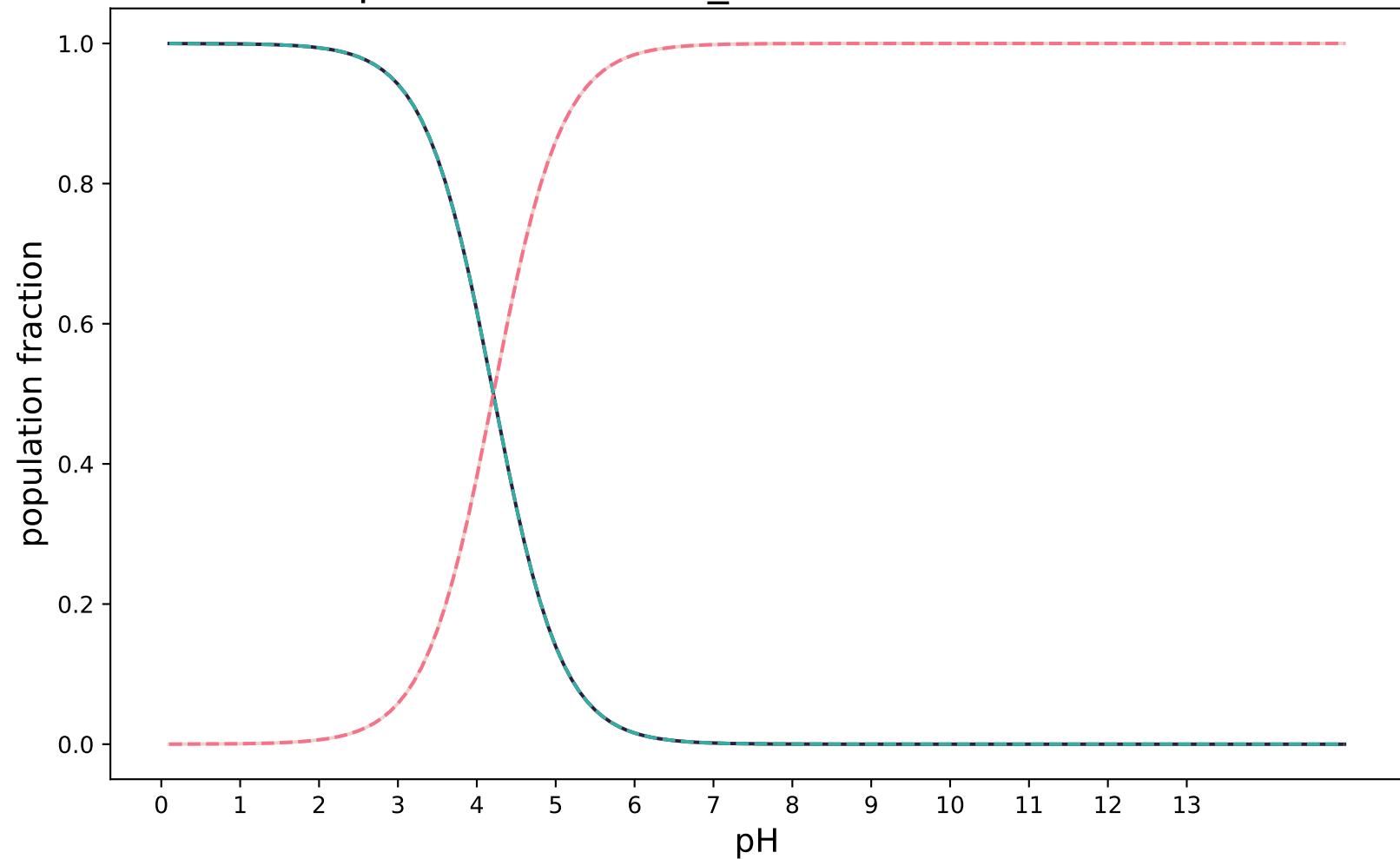


pKa-RobertRaddi_XGBoost:SAMPL8-18



-1.0 0.0 SAMPL8-18_micro005 reference