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PeakNet: Peak Finding for Serial Crystallography

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In recent years, serial femtosecond crystallography has made remarkable progress for the measurement of macromolecular structures and dynamics using intense femtosecond duration pulses from X-ray Free Electron Laser (FEL). In these experiments, FEL X-ray pulses are fired at a jet of protein crystals, and the resulting diffraction pattern is measured for each pulse. If the pulse hits protein crystals, the resulting diffraction pattern is recorded. However, most of the time the beam does not hit a crystal. As a result, out of the hundreds of thousands of diffraction patterns, only a small fraction is useful, so there is tremendous potential for data reduction. Diffraction from a protein crystal produce distinctive patterns known as Bragg peaks. Thus, recent years have seen an increased interest in artificial intelligence or more specifically machine learning to process diffraction patterns, resulting considerable data reduction.

Existing statistical methods utilize peak finding to identify and discriminate diffraction patterns that contains Braggs peaks and remove any patterns which only contain empty shots, resulting in considerable data reduction. Typically, peak finding methods require carefully crafted parameters from domain experts. Thus, we leverage the "You only look once" (YOLO) object detection network to detect Bragg peaks in diffraction patterns with no parameters from users. In addition, we develop a pixel level labeling mechanism based on feature extractors to extract bounding boxes information to train the object detector.

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