

# BRUNO: A Deep Recurrent Model for Exchangeable Data

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# EXCHANGEABILITY

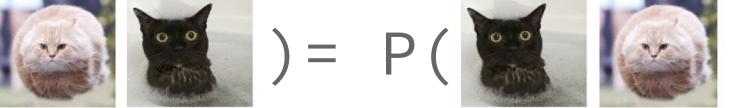
A stochastic process  $x_1, x_2, x_3 \dots$  is **exchangeable** if for all  $n$  and all permutations  $\pi$ :

$$p(x_1, \dots, x_n) = p(x_{\pi(1)}, \dots, x_{\pi(n)})$$

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...

# EXCHANGEABILITY. IID EXAMPLE

A stochastic process  $x_1, x_2, x_3 \dots$  is **exchangeable** if for all  $n$  and all permutations  $\pi$ :

$$p(x_1, \dots, x_n) = p(x_{\pi(1)}, \dots, x_{\pi(n)})$$

**IID random variables  
are exchangeable:**

$$p(x_1, \dots, x_n) = \prod_{i=1}^n p(x_i)$$

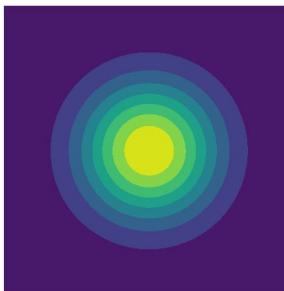
# EXCHANGEABILITY. NON-IID EXAMPLE

$$p(x_1, \dots, x_n) = \mathcal{N}_n(\mu, \Sigma)$$

$$\mu = \begin{bmatrix} \mu \\ \mu \\ \vdots \\ \mu \end{bmatrix} \quad \Sigma = \begin{bmatrix} v & \rho & \rho & \dots & \rho \\ \rho & v & \rho & \dots & \rho \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \rho & \dots & v \end{bmatrix} \quad 0 \leq \rho < v$$

compound symmetry  
covariance structure

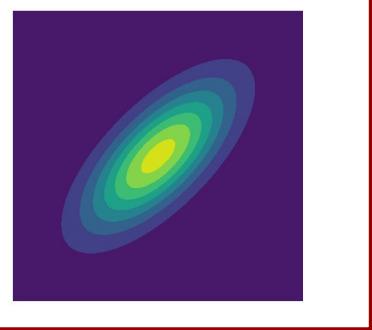
i.i.d



$$v = 1 \quad \rho = 0$$

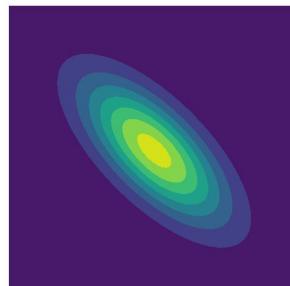
exchangeable

$$v = 1 \quad \rho = 0.7$$



not  
exchangeable

$$v = 1 \quad \rho = -0.7$$



# EXCHANGEABILITY AND BAYESIAN COMPUTATIONS

De Finetti's theorem says that every exchangeable process is a mixture of i.i.d. processes:

$$p(x_1, \dots, x_n) = \int p(\theta) \prod_{i=1}^n p(x_i | \theta) d\theta$$

where  $\theta$  is some parameter conditioned on which the data is i.i.d.

# DEFINETTI'S THEOREM. EXAMPLE

Assume we have a process, where  $x_1, \dots, x_n \sim \mathcal{N}_n(0, \Sigma)$

with an exchangeable covariance structure:

$$\Sigma = \begin{bmatrix} v & \rho & \rho & \dots & \rho \\ \rho & v & \rho & \dots & \rho \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \rho & \dots & v \end{bmatrix} \quad 0 \leq \rho < v$$

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Then  $x_1, \dots, x_n$  are i.i.d

with  $x_i \sim \mathcal{N}(\theta, v - \rho)$  conditionally on  $\theta \sim \mathcal{N}(0, \rho)$

# DE FINETTI'S THEOREM. WHY?



Bayesian

$x_1, x_2, x_3, \dots$   
successive coin tosses

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# DE FINETTI'S THEOREM. WHY?



Bayesian

$x_1, x_2, x_3, \dots$   
successive coin tosses

If we assume  $x_1, x_2, x_3, \dots$  are iid:

$$p(x_n | x_{1:n-1}) = p(x_n)$$

=> results of the first  $n-1$  tosses do not change the uncertainty about the result of  $n$ -th tosses

# EXCHANGEABILITY AND BAYESIAN COMPUTATIONS #2

$$p(x_1, \dots, x_n) = \int p(\theta) \prod_{i=1}^n p(x_i|\theta) d\theta$$

rewrite in terms of predictive distributions


$$p(x_n|x_{1:n-1}) = \int \underbrace{p(x_n|\theta)}_{\text{likelihood}} \underbrace{p(\theta|x_{1:n})}_{\text{posterior}} d\theta$$

# EXCHANGEABILITY AND BAYESIAN COMPUTATIONS #3

$$p(x_n|x_{1:n-1}) = \int \underbrace{p(x_n|\theta)}_{\text{likelihood}} \underbrace{p(\theta|x_{1:n})}_{\text{posterior}} d\theta$$

Gives 2 ways for defining models of exchangeable sequences

# EXCHANGEABILITY AND BAYESIAN COMPUTATIONS #3

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Gives 2 ways for defining models of exchangeable sequences:

1. via explicit Bayesian modelling => **VAE-based models**

# EXCHANGEABILITY AND BAYESIAN COMPUTATIONS #3

$$p(x_n|x_{1:n-1}) = \int \underbrace{p(x_n|\theta)}_{\text{likelihood}} \underbrace{p(\theta|x_{1:n})}_{\text{posterior}} d\theta$$

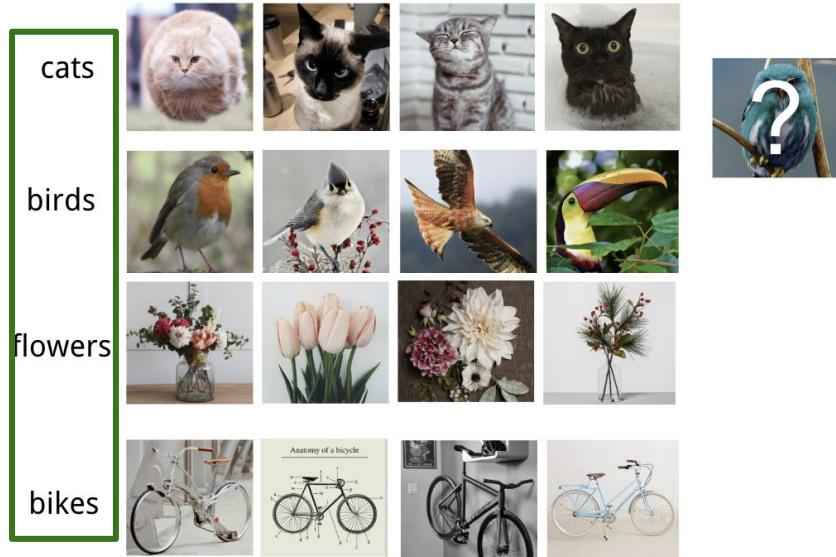
Gives 2 ways for defining models of exchangeable sequences:

1. via explicit Bayesian modelling => **VAE-based models**
2. via exchangeable processes => **BRUNO**



# META-LEARNING. EPISODE

**L~T**



# META-LEARNING. EPISODE

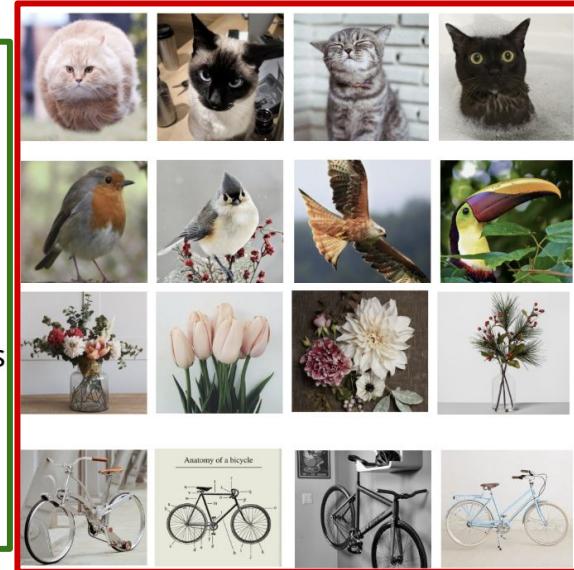
**L~T**

cats

birds

flowers

bikes



**S~L**

# META-LEARNING. EPISODE

$L \sim T$

cats



birds



flowers



bikes

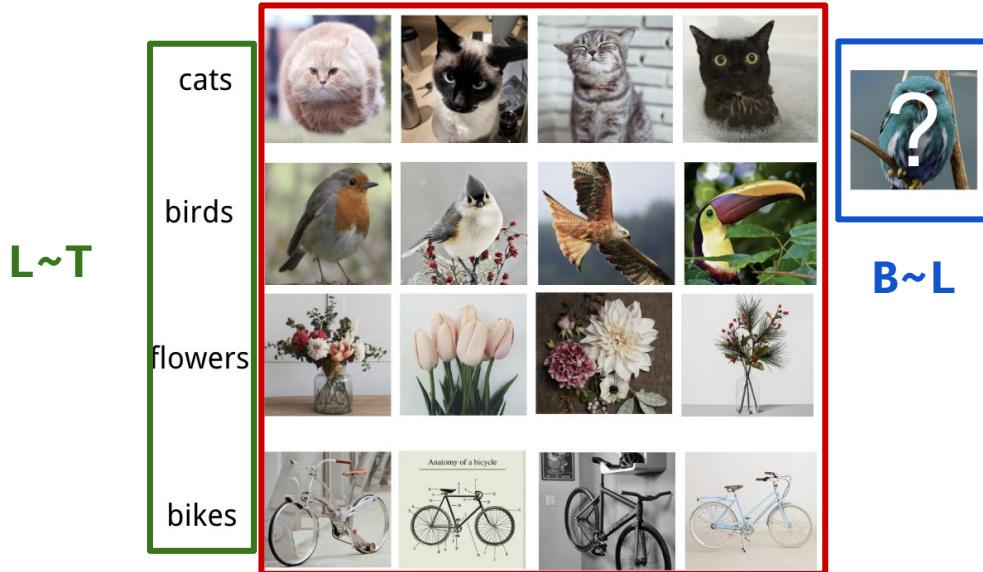


$B \sim L$



$S \sim L$

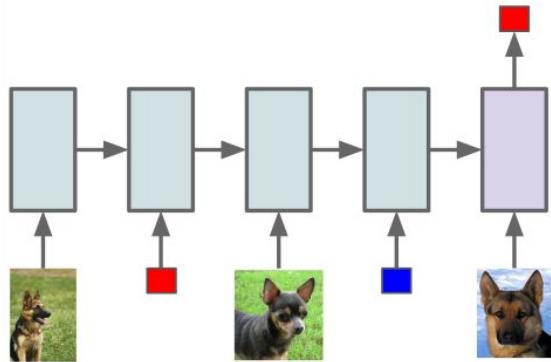
# META-LEARNING. EPISODE



$$\theta^* = \arg \max_{\theta} \mathbb{E}_{L \sim T} \left[ \mathbb{E}_{S \sim L, B \sim L} \left[ \sum_{(x,y) \in B} \log p_{\theta}(y|x, S) \right] \right]$$

# META-LEARNING MODELS. TAXONOMY

## Model Based

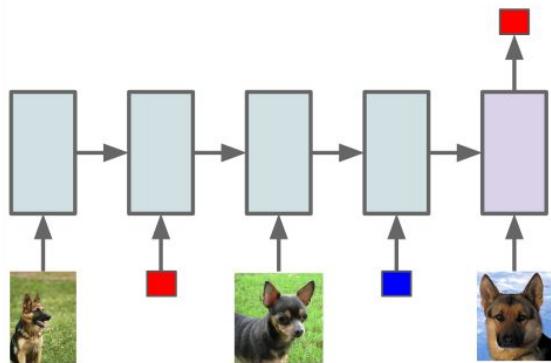


$$p_{\theta}(y|x, S) = f_{\theta}(x, S)$$

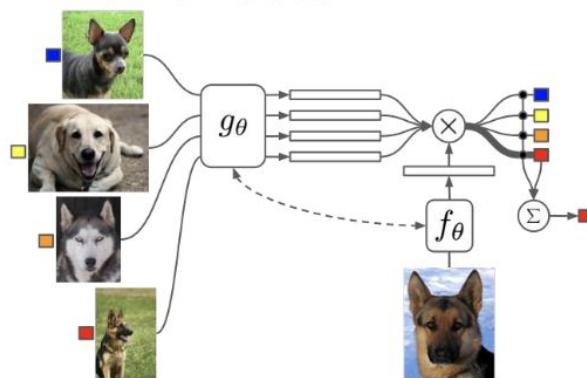
Memory-Augmented Neural Network  
Neural Processes  
BRUNO

# META-LEARNING MODELS. TAXONOMY

## Model Based



## Metric Based



$$p_{\theta}(y|x, S) = f_{\theta}(x, S)$$

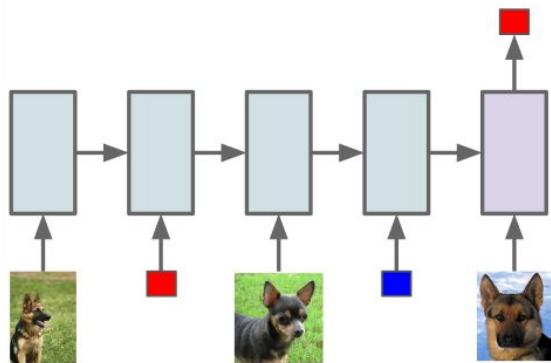
$$p_{\theta}(y|x, S) = \sum_{(x_i, y_i) \in S} k(x_i, x) y_i$$

Memory-Augmented Neural Network  
Neural Processes  
BRUNO

Siamese Neural Networks  
Matching Networks  
Relation Network  
Prototypical Networks

# META-LEARNING MODELS. TAXONOMY

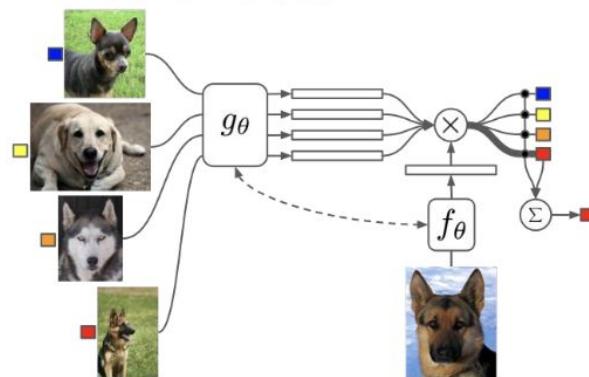
## Model Based



$$p_{\theta}(y|x, S) = f_{\theta}(x, S)$$

Memory-Augmented Neural Network  
 Neural Processes  
 BRUNO

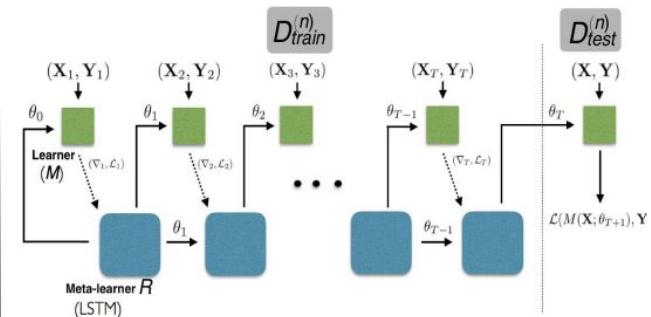
## Metric Based



$$p_{\theta}(y|x, S) = \sum_{(x_i, y_i) \in S} k(x_i, x) y_i$$

Siamese Neural Networks  
 Matching Networks  
 Relation Network  
 Prototypical Networks

## Optimization Based



$$\begin{aligned} p_{\theta}(y|x, S) &= f_{\theta(S)}(x, S) \\ \theta(S) &= g_{\phi}(\theta_0, \{\nabla_{\theta_0} L(x_i, y_i)\}_{(x_i, y_i) \in S}) \end{aligned}$$

LSTM meta-learner  
 Model-agnostic meta-learning (MAML)

# EXCHANGEABILITY AND META-LEARNING

## 1. Order-invariance

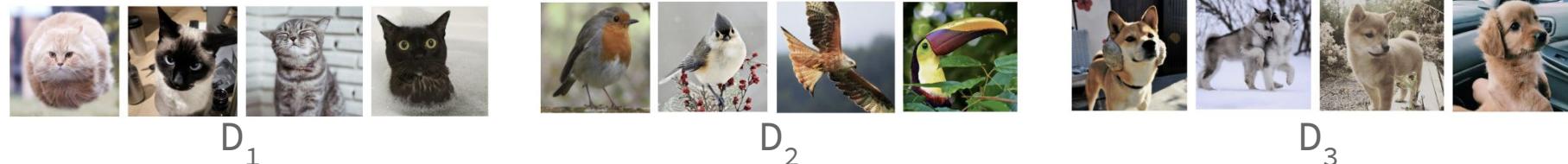


# EXCHANGEABILITY AND META-LEARNING

## 1. Order-invariance



## 2. Correlation



$\{D_1, D_2, \dots, D_k\}$  are i.i.d.

$\{x_1, x_2, \dots, x_n\}$  are correlated

# SIMPLE

$$p(x_1, \dots, x_n) = \mathcal{N}_n(\mu, \Sigma)$$

$$\mu = \begin{bmatrix} \mu \\ \mu \\ \vdots \\ \mu \end{bmatrix} \quad \Sigma = \begin{bmatrix} v & \rho & \rho & \dots & \rho \\ \rho & v & \rho & \dots & \rho \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \rho & \dots & v \end{bmatrix} \quad 0 \leq \rho < v$$

# DIFFICULT



$$p(x_1, \dots, x_n) = ?$$

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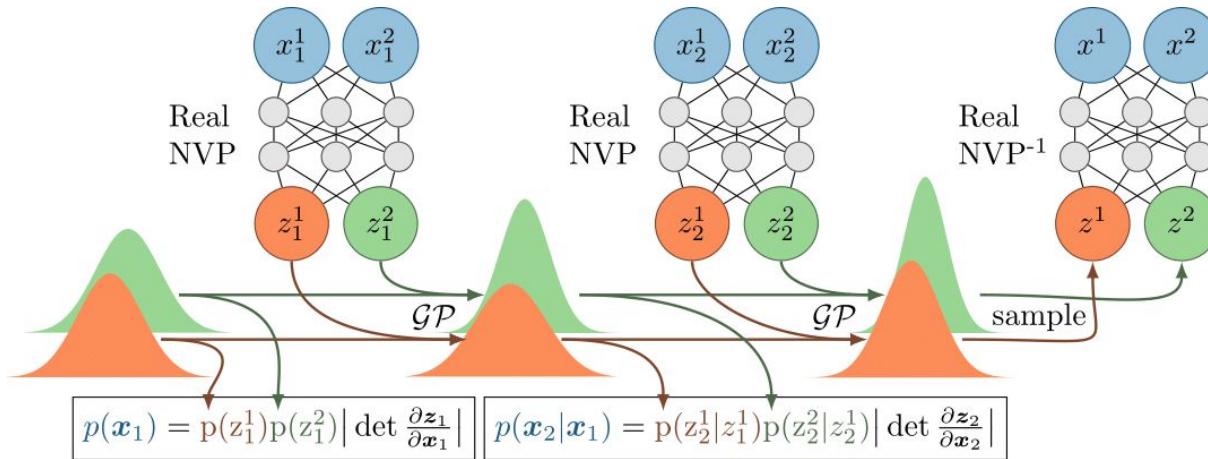
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DIFFICULT



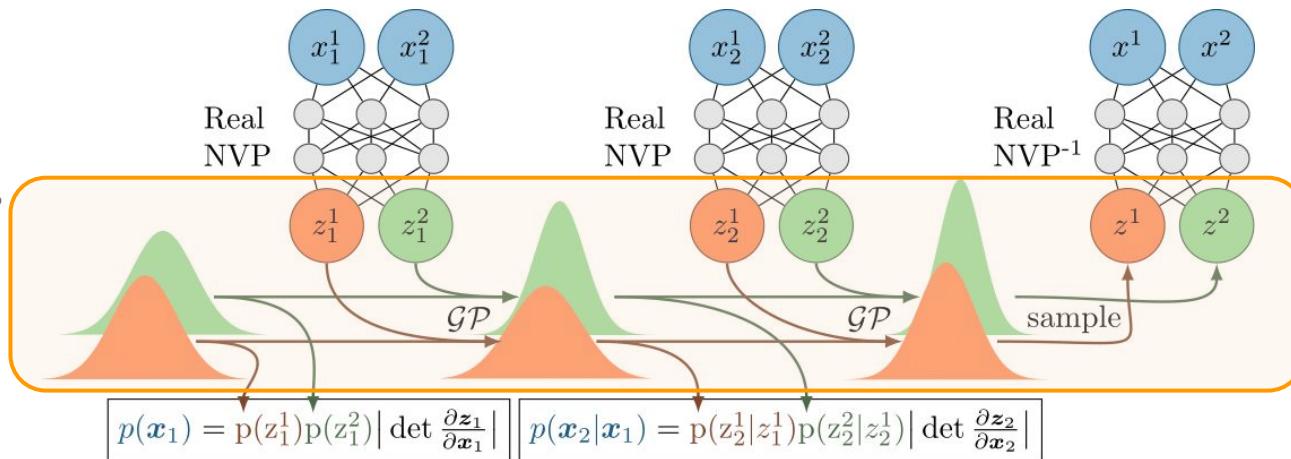
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# BRUNO: BAYESIAN RECURRENT NEURAL MODEL



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Process  
in the  
latent  
space



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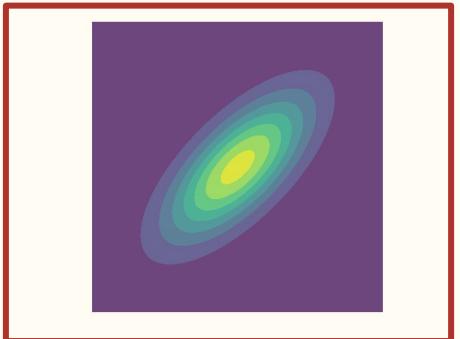
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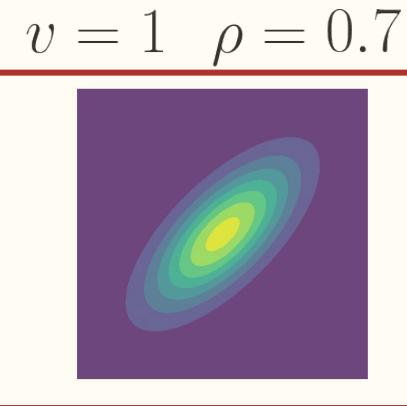
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Defines an exchangeable Gaussian process

# GAUSSIAN PROCESSES

**Definition.**  $f$  is a Gaussian process on  $\mathcal{X}$  with

mean function  $\Phi : \mathcal{X} \mapsto \mathbb{R}$

kernel function  $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$

if any finite collection of function values have a joint multivariate Gaussian distribution, i.e.  $(f(x_1), \dots, f(x_n)) \sim \mathcal{N}_n(\mu, \Sigma)$  where

$\mu \in \mathbb{R}^n$  with  $\mu_i = \Phi(x_i)$

$\Sigma \in \Pi(n)$  with  $\Sigma_{ij} = k(x_i, x_j)$

# EXCHANGEABLE GAUSSIAN PROCESSES

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# EXCHANGEABLE GAUSSIAN PROCESSES

$$(z_1, \dots, z_n) \sim \mathcal{N}_n(\mu, \Sigma) \quad \mu = \begin{bmatrix} \mu \\ \mu \\ \vdots \\ \mu \end{bmatrix} \quad \Sigma = \begin{bmatrix} v & \rho & \rho & \dots & \rho \\ \rho & v & \rho & \dots & \rho \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \rho & \dots & v \end{bmatrix} \quad 0 \leq \rho < v$$

Predictive distribution?

$$p(z_{n+1} | z_{1:n}) = \mathcal{N}(\mu_{n+1}, v_{n+1})$$

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Predictive distribution?

$$p(z_{n+1} | z_{1:n}) = \mathcal{N}(\mu_{n+1}, v_{n+1})$$

$$\begin{aligned} \mu_{n+1} &= (1 - d_n)\mu_n + d_n z_n \\ v_{n+1} &= (1 - d_n)v_n + d_n(v - \rho) \end{aligned}$$

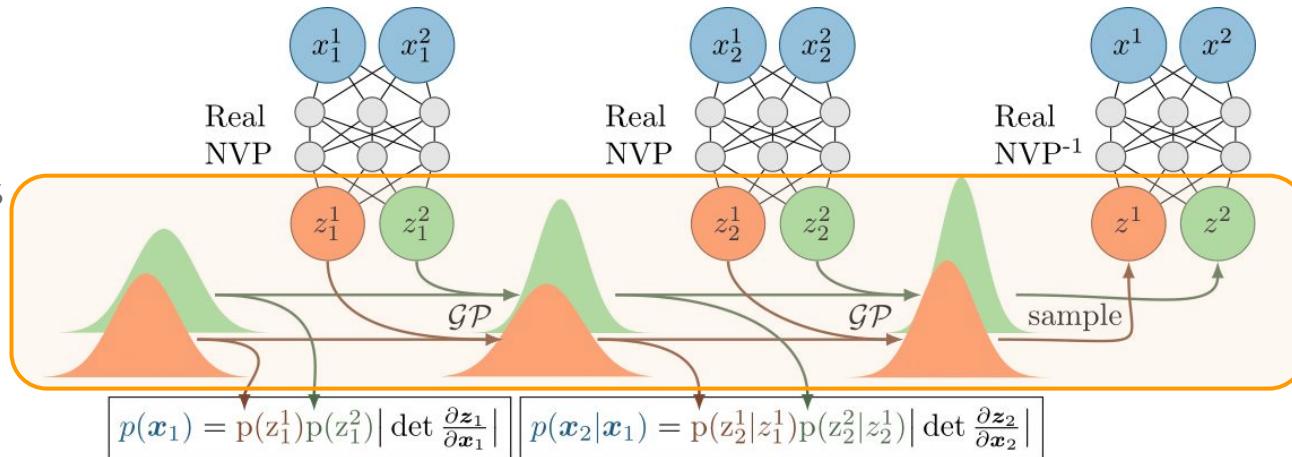
$$d_n = \frac{\rho}{v + \rho(n-1)}$$

$$\mu_1 = \mu, \quad v_1 = v$$

recurrence

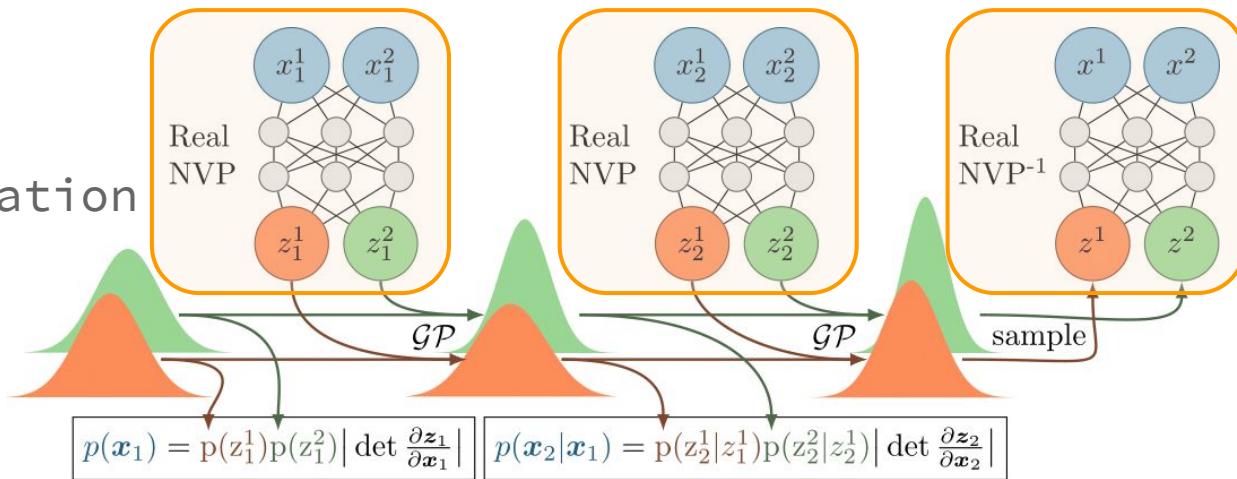
# BRUNO

Process  
in the  
latent  
space



# BRUNO

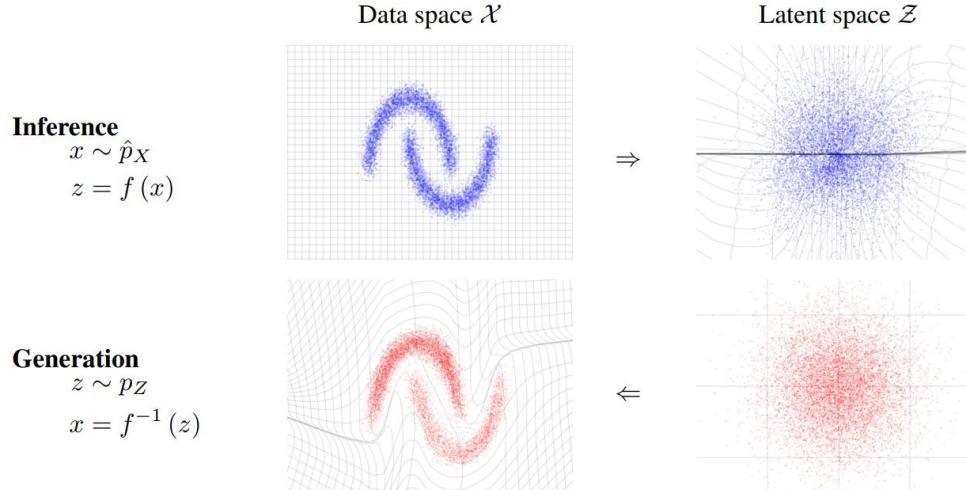
Powerful  
bijective  
transformation



# REAL NVP

$$f : \mathcal{X} \mapsto \mathcal{Z} \text{ with } \mathcal{X} = \mathbb{R}^D$$

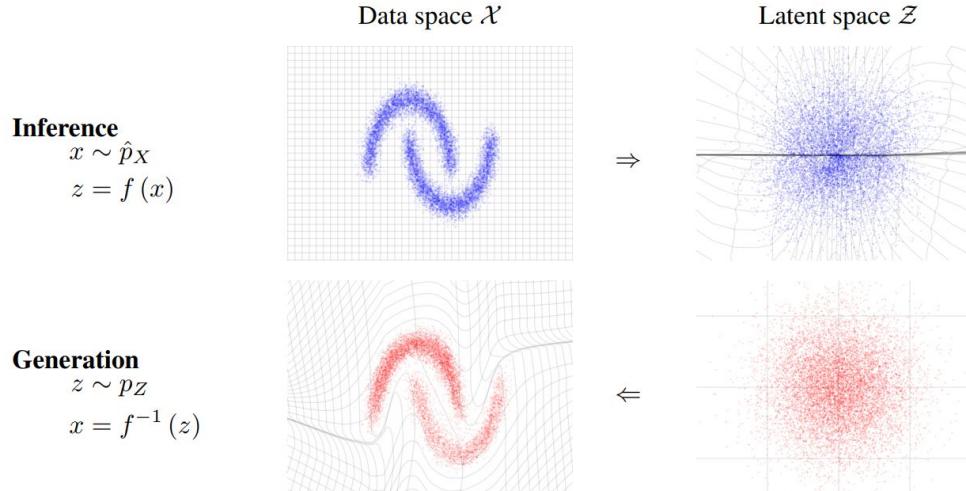
- bijective
- forward and the inverse mappings are equally expensive
- computing the log determinant of the Jacobian is  $O(D)$



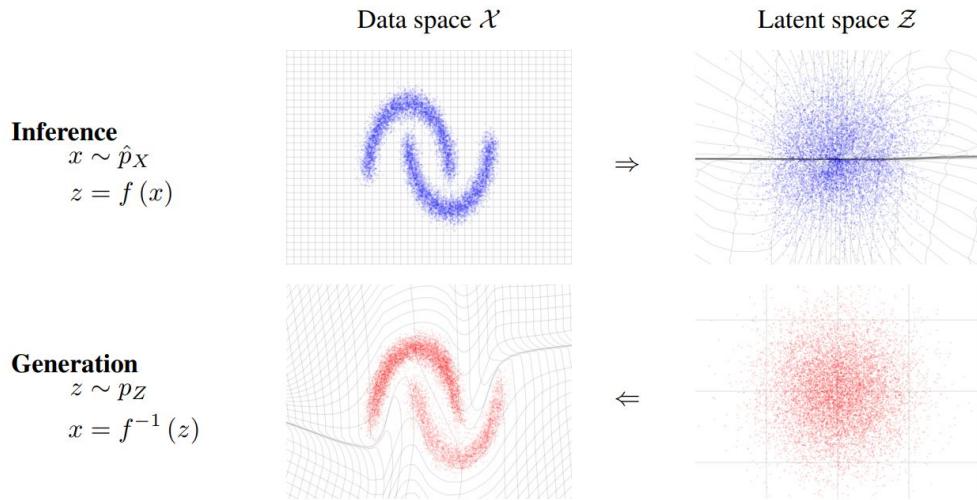
# REAL NVP

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- bijective
- forward and the inverse mappings are equally expensive
- computing the log determinant of the Jacobian is  $O(D)$



# REAL NVP. CHANGE OF VARIABLES



Likelihood evaluation:

$$p(\mathbf{x}) = p(\mathbf{z}) \left| \det \left( \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right) \right|$$

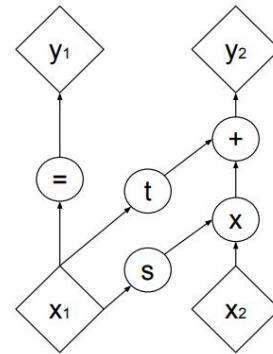
# REAL NVP'S COUPLING LAYER

$$y_{1:d} = x_{1:d}$$

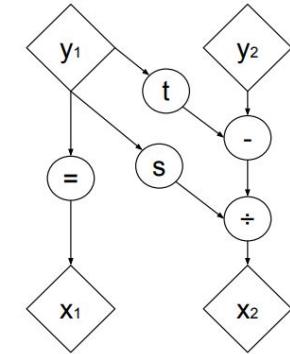
$$y_{d+1:D} = x_{d+1:D} \odot \exp(s(x_{1:d})) + t(x_{1:d})$$

Jacobian:

$$\frac{\partial y}{\partial x^T} = \begin{bmatrix} \mathbb{I}_d & 0 \\ \frac{\partial y_{d+1:D}}{\partial x_{1:d}^T} & \text{diag}(\exp[s(x_{1:d})]) \end{bmatrix}$$



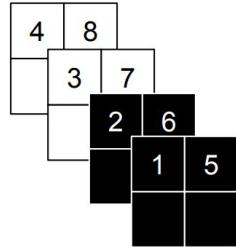
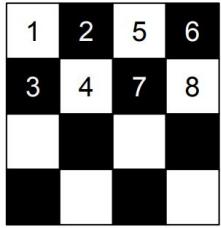
(a) Forward propagation



(b) Inverse propagation

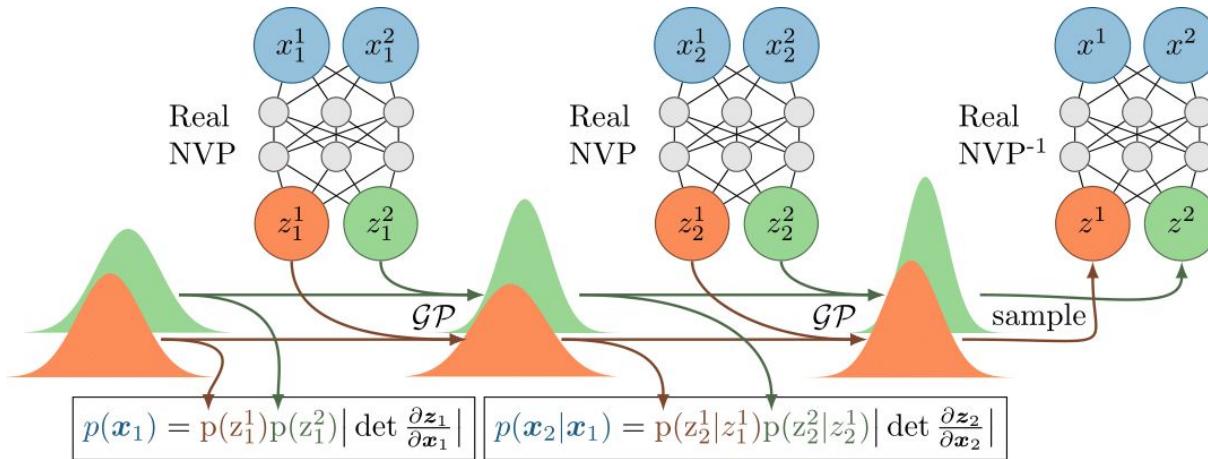
# CONVOLUTIONAL REAL NVP

Schemes to partition the dimensions when using convolutions



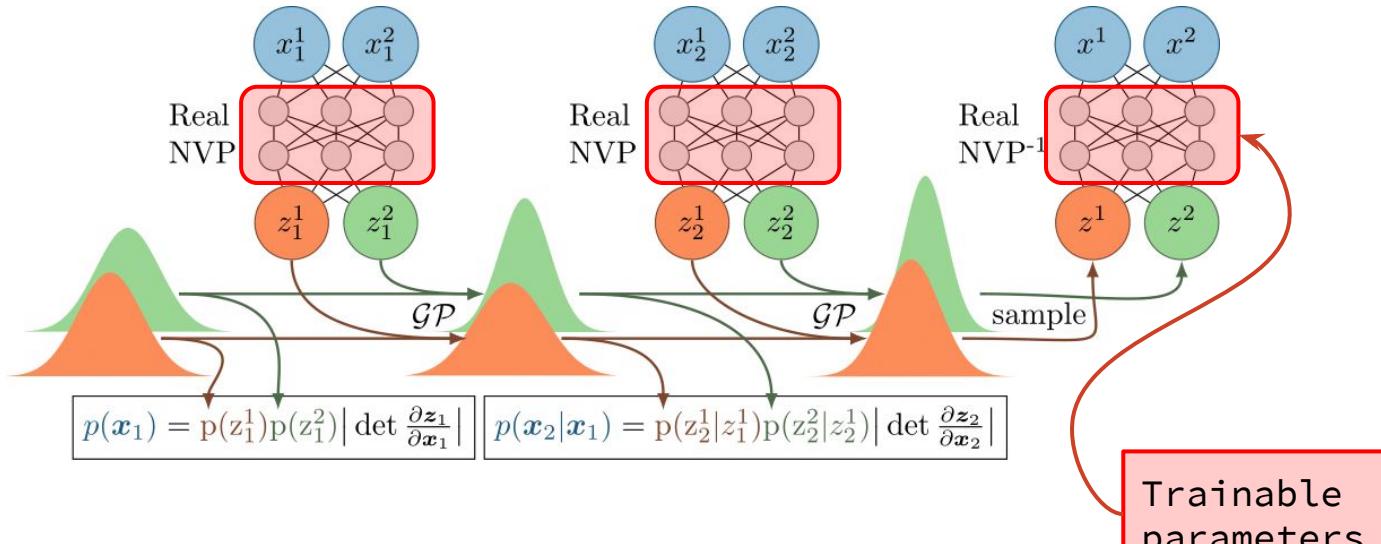
Samples from Real NVP  
trained on CelebA and LSUN

# BRUNO



- ★ Latent dimensions are independent, so  $p(\mathbf{z}) = \prod_{d=1}^D p(z^d)$
- ★ For every latent dimension  $d$ :  $(z_1^d, \dots, z_n^d) \sim \mathcal{N}_n(\mu^d \mathbf{1}, \mathbf{K}^d)$  with an exchangeable  $\mathbf{K}^d$

# TRAINING BRUNO

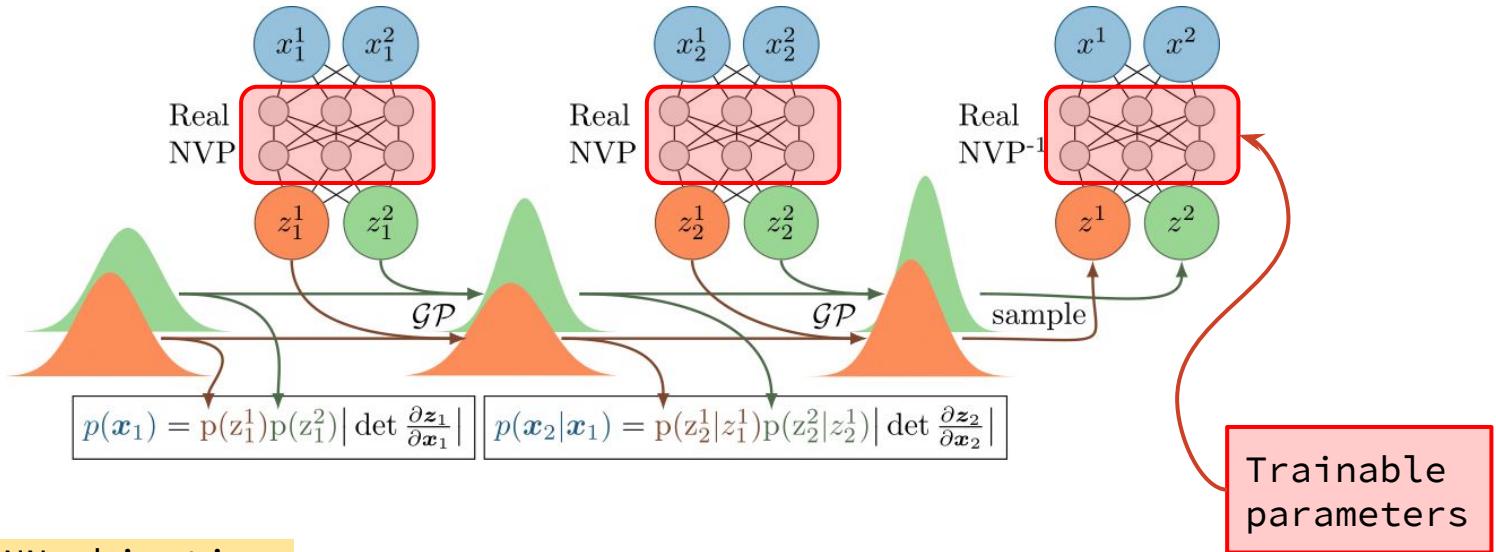


$$\star p(\mathbf{z}) = \prod_{d=1}^D p(z^d)$$

$$\star (z_1^d, \dots, z_n^d) \sim \mathcal{N}_n(\mu^d \mathbf{1}, \mathbf{K}^d) \text{ with }$$

$$\mathbf{K}_{ij}^d = \begin{cases} v^d, & i = j \\ \rho^d, & i \neq j \end{cases}$$

# TRAINING BRUNO



Classical RNN objective:

$$\mathcal{L} = \sum_{n=0}^{N-1} \log p(\mathbf{x}_{n+1} | \mathbf{x}_{1:n})$$

$$\mathbf{K}_{ij}^d = \begin{cases} v^d, & i = j \\ \rho^d, & i \neq j \end{cases}$$

# EXPERIMENTS: FASHION MNIST

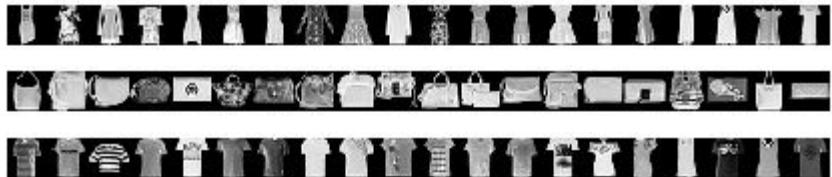


Random samples from the dataset

# EXPERIMENTS: FASHION MNIST



Random samples from the dataset

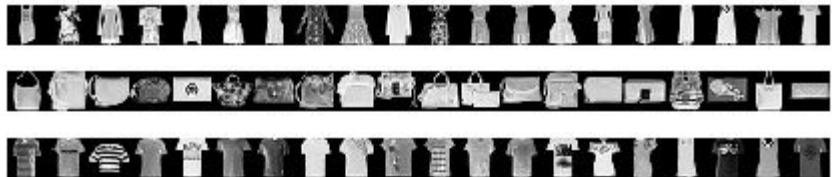


Training sequences

# EXPERIMENTS: FASHION MNIST



Random samples from the dataset



Training sequences



BRUNO samples from  
the prior  $p(x)$

# EXPERIMENTS: FASHION MNIST



# LEARNING TO CORRELATE



28x28 inputs  $\rightarrow$  784 latent dimensions  
with own variances and covariances:

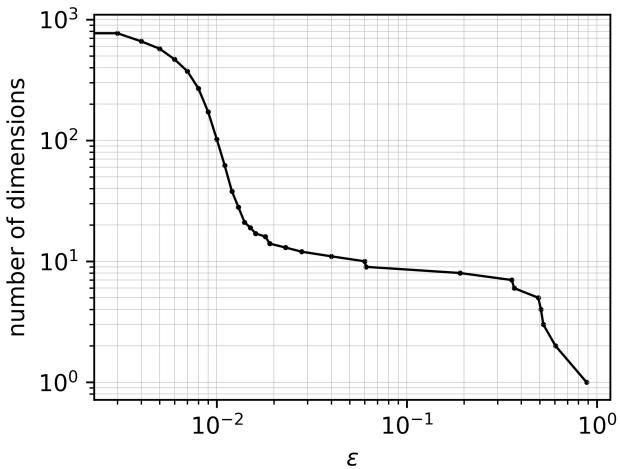
$$\Sigma = \begin{bmatrix} v & \rho & \rho & \dots & \rho \\ \rho & v & \rho & \dots & \rho \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \rho & \rho & \rho & \dots & v \end{bmatrix} \quad 0 \leq \rho < v$$

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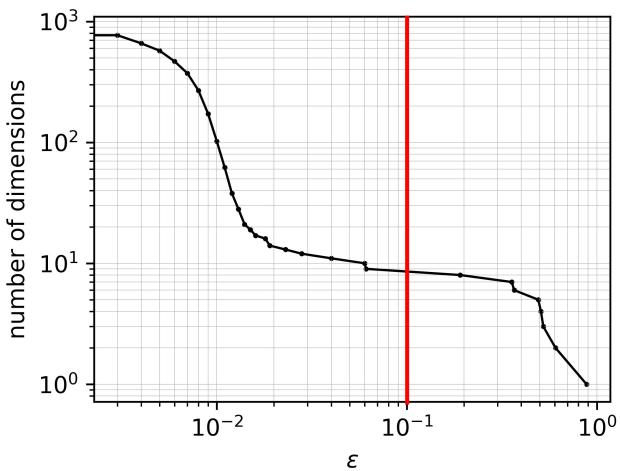


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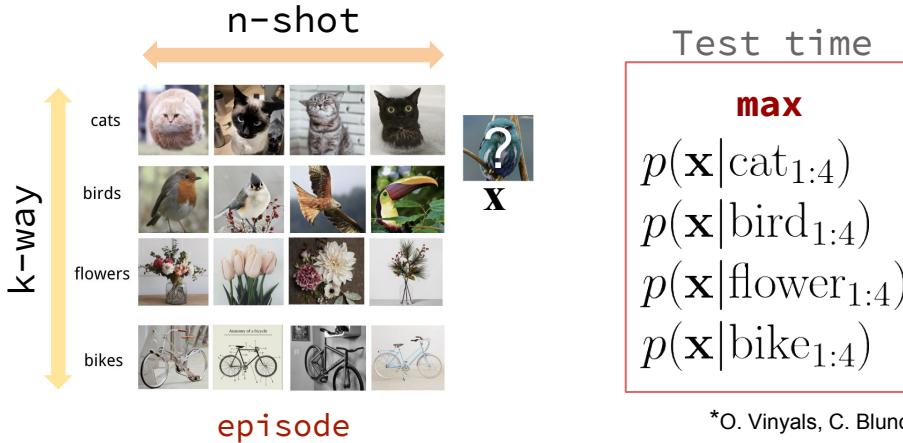


# EXPERIMENTS: OMNIGLOT FEW-SHOT GENERATION

**Omniglot:** 1623 different handwritten characters from 50 different alphabets.  
Each of the characters was drawn by 20 different people.

# EXPERIMENTS: OMNIGLOT FEW-SHOT CLASSIFICATION

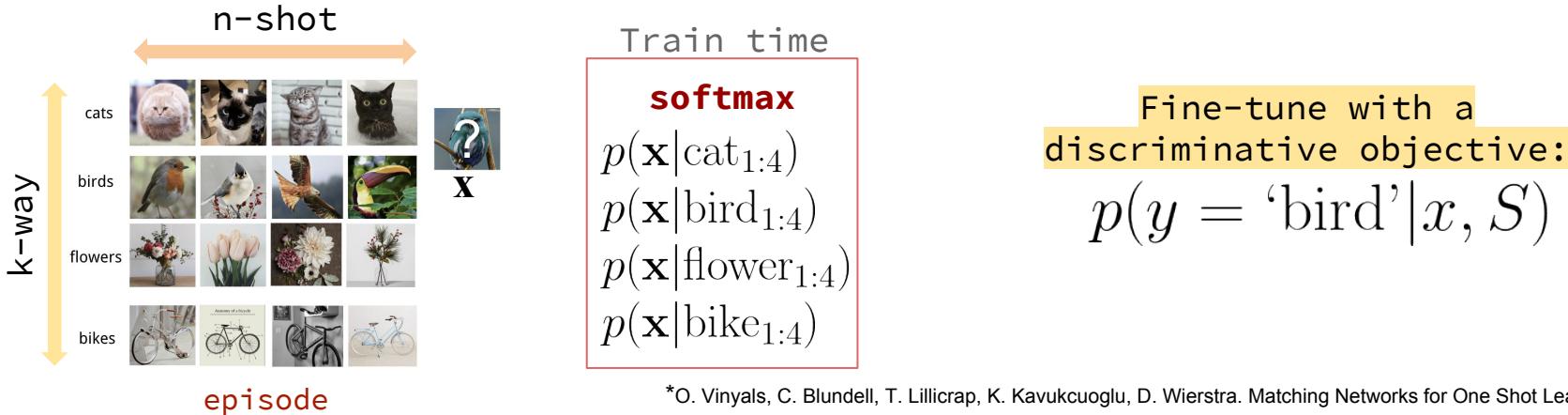
Model	5-way		20-way	
	1-shot	5-shot	1-shot	5-shot
<b>BASELINE CLASSIFIER*</b>	80.0	95.0	69.5	89.1
<b>MATCHING NETS*</b>	98.1	98.9	93.8	98.5
<b>BRUNO</b>	86.3	95.6	69.2	87.7
<b>BRUNO</b> (discriminative fine-tuning)	97.1	99.4	91.3	97.8



\*O. Vinyals, C. Blundell, T. Lillicrap, K. Kavukcuoglu, D. Wierstra. Matching Networks for One Shot Learning. NIPS'16

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# BRUNO

- \* Likelihoods  $p(\mathbf{x}_{n+1} | \mathbf{x}_{1:n})$
- \* Easy sampling from  $p(\mathbf{x}_{n+1} | \mathbf{x}_{1:n})$

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# CONDITIONAL BRUNO

Can we model  $p(\mathbf{x}_{n+1} | \mathbf{h}_{n+1}, \mathbf{x}_{1:n}, \mathbf{h}_{1:n})$  ?

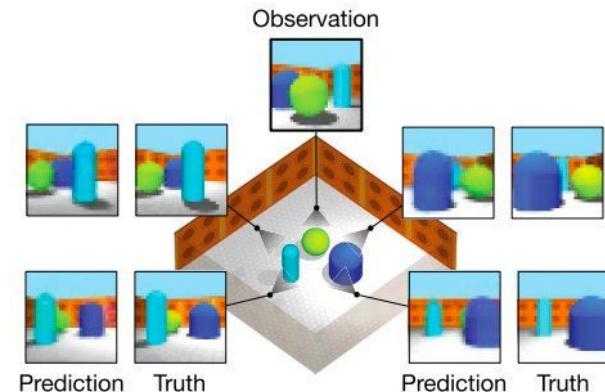
# BRUNO

- \* Likelihoods  $p(\mathbf{x}_{n+1} | \mathbf{x}_{1:n})$
- \* Easy sampling from  $p(\mathbf{x}_{n+1} | \mathbf{x}_{1:n})$

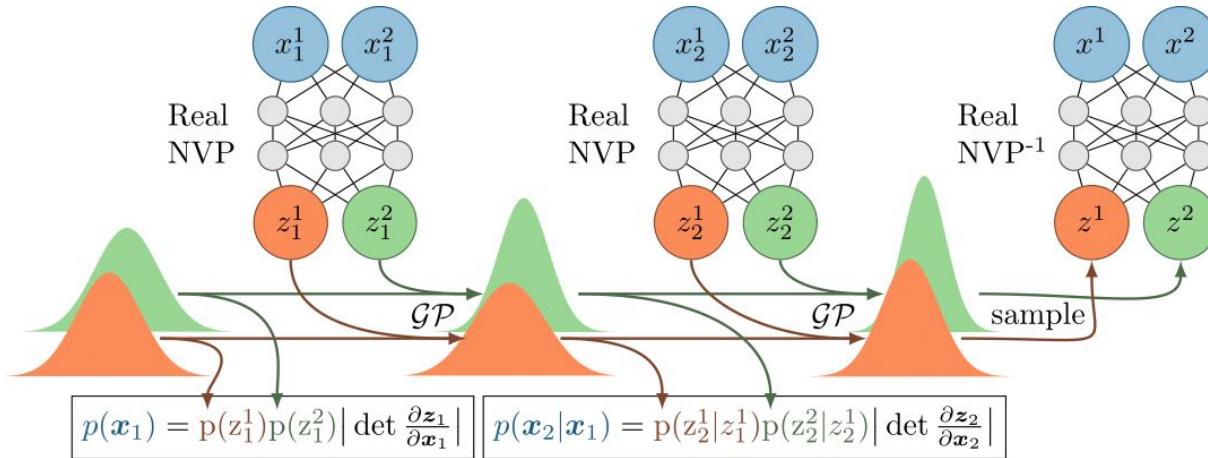
## CONDITIONAL BRUNO

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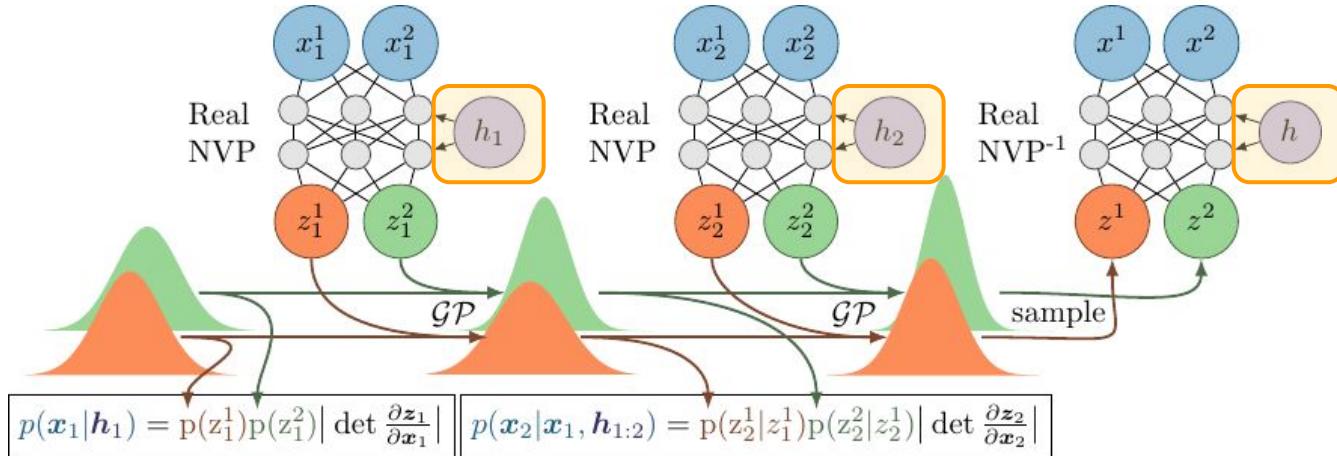
observations  
scene view-  
point



# BRUNO



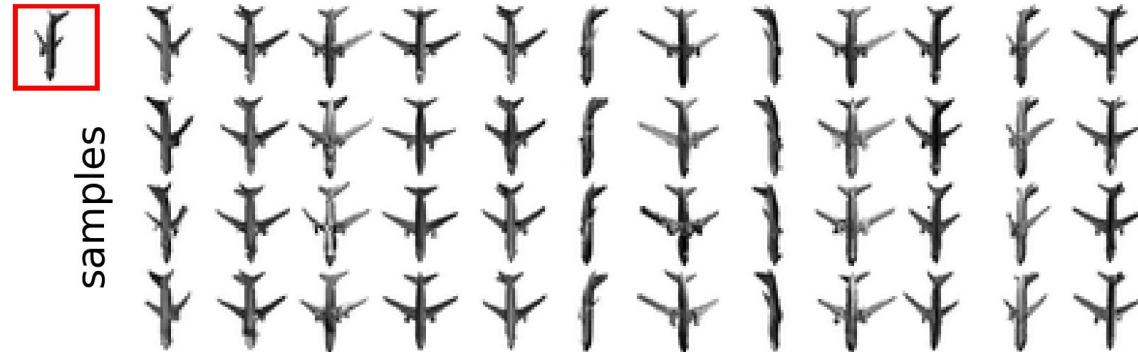
# CONDITIONAL BRUNO



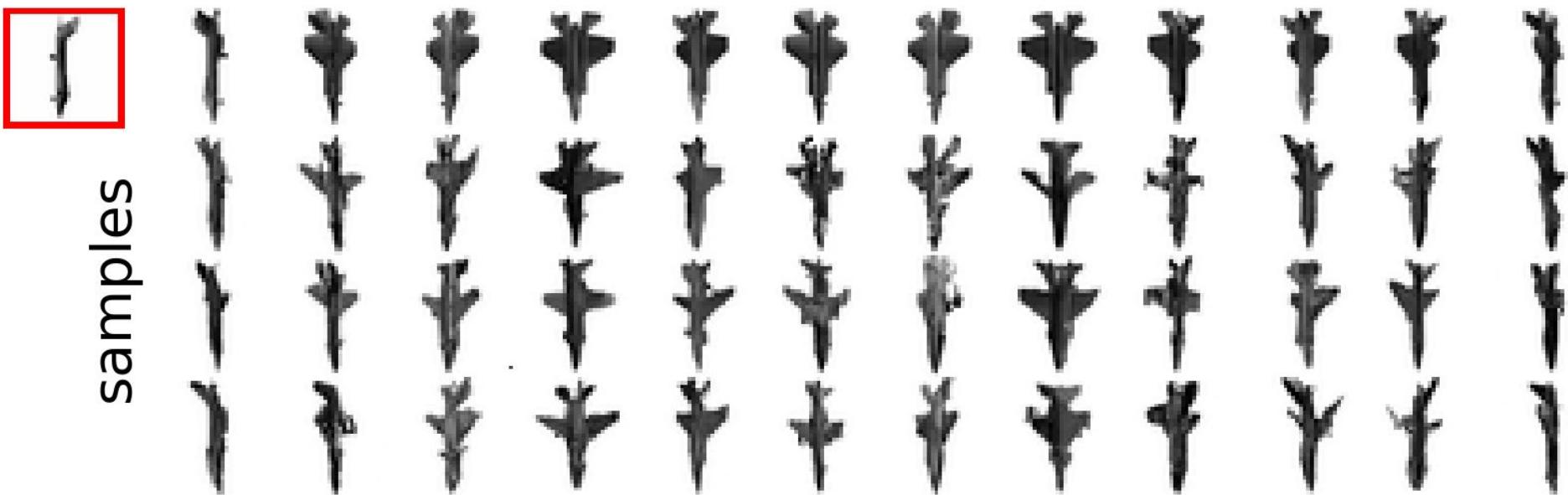
# EXPERIMENTS: SHAPENET CHAIRS & AIRPLANES



samples from  
 $p(x|x_1, h=45^\circ)$



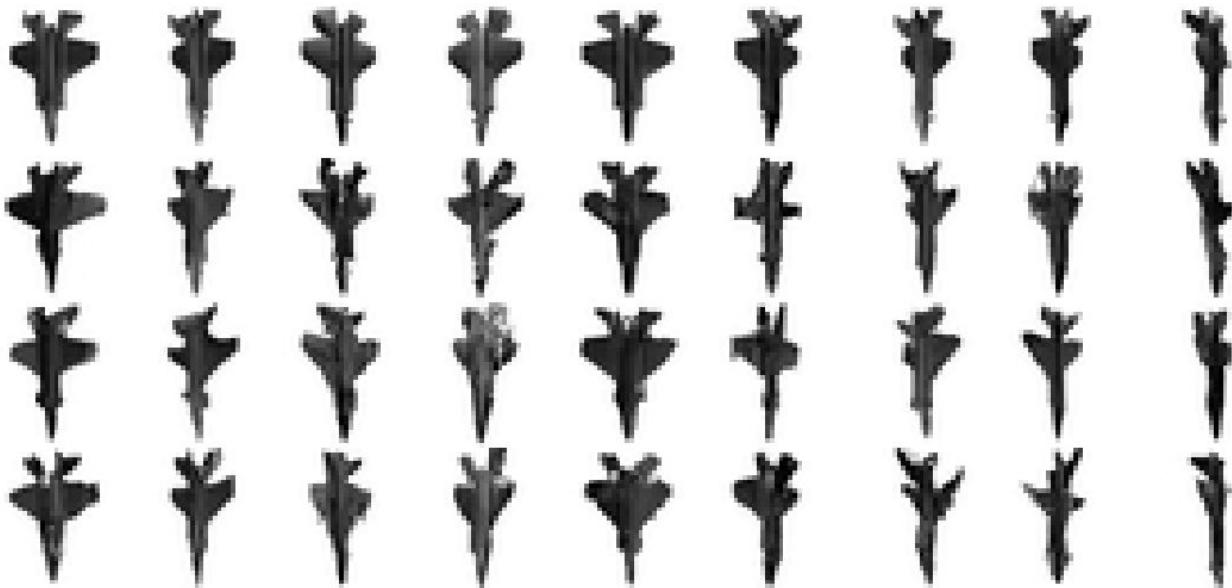
# EXPERIMENTS: SHAPENET CHAIRS & AIRPLANES



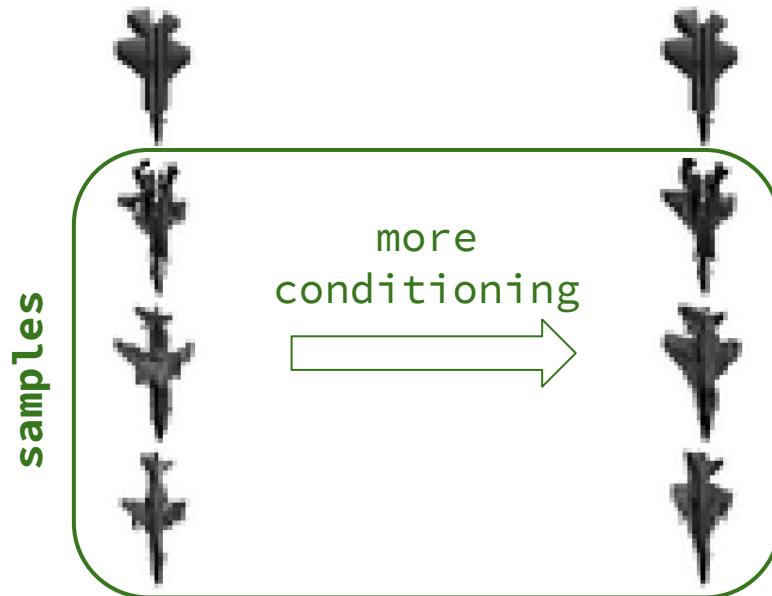
# EXPERIMENTS: SHAPENET CHAIRS & AIRPLANES



samples



# EXPERIMENTS: SHAPENET CHAIRS & AIRPLANES



# CONCLUSION

BRUNO = expressiveness of DNNs + data-efficiency of GPs

A meta-learning exchangeable model with

- exact likelihoods
- fast sampling and inference
- no retraining or changes to the architecture at test time
- recurrent formulation