Variational principles & efficient subspace emulation

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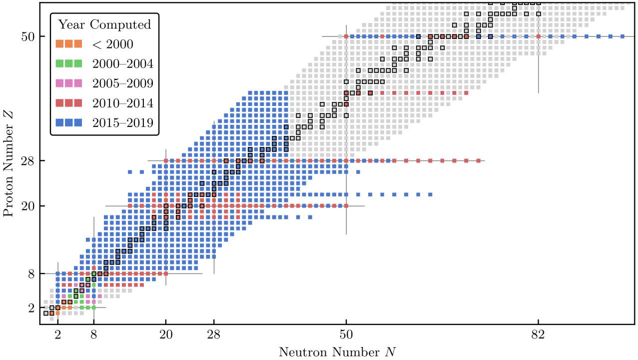
There is code to accompany these slides!

github.com/jordan-melendez/quantum-emulator-examples

Background

Progress in heavy nuclei

- Great progress has been made
- Growth in computing power and algorithms is pushing to heavier systems
- But statistics requires more than one prediction



Why we need emulators

Complexity:

1. 🤔 Forward UQ
2. 😰 Inverse UQ
3. 😱 Experimental Design

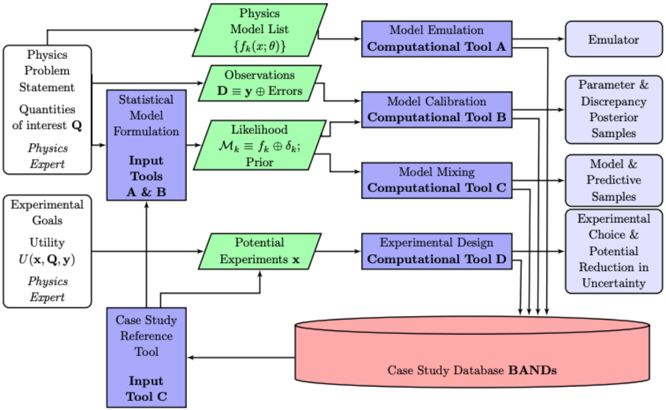
- r-process, $0\nu\beta\beta$ simulations, & optimizing FRIB experiments can each be compute intensive — but important!
- Emulator: An algorithm capable of accurately approximating the exact solution while requiring only a fraction of the computational resources

Relation to BAND

BAND

The goal of BAND is to translate novel statistical methods of UQ into software tools that address prominent current problems in nuclear physics.

- Subspace emulation could play a key role in Tool A.
- An emulator can feed into all subsequent tools

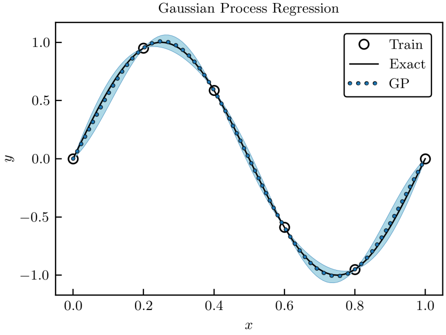


Emulators

Gaussian processes as emulators

```python
import numpy as np
from sklearn.gaussian_process \
    import GaussianProcessRegressor
from sklearn.gaussian_process.kernels \
    import RBF, ConstantKernel as C

x_train = np.arange(0, 1.1, 0.2)
x_valid = np.linspace(0, 1, 101)
y_train = np.sin(2 * np.pi * x_train)
y_valid = np.sin(2 * np.pi * x_valid)

kernel = C(1) * RBF(length_scale=0.2)
gp = GaussianProcessRegressor(kernel)
gp.fit(x_train[:, None], y_train)
y_pred, y_stdv = gp.predict(
    x_valid[:, None], return_std=True)
```

- Forward Problem: Train at "kinematic" points
- Inverse Problem: + train at parameter values
- Modern libraries make it easy



Gaussian processes: pros & cons

Pros

- Non-intrusive (can leave legacy code untouched)
- Easy to use
- Flexible (non-parametric)
- Error bands for free
- ...

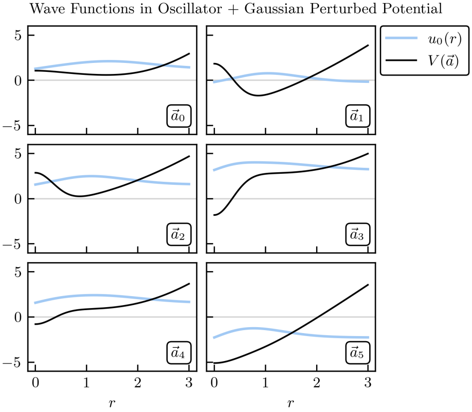
Cons

- Not great at extrapolating
- Choosing a kernel — not always straightforward
- Numerical instabilities can arise
- Parameter space can be large!
- Does not necessarily take advantage of structure of the system (more on this later...)

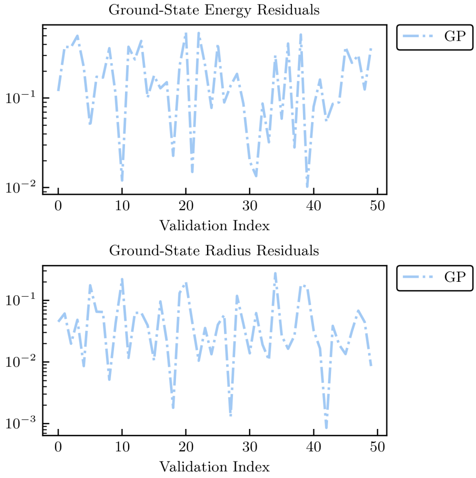
Example: GPs for the Schrödinger equation

$$V(\vec{a}) = V_{h.o.}(\omega) + \sum a_i \exp\left[-(r/b_i)^2\right]$$

for fixed $\{b_i\} = \{0.5, 2, 4\}$.



Fit separate GP to E and radius $R = \mathbb{E}[r]$.



Ritz subspace method: the basics

Instead of solving the Schrödinger eq. (an eigenvalue problem for bound states)

$$H(\vec{a})\,|\psi(\vec{a})\rangle = E(\vec{a})\,|\psi(\vec{a})\rangle$$

write down a trial wave function as a linear combination

$$|\widetilde{\psi}\rangle = \sum_i \beta_i\,|\psi_i\rangle$$

and use a variational method to determine the best β_i:

Bound state variational method

Minimize $\langle\widetilde{\psi}|H(\vec{a})|\widetilde{\psi}\rangle$ such that $\langle\widetilde{\psi}|\widetilde{\psi}\rangle = 1$.

The problem has then been reduced from determining an infinite-dimensional (or, at least large) $|\psi(\vec{a})\rangle$ to determining a couple coefficients β_i.

Ritz subspace method for eigenvalue problems (arXiv:2104.04441)

Problem: $H(\vec{a})$ is $N \times N$ and $N \gg 1$

$$H(\vec{a})\,|\psi(\vec{a})\rangle = E(\vec{a})\,|\psi(\vec{a})\rangle \tag{17}$$

such that $\quad H(\vec{a}) = H_0 + \sum a_j H_j$

Solution: Choose a basis with $N_b \ll N$:

$$X \equiv \begin{pmatrix} | & | & & | \\ |\psi_1\rangle & |\psi_2\rangle & \cdots & |\psi_{N_b}\rangle \\ | & | & & | \end{pmatrix} \tag{18}$$

$$\widetilde{H}(\vec{a}) = X^\dagger H(\vec{a}) X, \qquad \mathcal{N} = X^\dagger X \tag{19}$$

Finally, solve smaller problem:

$$\widetilde{H}(\vec{a})\beta(\vec{a}) = \widetilde{E}(\vec{a})\mathcal{N}\beta(\vec{a}) \tag{20}$$

```python
def setup_projections(self, X):
    # Project matrices once
    H0_sub = X.T @ self.H0 @ X # const.
    H1_sub = X.T @ self.H1 @ X # linear
    # Store for later
    self.X = X; self.N = X.T @ X
    self.H0_sub = H0_sub
    self.H1_sub = H1_sub
    return self

def solve_subspace(self, a):
    H = self.H0_sub + self.H1_sub @ a
    from scipy.linalg import eigh
    E, beta = eigh(H, self.N)
    return E[0], beta[:, 0] # g.s.
```

Ritz subspace method for eigenvalue problems (arXiv:2104.04441)

What is gained?

$$H(\vec{a})\,|\psi(\vec{a})\rangle = E(\vec{a})\,|\psi(\vec{a})\rangle \qquad (17)$$

v.s.

$$\widetilde{H}(\vec{a})\beta(\vec{a}) = \widetilde{E}(\vec{a})\mathcal{N}\beta(\vec{a}) \qquad (20)$$

Eq. (20) is much smaller, and

$$E(\vec{a}) \approx \widetilde{E}(\vec{a}) \qquad |\psi(\vec{a})\rangle \approx X\beta(\vec{a})$$

Emulator for both $E(\vec{a})$ and $|\psi(\vec{a})\rangle$! Thus:

$$\begin{aligned}\langle\hat{O}(\vec{a})\rangle &= \langle\psi(\vec{a})|\hat{O}(\vec{a})|\psi(\vec{a})\rangle \\ &\approx \beta(\vec{a})^\dagger[X^\dagger\hat{O}(\vec{a})X]\beta(\vec{a}) \qquad (21)\end{aligned}$$

```python
def solve_subspace(self, a):
    H = self.H0_sub + self.H1_sub @ a
    from scipy.linalg import eigh
    E, beta = eigh(H, self.N)
    # Get ground states:
    return E[0], beta[:, 0]

def predict(self, a):
    E, beta = self.solve_subspace(a)
    psi = self.X @ beta
    return E, psi

def expectation_value(self, a):
    op = self.op0_sub + self.op1_sub @ a
    E, beta = self.solve_subspace(a)
    return beta.T @ op @ beta
```

Subspace methods: pros & cons

Pros

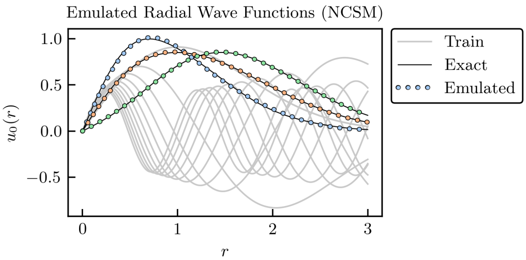
- Can radically reduce the size of the eigenvector problem
- If the basis is well chosen, one can get very accurate results
- Can emulate both the energy and the wave function
- Gets emulator for downstream observables $\langle \hat{O}(\vec{a}) \rangle$ for free

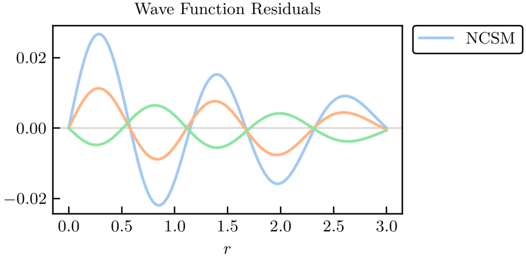
Cons

- Intrusive (Requires writing new solver code, but it fits in these slides!)
- Not clear how to choose the basis $\{ |\psi_i\rangle \}$. (Will fix right now.)
- No free uncertainty quantification
- Emulating excited states will require enlarging basis

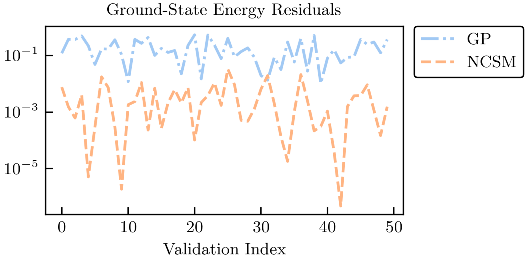
A comparison: GPs vs Ritz (NCSM) subspace emulators

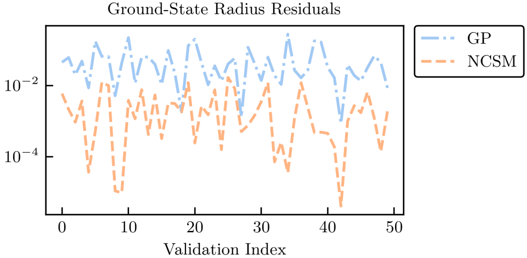
Use 6 lowest oscillator states as basis.





Fit a separate GP to E and the radius R.





Efficient Subspace Emulators
aka Eigenvector Continuation
aka Reduced Basis Method

Efficient subspace emulators for bound states: the basics

Remember, write down a trial wave function: $|\widetilde{\psi}\rangle = \sum \beta_i |\psi_i\rangle$

Bound state variational method

Minimize $\langle\widetilde{\psi}|H(\vec{a})|\widetilde{\psi}\rangle$ such that $\langle\widetilde{\psi}|\widetilde{\psi}\rangle = 1$.

But how to choose the basis $\{\,|\psi_i\rangle\}$? For parameter-dependent problems:

Efficient Subspace Emulation

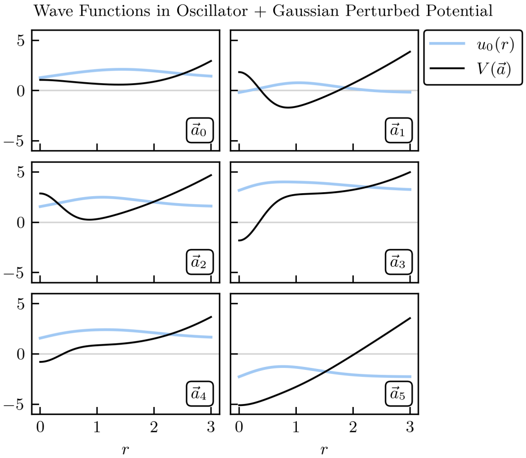
The insight: Use exact solutions $|\psi(\vec{a}_i)\rangle$ at a set of training parameters $\{\vec{a}_i\}$ as the basis for the variational calculation.

The intuition: As the $\vec{a}$ are varied, the eigenvectors only trace a small subspace compared to the full Hilbert space. Using exact solutions thus automatically finds an incredibly effective basis for subsequent emulation.

Efficient subspace emulators for bound states: the code

$$V(\vec{a}) = V_{h.o.}(\omega) + \sum a_i \exp\left[-(r/b_i)^2\right]$$

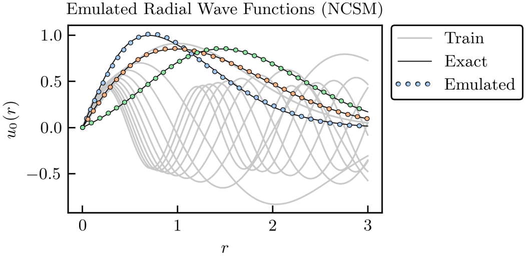
for fixed $\{b_i\} = \{0.5, 2, 4\}$.



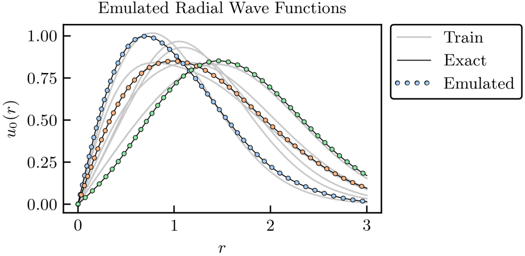

```python
import numpy as np

def fit(self, a_train):
    # Create subspace from exact |ψ(a⃗)⟩
    X = []
    for a in a_train:
        E, psi = self.solve_exact(a)
        X.append(psi)
    # Stack them as columns
    X = np.stack(X, axis=1)

    # The same function as before:
    self.setup_projections(X)
    # Store the training points
    self.a_train = a_train
    return self
```

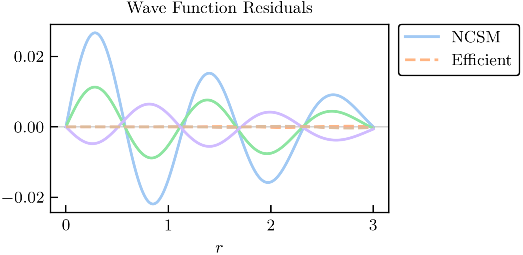
Another comparison: GPs vs NCSM vs efficient emulators

Inefficient! Most training wave functions do not look like the emulated states

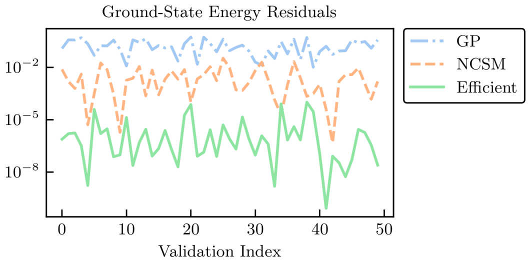


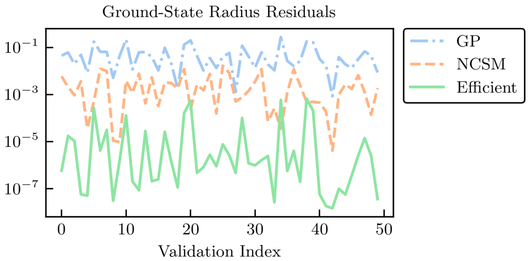
Much smaller basis span, but much more efficient!





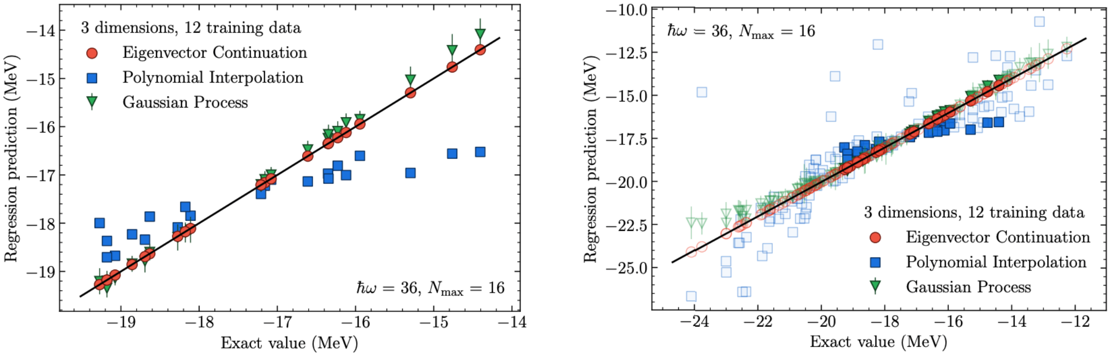
Another comparison: GPs vs NCSM vs efficient emulators





Comparing GP, NCSM, and the efficient emulators: the efficient emulator wins!

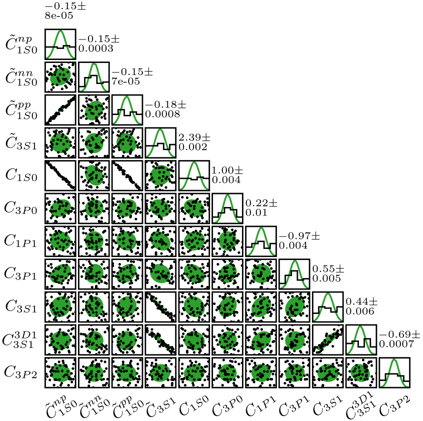
Bound state emulators in the wild (König *et al.* arXiv:1909.08446)

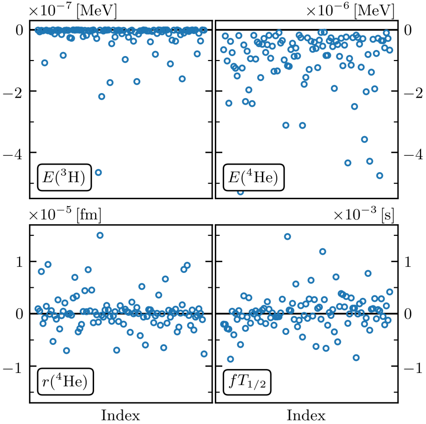


Eigenvector continuation (the efficient subspace emulator) beats both polynomials and GPs on interpolation and extrapolation in parameter space.

Observable: ^{4}He g.s. energy. Uses 12 training points with 3 parameters.

Bound state emulators in the wild: inverse problem (arXiv:2104.04441)



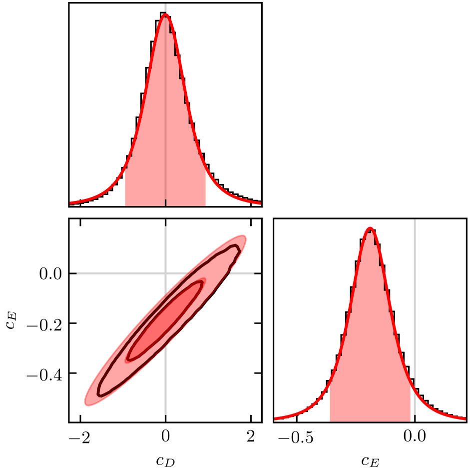


Sampling 15 different parameters (some not shown). 50 training points.

Negligible residuals on validation data

Bound state emulators in the wild: inverse problem (arXiv:2104.04441)

Able to rapidly perform sampling on laptop in minutes, rather than on supercomputer for hours



Bound state emulators in the wild: uncertainties (Sarkar, Lee: arXiv:2107.13449)

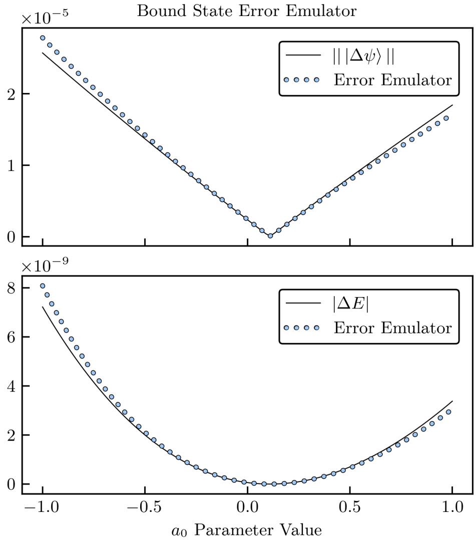
Uncertainty in the emulator:

$$\text{Error}[\,|\widetilde{\psi}\rangle] \propto \left[\frac{\langle\widetilde{\psi}|[H-\widetilde{E}]^2|\widetilde{\psi}\rangle}{\langle\widetilde{\psi}|H^2|\widetilde{\psi}\rangle}\right]^{1/2}$$

If H is linear in $\vec{a}$, this can be computed in the small space.

Can obtain proportionality constant if needed

$\text{Error}[E] \sim \text{Error}[\,|\widetilde{\psi}\rangle]^2$



Beyond Bound States

Efficient trial scattering wave functions: the basics (arXiv:2007.03635)

Again, write down a trial wave function: $|\widetilde{\psi}\rangle = \sum \beta_i |\psi_i\rangle$.

For scattering, it is convenient to work with the radial wave function $u_\ell(r)$ for partial wave ℓ, which in asymptotic form is

$$u_\ell(r) \xrightarrow[r\to\infty]{} \sin\left(pr - \frac{1}{2}\ell\pi\right) + K_\ell \cos\left(pr - \frac{1}{2}\ell\pi\right)$$

Kohn variational principle (KVP)

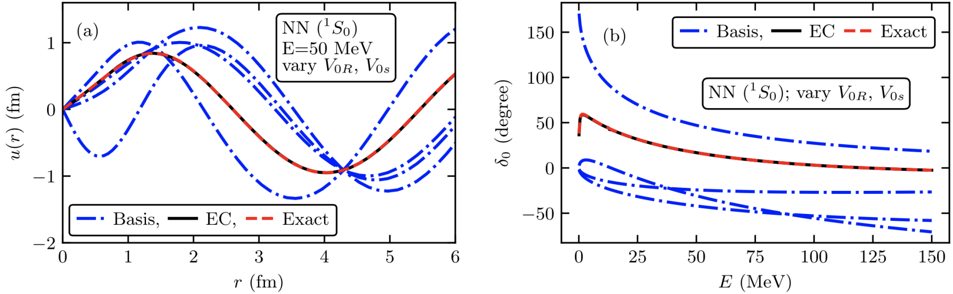
Minimize $\mathcal{K}_{KVP}[\widetilde{\psi}_\ell] = K_\ell - \langle\widetilde{\psi}_\ell|H(\vec{a}) - E|\widetilde{\psi}_\ell\rangle$ such that $\langle\widetilde{\psi}_\ell|\widetilde{\psi}_\ell\rangle = \delta(\cdots)$.

Again, use exact $u_\ell(r)$ at training points $\{\vec{a}_i\}$ as the basis.

It is a linear problem, can solve for β analytically and quickly.

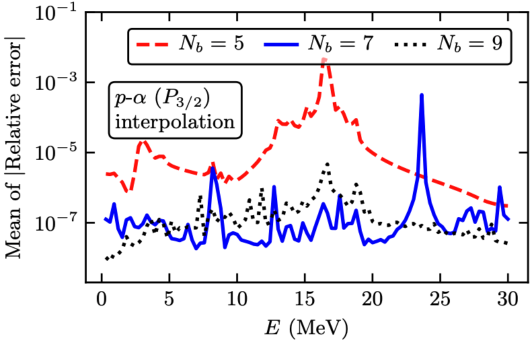
Trial scattering wave functions in the wild (arXiv:2007.03635)

Can emulate entire scattering wave function and its phase shifts



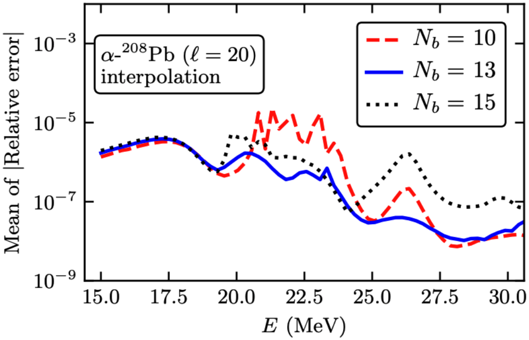
Trial scattering wave functions in the wild (arXiv:2007.03635)

Can accurately emulate with Coulomb



Trial scattering wave functions in the wild (arXiv:2007.03635)

Also works with optical potentials



Efficient trial K or T matrices (arXiv:2106.15608)

Rather than solve the Schrödinger equation, use the Lippmann–Schwinger (LS) equation

$$K = V + VG_0K$$

Propose trial K matrix

$$\widetilde{K} = \sum \beta_i K_i$$

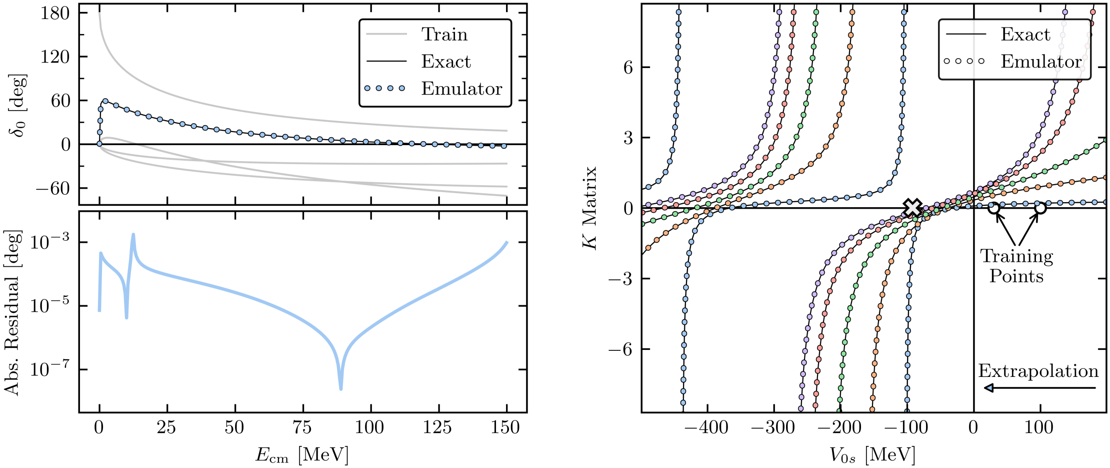
Newton variational principle (NVP)

Minimize $\mathcal{K}_{NVP}[\widetilde{K}] = V + VG_0\widetilde{K} + \widetilde{K}G_0V - \widetilde{K}G_0\widetilde{K} + \widetilde{K}G_0VG_0\widetilde{K}$ (no constraints!)

As usual, take the matrix basis $\{K_i\}$ from exact solutions of the LS equation.

It is a linear problem, can solve for β analytically and quickly.

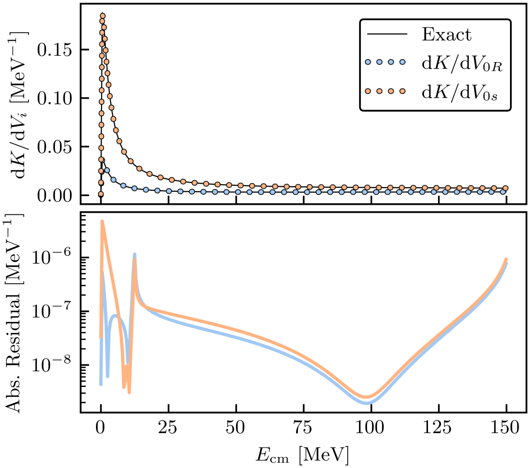
Trial K matrices in the wild (arXiv:2106.15608)



Can extrapolate very far from support of data, even across singularities

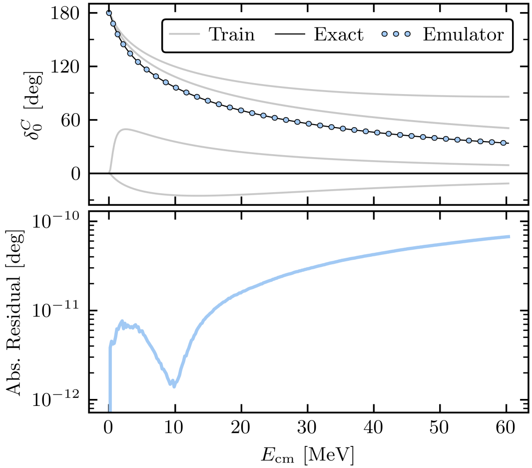
Trial K matrices in the wild (arXiv:2106.15608)

Can accurately & efficiently emulate gradients with respect to parameters

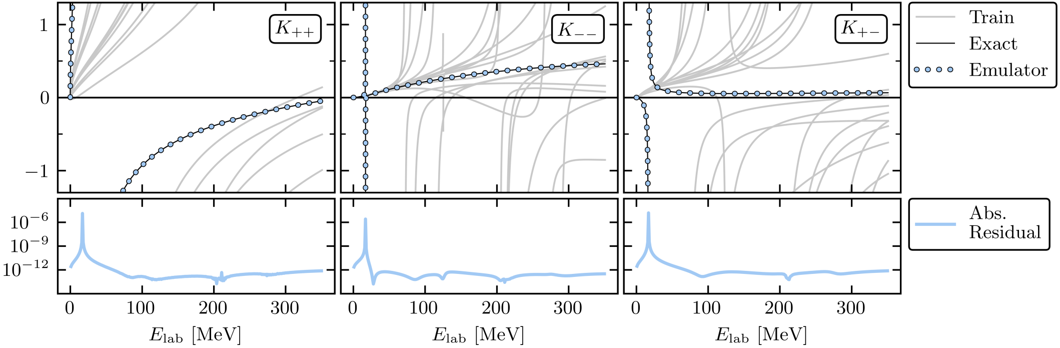


Trial K matrices in the wild (arXiv:2106.15608)

Can easily handle the Coulomb interaction



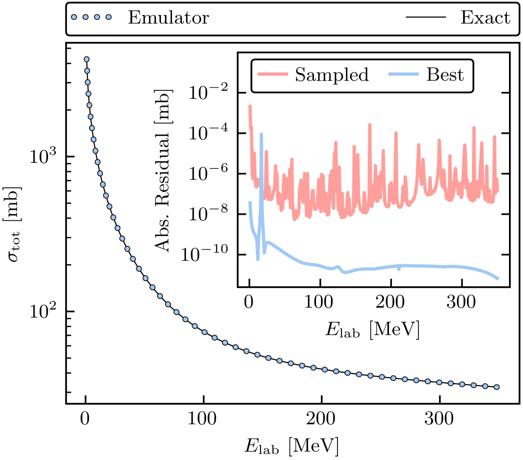
Coupled channels get major speedups with emulation



Trial K matrices in the wild (arXiv:2106.15608)

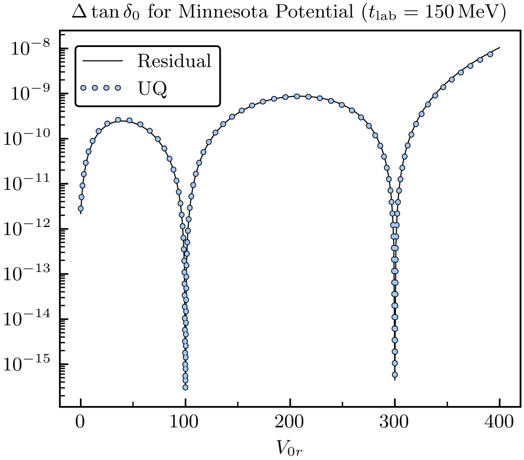
$$\sigma_{\text{tot}}(q) = -\frac{\pi}{2q^2}\sum_{j=0}^{j_{\text{max}}}(2j+1)\,\text{Re}\left\{\text{Tr}\left[S_j(q) - \mathbb{1}\right]\right\}$$

Multiple emulators across partial waves can be combined to emulate scattering observables. Over 300x improvement in CPU time.



Trial K matrices in the wild: uncertainties (In progress)

- By following reduced basis approach, UQ for $\widetilde{K}$ is possible
- Determined up to proportionality constant
- Can help propose next training point
- Can be added to error budget if using emulator in the wild



Density functional theory?! (In progress)

Two reasonable approaches

1. The Kohn-Sham formalism requires self-consistently solving Schrödinger equations for orbitals. One could emulate this step.
2. The ground state energy is minimized as a functional of the density. Just write down a trial density and turn the crank.

I took the latter approach

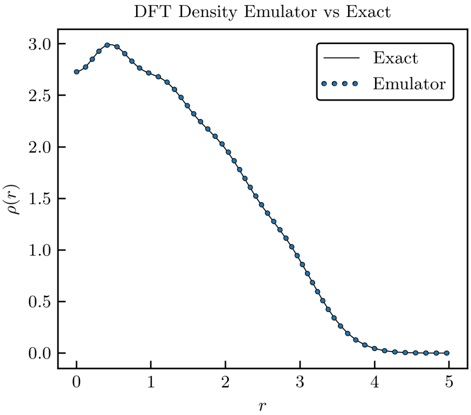
$$\widetilde{\rho} = \sum \beta_i \rho_i$$

and minimized

$$E[\widetilde{\rho}] = g \sum \epsilon - a \int \mathrm{d}^3x \, [\widetilde{\rho}(x)]^2 - b \int \mathrm{d}^3x \, [\widetilde{\rho}(x)]^{7/3} - c \int \mathrm{d}^3x \, [\widetilde{\rho}(x)]^{8/3}$$

Non-linear means there is no “nice” solution for β. Use an optimizer.

Density functional theory?! (In progress)



Emulators for generic differential equations

1. Derive the Galerkin weak formulation of the PDE
2. Apply the reduced basis method

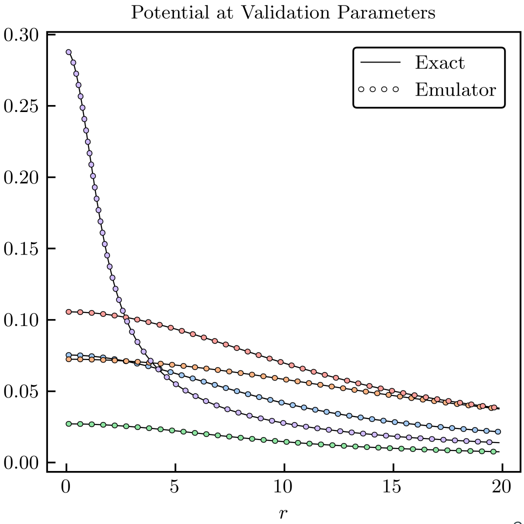
Example [Gaussian $\rho(\vec{a})$ for parameters $\vec{a}$]:

- Poisson equation

$$\nabla^2\phi = -\rho$$

- Weak form:

$$\int_\Omega \nabla\phi\nabla\psi \mathrm{d}x = -\int_\Omega \rho\psi \mathrm{d}x$$



Concluding Remarks

Conclusions

BAND

The goal of BAND is to translate novel statistical methods of UQ into software tools that address prominent current problems in nuclear physics.

Subspace emulation could play a key role in this effort

Benefits

- Can radically reduce the size of the problem (not just eigenvectors!)
- An extremely effective basis can be chosen automatically
- Gets emulator for downstream observables $\langle \hat{O}(\vec{a}) \rangle$ for free

- Promising directions: heavy systems, beyond eigenvalues, DFT, PDEs, etc.
- Error bands are in the works!

Thank you!

buqeye.github.io