Comparison metrics

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DSFP Session 16

Adapted from a lesson at the Winter 2020 LSST-DESC collaboration meeting's "DE School"



Overview



The problem set aims to be specific to Bayesian model comparison, but this lecture is to give you some context for what metrics mean in the context of working with probabilities as the end goal. How do we know if/when any estimated probabilities are good enough?





Conditional probability & forward models Clence

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The universe has <u>true</u> physical parameters θ .

Conditional probability & forward models



The universe has true physical parameters θ .

There is a <u>causal</u> relationship $p(x \mid \theta)$ between data and the physical parameters; the parameters θ determine the data x.

Probability distribution function (PDF)

Conditional probability & forward models



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We observe instances of data x generated by that model.

A tangible example of astrophysical parameter estimation under Bayesian statistics

Context: photo-zs



Spectroscopic redshift determination



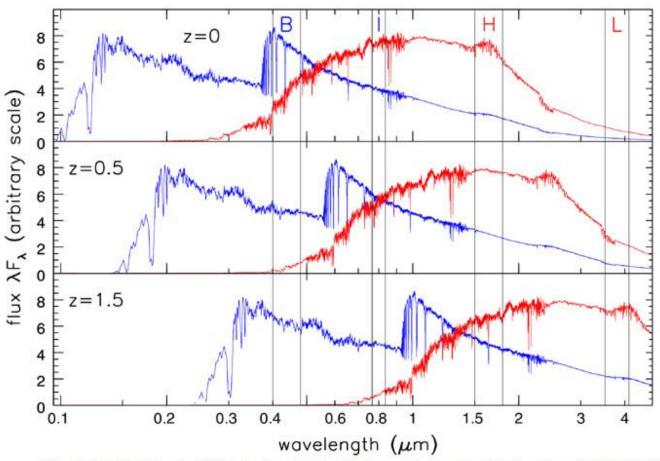
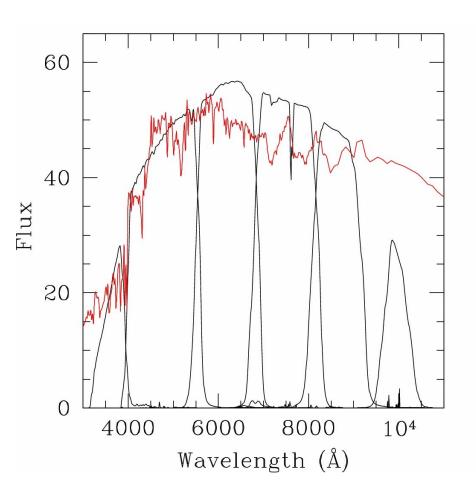
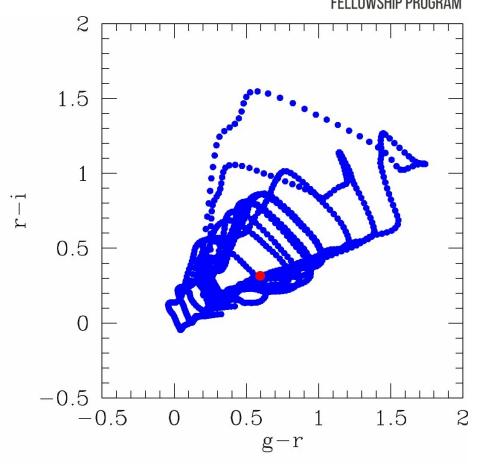
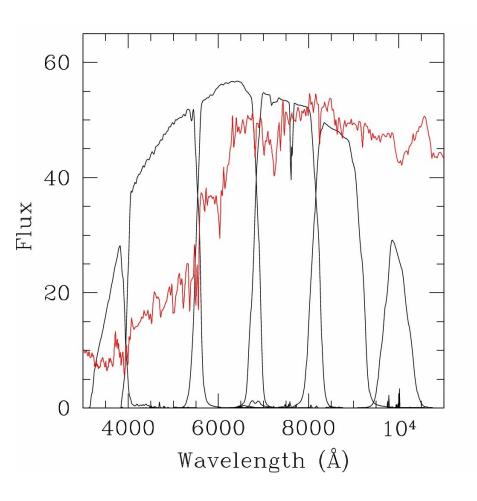
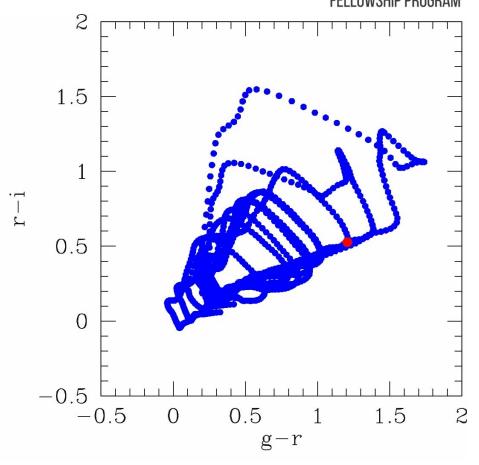


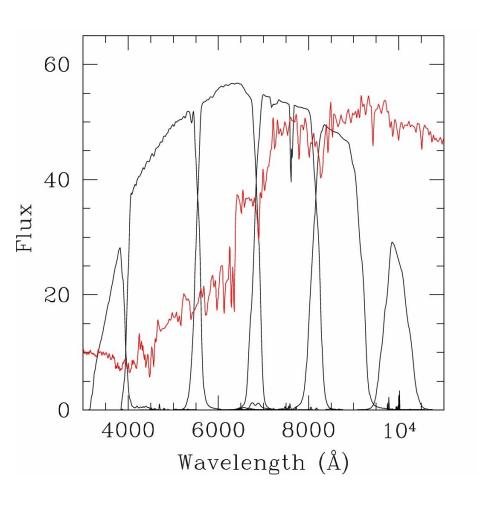
Fig 8.12 (S. Charlot) 'Galaxies in the Universe' Sparke/Gallagher CUP 2007

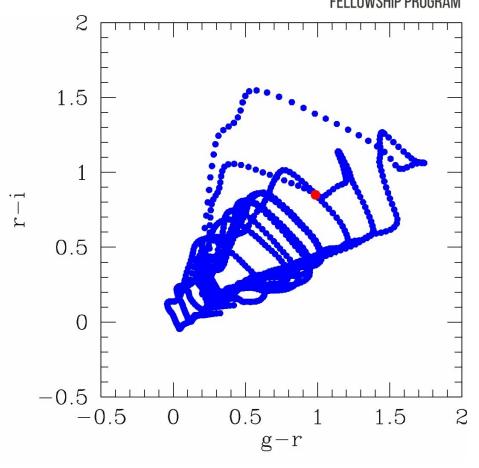


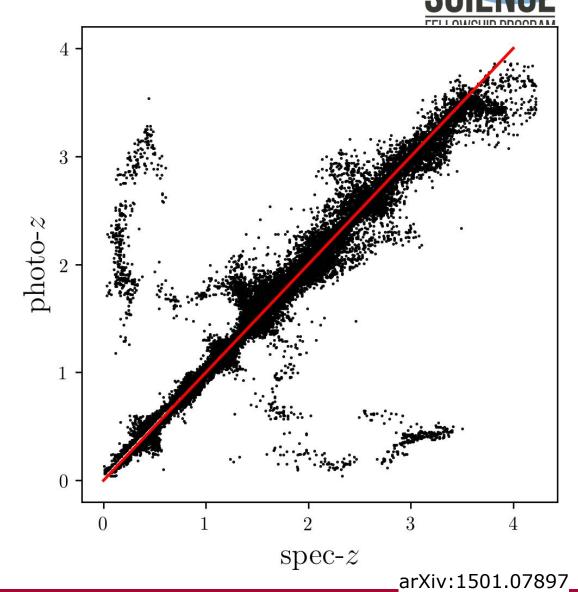
















Intrinsic scatter

$$\sigma_z < 0.02(1+z)$$

Bias

$$\langle |z - \hat{z}| \rangle < 0.003(1+z)$$

Catastrophic outlier rate

$$N_{|z-\hat{z}|>3\sigma_z} < 0.1N_{LSST}$$





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Catastrophic outlier rate

$$N_{|z-\hat{z}|>3\sigma_z} < 0.1N_{LSST}$$

What do these metrics miss?



Intrinsic scatter

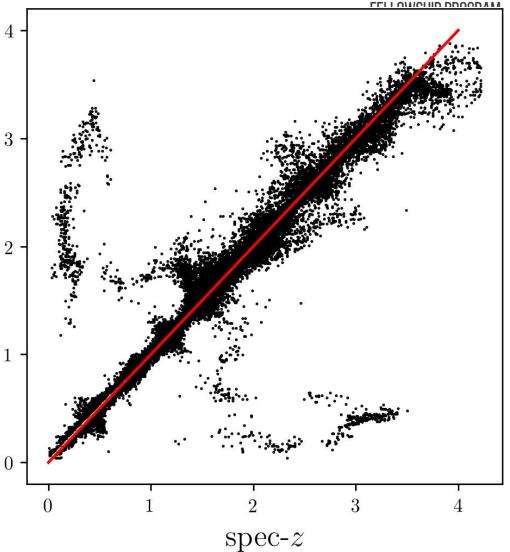
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$$N_{|z-\hat{z}|>3\sigma_z} < 0.1N_{LSST}$$
 of open $\frac{\aleph}{2}$



arXiv:1501.07897_

Conditional probability & forward models



The universe has true physical parameters θ .

There is a causal relationship $p(x \mid \theta)$ between data and the physical parameters; the parameters θ determine the data x.

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Conditional probability & forward models



The universe has true physical parameters θ .

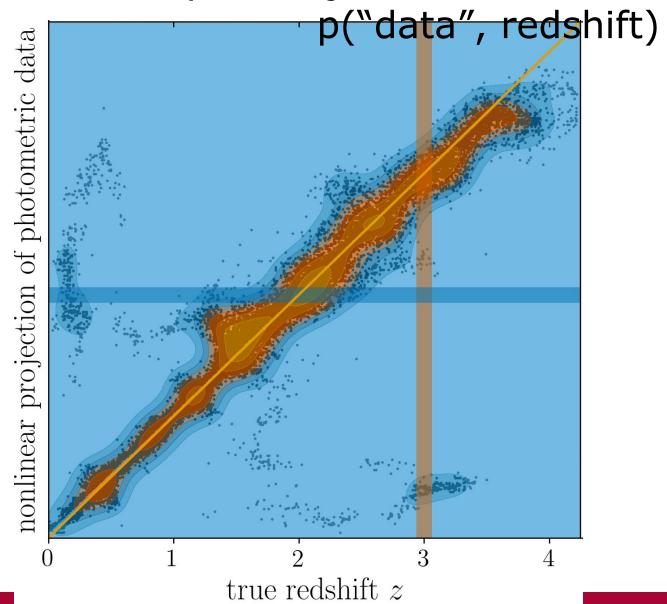
There is a causal relationship $p(x \mid \theta)$ between data and the physical parameters; the parameters θ determine the data x.

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We want to constrain the physical parameters θ that determined the observed data x, i.e. $p(\theta \mid x)$.

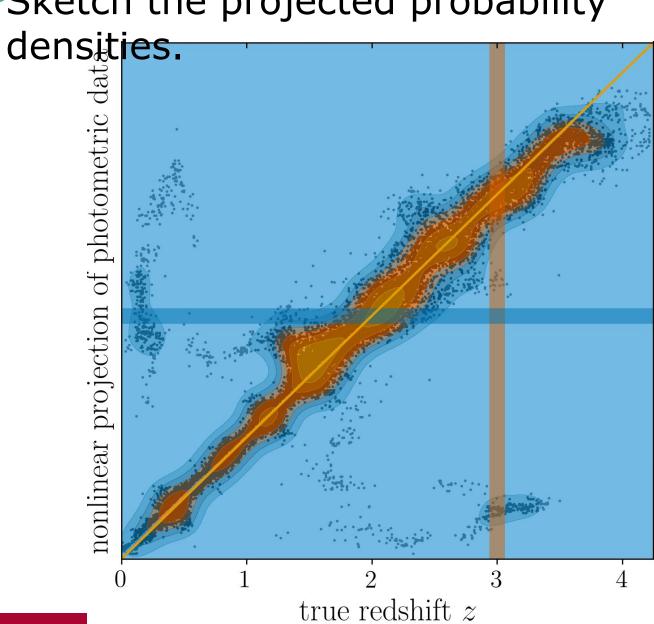
Photo-zs sample the joint PDF



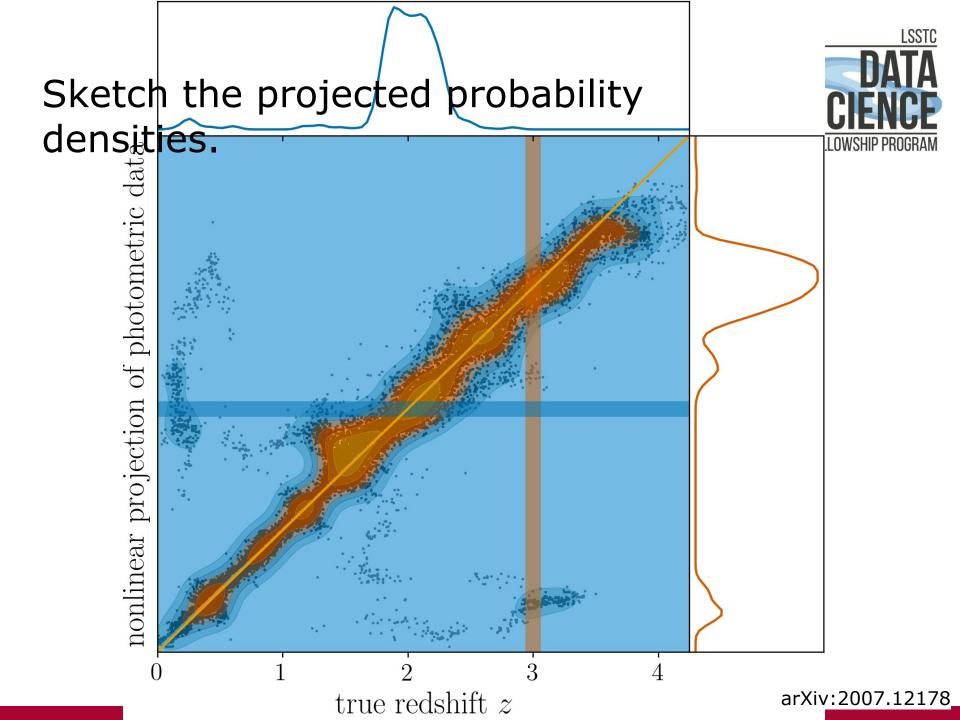


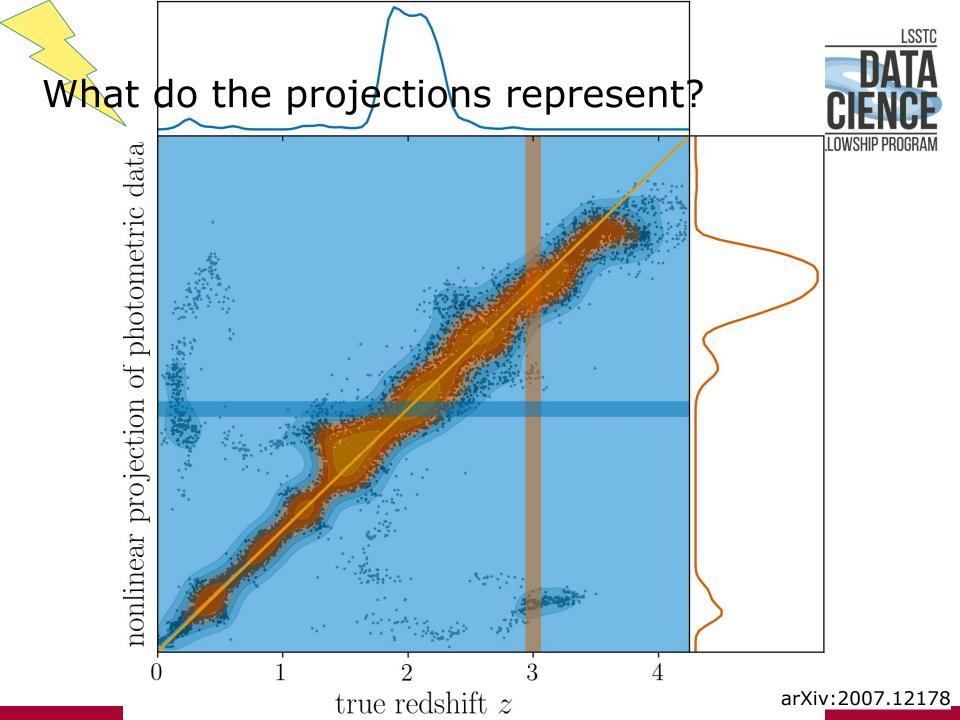
Sketch the projected probability

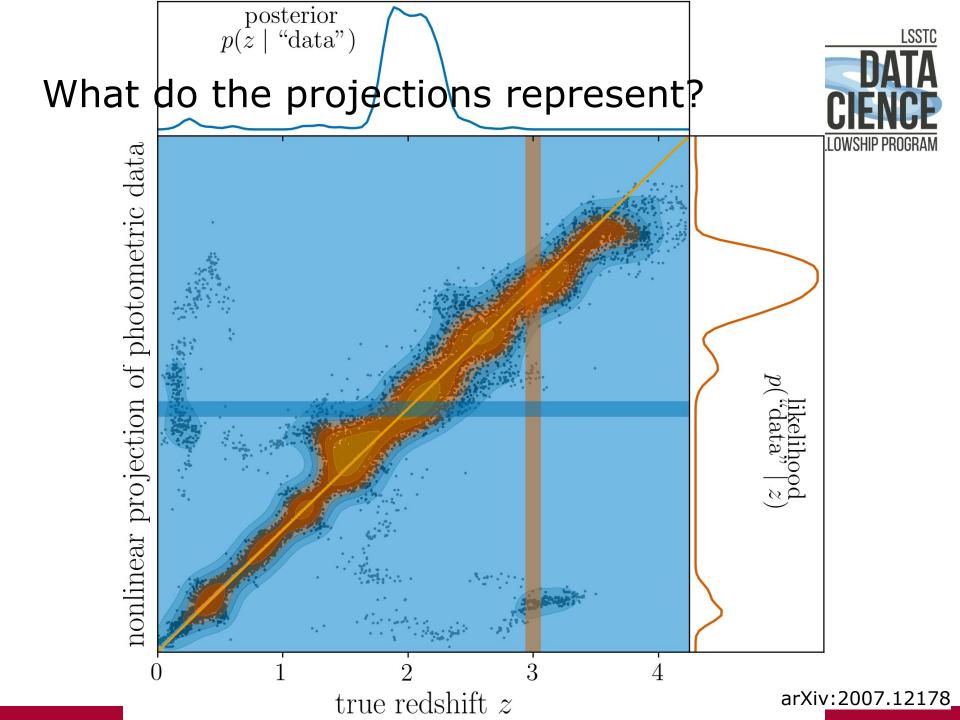


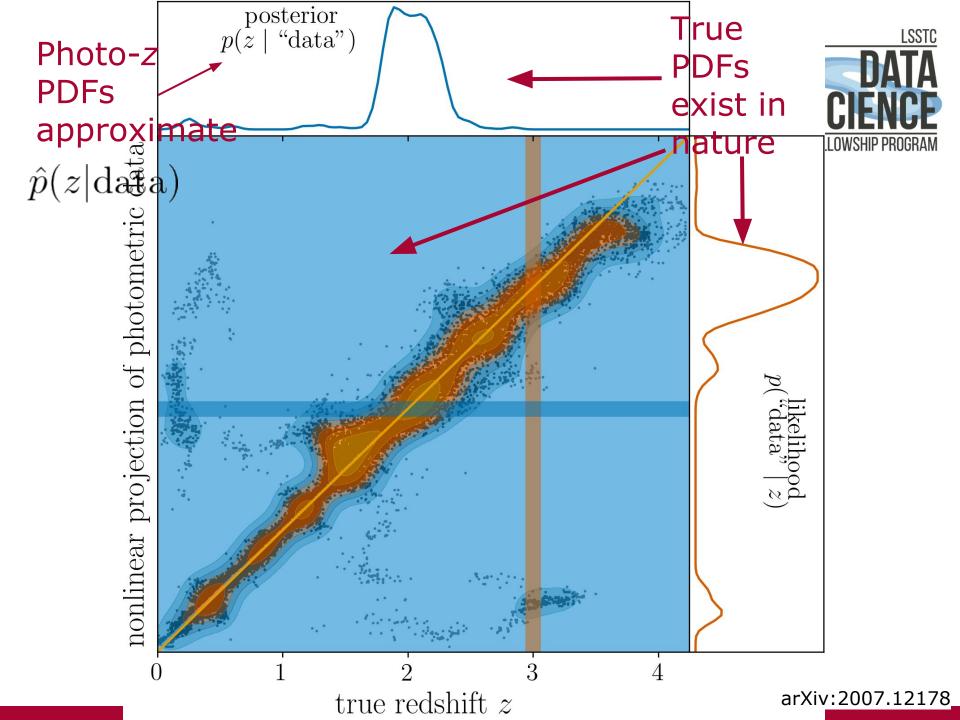


arXiv:2007.12178









How do we compare PDFs?



Quantitative metrics of 1D PDFs



Root-mean-square Error (RMSE)

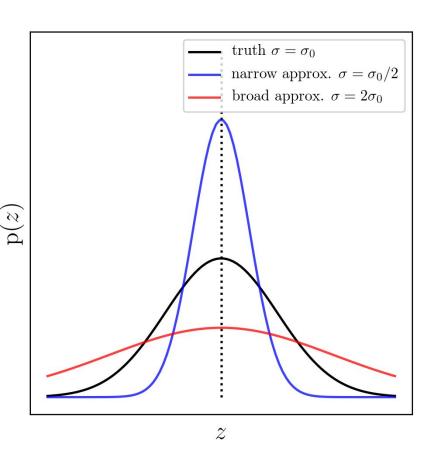
RMSE =
$$\sqrt{\int (p_{\text{true}}(z) - \hat{p}_{\text{est}}(z))^2 dz}$$

Kullback-Leibler Divergence (KLD)

$$\mathrm{KLD}[\hat{p}_{\mathrm{est}}(z); p_{\mathrm{true}}(z)] = \int_{-\infty}^{\infty} p_{\mathrm{true}}(z) \log \left[\frac{p_{\mathrm{true}}(z)}{\hat{p}_{\mathrm{est}}(z)} \right] dz$$

Gaussian example: precision⁻¹ = σ/σ_0

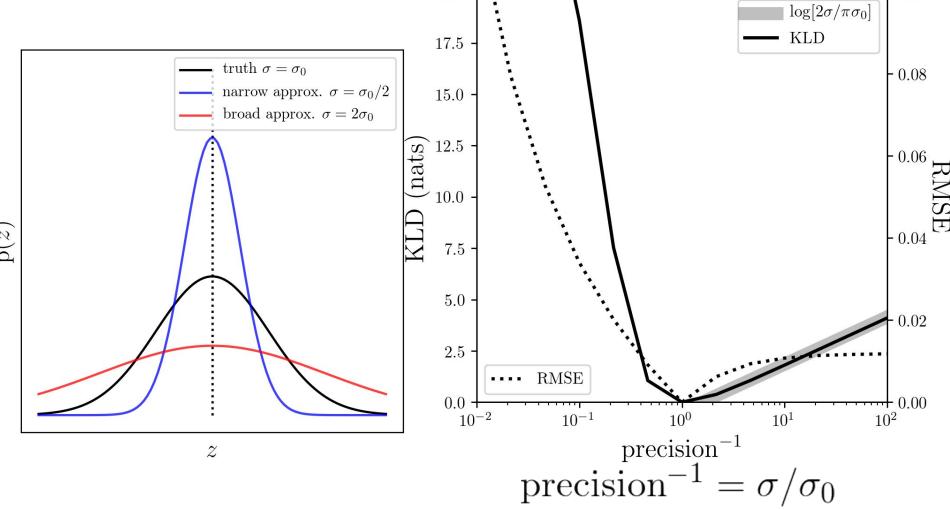




Interpret the asymptotic behavior of the

20.0

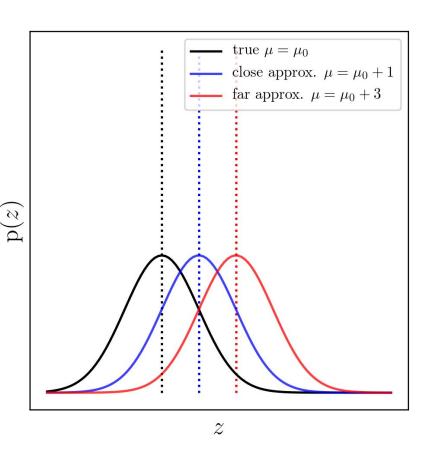




arXiv:1806.00014







Interpret the asymptotic behavior of the

20.0

LSSTC

0.05

- 0.04

- 0.03 ${\Bbb Z}$

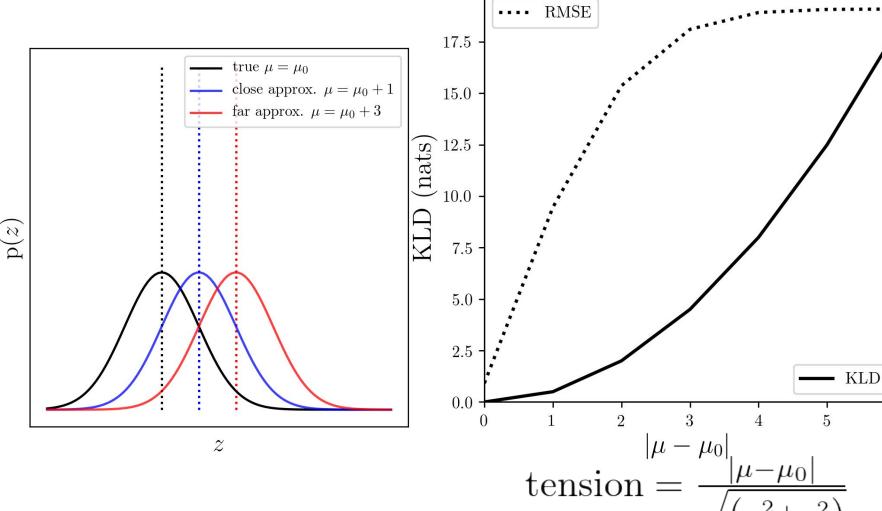
0.02

- 0.01

-0.00

arXiv:1806.00014_

metrics.



What does this have to do with Bayesian model comparison?

Example: PZ DC1



The PZ DC1 experiment



Motivation: identify the best photo-z posterior code for LSST-DESC

<u>Data</u>: cosmological redshifts & photometry catalog painted on N-body simulation

Control: idealized, shared

prior information

The PZ DC1 experiment



Motivation: identify the best photo-z posterior code for LSST-DESC

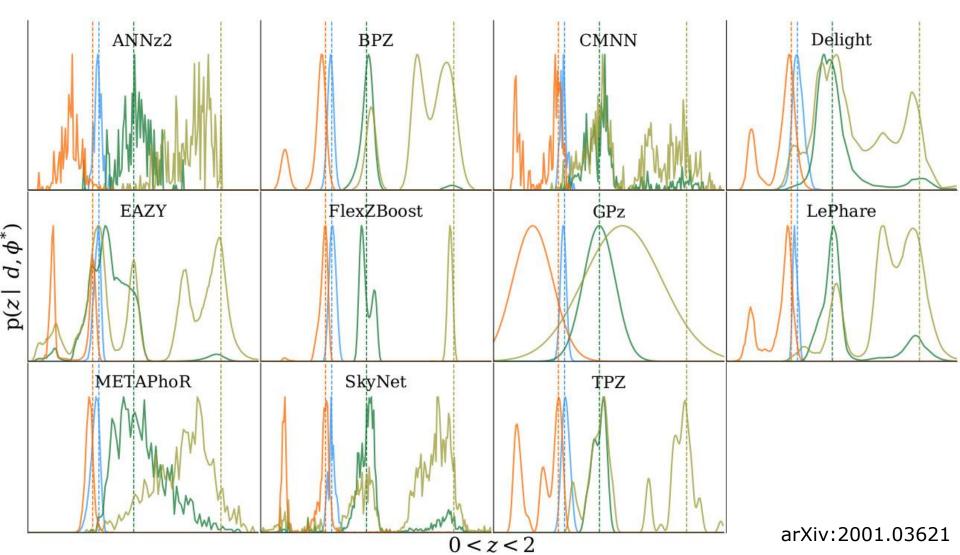
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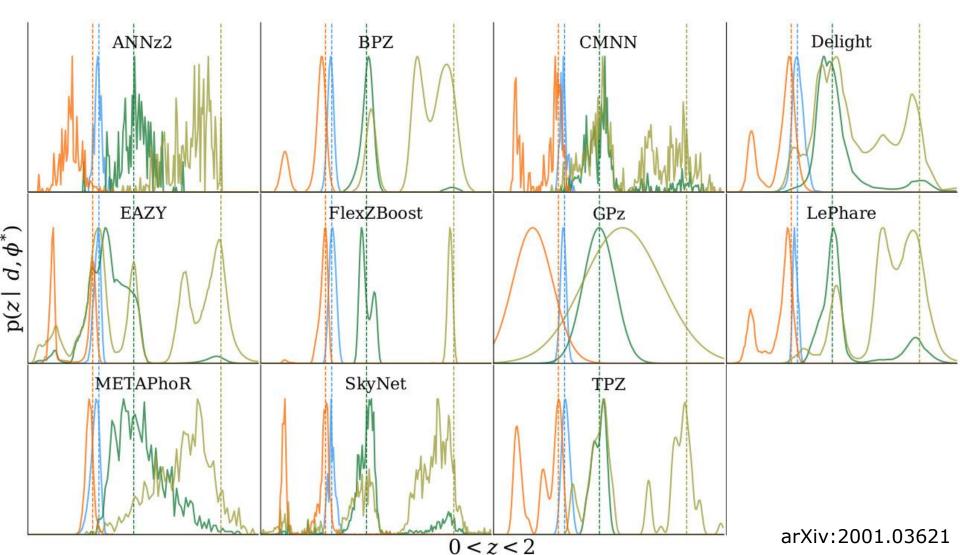
Suggest possible causes for differences between photo-z posterior estimates.

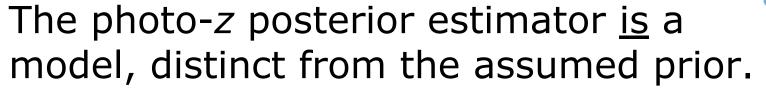




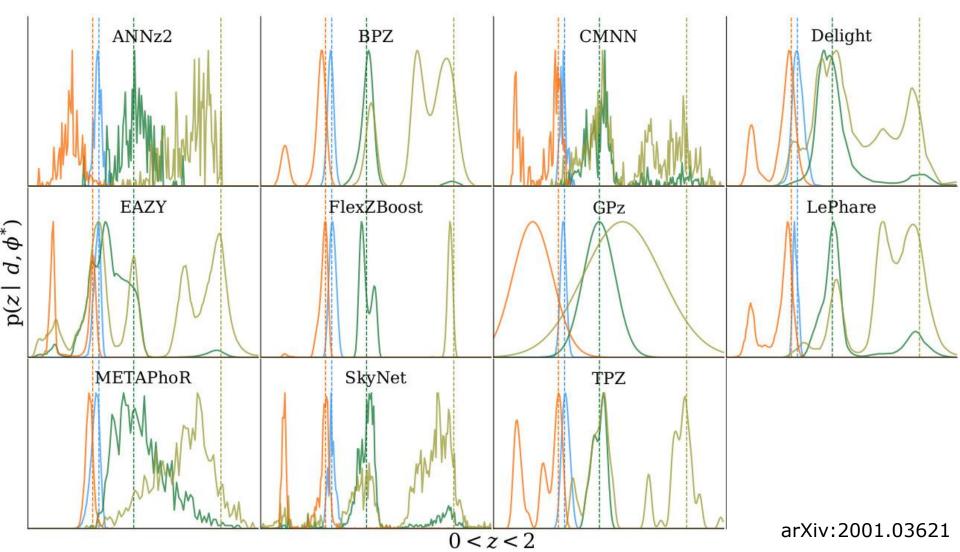
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There is a causal relationship $p(x \mid \theta)$ Data: cosmological redshifts & between data and the physical parameters; photometry catalog painted the parameters θ determine the data x.

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We observe instances of data *x* generated by that model.

<u>Control</u>: idealized, shared prior information

Quantitative metrics of 1D PDFs



Root-mean-square Error (RMSE)

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$$\sqrt{\int (p_{\text{true}}(\mathbf{p}_{0})^{2}dz}$$

Kullback-Leibler Divergence Resteriors

$$\text{KLD}[\hat{p}_{\text{est}}(z); p_{\text{true}}(z)] = \int_{-\infty}^{\infty} p_{\text{true}}(z) \log \left[\frac{p_{\text{true}}(z)}{\hat{p}_{\text{est}}(z)} \right] dz$$

Quantitative metrics of 1D PDF ensembles



Root-mean-square Error (RMSE)

RMSE =
$$\sqrt{\int (p_{\text{true}}(\mathbf{p}_0 \cdot \hat{\mathbf{p}}_{\text{rest}}(\mathbf{z}))^2 dz}$$

Kullback-Leibler Divergence (KDS) teriors

$$ext{KLD}[\hat{p}_{ ext{est}}(z); p_{ ext{true}}(z)] = \int_{-\infty}^{\infty} p_{ ext{true}}(z) \log \left[rac{p_{ ext{true}}(z)}{\hat{p}_{ ext{est}}(z)}
ight] dz$$

Cumulative Distribution Function (CDF)

$$CDF[\hat{p}, z'] \equiv \int_{-\infty}^{z'} \hat{p}(z) dz$$

Quantitative metrics of 1D PDF ensemble



Root-mean-square Error (RMSE)

RMSE =
$$\sqrt{\int (p_{\text{true}}(\mathbf{p_{o}})^2 dz}$$

Kullback-Leibler Divergence Resteriors

$$\mathrm{KLD}[\hat{p}_{\mathrm{est}}(z); p_{\mathrm{true}}(z)] = 0$$

$$\mathrm{KLD}[\hat{p}_{\mathrm{est}}(z); p_{\mathrm{true}}(z)] = \int_{-\infty}^{\mathbf{a}} p_{\mathrm{true}}(z) \, \log \left[\frac{p_{\mathrm{true}}(z)}{\hat{p}_{\mathrm{est}}(z)} \right] \, dz$$

Cumulative Distribution Function (CDF)

$$CDF[\hat{p}, z'] \equiv \int_{-\infty}^{z'} \hat{p}(z) dz$$

Probability Integral Transform (PIT)

$$P(PIT \equiv CDF[\hat{p}, z_{true}])$$

Sketch the PIT histogram of an ideal photo-z posterior estimator.



$$CDF[\hat{p}, z'] \equiv \int_{-\infty}^{z'} \hat{p}(z)dz$$

$$P(PIT \equiv CDF[\hat{p}, z_{true}])$$

Sketch the PIT histogram of an ideal photo-z posterior estimator.



ideal PIT

count

$$CDF[\hat{p}, z'] \equiv \int_{-\infty}^{z'} \hat{p}(z) dz$$

$$P(PIT \equiv CDF[\hat{p}, z_{true}])$$

$$PIT = 0 < \int_0^{z_{\text{true}}} \hat{p}(z) dz < 1$$

What might the PIT look like for these photo-z posterior estimators?



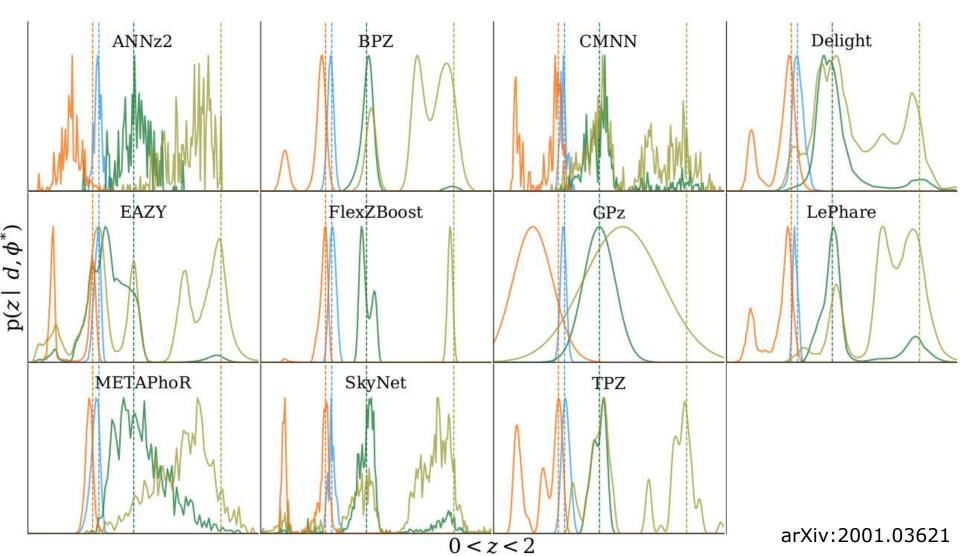
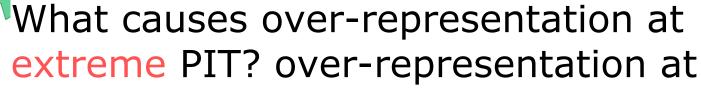


Photo-z posterior ensemble metrics

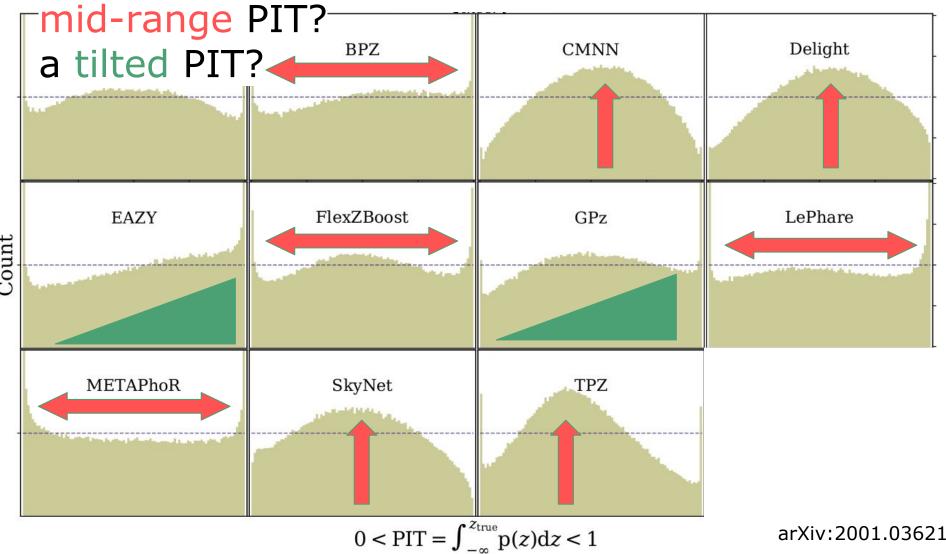


-	ANNz2	BPZ	CMNN	Delight
Count	EAZY	FlexZBoost	GPz	LePhare
-	METAPhoR	SkyNet	TPZ	

 $0 < PIT = \int_{-\infty}^{z_{true}} p(z) dz < 1$ arXiv:2001.03621

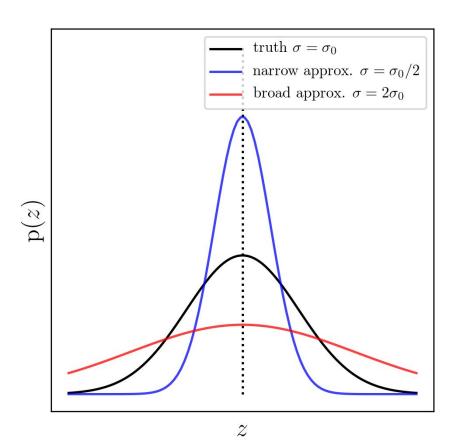






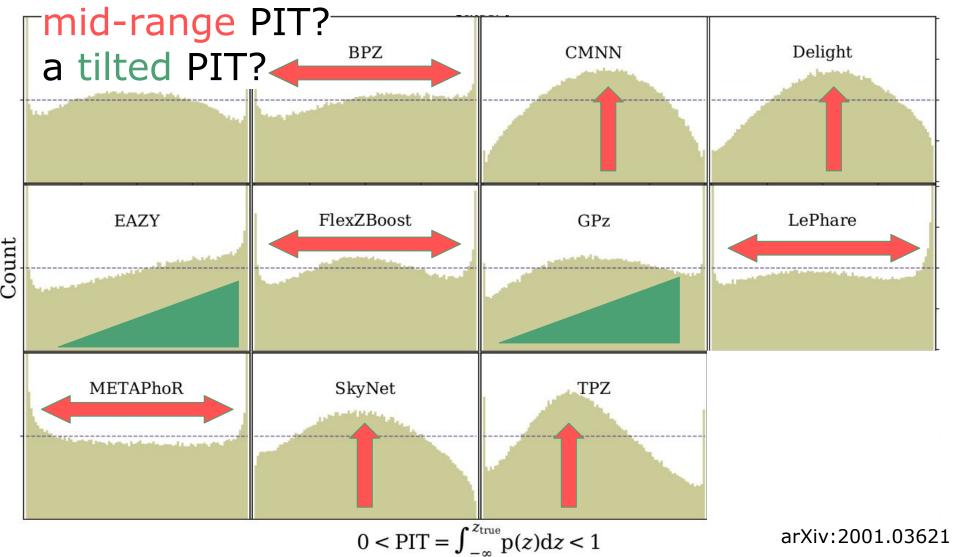
(Hint: Imagine the PIT histograms in the Gaussian example.)

LSSTC



DATA SCIENCE FELLOWSHIP PROGRAM

What causes over-representation at extreme PIT? over-representation at



Quantitative metrics of 1D PDF ensemble



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$$\mathrm{KLD}[\hat{p}_{\mathrm{est}}(z); p_{\mathrm{true}}(z)] = \int_{-\infty}^{\infty} p_{\mathrm{true}}(z) \, \log \left[\frac{p_{\mathrm{true}}(z)}{\hat{p}_{\mathrm{est}}(z)} \right] \, dz$$

Cumulative Distribution Function (CDF)

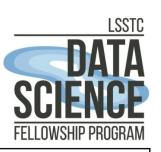
$$CDF[\hat{p}, z'] \equiv \int_{-\infty}^{z'} \hat{p}(z) dz$$

Probability Integral Transform (PIT)

$$P(PIT \equiv CDF[\hat{p}, z_{true}])$$

Quantile-quantile (QQ) Plot $\sim \int p(PIT)dPIT$

Sketch the Q-Q Plot of a hypothetical perfect photo-z estimator.



ideal PIT

count

$$CDF[\hat{p}, z'] \equiv \int_{-\infty}^{z'} \hat{p}(z) dz$$

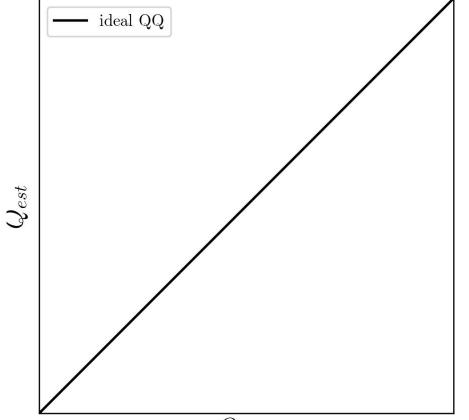
$$P(PIT \equiv CDF[\hat{p}, z_{true}])$$

$$PIT = 0 < \int_0^{z_{\text{true}}} \hat{p}(z)dz < 1$$

 $\sim \iint p(PIT)dPIT$

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$$CDF[\hat{p}, z'] \equiv \int_{-\infty}^{z'} \hat{p}(z) dz$$

$$P(PIT \equiv CDF[\hat{p}, z_{true}])$$

$$\sim \int p(PIT)dPIT$$

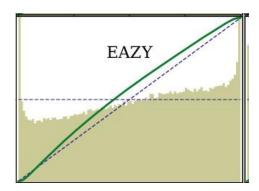


r		$0 < Q_{th}$	eorv < 1	
_	ANNz2	BPZ	CMNN	Delight
ınt	EAZY	FlexZBoost	GPz	LePhare A
Count				Q _{data} < 1
	METAPhoR	SkyNet	TPZ	

0 < 0

 $0 < PIT = \int_{-\infty}^{z_{\text{true}}} p(z) dz < 1$



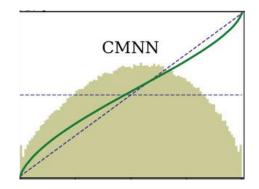




	$0 < Q_{theorv} < 1$			
	ANNz2	BPZ	CMNN	Delight
Count	EAZY	FlexZBoost	GPz	LePhare
Col				
	METAPhoR	SkyNet	TPZ	

 $0 < PIT = \int_{-\infty}^{z_{\text{true}}} p(z) dz < 1$





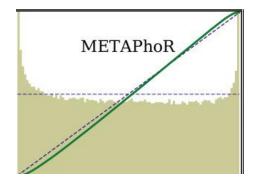
Sketch the QQ plot. p(PIT)dPIT



		$0 < Q_{th}$	eorv < 1	-	
	ANNz2	BPZ	CMNN	Delight	
Count	EAZY	FlexZBoost	GPz	LePhare	$0 < Q_d$
Co					$Q_{data} < 1$
	METAPhoR	SkyNet	TPZ		

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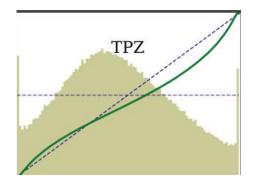
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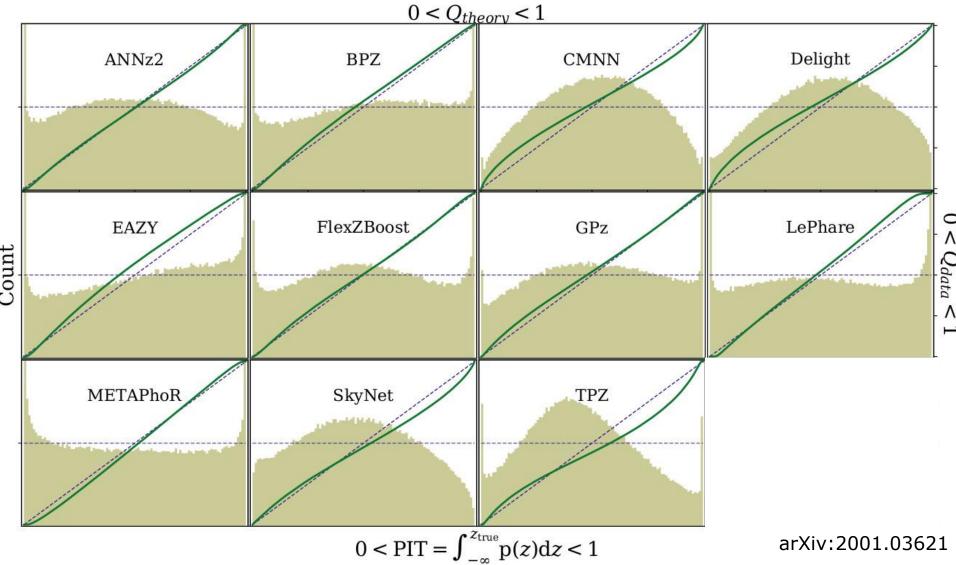
	$0 < Q_{theory} < 1$				
	ANNz2	BPZ	CMNN	Delight	
Count	EAZY	FlexZBoost	GPz	LePhare C & Qdata & L	
-	METAPhoR	SkyNet	TPZ		

 $0 < PIT = \int_{-\infty}^{z_{\text{true}}} p(z) dz < 1$









Where is this going?



These metrics tell us about ensembles of 1D PDFs that correspond to different models.

In the problem session, we'll go over samples from 2D PDFs that correspond to different models (and data).