4.3 Direct problem

For the direct problem, there are several possible mappings $X \to Y$ to consider. For all these mappings the goal is to find the energy bands (i.e. eigenvalues of $\boldsymbol{H}$) for a given set of hopping parameters $\boldsymbol{t}$ and Brillouin zone position $\boldsymbol{k}$. However, the mappings replace different stages of the tight binding calculation, as shown schematically in Figure 4.6. For example, if the map leads to characteristic polynomial coefficients, a traditional algorithm is used to obtain the roots of the polynomial.

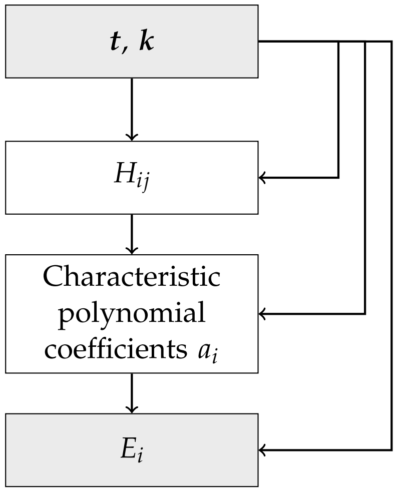

Figure 4.6: Bypassing parts of the tight-binding calculation with a mapping.

The three alternatives displayed above are mapping the tight binding parameters $\boldsymbol{t}, \boldsymbol{k}$ to

1. the (sometimes complex-valued) matrix elements H_{ij};
2. the real coefficients of the characteristic monic polynomial

$$a_0 + a_1\lambda + a_2\lambda^2 + a_3\lambda^3 + \lambda^4 = 0;$$

3. the real eigenvalues of $\boldsymbol{H}$, i.e. the roots of the polynomial above.

The first approach means predicting complex numbers which could be technically implemented by considering the real and imaginary part separately, but it will not be pursued in this thesis.

The second and third approach both mean predicting four real numbers (coefficients a_0, a_1, a_2, a_3 or the eigenvalues E_1, E_2, E_3, E_4) and these numbers respond differently to changes in $\boldsymbol{t}$ (and $\boldsymbol{k}$). Before applying one of the Machine Learning methods, it is helpful to take a closer look at the data to gain an intuitive understanding of the task.