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Precision analysis and the determination of outliers

Precision was determined by analyzing replicate samples drawn from one Niskin.

Outliers are discarded on the basis of Chauvenet's criteria. The statistic is calculated by finding the Chauvenet critical value (Z-critical) for the total degrees of freedom (v) of the dataset:

$$Z\text{-critical} = \text{ABS}(\text{NORM.S.INV}(1/(4*v)))$$

The maximum deviation, D_{max} , is compared with the individual residuals from the original concentrations.

If a replicate's residual is greater than D_{max} this value can be rejected. D_{max} is determined by the following formula:

$$D_{max} = Z\text{-critical} * \sigma$$

where σ is the standard deviation of residuals

Precision is assessed by calculating the pooled standard deviation (S_p).

Pooled standard deviation is calculated for a combination of duplicates and triplicates using the following formula:

$$s_p = \sqrt{\frac{SS_1 + SS_2 + \dots + SS_k}{v_1 + v_2 + \dots + v_k}}$$

where: v = total degrees of freedom (1 for duplicates, 2 for triplicates).

SS = sum of squares of the residuals.

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Precision statement for replicate samples drawn from a single Niskin bottle:

Salinity: Bottle duplicates ranged from 31.8403 to 34.6719 with a pooled standard deviation of 0.0008 from 19 replicates - after the removal of 1 outlier sample using the Chauvenet criteria.

The pooled standard deviation was 0.0114 when using the complete set of 20 replicates.

Duplicate samples from a single Niskin bottle

Event Number	Sample Number	Station	Pressure dbar	Salinity 1	Salinity 2	Rejected yes / no	Comment
28	115	P4	1250.4	34.4645	34.4648		
28	116	P4	1000.6	34.3718	34.3726		
39	208	P8	2000.8	34.5792	34.5793		
39	211	P8	1000.4	34.3564	34.3568		
47	323	P12	3001.7	34.6473	34.6466		
47	325	P12	2500.6	34.6275	34.6274		
47	327	P12	1500.2	34.4992	34.4997		
47	329	P12	1000.4	34.3566	34.3534		
70	551	P16	3500.0	34.6657	34.6674		
70	555	P16	1999.2	34.5860	34.5863		
70	557	P16	1251.8	34.4394	34.3677	yes	Very poor replication. Possibly mis-sampled?
79	645	P20	3000.0	34.6512	34.6520		
79	647	P20	1999.4	34.5771	34.5759		
79	650	P20	1000.9	34.3558	34.3539		
99	811	P26	3500.8	34.6719	34.6717		
99	813	P26	2501.4	34.6264	34.6275		
115	971	P4	1000.4	34.3689	34.3686		
115	972	P4	802.0	34.2651	34.2646		
115	976	P4	10.4	31.8427	31.8426		
115	977	P4	4.9	31.8403	31.8404		