Fitting Computer Models

David C. Stenning

Department of Statistics, University of California, Irvine

Computer Model for Stellar Evolution



- We observe a star's *photometric magnitudes*—the apparent brightness of a star in several wide wavelength bands.
 - Magnitudes observed with Gaussian measurement error.
- Computer models to predict the photometric magnitudes of a star given a set of input parameters that describe certain characteristics about the star.
- Embed these models in a multilevel model for statistical inference.

Combining Computer Models and Statistical Models



- Observe photometric magnitudes through *n* different filters per star.
- Model photometric magnitudes as *n* independent Gaussians.
 - Means involve the computer models for stellar evolution; depend on the stellar evolution parameters.
 - Known Gaussian measurement errors in the covariance matrix.
- Data is contaminated by non-cluster *field stars*.
 - Use a finite mixture model, with field star magnitudes assumed uniform over the range of the data.

(日) (同) (三) (

Final Combined Computer/Statistical Model



- We take a Bayesian approach to model fitting.
 - Informative prior distributions are constructed based on previous studies and astrophysical theory.

< ロ > < 同 > < 回 > < 回 > < 回 > <

э

- Specifying a Bayesian statistical model:
 - Likelihood Function: the distribution of the data, Y, given model parameters, Θ. Denoted by L(Θ) = P(Y | Θ).
 - Θ may contain computer model inputs.
 - Prior Distribution: represents knowledge about the parameters obtained *prior* to the current data. Denoted by P(Θ).
 - Posterior Distribution: represents knowledge about the parameters in light of the data. Denoted by $P(\Theta | Y)$.
- From Bayes' Theorem:

```
P(\Theta \mid Y) \propto P(Y \mid \Theta) P(\Theta)
```

Complex Posterior Distributions



ヘロト ヘヨト ヘヨト ヘ

э

Exploring $P(\Theta \mid Y)$



source: http://commons.wikimedia.org/wiki/File:3dRosenbrock.png#mediaviewer/File:3dRosenbrock.png

- We explore the posterior distribution, P(Θ | Y), using Markov chain Monte Carlo (MCMC) methods.
- MCMC produces (correlated) samples from $P(\Theta | Y)$.
- Fitted values, 95% CIs, etc. computed using MCMC draws.

The Metropolis Algorithm

Draw $\Theta^{(0)}$ from some starting distribution.

For $t = 1, 2, \ldots$

• Draw "proposed state" $\Theta^{(*)} = \Theta^{(t-1)} + random perturbation.$

• random perturbation must be symmetric

• e.g.
$$\Theta^{(*)} \sim N\left(\Theta^{(t-1)},\xi\right)$$

• Compute
$$a = \min\left(1, \frac{P\left(\Theta^{(*)} \mid Y\right)}{P\left(\Theta^{(t-1)} \mid Y\right)}\right).$$

• Set $\Theta^{(t)} = \Theta^{(*)}$ with probability *a*, else set $\Theta^{(t)} = \Theta^{(t-1)}$.

Note that proposed states "uphill" are always accepted, while proposed states "downhill" are only sometimes accepted.

The Metropolis Algorithm: Step-Size Effect



< 一型

Adaptive Metropolis Algorithm

- How to choose an "optimal" proposal distribution?
- For a $N(0, \Sigma)$ target distribution, the optimal proposal distribution is $N(0, [(2.38)^2/d]\Sigma)$, where Σ is a d-dimensional covariance matrix (Gelman *et al.* 1996).
- Adaptive Metropolis (AM) algorithm (e.g., Haario et al. 2001):
 - At iteration t, draw $\Theta^{(*)} \sim N\left(\Theta^{(t-1)}, \left[(2.38)^2/d\right]\xi_{t-1}\right)$.
 - ξ_{t-1} is the empirical covariance matrix of $\Theta^{(0)}, \dots, \Theta^{(t-1)}$.

Key condition: the amount of adaptation at iteration t goes to 0 as $t \rightarrow \infty$ (Diminishing Adaptation Condition).

Adaptive Metropolis Advantage



- Exploring a (marginal) posterior distribution using an AM algorithm.
- Improved efficiency and convergence compared to non-adaptive Metropolis implementation.
 - Same data and setup used for both algorithms.
 - AM algorithm adapts the proposal distribution starting at iteration 1000.

CMD Matrix with Fitted Computer Models



Stenning, David Fitting Computer Models

Thanks!

- David A. van Dyk
- Ted von Hippel
- Nathan Stein
- Rachel Wagner-Kaiser
- Elliot Robinson
- Elizabeth Jeffery
- William H. Jefferys
- Steven DeGennaro