How do initial diffraction images get turned into a unit cell and what can I do when it doesn't work?

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One of the most mysterious black boxes is the fully automatic generation of a unit cell, together with crystal orientation, from the initial images obtained on a single-crystal diffractometer. Often there are few user options and only one or just a small number of possible solutions are offered. How does it work, what problems might there be, and what can be done when a sensible answer isn't provided? To understand this, a few basic properties of direct-space (crystal structure) lattices and reciprocal-space (diffraction pattern) lattices need to be known, and how these relate to the mounting of the sample crystal on the goniometer head (the required level of mathematics is not particularly high!). Various procedures developed over several decades are embedded in current software and I will describe and illustrate the fundamentals of the ways they operate, together with more recent developments and improvements. Most of the problems arise from samples that are not really single crystals, such as twins, conglomerates, and other multiple crystals that generate contaminated diffraction patterns for which a single reciprocal lattice cannot be found. Automatic software can be helped by various kinds of manual intervention, particularly ways of influencing the selection of observed diffraction peaks (reflections) to be used in the calculations. A degree of transparency is actually possible for this particular black box.