Grid Computing and the TeraGrid GI Science Gateway

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Outline

1. Example data
2. Grid computing
3. The TeraGrid
4. TeraGrid Science Gateways
5. GISolve
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Example data

Sulfur dioxide concentration data from the EPA Air Quality System database
Example data

\( n = 4711 \) observations from 870 sites in the years 1998–2005
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Grid computing

- several different definitions, all involving distributed computing
- networking together computing clusters at different geographic locations to harness computing and storage resources
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The Teragrid

- the world’s largest, most comprehensive distributed cyberinfrastructure for open scientific research
- began in 2001 when NSF awarded $45 million to establish a Distributed Terascale Facility (DTF)
  - to NCSA, SDSC, Argonne National Laboratory, and the Center for Advanced Computing Research (CACR) at California Institute of Technology
- coordinated through the Grid Infrastructure Group (GIG) at the University of Chicago
more than 250 teraflops of computing capability (May 2007)
  - teraflop: trillion \((10^{12})\) floating point operations per second
more than 30 petabytes of online and archival data storage (May 2007)
  - petabyte: quadrillion \((10^{15})\) bytes
rapid access and retrieval over high-performance networks.
TeraGrid Resource Provider sites

- Indiana University
- Oak Ridge National Laboratory
- National Center for Supercomputing Applications
- Pittsburgh Supercomputing Center
- Purdue University
- San Diego Supercomputer Center
- Texas Advanced Computing Center
- University of Chicago/Argonne National Laboratory
- the Joint Institute for Computational Sciences
- the Louisiana Optical Network Initiative
- the National Center for Atmospheric Research
Communication among TeraGrid sites

- Each resource provider maintains 10+ Gbps to one of three TeraGrid hubs (Chicago, Denver or Los Angeles).
- The hubs are interconnected via 10 Gbps lambdas (fiber-optic communications lines).
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TeraGrid Science Gateways

- enable users with a common scientific goal to use national resources through a common interface
- account management, accounting, certificates management, and user support is delegated to the gateway developers
- three common forms:
  - A gateway that is packaged as a web portal with users in front and TeraGrid services in back.
  - Grid-bridging Gateway: Science gateway is a mechanism to extend the reach of the community’s existing Grid so it may use the resources of the TeraGrid.
  - A gateway that involves application programs running on users’ machines (i.e. workstations and desktops) and accesses services in TeraGrid (and elsewhere).
Current TeraGrid Science Gateways

http://www.teragrid.org/programs/sci_gateways/
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GISolve

- Geographic Information Science gateway
- web portal
- “The purpose of this project is to develop a TeraGrid Science Gateway toolkit for GIScience. Our gateway toolkit provides user-friendly capabilities for performing geographic information analysis using computational Grids, and help non-technical users directly benefit from accessing cyberinfrastructure capabilities.”
- current modules
  1. random spatial point generator
  2. distance-weighted interpolation of surfaces
  3. cluster detection algorithm ($G_i^*$)
  4. Bayesian geostatistical spatial model fitting using MCMC
Scheduling on TeraGrid Science Gateway web portals

- local job scheduler manages individual TeraGrid resource
  - Condor
  - Portable Batch System (PBS)

- Globus Resource Access and Management (GRAM)
  - interacts with local job schedulers to allocate computational resources for applications
  - monitors and controls computing processes

- user interactions with Science Gateways through TeraGrid software supporting Web Services Globus Toolkit
Geostatistical models

- natural and interpretable way to model spatial correlation for data measured at irregularly-spaced point sites
- correlation is a function of the distance, and possibly orientation, between sites
Simple geostatistical model with spatial correlation and additive measurement error

\[ Y \sim N \left( X^T \beta, \sigma_s^2 \Sigma(\phi) + \sigma_e^2 I \right) \]

- \( X \) is a matrix of location-specific covariates
- \( \beta \) is a vector of coefficients to be estimated
- \( \Sigma(\phi) \) is spatial correlation matrix
  - entries are calculated from correlation function
- \( \sigma_s^2 \) is spatial variance
- \( \sigma_e^2 \) is random variance (measurement error variance)
- \( I \) is identity matrix
- Bayesian model completed by specification of prior distributions on \( \phi, \sigma_s^2, \sigma_e^2 \), and \( \beta \)
Our alternative reparameterization

- facilitates prior specification and computing algorithm
- reparameterized covariance matrix

\[
\sigma_s^2 \Sigma(\phi) + \sigma_e^2 I = \sigma_{tot}^2 \left[ (1 - S) \Sigma(\phi) + S I \right]
\]

where

\[
\sigma_{tot}^2 = \sigma_s^2 + \sigma_e^2
\]

\[
S = \frac{\sigma_e^2}{\sigma_s^2 + \sigma_e^2}
\]
Prior densities

- continuous uniform prior on \( \phi \)
  - endpoints chosen to reflect belief as to largest and smallest possible distances at which spatial correlation could decay to 0
- joint prior on \( S \) and \( \sigma_{tot}^2 \) obtained by change-of-variable from inverse gamma priors on \( \sigma_e^2 \) and \( \sigma_s^2 \)
- multivariate normal or flat prior on \( \beta \)
Spatiotemporal model with separable correlation structure

\[
Y \sim N \left( X^T \beta, \sigma^2_{tot} \left\{ (1 - S) K \left[ \Sigma(\phi) \otimes \Sigma(\rho) \right] K^T + S I \right\} \right)
\]

- where \( \Sigma(\rho) \) is an AR(1) matrix representing temporal correlation
- \( K \) is a matrix of 1’s and 0’s that matches each observation \( Y_i \) with the correct row and column of \( \Sigma(\phi) \otimes \Sigma(\rho) \)
  - \( K \) is not needed if data are “rectangular"
- prior on \( \rho \) uniform on (-1,1) or (0,1), slightly bounded away from endpoints
Computing algorithm in GISolve MCMC module

- very efficient MCMC computing algorithm that produces low autocorrelation in MCMC output
- computational bottleneck is linear algebra operations on big matrices, especially cholesky decomposition
- single-chain and multi-chain parallelization
  - linear algebra operations for each chain are parallelized using PlaPACK
  - all CPUs for an individual chain must be on same TeraGrid resource
  - multiple chains may be run simultaneously
    - "embarrassingly parallel"
    - different chains may be run on different TeraGrid resources
    - SPRNG used to make sure random number streams for different chains are independent
Challenges in TeraGrid implementation

- different TeraGrid sites have different software, libraries, and batch scheduling programs installed
- had to get PLAPACK installed and working on all sites where GISolve could be used
details of model and algorithm currently implemented in GISolve are in Yan, Cowles, Wang, and Armstrong, *Statistics and Computing*, 2007

extension of the sequential version of algorithm to handle prediction, areal data, fusion of areal and point source data, complicated spatial and nonspatial covariance structure

- implemented in *ramps* package for R
- explained in Cowles, Yan, and Smith 2007 and Smith, Yan, and Cowles 2007 (available as tech reports on stats dept web page)

not yet incorporated into GISolve
Using MCMC module in GISolve

- in advance of your session
  - get account on GISolve
  - request to reserve TeraGrid resources
- go to www.gisolve.org to log in
- upload file of spatiotemporal data you want to analyze
- upload configuration file
- select which TeraGrid partner sites you want to use
  - how many CPUs at each
  - how many parallel MCMC chains to run
  - number of iterations
• specify maximum wall clock time
  • must be long enough for the number of requested iterations to finish
  • must not run past the end of the reserved time on resource

• submit job

• click “Visualize output" to view plots of accumulating samples

• download zip files of plots and numeric output
Data files must be plain text files

First line is two integers:
- number of rows of data
- number of regression coefficients in model, including intercept

Data itself in rectangular format with the following columns (in order):
- response variable
- values of predictor variables, including a column of ones if intercept is required
- x coordinate of spatial location (longitude)
- y coordinate of spatial location (latitude)
- integer representing measurement time
Data file example: sim2000.dat

2000 4
-0.0665 1 0.8056 0.9732 1 0.8056 0.9732 1
-3.0575 1 0.6244 0.4855 1 0.6244 0.4855 1
-2.1376 1 0.7375 0.3452 1 0.7375 0.3452 1

-9.9081 1 0.2165 0.4516 20 0.2165 0.4516 20
-9.9882 1 0.7621 0.0421 20 0.7621 0.0421 20
-8.8069 1 0.4893 0.4964 20 0.4893 0.4964 20
-8.6049 1 0.4142 0.9086 20 0.4142 0.9086 20
Configuration file

- specifies model to be fit
  1. choice among three spatial correlation functions
  2. specification of parameters of prior distributions on $\sigma_e^2$, $\sigma_Z^2$, $\phi$, $S$, $\rho$
- provides initial values for each MCMC chain
content of individual lines

1. Correlation type (1 = spherical; 2 = exponential; 3 = Gaussian)
2. Distance metric (1 = great circle distance; 2 = euclidean distance)
3. The unit of distance: for example, distunit = 10 means that the distances are in 10s.
4. $\alpha_e, \beta_e, \alpha_z, \beta_z$ (parameters of IG priors for $\sigma^2_e$ and $\sigma^2_z$)
5. Left right endpoints of uniform prior distribution for phi
6. Left right endpoints of support of distribution for S
7. Left right endpoints of uniform prior distribution for rho
8. block_size block_size_alg (PlaPACK configuration; leave as in example)
9. Chain index (from 0 to (number of chains - 1)) and initial values for phi, S, and rho
   - as many rows of this kind as there are chains
Configuration file example

1
2
1.0
0.5 0.5 0.5 0.5
0.05 2.0
0.01 0.99
0.01 0.99
200 400
0 0.5 0.75 0.75
1 1.0 0.5 0.5
2 1.5 0.25 0.25
Specifying number of CPUs and number of chains at each site

- number of CPUs is total number to be divided among all the chains at the site
- make number of CPUs *per chain* a perfect square to use PLAPACK efficiently
  - how big a perfect square determined by size of dataset (see graph of speedups in next slide)
- running parallel chains
  - helps in assessing convergence
  - generates more samples per unit time if CPUs are available
  - samples from different chains are independent
- efficient MCMC algorithm results in short burn-in, so a relatively small number of iterations are "wasted"
choosing numbers of CPUs and chains

- for dataset of 10000 observations, if you have 32 CPUs available at each of 3 sites, perhaps run 1 chain using 25 CPUs at each site
- for dataset of 2000 observations, perhaps 3 chains at each site, each chain using 9 CPUs

ability to extend chains from where they left off is being added