Reassessment of impurity transport coefficients in Alcator C-Mod

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Measuring impurity transport and testing simulations: making sure we know what we think we know

Impurity transport coefficients D, V are often used in validation metrics

$$\frac{\partial n_Z}{\partial t} = -\nabla \cdot \Gamma_Z + Q_Z$$

Model impurity flux Γ_Z with diffusion coefficient D, convective velocity V:

$$\Gamma_Z = -D\nabla n_Z + V n_Z$$

D, V are often used to validate impurity transport simulations:
Important to measure D, V properly to have a strong test of the code.

Measuring impurity transport and testing simulations: making sure we know what we think we know

$$\Gamma_Z = -D\nabla n_Z + V n_Z$$

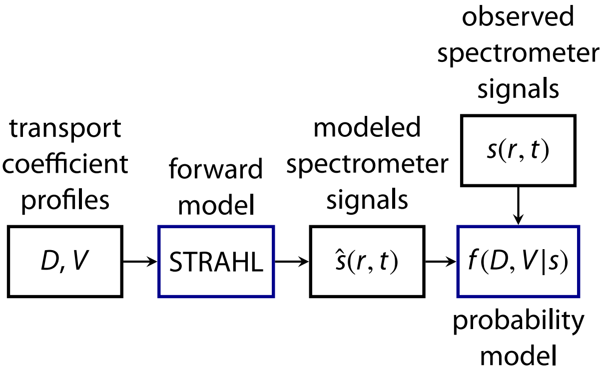
Current approaches for measuring *D*, *V* have considerable shortcomings

- Error bars not consistent with intuition.
- Different starting points give different results:
  - Multiple solutions?
  - Broad region of acceptable solutions?

New approach fixes these issues

- Use advanced inference techniques to find $D(r)$, $V(r)$.
- Rigorous selection of level of complexity in $D(r)$, $V(r)$ is critical.

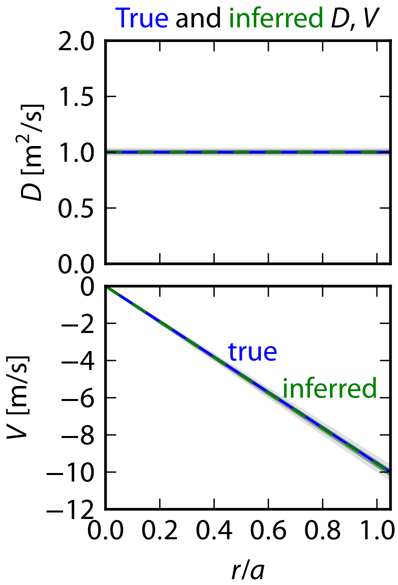
Inferring impurity transport coefficients: a nonlinear inverse problem



- Inject impurity with laser blow-off
- Can only observe s, want to know D, V.
- Need to assume a parameterization for $D(r), V(r)$.
- Two steps:
  1. Find D, V consistent with s for given parameterization.
  2. Find best parameterization.
- Do both steps simultaneously with **MultiNest** [Feroz MNRAS 2008, 2009]: Bayesian inference algorithm.

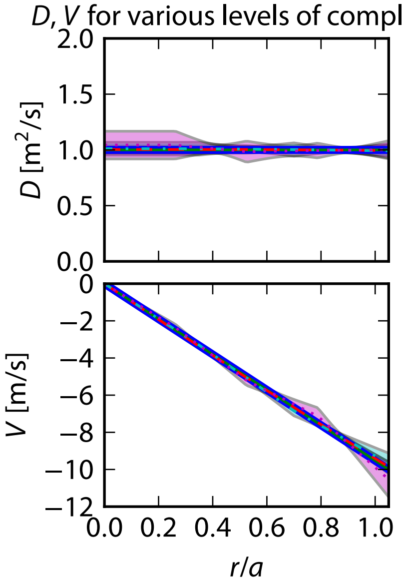
MultiNest successfully reconstructs simple *D*, *V* profiles

(synthetic data)

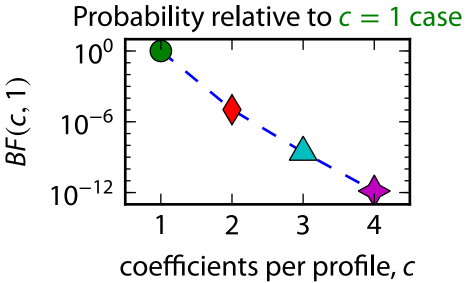


- Five local measurements, uniformly spaced over $0 \leq r/a \leq 1$
- $\Delta t = 6$ ms, 5% noise
- Have also tested with 32 x-ray spectrometer chords: can handle tomographic inversion

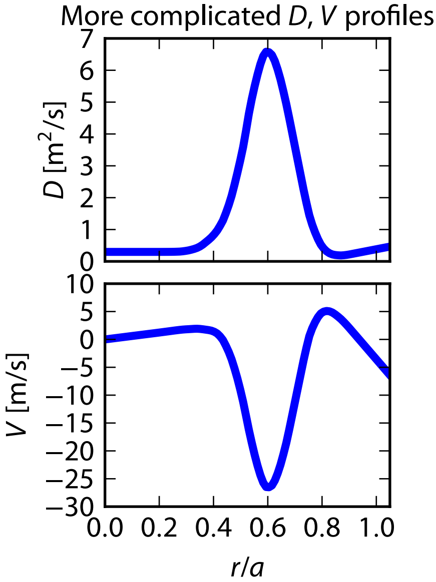
MultiNest successfully determines how many spline coefficients to use



- MultiNest estimates the evidence $f_{s|c}(s|c)$: probability of observing the data given c.
- Ran with various numbers of free parameters: correctly selected $c = 1$ case.
- Bayes factors: $BF(c, 1) = f_{s|c}(s|c)/f_{s|1}(s|1)$

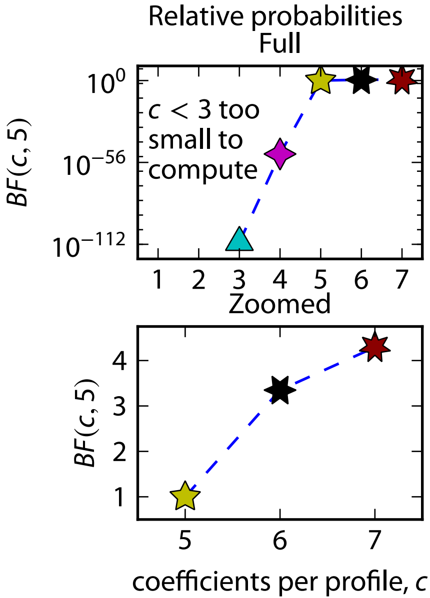


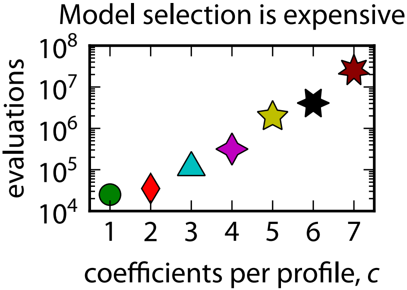
Testing with more complicated synthetic data



- Need to test with data representative of reality.
- Used result from [Howard NF 2012, Chilenski NF 2015] as true profile.
- Realistic diagnostic configuration:
  - 32 x-ray spectrometer chords (Ca^{18+}), 6 ms time resolution, 5% noise
  - 2 VUV spectrometer chords (Ca^{17+}, Ca^{16+}), 2 ms time resolution, 5% noise

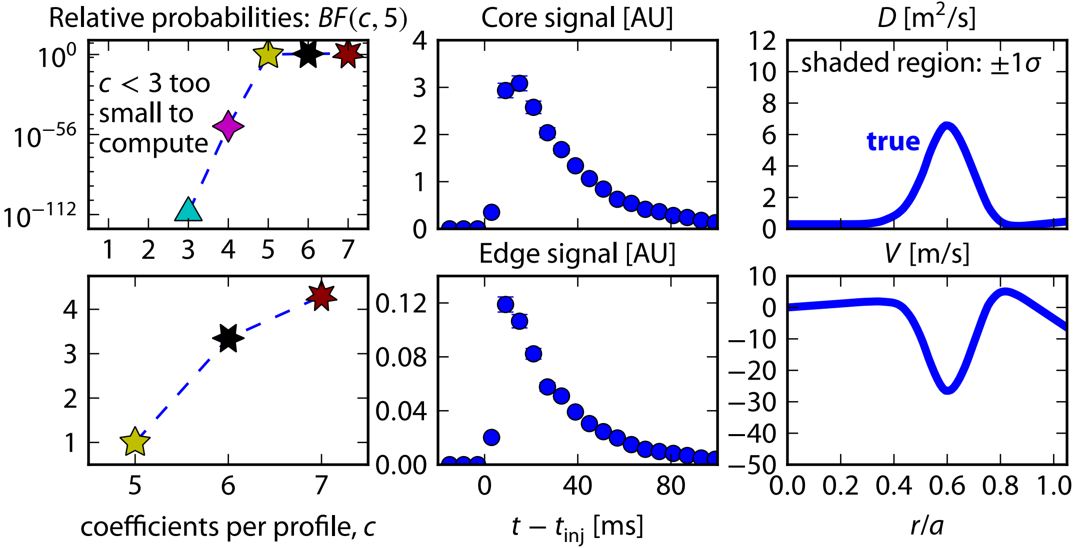
More complicated synthetic data pose a challenge





- 7 coefficient case took 7000 CPU-hours = 15 wall-clock days!
- Need to speed up model, deploy on cluster to make this practical.
- (Recall: $BF(c, 5) = f_{s|c}(s|c)/f_{s|5}(s|5)$)

Results only resemble true profile when a minimum level of complexity is obtained…despite “good” match to data: “eyeballing” does not work!



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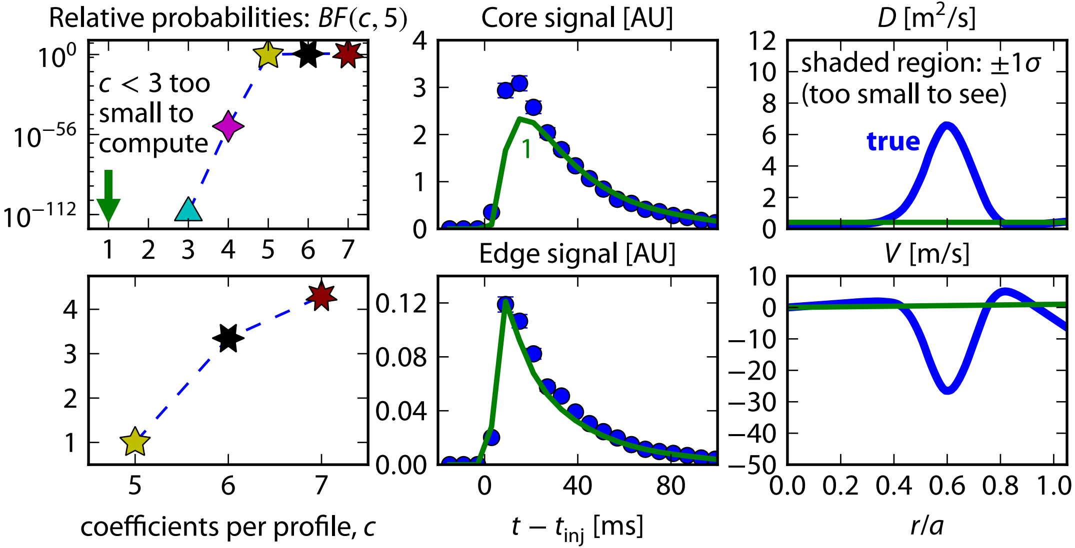

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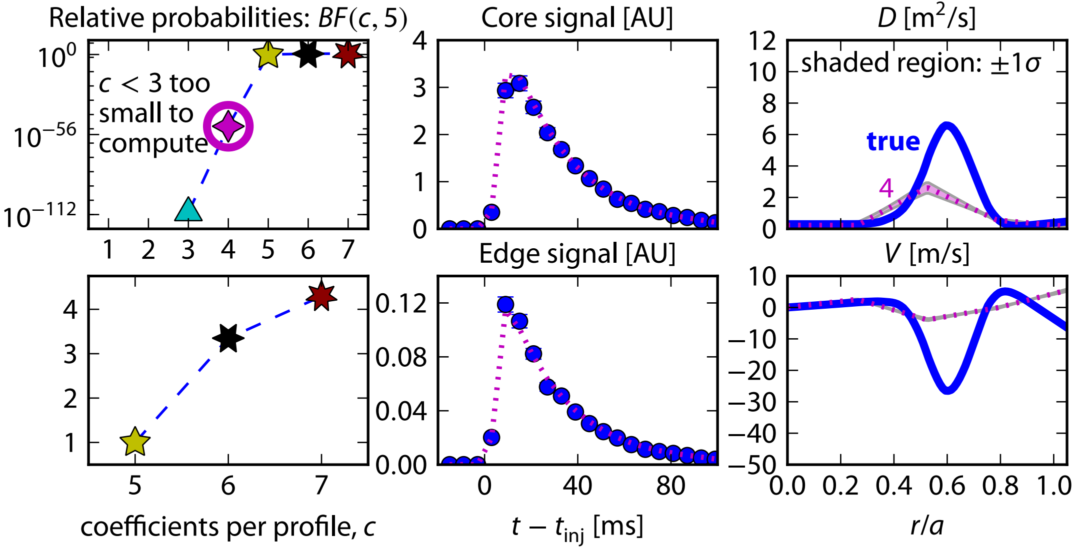

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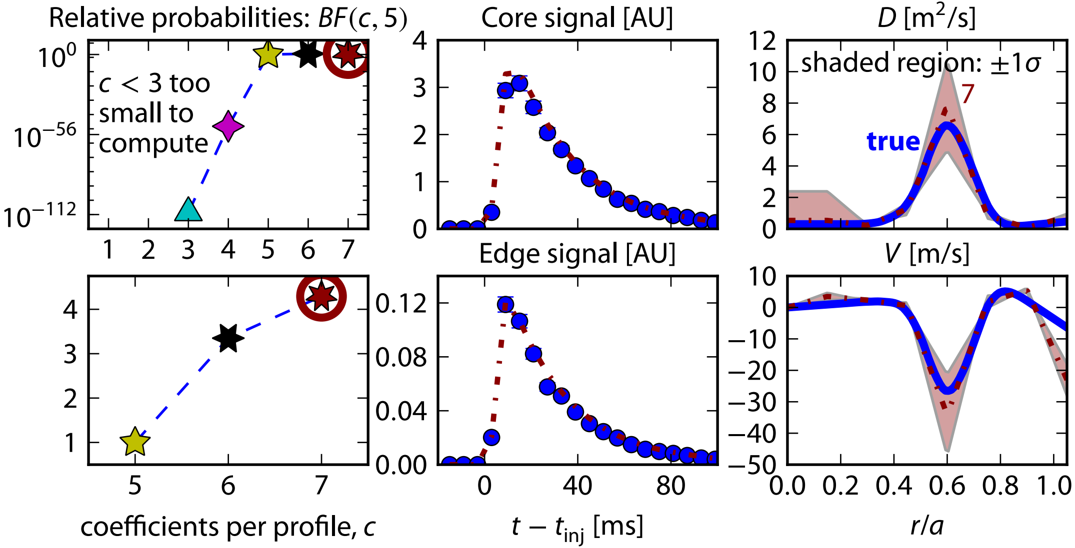

Getting *D*, *V* right requires careful statistical analysis

Conclusions

- ***Need*** to select right level of complexity:
  - Can appear to match data well while not matching the real *D* and *V* at all.
  - New approach rigorously selects the most likely model.
- Can also estimate/verify diagnostic requirements.
- Validation of impurity transport simulations is still an open question, but we have a path forward.

Future work

- Speed up, parallelize analysis.
- Improve handling of sawteeth.
- Develop more efficient ways of selecting basis functions.
- Re-assess previous results from Alcator C-Mod and other tokamaks.

Additional details are in my PhD thesis: markchil.github.io/pdfs/thesis.pdf

Open-source software: github.com/markchil/bayesimp

Backup slides

Inferring impurity transport coefficients: a nonlinear inverse problem

inject impurity → diffusion, convection move impurity → observe signals

Finding D, V with Bayesian inference

$$\underbrace{f_{D,V|s}(D,V|s)}_{\text{posterior distribution}} = \frac{\overbrace{f_{s|D,V}(s|D,V)}^{\text{likelihood: from STRAHL + data}} \; \overbrace{f_{D,V}(D,V)}^{\text{prior distribution } (D>0,\, V(0)=0, \text{ etc.})}}{\underbrace{f_s(s)}_{\text{evidence}}}$$

- f: probability density function
- s: measured signals
- D, V: parameters describing radial profiles of diffusion, convection

Parameter estimation: Find D, V: characterize $f_{D,V|s}(D,V|s)$.

Model selection: Find best way of parameterizing D, V: maximize $f_s(s)$.

$\mathcal{M}$: functional form (model) used to parameterize $D(r)$, $V(r)$.

Use **MultiNest** [Feroz MNRAS 2008, 2009]: samples $f_{D,V|s}(D,V|s)$ *and* estimates $f_s(s)$.

Inferring impurity transport coefficients: a nonlinear inverse problem

inject impurity → diffusion, convection move impurity → observe signals

Finding *D*, *V* with Bayesian inference

$$\underbrace{f_{D,V|s,\mathcal{M}}(D,V|s,\mathcal{M})}_{\text{posterior distribution}} = \frac{\overbrace{f_{s|D,V,\mathcal{M}}(s|D,V,\mathcal{M})}^{\text{likelihood: from STRAHL + data}}\ \overbrace{f_{D,V|\mathcal{M}}(D,V|\mathcal{M})}^{\text{prior distribution } (D>0,\ V(0)=0,\text{ etc.})}}{\underbrace{f_{s|\mathcal{M}}(s|\mathcal{M})}_{\text{evidence}}}$$

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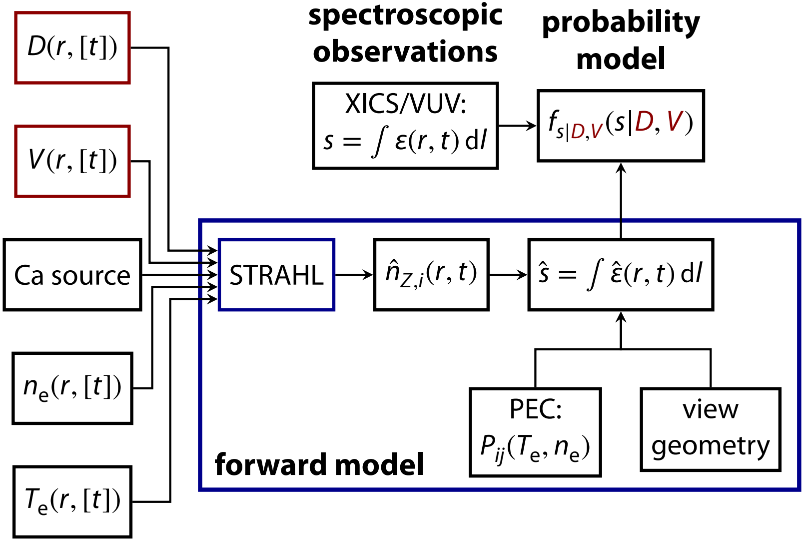
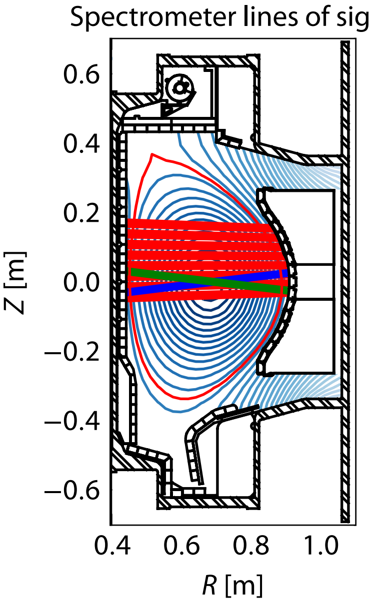
Inferring impurity transport coefficients is a difficult inverse problem



Spectrometer chords on Alcator C-Mod



HiReX-SR X-ray imaging crystal spectrometer (XICS) with 32 chords split into 8 groups. Views He-like Ca (0.32 nm) with 6 ms time resolution.

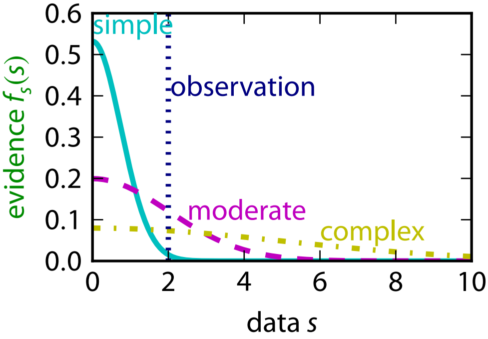
XEUS Vacuum ultraviolet (VUV) spectrometer with one chord. Views Li-like Ca (1.9 nm) with 2 ms time resolution.

LoWEUS Vacuum ultraviolet (VUV) spectrometer with one chord. Views Be-like Ca (19 nm) with 2 ms time resolution.

Model selection using the evidence (a.k.a. the marginal likelihood)

$$\underbrace{f_{D,V|s}(D,V|s)}_{\text{posterior}} = \frac{\overbrace{f_{s|D,V}(s|D,V)}^{\text{likelihood}}\,\overbrace{f_{D,V}(D,V)}^{\text{prior}}}{\underbrace{f_s(s)}_{\text{evidence}}}$$

$$f_s(s) = \int f_{s|D,V}(s|D,V) f_{D,V}(D,V)\,\mathrm{d}D\,\mathrm{d}V$$



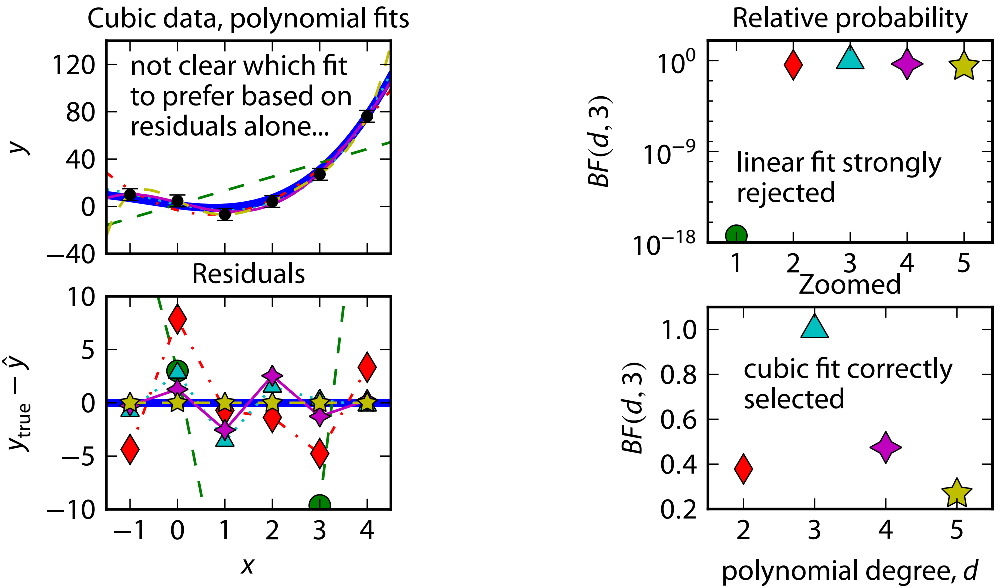
Tradeoff between goodness of fit, complexity [Schwarz AS 1978]:

$$\ln f_s(s) \approx \underbrace{\ln f_{s|\hat{\theta}}(s|\hat{\theta})}_{\text{goodness-of-fit}} - \underbrace{\frac{d}{2}\ln N}_{\text{complexity}}$$

(d is number of parameters, N number of datapoints)

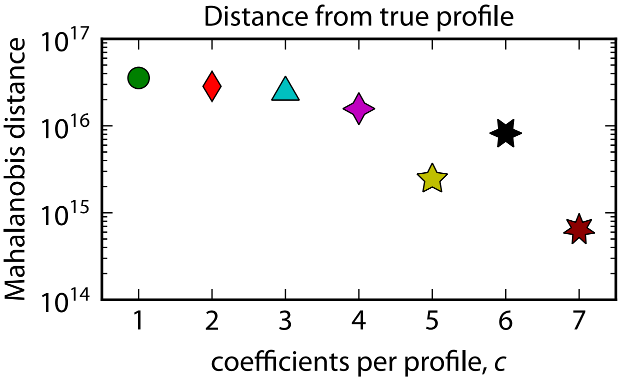
- $f_s(s)$ is maximized by model with "right" level of complexity.
- Simple models can only explain a few data sets, low evidence for most s.
- Complex models can explain many data sets, any given s has low probability.

Simple example: fitting noisy data from $y = x^3 + 2x^2 - 5x + 1$

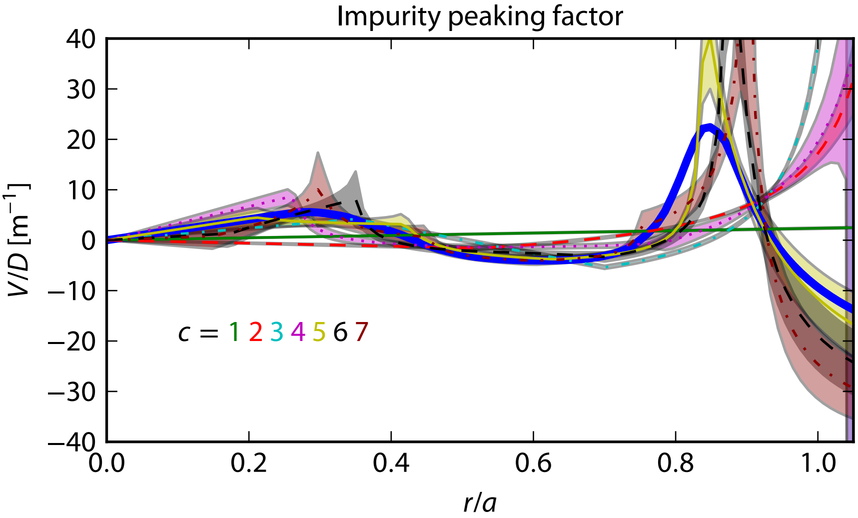


More complex models match the true profiles better

Mahalanobis distance: $M = \sqrt{(\boldsymbol{T}_{\text{true}} - \boldsymbol{\mu})^{\top} \boldsymbol{\Sigma}^{-1} (\boldsymbol{T}_{\text{true}} - \boldsymbol{\mu})}$, $\boldsymbol{T} = [D, V]$



V/D is captured for $r/a \lesssim 0.7$, $c \geq 5$



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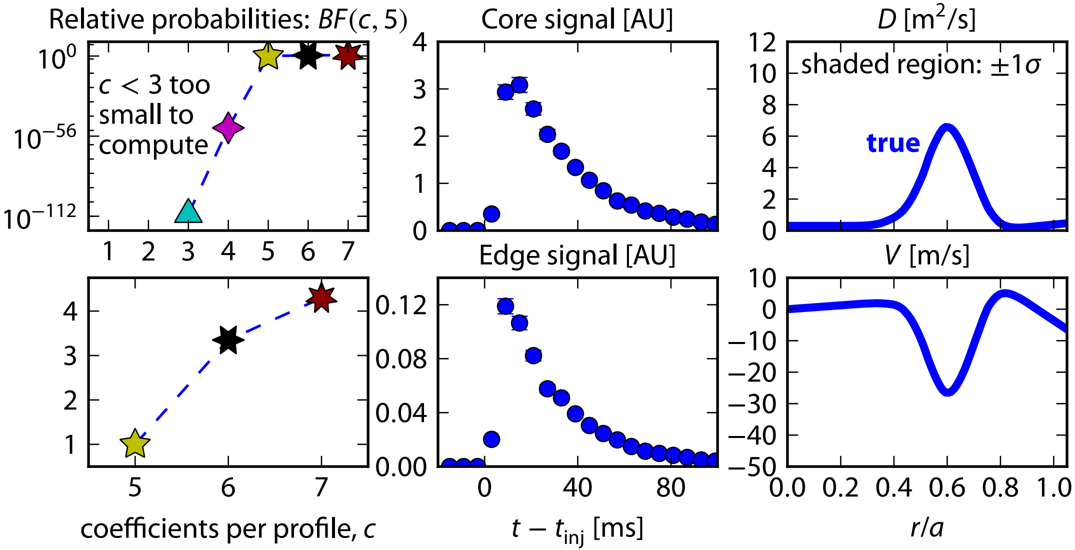

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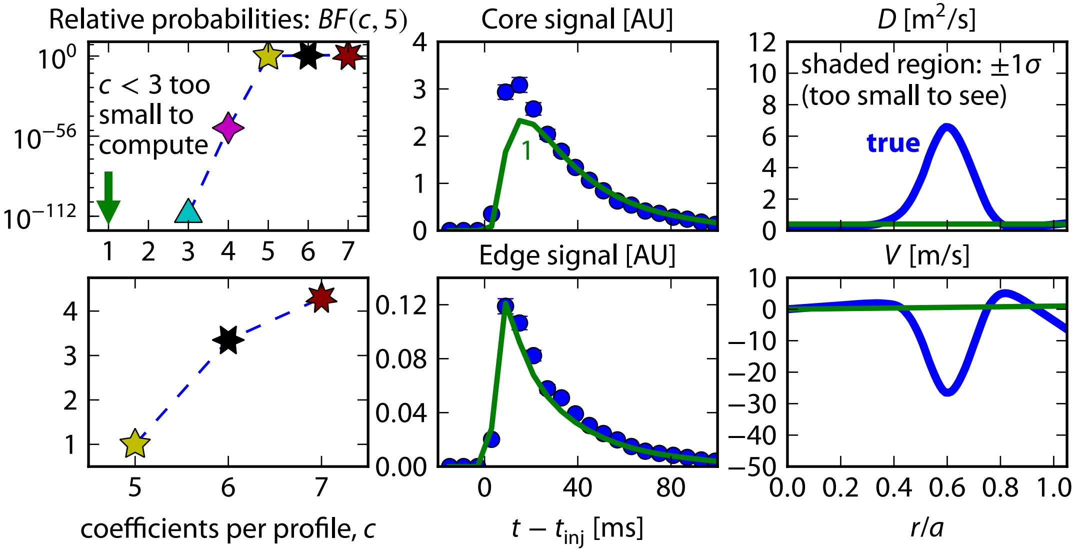

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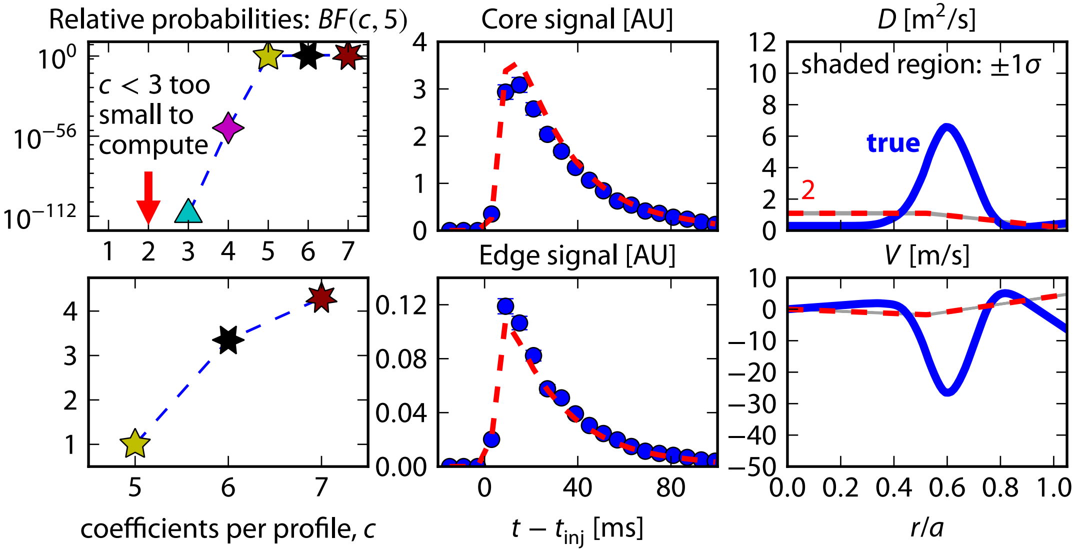

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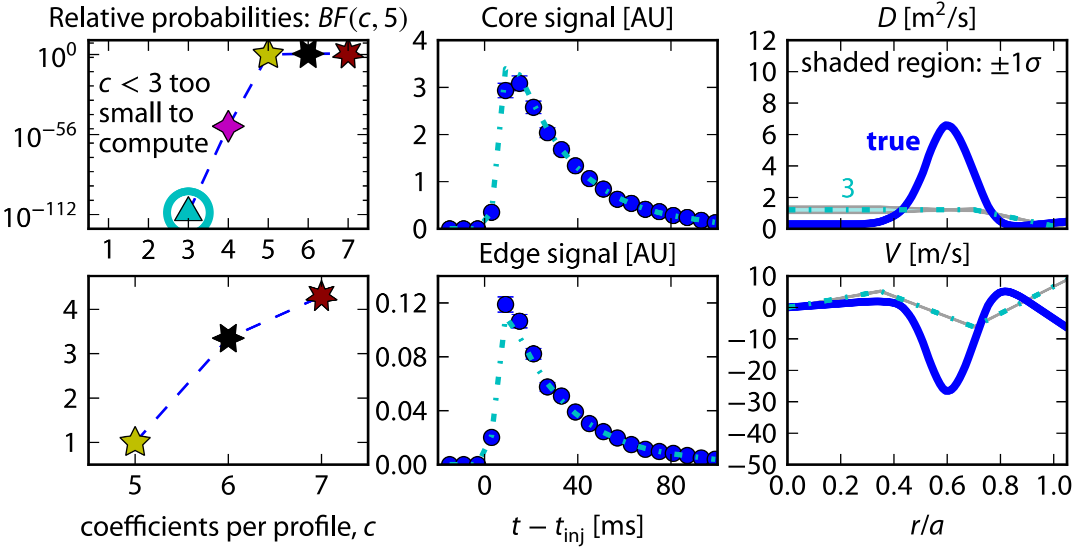

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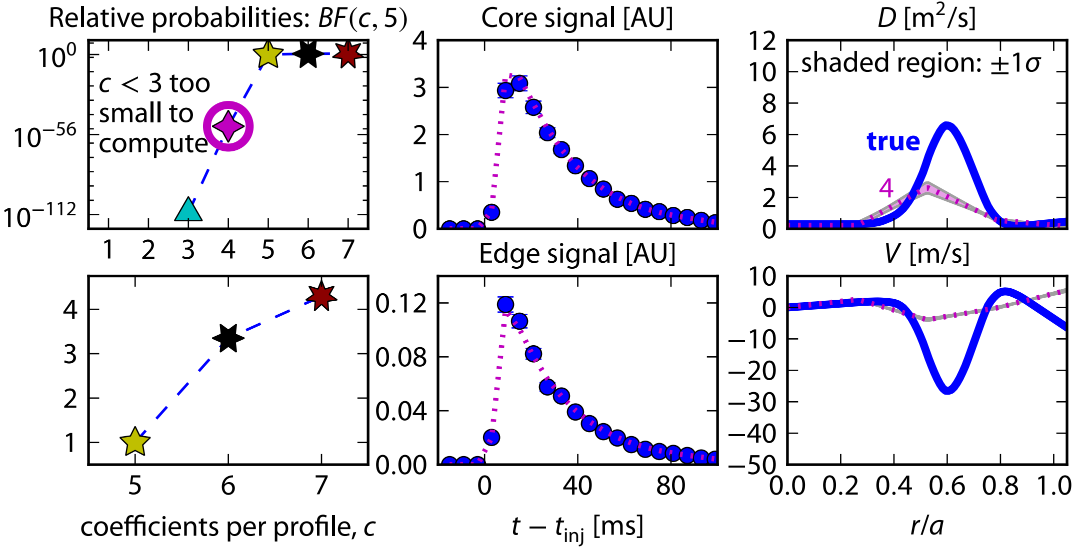

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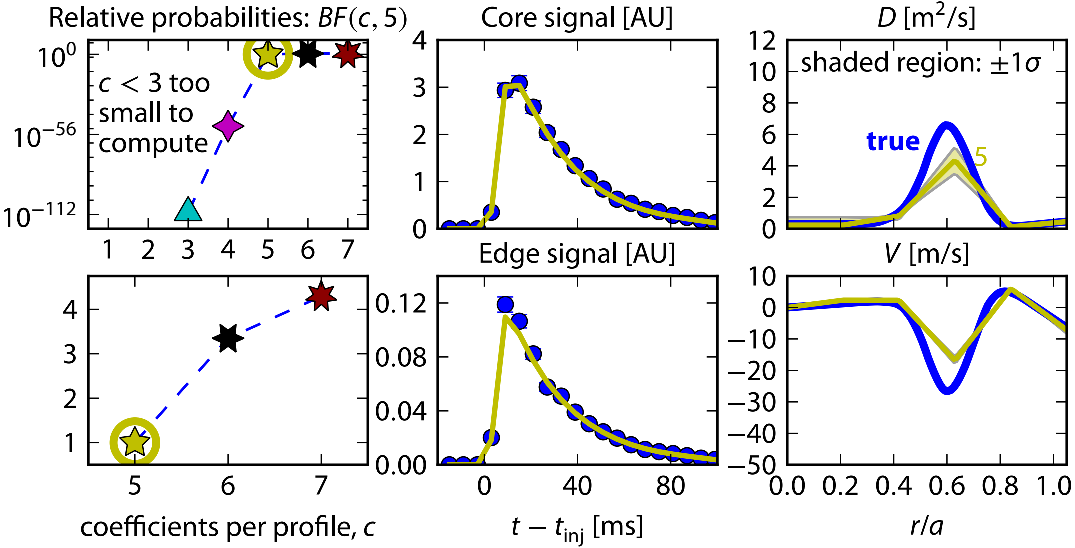

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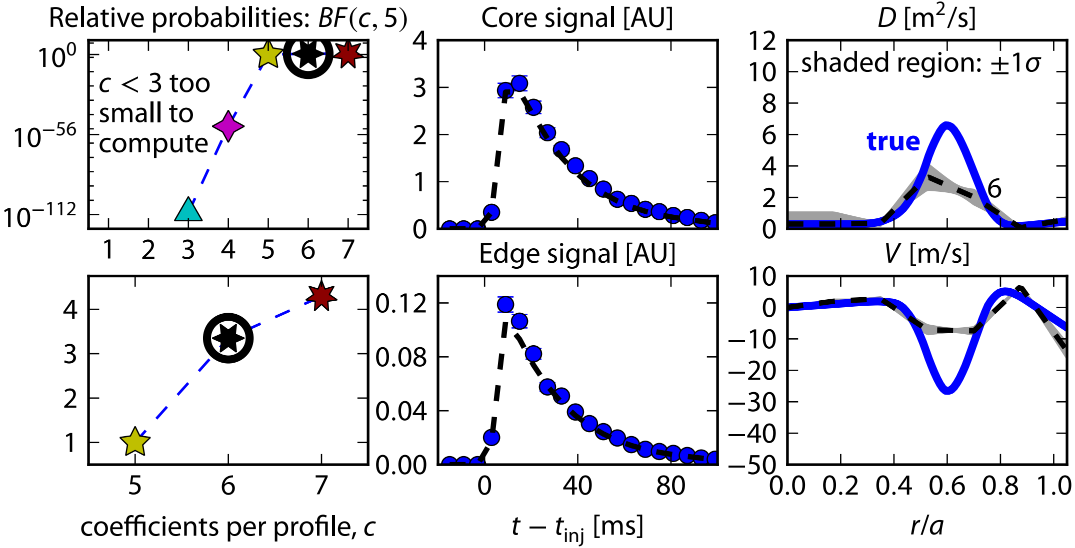

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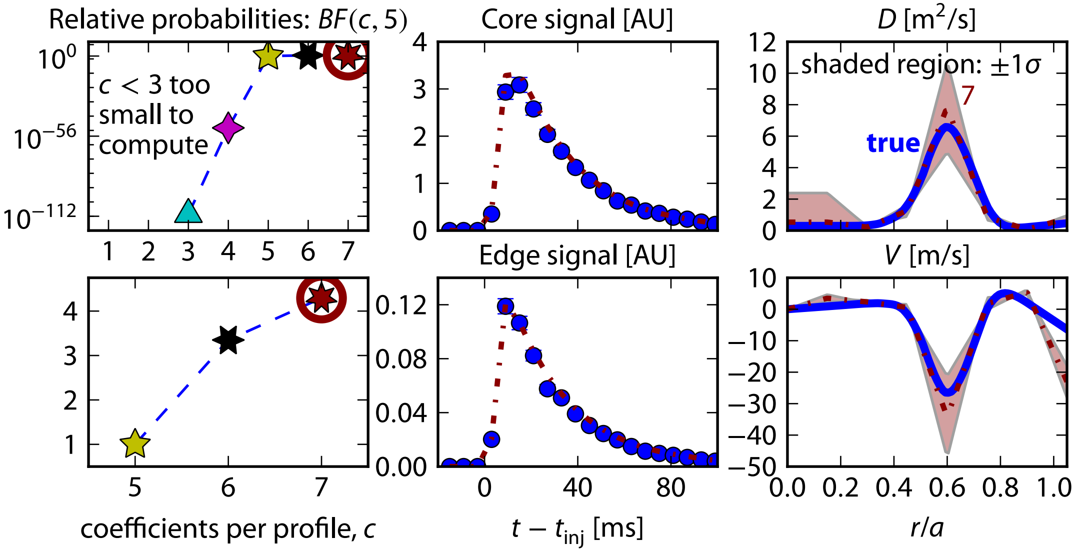

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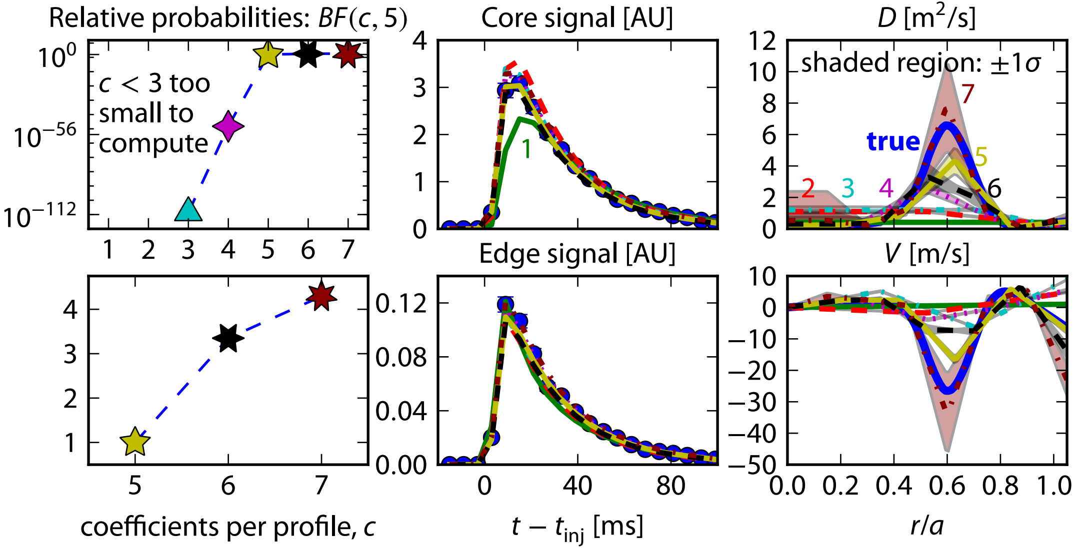
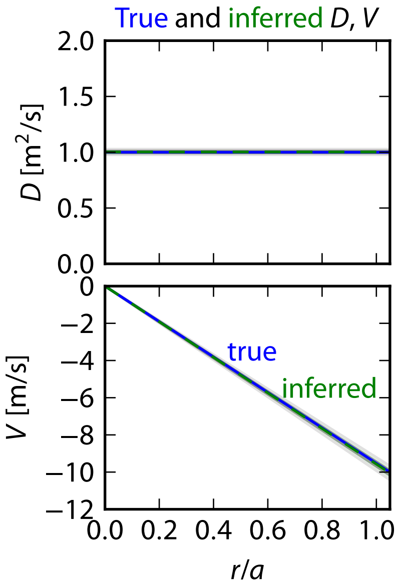
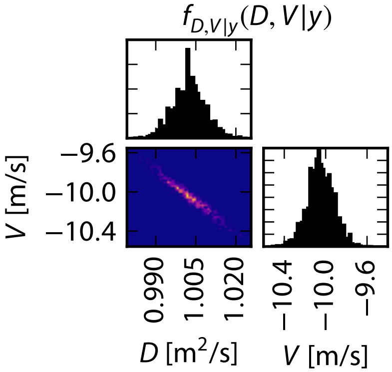


MultiNest successfully reconstructs simple *D*, *V* profiles

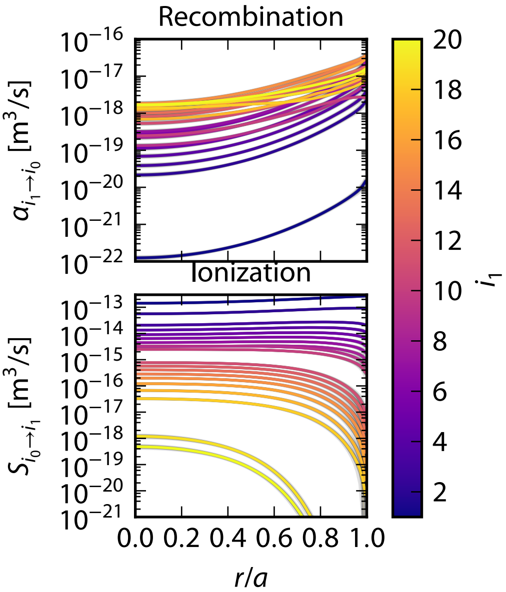
(synthetic data)



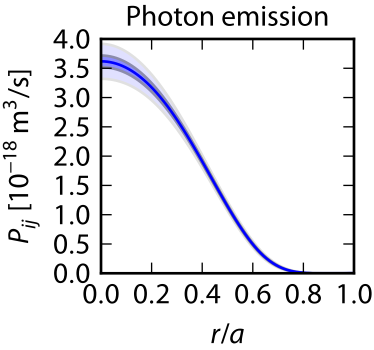
- Five local measurements
- $\Delta t = 6$ ms, 5% noise
- Have also tested with 32 XICS chords



Rate coefficients have low sensitivity to n_e, T_e over their uncertainties



- 1000 samples from n_e, T_e
- $\pm 3\sigma$ band on α, S not even visible!
- These are the only ways that n_e, T_e enter the calculation.

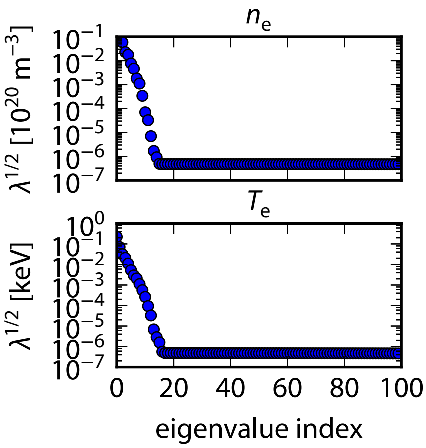


GPR permits efficient propagation of uncertainty [Chilenski NF 2015]

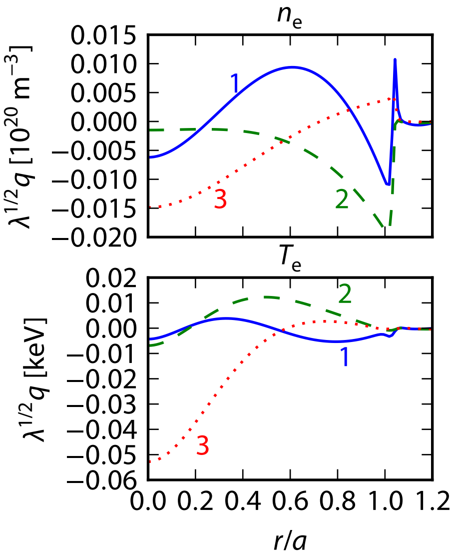
Drawing samples of the profile $\boldsymbol{y}$:

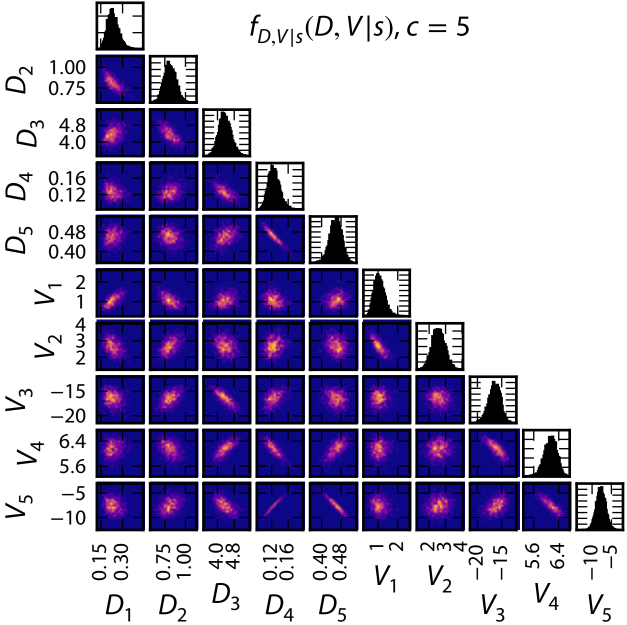
$$\boldsymbol{y} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}), \quad \boldsymbol{\Sigma} = \mathbf{Q}\boldsymbol{\Lambda}\mathbf{Q}^{-1}$$

$$\tilde{\boldsymbol{y}} = \mathbf{Q}\boldsymbol{\Lambda}^{1/2}\boldsymbol{u} + \boldsymbol{\mu}, \quad \boldsymbol{u} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

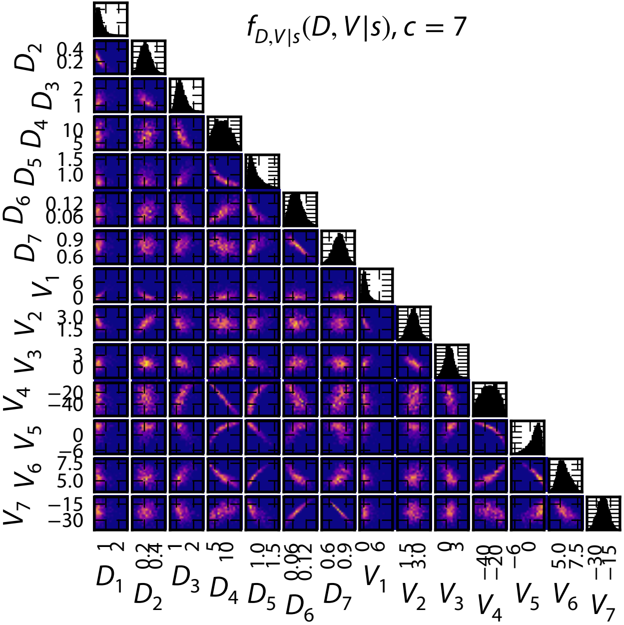


n_e, T_e eigenvectors





$f_{D,V|s}(D, V|s), c = 5$
D_1 D_2 D_3 D_4 D_5 V_1 V_2 V_3 V_4 V_5


$f_{D,V|s}(D,V|s), c = 7$
D_1
D_2
D_3
D_4
D_5
D_6
D_7
V_1
V_2
V_3
V_4
V_5
V_6
V_7