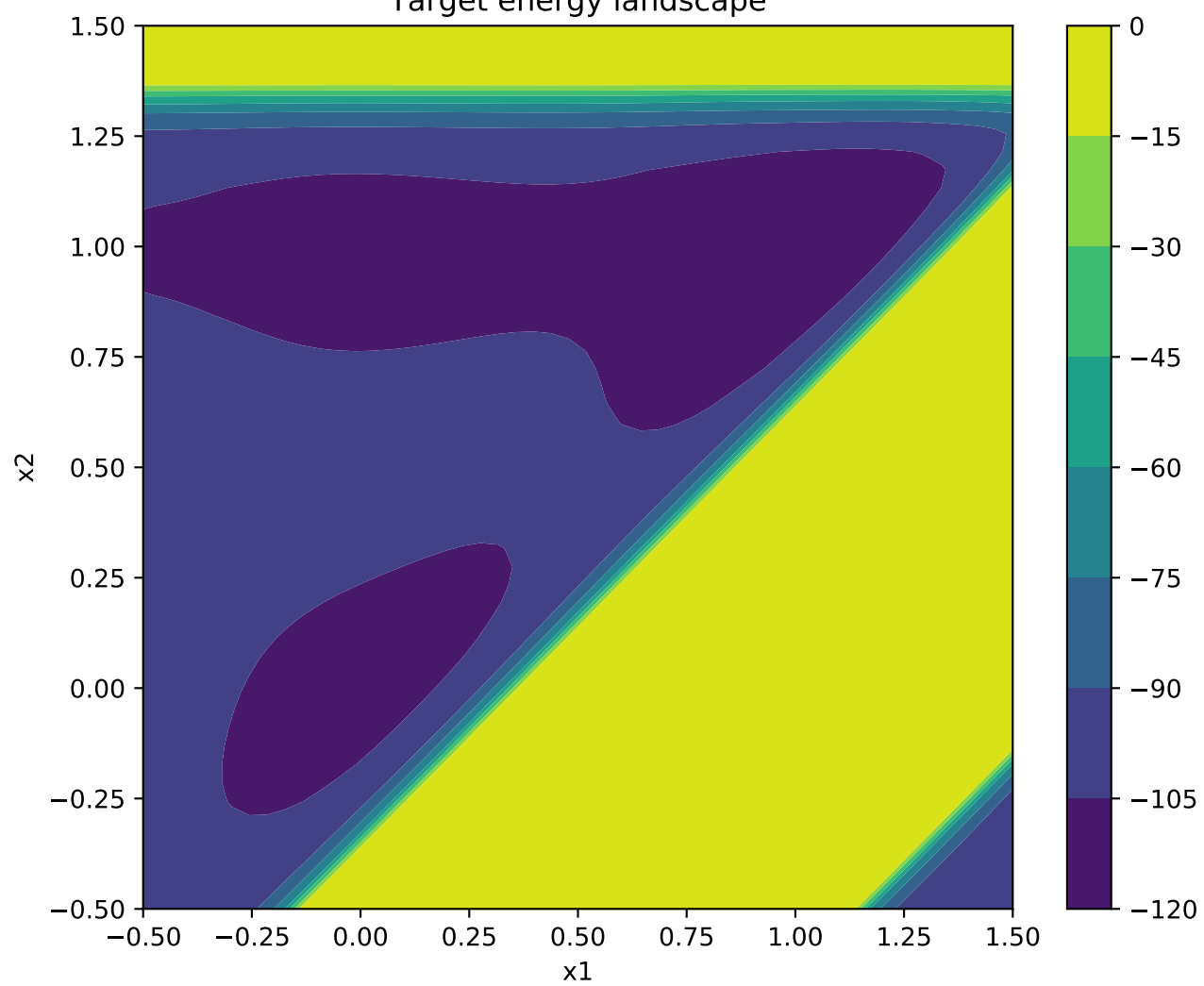
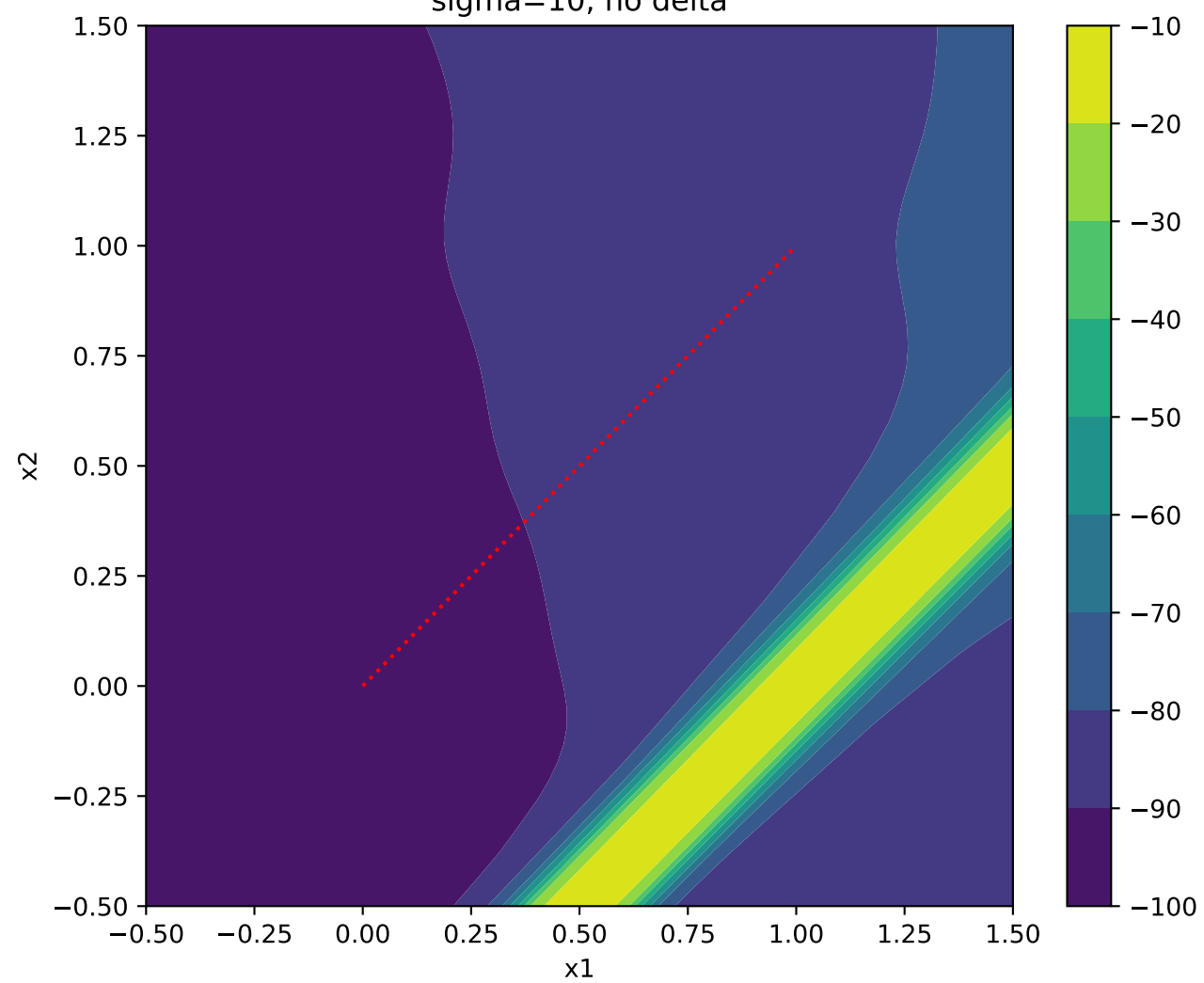


Target energy landscape



Predicted energy landscape
sigma=10, no delta



Energy of linear path
sigma=10 for ML models, bias=mean(Etrain)=-18.020312060028687

