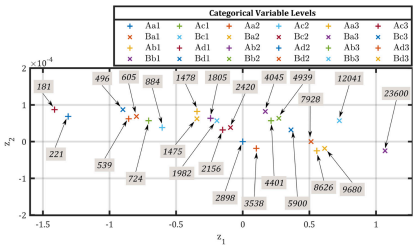
Multi-task Multi-output Drug Formulation

Tuesday, May 14, 2024 1:16 PM



https://bpb-us-e2.wpmucdn.com/faculty.sites.uci.edu/dist/1/863/files/2023/01/LMGP-Paper.pdf

X = [Xr, Xs]

Z=**A** Xr

X' = [Z, Xs]

Input

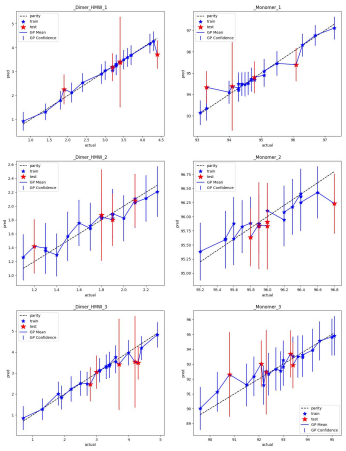
Formulation #	Buffer Type	pH	Sugar/ Salt	Additive	Additive Conc (mM)	PS20 Conc (%)
1	Ace	4.5	4% Sorbitol	Arginine	40	0.02
2	Ace	4.5	4% Sorbitol	Glycine	40	0.02
3	Ace	5	4% Sorbitol	Arginine	40	0.02
4	Ace	5	4% Sorbitol	Glycine	40	0.02
5	Ace	5	0.1M NaCl	Glycine	40	0.02
6	Ace	5.5	4% Sorbitol	Glycine	40	0.02
7	His	5.5	4% Sorbitol	Arginine	40	0.02
8	His	6	4% Sorbitol	Arginine	40	0.02
9	His	6	4% Sorbitol	Glycine	40	0.02
10	His	6	0.1M NaCl	Glycine	40	0.02
11	His	6.5	4% Sorbitol	Arginine	40	0.02
12	His	6.5	4% Sorbitol	Glycine	40	0.02
13	Cit	5	4% Sorbitol	Arginine	40	0.02
14	Cit	5	0.1M NaCl	Glycine	40	0.02
15	Cit	6	4% Sorbitol	Glycine	40	0.02
16	Cit	6.5	4% Sorbitol	Arginine	40	0.02
17	Cit	6.5	4% Sorbitol	Glycine	40	0.02
18	Cit	7	0.1M NaCl	Glycine	40	0.02
19	Cit	7	4% Sorbitol	Glycine	40	0.02
20	Cit	7	4% Sorbitol	Arginine	40	0.02
21	Phos	6.5	4% Sorbitol	Arginine	40	0.02
22	Phos	6.5	4% Sorbitol	Glycine	40	0.02
23	Phos	7	4% Sorbitol	Arginine	40	0.02
24	Phos	7	4% Sorbitol	Glycine	40	0.02

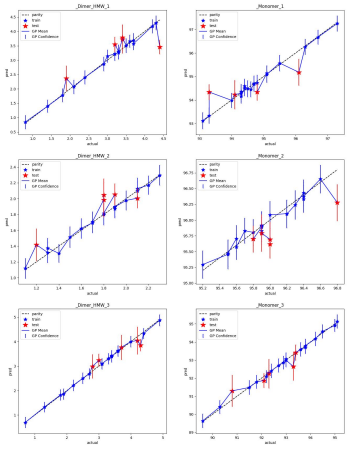
Output

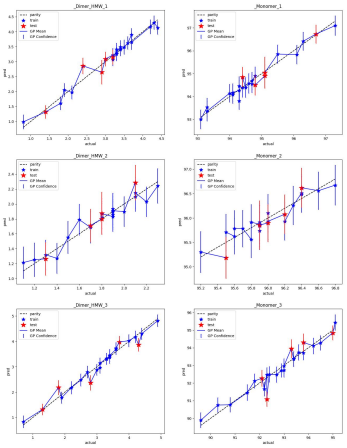
	%Dimer (HMW)			%Monomer			%LMW		
	T0	*FT*	*40°C*	*T0*	*FT*	*40°C*	*T0*	*FT*	*40°C*
1	2.4	1.6	1.8	95.1	96.2	93.8	2.5	2.2	4.4
2	0.8	1.1	0.7	97.3	96.6	95.1	2.0	2.2	4.2
3	3.2	2.0	2.7	94.3	95.6	93.4	2.6	2.4	3.9
4	1.4	1.4	1.3	96.7	96.4	95.0	1.9	2.3	3.6
5	4.2	2.3	3.4	93.3	95.2	**92.7**	2.5	2.4	4.0
6	1.8	1.3	1.9	96.3	96.4	94.5	2.0	2.3	3.6
7	3.6	2.2	3.1	94.0	95.5	93.8	2.4	2.3	3.1
8	3.7	2.1	3.4	94.3	95.6	93.0	1.9	2.4	3.5
9	2.1	1.3	2.2	95.5	96.4	94.2	2.4	2.3	3.6
10	4.3	2.1	4.9	93.1	95.5	**89.6**	2.6	2.4	**5.5**
11	4.4	2.1	4.3	93.3	95.8	**92.1**	2.4	2.1	3.6
12	1.9	1.2	2.8	96.1	96.8	93.3	2.0	2.0	3.9
13	2.9	1.5	2.5	95.1	96.3	93.6	2.0	2.2	4.0
14	3.5	1.8	3.4	94.5	95.9	**92.4**	2.0	2.3	**4.2**
15	3.2	1.9	3.0	94.8	96.0	93.4	2.0	2.1	3.6
16	3.2	1.7	3.1	94.8	96.0	**93.0**	1.9	2.2	**3.9**
17	3.3	1.9	3.3	94.7	95.8	**92.9**	2.0	2.3	3.9
18	3.7	1.9	4.0	94.3	95.9	**91.5**	2.0	2.2	**4.5**
19	3.3	1.8	3.6	94.7	95.9	**91.8**	2.0	2.3	**4.6**
20	3.3	1.7	3.3	94.4	96.2	**92.3**	2.4	2.1	4.4
21	3.4	1.8	3.7	94.1	96.0	**92.3**	2.5	2.2	4.0
22	3.0	1.9	3.6	94.4	95.7	**92.2**	2.5	2.5	4.2
23	3.4	1.8	4.2	94.1	95.9	**90.8**	2.5	2.3	**5.0**
24	3.3	1.9	4.4	94.6	95.9	**90.3**	2.2	2.2	**5.3**

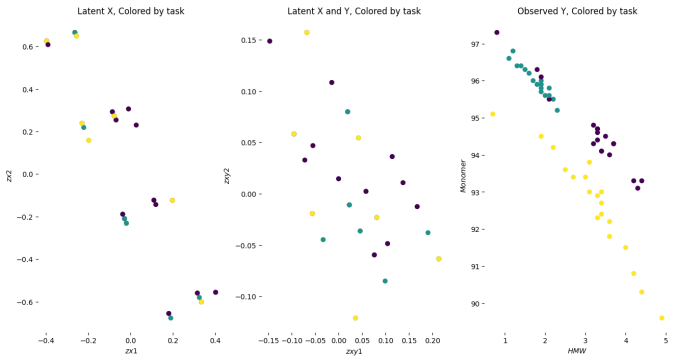
MAE	_Dimer_HMW_1	_Monomer_1	_Dimer_HMW_2	_Monomer_2	_Dimer_HMW_3	_Monomer_3
Multitask-singleoutput (task rank 0, lik rank 0)	0.22	0.46	0.1	0.21	0.43	0.69
LMGP	0.49	0.54	0.18	0.28	0.22	0.29
Hier LMGP	0.19	0.21	0.06	0.16	0.31	0.54
Multitask-Multioutput (task rank 1, lik rank 1)	0.2	0.2	0.16	0.13	0.31	0.36
Multitask-singleoutput (task rank 1, lik rank 1)	0.36	0.51	0.19	0.21	0.39	0.48
Multitask-Multioutput (task rank 3, lik rank 2, ohe, per task scale)	0.30	0.19	0.05	0.10	0.36	0.46

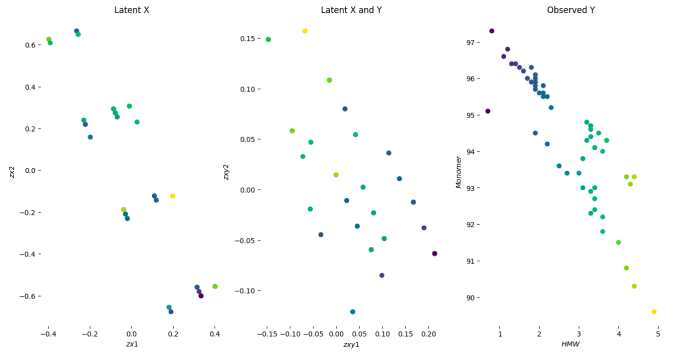
Avg STD	_Dimer_HMW_1	_Monomer_1	_Dimer_HMW_2	_Monomer_2	_Dimer_HMW_3	_Monomer_3
Multitask-singleoutput (task rank 0, lik rank 0)	1.1	1.27	0.49	0.61	1.34	2.06
LMGP	0.37	0.49	0.18	0.26	0.41	0.66
Hier LMGP	0.27	0.49	0.23	0.42	0.26	0.46
Multitask-Multioutput (task rank 1, lik rank 1)	0.43	0.75	0.3	0.57	0.46	0.78
Multitask-singleoutput (task rank 1, lik rank 1) IN PCT	0.36	0.01	0.3	0.01	0.36	0.02
Multitask-singleoutput (task rank 0, lik rank 0) IN PCT	0.34	0.01	0.28	0.01	0.37	0.02







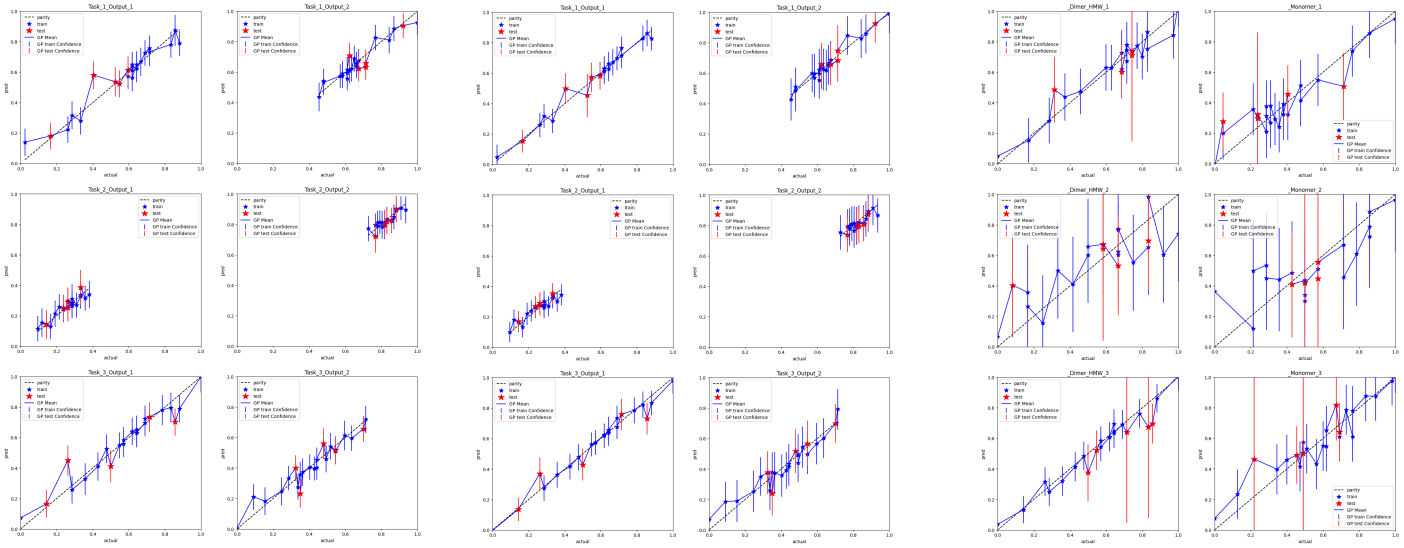




Lmgp reduce cate multitask

multitask

Non-hierarchical


Task_1_Output_1
Task_1_Output_2
Task_1_Output_1
Task_1_Output_2
_Dimer_HMW_1
_Monomer_1
Task_2_Output_1
Task_2_Output_2
Task_2_Output_1
Task_2_Output_2
_Dimer_HMW_2
_Monomer_2
Task_3_Output_1
Task_3_Output_2
Task_3_Output_1
Task_3_Output_2
_Dimer_HMW_3
_Monomer_3
parity
train
test
GP Mean
GP train Confidence
GP test Confidence
pred
actual