

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 π :

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

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$$P(\text{img1} \text{ img2}) = P(\text{img2} \text{ img1})$$

$$P(\text{img3} \text{ img4} \text{ img5}) = P(\text{img3} \text{ img5} \text{ img4}) = P(\text{img5} \text{ img3} \text{ img4}) = \dots$$

...

EXCHANGEABILITY. IID EXAMPLE

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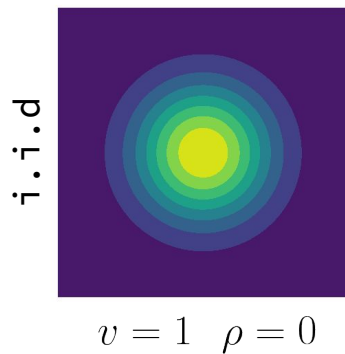
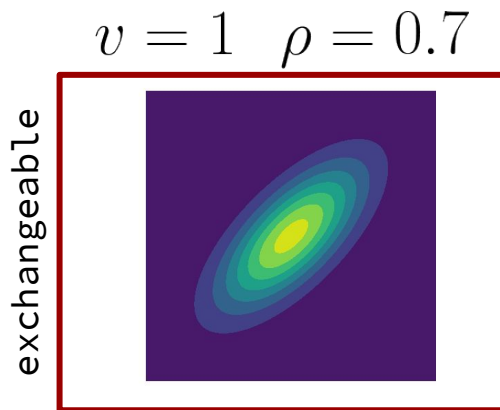
IID random variables are exchangeable:

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

EXCHANGEABILITY. NON-IID EXAMPLE

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

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



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 θ is some parameter conditioned on which the data is i.i.d.

DE FINETTI'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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x_1, x_2, x_3, \dots

successive coin tosses

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

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

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Gives 2 ways for defining models of exchangeable sequences:

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

A KILLER APPLICATION: META-LEARNING

dogs

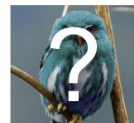
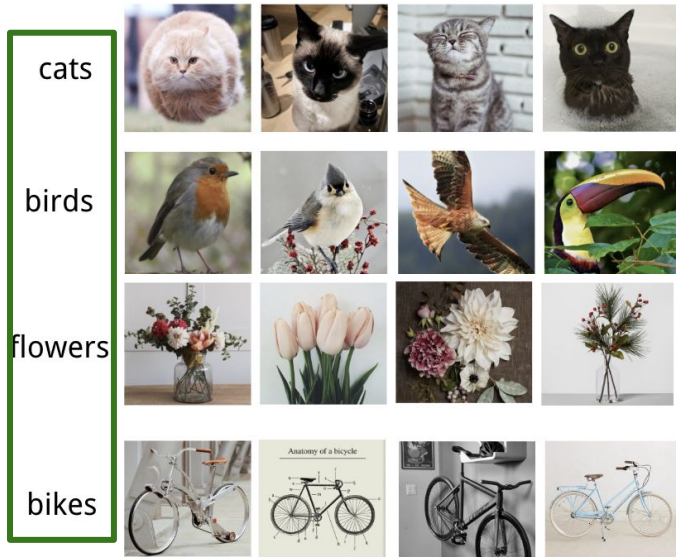


otters



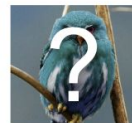
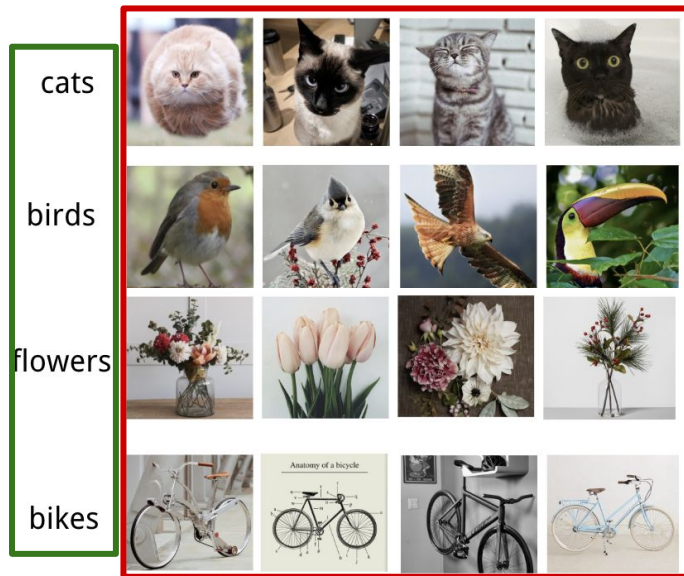
META-LEARNING. EPISODE

L~T



META-LEARNING. EPISODE

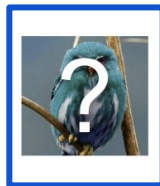
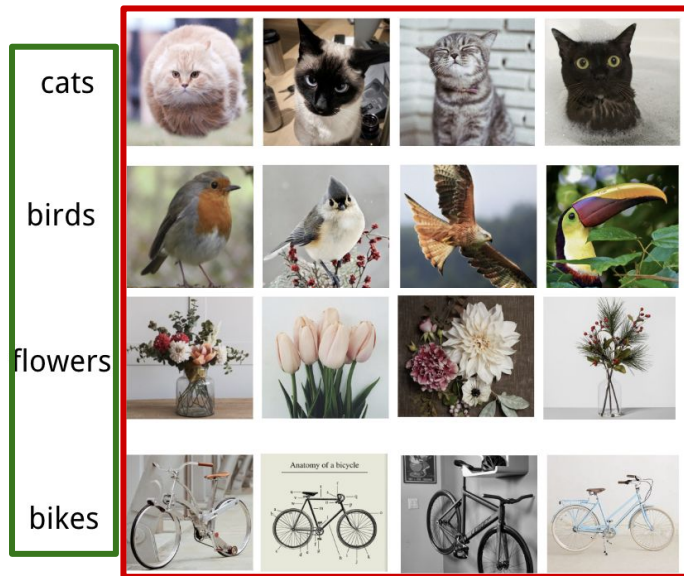
L~T



S~L

META-LEARNING. EPISODE

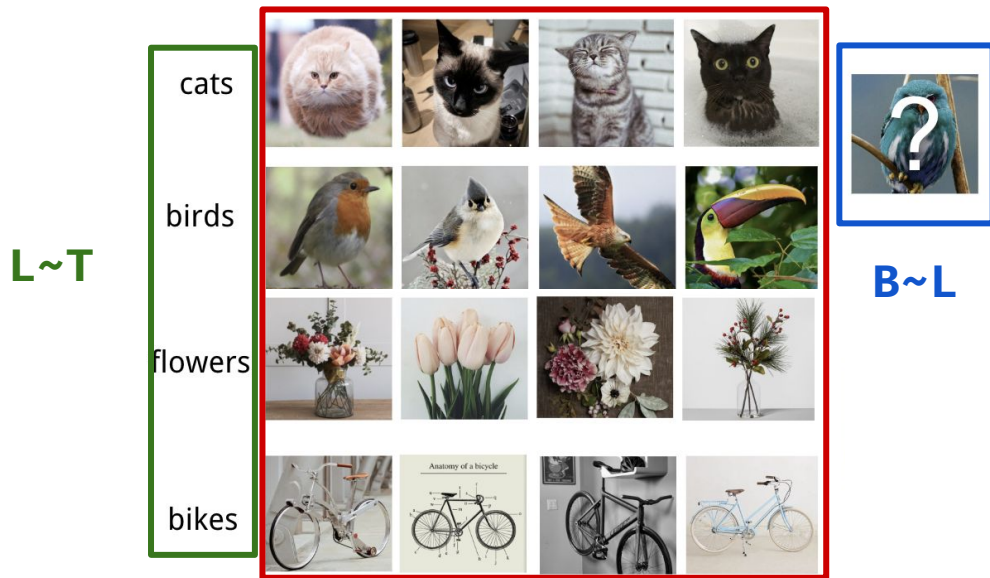
L~T



B~L

S~L

META-LEARNING. EPISODE

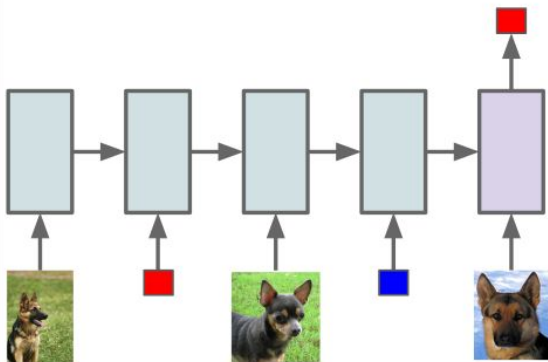


$S \sim L$

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

META-LEARNING MODELS. TAXONOMY

Model Based

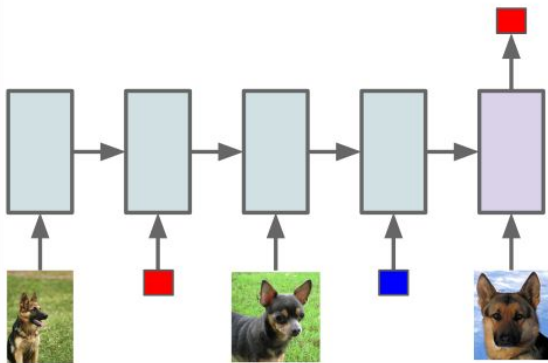


$$p_{\theta}(y|x, S) = f_{\theta}(x, S)$$

Memory-Augmented Neural Network
Neural Processes
BRUNO

META-LEARNING MODELS. TAXONOMY

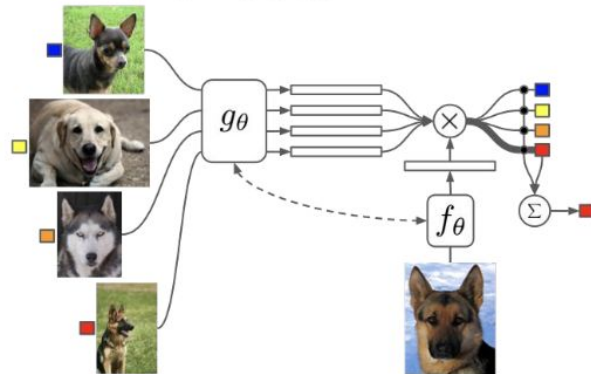
Model Based



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

Memory-Augmented Neural Network
Neural Processes
BRUNO

Metric Based

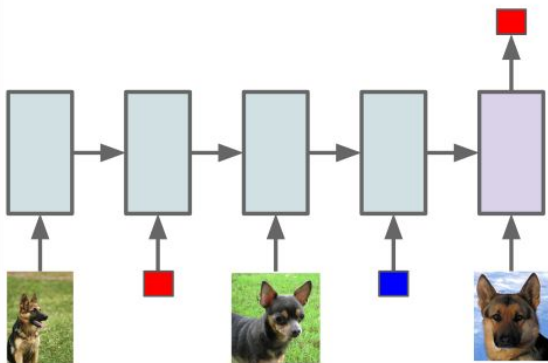


$$p_{\theta}(y|x, S) = \sum_{(x_i, y_i) \in S} k(x_i, x) y_i$$

Siamese Neural Networks
Matching Networks
Relation Network
Prototypical Networks

META-LEARNING MODELS. TAXONOMY

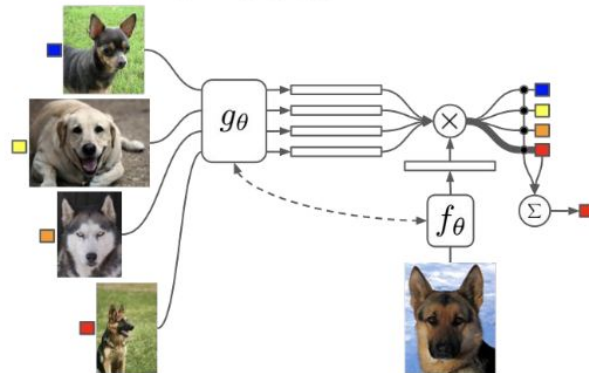
Model Based



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Neural Processes
BRUNO

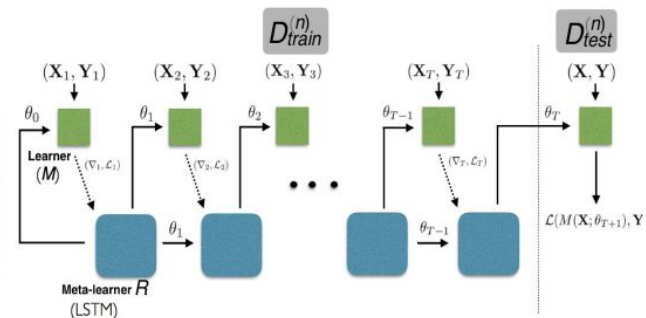
Metric Based



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

Siamese Neural Networks
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Relation Network
Prototypical Networks

Optimization Based



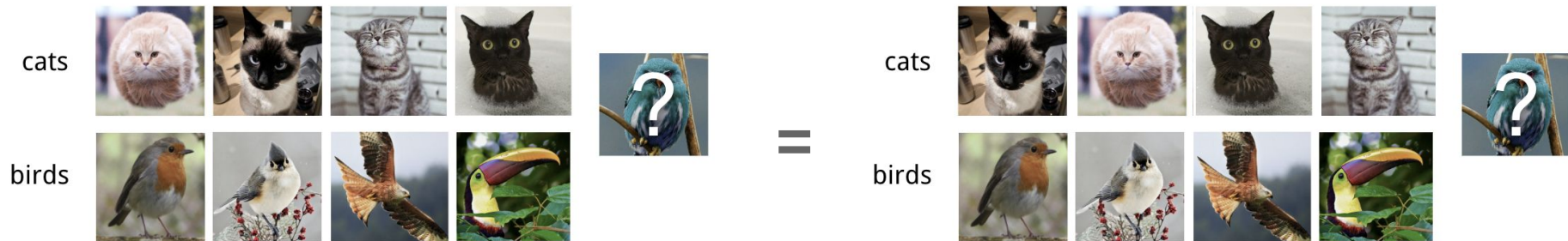
$$p_{\theta}(y|x, S) = f_{\theta(S)}(x, S)$$

$$\theta(S) = g_{\phi}(\theta_0, \{\nabla_{\theta_0} L(x_i, y_i)\}_{(x_i, y_i) \in S})$$

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

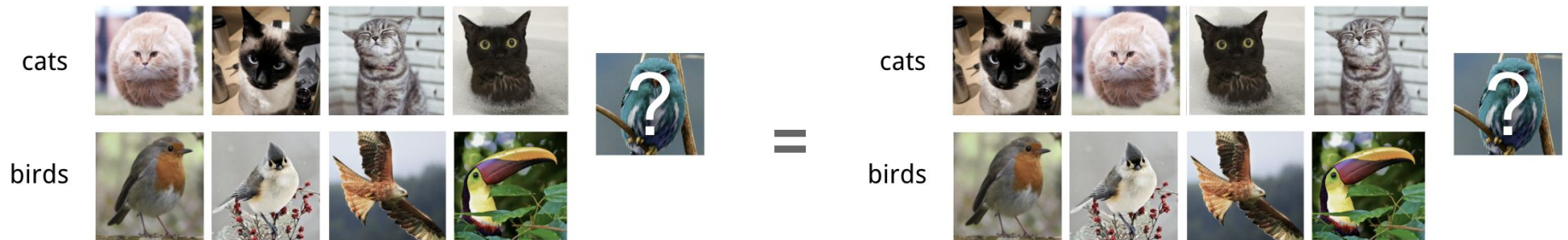
EXCHANGEABILITY AND META-LEARNING

1. Order-invariance



EXCHANGEABILITY AND META-LEARNING

1. Order-invariance



2. Correlation



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

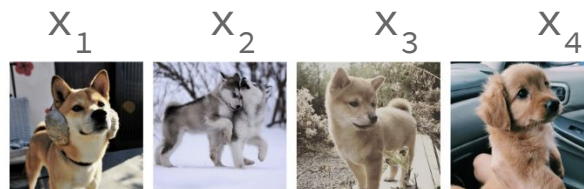
$\{x_1, x_2, \dots, x_n\}$ are correlated

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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bijection

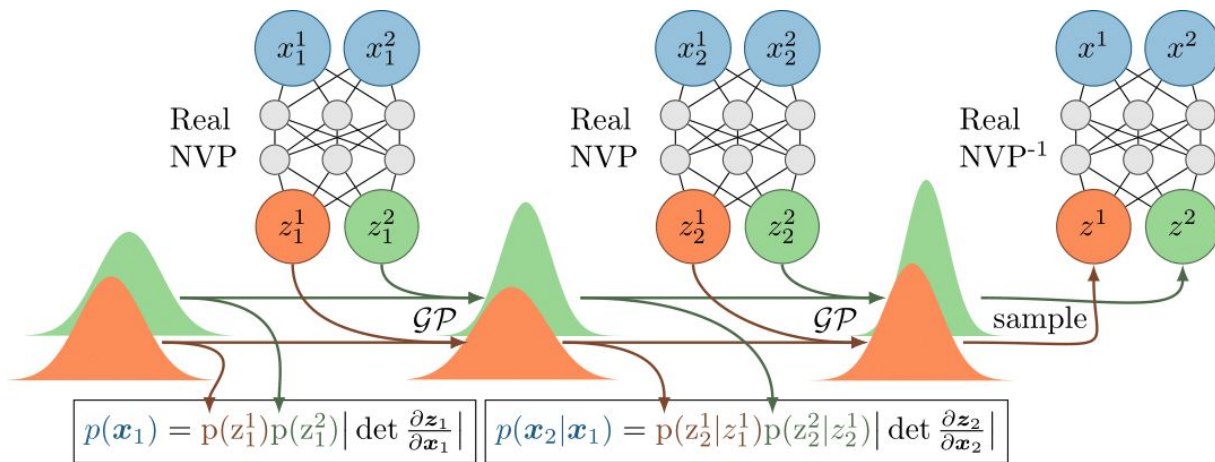


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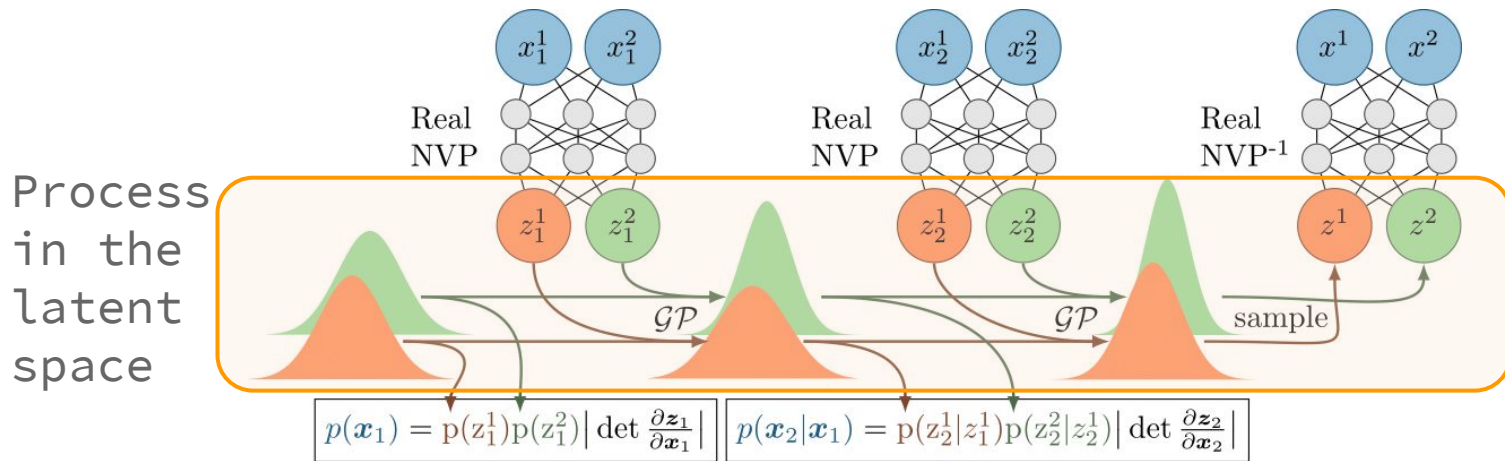


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BRUNO: BAYESIAN RECURRENT NEURAL MODEL



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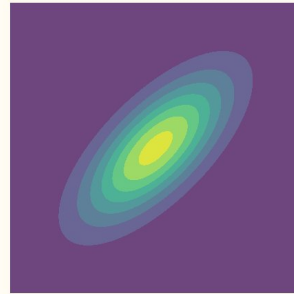
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$$v = 1 \quad \rho = 0.7$$



EXCHANGEABILITY

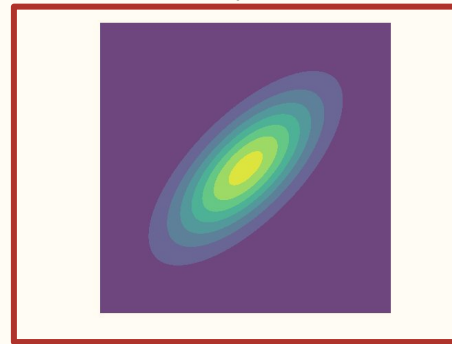
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Defines an
exchangeable
Gaussian
process

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

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

Predictive distribution?

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

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EXCHANGEABLE GAUSSIAN PROCESSES

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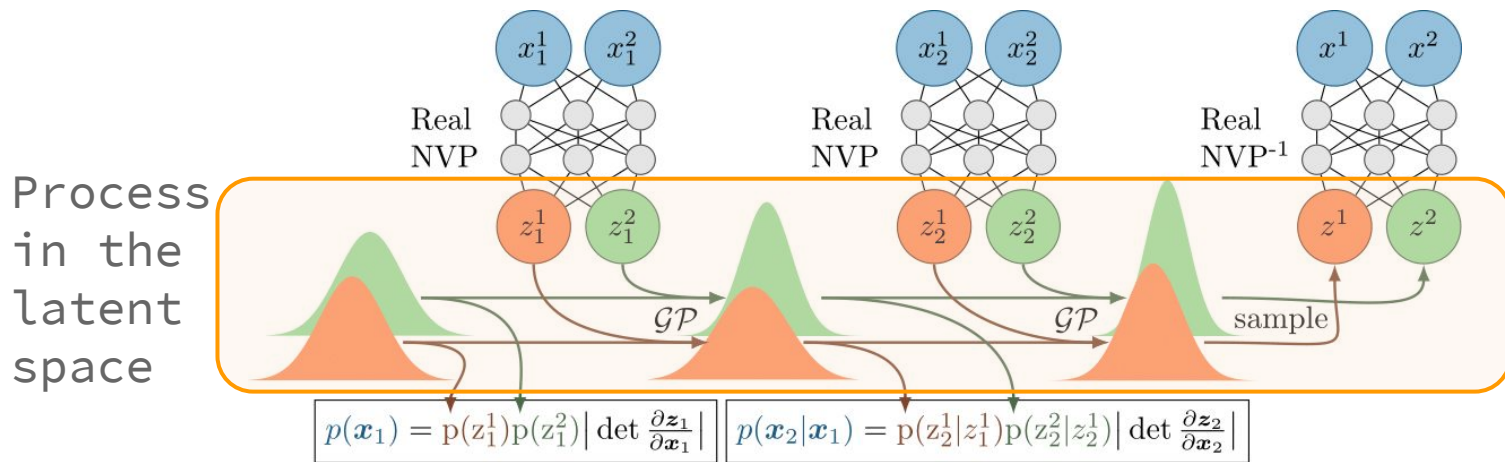
$$\begin{aligned} \mu_{n+1} &= (1 - d_n)\mu_n + d_n z_n \\ v_{n+1} &= (1 - d_n)v_n + d_n(v - \rho) \end{aligned}$$

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

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

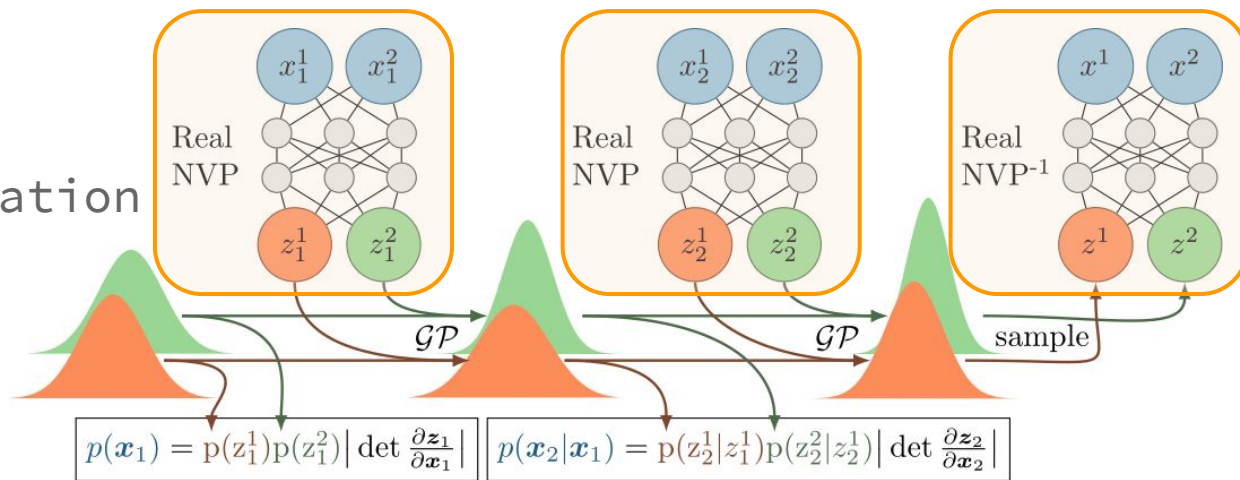
recurrence

BRUNO



BRUNO

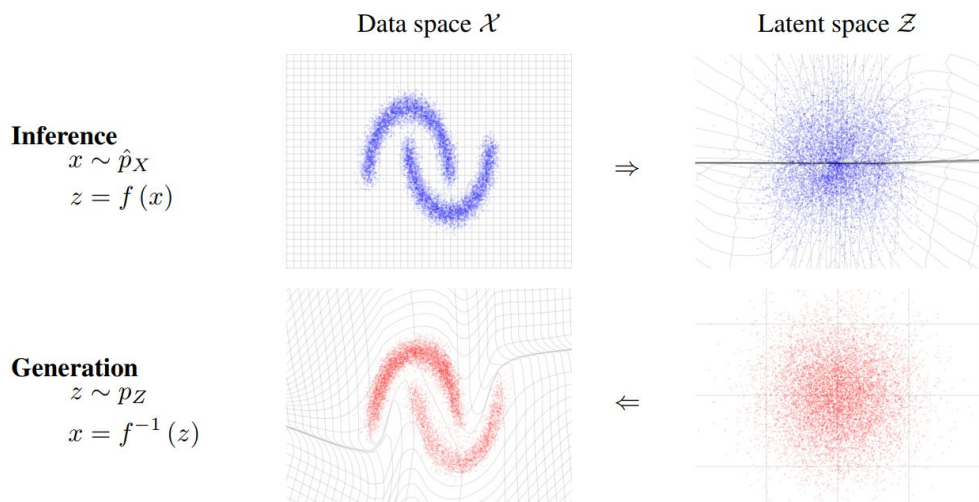
Powerful
bijective
transformation



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 $O(D)$



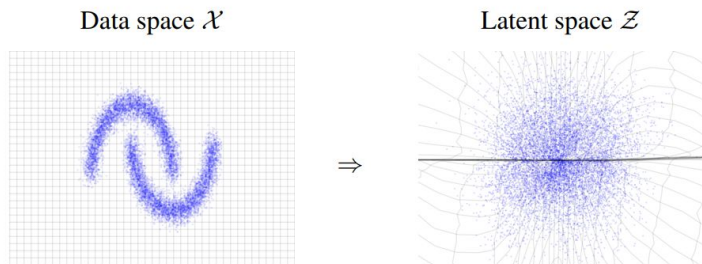
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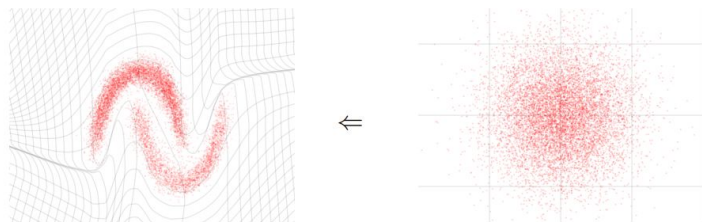
Inference

$$x \sim \hat{p}_X \\ z = f(x)$$



Generation

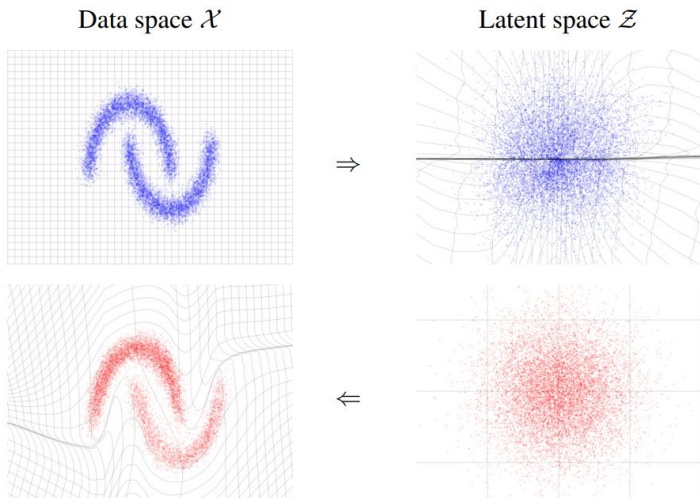
$$z \sim p_Z \\ x = f^{-1}(z)$$



REAL NVP. CHANGE OF VARIABLES

Inference

$$x \sim \hat{p}_X \\ z = f(x)$$



Generation

$$z \sim p_Z \\ x = f^{-1}(z)$$

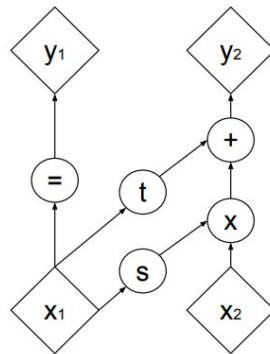
Likelihood evaluation:

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

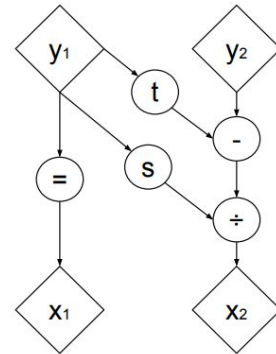
REAL NVP'S COUPLING LAYER

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

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



(a) Forward propagation



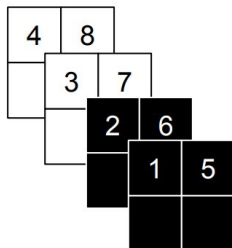
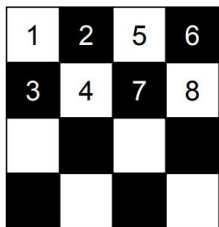
(b) Inverse propagation

Jacobian:

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

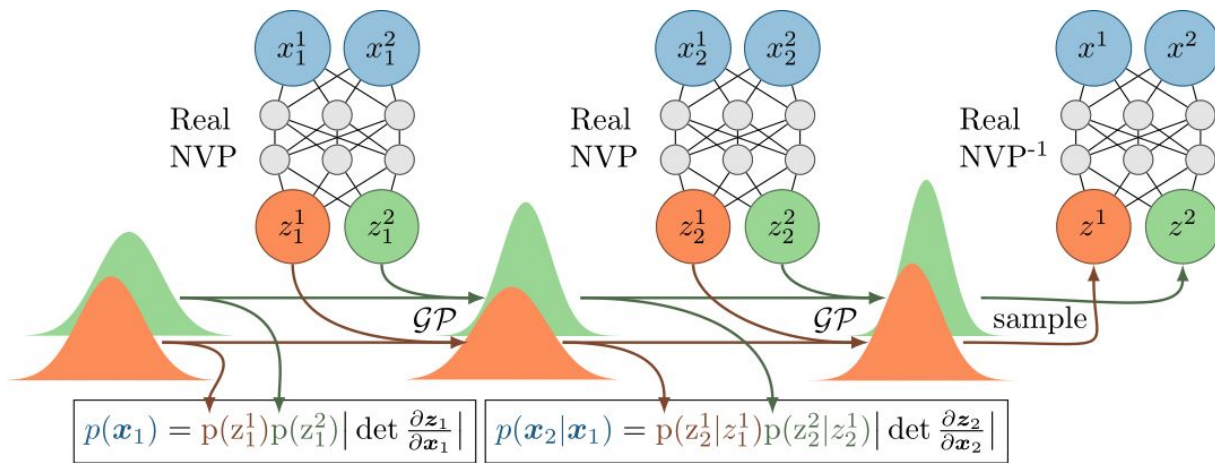
CONVOLUTIONAL REAL NVP

Schemes to partition
the dimensions when
using convolutions



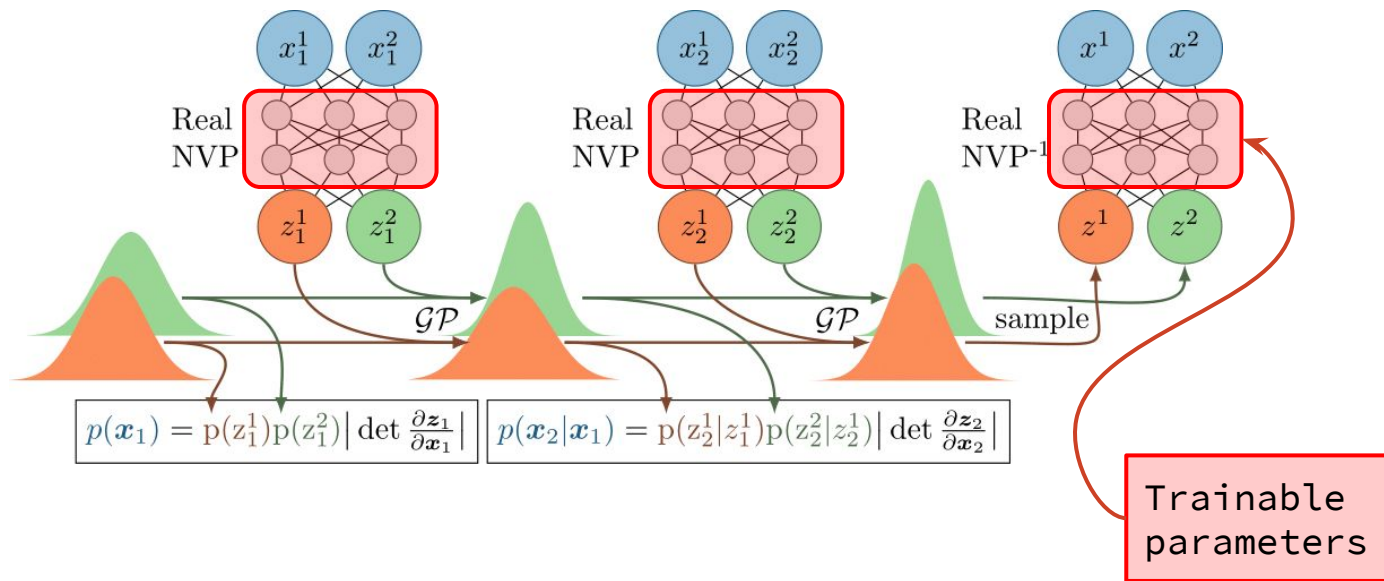
Samples from Real NVP
trained on CelebA and LSUN

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

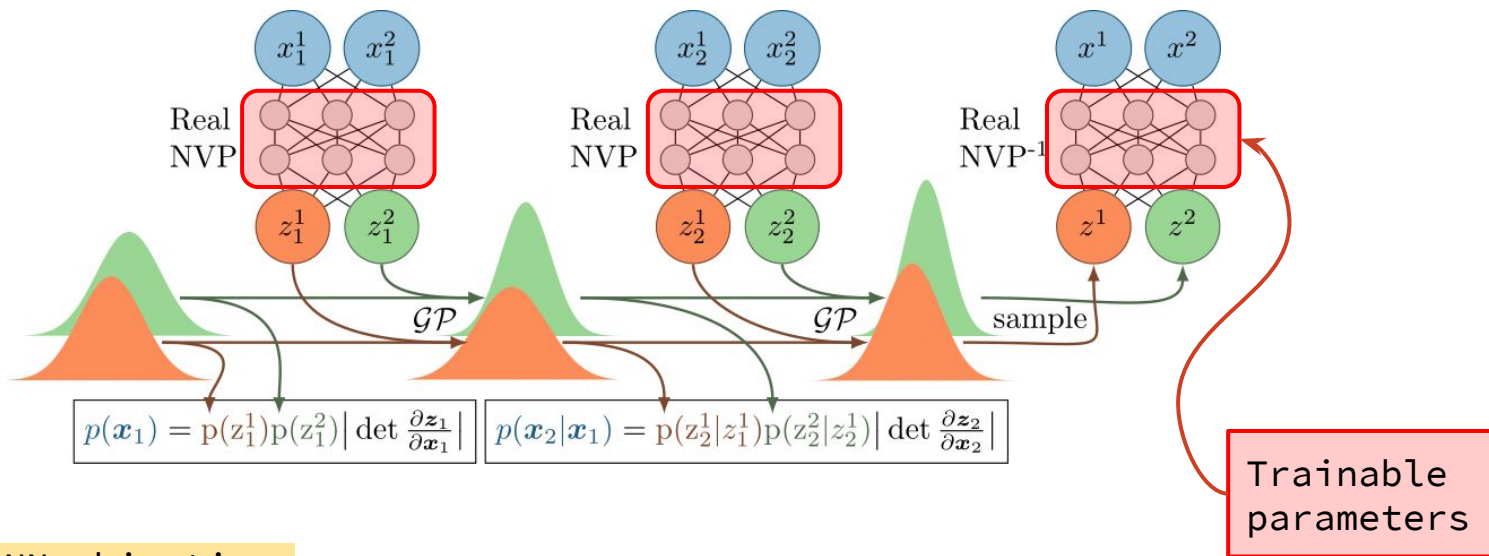
TRAINING BRUNO



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

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

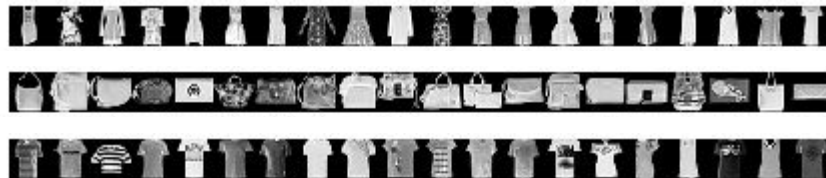


Training sequences

EXPERIMENTS: FASHION MNIST



Random samples from the dataset



Training sequences



BRUNO samples from the prior $p(x)$

EXPERIMENTS: FASHION MNIST

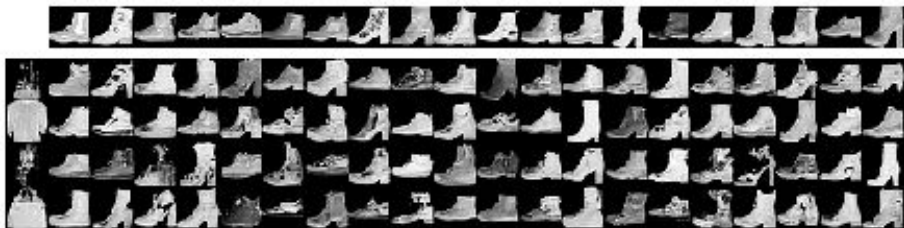
conditioning
inputs x_1, x_2, \dots



samples from
the prior $p(x)$

samples from
 $p(x|x_1)$

samples from
 $p(x|x_1, \dots, x_{20})$



LEARNING TO CORRELATE

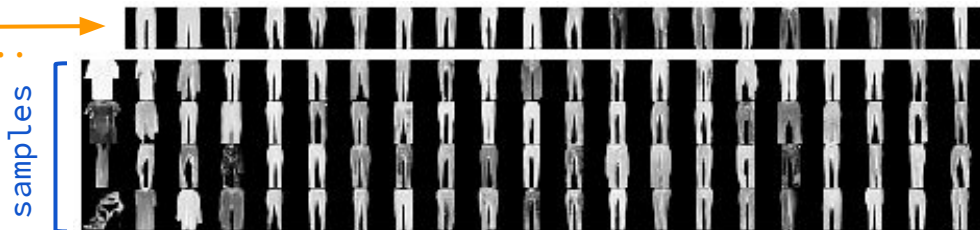


28x28 inputs \rightarrow 784 latent dimensions
with own variances and covariances:

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

LEARNING TO CORRELATE

conditioning
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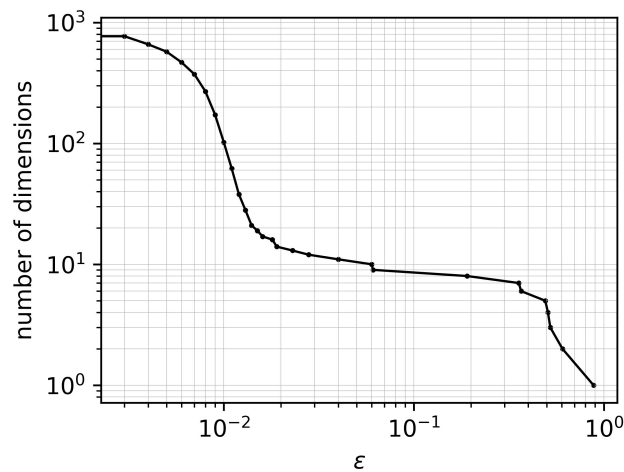


samples from the prior $p(x)$ samples from $p(x|x_1)$

samples from $p(x|x_1, \dots, x_{20})$

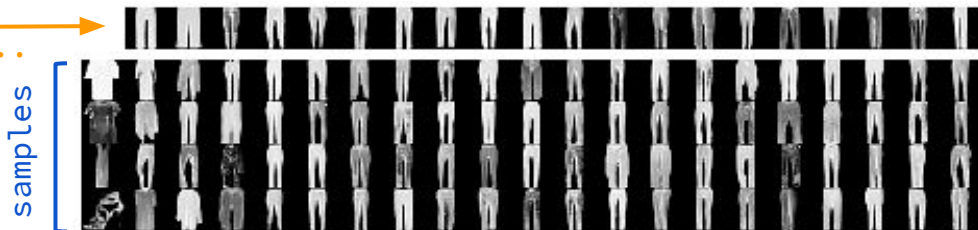
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LEARNING TO CORRELATE

conditioning
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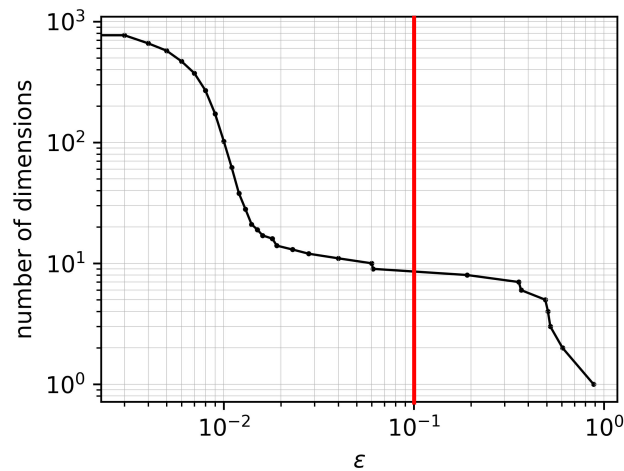


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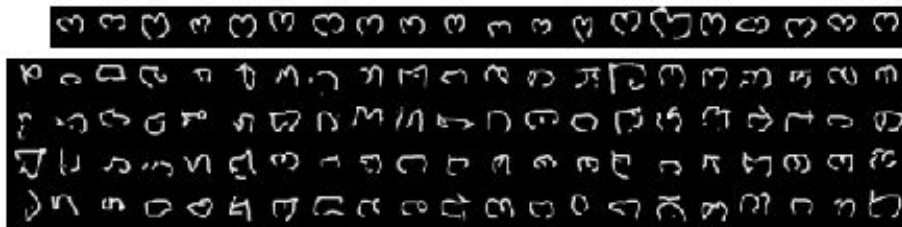
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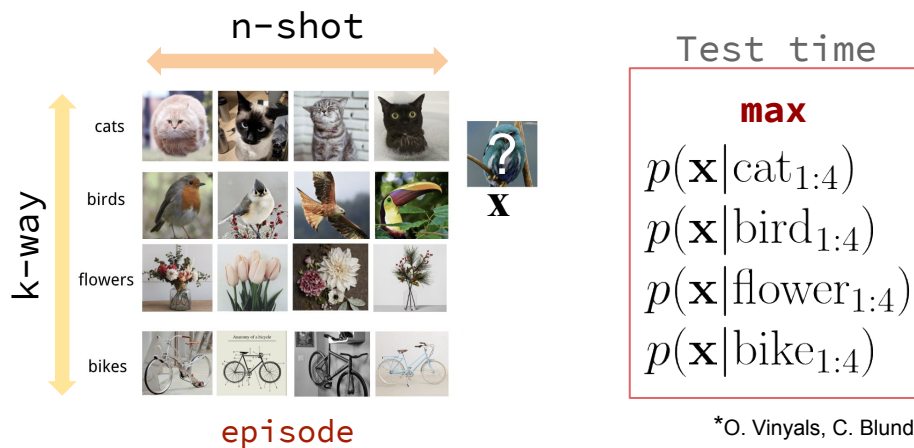
EXPERIMENTS: OMNIGLOT FEW-SHOT GENERATION

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



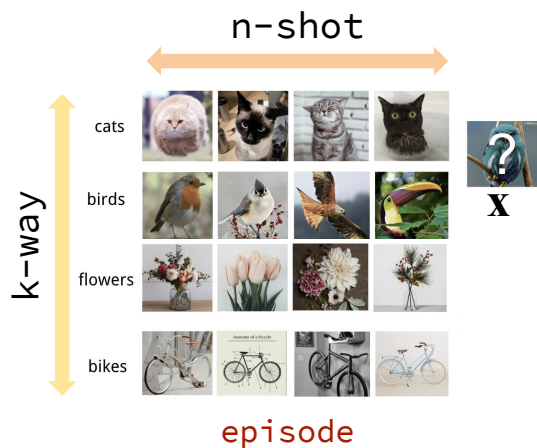
EXPERIMENTS: OMNIGLOT FEW-SHOT CLASSIFICATION

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



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Train time

softmax

$$\begin{aligned}
 & p(\mathbf{x} | \text{cat}_{1:4}) \\
 & p(\mathbf{x} | \text{bird}_{1:4}) \\
 & p(\mathbf{x} | \text{flower}_{1:4}) \\
 & p(\mathbf{x} | \text{bike}_{1:4})
 \end{aligned}$$

Fine-tune with a discriminative objective:

$$p(y = \text{'bird'} | x, S)$$

BRUNO

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

BRUNO

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CONDITIONAL BRUNO

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

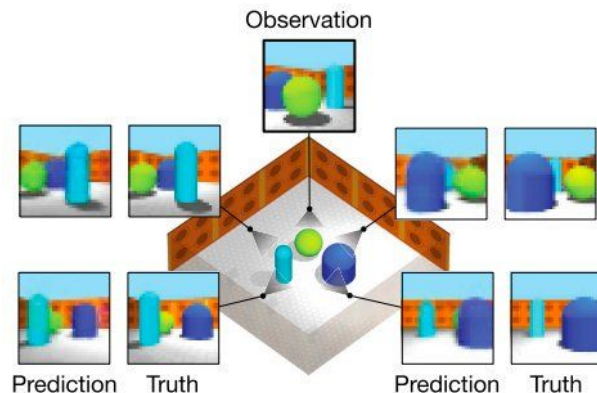
BRUNO

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

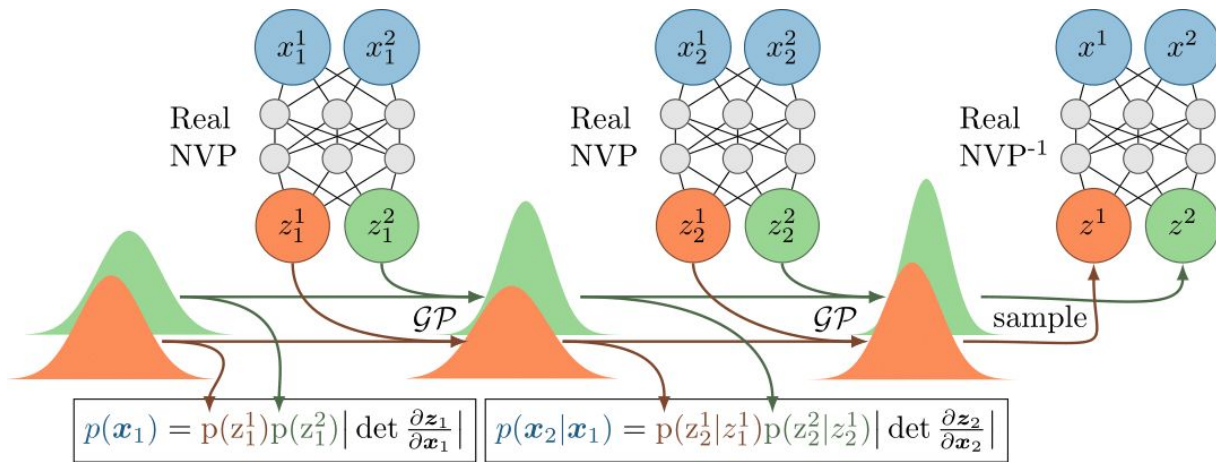
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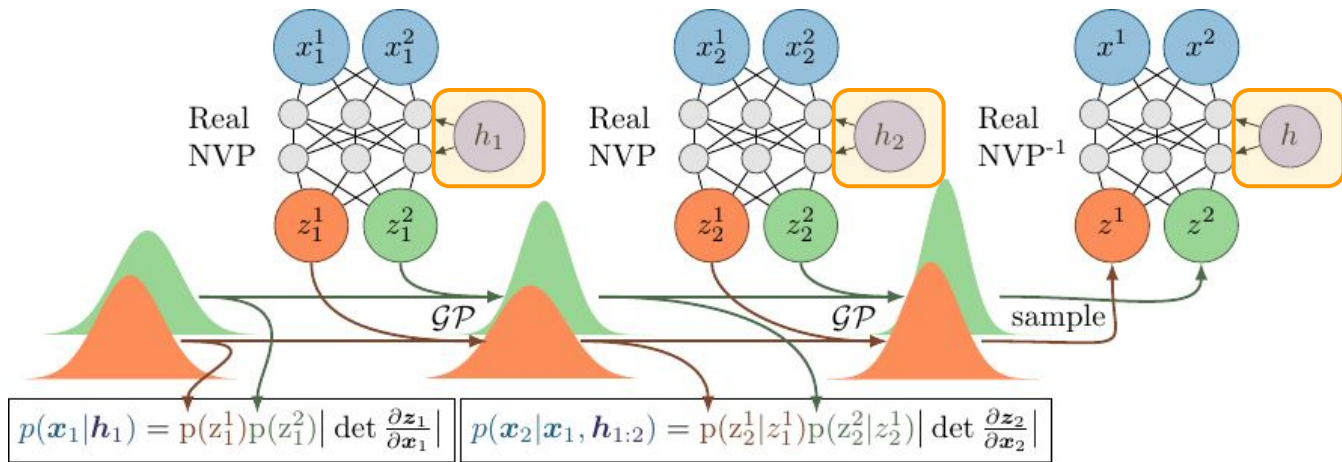
observations
scene view-point



BRUNO



CONDITIONAL BRUNO



EXPERIMENTS: SHAPENET CHAIRS & AIRPLANES

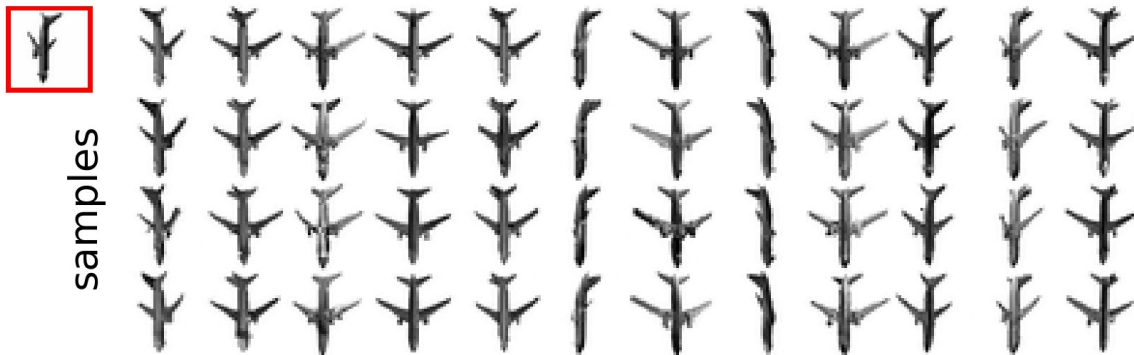
observation x_1 ] ground truth

samples



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

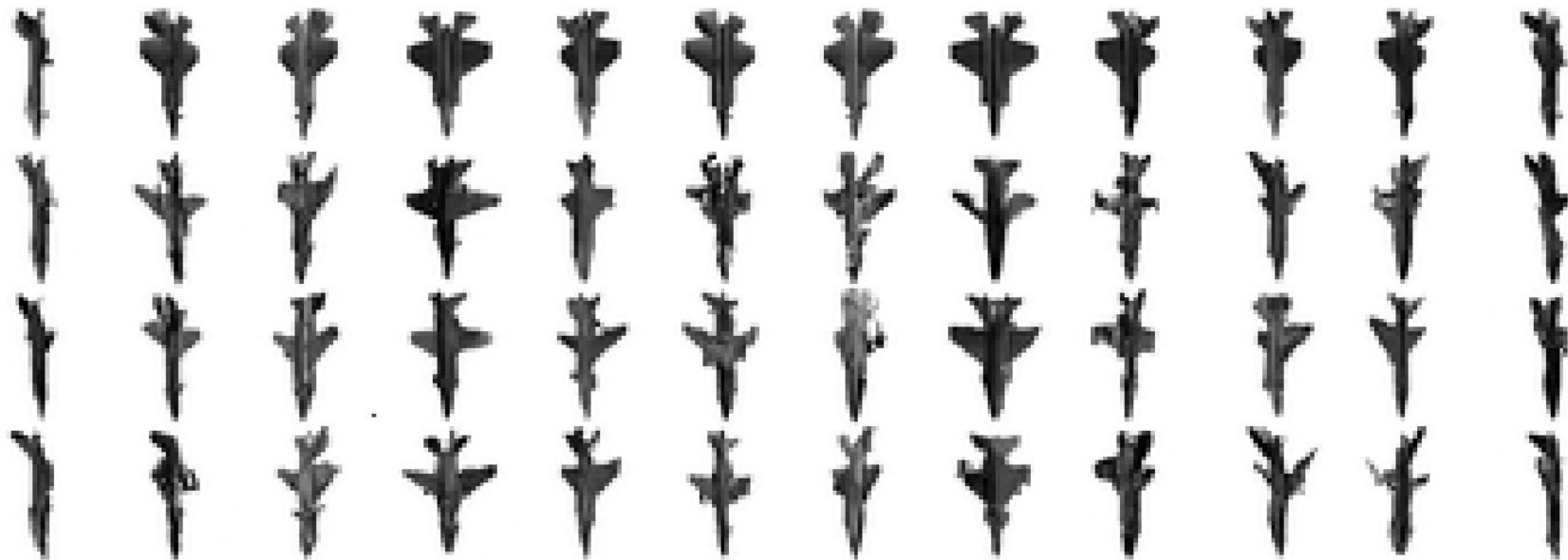
samples



EXPERIMENTS: SHAPENET CHAIRS & AIRPLANES



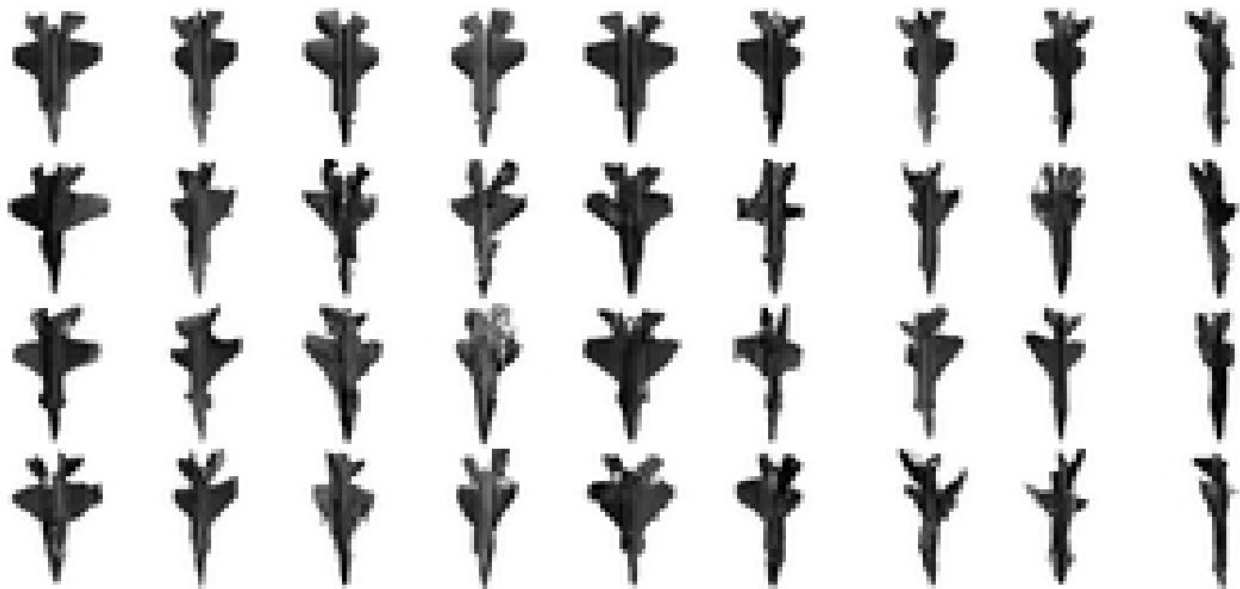
samples



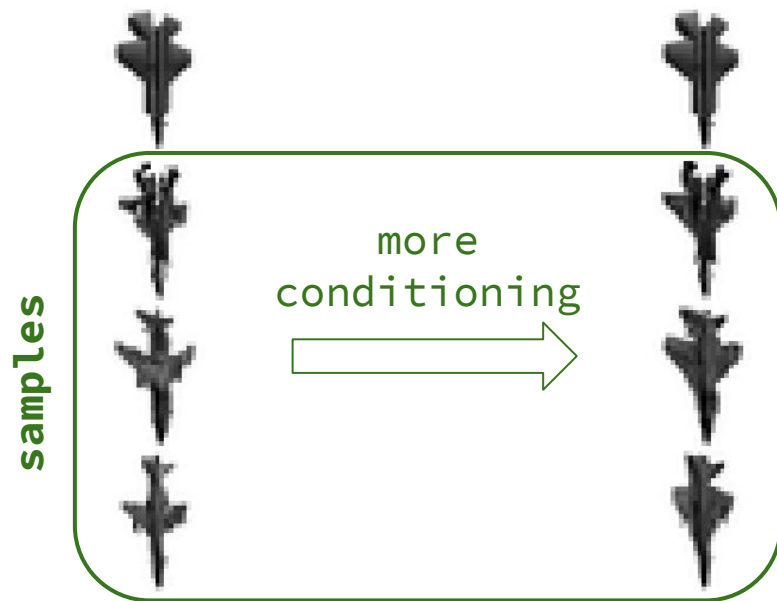
EXPERIMENTS: SHAPENET CHAIRS & AIRPLANES



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