Supplementary materials for: Estimating the spectrum in computed tomography via Kullback-Leibler divergence constrained optimization

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ADDITIONAL SIMULATION RESULTS

Here, we provide simulation results that investigate the effect of early stopping on the x-ray spectrum reconstruction using the EM algorithm. Figure 1 shows the spectral curves estimated by EM for different numbers of iterations. The transmission data are simulated as described in the simulation study (see Section III.A in the main text). As seen in the figure, by stopping after 300 iterations, the EM method recovers the ground truth spectrum remarkably well and both spectra are indistinguishable in the plot; however, for low iteration number (e.g. 10 iterations), the resulting spectrum is still biased towards the initial value, and for high iteration number (e.g. $5,000$ iterations), the EM method appears to overfit to the transmission data and therefore cannot generalize to transmission measurements beyond the given data set. While determining a good iteration number is crucial to implement the EM method, Sidky et al.[1] demonstrates the robustness of the EM method, i.e. the estimated x-ray spectrum is not strongly sensitive to the choice of number of iterations. In practice, the number of iterations can be determined by preliminary simulation studies.

Next, we investigate how the choice of the initial spectrum affects on the performance of the proposed KL-

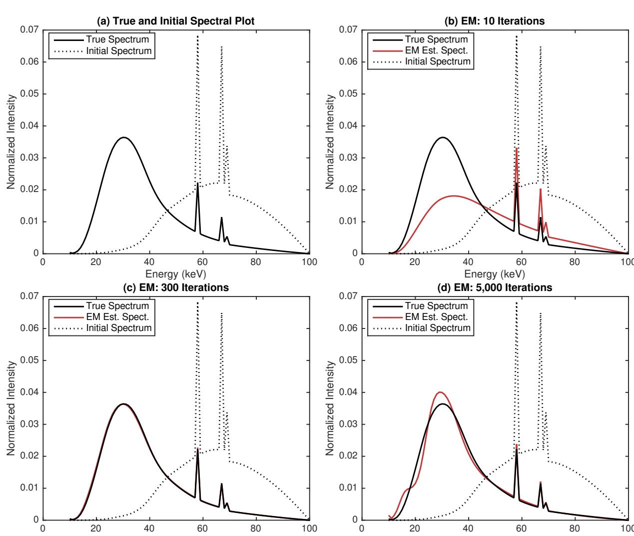

FIG. 1 Spectrum estimation from simulated transmission measurements by use of EM. A detailed description of the simulation setting is given in the main text. Panel (a) shows the ground truth x-ray spectrum (black solid line) and the initial x-ray spectrum (black dotted line). The remaining three panels show the estimated spectra by EM for different number of iterations.

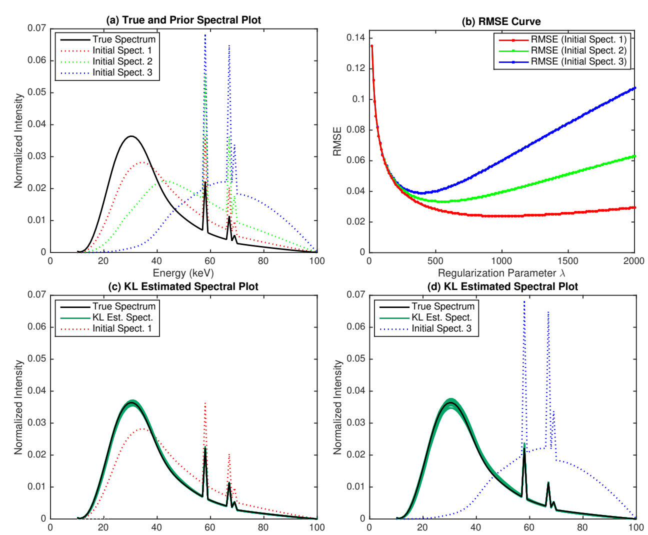

FIG. 2 Spectrum estimation from simulated transmission measurements by use of KL. Different types of true and initial x-ray spectrum are employed as depicted in panel (a). In each setting, spectrum reconstruction is performed for 20 independent sets of transmission measurements. Panel (b): Spectral curves for 20 different trials. The band formed by the curves shows variation between the reconstructed x-ray spectra. Panels (c),(d): The RMSE curves for different regularization parameters. Each point represents an average over 20 trials.

divergence based method. We fix the ground truth spectrum as depicted in Figure 2(a) with black solid line, and vary the initial spectrum as shown in Figure 2(a). We repeat the estimation process as done in Section III.A, but now with a wider range of $\lambda \in \{20, 30, \ldots, 2000\}$ as larger regularization parameters are likely to be chosen when the initial spectrum is more precise. Figure 2(b) shows the RMSE plots for the three initial values, each of which are averaged over 20 trials. As clearly indicated by the plot, spectrum estimation with better initial guess leads to improvements in the accuracy and appears to be more stable against λ, compared to the poor initial guess. This finding is further confirmed by comparing Figure 2(c) and (d), where using better initial guess, Figure 2(c), results in narrower band between the spectral curves than the poor initial guess, Figure 2(d).

[1] E. Y. Sidky, L. Yu, X. Pan, Y. Zou, and M. Vannier, "A robust method of x-ray source spectrum estimation from transmission measurements: Demonstrated on computer simulated, scatter-free transmission data," *J. Appl. Phys.*, vol. 97, art. no. 124701, 2005.