Geo 327G Semester Project

GIS Analysis of Ion Concentrations in the Queen City Aquifer

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Objective

The goal of this project was to create various lon Concentration probability maps of the Queen City Aquifer in Texas. Coupled with other geochemical analysis methods, these probability maps could be used to provide useful insights into the geochemisty of the aquifer.

Methods

To produce ion concentration probability maps I will obtain and manipulate data available on the Texas Water Development Board website. Then I will use a geostatistical interpolation method to predict the concentration of a specific ion across the Queen City Aquifer from 20 years' worth of well concentration data.

Data Collection

The majority of the data required for this project can be obtained from the Texas Water Development Board website.

- <u>http://www.twdb.state.tx.us/groundwater/data/gwdbrpt.asp</u>
 - From here download the "Entire Groundwater Database (mdb)" and also the "GWDB well locations"
- <u>http://www.twdb.state.tx.us/mapping/gisdata.asp</u>
 - o Download the "Minor Aquifers Shapefile"

Data Processing

The objective of data processing is to create a shapefile of Queen City Aquifer wells that has millimole ion concentrations.

- 1. Start ArcGIS and create a new map. Load the "GWDB_well_locations" shapefile into the table of contents.
- 2. Isolate all of the Queen City Aquifer wells
 - a. On the top bar of ArcGIS hit the selection tab and click "select by attribute"
 - b. The layer selected is the "GWDB_well_locations". In the box that contains the various fields for the layer, Click "Aquifer_id" and click then "Get Unique Values"

c. Create the query "Aquifer_id" = "QUEEN CITY". This should look like Figure 1. Hit okay.

Select By Attributes
Layer: SGWDB_well_locations Only show selectable layers in this list Method: Create a new selection
"aquifer_co" "aquifer_id" "elev_of_ls" "elev_meth" "date_drill" = Like 'Marble Falls' 'Nacatoch' 'Ogallala' 'Other' 'Pecos Valley' 'Queen City' 'Is Get Unique Values SELECT * FROM GWDB_well_locations WHERE:
Clear Venfy Help Load Save
OK Apply Close

- d. To extract the Queen City wells from the "GWDB_well_locations" go to the toolbox > Analysis Tools > Extract > Select.
- e. The input feature is the "GWDB_well_locations". Name the output feature "QC_wells" and save it into your project folder. Hit OK
- 3. Next obtain the water quality data
 - a. Open Excel and go to the Data Tab
 - b. Using the Import from Microsoft Access feature select the "GWDB" Access file that you downloaded. A "Select Table" will pop-up and select "waterqua" from this list. See Figure 2. Click okay and import the data into a table.

Enable selection of <u>m</u> ultip	le tables			
Name		Description	Modified	Crea [®] 1
III typelift			4/29/2009 8:50:21 AM	4/29/
III typepower			4/29/2009 8:50:21 AM	4/29,
III usgswl			3/7/2012 8:06:48 AM	4/29/
III waterlev			3/7/2012 8:06:57 AM	4/29/
III waterqua			3/7/2012 8:07:16 AM	4/29,
III wateruse			6/26/2012 11:40:48 A	11/3/
iii wdremarks			3/7/2012 8:07:03 AM	4/29,
•	III			•
				Concol

- 4. Furthermore, manipulate the well quality data so we can get Queen City Aquifer for the past 20 years.
 - a. In excel use the "Filter" function and select all the years from 2013-1993
 - b. Highlight all the cells and copy and paste them into a new sheet. Name this sheet "20yr"
 - c. In this new sheet, highlight all of the cells and use the custom sort feature. Sort by "yydate" and have them ordered largest to smallest.
 - i. This will ensure that if there is multiple data for a single well in this time frame the most recent well quality data will be chosen when we join this table to the Isolated Queen city wells in ArcGIS.
- 5. Next, we use the manipulated well quality data in excel to obtain the Queen City well quality data in this 20 year time span.
 - a. In ArcGIS, right click on "QC_Wells" shapefile and go to the Join and Relate section and select join table
 - b. You want to join attributes from a table, based on "state_well" field. In the "choose a table to join section" browse to your well quality spreadsheet and select the "20yr" sheet. The Field in the table to base the join on is the state_well_number". Also we only want to keep matching records. See Figure 3.

Vhat	do vou want to join to this laver?
Join a	attributes from a table
1.	Choose the field in this layer that the join will be based on:
	state_well
2.	Choose the table to join to this layer, or load the table from disk:
	'20 yr\$'
	Show the attribute tables of layers in this list
ſ	state_well_number
	All records in the target table are shown in the resulting table. Unmatched records will contain null values for all fields being appended into the target table from the join table.
	Keep only matching records
	If a record in the target table doesn't have a match in the join table, that record is removed from the resulting target table.
	Validate Join

Figure 3

- 6. Convert the well quality ion concentration data from mg/l of the ions to millimoles.
 - a. In ArcGIS, Open "QC_wells" attribute table and select all the data. Then copy and paste this into a new sheet on your existing excel spreadsheet. Name this sheet "20yr_mg".
 - b. Next create a new sheet and name it "mmol" and copy and paste the well numbers from "20yr_mg" plus the desired column headings. Using excel

functions convert mg/l to millimoles. The end result should be that your "mmol" sheet has all of the converted values.

- 7. Join the "QC_mmol" sheet to QC_Wells
 - a. In ArcGIS, right click on "QC_Wells" shapefile and go to the Join and Relate section and select join table
 - b. You want to join attributes from a table, based on "state_well" field. In the "choose a table to join section" browse to your well quality spreadsheet and select the "mmol" sheet. The Field in the table to base the join on is the "state_well". Also we only want to keep matching records.
- 8. Make this join permanent and create a separate shapefile for the mmol well data.
 - a. Right click on "QC_Wells" select "data" then "export data".
 - b. Export all features and use the same coordinate system as the layer.
 - c. Under output, browse to your project folder, name it "QC_mmol" and then make sure you save it as a shape file. See figure 4

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									-
Name									
Name:	QC_mmol						S	Save	



- 9. Extract the Queen City Aquifer shapefile from the "New_minor_aquifers" shapefile
 - a. Place the "New_minor_aquifers_dd" shapefile onto the table of contents
 - b. On the top bar of ArcGIS hit the selection tab and click "select by attribute"
 - c. Choose the "New_minor_aquifers_dd" layer
 - d. In the box that contains the various fields for the layer, Click "AQU_NAME" and click then "Get Unique Values"

e. Create the query "AQU_NAME" = "QUEEN CITY". This should look like Figure 5. Hit okay

Select By Attributes	23
Layer: NEW_minor_aquifers_dd	•
Method: Create a new selection	-
"FID" "AREA" "PERIMETER" "AQU_NAME" "AQUIFER"	
= <> Like 'MARATHON' > >= And 'MARBLE FALLS' 'NACATOCH' 'QUEEN CITY' 'QUEEN CITY' 'RITA BLANCA' _% () Not Is Get Unique Values Go To:	•
SELECT * FROM NEW_minor_aquifers_dd WHERE: "AQU_NAME" = 'QUEEN CITY'	*
Clear Venfy Help Load Sa OK Apply Ch	ve



- f. Next go to the toolbox > Analysis Tools > Extract > Select.
- g. The input feature is the "New_minor_aquifers_dd". Name the output feature "QC_aquifer" and save it into your project folder. Hit OK

ArcGIS Processing

Once we have our data all sorted, we can now start to construct our probability maps of ion concentrations. We will utilize the Kriging method in the Geostatistical Analyst Extension. Kriging an

interpolation method that is based statistically. So before we start kriging you must check if your data set has a few important characteristics:

- 1. Is the data in a Gaussian distribution?
 - a. Kriging predictions are best if the data are Gaussian, and Gaussian distribution is needed to produce confidence intervals for prediction and probability mapping.
 - b. Within the Explore data feature of the geostatistical analyst, you may use the Histogram feature to check the data's distribution. If it is not we will have to use a transformation method during Kriging to make our data Gaussian.
- 2. Are there any trends in the data?
 - a. If trends exists, the mean data value will not be the same everywhere, violating one of the assumptions of data stationarity of the kriging model.
 - b. Within the Explore data feature of the geostatistical analyst, the Trend Analysis tool can be used to determine if there are any trends.
 - c. It is important to note any trends as we can try and remove them through the kriging process.
- 3. Are there any spatial autocorrelation and directional influences in the data?
 - a. The Semivariogram feature, within the explore data section of the Geostatistical Analyst, is a graph that displays the distance between the location of points versus the difference of their values squared.
 - i. Points that are close together should have a small difference squared values indicating that these points have similar values. It is expected however that as points get further away their difference of their values squared should start to vary more.
 - b. So an assumption for geostatistics is that any two locations that have a similar distance and direction from each other should also have similar values for their differences of their values squared.
 - i. Directional relationships are important. If in one direction, values change more rapidly or slowly compared to another direction there is an anisotropy. We must note this and take account of it when Kriging.

With this in mind, and after going through all of the ion concentration data, I found that each ion did not have a Gaussian distribution, contained trends, and had anisotropies associated with them. As a consequence, the kriging method explained here for the Chloride concentration can be applied to all of the other ions.

- 1. Go into the Geostatistical Analysts and select the Geostatistical Wizard.
- 2. Select the "Kriging/CoKriging" method.
- 3. The Source Dataset is the "QC_mmol" shapefile and select the data field corresponding to the chloride concentration. See figure 6. Then click next.

Methods	Ir	nput Data			
Deterministic methods	Ε	Dataset			
Inverse Distance Weighting		Source Dataset	QC mmol		· ·
Global Polynomial Interpolation		Data Field	chloride m		
Radial Basis Functions Local Polynomial Interpolation Geostatistical methods	Ξ	Dataset 2			_
Local Polynomial Interpolation		Source Dataset	<none></none>		÷.
Geostatistical methods	Ξ	Dataset 3			
Kriging / CoKriging		Source Dataset	<none></none>		Ξ.
Areal Interpolation	Ξ	Dataset 4			
Empirical Bayesian Kriging		Source Dataset	<none></none>		
Kriging / CoKriging					
riging is an interpolator that can be exe llows you to investigate graphs of spat utput surfaces including predictions, pr lot of decision-making. Kriging assumes <u>bout Kriging / CoKriging</u>	act ial a edio s th	or smoothed depending on th auto- and cross-correlation. K ction standard errors, probabi e data come from a stationary	e measurement error model riging uses statistical models lity and quantile. The flexibi y stochastic process, and so	. It is very flexible that allow a varie lity of kriging can r me methods assun	and ty of equire

Figure 6

4. We will use simple kriging with a transformation type of "Normal Score". Also we want to decluster the data before this transformation and remove second order trends. Kriging Step 2 of 8 should look like figure 7.

Kriging Type	Dataset #1		
Drdinary	 Transformation type	Normal Score	
Simple	Decluster before transformation	True	
Jniversal indicator robability Disjunctive	Order of trend removal	Second	
Output Surface Type			
Prediction Quantile Probability Prediction Standard Error			
	< Back Next	> Finish	Cancel

- Figure 7
- 5. In step 3 of 8, we leave all of the default setting except that we will set "Advanced mode" to true. Then in the advanced properties we will only change the sector type to 4 Sectors. After these changes your window should look like figure 8. Click next

Seostatistical wizard - Kriging step 3 of 8 - Method Proper	ties	;		23
		Trend	[QC_mmol - chloride_m]	*
	Ξ	General Properties		=
		Exploratory Trend S		
		Order of polynomial	2	
		Kernel Function	Exponential	
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1		Goodness of Fit	0.2903374	
		Optimize Model	<u>b/</u>	
		Advanced mode	True	
	Ξ	Advanced Propertie	25	
		Neighborhood type	Standard	
		Maximum neighbors	1000	
		Minimum neighbors	10	
		Sector type	🕀 4 Sectors 🗸	
		Angle	0	
		Major semiaxis	8.146546	
		Minor semiaxis	8.146546	
a de la companya de la		Anisotropy factor	1	
		Bandwidth	6.517237	
59-9 2.2		Use Spatial Conditio	False	
		Spatial Condition Nu		
		Predicted Value		*
	A	ector type lows a choice of 1, 4, 4	with an offset of 45°, or 8 secto	ors.
	<	Back Next >	Finish Cancel	

Figure 8

6. Step 4 of 8 involves declustering the data. We will use the polygonal method and our clip layer will be "QC_aquifer". It should appear similar to figure 9.





- 7. Step 5 of 8 involves normalizing the data set to a Gaussian distribution. No fields were touched here. The data appears to have been successfully adapted to the Gaussian distribution.
- 8. Step 6 of 8 involves Semivariograms. The important thing to note here is if there is any anisotropies in our data. Within the Covariance map we can see that the data changes rapidly in the N-S direction but really slow in the E-W. This is an anisotropy so to take

account of this we may turn the "Anisotropy" field under Model#1 to "true". It should look simil8ar to figure 10.

ovariance	🗆 Gener	al			
	Optimize	e model	N/		
C	Examine	e bivariate di	False		
1.453	Variable		Covariance		
1.09	🗉 Model	Nugget			
1727	Enable		True		1
	Calculat	e Nugget	True		
1.363			0		
0 1246 2692 4.027 5.292 6	720 Measure	ement Error	100	%	
Madal A Pinnad A AvaraBintanaa (Dagraa) h.	103 E Model	#1			
dol: 0*Nuccot 1 2052*Stoble/0 005729 0 0044964 11	212 Type		Stable		
del : 0 Nugget+1.5005 Stable(0.000725,0.0044804,11	Parame	ter	1.216016		晟
1.4531 View Settings	Major R	ange	0.00672899		2
1 2109 Show se False	Anisotro	ру	True		-
Show all False	Minor R	ange	0.004486402		2
0.9687 Show poi Binned a	Directio	n	11.25		2
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0 View Settings	only with d	ariogram and co listance but wit	variance functions h direction as well.	may chang This is calle	je n id a
	C Park	Neut 2	Einich		

Figure 10

- 9. Step 7 of 8 involves the Searching Neighborhood. I did not change anything in this section.
- 10. Step 8 of 8 displays the cross validation plot and the prediction errors. Ideally we want the mean close to zero, the Root Mean Square error and Standard error to be minimized, and the Root Mean Standardized error close to one. As we can see in Figure

Source ID	Included	Measured	Predicted	Error	St	^	Predicted
D	Yes	0.00939	0.006	-0	0.	Ξ	3.547
1	Yes	0.001591	0.013	0	0.	-	2051
2	Yes	0.001814	0.013	0	0.		2.951
3	Yes	0.014482	0.010	-0	0.		2.356
4	Yes	0.002292	0.003	0	0.		
5	Yes	0.006191	0.002	-0	0.		1.761
6	Yes	0.003183	0.003	0	0.		1 166
7	Yes	0.000796	0.000	-0	0.		1.100
в	Yes	0.004774	0.003	-0	0.		0.571
9	Yes	0.001591	0.004	0	0.		
10	Yes	0.006302	0.018	0	0.		-0.024 0.69 1.404 2.118 2.832 3.547
11	Yes	0.01687	0.015	-0	0.		Measured
12	Yes	0.004918	0.021	0	0.		Predicted (Error) Standardized Error) Normal QQPlot
13	Yes	0.01114	0.010	-0	0.		
14	Yes	0.020689	0.009	-0	0.		Regression function 0.347253233399894 *
15	Yes	0.018461	0.009	-0	0.		Prediction Errors
16	Yes	0.000796	0.012	0	0.		Samples 217 of 217
17	Yes	0.02427	-0.004	-0	0.		Mean -0.01538939
18	Yes	0.00265	-0.010	-0	0.		Root-Mean-Square 0.2900025
19	Yes	0.011538	0.000	-0	0.		Mean Standardized -0.1171342
20	Yes	0.034853	-0.008	-0	0.	Ŧ	Root-Mean-Square Stan 2.195465
•					•		Average Standard Error 0.1298204
						_	

Figure 11

11, our result coincides well with these values except for the Root Mean Square Standardized error. Click finish.

With the kriging done we now have a probability map for a large Area. To be more useful we want the probability map to be fit to just the shape of the aquifer. The steps are as follows:

- 1. Right click on the CL- prediction map and go to data, then export to vector.
- 2. Keep the input as "Cl-", change the contour type to "Filled Contour", and change the contour quality to "Presentation". In the output section select your project folder and name it "Cl_contour". This should look similar to figure 12. Click OK.

🔨 GA Layer To Contour		x
Input geostatistical layer		*
CI-	I 🖻	
Contour type FILLED CONTOUR	•	
Output feature dass		
\\austin.utexas.edu\disk\geoprofiles\default\jpm2786\My Documents\ArcGIS\Default.gdb\GALa	yerToC 🔁	
Contour quality (optional)		
PRESENTATION	•	
		-
OK Cancel Environments	Show Help >>	



- Next, go into the toolbox, and select clip, within the Extract feature of the Analysis Tools. Select "Cl_contour" as your input feature. Select "QC_aquifer" as your clip feature. In the output feature class select your project folder and name it "CL_prob_clip". See Figure 13.
- 4. The last step is to set the symbology of this clipped probability map. To do this, right click on the "Cl_prob_clip" in the table of contents. Select properties and click on the symbology tab. Click the "import" box in the right hand corner of this window. Within the Import symbology window we want to import from another layer in the map, which

in this case would be the "Cl_contour" shape file. Click ok. The keep the default settings in the "Import Symbology Matching Dialog" window and click OK.

5. Your final product should look like figure 14.

Clip		
Input Features		A
Cl_contour		
Clip Features		
QC_aquifer		
Output Feature Class		
\\austin.utexas.edu\disk\ge	oprofiles\default\jpm2786\My Documents\ArcGIS\De	efault.gdb\Cl_contour_I 🞽
XY Tolerance (optional)		
		Decimal degrees 🔻
	OK Cancel Envi	rooments Show Help 22
	🖂 🛤 Geocoding Tools	
	Figure 13	

To complete the rest of the probability maps replicate all of the steps explained in the ArcGIS

processing section over again. However there is one important difference. When you go to Krig, the Source Data set remains the "QC_mmol" shapefile but the Data field selection will be changed to the desired ion.

Jacob Makis 5/1/2014

lon Concentration Map of the Queen City Aquifer, TX



Conclusion

Using the geostatistical interpolation method of Kriging for ion concentration maps can give you a broad sense of the geochemical reactions that may be taking place. For instance, you could compare the Sodium and Chloride concentrations and see if they coincide. This would indicate a 1:1 ratio between these ions which we would expect. However, a thing to note about these maps, is that they were done with a 20 year span of data. Surely, ion concentrations will vary by location over this time scale. Therefore making any assumptions made from these have a high amount of uncertainty. Additionally, much of the Kriging that was done did came close but did not fit the error parameters discussed perfectly. Consequently, this increases the uncertainty of any assumptions made.