# How cryptic is cryptic diversity? Machine learning approaches to fine scale variation in the morphology of *Emys marmorata*.

Peter D Smits<sup>1</sup>, Kenneth D Angielczyk<sup>2</sup>, James F Parham<sup>3</sup>

<sup>1</sup>Committee on Evolution Biology, University of Chicago, <sup>2</sup>Department of Geology, Field Museum of Natural History, <sup>3</sup>Department of Geological Sciences, California State University – Fullerton

June 22, 2013

## Cryptic diversity

Cryptic species are species which were first delimited via molecular means. Were not/cannot be identified via morphology.

How much of cryptic diversity is just a function of sample size and/or method?

# Emys marmorata



wikimedia

# Morphological hypothesis

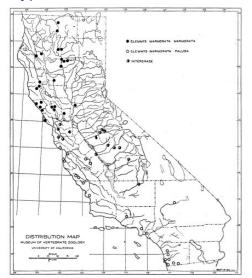
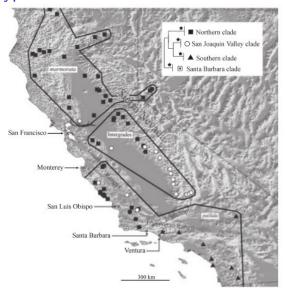


Fig. 4. California localities from which specimens have been examined.

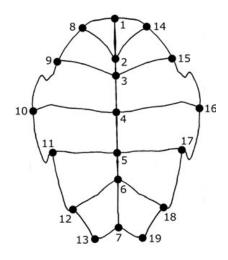
## Molecular hypotheses



Spinks et al. 2010 Molec. Ecol

## Methods: morphometrics

- ▶ 524 adult individuals
- plastral ("belly") shape
- landmarks averaged across bilat axis
- ► total 13 landmarks, 7 on bilat axis, 6 off
- geographic information known/inferred



Angielczyk et al. 2011 Evolution

## Unsupervised learning

Fancy way of saying clustering or density estimation.

Partitioning around mediods (PAM) compared with "gap" statistic.

Analogous to k-means clustering, a divisive clustering algorithm.

Minimize sum of dissimilarities between points and medoids.

"Gap" is analogous to goodness-of-clustering.

## Supervised learning

Fancy way of saying classification (and regression).

Features (principal components) predict class (subspecific assignment).

Multinomial logistic regression and random forests.

## Model training and selection

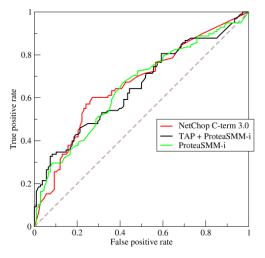
- split into training and testing sets, 75-25.
- tuning parameters via grid-search
- uncertainty via 10-fold CV
- model selection
  - multinomial logistic regression: min AICc
  - ► random forest: max ROC

#### ROC and confusion matrices

		Predicted class	
		1	0
Actual class	1	TRUE	FALSE
		POSITIVE	NEGATIVE
	0	FALSE	TRUE
		POSITIVE	NEGATIVE

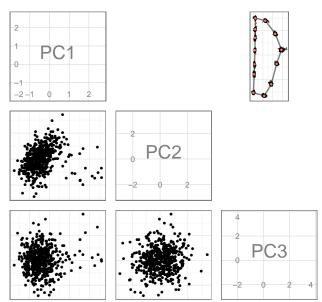
#### **ROC**

- true positive rate or sensitivity: TP TP+FN
- ▶ false positive rate or 1 - specificity: <sup>FP</sup>/<sub>FP+TN</sub>
- multiclass, all-against one (Hand and Till 2001 Machine Learning)

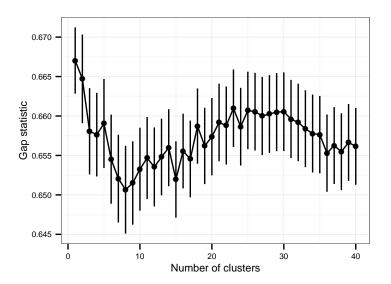


wikimedia

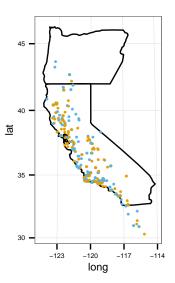
# Results: mophometrics



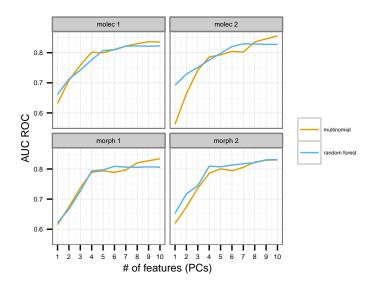
## Results: gap clustering



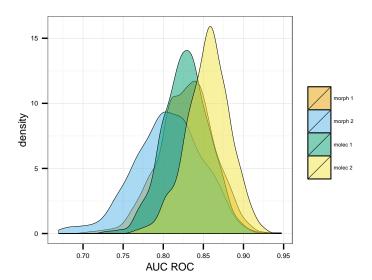
#### Second best cluster



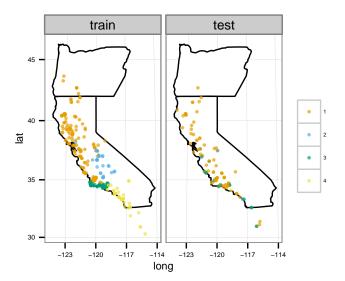
#### Model selection via ROC



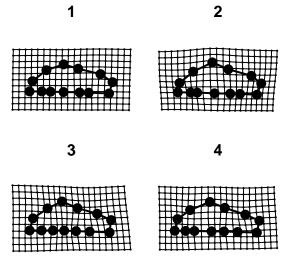
# Generalize using best random forest model



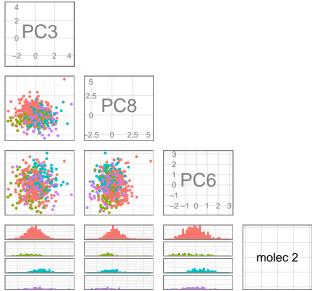
#### Best classification scheme via RF model results



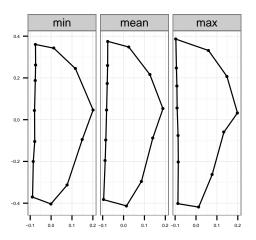
# Mean shape of classes



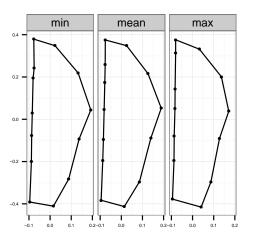
# Variable importance of random forest model



# Shape across PC3



# Shape across PC8



#### **Future**

- illustration of morphological validation of previously cryptic variation
  - the concordance is remarkable
  - large sample sizes can be difficult
- utility of large data, machine learning methods
- unsupervised methods for when no explicit hypothesis nonparametric Bayes
- cause of interclass variation local adaptation? pure isolation?

## Acknowledgements

- Ben Frable, Dallas Krentzel, Michael Foote, David Bapst
- collections at CAS, FMNH, LACM, LSUMNS, MSE, MVZ, NMNH, SBMNH, SDMNH, UCMP, UMZC
- ► NSF DBI-0306158 to KDA

