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Leveraging Automatic Differentiation in Complex Model Fitting

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Understanding laser-solid interactions is important for the development of laser-driven particle and photon sources, e.g., tumor therapy, astrophysics, and fusion. Currently, these interactions can only be modeled by simulations that need to be verified experimentally. Consequently, pump-probe experiments were conducted to examine the laser-plasma interaction that occurs when a high intensity laser hits a solid target. Since we aim for a femtosecond temporal and nanometer spatial resolution at European XFEL, we employ Small-Angle X-ray Scattering (SAXS) and Phase Contrast Imaging (PCI) that can each be approximated by an analytical propagator. In our reconstruction of the target, we employ a gradient descent algorithm that iteratively minimizes the error between experimental and synthetic patterns propagated from proposed target structures. By implementing the propagator in PyTorch we leverage the automatic differentiation capabilities, as well as the speed-up by computing the process on a GPU. We perform a scan of different initial parameters to find the global minimum, which is accelerated by batching multiple parallel reconstructions. The fully differentiable implementation of a forward function may serve as a physically-constraining loss, enabling training with unpaired data or unsupervised training of neural networks to predict the initial parameters for the gradient descent fit.

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