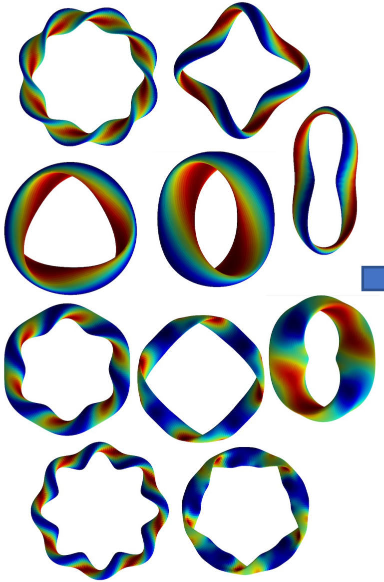
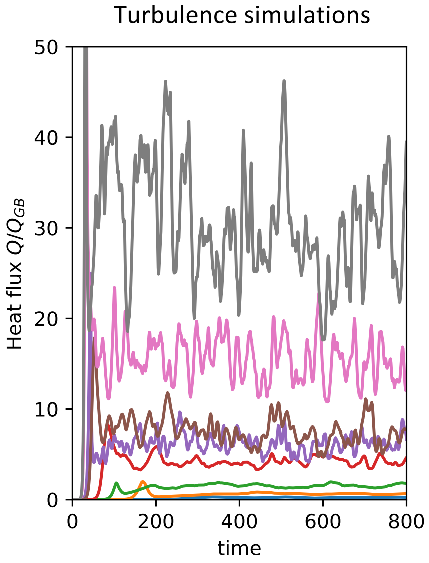
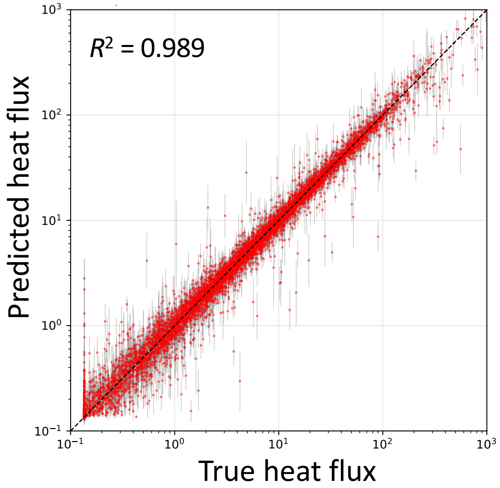
How does magnetic geometry affect ITG turbulence? Insights from data & machine learning





Regression



Feature importance

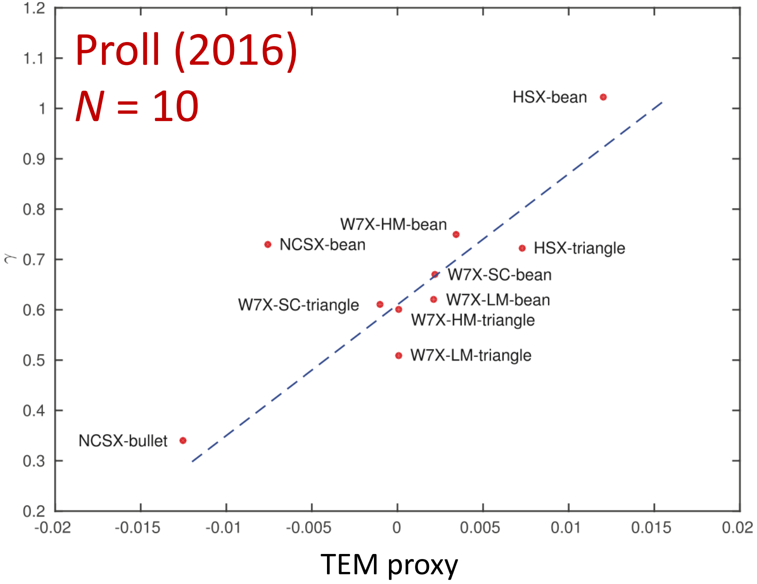
$$\mathrm{mean}([\Theta(\mathbf{B}\times\kappa\cdot\nabla y)+0.2]|\nabla x|^3/B)$$

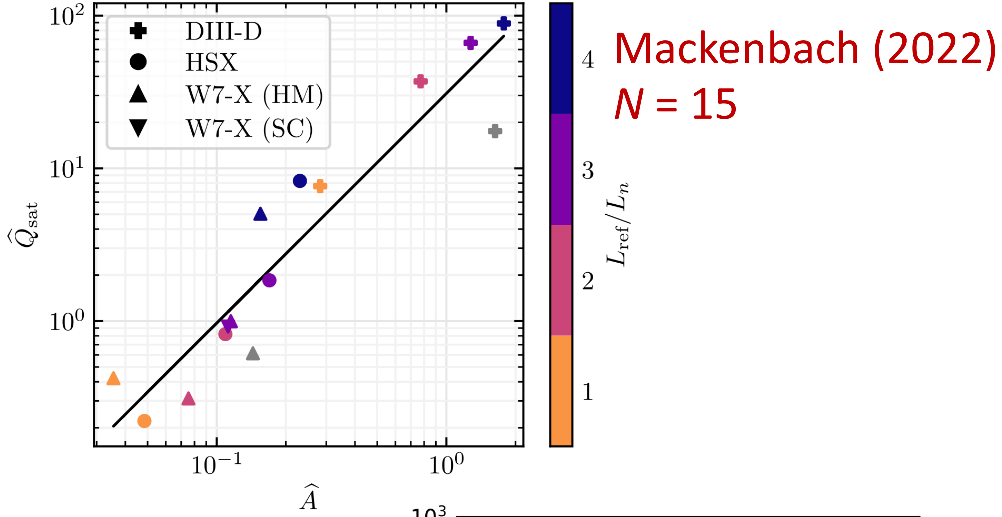
$$\mathrm{median}((\mathbf{B}\times\nabla B\cdot\nabla x)^2|\nabla x|^8/B^8)$$

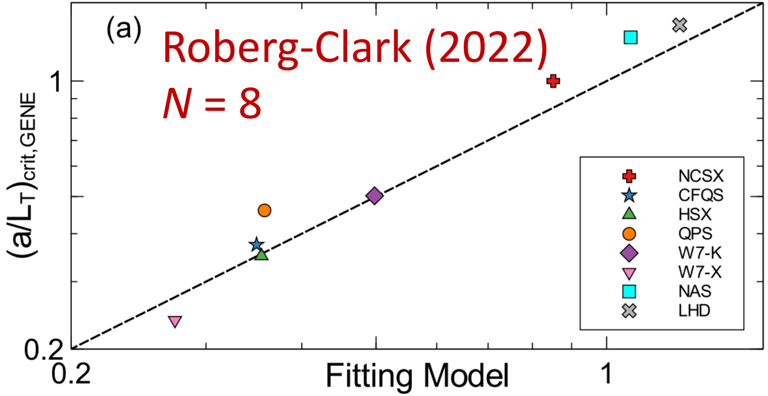
M Landreman, J Y Choi, C Alves, P Balaprakash, R M Churchill , R Conlin, G Roberg-Clark **arXiv:2502.11657**

Thanks to many others who gave suggestions

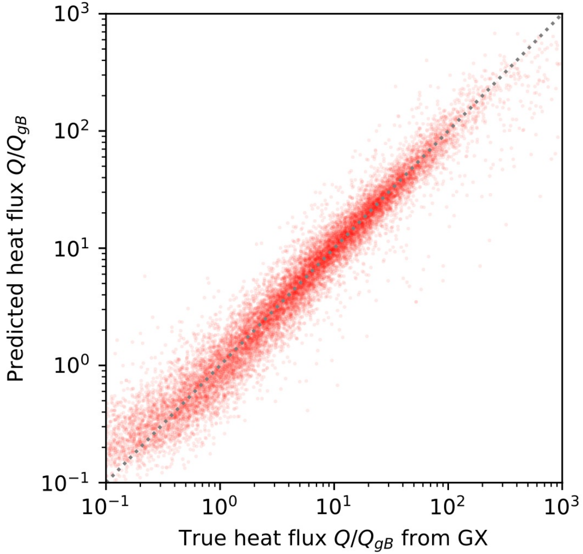
Supported by the US DOE StellFoundry SciDAC







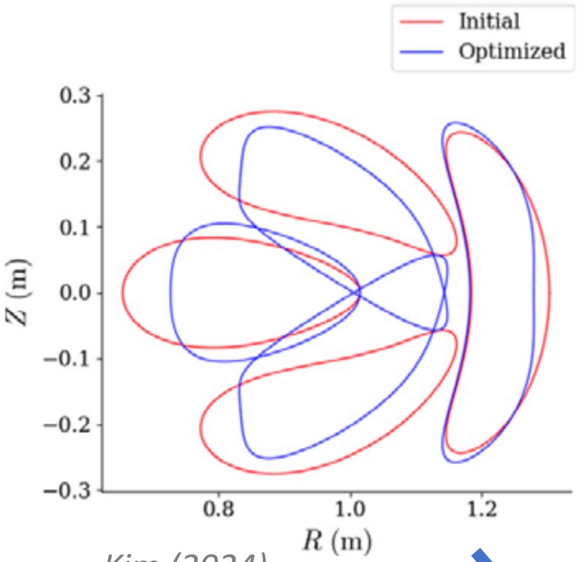
This work:
N = 100,705



Motivations

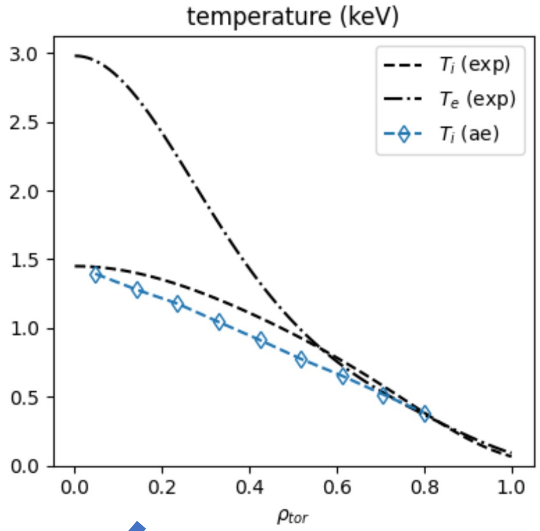
Understanding

Optimization



Kim (2024)

Profile prediction

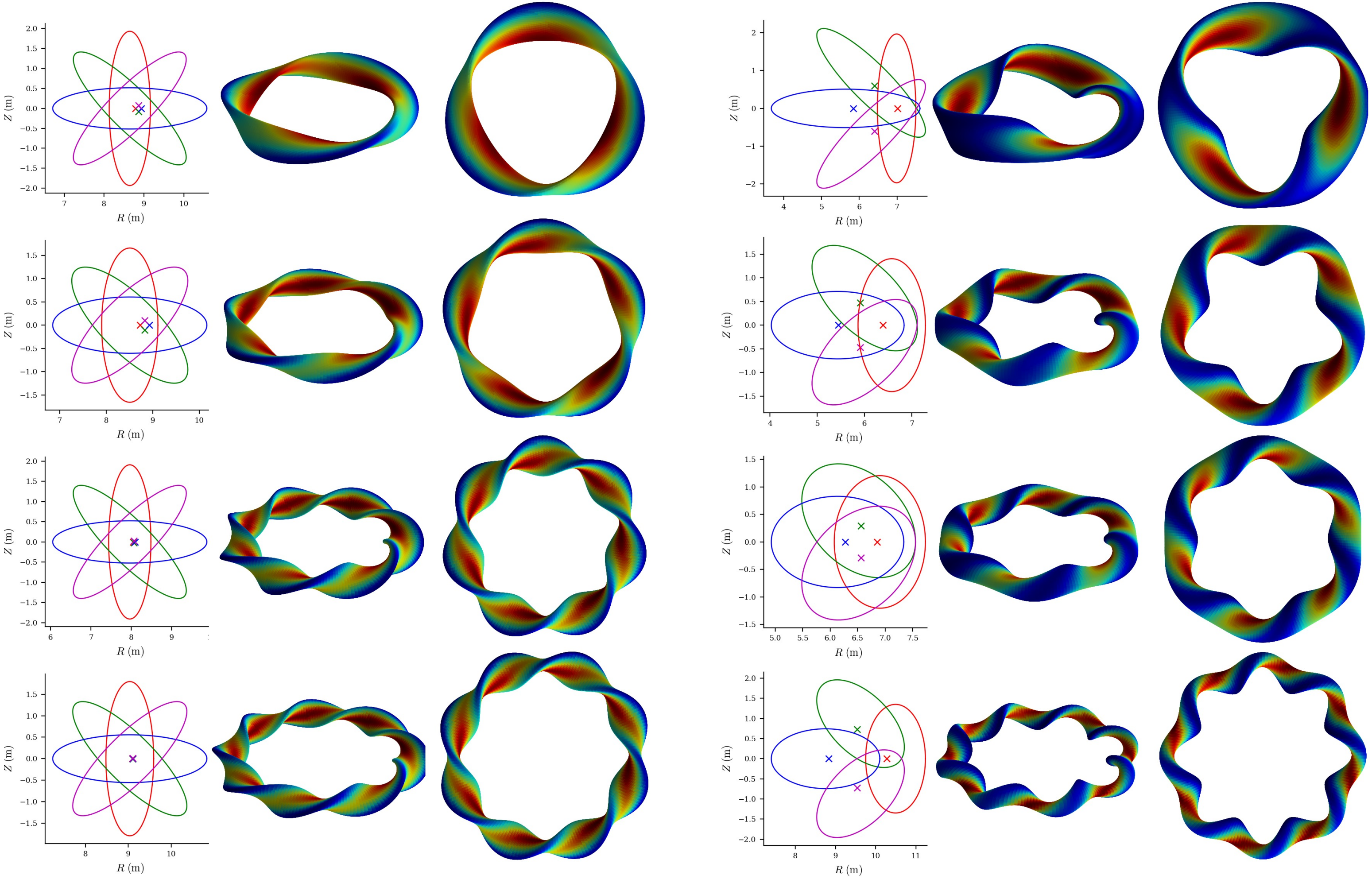


Mandell (2024)

Optimize geometry for maximum fusion power

Turbulence simulations
Heat flux Q/Q_{GB}
time
Regression
R^2 = 0.989
Predicted heat flux
True heat flux
Feature importance
$\mathrm{mean}([\Theta(\mathbf{B}\times\kappa\cdot\nabla y)+0.2]|\nabla x|^3/B)$
$\mathrm{median}((\mathbf{B}\times\nabla B\cdot\nabla x)^2|\nabla x|^8/B^8)$

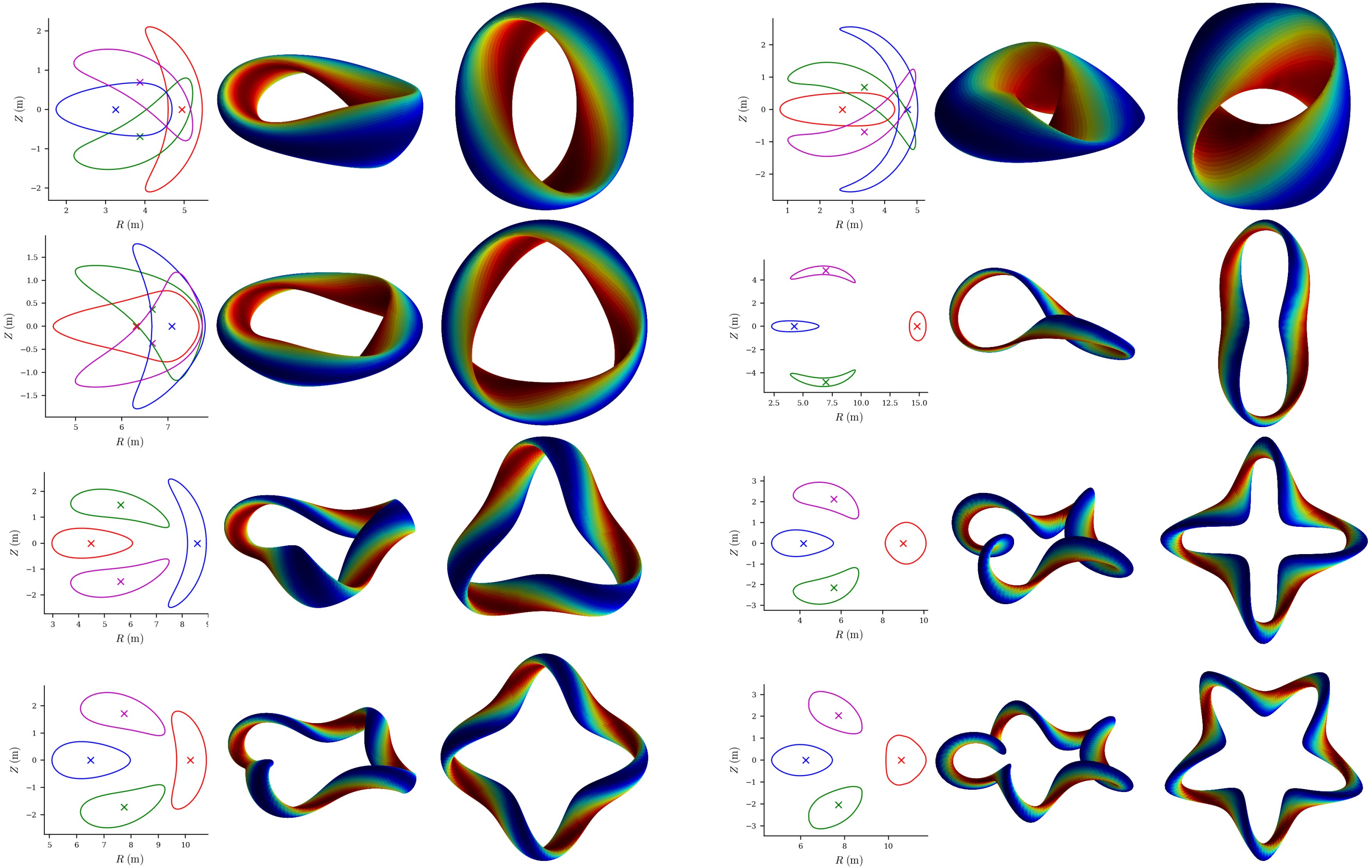
Equilibria group 1: random rotating ellipses



Nfp,
aspect ratio,
elongation,
axis torsion,
and beta are
all random.

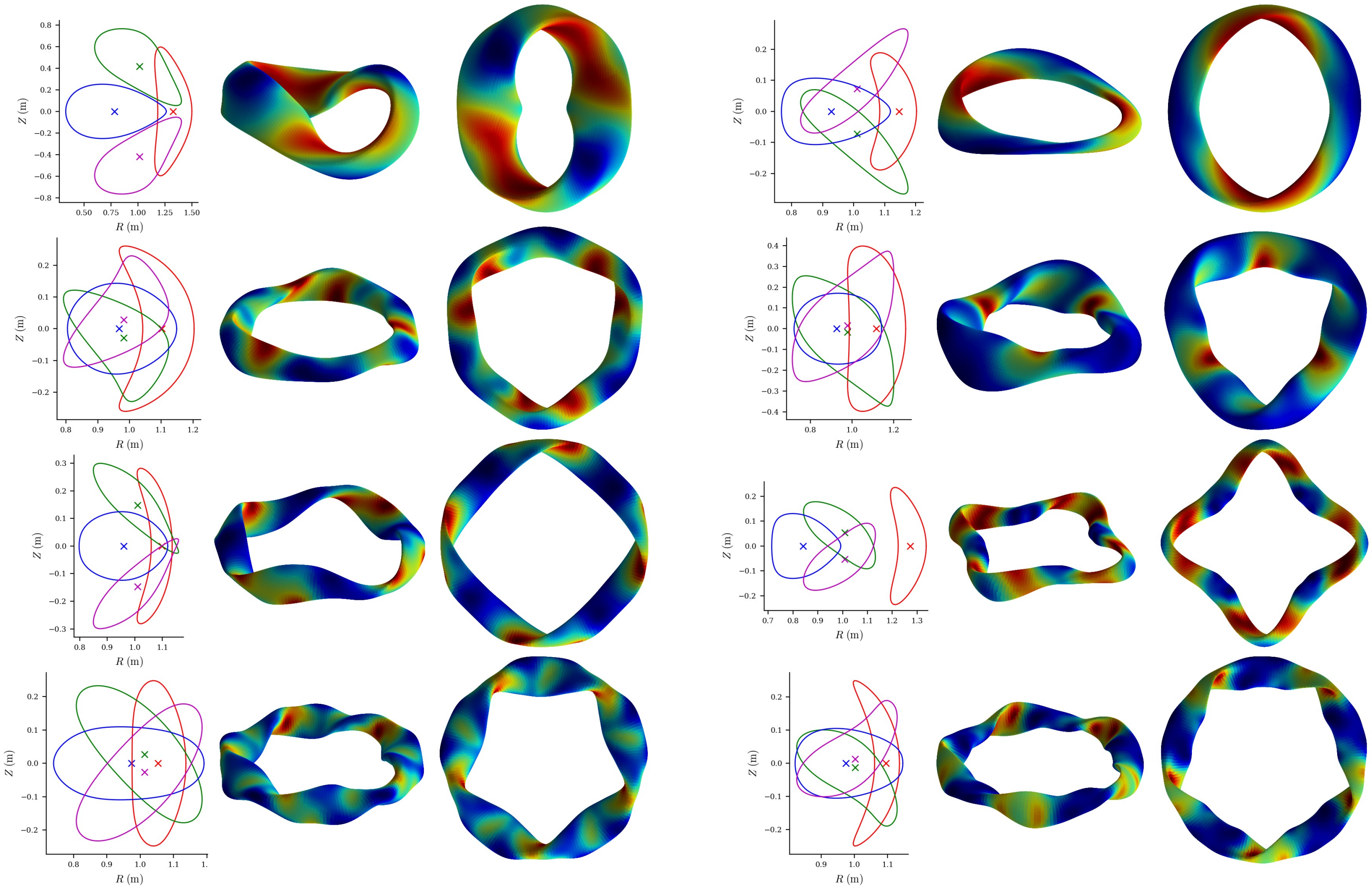
All
configurations
have same
minor radius &
toroidal flux,
so same
gyroBohm
normalization

Equilibria group 2: QUASR QA & QH (Giuliani 2024)

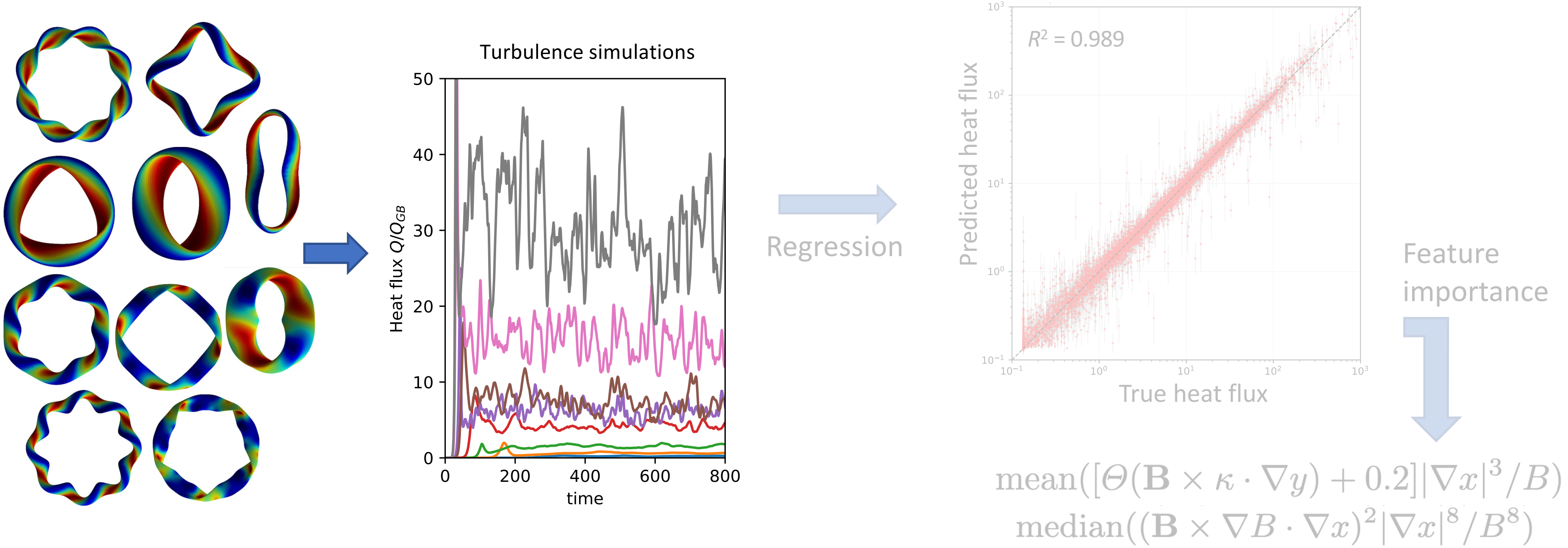


Random pressure added for even more diversity

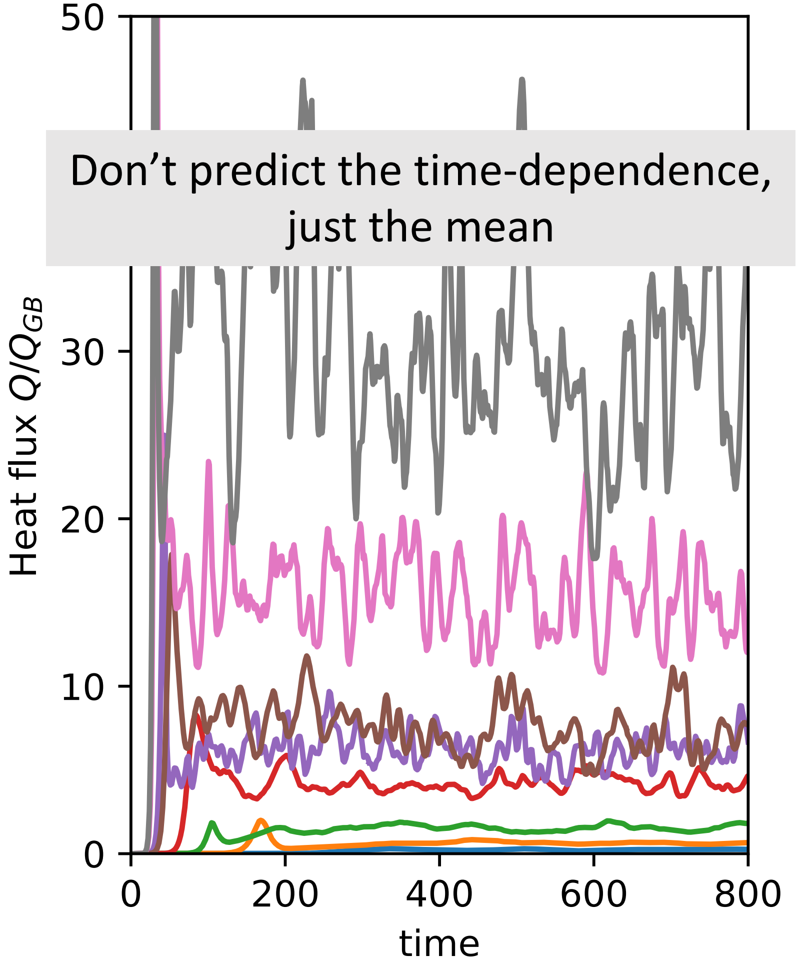
Equilibria group 3: random boundary modes



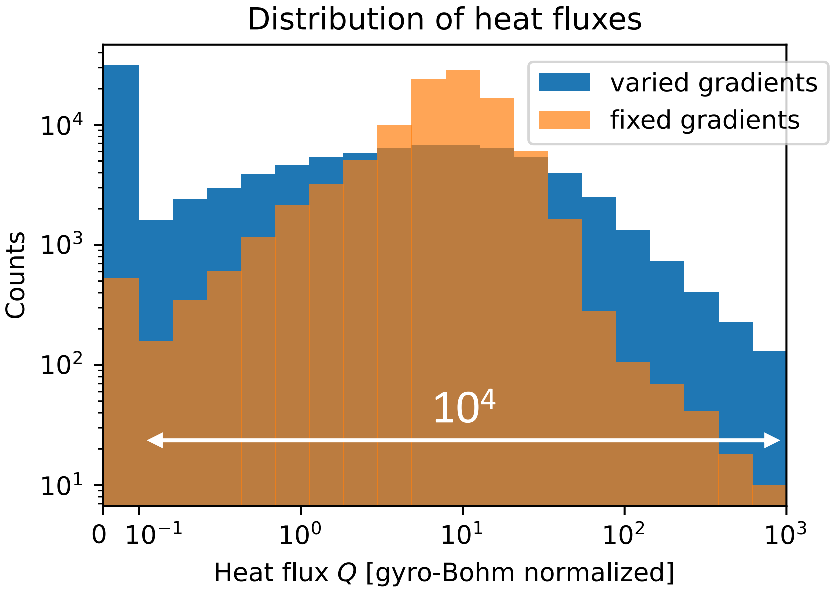
RBC and ZBS boundary Fourier modes sampled from normal distributions, fit to 44 “real” stellarators


Turbulence simulations
Heat flux Q/Q_{GB}
time
0
10
20
30
40
50
200
400
600
800
Regression
R^2 = 0.989
Predicted heat flux
True heat flux
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Feature importance
$\mathrm{mean}([\Theta(\mathbf{B}\times\kappa\cdot\nabla y)+0.2]|\nabla x|^3/B)$
$\mathrm{median}((\mathbf{B}\times\nabla B\cdot\nabla x)^2|\nabla x|^8/B^8)$

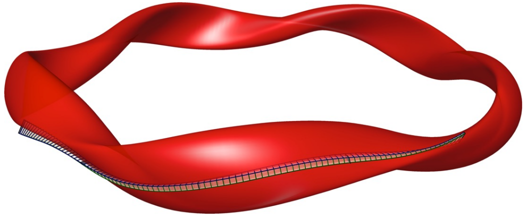
Nonlinear turbulence simulations were run with GX in every equilibrium

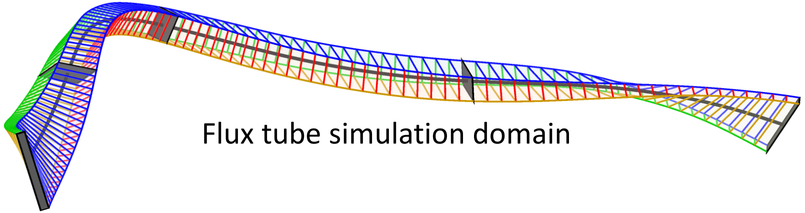


- Electrostatic, adiabatic electrons.
- 1 simulation in each tube with random dT/dx and dn/dx.
- 1 simulation in each tube with (a/T) dT/dx = 3, (a/n) dn/dx=0.9
- 8 minutes to get heat flux on 1 GPU
- $2{\times}10^5$ nonlinear simulations took < 7000 node-hours (1/8 allocation)



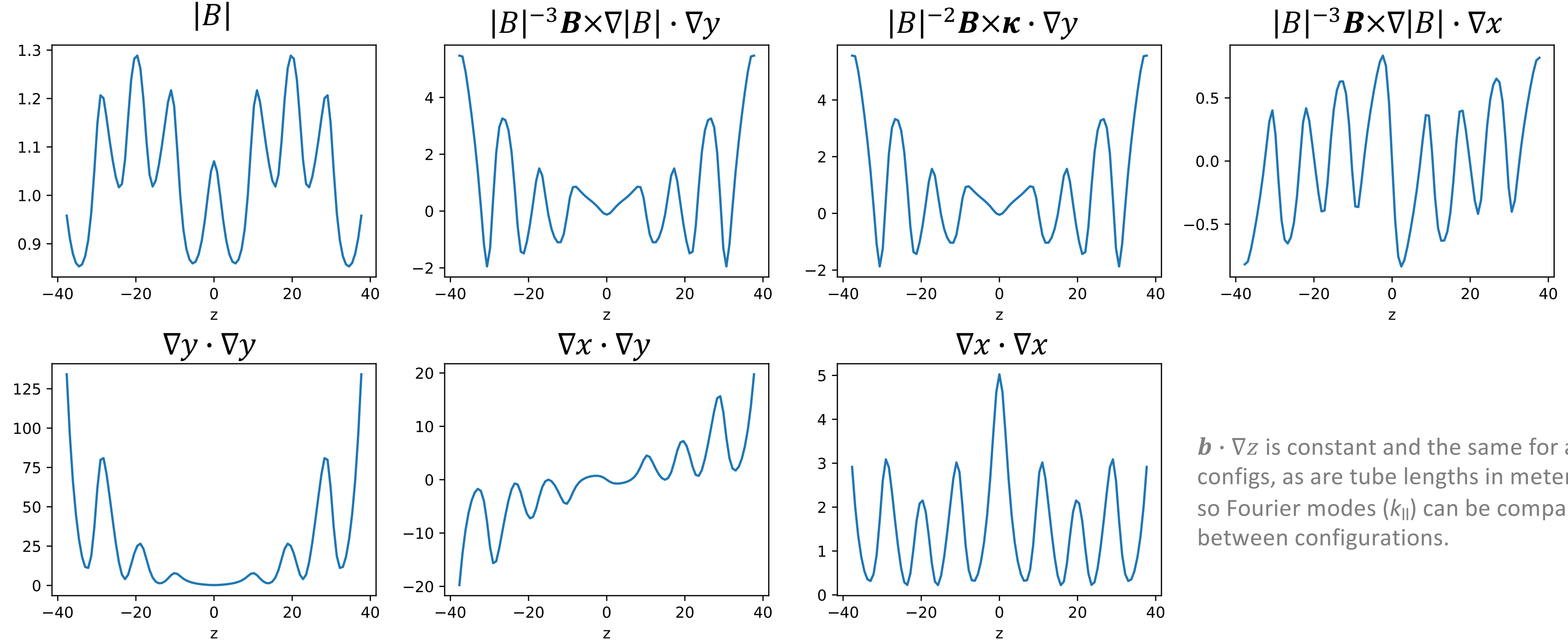
Raw feature space: 7x 1D functions that enter the turbulence simulations



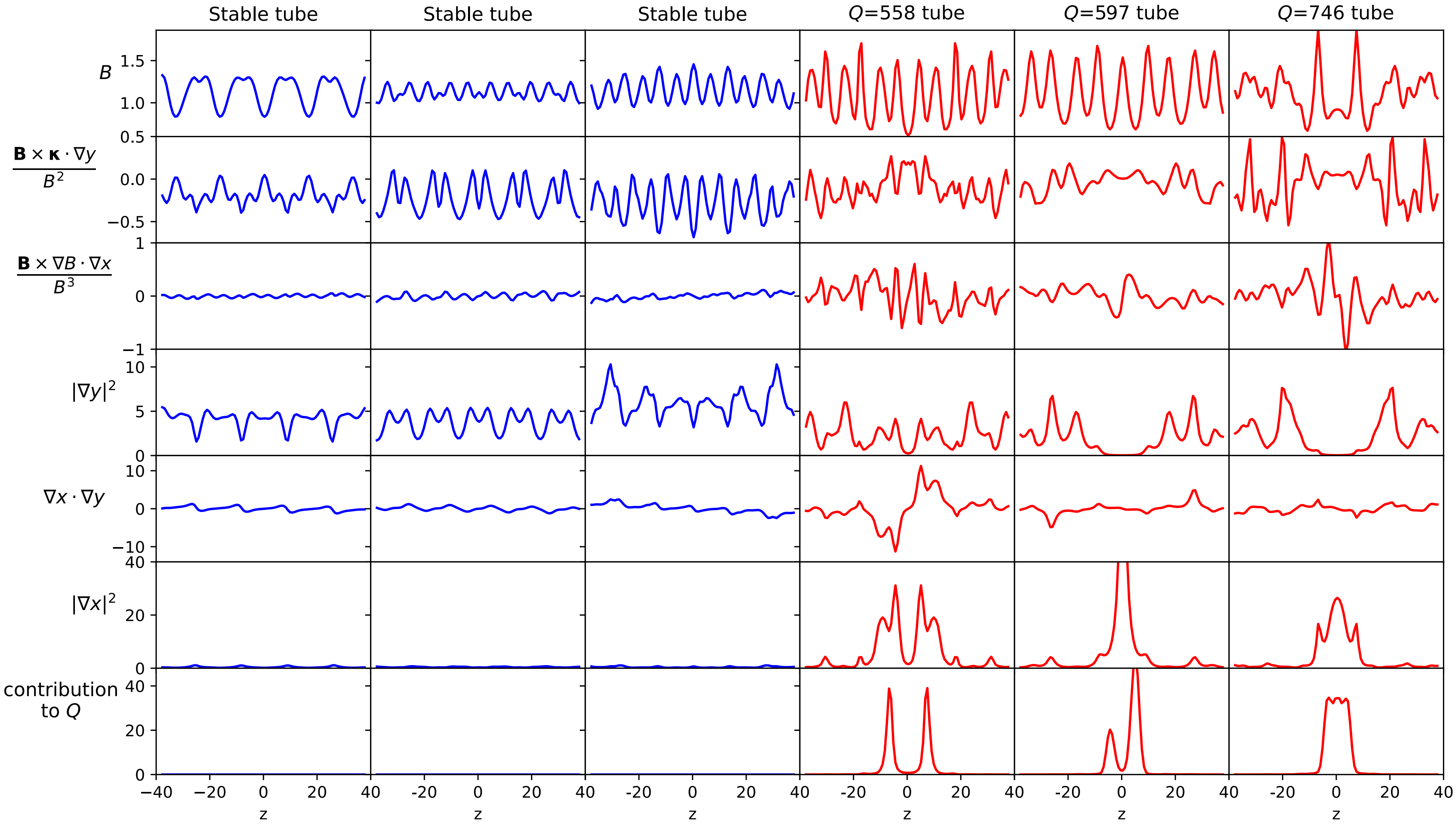


$$\boldsymbol{B} = B_{ref} \nabla x \times \nabla y$$

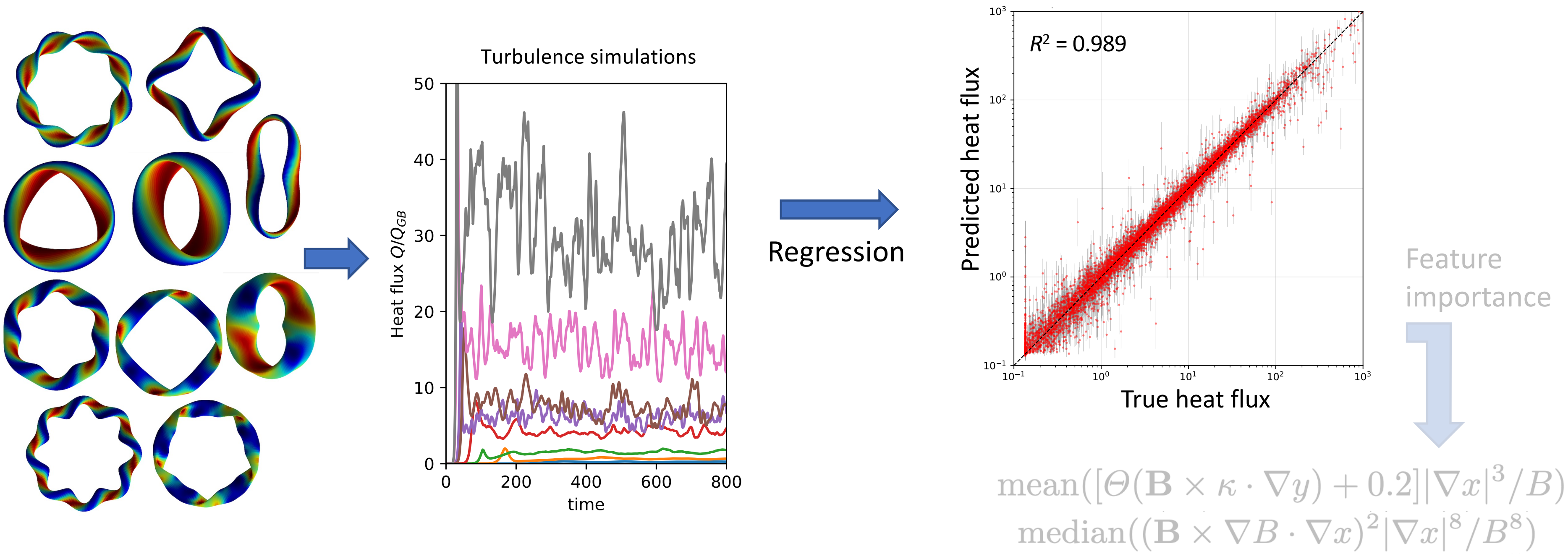
$$x = a\sqrt{\psi/\psi_{edge}}$$



$\boldsymbol{b} \cdot \nabla z$ is constant and the same for all configs, as are tube lengths in meters, so Fourier modes ($k_{\|}$) can be compared between configurations.



Stable tube
Stable tube
Stable tube
Q=558 tube
Q=597 tube
Q=746 tube
B
$\frac{\mathbf{B}\times\boldsymbol{\kappa}\cdot\nabla y}{B^2}$
$\frac{\mathbf{B}\times\nabla B\cdot\nabla x}{B^3}$
$|\nabla y|^2$
$\nabla x\cdot\nabla y$
$|\nabla x|^2$
contribution to Q
z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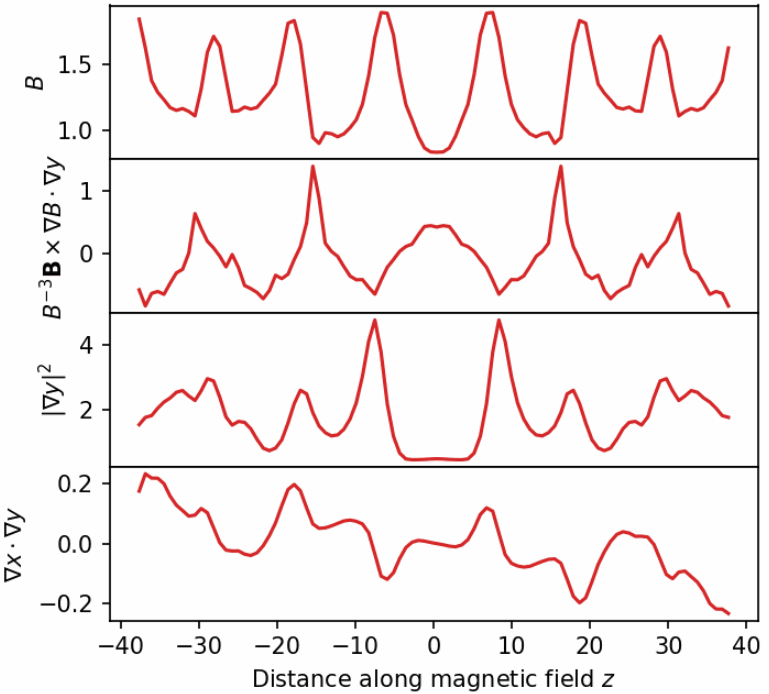
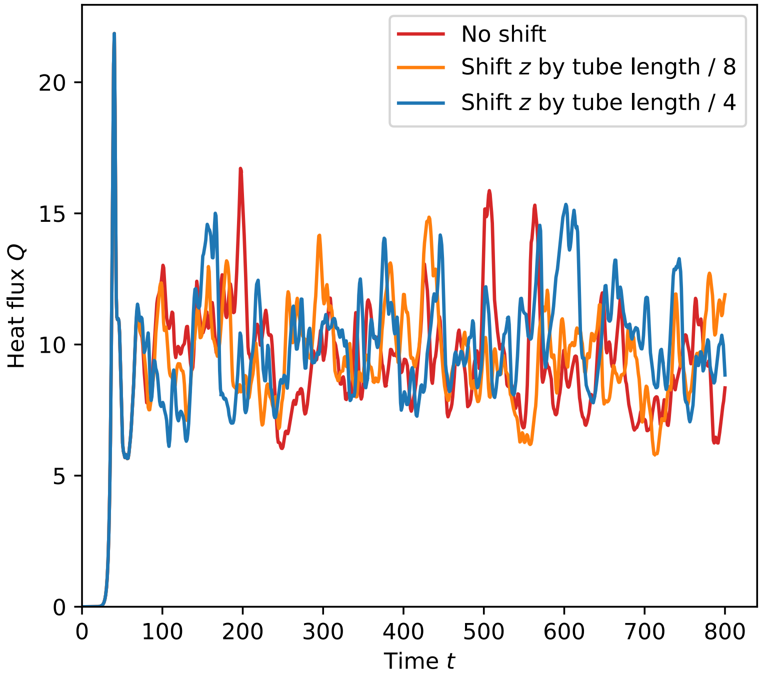
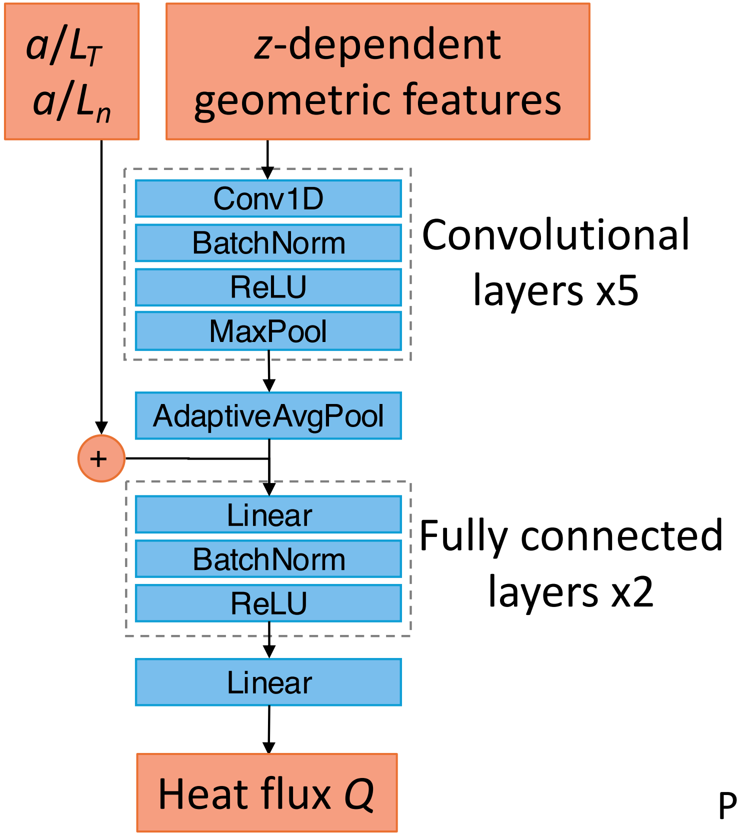
Raw features should *not* be directly fed to classical regression or fully-connected neural network, since model should be translation-invariant

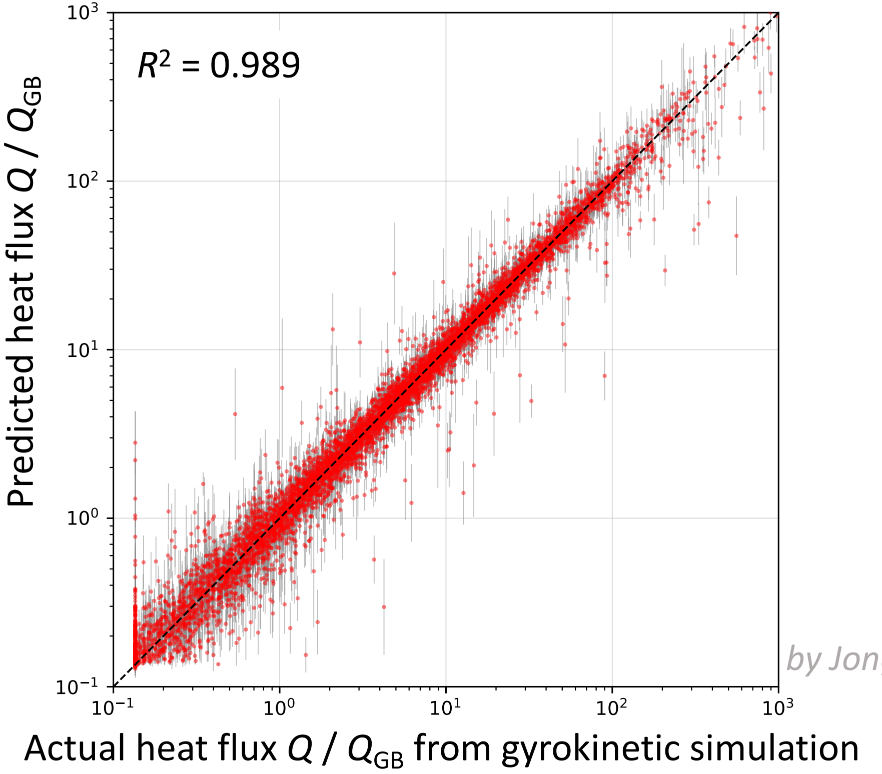
- GK equation, hence heat flux, is invariant under periodic translation of the raw features in z.
- Similar to computer vision, where convolutional neural networks give approximate translation-invariance.





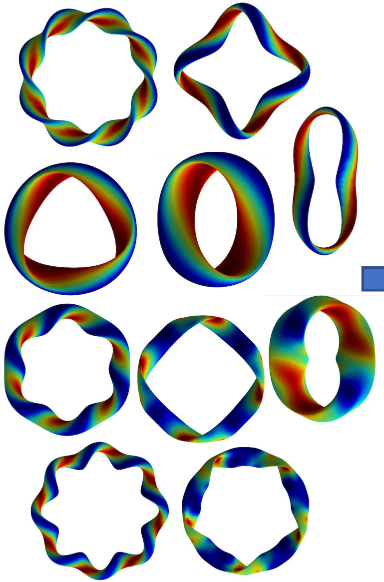
Convolutional neural networks give accurate prediction of the turbulence

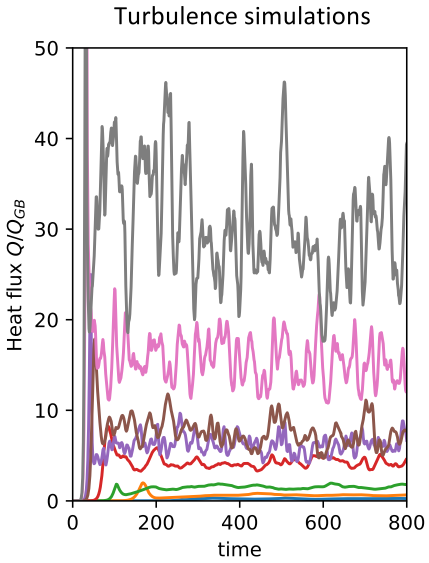




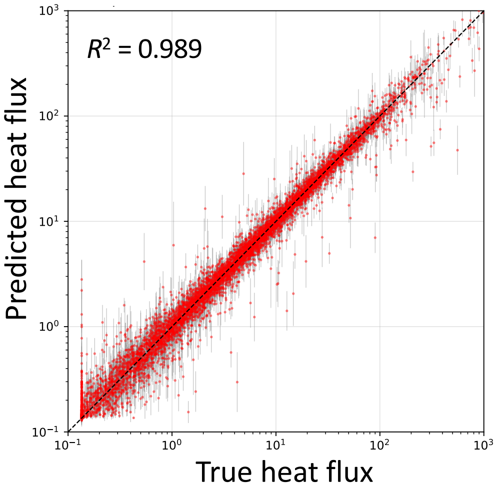
by Jong Choi, ORNL

Prediction in 0.001 sec for single network, 0.1 sec for ensemble





Regression



Feature importance

$$\mathrm{mean}([\Theta(\mathbf{B} \times \kappa \cdot \nabla y) + 0.2] |\nabla x|^3 / B)$$

$$\mathrm{median}((\mathbf{B} \times \nabla B \cdot \nabla x)^2 |\nabla x|^8 / B^8)$$

- Spearman correlation
- Sequential feature selection
- Shapley values
- Testing physics-based surrogates

Our interpretable models use a large library of candidate features, all translation-invariant

Start with inputs to the gyrokinetic equation & local shear:
$F = \{B,\ B^{-3}\mathbf{B}\times\nabla B\cdot\nabla y,\ B^{-2}\mathbf{B}\times\boldsymbol{\kappa}\cdot\nabla y,\ B^{-3}\mathbf{B}\times\nabla B\cdot\nabla x,\ |\nabla x|^2,\ \nabla x\cdot\nabla y,\ |\nabla y|^2,\ d/dz(\nabla x\cdot\nabla y\ /\ |\nabla x|^2)\}$.

U = unary operations on f(z): identity, df/dz, Heaviside(f), Heaviside(-f), ReLU(f), ReLU(-f), 1/f, f^2, f/B (Jacobian), f*B

C(U(F)) = U(F) and all pairwise products of functions in U(F)

Reductions: R = {min, max, max-min, mean, median, mean square, variance, skewness, L_1 norm, quantiles 0.1, 0.25, 0.75, or 0.9, abs of fft coefficients 1-3, $k_{||}$ with largest amplitude, expected $k_{||}$, count above [-2, -1, 0, 1, 2]}

Features: R(U(C(U(F)))) $\Longrightarrow$ > 1 million combinations

Spearman correlation is a quick tool to find the most important feature

- Spearman correlation is the regular Pearson correlation of the the sorted rank of the target with the sorted rank of the feature.
- Its magnitude is invariant to any monotonic nonlinear function, e.g. corr(x, exp(x)) = 1
- No regression model required.
- Features with highest correlation to heat flux *Q* at fixed dT/dx & dn/dx:

Feature	Correlation
$\text{variance}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^2/B)$	0.775
$\text{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^8/B^2)$	0.774
$\text{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^4/B)$	0.772
$\text{variance}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^4/B)$	0.769
$\text{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^4/B^2)$	0.769

Heaviside function: Where there is bad curvature,

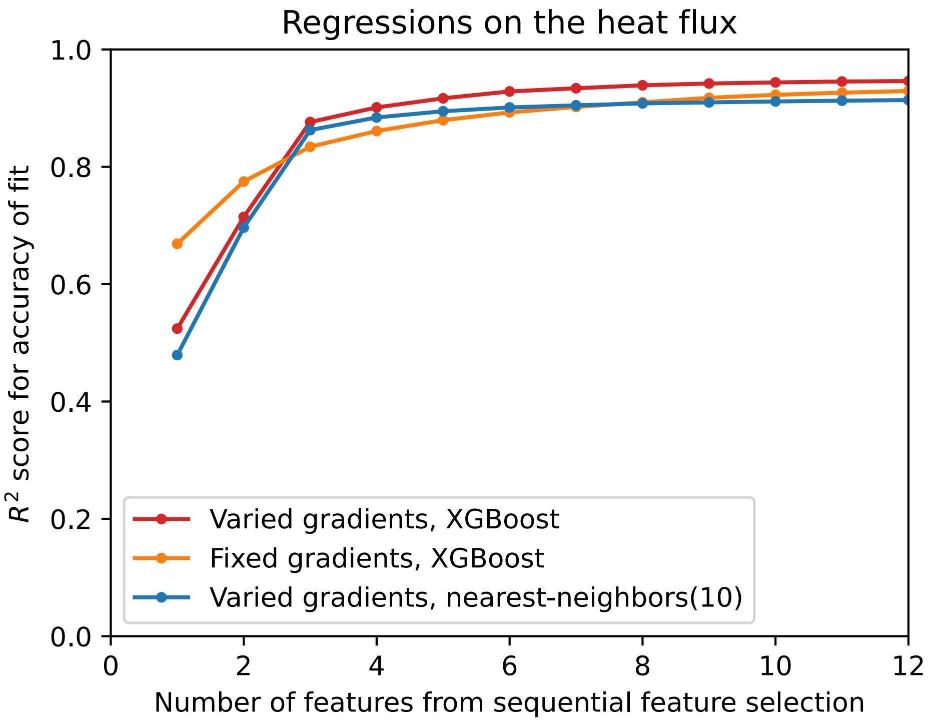
Jacobian (maybe squared)

local temperature gradient in real space (to various powers) $|\nabla T| = (dT/dx)\ |\nabla x|$

Extremely similar to Mynick (2010), Xanthopoulos (2014), Stroteich (2022), Goodman (2024)!

Forward sequential feature selection: ~3 features can be almost as predictive as all features

Stiffness



Critical gradient

Most important features from sequential feature selection

Regression on heat flux

Feature	R^2
a/L_T	0.524
a/L_n	0.714
$\mathrm{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^4/B^2)$	0.876
$\mathrm{median}((\mathbf{B} \times \nabla B \cdot \nabla x)^2\lvert\nabla x\rvert^8/B^8)$	0.901
$\mathrm{absFFTCoeff1}(\mathrm{ReLU}(\mathbf{B} \times \nabla B \cdot \nabla x)/B^5)$	0.917

Classification (stability vs instability)

Feature	log-loss
a/L_T	0.361
a/L_n	0.189
$\mathrm{mean}(\Theta(\mathbf{B} \times \nabla B \cdot \nabla y)\lvert\nabla x\rvert^2/B)$	0.122
$\mathrm{mean}(\Theta(-\mathbf{B} \times \nabla B \cdot \nabla x)\lvert\nabla x\rvert^2 B)$	0.105
$\mathrm{mean}((\mathbf{B} \times \kappa \cdot \nabla y)/B)$	0.094

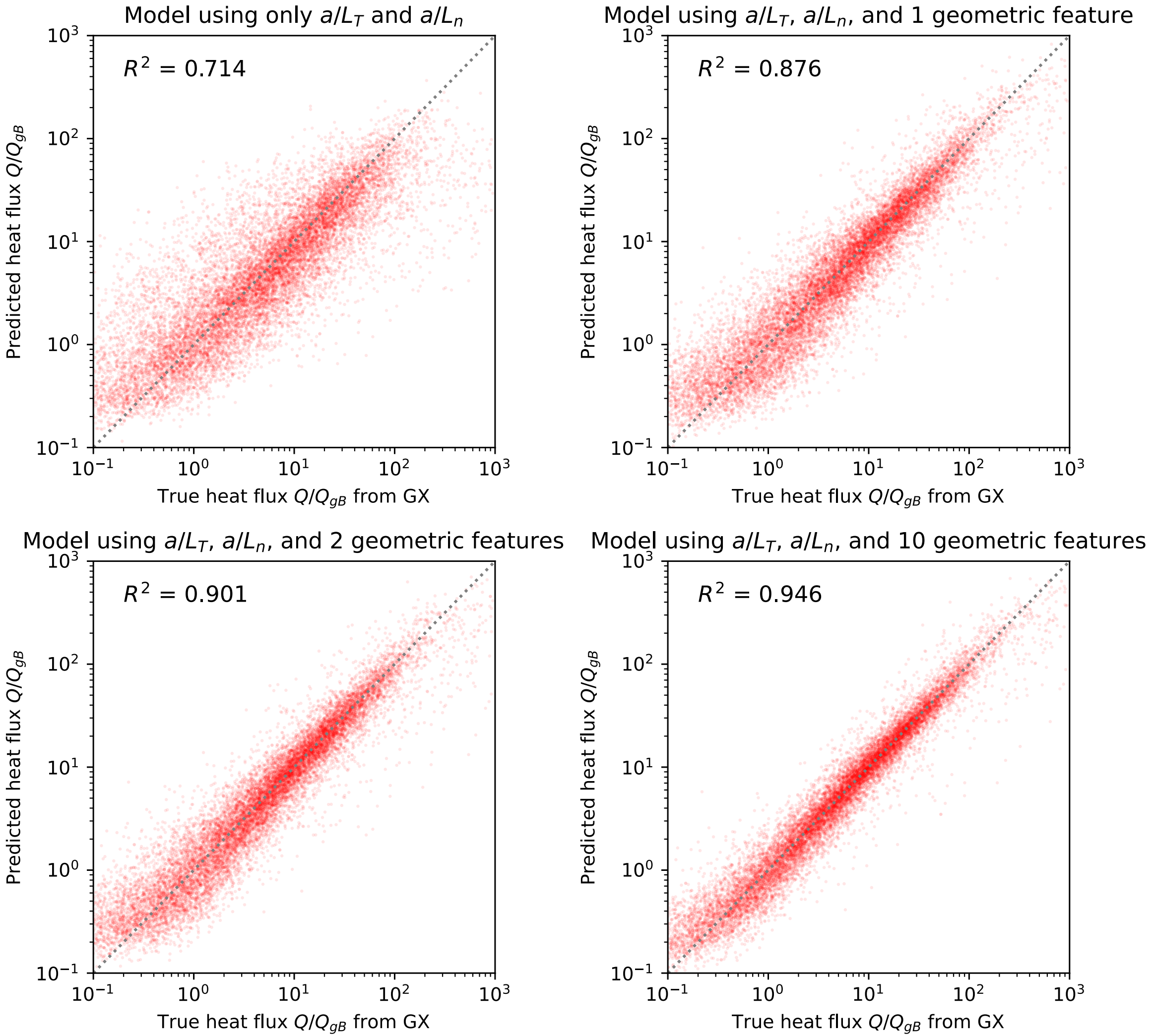
The 2nd most important geometric feature involves flux surface compression and radial ∇B drift

The most important geometric feature is where curvature is bad

The gradients are more important than any geometric feature

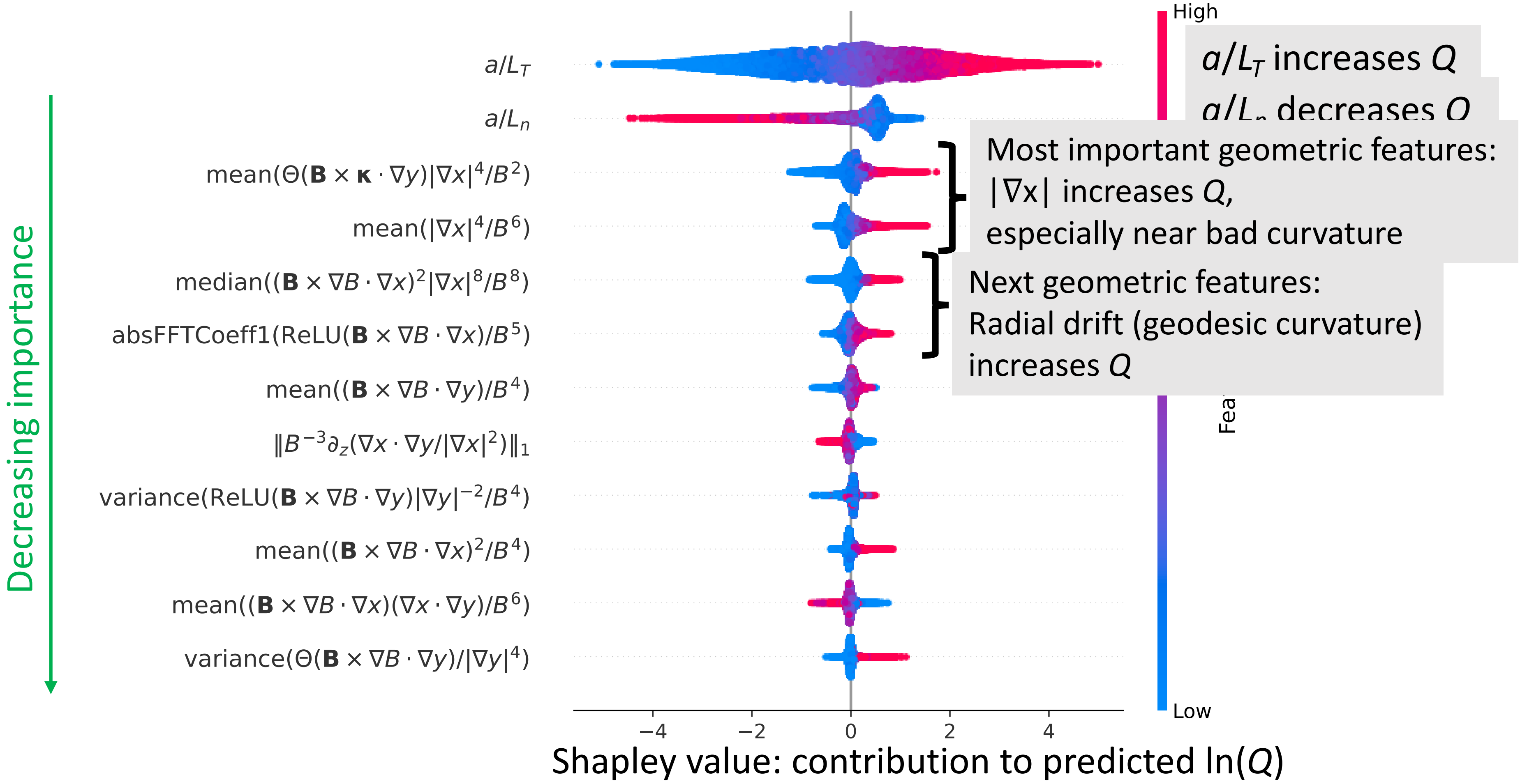
Xanthopoulos et al (2011), Nakata & Matsuoka (2022):
Larger geodesic curvature (= radial drift) ⇒ Stronger damping of zonal flows ⇒ higher heat flux

Sequential feature selection allows closer fit to the data as more geometric features are included

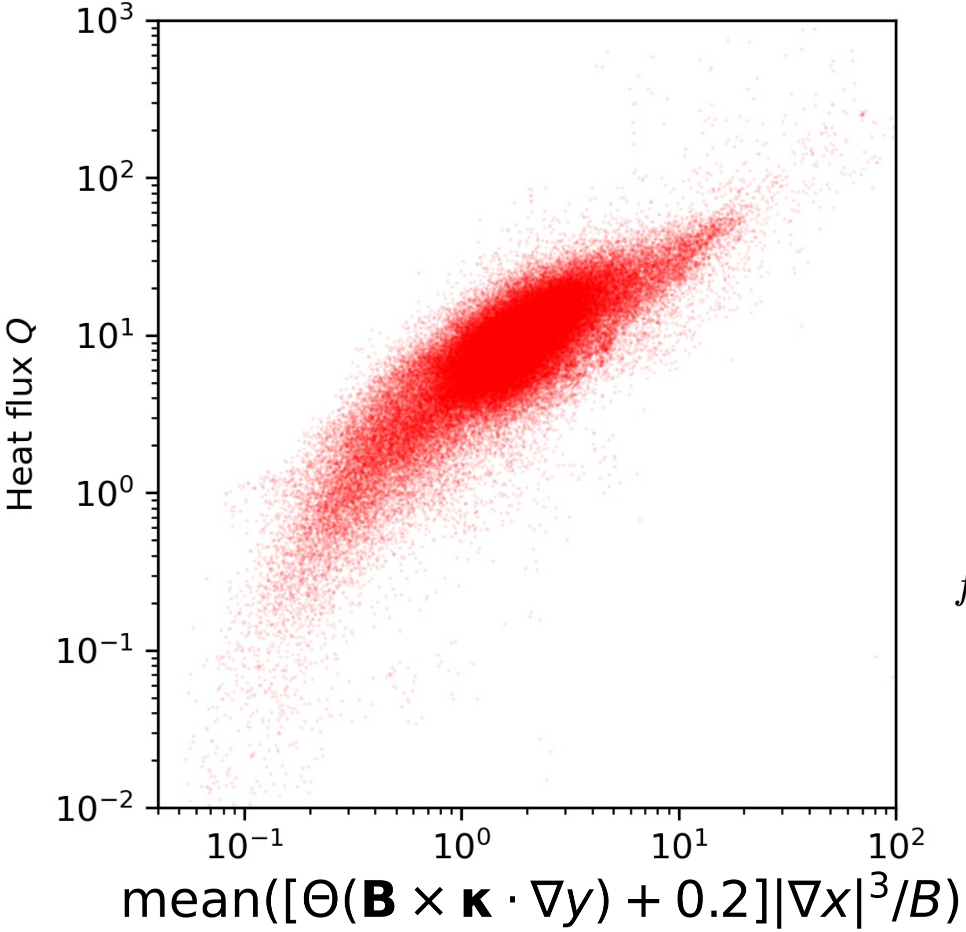


Performance shown on 20% held-out test data

Shapley values show the sign and magnitude of each feature's effect



The first geometric feature can be fine-tuned for even better fit



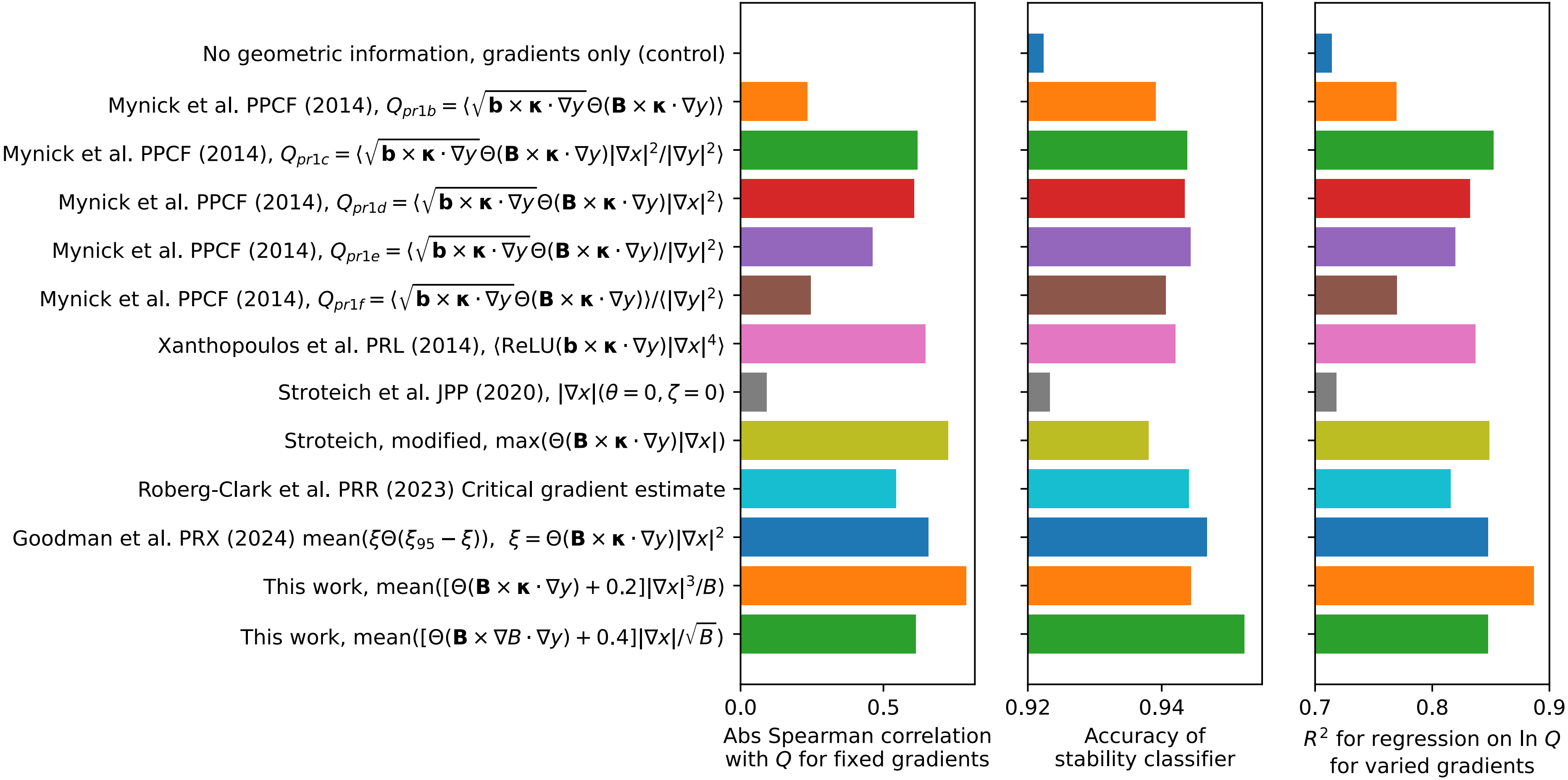
Fixed-gradient dataset.

No regression model used here.

Feature fine-tuned for stability classifier:

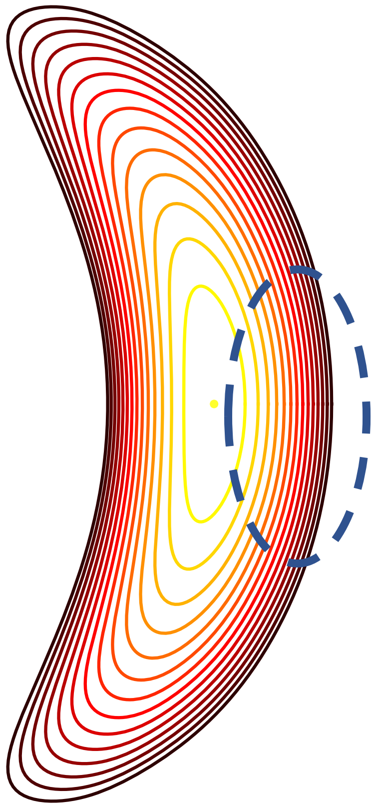
$$f_{\text{stab}} = \text{mean}([\Theta(\mathbf{B} \times \nabla B \cdot \nabla y) + 0.4]|\nabla x|/\sqrt{B})$$

Previously proposed proxies can be tested



Multiple lines of evidence agree that the most important geometric feature is $|\nabla\psi|$ in regions of bad curvature

- Highest Spearman correlation at fixed gradients.
- Consistently the first geometric feature chosen in sequential feature selection:
  - In regression on the heat flux above the critical gradient
  - And in the classifier for stability vs instability (i.e. determines critical gradient)
  - Chosen by XGBoost, nearest-neighbors, & other algorithms
- Also the largest Shapley values



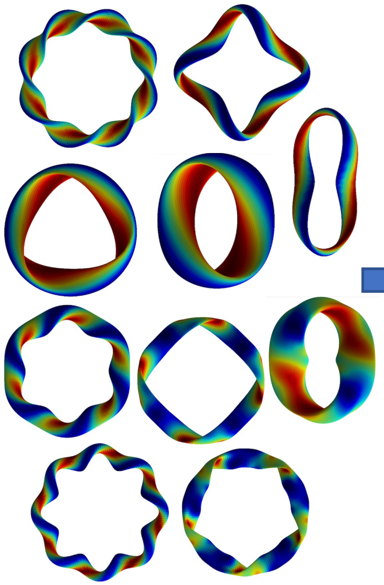
There are many extensions possible

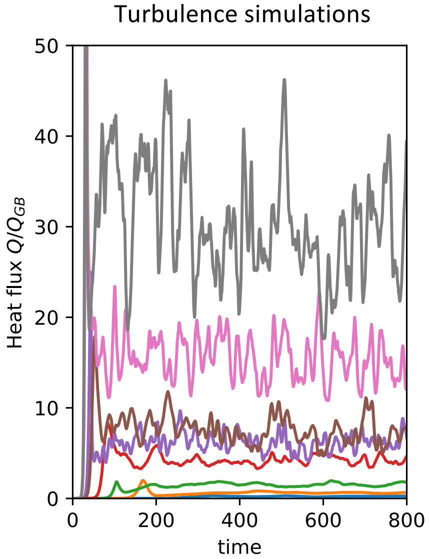
- Try larger sets of possible features
- From the gyrokinetic equation, understand how these features affect turbulence.
- Kinetic electrons, magnetic fluctuations.
- Saliency maps to understand the features learned by the neural networks.
- Symbolic regression.
- Kolmogorov-Arnold Networks.
- Optimization, profile prediction.
- Include & test other physics-motivated features.

Data is online at doi:10.5281/zenodo.14867776, so have a go at it!

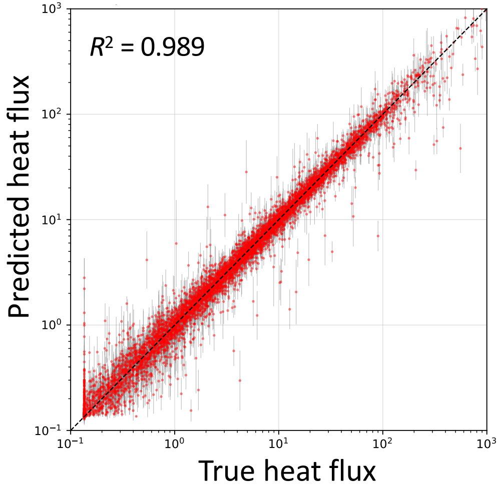
Paper: arXiv:2502.11657

Dataset doi:10.5281/zenodo.14867776





Regression



Feature importance

$$\mathrm{mean}([\Theta(\mathbf{B}\times\kappa\cdot\nabla y)+0.2]|\nabla x|^3/B)$$

$$\mathrm{median}((\mathbf{B}\times\nabla B\cdot\nabla x)^2|\nabla x|^8/B^8)$$

Extra slides

At each step, the top features are variations on a theme

Sequential feature selection step 3

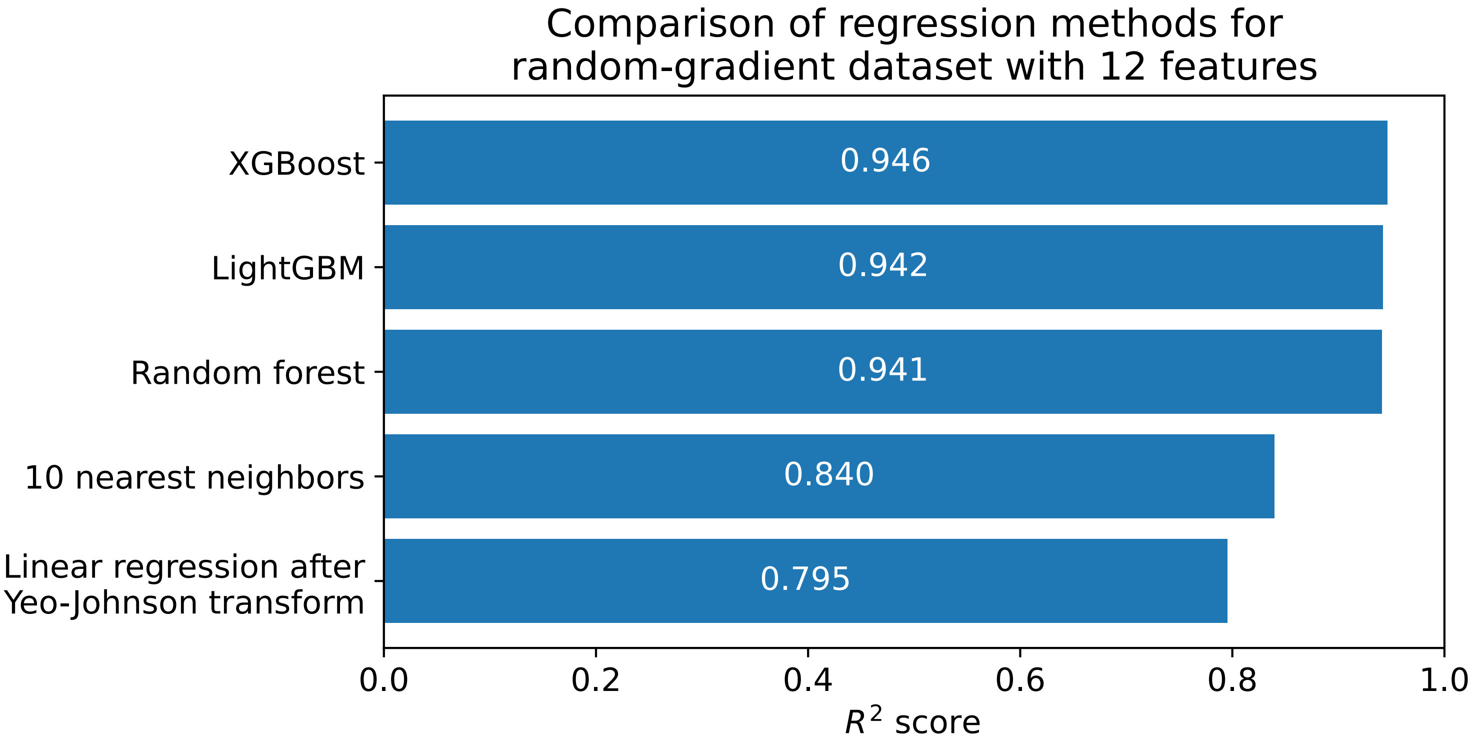
Feature	R^2
$\text{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^4/B^2)$	0.876
$\text{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^4/B)$	0.874
$\text{variance}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^2/B)$	0.871
$\text{quantile0.9}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^2/B)$	0.870
$\text{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\lvert\nabla x\rvert^8/B^4)$	0.869

Sequential feature selection step 4

Feature	R^2
$\text{median}((\mathbf{B} \times \nabla B \cdot \nabla x)^2\lvert\nabla x\rvert^8/B^8)$	0.901
$\text{quantile0.75}(\text{ReLU}(-\mathbf{B} \times \nabla B \cdot \nabla x)^2\lvert\nabla x\rvert^8/B^6)$	0.901
$\text{median}((\mathbf{B} \times \nabla B \cdot \nabla x)^2\lvert\nabla x\rvert^8/B^6)$	0.901
$\text{median}(\lvert\mathbf{B} \times \nabla B \cdot \nabla x\rvert\lvert\nabla x\rvert^4/B^4)$	0.901
$\text{quantile0.75}(\text{ReLU}(-\mathbf{B} \times \nabla B \cdot \nabla x)\lvert\nabla x\rvert^4/B^3)$	0.901

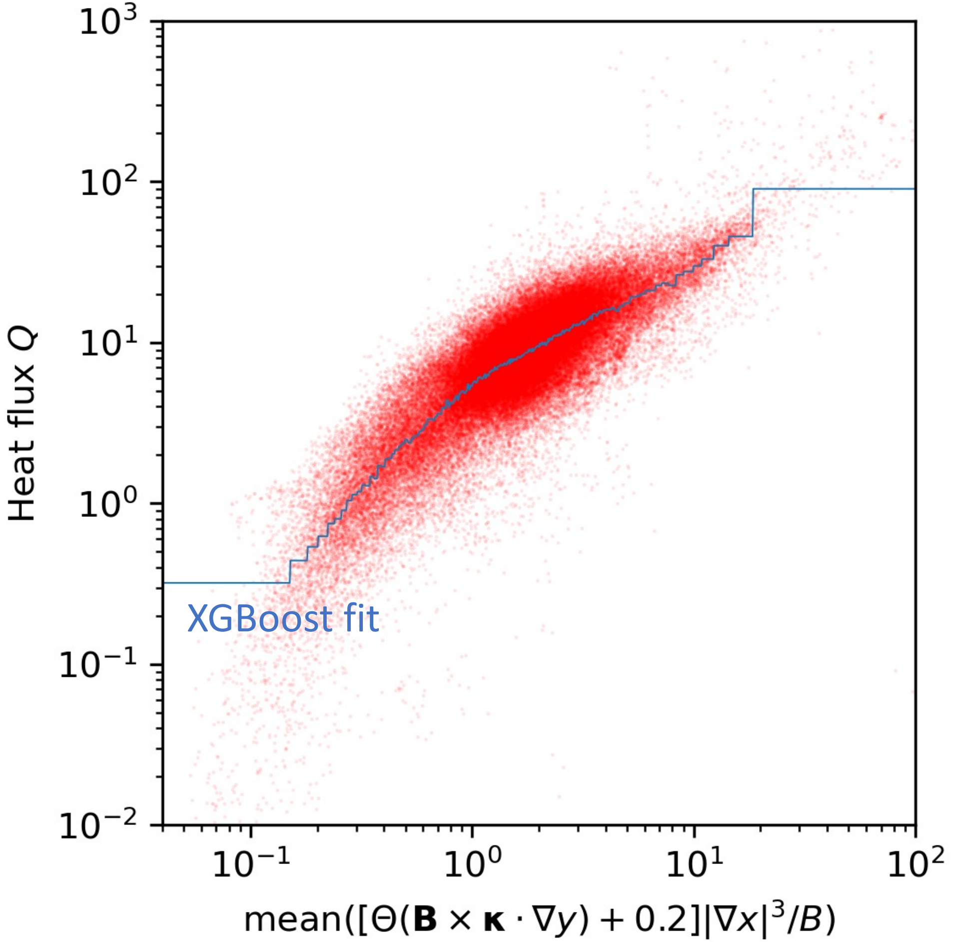
Regression for the random-gradient dataset

Other machine learning regression methods work also



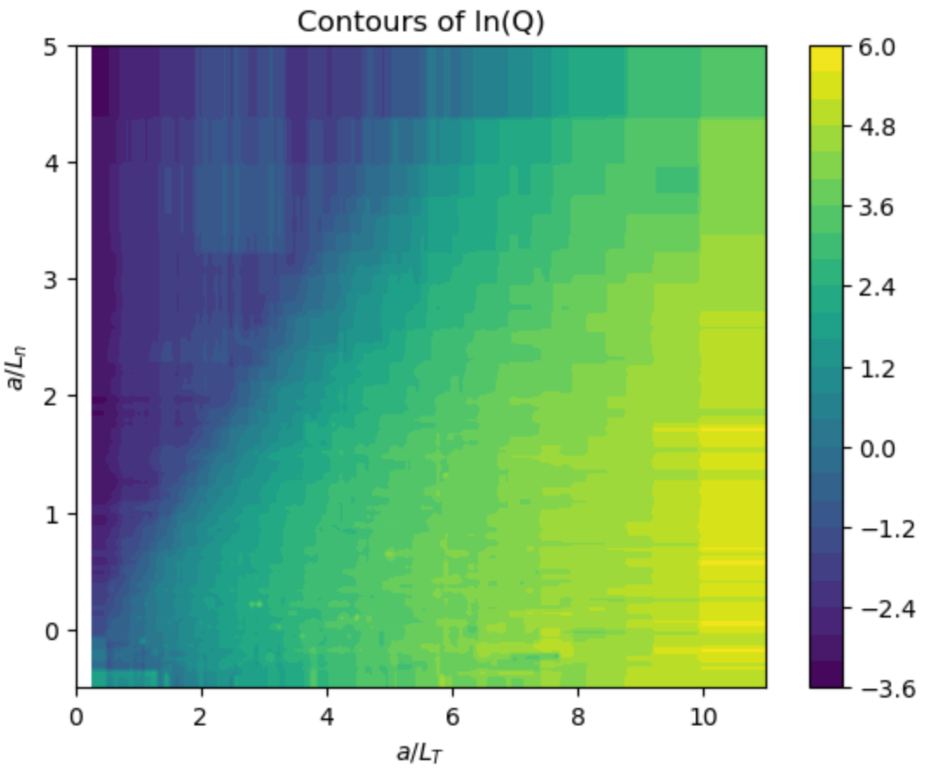
All using a/L_T, a/L_n, and the top 10 geometric features selected via XGBoost

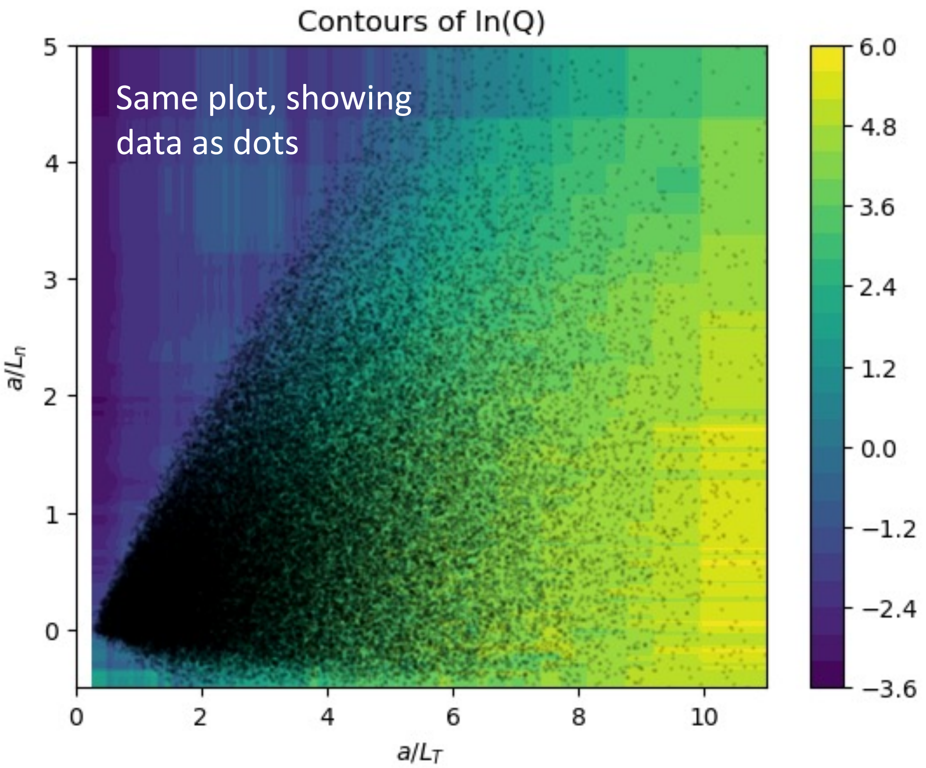
XGBoost regression model with 1 feature



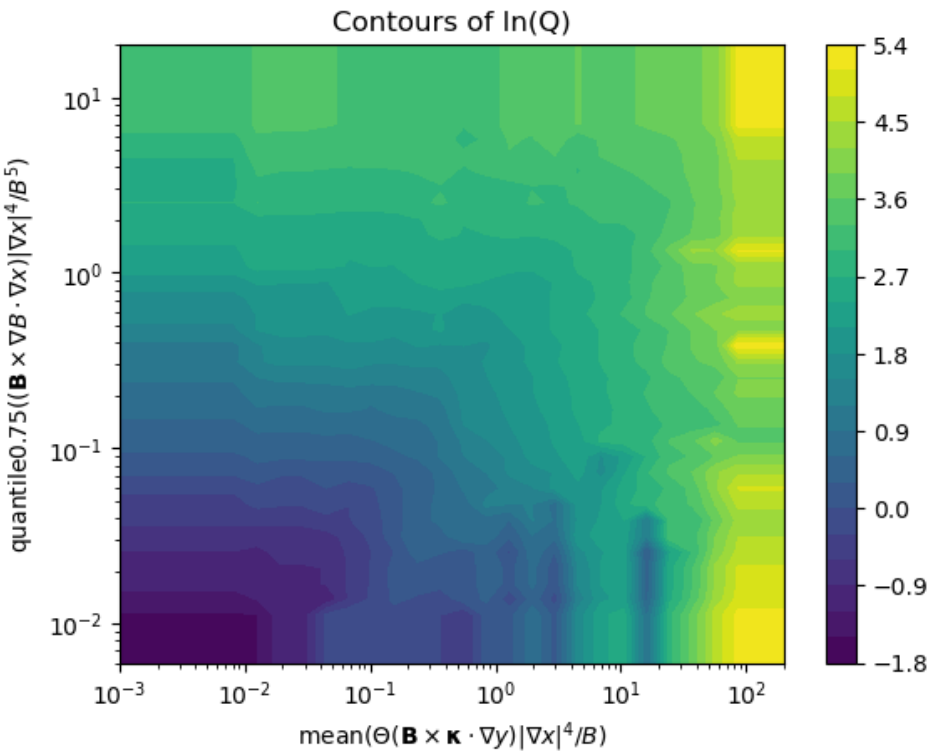
Fixed-gradient dataset

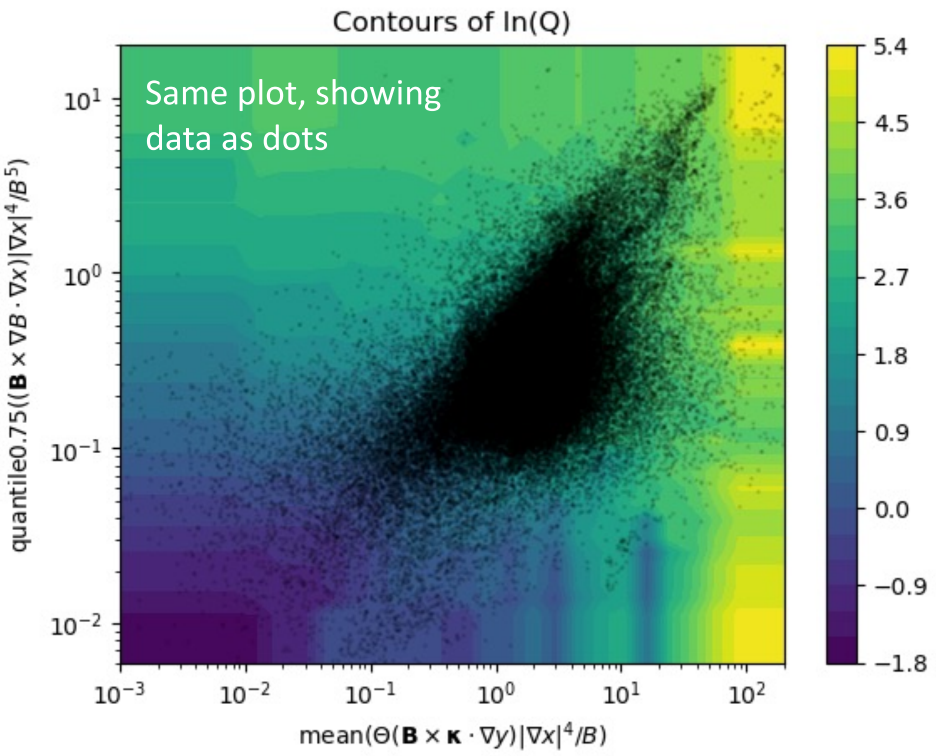
XGBoost regression model using only a/LT and a/Ln

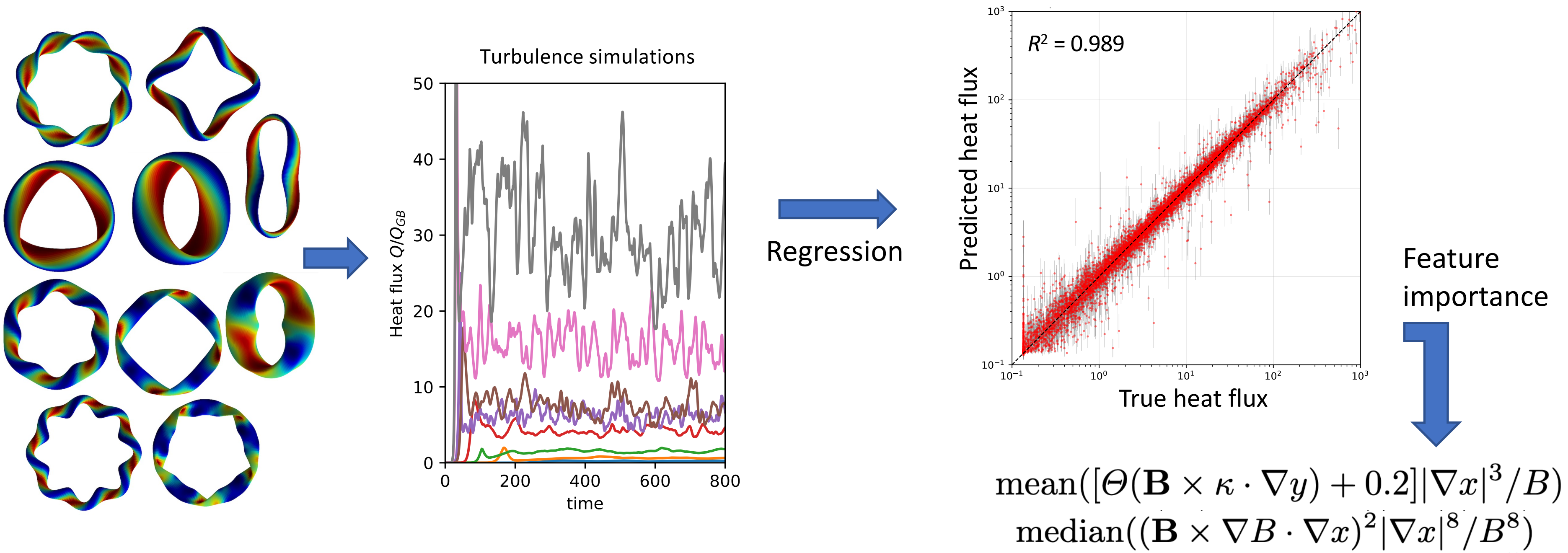




XGBoost regression model for fixed gradients using 2 features



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