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1. Matchup Criteria

1.1. Parameters of Interest

1.1.1. Primary

- Water quality parameter (e.g., chl-a, Turbidity)
- Lat/Lon geolocation
- Date and Time (hours, minutes) of in situ
- Date and Time (hours, minutes) of satellite overpass (sensing)

1.1.2. Auxiliary

- Lat/Lon geolocation error
- Wind
- Masks (water, clouds, cirrus clouds etc.)
- Distance from the coast
- Sensor zenith (viewing) angle
- Sensor azimuth angle
- Sun zenith angle
- Sun azimuth angle
- Water quality parameter uncertainty/error from in situ

- Water quality parameter uncertainty/error from satellite retrieval
- Aerosol Optical Thickness (AOT)
- Measurement water depth (if sampling not from first centimeters-meter)

1.2. Exclusion Thresholds

Parameter	**Units**	**Pass Criterion**
Time difference	hours	[-3, 3]
Geolocation error	m	< 10
Wind	m/s	<= 5.4
Distance from the coast	m	>= 60 (TBD)
Relative azimuth angle	Degrees	[70-120]
Sun-Sensor (phase) angle	Degrees	>= 40
Aerosol Optical Depth (AOT)		
Observation water depth	m	< 1

2. Matchup Workflow Protocol

2.1. Things to keep in mind

- If water body or specific region of water body is highly dynamic, keep exclusion restrictions tighter
- If we know that the water body has significant stratification, then it makes sense to exclude measurements in higher depths (here it would make sense to check if water column profiles exist for different variables)
- Categorization of matchups per optical water type to see if regression error metrics change. Pay attention to the qualitative parameters per in situ measurement, as every single measurement is important
- Clouds (e.g, Cirrus) (Check existing masks etc.)
- Haze (check if it’s taken into account during the atmospheric correction)
- Sun glint regions (check if it’s taken into account during the atmospheric correction)
- Regions close to shoreline/adjacency effect (check if it’s taken into account during the atmospheric correction)
- Specific satellite image geolocation error. For example, if the geolocation error of the image is 1-2 pixels (i.e., 10-20m) and the measurement is close to the shoreline then there may be a mismatch between them, which means that this measurement should be excluded

2.2. Protocol

<FIGURE>

Time criteria

- You can incorporate the time difference between in situ measurement and satellite overpass as a source of error or simply visualize it.
  Note: Caution when calculating the time differences. The satellite sensing times are in UTC, while the in situ measurements may be in local times. Local times change in winter and summer, so they depend on whether the state authorities of the country follow this regulation.
- Acceptable: Depends on other conditions e.g.,
  - wind → which may give waves and wakes or fast change of mixing of water in coastal regions of the water body
  - Haze/High atmospheric particles (e.g., african dust) → which cannot be entirely corrected
  - Cirrus clouds → which cannot always detected (let alone corrected)
  - Tides → if you have in situ measurement in a region which has significant tides, this means that if you take the measurement at X time, and the satellite passes after 2hrs, then the point you took the measurement will have become land
  - Flag or Exclude matchups with >2-hour differences, especially if dynamic conditions are expected

Spatial window

- In situ and image overlap approach
  - Exact pixel
  - 3x3 window
  - 5x5 window
    Note: Size of window depends on the spatial resolution, among others (e.g., for the 10m of Sentinel-2 the 3x3 may be sufficient)
- Calculate statistics inside the above windows (mean, median, std etc.)
- Rule of thumb for measurement depth is to be as close to the surface as possible
- If there are depth profile measurements, we can extrapolate to the water surface
- If there is a single measurement per point
  - Either assume that the depth measurement is representative of the water surface, thus it's a good measurement
  - Or incorporate the depth as an error source
  - Or exclude the measurement
  - Or other?
- Pay attention to measurements that are close to the coastline of the water body, because the adjacency effect will take place
  - Either assume there is no adjacency effect (e.g., if the atmospheric correction is supposed to have corrected for it)
  - Or incorporate it as a source of error e.g., devise a rule such as the distance from the shoreline
  - The statistics of the spatial window (if it has high standard deviation or the mean is very different from the median)
  - Or exclude the measurement (again based on some devised reasonable rule)
- Pay attention to measurements that have been conducted close to the coastline which usually has low water depth (shallow regions). If water is relatively clear, then in this case the signal the sensor sees is mixed between water and the bottom of the

water body. Pay attention if the atmospheric correction somehow corrects for bottom effects, otherwise consider it as a source of error at least qualitatively

3. Reporting

3.1. Statistical Analysis

3.1.1. Outlier Detection methodology

3.1.2. Linear Regression model

3.2. Metrics Definition

3.2.1. Pearson’s rho

3.2.2. Spearman’s rho

3.2.3. R-Squared

3.2.4. Root Mean Squared Error (RMSE)

3.2.5. Mean Absolute Error (MSE)

3.2.6. Model Residuals

3.2.7. Bias

3.3. What to include

Reporting needs at least:

- Raw data (link)
- Detailed preparation (corrections etc.) that was applied
- ARD data (link or table)
- Number of matchups
- Flags on excluded matchups (and why)
- Time differences
- Depths of in situ samples (if needed)
- Histograms
- Scatter plots with regression model and 1:1 line
- Error bars if possible (e.g. uncertainties from in-situ/satellite-retrieved)
- Regression residuals plots