Correlations are important!

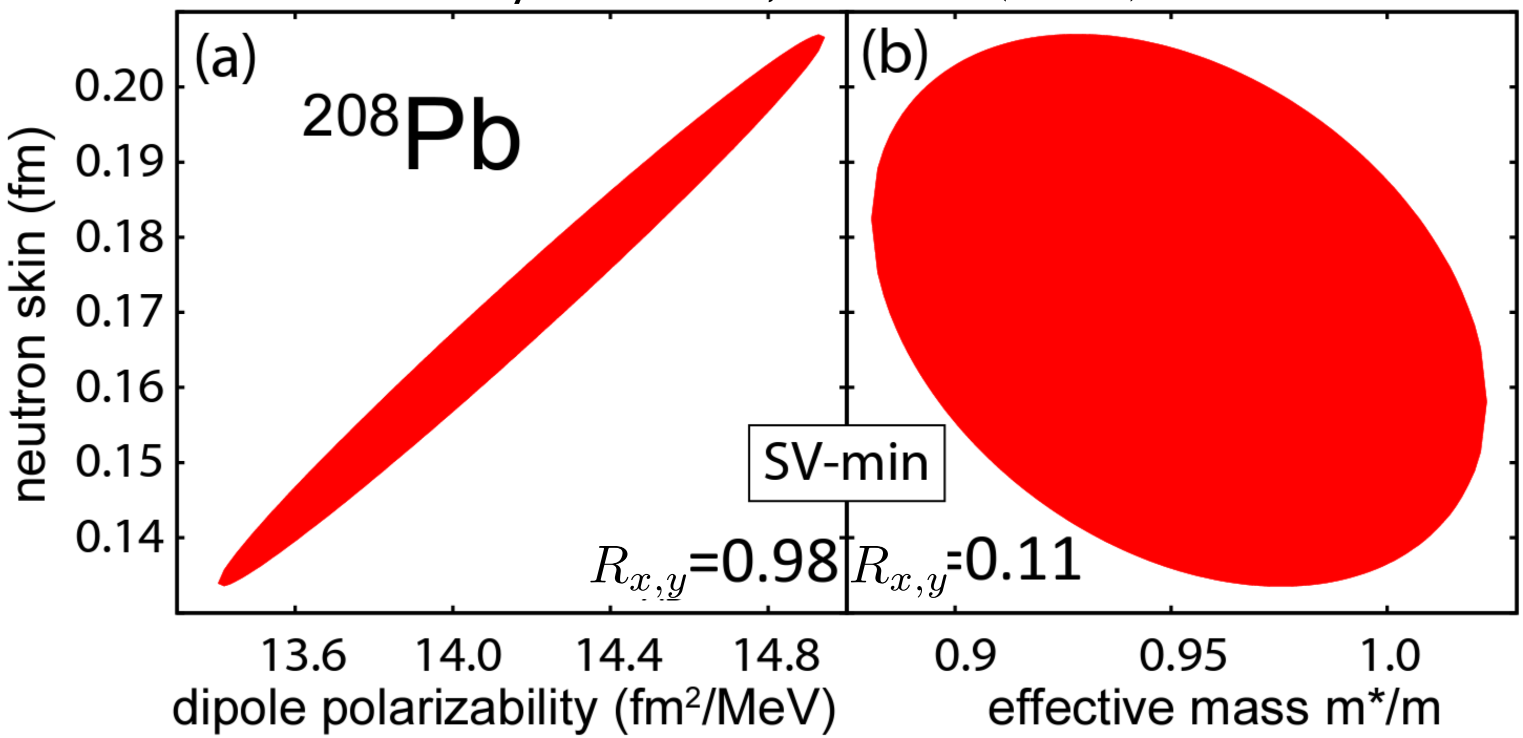
$$R_{x,y} = \frac{\text{cov}(x,y)}{\sigma_x \sigma_y}$$

bivariate correlation coefficient

$$\text{CoD}(x,y) = R^2_{x,y}$$

coefficient of determination

Phys.Rev.C81, 051303 (2010)



Consider observable $z = x - y$

Variance of difference: $\sigma_z^2 = \sigma_x^2 + \sigma_y^2 - 2R_{x,y}\sigma_x\sigma_y$

$R_{x,y} \approx 1$ ➡ $\sigma_z \approx |\sigma_x - \sigma_y|$ reduced

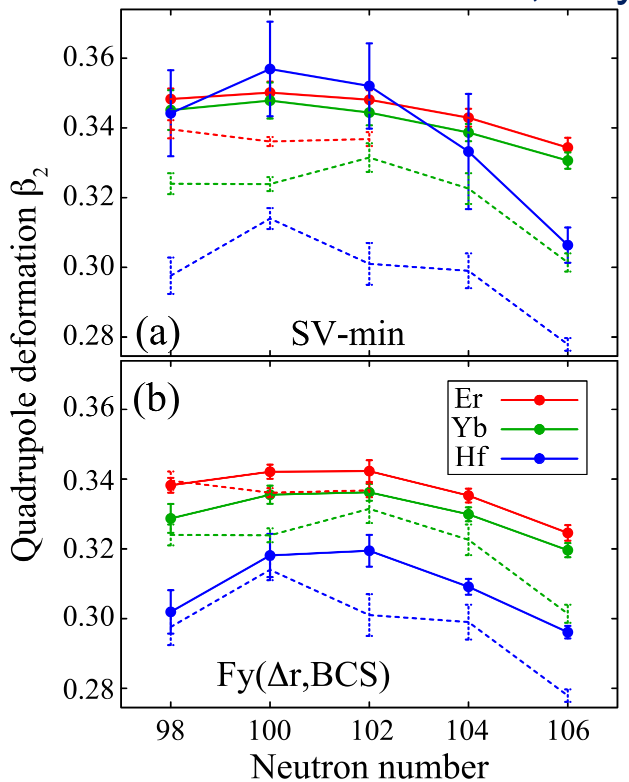
$R_{x,y} \approx 0$ ➡ $\sigma_z \approx \sqrt{\sigma_x^2 + \sigma_y^2}$ large

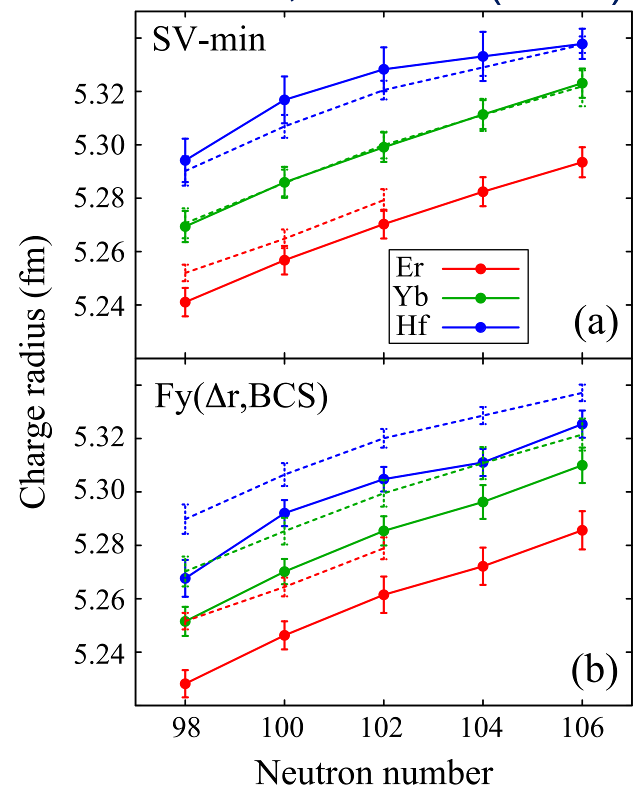
Are variances of differences of smoothly varying observables small? One needs to know the value of $R_{x,y}$!

Statistical correlations of nuclear quadrupole deformations and charge radii

P.-G. Reinhard & WN, Phys. Rev. C 106, 014303 (2022)

nuclear shapes





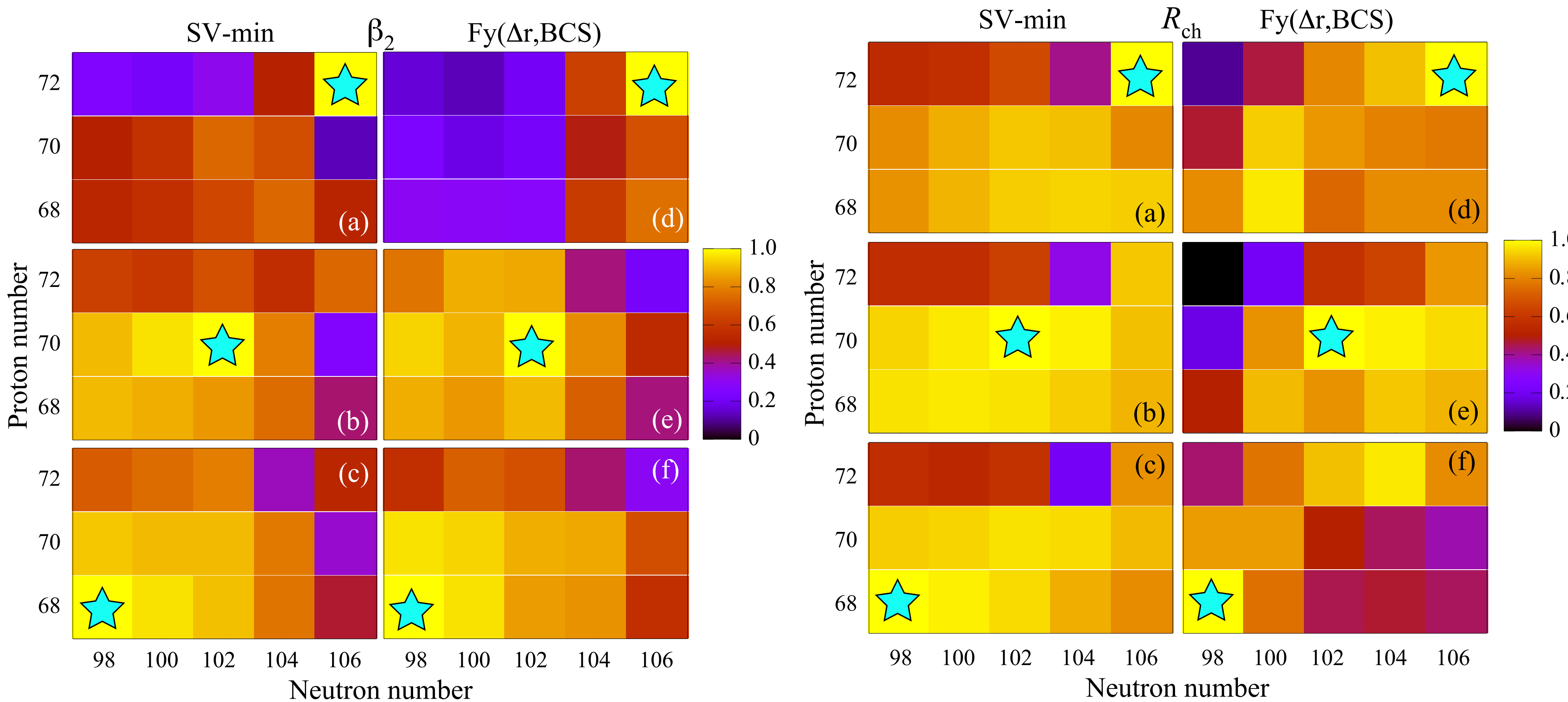
nuclear sizes

Quadrupole deformations and charge radii vary smoothly! But what about correlations?

Until you calculate you do not know!

- The smooth
  enough that differences have small errors.
- Because the points did not jump around, the *errors must be correlated*.

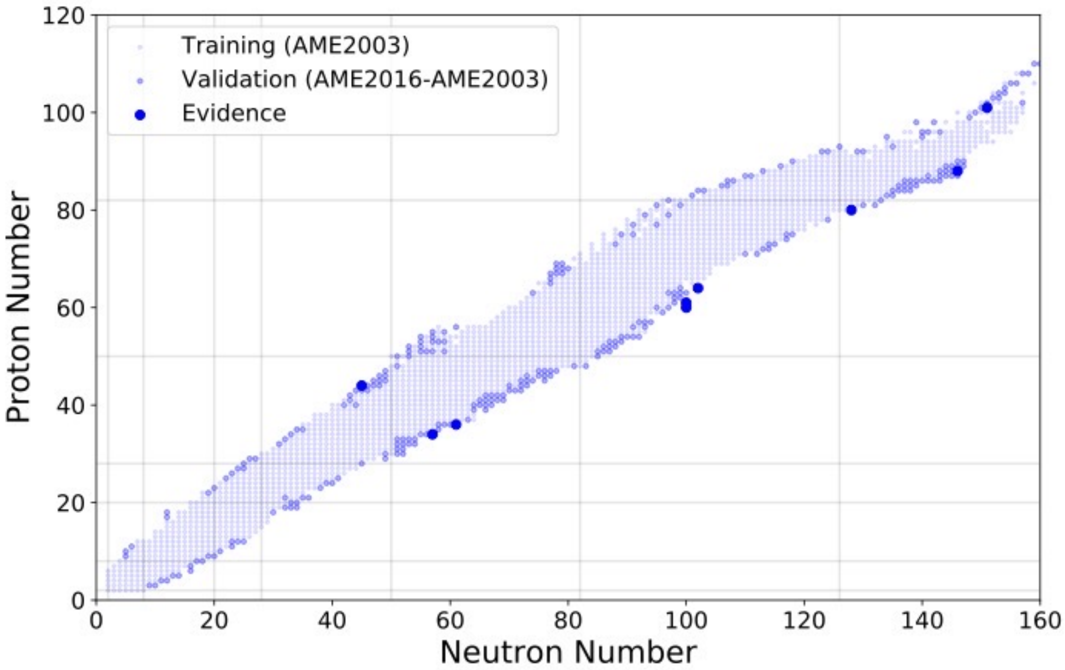
?



- The calculated CoD diagrams show patterns that are fairly localized as compared to the smooth trends of observables.
- The local variations of CoDs reflect the underlying deformed shell structure and changes of single-particle configurations.
- The errors on radii differences are actually important to know!

We (R. Jain, L. Neufcourt, S.A. Giuliani, and WN) are currently finalizing the BMA mass table based on predictions of several global DFT mass models. The results will be stored at

BMEX



The results of our analysis (masses and covariances) will allow user to extract mass differences (Q-values) and reliable uncertainties for them

Bayesian Model Mixing (BMM) for masses

V. Kejzlar, L. Neufcourt, and WN

See M. Pratola's Tawaret presentation for definitions

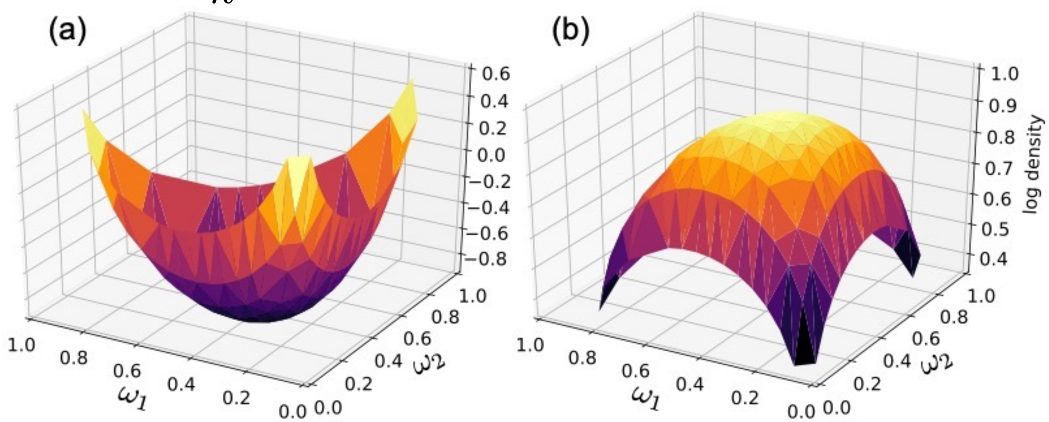
Global linear model: $$y^*(x) = \sum_{k=1}^{p} \omega_k^* f_k(x) \qquad \omega_k^* \geq 0, \quad \sum_k \omega_k^* = 1$$

Dirichlet model. The weights are given hierarchically by a Dirichlet distribution:

$$p(\boldsymbol{\omega}|\boldsymbol{\alpha}) \propto \prod_k \omega_k^{\alpha_k - 1}$$

$$\omega_1, \ldots, \omega_p \geq 0 : \sum_k \omega_k = 1 \qquad \langle \omega_k \rangle = \alpha_k / \sum_k \alpha_k$$

α= (0.3,0.3,0.3)



α= (1.3,1.3,1.3)

α < 1 leads to model selection while α > 1 encourages true mixing

Local BMM models, weights vary in the domain *x*

$$y^*(x) = \sum_{k=1}^{p} \omega_k^*(x) f_k(x).$$

We assume that at every location *x* the model weights follow jointly a Dirichlet distribution:

$$\omega_1(x), \ldots, \omega_p(x) | x \sim Dir(\alpha_i(x), \ldots, \alpha_p(x))$$

The test case: two-neutron separation energies

model	train	test	calibrated σ
/w δ_f			
SkM*	1.19	1.14	1.19(4)
SkP	0.84	0.74	0.83(3)
SLy4	0.99	0.81	0.99(3)
SV-min	0.77	0.63	0.77(2)
UNEDF0	0.77	0.63	0.77(2)
UNEDF1	0.75	0.50	0.75(2)
UNEDF2	0.85	0.67	0.84(3)
FRDM-2012	0.48	0.45	0.47(1)
HFB-24	0.42	0.40	0.42(1)
rms rms	0.81	0.70	
BMA (Full train)	0.42	0.40	0.42(1)
BMA (S + MC)	0.36	0.36	0.49(14)
BMA (S + Laplace)	0.36	0.35	0.52(16)
BMA (S + Exact)	0.37	0.37	0.47(13)
Dirichlet + GPM	0.25	0.33	0.26(1)

different evidences calculations

BMM based on Dirichlet

A useful online tool for mass predictions!