

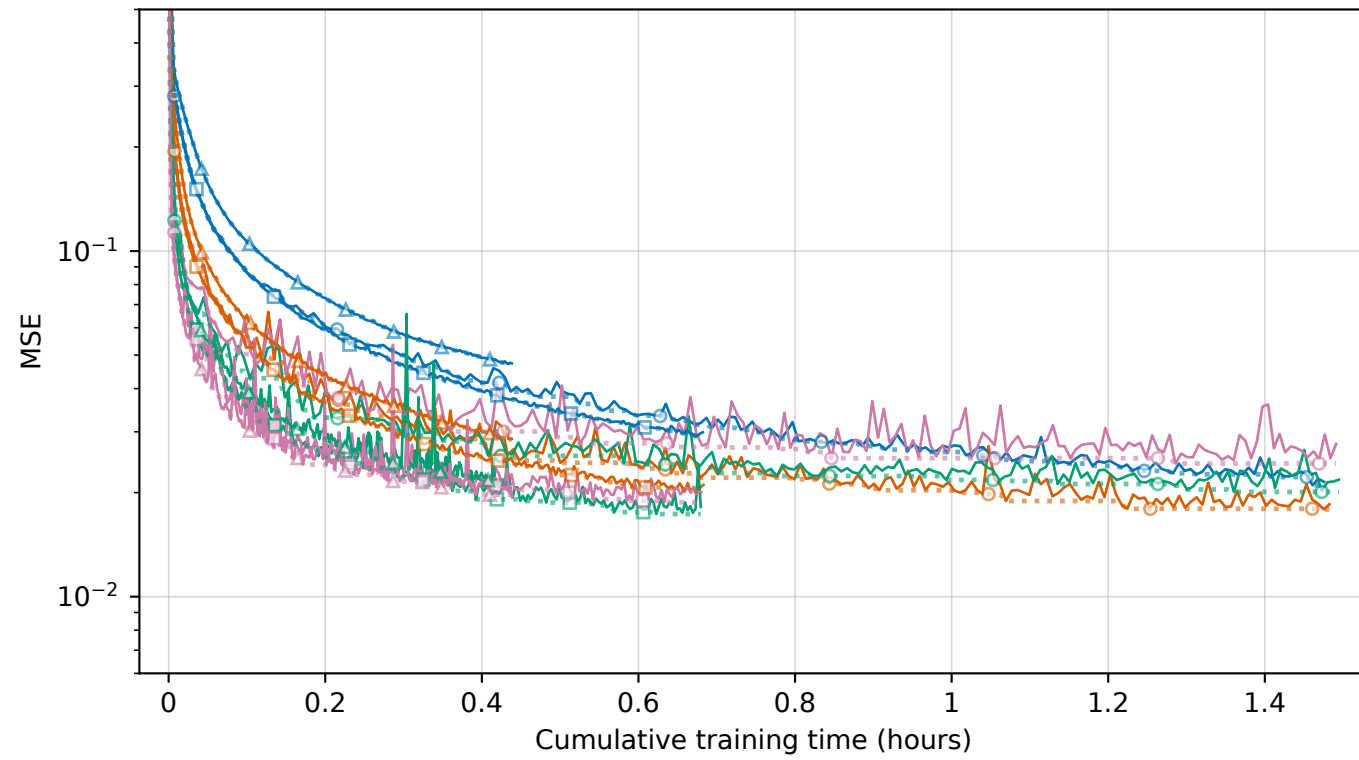
Validation metrics: batch-size and learning-rate comparison

Initialization seed 125672 | 12 runs | through epoch 2,000

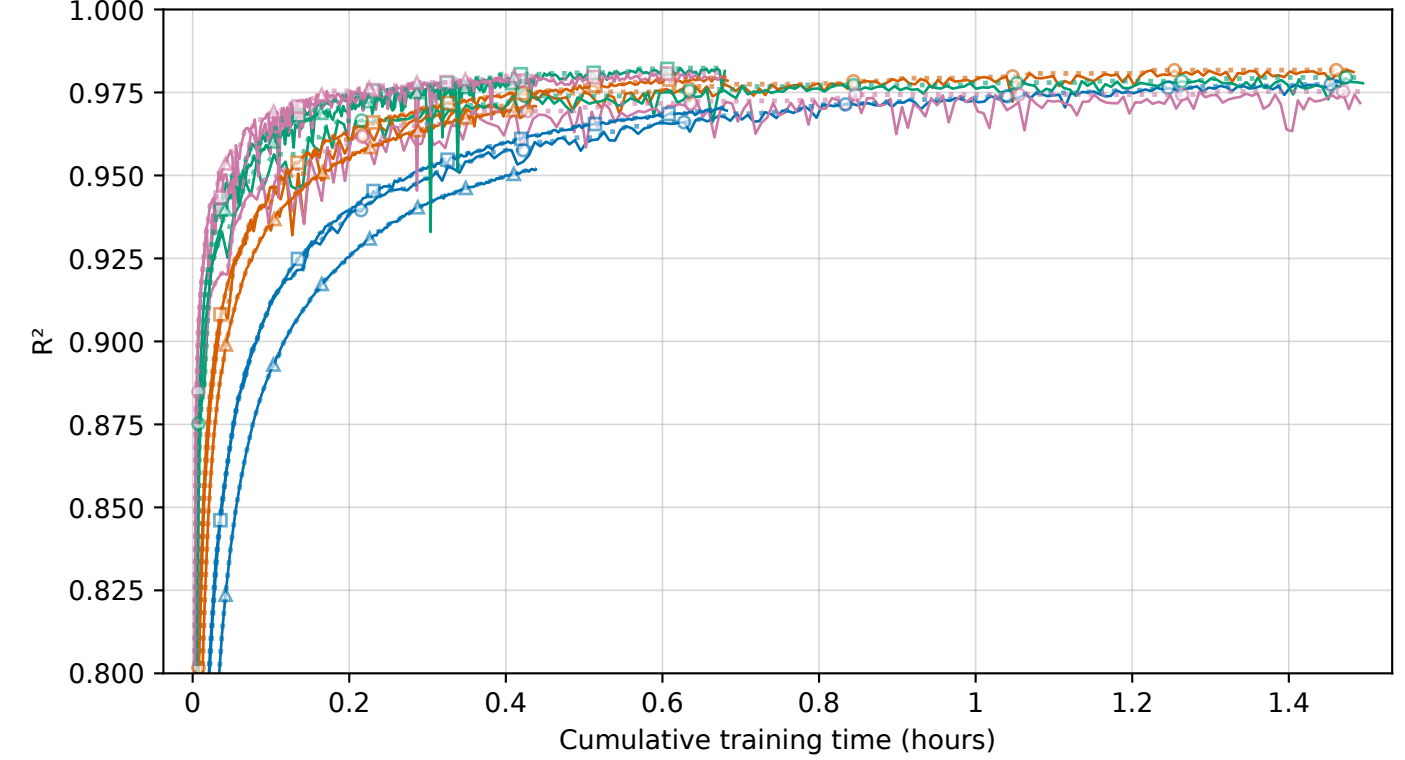
— valid: current checkpoint

····· best_valid: best checkpoint so far

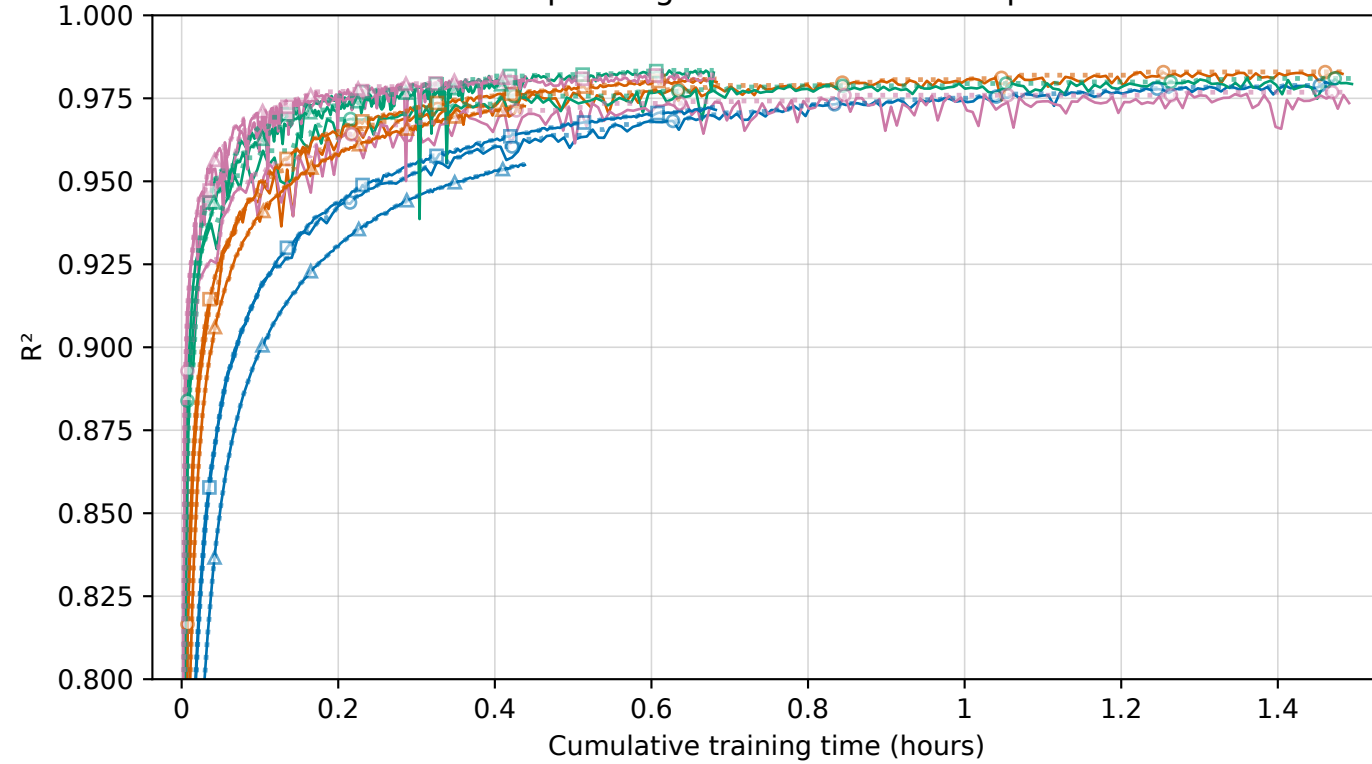
Pooled MSE in normalized space



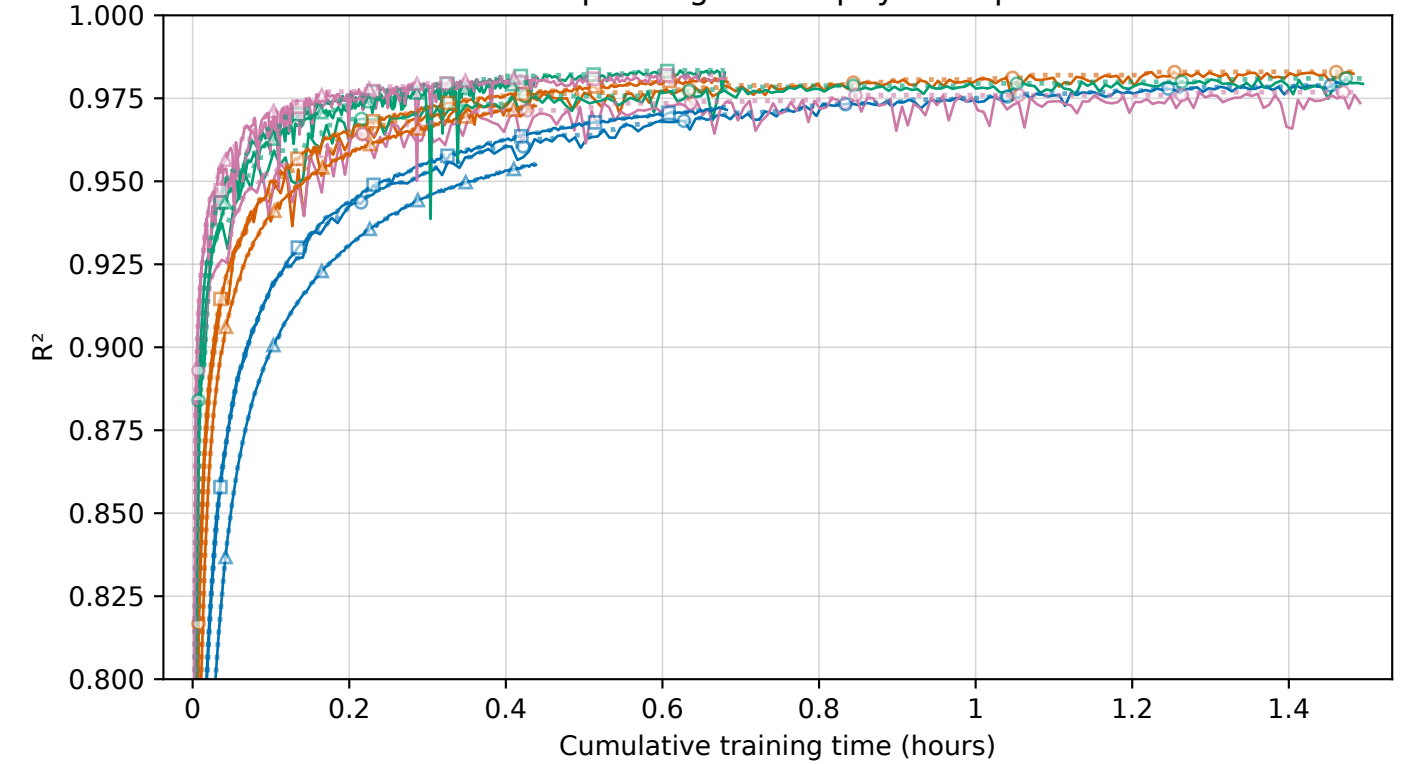
Pooled R² in normalized space



Mean per-target R² in normalized space



Mean per-target R² in physical space



····· B=4,096, LR=0.0001
····· B=16,384, LR=0.0001
····· B=65,536, LR=0.0001

····· B=4,096, LR=0.0003
····· B=16,384, LR=0.0003
····· B=65,536, LR=0.0003

····· B=4,096, LR=0.001
····· B=16,384, LR=0.001
····· B=65,536, LR=0.001

····· B=4,096, LR=0.003
····· B=16,384, LR=0.003
····· B=65,536, LR=0.003

Best checkpoint selected by minimum pooled validation MSE in normalized space.