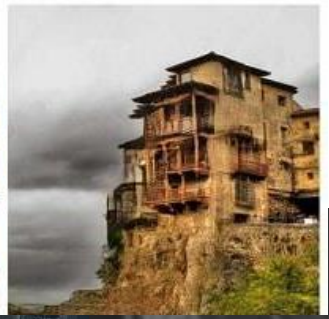
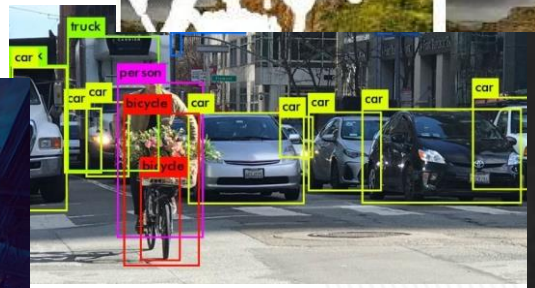
Inverse Problems in Computational Imaging and Chemistry

Tomer Weiss

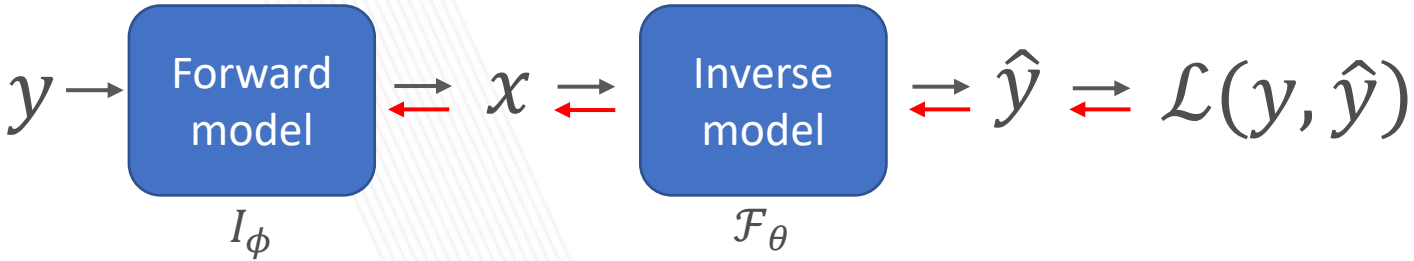
IMVC 2024

Neural networks are great



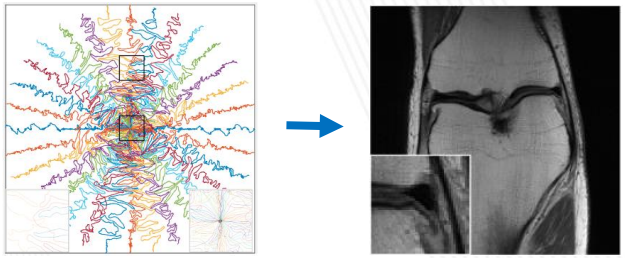


Can we use them in additional ways?

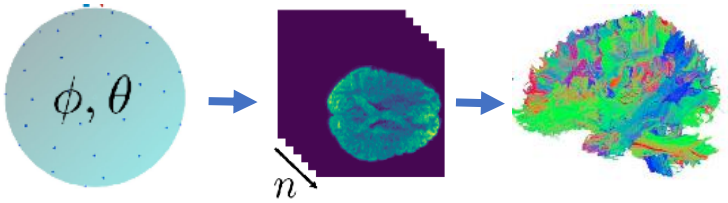


$$\theta^*, \phi^* = argmin_{\theta,\phi} \mathcal{L}(y, \hat{y})$$

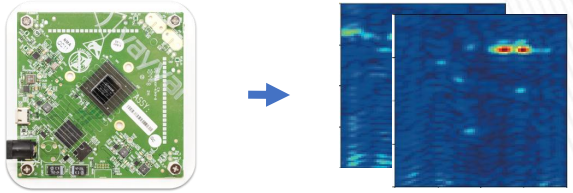
MRI



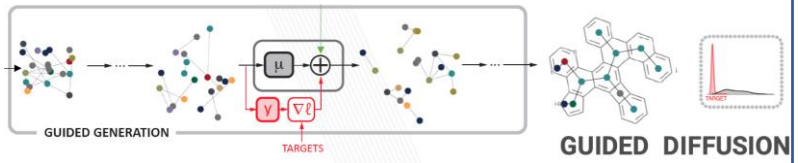
Diffusion MRI



MIMO Radar



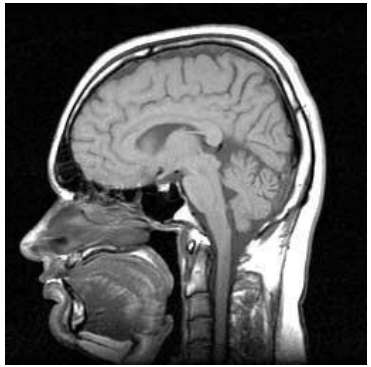
Molecular Design



MRI

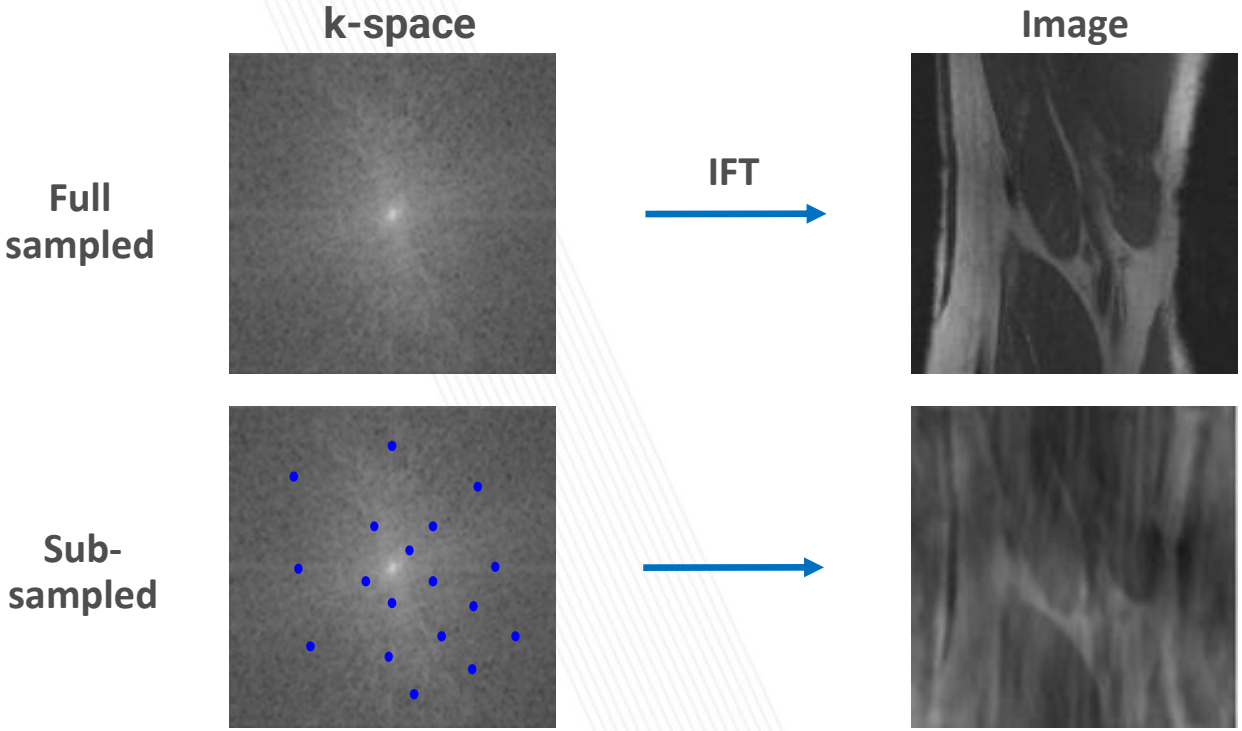
3D medical imaging technique

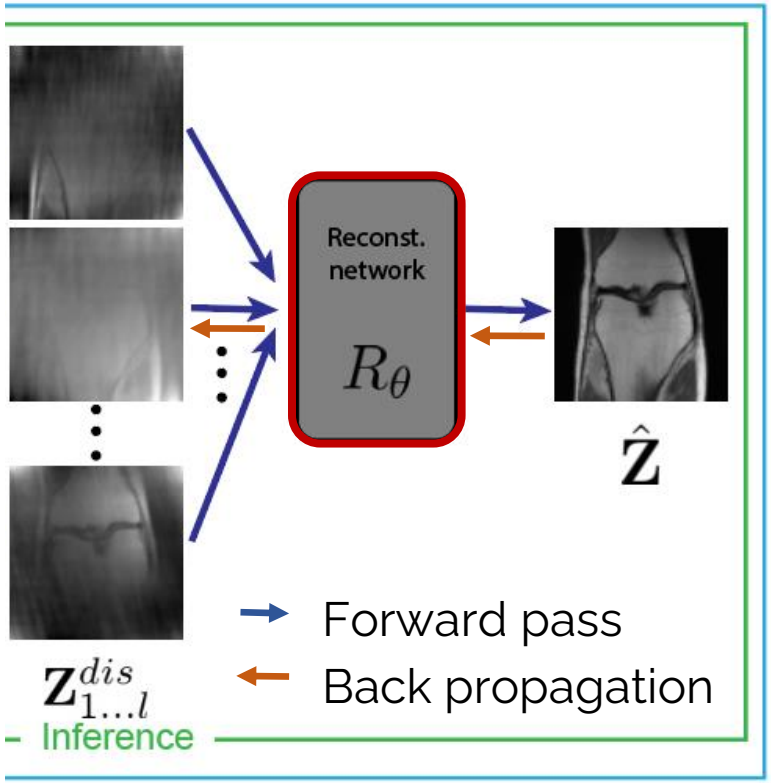
- Noninvasive
- Without harmful radiation
- Superb imaging contrast and resolution



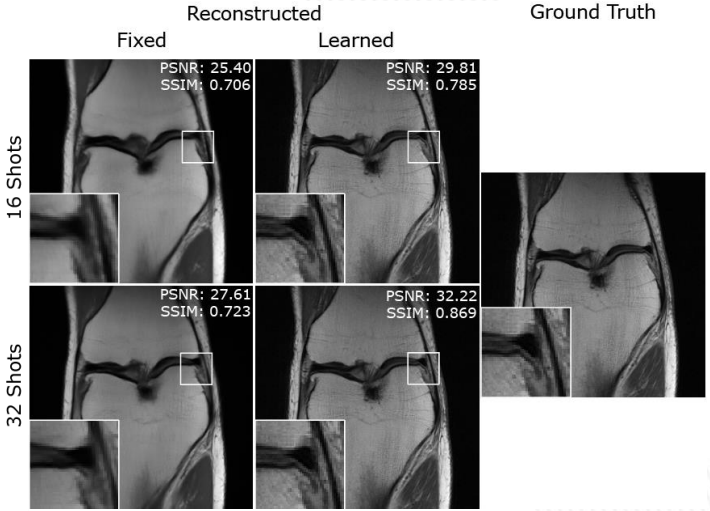
Long acquisition times (30-60 mins)

Acceleration through undersampling

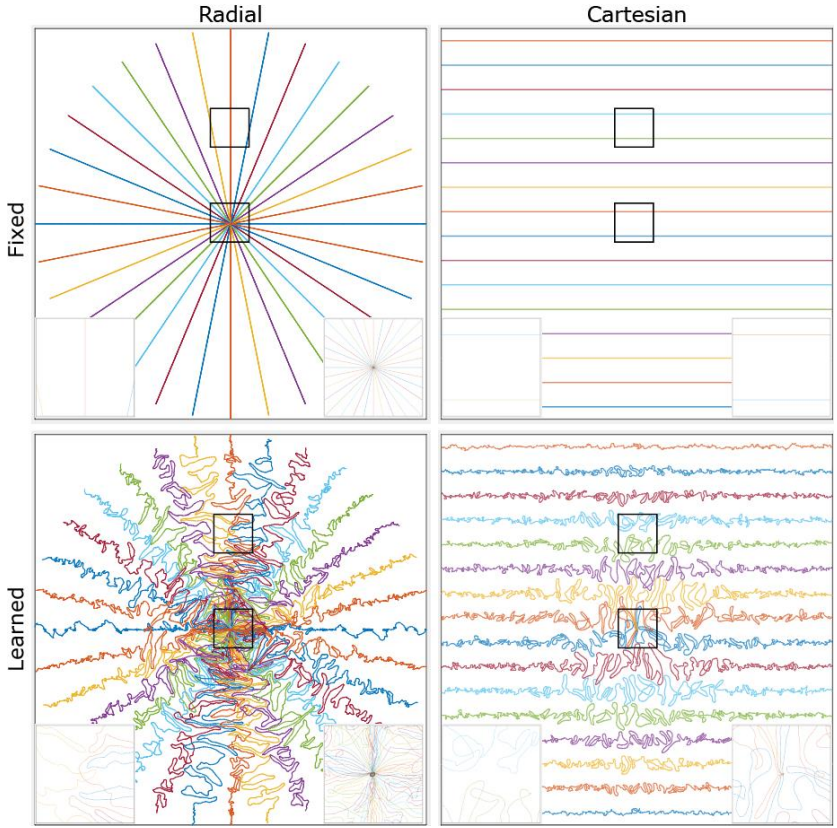



Reconst. network
R_θ
$\hat{\mathbf{Z}}$
$\mathbf{Z}^{dis}_{1\ldots l}$
Inference
Forward pass
Back propagation

Results

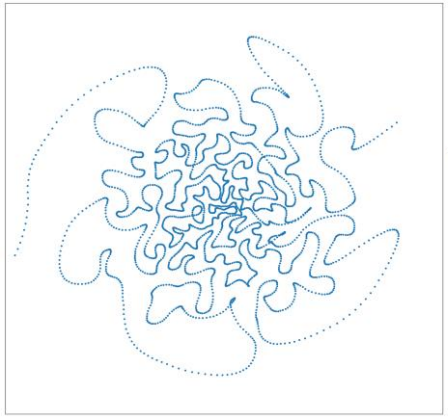


N. of shots	16	
Trajectory	PSNR	SSIM
Cartesian-Fixed	18.57±1.67	0.427±0.051
Cartesian-PILOT	31.43±1.48	0.806±0.036
Radial-Fixed	29.09±1.43	0.741±0.040
Radial-PILOT	33.71±1.58	0.863±0.032
Spiral-Fixed	33.89±1.56	0.874±0.030
Spiral-PILOT	**35.55±1.59**	**0.903±0.026**

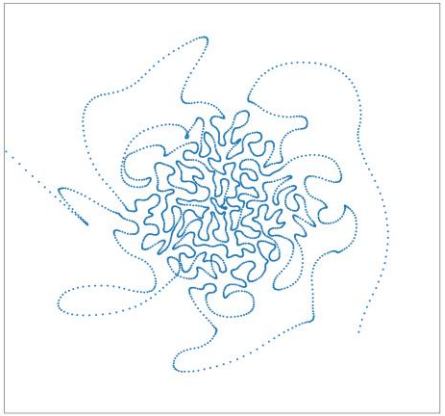


Different end task or organ

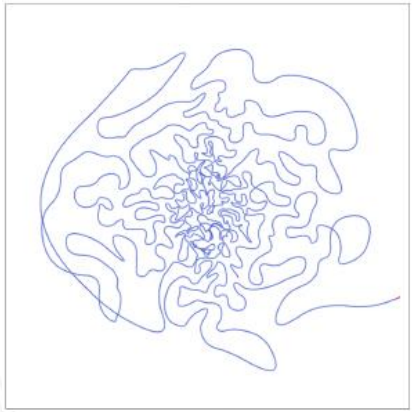
Segmentation



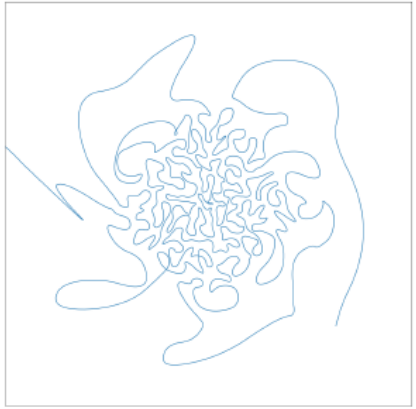
Reconstruction



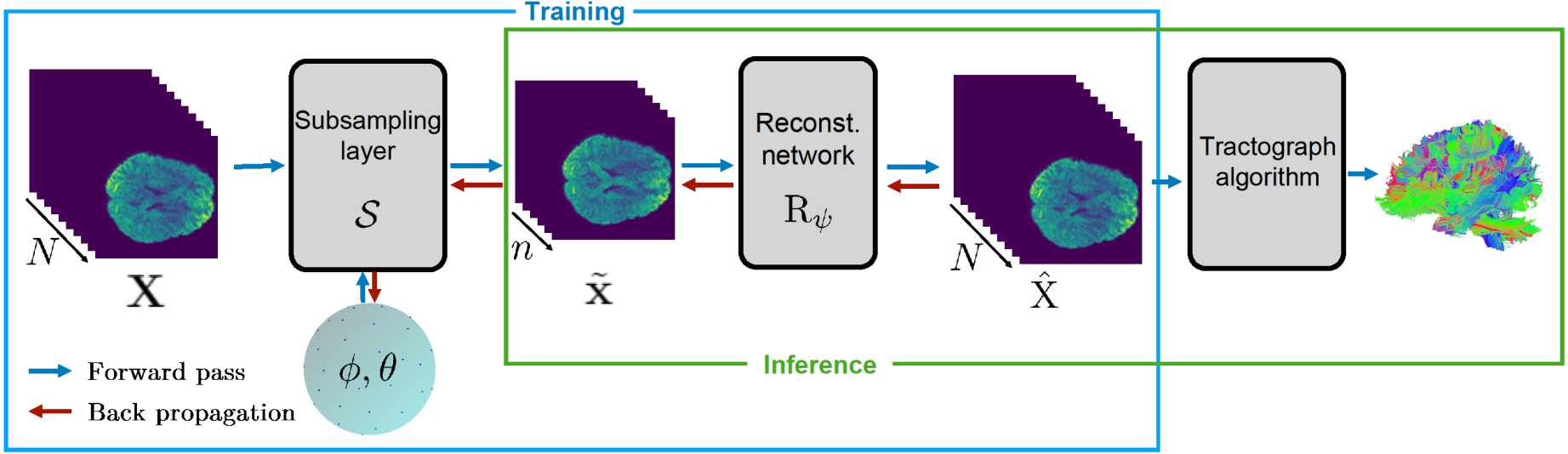
Knee



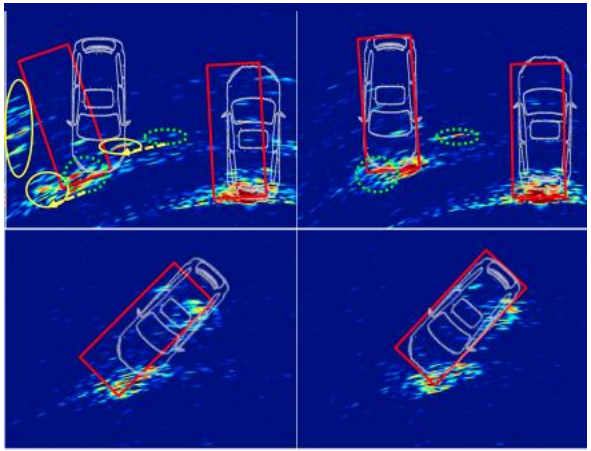
Brain



Diffusion MRI



MIMO radar imaging



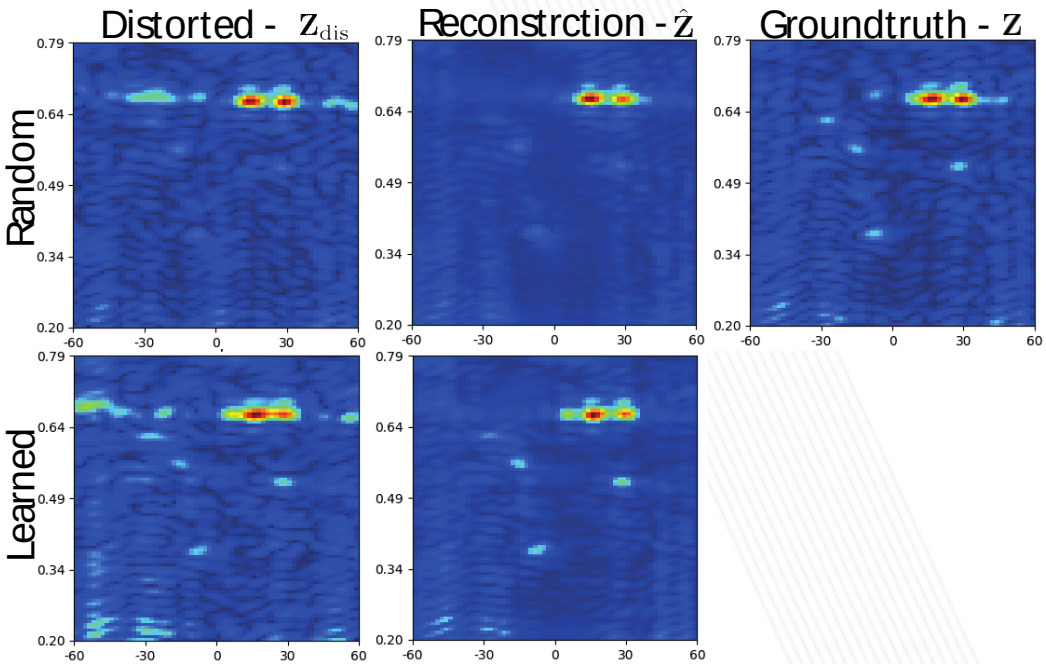
Pros

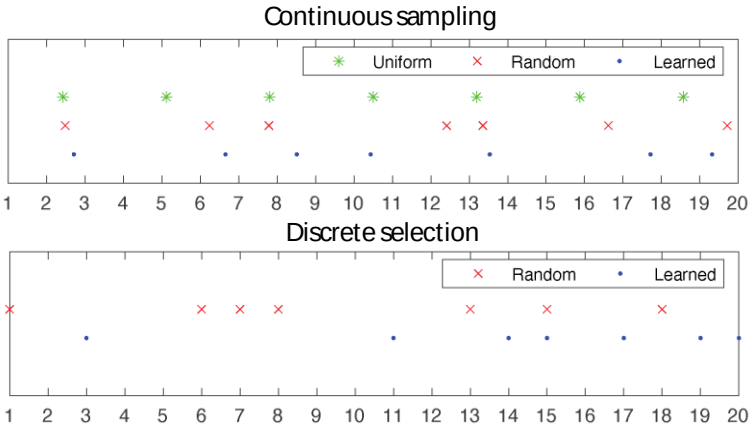
- Accurate range, velocity and direction of arrival (DOA) estimation at relatively long distances
- Automotive - penetrate much denser fog and rain compared to the optical counterparts

Cons

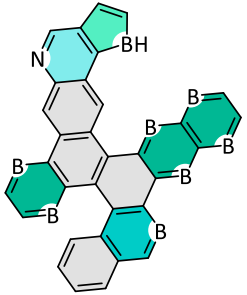
- multiple receive channels -> high cost and power
- Low frame rate

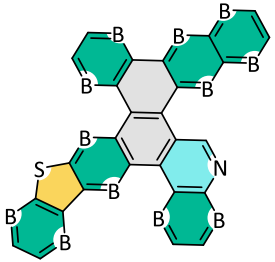
Results - MIMO radar imaging

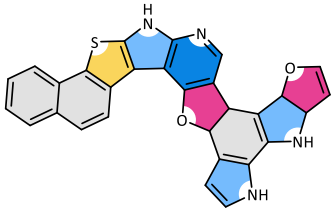




Molecular design

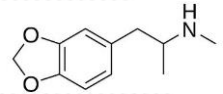




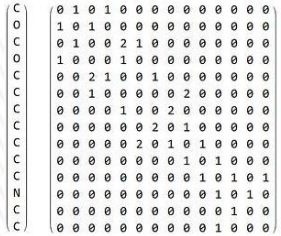


Can we use the gradients of a prediction network?

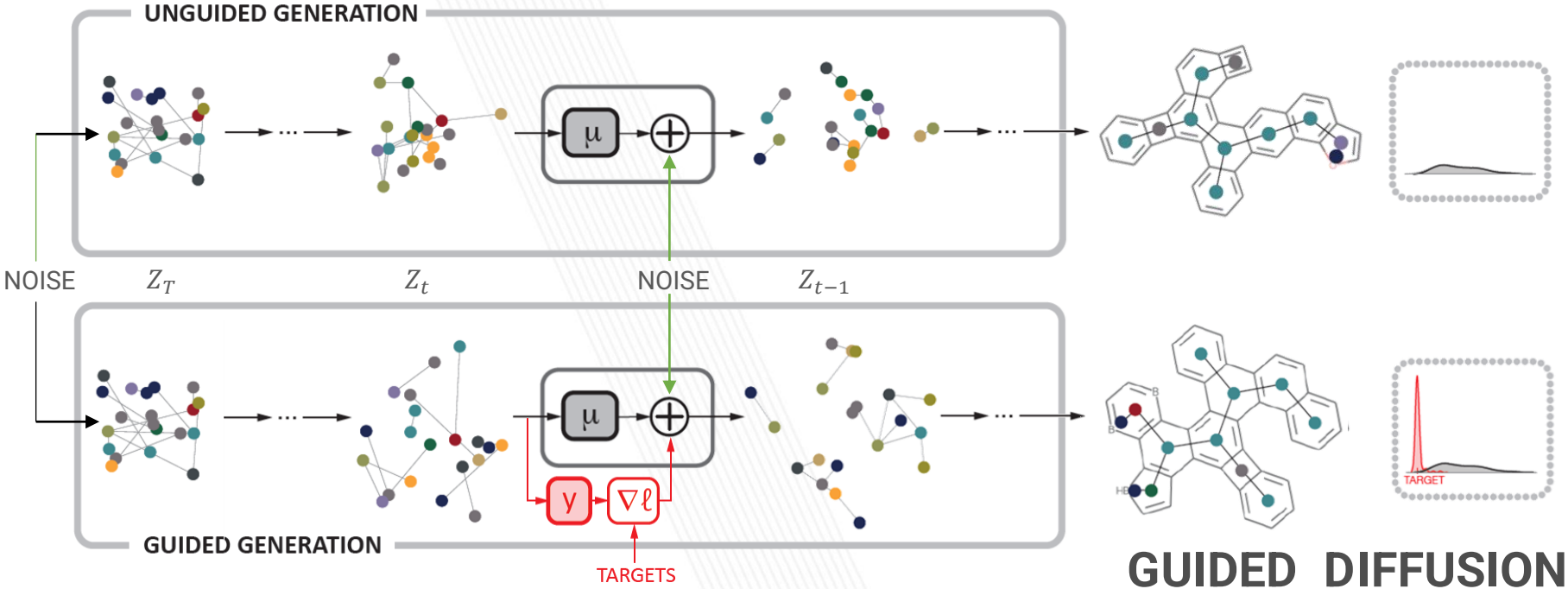
$\epsilon \sim \mathcal{N}(0, I)$ ⇄ Generator ⇄ x ⇄ Properties predictor ⇄ $\hat{y}$ ⇄ $\mathcal{L}(\hat{y})$



CC(CC1=CC2=C(C=C1)OCO2)NC

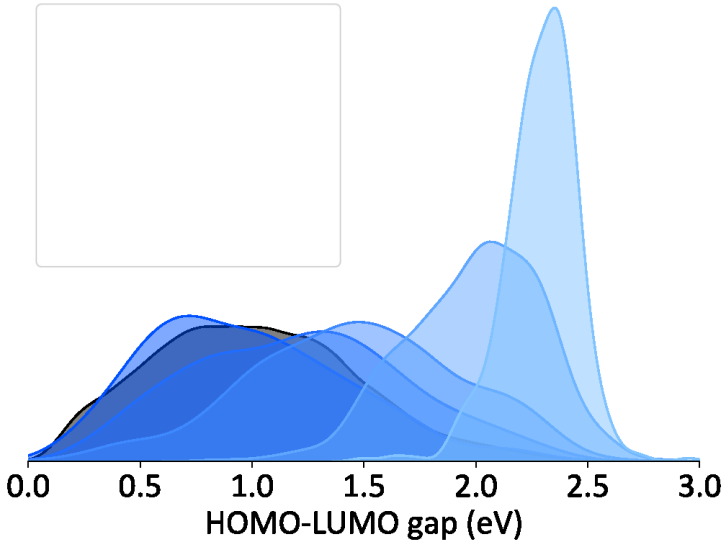


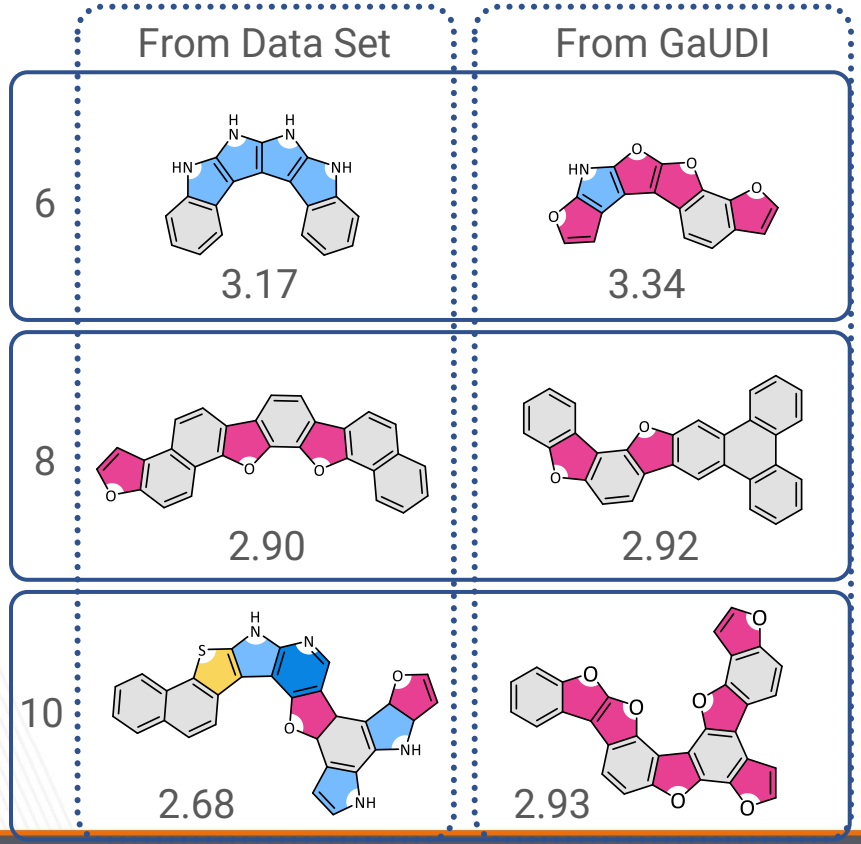
Guided Diffusion Models

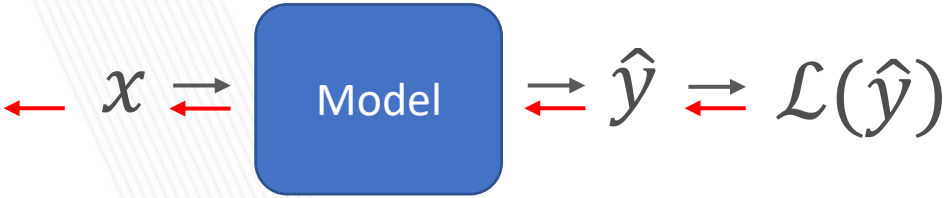


GaUDI – Out of Distribution

Target: Maximize HOMO-LUMO gap







- There are many interesting ways we can use Neural-Networks

Thanks!