For Monte Carlo linac simulation and patient dose calculation, it is important to accurately determine the phase space parameters of the initial electron beam incident on the target. These parameters, such as mean energy and radial intensity distribution, have traditionally been determined by matching the calculated dose distributions with the measured dose distributions through a trial and error process. In this work, we have treated this issue as an optimization problem and systematically investigated various aspects of it. A 6 MV beam from a 21EX Varian linac was simulated with initial mean energy from 5 to 7 MeV with increment of 0.25 MeV, and with the standard deviation of the initial Gaussian intensity distribution from 0.4 to 2.5 mm with increment of 0.3 mm. The depth dose profiles and cross beam dose profiles at various depths were calculated and compared with the measured data for the field sizes of 4×4, 10×10 and 40×40 cm². Three cost functions, the χ^2 , mean absolute error, and the κ -factor (defined as the fraction of the voxels with absolute error less than 1 %), were evaluated to find the best way for dose comparison. It is found that all of them can be used as the cost functions with slight preference on the κ -factor. We also found that the minimum data set required for dose comparison are the dose profiles at various depths for 40×40 cm² field size, and there are multiple combinations of the phase space parameters that yield good dose distributions.