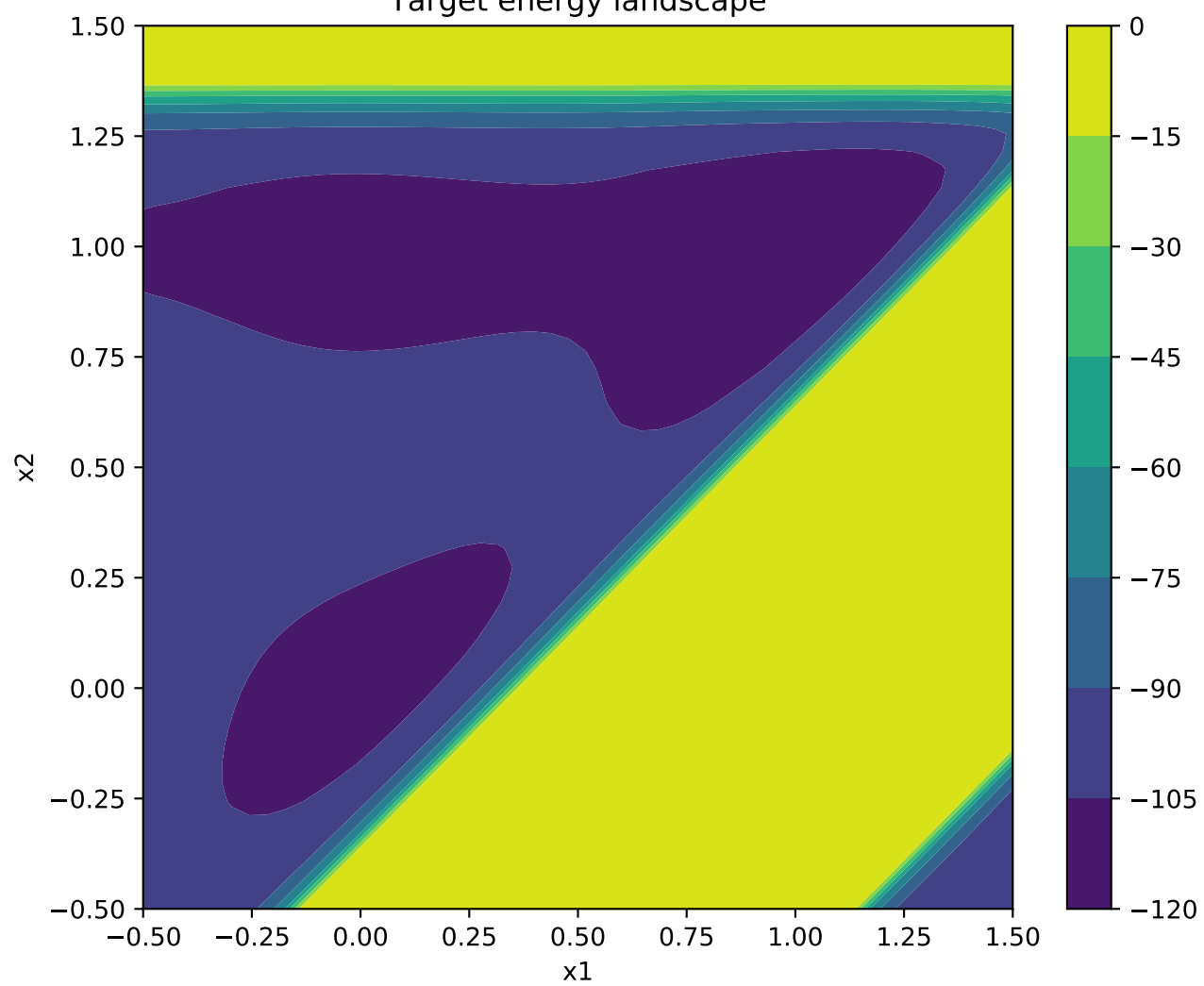
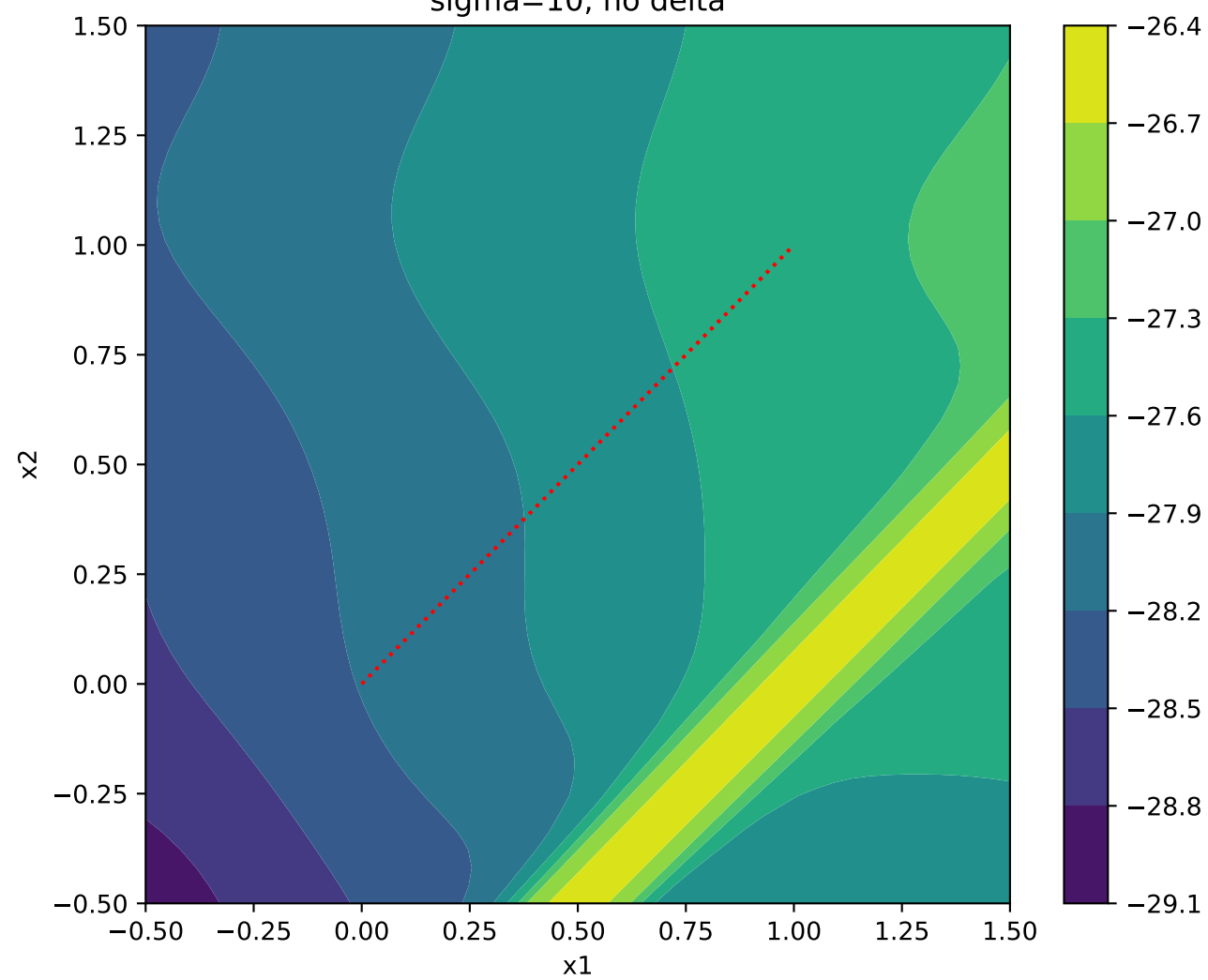


Target energy landscape

Predicted energy landscape  
sigma=10, no deltaEnergy of linear path  
sigma=10 for ML models, bias=mean(Etrain)=-26.68485089967415