

Figure 4.10: The maximum and mean absolute error for all the eigenvalues in the test set (20 000 calculations) for varying size of training set.

The large difference in test error in Figure 4.10 indicates there is a problem with mapping the eigenvalues directly. The problem is clearly visible when plotting the solutions for both maps at a crossing (correct outcome is shown Figure 4.8), see Figure 4.11. The kernel ridge regression method with a Gaussian kernel is only able to model smooth relations and fails at the crossing of the eigenvalues. However, the polynomial coefficients a_i behave smoothly even at a crossing and produce the right result.

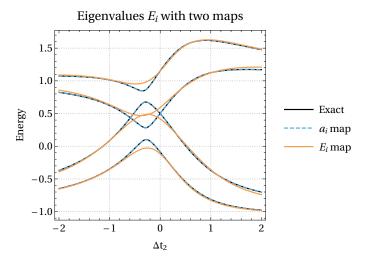


Figure 4.11: Visual example that mapping the eigenvalues directly leads to difficulty with crossings. The exact solution and the a_i map are identical while the E_2 and E_3 fail to capture the crossings and E_1 and E_4 the sharp turns.

To conclude, mapping the characteristic polynomial coefficients for a single