

Table 1: **High dimensional (dim = 43)** experimental results on the organoid drug-screen dataset across *replicate* populations.

	Train				Test			
	$\mathcal{W}_1(\downarrow)$	$\mathcal{W}_2(\downarrow)$	MMD ($\times 10^{-3}$) ($\downarrow$)	$r^2(\uparrow)$	$\mathcal{W}_1(\downarrow)$	$\mathcal{W}_2(\downarrow)$	MMD ($\times 10^{-3}$) ($\downarrow$)	$r^2(\uparrow)$
FM	3.925 $\pm$ 0.019	4.041 $\pm$ 0.023	3.76 $\pm$ 0.26	0.952 $\pm$ 0.007	3.961 $\pm$ 0.036	4.089 $\pm$ 0.042	5.90 $\pm$ 0.25	0.941 $\pm$ 0.010
FM ^w / $\mathcal{N}$	6.908 $\pm$ 0.037	7.181 $\pm$ 0.033	57.70 $\pm$ 0.75	0.639 $\pm$ 0.005	6.972 $\pm$ 0.022	7.244 $\pm$ 0.022	60.39 $\pm$ 0.98	0.642 $\pm$ 0.007
CGFM	3.864 $\pm$ 0.064	3.975 $\pm$ 0.069	3.16 $\pm$ 0.89	0.964 $\pm$ 0.006	4.087 $\pm$ 0.063	3.066 $\pm$ 0.066	8.84 $\pm$ 0.75	0.938 $\pm$ 0.006
CGFM ^w / $\mathcal{N}$	4.187 $\pm$ 0.008	4.340 $\pm$ 0.009	8.69 $\pm$ 0.50	0.936 $\pm$ 0.002	6.852 $\pm$ 0.045	7.114 $\pm$ 0.044	71.24 $\pm$ 3.71	0.666 $\pm$ 0.016
ICNN	4.286 $\pm$ 0.018	4.313 $\pm$ 0.112	38.6 $\pm$ 0.212	0.897 $\pm$ 0.031	4.194 $\pm$ 0.110	4.313 $\pm$ 0.112	37.9 $\pm$ 2.84	0.897 $\pm$ 0.008
MFM ^w / $\mathcal{N}$ ($k=0$)	3.940 $\pm$ 0.022	4.047 $\pm$ 0.023	3.91 $\pm$ 0.18	0.959 $\pm$ 0.006	3.896 $\pm$ 0.026	4.002 $\pm$ 0.030	4.35 $\pm$ 0.18	0.950 $\pm$ 0.005
MFM ^w / $\mathcal{N}$ ($k=10$)	3.976 $\pm$ 0.044	4.086 $\pm$ 0.049	4.52 $\pm$ 0.42	0.961 $\pm$ 0.002	3.943 $\pm$ 0.032	4.051 $\pm$ 0.034	5.28 $\pm$ 0.25	0.952 $\pm$ 0.001
MFM ^w / $\mathcal{N}$ ($k=50$)	3.968 $\pm$ 0.013	4.075 $\pm$ 0.014	4.36 $\pm$ 0.44	0.961 $\pm$ 0.002	3.934 $\pm$ 0.007	4.041 $\pm$ 0.008	4.99 $\pm$ 0.35	0.954 $\pm$ 0.000
MFM ^w / $\mathcal{N}$ ($k=100$)	3.937 $\pm$ 0.014	4.040 $\pm$ 0.015	3.94 $\pm$ 0.00	0.963 $\pm$ 0.001	3.908 $\pm$ 0.030	4.011 $\pm$ 0.033	4.68 $\pm$ 0.52	0.953 $\pm$ 0.002
MFM ($k=0$)	3.874 $\pm$ 0.015	3.973 $\pm$ 0.020	3.37 $\pm$ 0.14	0.967 $\pm$ 0.003	3.880 $\pm$ 0.009	3.990 $\pm$ 0.011	4.68 $\pm$ 0.16	0.955 $\pm$ 0.002
MFM ($k=10$)	3.896 $\pm$ 0.021	4.000 $\pm$ 0.021	3.82 $\pm$ 0.12	0.964 $\pm$ 0.001	3.899 $\pm$ 0.013	4.012 $\pm$ 0.011	5.13 $\pm$ 0.48	0.955 $\pm$ 0.001
MFM ($k=50$)	3.888 $\pm$ 0.038	3.991 $\pm$ 0.030	3.59 $\pm$ 0.41	0.963 $\pm$ 0.001	3.900 $\pm$ 0.038	4.013 $\pm$ 0.034	5.06 $\pm$ 0.22	0.954 $\pm$ 0.003
MFM ($k=100$)	3.906 $\pm$ 0.010	4.008 $\pm$ 0.005	4.05 $\pm$ 0.38	0.964 $\pm$ 0.002	3.898 $\pm$ 0.008	4.009 $\pm$ 0.009	5.19 $\pm$ 0.05	0.957 $\pm$ 0.000

Table 2: **High dimensional (dim = 43)** experimental results on the organoid drug-screen dataset across *patient* populations.

	Train				Test			
	$\mathcal{W}_1(\downarrow)$	$\mathcal{W}_2(\downarrow)$	MMD ($\times 10^{-3}$) ($\downarrow$)	$r^2(\uparrow)$	$\mathcal{W}_1(\downarrow)$	$\mathcal{W}_2(\downarrow)$	MMD ($\times 10^{-3}$) ($\downarrow$)	$r^2(\uparrow)$
FM	3.985 $\pm$ 0.054	4.115 $\pm$ 0.067	4.64 $\pm$ 0.43	0.938 $\pm$ 0.014	4.340 $\pm$ 0.078	4.564 $\pm$ 0.111	13.00 $\pm$ 0.67	0.865 $\pm$ 0.034
FM ^w / $\mathcal{N}$	6.892 $\pm$ 0.027	7.164 $\pm$ 0.033	57.03 $\pm$ 1.00	0.655 $\pm$ 0.003	7.114 $\pm$ 0.1001	7.404 $\pm$ 0.086	64.97 $\pm$ 3.79	0.613 $\pm$ 0.008
CGFM	3.882 $\pm$ 0.019	3.999 $\pm$ 0.020	3.16 $\pm$ 0.59	0.952 $\pm$ 0.004	4.443 $\pm$ 0.033	4.621 $\pm$ 0.041	17.00 $\pm$ 1.03	0.899 $\pm$ 0.008
CGFM ^w / $\mathcal{N}$	4.313 $\pm$ 0.077	4.480 $\pm$ 0.081	11.51 $\pm$ 1.96	0.918 $\pm$ 0.004	7.135 $\pm$ 0.045	7.390 $\pm$ 0.037	79.78 $\pm$ 4.67	0.637 $\pm$ 0.010
ICNN	4.289 $\pm$ 0.020	4.382 $\pm$ 0.021	37.0 $\pm$ 2.84	0.913 $\pm$ 0.003	4.525 $\pm$ 0.051	4.681 $\pm$ 0.054	74.0 $\pm$ 0.570	0.862 $\pm$ 0.127
MFM ^w / $\mathcal{N}$ ($k=0$)	3.982 $\pm$ 0.014	4.095 $\pm$ 0.015	5.04 $\pm$ 0.36	0.951 $\pm$ 0.002	4.177 $\pm$ 0.042	4.355 $\pm$ 0.048	10.53 $\pm$ 0.59	0.911 $\pm$ 0.001
MFM ^w / $\mathcal{N}$ ($k=10$)	4.006 $\pm$ 0.008	4.119 $\pm$ 0.012	5.13 $\pm$ 0.30	0.948 $\pm$ 0.001	4.156 $\pm$ 0.065	4.324 $\pm$ 0.067	9.58 $\pm$ 1.63	0.912 $\pm$ 0.003
MFM ^w / $\mathcal{N}$ ($k=50$)	3.982 $\pm$ 0.018	4.095 $\pm$ 0.016	4.74 $\pm$ 0.21	0.951 $\pm$ 0.002	4.153 $\pm$ 0.069	4.324 $\pm$ 0.070	9.63 $\pm$ 1.45	0.912 $\pm$ 0.002
MFM ^w / $\mathcal{N}$ ($k=100$)	4.004 $\pm$ 0.012	4.119 $\pm$ 0.014	5.19 $\pm$ 0.43	0.949 $\pm$ 0.002	4.166 $\pm$ 0.001	4.341 $\pm$ 0.003	9.52 $\pm$ 0.33	0.915 $\pm$ 0.005
MFM ($k=0$)	3.905 $\pm$ 0.005	4.012 $\pm$ 0.006	4.18 $\pm$ 0.25	0.958 $\pm$ 0.001	4.209 $\pm$ 0.007	4.380 $\pm$ 0.012	12.34 $\pm$ 0.50	0.918 $\pm$ 0.002
MFM ($k=10$)	3.896 $\pm$ 0.033	4.005 $\pm$ 0.036	3.89 $\pm$ 0.44	0.957 $\pm$ 0.005	4.216 $\pm$ 0.090	4.395 $\pm$ 0.098	11.99 $\pm$ 2.36	0.917 $\pm$ 0.005
MFM ($k=50$)	3.902 $\pm$ 0.018	4.008 $\pm$ 0.022	4.20 $\pm$ 0.17	0.958 $\pm$ 0.000	4.214 $\pm$ 0.017	4.396 $\pm$ 0.020	12.09 $\pm$ 0.75	0.916 $\pm$ 0.002
MFM ($k=100$)	3.884 $\pm$ 0.039	3.986 $\pm$ 0.044	3.77 $\pm$ 0.49	0.955 $\pm$ 0.001	4.100 $\pm$ 0.093	4.269 $\pm$ 0.104	8.96 $\pm$ 1.88	0.917 $\pm$ 0.004

Algorithm 1: Meta Flow Matching (training)

Input: Dataset of populations $\{(\pi(x_0, x_1 | i), c^i)\}_{i=1}^N$ and treatments c^i , and parametric models $v_t(\cdot; \omega), \varphi(\cdot; \theta)$.

for training iterations do

$i \sim \mathcal{U}_{\{1, N\}}(i)$ // sample a batch of n populations ids

$(x_0^j, x_1^j, t^j) \sim \pi(x_0, x_1 | i) \mathcal{U}_{[0, 1]}(t)$ // sample batch of n_i particles for every population i

$f_t(x_0^j, x_1^j) \leftarrow (1 - t^j)x_0^j + t^j x_1^j$,

$h^i(\theta) \leftarrow \varphi(\{x_0^j\}_{j=1}^{N_i}; \theta)$ // embed the entire population $\{x_0^j\}_{j=1}^{N_i}$ into $h^i(\theta)$. In CGFM $h \leftarrow i$. In FM $h \leftarrow \emptyset$.

$\mathcal{L}_{\text{MFM}}(\omega, \theta) \leftarrow \frac{1}{n} \sum_i \frac{1}{n_i} \sum_j \left\| \frac{\partial}{\partial t} f_t(x_0^j, x_1^j) - v_{t^j}(f_t(x_0^j, x_1^j) | h^i(\theta), c^i; \omega) \right\|^2$

$\omega' \leftarrow \text{Update}(\omega, \nabla_{\omega} \mathcal{L}_{\text{MFM}}(\omega, \theta))$ // evaluate new parameters of the flow model

$\theta' \leftarrow \text{Update}(\theta, \nabla_{\theta} \mathcal{L}_{\text{MFM}}(\omega, \theta))$ // evaluate new parameters of the embedding model

$\omega \leftarrow \omega', \theta \leftarrow \theta'$ // update both models

return $v_t(\cdot; \omega^*), \varphi(\cdot; \theta^*)$

Table 3: Synthetic letters experiment for population prediction on fully unseen test populations (Y's).

	$\mathcal{W}_1$	Test $\mathcal{W}_2$	MMD ($\times 10^{-3}$)
FM	0.238 $\pm$ 0.000	0.316 $\pm$ 0.000	3.32 $\pm$ 0.01
FM ^w / $\mathcal{N}$	1.030 $\pm$ 0.000	1.228 $\pm$ 0.000	45.36 $\pm$ 0.00
CGFM	0.327 $\pm$ 0.000	0.405 $\pm$ 0.000	6.85 $\pm$ 0.00
CGFM ^w / $\mathcal{N}$	1.062 $\pm$ 0.011	1.229 $\pm$ 0.010	55.66 $\pm$ 0.76
MFM ^w / $\mathcal{N}$ ($k=0$)	0.402 $\pm$ 0.011	0.485 $\pm$ 0.010	10.92 $\pm$ 0.18
MFM ^w / $\mathcal{N}$ ($k=1$)	0.391 $\pm$ 0.035	0.477 $\pm$ 0.041	10.71 $\pm$ 1.86
MFM ^w / $\mathcal{N}$ ($k=10$)	0.413 $\pm$ 0.018	0.502 $\pm$ 0.024	11.93 $\pm$ 1.14
MFM ^w / $\mathcal{N}$ ($k=50$)	0.446 $\pm$ 0.021	0.536 $\pm$ 0.028	13.40 $\pm$ 0.23
MFM ($k=0$)	0.218 $\pm$ 0.001	0.262 $\pm$ 0.002	3.79 $\pm$ 0.11
MFM ($k=1$)	0.215 $\pm$ 0.006	0.258 $\pm$ 0.007	3.78 $\pm$ 0.25
MFM ($k=10$)	0.208 $\pm$ 0.003	0.252 $\pm$ 0.002	3.55 $\pm$ 0.06
MFM ($k=50$)	0.204 $\pm$ 0.005	0.249 $\pm$ 0.006	3.14 $\pm$ 0.18

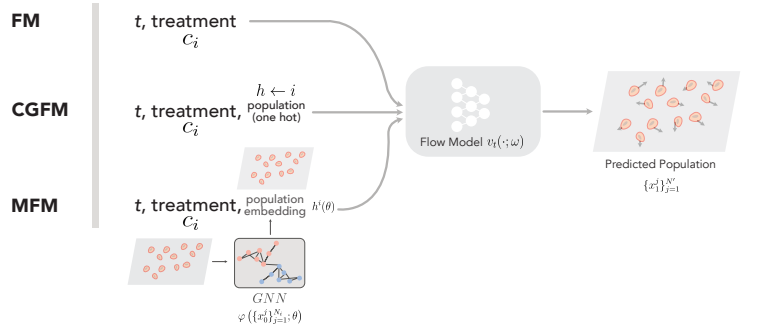


Figure 1: Illustrative comparison between Flow Matching (FM), conditional flow matching (CGFM), and Meta Flow Matching (MFM).