Readme for:

Locally Interpolated Alkalinity Regression (LIAR) for MATLAB: Estimates alkalinity and alkalinity uncertainty from 16 possible combinations of other parameter measurements. The Locally Interpolated Alkalinity Regression method is described in detail in the paper:

Carter et al. (to be filled in upon final submission).

For questions not addressed by the paper or this readme file, please contact Brendan Carter, Brendan.carter@gmail.com, and he will get back to you as he is able. Suggestions, bug reports, and queries regarding code updates are welcome.

Running the LIAR estimation routines in MATLAB is a 3 step procedure:

1. Download the required files: LIAR.m and LIAR_files.mat (note, the seawater package from CSIRO, link below, is also required for some applications).
2. Put all needed files into the current working MATLAB directory or a directory on the MATLAB path,
3. Call the LIAR function according to the detailed instructions below.

Updates: We intend to update regression coefficients as new quality controlled datasets become available. Please indicate if you use an updated regression coefficient set for reproducibility. Contact the corresponding author for updates or look for them and their descriptions online at: https://drive.google.com/open?id=0Bw_dE1twlSIIYWtUQUlQMmdxUDQ

Objects in LIAR_files.mat include:

`Coords`: Latitudes, longitudes, depths, and approximate potential densities of seawater at each of the LIAR grid coordinate locations.

`L*Poly/L*PolyExtra`: Polygons defining subregions of the Atlantic and Arctic Oceans (NA: North Atlantic, SA: South Atlantic, NO: Arctic). "Extra" polygons for the North and South Atlantic cover the subsets of these ocean basins from 0 to 180° E (as opposed to 0 to 180° W).

`Cs`: α coefficients at the coordinates in `Coords`.

`AAindsCs`: a boolean array indicating whether various coordinates in `Coords` are in either the Arctic or Atlantic Oceans.

`EMLRrec`: 16 histograms of E_{MLR} against salinity for the 16 different possible regressions (see paper for a full explanation).

The remainder of this document covers how to call the LIAR function correctly, and contains information that is duplicated as comments in the MATLAB code.

LIAR call syntax:
```
[AlkalinityEstimates, UncertaintyEstimates]=LIAR( Coordinates, Measurements, MeasIDVec, Equations, MeasUncerts, MolalityTF)
```

This function needs the CSIRO seawater package to run if measurements are povided in molar units, or if potential temperature or AOU are needed but not provided by the user. Scale differences from TEOS-10 are a negligible component of alkalintiy estimate error. The seawater package is distributed freely by CSIRO:

http://www.cmar.csiro.au/datacentre/ext_docs/seawater.htm

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Input/Output dimensions:
n: Integer number of desired estimate locations
e: Integer number of equations used at each location
y: Integer number of parameter measurement types provided by the user.
n*e: Total number of estimates returned

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Input descriptions:

Coordinates (required n by 3 array): Coordinates at which estimates are desired. The first column should be longitude (degrees E), the second column should be latitude (degrees N), and the last column should be depth (m). NaN coordinate values will return NaN estimates.

Measurements (required n by y array): Parameter measurements that will be used to estimate alkalinity. The column order is arbitrary, but specified by MeasIDVec. Concentrations (including AOU) should be expressed as micromol per kg unless MolalityTF is set to 0, temperature should be expressed as degrees C, and salinity should be specified with the unitless convention. NaN inputs are acceptable, but will lead to NaN estimates for any equations that depend on that parameter.

MeasIDVec (required 1 by y vector): Vector indicating which parameter is placed in each column of the 'Measurements' input. Note that salinity is required for all equations. If O2 is provided instead of AOU, then temperature or potential temperature must also be provided to convert O2 to AOU. For example, if the first three columns of 'Measurements' contain salinity, silicate, and temperature, then MeasIDVec should equal [1 5 7].

Parameter Key:
1. Salinity
2. Potential temperature
3. Nitrate
4. AOU
5. Silicate
6. O2
7. Temperature

Equations (optional 1 by e vector, default 1:16): Vector indicating which equations will be used to estimate alkalinity. This input also determines the order of the columns in the 'AlkalinityEstimates' output.

(S=salinity, Theta=potential temperature, N=nitrate, Si=silicate, AOU=apparent oxygen utilization... see 'Measurements' for units).

Equation Key:
1. S, Theta, N, AOU, Si
2. S, Theta, N, Si
3. S, Theta, AOU, Si
4. S, Theta, Si
5. S, Theta, N, AOU
6. S, Theta, N
7. S, Theta, AOU
8. S, Theta
9. S, N, AOU, Si
10. S, N, Si
11. S, AOU, Si
12. S, Si
13. S, N, AOU
14. S, N
15. S, AOU
16. S

MeasUncerts (Optional n by y array or 1 by y vector, default 1 by y vector of uncertainties specified in paper): Array of measurement uncertainties (see 'Measurements' for units). Uncertainties should be presented in order indicated by MeasIDVec. Providing these estimates will improve LIAR estimate uncertainties in 'UncertaintyEstimates'. Measurement uncertainties are a small part of LIAR estimate uncertainties for WOCE-quality measurements. However, estimate uncertainty scales with measurement uncertainty, so it is recommended that measurement uncertainties be specified for sensor measurements. If this optional input argument is not provided, the default WOCE-quality uncertainty is assumed. If a 1 by y array is provided then the uncertainty estimates are assumed to apply uniformly to all input parameter measurements. If default values are desired but you want to specify MolalityTF, then input "[]".

MolalityTF (Optional boolean, default true): Many sensors provide measurements in micromol per L (molarity) instead of micromol per kg (molality). Indicate false or 0 if provided measurements are expressed in molar units (concentrations must be micromol per L if so).

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Output descriptions:

AlkalinityEstimates: A n by e array of LIAR estimates specific to the coordinates and parameter measurements provided. Units are micromoles of total seawater titration alkalinity per kg of seawater regardless of whether MolalityTF is 0 or 1.

UncertaintyEstimates: A n by e array of LIAR uncertainty estimates specific to the coordinates, parameter measurements, and parameter uncertainties provided. Units are standard deviations of total seawater titration alkalinity in micromoles per kg of seawater regardless of whether MolalityTF is true or false.

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Missing data: should be indicated with a NaN. A NaN coordinate will yield NaN estimates for all equations at that coordinate. A NaN parameter value will yield NaN estimates for all equations that require that parameter.

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