Darwin Harbour Water Quality monitoring program analysis application manual

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About

This document comprises the manual for the Darwin Harbour Water Quality monitoring program analysis application. It provides information on:

- a broad overview of the structure of the application
- the application dependencies and how to install them
- starting the application
- progressing through the analysis pipeline
- visualising, interpreting and extracting outputs

Structural overview

R Graphical and Statistical Environment offers an ideal platform for developing and running complex statistical analyses as well as presenting the outcomes via professional graphical/tabular representations. As a completely scripted language it also offers the potential for both full transparency and reproducibility. Nevertheless, as the language, and more specifically the extension packages are community developed and maintained, the environment evolves over time. Similarly, the underlying operating systems and programs on which R and its extension packages depend (hereafter referred to as the *operating environment*) also change over time. Consequently, the stability and reproducibility of R codes have a tendency to change over time.

Docker containers

One way to attempt to future proof a codebase that must be run upon a potentially unpredictable operating environment is to **containerise** the operating environment, such that it is preserved to remain unchanged over time. Containers (specifically docker containers) are lightweight abstraction units that encapsulate applications and their dependencies within standardized, self-contained execution environments. Leveraging containerization technology, they package application code, runtime, libraries, and system tools into isolated units (*containers*) that abstract away underlying infrastructure differences, enabling consistent and predictable execution across diverse computing platforms.

Containers offer several advantages, such as efficient resource utilization, rapid deployment, and scalability. They enable developers to build, test, and deploy applications with greater speed and flexibility. Docker containers have become a fundamental building block in modern software development, enabling the development and deployment of applications in a consistent and predictable manner across various environments.

Shiny applications

Shiny is a web application framework for R that enables the creation of interactive and data-driven web applications directly from R scripts. Developed by Rstudio, Shiny simplifies the process of turning analyses into interactive web-based tools without the need for extensive web development expertise.

What makes Shiny particularly valuable is its seamless integration with R, allowing statisticians and data scientists to build and deploy bespoke statistical applications, thereby making data visualization, exploration, and analysis accessible to a broader audience. With its interactive and user-friendly nature, Shiny serves as a powerful tool for sharing insights and engaging stakeholders in a more intuitive and visual manner. ## Git and github

Git, a distributed version control system, and GitHub, a web-based platform for hosting and collaborating on Git repositories, play pivotal roles in enhancing reproducibility and transparency in software development. By tracking changes in source code and providing a centralized platform for collaborative work, Git and GitHub enable developers to maintain a detailed history of code alterations. This history serves as a valuable asset for ensuring the reproducibility of software projects, allowing users to trace and replicate specific versions of the codebase.

GitHub Actions (an integrated workflow automation feature of GitHub), automates tasks such as building, testing, and deploying applications and artifacts. Notably, through workflow actions, GitHub Actions can build docker containers and act as a container registry. This integration enhances the overall transparency of software development workflows, making it easier to share, understand, and reproduce projects collaboratively.

Figure 1 provides a schematic overview of the relationship between the code produced by the developer, the Github cloud repositiory and container registry and the shiny docker container run by user.

Installation

Installing docker desktop

To retrieve and run docker containers requires the installation of Docker Desktop on Windows and MacOSx

Windows

The steps for installing Docker Desktop are:

- **Download the Installer:** head to https://docs.docker.com/desktop/install/windows-install/ and follow the instructions for downloading the appropriate installer for your Windows version (Home or Pro).
- **Run the Installer:** double-click the downloaded file and follow the on-screen instructions from the installation wizard. Accept the license agreement and choose your preferred installation location.
- **Configure Resources (Optional):** Docker Desktop might suggest allocating some system resources like CPU and memory. These settings can be adjusted later, so feel free to use the defaults for now.
- **Start the Docker Engine:** once installed, click the "Start Docker Desktop" button. You may see a notification in the taskbar - click it to confirm and allow Docker to run in the background.
- **Verification:** open a terminal (or Powershell) and run `docker --version`. If all went well, you should see information about the installed Docker Engine version.

Additional Tips:

- Ensure Hyper-V (virtualization) is enabled in your BIOS settings for optimal performance.

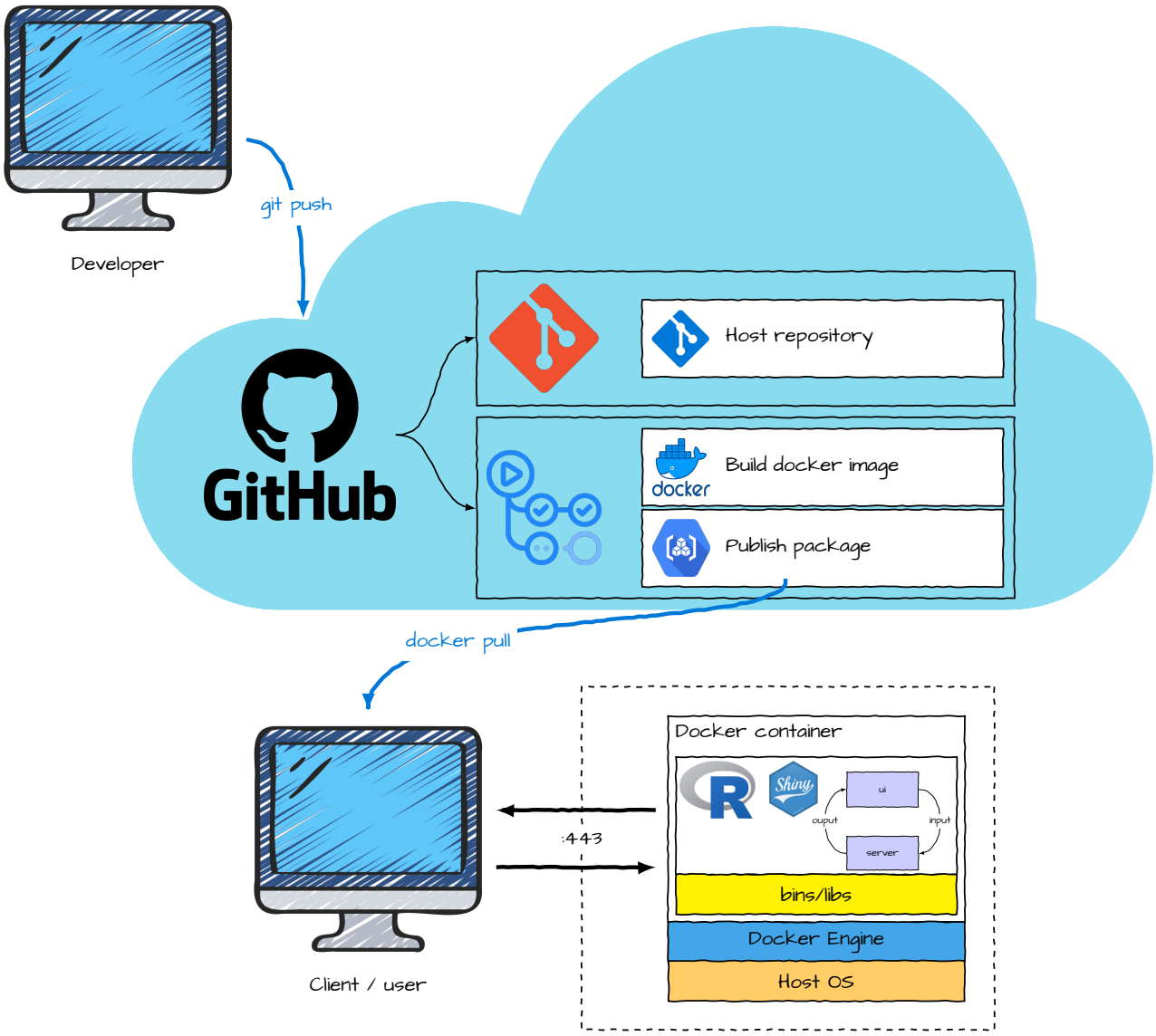


Figure 1: Diagram illustrating the relationship between the code produced by the developer and the shiny docker container utilised by user with a Github cloud conduit. The developed codebase includes a Shiny R application with R backend, `Dockerfile` (instructions used to assemble a full operating environment) and github workflow file (instructions for building and packaging the docker image on github via `actions`).

Installing the and running the app

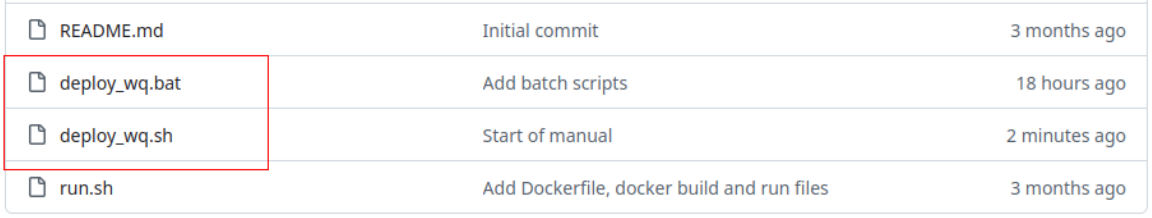
The task of installing and running the app is performed via a single **deploy script** (`deploy_wq.bat` on Windows or `deploy_wq.sh` on Linux/MacOSX/wsl). For this to work properly, the deploy script should be placed in a folder along with two additional folders (one called `input` and the other called `parameters`) that contains the input datasets (in csv format) and run time parameters. This structure is illustrated below for Windows.

```
\
|- deploy_wq.bat
|- input
   |- 16_wq.csv
   |- 17_wq.csv
   |- overwrites.csv
   |- weights_m.csv
   |- weights_s.csv
|- parameters
   |- config.ini
   |- water_quality_guidelines.csv
   |- spatial.csv
   |- GIS
      |- RCZ_rev24.*
      |- SBZone_upper.*
      |- Middle_Harbour_Upper.*
```

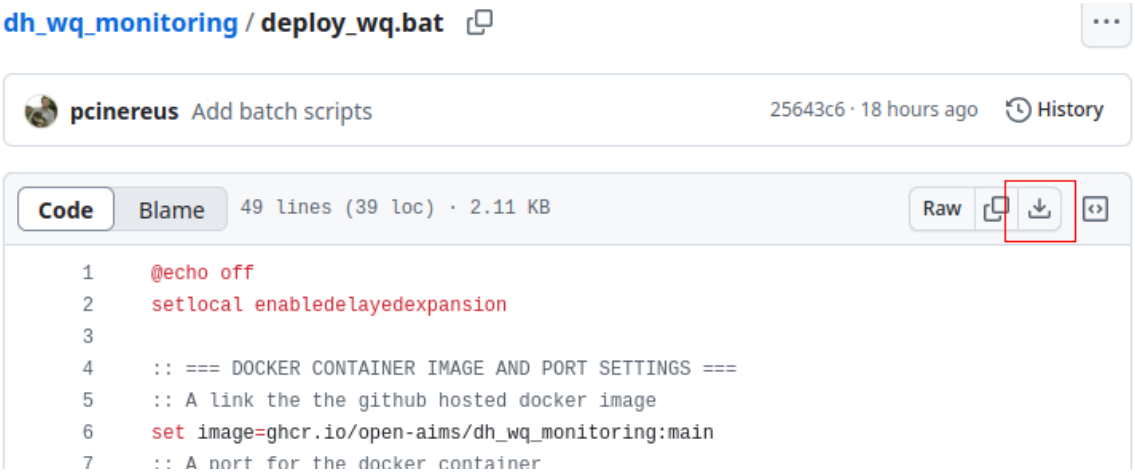
> **Note**
>
> In the above illustration, there are two example water quality datasets (`16_wq.csv` and `17_wq.csv`). To ensure that the application correctly identifies them as water quality datasets, it is important that they are named according to the following format: `<yy>_wq.csv` where the `<yy>` represents a two digit year (e.g. 16 for 2016). For additional information on the contents of these files, please see Section .

To set up the above structure:

1. create a new folder on your computer in a location of your choice that you are likely to remember and easily locate (e.g. on the desktop). Whilst the name of the folder is not important, it is recommended that it be named after the project (e.g. `darwin_harbour_wq_monitoring`).
2. download the deploy script from the projects github repository
   a. go to the projects github repository (https://github.com/open-AIMS/dh_wq_monitoring.git) in a browser
   b. click on either the `deploy_wq.bat` (Windows) or `deploy_wq.sh` (Linux/MacOSX/wsl).



   c. click on the download button and select the project folder as the location to download the file to. If the file is automatically downloaded to a downloads folder, move the file to the project folder.



3. within the project folder, create folders called `inputs` and `parameters` (as outlined above) and place all the appropriate data sets into these folders

To run the app, navigate inside of the project folder and run (typically double click) on the deploy script. Upon doing so, you will be presented with a directory selection window that is prompting for the path of the project folder. Navigate to and select the project folder before clicking the "OK" button. Shortly thereafter, the application will appear in a browser tab.

> More specific information about the `deploy_wq.bat` script
>
> The `deploy_wq.bat` script performs the following:
>
> 1. defines paths to the project repository and local project folder
> 2. checks if `docker` is installed and available from the command line for the current user
> 3. checks if `docker` is running
> 4. query the user for the location of the project folder
> 5. determine whether there are any updates to the `docker` image and if so pull them down
> 6. run the `docker` container
> 7. open the shiny app in a browser

The Darwin Harbour Water Quality Monitoring Program Analysis App

This Shiny application is designed to ingest very specifically structured water quality datasets containing Darwin Harbour Water Quality monitoring data and produce various analyses and visualisations. The application is served from a docker container to the localhost and the default web browser.

Docker containers can be thought of a computers running within other computers. More specifically, a container runs an instance of image built using a series of specific instructions that govern the entire software environment. As a result, containers run from the same image will operate (virtually) identically regardless of the host environment. Furthermore, since the build instructions can specify exact versions of all software components, containers provide a way of maximising the chances that an application will continue to run as designed into the future despite changes to operating environments and dependencies.

This shiny application comprises five pages (each accessable via the sidebar menu on the left side of the screen):

1. a **Landing** page (this page) providing access to the settings and overall initial instructions
2. a **Dashboard** providing information about the progression of tasks in the analysis pipeline
3. a **Data** page providing overviews of data in various stages
4. a **QAQC** page providing graphical QAQC outputs
5. a **Summaries** page providing summaries of the bootstrap aggregation of indices
6. a **Manual** page that displays the online manual for the application

Each page will also contain instructions to help guide you through using or interpreting the information. In some cases, this will take the from of an info box (such as the current box). In other cases, it will take the form of little symbols whose content is revealed with a mouse hover.

There are numerous stages throughout the analysis pipeline that may require user review (for example examining any data validation issues as well as the QAQC figures to confirm that the data are as expected). Consequently, it is advisable for the user to manually trigger each successive stage of the pipeline. The stages are:

- Stage 1 - Prepare environment

  More info

  This stage is run automatically on startup and essentially sets up the operating environment.

  - load any R package dependencies
  - get runtime settings from `../params/config.ini`. These include:
    * `focal_year`: usually the final year of sampling, all artifacts (data/graphics) will be stored in a folder reflecting this year
    * `method`: the index method to apply when calculating indices
    * `foldcap`: the folding cap to apply when calculating indices
    * `tuning`: the tuning to apply when calculating indices
    * `size`: the number of bootstrapp samples
    * `seed`: the random seed to apply to bootstrapping

- Stage 2 - Obtain data

  More info

  This stage comprises of the following steps:

  - read in the water quality guidelines from `../parameters/water_quality_guidelines.csv`.
  - read in each of the water quality data files from `../input/`. These files are in the format of `<number>_wq.csv`, where `<number>` is a two digit number representation of the sampling year.
  - read in each of the overwrites file from `../input/overwrites.csv`.
  - read in each of the measures weights file from `../input/weights_m.csv`.
  - read in each of the spatial weights file from `../input/weights_s.csv`.
  - read in the aggregation hierarchy file from `../input/hierarchy.csv`.
  - read in the spatial settings file from `../parameters/spatial.csv`.
  - validating each of the sources of input data according to a set of validation rules

  The tables within the **Raw data** tab of the **Data** page will also be populated (but wont be available for review until after the data have been processed in Stage 3).

- Stage 3 - Prepare spatial data

  More info

  This stage comprises of the following steps:

  - read in individual shapefiles from `../parameters/GIS`. The files are:
    * `RCZ_rev24.shp`
    * `SBZone_upper.shp`
    * `Middle_Harbour_Upper.shp`
  - combine all shapefiles into a single shapefile

  The tables within the **Processed data** tab of the **Data** page will also be populated.

- Stage 4 - Process data

  More info

  This stage comprises of the following steps:

  - combine all the water quality data into a single data set
  - process the dates from strings into genuine date objects
  - filter data to the bounds either defined in `../parameters/config.ini` or the data
  - select only measures for which there are guideline values
  - if the `focal_year` is undefined, define it based on the maximum date

  - pivot the data into a longer format that is more suitable for analysis and graphing
  - join in the guidelines information
  - use the spatial information in the shapefiles to assign spatial domains such as Regions and Zones.
  - apply any unit conversions to the values
  - apply limit of detection rules (to Dissolved Oxygen)
  - join in the aggregation hierarchy

  The tables within the **Processed data** tab of the **Data** page will also be populated and the `Data` page will be available for review.

- Stage 5 - Calculate indices

  More info

  This stage comprises of the following steps:

  - retrieve the processed data.
  - calculate the indices
  - prepare for bootstrapping

- Stage 6 - QAQC

  More info

  This stage comprises of the following steps:

  - retrieve the processed data.
  - construct outlier plots
  - contruct an LOR table
  - contruct boxplots for each Measure for the Focal Year for each Zone
  - construct timeseries boxplots for each Measure/Zone
  - construct boxplots for each Measure for the Focal Year conditional on Zone

  The QAQC figures of the **QAQC** page will also be populated.

- Stage 7 - Bootstrapping

  More info

  This stage comprises of the following steps:

  - generate bootsrapping schematic diagram
  - retrieve the processed data
  - retrieve the indices
  - process the overwrites
  - process the weights
  - aggregate to Zone/Measure/Source level
  - aggregate to Zone/Measure level
  - aggregate to Zone/Subindicator level
  - aggregate to Zone/Indicator level
  - aggregate to Region/Measure level
  - aggregate to Region/Subindicator level
  - aggregate to Region/Indicator level
  - aggregate to WH/Measure level
  - aggregate to WH/Subindicator level
  - aggregate to WH/Indicator level

- Stage 8 - Summaries

  More info

  This stage comprises of the following steps:

  - retrieve the processed data
  - compile all the indice scores
  - generate Zone/Measure/Source level
  - collate Zone/Measure level scores
  - collate Zone/Subindicator level scores

- collate Zone/Indicator level scores
- collate Region/Measure level scores
- collate Region/Subindicator level scores
- collate Region/Indicator level scores
- collate WH/Measure level scores
- collate WH/Subindicator level scores
- collate WH/Indicator level scores
- generate trend plots
- calculate effects (between years)
- generate effects plots

The trend and effects figures of the **Summaries** page will also be populated.

Underneath the sidebar menu there are a series of buttons that control progression through the analysis pipeline stages. When a button is blue (and has a play icon), it indicates that the Stage is the next Stage to be run in the pipeline. Once a stage has run, the button will turn green. Grey buttons are disabled.

Clicking on button will run that stage (or stages in some cases). While the stage is in progress, a popup will be displayed over the buttons. This popup serves two purposes. Firstly, some tasks within some stages are computationally intense and thus take some time to perform. For such tasks, a progress bar will be displayed in the popup to inform you of the progress through this task. Secondly, as some stages/tasks are slow, it provides visual feedback about when a stage has truly started and completed and prevents the temptation to repeatedly click on a button when nothing appears to be happening.

Once a stage is complete, the button will change to either green (success), yellow (orange) or red (failures) indicating whether errors/warnings were encountered or not. If the stage was completed successfully, the button corresponding to the next available stage will be activated.

Sidebar menu items that are in orange font are active and clicking on an active menu item will reveal an associated page. Inactive menu items are in grey font. Menu items will only become active once the appropriate run stage has been met. The following table lists the events that activate a menu item.

Menu Item	Trigger Event
Landing	Always active
Dashboard	Always active
Data	After Stage 4
QAQC	After Stage 6
Summaries	After Stage 8
Manual	Always active

Note, it is also possible to make all menu and buttons active using the **Run in sequence** toggle, however this should only be used if the full sequence of stages has already been run and you are returning to the analyses in a later session

Figure 2 provides a schematic overview of the sequence of filesystem events that occur during the development, deployment and running of this app.

1. the developed codebase is pushed to github and if necessary continuous integration (github actions) is triggered. The continuous integration will re-build and host a docker image as well as rebuild the manual.
2. when the client runs the `deploy_wq.bat` (or `deploy_wq.sh`) script, it will check whether docker is running and get input from the user about the location of the project directory.
3. github will be queried to discover if a new docker image is available. If so, then the new image will be pulled down locally and run (if docker is runnning).
4. the docker container will be run and this will trigger git within the container to pull down the latest version of the codebase from github to a temporary repo in the container. As the container is starting up, it will mount the project folder so that its contents are available to the environment within container and outputs produced within the container are available to the host.
5. some of the files in the temporary repo will be copied to a folder within the project folder.
6. the shiny app will start up on `port 3838` of the localhost and this will be offered to the default browser.
7. as the shiny app progresses through each of the analysis stages, more data will be added to various folders of the project directory.

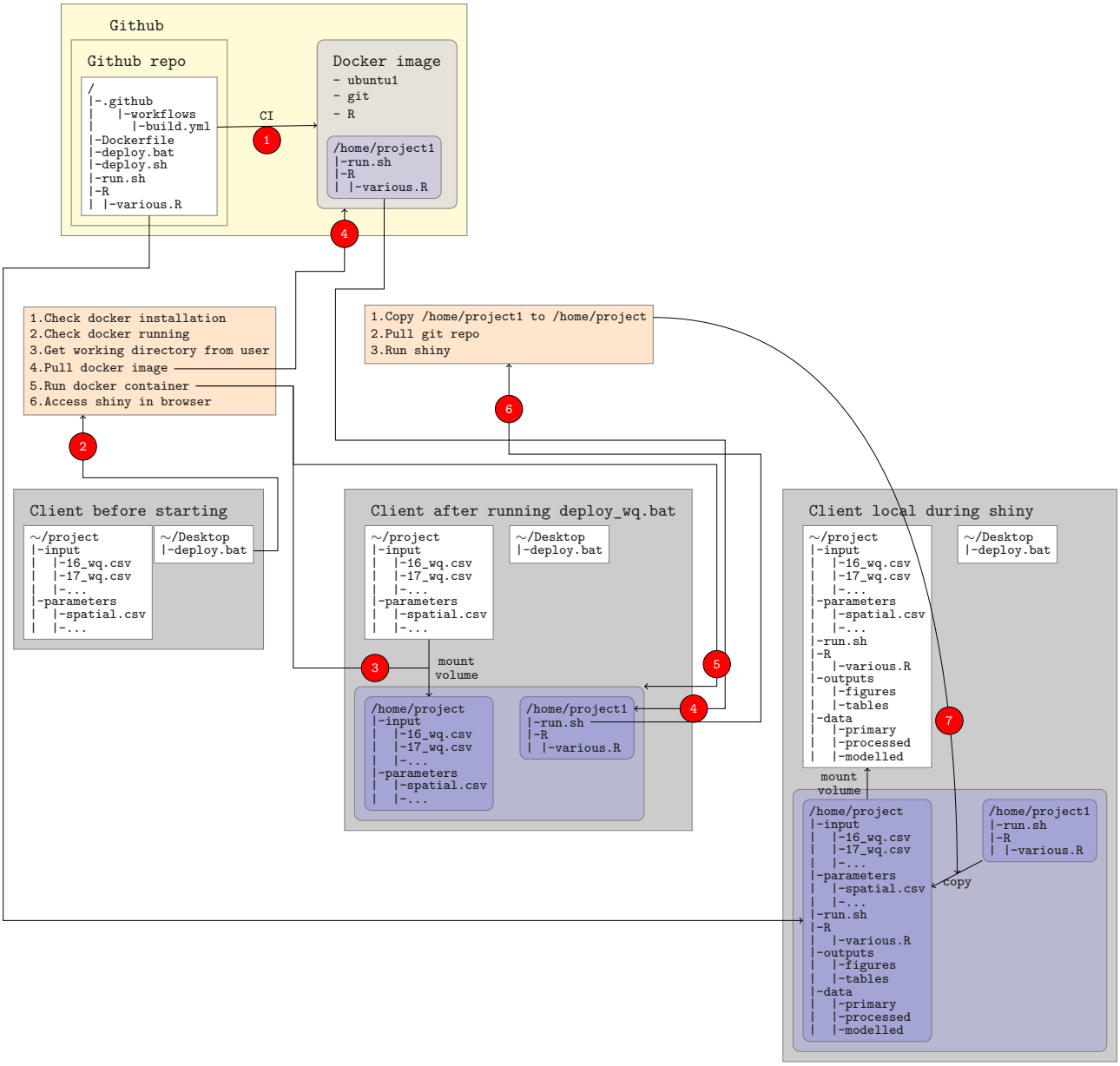


Figure 2: Diagram illustrating the sequence of filesystem events that occur during the development, deployment and running of this app.

Prior to starting the application

Before starting the application, it is important that you review the following files:

- `../parameters/config.ini`. Specifically, review the following fields:
  - `focal_year=`: indicates the year that will be considered the focal sampling year. All outputs will be stored in a folder reflecting this display diagnostics for this the focal year is the most recent sampling year. Furthermore, many of the QAQC diagnostics pertain specifically to this focal year alone.
  - `method=`: indicates the index method to employ (see Section for more information).
  - `foldcap=`: indicates the value (on the fractional/fold scale) to cap indices (see Section for more information)
  - `tuning=`: indicates the tuning value used in specific index calculations (see Section for more information)
  - `size=`: indicates the number of bootstrapp aggregations to use
  - `seed`: indicates the random seed to use during any stoichastic process
  - `start_date`: the minimum date for analysed data. This allows the lower bound year of the data to be restricted (to omit earlier data if necessary). If this item is missing, the start_date will be determined from the observed data.
  - `end_date`: the maximum date for the analysed data. This allows the upper bound year of the data to be restricted (to omit later data if necessary). If this item is missing, the end_date will be determined from the observed data.
- `../parameters/water_quality_guidelines.csv`. This file defines the guideline values associated with each measure as well as the labels to be used in tables/figures.
- `../parameters/spatial.csv`. This file defines the names used for Zones and Areas.
- `../input/overwrites.csv`. This file defines any expert overwrites that should be applied (in the event that the observed values are considered unrepresentative or unsuitable for some justifiable reason).
- `../input/weights_m.csv`. This file provides any specific weights that should be applied when aggregating items together on the Measure scale.
- `../input/weights_s.csv`. This file provides any specific weights that should be applied when aggregating items together on the spatial scale.

Analyses

Before describing the sequence of steps in the analysis pipeline, it is necessary to outline the major conceptual phases of the analyses.

Index computation

Water Quality indices (which are standardized measures of condition) are typically expressed relative to a guideline (see Appendix Section) or benchmark. Of the numerous calculation methods available, those that take into account the distance from the guideline (i.e. incorporate *difference-to-reference*) rather than simply an indication of whether or not a guideline value has been exceeded are likely to retain more information as well as being less sensitive to small changes in condition close to the guidelines.

The challenging aspect of distance (or amplitude) based index methodologies is that what constitutes a large deviation from a benchmark depends on the scale of the measure. For example, a deviation of 10 units might be considered relatively large of turbidity (NTU) or salinity (ppt), yet might be considered only minor for the Total Nitrogen ($\mu g/L$). In order to combine a range of such metrics together into a meaningful index, the individual scores must be expressed on a common scale. Whilst this is automatically the case for Binary compliance, it is not necessarily the case for distance based indices.

Table 2 describes and compares the formulations and response curves of the Binary compliance method as well as a number of amplitude (distance based) indexing methods.

The Modified Amplitude and Logistic Modified Amplitude are both based on a base 2 logarithm of the ratio of observed values to the associated be benchmark (see Table 2). This scale ensures that distances to the

benchmark are symmetric (in that a doubling and halving equate to the same magnitude - yet apposing sign). Furthermore, the logarithmic transformation does provide some inbuilt capacity to accommodate log-normality (a common property of measured values).

By altering the sign of the exponent, the Modified Amplitude methods can facilitate stressors and responses for which a failure to comply with a benchmark would be either above or below the benchmark (e.g. NTU vs Secchi depth). Further modifications can be applied to accommodate measures in which the benchmark represents the ideal and deviations either above or below represent increasingly poorer conditions (e.g. pH and dissolved oxygen).

The raw Modified Amplitude scores are relatively insensitive to small fluctuations around a benchmarks and sensitivity increases exponentially with increasing distance to the benchmark. The resulting scores can take any value in the real line $[-\infty, \infty]$ and hence are not bounded\footnote{Unbounded indices are difficult to aggregate, since items that have very large magnitude scores will have more influence on the aggregation than those items with scores of smaller magnitude. Furthermore, unbounded scores are difficult to convert into alphanumeric Grades. Consequently, the Scores need to be scaled before they can be converted to alphabetical grading scale. There are two broad approaches to scaling (see Table 2):

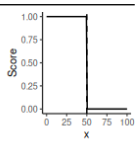
a. Capping and scaling: The log_2 scale can be capped to a range representing either a constant extent of change (e.g. twice and half the benchmark - a cap factor of 2) or else use historical quantiles (10th and 90th percentiles) to define the upper and lower bounds to which to cap the scale. Note historical quantiles are unavailable for the current application. Thereafter, either can be scaled to the range [0,1] via a simple formula (see Table 2 III.Scaled).

b. Logistic Modified Amplitude: By expressing the scores on a logistic scale, the range of scores can be automatically scaled to range [0,1]. Moreover, this method allows the shape of the response curve to be customized for purpose. For example, the relative sensitivity to changes close or far from the benchmarks can be altered by a tuning parameter.

Rather than aggregating across sites before calculating indices, we would suggest that indices should be calculated at the site level. This is particularly important when different measures are measured at different sites. Spatial variability can be addressed via the use of a bootstrapping routine (see below). We would recommend that measurements collected throughout the reporting year be aggregated together into a single annual value. This is primarily because most water quality guidelines pertain specifically to annual averages rather than single time samples. Although it is possible to incorporate uncertainty due to temporal variability, the low sparse temporal frequency of sample collection is likely to yield uncertainty characteristics that will swamp the more interesting spatial sources of uncertainty.

A useful metric for comparing the sensitivity of one indexing method over another is to take some representative longitudinal data and calculate indices based on the actual data as well as data that introduces progressively more noise.

Table 2: Formulations and example response curves for a variety of indicator scoring methods that compare observed values (x_i) to associated benchmark, guidelines or references values ($benchmark_i$ and dashed line). The Scaled Modified Amplitude Method can be viewed as three Steps: I. Initial Score generation, II. Score capping (two alternatives are provided) and III. Scaling to the range [0,1]. The first of the alternative capping formulations simply caps the Scores to set values (on a log_2 scale), whereas the second formulation (Quantile based, where $Q1$ and $Q2$ are quantiles) allows guideline quantiles to be used for capping purposes. Dotted lines represent capping boundaries. In the Logistic Scaled Amplitude method, T is a tuning parameter that controls the logistic rate (steepness at the inflection point). For the purpose of example, the benchmark was set to 50.

Method	Formulation	Response curve
Binary	$score_i = \begin{cases} 1 & \text{if } x_i \leq benchmark_i \\ 0 & \text{if } x_i \text{ else} \end{cases}$	

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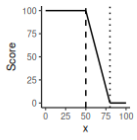
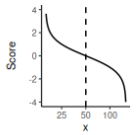
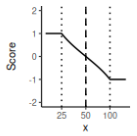
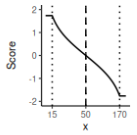
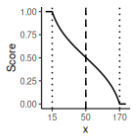
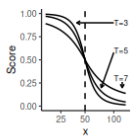
Method	Formulation	Response curve
Benchmark and WCS Modified Amplitude	$score_i = \begin{cases} 100 & \text{if } x_i \leq benchmark_i \\ 0 & \text{if } x_i \geq WCS_i \\ \left[1.0 - \left\lvert \frac{x_i - benchmark_i}{WCS_i - benchmark_i} \right\rvert\right].100 & \text{else} \end{cases}$	
I. Raw (MAMP)	$score_i = \begin{cases} log_2(\frac{x_i}{benchmark_i})^{-1} & \text{if} > benchmark_i = \text{fail} \\ log_2(\frac{x_i}{benchmark_i})^{1} & \text{if} < benchmark_i = \text{fail} \end{cases}$	
II. Fixed caps (-1, 1)	$Score_i = \begin{cases} log_2(-1) & \text{if } Score_i < -1 \\ log_2(1) & \text{if } Score_i > 1 \\ Score_i & otherwise \end{cases}$	
II. Quantile based caps	$Score_i = \begin{cases} log_2(\frac{Q1}{benchmark_i})^{-1} & \text{if } x_i < Q1 \\ log_2(\frac{Q2}{benchmark_i})^{1} & \text{if } x_i > Q2 \\ Score_i & otherwise \end{cases}$	
III. Scaled	$Score_i = \frac{Score_i - min(Score_i)}{max(Score_i) - min(Score_i)}$	
Logistic Scaled Modified Amplitude	$\lambda_i = \begin{cases} -1 & \text{if} > benchmark_i = \text{fail} \\ 1 & \text{if} < benchmark_i = \text{fail} \end{cases}; R_i = \begin{cases} -1 & \text{if} > benchmark_i = \text{fail} \\ 1 & \text{if} < benchmark_i = \text{fail} \end{cases};$ $Score_i = \frac{1}{1+e^{\lambda R_i T}}$	

Bootstrapping

Bootstrapping is a statistical resampling method that involves repeatedly sampling with replacement from a dataset to estimate the sampling distribution of a statistic. By generating multiple "bootstrap samples,"

this technique allows for the computation of measures such as confidence intervals, standard errors, and other uncertainty metrics without relying on strong parametric assumptions.

Bootstrapping is particularly useful for aggregating collections of data while retaining the combined uncertainty through the aggregation process. When data from multiple sources or experiments are combined, the uncertainty associated with each dataset must be accounted for to avoid underestimating the variability in the aggregated result. Bootstrapping achieves this by:

- *Resampling with replacement*: This ensures that the variability within each dataset is preserved and propagated into the aggregated result.
- *Estimating uncertainty*: By calculating statistics (e.g., means, medians, or other metrics) across bootstrap samples, bootstrapping provides a robust way to quantify the uncertainty in the aggregated data.
- *Non-parametric flexibility*: Bootstrapping does not require assumptions about the underlying distribution of the data, making it suitable for complex or non-standard datasets.

In summary, bootstrapping is a powerful tool for combining data while retaining all sources of uncertainty, ensuring that the aggregated results accurately reflect the variability inherent in the original datasets.

Hierarchical aggregation

To facilitate the integration of additional input Measures into the report card scores (such as additional Physico-chem or nutrients), or even additional Sub-indicators (such as sediment metals, seagrasses and mangroves), we can defined a hierarchical structure in which Measures (such as Turbidity, NOx, etc) are nested within appropriate Sub-indicators. In turn, these Sub-indicators are nested within Indicators.

By progressively abstracting away the details of the Measures and Sub-indicators, a more focused narrative can be formulated around each level of the hierarchy. For example, when discussing the current state (and trend in state) of the Water Quality Indicator, rather than needing to discuss each individual constituent of Water Quality, high-level Grades are available on which to base high-level interpretations. More detailed explorations are thence revealed as required by exploring the Grades at progressively finer scales of the hierarchy. Moreover, the hierarchical structure offers great redundancy and thus flexibility to add, remove and exchange individual measures.

Similar arguments can be made for a spatial hierarchy in which Zones are nested within Regions which in turn are nested within the Whole Harbour.

The current hierarchical structure comprises two physico-chemical Measures (Dissolved Oxygen and Turbidity) that are nested within a single Physico-chem Sub-indicator and four nutrient Measures (Ammonia, Chlorophyll-a, Filterable Reactive Phosphate and NOx) that are nested within a single Nutrient Sub-indicator.

There is future scope to add additional nutrient or physico-chemical Measures as well as metals and sediments. This hierarchy can be extended down to include other environmental indicators pertaining to habitats (mangroves, seagrass, corals) or other perspectives (cultural and economic).

The purpose of aggregation is to combine together multiple items of data. The current proposed Darwin Harbour report card is informed by a double hierarchical data structure in which Measures are nested within Sub-indicators which are nested in Indicators and Zones are nested within Regions which are nested within Whole of Harbour (see Figure 3).

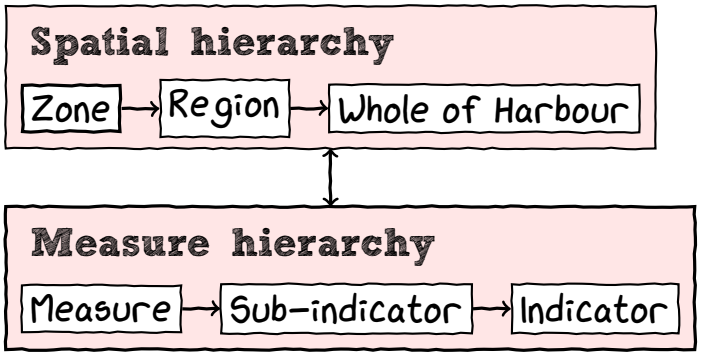


Figure 3: Schematic illustrating the Spatial and Measure aggregation hierarchies.

Table 3: Fabricated illustration of the discrepancies between total means (i.e. Whole of Harbour Indicator Score) generated from row means (Region Sub-indicator Scores) and column means (Whole of Harbour Sub-indicator Scores).

	Sub-Indicators		
Region	Physico - chem	Nutrients	Indicator
1	5.00	2	3.50
2	6.00		6.00
3	6.00	4	5.00
Whole of Harbour	5.67	3	X

Although the double hierarchy (Spatial and Measurement), does offer substantial redundancy and power advantages, it also introduce the complexity of how to combine the hierarchies into a single hierarchical aggregation schedule. Table 3 (a fabricated example), illustrates this complexity for aggregating across Spatial and Measure scales when data availability differs. This simple example demonstrates how different aggregation schedules can result in different Whole of Harbour Component Scores:

- calculating Whole of Harbour Component Score as the average of the Region level Water Quality Scores prioritizes that the Whole of Harbour Component Score should reflect the average of the Water Quality Indicator Scores for the Regions. This schedule will bias the resulting Whole of Harbour Water Quality Indicator Score towards Sub-indicators represented in more Regions. Although the entire Darwin Harbour sampling design is currently balanced, there is no guarantee that this will always be the case. If for example, Nutrients were not available for certain Regions, then the Whole of Harbour Indicator Score will be biased towards Physico-chemical Sub-indicators.
- calculating Whole of Harbour Water Quality Indicator Score as the average of the Whole of Harbour level Sub-indicator Scores prioritizes equal contributions of Sub-indicators to the Indicator Score at the expense of being able to relate Whole of Harbour Scores to the corresponding Region Scores.

If X (mean) is calculated from the three row means = 4.83, If X (mean) is calculated from the two column means = 4.33

Figure 4 illustrates the proposed aggregation schedule for Darwin Report Cards. Importantly, all *Indicator* Scores are generated from *Zone* level data and separate *Zone* and *Whole of Harbour* level Measure aggregations are maintained in parallel starting at the level of *Indicator*.

Important notes on this aggregation schedule:

- Water Quality Indicator Scores (and thus Grades) should be the aggregate of the constituent Sub-indicator Scores for the appropriate spatial scale and thus, both derived directly from Sub-indicator level data.
- Sub-indicator and Indicator level data often comprise data from differing numbers of Zones. To avoid biases towards Indicators from more Zones, Region and Whole of Harbour Indicator Scores should be calculated from Region and Whole of Harbour Indicator level data respectively.
- That is, Whole or Harbour Indicator Scores should not be calculated from Region Indicator Scores.
- As such, at the Indicator level Whole of Harbour Scores cannot be viewed as the average of the Region level Indicator data as they are both based on Sub-indicator data from different spatial scales (Regions vs Whole of Harbour).
- Consequently, Sub-indicator level data are the transferable level data through the spatial hierarchy.
- Region and Whole of Harbour Measure level data can be derived by aggregating down the spatial hierarchy, yet these are end of line derivatives that do not inform their respective Sub-indicator level data.

To maximize information retention throughout a series of aggregations, it is preferable to aggregate distributions rather than single properties of those distributions (such as means). The simplest way to perform a hierarchy of aggregations is to interactively calculate the means (or median) of items (means of means etc). At each successive aggregation level only very basic distributional summaries (such as the mean and perhaps standard deviation) are retained, the bulk of upstream information is lost. Alternatively, more complex methods that involve combining data or probability distributions can be effective at aggregating data in a way that propagates rich distributional properties throughout a series of aggregations.

Importantly, if the purpose of aggregation is purely to establish a new point estimate of the combined items, a large variety of methods essentially yield the same outcomes. On the other hand, if the purpose of aggregation is also to propagate a measure of uncertainty or confidence in the point estimate through multiple hierarchical

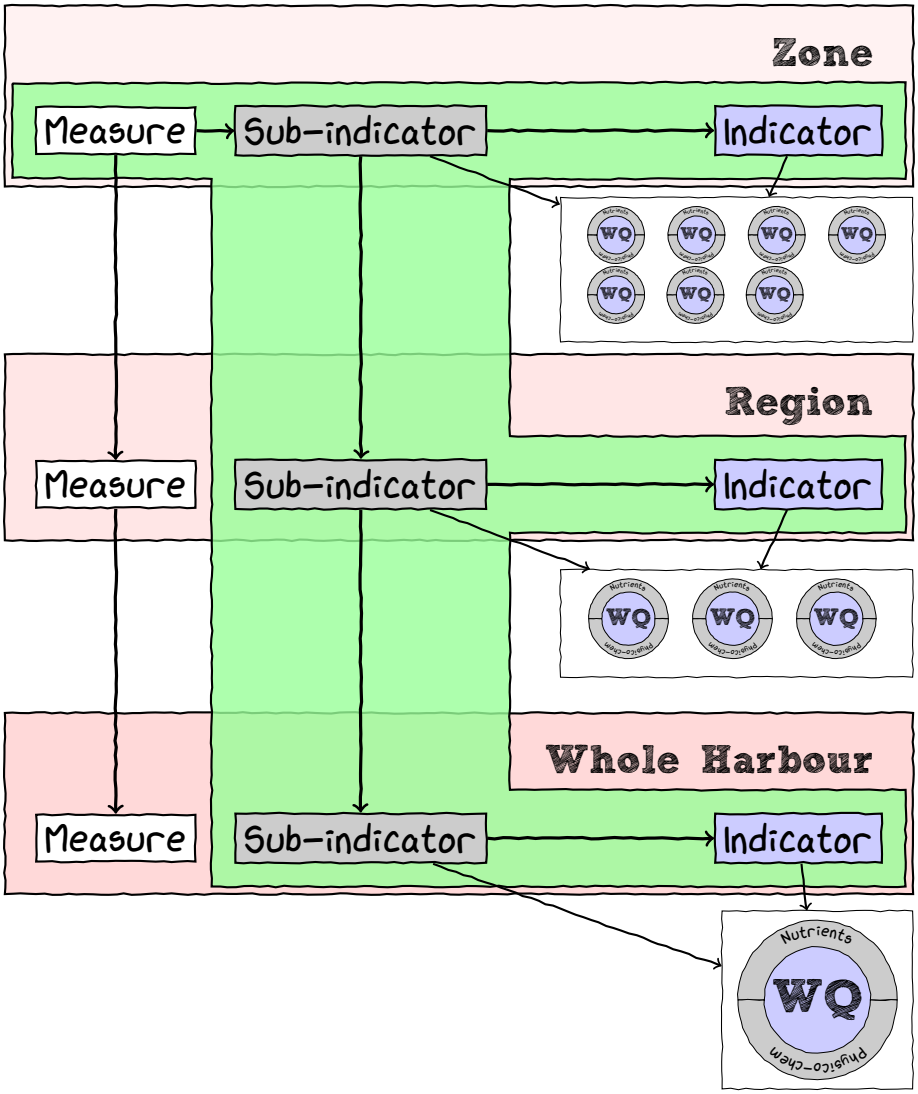


Figure 4: Schematic illustrating the combination of Spatial (Zone, Region and Whole of Harbour) and Measure (Measure, Sub-indicator, Indicator) nodes of the double hierarchical aggregation schedule associated with the Darwin Harbour Report Card. Aggregation directions between nodes are signified by arrows and the main aggregation pathway through the schedule is illustrated by the green polygon. Tabular summaries are produced at each node, and Water Quality Status discs (comprising Sub-indicators around a central Indicator Grade indicate where in the hierarchy they are generated.

levels of aggregation (as is the case here), then the different methodologies offer differing degrees of flexibility and suitability.

Hierarchical aggregations are essentially a series of steps that sequentially combine distributions (which progressively become more data rich). The resulting distribution formed at each step should thereby reflect the general conditions typified by its parent distributions and by extension, each of the distributions higher up the hierarchy.

Numerous characteristics can be estimated from a distribution including the location (such as mean and median) and scale (such as variance and range). For the current project, the mean and variance were considered the most appropriate[1] distributional descriptions and from these estimates Grades and measures of confidence can be respectively derived. Hence the numerical summaries (mean and variance) at any stage of the hierarchical aggregation are a byproduct rather than the sole property of propagation.

Bootstrap aggregation

Although some of the items to be aggregated together might initially comprise only a few values (or even a single value), it is useful to conceptualize them as continuous distributions. For example, when aggregating multiple *Measures* (such as all Water Quality Metals) together to generate a *Site* level) _Sub_indicator average, each *Measure* in each *Site* can be considered a distribution comprising the single Score for that *Measure*. Aggregation then involves combining together the multiple distributions into a single amalgam (by adding the distributions together, see Figure Figure 5). Similarly, when aggregating at the *Indicator* level across *Site* to generate *Zone* summaries for each *Indicator*, *Site* distributions are respectively added together to yield a single distribution per *Zone*.

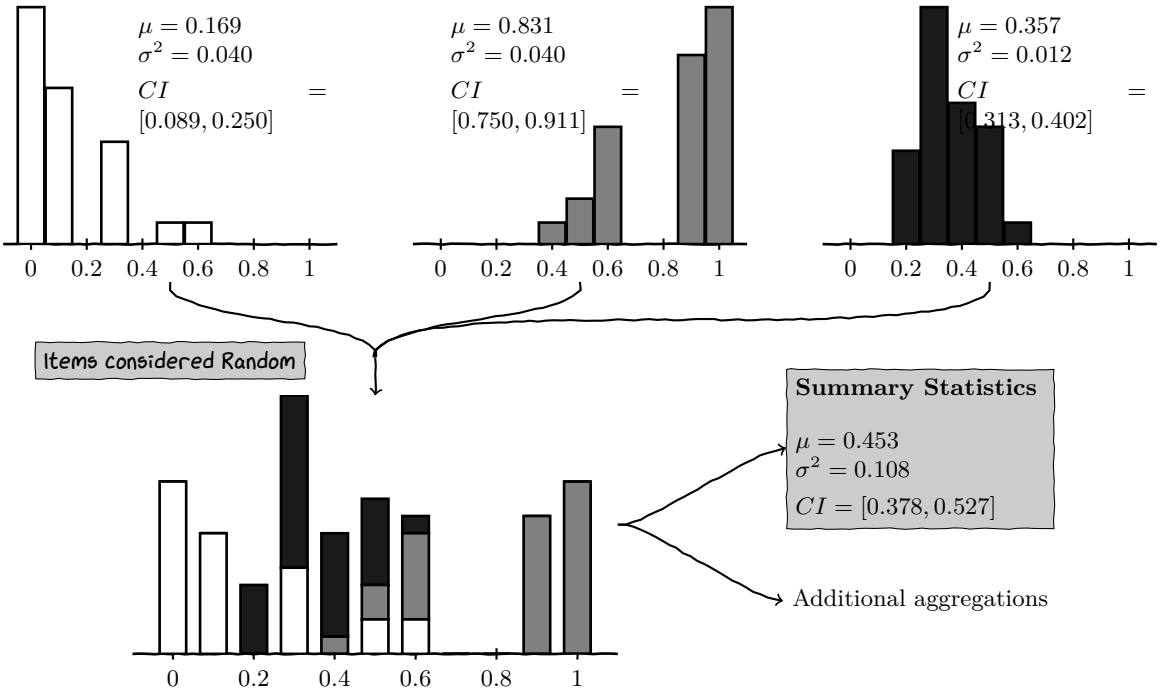


Figure 5: Illustration of Bootstrapped aggregation of three distributions. Simple summary statistics (mean, variance and 95% confidence interval presented for each distribution.

If the distributions being aggregated are all proportional distributions (e.g.~density distributions), adding them altogether is trivially simple. However, if, rather than actual distributions, the items to be aggregated are actually just small collections of values (as is the case for many of the measures here) or even large, yet unequally populous collections of values (as could be the case for Continuous Flow Monitoring with missing or suspect observations), then simply aggregating the distributions together will result in amalgams that are weighted according to the size of the collections (larger collections will have more influence). For example, if we were aggregating together three *Regional* (to yield Whole of Harbour estimates), one of which comprised

[1]The aggregations typically involve some Measures with a small number of unique observations (and thus indices) and thus means and variances provide greater sensitivity than medians and ranges. Moreover, the indexing stage effectively removes outliers and standardizes the scale range thereby reducing the need for robust estimators.

twice as many Zones, simple aggregation of distributions would result in a distribution that was more highly influenced by the Region with the more *Zones*. Similarly, when aggregating from the level of Sub-indicator to the level of Indicator, the resulting Indicator would be biased towards the Sub-indicator with the most Measures. Whilst this may well be a useful property (e.g.~stratified aggregation), it may also be undesirable.

Bootstrapping is a simulation process that involves repeated sampling (in this case with replacement) of a sample set with the aim of generating a bootstrap sample from a distribution. This bootstrap sample can be used to estimate the underlying probability distribution function that generated the data as well as any other summary statistics. Importantly, bootstrapping provides a way to generate distributions that are proportional and thus un-weighted by the original sample sizes thereby facilitating un-weighted aggregation. Bootstrapped distributions can be aggregated (added together) to yield accumulated child distributions that retain the combined properties of both parents (see Figure 5). As a stochastic process, repeated calculations will yield slightly different outcomes. Nevertheless, the more bootstrap samples are collected, the greater the bootstrap distributions will reflect the underlying Score distribution and provided the number of drawn samples is sufficiently large (e.g. 10,000 re-samples), repeated outcomes will converge.

Weights

Standard bootstrapping yields equally weighted distributions, however, specific weighting schemes can also be easily applied by bootstrapping in proportion to the weights. For example, to weight one parent twice as high as another, simply collect twice as many re-samples from the first distribution. To ensure that all resulting distributions have the same size (by default 10,000 items), the number of bootstrap samples collected (n) from each of the (p) parent distributions (i), given the weights (w_i) is calculated as:

$$n_i = \lceil (S/p) \times w_i \rceil$$

where S is the target size (10,000) and $\lceil . \rceil$ indicates the ceiling. Qualitative data (such as ratings) can also be incorporated by enumerating the categories before bootstrapping.

In addition to allowing expert driven weights that govern the contribution of different items during aggregations, it is possible to weight according to relative spatial areas during spatial aggregations. Currently, all Zones are equally weighted when aggregating to Region level and all Regions equal when aggregating to Whole of Harbour level. That means that small Zones have an equal contribution as large Zones despite representing a smaller fraction of the water body. Area based weights could be applied such that Zones and Regions contribute in proportion to relative areas.

Weights are defined by a user editable configuration file that is similar in structure to the Water Quality guidelines file.

Expert interventions

The ability for experts and Report Card managers to intervene (exclude or overwrite) Scores/Grades at any Spatial/Measure scale is essential to maintain the quality of a Report Card in the event of unrepresentative or suspect data. The current system is able to support expert interventions in the form of exclusions and overwrites. For example, after reviewing the QAQC, an expert can elect to exclude one or more Measures (or Subindicators etc) from one or more spatial scales. Such interventions are specified via a user editable configuration files[2] (csv) that is similar in structure to the Water Quality guidelines file.

The essential component of this configuration file is that it allows a user to specify what Data are to be excluded or replaced. These can be at any of the levels of the Measure hierarchy (Measures, Sub-indications and Indicators) and any level of the Spatial hierarchy (Zones, Regions and Whole of Harbour). Settings pertaining to levels further along the aggregation hierarchies have precedence. For example, if Nutrients are excluded (or overridden) in a particular Region, then all Nutrient Measures within all Zones will be excluded irrespective of what the settings are for any specific Measure/Zone.

To reiterate, the advantage of bootstrapping data before concatenating (or averaging) versus simply concatenating data from multiple sources together, is to ensure that source data are all of exactly the same sample size (so as to not weight more heavily towards the more populous source(s)[3]). Bootstrapping also provides a

[2]Since aggregation occurs across two hierarchies (the Measure hierarchy and the Spatial hierarchy - see @fig-hierarchies and @fig-hier), two configuration files are necessary.

[3]Such weightings should be handled in other ways if at all

mechanism for propagating all distribution information throughout an aggregation hierarchy and ensures that estimates of variance derived from child distributions are on a consistent scale[4]. The latter point is absolutely critical if variance is going to be used to inform a Confidence Rating system and confidence intervals.

Minimum operator procedures are supported by filtering on the lowest performed indicator prior to bootstrapping. Importantly, the bootstrapping routine simply provides a mechanism to collate all sources together to yield a super distribution. Thereafter, the joint distribution can be summarized in what ever manner is deemed appropriate (arithmetic, geometric, harmonic means, medians, variance, range, quantiles etc). Moreover, different levels of the aggregation can be summarized with different statistics if appropriate.

Scores and Grades

The double hierarchy Bootstrap aggregation described above, yields *Score* distributions for each Measure-level/Spatial-level combination. The location and scale of each distribution can thus be described by its mean and variance. Mean *Score* are then converted into a simple five-point alphanumeric *Grade* scale (and associated colors) using a control chart (see Table Table 4).

Table 4: Darwin Harbour Report Card Grade scale control chart

Score	Grade	Description
≥ 0.85	A	Very good
$\geq 0.65, < 0.85$	B	Good
$\geq 0.5, < 0.65$	C	Satisfactory
$\geq 0.25, < 0.5$	D	Poor
< 0.25	E	Very poor

The control chart grade boundaries adopted for the current report (presented in Table 4) are consistent with the Gladstone Healthy Harbour Partnership Report Card. Broadly, they represent two levels (Poor and Very Poor) under the Guideline values and three above (Satisfactory, Good and Very Good). The grade boundaries are usually determined by expert panel to ensure that the range of indices represented by each grade classification is congruent with community interpretation of a letter grade report cards. It is far less clear how estimates of uncertainty can be incorporated into such a grading scheme in a manner that will be intuitive to non-technical audiences. That said, statistical uncertainty is just one of many sources of un- certainty that should be captured into a confidence or certainty rating. Hence any expectations of presenting uncertainty in a quantitative manner may well be unrealistic anyway.

Certainty rating

Incorporating an estimate of scale (variance) into a certainty or confidence rating necessitates re-scaling the estimates into a standard scale. In particular, whereas a scale parameter of high magnitude indicates lower degrees of certainty, for a certainty rating to be useful for end users, larger numbers should probably represent higher degrees of certainty. Thus, the scaling process should also reverse the scale. Furthermore, variance is dependent on the magnitude of the values.

In order to re-scale a scale estimate into a certainty rating, it is necessary to establish the range of values possible for the scale estimate. Whilst the minimum is simple enough (it will typically be 0), determining the maximum is a little more challenging depending on the aggregation algorithm (bootstrapping, Bayesian Network etc). One of the advantages in utilizing proportional distributions (such as is the case for a Bayesian Network or a re-sampled bootstrap distribution) is that the scale parameter for the single worst case scenario can be devised (once the worst case scenario has been determined) independent of sample sizes or weightings. In most situations this is going to be when the distribution comprises equal mass at (and only at) each of the two extremes (for example, values of just 0 and 1).

The measure of confidence rating discussed above is purely an objective metric derived from the variance in the aggregation hierarchy. It is completely naive to issues such as missing data, outliers and Limit of Detection issues - the influences of which on a confidence rating are necessarily subjective. A full Confidence Rating would combine these objective variance component with additional subjective considerations such as climatic and disturbance information, and the perceived influence of missing, Limit of Detection and outlying data.

[4]Variance is inversely proportional to sample size

Hence, the statistical scaled statistical variance would form just one component in the Confidence Rating system.

The bootstrap aggregation method provides a mechanism for estimating variance from which to build such an expert considered Confidence Rating system.

Confidence intervals

Confidence intervals (CI) represent the intervals in which we have a certain degree of confidence (e.g. 95%) that repeated estimates will fall. Hence the 95% CI of the mean is the range defined by the quantiles representing 95% of repeated estimates of the mean.

To calculate 95% confidence intervals for bootstrap aggregated distributions (e.g. Zone 1/Nutrient distribution), we repeatedly[5] draw a single sample from each of the constituent distributions (e.g. a single value from the Zone 1 Ammonia, Chlorophyll-a, Filterable Reactive Phosphate and NOx distributions) and from each set of draws, calculate the weighted [6] mean of the values. The 95% CI is thus calculated as the quantiles (p=0.025 and p=0.975) of the means.

Aggregation schedule

A. Calculation of Zone level Scores and Grades

1. Collect raw data (= **Measures**) at each fixed monitoring site or along a Continuous Flow Monitoring (CFM) transect and compare individual observations to associated guideline/benchmark/reference
2. Create indexed data as an expression of degree of difference *scaled modified amplitude method*) to yield a **Score** for each **Measure** per sampling location (e.g. site or location along CFM transect) (applies to *Measures* in all *Indicators*, Water Quality)
3. Apply any expert opinion interventions
4. Combine **Measure** Scores into **Zone**-level **Sub-indicator** Scores by averaging taking into account any weightings, i.e. aggregate into observation-level Sub-indicator Scores. This step involves **Bootstrapping** each input to distributions of 10,000 re-samples (or fewer if weighted), combining distributions and finally Bootstrapping again into a single 10,000 size distribution.
5. Combine **Sub-indicator** Scores into **Zone**-level **Indicator** Scores by averaging, i.e. aggregate into Zone-level Indicator Scores.
6. Convert Scores into coloured **Grades** (A-E) for visual presentation in report card

B. Calculation of Region level Grades

1. Aggregate **Zone**-level _Sub-indicator** Scores from step A.5 into **Region**-level *Sub-Indicator* Scores by averaging (incorporating spatial weights)
2. Aggregate **Region**-level *Sub-indicator* Scores into **Region**-level *Indicator* Scores by averaging (incorporating weights)

C. Calculation of Whole Of Harbour Grades

1. Aggregate **Region**-level *Sub-Indicator* Scores from step B.1 into **Whole of Harbour**-level *Sub-Indicator* Scores by averaging (incorporating spatial weights)
2. Aggregate **Whole of Harbour**-level *Sub-Indicator* Scores into **Whole of Harbour**-level *Indicator* Scores by averaging (incorporating weights)

[5] The more repeated draws the closer the distribution of means will converge. For the current project, the number of repeated draws is 10,000.

[6] Weights according to the weights defined for that level of the aggregation hierarchy

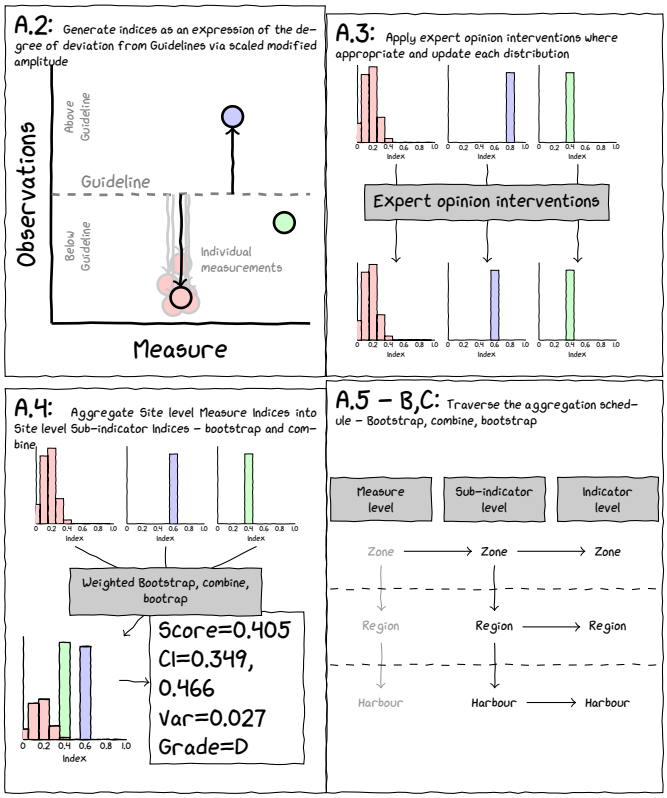


Figure 6: Schematic illustrating the major steps of the Darwin Harbour Report Card. In this fabricated example, there are three Measures (Red, Green and Blue). Each of the Blue and Green Measures are represented by a single discrete observation, whereas the Red Measure is represented by a large collection of observations. Expert option intervened to lower the blue Measure distribution from observed values at 0.8 to 0.6.

Temporal changes

A key goal of any monitoring program is to be able to report on status and trends. The above methodologies provide the tools for reporting on the status in any given year. What is also required is the ability to compare the status between years - that is to report on the changes in status over time.

The bootstrapp aggregations yield full empirical distributions for each Measure/Space unit per year. Typically we summarise these distributions via a mean and confidence interval to simplify their presentation. Then, if we simply wanted to calculate the change in a score between two years, we could simply subtract the mean of one year from the other. However, doing so would loose the information we had on uncertainty. If on the other hand, we subtracted the distribution for one year from that of another year, we would obtain a distribution of change values from which we could provide summaries like mean and confidence intervals.

Since each of the values in the distributions are produced via bootstrapping, they are not in any specific order (that is they are not ranked from lowest to highest value) and there are the same number (n) of bootstrapp samples in each distribution. Hence, if we line up the values of two distributions side by side, we can calculate the difference between each pair of values down the line. This will yield n differences. Collectively, these n differences now represent the distribution of change values.

In addition to summarising the distribution of change by properties such as mean and confidence interval, we can also estimate the probability that the change exceeds a certain value (typically zero). This calculation is simply the number of values that exceed (zero) divided by the total number of values and hereafter will be referred to as an exceedance probability (P_E).

Between two particular years, scores might generally increase, decrease or stay the same. To explore an increase, we would report on the probability that the change values were positive ($P_E > 0$) and to report on a decline we would focus on the probability that the change values were negative ($P_E < 0$). Note, we cannot report on the probability that the change values are zero (logically this is infinitely small). Herein, these exceedance probabilities are interpreted according to:

- $P_E \geq 0.95$: strong evidence of change

- $P_E \geq 0.90$: evidence of change
- $P_E \geq 0.85$: weak evidence of change
- $P_E < 0.85$: no evidence of change

Within this application, change is explored two ways:

1. annual change - the change between each successive pairs of years (e.g. 2016 vs 2017, 2017 vs 2018, etc).
2. quinquennial (half-decadal) change - the change between each pair of five year blocks of time. This is calculated by first aggregating together the blocks of years into single distributions before subtracting those distributions.

These changes can then by presented graphically and in tabular form.

Analysis stages

Stage 2 - obtaining the data

At the completion of this stage, the Data sidebar menu and Stage 3 & 4 button will become active and the Data page will be populated with the raw data and be available for review.

Read water quality guidelines data

This task will read in the water quality guidelines information from the `../parameters/water_quality_guidelines.csv` file.

Read input data

This task will sequentially read in each of the water quality data files from `../input/`. These files are in the format of `<number>_wq.csv`, where `<number>` is a two digit number representation of the sampling year.

Read in overwrites data

This task will read in each of the overwrites file from `../input/overwrites.csv`. The purpose of overwrites is to provide a mechanism for expert elicitation, whereby grades can be overwritten in the event that the expert strongly believes that the observed data are a poor reflection of the genuine health of the sampling unit.

Read in the weights data

There are two tasks to read read in the measures weights file from `../input/weights_m.csv` and the spatial weights file from `../input/weights_s.csv`. These files provide a mechanism to control how much weight different items have in an aggregation. If no weights are given, then all items are equally weighted during aggregation.

Read in aggregation hierarchy data

This task will read in the aggregation hierarchy file from `../input/hierarchy.csv`. The aggregation hierarchy determines the child items for each aggregation.

Read in the spatial settings data

This task will read in the spatial settings file from `../parameters/spatial.csv`. These data form a lookup that relate zone and area numbers to their names and provides some settings for the location and colour of labels on maps.

Validate input data

This task performs data validation in accordance with the rules set out in the following section.

Data requirements

To be valid, input data must be flat text files (*.csv) comprising:

- `../input/*_wq.csv`

Field	Description	Validation conditions
Zone	Spatial zone	must be numeric or factor
Region	Spatial region	must be numeric or factor
Source	Source of samples (CFM or Discrete)	must be character or factor of either (CFM or Discrete)
Date	Sample data	must be a valid string
Latitude	Latitude of sample	must be a numeric of format -d.d
Longitude	Longitude of sample	must be a numeric of format d.d
Chla_mug_PER_L	Chlorophyll-a concentration	must contain only numbers or start with a '<' symbol
Turbidity_NTU	Turbidity concentration	must contain only numbers or start with a '<' symbol
Turbidity_NTU		should not exist for Discrete source
DO_PERCENT_saturation	Percentage dissolved oxygen	must contain only numbers or start with a '<' symbol
NH3_mug_PER_L	Ammonium concentration	must contain only numbers or start with a '<' symbol
NH3_mug_PER_L		should not exist for CFM source
PO4_mug_PER_L	Phosphate concentration	must contain only numbers or start with a '<' symbol
PO4_mug_PER_L		should not exist for CFM source
Nox_mug_PER_L	Nox (nitrate and nitrite) concentration	must contain only numbers or start with a '<' symbol
Nox_mug_PER_L		should not exist for CFM source

- `../input/hierarchy.csv`

Field	Description	Validation conditions
Component	Highest level of measure hierarchy (always Environmental)	must contain characters
IndicatorGroup	Next measure level (always Water Quality)	must contain characters
Indicator	Next measure level (always Water Quality)	must contain characters
Subindicator	Either Nutrients or Physico-chem	must contain characters
Measure	Name of the Measure	must contain characters

- `../input/weights_*.csv`

Field	Description	Validation conditions
Component	Highest level of measure hierarchy (always Environmental)	must contain characters
IndicatorGroup	Next measure level (always Water Quality)	must contain characters
Indicator	Next measure level (always Water Quality)	must contain characters
Subindicator	Either Nutrients or Physico-chem	must contain characters
Measure	Name of the Measure	must contain characters
Zone	Spatial zone	must be numeric or factor
Region	Spatial region	must be numeric or factor
Site	Spatial site	must be numeric or factor

Field	Description	Validation conditions
Weight	Spatial site	must be numeric

Could be empty {tbl-colwidths="[25,35,40]"}

- `../input/overwrites.csv`

Field	Description	Validation conditions
Component	Highest level of measure hierarchy (always Environmental)	must contain characters
IndicatorGroup	Next measure level (always Water Quality)	must contain characters
Indicator	Next measure level (always Water Quality)	must contain characters
Subindicator	Either Nutrients or Physico-chem	must contain characters
Measure	Name of the Measure	must contain characters
Source	Source of samples (CFM or Discrete)	must be character or factor of either (CFM or Discrete)
Region	Spatial region	must be numeric or factor
Zone	Spatial zone	must be numeric or factor
Site	Spatial site	must be numeric or factor
overwrittenGrade	Grade to apply (overwrite observations)	must contain characters (A, B, C, D or E)

Could be empty {tbl-colwidths="[25,35,40]"}

- `../parameters/water_quality_guidelines.csv`

Field	Description	Validation conditions
ZoneName	Zone name	must contain characters
HydstraName	Name in hydstra	must contain characters
Conversion	Unit conversion factor	must be numeric
Measure	Name of the Measure	must contain characters
UnitsLabel	Name of the Measure including units	must contain characters
Label	Name of the Measure including units (formatted for LaTeX)	must contain characters
DirectionOfFailure	Direction of failure relative to guideline value	must be a single character (B or H)
GL	Water quality guideline value	must contain only numbers or start with a '<' symbol
RangeFrom	Water quality guideline lower limit of range (for DO)	must contain only numbers or start with a '<' symbol
RangeTo	Water quality guideline upper limit of range range (for DO)	must contain only numbers or start with a '<' symbol
DetectionLimit	Limit of detection value	must contain only numbers or start with a '<' symbol

- `../parameters/spatial.csv`

Field	Description	Validation conditions
Region	Spatial region	must be numeric or factor
RegionName	Region name	must contain characters
Zone	Spatial zone	must be numeric or factor
ZoneName	Zone name	must contain characters
Lab_lat	Latitude of zone label on maps	must be a numeric of format -d.d
Lab_long	Longitude of zone label on maps	must be a numeric of format d.d
HexColor	Hexidecimal colour code for zone labels on maps	must be a six digit hex code proceeded by a '#'

Stage 3 - Prepare spatial data

Read in shapefiles

This task will read in individual shapefiles from `../parameters/GIS`. The files are: - `RCZ_rev24.shp` - `SBZone_upper.shp` - `Middle_Harbour_Upper.shp`

Combine shapefiles

This task will combine all shapefiles into a single shapefile

Stage 4 - processing the data

Combine water quality data

The water quality data are read in as separate csv files. Although technically they could have been consolidated into a single file before opening this application, maintaining separate files for each year does allow the user to isolate any validation issues to a single year (thereby making them easier to located and correct).

The current task will combine all the water quality data into a single data set.

Process dates

Spreadsheets often display dates in different formats from what they actually store internally and what they export. It is always advisable when exporting dates from spreadsheets to export them as strings (words) rather than numbers (number of seconds past a reference date) as these are typically less ambiguous.

The current task will process the dates from strings into genuine date objects

Filter the date range of the data

It is possible to restrict the analyses to a narrower range of dates than those that appear in the observed data. For example, the observed data might include some samples from an otherwise incomplete sampling year, and it might be desirable to exclude these samples. Hence, this task determines whether a `start_date` or `end_date` have been defined in `../parameters/config.ini` and if so, uses them to trim the temporal range of the data.

The tables within the **Processed data** tab of the **Data** page will also be populated and the `Data` page will be available for review.

Select Measures

In order to compute indices, it is necessary to compare observed values to associated guideline values. In the current context a **Measure** is an observable property of water quality (such as Chlorophyl-a, Turbidity, Nox etc) - it is the analyte that is measured. This current task will exclude any measures for which there are no guideline values as these cannot be analysed further.

Define the focal year

The **focal year** represents the year that will be considered the focal sampling year for the analyses. All outputs will be stored in a folder reflecting this display diagnostics for this the focal year is the most recent sampling year. Furthermore, many of the QAQC diagnostics pertain specifically to this focal year alone.

Pivot data into longer format

Although it is often convenient to transcribe and store data in *wide* format (one in which each measure has its own column and each row represents a single sample collection), this format is illsuited for analyses and graphics in R. Analyses and graphics prefer data to be in *long* format. The following two tables highlight the differences between wide (top table) and long (bottom table) formats:

Zone	Date	Source	Chla_mug_PER_L	Turbidity_NTU	Nox_mug_PER_L
1	01/06/2016	CFM	1.338	2.68	NA
1	01/06/2016	CFM	1.376	2.63	NA
1	02/06/2016	Discrete	0.279	NA	0.013
1	02/06/2016	Discrete	0.178	NA	0.017

Zone	Date	Source	Measure	Value
1	01/06/2016	CFM	Chla_mug_PER_L	1.338
1	01/06/2016	CFM	Chla_mug_PER_L	1.376
1	02/06/2016	Discrete	Chla_mug_PER_L	0.279
1	02/06/2016	Discrete	Chla_mug_PER_L	0.178
1	01/06/2016	CFM	Turbidity_NTU	2.68
1	01/06/2016	CFM	Turbidity_NTU	2.63
1	02/06/2016	Discrete	Turbidity_NTU	NA
1	02/06/2016	Discrete	Turbidity_NTU	NA
1	01/06/2016	CFM	Nox_mug_PER_L	NA
1	01/06/2016	CFM	Nox_mug_PER_L	NA
1	02/06/2016	Discrete	Nox_mug_PER_L	0.013
1	02/06/2016	Discrete	Nox_mug_PER_L	0.017

This task will therefore pivot the data from wide to long format.

Join the guidelines data to the water quality data

This task will join (merge) the guideline data with the water quality data based on the Zones.

Apply spatial information

This task will use the shapefiles to assign spatial information (Zones and Regions) based on the latitude and longitude of the samples.

Make spatial lookup

This stage creates a lookup table that relates each of the spatial scales to one another. This lookup is used to inject the spatial information into the data and modelled derivatives after they are created and in so doing prevents the need to spatially join the data each time it is required.

Apply unit conversions

In addition to defining the guideline values, the `../input/water_quality_guidelines.csv` file defines any unit conversions that need to be applied. This task applies those unit conversions.

Apply limit of detection rules

This task applies limit of detection rules. Specifically, for all measures other than dissolved oxygen, if the observed value is below the detection limit, then the observed value is replaced by the detection limit. In the case of dissolved oxygen, if the observed value is less than 50, the observed value is replaced by NA (a missing value). In either case, a flag is added if a limit of detection replacement is made.

Join the aggregation hierarchy

The aggregation hierarchy determines what items are aggregated together during the bootstrapp aggregation process. This task joins the aggregation schedule into the data.

Stage 5 - Calculate indices

Load the data

This task loads the processed data in preparation for indice calculations.

Calculate indices

Prepare for bootstrapping

This current step prepares the Site/Year/Source level data for bootstrapp aggregation by repeatedly sampling these data (according to the nominated number of bootstrapp samples, n, set in the `../parameters/config.ini` file). In the case that only a single observation was collected at a specific site in a specific year for a specific source, then this observation will be repeated n times.

Stage 6 - QAQC

Stage 7 - Bootstrapping

Load data

This task will load the processed data.

Load the indices

This task will load the indices ready for bootstrapping.

Process the overwrites

This task will determine what overwrites have been defined in the `../input/overwrites.csv` file and make those specific changes to the indices prior to bootstrapping. Essentially, this task involves replacing the indices and grades calculated in Stage 5 (for the nominated measure/spatial scale) with those nominated the overwrites.

Process the weights

This task will determine what weights (measure or spatial) have been defined in `../input/weights_m.csv` and `../input/weights_s.csv` respectively and prepare for applying these weights during the appropriate aggregation phase.

Series of aggregations

There will then be a series of tasks that perform each of the hierarchical bootstrapp aggregations outlined in Figure 4.

Stage 8 - Summaries

This stage will generate a series of summary plots in the form of temporal trend plots and effects plots. At the end of this stage, the *Summaries* page will be enabled for review.

Load the data

This task will load the processed data.

Compile the scores

During the hierarchical boostrapp aggregation process, each Measure/Space combination is stored as its own data artifact. The current task will read each of these in an compile them together into a single object.

Series of trend plots

For each of the Measure/Space combinations, a temporal trend figure will be produced.

Calculate effects

This task will loop through each Measure/Space combination and calculate the annual and quinquennial (half-decadal) changes.

Effects plots

This task will generate effects plots for each Measure/Space/Change combination.

Application pages

Landing page

To run this tool, please adhere to the following steps:

1. review the *Path Settings* (specifically checking the **"Data input dir"**) and ensuring that there is at least one data file listed in the box under this setting
2. review the *Run Settings*. In particular,
    - consider whether you need to **Clear the previous data** - clicking the button to do so. Clearing the previous data deletes all cache and ensure that the analyses are performed fresh. **This is recommended whenever the input data changes**. Not clearing the previous data allows the user to skip directly to later run stages if earlier stages have already been run.
3. navigate the *Dashboard* via the menu on the left sidebar

In the *Run settings* panel, there is a **Run in sequence** toggle. By default, this toggle is set to "Yes" which ensures that all stages must be run in sequence and the various pages will become active once the appropriate stages have been complete. Toggling this switch to "NO" will instantly make all side menus, pages and run buttons become available. The purpose of this is to allow the user to re-visit the outcomes of analyses without the need to completely re-run the entire analysis. This is particularly useful if the user is returning to the analyses at a later date.

> Note
> Toggling the **Run in sequence** switch to "No" assumes that numerous artifacts (data saved throughtout the analysis process) are available and thus should only be considered after the analyses have been run through completely at some time. Never toggle this switch straight after clicking the "Clear previous data" button.

Dashboard

The analysis pipeline comprises numerous **Stages**, each of which is made up of several more specific **Tasks**. The individual Tasks represent an action performed in furtherance of the analysis and of which there are reportable diagnostics. For example, once the application loads, the first Stage of the pipeline is to prepare the environment. The first Task in this Stage is to load the necessary R packages used by the codebase. Whilst technically, this action consists of numerous R calls (one for each package that needs to be loaded), the block of actions are evaluated as a set.

Initially, all upcoming tasks are reported as "pending" (). As the pipeline progresses, each Task is evaluated and a status is returned as either "success" () or "failure" ().

The Stage that is currently (or most recently) being run will be expanded, whereas all other Stages will be collapsed (unless they contain errors). It is also possible to expand/collapse a Stage by double clicking on its title (or the small arrow symbol at the left side of the tree).

As the pipeline progresses, Task logs are written to a log file and echoed to the **Logs** panel. Each row represents the returned status of a specific Task and are formatted as:

- the time/date that the Task was evaluated
- the Task status, which can be one of:
  - `SUCCESS` the task succeeded
  - `FAILURE` the task failed and should be investigated
  - `WARNING` the task contained a warning - typically these can be ignored as they are usually passed on from underlying routines and are more targetted to developers than users.
- the Stage followed by the Task name
- in the case of errors and warnings, there will also be the error or warning message passed on from the underlying routines. These can be useful for helping to diagnose the source and cause of issues.

The Logs in the Log panel are presented in chronological order and will autoscroll such that the most recent log is at the bottom of the display. If the number of Log lines exceeds 10, a scroll bar will appear on the right side of the panel to help reviewing earlier Logs.

> Note
> The Status and Logs are completely refreshed each time the application is restarted.

The Progress panel also has a tab (called **Terminal-like**) which provides an alternative representation of the status and progress of the pipeline.

Data

The Data page comprises two panels or subpages accessable by tabs named "Raw data" and "Processed data" at the top of the page.

> **i** Note
>
> The contents of the Processed data subpage will not be revealed until the completion of Stage 3.

Raw data panel

The **Raw data** panel displays the input data and associated validation summaries (once the data have been loaded - that is, once Stage 2 has been complete). The table (main metadata table) above initially has a row for each of the input files.

The title of each input file name is displayed in the first column (**File**). The size and file creation time in the next two columns (fields). The **Status** field indicates whether the data in the various files are considered valid () or not ().

Clicking anywhere in a row containing will select the row and once a row is selected, information in both the *Data* and *Validation issues* tabs will be populated.

Initially, the *Instructions* tab will be active and visible (providing these instructions). The other two tabs are:

- **Data**: provides a view of the data beyind the selected row in the main metadata table and a mechanism to download those data. Only the first 10 rows are displayed in the table, the others being accessable via the controls under the table.

  Note, all numerical values are displayed only to three decimal places, yet the actual underlying data is full resolution.

- **Validation issues**: highlights and displays a description any validation issues associated with the selected row in the main metadata table.

  If there were no validation issues, this table will be empty. Otherwise, the description field will indicate the nature of the violation and in the case of issues with an individual record, the offending row will be presented across the remaining cells in the row. For more information about the validation tests, please refer to the **Data requirements** box (to the right of this box in the app).

Underneath both the Data and Validation tables, there is a **Download as csv** button. Via this button, you can download a comma separated text file version of the data in the table for further review in a spreadsheet of your choice. Once you click this button, you will be prompted to navigate to a suitable location to store the file.

Processed data panel

The Processed data panel displays the first 10 rows of the complete, compiled and processed data set. Descriptions of each field of these data are provided in the table below.

> **Note**
>
> This panel will not become active until the completion of Stage 3.

The **Processed data** panel displays the processed data. As part of the processing, the following new fields will be created:

Field	Description
Source	Source of samples (CFM or Discrete)
Date	Sample data
Latidude	Latitude of sample
Longitude	Longitude of sample
Focal_Year	Year in which analyses are logged (typically the most recent year)
Year	Year of sample
Measure	Name of the Measure
Value	Observed measure value
OldZone	Old Zone name
Region	Darwin Harbour Region number
Zone	Darwin Harbour Zone number
ZoneName	Name of the Darwin Harbour Zone
HydstraName	Name of the measure in hydstra
Conversion	Unit conversion factor
UnitsLabel	Name of the Measure including units
Label	Name of the Measure including units (in LaTeX format)
DirectionOfFailure	Direction of failure relative to guideline value
GL	Water quality guideline value
RangeFrom	Water quality guideline lower limit of range (for DO)
RangeTo	Water quality guideline upper limit of range range (for DO)
DetectionLimit	Limit of detection value
Flag	Limit of detection flag (when limit of detection applied)
Component	Highest level of measure hierarchy (always Environmental)
IndicatorGroup	Next measure level (always Water Quality)
Indicator	Next measure level (always Water Quality)

Field	Description
Subindicator	Either Nutrients or Physico-chem

Under the column (field) headings in the Processed data panel table, there are input boxes that act as filters. The data presented in the table will be refined to just those cases that match the input string as it is being typed. It is possible to engage with any or all of these filters to help refine the search.

Under the table there is a **Download as csv** button. Via this button, you can download a comma separated text file version of the data in the table for further review in a spreadsheet of your choice. Once you click this button, you will be prompted to navigate to a suitable location to store the file.

QAQC

The QAQC page comprises two panels or subpages accessable by tabs at the top of the page and named "Observations" and "Boxplots".

Observations

This page displays multi-panel figures depicting the observed data for a selected year conditional on Measures (columns) and Zones (rows). These figures at organised according to three *Source* types (all, CFM and Discrete) and these are activated via three large tab buttons down the left side of the panel. The sampling year is selected via a dropdown box in a panel above the figures.

The individual figures depict the observed Measures (columns) of all Water Quality data from each of eleven Zones (rows). The red vertical line indicates associated Water Quality Guideline value. The transparent red band indicates a range of values represented by half and twice the guideline value (equivalent to the Scaled Modified Amplitude index capping domain). The blue band represents the Guideline range for Dissolved Oxygen. Note, the y-axis only represents jittered and unordered space. temporal sampling design.

Boxplots

This page displays multi-panel figures depicting boxplots for the observed data for a selected year conditional on Measures (columns) and Zones (x-axes).

These figures at organised according to three types (all, timeseries and zones) and these are activated via three large tab buttons down the left side of the panel. The sampling year is selected via a dropdown box in a panel above the figures.

- all: the figure depicts the boxplots of the observed Measures (panels) of Water Quality data from each of eleven Zones (x-axes) for each source. The horizontal dashed lines indicate the associated Water Quality Guideline values.
- timeseries: the figure depicts the boxplots of the observed Measures (panels) of Water Quality data from each of the eleven Zones (x-axes) across all sampling years. The horizontal dashed lines indicate the associated Water Quality Guideline values.
- zones: the figure depicts the boxplots of the observed Measures (panels) of Water Quality data from selected zones for the selected sampling year. The dropdown is used to select the zones. The horizontal dashed lines indicate the associated Water Quality Guideline values.

Summaries

The Summaries page comprises a horizontal selector panel along with three three panels or subpages accessable by tabs at the tabs and named "Trends", "Annual effects" and "Contrast effects".

Within the selector panel, there are a series of dropdown selection boxes for choosing between a set of candidates for each of the following:

- Subindicator
- Measure

- Region
- Zone
- Source

In each case, in addition to candidates created from the unique values observed in the data, there is also an "All" candidate. The All candidate represents the aggregation of the other candidates. For example, the All *Region* candidate allows for the selection of the Whole of Harbour. Similarly, the All candidate in the *Measures* selector when the *Subindicator* selector has the "Physico-chem" candidate selected indicates the aggregate of all Measures across Physico-chem.

The selectors are linked such that selecting a candidate from one dropdown (e.g. *Region*) will determine what candidates are available in other selector dropdowns (e.g. *Zones* and *Source*). By default, the All candidate is selected for all selectors. This equates to the Whole of Harbour Indicator scores (i.e. the highest level of aggregation).

Trends

The trend plots display the temporal trend in indicator scores. Uncertainty (95% confidence intervals) in the scores are depicted by vertical whiskers and the open symbols are coloured according to the grade associated with the mean score. Dashed horizontal lines indicate the grade boundaries.

Annual effects

The distribution of comparisons (absolute change in indicator score) of each sampling year to the previous sampling year are depicted by density plots with point and whiskers (mean and 95% confidence intervals) below. Exceedance probabilitys for increase ($P(\Delta > 0)$) and decrease ($P(\Delta < 0)$) are overlayed onto the density plots. Density distributions are coloured according to whether there is strong evidence for an increase (green) or decrease (red) or no evidence of change (gray).

Contrast effects

The distribution of comparisons (absolute change in indicator score) of each half-decade to the previous half-decade are depicted by density plots with point and whiskers (mean and 95% confidence intervals) below. Exceedance probabilitys for increase ($P(\Delta > 0)$) and decrease ($P(\Delta < 0)$) are overlayed onto the density plots. Density distributions are coloured according to whether there is strong evidence for an increase (green) or decrease (red) or no evidence of change (gray).

Appendix

Guideline values

ZoneName	HydstraName	Conversion	Measure	Units	Label	Label	Direction	GL	Range From	Range To	DetectionLimit
Blackmore River	Chlorophyll-a (ug/L)	1	Chla_mug_PERL	Phytoplankton Chlorophyll-a (µg/L)	Chlorophyll-a~(mu*g/L)	H	4			0.1
Blackmore River	turbidity (NTU)	1	Turbidity_NTU	Turbidity (NTU)	Turbidity~(NTU)	H	5			1.0
Blackmore River	dissolved oxygen (%)	1	DO_PERCENT_SAT	Dissolved Oxygen (% Saturation)	$Dissolved_{Oxygen}$(‘%’~Saturation)	B	80	100		0.1
Blackmore River	Ammonia as N (mg/L)	1000	NH3_mug_PERL	Ammonia (µg/L)	$Ammonia_{as}$N~(mu*g/L)	L	20			1.0
Blackmore River	Reactive Phosphate (mg/L)	1000	PO4_mug_PERL	Filterable Reactive Phosphorus (µg/L)	$Filterable_{Reactive}$Phosphorus~(mu*g/L)	L	10			1.0

ZoneName	HydstraName	Conversion	Measure	Units	Label	Label	Direction	Off	Range	Range	Detection	Limit
Blackmore River	NOx (mg/L)	1000	Nox_mug_PER_L	NOx as N (µg/L)	NOx as N (µg/L)	$NOx_{as}N$~(mu*g/L)	H		20			1.0
East Arm	Chlorophyll-a (ug/L)	1	Chla_mug_PER_L	Chlorophyll-a (µg/L)	Chlorophyll-a (µg/L)	Chlorophyll-a~(mu*g/L)	H		4			0.1
East Arm	turbidity (NTU)	1	Turbidity_NTU	Turbidity (NTU)	Turbidity (NTU)	Turbidity~(NTU)	H		5			1.0
East Arm	dissolved oxygen (%)	1	DO_PERCENT_Sat	Dissolved Oxygen (% Saturation)	Dissolved Oxygen (% Saturation)	$Dissolved_{Oxygen}$(%Saturation)	B		80	100		0.1
East Arm	Ammonia as N (mg/L)	1000	NH3_mug_PER_L	Ammonia (µg/L)	Ammonia (µg/L)	$Ammonia_{as}N$~(mu*g/L)	H		20			1.0
East Arm	Reactive Phos-phate (mg/L)	1000	PO4_mug_PER_L	Filterable Reactive Phosphorus (µg/L)	Filterable Reactive Phosphorus (µg/L)	$Filterable_{Reactive}Phosphorus$~(mu*g/L)	H		10			1.0
East Arm	NOx (mg/L)	1000	Nox_mug_PER_L	NOx as N (µg/L)	NOx as N (µg/L)	$NOx_{as}N$~(mu*g/L)	H		20			1.0
Elizabeth River	Chlorophyll-a (ug/L)	1	Chla_mug_PER_L	Chlorophyll-a (µg/L)	Chlorophyll-a (µg/L)	Chlorophyll-a~(mu*g/L)	H		4			0.1
Elizabeth River	turbidity (NTU)	1	Turbidity_NTU	Turbidity (NTU)	Turbidity (NTU)	Turbidity~(NTU)	H		5			1.0
Elizabeth River	dissolved oxygen (%)	1	DO_PERCENT_Sat	Dissolved Oxygen (% Saturation)	Dissolved Oxygen (% Saturation)	$Dissolved_{Oxygen}$(%Saturation)	B		80	100		0.1
Elizabeth River	Ammonia as N (mg/L)	1000	NH3_mug_PER_L	Ammonia (µg/L)	Ammonia (µg/L)	$Ammonia_{as}N$~(mu*g/L)	H		20			1.0
Elizabeth River	Reactive Phos-phate (mg/L)	1000	PO4_mug_PER_L	Filterable Reactive Phosphorus (µg/L)	Filterable Reactive Phosphorus (µg/L)	$Filterable_{Reactive}Phosphorus$~(mu*g/L)	H		10			1.0
Elizabeth River	NOx (mg/L)	1000	Nox_mug_PER_L	NOx as N (µg/L)	NOx as N (µg/L)	$NOx_{as}N$~(mu*g/L)	H		20			1.0
West Arm	Chlorophyll-a (ug/L)	1	Chla_mug_PER_L	Chlorophyll-a (µg/L)	Chlorophyll-a (µg/L)	Chlorophyll-a~(mu*g/L)	H		4			0.1
West Arm	turbidity (NTU)	1	Turbidity_NTU	Turbidity (NTU)	Turbidity (NTU)	Turbidity~(NTU)	H		5			1.0
West Arm	dissolved oxygen (%)	1	DO_PERCENT_Sat	Dissolved Oxygen (% Saturation)	Dissolved Oxygen (% Saturation)	$Dissolved_{Oxygen}$(%Saturation)	B		80	100		0.1
West Arm	Ammonia as N (mg/L)	1000	NH3_mug_PER_L	Ammonia (µg/L)	Ammonia (µg/L)	$Ammonia_{as}N$~(mu*g/L)	H		20			1.0
West Arm	Reactive Phos-phate (mg/L)	1000	PO4_mug_PER_L	Filterable Reactive Phosphorus (µg/L)	Filterable Reactive Phosphorus (µg/L)	$Filterable_{Reactive}Phosphorus$~(mu*g/L)	H		10			1.0
West Arm	NOx (mg/L)	1000	Nox_mug_PER_L	NOx as N (µg/L)	NOx as N (µg/L)	$NOx_{as}N$~(mu*g/L)	H		20			1.0
Buffalo Creek	Chlorophyll-a (ug/L)	1	Chla_mug_PER_L	Chlorophyll-a (µg/L)	Chlorophyll-a (µg/L)	Chlorophyll-a~(mu*g/L)	H		4			0.1
Buffalo Creek	turbidity (NTU)	1	Turbidity_NTU	Turbidity (NTU)	Turbidity (NTU)	Turbidity~(NTU)	H		5			1.0
Buffalo Creek	dissolved oxygen (%)	1	DO_PERCENT_Sat	Dissolved Oxygen (% Saturation)	Dissolved Oxygen (% Saturation)	$Dissolved_{Oxygen}$(%Saturation)	B		80	100		0.1

ZoneName	HydstraName	Conversion	Measure	Units	Label	Label	Direction	Off	Range	Range	Detection	Limit
Buffalo Creek	Ammonia as N (mg/L)	1000	NH3_mug_AMMONIA	PERIOD (µg/L)	Ammonia	$Ammonia_{as}N$~(mu*g/L)	H		20			1.0
Buffalo Creek	Reactive Phosphate (mg/L)	1000	PO4_mug_FILTERED	PERIOD (µg/L)	Filterable Reactive Phosphorus	$Filterable_{Reactive}Phosphorus$~(mu*g/L)	H		10			1.0
Buffalo Creek	NOx (mg/L)	1000	Nox_mug_NOX_AS_N	PERIOD (µg/L)	$NOx_{as}N$~(mu*g/L)		H		20			1.0
Myrmidon Creek	Chlorophyll-a (ug/L)	1	Chla_mug_CHLOROPHYLL_A	PERIOD (µg/L)	Chlorophyll-a	Chlorophyll-a~(mu*g/L)	H		4			0.1
Myrmidon Creek	turbidity (NTU)	1	Turbidity_NTU	PERIOD (NTU)	Turbidity	Turbidity~(NTU)	H		5			1.0
Myrmidon Creek	dissolved oxygen (%)	1	DO_PERCENT_SAT	PERIOD (% Saturation)	Dissolved Oxygen	$Dissolved_{Oxygen}$(%~Saturation)			80	100		0.1
Myrmidon Creek	Ammonia as N (mg/L)	1000	NH3_mug_AMMONIA	PERIOD (µg/L)	Ammonia	$Ammonia_{as}N$~(mu*g/L)	H		20			1.0
Myrmidon Creek	Reactive Phosphate (mg/L)	1000	PO4_mug_FILTERED	PERIOD (µg/L)	Filterable Reactive Phosphorus	$Filterable_{Reactive}Phosphorus$~(mu*g/L)	H		10			1.0
Myrmidon Creek	NOx (mg/L)	1000	Nox_mug_NOX_AS_N	PERIOD (µg/L)	$NOx_{as}N$~(mu*g/L)		H		20			1.0
Outer Harbour	Chlorophyll-a (ug/L)	1	Chla_mug_CHLOROPHYLL_A	PERIOD (µg/L)	Chlorophyll-a	Chlorophyll-a~(mu*g/L)	H		1			0.1
Outer Harbour	turbidity (NTU)	1	Turbidity_NTU	PERIOD (NTU)	Turbidity	Turbidity~(NTU)	H		5			1.0
Outer Harbour	dissolved oxygen (%)	1	DO_PERCENT_SAT	PERIOD (% Saturation)	Dissolved Oxygen	$Dissolved_{Oxygen}$(%~Saturation)			80	100		0.1
Outer Harbour	Ammonia as N (mg/L)	1000	NH3_mug_AMMONIA	PERIOD (µg/L)	Ammonia	$Ammonia_{as}N$~(mu*g/L)	H		20			1.0
Outer Harbour	Reactive Phosphate (mg/L)	1000	PO4_mug_FILTERED	PERIOD (µg/L)	Filterable Reactive Phosphorus	$Filterable_{Reactive}Phosphorus$~(mu*g/L)	H		10			1.0
Outer Harbour	NOx (mg/L)	1000	Nox_mug_NOX_AS_N	PERIOD (µg/L)	$NOx_{as}N$~(mu*g/L)		H		10			1.0
Shoal Bay	Chlorophyll-a (ug/L)	1	Chla_mug_CHLOROPHYLL_A	PERIOD (µg/L)	Chlorophyll-a	Chlorophyll-a~(mu*g/L)	H		1			0.1
Shoal Bay	turbidity (NTU)	1	Turbidity_NTU	PERIOD (NTU)	Turbidity	Turbidity~(NTU)	H		5			1.0
Shoal Bay	dissolved oxygen (%)	1	DO_PERCENT_SAT	PERIOD (% Saturation)	Dissolved Oxygen	$Dissolved_{Oxygen}$(%~Saturation)			80	100		0.1
Shoal Bay	Ammonia as N (mg/L)	1000	NH3_mug_AMMONIA	PERIOD (µg/L)	Ammonia	$Ammonia_{as}N$~(mu*g/L)	H		20			1.0
Shoal Bay	Reactive Phosphate (mg/L)	1000	PO4_mug_FILTERED	PERIOD (µg/L)	Filterable Reactive Phosphorus	$Filterable_{Reactive}Phosphorus$~(mu*g/L)	H		10			1.0

ZoneName	HydstraName	Conversion	Measure	UnitsLabel	Label	Direction	GL	RangeFrom	RangeTo	DetectionLimit
Shoal Bay	NOx (mg/L)	1000	Nox_mug_PER_L	NOx as N (µg/L)	$NOx_{as}N$~(mu*g/L)	H	10			1.0
Shoal Bay Upper	Chlorophyll-a (ug/L)	1	Chla_mug_PER_L	Chlorophyll-a (µg/L)	Chlorophyll-a~(mu*g/L)	H	4			0.1
Shoal Bay Upper	turbidity (NTU)	1	Turbidity_NTU	Turbidity (NTU)	Turbidity~(NTU)	H	5			1.0
Shoal Bay Upper	dissolved oxygen (%)	1	DO_PERCENT_saturation	Dissolved Oxygen (% Saturation)	$Dissolved_{Oxygen}$(`%~Saturation)	B		80	100	0.1
Shoal Bay Upper	Ammonia as N (mg/L)	1000	NH3_mug_PER_L	Ammonia (µg/L)	$Ammonia_{as}N$~(mu*g/L)	H	20			1.0
Shoal Bay Upper	Reactive Phosphate (mg/L)	1000	PO4_mug_PER_L	Filterable Reactive Phosphorus (µg/L)	$Filterable_{Reactive}$Phosphorus~(mu*g/L)	H	10			1.0
Shoal Bay Upper	NOx (mg/L)	1000	Nox_mug_PER_L	NOx as N (µg/L)	$NOx_{as}N$~(mu*g/L)	H	20			1.0
Middle Harbour	Chlorophyll-a (ug/L)	1	Chla_mug_PER_L	Chlorophyll-a (µg/L)	Chlorophyll-a~(mu*g/L)	H	2			0.1
Middle Harbour	turbidity (NTU)	1	Turbidity_NTU	Turbidity (NTU)	Turbidity~(NTU)	H	5			1.0
Middle Harbour	dissolved oxygen (%)	1	DO_PERCENT_saturation	Dissolved Oxygen (% Saturation)	$Dissolved_{Oxygen}$(`%~Saturation)	B		80	100	0.1
Middle Harbour	Ammonia as N (mg/L)	1000	NH3_mug_PER_L	Ammonia (µg/L)	$Ammonia_{as}N$~(mu*g/L)	H	20			1.0
Middle Harbour	Reactive Phosphate (mg/L)	1000	PO4_mug_PER_L	Filterable Reactive Phosphorus (µg/L)	$Filterable_{Reactive}$Phosphorus~(mu*g/L)	H	5			1.0
Middle Harbour	NOx (mg/L)	1000	Nox_mug_PER_L	NOx as N (µg/L)	$NOx_{as}N$~(mu*g/L)	H	20			1.0
Middle Harbour Upper	Chlorophyll-a (ug/L)	1	Chla_mug_PER_L	Chlorophyll-a (µg/L)	Chlorophyll-a~(mu*g/L)	H	2			0.1
Middle Harbour Upper	turbidity (NTU)	1	Turbidity_NTU	Turbidity (NTU)	Turbidity~(NTU)	H	5			1.0
Middle Harbour Upper	dissolved oxygen (%)	1	DO_PERCENT_saturation	Dissolved Oxygen (% Saturation)	$Dissolved_{Oxygen}$(`%~Saturation)	B		80	100	0.1
Middle Harbour Upper	Ammonia as N (mg/L)	1000	NH3_mug_PER_L	Ammonia (µg/L)	$Ammonia_{as}N$~(mu*g/L)	H	20			1.0

ZoneName	HydstraName	Conversion	Measure	UnitsLabel	Label	DirectionOfTarget	TargetRange	RangeDetection	Limit
Middle Harbour Upper	Reactive Phosphate (mg/L)	1000	PO4_mug_FILTERED	Filterable Reactive Phosphorus (µg/L)	$Filterable_{Reactive}$ Phosphorus (mu*g/L)	L	5	H	1.0
Middle Harbour Upper	NOx (mg/L)	1000	Nox_mug_FILTERED	NOx as N (µg/L)	NOx_{as} N~(mu*g/L)	L	20	H	1.0