

Unsupervised Deep Learning

Tutorial – Part I

Alex Graves



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Artificial Intelligence Research

Part I – Alex Graves

- Introduction to unsupervised learning
- Autoregressive models
- Representation learning
- Unsupervised reinforcement learning
- 10-15 minute break

Part 2 – Marc’Aurelio Ranzato

- Practical Recipes of Unsupervised Learning
- Learning representations
- Learning to generate samples
- Learning to map between two domains
- Open Research Problems
- 10-15 minutes questions (both presenters)

Introduction to Unsupervised Learning

Types of Learning

	With Teacher	Without Teacher
Active	Reinforcement Learning / Active Learning	Intrinsic Motivation / Exploration
Passive	Supervised Learning	Unsupervised Learning

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1. Targets / rewards can be **difficult to obtain** or define
2. Unsupervised learning feels more **human**
3. Want rapid **generalisation** to **new tasks** and situations

Transfer Learning

- Teaching on one task and **transferring** to another (multi-task learning, one-shot learning...) *kind of works*
- E.g. **Retraining** speech recognition systems from a language with lots of data can improve performance on a related language with little data
- But never seems to transfer as **far** or as **fast** as we want it to
- Maybe there just isn't enough **information** in the targets/rewards to learn transferable **skills**?

Stop learning tasks, start learning skills – Satinder Singh

The Cherry on the Cake

- The **targets** for supervised learning contain **far less** information than the input data
- RL **reward signals** contain even less
- Unsupervised learning gives us an essentially **unlimited** supply of information about the world: surely we should exploit that?

If intelligence was a cake, unsupervised learning would be the cake, supervised learning would be the icing on the cake, and reinforcement learning would be the cherry on the cake.

– Yann LeCun

Example

- ImageNet training set contains $\sim 1.28M$ images, each assigned one of 1000 labels
- If labels are equally probable, complete set of randomly shuffled labels contains $\sim \log_2(1000) * 1.28M \approx 12.8$ Mbits
- Complete set of images uncompressed at 128×128 contains ~ 500 Gbits: > 4 orders of magnitude more
- A large conv net ($\sim 30M$ weights) can memorise randomised ImageNet labellings. Could it memorise randomised pixels?

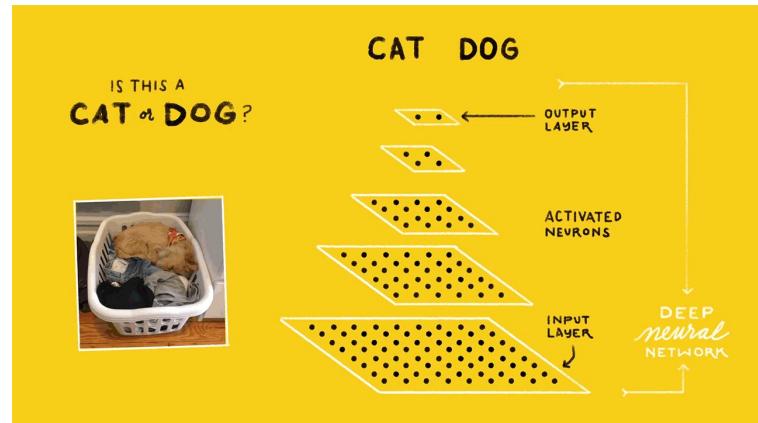
Supervised Learning

- Given a dataset D of **inputs x** labelled with **targets y** , learn to predict y from x , typically with **maximum likelihood**:

$$\mathcal{D} = \{(x, y)\}$$

$$L(\mathcal{D}) = \sum_{(x,y) \in \mathcal{D}} -\log p(y|x)$$

- (Still) the dominant paradigm in deep learning: image classification, speech recognition, translation...

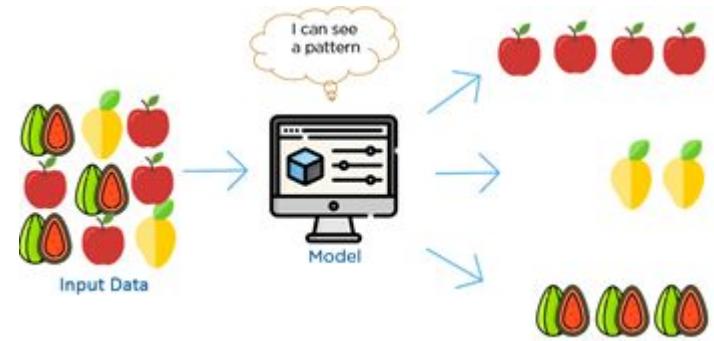


Unsupervised Learning

- Given a dataset D of inputs x , learn to predict... what?

$$\mathcal{D} = \{x\}$$

$$L(\mathcal{D}) = ???$$



- Basic challenge of unsupervised learning is that the task is **undefined**
- Want a single task that will allow the network generalise to many other tasks (**which ones?**)

Density Modelling

- Simplest approach: do **maximum likelihood** on the data instead of the targets

$$\mathcal{D} = \{x\}$$

$$L(\mathcal{D}) = \sum_{x \in \mathcal{D}} -\log p(x)$$

- Goal is to learn the '**true distribution**' from which the data was drawn
- Means attempting to learn **everything** about the data

Where to Look

Not everyone agrees that trying to understand everything is a good idea. Shouldn't we instead **focus** on things that we believe will one day be **useful** for us?

... we lived our lives under the constantly changing sky without sparing it a glance or a thought. And why indeed should we? If the various formations had had some meaning, if, for example, there had been concealed signs and messages for us which it was important to decode correctly, unceasing attention to what was happening would have been inescapable...

– Karl Ove Knausgaard, *A Death in the Family*

Problems with Density Modelling

- **First problem:** density modelling is **hard!** From having too few bits to learn from, we now have too many (e.g. video, audio), and we have to deal with complex interactions between variables (**curse of dimensionality**)
- **Second Problem:** **not all bits are created equal.** Log-likelihoods depend much more on low-level details (pixel correlations, word N-Grams) than on high-level structure (image contents, semantics)
- **Third problem:** even if we learn the underlying structure, it isn't always clear how to access and exploit that knowledge for future tasks (**representation learning**)

Generative Models

- Modelling densities also gives us a **generative model** of the data (as long as we can draw samples) $\hat{x} \sim p(x)$
- Allows us to ‘see’ what the model has and hasn’t learned
- Can also use generative models to **imagine** possible scenarios, e.g. for **model-based RL**

What I cannot create, I do not understand

– Richard Feynman

Autoregressive Models

The Chain Rule for Probabilities

$$P(w_1, w_2, \dots, w_{T-1}, w_T) = \prod_{t=1}^T P(w_t | w_{t-1}, w_{t-2}, \dots, w_1)$$

the	cat	sat	on	the	mat	$P(w_1)$
the	cat	sat	on	the	mat	$P(w_2 w_1)$
the	cat	sat	on	the	mat	$P(w_3 w_2, w_1)$
the	cat	sat	on	the	mat	$P(w_4 w_3, w_2, w_1)$
the	cat	sat	on	the	mat	$P(w_5 w_4, w_3, w_2, w_1)$
the	cat	sat	on	the	mat	$P(w_6 w_5, w_4, w_3, w_2, w_1)$

Autoregressive Networks

- Basic trick: split high dimensional data up into a sequence of small pieces, predict each piece from those before (~~curse of dimensionality~~)
- Conditioning on past is done via network state (LSTM/GRU, masked convolutions, transformers...), output layer parameterises predictions

$$\mathcal{D} = \{\mathbf{x}\}$$

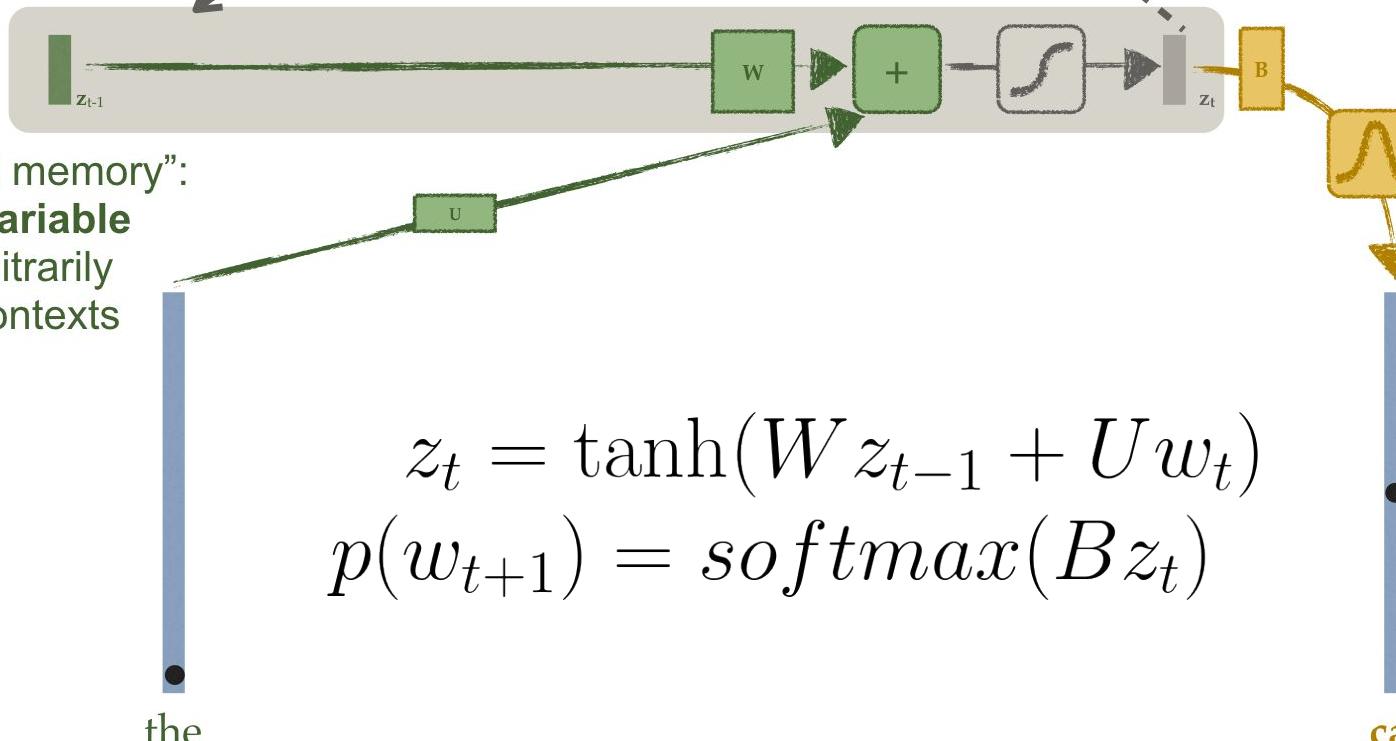
$$\mathbf{x} = (x_1, \dots, x_T)$$

$$p(\mathbf{x}) = \prod_{t=1}^T p(x_t | x_{<t})$$

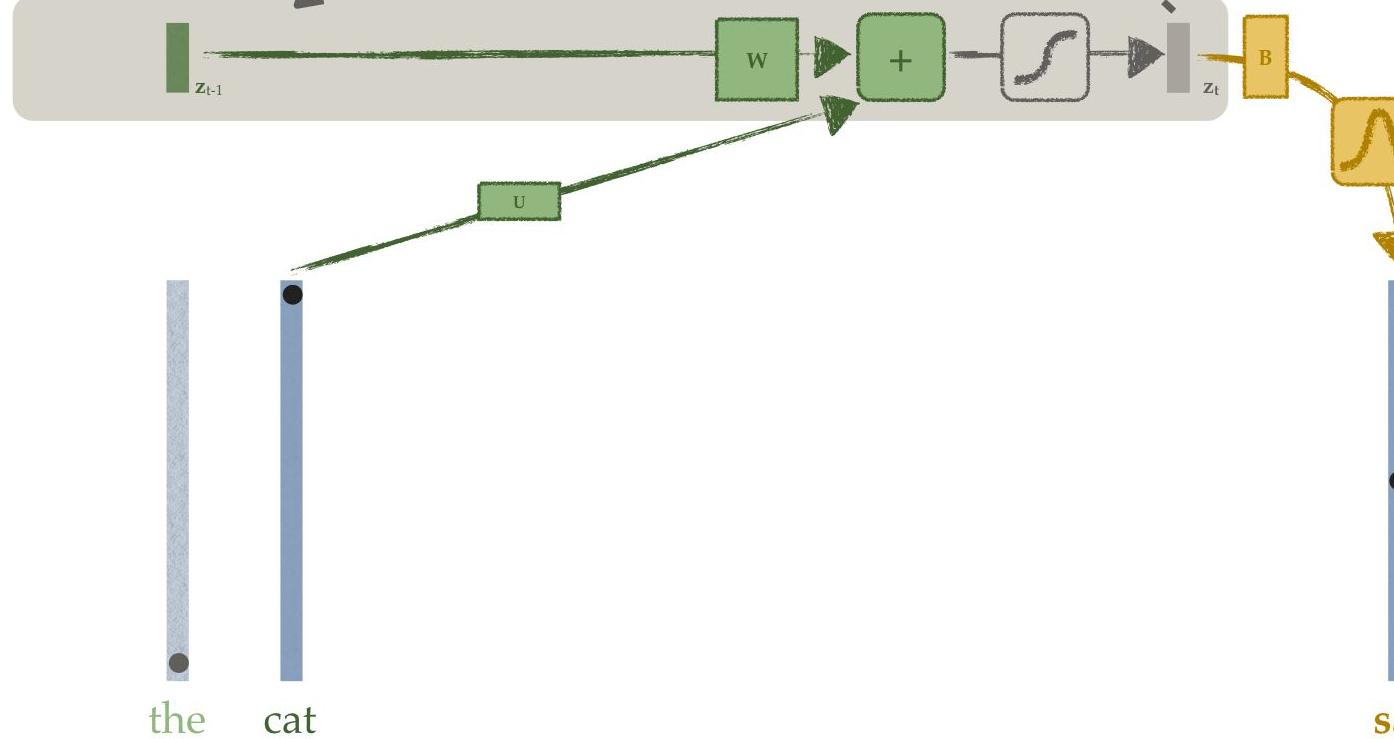
$$L(\mathcal{D}) = \sum_{\mathbf{x} \in \mathcal{D}} \sum_{t=1}^T -\log p(x_t | x_{<t})$$

Recurrent Neural Network Language Models

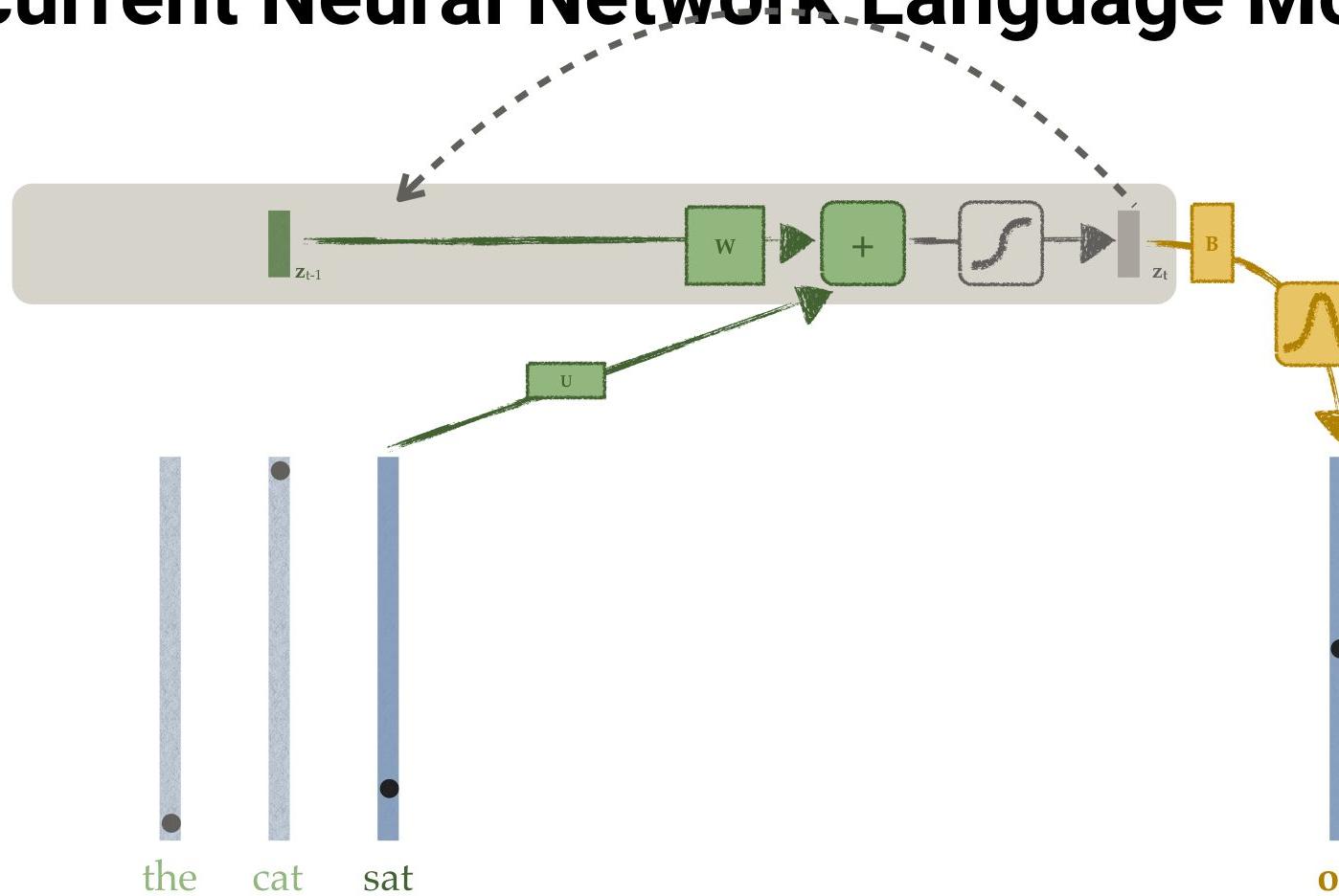
[Jeffrey L Elman (1991) "Distributed representations, simple recurrent networks and grammatical structure", *Machine Learning*;
Tomas Mikolov et al. (2010) "Recurrent neural network based language model", *INTERSPEECH*]



Recurrent Neural Network Language Models



Recurrent Neural Network Language Models

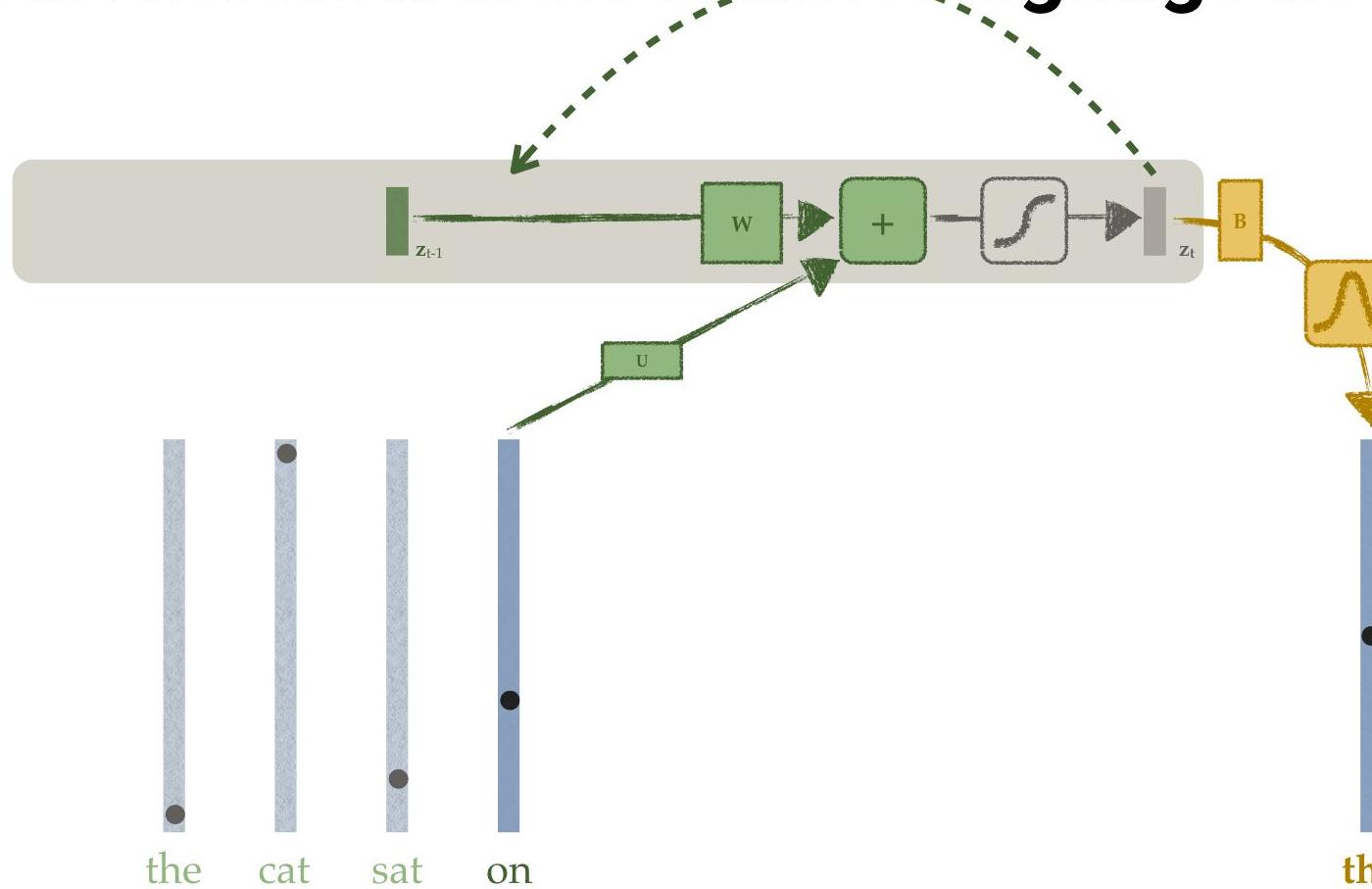


the cat sat

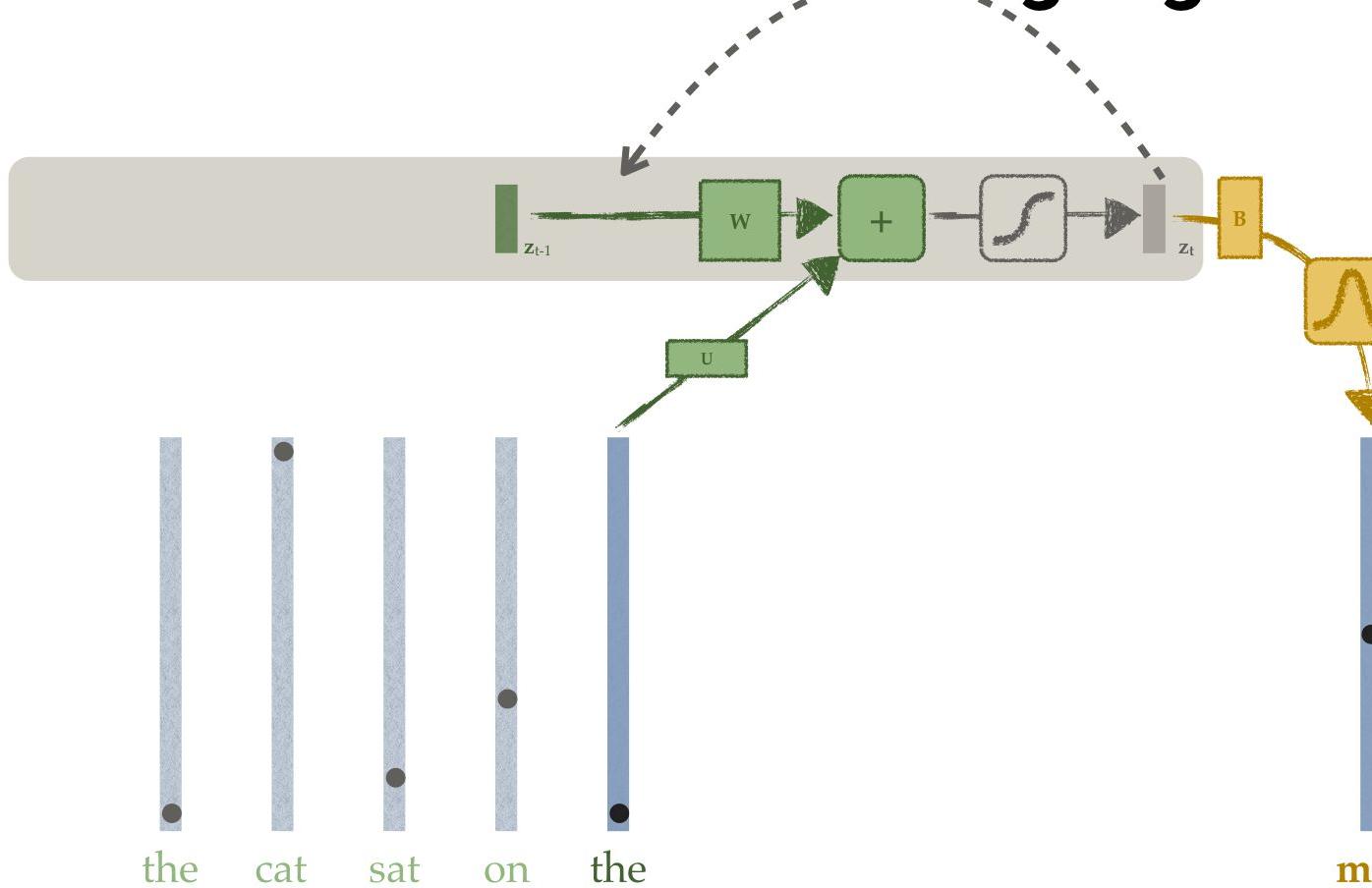
on

Slide Credit: Piotr Mirowski

Recurrent Neural Network Language Models



Recurrent Neural Network Language Models



Advantages of Autoregressive Models

- **Simple to define:** just have to pick an ordering
- **Easy to generate samples:** just sample from each predictive distribution, then feed in the sample at the next step as if it's real data (dreaming for neural networks?)
- **Best log-likelihoods for many types of data:** images, audio, video, text...

Disadvantages of Autoregressive Models

- **Very expensive** for high-dimensional data (e.g millions of predictions per second for video); can mitigate with **parallelisation** during training, but **generating** still slow
- **Order dependent**: get very different results depending on the order in which predictions are made, and can't easily **impute** out of order
- **Teacher forcing**: only learning to predict one step ahead, not many (potentially brittle generation and myopic representations)

Language Modelling

Some of the obese people lived five to eight years longer than others.

Abu Dhabi is going ahead to build solar city and no pollution city.

Or someone who exposes exactly the truth while lying.

VIERA , FLA . -- Sometimes, Rick Eckstein dreams about baseball swings.

For decades, the quintessentially New York city has elevated its streets to the status of an icon.

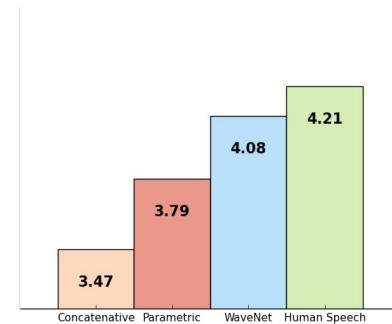
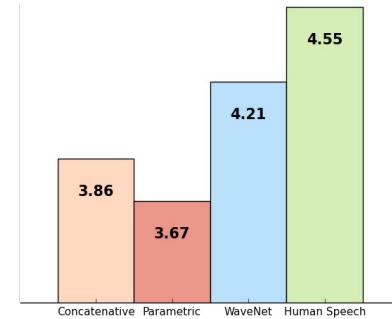
The lawsuit was captioned as United States ex rel.

MODEL	TEST PERPLEXITY
LARGE ENSEMBLE (CHELBA ET AL., 2013)	43.8
RNN+KN-5 (WILLIAMS ET AL., 2015)	42.4
RNN+KN-5 (JI ET AL., 2015A)	42.0
RNN+SNM10-SKIP (SHAZEER ET AL., 2015)	41.3
LARGE ENSEMBLE (SHAZEER ET AL., 2015)	41.0
OUR 10 BEST LSTM MODELS (EQUAL WEIGHTS)	26.3
OUR 10 BEST LSTM MODELS (OPTIMAL WEIGHTS)	26.1
10 LSTMS + KN-5 (EQUAL WEIGHTS)	25.3
10 LSTMS + KN-5 (OPTIMAL WEIGHTS)	25.1
10 LSTMS + SNM10-SKIP (SHAZEER ET AL., 2015)	23.7

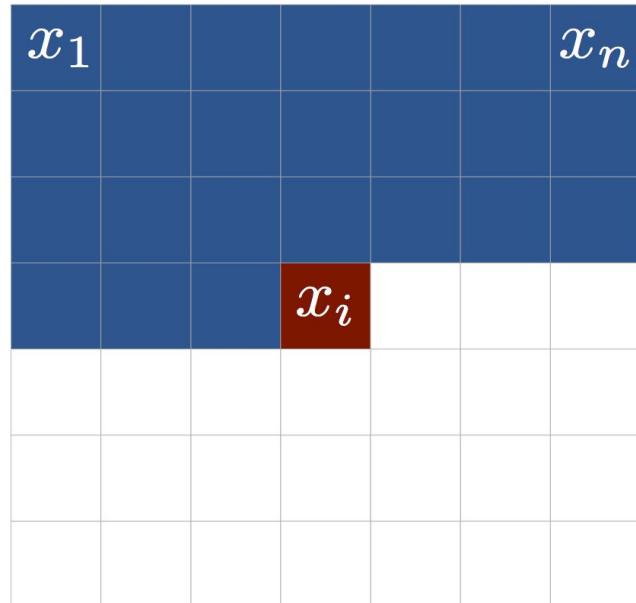
WaveNets



1 Second



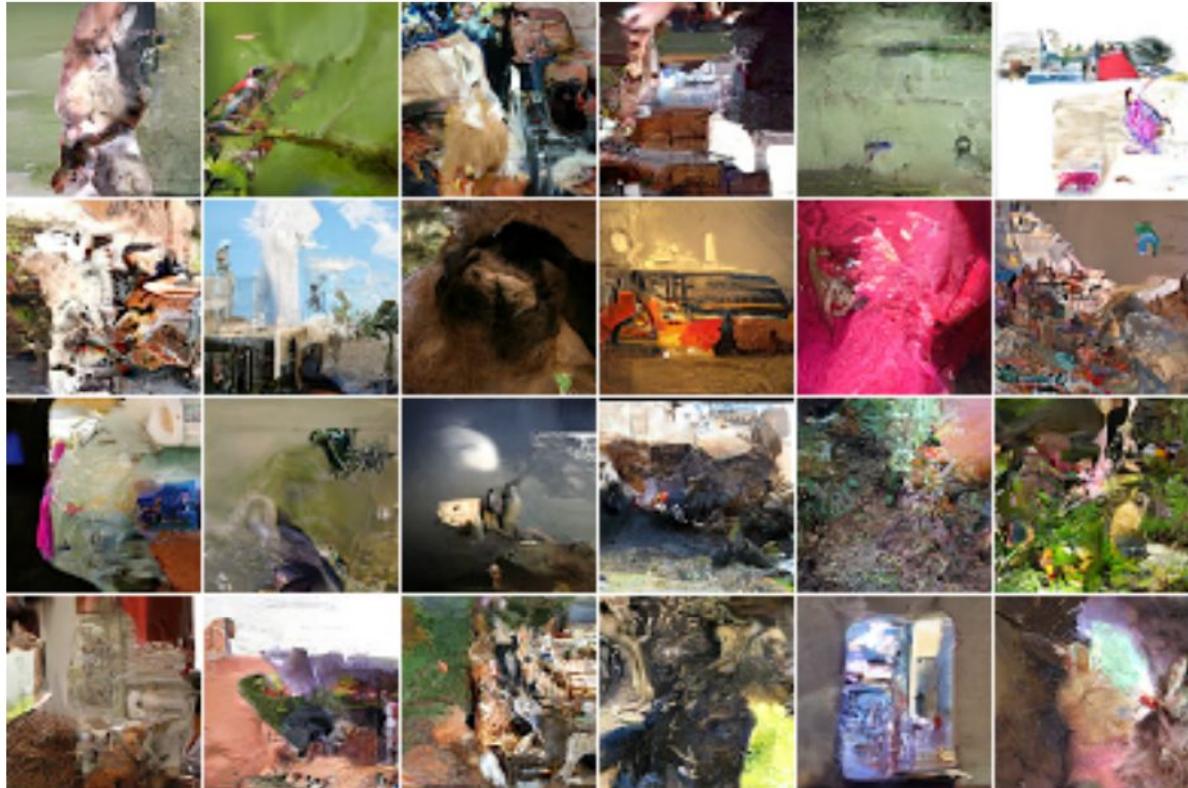
PixelRNN - Model



$$p(\mathbf{x}) = \prod_{i=1}^{n^2} p(x_i | x_1, \dots, x_{i-1})$$

- Fully visible
- Model pixels with **Softmax**
- ‘Language model’ for images

Pixel RNN - Samples



van den Oord, A., et al. "Pixel Recurrent Neural Networks." *ICML* (2016).

Conditional Pixel CNN



Geyser



Hartebeest

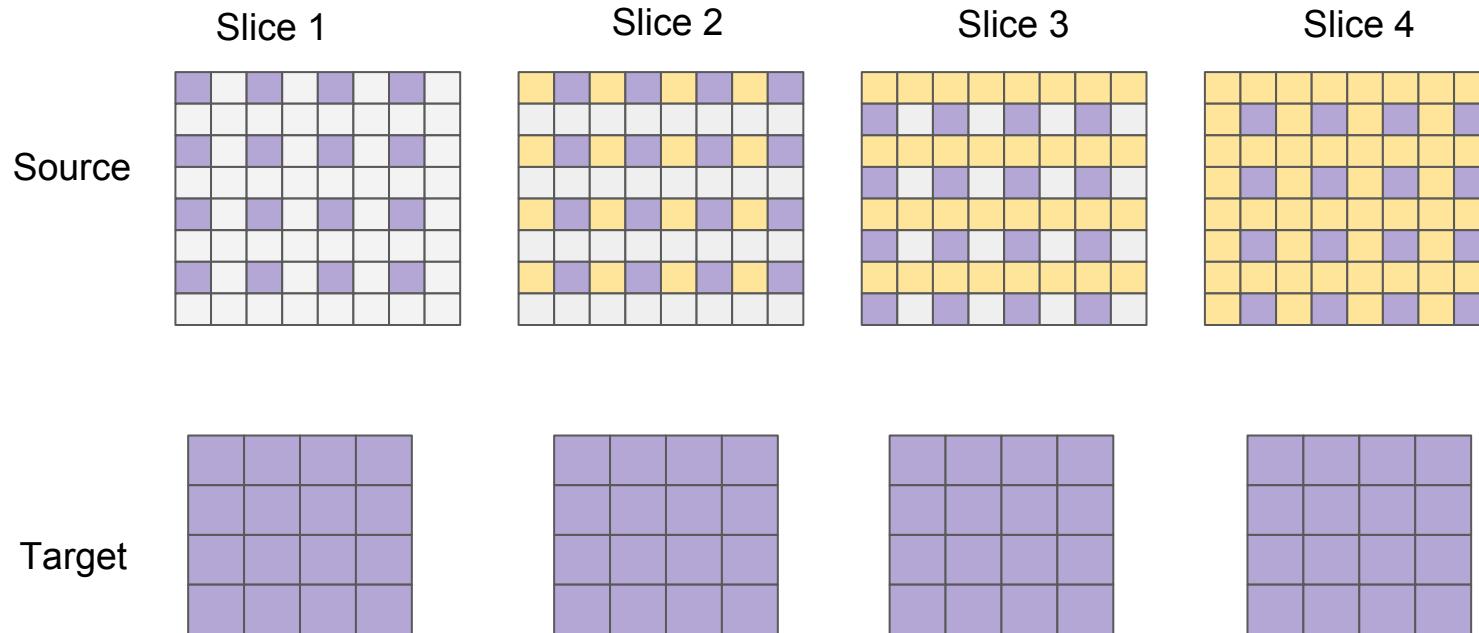


Grey whale



Tiger

Autoregressive over slices, then pixels within a slice



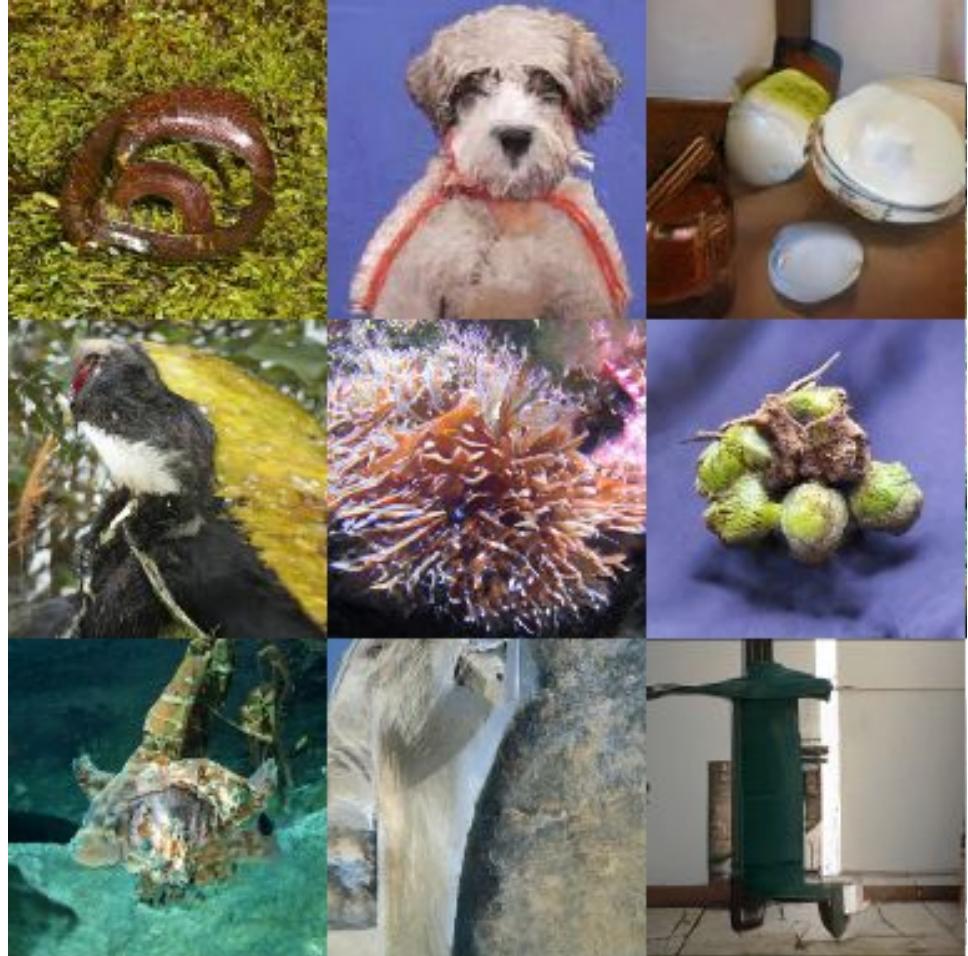
256 x 256 CelebA-HQ



J. Menick et. al. *Generating High Fidelity Images with subsample pixel networks and multidimensional upscaling* (2018)

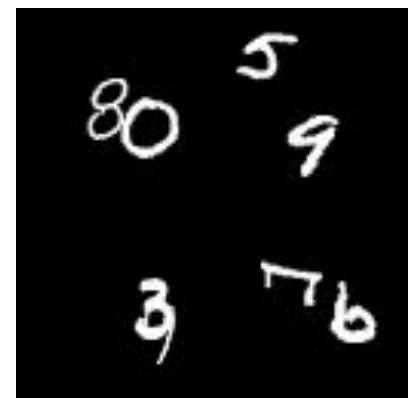
128 × 128 ImageNet

J. Menick et. al. *Generating High Fidelity Images with subsample pixel networks and multidimensional upscaling* (2018)



Video Pixel Network (VPN)

Model	Test
(Shi et al., 2015)	367.2
(Srivastava et al., 2015a)	341.2
(Brabandere et al., 2016)	285.2
(Patraucean et al., 2015)	179.8
Baseline model	110.1
VPN	87.6
Lower Bound	86.3

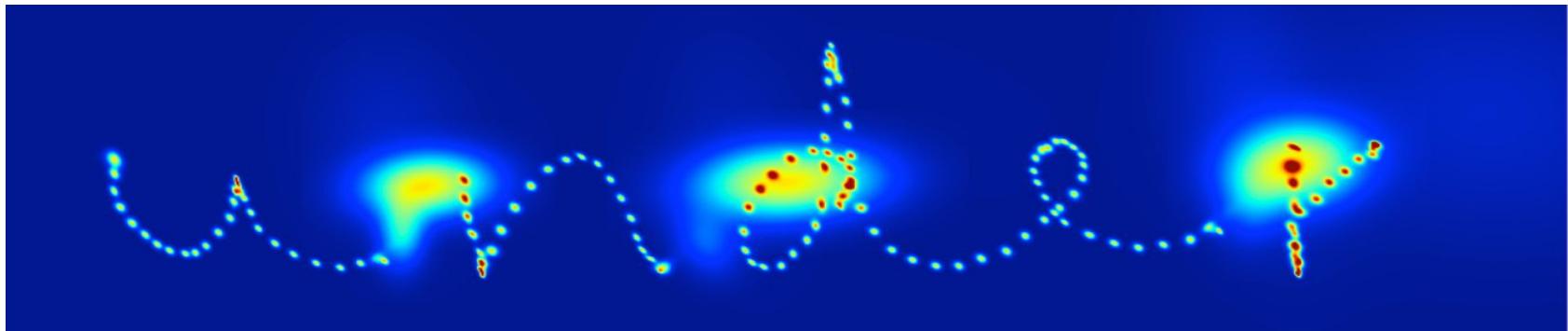


Handwriting Synthesis

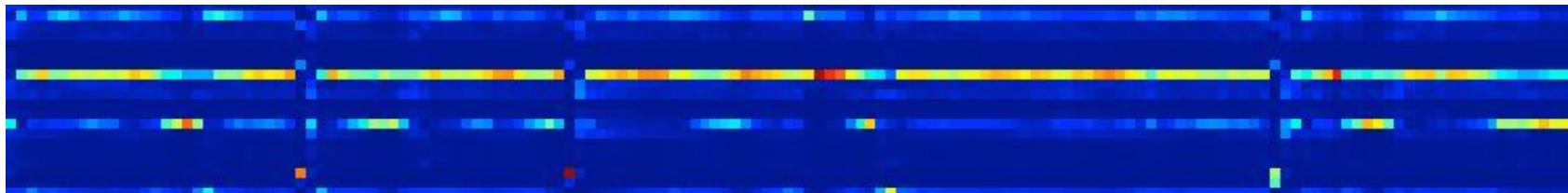
from his travels it might have been

Autoregressive Mixture Models

Co-ordinate Density



Component Weights



Distribution over Sequences

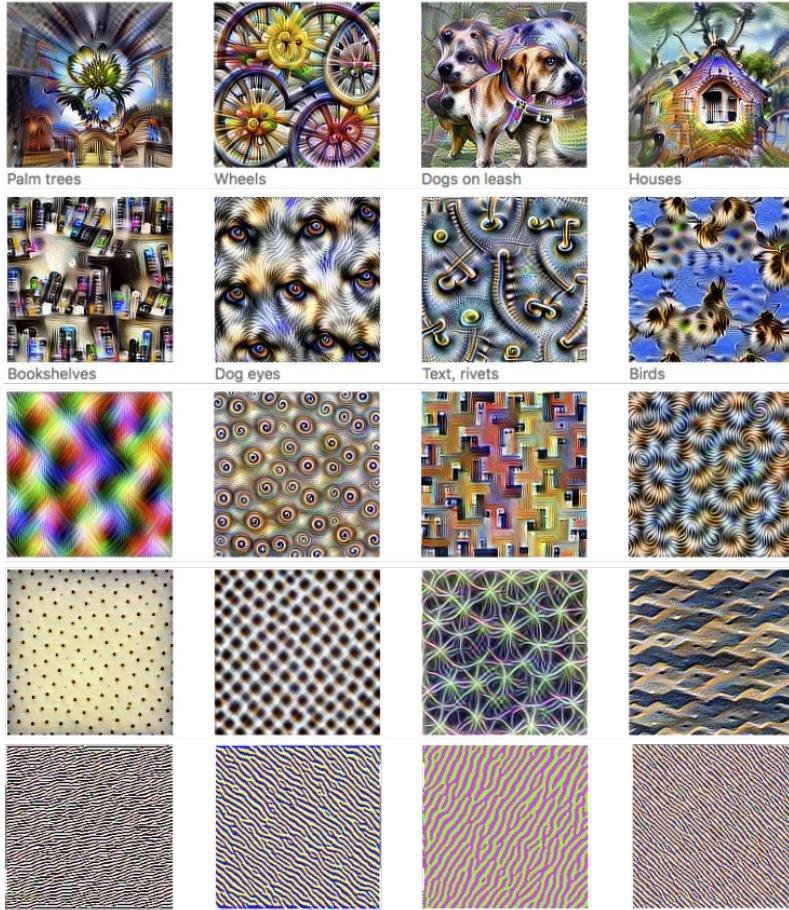


Carter et. al., *Experiments in Handwriting with a Neural Network* (2016)

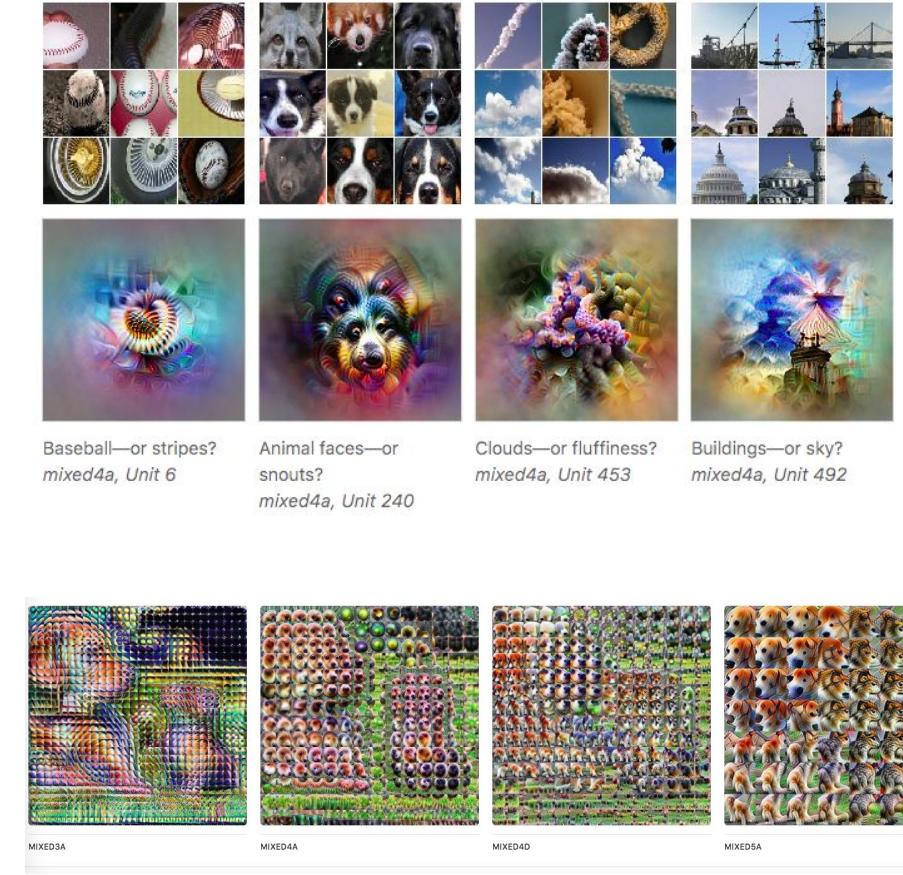
Representation Learning

The Language of Neural Networks

- Deep networks work by learning complex, often hierarchical internal **representations** of input data
- These form a kind of **language** the network uses to describe the data
- Language can **emerge** from **tasks** like object recognition:
has pointy ears, whiskers, tail => cat (c.f. **Wittgenstein**)



The visual vocabulary of a convolutional neural network. For each layer of the network, images are generated that maximally activate particular neurons. The response of these neurons to other images can then be interpreted as the presence or absence of visual "words": textures, bookshelves, dog snouts, birds



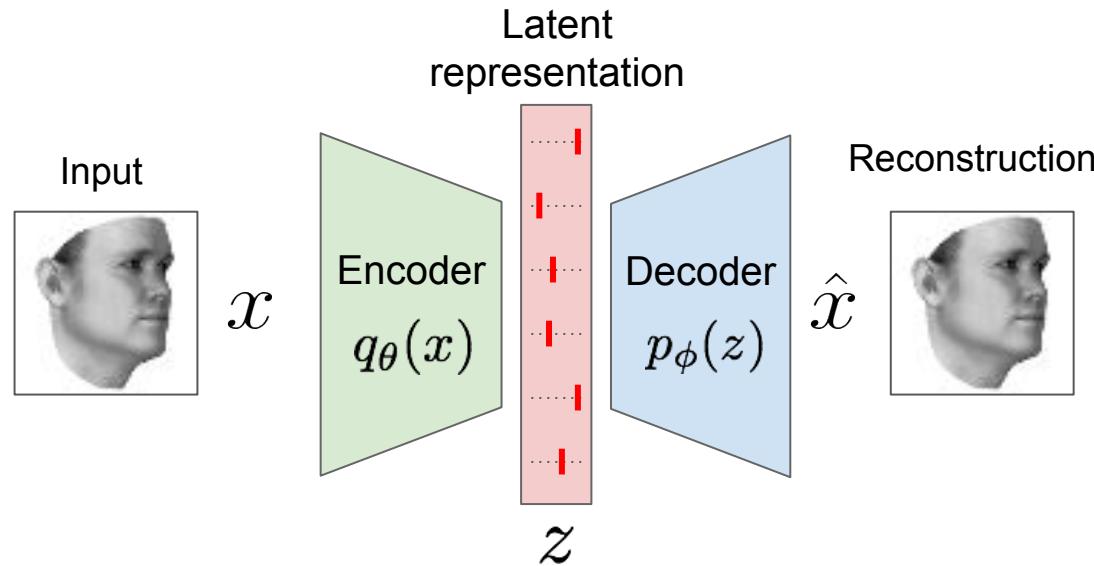
Unsupervised Representations

- Task-driven representations are limited by the **requirements** of the task: e.g. don't need to internalise the laws of physics to recognise objects
- Unsupervised representations **should** be more general: as long as the laws of physics help to model observations in the world, they are worth representing

Reading the Latent Language

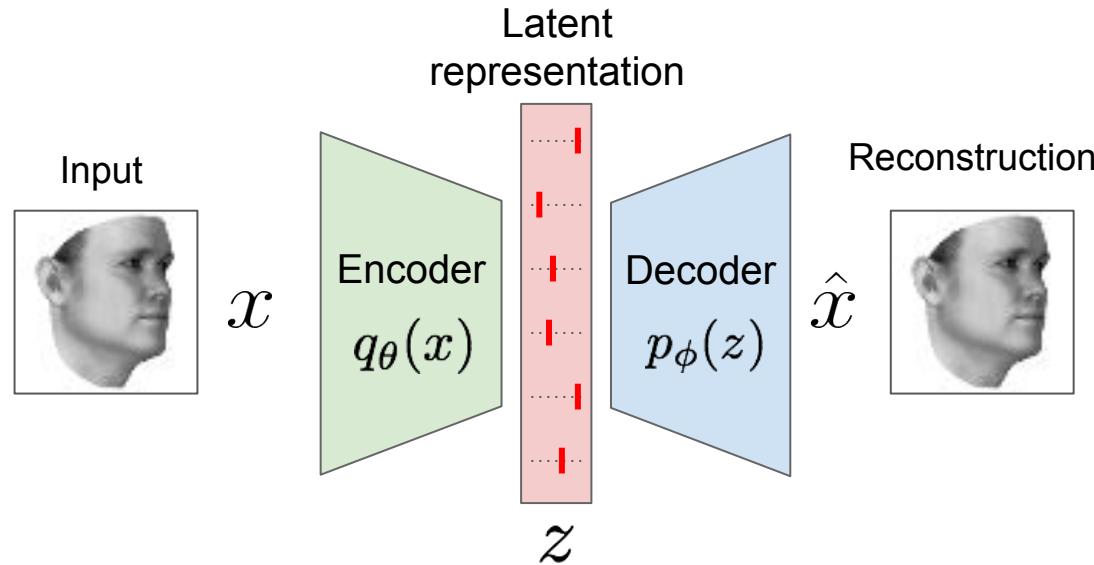
- We want neural networks to **describe** the data to us (image captioning without the captions?)
- Then we can **re-use** the descriptions to **plan**, **reason**, and **generalise** at a more abstract level
- Good density models **must** learn a rich internal language, but we can't read it (distil for WaveNet?): we need to break open the black box
- One way to make representations more **accessible** is to force them through a **bottleneck**

Autoencoder



$$\mathcal{L}^{AE}(\mathbf{x}; \theta, \phi) = \frac{[\mathbf{x} - p_\theta(q_\phi(\mathbf{x})]^2}{\text{Reconstruction cost}}$$

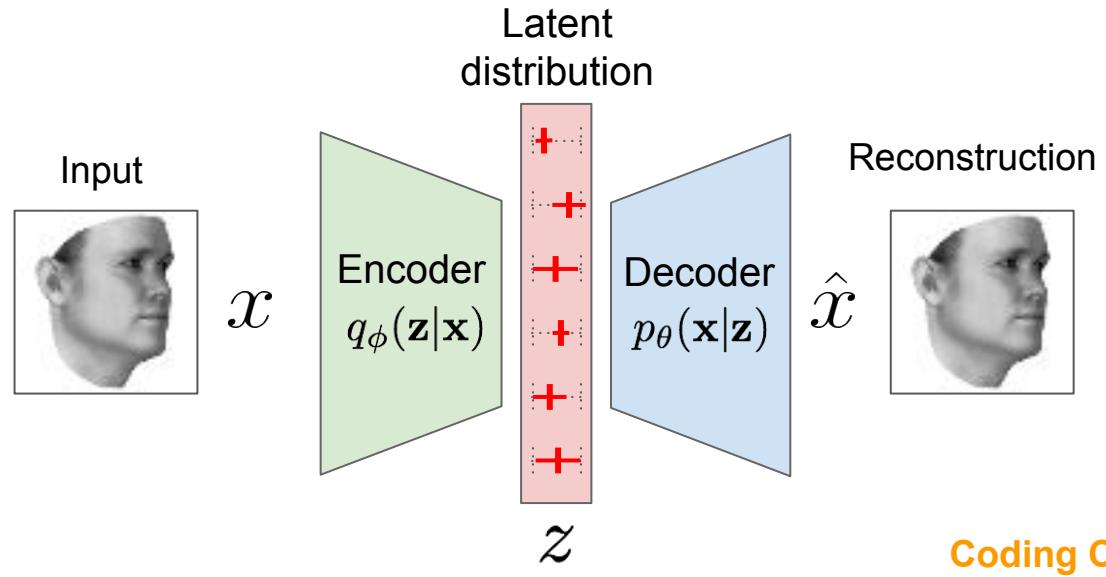
Autoencoder



$$\mathcal{L}^{AE}(\mathbf{x}; \theta, \phi) = \frac{\left[\mathbf{x} - p_\phi(q_\phi(\mathbf{x})) \right]^2 - \log p_\theta(q_\phi(\mathbf{x}))}{\text{Reconstruction cost}}$$

Variational AutoEncoder

Kingma et al, 2014
Rezende et al, 2014



$$\mathcal{L}_{VAE}(\mathbf{x}; \theta, \phi) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})} [-\log p_\theta(\mathbf{x}|\mathbf{z})] + KL(q_\phi(\mathbf{z}|\mathbf{x}) || p(\mathbf{z}))$$

Reconstruction cost

Minimum Description Length for VAE

- Alice wants to transmit \mathbf{x} as compactly as possible to Bob, who knows only the prior $p(\mathbf{z})$ and the decoder weights
- The **coding cost** is the number of bits required for Alice to transmit a sample from $q_{\theta}(\mathbf{z}|\mathbf{x})$ to Bob (e.g. **bits-back** coding)
- The **reconstruction cost** measures the number of additional error bits Alice will need to send to Bob to reconstruct the data given the latent sample (e.g. **arithmetic** coding)
- The sum of the two costs is the total length of the message Alice needs to send to Bob to allow him to recover \mathbf{x} (c.f. **variational inference**)

Code Collapse

- Ideally a VAE would put **high-level** information in the codes, leave **low-level** information to the decoder
- **But** when the decoder is sufficiently powerful (e.g. autoregressive) the coding distribution tends to ‘collapse’ to the prior $p(z)$
- This means no information is passed through the bottleneck and no latent representation is learned
- **MDL** suggests a reason: **a powerful decoder can implicitly learn $p(z)$** , meaning that if each x is **independently** transmitted, the number of bits saved by the decoder by conditioning on $z \approx$ the cost of transmitting z

Thought Experiments

- **Experiment 1:** An MNIST Decoder learns a uniform mixture over 10 disjoint models. Prior is uniform over 10 classes. Conditioning on the image class saves $\sim \log_2(10)$ bits, encoding the class costs $\sim \log_2(10)$ bits
- **Experiment 2:** Pick 100 character strings at random from an encyclopedia. The context from the paragraph, article etc. is missing. Is it worth appending that information to each of the strings?

Learn the Dataset, Not the Datapoints

- Suggests a fundamental flaw with using log-likelihoods to find representations: never worth encoding high-level information
- Example: conditioning on ImageNet labels makes a huge difference to samples, tiny difference to log-probs ($\approx \log_2(1000)$ bits)
- **But** one label applies to many data, so worth encoding high-level information **if we only encode it once for the whole dataset** ($\approx 1000 \times \log_2(1000)$ bits)
- Want to **amortise** the coding cost over the whole dataset
- Use high level information to **organise** low level data, not **annotate** it

...one must take seriously the idea of working with datasets, rather than datapoints, as the key objects to model.

– Edwards & Storkey, *Towards a Neural Statistician*, (2017)

Associative Compression Networks

- ACNs modify the VAE loss by replacing the **unconditional** prior $p(z)$ with a **conditional** prior $p(z|z')$, where z' is the latent representation of an **associated** data point (one of the **K nearest Euclidean neighbours** to z)
- $p(z|z')$ – parameterised by an MLP – models only part of the latent space, rather than the whole thing, which **greatly reduces the coding cost**
- **Implicit amortisation:** the more clustered the codes, the cheaper they are
- **Result:** rich, informative codes are learned, even with powerful decoders.

MDL for ACN

- Alice now wants to transmit the entire ***dataset*** to Bob, **in any order** (justified for **IID** data?)
- Bob has the weights of the associative prior, decoder **and encoder**
- Alice chooses an ordering for the data that minimises total coding cost (**travelling salesman**) and sends the data to Bob **one at a time**.
- After receiving each latent code + error bits, he decodes the datapoint, then re-encodes it and uses the result to determine the **associative prior** for the next code

Algorithm 1 Associative Compression Network Training

Initialise \mathbf{C} : $c(x) \sim \mathcal{N}(0, 1) \forall x \in \mathbf{X}$

repeat

 Sample x uniformly from \mathbf{X}

 Run encoder network, get $q(z|x)$

 Update \mathbf{C} with new code: $c(x) \leftarrow \mathbb{E}_{z \sim q(z|x)} [z]$

$KNN(x) \leftarrow K$ nearest Euc. neighbours to $c(x)$ in \mathbf{C}

 Pick \hat{c} randomly from $KNN(x)$

 Run prior network, get $r(z|\hat{c})$

$z \sim q(z|x)$

 Run decoder network, compute $-\log p(x|z)$

$L^{ACN}(x) = KL(q(z|x)||r(z|\hat{c})) - \log p(x|z)$

 Compute gradients, update network weights

until convergence

Red bits are
different from
standard VAE,
The rest is the
same

Table 3. Binarized MNIST linear classification results

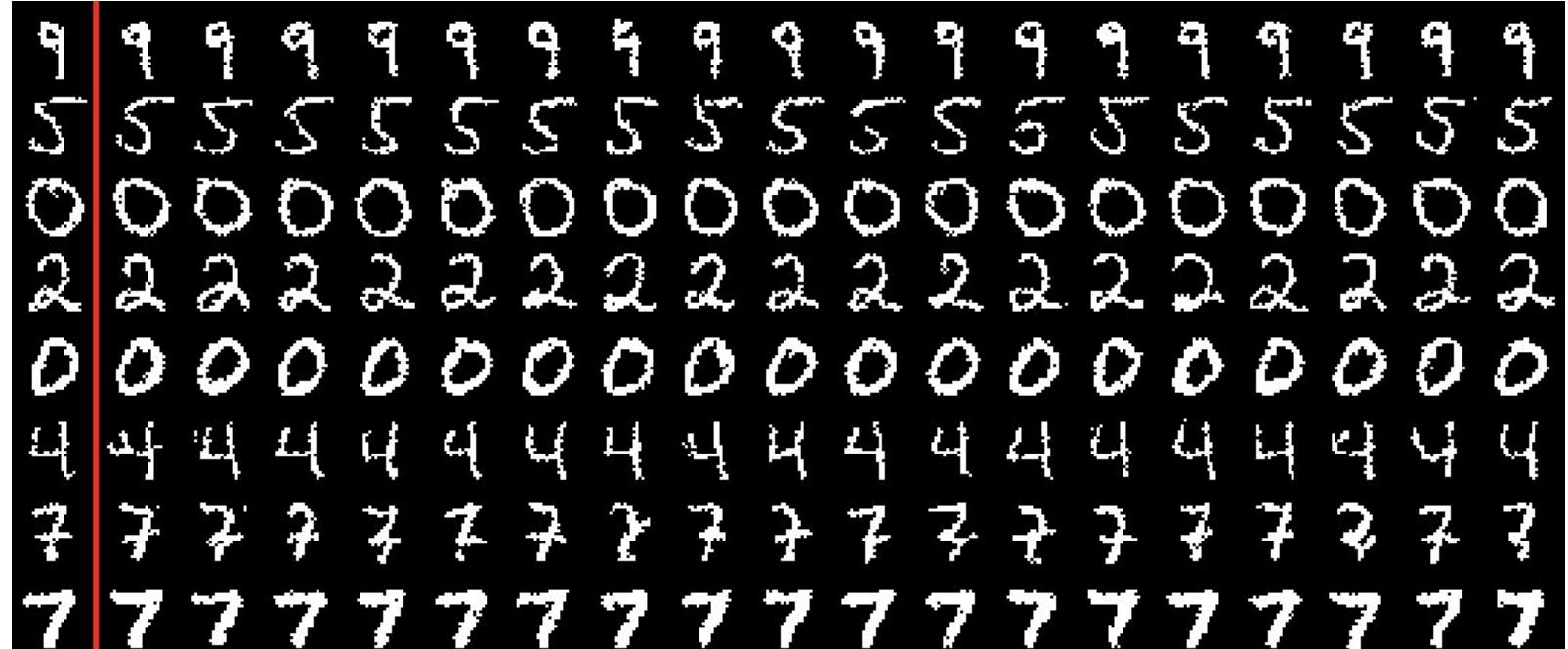
INPUT	ACCURACY (%)
PCA (16 COMPONENTS)	82.8
PIXELS	89.4
STANDARD VAE CODES	95.4
GATED PIXELVAE CODES	97.9
ACN CODES	98.5

Table 1. Binarized MNIST test set compression results

MODEL	NATS / IMAGE
GATED PIXEL CNN (OURS)	81.6
PIXEL CNN (OORD ET AL., 2016A)	81.3
DISCRETE VAE (ROLFE, 2016)	81.0
DRAW (GREGOR ET AL., 2015)	≤ 81.0
PIXEL RNN (OORD ET AL., 2016A)	79.2
VLAE (CHEN ET AL., 2016B)	79.0
GLN (VENESS ET AL., 2017)	79.0
MATNET (BACHMAN, 2016)	≤ 78.5
ACN (UNORDERED)	≤ 80.9
ACN (ORDERED)	≤ 73.9

Unordered: KL from unconditional prior

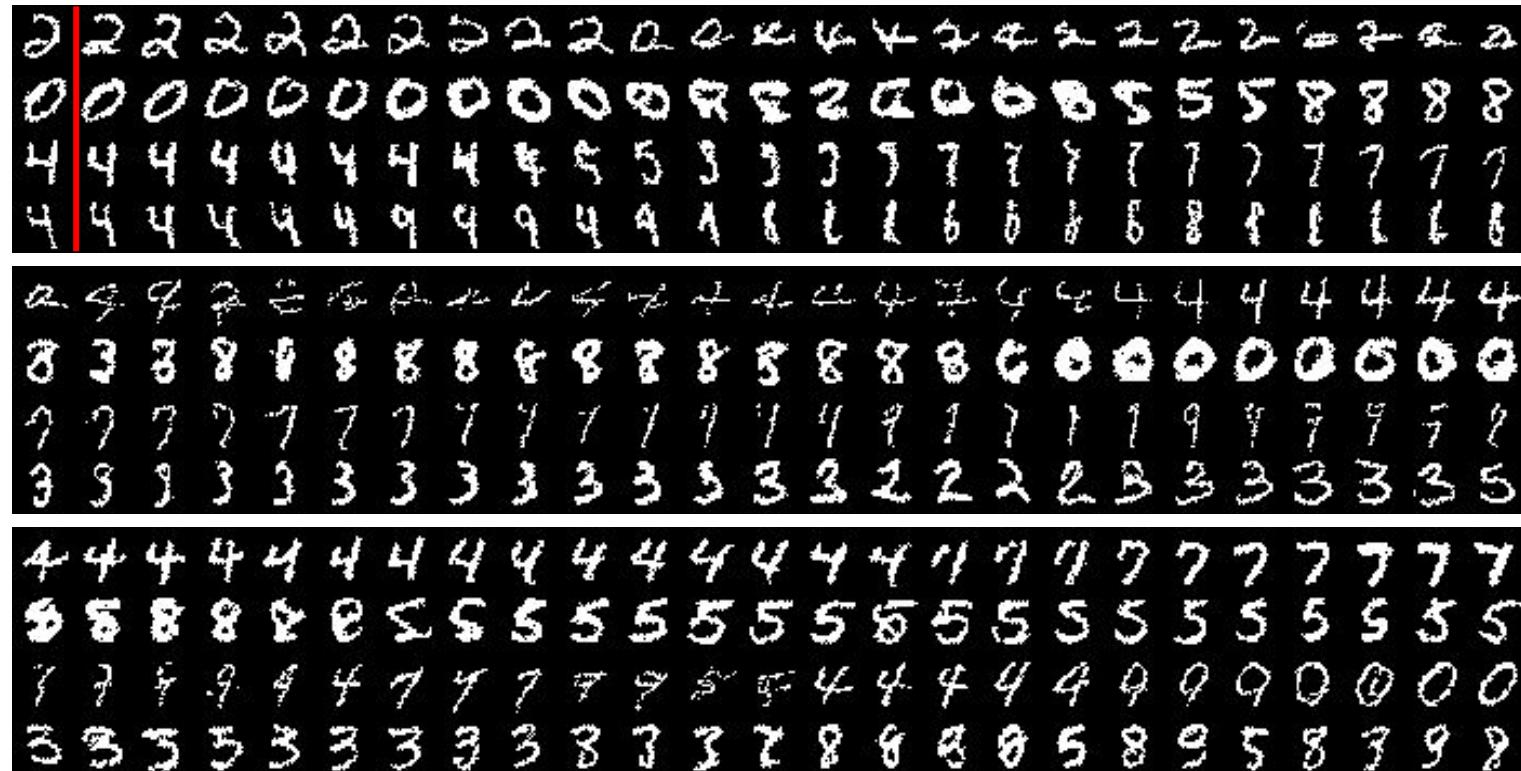
Ordered: KL from conditional ACN prior



Binary MNIST reconstructions: leftmost column are test set images



CelebA Reconstructions: leftmost column from test set



'Daydream' sampling: encode data, sample latent from conditional prior, generate new data conditioned on latent, repeat

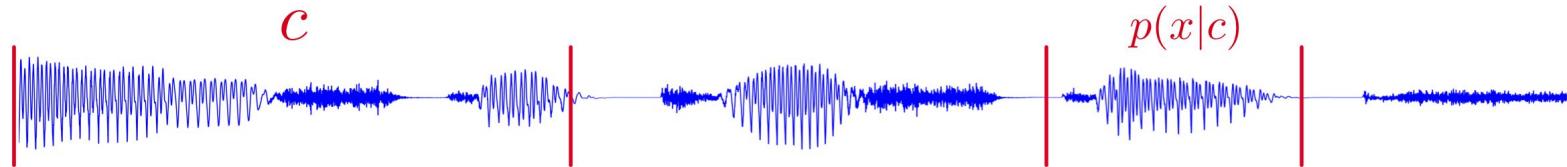
Mutual Information

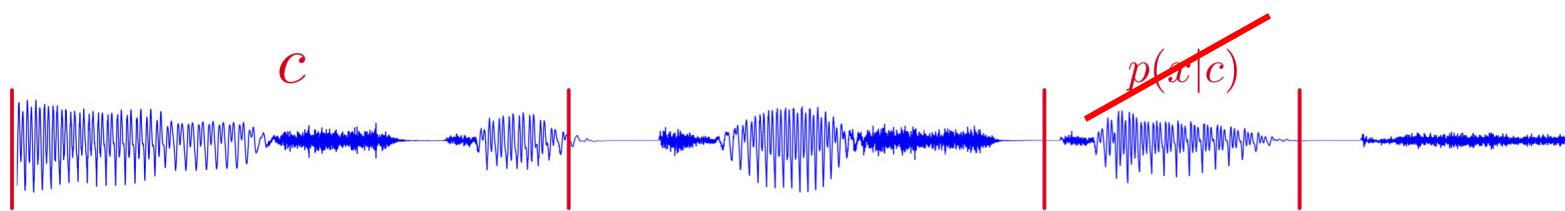
- Want codes that ‘**describe**’ the data as well as possible
- Mathematically, we want to maximise the **mutual information** between the code \mathbf{z} and the data \mathbf{x}

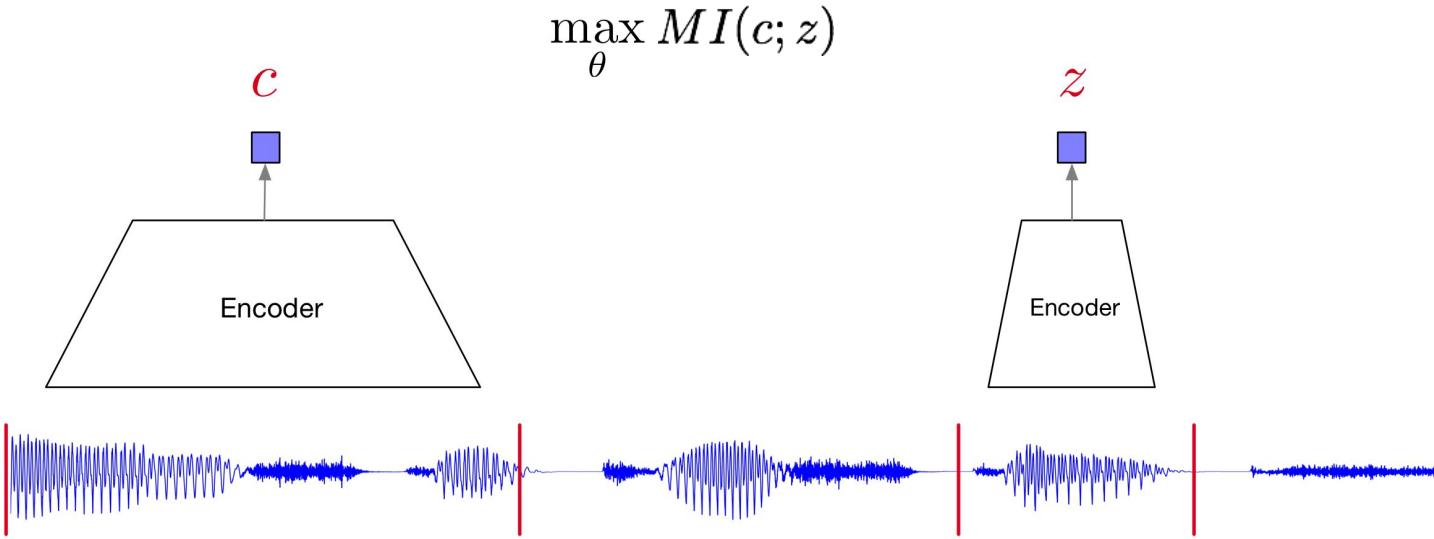
$$MI(z, x) = KL(p(z, x) || p(z)p(x))$$

- For an autoencoder, the difference between decoding \mathbf{x} with \mathbf{z} and (optimally) decoding without \mathbf{z} is a **lower bound** on $MI(x, z)$, so minimising the **reconstruction** cost maximises **MI**
- But decoding is very **expensive** if we just want codes
- Are there other ways to maximise **MI**?

Contrastive Predictive Coding

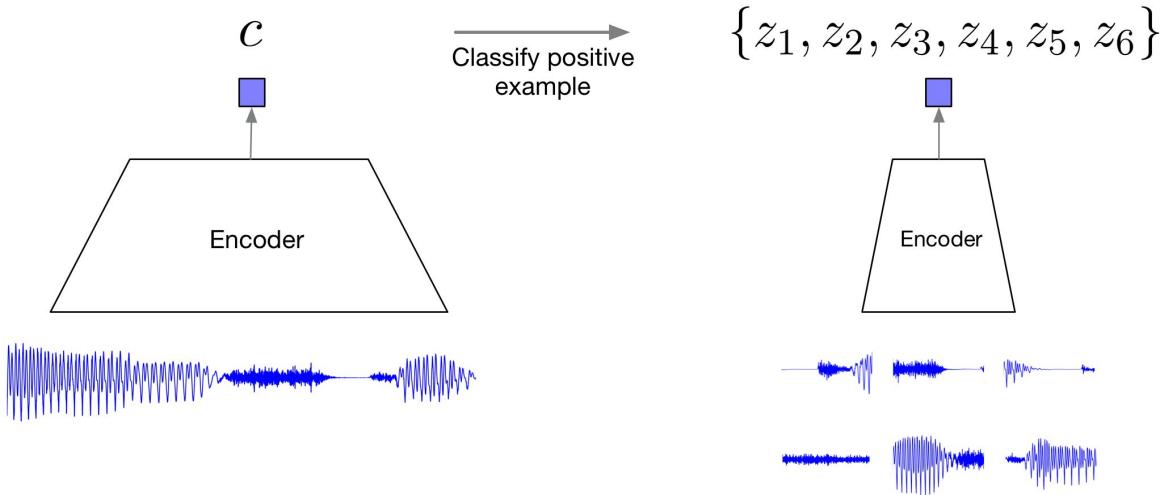




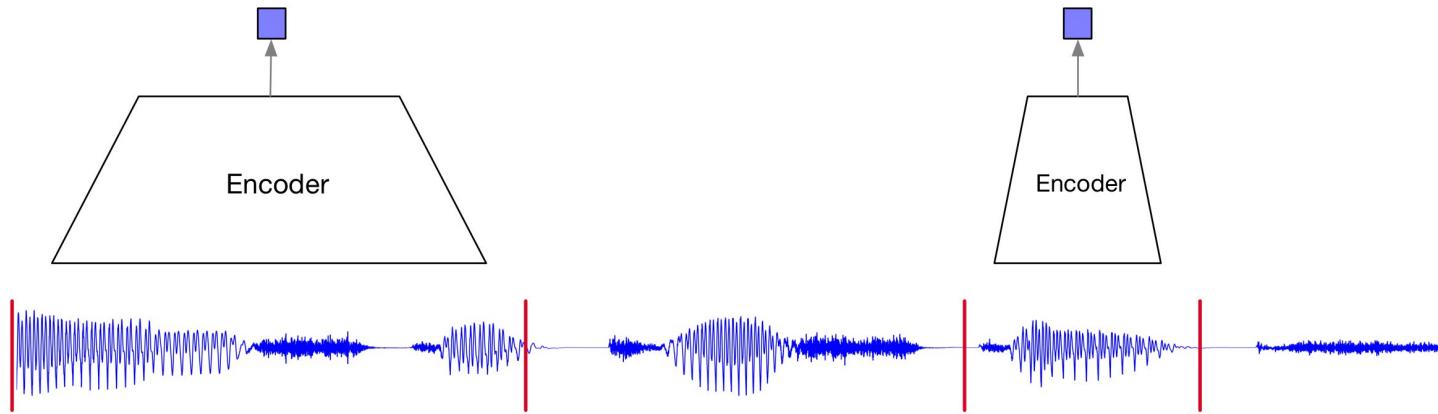


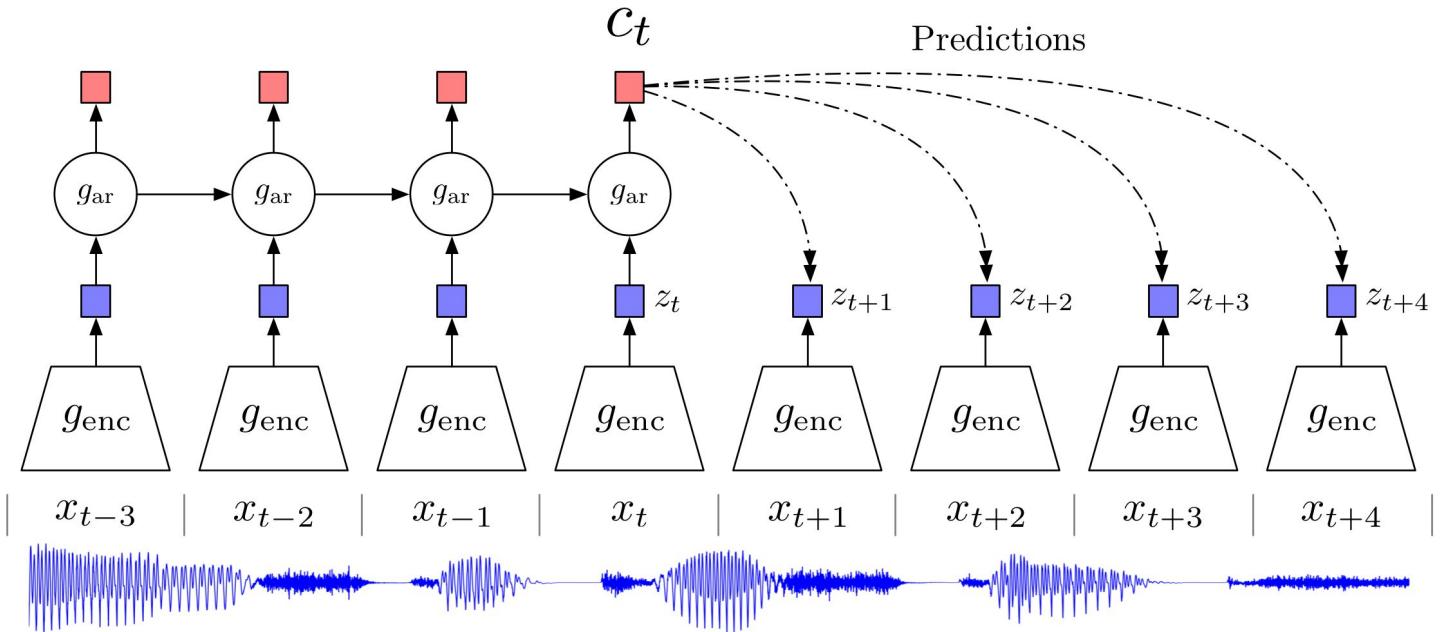
$$\frac{\exp f(c, z_i)}{\sum_j \exp f(c, z_j)}$$

$$f_k(x_{t+k}, c_t) = \exp \left(z_{t+k}^T W_k c_t \right)$$



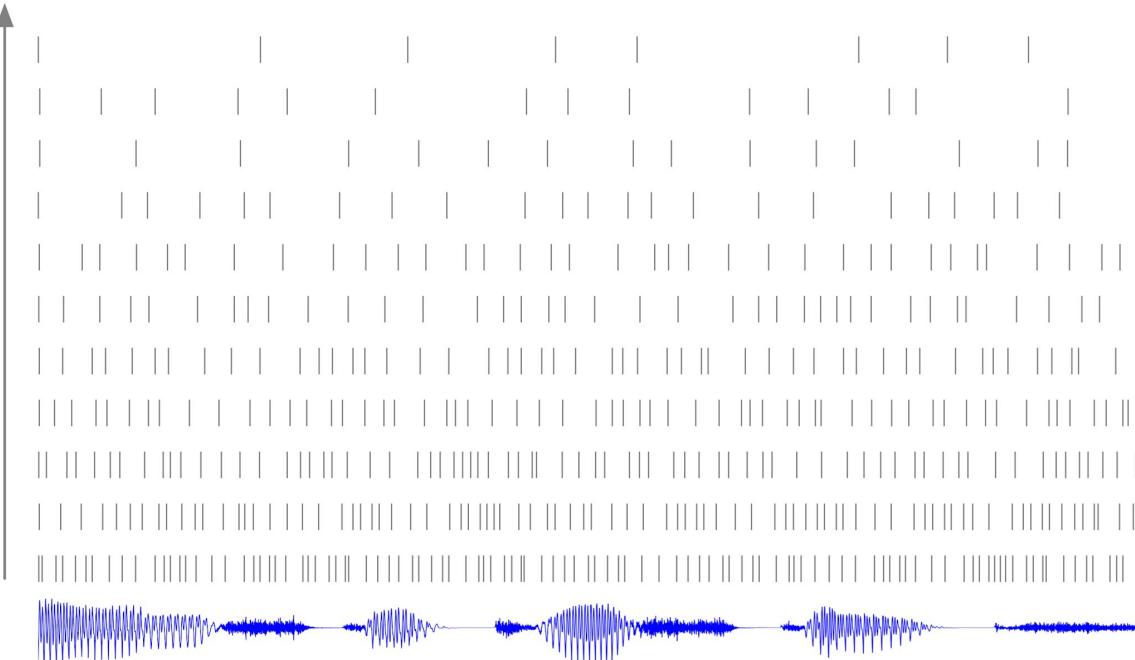
$$MI(x_t, c_t) \geq \log N - \mathcal{L}_N$$

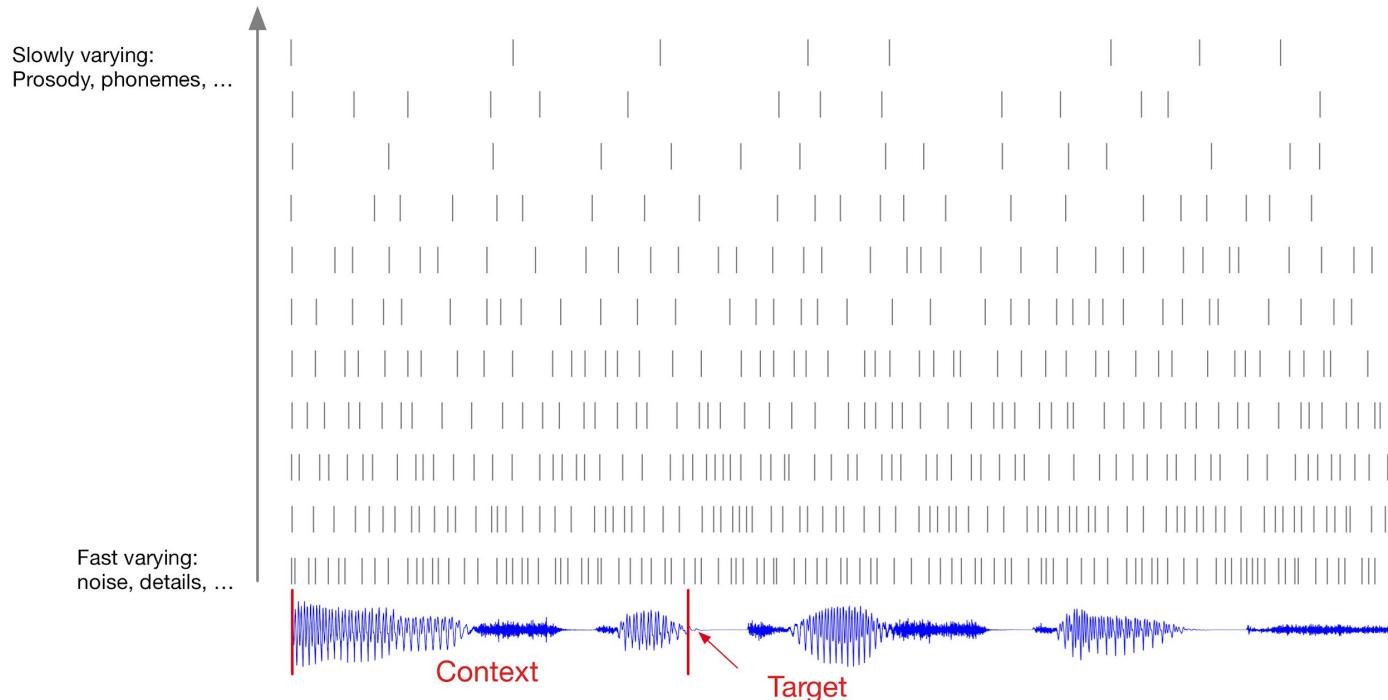


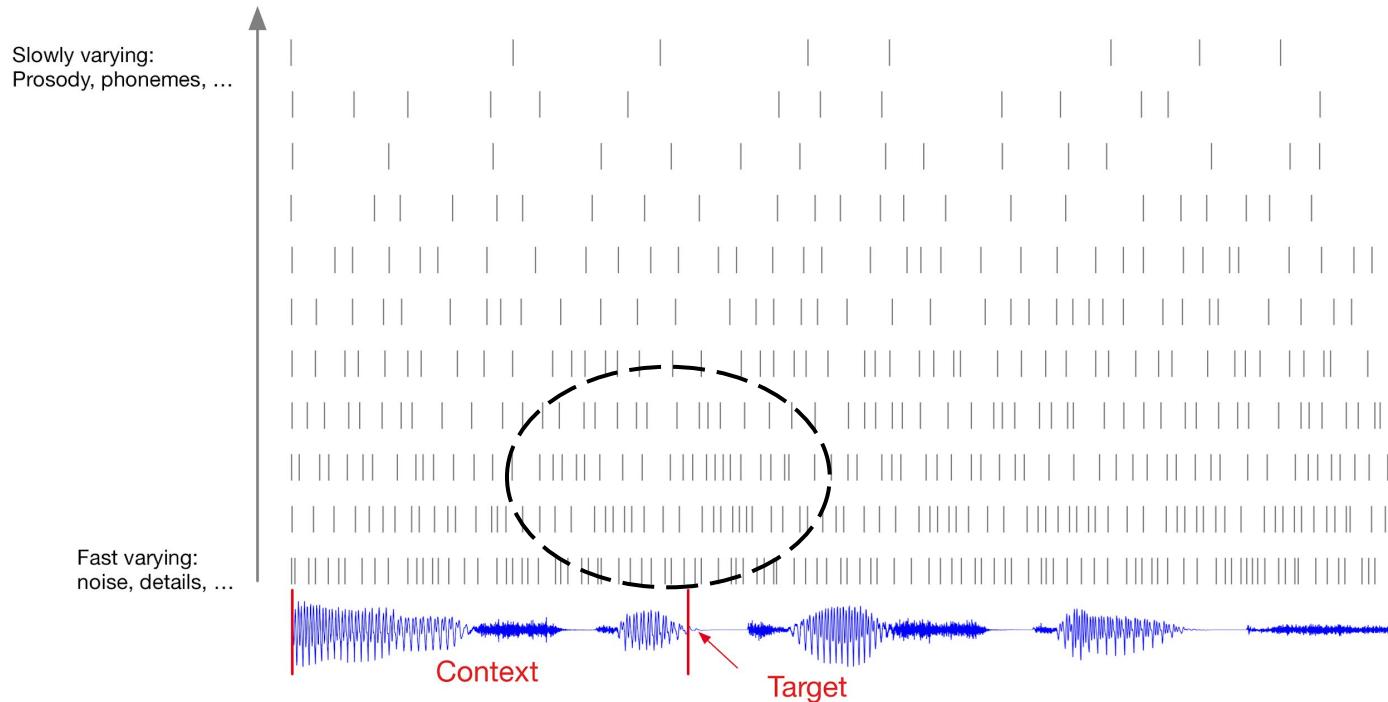


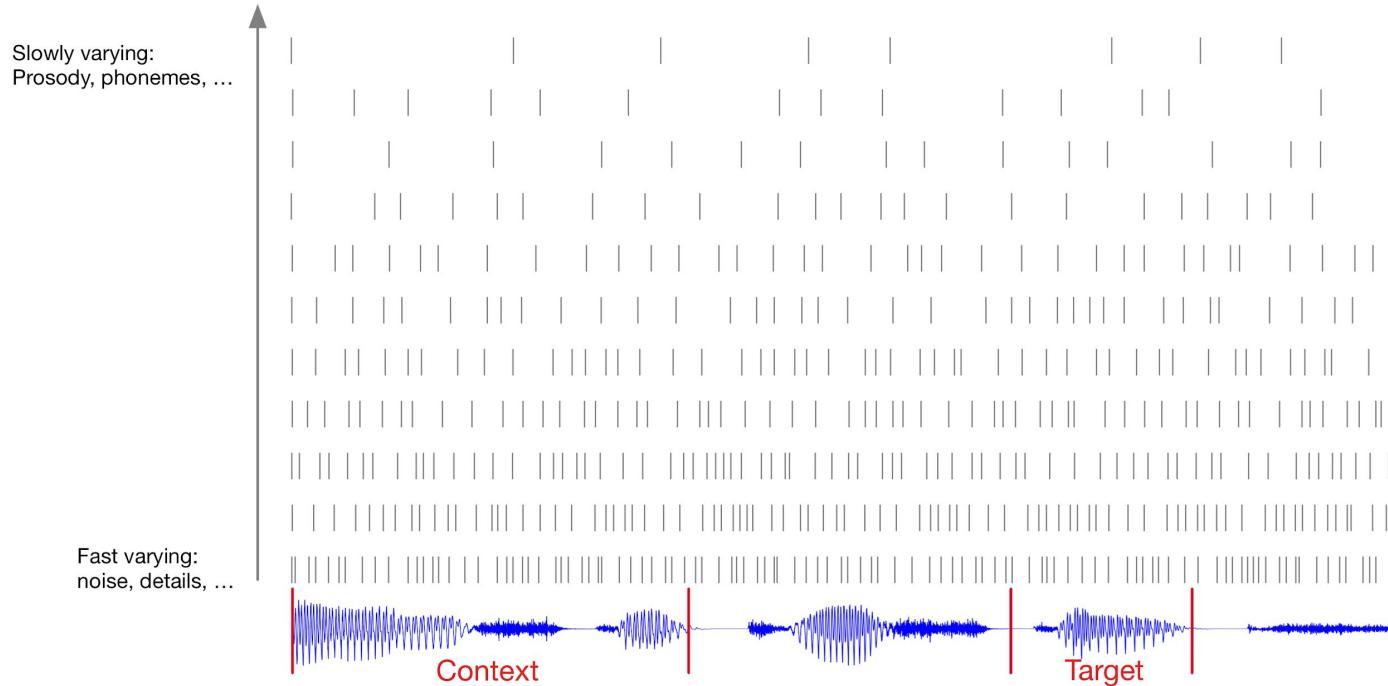
Slowly varying:
Prosody, phonemes, ...

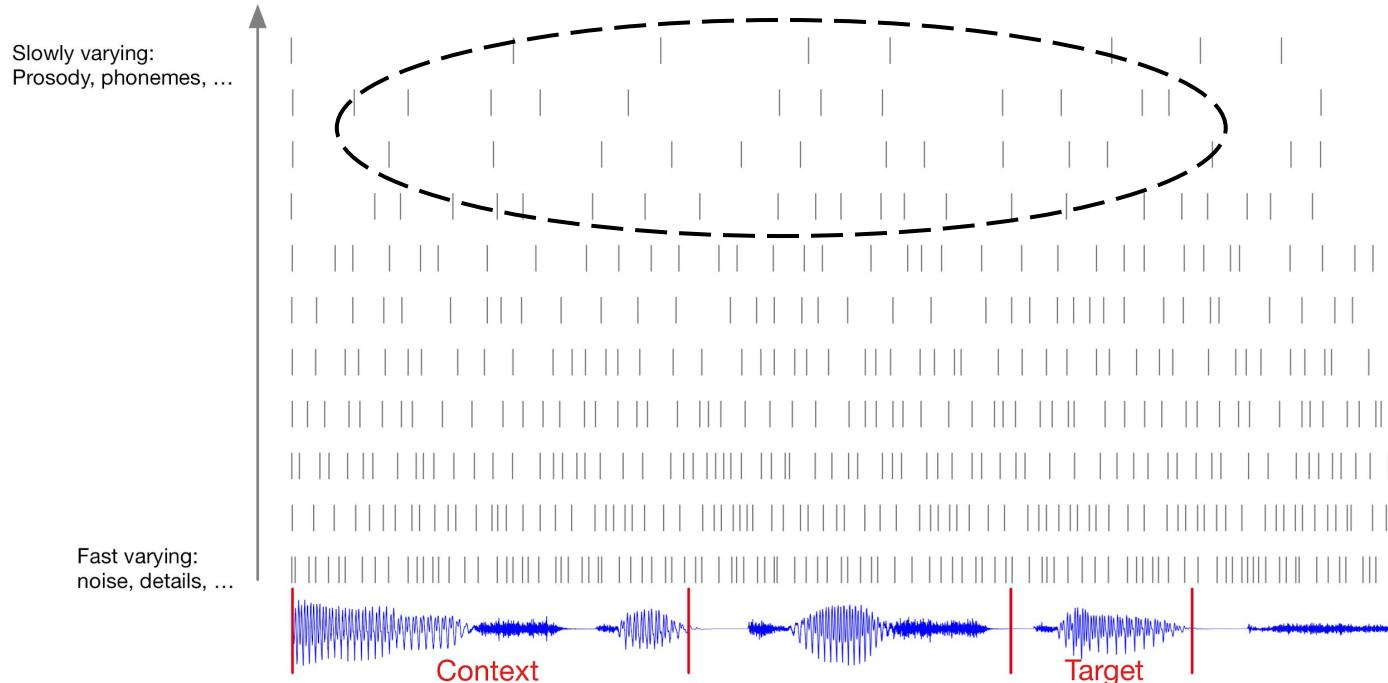
Fast varying:
noise, details, ...





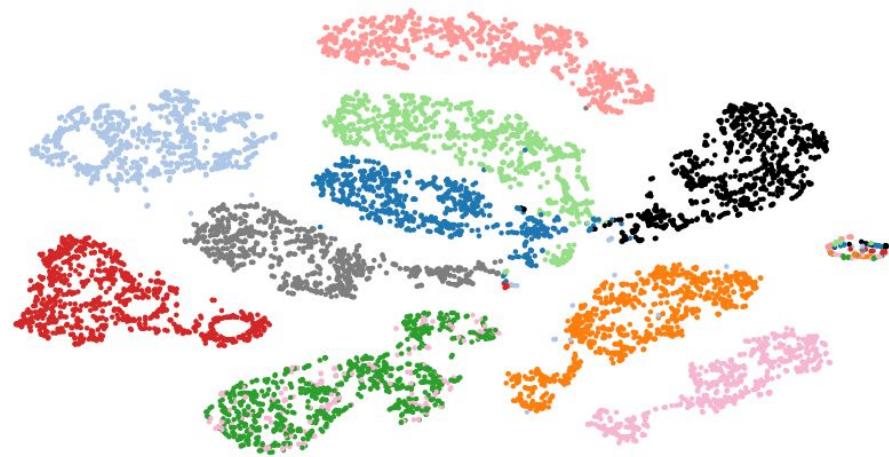






Speech - LibriSpeech

Method	ACC
Phone classification	
Random initialization	27.6
MFCC features	39.7
CPC	64.2
Supervised	74.6
Speaker classification	
Random initialization	1.87
MFCC features	17.6
CPC	97.4
Supervised	98.5



t-SNE on codes coloured by speaker identity

Images - ImageNet

Method	Top-1 ACC	Method	Top-5 ACC
Using AlexNet conv5		Motion Segmentation (MS)	48.3
Video [24]	29.8	Exemplar (Ex)	53.1
Relative Position [10]	30.4	Relative Position (RP)	59.2
BiGan [25]	34.8	Colorization (Col)	62.5
Colorization [9]	35.2	Combination of MS + Ex + RP + Col	69.3
Jigsaw [26] *	38.1	CPC	73.6
Using ResNet-V2			
Motion Segmentation [27]	27.6		
Exemplar [27]	31.5		
Relative Position [27]	36.2		
Colorization [27]	39.6		
CPC	48.7		

NLP - BookCorpus

Method	MR	CR	Subj	MPQA	TREC
Paragraph-vector [31]	74.8	78.1	90.5	74.2	91.8
Skip-thought vector [32]	75.5	79.3	92.1	86.9	91.4
Skip-thought + LN [33]	79.5	82.6	93.4	89.0	-
CPC	76.9	80.1	91.2	87.7	96.8

Unsupervised Reinforcement Learning

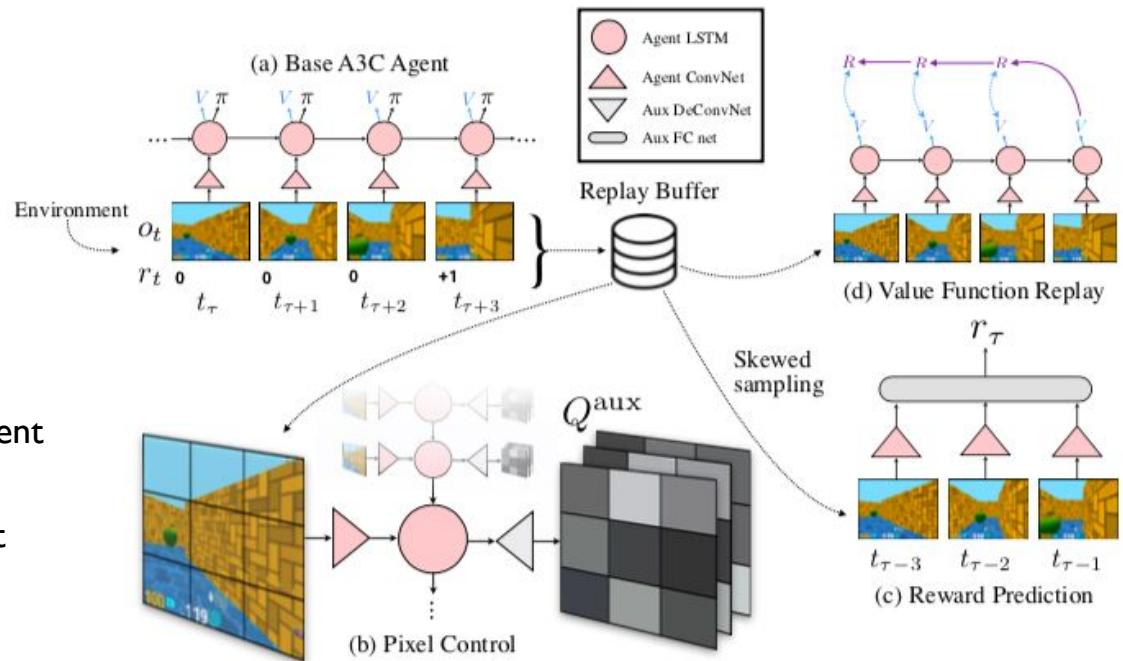
Auxiliary Tasks

- How can unsupervised learning help reinforcement learning?
- Simplest way is as an **auxiliary task**: maximise reward and minimise unsupervised loss with the **same network**
- Hope is that the **representations** learned for the unsupervised task will help with the RL task
- Also applies to supervised learning (e.g. **semi-supervised** learning, unsupervised **pre-training**)

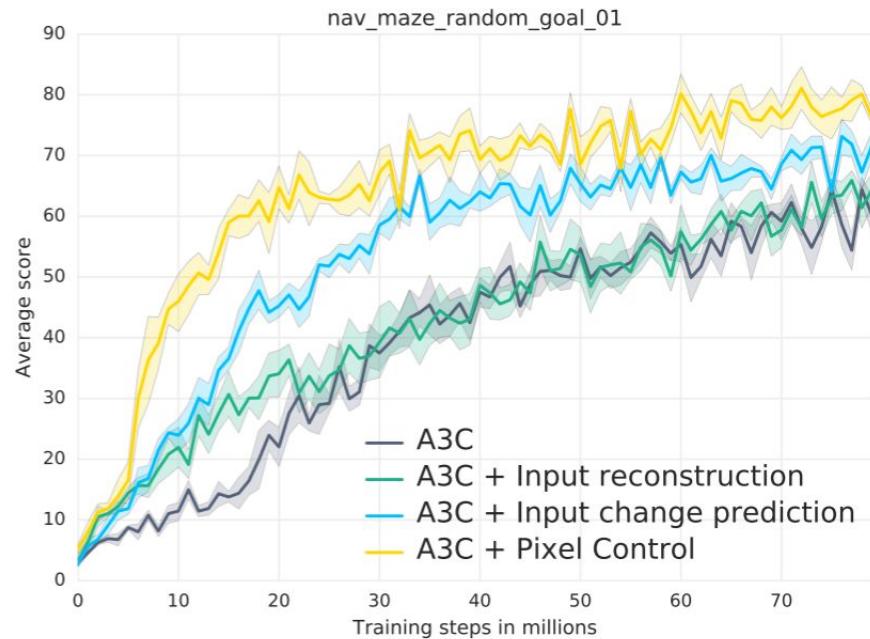
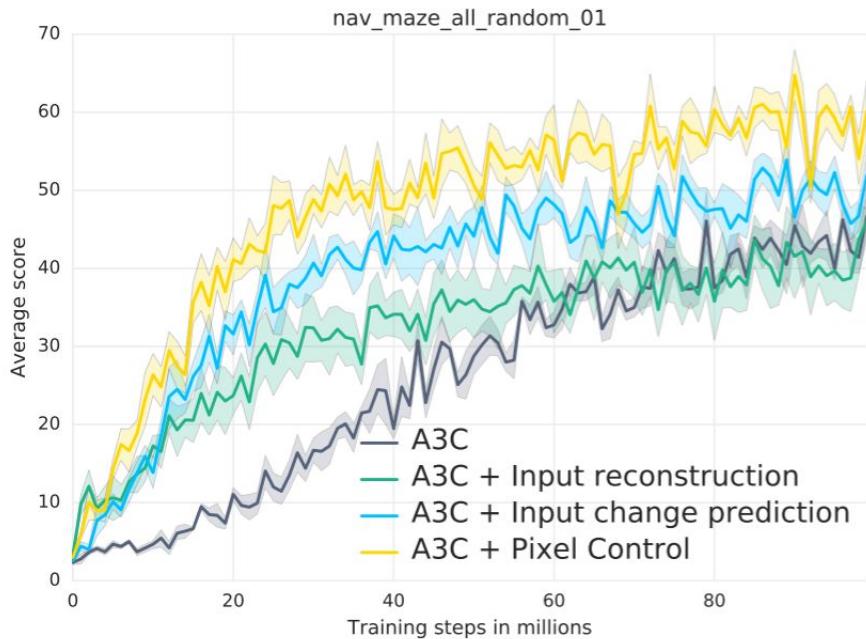
UNREAL Agent

Pixel Control – auxiliary policies are trained to maximise change in pixel intensity of different regions of the input

Reward Prediction – given three recent frames, the network must predict the reward that will be obtained in the next unobserved timestep.



Unsupervised RL Baselines



Sparse Rewards? More Cherries!

Single scalar reward signal

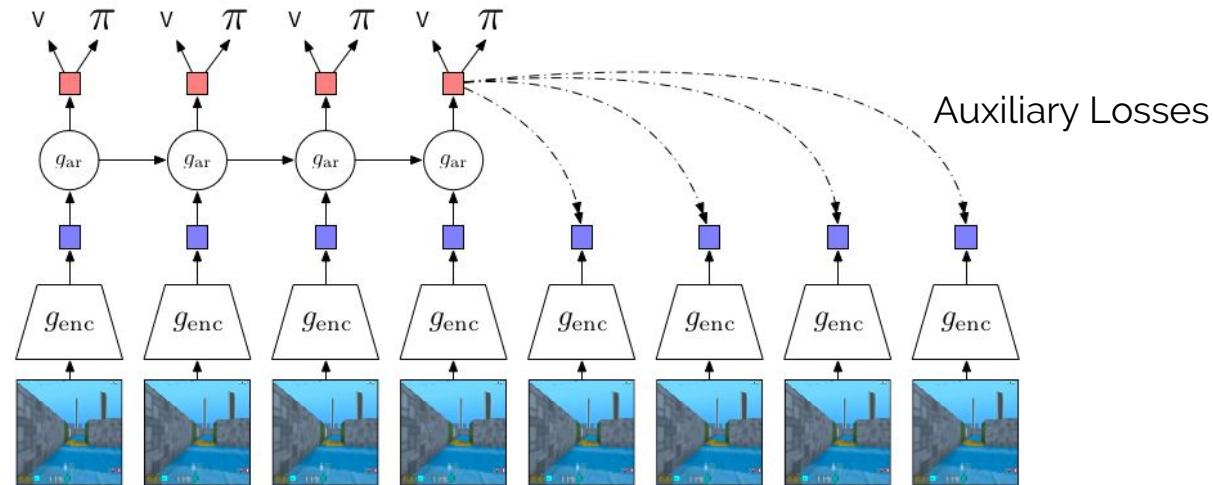


Many reward signals

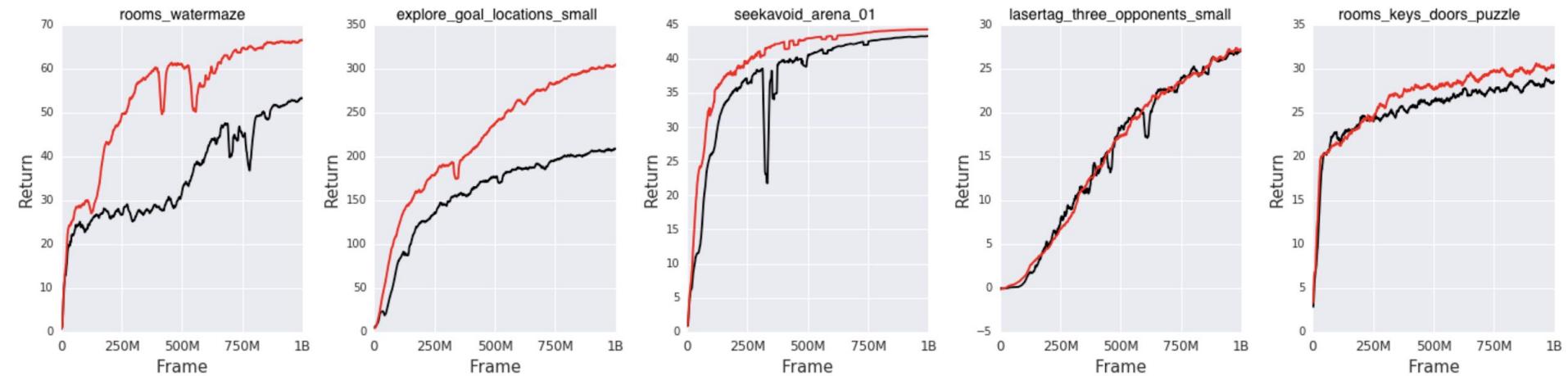


Reinforcement Learning on DM-Lab

Auxiliary loss is on policy
Predict 30 steps in the future



Reinforcement Learning on DM-Lab



-- Batched A2C
-- Aux loss

Intrinsic Motivation

- Unsupervised learning can guide the policy of an RL agent as well as shaping the representations
- Agent becomes **intrinsically motivated to discover** or **control** aspects of the environment, with or without an **extrinsic reward**
- Many variants, no consensus...

Curious Agents

Can reward the agent's **curiosity** by guiding it towards 'novel' observations from which it can rapidly learn. Many curiosity signals can be used:

- **Prediction Error:** choose actions to maximise prediction error in observations.
Problem is **noise addiction**: inherently unpredictable environments become unreasonably interesting. One solution is to make predictions in **latent space** instead: network doesn't import noise into latent representations, only useful structure



(a) learn to explore on Level-1

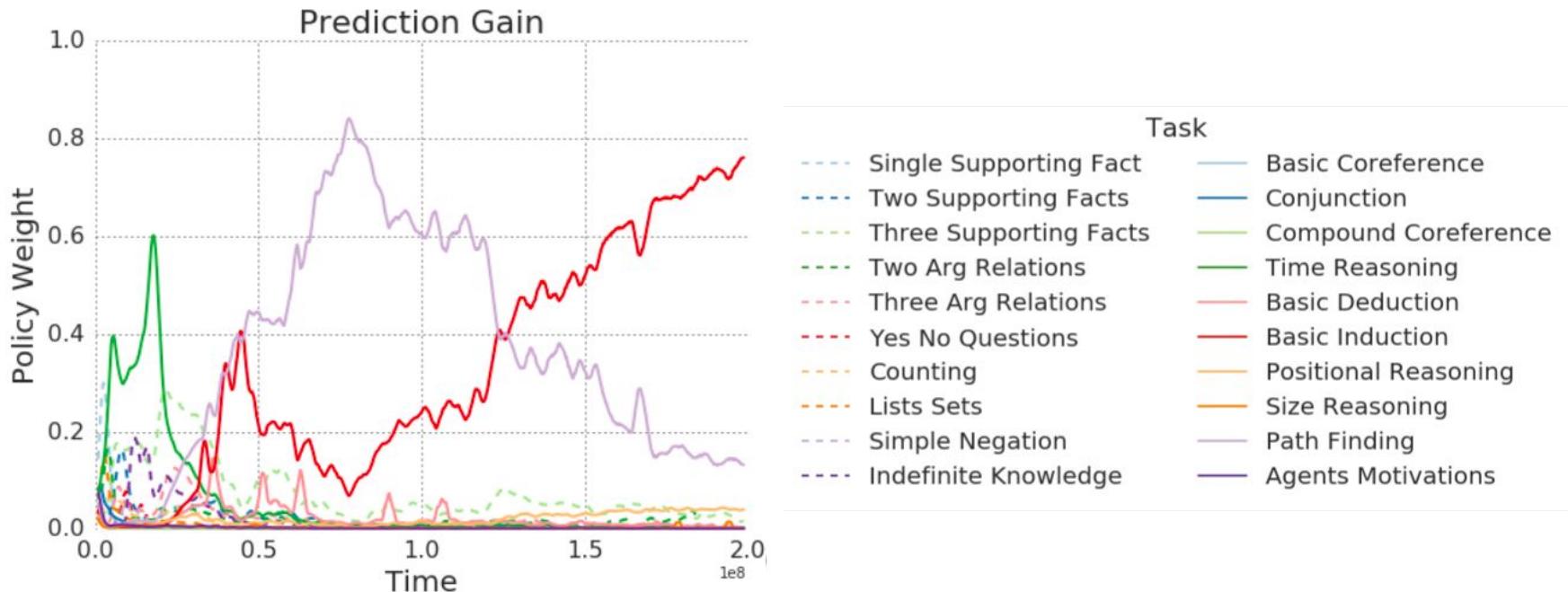


(b) explore faster on Level-2

Curious Agents (cotd.)

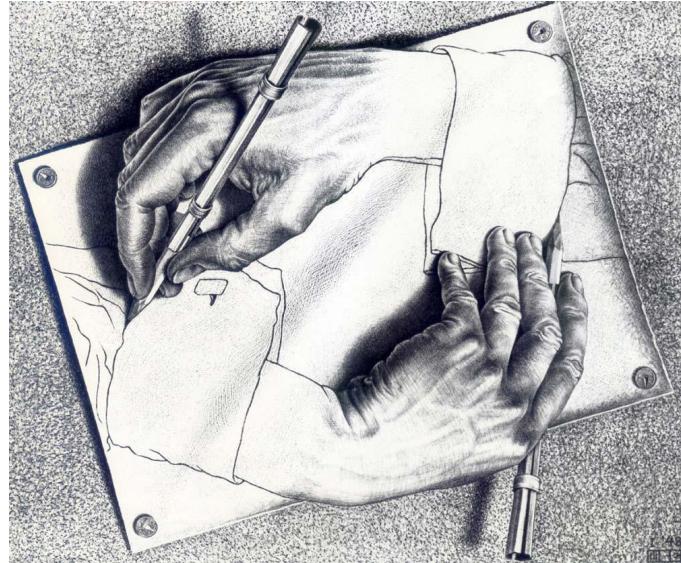
- **Bayesian Surprise:** maximise **KL** between posterior (after seeing observation) and prior (before seeing it)
Baldi et. al., *Bayesian Surprise Attracts Human Attention.* (2005)
- **Prediction Gain:** maximise **change** in prediction error before and after seeing an observation. Approximates Bayesian surprise.
Bellemare et. al. (*Unifying Count-Based Exploration and Intrinsic Motivation.* 2016)
- **Complexity Gain:** maximise increase in complexity of (regularised) predictive **model**. Assumes a parsimonious model will only increase complexity if it discovers a meaningful regularity. Needs a way of measuring complexity (e.g. VI).
Graves et. al. *Automated Curriculum learning For Neural Networks.* (2017)

Prediction Gain Syllabus



Curiouser and Curiouser...

- **Complexity Gain:** Seek out data that maximise the decrease in bits of **everything** the agent has **ever observed** (!). In other words find (or create) the thing that **makes the most sense of the agent's life so far**: science, art, music, jokes...



Driven by Compression Progress: A Simple Principle Explains Essential Aspects of Subjective Beauty, Novelty, Surprise, Interestingness, Attention, Curiosity, Creativity, Art, Science, Music, Jokes, Schmidhuber, 2008

Empowered Agents

Instead of curiosity, agent can be motivated by **empowerment**: attempt to maximise the **Mutual Information** between the agent's actions and the consequences of its actions (e.g. the **state** the actions will lead to). Agent wants to have as much **control** as possible over its future.

Klyubin et. al. *Empowerment: A Universal Agent-Centric Measure of Control* (2005)

One way to maximise mutual information is to **classify** the high level '**option**' that determined the actions from the final state (while keeping the option **entropy** high): contrastive estimation again?

Gregor et. al. *Variational Intrinsic Control* (2016)

Conclusions

- Unsupervised learning gives us much more signal to learn from
- But it isn't clear what the learning objective should be
- Density modelling is one option
- Autoregressive neural networks are a powerful family of density model
- Methods such as autoencoding and predictive coding can yield useful latent representations
- RL can benefit from unsupervised learning as an auxiliary loss, and from intrinsic motivation signals such as curiosity