

A DATA-DRIVEN MARKOV CHAIN MONTE CARLO METROPOLIS-HASTINGS ALGORITHM FOR A MODEL OF THE HUMAN THUMB

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INTRODUCTION

Monte Carlo techniques are gaining acceptance in complex biomechanical modeling to explore the effects of anatomical variability and measurement uncertainty on model predictions in an open-loop manner (e.g., Langenderfer *et al.*, 2006; Santos and Valero-Cuevas, 2006). However, creating realistic models will require advanced stochastic methods to perform closed-loop, data-driven searches when model parameter spaces are large. We present what, to our knowledge, is the first use of Markov chain Monte Carlo (MCMC) techniques in biomechanics with synthetic data from a model of the human thumb as a proof-of-concept of the MCMC Metropolis-Hastings algorithm to explore a complex 36-dimensional (36D) model parameter space.

METHODS

Previously, we described an MCMC Metropolis-Hastings algorithm (Santos and Valero-Cuevas, 2004) that uses the single-site updating technique to explore a 36D model parameter space in a manner similar to a biased random walk: thumb bone dimensions (8), kinematic axes of rotation (16) (Giurintano *et al.*, 1995), and frame transformations at the proximal base (6) and distal tip (6) of the thumb. Here, we apply the algorithm to a model with 36 arbitrarily defined model parameters. To validate the algorithm, we used a truth model to simulate experimental data (thumbnail location, orientation, and linear and angular velocities) for nine active motions (e.g.,

flexion/extension). We also added zero-mean, uncorrelated multivariate Gaussian “measurement noise” to our deterministic truth model outputs. Ten independent Markov chains driven by these noisy data searched the 36D model parameter space for the subspace that best fit the data (i.e., the posterior distribution) until the Gelman-Rubin convergence diagnostic fell below a threshold of 1.2. We used posterior-predictive sampling to compare the MCMC results to the truth model and cross-validated the results using a separate set of simulated experimental data that were not used to drive the MCMC simulations.

RESULTS AND DISCUSSION

We ran each Markov chain for 105,000 iterations on 2.4GHz dual Intel[®] Xeon[®] machines, which took 255.5 hours (49 hrs. for MCMC simulations in C and 206.5 hrs. for post-analysis in MATLAB[®]). Six chains converged to the true posterior distribution while the remaining four chains located other local minima in the 36D landscape (Figure 1).

The errors in the posterior predictive samples for the six chains were minimal (Figure 2). Despite the fact that we provided noisy simulated data to our Metropolis-Hastings algorithm, the algorithm estimated and accounted for the noise to find the true values and successfully locate the true posterior distribution. The errors in the posterior predictions for the cross-validation data set were also minimal, demonstrating

that the algorithm did not simply over fit the data given, but actually found the true parameters in the 36D space.

CONCLUSIONS

We have successfully demonstrated the unprecedented use of our Metropolis-Hastings sampling algorithm to a large 36D biomechanical model parameter space with practical application to experimental data. MCMC techniques in biomechanics may provide clinical benefits such as the ability to determine sensitivity of model predictions and functional clinical outcomes to changes in model parameters, and to categorize clinically-relevant subpopulations. Convergence of a majority of chains to the true values demonstrates that the method is able to accommodate the expected redundancies of large parameter spaces.

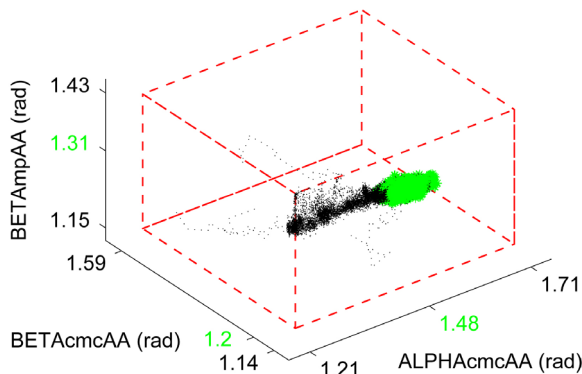


Figure 1: Convergence (green points) of the six Markov chains for three representative parameters. The chains located the true posterior distribution in the cuboid defined by the bounds on the prior distributions (red dashed lines). A Monte Carlo integrator must randomly sample from the entire volume. The MCMC simulations, in contrast, are more computationally efficient because they behave like biased random walks that converge to the model parameter subspace that best fits the data (true values in green). While only 3D results are shown here, convergence occurred in 36D.

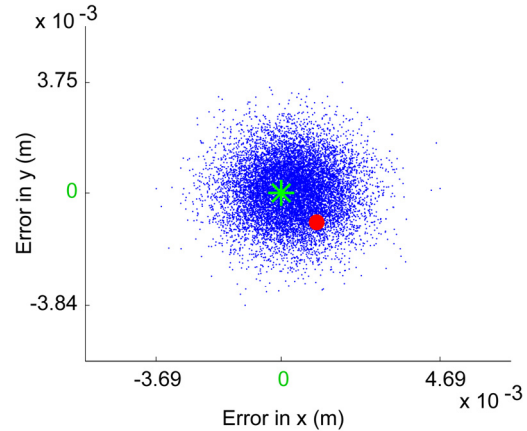


Figure 2: The posterior predictive sample errors (blue points) are shown for two experimental outputs (x and y coordinates for thumbnail location) for a single representative data point. The green asterisk indicates the true error value of zero. The red circle is the offset of the noisy simulated data point actually used to drive the MCMC simulations. Note that the algorithm estimated the variance in the noisy simulated data and recovered the true parameter values (blue cloud of points is centered around the true error value of zero).

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ACKNOWLEDGEMENTS

NSF Graduate Research Fellowship (to V.J. Santos), Grant Nos. AR050520 and AR052345 from the NIH, and NSF CAREER Award BES-0237258 (to F.J. Valero-Cuevas).