CSXR W line analysis validation and error quantization

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Unknown Tungsten line determined to be W^{45+}

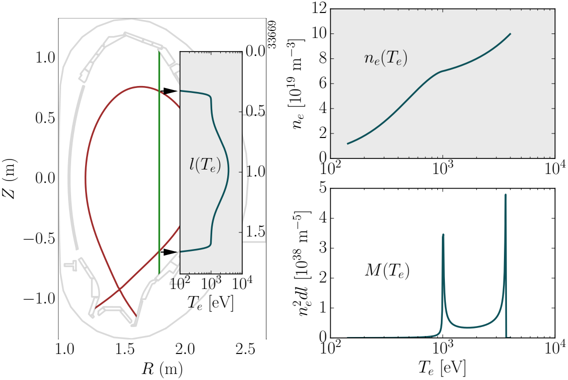
- The Compact Soft X-ray spectrometer (CSXR) observes several tungsten lines in high T_e discharges
- Correlation to other tungsten (W) measurements characterized the brightest unknown line in wavelength range as W^{45+}
- Error bars were characterized for this analysis using Fisher Information of the expected error distribution
- To validate this workflow, a known but 'weaker' tungsten line (W^{44+} at .39895) was also characterized

Method used matrix formulation to determine charge state

$$\mathbf{M}_{ij} = n_{e,i}^2(T_{e,j})\Delta l_i(T_{e,j})$$

$$\vec{I}_{CSXR} = \frac{G}{4\pi}\vec{c}_W \circ \left(\mathbf{M} \cdot \vec{\tilde{f}}_Z(T_e)\right)$$

- $c_{W,i}$ is determined by GI spectrometer, for shot i
- M_{ij} developed from EQH shotfiles with CSXR sightline
- Same n_e and T_e profiles were used for original $c_{W,i}$ calculation



Spectra from 3000 discharges (campaigns 2014-2018) were collated into a dataset for the inverse problem

Error propagation difficulties occur with chosen objective function

- Using L-BFGS algorithm, objective $(\log(I_{CSXR}) - \log(c_W M \tilde{f}_Z))^2$ was minimized, which assumes that the logarithms of the data are normally distributed
- Solutions are derived nonlinearly, meaning covariance matrix is not immediately specified on output
- the variances of $\hat{\tilde{f}}_z$ are complicated
  - the estimators are a sum within a logarithm when compared to the data
  - The use of regularization implies solution is biased with initial dataset
  - Least-squares with regularization variance calculations cannot be used

The impact of bias makes variance-based confidence intervals in estimators misleading

Bootstrapping only estimates confidence from variance

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- For complex non-linear problems, often a *bootstrapping* approach is used in estimating confidence intervals
- Bootstrapping works by generating sets of estimators from resampled data
- However, it only estimates confidence from variance and confidence intervals will shrink with higher bias (*i.e.* with stronger regularization)

Other methods, such as bootstrapping, cannot separate variance from bias and a Bayesian approach is needed for this task

Validity of methods tested with known line (W^{44+})

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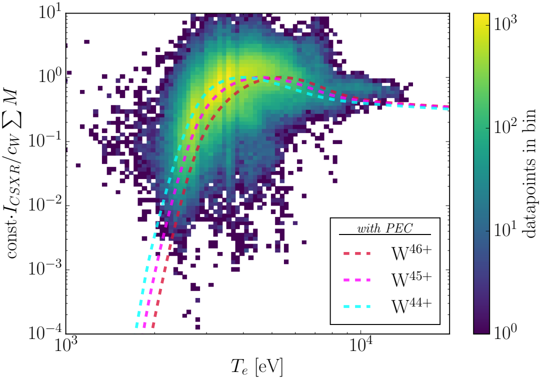
- Testing the methods on a known line will give a rough estimation of the $\tilde{f}_Z$ recovery
- The next brightest tungsten line is a known $44+$ near the Ar He-like Z line (at .39895 nm)
- Observations of this line have been seen on similar spectrometers at other facilities
- Forward model results cannot separate between W^{44+} and W^{45+} for this line

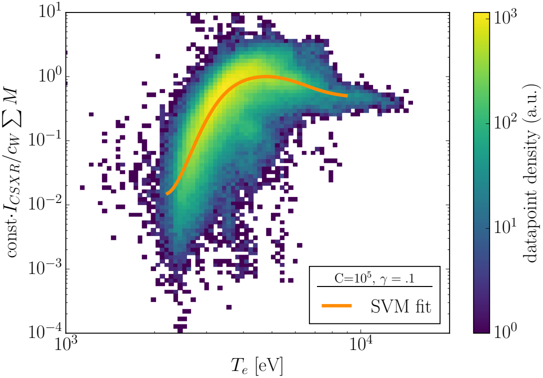


Secondary method determines $\tilde{f}_z$ from $T_{e,max}$ model

- SVM was used to regress $I_{CSXR}/(c_W \sum M)$ vs $T_{e,max}$ without a discritized T_e base
- Instead of the complicated $\mathbf{M}$ matrix, the simplified $\hat{M}$ model allows for simple inverses (It is inherently square and one-to-one)
- This allows for a non-inverse problem like approach in determining $\tilde{f}_Z$
- The method mostly treats the equilibrium variability and spectral fitting variability separately

SVM determines nonlinear regression of $I_{CSXR}/\left(c_W \sum M\right)$ vs $T_{e,max}$

- SVM (*Support Vector Machines*) can regress or classify very nonlinear datasets with minimal assumptions
- Using a radial-basis function kernel, a representation of the dataset can be easily determined
  - Smoothness of the fit and influence of points can be determined by free parameters C and γ respectively
  - the values are easily determined by cross-correlation



'Unknown' line (W^{45+})

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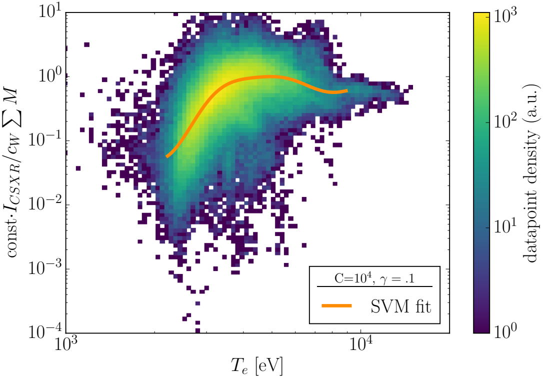
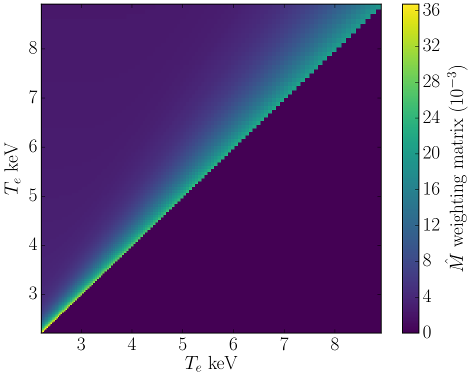


'known' line (W^{44+})

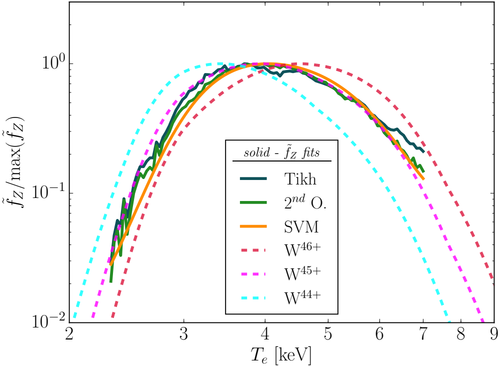
$\hat{M}^{-1}(T_e, T_{e,max})$ is used to yield $\tilde{f}_Z$

- Remember that the forward model uses the equation $\hat{M}\tilde{f}_Z \propto I_{CSXR}/(c_W \sum M)$
- $\tilde{f}_z$ can be recovered by multiplying the SVM regression of $I_{CSXR}/(c_W \sum M)$ by $\hat{M}^{-1}$, each of which as functions of $T_{e,max}$
- $\hat{M}$ essentially contains the weights of the fractional abundance for a given $T_{e,max}$, the inverse translates $T_{e,max}$ weights to T_e values
- The $\hat{M}$ model has a fixed $T_{e,ped}$ which possibly affects low $T_{e,max}$ data



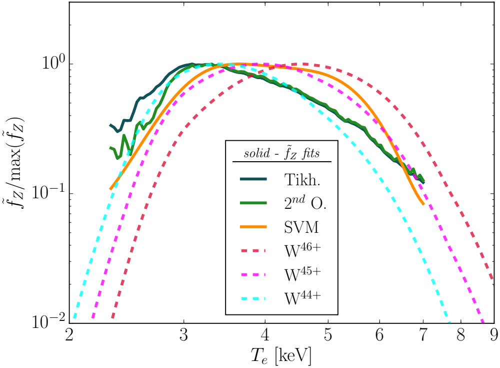
Methods tested on strong W^{45+} line for understanding variation

- The 3 methods utilized are:
  - Tikhonov regularization (Tikh.)
  - 2^{nd}-order Tikhonov regularization (2^{nd} O.)
  - SVM method with M^{-1} (SVM)
- All yield similar results, suggesting W^{45+}
- All end results cross-validated for smoothing parameters



Methods tested on W^{44+} lines for validity

- Much poorer fits are observed with the known W^{44+} line, larger bias in all cases (this would surprisingly yield smaller errorbars using traditional methods)
- Likely due to less intense measure of this line due to vignetting, significantly more variation in data observed
- SVM model issues can be observed in forward model (large spread in data)
- Matrix methods faithfully suggest line of correct charge state



Conclusions and future work

- Compilicated nature of the chosen nonlinear fit and regularization makes confidence intervals useless, as bias corrupts variance calculations
- A secondary method using the 'Forward' model and SVMs determines a similar result in the intense line, but is impacted by assumptions and variability in the known line
- I would like to get a hold of similar data on imaging spectrometers

Bootstrapping results

Comparison of Confidence Intervals (W^{45+})

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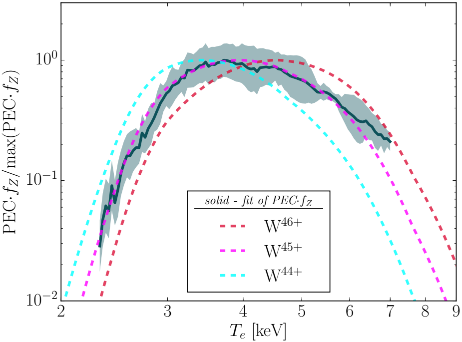
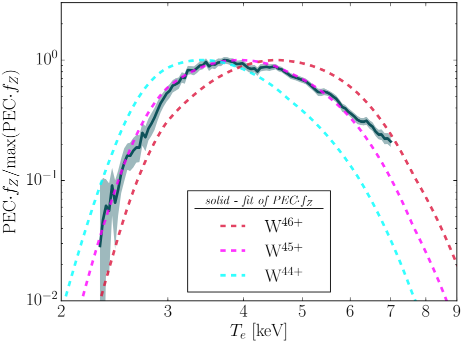


Hessian inverse-based



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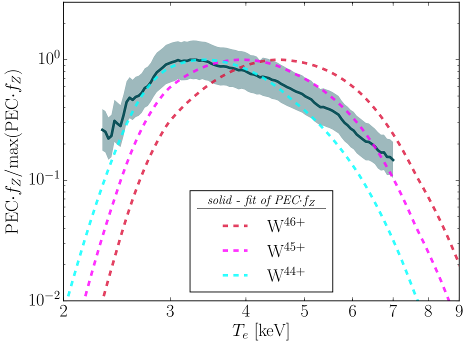
Comparison of Confidence Intervals (W^{44+})



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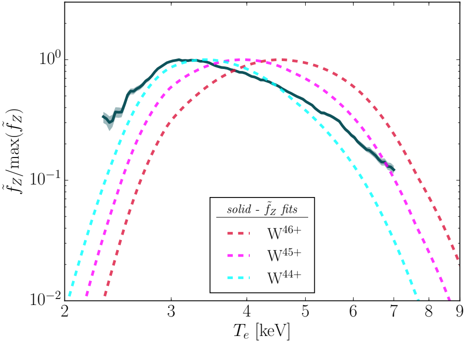

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Variance issues highlighted in differences

- Forward model demonstrably shows higher variability in known line, but is not reflected in solutions
- Bias reduces variance (known line has an order of magnitude higher regularization), hence difference in bootstrapping solution
- The hessian solution assuming log-normality is substantially different from bootstrapping

Forward model explanation

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Forward model derivation

$$I_{CSXR} = \frac{Gc_W}{4\pi} \sum_j M_j \tilde{f}_Z(T_{e,j})$$

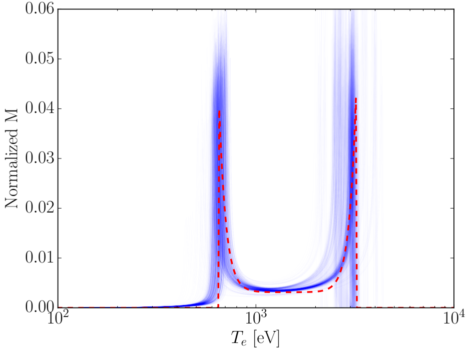
$$\frac{4\pi I_{CSXR}}{Gc_W \sum M} = \sum_j \frac{M_j}{\sum M} \tilde{f}_Z(T_{e,j}) = \sum_j \hat{M}_j \tilde{f}_Z(T_{e,j})$$

- We solve for a simplified $\hat{M}$ which is only a function of $T_{e,max}$, this assumes a low pedestal temperature and rigid profile shapes. This is knowingly approximate
- The $I_{CSXR}/c_W \sum M$ term is histogrammed based on the peak observed sightline temperature $T_{e,max}$.
- Various $\tilde{f}_Z$ can be applied in order to see which minimizes a log squared objective function.

Model of M allows for understanding of dataset

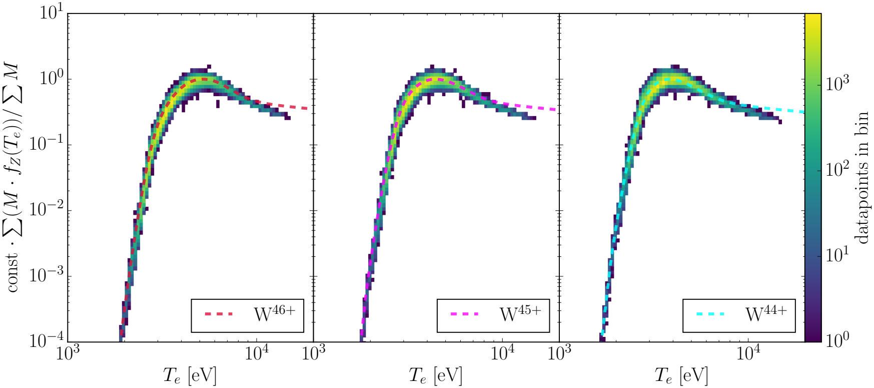
- A simple normalized model M is used to represent the sightline in T_e space
  - $T_{e,ped}$ - fixed value of 600eV (value is relatively unimportant)
  - $T_{e,max}$ - Maximum temperature for sightline
  - λ - decay length
  - a - baseline value

- This function can be used to generate forward models, due to the simplification to 4 variables



$$\hat{M}(T_e) = \frac{a + \left(\frac{T_{e,ped}}{T_e}\right)^{1/\lambda} + \left(\frac{T_e}{T_{e,max}}\right)^{1/\lambda}}{\sum_{j=T_{e,ped}}^{T_{e,max}} a + \left(\frac{T_{e,ped}}{T_j}\right)^{1/\lambda} + \left(\frac{T_j}{T_{e,max}}\right)^{1/\lambda}}$$

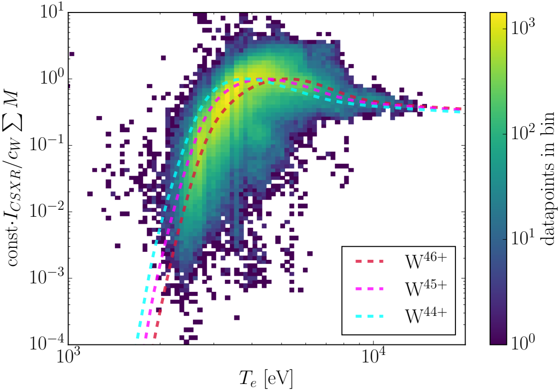
Model $\hat{M}$ reasonably describes M



the model function $\sum \hat{M} f_Z(T_e)$ is compared to a heat map of experimental $\frac{\sum M f_Z(T_e)}{\sum M}$ for various charge states

Expected I_{CSXR} can visualize data variance as a function of $T_{e,max}$

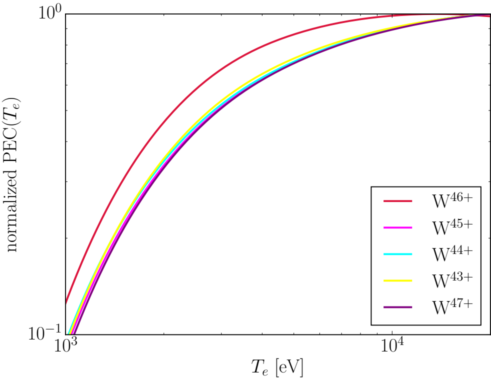
- Data and forward model can be compared for total intensity as a function of $T_{e,max}$ (see equation)
- This is a powerful tool to understand dataset dependencies/limitations
- At lower T_e, I_{CSXR} is dominated by the rise in $f_Z(T_e)$
- At higher T_e, peak emission region moves off-axis and emitting region shrinks



$$\sum_j \hat{M}(T_{e,max}) f_Z(T_{e,j}) \propto \frac{I_{CSXR}(T_{e,max})}{c_W \sum_j M(T_{e,j})}$$

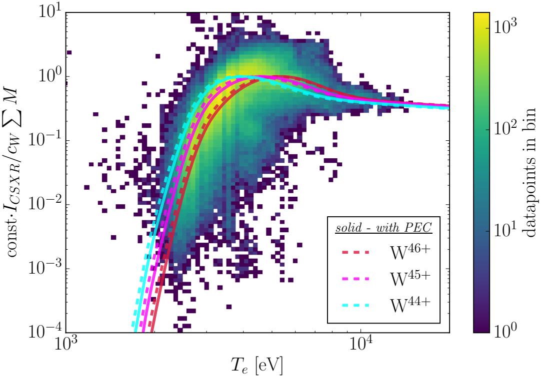
Photon Emissivity Coefficient modifies forward model projections

- Original work assumed that the Photon Emissivity Coefficient (PEC) was a constant
- It is actually also a function of n_e and T_e, and will impact forward model
- All curves relatively similar, with 1 order of magnitude variation across T_e range
- Data taken from ADAS for highest emitting lines in .38-.41 nm wavelength range

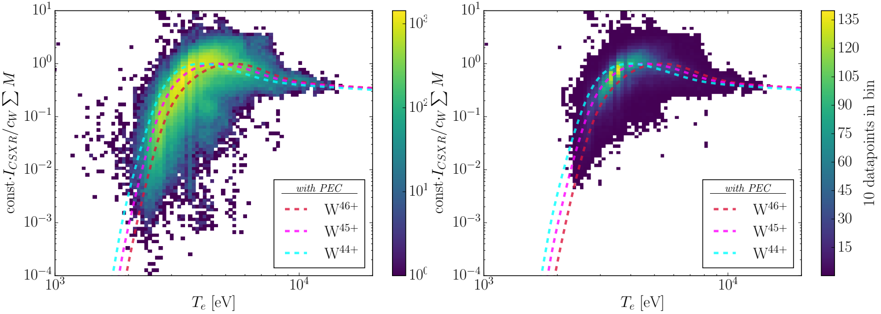


Forward model fits data better with non-constant PEC

- As PEC curves were monotonically increasing, it serves to shift modelled data to higher T_e
- The order of magnitude change in PEC shifts data only slightly, as change in f_Z is greater
- Peak of model also shifts slightly in all cases to slightly higher T_e



Forward model fits to W^{45+} with PEC



- Both plots show the PEC solutions with a linear and logarithmic color scheme (linear with lower cutoff of 100)
- Across electron temperatures with substantial data the best fit is W^{45+} with PEC
- At temperatures below 2 keV, c_W dataset is limited and distorts T_e dependence