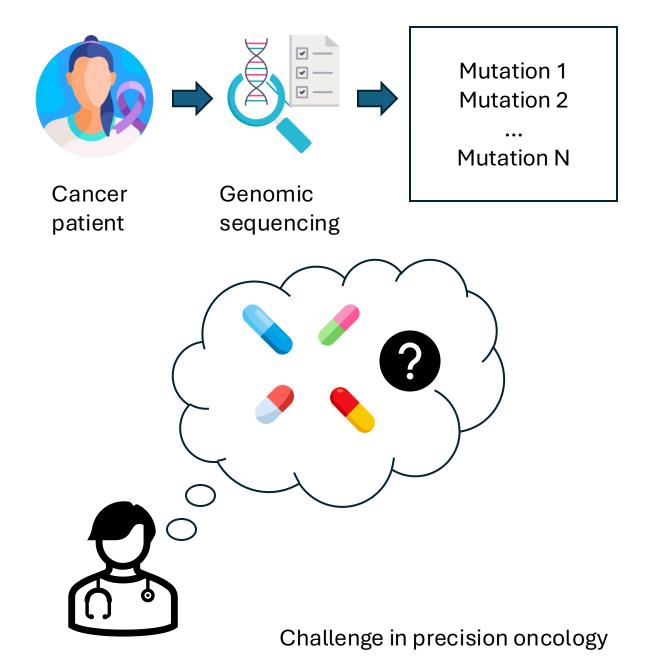
**GANDALF:** Generative AttentioN based Data Augmentation and predictive modeLing Framework for personalized cancer treatment

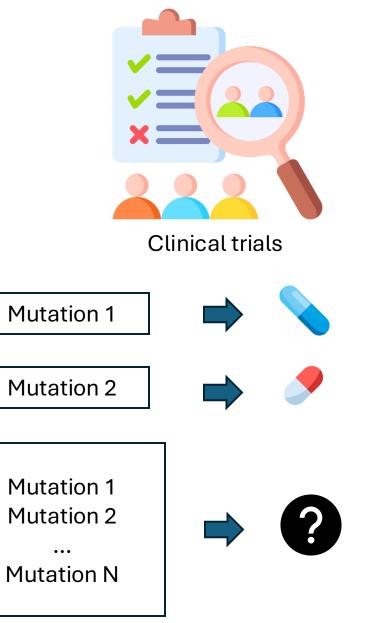
Aishwarya Jayagopal<sup>1</sup>, Yanrong Zhang<sup>1</sup>, Robert J. Walsh<sup>2</sup>, Tuan Zea Tan<sup>3</sup>, Anand D. Jeyasekharan<sup>3</sup>, Vaibhav Rajan<sup>1</sup>



<sup>&</sup>lt;sup>1</sup> National University of Singapore, <sup>2</sup> National University Cancer Institute,

<sup>&</sup>lt;sup>3</sup> Cancer Science Institute of Singapore



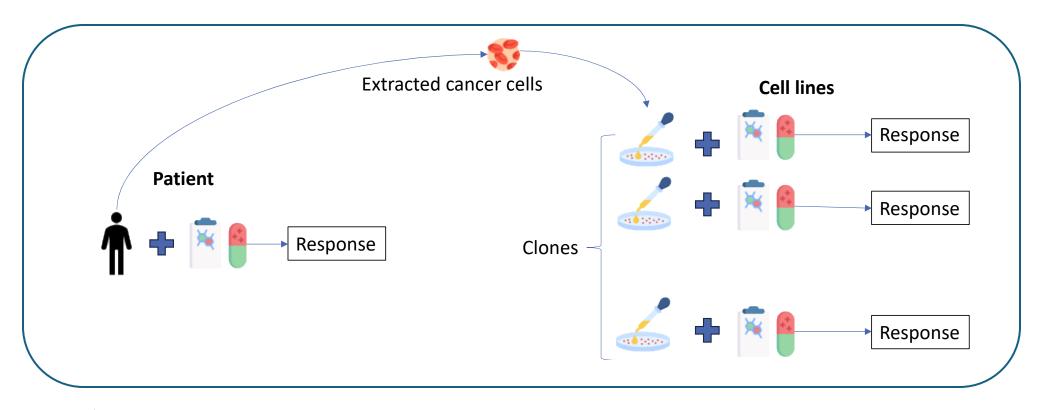


Clinical trials intractable!

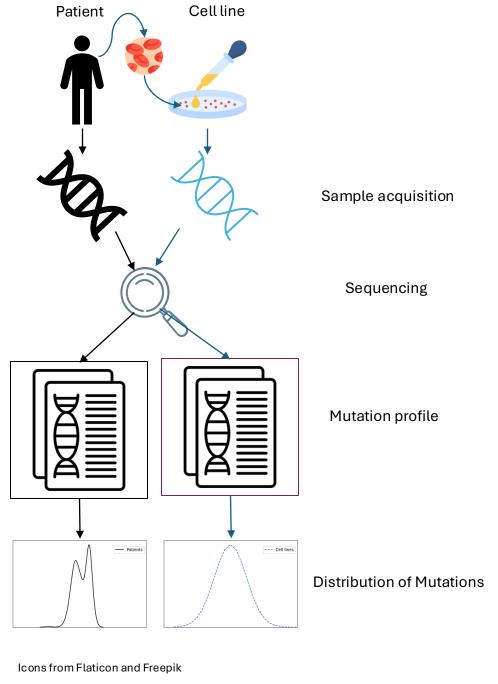
# Recommendations Mutation 1 Mutation 2 Mutation N Deep learning methods

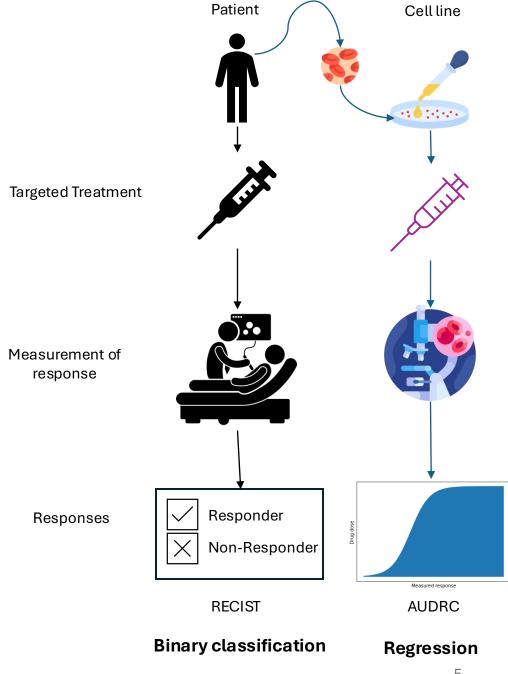
Clinical standard of care treatment uses only subset of drugs

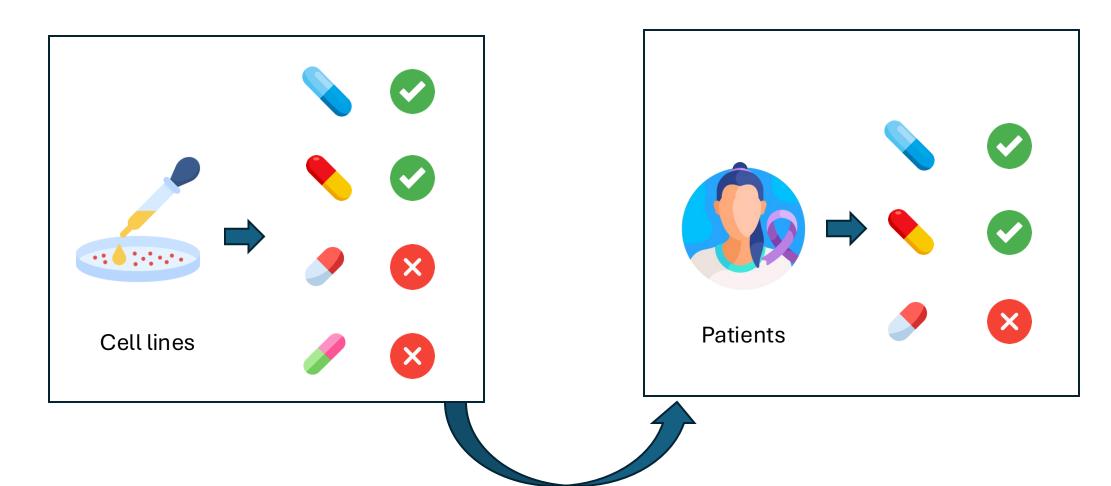
#### Cell lines: A Related "Domain"



- > Extract cancer cells and clone them in lab (living cells, continue growing)
  - $\triangleright$  Ensures each cell has same genomic data (X)
  - $\triangleright$  Administer multiple drugs on cell lines, measure response (Y)

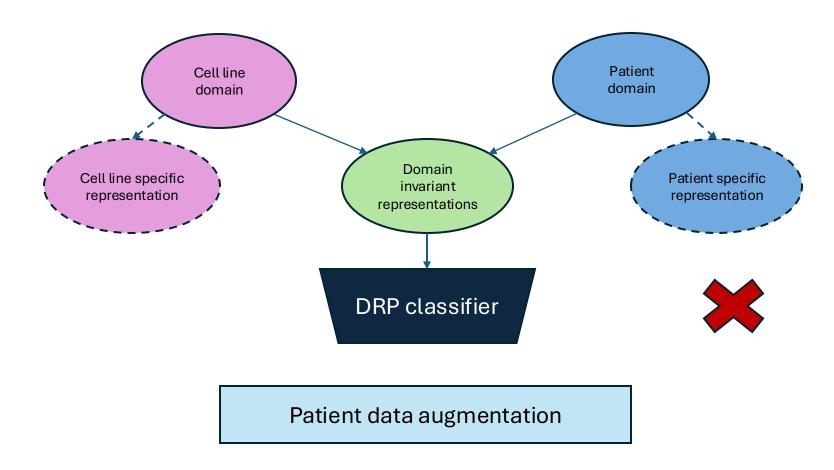






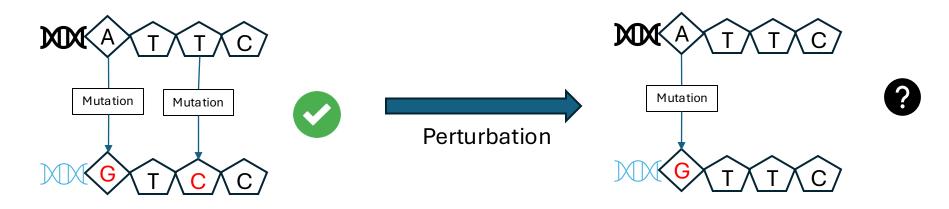
Transfer learning

#### Modeling patient specific representations



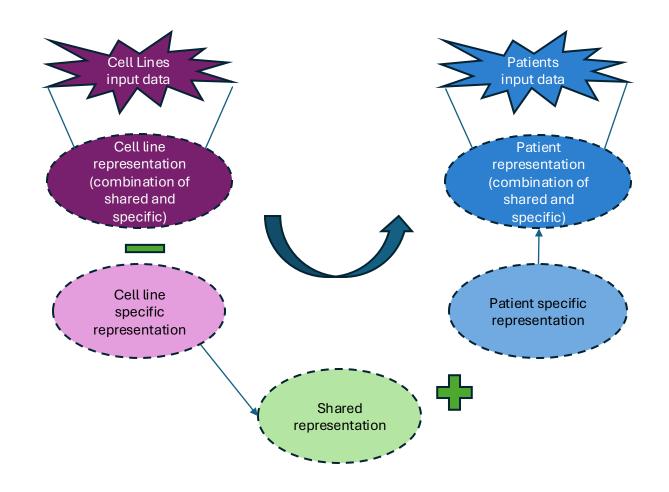
#### Genomic Data Augmentation

- No 'label-invariance' guarantee
- "Nearby" data points can respond differently to drugs
  - Perturbation ⇒ addition/removal of mutation



Use labelled cell lines to generate patient-like samples and assign labels to them.

#### Intuition



#### **Model Training**

Pretraining diffusion models Generating new patient-like samples Training a multi-task learning network Assigning pseudo labels and selection of confident samples Training a drug response prediction classifier

### Results: Comparison against SOTA

AUROC (M	AUROC (Mean / Standard deviation)						AUPRC (Mean / Standard deviation)					
Method	Cis	Flu	Gem	Pac	Tem		Method	Cis	Flu	Gem	Pac	Tem
GANDALF	0.6343	0.7309	0.6188	0.7728	0.6451		GANDALF	0.9093	0.8483	0.5874	0.9558	0.2535
	±	1 ±	±	±	±			<b>±</b>	±	$\pm$ 0.175	$\pm$ 0.024	±
	0.0306	0.0664	0.0674	0.1253	0.0776			0.0355	0.0933			0.1108
DruID	0.6764	0.6071	0.5092	0.5119	0.6194		DruID	0.9176	0.7588	0.4515	0.8897	0.3104
	±	±	<u>+</u>	±	±			<b>±</b>	±	±	土	±
	0.1447	0.1988	0.1005	0.2324	0.0420			0.0671	0.1484	0.1297	0.0223	0.1039
PANCDR	0.6278	0.4762	0.4429	0.4236	0.6436		PANCDR	0.9018	0.6951	0.4562	0.8561	0.3049
	±	±	<u>±</u>	±	<u> </u>			土	±	土	土	±
	0.0308	0.1798	0.2268	0.4168	0.2310			0.0324	0.1530	0.2270	0.1019	0.2653
PREDICT-	0.5072	0.3869	0.5046	0.6815	0.5350		PREDICT-	0.8622	0.5885	0.3873	0.8687	0.1373
AI	±	±	<u> </u>	±	±		AI	<b>±</b>	±	<u>+</u>	土	±
	0.0331	0.0372	0.1181	0.1786	0.0606			0.0189	0.0581	0.0489	0.1090	0.0050
drug2tme	0.5243	0.7167	0.4568	0.3194	0.5951		drug2tme	0.8754	0.8092	0.4826	0.7824	0.3058
	±	<u> </u>	<u>+</u>	±	±			土	±	土	土	±
	0.1301	0.1957	0.0857	0.3127	0.2541			0.0523	0.1722	0.0947	0.1023	0.1327
CODE-AE	0.6322	0.5381	0.5085	0.3611	0.4332		CODE-AE	0.9059	0.6665	0.4735	0.8208	0.1756
	±	±	土	±	<u>+</u>			土	±	土	土	±
	0.1872	0.1606	0.0503	0.3155	0.3123			0.0521	0.1435	0.0701	0.0574	0.0929

Max Improvement in AUROC: 10.96% Max Improvement in AUPRC: 3.91%

#### Advantages of GANDALF

Model is generative

Allows use of prior information from cell lines

Avoiding overfitting when using augmented patient data

## Thank you!

#### Paper



Code repo

