## Blackwell-Tapia Conference
## November 14-15, 2008

### SPEAKER TITLES/ABSTRACTS

**Angela Gallegos**
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"Crocodilia, Sex Determination and Delay Differential Equations"

The crocodilia have multiple interesting characteristics that affect their population dynamics. They are among several reptile species which exhibit temperature-dependent sex determination (TSD) in which the temperature of egg incubation determines the sex of the hatchlings. Their life parameters, specifically birth and death rates, exhibit strong age-dependence. We develop delay-differential equation (DDE) models describing the evolution of a crocodilian population. In using the delay formulation, we are able to account for both the TSD and the age-dependence of the life parameters while maintaining some analytical tractability. In our single-delay model we also find an equilibrium point and prove its local asymptotic stability. We numerically solve the different models and investigate the effects of multiple delays on the age structure of the population as well as the sex ratio of the population. For all models we obtain very strong agreement with the age structure of crocodilian population data as reported in Smith and Webb (Aust. Wild. Res. **12**, 541–554, 1985). We also obtain reasonable values for the sex ratio of the simulated population. This is joint work with Tenecia Plummer, David Uminsky, Cinthia Vega, Clare Wickman and Michael Zawoiski.

**Oscar Gonzalez**
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"Predicting Geometric Properties of DNA from Hydrodynamic Diffusion Data"

The sequence-dependent curvature and flexibility of DNA is critical for its packaging into the cell, recognition by other molecules, and conformational changes during biochemical processes. However, few methods are available for directly probing these properties at the basepair level. In this talk, a model for estimating sequence-dependent curvature and other geometric properties of DNA from hydrodynamic data on short sequences is described. The model is based on a generalized diffusion equation for DNA in dilute solution, with a coefficient matrix determined by the Stokes equations in the spatial domain around a single molecule. By comparing experimental measurements of this matrix with predictions based on direct numerical solution of the Stokes equations around sequence-dependent geometries, various structural features of DNA can be

studied. In a preliminary application, we use the model to predict the hydrated radius of DNA under different assumptions on DNA curvature. Our results indicate that previous estimates of the radius, which were based on an assumption of zero curvature, are likely to be underestimates.

**Rudy Horne**
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"Solitary Waves in Discrete Media in the Presence of Four-Wave Mixing Products"

In this talk, I will discuss solutions that arise in a vector discrete model of the Nonlinear Schr\"odinger equation where nonlinear inter-component coupling and four-wave mixing are taken into account. We show that the solutions to this model give rise to two single mode branch solutions as well as two mixed mode branch solutions. These solutions are obtained explicitly and their stability is analyzed in the so-called anti-continuum limit. Also, we connect this analysis to recent experiments that motivated this work.

**Gabriel Huerta**
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"Statistical Approaches for Parameter Estimation in Climate Models"

To quantify the uncertainties arising in climate prediction it is necessary to estimate a multidimensional probability distribution. This is known as the calibration problem. The computational cost of evaluating such a probability distribution for a climate model is impractical using traditional methods such as Gibbs/Metropolis algorithms. This talk will describe an optimization based method that has been applied for non-linear problems in geophysics and that is currently in use to calibrate parameters of an atmospheric general circulation model (ACGM).

Furthermore, we will also consider adaptive Monte Carlo based methods in the context of a climate model that is able to approximate the noise and response behavior of the AGCM. Comparisons and efficiency evaluations between approaches will be made. Another aspect of this talk is to overview the current role of spatial methods in providing emulators to climate model output and reducing computational burden. In particular we will discuss the use of Gaussian process (GP) in this context and on potential limitations and challenges for these methods.

**Jacqueline Hughes-Oliver**
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"Analysis of High-Dimensional Structure-Activity Screening Datasets Using the Optimal Bit String Tree"

A new classification method called the Optimal Bit String Tree (OBSTree) is proposed to identify quantitative structure-activity relationships (QSARs) in high-throughput screening studies. This recursive partitioning method introduces the concept of a chromosome to describe the simultaneous presence or absence of a combination of molecular features within a compound. Chromosomes are combined with a subset of descriptors (or predictor variables) to create a splitting variable, and these splitting variables form the search space for recursively splitting a compound collection in order to identify those compounds having both similar molecular structure and similar biological activity. Because of the resulting explosion in size of the search space, care is needed when exploring this space. We use a new stochastic searching scheme that consists of a weighted sampling scheme, simulated annealing, and a trimming procedure. Simulation studies and application to screening for monoamine oxidase (MAO) inhibitors show that OBSTree is advantageous in accurately and effectively identifying QSAR rules and finding different classes of active compounds.

**Juan Meza**
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"Optimization: The Difference Between Theory and Practice"

There's an old saying, "In theory, there's no difference between theory and practice, but in practice there is". In this talk, I will discuss some of the challenges one faces when trying to solve optimization problems arising in real-world applications and what roles theory and practice play in developing new optimization algorithms. Today, scientists are working on problems such as designing nanostructures with specific properties, predicting the structure of proteins, finding new supernovae, and determining vulnerabilities in the electric power grid. In part, this is due to an increased ability to mathematically model new physical and engineering processes and the rapid rise of computational modeling and simulation. The resulting simulation-based optimization problems, however, have very different characteristics than classical problems and usually do not fit within the standard theoretical assumptions. In many cases, for example, there is noise associated with the evaluation of the objective function, usually through numerical errors in the solution of the equations. In other cases, no derivative information is available or the function may not be sufficiently smooth for standard methods. I will discuss several optimization techniques for the solution of these types of problems and some lessons learned in applying theory to practical problems.

**Yolanda Munoz Maldonado**
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"Testing the Equality of Mean Functions for Continuous Time Stochastic Processes"

One of the most common activities in Statistics is the comparison of means for two or more groups. This task is usually carried out by the method called Analysis of Variance (ANOVA). When the analysis is done on functional data, the implementation of this technique becomes complicated due to the dimensionality of the problem. In this talk, we modify the test statistic of a permutation test used to compare the similarity between two sets of curves. The modified statistic is shown to be a U-statistic, and using its asymptotic distribution and following classical ANOVA reasoning, it allows for comparison of two or more groups of functions. A small Monte-Carlo simulation shows comparable power between the permutation test and our proposed approach when the number of groups analyzed is two. It also provides evidence that the U-statistic performs well for three sets of curves. We apply the U-statistic test to a ganglioside profile data set.

**Tanya Moore**
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"Using Mathematics to Transform Communities"

Can mathematics be used to empower a community? How does a biostatistician transfer math skills to work in the government and non-profit sectors? How is statistics really used in the field of public health? During this talk I will share highlights of my journey from studying mathematics to working in a city health department and for a non-profit that is committed to supporting and encouraging emerging scientist and mathematicians.

**Freda Porter**
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"Technologies for Addressing Environmental Challenges"

The protection of water resources is vital in today's environment. A number of environmental issues are presented along with the latest technologies including 1) corrosion control coatings and processes, industrial water recovery, and monitoring solutions; 2) EPA Brownfields properties and remediation technologies; 3) Leaky landfills and groundwater monitoring; and 4) UST removal and remediation, where EPA guidelines' function is to reduce leaking USTs that contaminate water supplies. Risk-based modeling of natural bioattenuation for groundwater contamination along with monitoring is suggested for measuring the extent of contamination. The mathematical underpinning of estimating the rate of natural bioattenuation is discussed.

**Richard Tapia**
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"Optimization: The Cradle of Contemporary Mathematics"

In contrast to other disciplines in mathematics, problems in optimization are usually quite easy to state and to understand—even for those with limited mathematical sophistication. As such, important optimization problems embedded in some controversy have played a major role in motivating and promoting mathematical activity.

Writing circa 200 BC, the Greek mathematician Zenodorus considered the so-called isoperimetric problem: Determine, from all simple closed planar curves of the same perimeter, the one that encloses the greatest area.

In this talk the speaker will argue that the isoperimetric problem has been the most influential mathematics problem of all time. It played a major role in motivating the calculus of variations activity credited to the Bernoullis, Newton, Euler, and Lagrange in the late 1600's and early 1700's. In turn the early calculus of variations led to the golden era of mathematics that we recognize as the 18th and 19th centuries. Yet a complete proof of the isoperimetric problem eluded these early pioneers. Indeed, it was Weierstrass who first gave a complete proof more than a century later. In this talk the speaker will demonstrate that Euler and later Lagrange in the derivation of their , now well-known, Euler-Lagrange equation necessary condition were one direct observation away from deriving a sufficiency condition that would have given a straightforward resolution of the isoperimetric problem. Finally the derivation of the Euler-Lagrange equation presented by Euler and Lagrange is well known to be flawed. A correct derivation was given by du Bois-Raymond some 150 years later. We argue quite surprisingly that the du Bois-Raymond's derivation can be viewed as presenting the Euler-Lagrange equation as a Lagrange multiplier rule. As such, it would be the worlds first Lagrange multiplier rule and would precede the very notion of Lagrange multiplier rules.

**Timothy Thornton**
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"Statistical Methods for Genetic Association Studies in Structured Populations"

Genetic association testing has proven to be a valuable tool for the mapping of complex diseases. Technological advances have made it feasible to perform case-control association studies on a genome-wide basis. Some of the characteristics of the data include missing information, and the need to analyze hundreds of thousands or millions of genetic markers in a single study, which puts a premium on computational speed of the methods. The observations in these studies can have several sources of dependence, including population structure and relatedness among the sampled individuals, where some of this structure may be unknown. We describe a new approach to this problem.

**Ulrica Wilson**
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"A Criterion for Finding Cyclic $k_p$((t))-division Algebra"

What are all of the different types of division algebras? This question is far from being answered, but there is much that can be said. One strategy is to identify all the possible constructions of division algebras over a particular field. For example, thanks to Frobenius, we know that there are exactly two $\mathbb{R}$-division algebras, $\mathbb{R}$ itself, and Hamilton's quaternions. This kind of classification is optimal because we have an explicit list of $\mathbb{R}$-division algebras (up to isomorphism). Classifying division algebras over other fields has proven to be much more difficult. Cyclic division algebras form a particularly nice class of division algebras. In this talk along with describing this special class of division algebras I will give a criterion for determining the cyclicity of division algebras over the Laurent series field $k_p((t))$.