

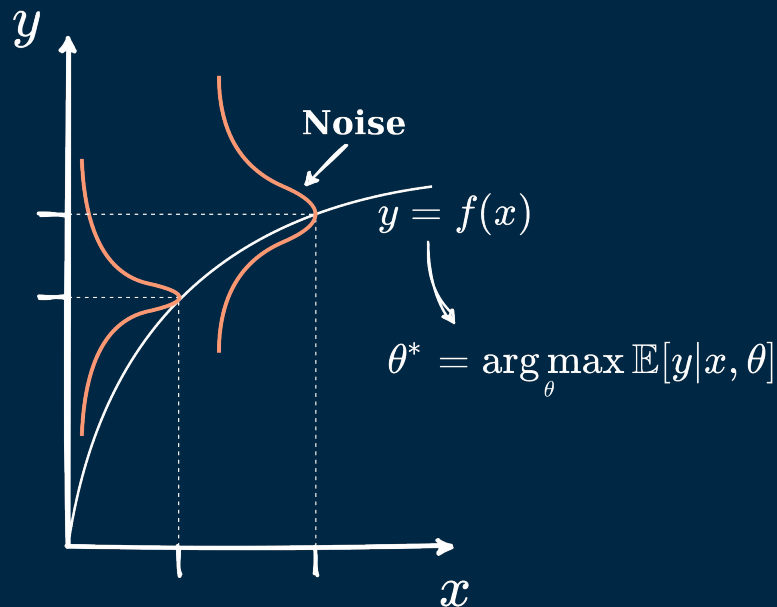
# GRAPH MIXTURE DENSITY NETWORKS

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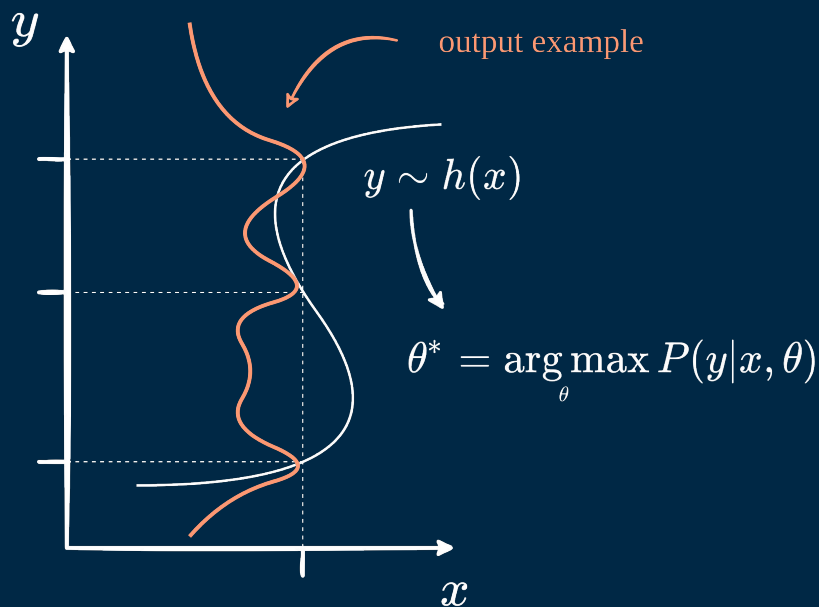


# Regression vs Density Estimation

Regression → **Unimodal** distribution around true target  
 Desired Output → **value**



Density Estimation → **Multimodal** distribution of true target  
 Desired Output → **distribution**

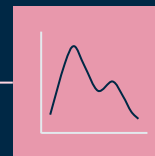


# Why GMDN



## Structure

Like Deep Graph Networks



## Uncertainty

- 1) Data Representation
- 2) Encoder Expressiveness



## Multimodality

Like Mixture Density Networks

## End-to-end

Get the best of **neural** and **probabilistic** worlds

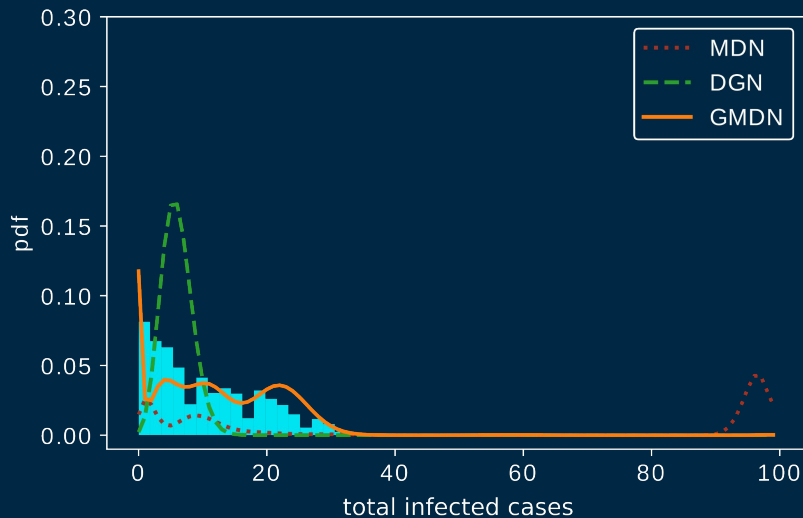




# Results

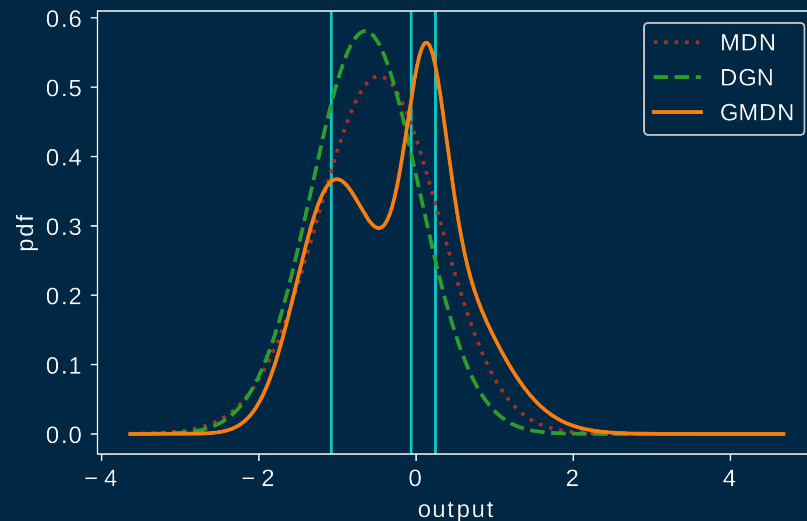
## Synthetic Epidemic Simulations

Model	BA-100	ER-100	Structure	Multimodal
RAND	-4.60	-4.60	✗	✗
HIST	-1.16	-2.32	✗	✓
MDN	-1.17(.05)	-2.54(.07)	✗	✓
DGN	-0.90(.35)	-1.96(.16)	✓	✗
GMDN	<b>-0.67(.02)</b>	<b>-1.56(.04)</b>	✓	✓



## Chemical Tasks

Model	alchemy_full		ZINC_full	
	log $\mathcal{L}$	MAE	log $\mathcal{L}$	MAE
RAND	-27.12	-	-4.20	-
HIST	-21.91	-	-1.28	-
MDN	-1.36(.90)	0.62(.01)	-1.14(.01)	0.67(.00)
DGN	-7.19(1.3)	0.62(.01)	-0.90(.10)	0.49(.03)
GMDN	<b>-0.57(1.4)</b>	<b>0.61(.02)</b>	<b>-0.75(.10)</b>	<b>0.49(.04)</b>



# Questions?



Thanks for listening!

See you at the live Q&A!

You can reach out via:

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The CIML Group  : [ciml.di.unipi.it](http://ciml.di.unipi.it)

Code: [github.com/diningphil/graph-mixture-density-networks](https://github.com/diningphil/graph-mixture-density-networks)

