

Experimental data analysis techniques for validation of tokamak impurity transport simulations

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Experimental data analysis techniques for validation of tokamak impurity transport simulations

- ① Motivation: validation of turbulent transport simulations
- ② Profile fitting with nonstationary Gaussian process regression
- ③ Inferring impurity transport coefficients: a very difficult inverse problem
- ④ Conclusions and future directions

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Motivation: nuclear fusion and impurity transport

Ideal situation

- Make plasma, heat it up.
- Energy is produced faster than it is lost.
- Impurities do not accumulate.
- Clean, sustainable energy for everyone! 😊

What actually happens

- Make plasma, heat it up.
- Turbulence causes energy to leak out.
- Impurities accumulate, further contributing to energy loss.
- No net energy gain. 😞

Options

- Build bigger and bigger tokamaks until we finally get one big enough to hold its energy in. \$\$\$ = 😞
- Develop predictive simulations, figure out how to optimize the configuration *before* building an expensive facility. \$\$ = 😊

Motivation: validation of impurity transport simulations

Options

- Build bigger and bigger tokamaks until we finally get one big enough to hold its energy in. \$\$\$ = ☹
- **Develop predictive simulations, figure out how to optimize the configuration before building an expensive facility.** \$\$ = ☺

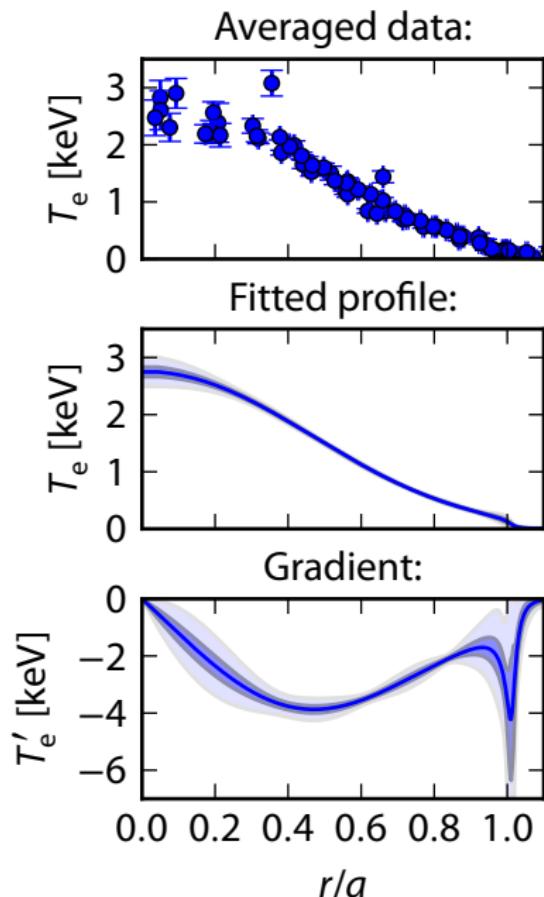
How do we get there?

- Need to test simulations against existing experiments.
- Highly sensitive to gradients: *all* validation work benefits from improved gradient measurements.
- Impurity transport measurements are key:
 - Of fundamental importance to setting the power balance.
 - Another channel to check turbulent transport simulations with.

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Profile fitting: a critical step for plasma data analysis



- Transport codes are highly sensitive to *gradients* in n_e , T_e , etc.
- Many codes require *entire profiles* as inputs.
- Need to propagate profile uncertainties efficiently.

Gaussian process regression (GPR) overcomes the many issues with previous approaches to profile fitting

Old: Splines

- Fit data with piecewise polynomial.
- Software readily available.

- Pick properties by eye:
subjective, time consuming.

- Inefficient propagation of profile uncertainty.


New: GPR

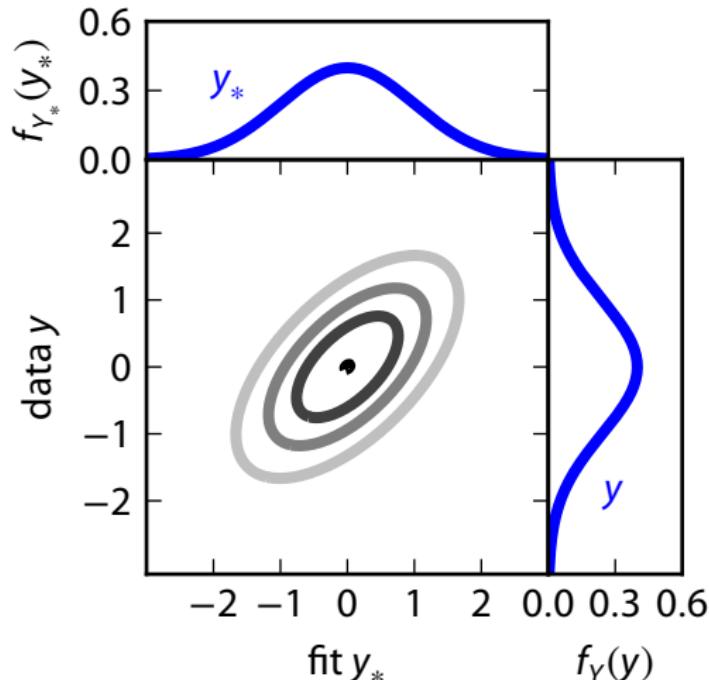
- Fit data with multivariate normal distribution.
- New software had to be written.

- Pick properties with statistically rigorous, automated procedure.

- Enables efficient uncertainty propagation.

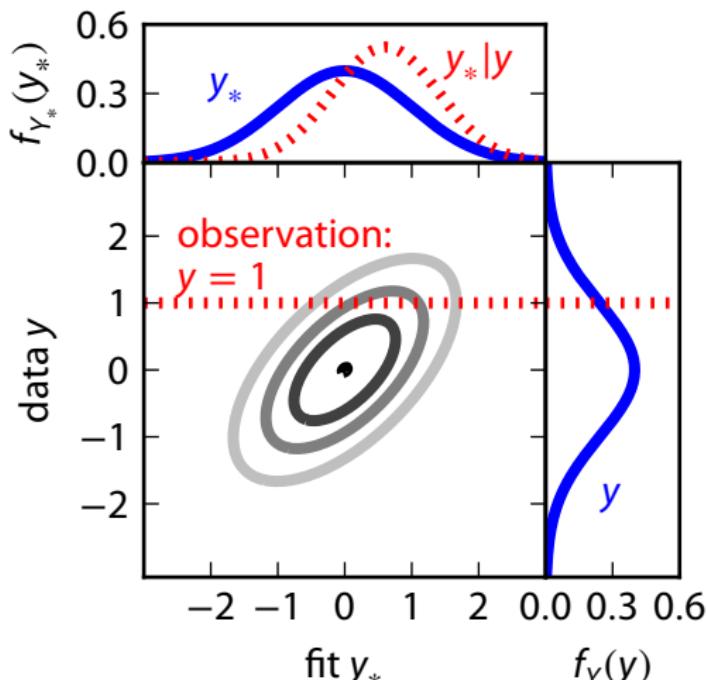

Gaussian process regression (GPR): a statistically rigorous method to fit profiles, propagate uncertainty

- Describe data y , fit y_* as a multivariate normal distribution.
- Can include derivatives, line integrals.



Gaussian process regression (GPR): a statistically rigorous method to fit profiles, propagate uncertainty

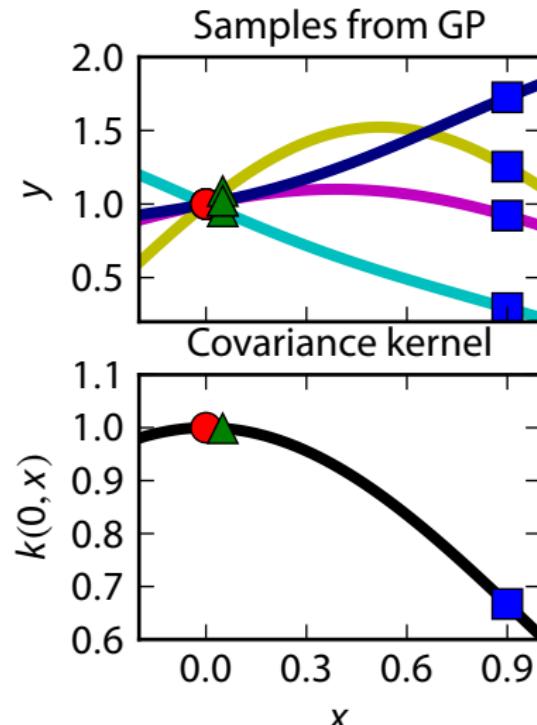
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The covariance kernel sets the smoothness

Covariance kernel

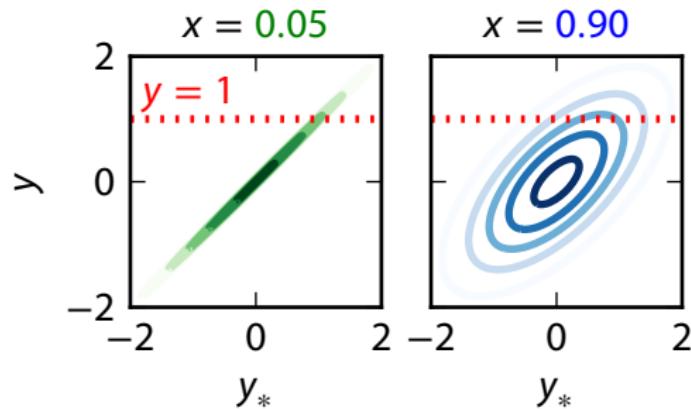
$k(x_1, x_2) = \text{cov}[y_1, y_2]$ sets how spatial covariance decays:



Key step: infer hyperparameters

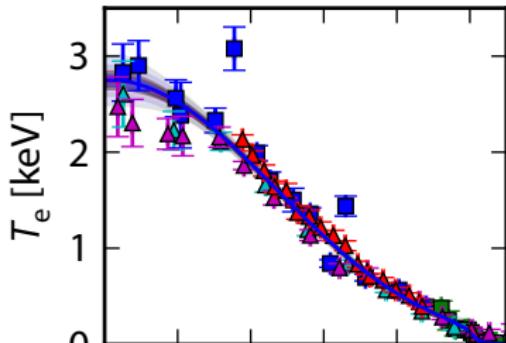
θ of covariance kernel:

- maximize $f_{\Theta|Y}(\theta|y)$, or
- sample $\tilde{\theta} \sim f_{\Theta|Y}(\theta|y)$

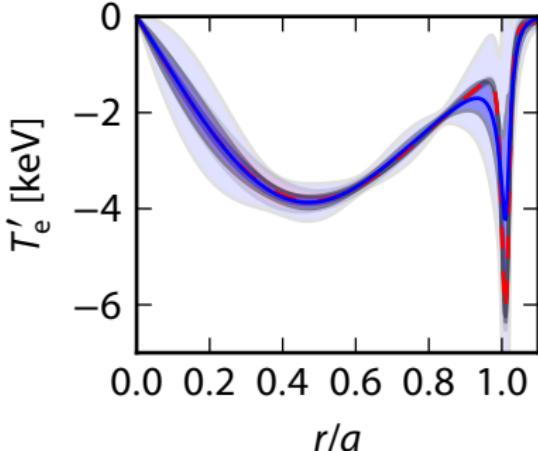


Demonstration: L-mode temperature profile

Profile:



Gradient:

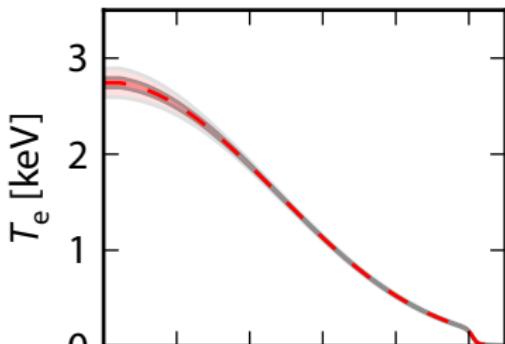


- Combine data from core TS, edge TS, GPC, GPC2, FRCECE
- Force $dT_e/dr = 0$ at $r = 0$
- Handling the hyperparameters θ :
 - MAP: $\hat{\theta} = \arg \max_{\theta} f_{\Theta|Y}(\theta|y)$
 - MCMC: $f_{Y_*|Y}(y_*|y) = \int f_{Y_*|Y, \theta}(y|y_*, \theta) f_{\Theta|Y}(\theta|y) d\theta$
- Key result: $\sigma_{T_{e,MCMC}} \approx \sigma_{T_{e,MAP}}$, $\sigma_{a/L_{T_{e,MCMC}}} \approx 2.6 \times \sigma_{a/L_{T_{e,MAP}}}$
- Can use fast MAP when only value matters 😊, but need slow MCMC when gradients matter 😞
- Software: gptools.readthedocs.io

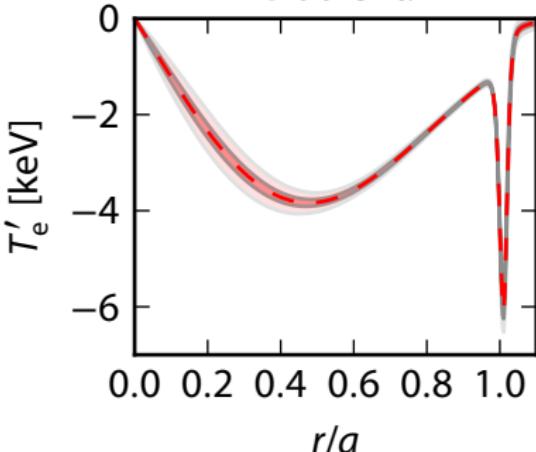
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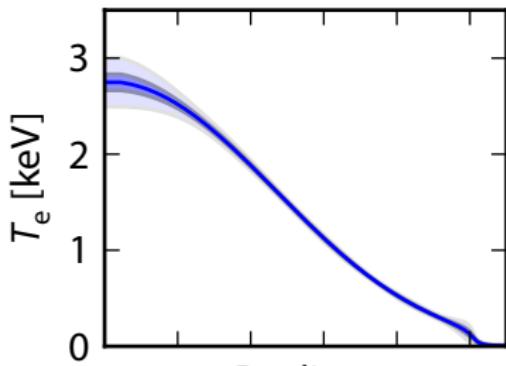


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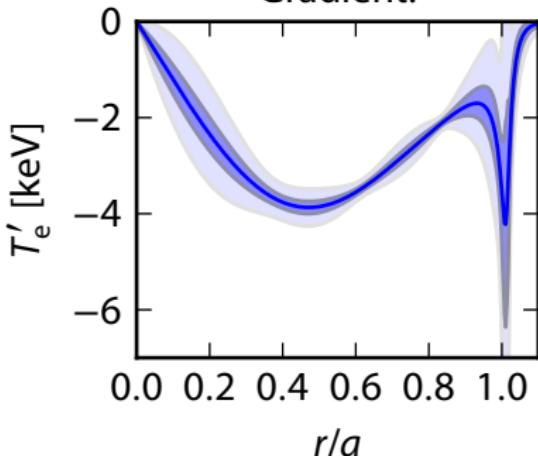
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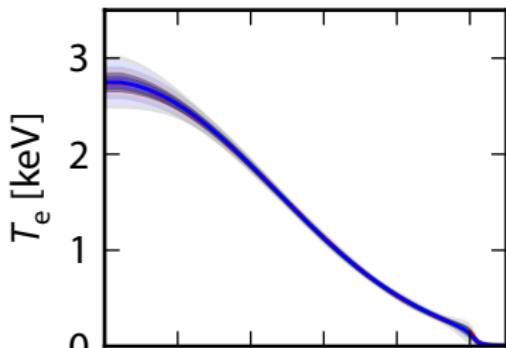


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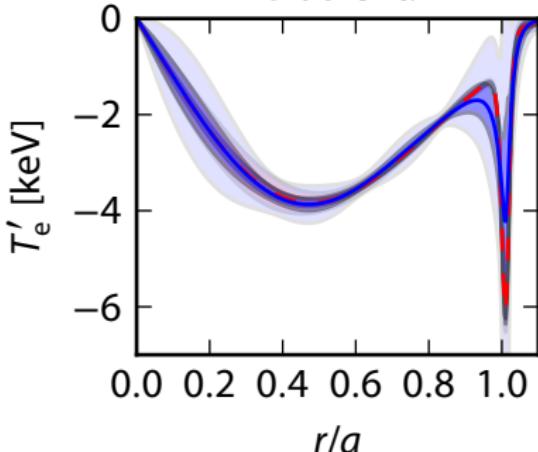
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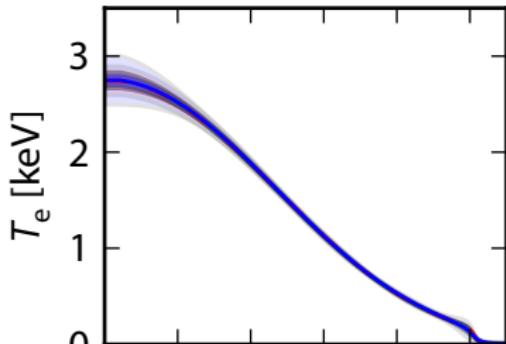


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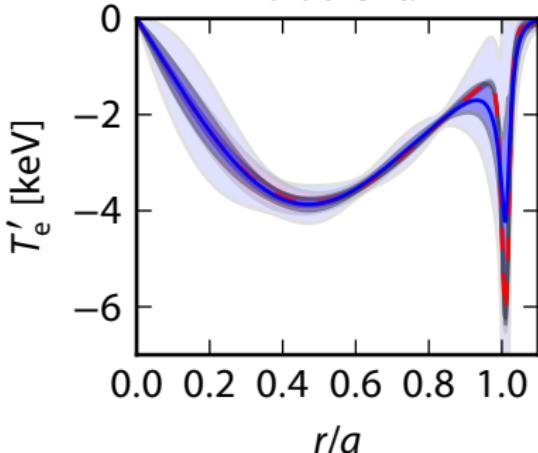
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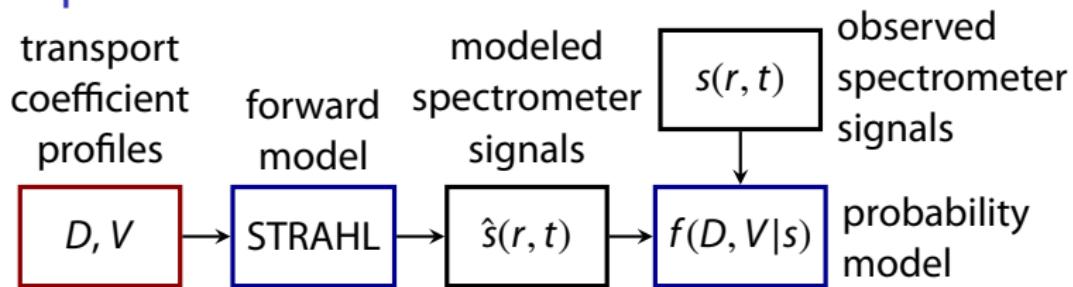
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Inferring impurity transport coefficients: a nonlinear inverse problem

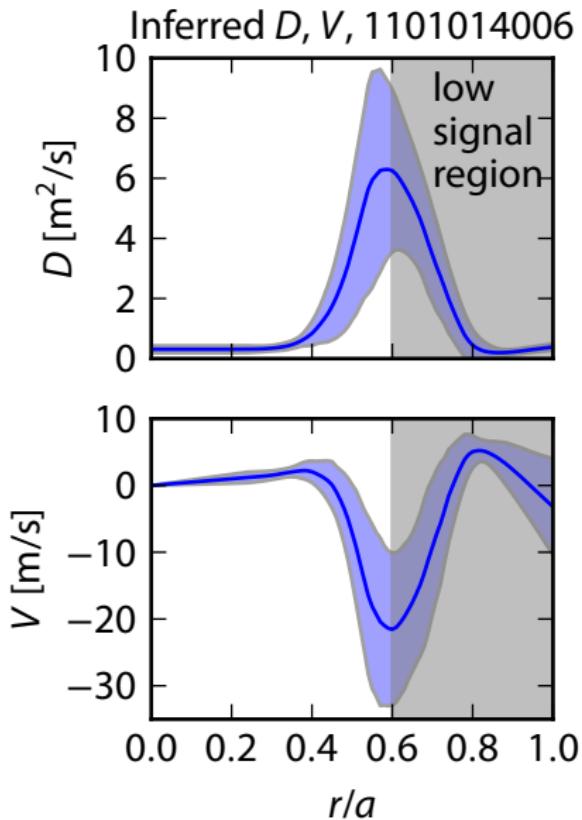


- Diffusion coefficient D , convective velocity V .
- Can only observe s , want to know D, V .
- Only know the forward mapping: $\hat{s} = m(D, V)$, but want $D, V = m^{-1}(s)$.
- Key questions:
 - Existence:** Is there a D, V such that $\hat{s} \approx s$?
 - Uniqueness:** How many D, V are there such that $\hat{s} \approx s$?
 - Stability:** How much do D, V change when I perturb s ?

What is wrong, and what I have done about it

Previous methods have substantial shortcomings

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



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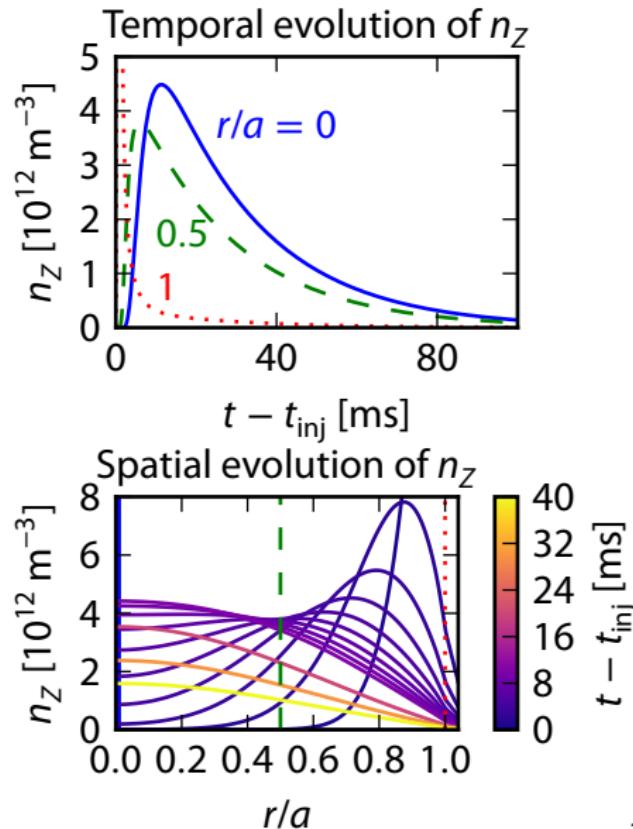
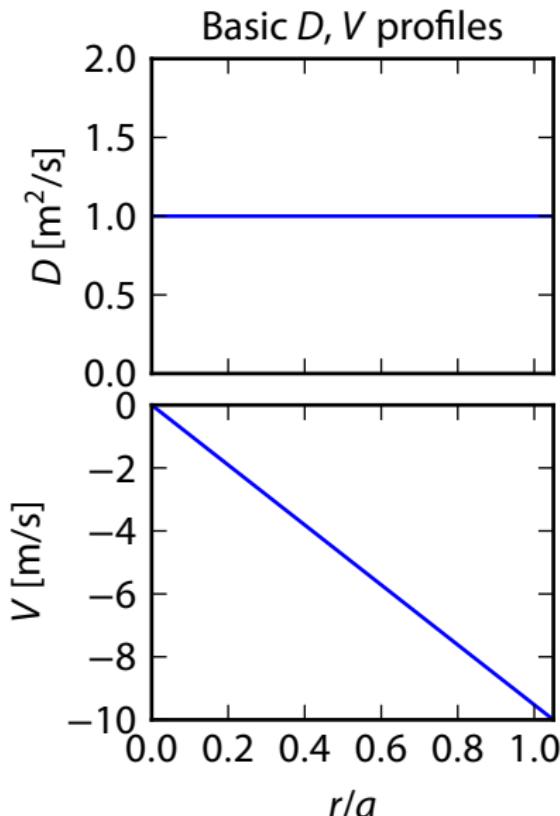
Attack the problem two ways

- **Fast, linearized model** to get order-of-magnitude
- **Slow, complete procedure**

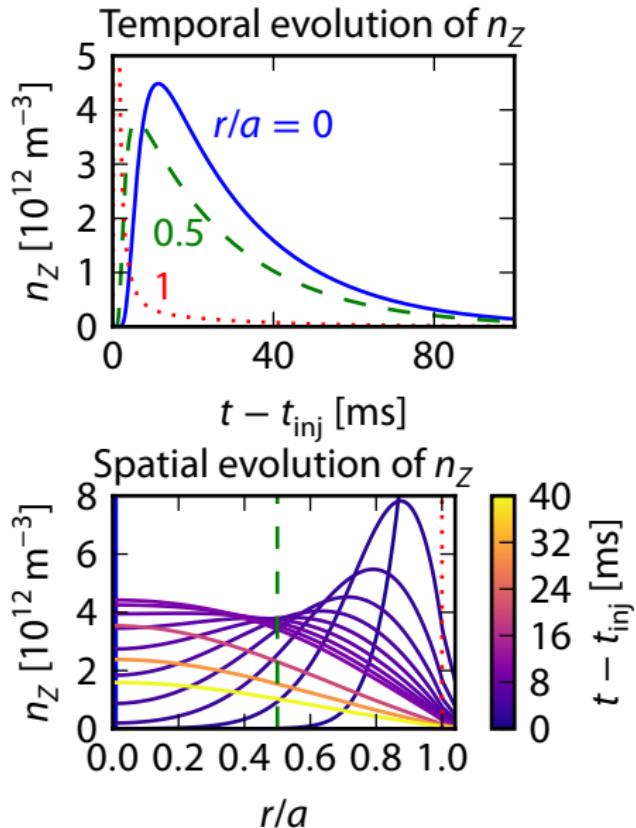
Surprising results

- Spatial resolution trumps temporal resolution.
- n_e, T_e do not matter.
- Selecting the appropriate complexity for D, V is really, really important.

Painfully simple transport coefficient profiles produce behaviors representative of what is seen experimentally

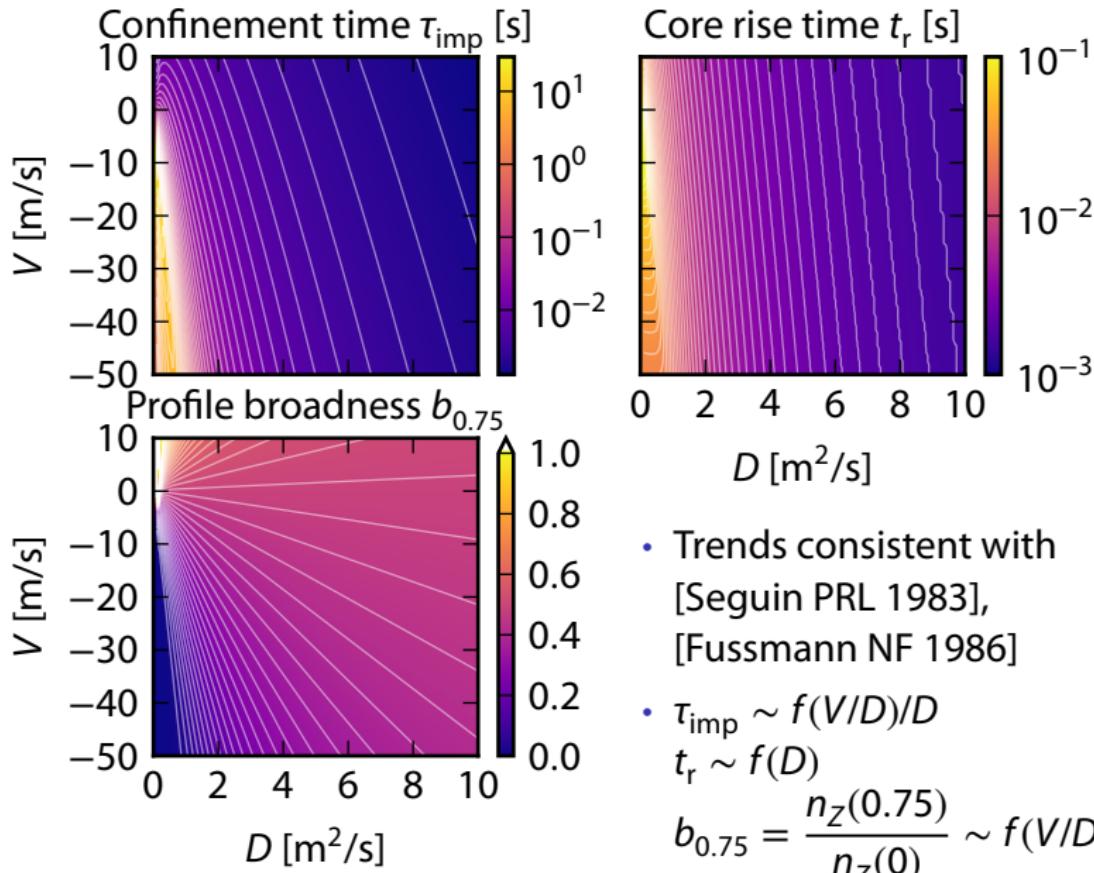


Three figures of merit capture most of the information



- Informed by theoretical analysis in [Seguin PRL 1983] and [Fussmann NF 1986].
- **Impurity confinement time:** $\tau_{\text{imp}} \sim f(V/D)/D$
- **Rise time** (of core): $t_r \sim f(D)$
- **Profile broadness** (during decay):
 $b_{r/a} = n_Z(r/a)/n_Z(0) \sim f(V/D)$

τ_{imp} , t_r , $b_{0.75}$ are all different functions of D , V

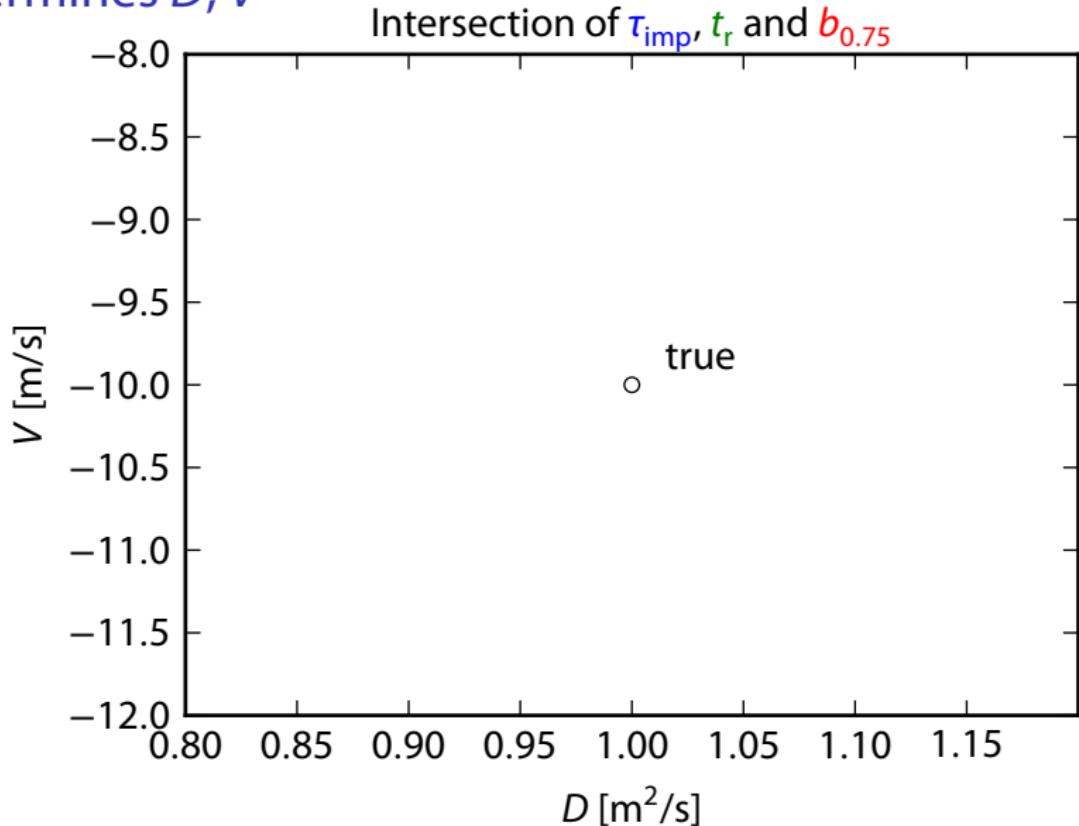


- Trends consistent with
[Seguin PRL 1983],
[Fussmann NF 1986]

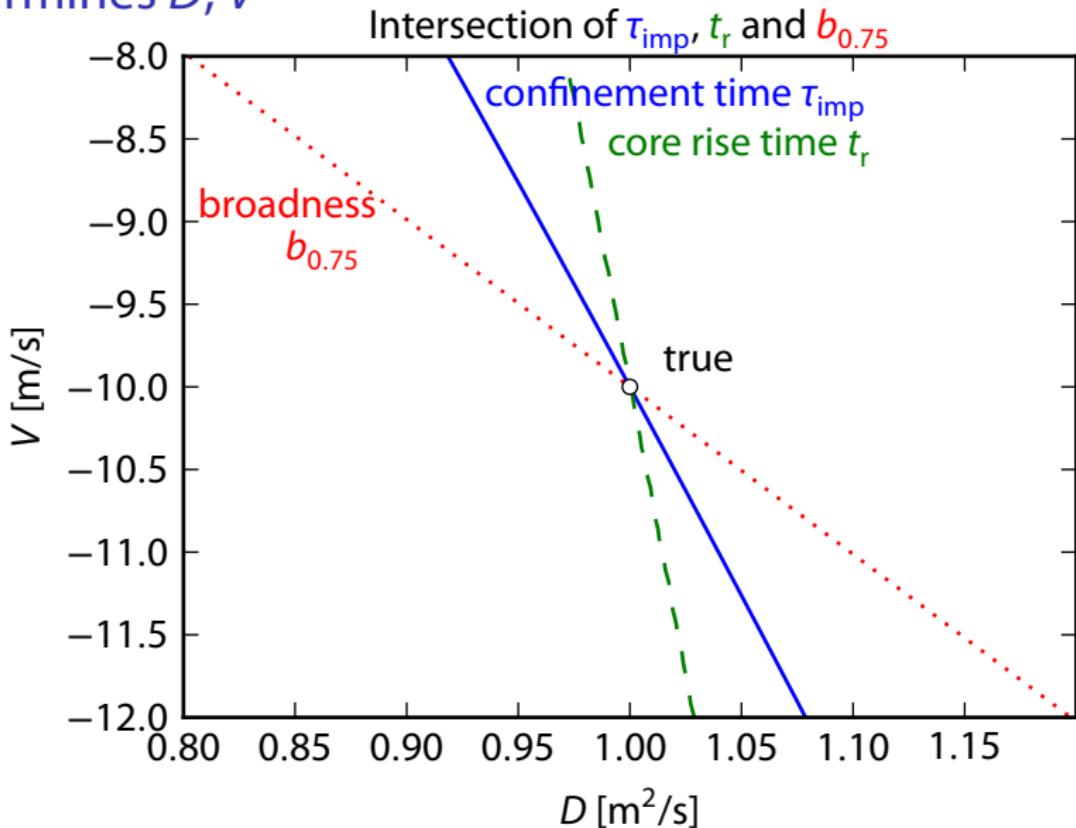
- $\tau_{\text{imp}} \sim f(V/D)/D$
 $t_r \sim f(D)$

$$b_{0.75} = \frac{n_Z(0.75)}{n_Z(0)} \sim f(V/D)$$

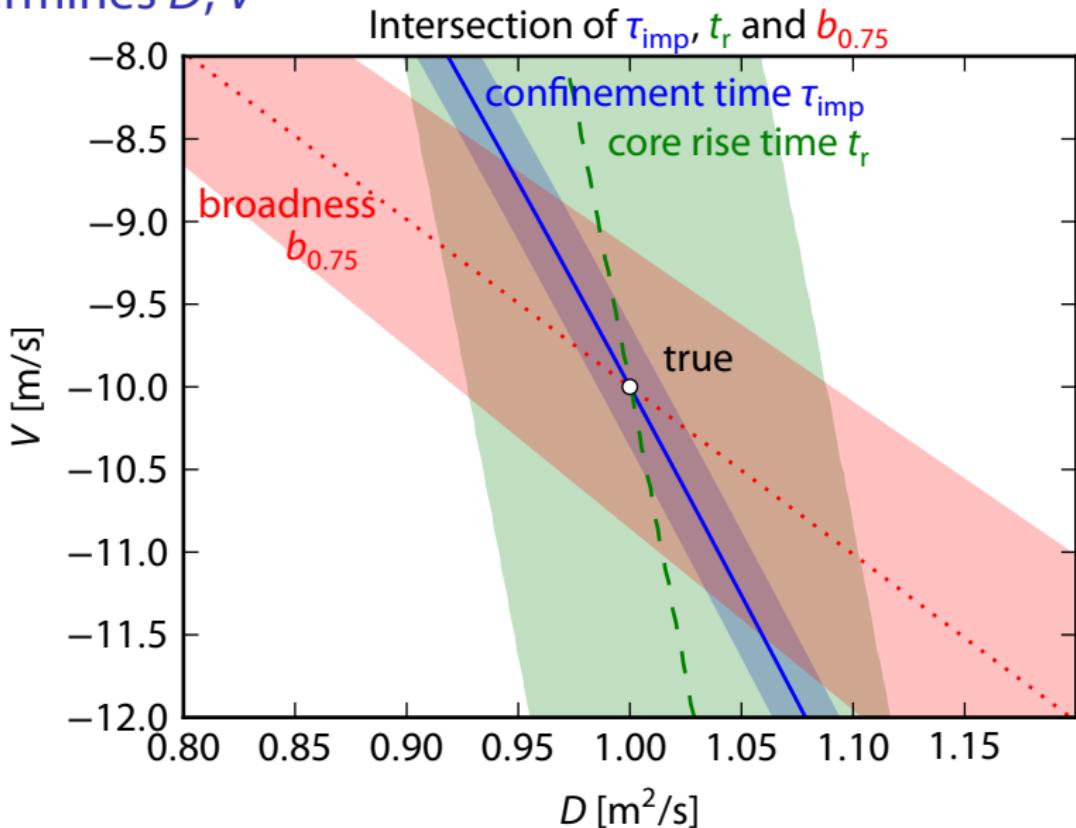
The unique intersection of the contours of τ_{imp} , t_r and $b_{0.75}$ determines D, V



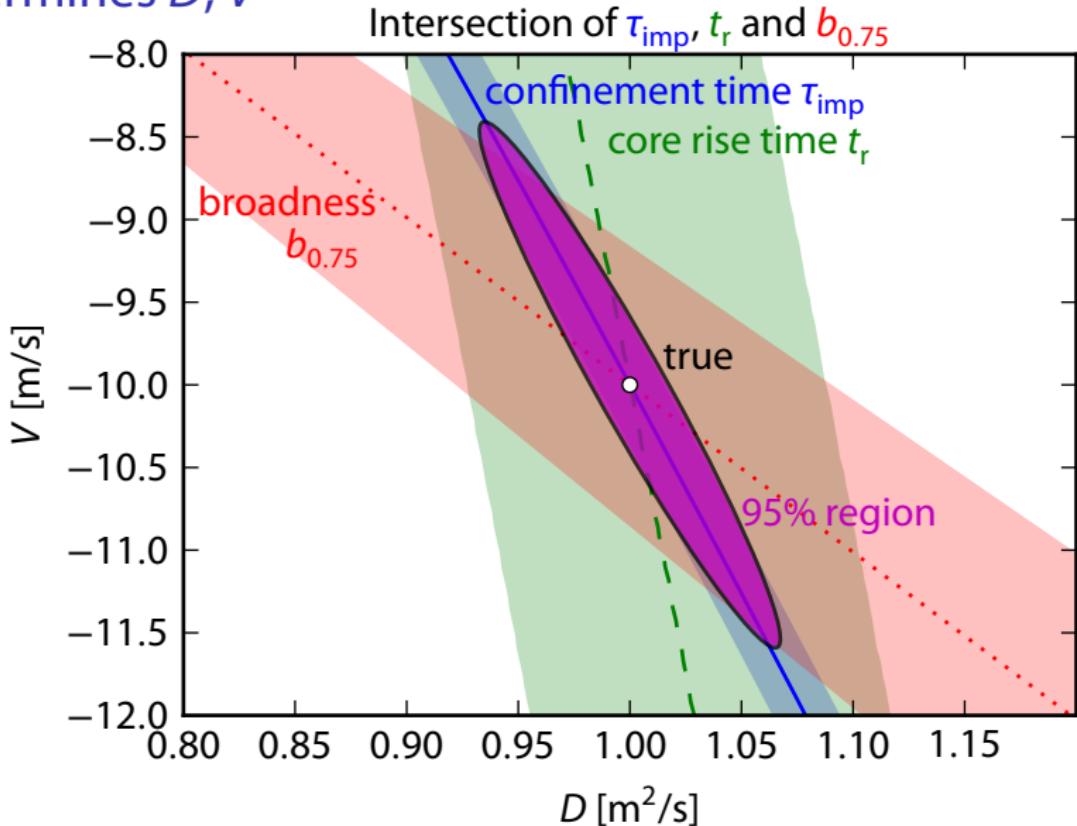
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Making the picture quantitative

- Linearize each figure of merit $y_i = g_i(D, V)$ with respect to D, V .
- Assume Gaussian noise: $y_i \sim \mathcal{N}(\mu_{y_i}, \sigma_{y_i}^2)$.
- Transport coefficient vector $\mathbf{T} = [D, V]^\top \sim \mathcal{N}(\boldsymbol{\mu}_{T|y}, \boldsymbol{\Sigma}_{T|y})$:

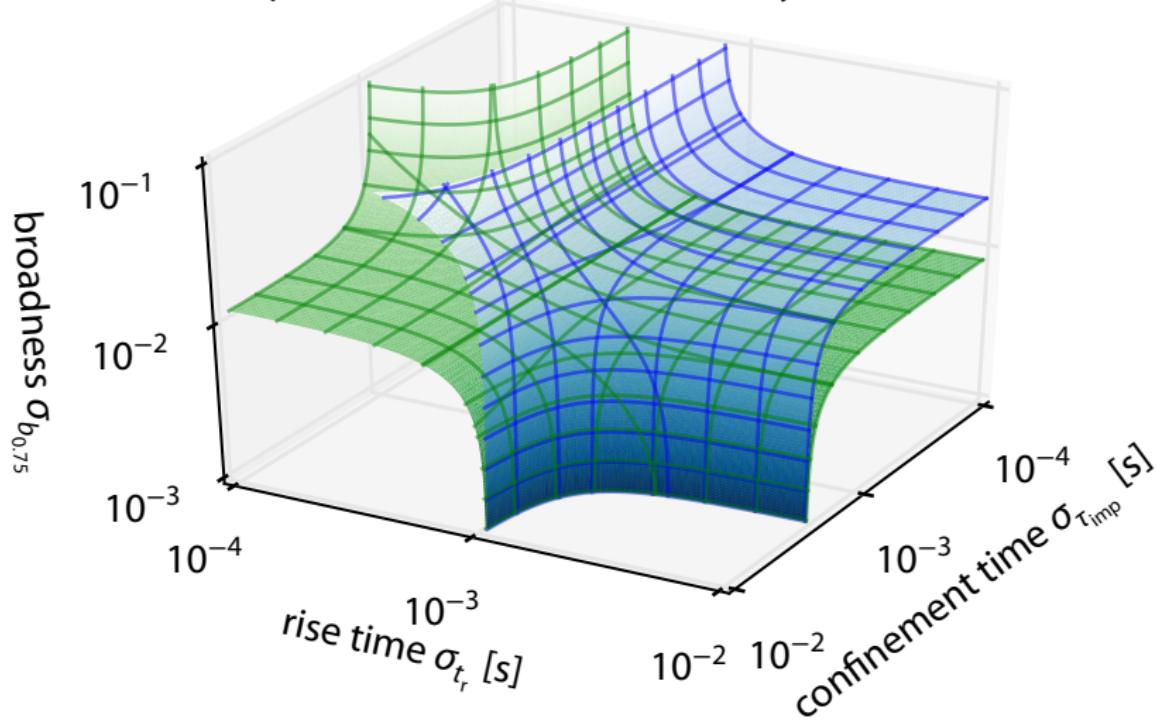
$$\boldsymbol{\mu}_{T|y} = (\mathbf{C}^\top \boldsymbol{\Sigma}_y^{-1} \mathbf{C})^{-1} (\mathbf{C}^\top \boldsymbol{\Sigma}_y^{-1} (\mathbf{y} - \mathbf{a}))$$
$$\boldsymbol{\Sigma}_{T|y} = (\mathbf{C}^\top \boldsymbol{\Sigma}_y^{-1} \mathbf{C})^{-1}$$

- $\boldsymbol{\mu}_{T|y}$ is the actual prediction of $\mathbf{T} = [D, V]^\top$,
- $\boldsymbol{\Sigma}_{T|y}$ contains the uncertainties.
- \mathbf{a} and \mathbf{C} come from the linearization.
- \mathbf{y} contains the actual observations,
- $\boldsymbol{\Sigma}_y$ contains the uncertainties.

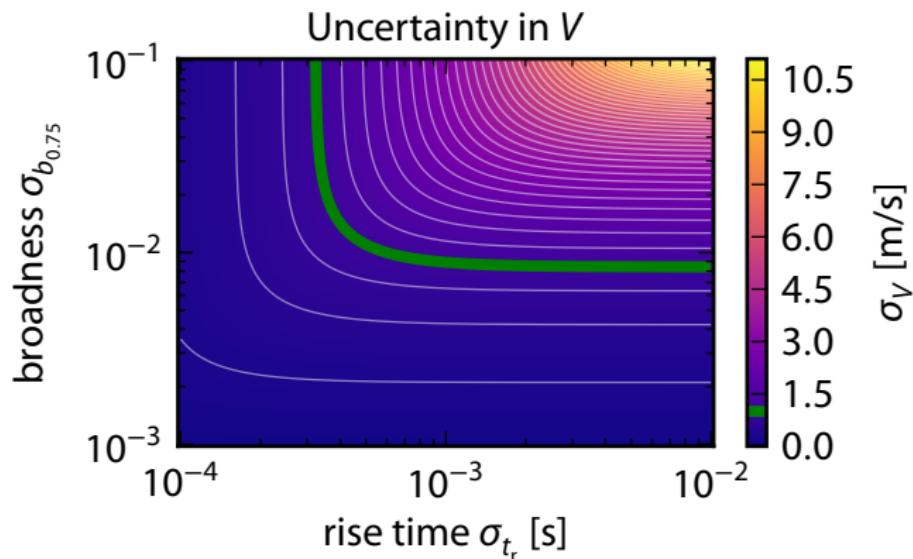
This is exactly the result of **weighted least squares regression**:
the analysis attempts to match the observations in the least squares sense.

The linearized model can estimate the uncertainties on D and V given the uncertainties on τ_{imp} , t_r and $b_{0.75}$

Requirements for 10% uncertainty in D and V



Either rise time or broadness needs to be known to high precision



- Green contour: $\sigma_V/V_0 = \pm 10\%$ (what previous plot gave).
- Assume confinement time is known precisely.
- **Only need to know one of t_r or $b_{0.75}$ to high precision:** only a limited window where they are on an equal footing.

Characterizing the diagnostic requirements

Three key parameters:

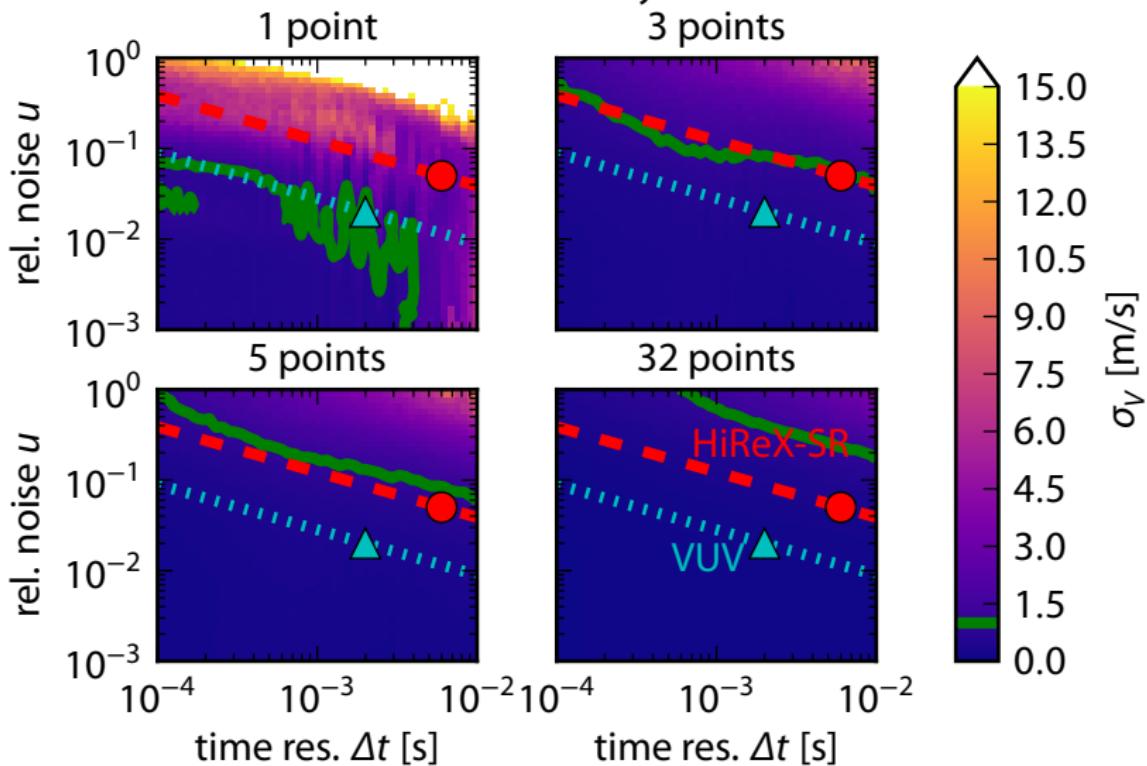
1. Number of channels, N
2. The time resolution, Δt
3. The relative noise level, $u = \sigma_s/s$

Method:

1. Generate many synthetic data sets with different realizations of Gaussian noise and phase with respect to injection.
2. Determine τ_{imp} , t_r and $b_{r/a} = n_Z(r/a)/n_Z(0)$ for each realization.
3. Compute $\sigma_{\tau_{\text{imp}}}$, σ_{t_r} and $\sigma_{b_{r/a}}$ from the ensemble of fits.
4. Compute σ_D and σ_V .

Spatial resolution is more important than time resolution

Uncertainty in V



Dashed lines: contours of constant photon rate

Green contours: $\sigma_V/V_0 = \pm 10\%$

Implications of the linearized model

- C-Mod's diagnostics appear to be sufficient to reproduce simple D, V profiles. 
- Spatial resolution is more important than time resolution:
 - Better to invest in *more* detectors than *fancier* detectors.  
 - Can handle sawteeth by using a *single* injection. 

Caveats

- Ignored details of tomographic inversion.
- Threw out lots of other information in the signals.
- Used painfully oversimplified D, V profiles.

Building the full analysis: two key steps to inference

Bayes' rule combines information from data with **prior knowledge/constraints**:

$$f_{D,V|y}(D, V|y) = \frac{\underbrace{f_{y|D,V}(y|D, V)}_{\substack{\text{likelihood:} \\ \text{information from data } y}} \cdot \underbrace{f_{D,V}(D, V)}_{\substack{\text{prior:} \\ \text{prior knowledge, constraints}}}}{\underbrace{f_y(y)}_{\substack{\text{evidence:} \\ \text{probability of data} \\ \text{under given parameterization, } \mathcal{M}}}}$$

$f_{D,V|y}(D, V|y)$
posterior:
everything known about D, V

Parameter estimation Find the values of D, V consistent with the data y : characterize $f_{D,V|y}(D, V|y)$.

Model selection Find the best way of parameterizing D, V by maximizing $f_y(y)$.

MultiNest [Feroz MNRAS 2008, 2009; Buchner AA 2014] produces samples from $f_{D,V|y}(D, V|y)$ and an estimate of $f_y(y)$.
Can handle multimodal posterior distributions.

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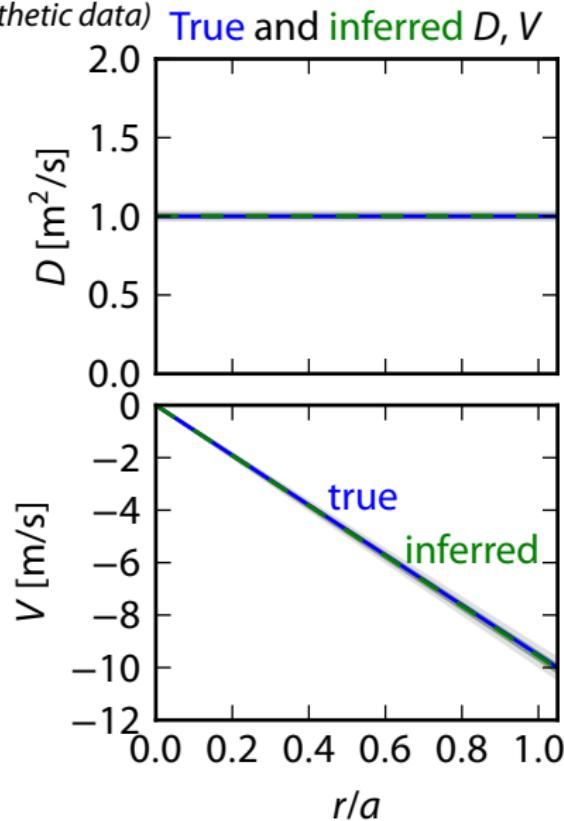
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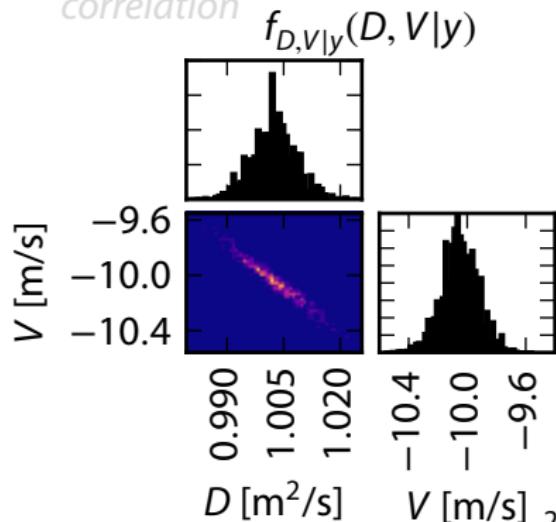
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MultiNest successfully reconstructs simple D, V profiles

(synthetic data)

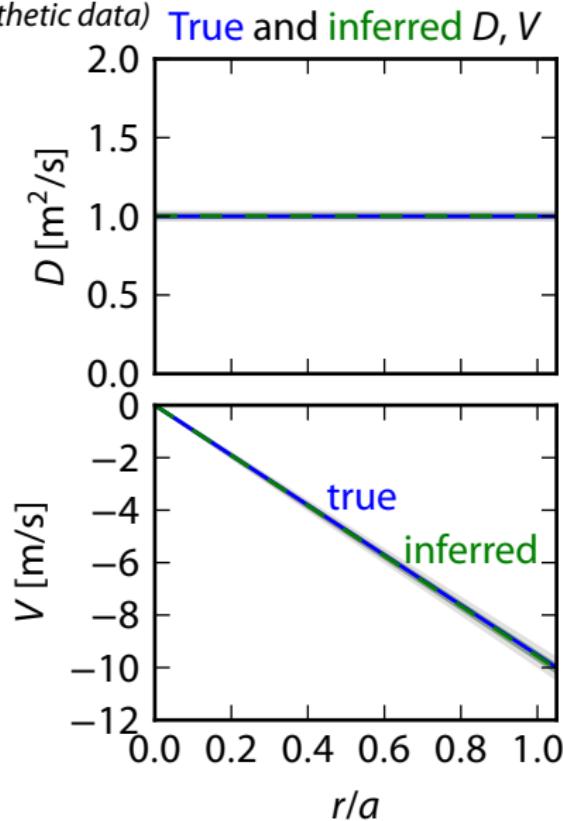


- Five local measurements
- $\Delta t = 6 \text{ ms}$, 5% noise
- Have also tested with 32 HiReX-SR chords
- 5x smaller σ_D, σ_V than linearized analysis, but same correlation



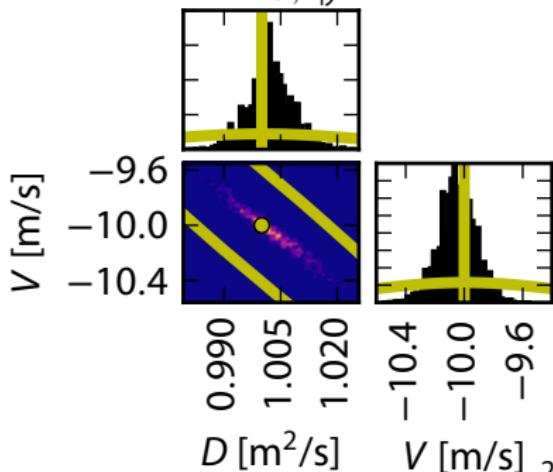
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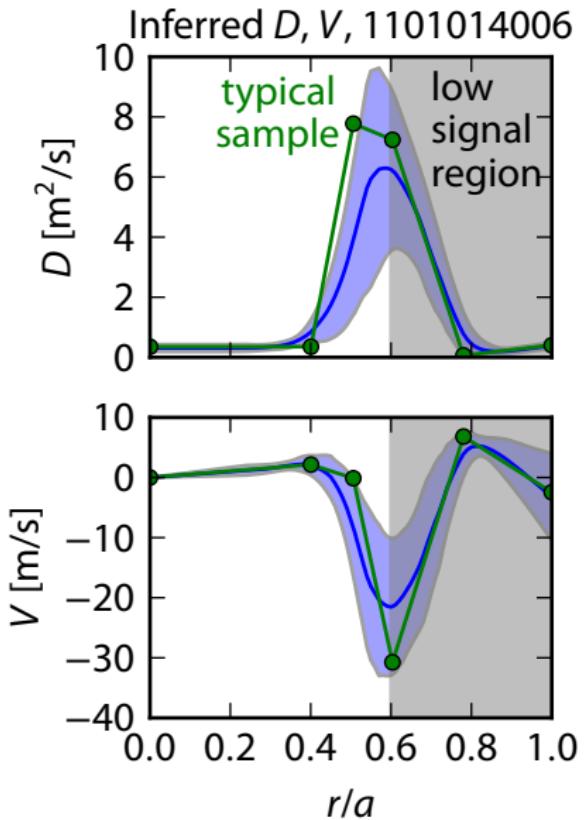
$$f_{D,V|y}(D, V|y)$$



Previous analysis ascribed all uncertainty in D , V to n_e , T_e (experimental data)

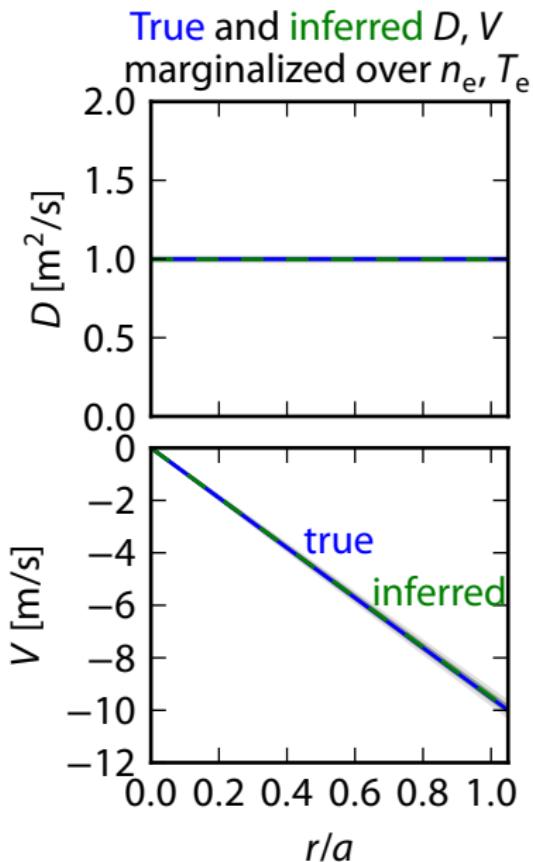
Previous approach [Howard NF 2012, Chilenski NF 2015]:

1. Model D , V with piecewise linear splines.
2. Generate random samples of n_e , T_e according to diagnostic uncertainties.
3. For each n_e , T_e realization, generate a random distribution of spline knots.
4. Given n_e , T_e and the spline knots, run an optimizer to find the best-fitting D , V profiles.
5. Find mean, standard deviation of resulting profiles.



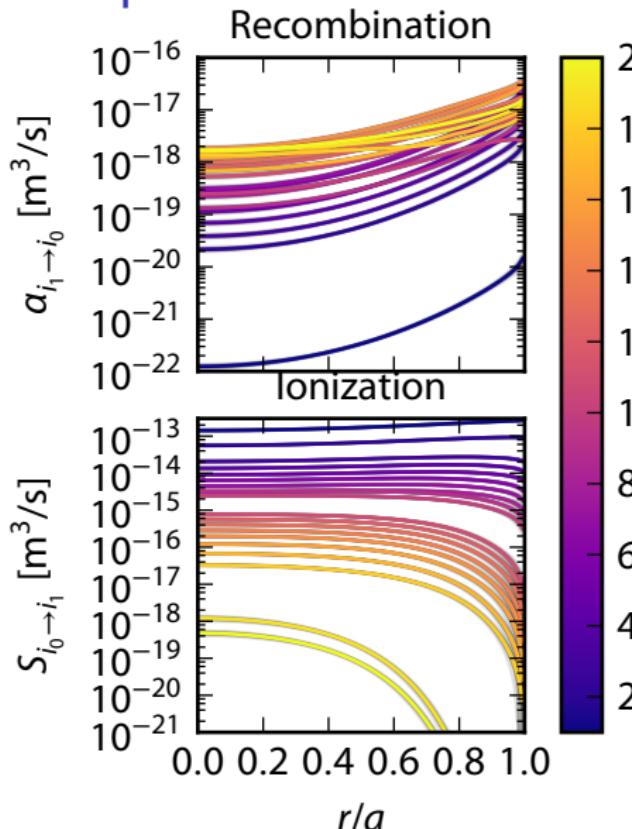
New result: n_e, T_e have little effect on D, V

(synthetic data)

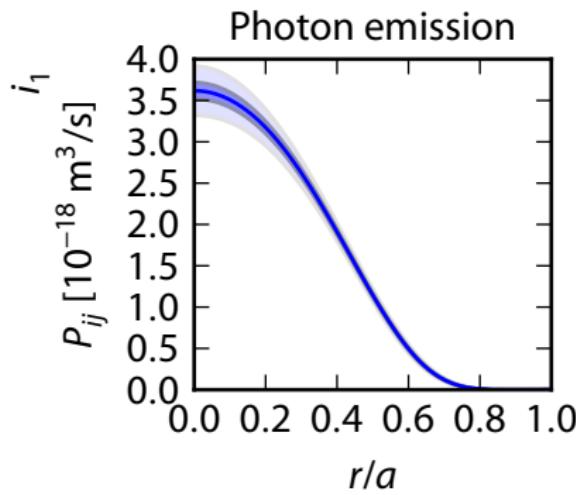


- 32 HiReX-SR chords, $\Delta t = 6 \text{ ms}$, 5% noise
- Fit n_e, T_e with GPR, propagated uncertainty using 3 eigenvalues for each.
- **Result is identical to fixed n_e, T_e case: exactly the opposite of what was expected from the previous work.**

The rate coefficients have limited sensitivity to n_e , T_e over the experimental uncertainties



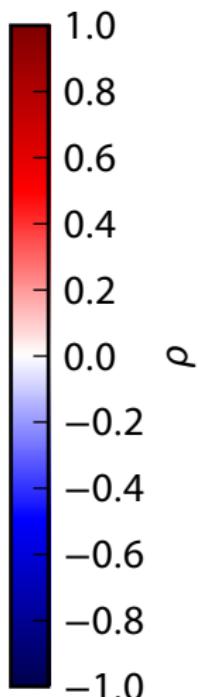
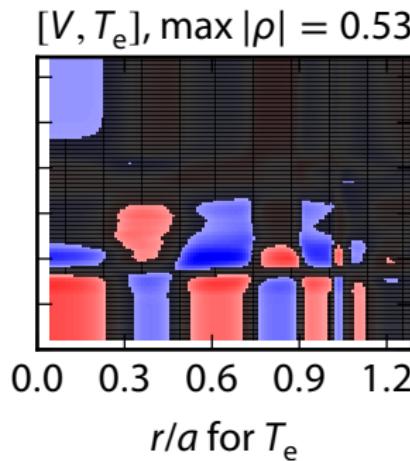
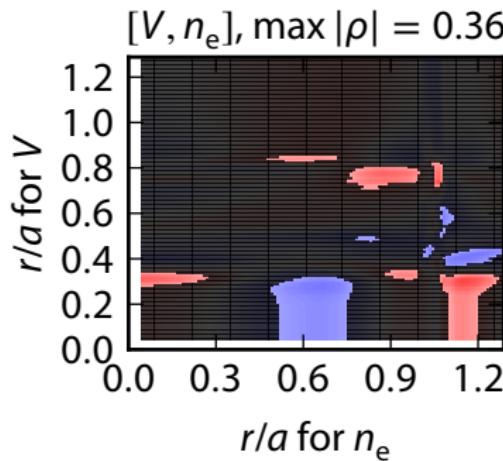
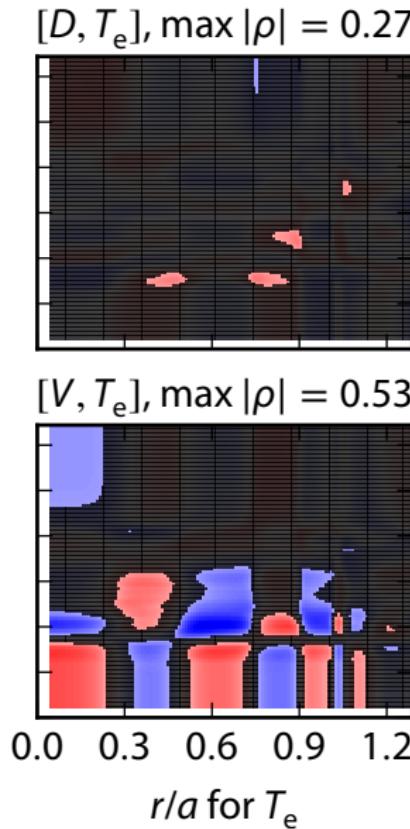
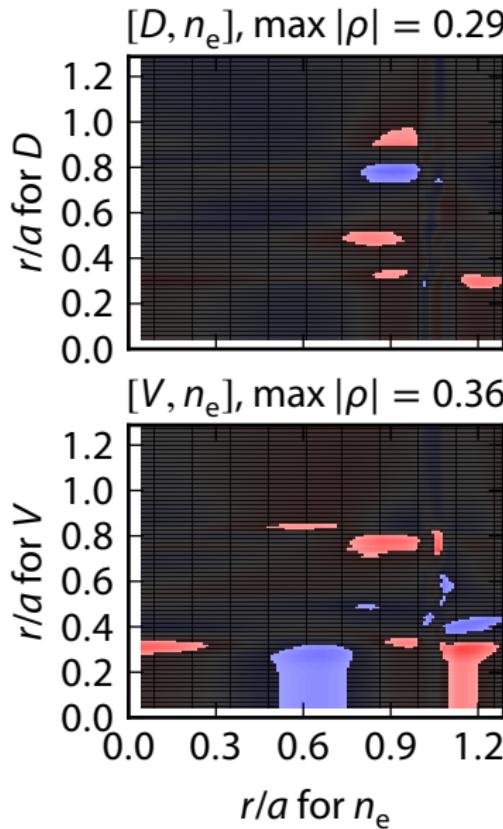
- 1000 samples from n_e , T_e
- $\pm 3\sigma$ band on a , S not even visible!
- These are the only ways that n_e , T_e enter the calculation.



How to explain the previous result? (1)

(experimental data)

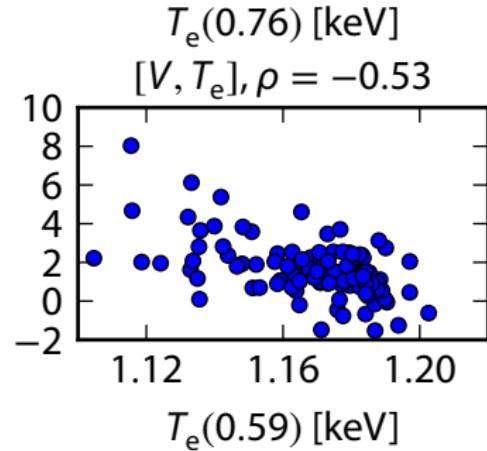
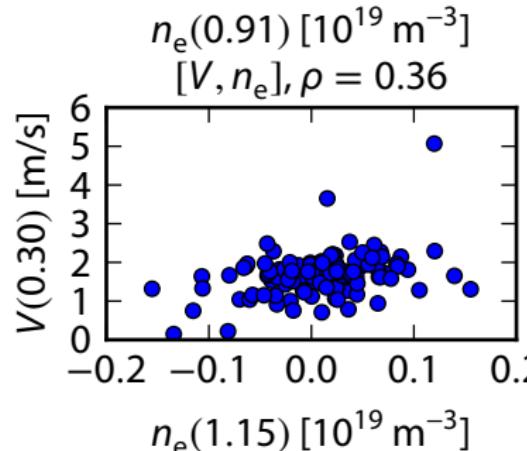
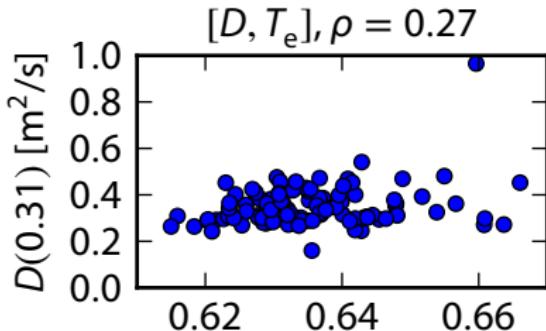
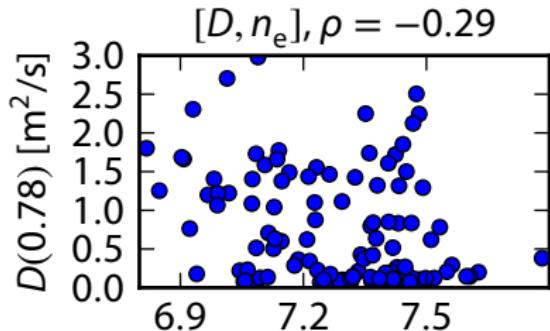
There is little correlation (ρ) between n_e , T_e and D, V



How to explain the previous result? (2)

(experimental data)

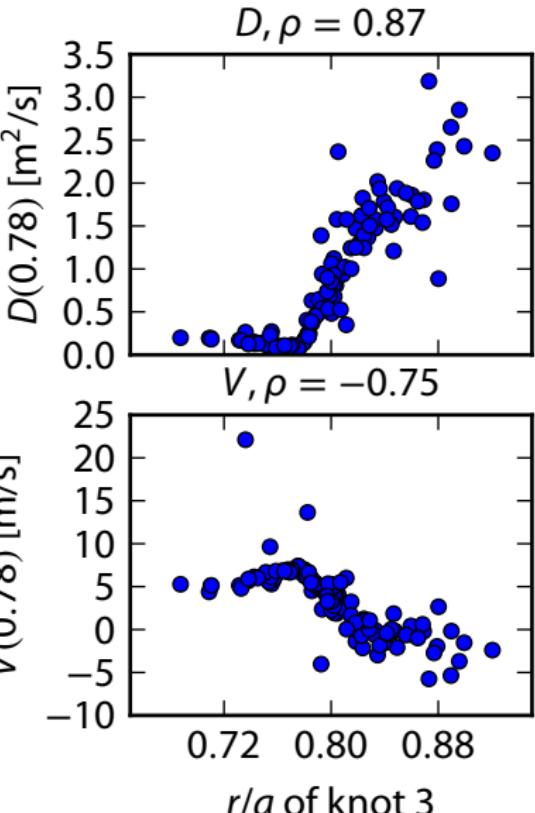
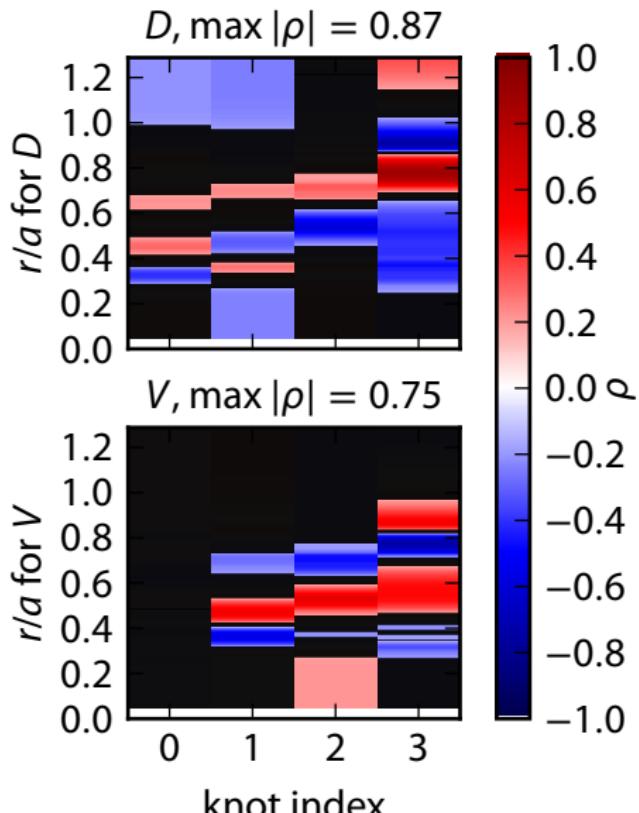
There is little correlation (ρ) between n_e , T_e and D , V



How to explain the previous result? (3)

(experimental data)

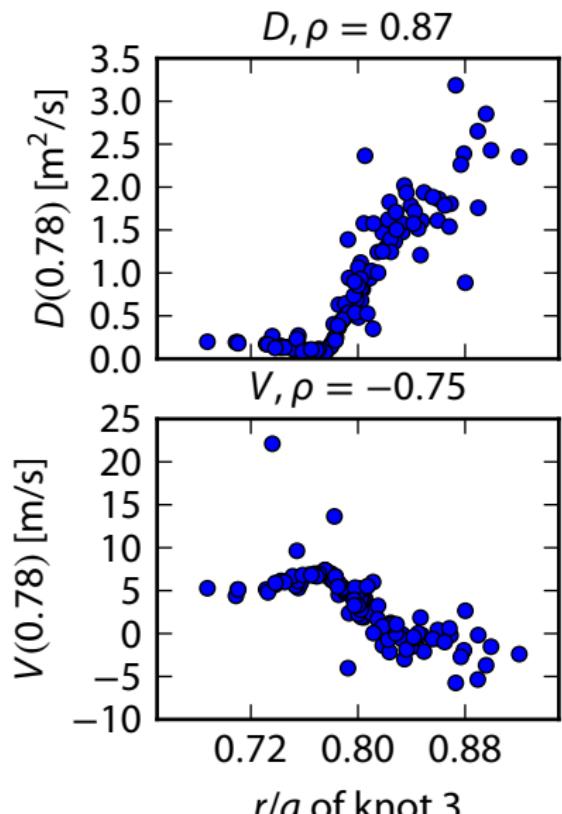
There is strong correlation (ρ) between knots and D, V



How to explain the previous result? (4)

(experimental data)

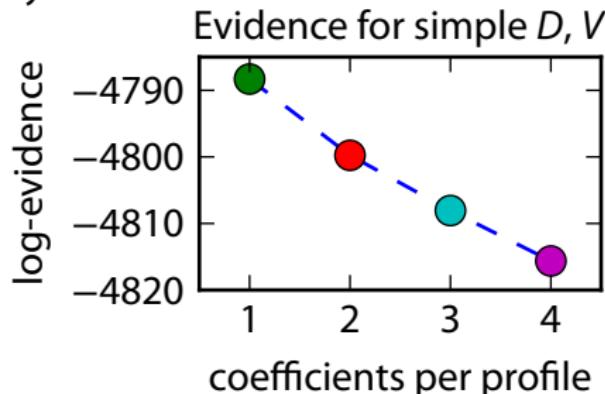
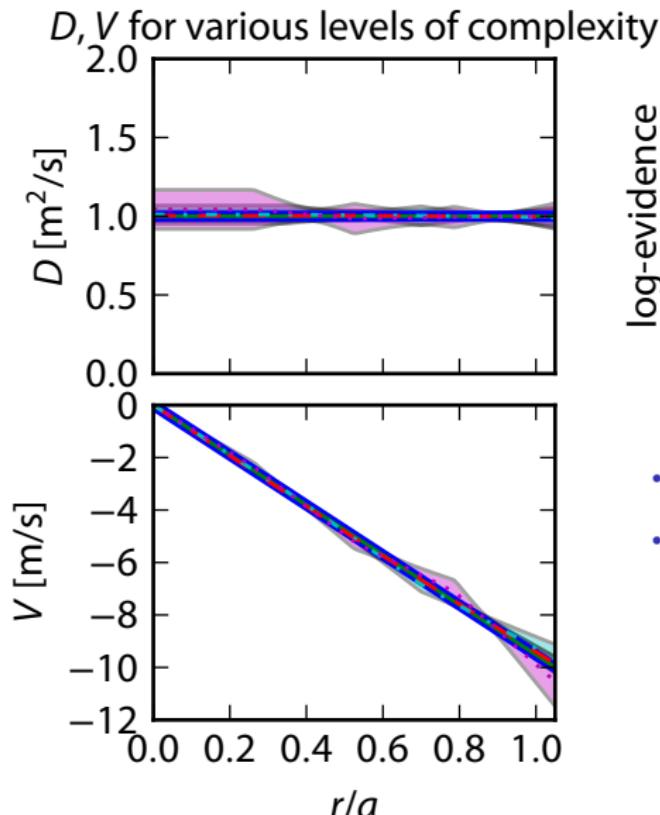
The variation seen before comes from moving the knots



- Correlation of D, V with knot locations is *much* higher than with n_e, T_e .
- Implies the previous parameterization is too inflexible.
- Free knots cause degenerate posterior distributions, need to add *fixed position* knots.
- **Selecting the right level of complexity is critical.**

Evidence $f_y(y)$ successfully selects simple model

(synthetic data)

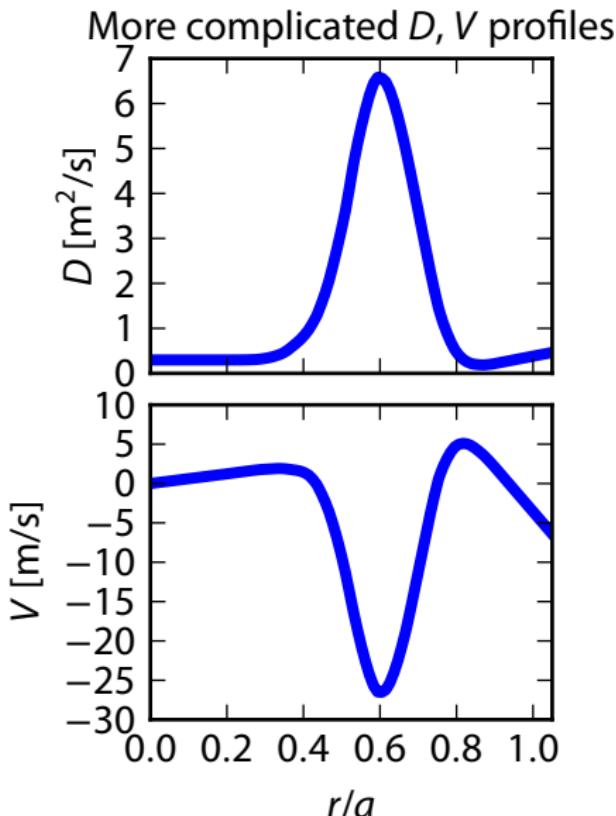


- True model has 1 coefficient.
- Linear trend is consistent with [Schwarz AS 1978]:

$$\ln f_y(y) \approx \ln f_{y|\hat{\theta}}(y|\hat{\theta}) - \frac{d}{2} \ln N$$

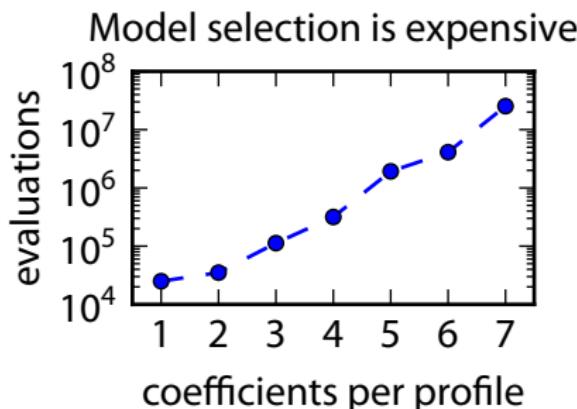
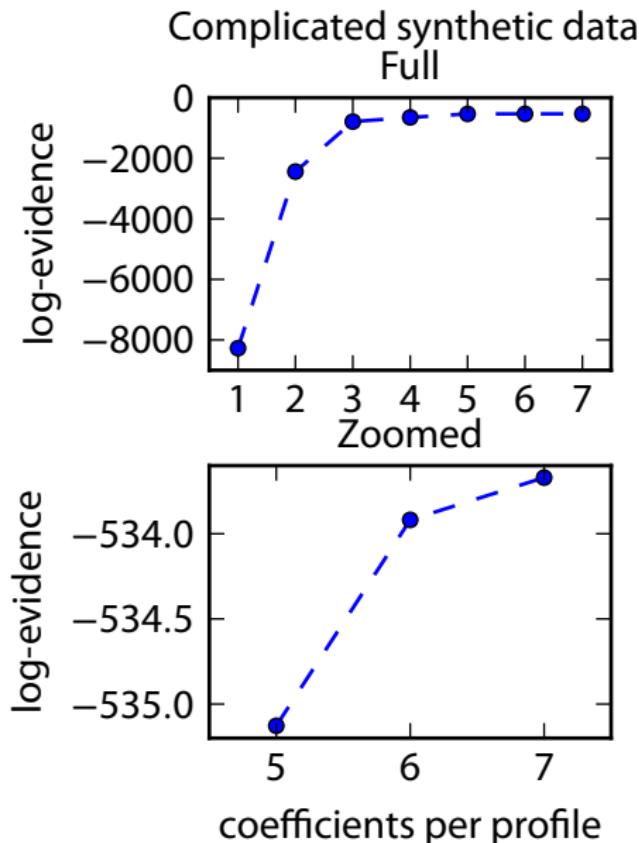
(d is number of parameters)

Testing with more complicated synthetic data



- Used result from old analysis as true profile:
 - Linear splines with 5 coefficients
 - Spline knots randomly varied to produce smooth curve
- Realistic diagnostic configuration:
 - 32 HiReX-SR chords (Ca^{18+}), 6 ms time resolution, 5% noise
 - 2 VUV chords ($\text{Ca}^{17+}, \text{Ca}^{16+}$), 2 ms time resolution, 5% noise

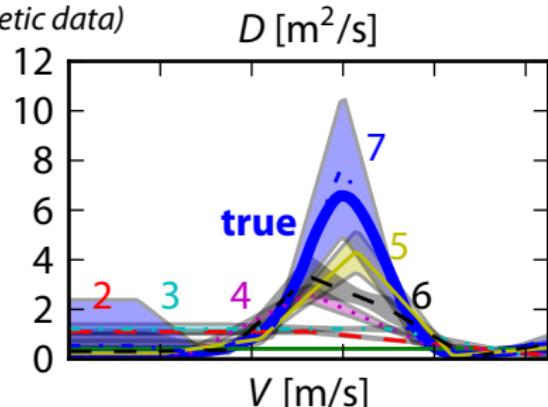
More complicated synthetic data pose a challenge



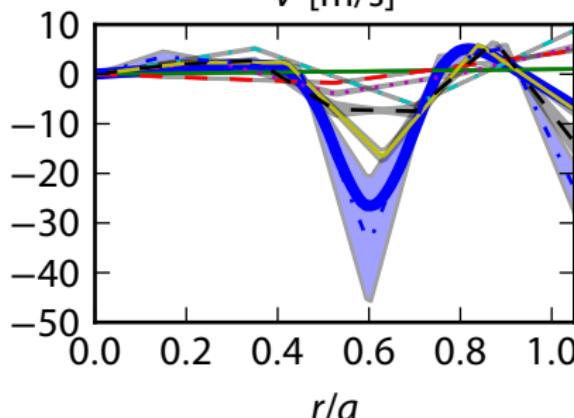
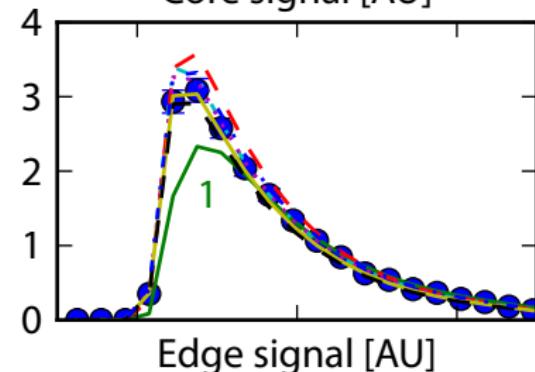
- 7 coefficient case took 7000 CPU-hours = 15 wall-clock days!
- Need to speed up STRAHL, deploy on cluster to make this practical.

Results only resemble true profile when a minimum level of complexity is obtained...despite "good" match to data

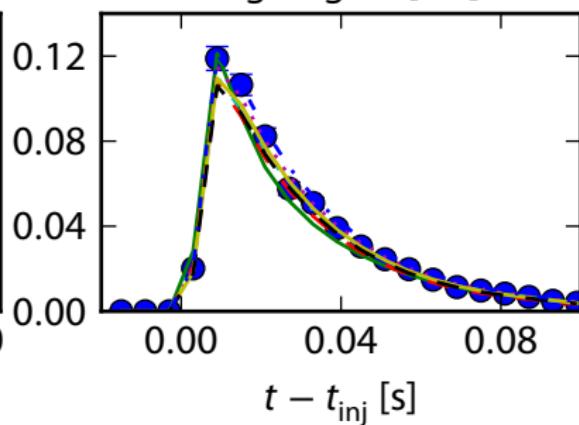
(synthetic data)



Core signal [AU]



Edge signal [AU]



Getting D, V right is very difficult

- Do not need to worry about n_e, T_e uncertainties. 😊
- **Need** to select appropriate model complexity rigorously:
 - Any result obtained using overly simple functions to describe D, V is questionable.
 - **There is now an opportunity to reassess our entire picture of how well gyrokinetics describes impurity transport.** 😊
 - Proper model selection is *very* time consuming. 😞

Always ask the following:

1. How is parameter estimation performed? How are parameter uncertainties estimated?
2. How is model selection performed? Is a reasonable level of complexity for D, V used?
3. Was the analysis procedure thoroughly verified with *realistic* synthetic data?

Experimental data analysis techniques for validation of tokamak impurity transport simulations

- 1 Motivation: validation of turbulent transport simulations
- 2 Profile fitting with nonstationary Gaussian process regression
- 3 Inferring impurity transport coefficients: a very difficult inverse problem
- 4 Conclusions and future directions

Publications

Published

Chilenski NF 2015 Use of nonstationary GPR to fit L-mode profiles, propagate uncertainty.

Chilenski CPC 2016 Open source Python code for working with magnetic reconstruction data.

In progress

- Inferring *second* derivatives to test theories of momentum transport.
- Profile fitting incorporating TCI data.
- Profile fitting incorporating mtanh mean function.
- New approaches for making nonstationary Gaussian processes.
- Linearized impurity transport analysis.
- Complete impurity transport analysis.

Conclusions, contributions, and future work

Contributions of this thesis work

- New procedure and accompanying software for fitting plasma profiles: **can improve all validation efforts.**
- Linearized model for estimating diagnostic requirements: **time resolution is not as important as was previously believed.**
- Full procedure for inferring D, V : **model selection is critical, n_e, T_e have minimal effect.**

Future directions to build on this work

- Streamline impurity transport analysis, deploy on cluster.
- Handle sawteeth properly.
- Reassess validation of impurity transport simulations.

"The Freidberg question" scorecard: ☺ = 8, ☻ = 1, ☹ = 3