MATT ARRAN

FOSS for large-dataset geostatistics

British Geological Survey

Outline

- Motivation
- New software for variogram calculation
- Existing software for model fitting
- Conclusions

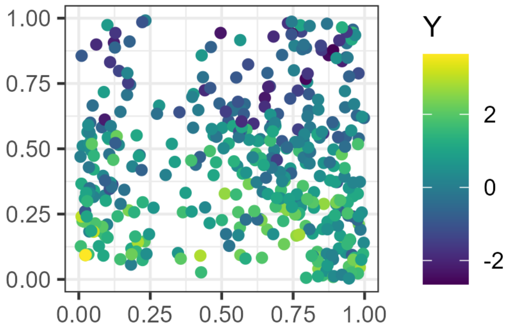
Motivation

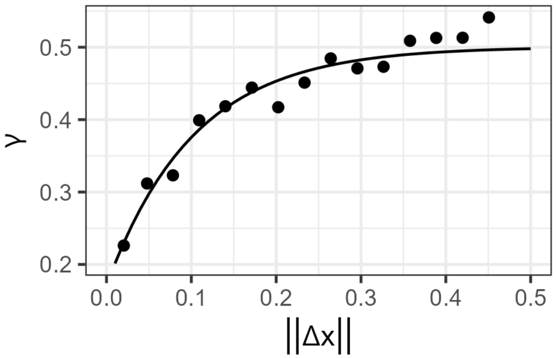
Geostatistics

- Tobler's first law of geography:

"everything is related to everything else, but near things are more related than distant things"

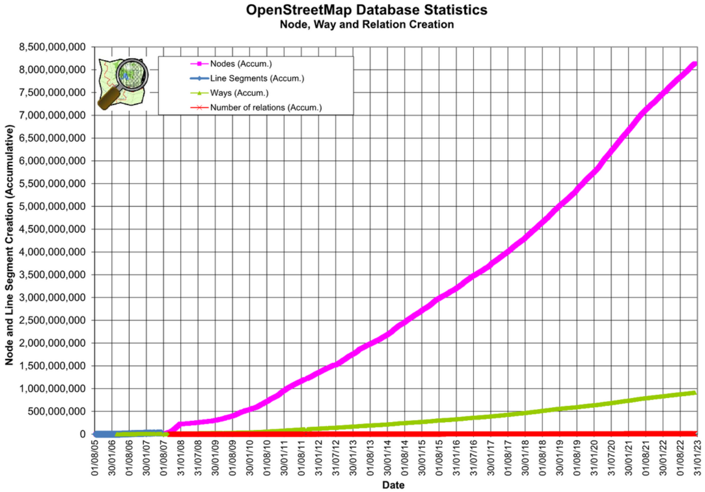
- Standard approach:
    1. Examine how correlation varies with distance, via an empirical variogram
    2. Fit a model, via an inferred spatial covariance matrix
    3. Predict values at new locations, via kriging





Large datasets

- Datasets are growing with increasing computing power
- Geostatistics' computational costs grow faster than dataset size n
  - # of inter-datapoint distances/covariance matrix entries: $O(n^2)$
  - # of operations for covariance matrix decomposition: $O(n^3)$

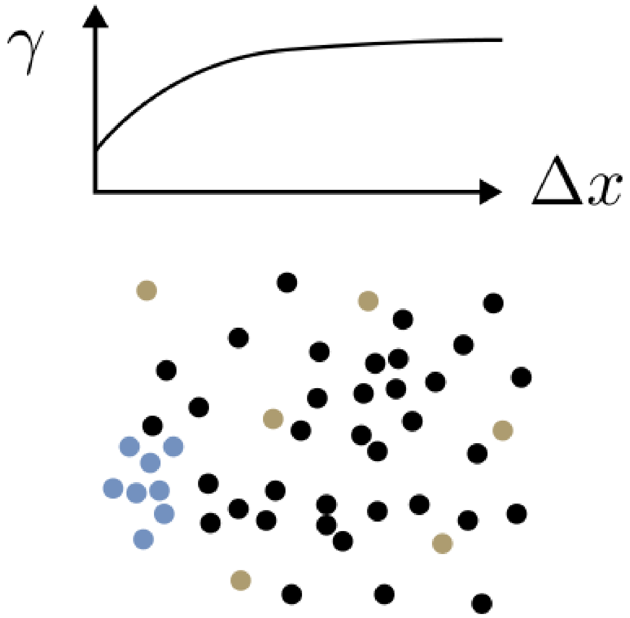


https://wiki.openstreetmap.org/wiki/Stats

Variogram calculation

Sampling risks

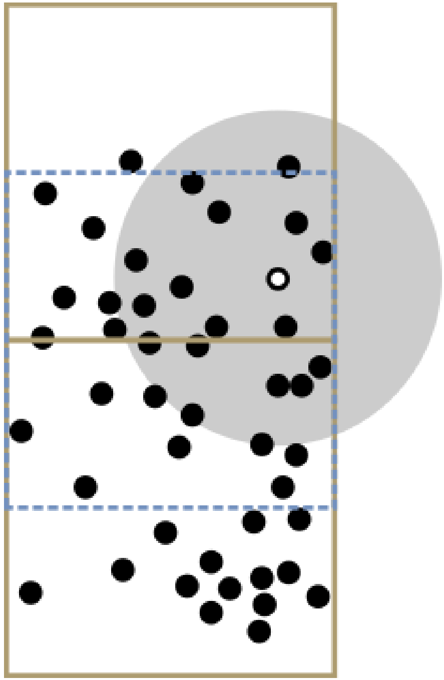
- Excessive spatial span:
  - Covariate variation dominates variability
  - Spatially correlated effect unconstrained
  - Inefficiency from low intercorrelation
- Insufficient spatial span:
  - Correlation dominates variability
  - Covariate dependence unconstrained
  - Inefficiency from high intercorrelation



Efficient sampling

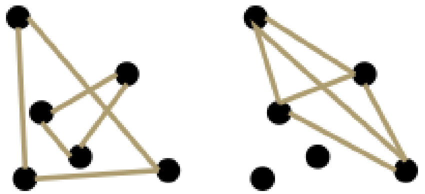
- Estimate maximum significant correlation length λ
- Divide datapoints into 2λ x 2λ boxes with overlaps λ
  - All significant pair-interactions within some box
- From each box, sample # pairs $\propto$ # datapoints
  - First approx. to Reilly and Gelman (2012)
- # of comparisons $O[A\lambda^2\rho\rho_{min}]$ rather than $O[(A\rho)^2]$

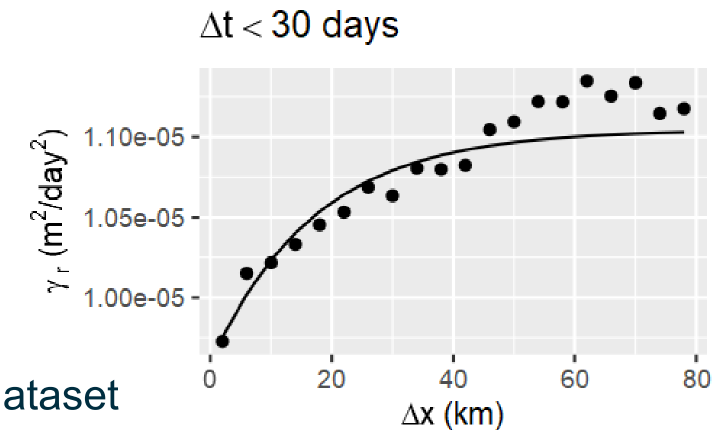
  (for Area A, typical and low datapoint density ρ, ρ_{min})



Variogram implementation

- Development version implemented in R
- Euclidean and WGS84 distances supported
- Options for subsampling:
  - Complete coverage
  - Complete network
- Options for estimator:
  - Matheron (1962)'s
  - Cressie & Hawkins (1980)'s
  - Genton (1998)'s
- Applied to 78,878-datapoint Punjab groundwater dataset
  - ~ 1 hour to identify ~ 1.6 million interacting pairs





ADD YOUR SUBTITLE HERE

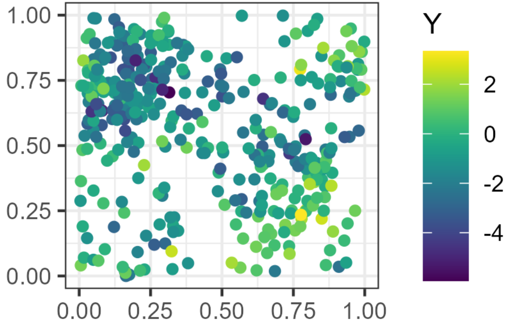
Model fitting

Published approaches

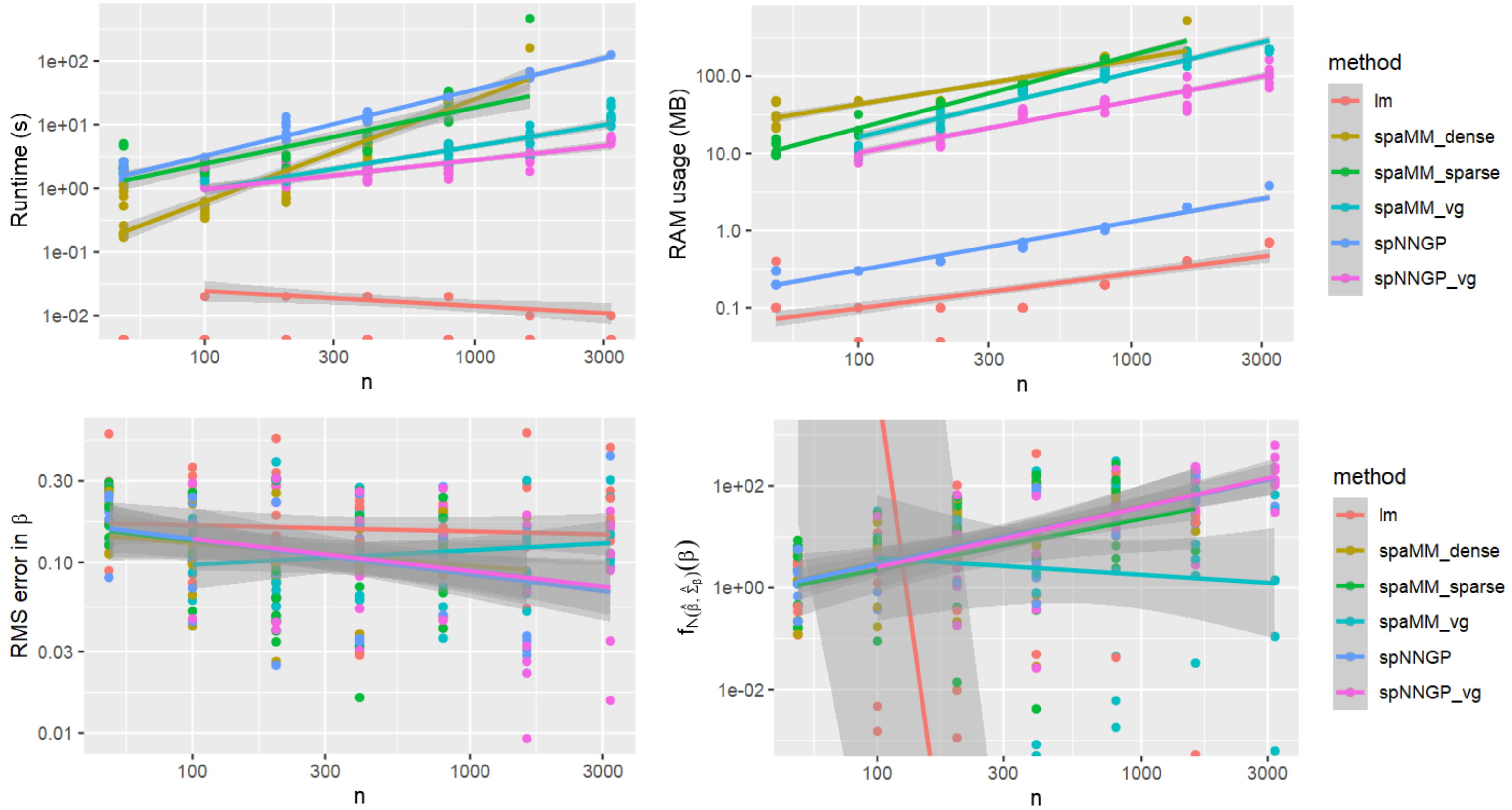
- Take advantage of low correlation at distance:
  - Tapered covariance matrices (e.g. with R package spaMM)
  - Nearest-Neighbour Gaussian Process (R package spNNGP)
- Take advantage of high correlation in proximity:
  - Fixed Rank Kriging (R package FRK)
  - Predictive Process (R package spBayes)
- Both: Multi-Resolution Approximation (Julia package MRA_JASA, Python pyMRA)
- Solve equivalent problem with more sparsity:
  - Lattice Kriging (R package LatticeKrig)
  - INLA for equivalent SPDE (R package R-INLA)
- Few direct comparisons between different approaches

Comparison method

- Simulate datapoints at n = 50, 100, …, 3200 locations in the unit square
  - *Locations*: mixture of three Gaussian clusters and a uniform distribution
  - *Covariates*: one uncorrelated, one spatially correlated
  - *Errors*: exponential correlation structure with nugget
- Estimate coefficients with linear regression lm, as control, &:
  - Dense covariance matrix, using spaMM
  - Sparse, spherically tapered covariance matrix, using spaMM
  - Nearest-Neighbours Gaussian Process, using spNNGP
- Specify correlation structure:
  - As part of the model fit
  - Using the empirical semivariogram

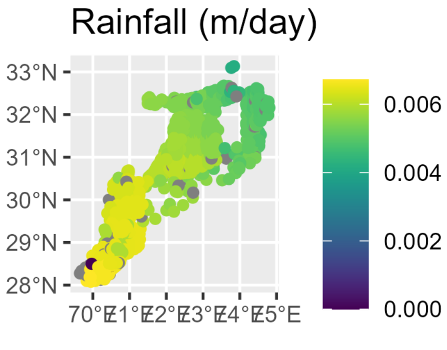


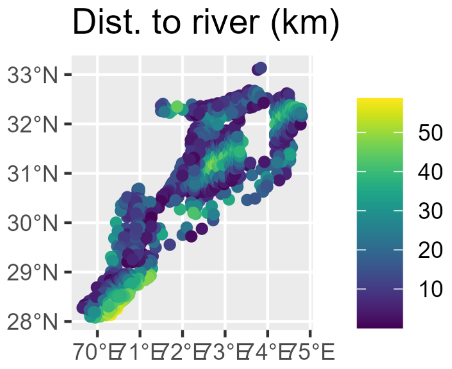
Comparison results

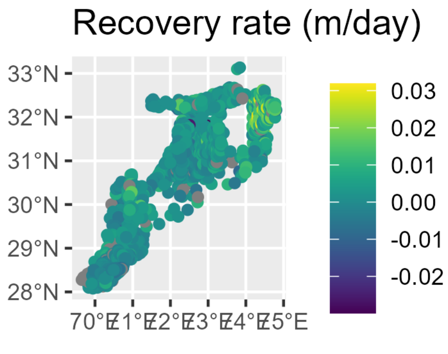


Application

- Consider monsoonal groundwater change rates in Punjab, Pakistan, 1979 – 2009
  - 41,852 records at 2,967 sites
  - Low residual inter-year temporal correlation
  - Spatially correlated covariates and errors
- Fit a linear model with a spatially correlated error term
  - Using spaMM, with a tapered covariance matrix specified from the variogram








```
 ------------ Fixed effects (beta) ------------
[one-time computation of covariance matrix, which may be slow]
                      Estimate  Cond. SE  t-value
(Intercept)          -0.001441 5.840e-04  -2.4670
prev_prec             1.307351 5.200e-02  25.1431
prev_pet              0.110728 9.814e-02   1.1282
tubewell_density    -58.908726 1.751e+01  -3.3642
prev_dWL             -0.001137 5.108e-05 -22.2523
prev_prec_anom        0.933084 1.780e-01   5.2423
prev_irrig            0.396764 6.611e-02   6.0020
prev_prec_anom:riv   -0.005685 6.968e-03  -0.8159
prev_irrig:canal     -0.004589 3.522e-03  -1.3031
 --------------- Random effects ---------------
Family: gaussian( link = identity )
           --- Variance parameters ('lambda'):
lambda = var(u) for u ~ Gaussian;
   id  :  1.982e-05
# of obs: 9039; # of groups: id, 9039
 -------------- Residual variance  ------------
phi estimate was 1.72108e-06
 ------------- Likelihood values  -------------
                        logLik
logL       (p_v(h)): 35846.38
```

Conclusions

Conclusions

- Computationally efficient methods key to large-dataset geostatistics
- Variety of free, open-source software available, especially in R
- New tool promising for empirical variogram calculation
- For model fitting and prediction, spNNGP’s the best option when applicable

Future work

- Rewrite variogram calculation as production code
  – Which language would be most useful?
- Test more existing methods
  – Which dataset complications are most important to model?
- Extend tests to prediction
  – Against which non-statistical methods would tests be most useful?