Improving Mass Predictions Throughout the Nuclear Chart

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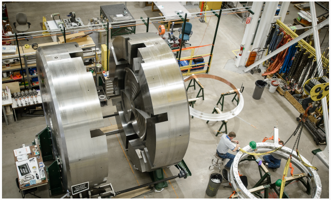
Tanthco seminar

San Diego State University

Uncertainty Quantification in nuclear physics

- Theory - Experiment feedback loop
  - FRIB, RIKEN, CERN, ...
- Nuclear applications
  - Description of astrophysical phenomena
  - Safety in nuclear reactors
- Estimate model errors
  - Meaningful comparisons
  - Extrapolate beyond the experiment
  - Required for publishing in PRA

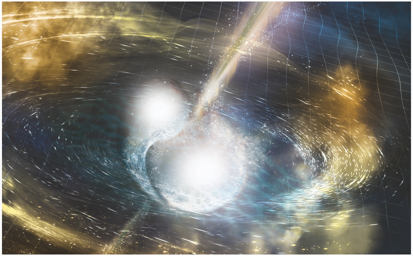
[http://www.nasa.gov/wise/pia18848]



[MSU Today. Photo by G.L. Kohuth]

r-process, still an open challenge

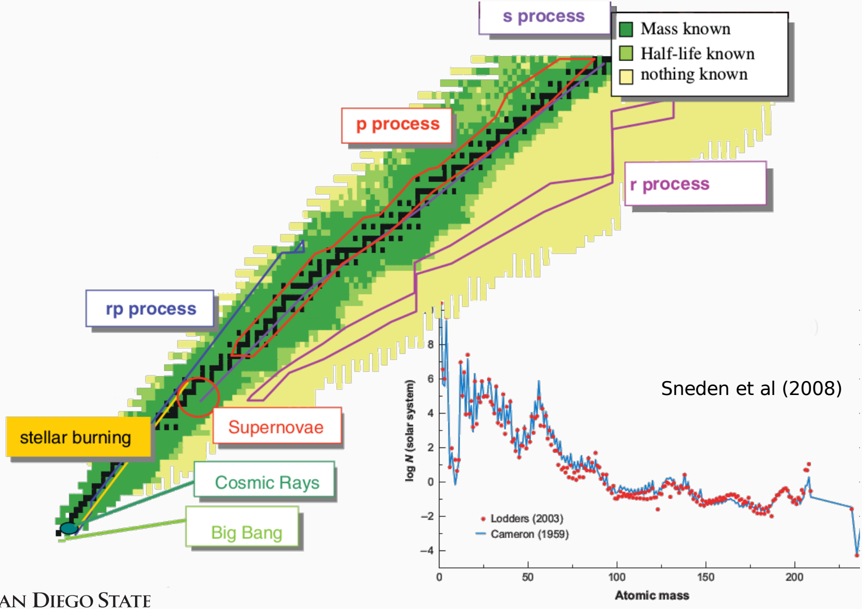
- GW170817/GRB170817a/SSS17a
- Multi-messenger observation of a neutron star merger
- 3674 researchers, 953 institutions, 1 paper
- confirmation of the r-process



[https://www.ligo.caltech.edu]

  - Responsible for half of the heavy elements
  - Several inputs
    - Masses of neutron-rich nuclei
    - β-decay rates
    - Astrophysical environment
  - Uncertainties from astrophysical and nuclear models

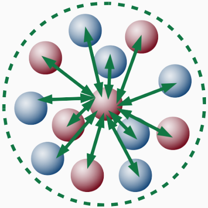
Many body calculations for astrophysical processes



Sneden et al (2008)

The nuclear many body problem

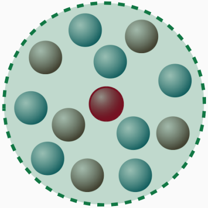
Ab-initio



$$(T + \sum_{ij}^{A} V_{ij})\Psi = E\Psi$$

- Every pair of nucleons is accounted for
- “Realistic”

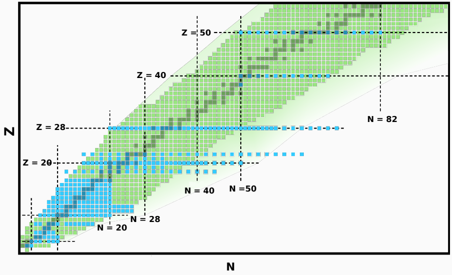
Mean field



$$(T + \sum_{i}^{A} \tilde{V}_i)\Psi = E\Psi$$

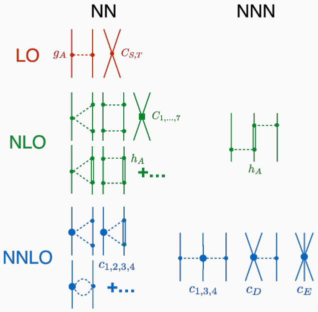
- An average interaction is used
- “Phenomenological”

Ab-initio methods with χ-EFT

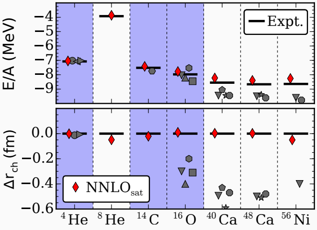


[Hergert et al. Phys. Rept. 621 (2016) 165]

- Systematic, order by order
- Light and medium nuclei ✓
- Heavy nuclei out of reach
  - A problem of scaling



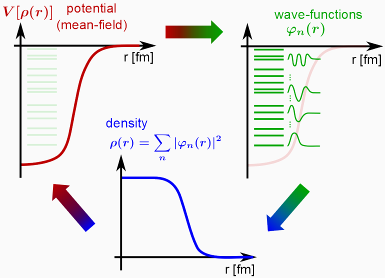
[Ekström et al. arXi:1707.09028]



[Hagen et al. Phys. Scr. 91 (2016) 063006]

Phenomenological DFT (A type of mean field)

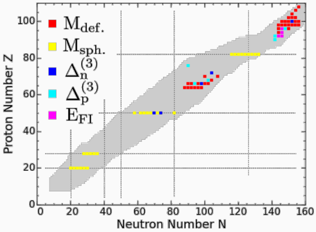
- DFT is based on Hartree-Fock-Bogoliubov theory
  - Non-linear eigenvalue problem
  - Iterative solution
  - Phenomenological interactions
- Good computational scaling
- Static and dynamic properties of nuclei
- No systematic improvement



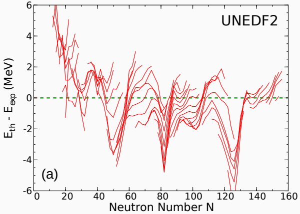
Self-consistent mean-field theory

State of the art in DFT: UNEDF family of functionals

- 12 to 14 parameters adjusted to selected nuclear properties
- UNEDF0
  - First optimization
  - Spherical and deformed nuclei
- UNEDF1
  - Focus on large deformations
  - Improved description of fission barriers
- UNEDF2
  - 2 Additional parameters
  - More experimental data
  - The limit for Mean field?



[Schunck et al. EPJA51 (2015) 169]



[Kortelainen et al. PRC89 (2014) 054314]

The best of both worlds

Mean Field Component

- Contact terms for short range physics
- Adjusted to nuclear properties
- Encodes many body correlations

$+$

Microscopic Component

- Derived from χ-EFT
- Long range physics, pions
- Adjusted to NN scattering
  - Fixed at the DFT level!
- Order by order
- Non-Local density!

A scalable framework with systematic improvements

Microscopically constrained EDF

- Non-local densities for finite range potentials

$$E_H^{NN} \sim \int dRdr \langle r|V^{NN}|r\rangle \rho_1\left(R+\frac{r}{2}\right)\rho_2\left(R-\frac{r}{2}\right)$$

$$E_F^{NN} \sim \int dRdr \langle r|V^{NN}|r\rangle \rho_1\left(R-\frac{r}{2}, R+\frac{r}{2}\right)\rho_2\left(R+\frac{r}{2}, R-\frac{r}{2}\right)\hat{P}_{12}$$

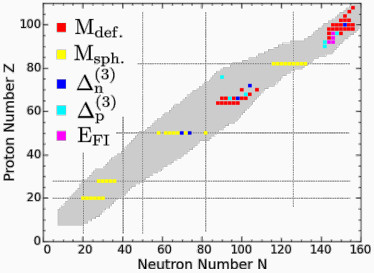
- Density Matrix Expansion (DME)

$$\rho\left(R+\frac{r}{2}, R-\frac{r}{2}\right) \approx \Pi_0^\rho(k_F r)\rho(R) + \frac{r^2}{6}\Pi_2^\rho(k_F r)\left[\frac{1}{4}\Delta\rho(R) - \tau(R) + \frac{3}{5}k_F^2\rho(R)\right]$$

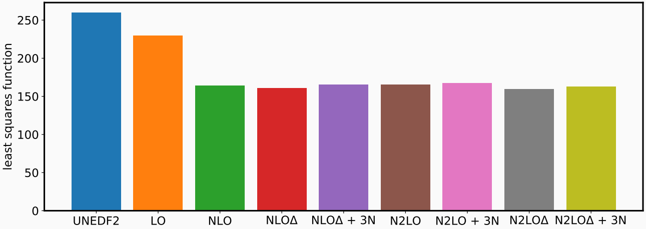
Like a Taylor expansion for the non-local density

Optimizing DFT component

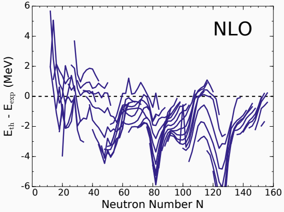
- UNEDF2 optimization protocol
- 130 data, 14 parameters
- Masses, radii, fission isomers, spin-orbit splittings, nuclear matter

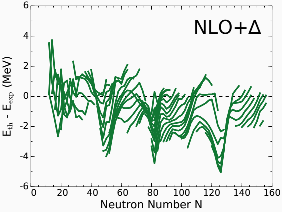


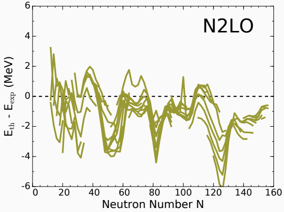
[Schunck et al. EPJA51 (2015) 169]

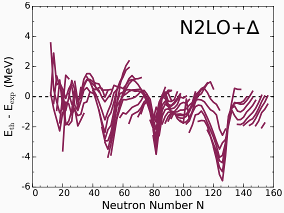


Mass Tables







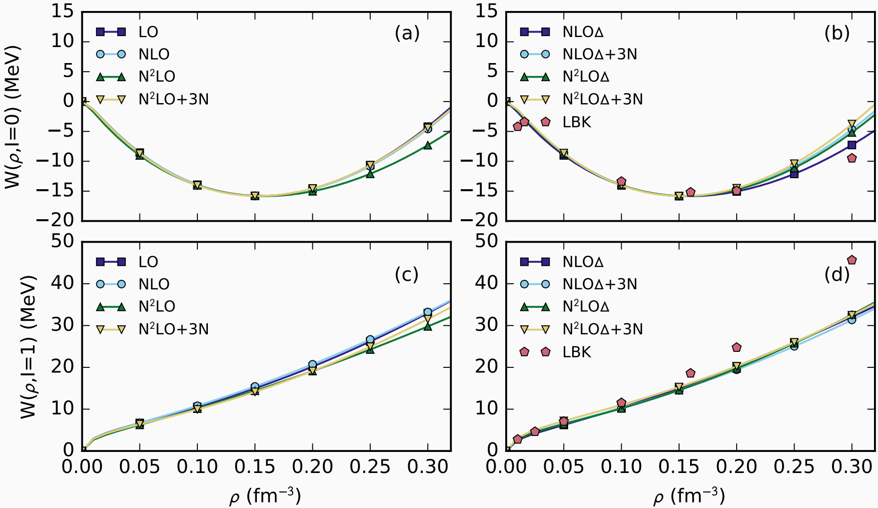


Order by order improvement

EDF	r.m.s. deviation
UNEDF2	1.98
LO	1.99
NLOΔ	1.41
N2LOΔ	1.26

[RNP, Schunck, Dyhdalo, Furnstahl, Bogner. PRC97 (2018) 05430]

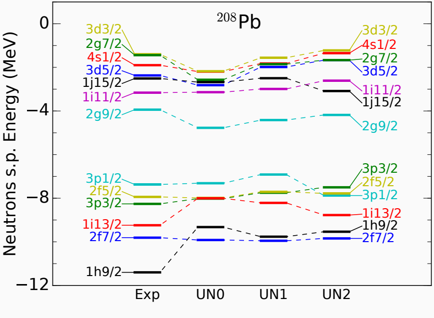
Nuclear Matter and Neutron Matter

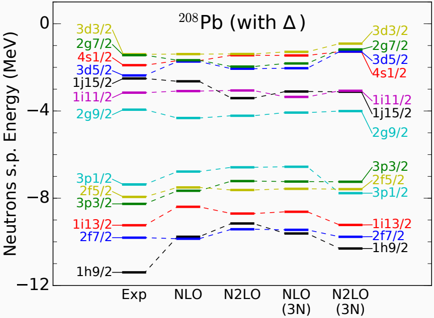


[RNP, Schunck, Dyhdalo, Furnstahl, Bogner. PRC97 (2018) 05430]

Single-Particle Spectra

Quantitatively comparable to UNEDF results



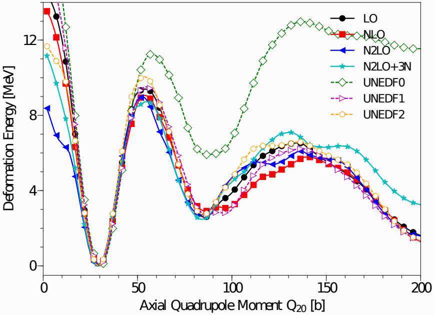


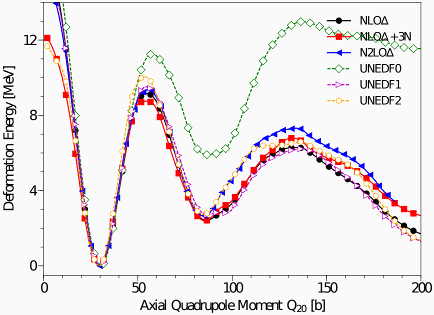
[RNP, Schunck, Dyhdalo, Furnstahl, Bogner. PRC97 (2018) 05430]

- Single-particle energies from blocking calculations
- Exactly the same conditions for all EDFs

Deformation Properties

Quality of fission barriers is comparable to other EDFs





[RNP, Schunck, Dyhdalo, Furnstahl, Bogner. PRC97 (2018) 05430]

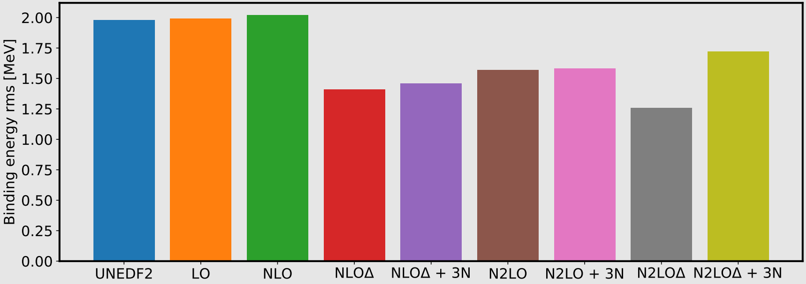
- Inclusion of fission isomers in fitting protocols constrains fission barriers
- Variations up to 2 MeV in height of fission barriers

Not everything is great …

Not everything is great ...

Δ's improve performance, 3N terms don't

rms for Binding energies



Similar pattern for proton radii

3N issue

Possible explanations:

- Implementation of the 3N terms
  - Derivation of density dependent couplings ✓
  - Calculation of density dependent couplings ✓?
  - Implementation in numerical code ✓
  - Optimization protocol ?

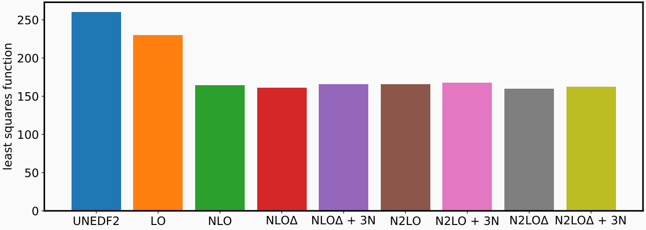
3N issue

Possible explanations:

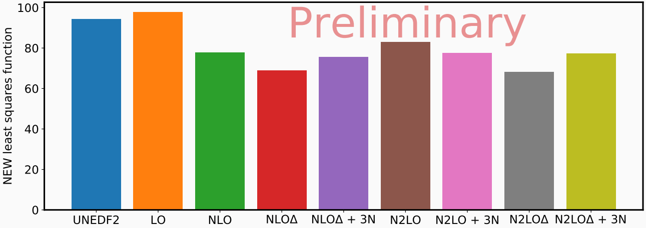
- Optimization protocol
  - Automated diagnostic tools from Argonne National Lab
    - Test that all observables are physically reasonable
    - Actinides are deformed, ^{208}Pb is doubly magic, ...
  - Some level of noise has been present in all optimizations
    - Including UNEDF
  - New objective function has been defined
    - Different weights for some binding energies.
  - Recalibration is necessary
    - Currently being done

New optimization protocol

Original optimization (least sqaures function)



Recalibrated functionals (least sqaures function)



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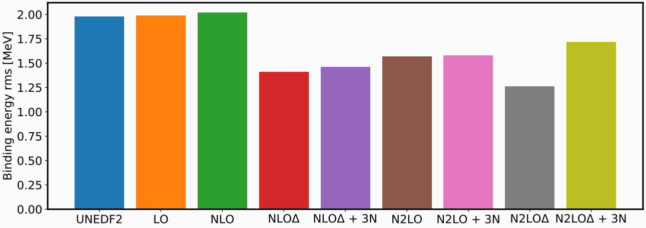
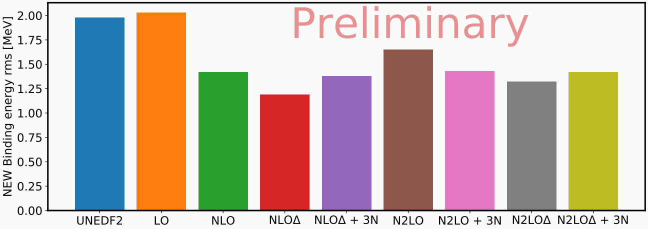
New optimization protocol

Original optimization (rms for all masses)



Recalibrated functionals (rms for all masses)



3N issue

Future possible explanations:

- Calculation of density dependent couplings.
- Issues in the calculation of mass tables.
    - Similar checks for physical solutions
- More terms in the DME?
- Is this specific flavor or DME appropriate for 3N terms?

Improving masses with Machine Learning

Collaborators

- Garret Gallear
    - M.S. Student, graduated in spring 2019
- Zach Barvian
    - Current M.S. Student.

Several new applications of ML to Nuclear Physics

Nuclear charge radii: density functional theory meets Bayesian neural networks

PHYSICAL REVIEW C **96**, 044308 (2017)

Refining mass formulas for astrophysical applications: A Bayesian neural network approach

PHYSICAL REVIEW C **97**, 014306 (2018)

Validating neural-network refinements of nuclear mass models

PHYSICAL REVIEW C **98**, 034318 (2018)

Editors' Suggestion

Bayesian approach to model-based extrapolation of nuclear observables

PHYSICAL REVIEW C **101**, 051301(R) (2020)

Rapid Communications

Predicting nuclear masses with the kernel ridge regression

PHYSICAL REVIEW LETTERS **122**, 062502 (2019)

Neutron Drip Line in the Ca Region from Bayesian Model Averaging

PHYSICAL REVIEW C **101**, 014304 (2020)

Predictions of nuclear charge radii and physical interpretations based on the naive Bayesian probability classifier

Machine learning-based inversion of nuclear responses

- An abundance of data collected over several decades
- The ultimate goal is to make reliable predictions

Machine Learning algorithms

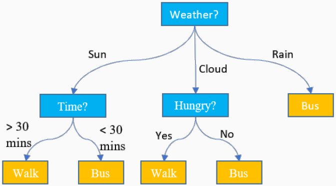
Typical process:

- Collect data
- Select target(s) (what you want to predict)
- Select features (independent variables)
- Split data in training and testing
- Train the algorithm (minimize a loss function)
- Benchmark against testing data (avoid over-fitting)
- Make new predictions

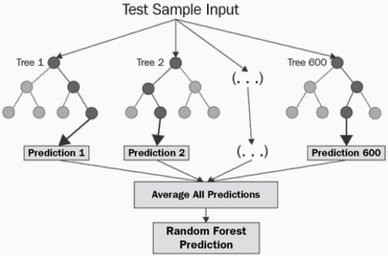
It's a fancy interpolator

Decision Trees

- A non-parametric approach
- A series of boolean questions to reach a prediction
- Features can be numerical or categorical
- More branches $\rightarrow$ better description of training data
- Very easy to over-fit



Random Forests: Avoiding Over-fitting

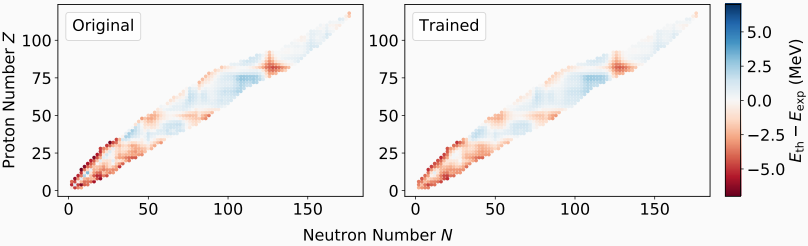


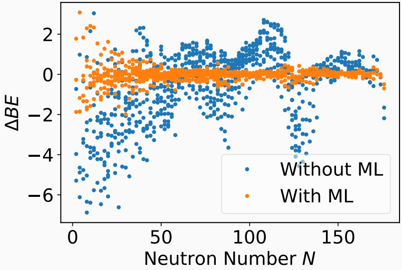
- Randomly select a subset from the training data
- Create a decision tree
- Repeat hundreds of times
- Each tree will ask slightly different questions
- Prediction will be the average of all predictions

Random Forests for Nuclear Model Discrepancy

- Collect data: Atomic Mass Evaluation 2016 and UNEDF0
- Select Target: $\Delta BE(Z,N) = BE_{\mathrm{theo}}(Z,N) - BE_{\mathrm{exp}}(Z,N)$
- Select Features: Number of protons Z and number of neutrons N
- Split data: 75% trainnig, 25% testing
- Train the random forest: Training score 0.972(3)
- Benchmark against testing data: Testing score 0.79(5)
- Improved Binding energy: $BE_{\mathrm{ML}}(Z,N) = BE_{\mathrm{theory}}(Z,N) - \Delta BE_{\mathrm{ML}}(Z,N)$

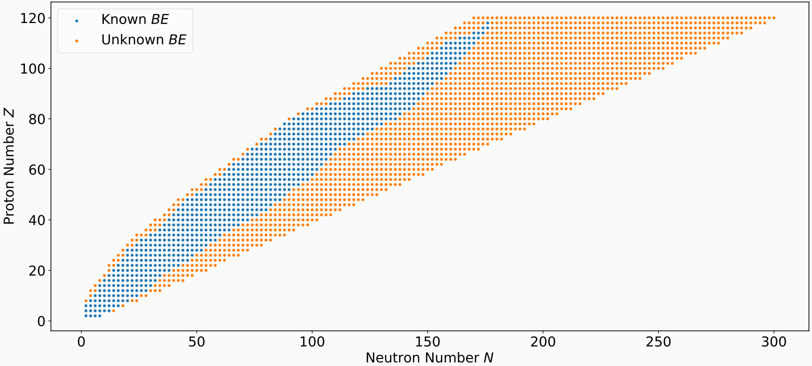
Random Forests for Nuclear Model Discrepancy





What about the neutron rich nuclei?

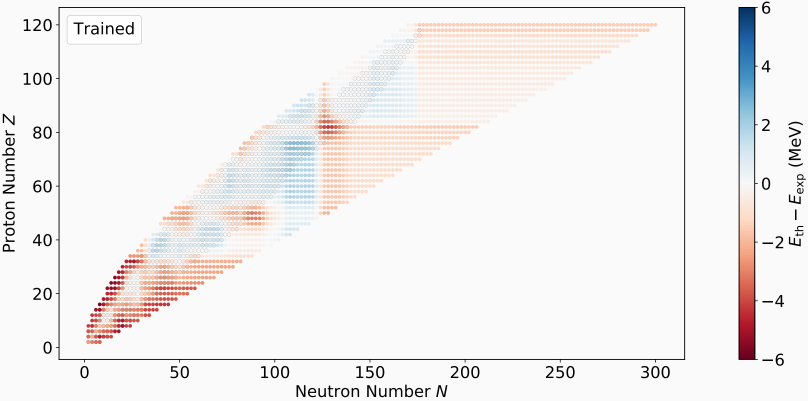
What about the neutron rich nuclei?



We will need to extrapolate our ML algorithm

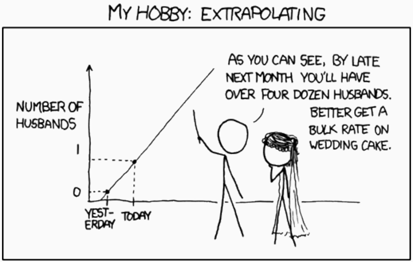
Is that reliable?

What about the neutron rich nuclei?



Least reliable where we need them the most!

Machine Learning is a terrible extrapolator



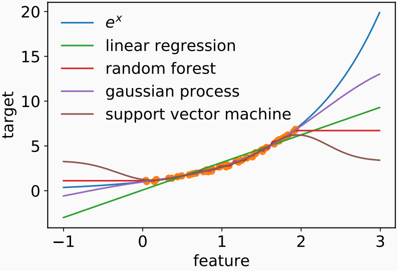
- Dogs vs Cats
- Dogs vs Cats vs Tables?
- Dogs vs Cats vs Wolfs?

- Benchmarking against testing data doesn't tell you anything about regions where there's no data

Machine Learning is a terrible extrapolator

Trying to reproduce e^x

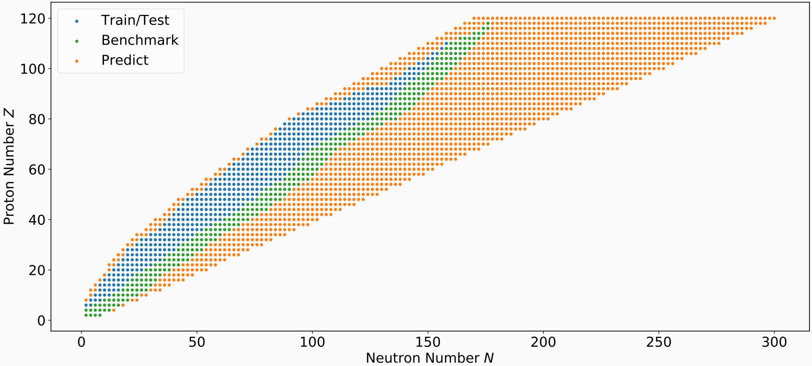
- Data in the $[0, 2]$ interval
- Predictions in the $[-1, 3]$ interval
- Different machine learning algorithms
- Completely incorrect results



This has been known for three decades!

Haley and Soloway, *Extrapolation limitations of multilayer feedforward neural networks*, in Proceedings 1992 International Joint Conference on Neural Networks

Testing extrapolation power



Drop the N most neutron rich nuclei from which there is known data

Testing extrapolation power

Performance decreases with extrapolation length

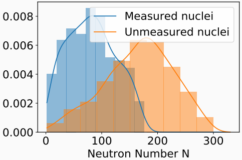
N drop	Training score	Testing score	Benchmark score
1	0.970(4)	0.79(5)	0.82(2)
2	0.967(4)	0.76(6)	0.79(2)
3	0.966(4)	0.74(6)	0.73(4)
4	0.966(4)	0.74(7)	0.67(4)
5	0.969(3)	0.77(5)	0.61(5)
6	0.967(3)	0.76(6)	0.50(5)

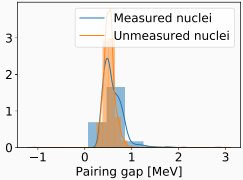
Solution: Use features that avoid extrapolations

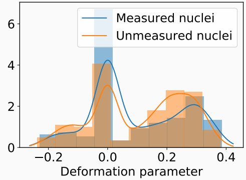
DFT produces additional properties for each nuclei

- Deformation parameters
- Nuclear radii
- Different contributions to the total energy
- Pairing energies
- Pairing gaps

Look for similar distributions between the in and out region







New extrapolation power

Random Forests for Nuclear Model Discrepancy

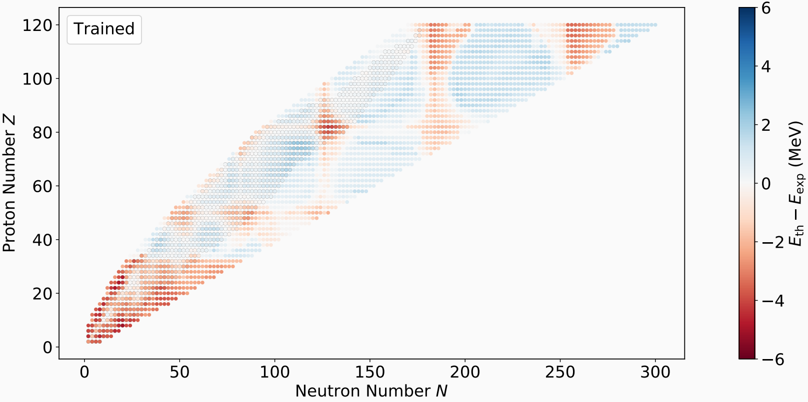
- Collect data: Atomic Mass Evaluation 2016 and UNEDF0
- Select Target: $\Delta BE(Z,N) = BE_{\mathrm{theo}}(Z,N) - BE_{\mathrm{exp}}(Z,N)$
- Select Features $\vec{F}(Z,N)$
  - Z, pairing gap, energy corrections, deformation, spin-orbit energy
- Split data: 75% trainnig, 25% testing
- Train the random forest: Training score 0.961(3)
- Benchmark against testing data: Testing score 0.71(5)
- Improved Binding energy:
  $BE_{\mathrm{ML}}(Z,N) = BE_{\mathrm{theory}}(Z,N) - \Delta BE_{\mathrm{ML}}(\vec{F})$

Testing extrapolation power

Benchmark remains consistent with testing

N drop	Training score	Testing score	Benchmark score
1	0.959(3)	0.68(9)	0.77(2)
2	0.955(3)	0.68(4)	0.77(2)
3	0.954(3)	0.67(8)	0.74(2)
4	0.953(4)	0.63(8)	0.66(4)
5	0.950(4)	0.69(6)	0.63(3)
6	0.949(2)	0.61(4)	0.63(3)

What about the neutron rich nuclei?



Nuclear structure patterns are now present

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Limitations

- There's a decrease in testing score with new features
- r-process nuclei are even farther from our training data
- Is the model discrepancy the same in both regions?
    - How reliable is our theory in the neutron rich side?
- Do our new features capture everything that we need?

Summary and outlook

Summary

Microscopically constrained Mean Field calculations

- New family of EDFs constrained by χ-EFT
- Quality EDFs with global predictive power
- Surprising improvement in mass calculations
- Δ's improve performance, 3N terms don't
- Optimization is under review

Model Discrepancy with Machine Learning

- Easy to estimate model discrepancy
- Direct extrapolations are not reliable
- Selecting features that avoid extrapolations is crucial

Outlook

Microscopically constrained Mean Field calculations

- Other possible checks for 3N under-performance:
  - Review calculation of DME couplings
  - Review calculation of mass tables
  - Extra terms in DME
  - DME Flavor
- Quantification and propagation of uncertainties

Model Discrepancy with Machine Learning

- Use different functionals (UNEDF1-2, DME, Skyrme, etc)
  - Do all corrections point in the same direction?
- New predictions in r-process simulations