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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Sulfur dioxide concentration data from the EPA Air Quality System database
$n = 4711$ observations from 870 sites in the years 1998–2005
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4. TeraGrid Science Gateways
5. GISolve
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.
The TeraGrid

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).
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/
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.

- Random spatial point generator
- Distance-weighted interpolation of surfaces
- Cluster detection algorithm ($G_i^*$)
- 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

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

- \( \mathbf{X} \) 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)
- \( \mathbf{I} \) 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
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
For more information

- 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 and right endpoints of uniform prior distribution for phi
6. Left and right endpoints of support of distribution for S
7. Left and 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