



Coot

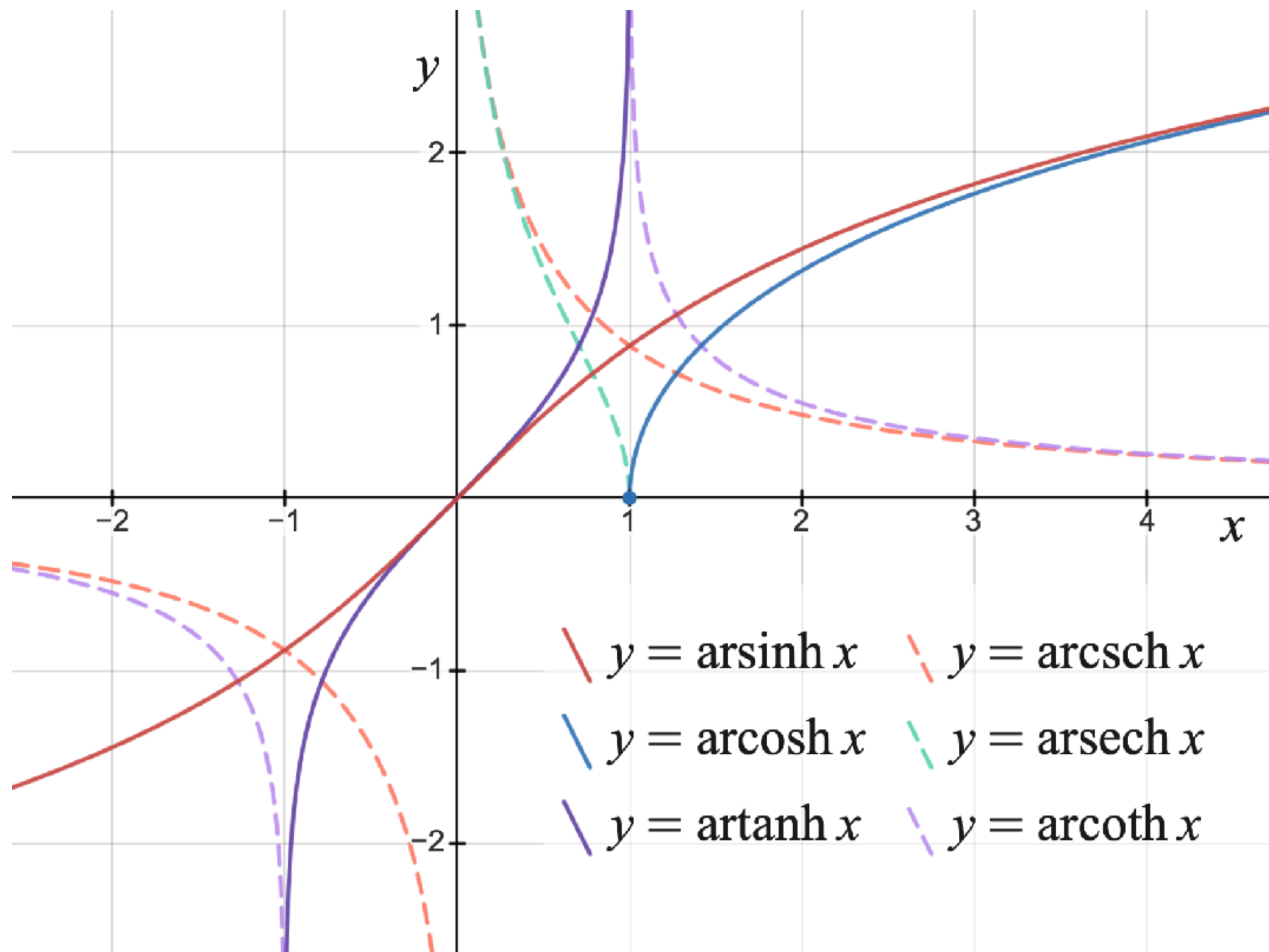
RamaRota: June 2026

- In what way, if any, is the Ramachandran Plot dependent on χ_1 (and χ_2)?
- In what way, if any, is τ dependent on χ_1 (and χ_2)?
- Are we making tools for model-building (what Coot does) or validation?

RamaRota Validation

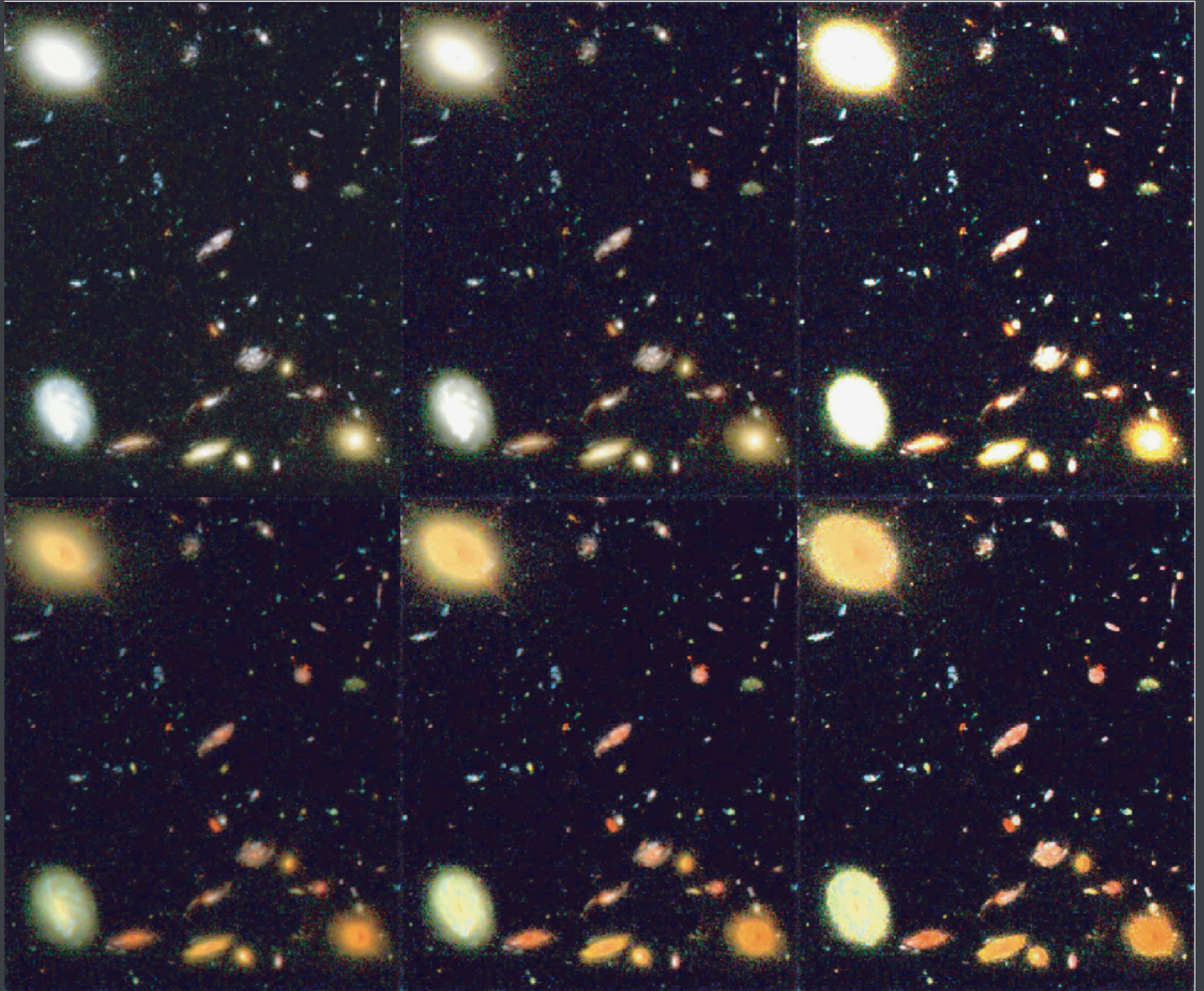
- So, we want to make a tool that reads a protein model, examines ϕ , ψ , τ , χ_1 , χ_2 residue by residue...
- and says “that’s improbable”

Lupton Stretch



$$\operatorname{arsinh} x = \ln\left(x + \sqrt{x^2 + 1}\right) \quad -\infty < x < \infty,$$

Lupton Stretch



Preparing Red-Green-Blue Images from CCD Data

Robert Lupton, Michael R. Blanton, George Fekete, David W. Hogg, Wil O'Mullane, Alex Szalay, and Nicholas Wherry

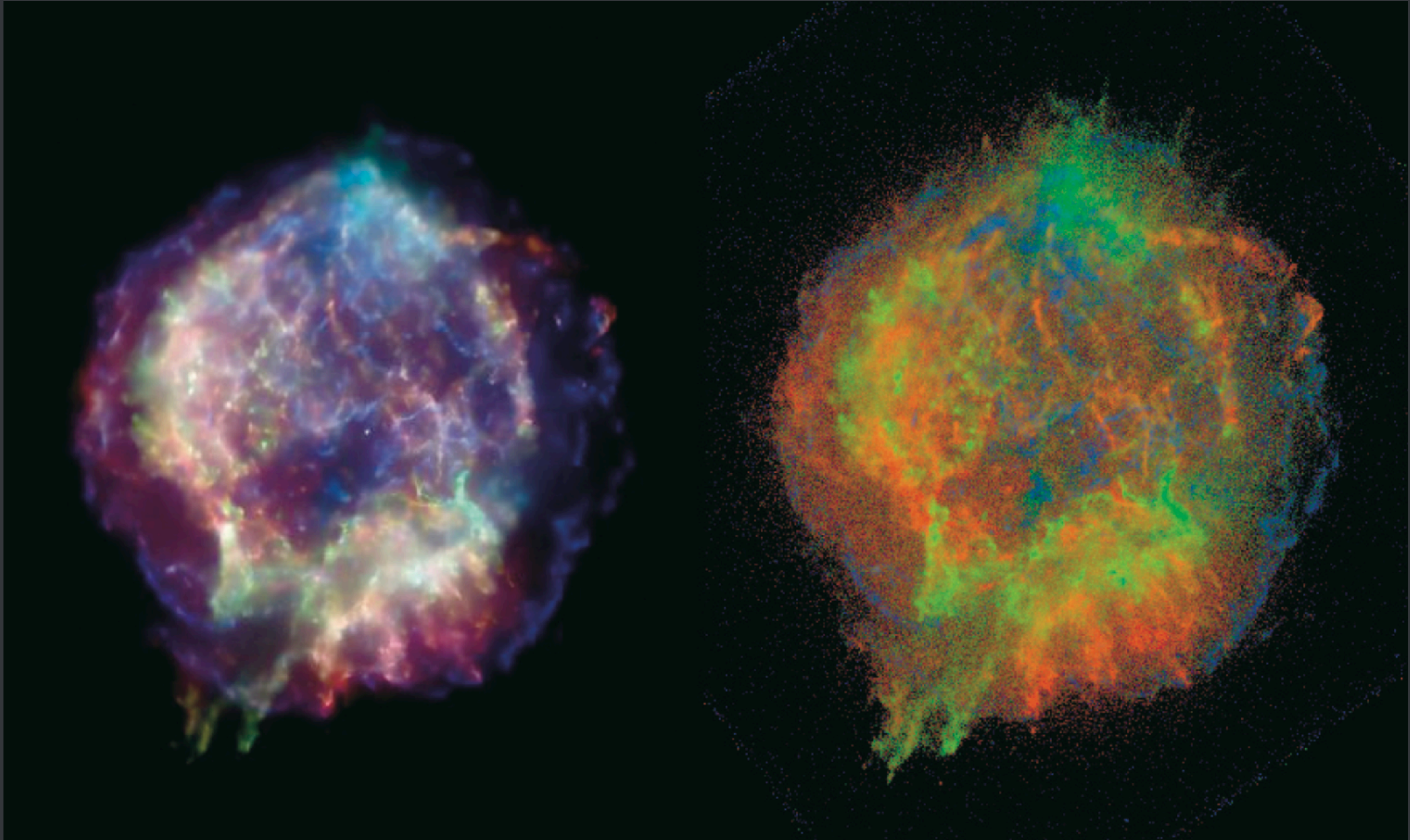
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[Publications of the Astronomical Society of the Pacific, Volume 116, Number 816](#)

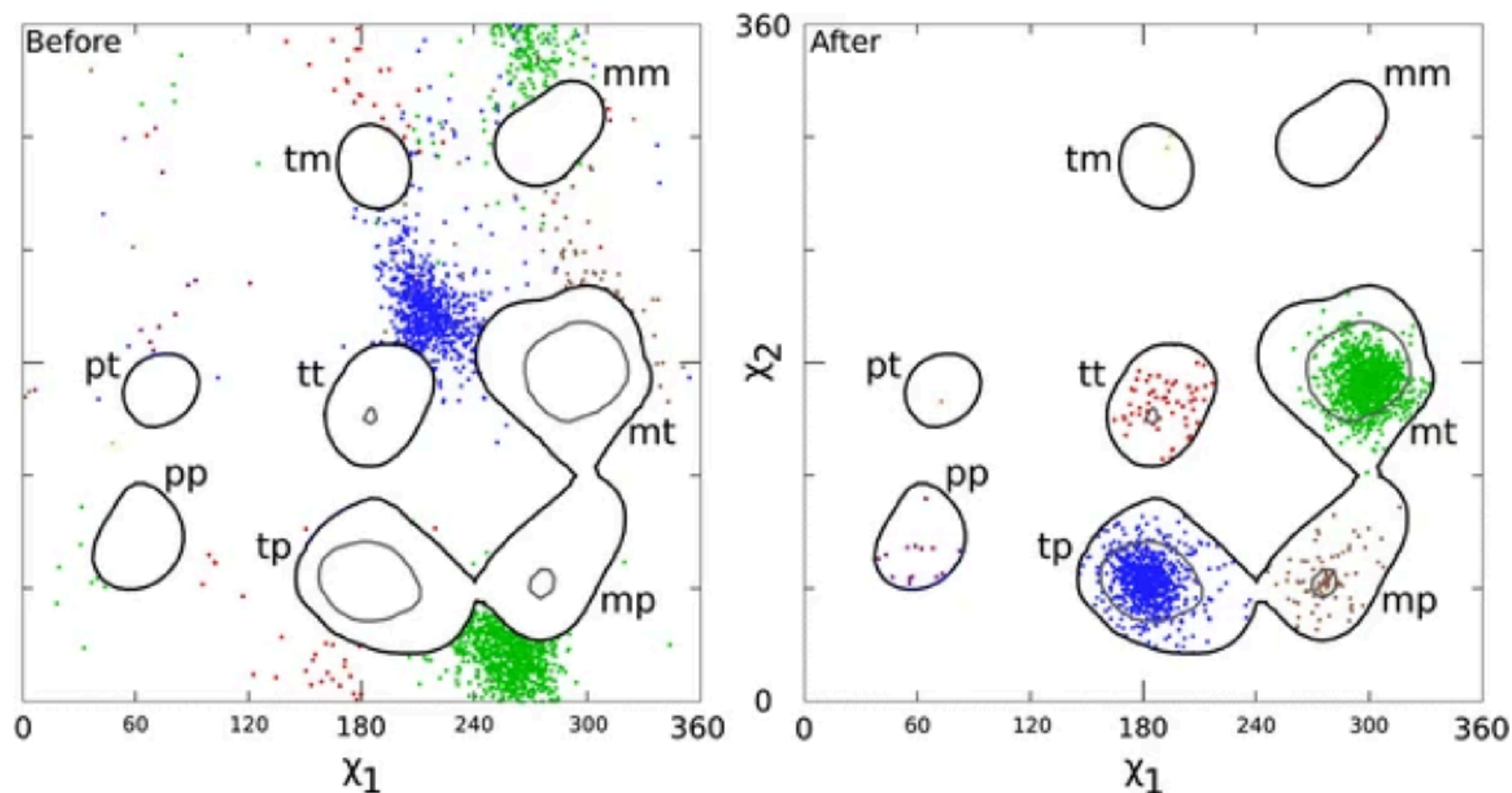
Citation Robert Lupton et al 2004 *PASP* 116 133

DOI 10.1086/382245

Lupton Stretch



“Autofix for backwards fit side chains...”



Before and after χ_1 – χ_2 plots of the 2,037 accepted Leu corrections, for those identified as rotamer outliers (<1%) in our 945-file dataset and successfully corrected by Autofix. Contours are taken from the Top500 Leu

Bayesian Statistical Studies of the Ramachandran Distribution*

Alexander Pertsemlidis, Jan Zelinka, John W. Fondon III, R. Keith
Henderson, and Zbyszek Otwinowski

The IDDT of the pIDDT:

JOURNAL ARTICLE

IDDT: a local superposition-free score for comparing protein structures and models using distance difference tests

Valerio Mariani, Marco Biasini, Alessandro Barbato, Torsten Schwede

[Author Notes](#)

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Maximum Mean Discrepancy

A Kernel Two-Sample Test

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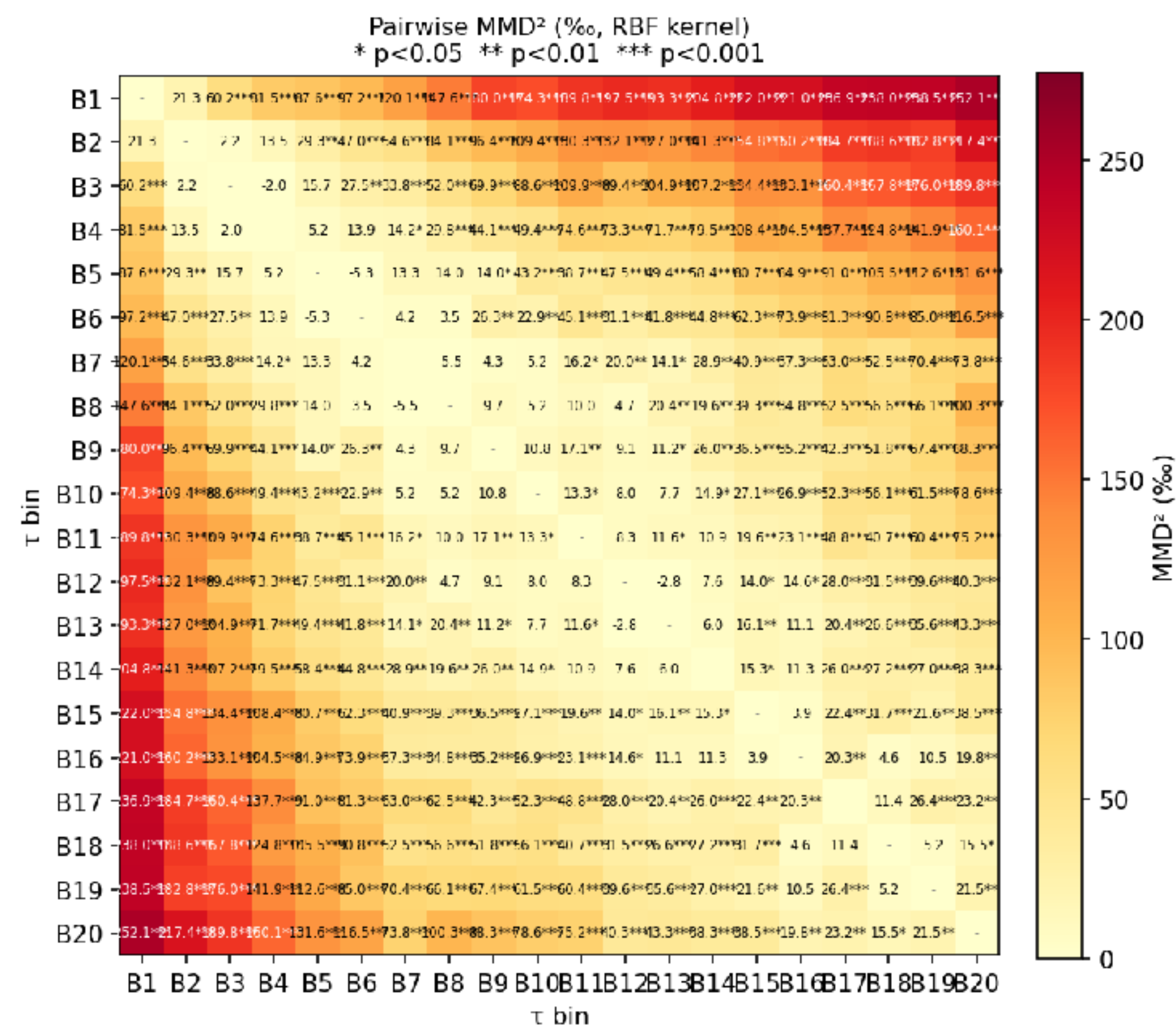
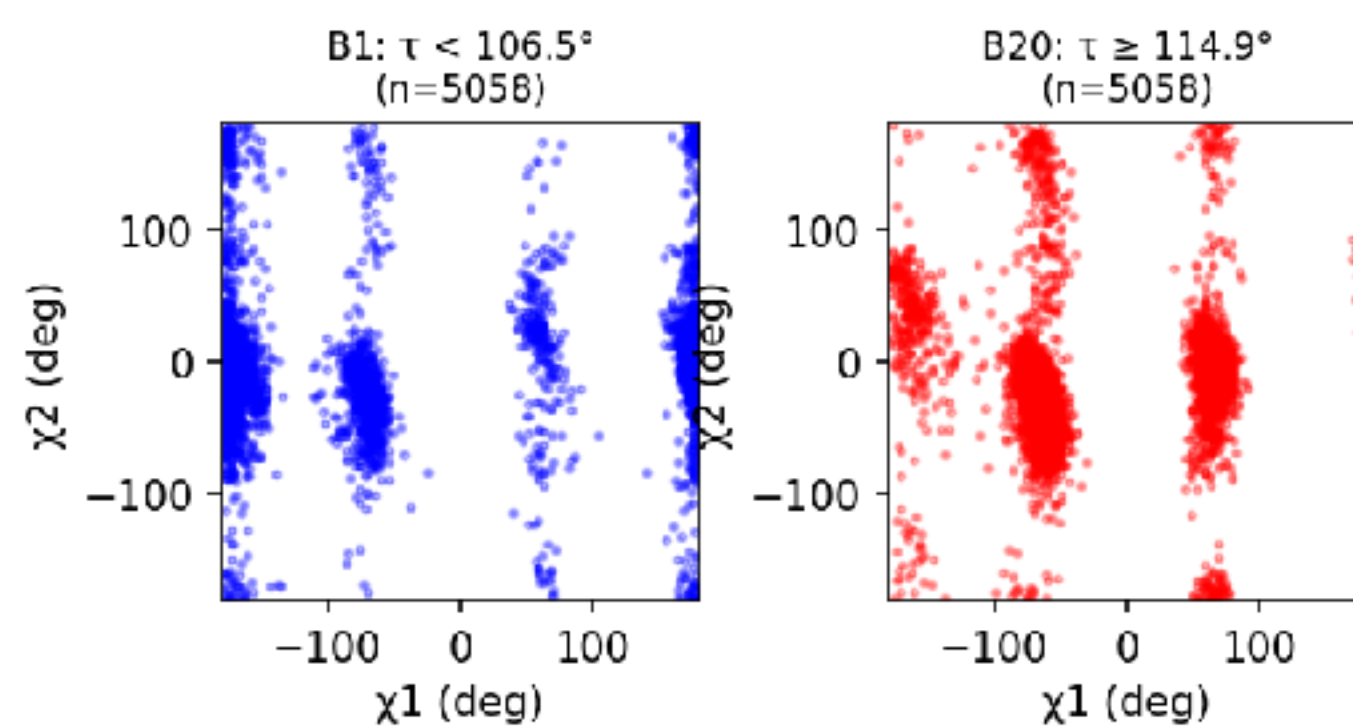
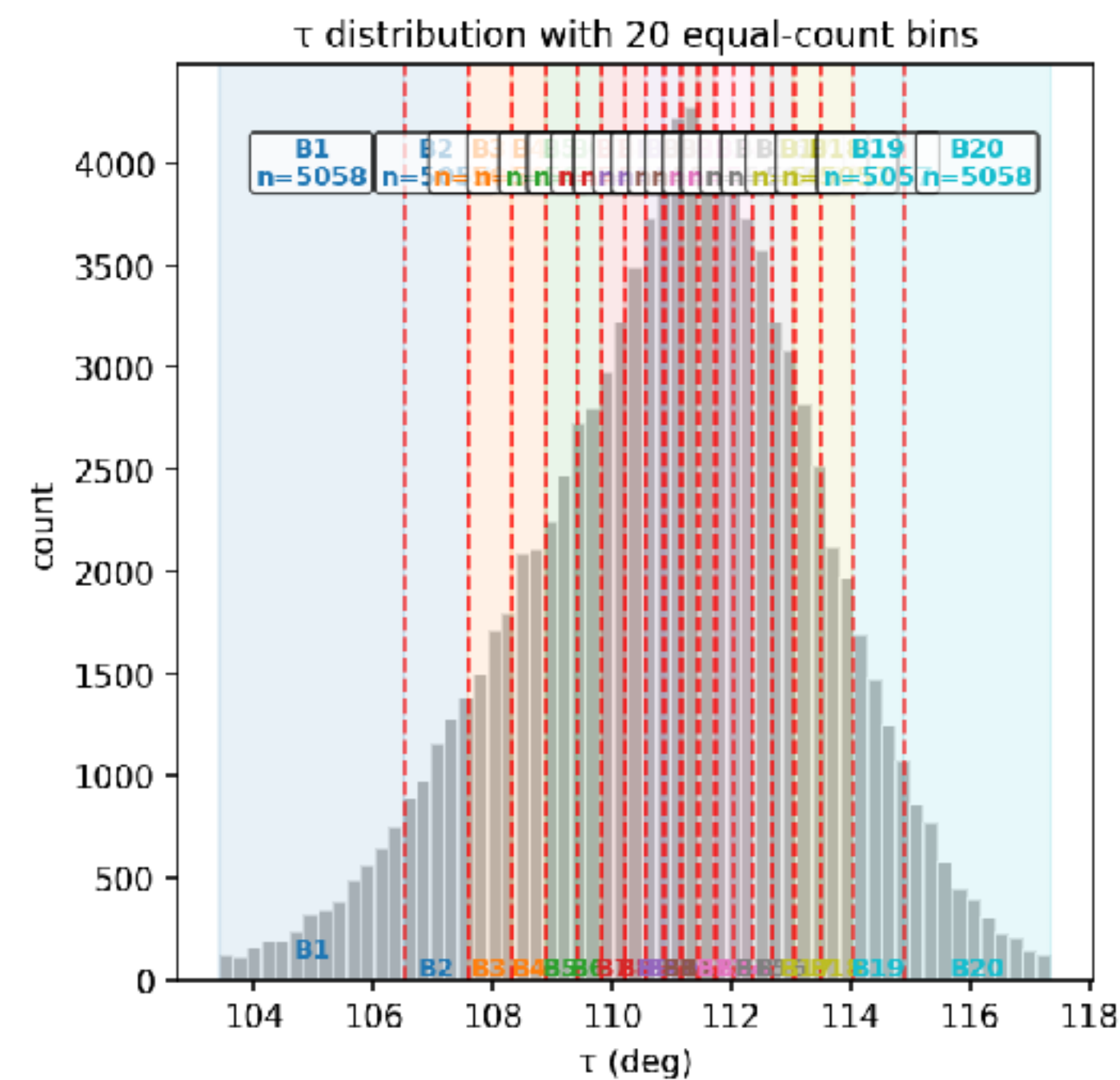
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Editor: Nicolas Vayatis

Abstract

We propose a framework for analyzing and comparing distributions, which we use to construct statistical tests to determine if two samples are drawn from different distributions. Our test statistic is the largest difference in expectations over functions in the unit ball of a reproducing kernel Hilbert space (RKHS), and is called the *maximum mean discrepancy* (MMD). We present two distribution-free tests based on large deviation bounds for the MMD, and a third test based on the asymptotic distribution of this statistic. The MMD can be computed in quadratic time, although efficient linear time approximations are available. Our statistic is an instance of an integral probability metric, and various classical metrics on distributions are obtained when alternative function classes are used in place of an RKHS. We apply our two-sample tests to a variety of problems, including attribute matching for databases using the Hungarian marriage method, where they perform strongly. Excellent performance is also obtained when comparing distributions over graphs, for which these are the first such tests.

ASP: Does the (χ_1 , χ_2) distribution depend on τ ?



ASN: Does the (χ_1 , χ_2) distribution depend on τ ?

