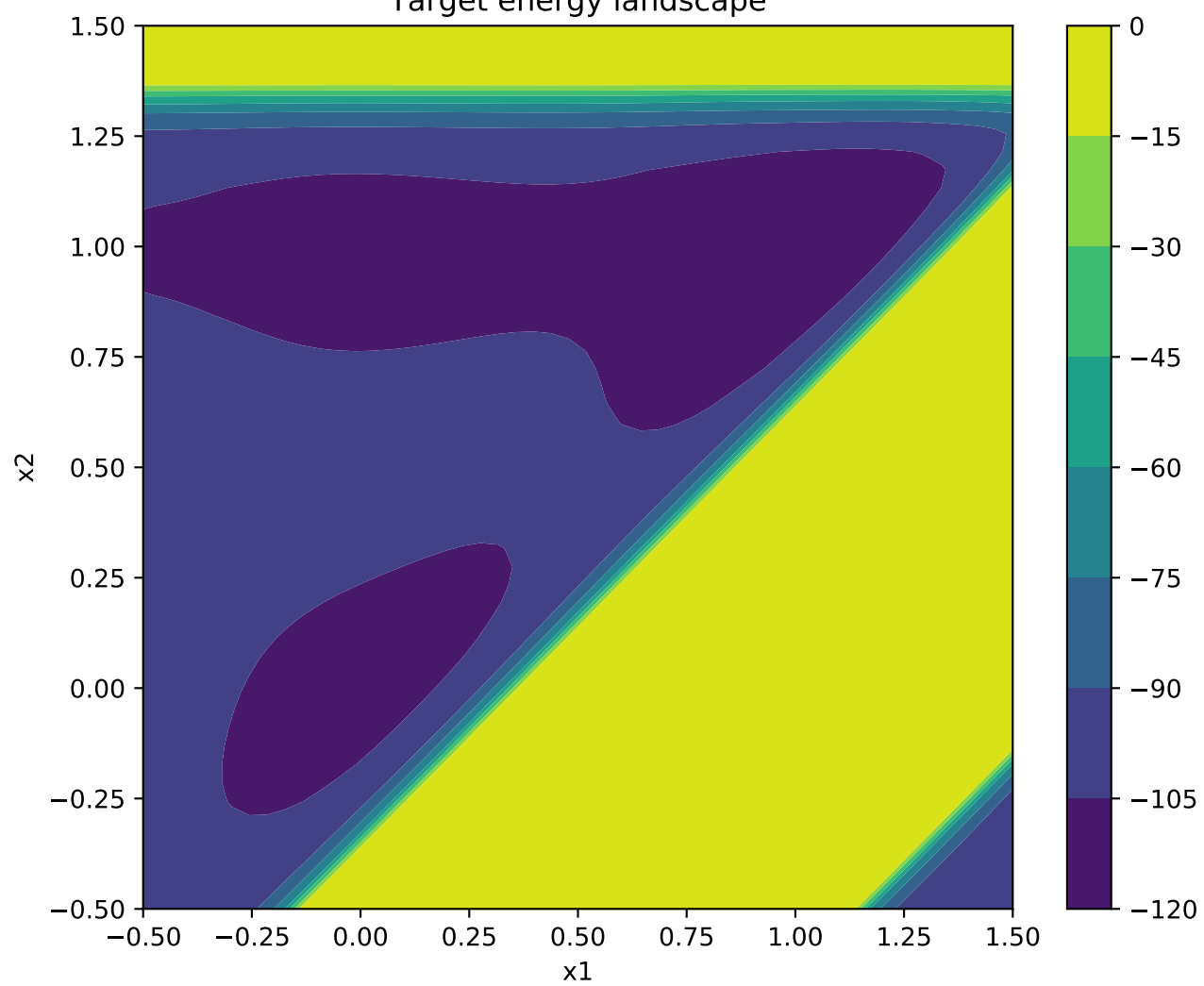
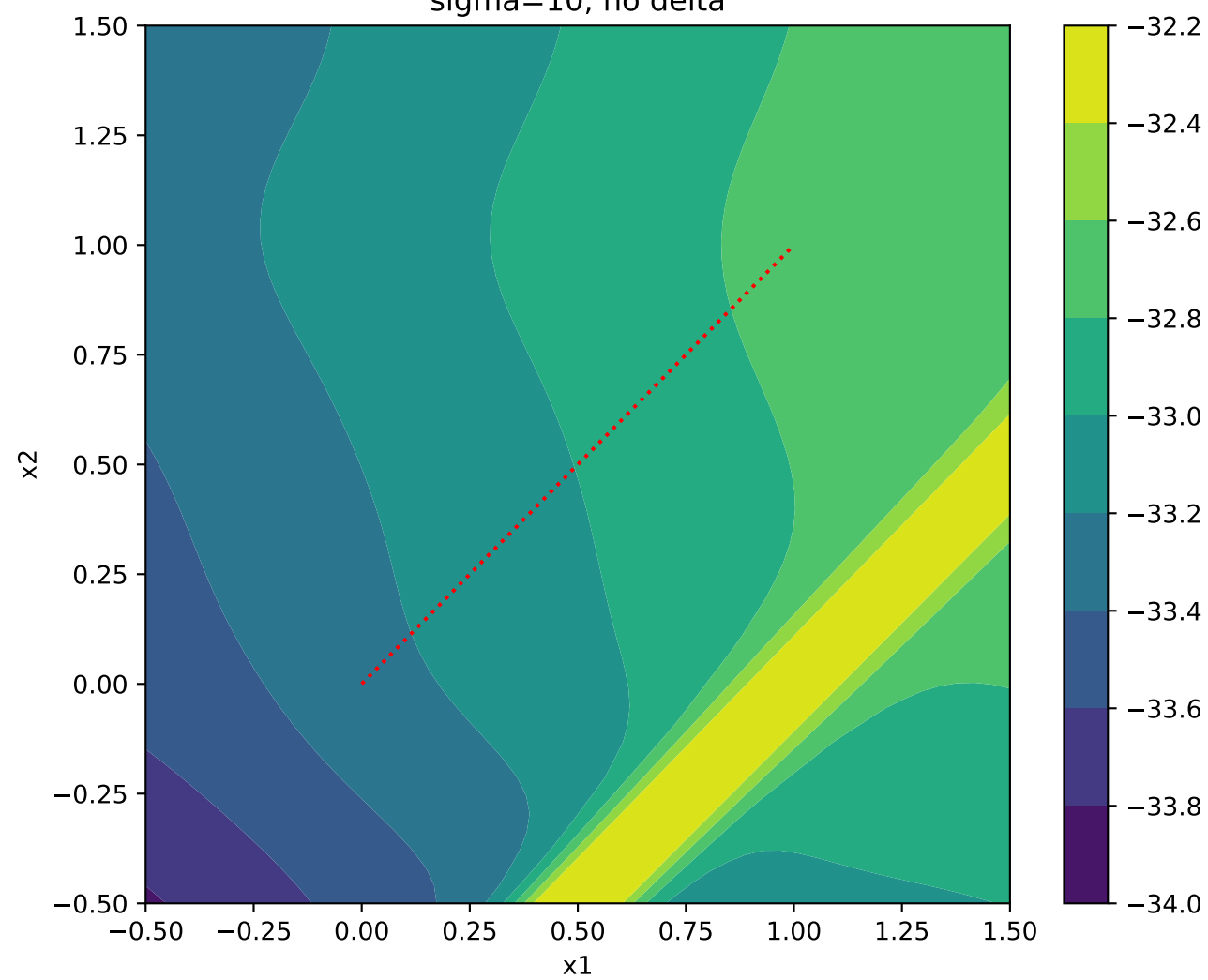


Target energy landscape

Predicted energy landscape
sigma=10, no deltaEnergy of linear path
sigma=10 for ML models, bias=mean(Etrain)=-32.33942389677859