DOWNLOAD PDF MONTE CARLO METHODS IN STATISTICAL PHYSICS NEWMAN

Chapter 1 : CiteSeerX â€” Citation Query Monte Carlo Methods

In particular, it is about Monte Carlo methods, which form the largest and most important class of numerical methods used for solving statistical physics problems.

Snijders - Journal of Social Structure , " This paper is about estimating the parameters of the exponential random graph model, also known as the p model, using frequentist Markov chain Monte Carlo MCMC methods. The exponential random graph model is simulated using Gibbs or Metropolis-Hastings sampling. The estimation procedures consider The estimation procedures considered are based on the Robbins-Monro algorithm for approximating a solution to the likelihood equation. Show Context Citation Context The existence of two or more regimes is reminiscent of the longrange dependence that is known to occur for certain parameter values in the Ising model cf. This also is related to the degeneracy problem discussed by Strauss for the transitivity model and other New specifications for exponential random graph models by Tom A. Handcock , " The strong point of these models is that they can represent a variety of structura The strong point of these models is that they can represent a variety of structural tendencies, such as transitivity, that define complicated dependence patterns not easily modeled by more basic probability models. Applying these models in their traditional specification to observed network data often has led to problems, however, which can be traced back to the fact that important parts of the parameter space correspond to nearly degenerate distributions, which may lead to convergence problems of estimation algorithms, and a poor fit to empirical data. This paper proposes new specifications of Exponential Random Graph Models. These specifications represent structural properties such as transitivity and heterogeneity of degrees by more complicated graph statistics than the traditional star and triangle counts. Three kinds of statistic are proposed: Examples are presented both of modeling graphs and digraphs, in which the new specifications lead to much better results than the earlier existing specifications of the ERGM. It is concluded that the new specifications increase the range and applicability of the ERGM as a tool for the statistical analysis of social networks. These distributions are not interesting in terms of transitivity. This near-degeneracy is related to the phase transitions known for the Ising and some other models e. J , " The protein conformation is described as a lattice chain connecting Ca atoms, with attached Cb atoms and side-chain centers of mass. The model force field includes various short-range and long-range knowle The model force field includes various short-range and long-range knowledge-based potentials derived from a statistical analysis of the regularities of protein structures. The combination of these energy terms is optimized through the maximization of correlation for 30 3 60, decoys between the root mean square deviation RMSD to native and energies, as well as the energy gap between native and the decoy ensemble. To accelerate the conformational search, a newly developed parallel hyperbolic sampling algorithm with a composite movement set is used in the Monte Carlo simulation processes. To fold larger-size proteins as well as to improve the folding yield of small proteins, we incorporate into the basic force field side-chain contact predictions from our threading program PROSPECTOR where homologous proteins were excluded from the data base. For native fold selection, we introduce quantities dependent on the cluster density and the combination of energy and free energy, which show a higher discriminative power to select the native structure than the previously used cluster energy or cluster size, and which can be used in native structure identification in blind simulations. These procedures are readily automated and are being implemented on a genomic scale. In recent work Zhang et al. It is believed that almost any pair of people in the world can be connected to one another by a short chain of intermediate acquaintances, of typical length about six. This phenomenon, colloquially referred to as the "six degrees of separation," has been the subject of considerable recent This paper provides a short review of the topic. The use of simulation for high-dimensional intractable computations has revolutionized applied mathematics. Designing, improving and understanding the new tools leads to and leans on fascinating mathematics, from representation theory through micro-local analysis.

DOWNLOAD PDF MONTE CARLO METHODS IN STATISTICAL PHYSICS NEWMAN

Chapter 2 : M. E. J. Newman's Monte Carlo Methods in Statistical Physics PDF | Badabble Publishing E-bo

Monte Carlo Methods in Statistical Physics / Edition 1 This book provides an introduction to Monte Carlo simulations in classical statistical physics and is aimed both at students beginning work in the field and at more experienced researchers who wish to learn more about Monte Carlo methods.

Computation of strained epitaxial growth in three dimensions by kinetic Monte by Giovanni Russo, Peter Smereka , " A numerical method for computation of heteroepitaxial growth in the presence of strain is presented. The model used is based on a solid-on-solid model with a cubic lattice. Elastic effects are incorporated using a ball and spring type model. The growing film is evolved using Kinetic Monte Carlo KMC and it is assumed that the film is in mechanical equilibrium. The strain field in the substrate is computed by an exact solution which is efficiently evaluated using the fast Fourier transform. The strain field in the growing film is computed directly. The resulting coupled system is solved iteratively using the conjugate gradient method. Finally we introduce various approximations in the implementation of KMC to improve the computation speed. Numerical results show that layer-by-layer growth is unstable if the misfit is large enough resulting in the formation of three dimensional islands. However, with the inclusion of elastic effects, the implementation of rejection-free KMC is not so straightforward. Here we shall outline various approximations of the model which lead to a much fas Simulation of wetting-layer and island formation in heteroepitaxial growth by F. Tp â€" Computer modeling and simulation. Ac â€" Nucleation and growth: Aj â€" Theory and models of crystal growth; physics of crystal growth, crystal morphology and orientation. We observe the appearance of strain-induced mounds upon a wetting layer, i. The transition from 2d to 3d islands occurs at a critical layer thickness and its dependence on the growth parameters is studied quantitatively. We find that for large enough deposition rates the layer thickness as well as the size and density of islands depend on the misfit between substrate and adsorbate, only. As a consequence, heteroepitaxial growth has been a matter of significant interest in both experimental and theoretical studies see, e. In particular, the strain-induced formation Show Context Citation Context In order to consider the deformation of the crystal, after each microscopic event diffu This paper addresses the problem of sampling from binary distributions with constraints. In particular, it proposes an MCMC method to draw samples from a distribution of the set of all states at a specified distance from some reference state. For example, when the reference state is the vector of ze We motivate the need for this algorithm with examples from statistical physics and probabilistic inference. Unlike previous algorithms proposed to sample from binary distributions with these constraints, the new algorithm allows for large moves in state space and tends to propose them such that they are energetically favourable. The algorithm is demonstrated on three Boltzmann machines of varying difficulty: A ferromagnetic Ising model with positive potentials , a restricted Boltzmann machine with learned Gabor-like filters as potentials, and a challenging three-dimensional spin-glass with positive and negative potentials. Here, fixing the number of active variables has the physical meaning of holding the magnetization of the system constant. In probabilistic inference, constraints on the number of active A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition. A well-defined, relatively complex Greek-key topology, groun A well-defined, relatively complex Greek-key topology, ground native conformations was found; however, the cooperativity of the folding transition was very low. It is demonstrated that the all-or-none transition arises from the interplay between local stiffness and properly defined tertiary interactions. The tertiary interactions are directional, mimicking the packing preferences seen in proteins. The model properties are compared with other minimal protein-like models, and we argue that the model presented here captures essential physics of protein folding structurally well-defined protein-like native conformation and cooperative all-or-none folding A new mathematical representation of game theory. In this paper, we introduce a framework of new mathematical representation of Game Theory, including static classical game and static quantum game. The idea is to find a set of base vectors in strategy space and to define their inner

product so as to form them as a Hilbert space, and then form a Hil The idea is to find a set of base vectors in strategy space and to define their inner product so as to form them as a Hilbert space, and then form a Hilbert space of system state. Basic ideas and formulas in Game Theory have been reexpressed in such a space of system state. This space provides more possible strategies than traditional classical game and quantum game. All the games have been unified in the new representation and their relation has been discussed. It seems that if the quantized classical game has some independent meaning other than traditional classical, a payoff matrix with non-zero off-diagonal elements is required. On the other hand, when such new representation is applied onto quantum game, the payoff matrix gives non-zero off-diagonal elements. Also in the new representation of quantum games, a set of base vectors are naturally given from the quantum strategy operator space. This gives a kind of support for our approach in classical game. Ideas and technics from Statistical Physics can be easily incorporated into Game Theory through such a representation. This incorporation gives an endogenous method for refinement of Equilibrium State and some hits to simplify the calculation of Equilibrium State. Kinetics Equation and thermal equilibrium has been introduced as an efficient way to calculate the Equilibrium State. Although we have gotten some successful experience on some trivially cases, the progress of such a dynamical equation for the general case is still waiting for more exploration.

DOWNLOAD PDF MONTE CARLO METHODS IN STATISTICAL PHYSICS NEWMAN

Chapter 3 : CiteSeerX â€” Citation Query Monte Carlo Methods in Statistical Physics

Monte Carlo Methods in Statistical Physics is well suited for classroom use and could be valuable as a reference or tool for self-study for both beginning and.

Equilibrium Monte Carlo calculations 1. The principles of equilibrium thermal Monte Carlo simulations 3. The Ising model and the Metropolis algorithm 4. Other algorithms for the Ising model 5. The conserved-order-parameter Ising model 6. Disordered spin models 8. Analysing Monte Carlo data II. Principles of out-of-equilibrium Monte Carlo simulation Non-equilibrium simulations of the Ising model Monte Carlo simulations in surface science The repton model Lattices and data structures Monte Carlo simulations on parallel computers Barkema A Clarendon Press Publication Reviews and Awards "This book is intended for those who are interested in the use of Monte Carlo simulations in classical statistical mechanics. Its primary goal is to explain how to perform such simulations efficiently. To this end, the authors discuss. The book is divided into three parts covering equilibrium Chapters and non-equilibrium Monte Carlo simulations, and implementations Each algorithm is introduced in the context of a particular model. For example, the Metropolis algorithm is illustrated by its application to the Ising model. A brief outline of the physics behind each model is always given. The present text discusses many of these algorithms. The book is well written and can be enjoyed at various levels. In summary, this book belongs in the personal library of all researchers in statistical physics regardless of whether they write Monte Carlo algorithms or not , computational scientists interested in Monte Carlo methods, and advanced undergraduates and graduate students wishing to learn about recent developments in statistical physics and Monte Carlo methods. Their writing is excellent throughout, and they cover a wide range of topics. Monte Carlo Methods in Statistical Physics is well suited for classroom use and could be valuable as a reference or tool for self-study for both beginning and experienced researchers. This book should give newcomers to Monte Carlo methods all the information and advice they need to get useful programs up and running. In addition to a basic presentation of the algorithms, Newman and Barkema discuss various implementation issues at length, give a wide range of programming advice, and discuss random number generators. This book also has an extensive treatment of data analysis techniques. In my opinion this book can be very useful for both graduate students and experienced researchers. Problems are clearly stated, solutions are accurately discussed and there are problems to solve after every chapter. This book is surely suitable for use as a textbook for a course on simulation methods, or as a supplementary text in a course on statistical physics. Although the overall technical level is that of a graduate text, I think even experienced researchers in the field would benefit from reading the detailed accounts of the most sophisticated new simulation techniques which have appeared in recent years. Cirillo, Mathematical Reviews Clippings m Share:

Chapter 4 : Monte Carlo methods in statistical physics | Search Results | IUCAT

An up-to-date introduction to Monte Carlo simulations in classical statistical physics. Covers both equilibrium and out of equilibrium systems and discusses in detail numerous algorithms, including Metropolis and heat-bath algorithms, continuous time Monte Carlo, cluster algorithms, and entropic.

Chapter 5 : Monte Carlo Methods in Statistical Physics

This book provides an introduction to Monte Carlo simulations in classical statistical physics and is aimed both at students beginning work in the field and at more experienced researchers who wish to learn more about Monte Carlo methods. It includes methods for both equilibrium and out of.

DOWNLOAD PDF MONTE CARLO METHODS IN STATISTICAL PHYSICS NEWMAN

Chapter 6 : Monte Carlo Methods in Statistical Physics - M. E. J. Newman, G. T. Barkema - Google Books

Monte Carlo Methods in Statistical Physics is published by Oxford University Press.. It can be purchased directly from the press, from good scientific bookstores or online from, amongst other places, blog.quintoapp.com or Barnes and Noble.

Chapter 7 : Simulation Methods in Physics I WS / - ICPWiki

This book provides an introduction to Monte Carlo simulations in classical statistical physics and is aimed both at students beginning work in the field and at more experienced researchers who wish to learn more about Monte Carlo methods.

Chapter 8 : Monte Carlo method in statistical physics - Wikipedia

Monte Carlo methods in statistical physics. Author Monte Carlo methods in statistical physics / M.E.J. Newman and G.T. Barkema. Monte Carlo method.

Chapter 9 : Barkema, G. T. [WorldCat Identities]

Overview. The general motivation to use the Monte Carlo method in statistical physics is to evaluate a multivariable integral. The typical problem begins with a system for which the Hamiltonian is known, it is at a given temperature and it follows the Boltzmann statistics.