Supplementary information

Measurements with Noise: Bayesian Optimization for Co-optimizing Noise and Property Discovery in Automated Experiments

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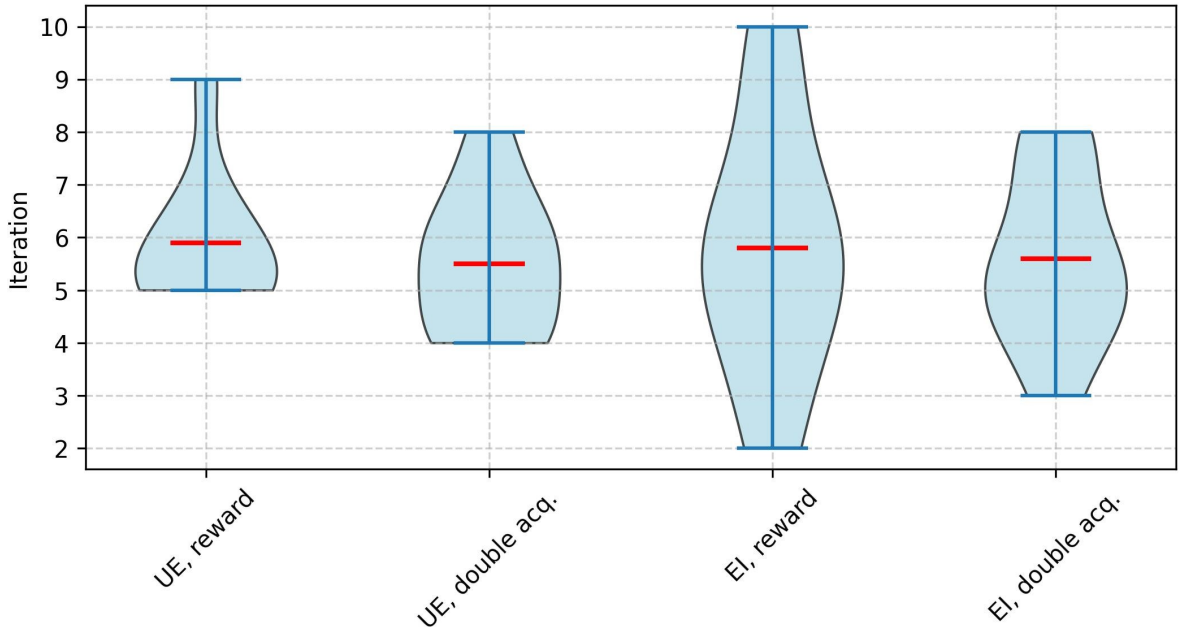

Figure S1: Violin plots showing the distribution of iteration numbers at which the noise model converges to the optimum. The simulations are driven by two acquisition functions (UE and EI) and different policies (pure reward-driven and double acquisition). Each violin represents data from 10 experiments, with red dashes indicating the mean values.

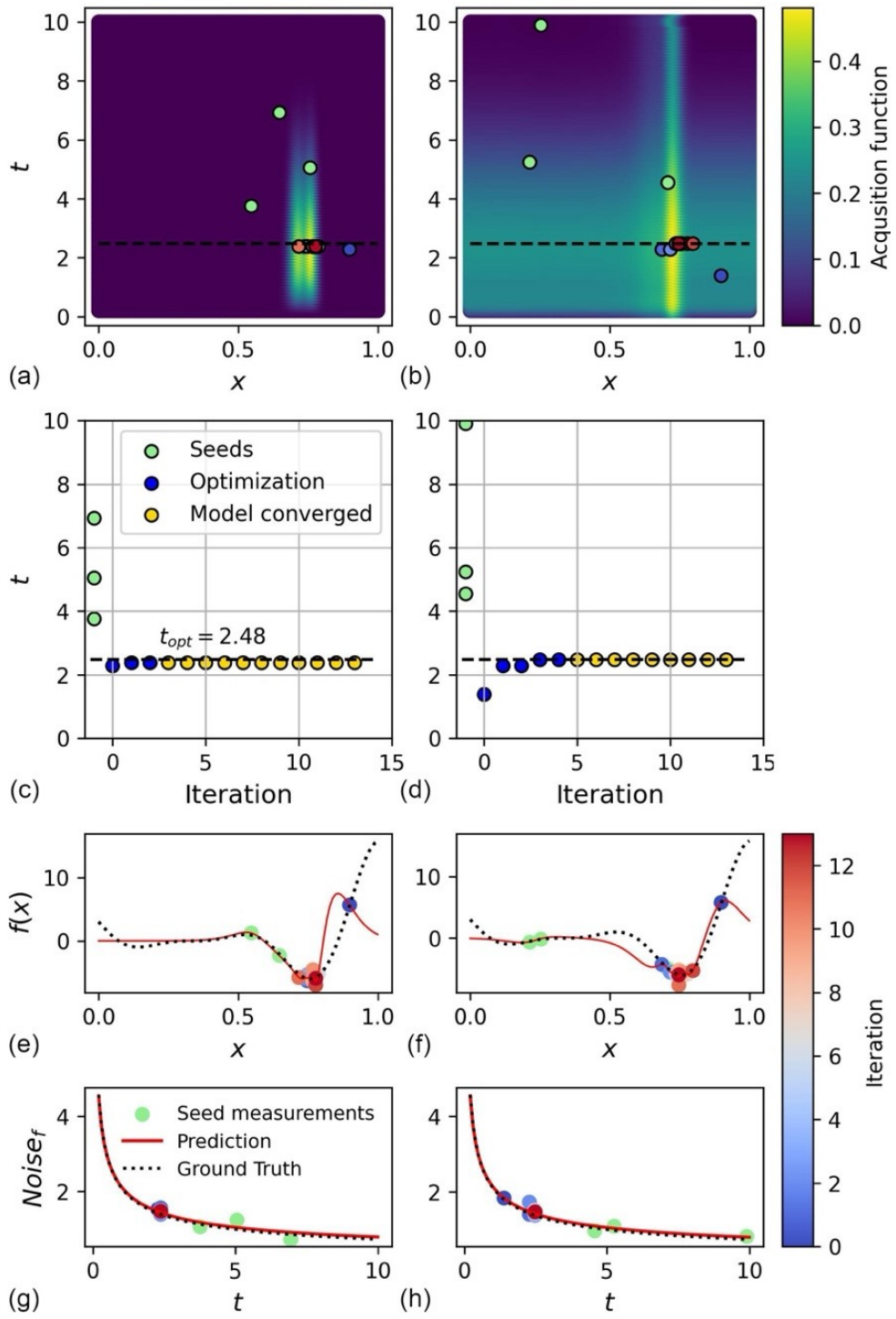

Figure S2: Automated experiment simulations using the (a, c, e, g) reward-driven approach and the (b, d, f, h) double-acquisition approach. (a, b) Experimental trajectories in the (x, t) exploration space. The background shading represents the acquisition function values. (c, d) Evolution of the optimal measurement time predictions with iteration number. (e, f) Predictions of $f(x)$ and (g, h) $Noise_f(t)$ at the final exploration step. Data points in (a, b, e-h) are color-coded based on iteration number, with light green indicating the initial seed measurements. The **EI** acquisition function drives function optimization in both simulations.

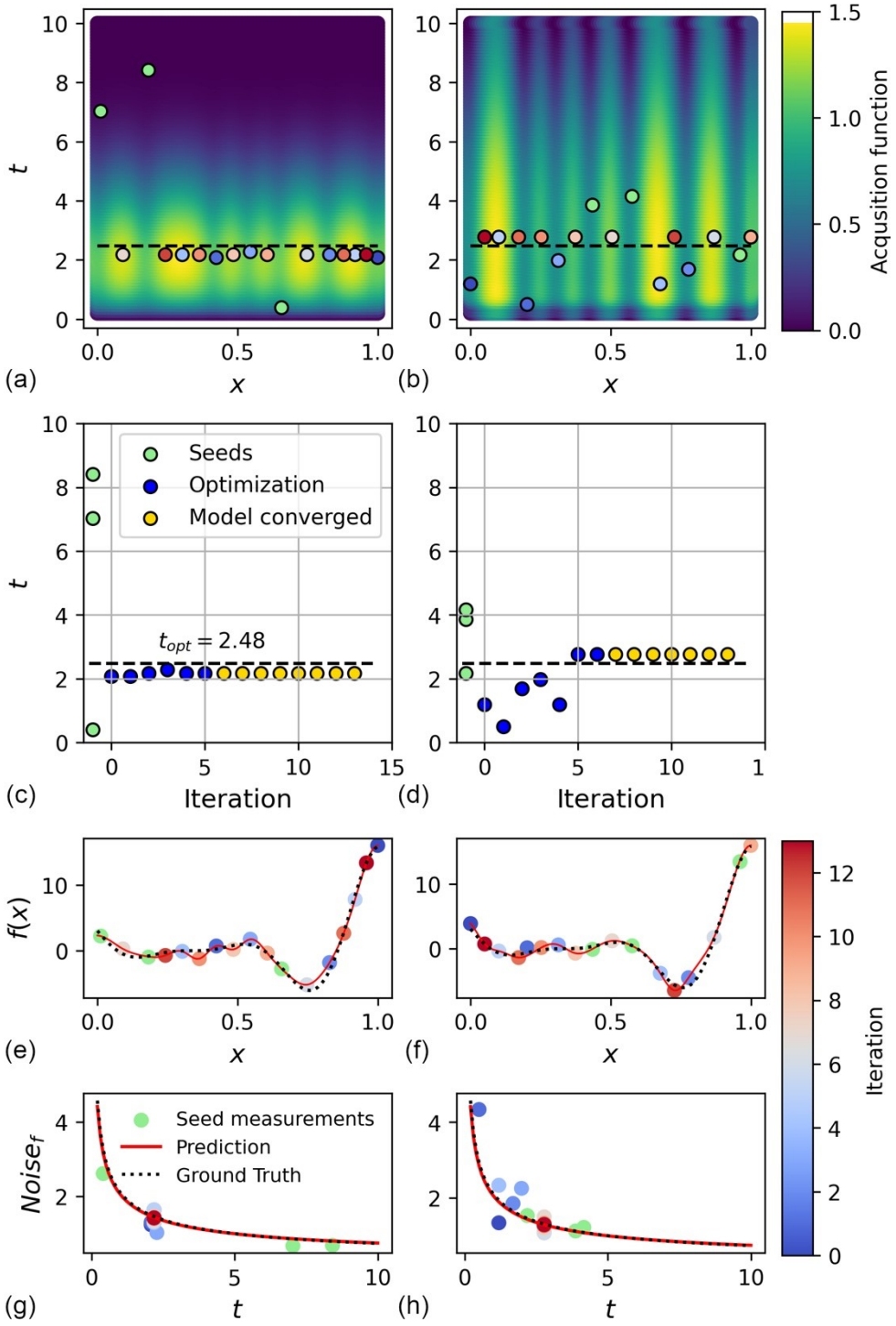

Figure S3: Automated experiment simulations using the (a, c, e, g) reward-driven approach and the (b, d, f, h) double-acquisition approach. (a, b) **Five** measurements are taken at each iteration to estimate both $f(x)$ and the $Noise$. Experimental trajectories in the (x, t) exploration space. The background shading represents the acquisition function values. (c, d) Evolution of the optimal measurement time predictions with iteration number. (e, f) Predictions of $f(x)$ and (g, h) $Noise_f(t)$ at the final exploration step. Data points in (a, b, e-h) are color-coded based on iteration number, with light green indicating the initial seed measurements.