Quality Assurance and Control in Oceanographic Observations

Dr. Matthias Lankhorst

SCRIPPS INSTITUTION OF OCEANOGRAPHY
UC San Diego

Motivation: Requirement Flowdown

- Our science objectives dictate how accurate our data have to be
- QA/QC methods to:
  - Collect data with the required accuracy
  - Identify and remove anomalies that do not meet the requirements

Motivation: Why Data QA/QC?

- Sensor behavior changes with time:
  - Aging
  - Biofouling
- Sensors or instruments can fail:
  - Transmission errors
  - Mechanical failure

…but then we do not meet our requirements!

Imperative to examine our end product (data) to mitigate the above effects → data QA/QC.

Example:
CTD Instrument SBE-37IM

Before:

After:

Biofouling example:
Can we trust data from this instrument?
Can we adjust it to meet specifications?

QA vs. QC: “Assurance” vs. “Control”

- Quality Assurance (QA) and Quality Control (QC) often used interchangeably
- QA: Part of quality management focused on providing confidence that quality requirements will be fulfilled
  - All the planned and systematic activities [...] that [...] provide confidence that a product or

QA: Focus on **planning**, e.g.: choice of sensors, sampling schemes, …

- QC: Part of quality management focused on fulfilling quality requirements

QC: Focus on **doing**, e.g.: following procedures, inspecting data, …

quality

Content credit (also a recommended resource): ASQ, https://asq.org/quality-resources/quality-assurance-vs-control

In an ideal observational system…

- … we have requirements that tell us how good the data have to be,
- … we design our observations such that they will deliver data of that quality (QA),
- … and we operate the system accordingly, with an inspection element that confirms meeting the quality requirements (QC).

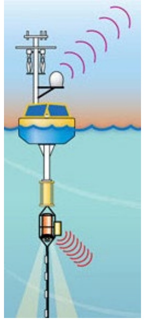
QC Output: Two Options, Two Goals

Options:

- Correct / adjust "bad" data
- Leave "bad" data as is but flag accordingly

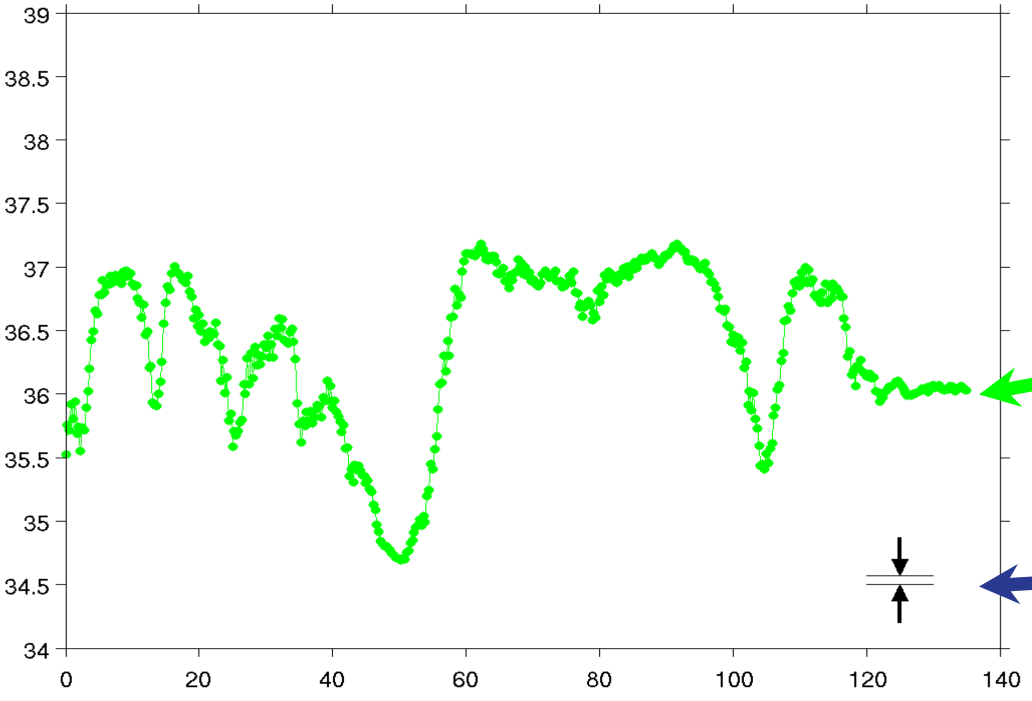
Goals:

- As few bad data points as possible
- As accurately flagged (good/bad) as possible



Raw data stream:	2.1	2.0	2.2	9.3	2.5	2.4	2.7
Operator figures out sensor drift, **Adjusted data set:**	2.1	2.0	2.2	9.2	2.1	2.0	2.1
QC flags:	1	1	1	1	0	1	1

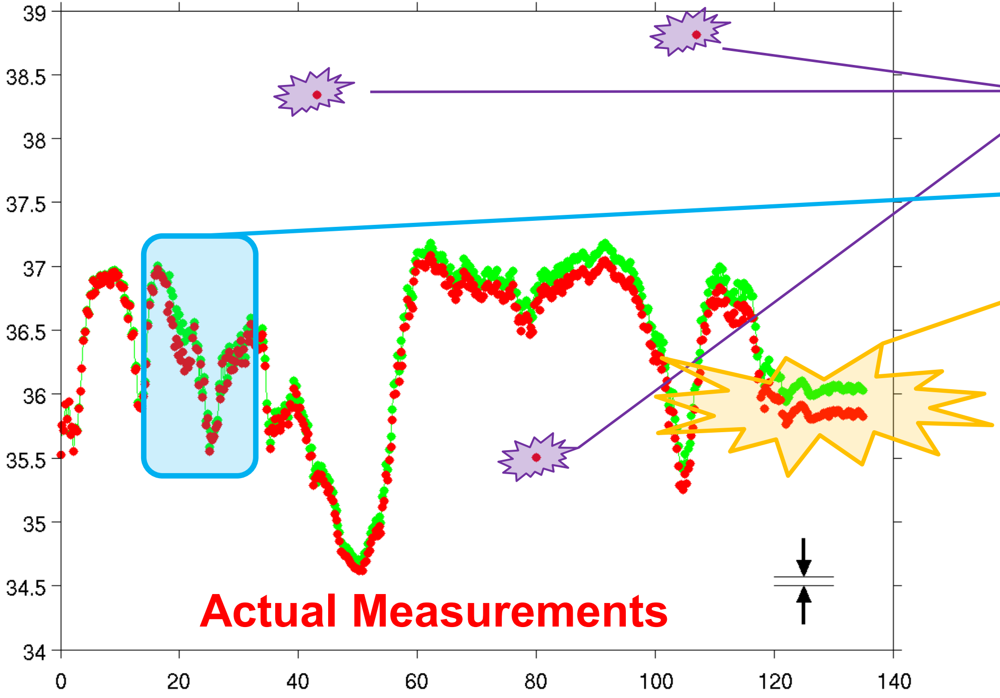
Example of Time Series



The “true” values

Target Accuracy

Example of Time Series



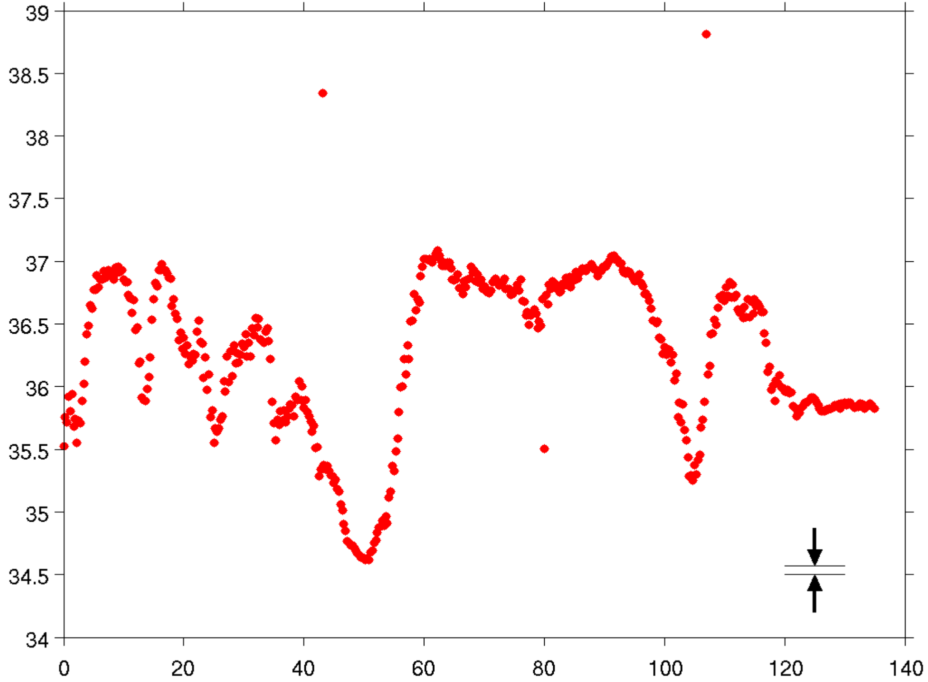
Degraded by:

- Large outliers / spikes
- Small outliers
- Small sensor drift

…where "small" means:

"small compared to natural variability but still **greater than target accuracy**"

Example of Time Series



Now…

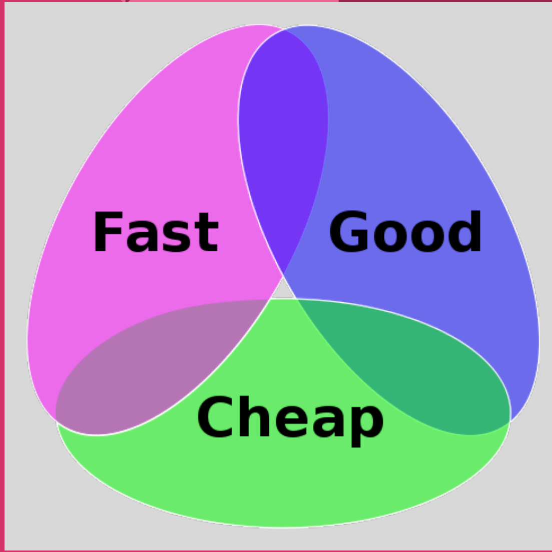
…can you…

- find ‘em?
- correct ‘em?

(Remember that target accuracy!)

Constraints

- Time
  - Real-time vs. delayed-mode data flow
  - Handling during instrument turn-around
- Technical
  - Is there a procedure to do this?
  - Does result meet requirements?
- Cost
  - Human-in-the-loop procedures have labor costs
  - Additional engineering features

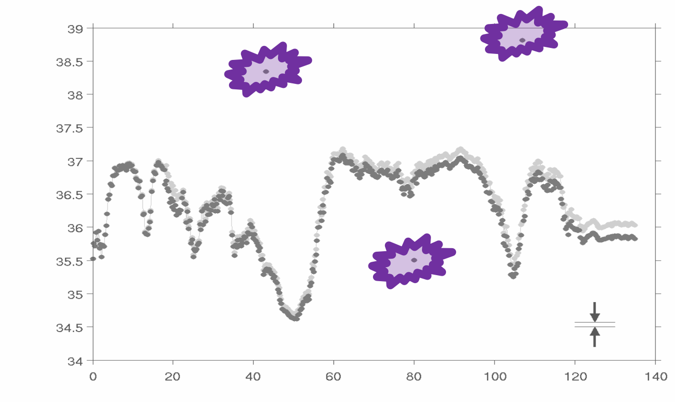


What is better: fewer data points of high quality, or more data points of lower/unknown quality?

Option to Address Gross Outliers

Automated algorithms to detect large anomalies:

- Global range test
- Local range test (by depth/time)
- Spike test
- Stuck value test
- Trend test
- Gradient test
- Propagate flags to derived data products

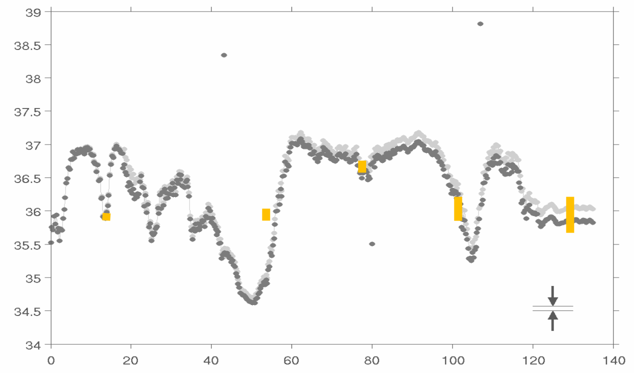


Need to identify algorithm and input parameters, good resource: QARTOD manuals, https://ioos.noaa.gov/project/qartod/

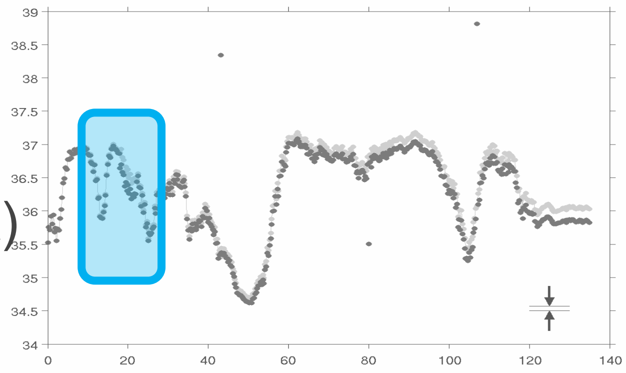
Option to Address Small Trend

Concept:

- Calibrations at mission start & end
- Interpolate over duration of mission
  - Calibration methods may be different between sensors or sites
  - Additional decision points during mission from inter-sensor comparison (e.g. glider flies by mooring)
- Human involvement in decision-making



Option to Address Small Outliers



Concepts:

- Human inspection:
  - Parameter-specific visualization (T -S plot)
  - Utilize neighboring sensors to check for consistency (Do all salinity sensors show same anomaly? Is salinity anomaly accompanied by anomaly in oxygen?)
- Develop software to explore inter-sensor correlations

Different Calibration/Verification Methods

Options for determining calibration/adjustment coefficients:

- Send back to manufacturer
- In home laboratory
- At sea via comparison against reference
- During mission via comparison against neighboring sensor

"Primary" calibration with many coefficients, spans full range of measurements

"Secondary" adjustment, simple equation (e.g. gain & offset), assumes that primary calibration is almost correct

Different Calibration/Verification Methods

Options for determining calibration/adjustment coefficients:

- Send back to manufacturer
- In home laboratory
- At sea via comparison against reference
- During mission via comparison against neighboring sensor

Need to trust calibration labs… are they certified, do they use methods traceable against some standard?

Need to trust references (e.g. water samples). Use documented methods & standards!

Uncertainty of the Final Data Product

Options for determining calibration/adjustment coefficients:

- Send back to manufacturer
- In home laboratory
- At sea via comparison against reference
- During mission via comparison against neighboring sensor

But how good (accuracy) is our data after all this???

Calibration against a standard of known accuracy (usually done by manufacturer). Derive nominal accuracy and precision from combination of:

- how good the standard itself is,
- how well the to-be-calibrated device matches the standard

Uncertainty of the Final Data Product

Where to find values for accuracy (for reference standards):

- Vendor-provided specifications that come with instruments
- Published alongside procedures/methods documentation

Important to indicate in metadata that comes with data:

- A reasonable estimate of uncertainty and/or accuracy
- A reasonable amount of documentation what methods/instruments were used

Example

Options for determining calibration/adjustment coefficients:

- Send back to manufacturer
- In home laboratory
- At sea via comparison against reference
- During mission via comparison against neighboring sensor

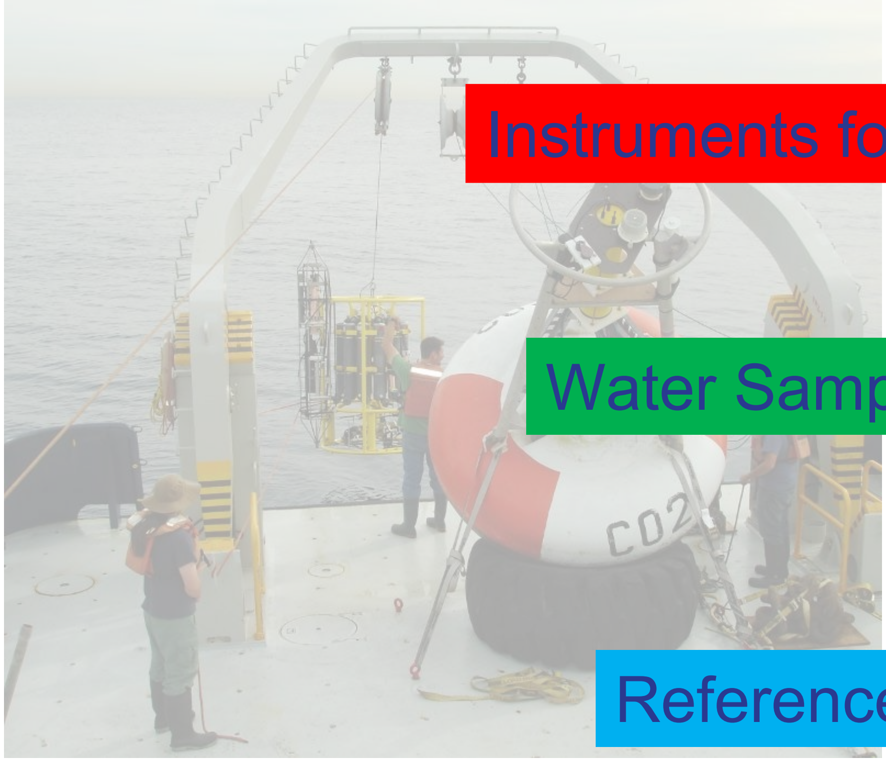
Mooring instruments attached to CTD rosette before deployment.

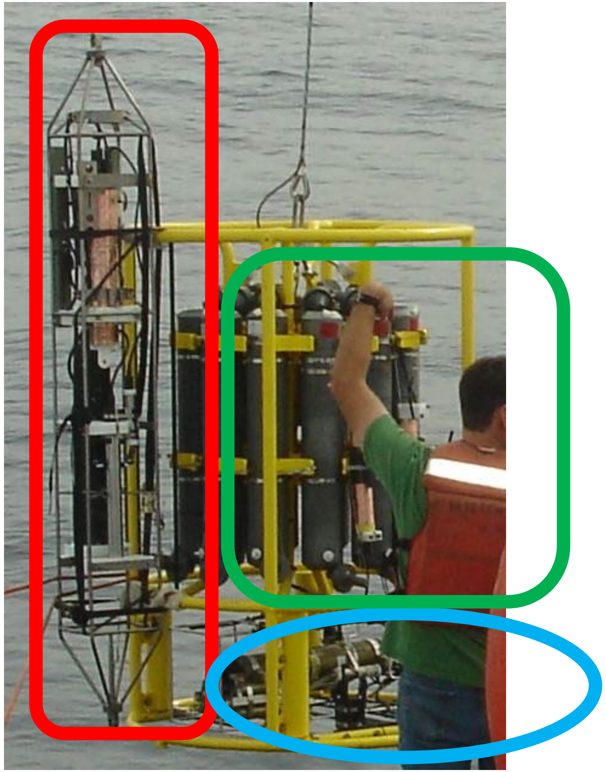
CTD system has “primary” factory calibration (roughly annually), plus water samples for “secondary” adjustments.

Moored CTD Walkthrough: Calibration

- Procedure:
  - Attach to-be-calibrated instrument to shipborne reference sensor (here: mooring instrument attached to CTD)
  - Lower this package into deep ocean (where water is very homogeneous)
  - Extract data from select depths
  - Determine gain/offset coefficients, as appropriate
- Routine method in deep-ocean observing community, e.g. RAPID-MOCHA, EuroSITES, MOVE
- Online resource for this and other procedures: **https://www.oceanbestpractices.org/**

Moored CTD Walkthrough: Calibration



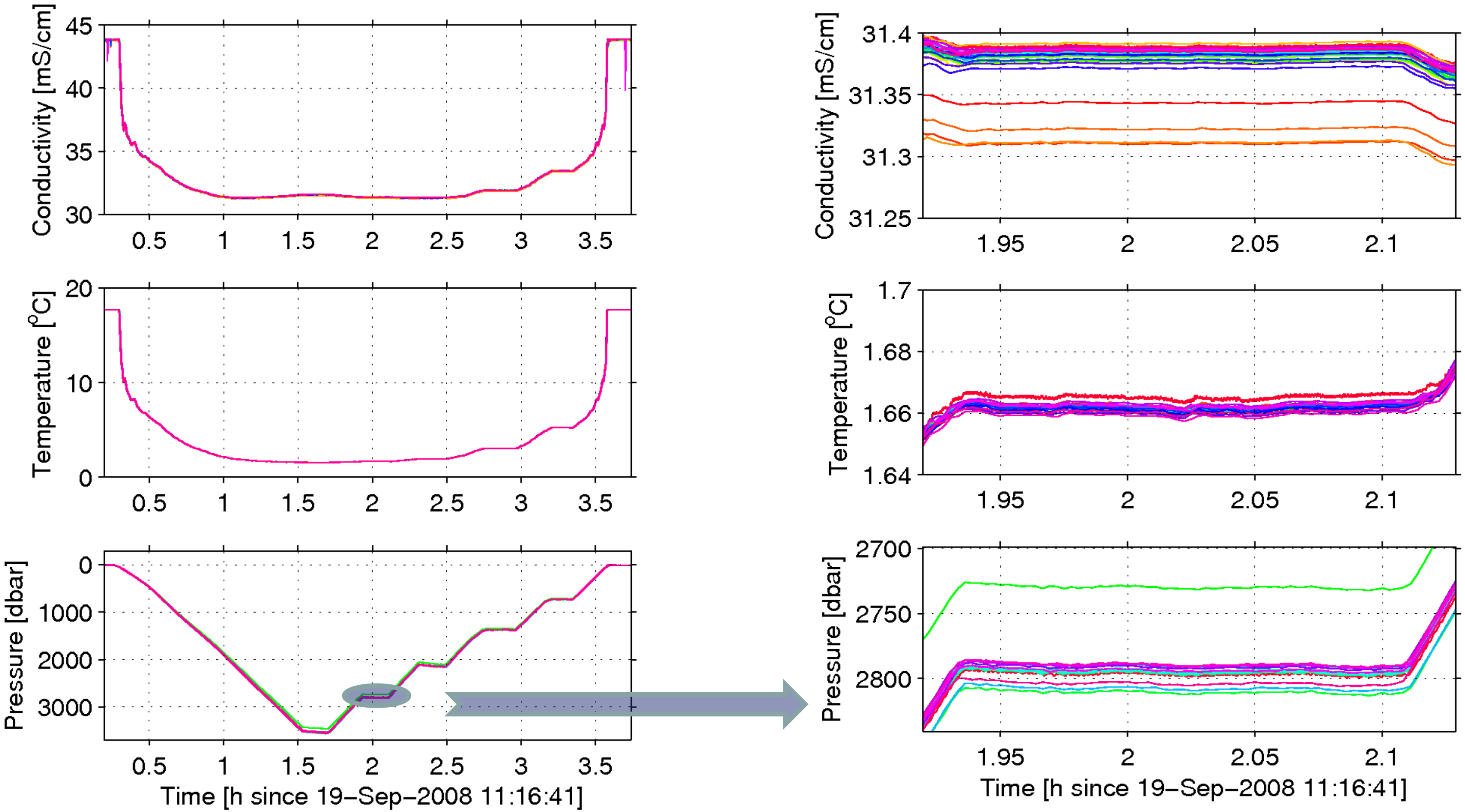


Instruments for mooring

Water Sample Bottles

Reference Sensors

Moored CTD Walkthrough: Calibration



Moored CTD Walkthrough: Calibration

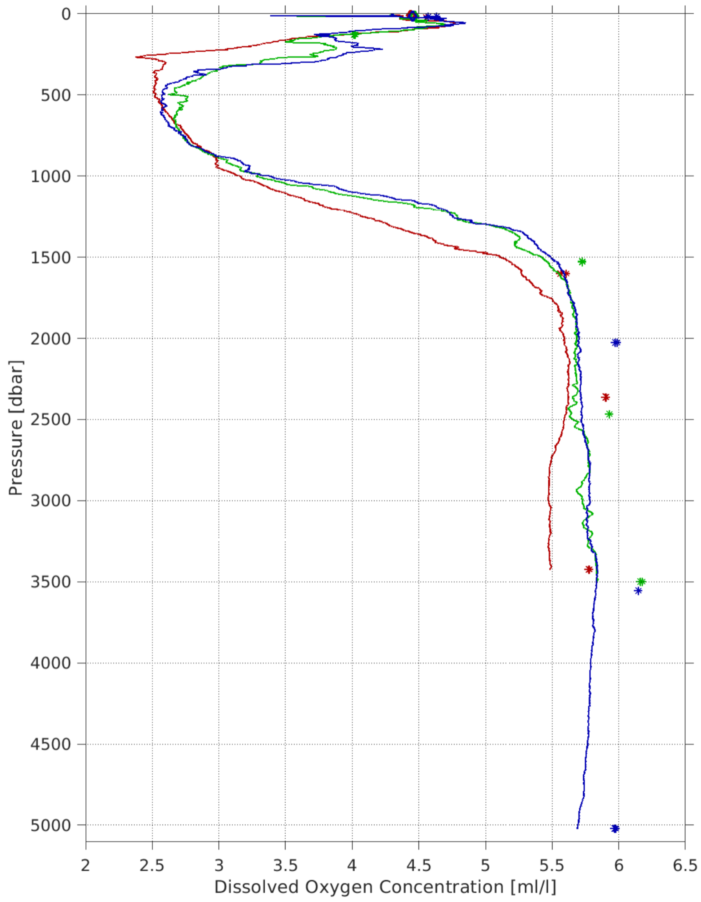
So, how good is the data?

- Can match the reference CTD within the vendor-specified accuracy limits, C: 0.003 mS/cm; T: 0.002 °C; P: depends on sensor, 1-7 dbar
- Therefore, the mooring data at/near the time when the comparison was made is basically as good as the vendor-specified reference accuracy
- But: interpolation between "before/after" CTD casts to cover an entire mooring deployment period - might not be drifting linearly

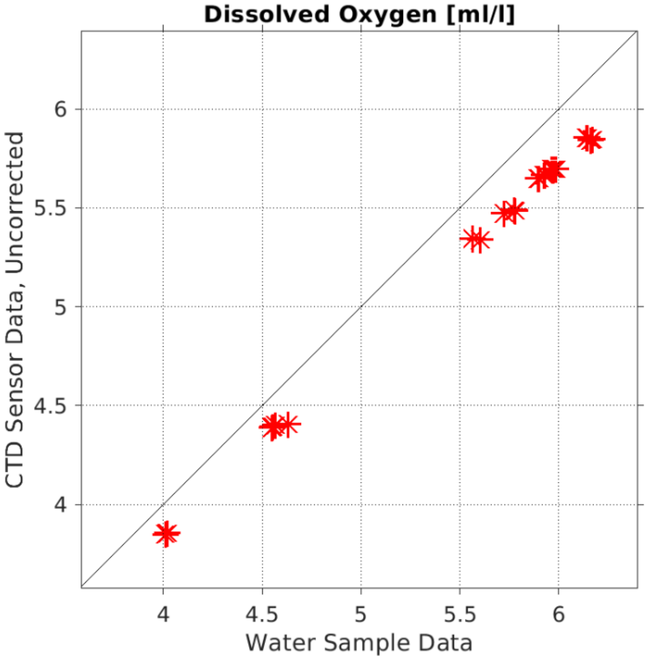
- Consistency check: can compare sensor drift over many years when this is done routinely - T and P very stable, C mostly affected by bio-fouling and more stable when deployed at depth

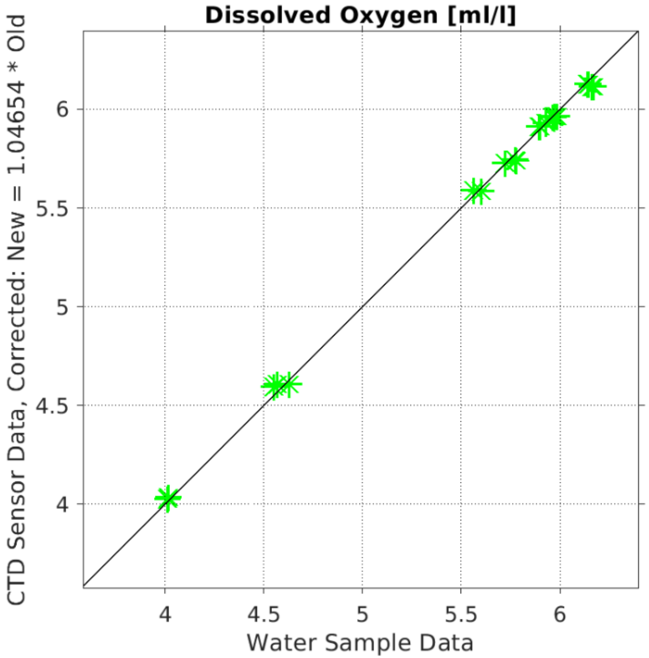
Hands-On Example 1: Adjust CTD Cast Oxygen Data

- Data given in **data_example01.mat**:
  - oxygen data from water samples collected during CTD cast
  - oxygen data from CTD sensors at the same times/locations/depth
- Plot the data!
- Assuming that the water sample data are correct, how could the CTD sensor data be adjusted such that they best match the samples?



Hands-On Example 1: Adjust CTD Cast Oxygen Data



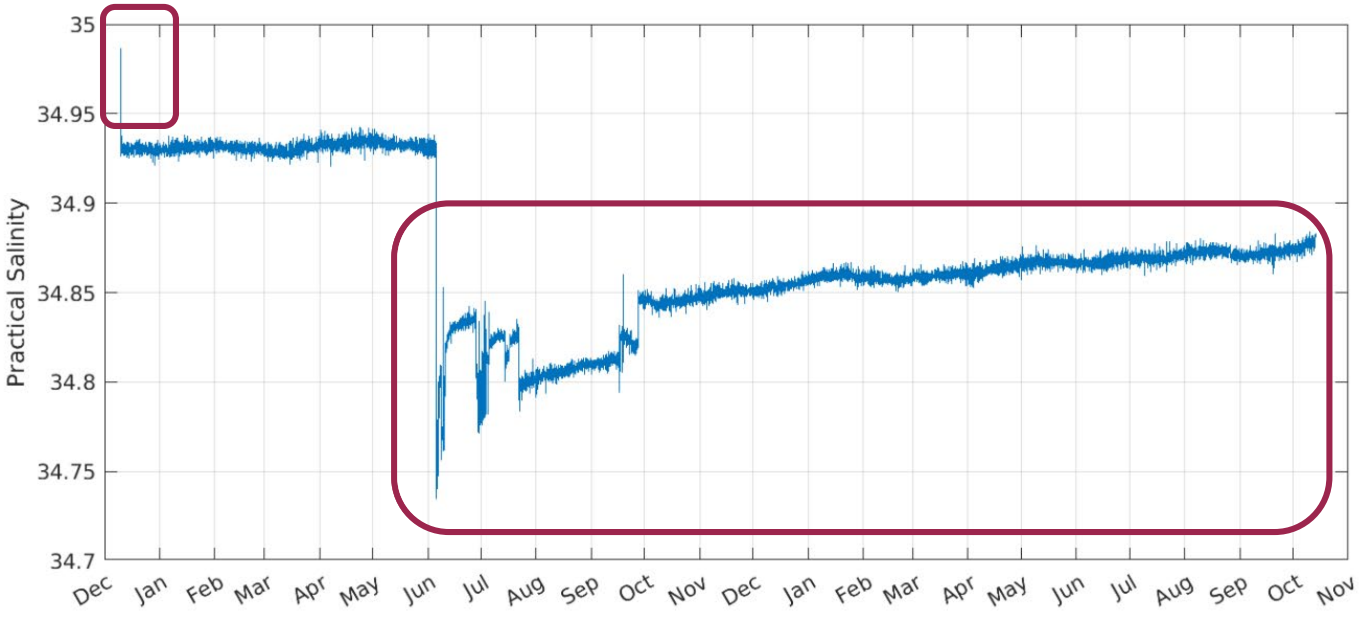


For this sensor type, recommended adjustment is gain only (no offset)

Hands-On Example 2: Identify Bad Data in Time Series

- Data given in data_example02.mat:
  - Time series of salinity from a mooring
- Plot the data!
- What part of the data look strange? What may have happened? Can perhaps some parts of the data still be used?

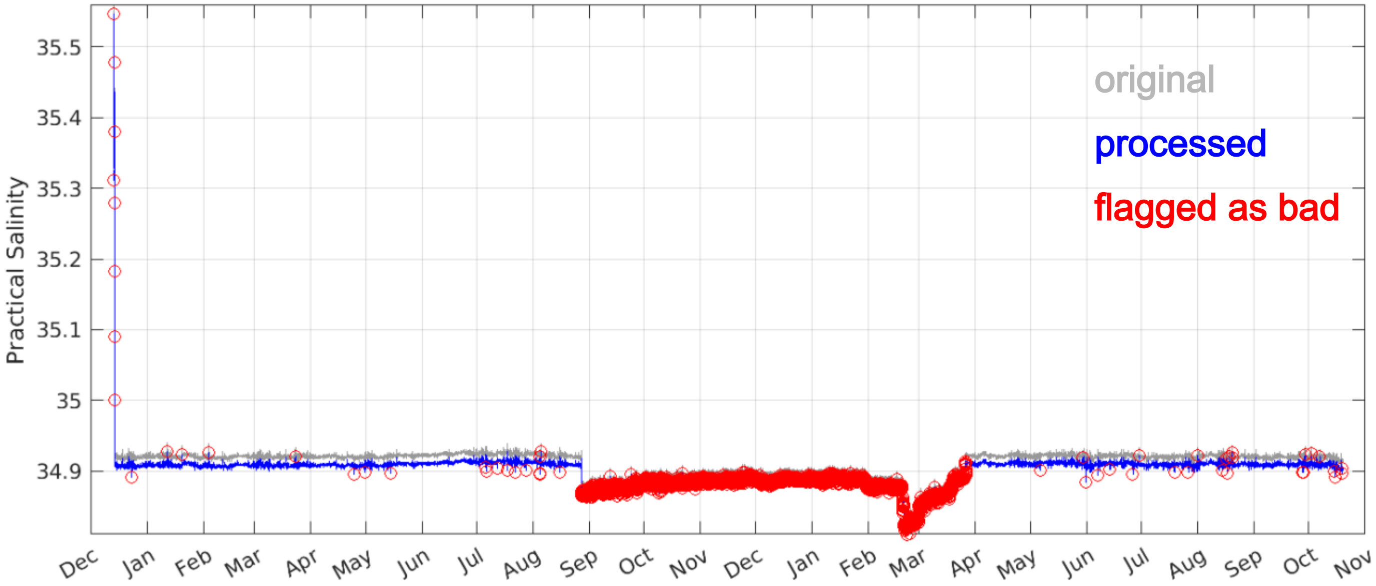
Hands-On Example 2: Identify Bad Data in Time Series



Hands-On Example 3: Inspect Time Series Processing

- Data given in data_example03.mat:
  - Time series of salinity from a mooring in an “original” and a “processed” version
  - Quality flag indicating which data points are bad
- Plot the data!
- What part of the data look strange? Is this reflected in the QC flags?
- What changed between the original and processed versions?

Hands-On Example 3: Inspect Time Series Processing



Data QA/QC

- …to make our data meet our requirements
- Options for gross outliers, small outliers, and small sensor drift
- Calibration/validation
- Uncertainty of final data (and documentation)
- Examples