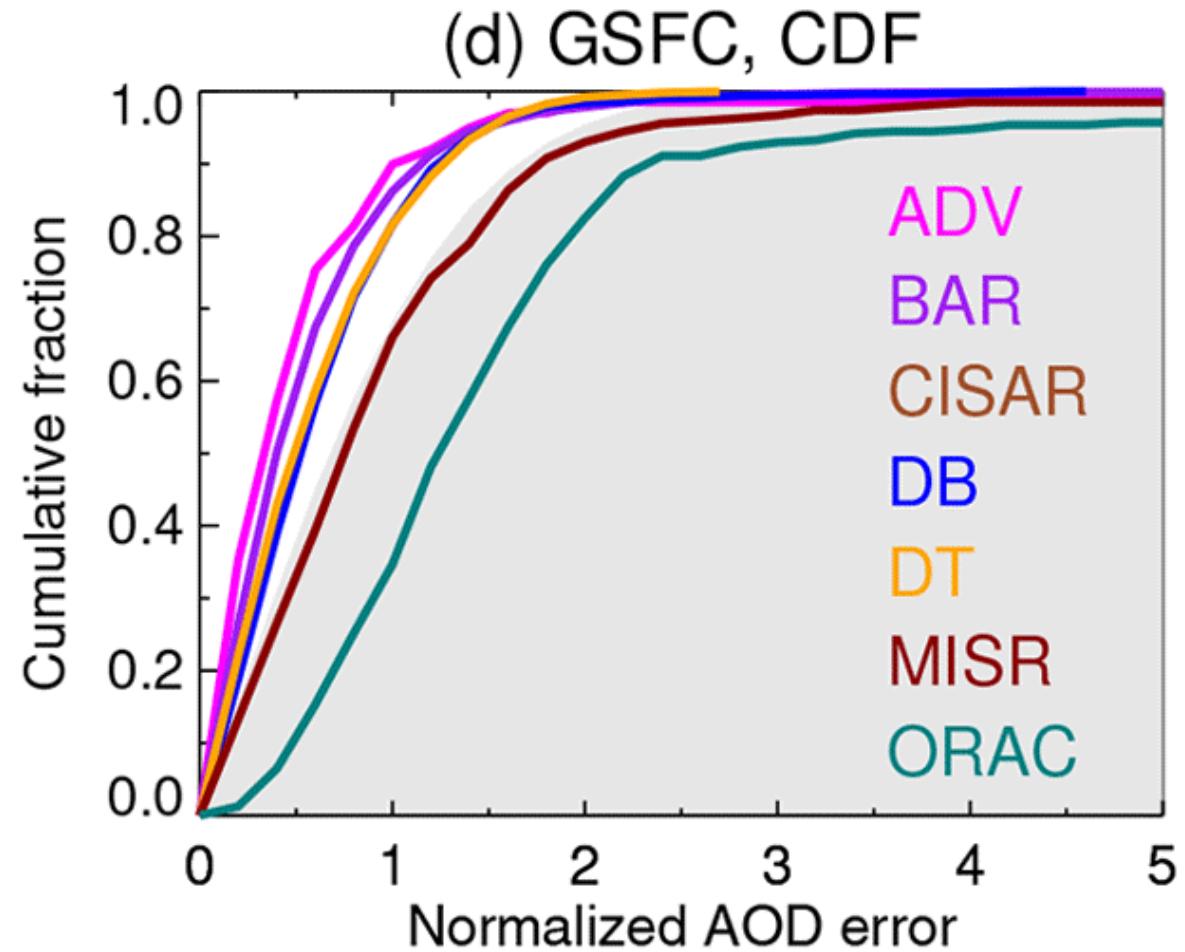
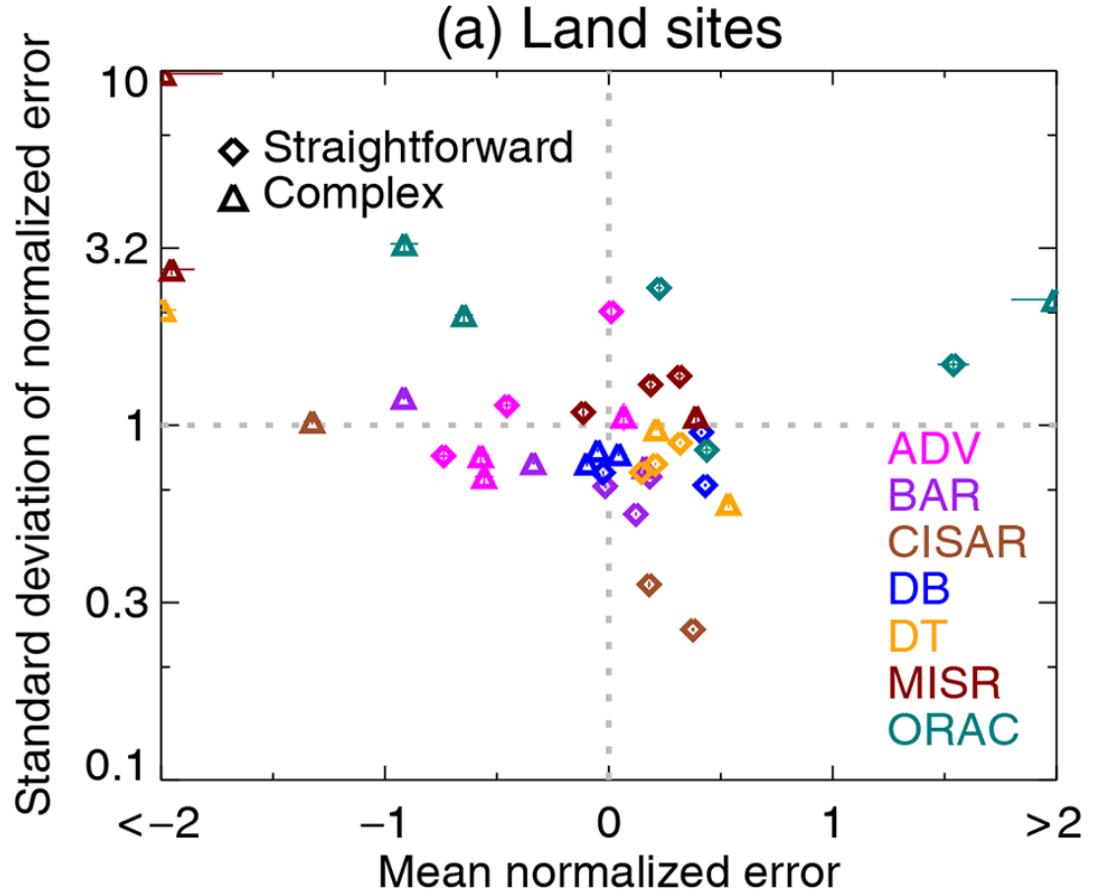
Look at distributions of normalised error



- Normalise as error/ED
- If unbiased and appropriate magnitude, distributions should follow $N(0,1)$

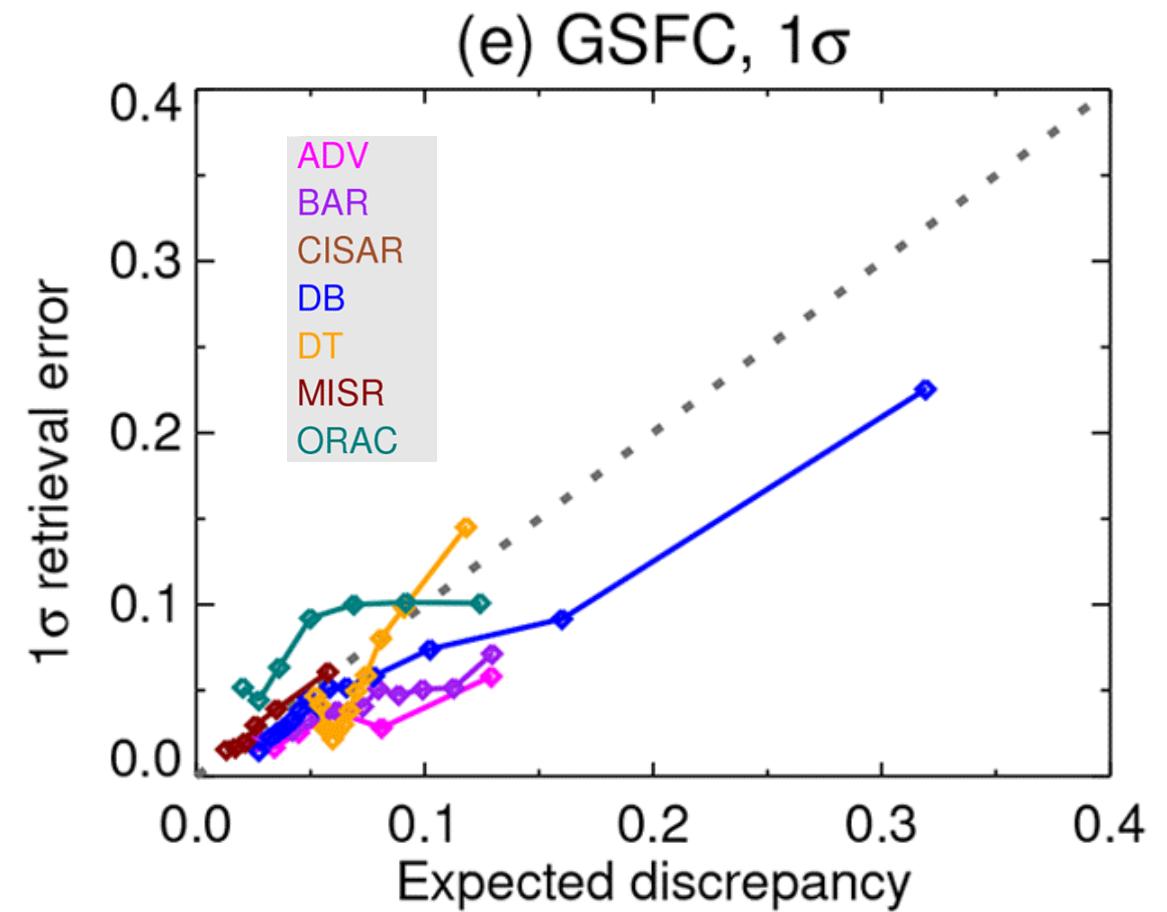
Sayer *et al.*, AMT (2020)

Examples on real aerosol data



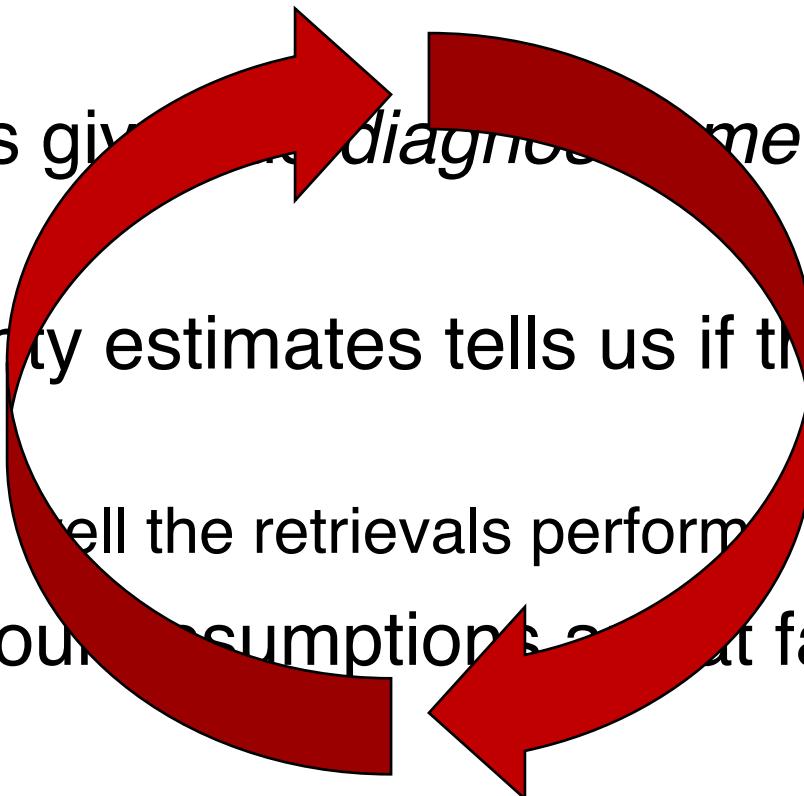
Can we tell low-uncertainty situations from high ones?

- Stratify by ED
- Look at 1σ point (68^{th} percentile) of absolute error
 - Additional percentiles can tell you more about *how Gaussian* the error distribution is for a given ED
- Similar to *forecast calibration, skill scores, etc*



Closing the loop

- Validating retrievals gives us *metrics of quality* to report uncertainty
- Validating uncertainty estimates tells us if things are *working as we expect*
 - Regardless of how well the retrievals perform
- Figure out where your assumptions go *out of fault*, then *refine* them!



References and resources

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- Sayer, A. M., Govaerts, Y., Kolmonen, P., Lipponen, A., Luffarelli, M., Mielonen, T., Patadia, F., Popp, T., Povey, A. C., Stebel, K., and Witek, M. L. (2020), A review and framework for the evaluation of pixel-level uncertainty estimates in satellite aerosol remote sensing, *Atmos. Meas. Tech.*, 13, 373–404, <https://doi.org/10.5194/amt-13-373-2020>
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