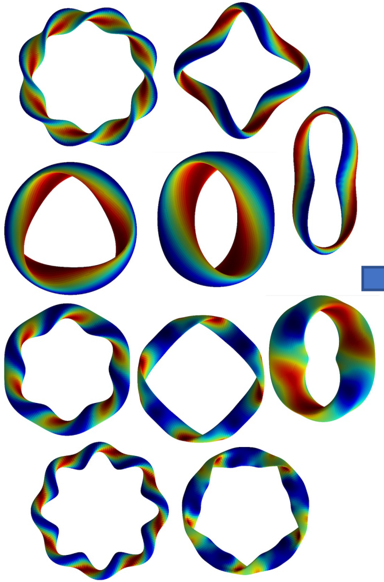
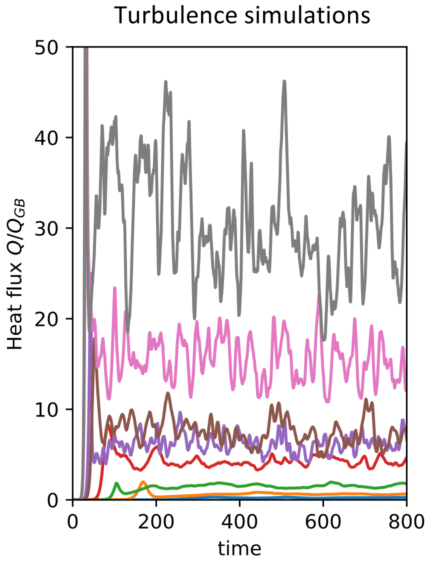
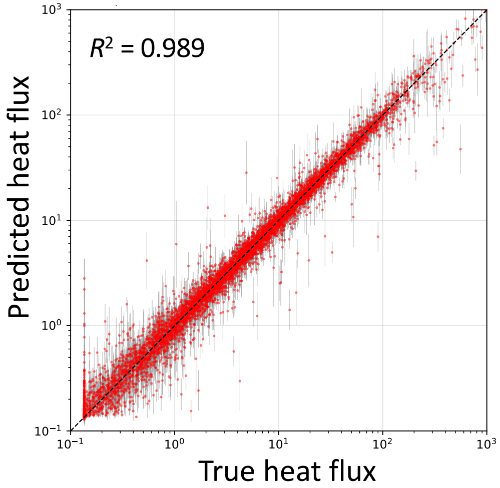
How does magnetic geometry affect ITG turbulence? Insights from data & machine learning





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**

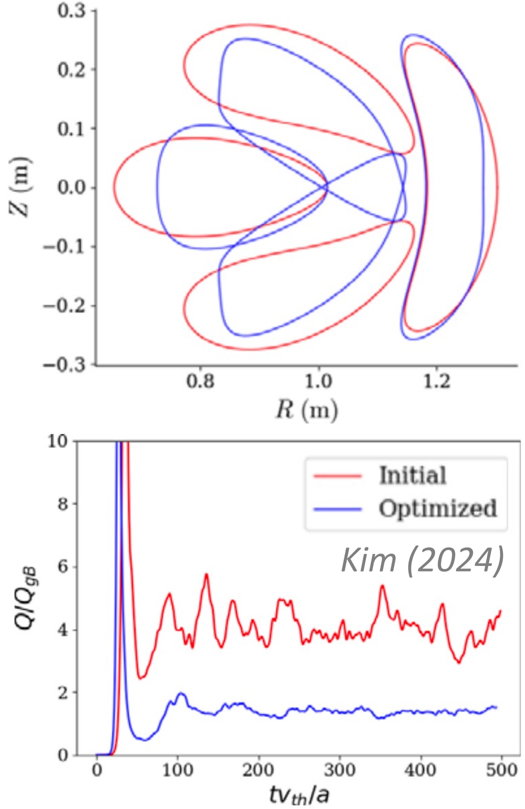
Thanks to many others who gave suggestions

Supported by the US DOE StellFoundry SciDAC

Motivations

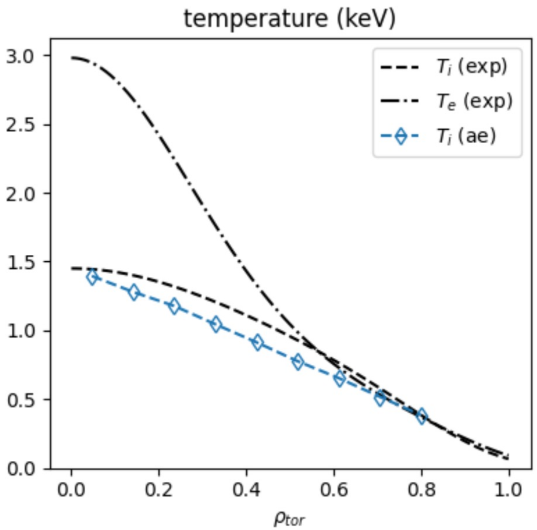
Understanding

Optimization

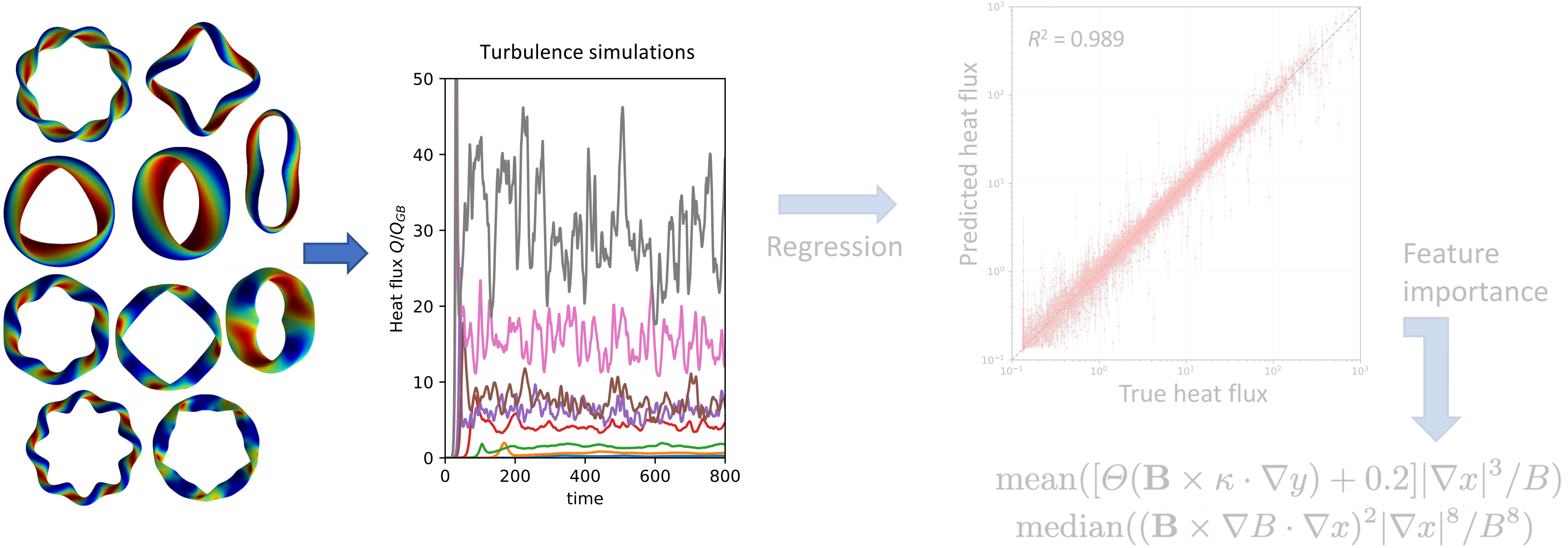


Kim (2024)

Profile prediction

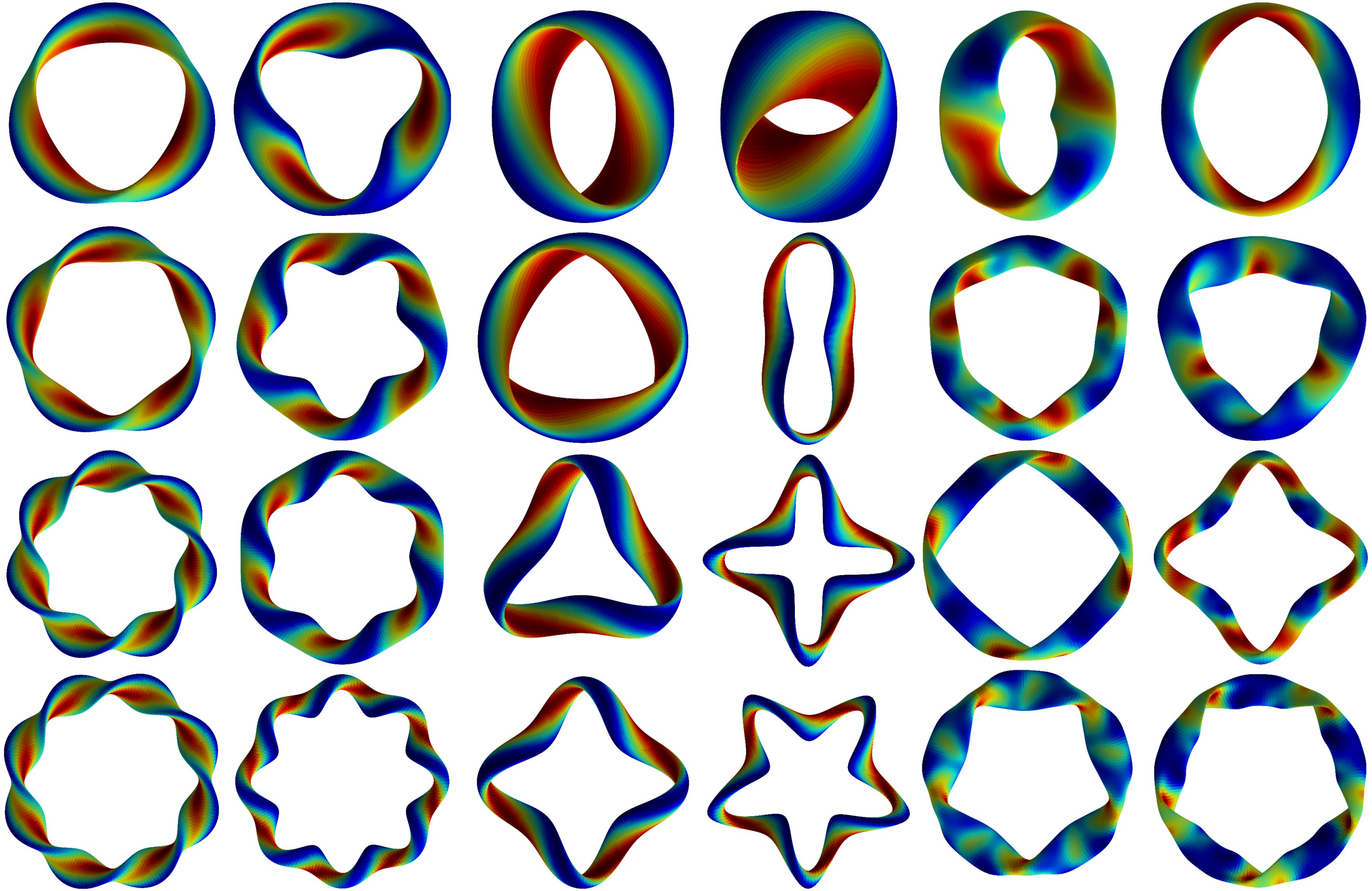


Mandell (2024)



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 include rotating ellipses, quasi-symmetric, and random shapes

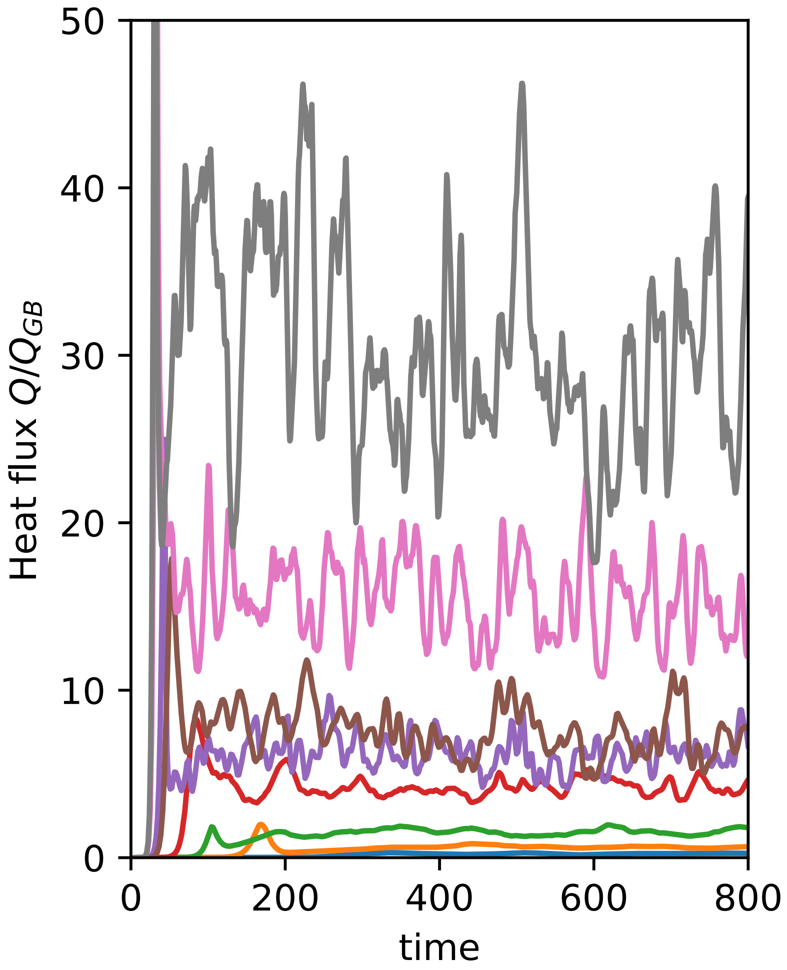


Aspect ratio, elongation, $q = 1 / \iota$, β, and number of field periods are all varied.

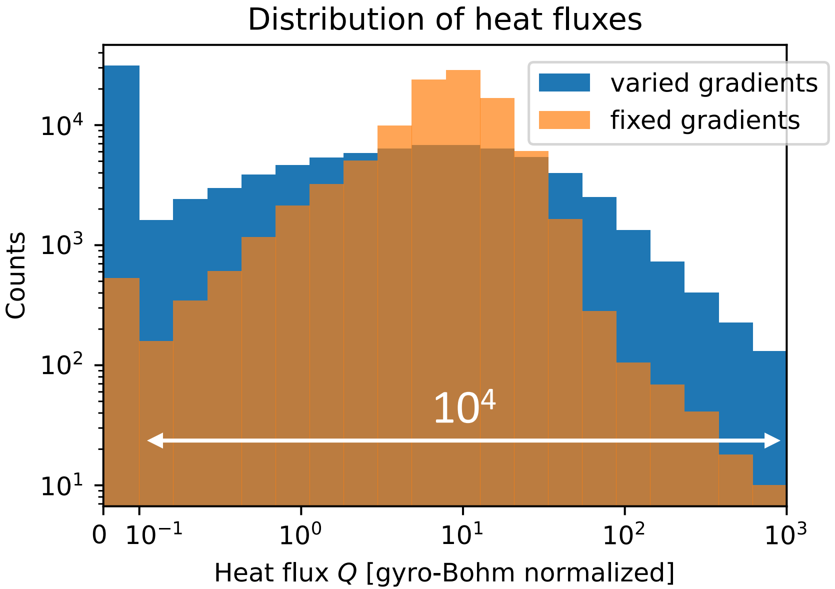
All configurations scaled to have same gyroBohm normalizations

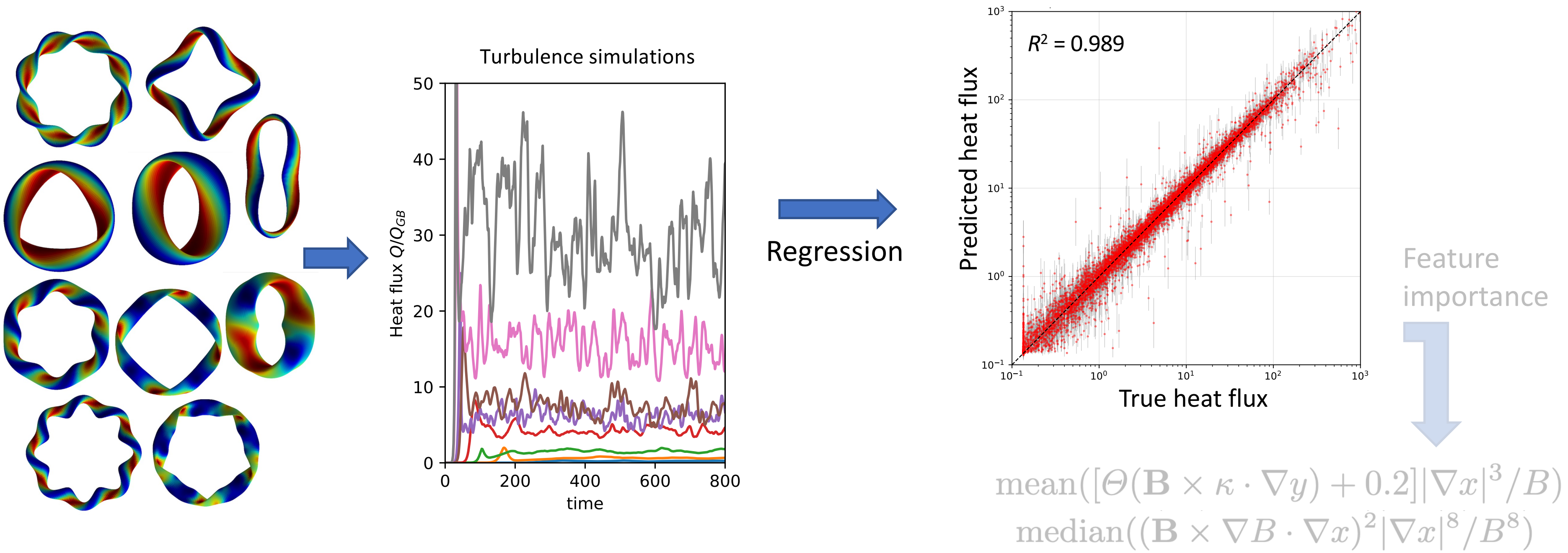
(Tokamak generation underway by Ralf Mackenbach)

Nonlinear turbulence simulations were run with GX in every equilibrium

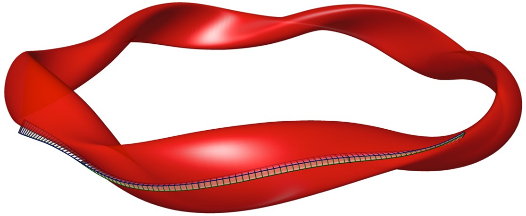


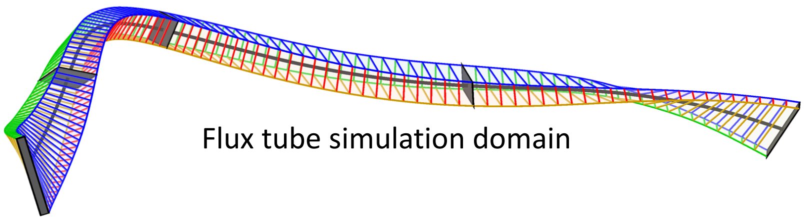
- Electrostatic, adiabatic electrons.
- 1 simulation in each tube with random dT/dx and dn/dx.
- 1 simulation in each tube with (a/T) dT/dx = 3, (a/n) dn/dx=0.9
- 8 minutes to get heat flux on 1 GPU
- 2×10^5 nonlinear simulations took < 7000 node-hours




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

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

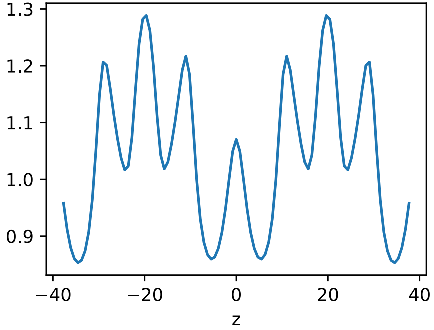




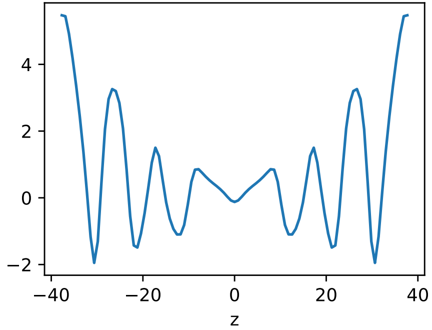
$$\boldsymbol{B} = B_{ref} \nabla x \times \nabla y$$

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

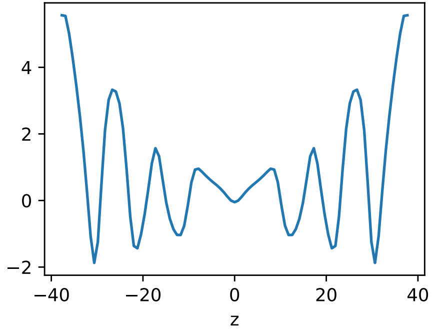
$|B|$



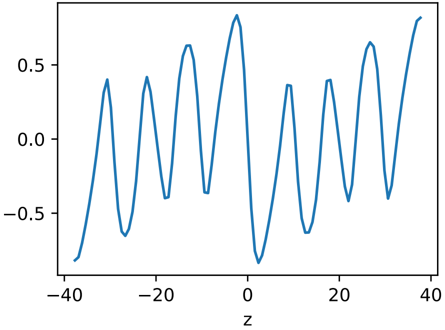
$|B|^{-3}\boldsymbol{B}\times\nabla|B|\cdot\nabla y$



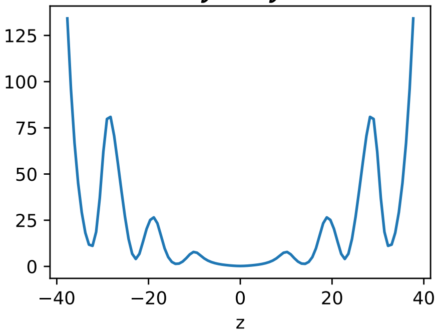
$|B|^{-2}\boldsymbol{B}\times\boldsymbol{\kappa}\cdot\nabla y$



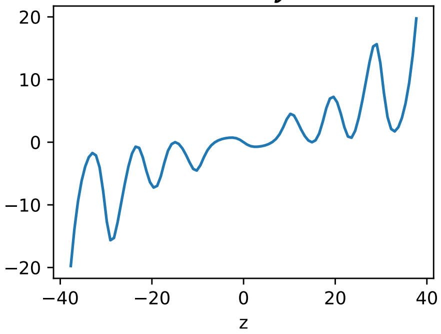
$|B|^{-3}\boldsymbol{B}\times\nabla|B|\cdot\nabla x$



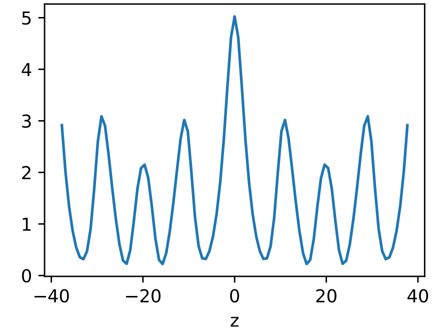
$\nabla y\cdot\nabla y$



$\nabla x\cdot\nabla y$



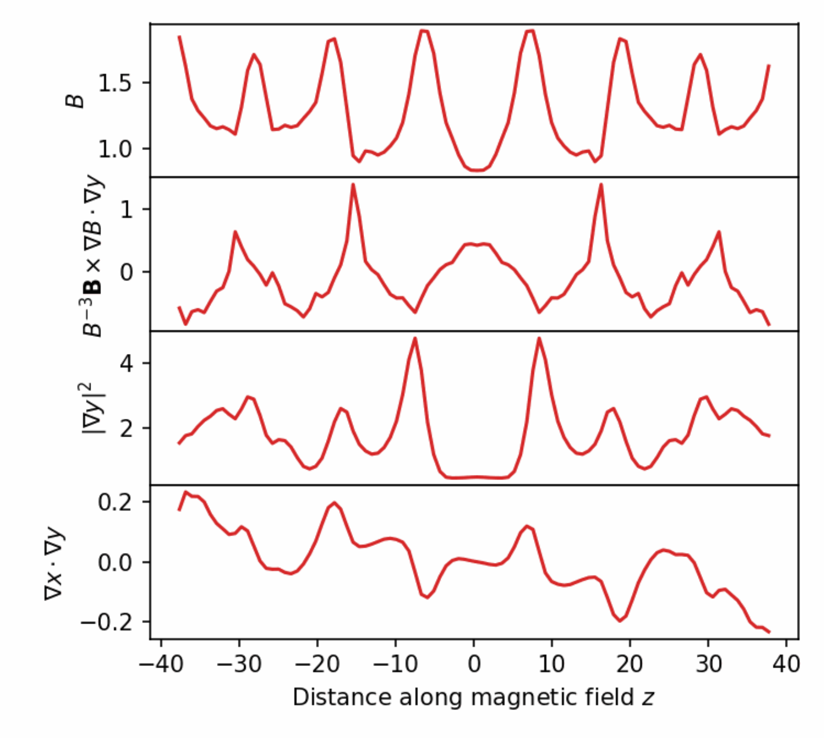
$\nabla x\cdot\nabla x$

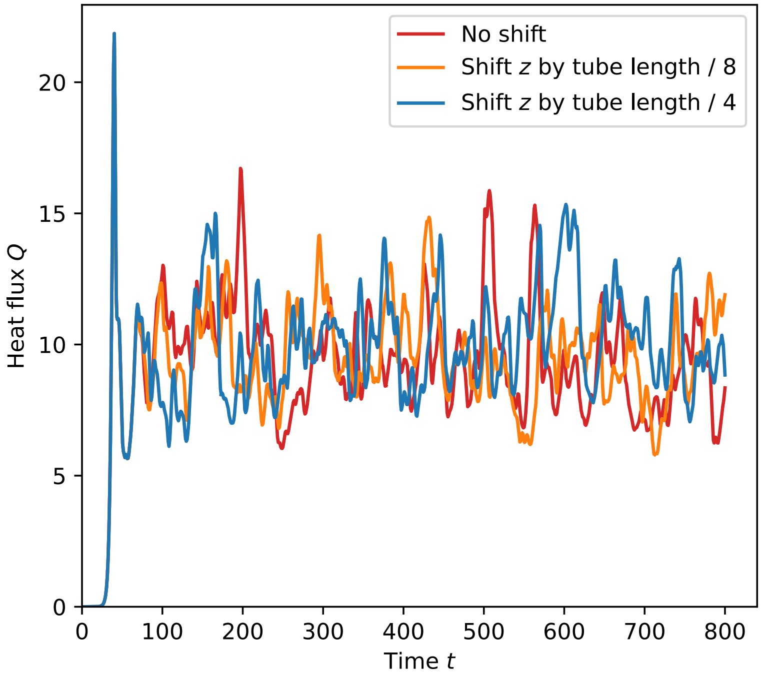


$\boldsymbol{b}\cdot\nabla z$ is constant and the same for all configs, as are tube lengths in meters, so Fourier modes ($k_{||}$) can be compared between configurations.

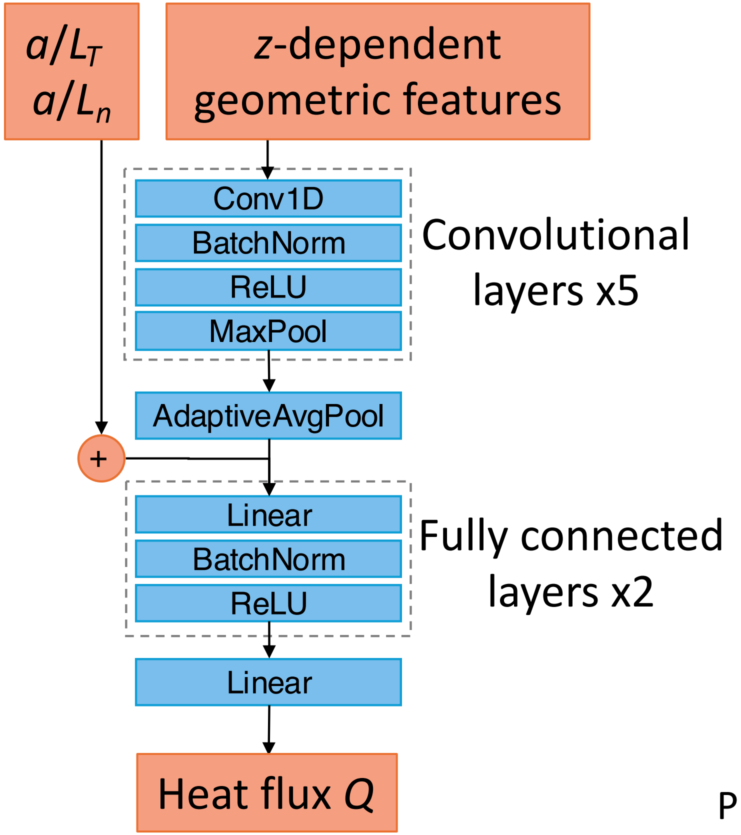
Raw features should *not* be directly fed to classical regression or fully-connected neural network, since model should be translation-invariant

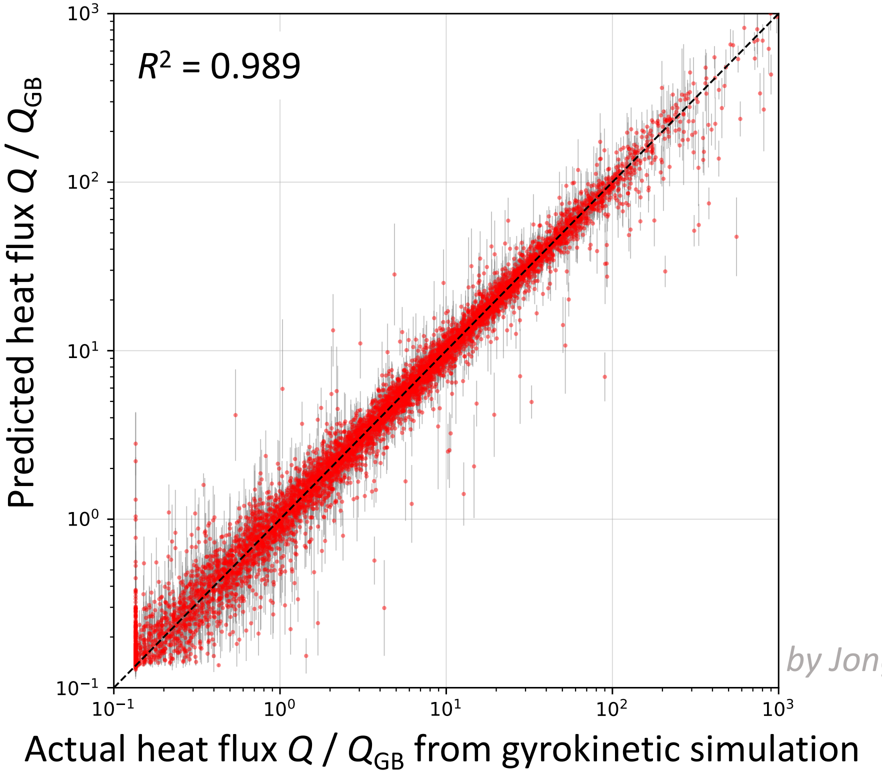
- GK equation, hence heat flux, is invariant under periodic translation of the raw features in z.
- Similar to computer vision, where convolutional neural networks give approximate translation-invariance.





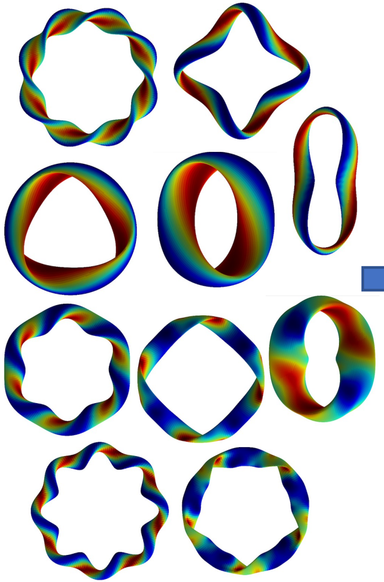
Convolutional neural networks give accurate prediction of the turbulence

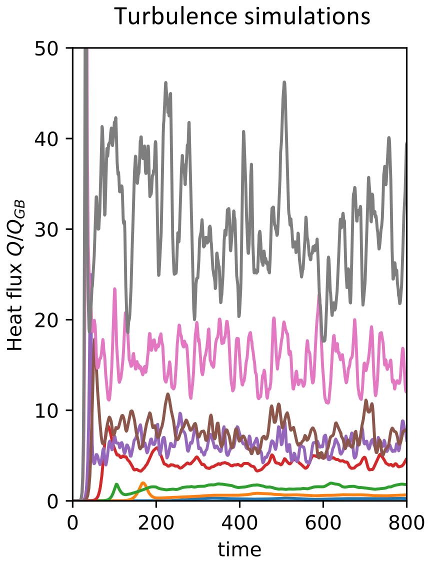




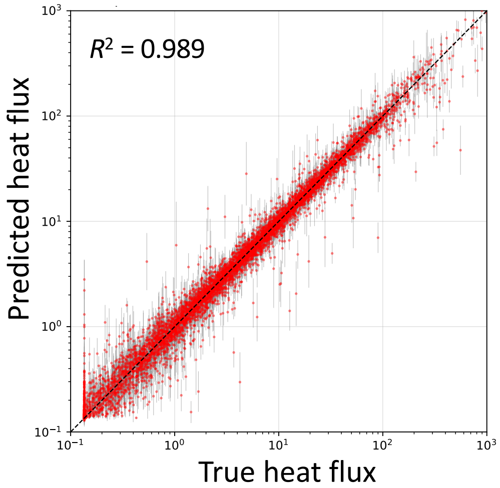
by Jong Choi, ORNL

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:
B, $B^{-3}\mathbf{B}\times\nabla B\cdot\nabla y$, $B^{-2}\mathbf{B}\times\boldsymbol{\kappa}\cdot\nabla y$, $B^{-3}\mathbf{B}\times\nabla B\cdot\nabla x$,
$|\nabla x|^2$, $\nabla x\cdot\nabla y$, $|\nabla y|^2$, $d/dz(\nabla x\cdot\nabla y / |\nabla x|^2)$.

Apply unary operations on $f(z)$: f^2, df/dz, Heaviside(f), etc.,

Include all pairwise products,

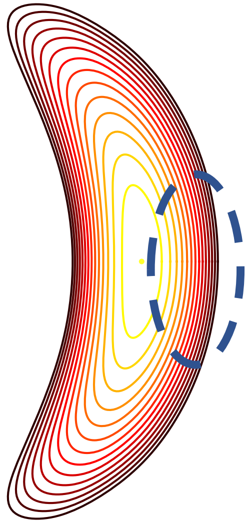
Reductions: max, median, abs of fft coefficients, $k_{||}$ with largest amplitude, etc.

$\Longrightarrow$ > 1 million combinations

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

- Unlike Pearson, Spearman is invariant to any monotonic function.
- Features with highest correlation to heat flux *Q* at fixed dT/dx & dn/dx:

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



Heaviside function: Where there is bad curvature,

local temperature gradient in real space (to various powers)

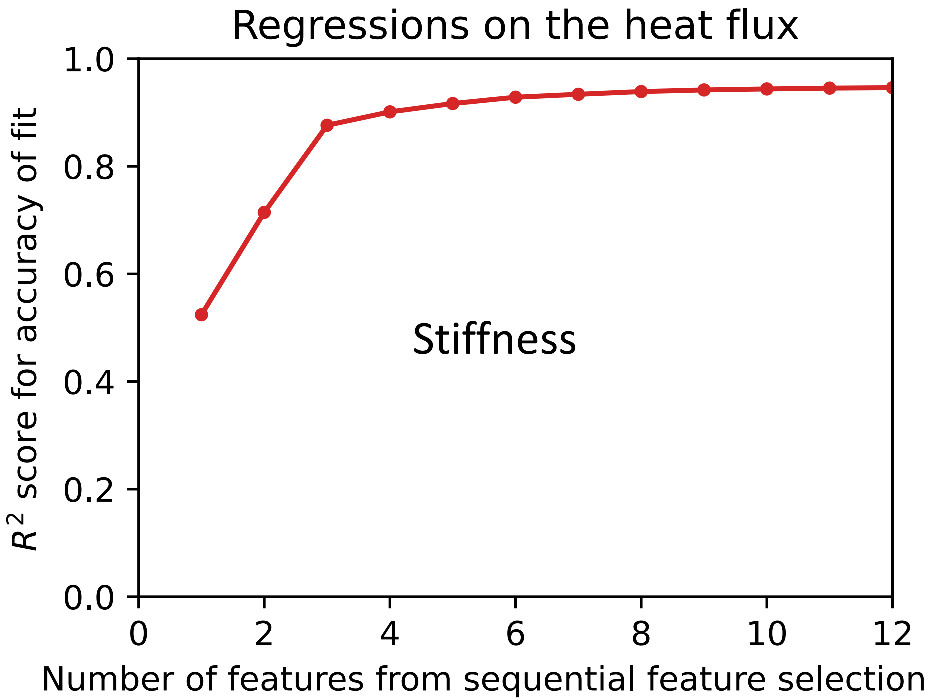
Jacobian (maybe squared)

$|\nabla T| = (dT/dx)\ |\nabla x|$

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

?!?! $|\nabla x|$ does not appear in gyrokinetic equation for $k_x = 0$ modes!

Another method to identify most important features: forward sequential feature selection



Stiffness

Critical gradient

Using decision trees (XGBoost library), varied-gradient dataset

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

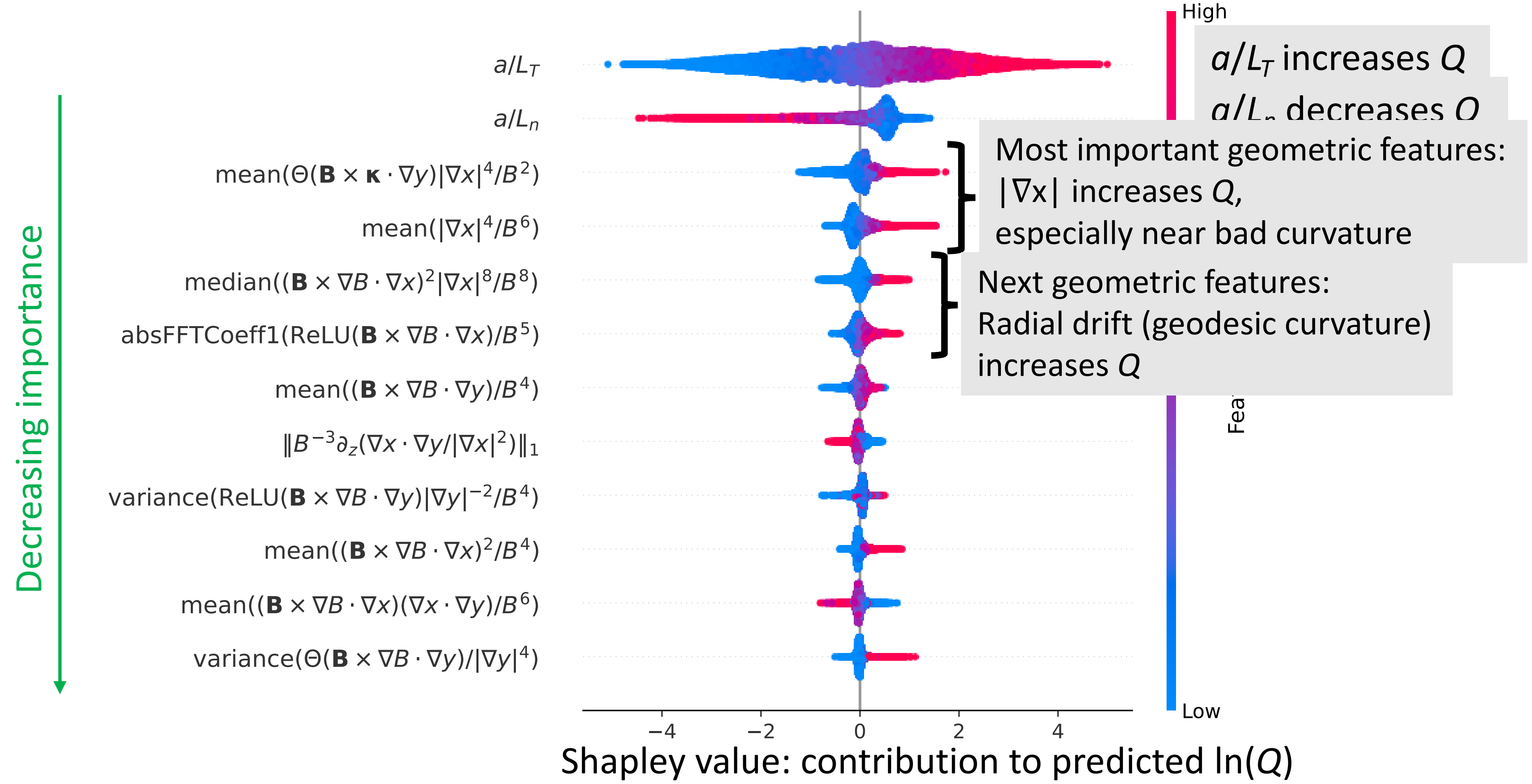
The gradients are more important than any geometric feature

The most important geometric feature is flux surface compression where curvature is bad

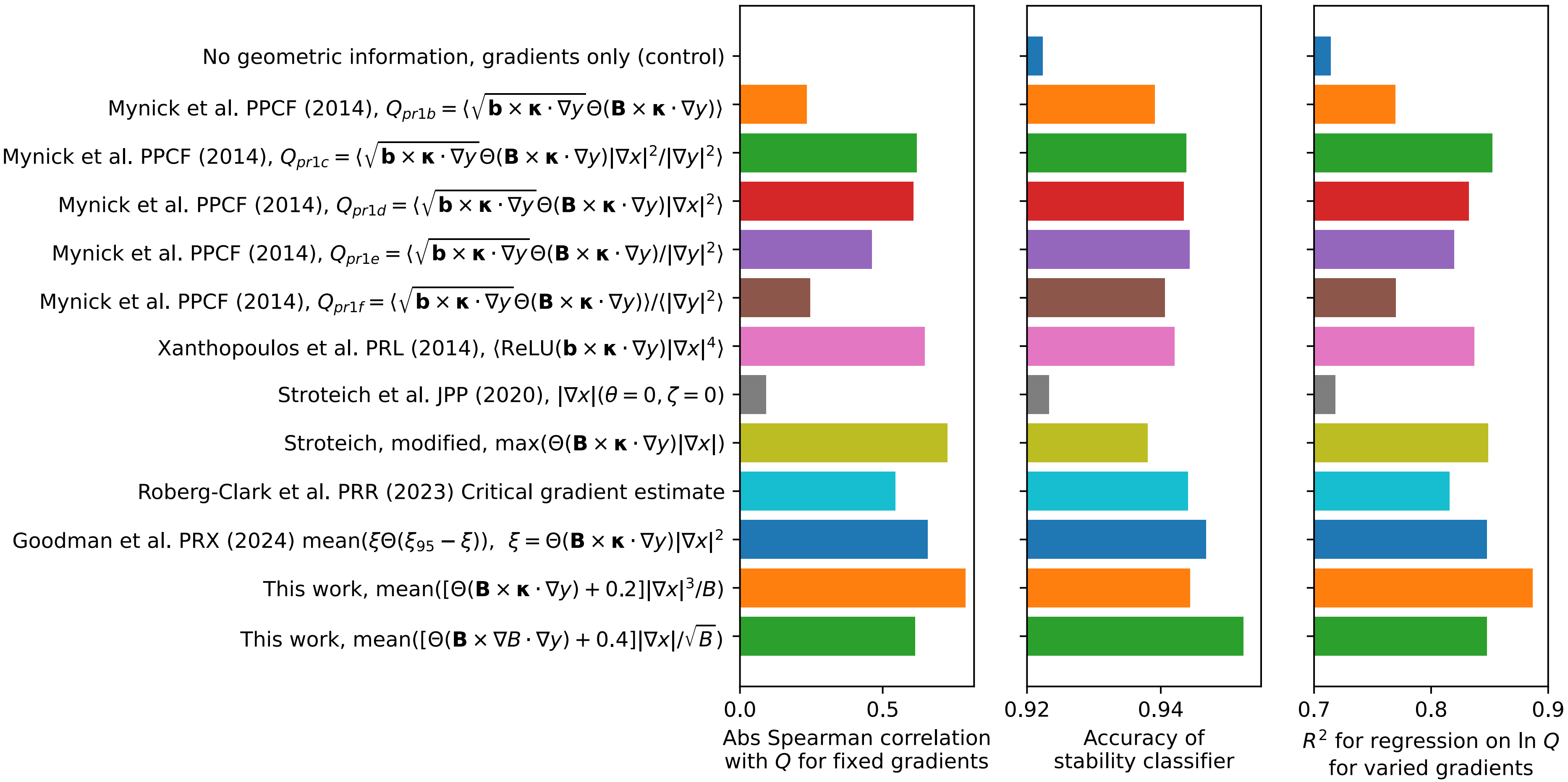
The 2nd most important geometric feature involves flux surface compression and radial ∇B drift

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

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



Previously proposed proxies can be tested



Summary

- Interpretable ML can reveal trends and stimulate theory.
- Most important feature for ITG seems to be $|\nabla\psi|$ in regions of bad curvature.

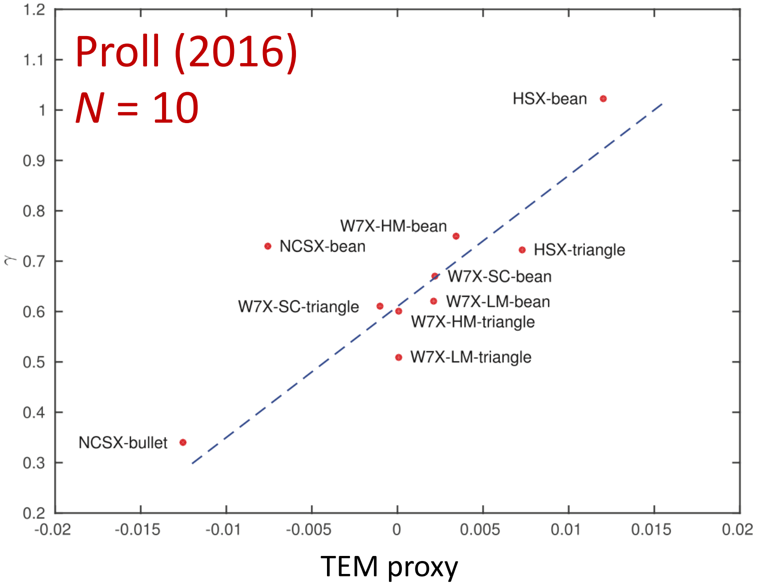
Future work

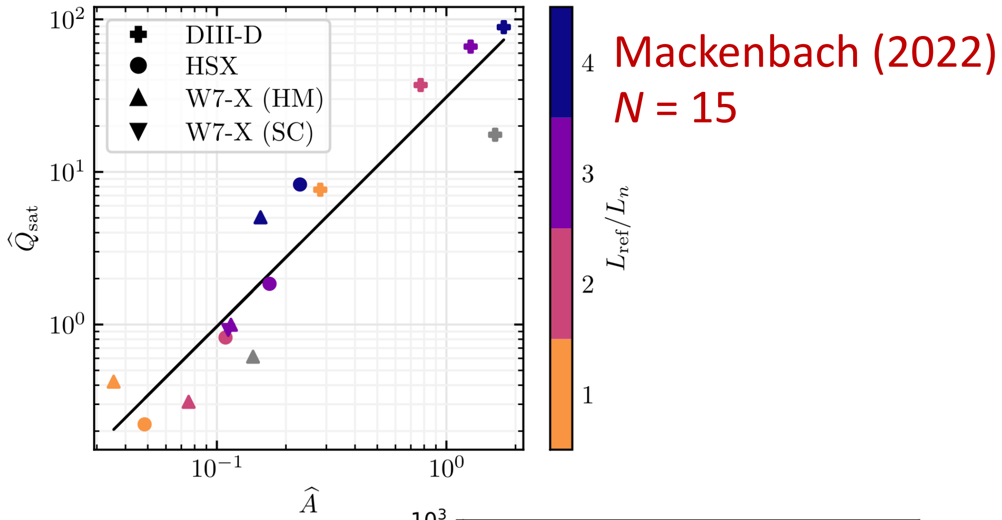
- From the gyrokinetic equation, understand how top features affect turbulence.
- Saliency maps to understand the features learned by the neural networks.
- Other interpretable methods (symbolic regression, Kolmogorov-Arnold Networks)
- Kinetic electrons, magnetic fluctuations.
- Optimization & profile prediction.

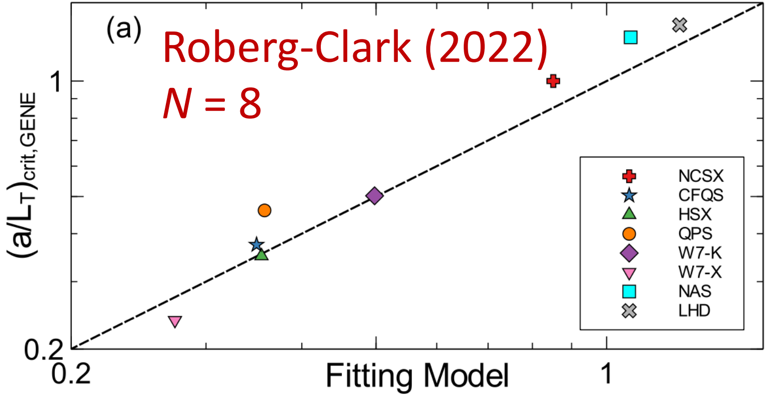
Paper:
arXiv:2502.11657

Dataset
doi:10.5281/zenodo.14867776

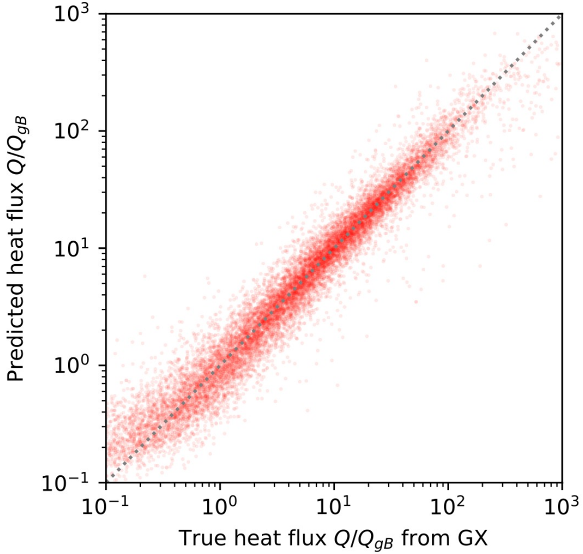
Extra slides







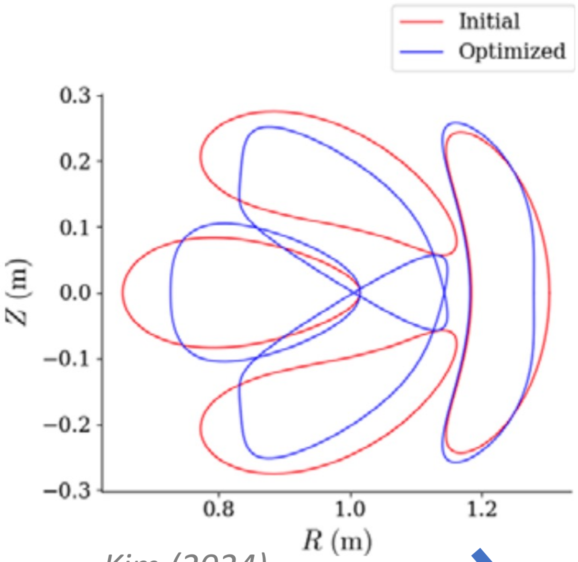
This work:
N = 100,705



Motivations

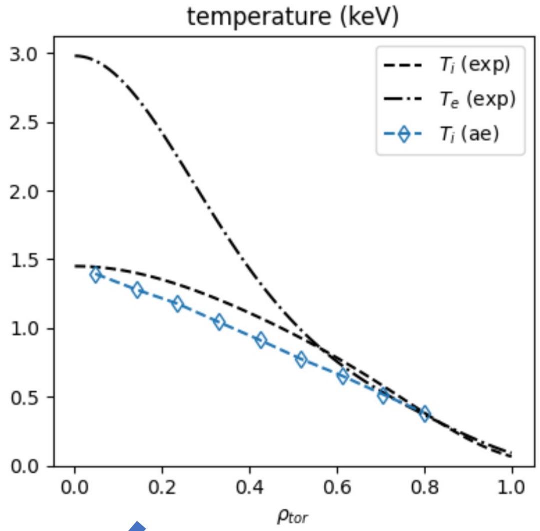
Understanding

Optimization



Kim (2024)

Profile prediction

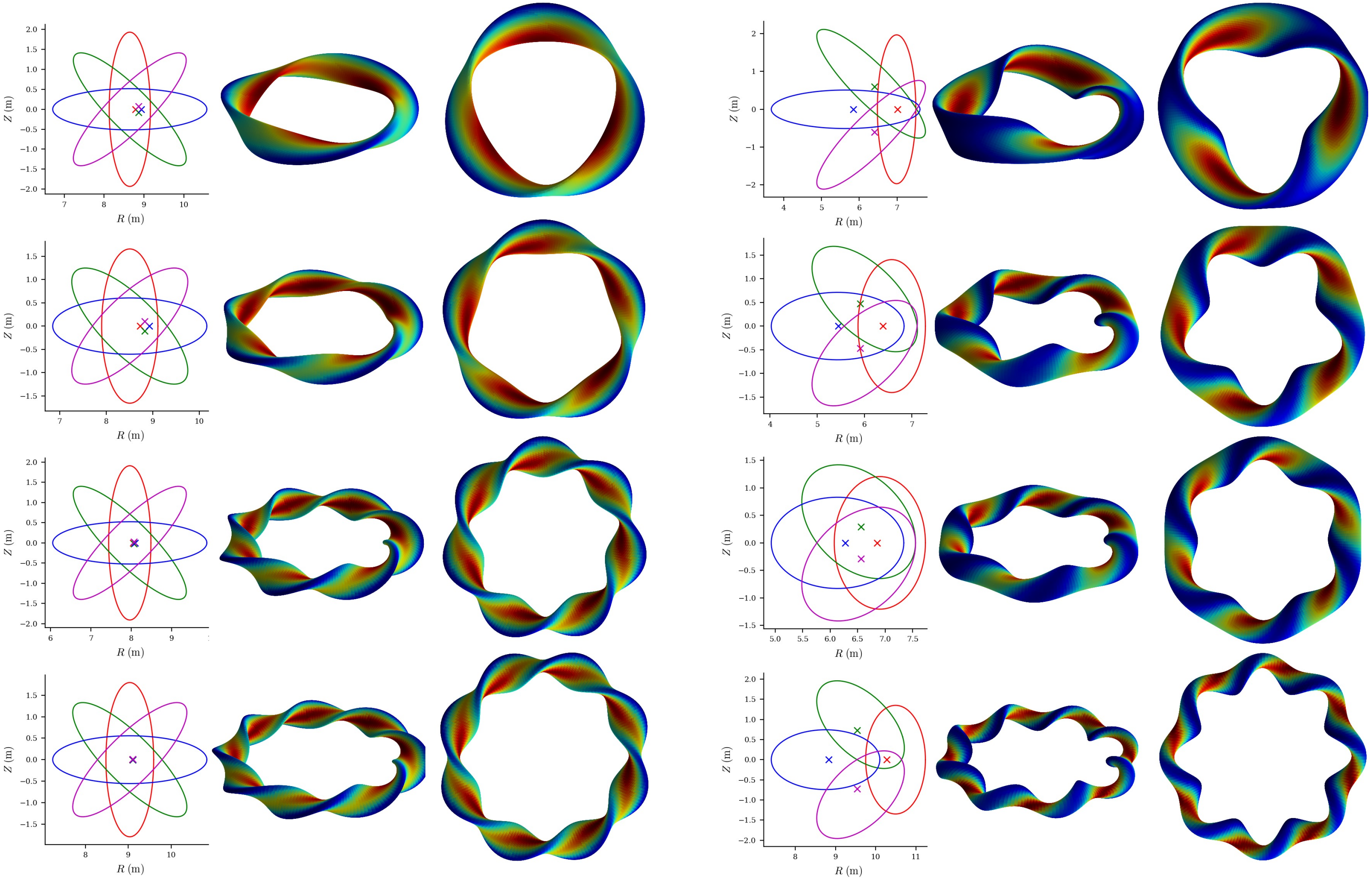


Mandell (2024)

Optimize geometry for maximum fusion power


Turbulence simulations
Heat flux Q/Q_GB
time
Regression
R² = 0.989
Predicted heat flux
True heat flux
Feature importance
mean([Θ(B × κ · ∇y) + 0.2]|∇x|³/B)
median((B × ∇B · ∇x)²|∇x|⁸/B⁸)

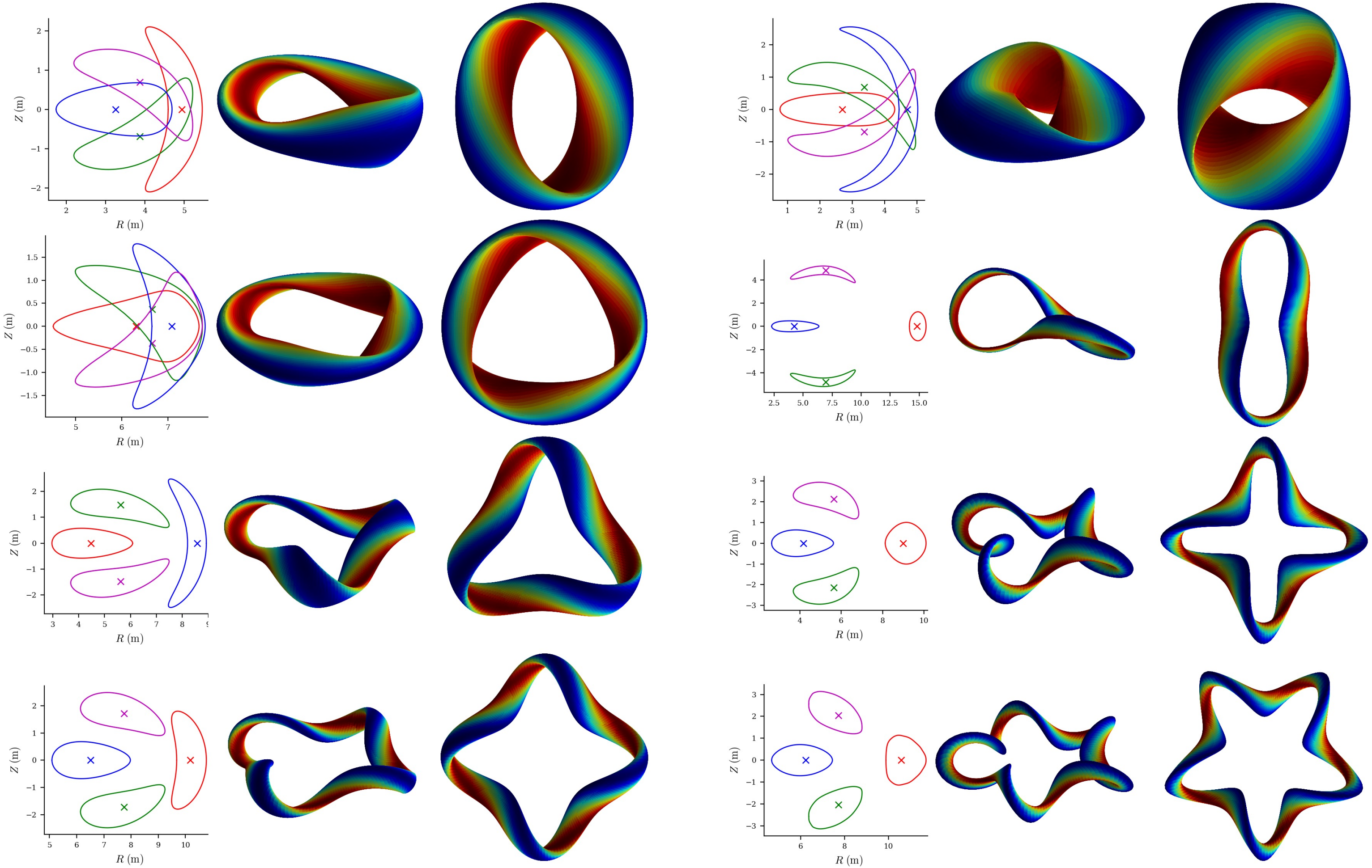
Equilibria group 1: random rotating ellipses



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

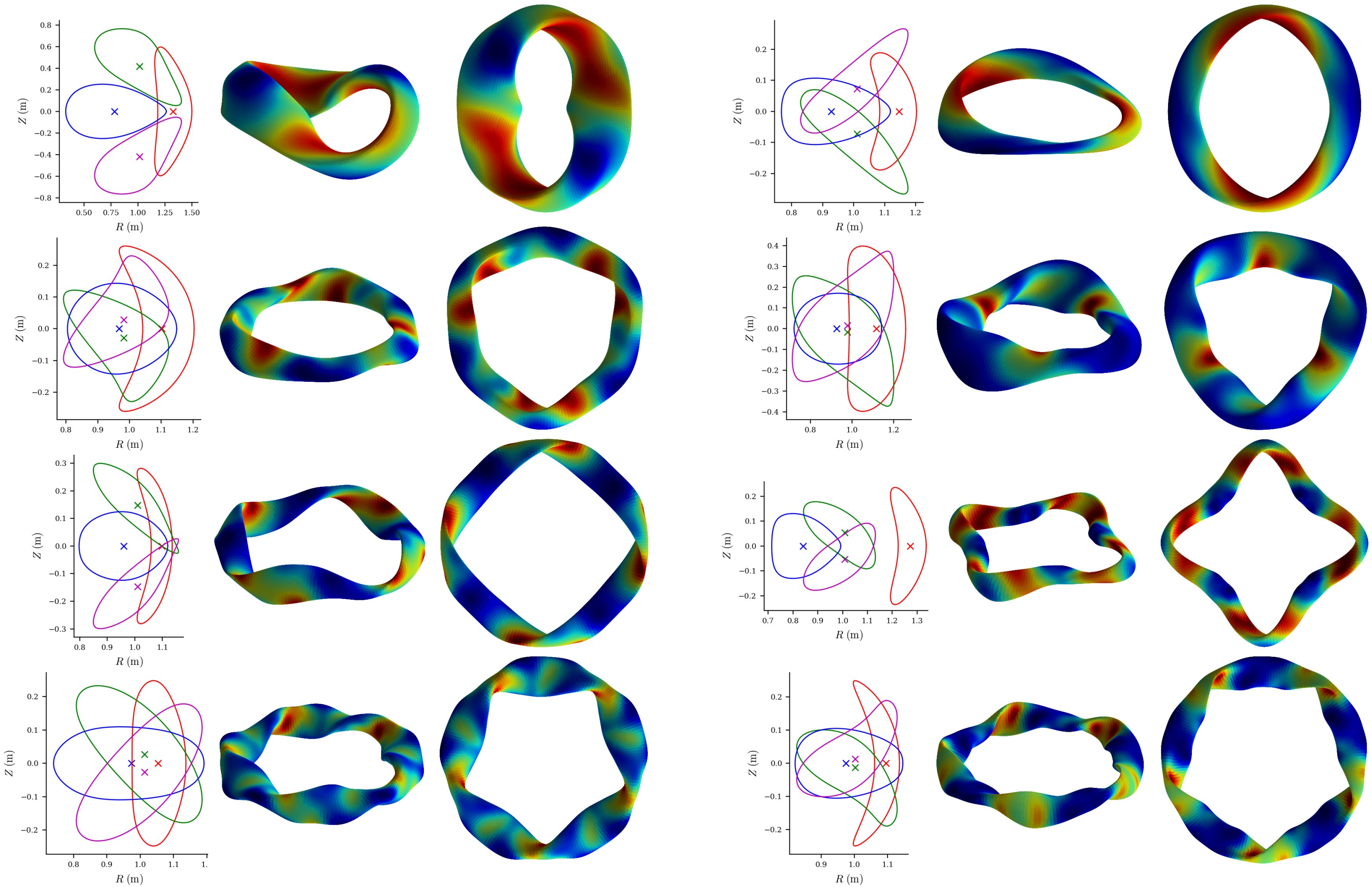
All configurations have same minor radius & toroidal flux, so same gyroBohm normalization

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

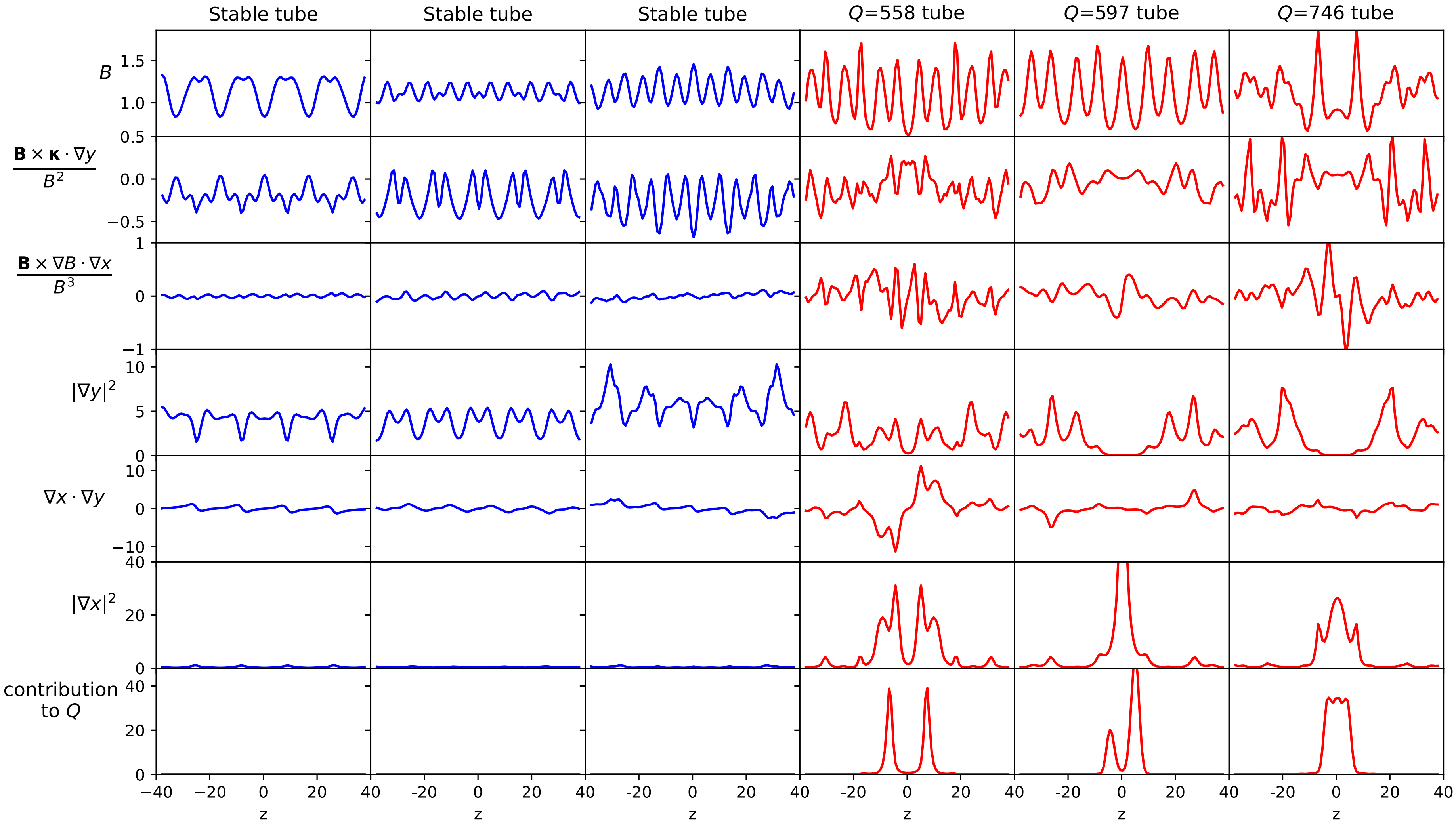


Random pressure added for even more diversity

Equilibria group 3: random boundary modes



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



Stable tube
Stable tube
Stable tube
Q=558 tube
Q=597 tube
Q=746 tube
B
B × κ · ∇y / B²
B × ∇B · ∇x / B³
|∇y|²
∇x · ∇y
|∇x|²
contribution to Q
z

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,

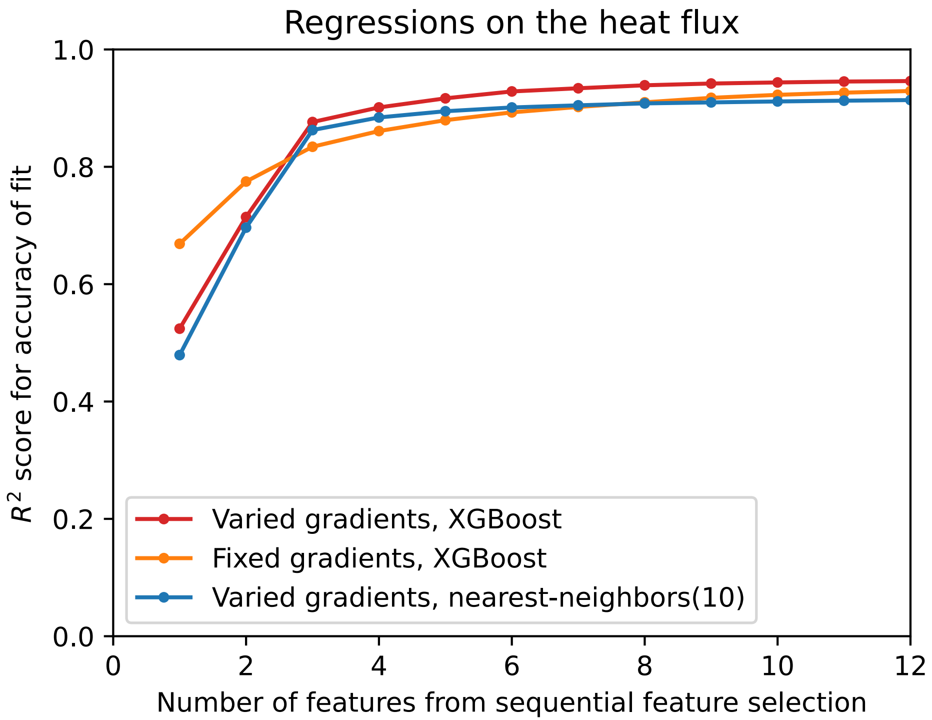
Jacobian (maybe squared)

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)!

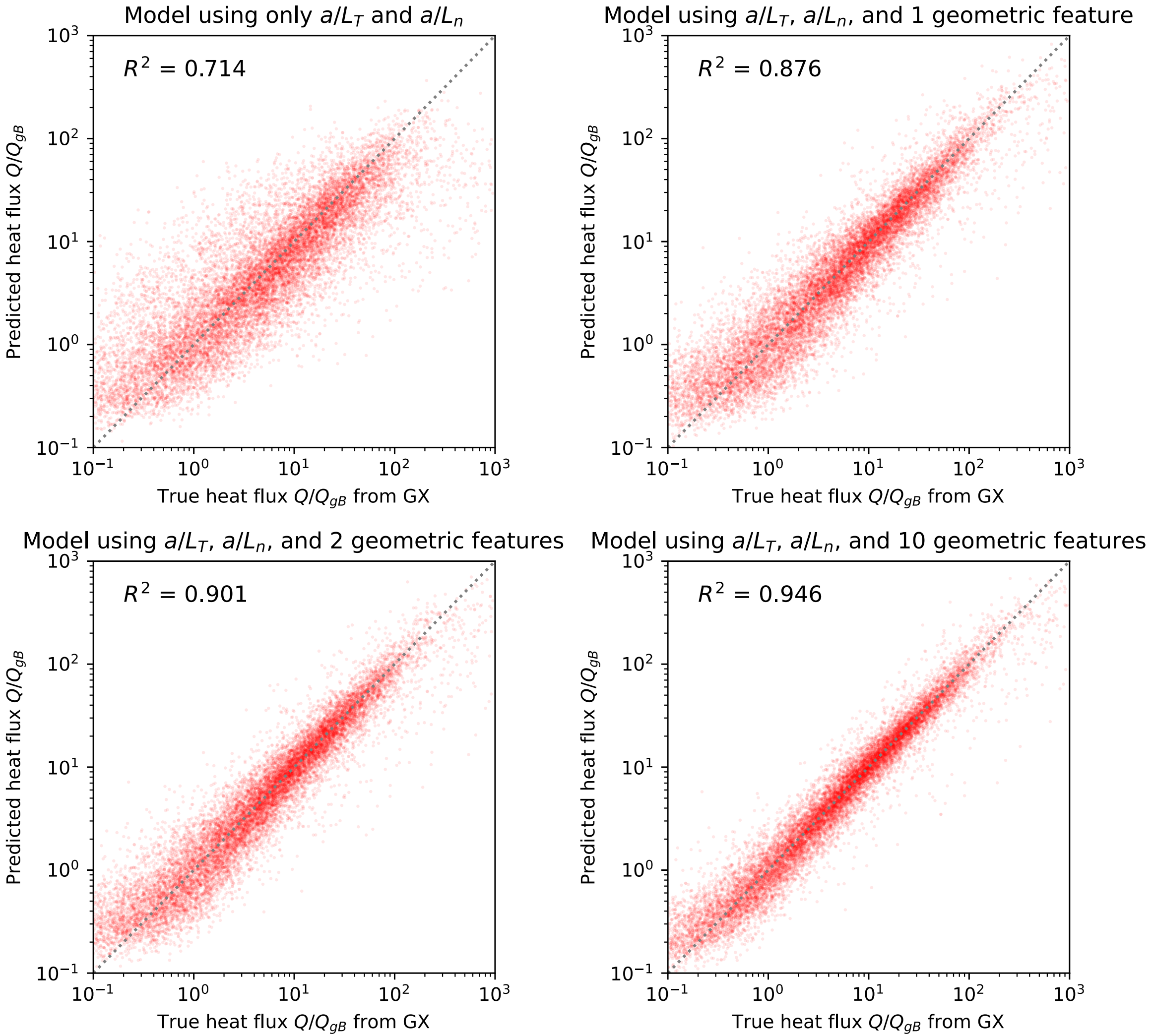
Forward sequential feature selection: ~3 features can be almost as predictive as all features

Stiffness



Critical gradient

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



Performance shown on 20% held-out test data

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

Sequential feature selection step 3

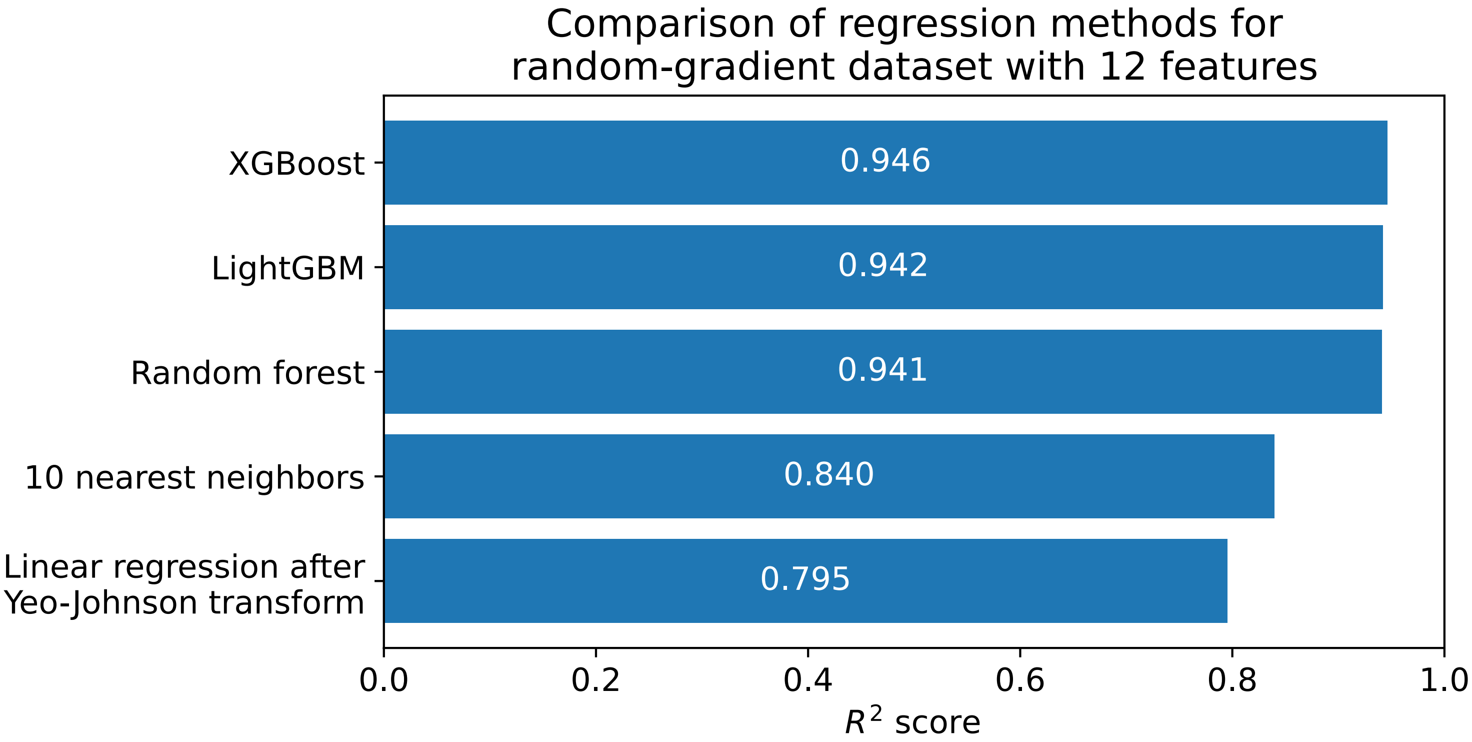
Feature	R^2
$\text{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\vert\nabla x\vert^4/B^2)$	0.876
$\text{mean}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\vert\nabla x\vert^4/B)$	0.874
$\text{variance}(\Theta(\mathbf{B} \times \kappa \cdot \nabla y)\vert\nabla x\vert^2/B)$	0.871
$\text{quantile0.9}(\Theta(\mathbf{B}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

Sequential feature selection step 4

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

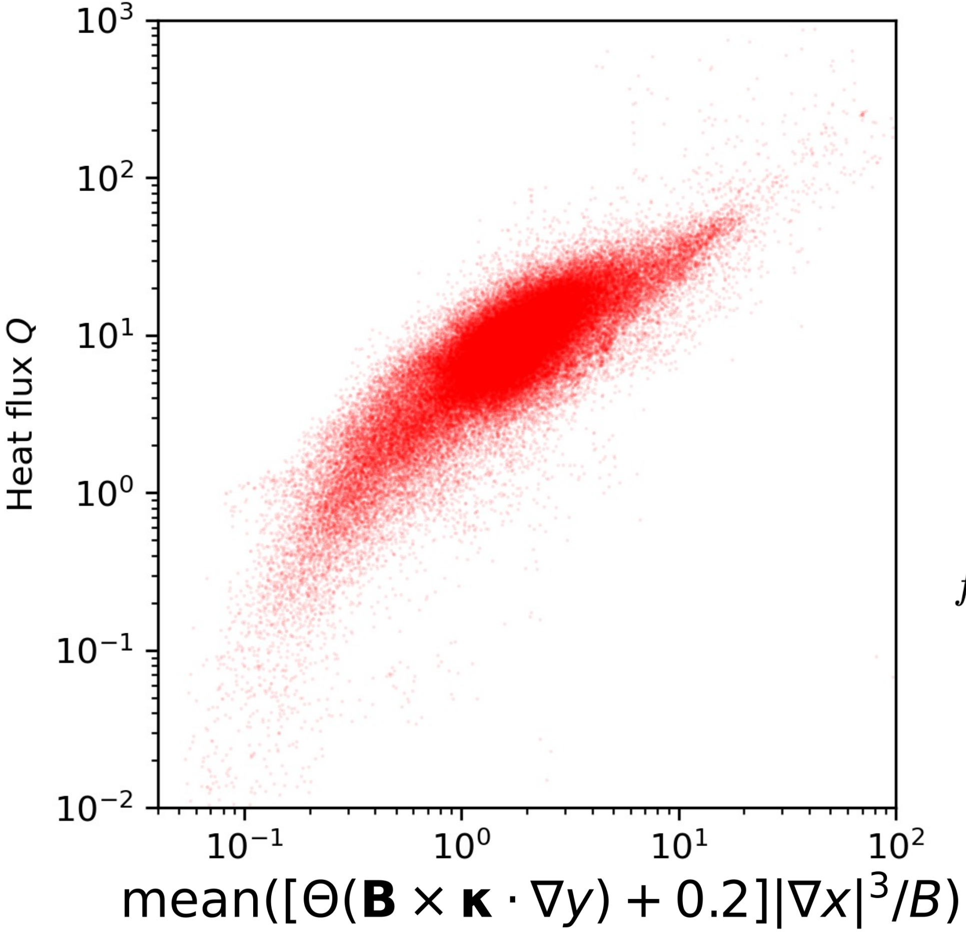
Regression for the random-gradient dataset

Other machine learning regression methods work also



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

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



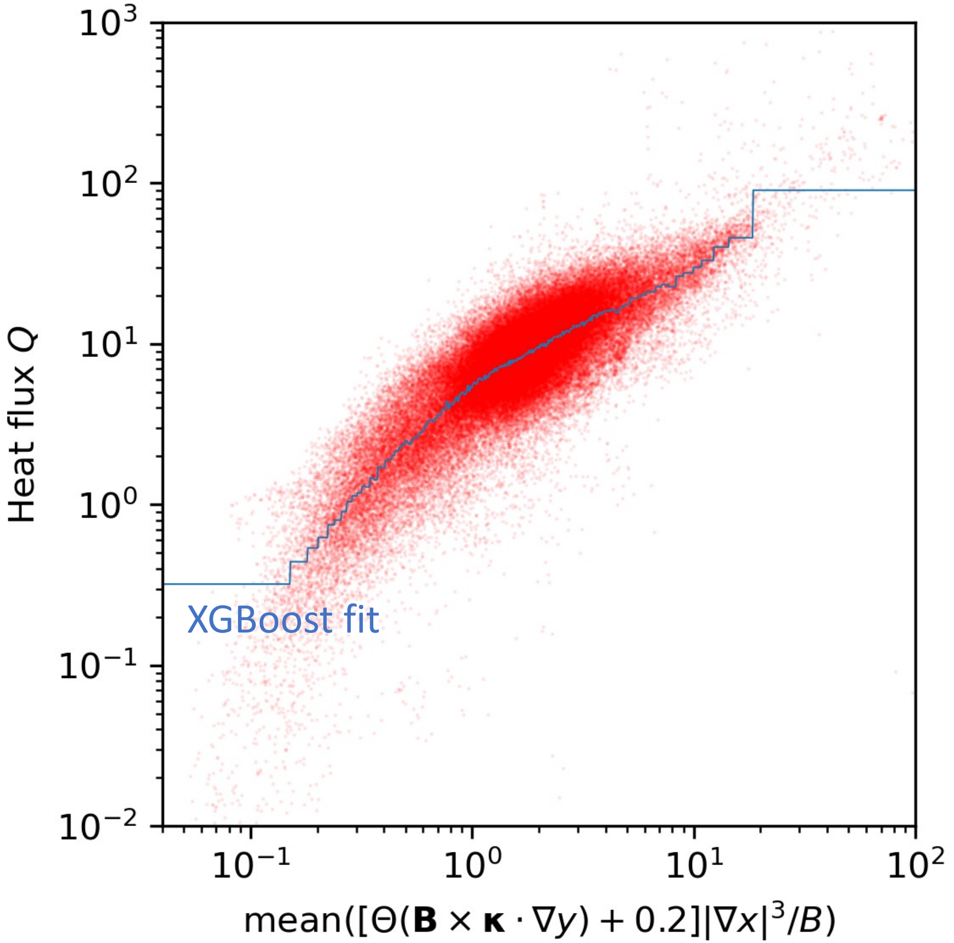
Fixed-gradient dataset.

No regression model used here.

Feature fine-tuned for stability classifier:

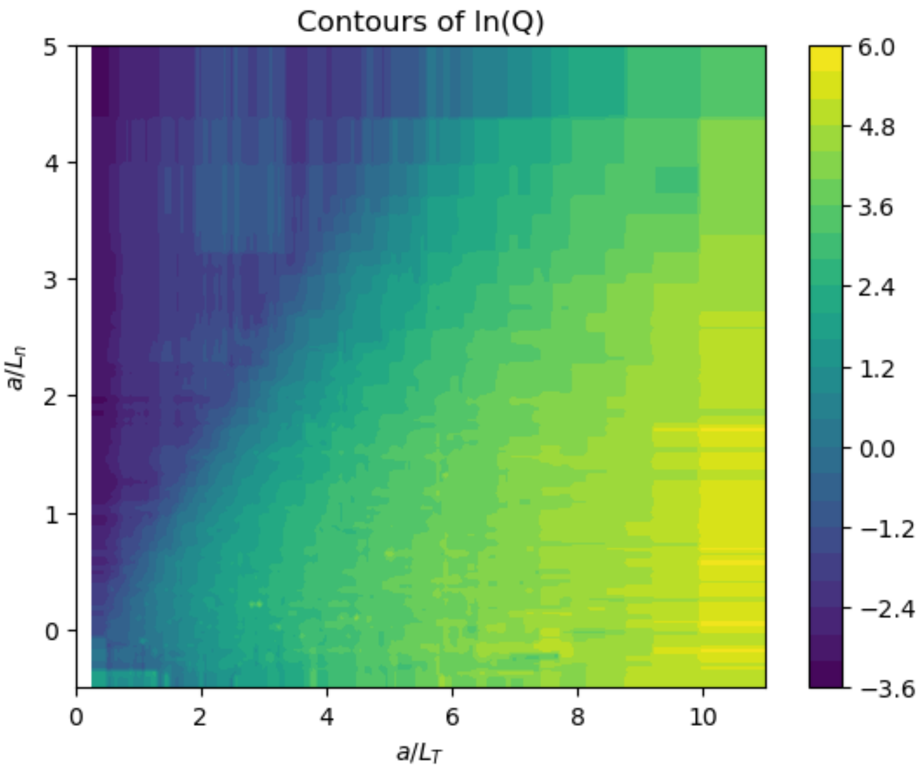
$$f_{\mathrm{stab}} = \mathrm{mean}([\Theta(\mathbf{B} \times \nabla B \cdot \nabla y) + 0.4]|\nabla x|/\sqrt{B})$$

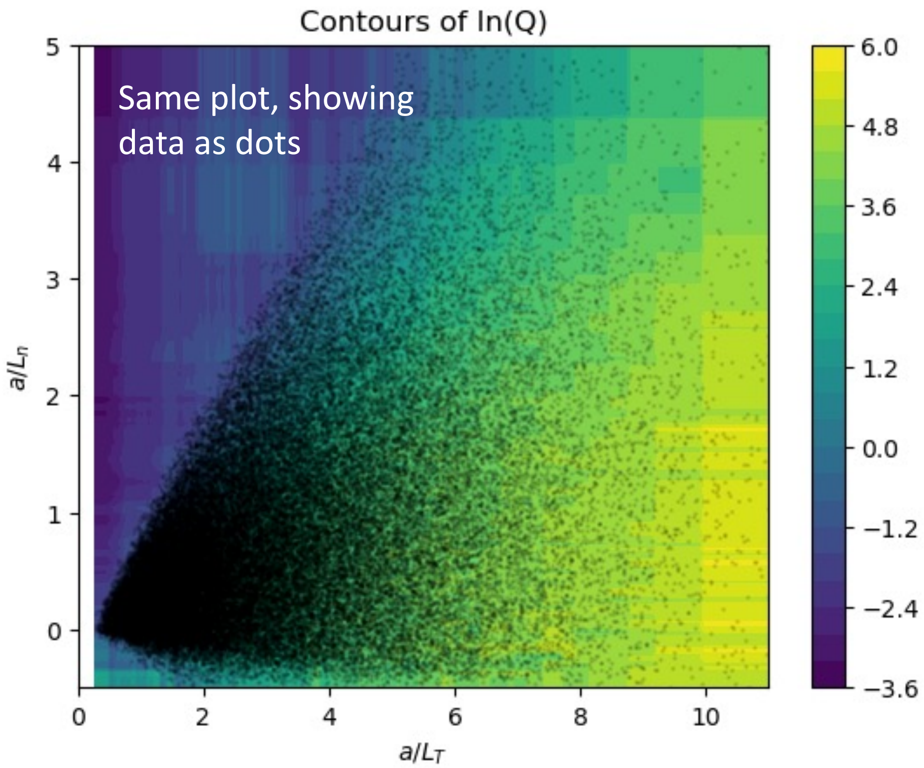
XGBoost regression model with 1 feature



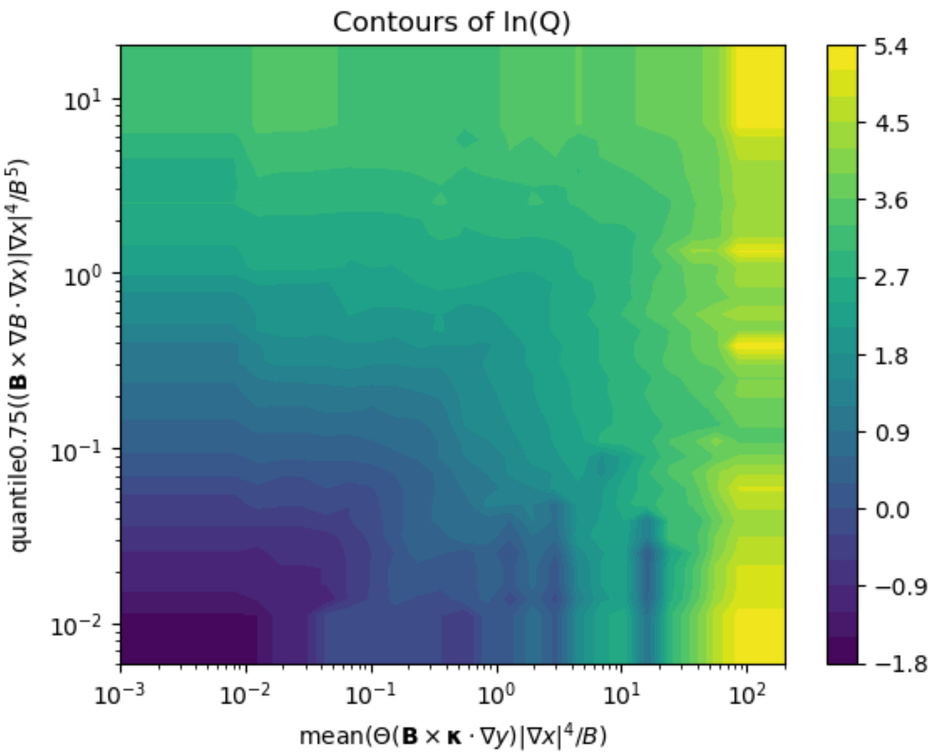
Fixed-gradient dataset

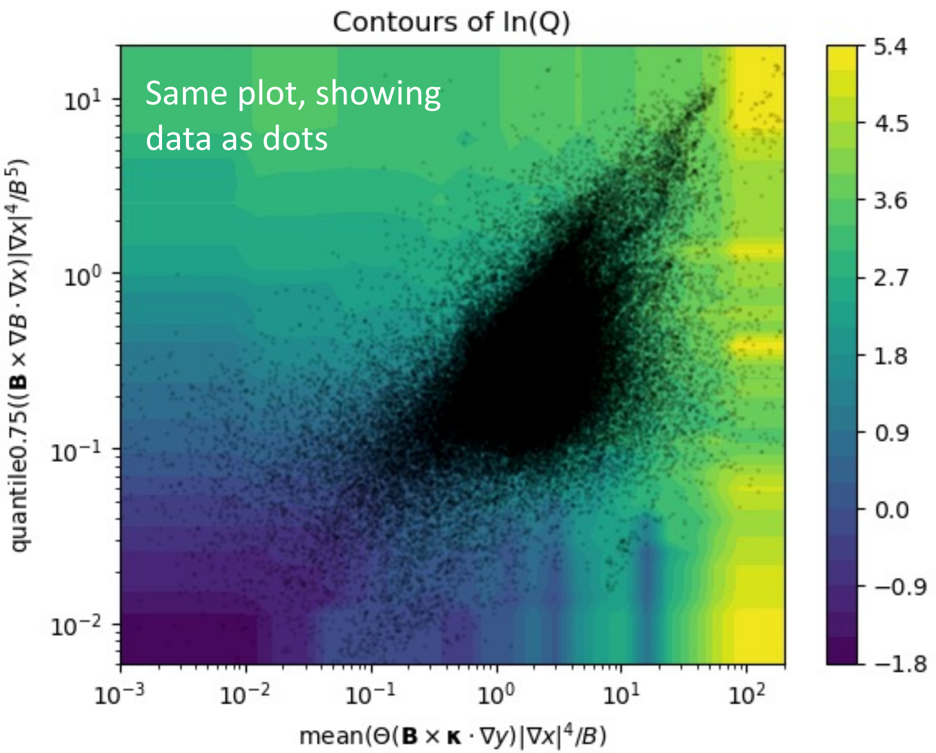
XGBoost regression model using only a/LT and a/Ln

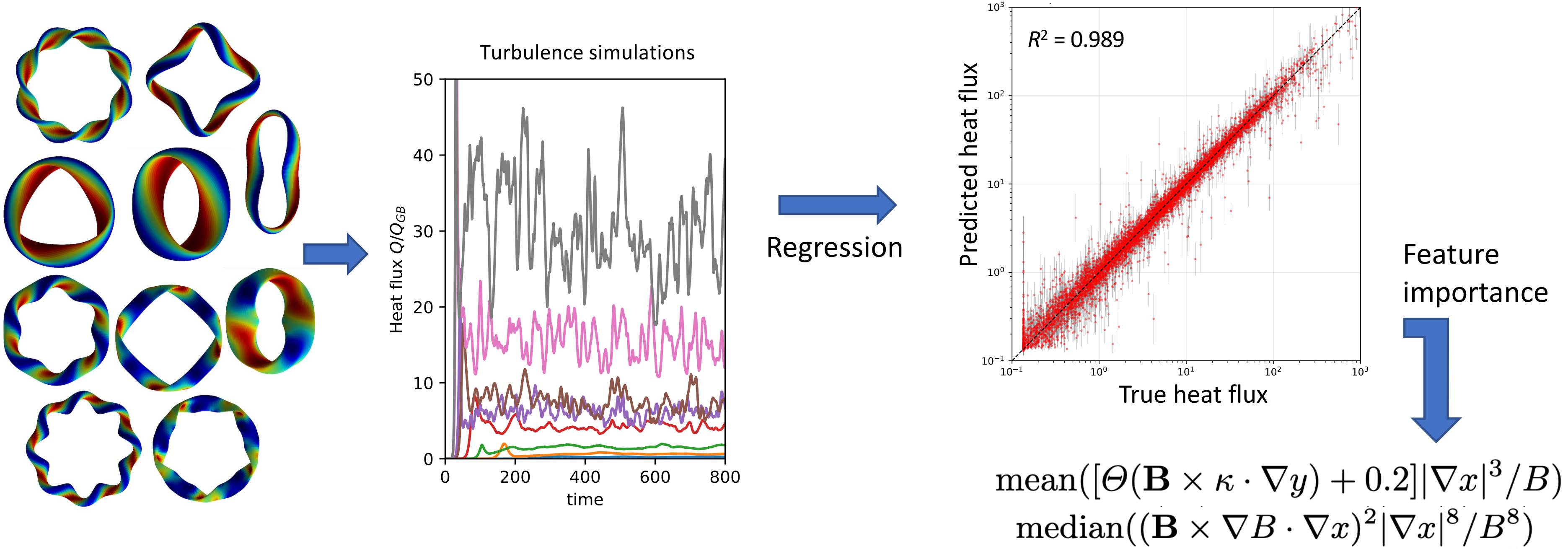




XGBoost regression model for fixed gradients using 2 features



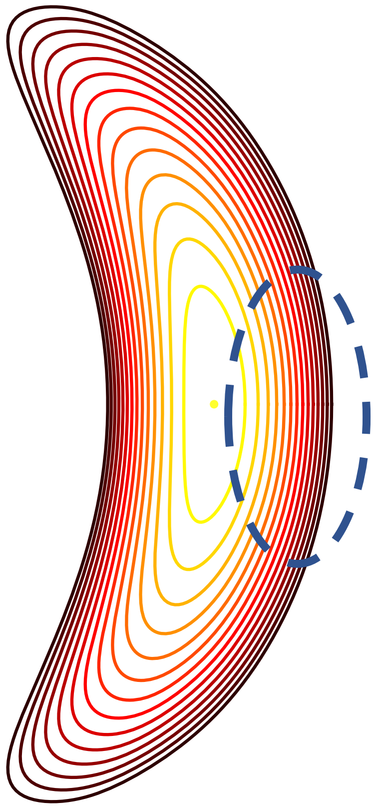




Turbulence simulations
Heat flux Q/Q_{GB}
0
10
20
30
40
50
0
200
400
600
800
time
Regression
$R^2 = 0.989$
Predicted heat flux
True heat flux
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
Feature importance
$\mathrm{mean}([\Theta(\mathbf{B} \times \kappa \cdot \nabla y) + 0.2] |\nabla x|^3 / B)$
$\mathrm{median}((\mathbf{B}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

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



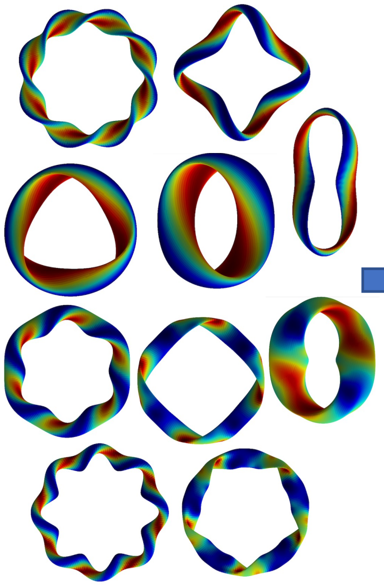
There are many extensions possible

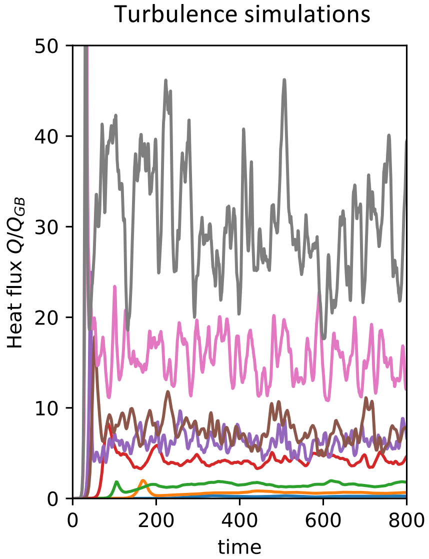
- Try larger sets of possible features
- From the gyrokinetic equation, understand how these features affect turbulence.
- Kinetic electrons, magnetic fluctuations.
- Saliency maps to understand the features learned by the neural networks.
- Symbolic regression.
- Kolmogorov-Arnold Networks.
- Optimization,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

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

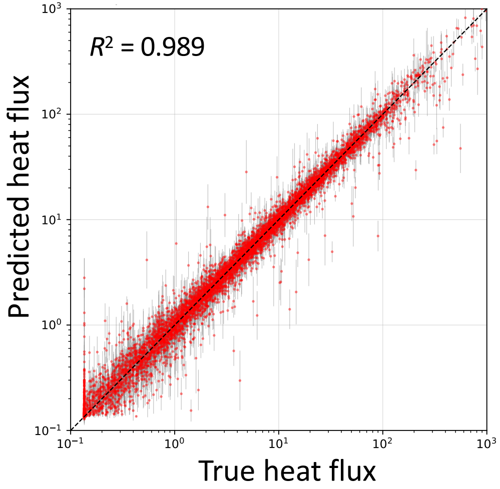
Paper: arXiv:2502.11657

Dataset doi:10.5281/zenodo.14867776





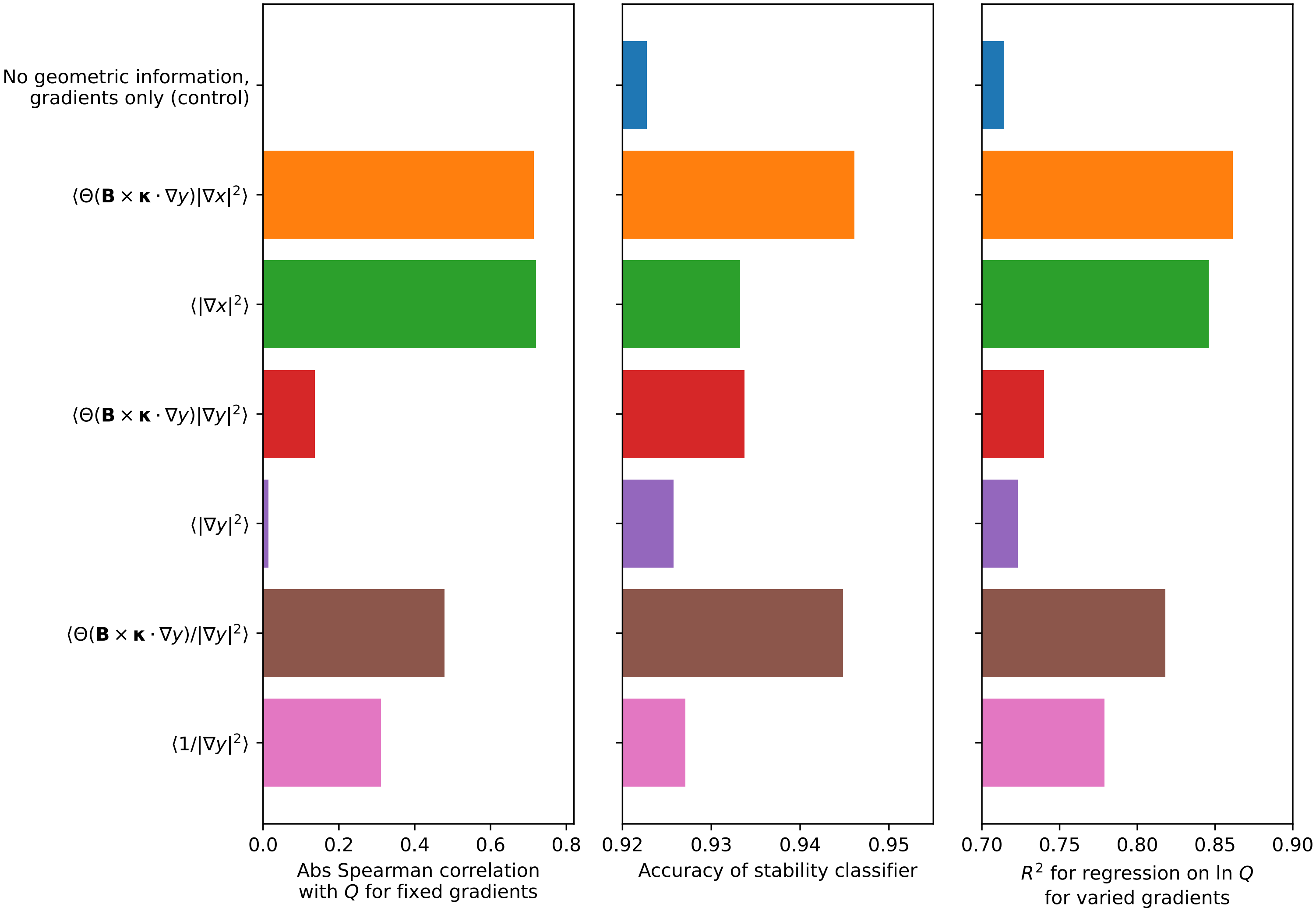
Regression



Feature importance

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

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


No geometric information, gradients only (control)
$\langle \Theta(\mathbf{B} \times \boldsymbol{\kappa} \cdot \nabla y) |\nabla x|^2 \rangle$
$\langle |\nabla x|^2 \rangle$
$\langle \Theta(\mathbf{B} \times \boldsymbol{\kappa} \cdot \nabla y) |\nabla y|^2 \rangle$
$\langle |\nabla y|^2 \rangle$
$\langle \Theta(\mathbf{B} \times \boldsymbol{\kappa} \cdot \nabla y) / |\nabla y|^2 \rangle$
$\langle 1/|\nabla y|^2 \rangle$
0.0
0.2
0.4
0.6
0.8
Abs Spearman correlation with Q for fixed gradients
0.92
0.93
0.94
0.95
Accuracy of stability classifier
0.70
0.75
0.80
0.85
0.90
R^2 for regression on ln Q for varied gradients