NEW YORK UNIVERSITY

Facebook AI Research

Deep Learning

Lecture 2 – Unsupervised Learning

Machine Learning Summer School – Madrid 2018

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Part 2 Schedule

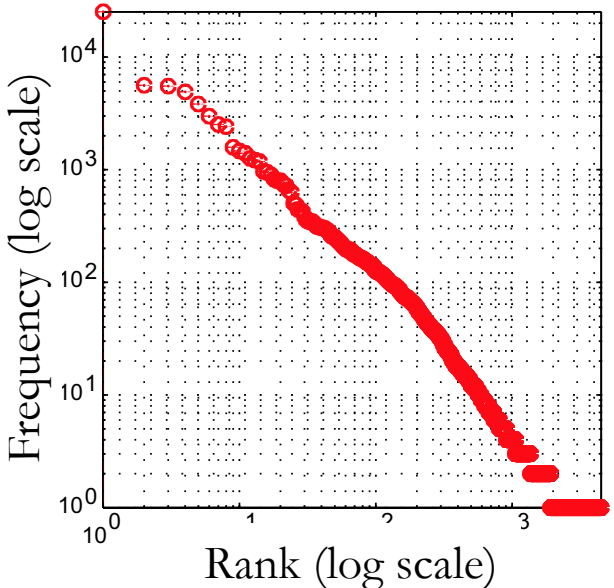
- Motivation
- Unsupervised Learning
  - Literature review
  - Generative models of video
    - [Stochastic Video Generation, Denton et al., ICML 2018]

- Self-supervised learning
  - Review of approaches from vision
  - [Unsupervised Learning by Predicting Noise, Bojanowski & Joulin, ICML 2017]

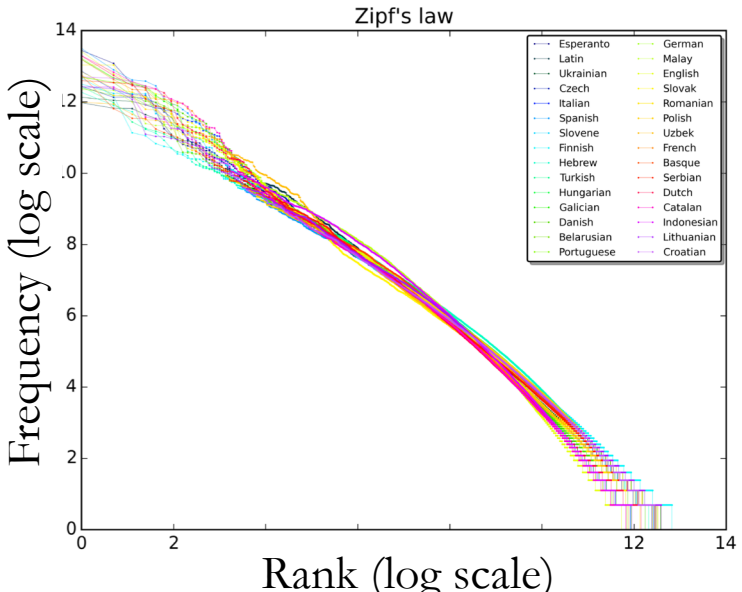
Unsupervised Learning

- Learning without labels (or from just a few)
  - Need to capture structure inherent in data
- Practical importance:
  - Very uneven distribution of categories in real-world (Zipf's law)
  - Lots of rare categories with few examples

Objects in Vision Dataset (LabelMe)



Words in Wikipedia Corpus



Arguments for Unsupervised Learning

- Want to be able to exploit unlabeled data
  - Vast amount of it often available
  - Essentially free
- Good regularizer for supervised learning
  - Helps generalization
  - Transfer learning
  - Zero/one/few - shot learning

Unsupervised Learning

- Biological argument [from G. Hinton]:
  - Our brains have 10^15 connections
  - We live for 10^9 secs
  - Need 10^6 bits/sec
  - Insufficient information from occasional high level label
  - Only source with enough information is input itself

- Challenging problem: big focus on many DL groups

Historical Note

- Deep Learning revival started in ~2006
  - Hinton & Salakhudinov Science paper on RBMs
- Unsupervised Learning was focus from 2006-2012
- In ~2012 great results in vision, speech with supervised methods appeared
  - Less interest in unsupervised learning

Overview of Unsupervised Approaches

- Given just data {X}
  - Unlike supervised learning there are no **provided** labels {Y}

1. Density modeling, i.e. build model of p(X)
   - Enables sampling of new data
   - Evaluate probability of a data point
   - Can be conditional model, e.g. p(X_t | X_{t-1},…)
   - Requires (deep) generative architectures

2. "Self supervised" learning

- Find supervision signal y **within the input data**
- This signal is then used as a target:

$$y : \mathcal{X} \to \mathcal{Y}$$

$$x \mapsto y(x)$$

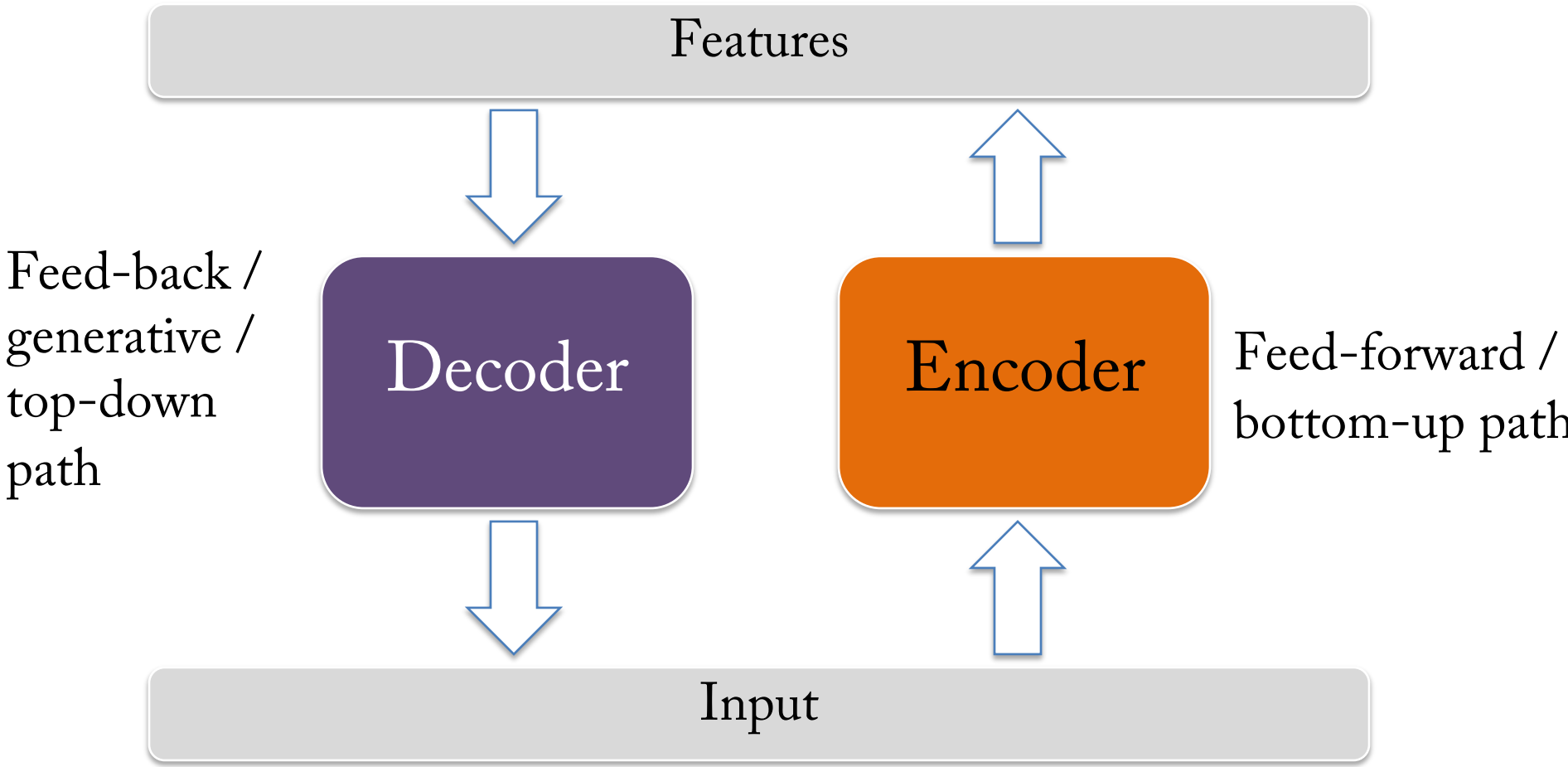
- Allows the use of standard supervised learning losses and architectures

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \ell(f_\theta(x_i), y(x_i))$$

- Pre-training of representation for subsequent task
- Typically involves some insight into domain to pick y
- Inspired by word2vec (Mikolov et al. 2013)
  - E.g. The cat sat on the mat
  - X = {The, cat, NULL, on the mat}
  - Y = {sat}

1. Density Modeling of Natural Signals using Deep Learning

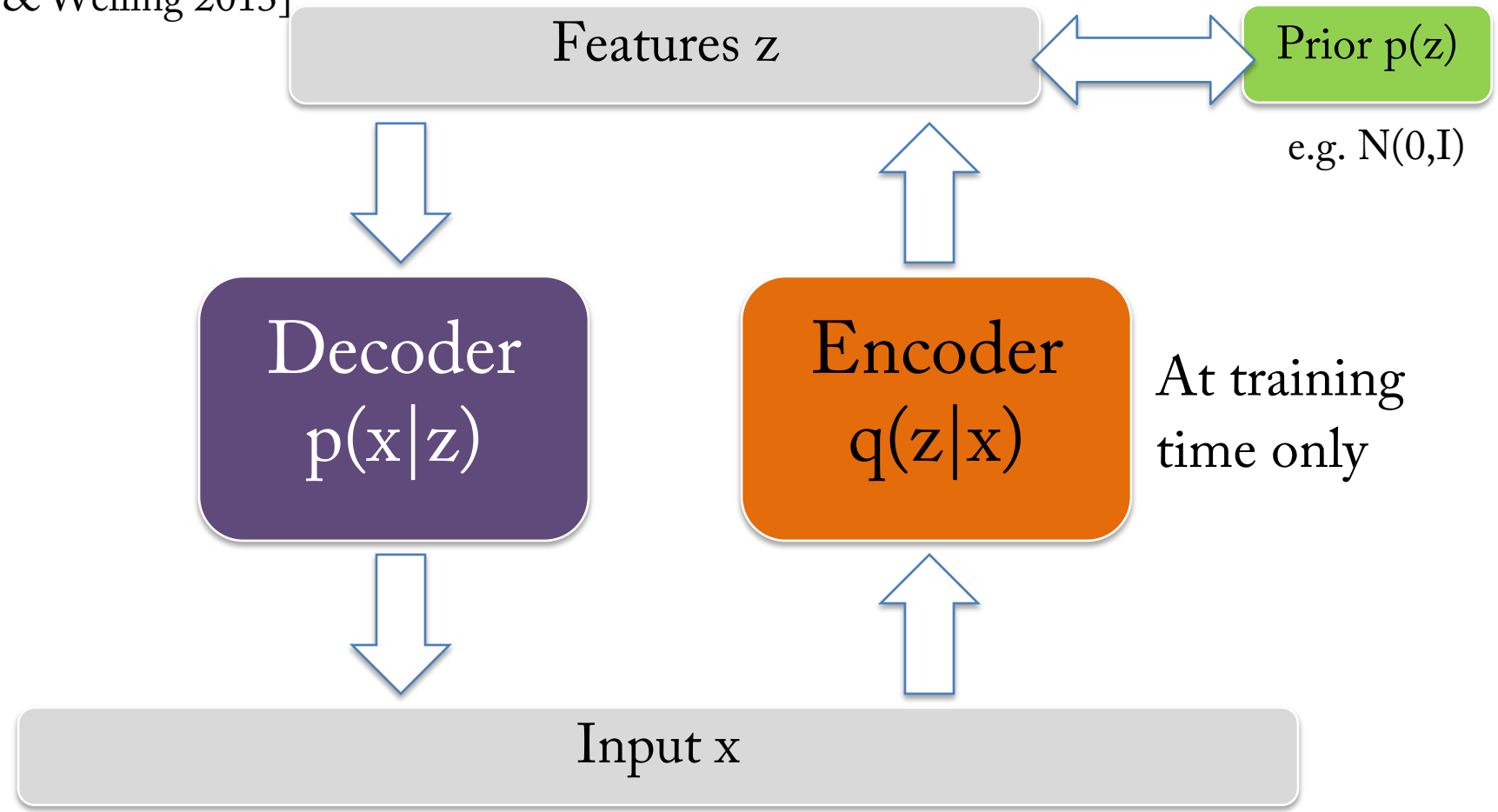
Auto-Encoder



- Encoder/Decoder will be deep network
- Slightly different architectures for decoder (needs to output image)
- Architecture depends on application

Variational Auto-Encoder

[Kingma & Welling 2013]

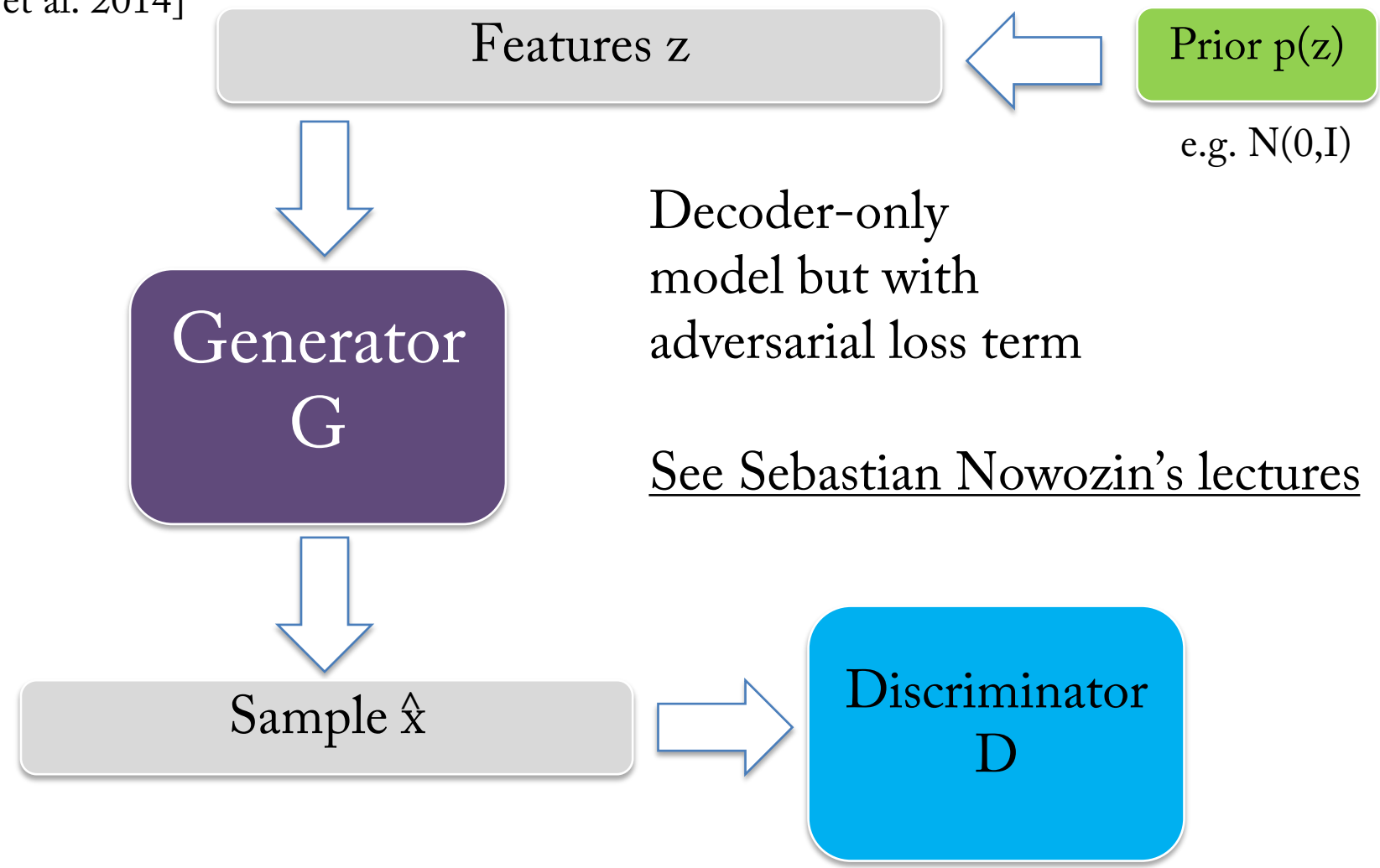


- Makes auto-encoder into a true generative model

$$\underbrace{\mathbb{E}_{q(z|x)} \log p(x|z)}_{\text{Reconstruction term}} - \underbrace{D_{KL}(q(z|x)||p(z))}_{\text{Prior term}}$$

Generative Adversarial Networks

[Goodfellow et al. 2014]



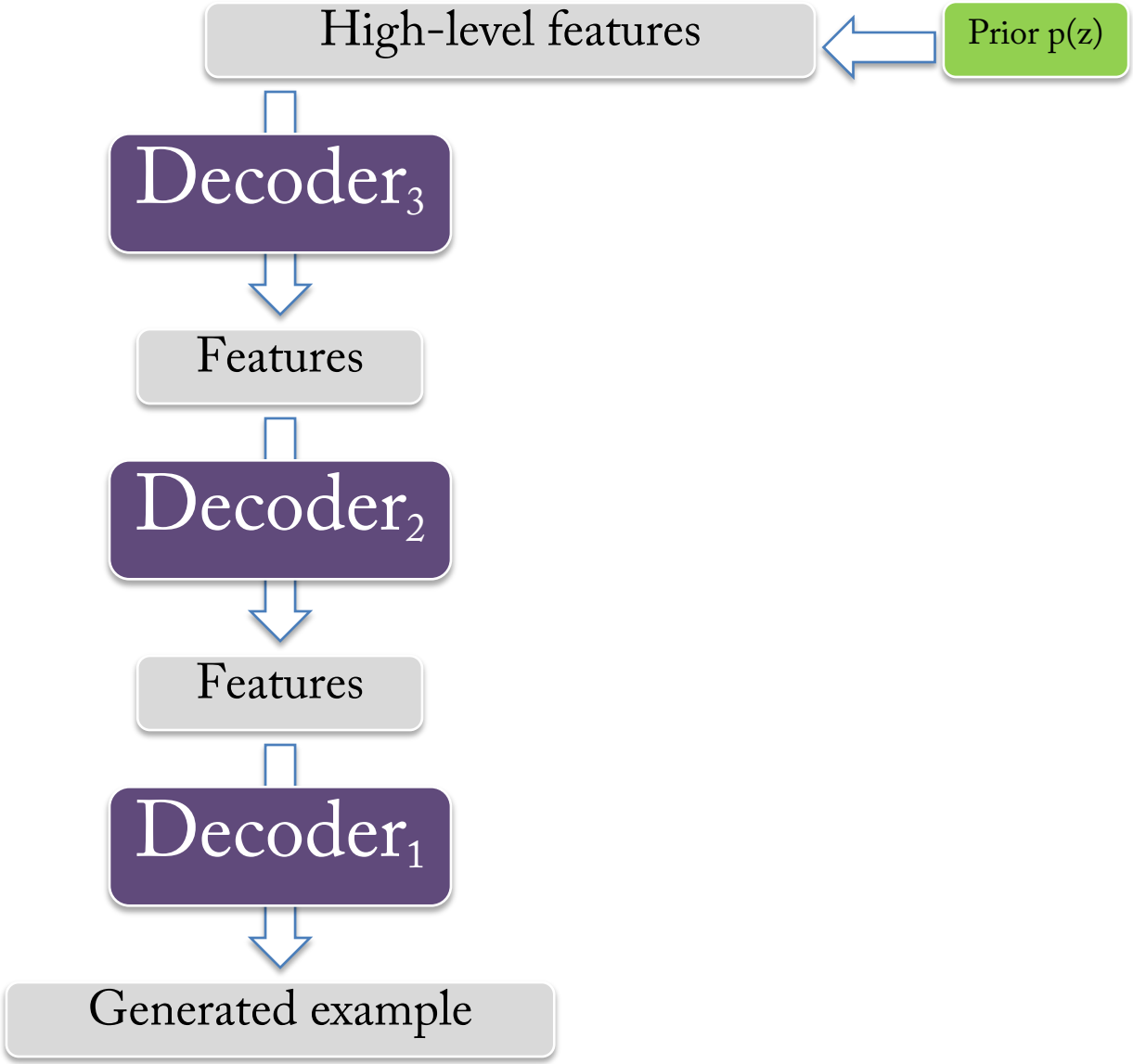
- Mini—max game between G and D

$$\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$

Generating Samples

- Sample from prior p(z)

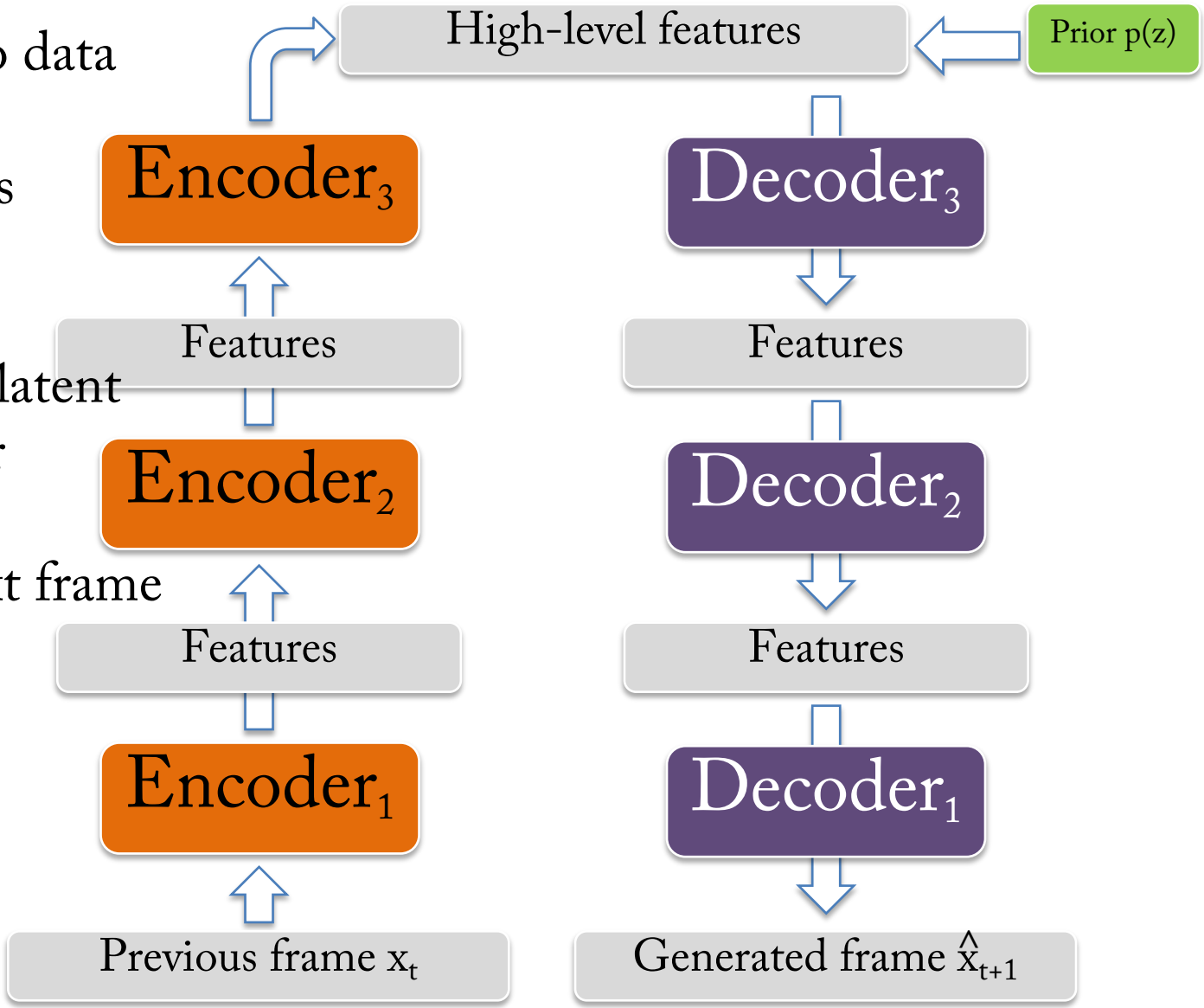
- Push through decoder network



Conditional Generation

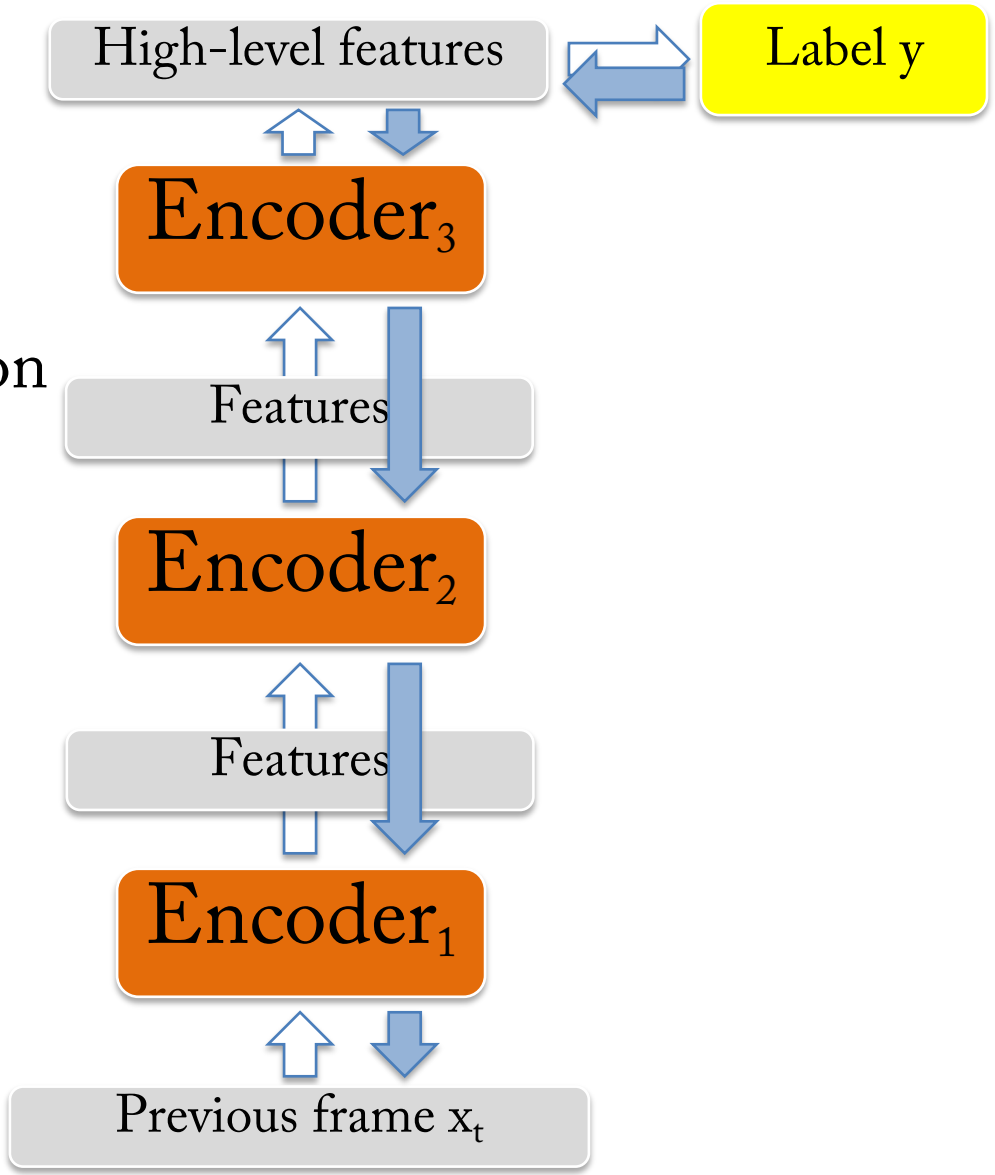
E.g. consider video data

- Encode previous frames(s)
- [Optional] add latent noise from prior
- Reconstruct next frame via decoder



Supervised Fine-Tuning

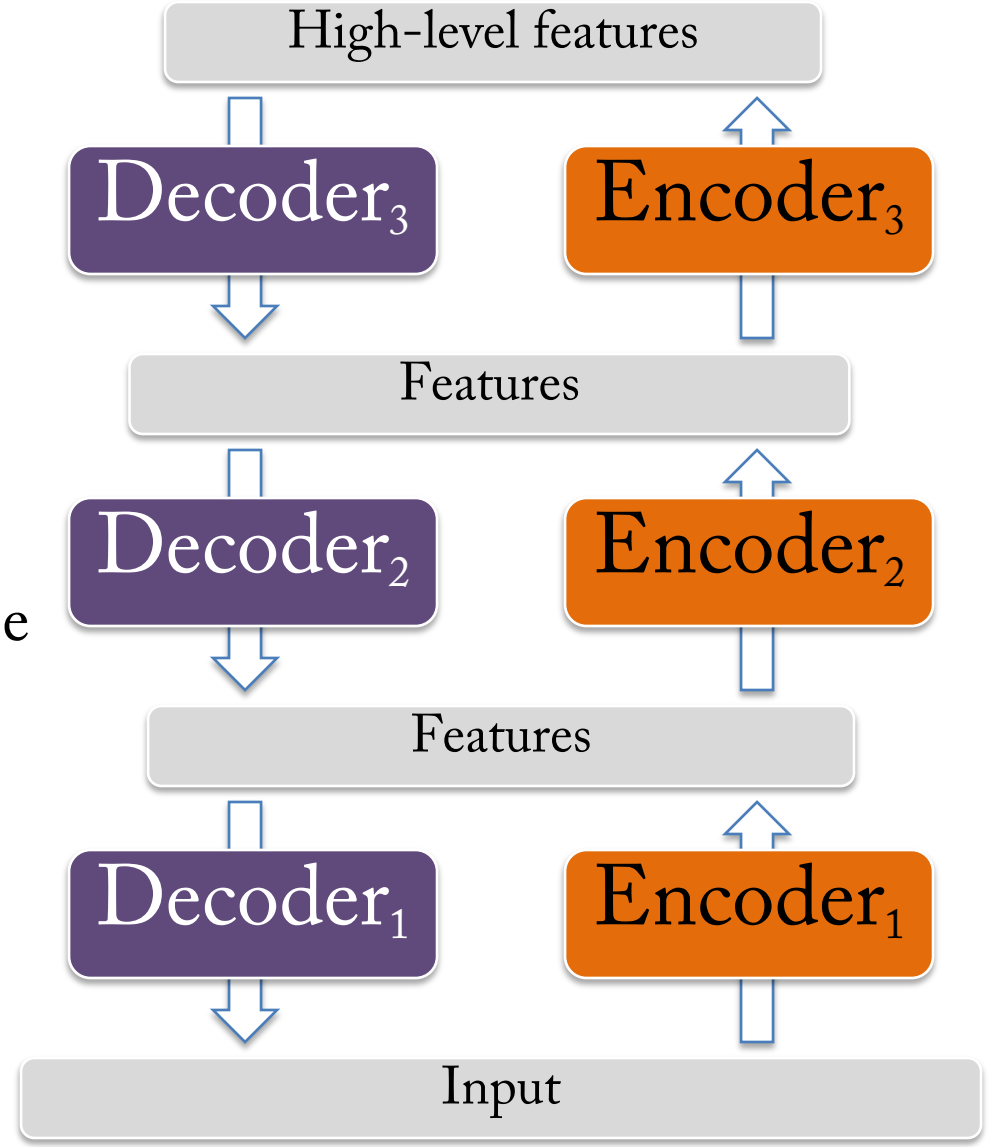
- After unsupervised "pre-training", refine model with few labels on target task
- Unsupervised training phase learns "good" representation



Stacked Auto-Encoders

- Ladder Networks
  [Rasmus et al. 2015]
  - Reconstruction constraint at each layer
  - Trained end-to-end

- Can be trained layer-wise
  - Stacked RBMs
  [Hinton & Salakhutdinov 2006]



Many Others Approaches

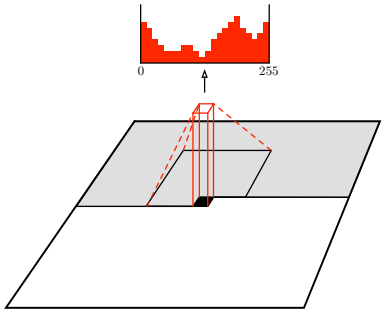
- Autoencoder (most unsupervised Deep Learning methods)
  - Restricted / Deep Boltzmann Machines
  - Denoising autoencoders
  - Predictive sparse decomposition
- Decoder-only
  - Sparse coding & hierarchical variants

Pixel-CNN

[van den Oord et al., arXiv 1606.05328, 2016]

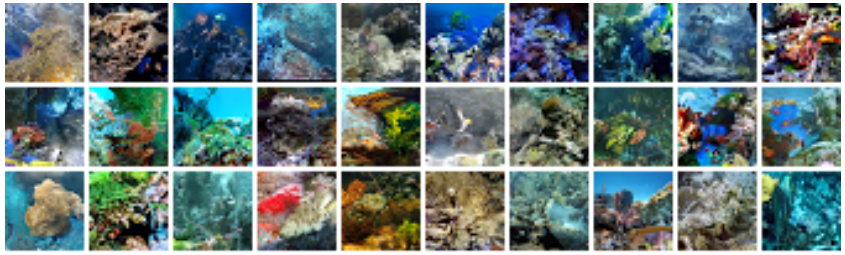
- Conditional generative model of images
- Generate each pixel, in raster-scan order
- Just predict distribution over a single pixel (can be multi-modal)
- See also Video Pixel Networks [Kalchbrenner et al., 2016],
- NADE [Larochelle & Murray 2011] & RIDE [Theis and Bethge, NIPS 2015].

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



1	1	1	1	1
1	1	1	1	1
1	1	0	0	0
0	0	0	0	0
0	0	0	0	0

African elephant

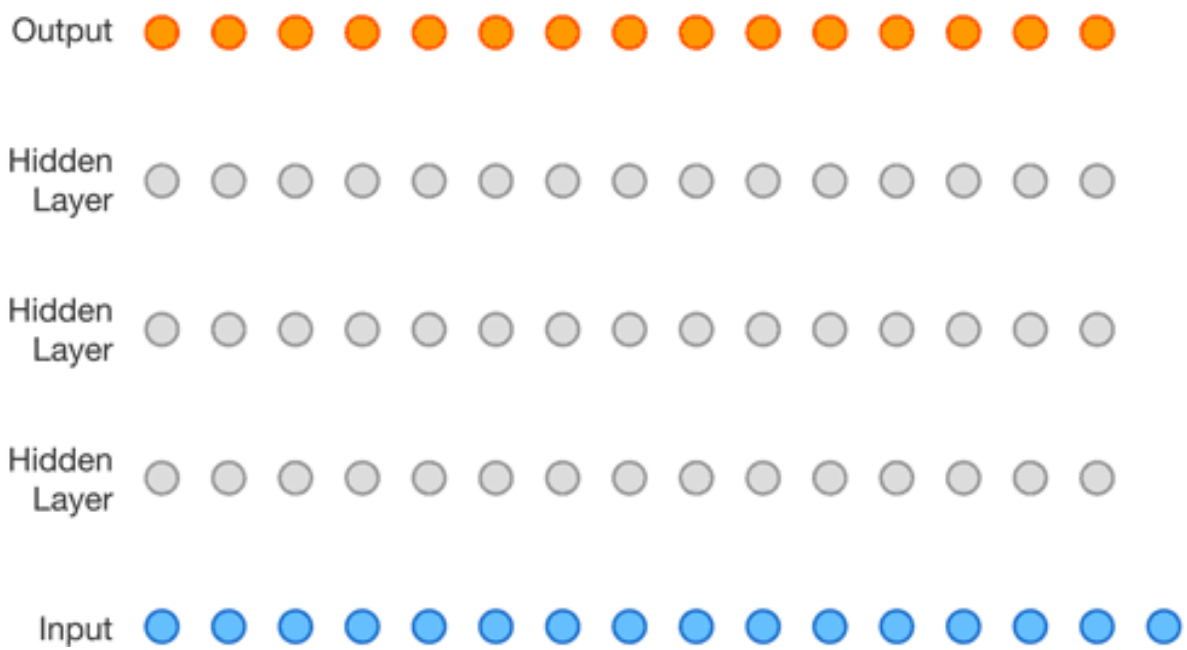


Coral Reef

Wavenet

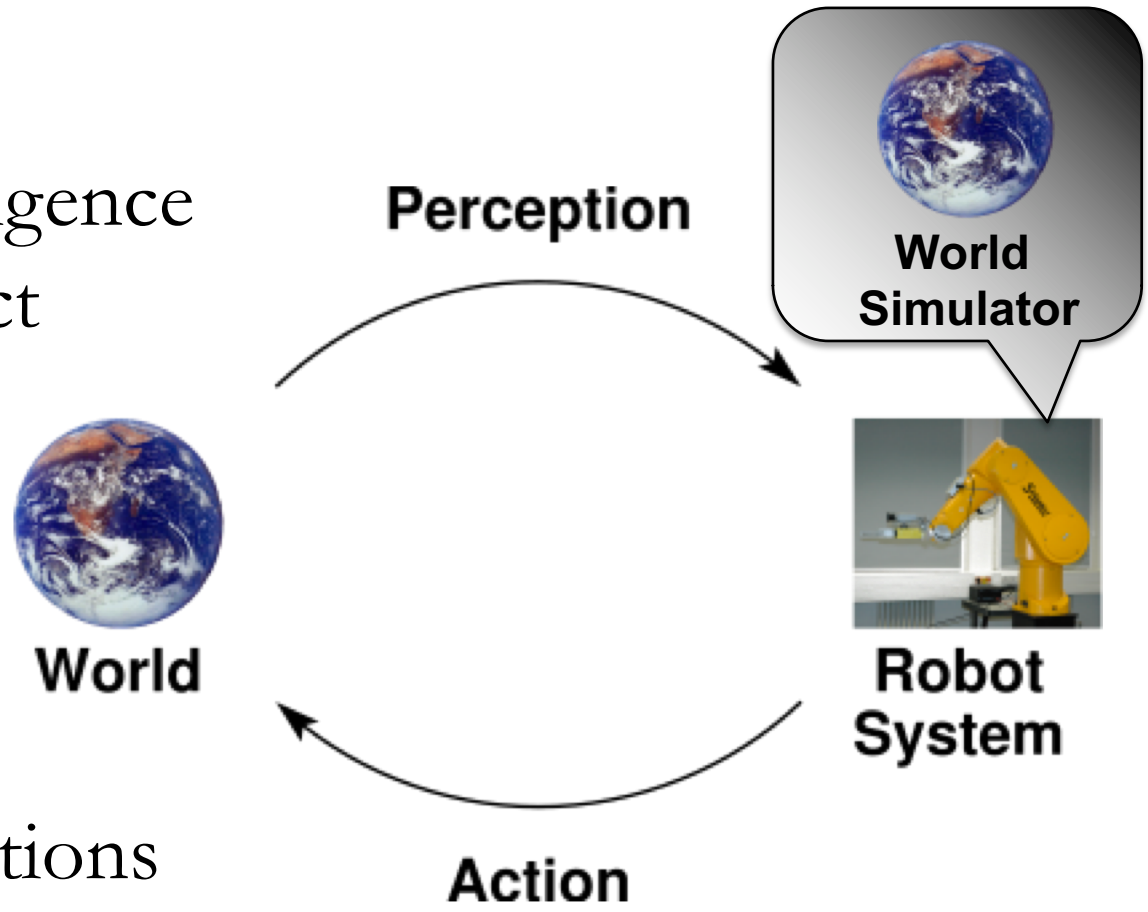
[van den Oord et al., arXiv 1609.03499, 2016]

- Generative model of raw speech waveform
- Condition on previous parts of waveform $p(\mathbf{x}) = \prod_{t=1}^{T} p(x_t \mid x_1, \ldots, x_{t-1})$
- Dilated causal convolution layers
- Discrete output distribution (use softmax)



An aside: Reasoning and Planning in World

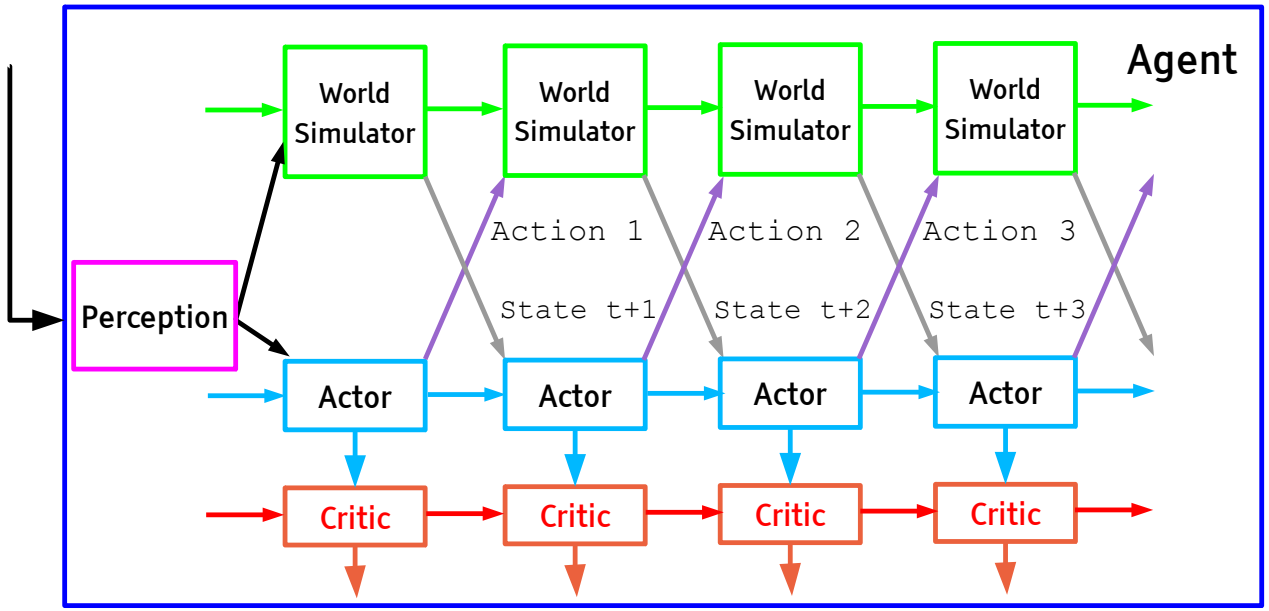
- Solving AI requires more than just perception
- Essence of intelligence is ability to predict
- To plan ahead need to simulate world & reason about possible actions



[Craik 1943; Dennett 1978; Sutton & Barto 1981; Sutton 1991]

Planning in the World

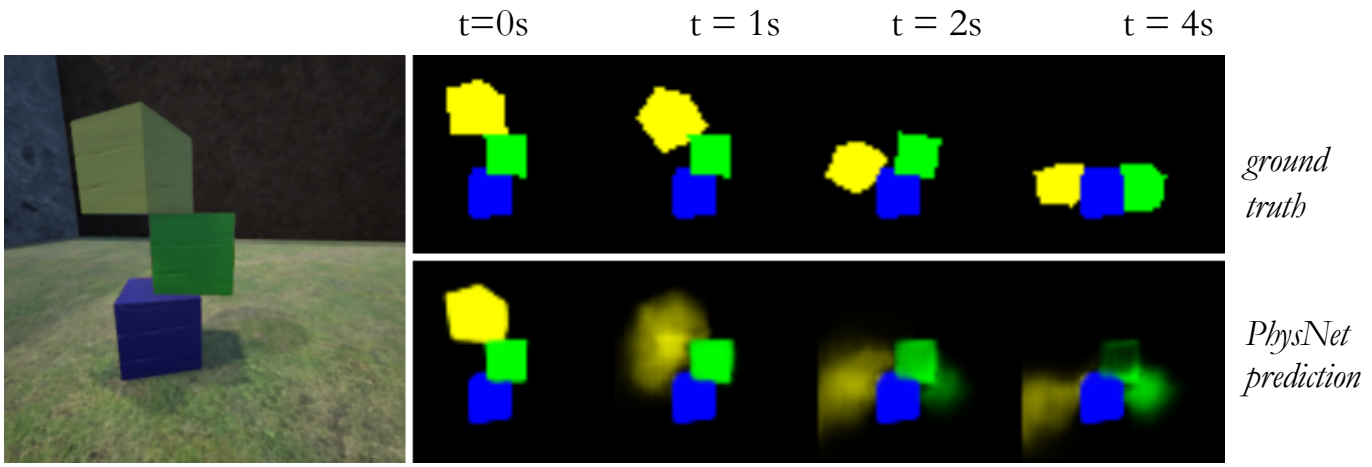
- Try out different action sequences in mind of robot/agent
- Need accurate world simulator



[Yann LeCun]

Video Prediction

- Predict pixels of next frame, given previous ones
- Enables learning of world model/simulator
- Challenging due to inherent uncertainty in the dynamics of the world
  - Pixel wise loss functions can cause blurring due to multiple futures being accounted for



[Lerer, Gross, Fergus ICML 2016]

Video Prediction

- Lots of prior work, e.g.:
  - LSTMs: Srivastava et al. (2015); Finn et al. (2016)
  - Discrete latent variables: Ranzato et al. (2014)
  - Optical flow: Xue et al. (2016); Walker et al. (2015)
  - Action-conditional: Chiappa et al. (2017) and Oh et al. (2015)

[Mathieu, Couprie, LeCun, ICLR 2016]

Handling Uncertainty

- Video prediction is challenging due to inherent uncertainty in the dynamics of the world
- Pixel wise loss functions can cause blurring due to multiple futures being accounted for

- Two broad approaches:
  - GANs (Mathieu et al. 2015; Vondrick et al. 2016)
  - Latent variables (Henaff et al., 2017; Babaeizadeh et al. 2018; Denton & Fergus 2018)

Stochastic Video Generation with a Learned Prior

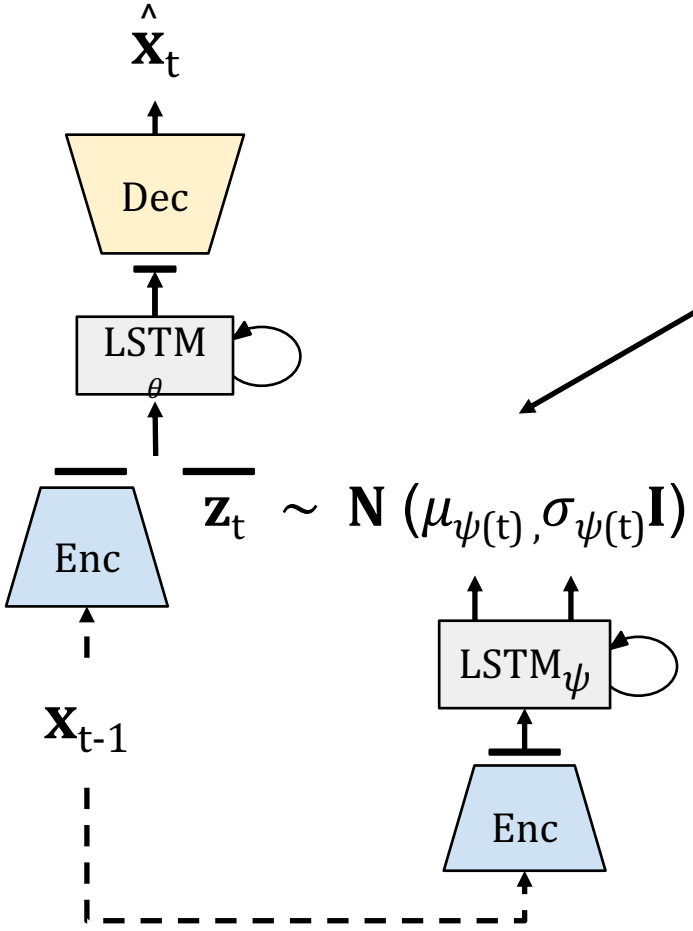
ICML 2018

Emily Denton[1] and Rob Fergus[12]

1

2

Stochastic video generation, Denton & Fergus 2018

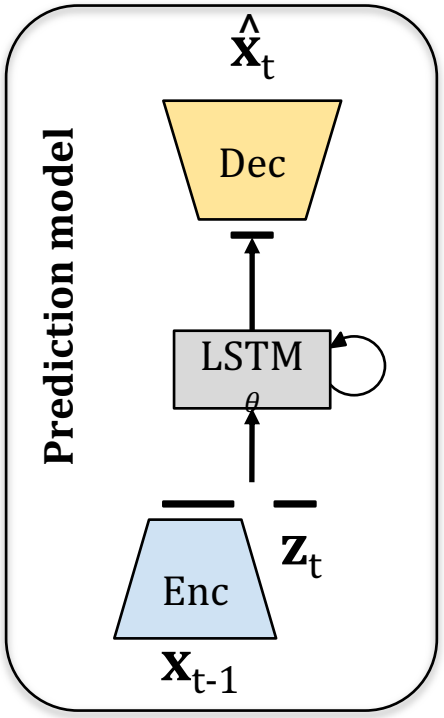


Learned prior dependent on all previous frames

- Combines a deterministic frame predictor with time-dependent stochastic latent variables
- Learned prior over the latent variables can can be interpreted as a predictive model of uncertainty

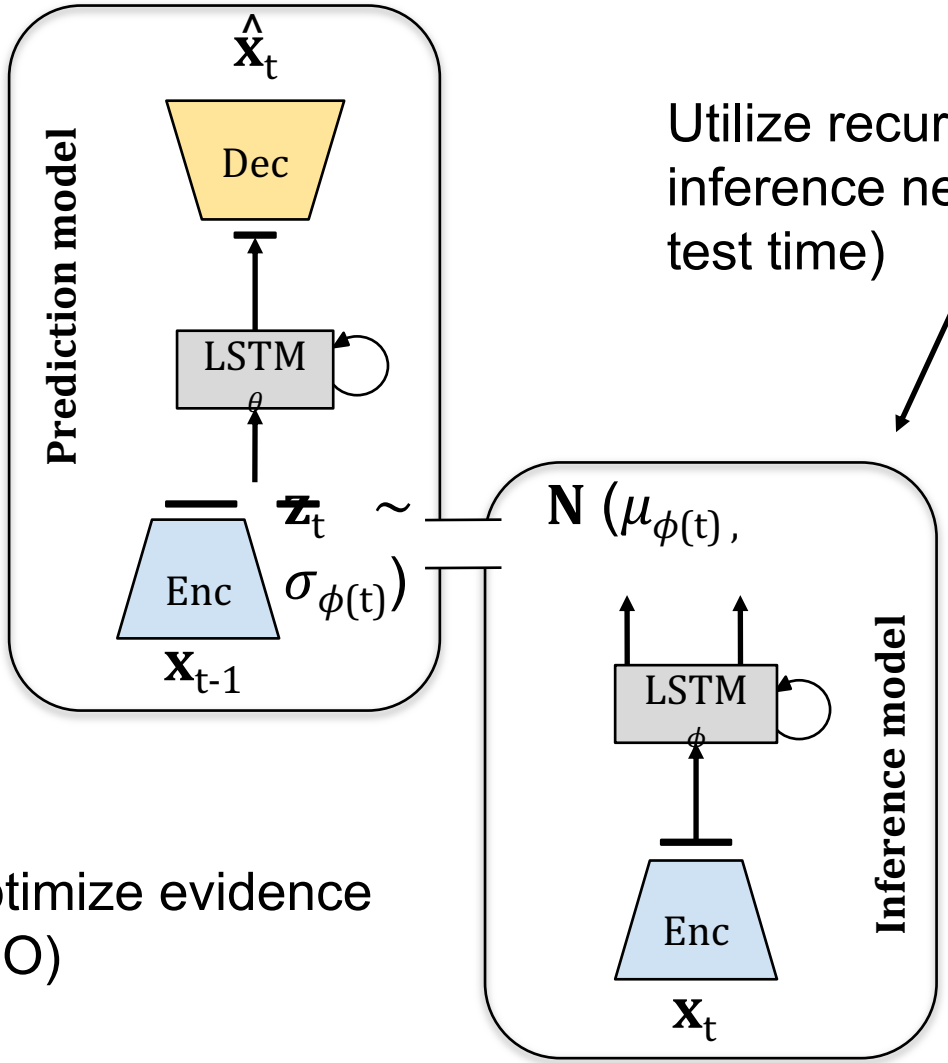
[Denton et al. ICML 2018]

Training at time *t*:



[Denton et al. ICML 2018]

Training at time *t*:

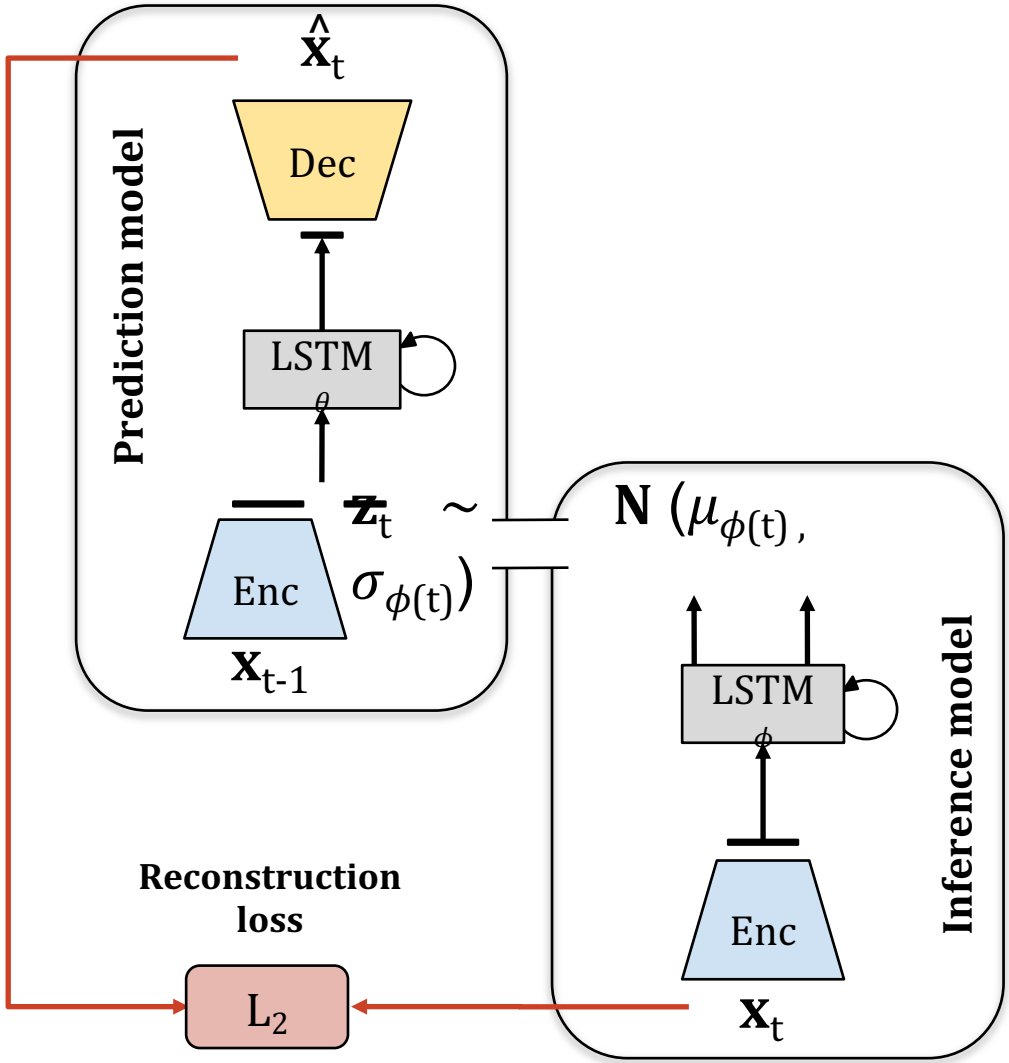


Utilize recurrent approximate inference network (not used at test time)

Train model by optimize evidence lower bound (ELBO)

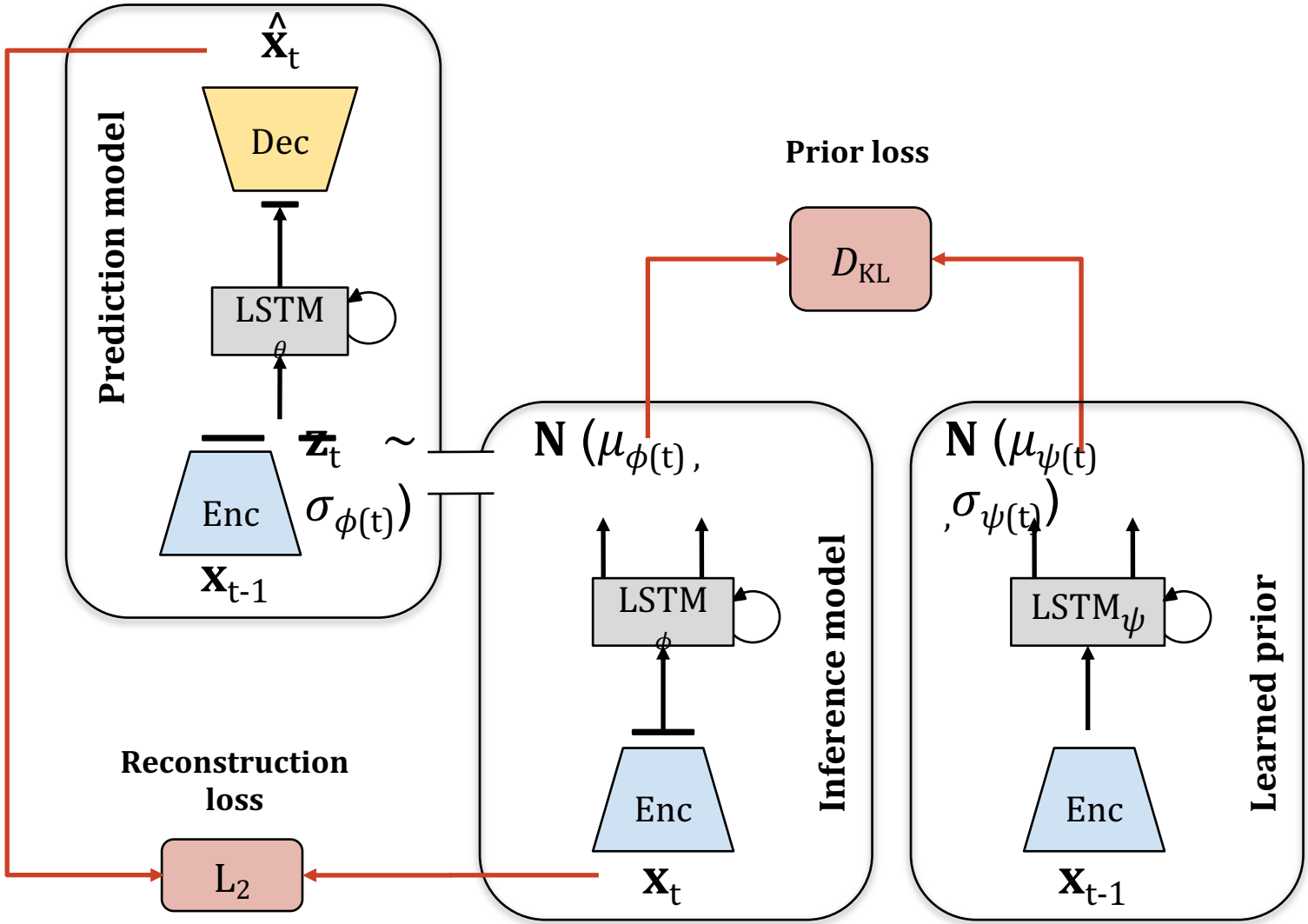
[Denton et al. ICML 2018]

Training at time *t*:



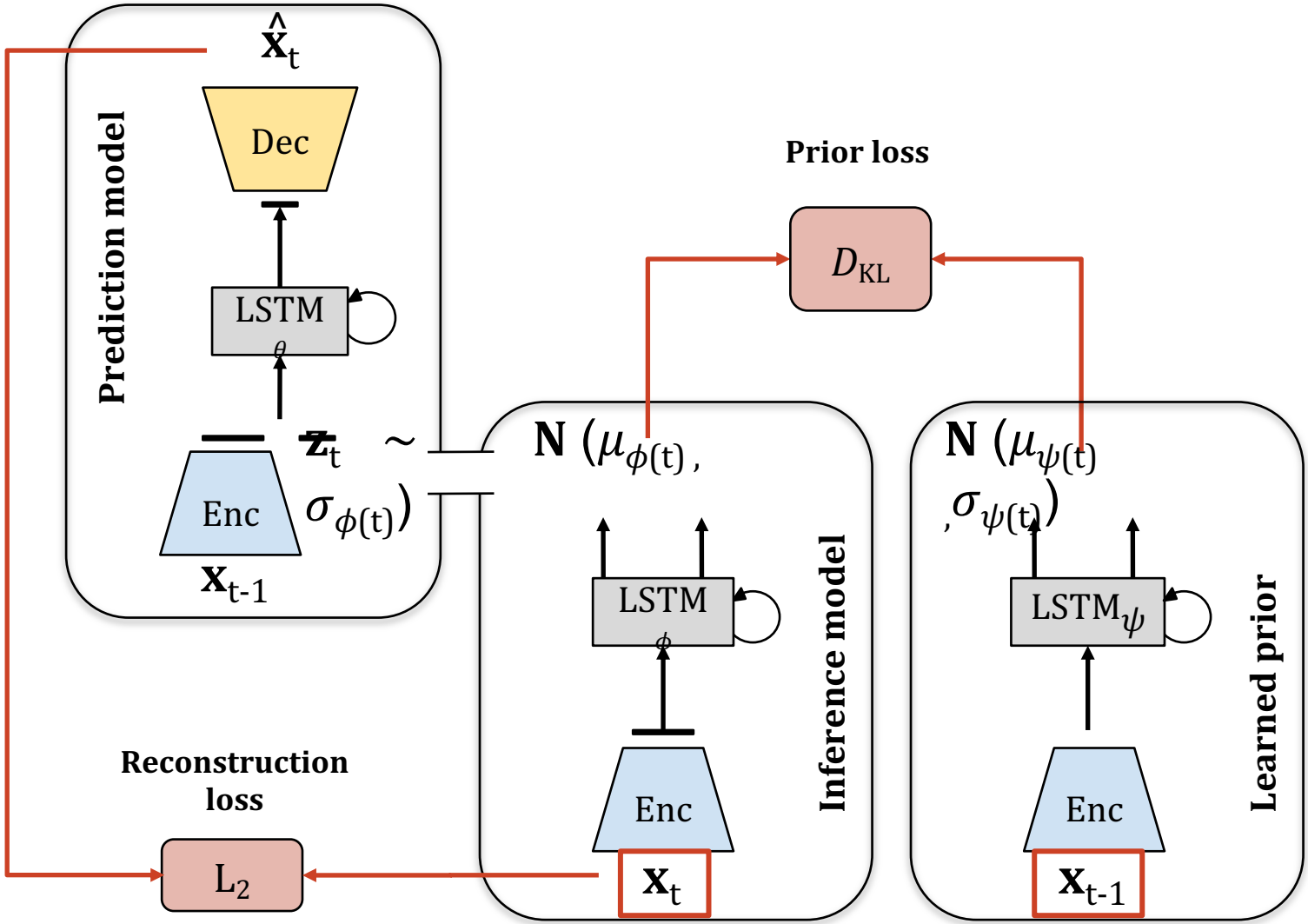
[Denton et al. ICML 2018]

Training at time *t*:



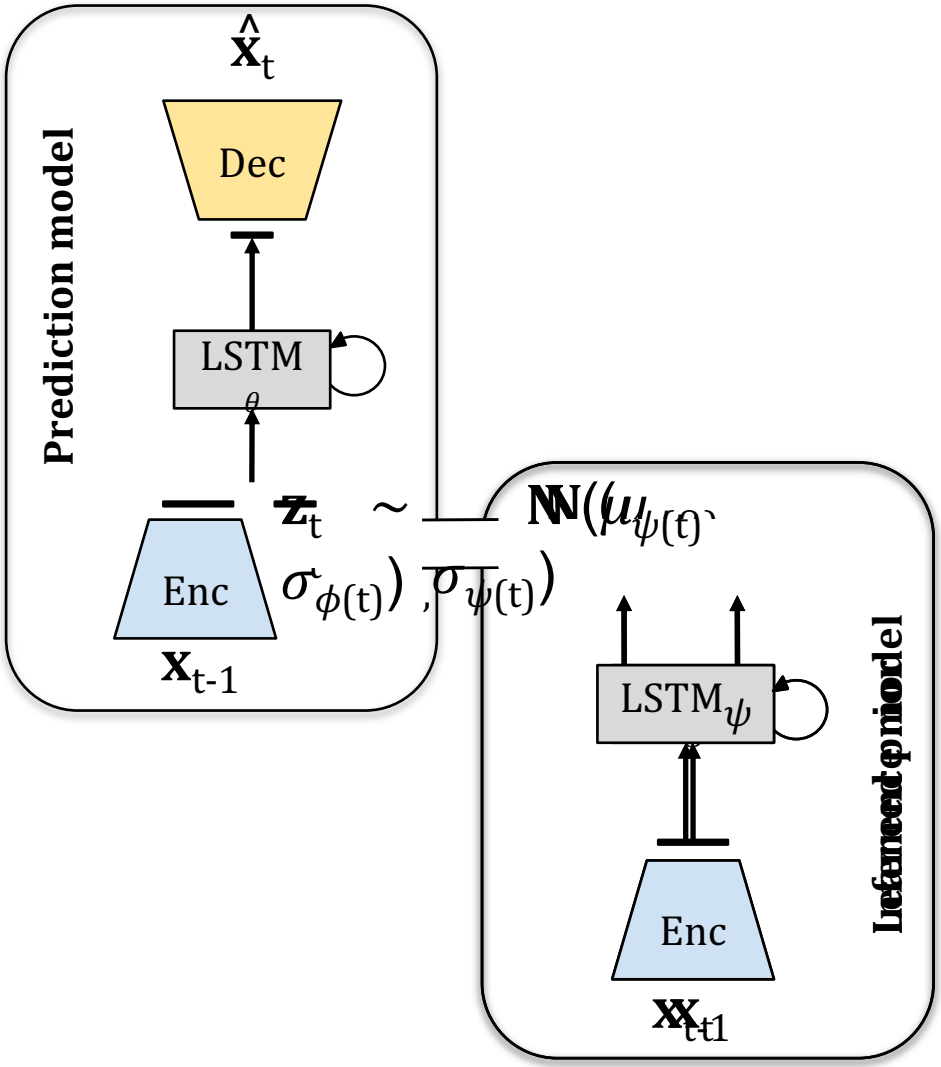
[Denton et al. ICML 2018]

Training at time *t*:



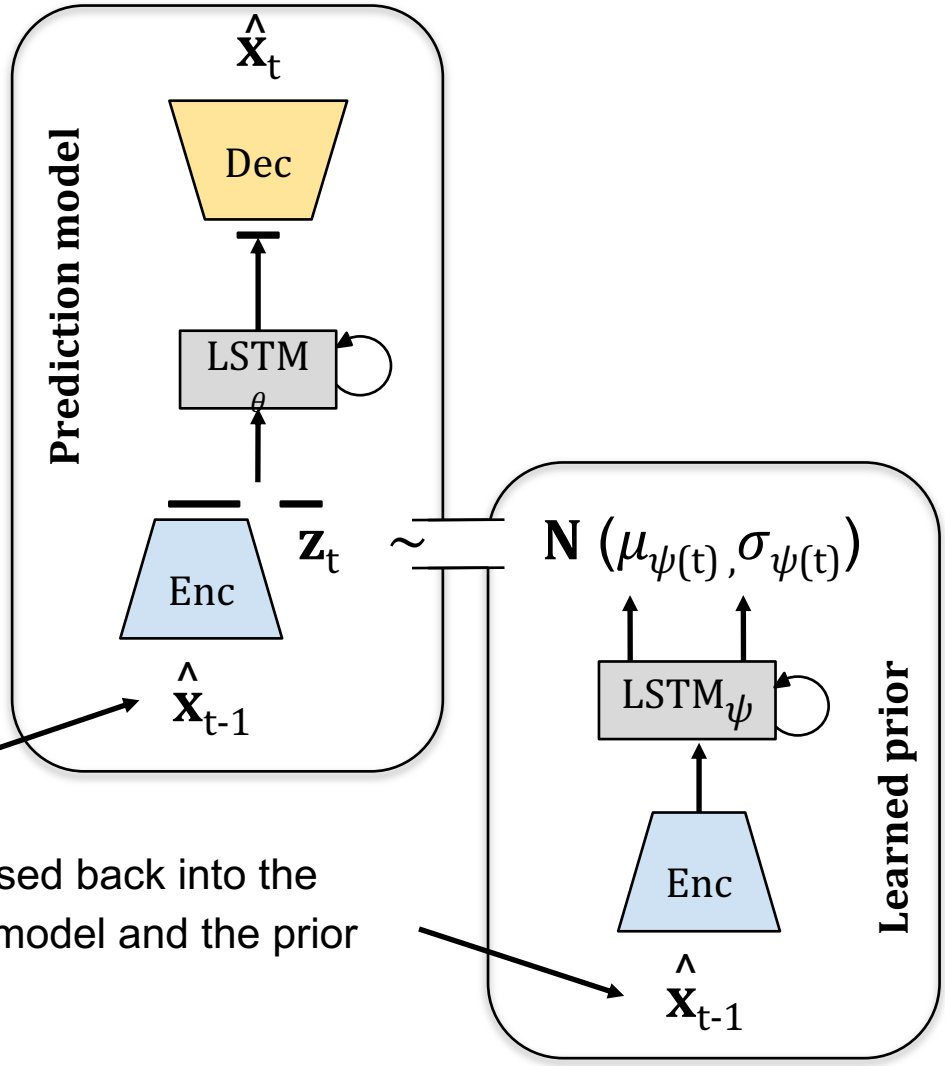
[Denton et al. ICML 2018]

Generation at time *t*:



[Denton et al. ICML 2018]

Generation at time *t*:



Generated frames passed back into the input of the prediction model and the prior

[Denton et al. ICML 2018]

Babaeizadeh et al. (2018)

Inference

Feed forward net encodes entire video sequence:

$$\boldsymbol{z}_t \sim q_\phi(\boldsymbol{z} \mid \boldsymbol{x}_{1:T})$$

Denton et al. (2018)

Inference

Recurrent net produces different distribution for every *t*:

$$q_\phi(\mathbf{z} \mid \mathbf{x}) = \prod_t q_\phi^{(t)}(\mathbf{z}_t \mid \mathbf{x}_{1:t})$$

$$\mathbf{z}_t \sim q_\phi^{(t)}(\mathbf{z}_t \mid \mathbf{x}_{1:t})$$

[*Babaeizadeh et al. Stochastic variational video prediction. ICLR, 2018.*]

[Denton et al. ICML 2018]

Babaeizadeh et al. (2018)

Inference

Feed forward net encodes entire video sequence:

$$\boldsymbol{z}_t \sim q_\phi(\boldsymbol{z} | \boldsymbol{x}_{1:T})$$

Generation

$$\boldsymbol{z}_t \sim \mathbf{N}(\mathbf{0}, \mathbf{I})$$

Denton et al. (2018)

Inference

Recurrent net produces different distribution for every *t*:

$$q_\phi(\mathbf{z} \mid \mathbf{x}) = \prod_t q_\phi^{(t)}(\mathbf{z}_t \mid \mathbf{x}_{1:t})$$

$$\mathbf{z}_t \sim q_\phi^{(t)}(\mathbf{z}_t \mid \mathbf{x}_{1:t})$$

Generation

$$\mathbf{z}_t \sim \mathbf{N}(\mu_\psi(\mathbf{x}_{1:t-1}), \sigma_\psi(\mathbf{x}_{1:t-1})\mathbf{I})$$

[*Babaeizadeh et al. Stochastic variational video prediction. ICLR, 2017.*]

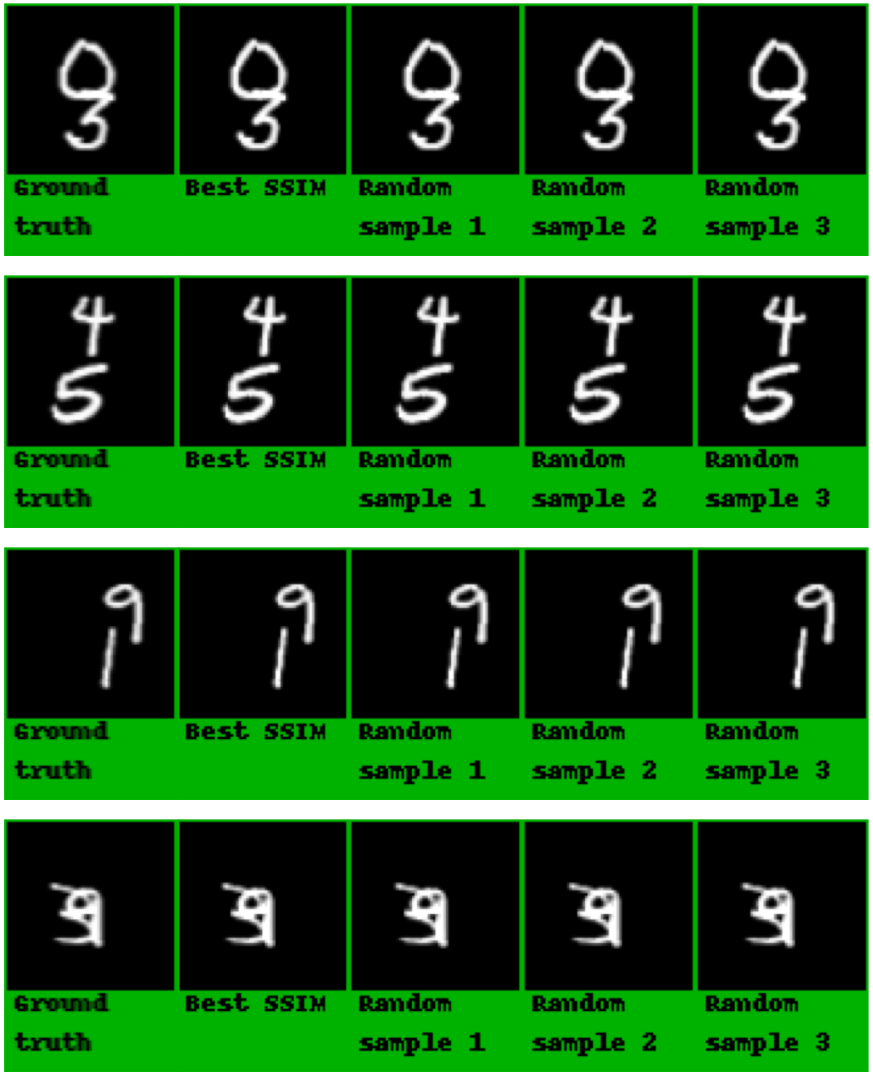
[Denton et al. ICML 2018]

Stochastic Moving MNIST

- Stochastic variant of the Moving MNIST dataset (*Srivastava et al.*, 2015)

Green: Ground truth input
Red: generated frames

- Model conditioned on 5 frames and trained to predict next 10 frames
- Best SSIM chosen from 100 samples



[Denton et al. ICML 2018]

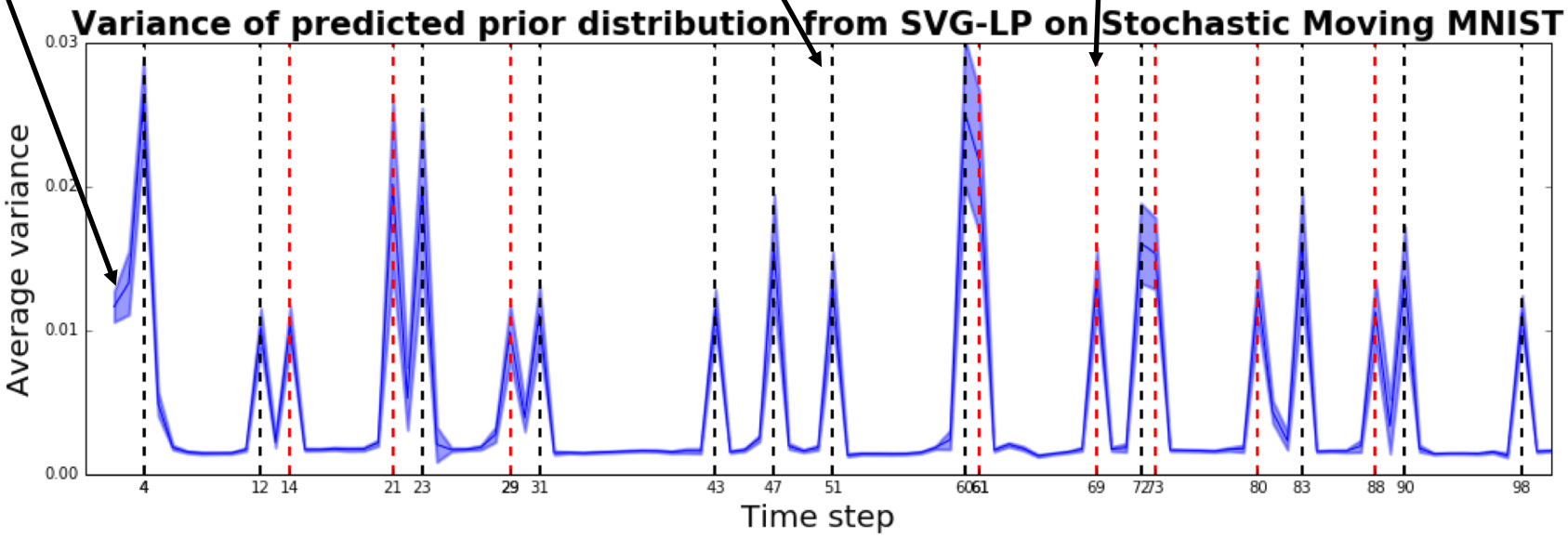
Learned prior can be interpreted as a model of uncertainty

Prior predicts *low variance distribution for deterministic parts of the video*, *high variance distribution as points of uncertainty*

Predicted variance from our models learned prior

Black dashed lines:
digit 1 collides with wall

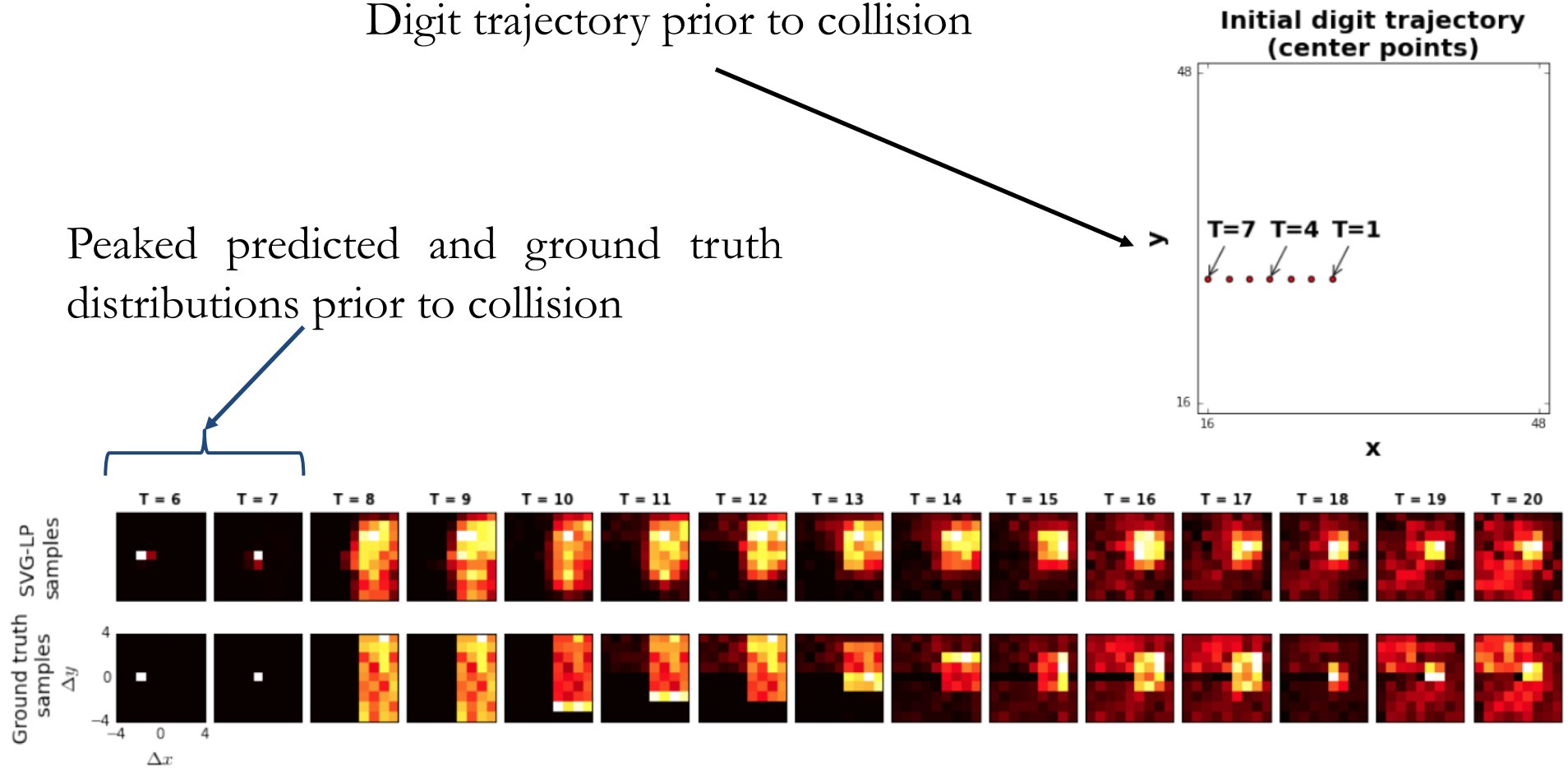
Red dashed lines:
digit 2 collides with wall



[Denton et al. ICML 2018]

Digit trajectory prior to collision

Peaked predicted and ground truth distributions prior to collision



[Denton et al. ICML 2018]

BAIR robot push dataset (Ebert et al., 2017)

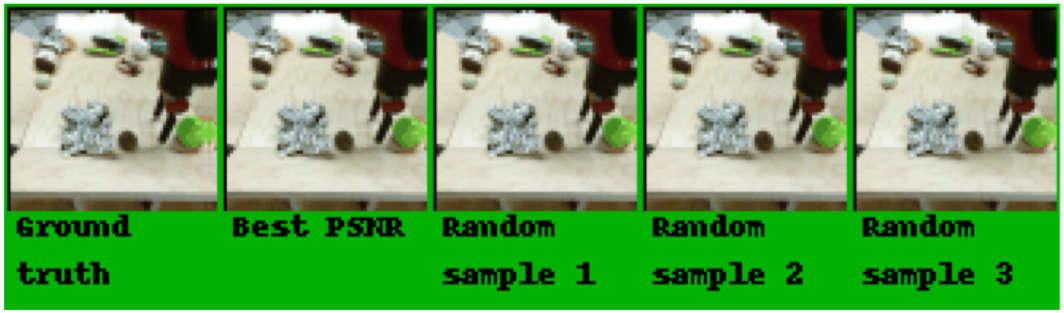
- Sawyer robotic arm pushing a variety of objects around a table top
- 30 frames in sequence, 64x64 resolution
- Movements of the arm are highly stochastic

[Ebert et al. Self-supervised visual planning with temporal skip connections. CoRL, 2017.]

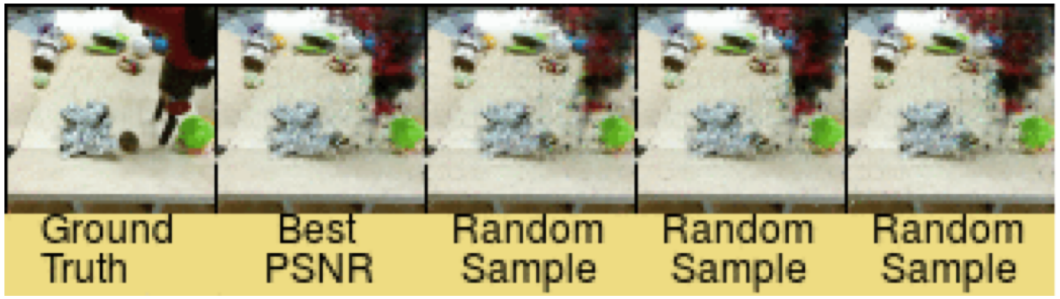
[Denton et al. ICML 2018]

BAIR robot push dataset

SVG-LP (ours)



Babaeizadeh et al. (2018)



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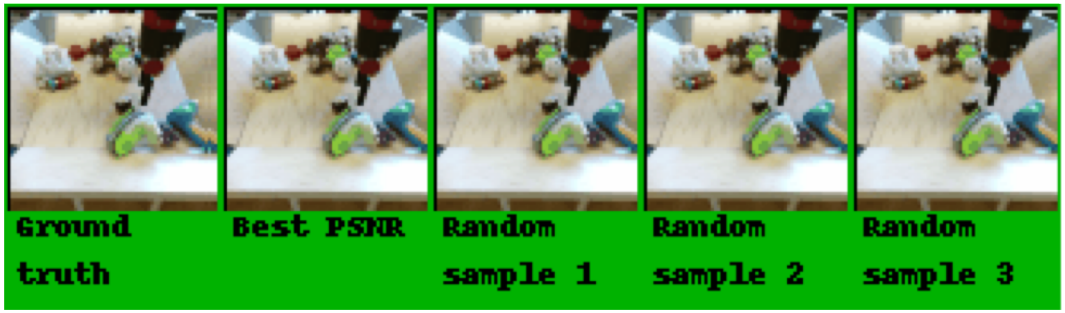
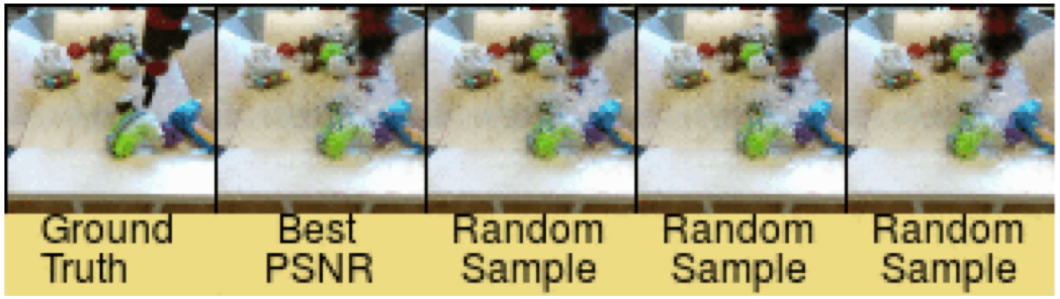


Babaeizadeh et al. (2018)



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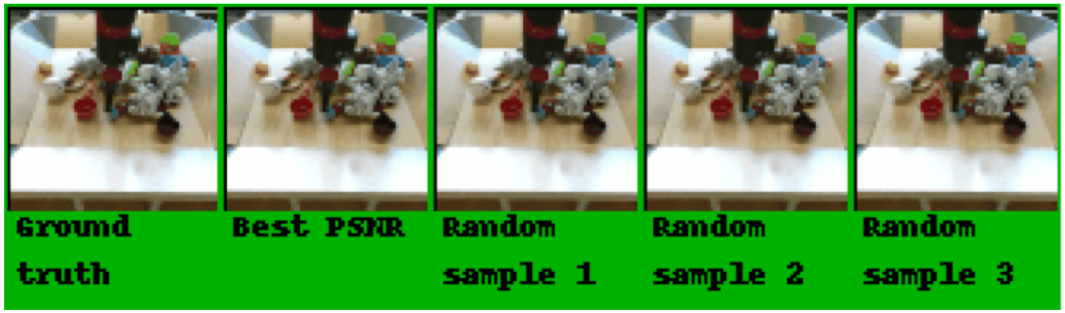
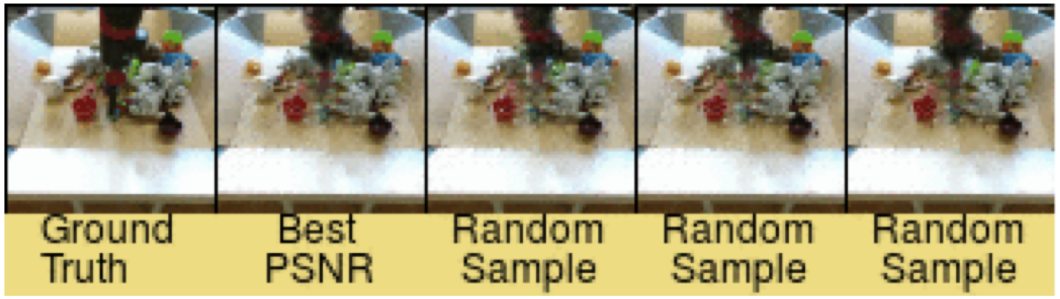


Babaeizadeh et al. (2018)



[*Babaeizadeh et al. Stochastic variational video prediction. ICLR, 2018.*]

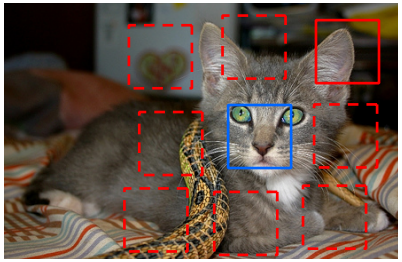
[Denton et al. ICML 2018]

2. Self-supervised Learning

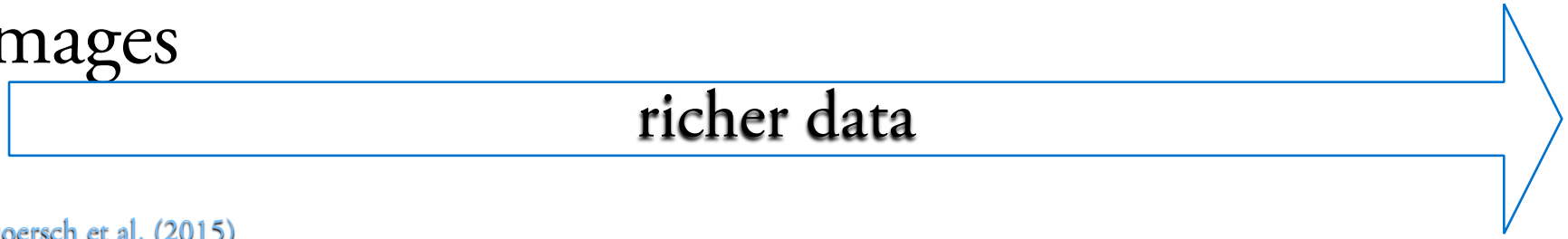
Unsupervised learning as a pre-training step

- Target task is high-level understanding of signal
  - E.g. Classification, detection
- Unsupervised learning to pre-train models
  - Then fine-tune with labels on target task
- Some success in NLP
  - Word2vec for word embeddings
  - Language modeling for machine translation
- No equivalent success in computer vision or other domains
- But there are a lot of attempts!

Range of self-supervised systems

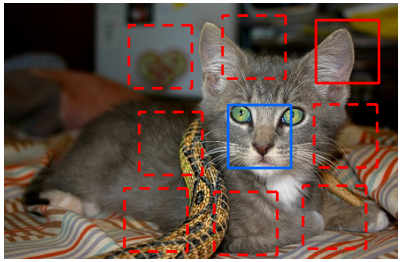


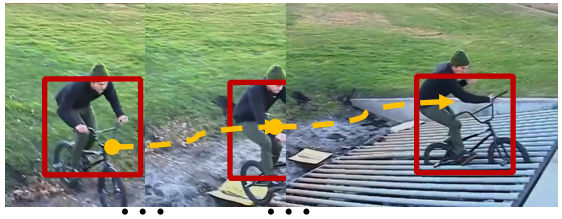
images



- Doersch et al. (2015)
- Zhang et al. (2016)
- Zhang et al. (2017)
- Noroozi et al. (2016)
- Pathak et al. (2016)

Range of self-supervised systems





images videos

richer data

- Doersch et al. (2015)
- Zhang et al. (2016)
- Zhang et al. (2017)
- Noroozi et al. (2016)
- Pathak et al. (2016)

- Wang et al. (2015)
- Misra et al. (2016)
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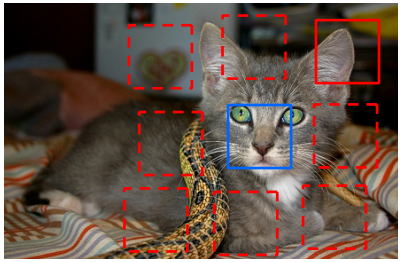
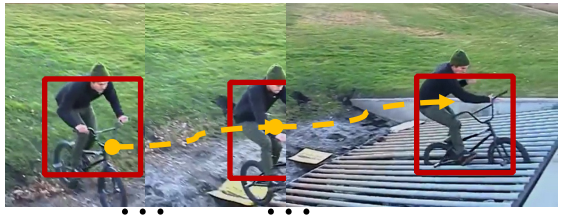
Range of self-supervised systems





images videos sound & depth

richer data

- Doersch et al. (2015)
- Zhang et al. (2016)
- Zhang et al. (2017)
- Noroozi et al. (2016)
- Pathak et al. (2016)

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- Zhang et al. (2017)
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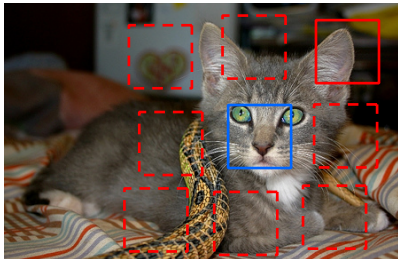
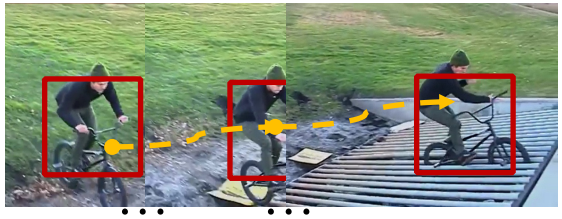
Range of self-supervised systems





images videos sound & depth actions

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- Pathak et al. (2017)

- Owens et al. (2016)
- Zhang et al. (2017)
- Bansal et al. (2016)

- Agarwal et al. (2015)
- Jayaraman et al. (2015)
- Pinto et al. (2016)
- Agarwal et al. (2016)
- Pinto et al. (2017)
- Pinto et al. (2016)

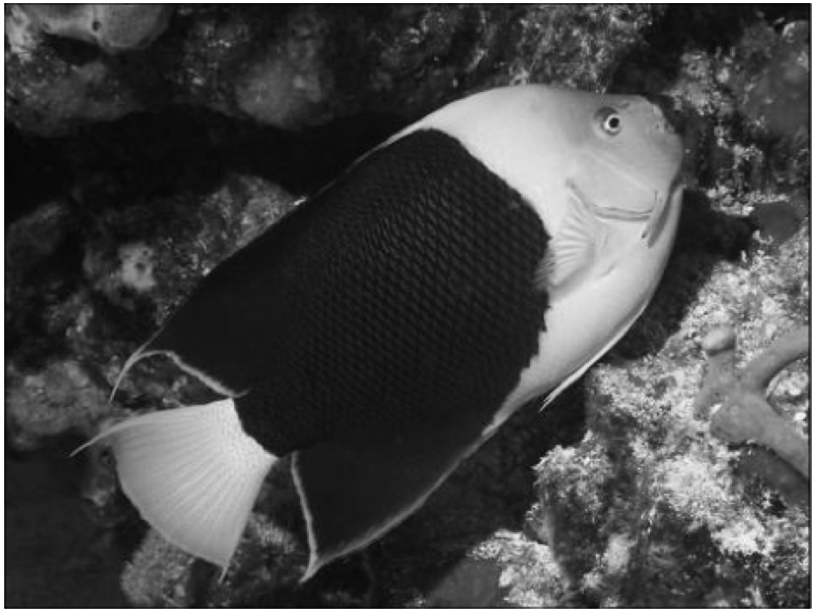
Image colorization

Colorful Image Colorization

Richard Zhang, Phillip Isola, Alexei (Alyosha) Efros

slides from Zhang

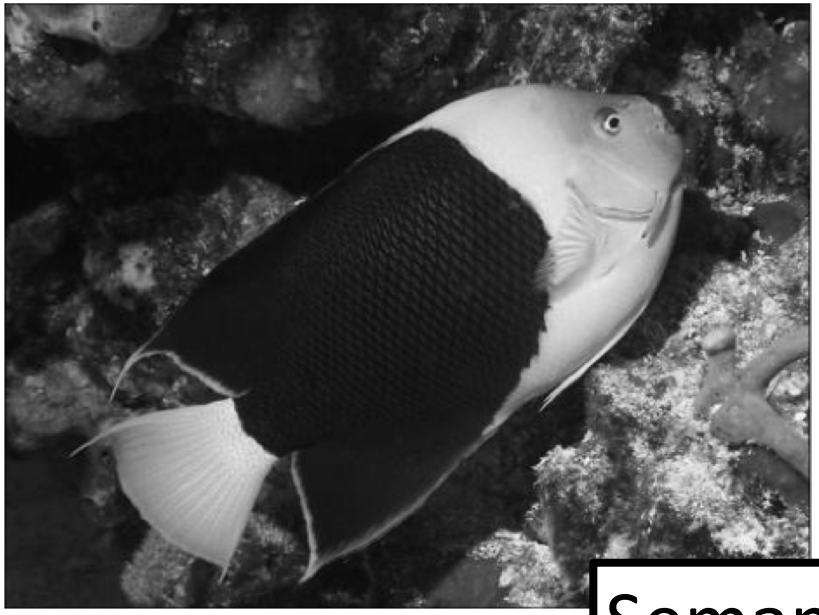
http://richzhang.github.io/colorization/



$\mathcal{F}$

Grayscale image: *L* channel $\mathbf{X} \in \mathbb{R}^{H \times W \times 1}$

Color information: *ab* cha $\hat{\mathbf{Y}} \in \mathbb{R}^{H \times W \times 2}$



$\mathcal{F}$

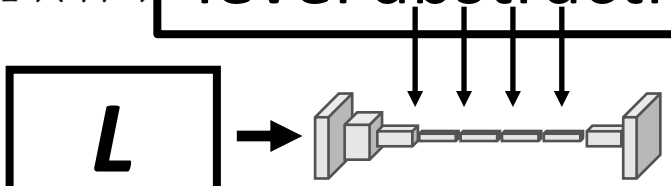
Grayscale image

$\mathbf{X} \in \mathbb{R}^{H \times W \times$

Semantics? Higher-level abstraction?

oncatenate (L,ab)

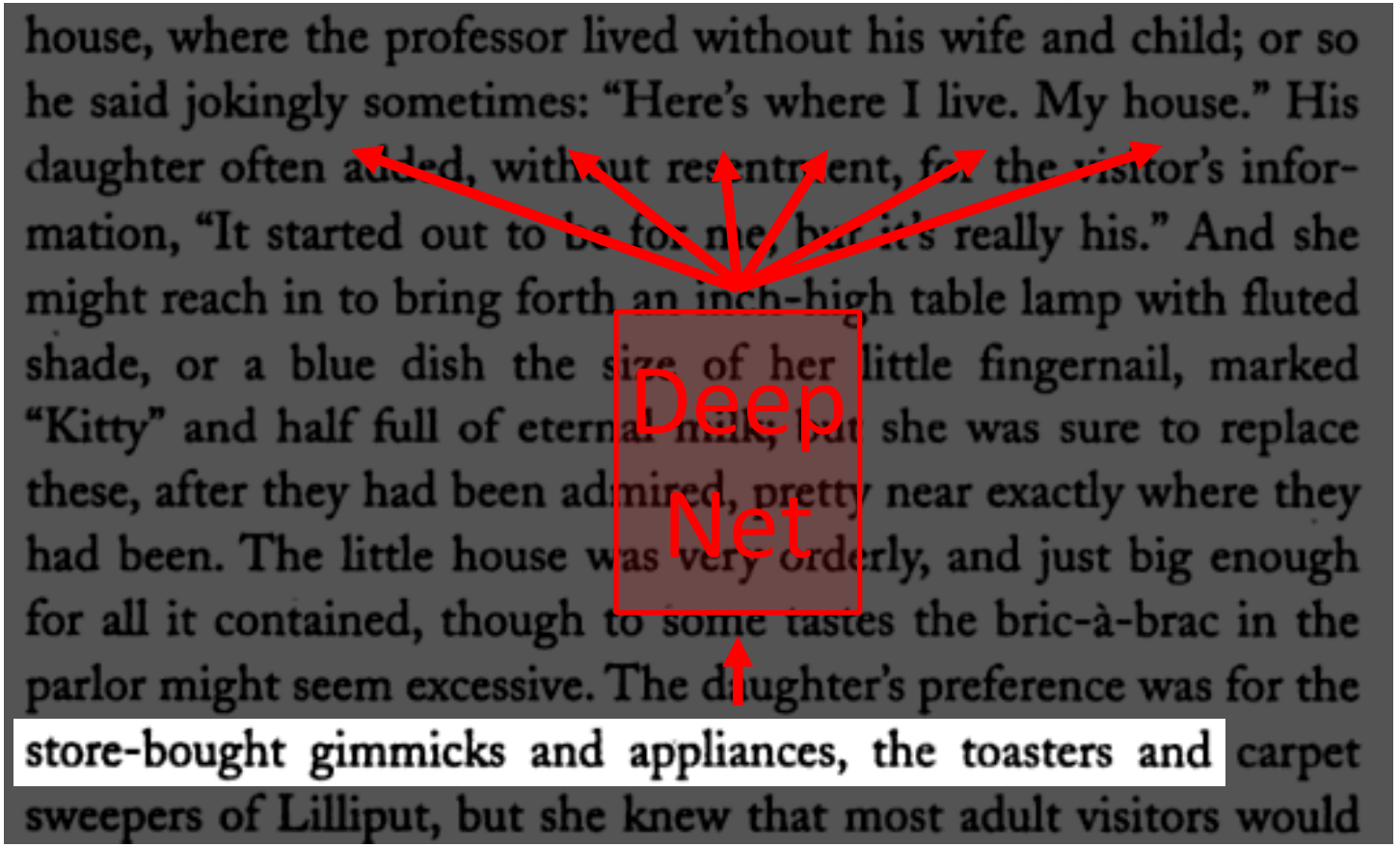
$(\mathbf{X}, \hat{\mathbf{Y}})$



"Free" supervisory signal

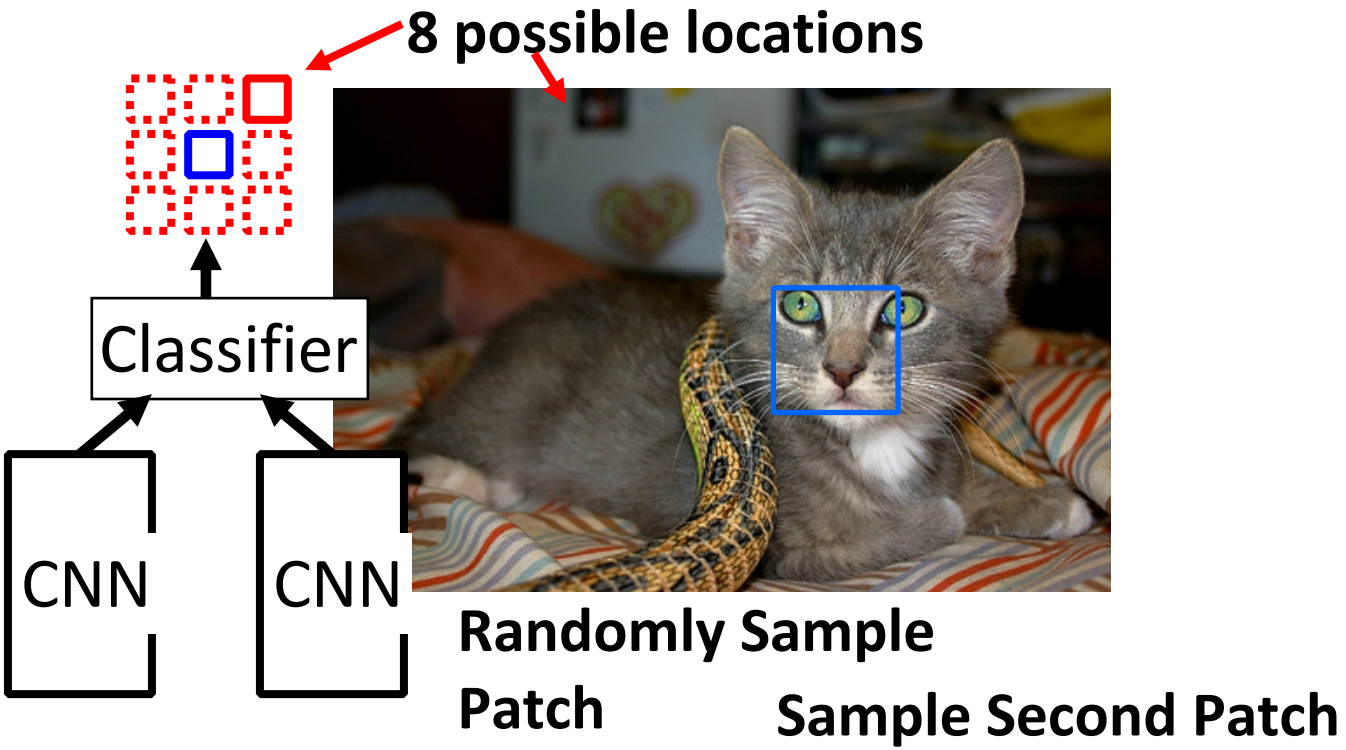
Context as supervision

Collobert & Weston 2008; Mikolov et al. 2013



Unsupervised Visual Representation Learning by Context Prediction
[Doersch et al. ICCV 2015]

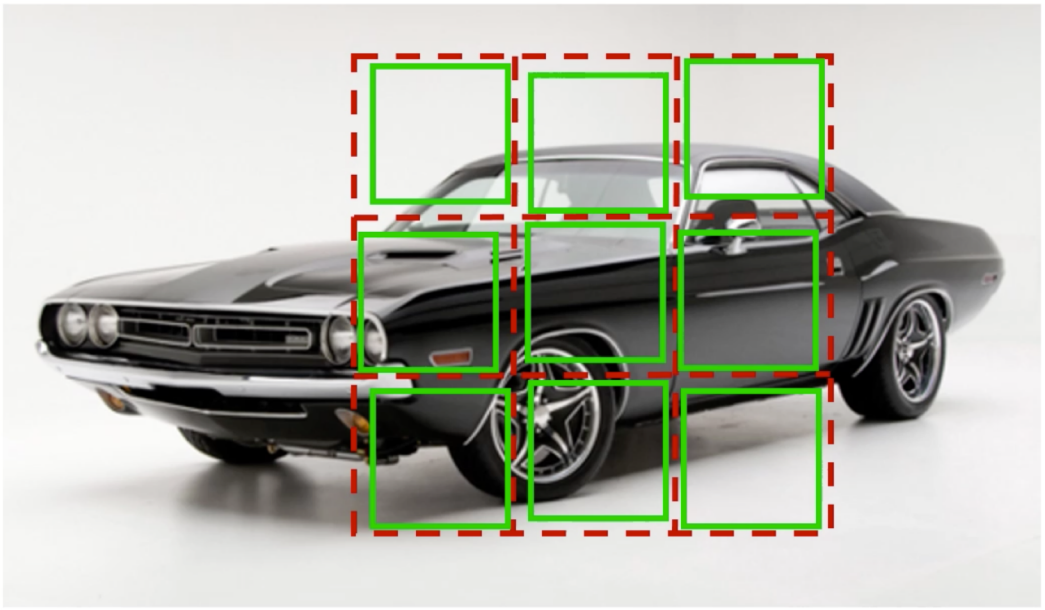
Relative Position Task



Unsupervised Learning of Visual Representations by Solving Jigsaw Puzzles, Noorozi et al. (2016)

What do we learn when we solve a Jigsaw puzzle?

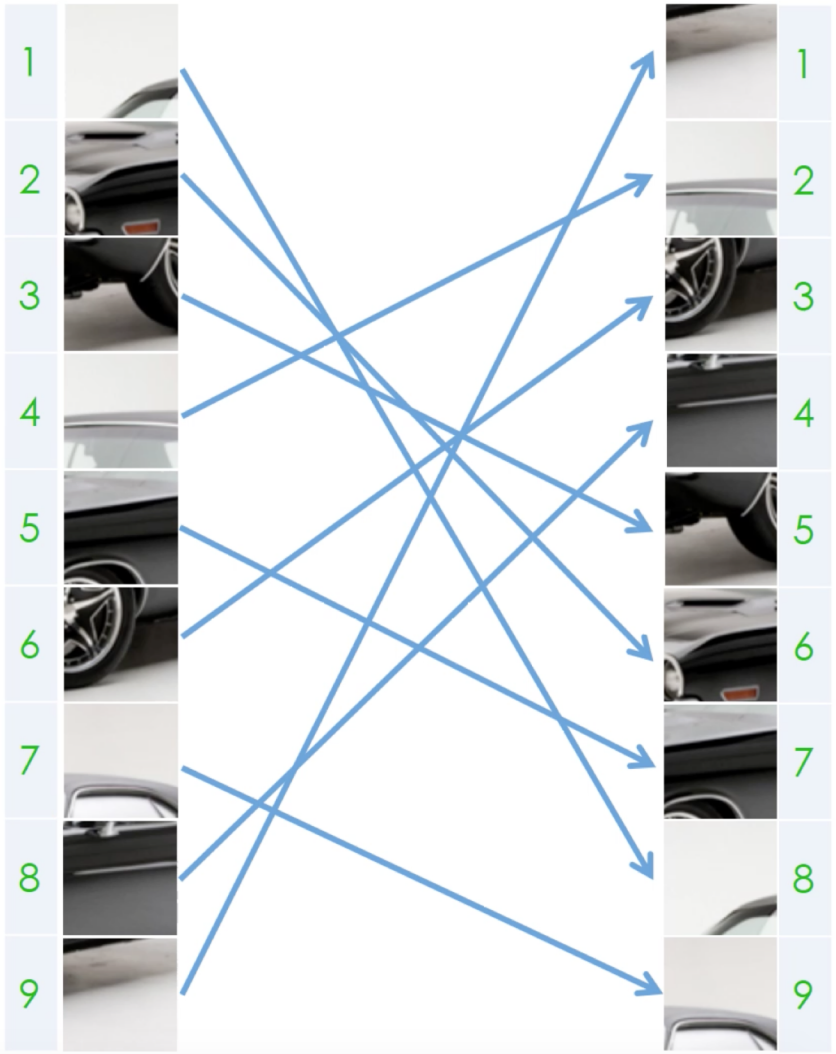
[Noorozi et al. (2016)]



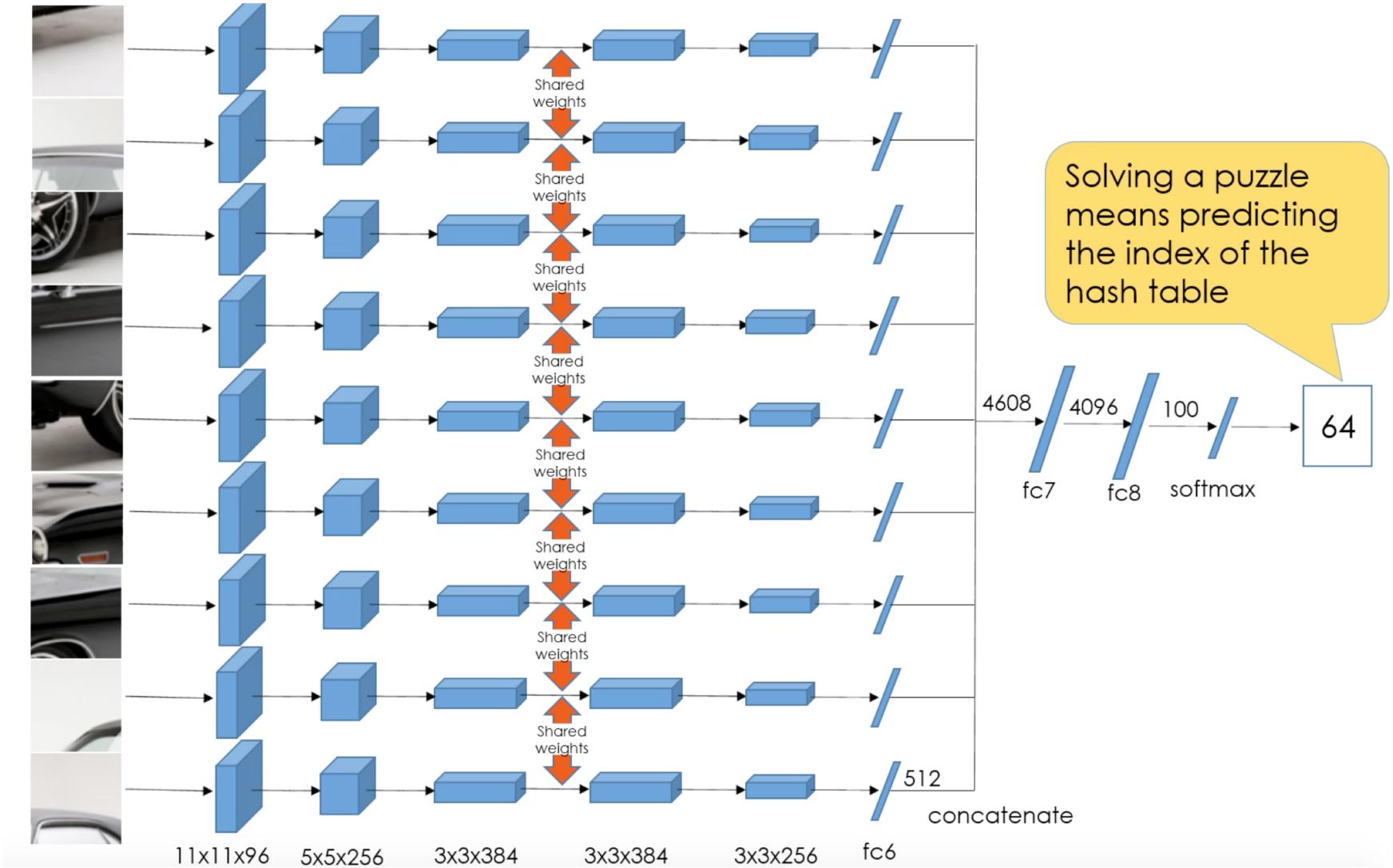
Hash Set

index	table
64	9,4,6,8,3,2,5,1,7

Reorder patches according to the selected hash table



[Noorozi et al. (2016)]



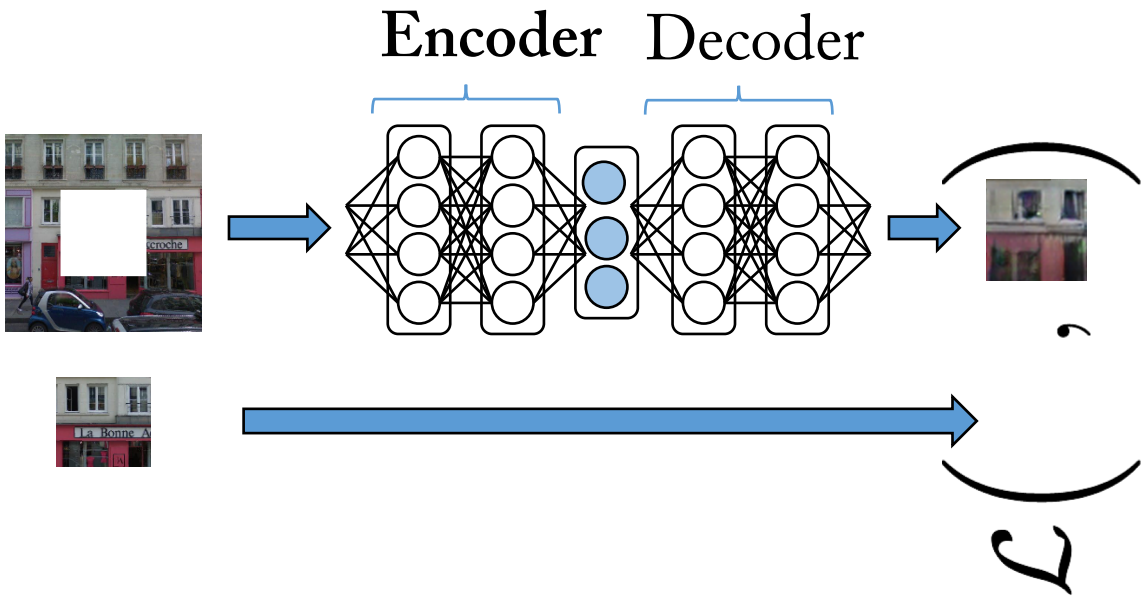
[Noorozi et al. (2016)]

Feature Learning by Inpainting

[Context Encoders: Feature Learning by Inpainting, Pathak et al. (2016)]

[Pathak et al. (2016)]

Context Encoders



- Encoder can be substituted with any network architecture like AlexNet etc.
- Decoder is a set of UpConv/deconv/frac-strided-conv layers

[Pathak et al. (2016)]

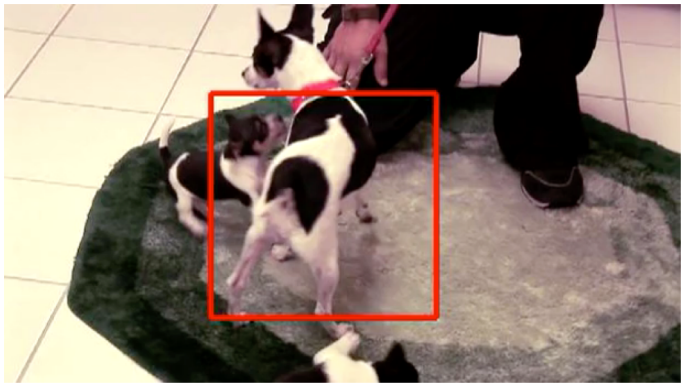
Combined L2 + GAN loss

Input Image L2 Loss Adversarial Loss Joint Loss

[Pathak et al. (2016)]

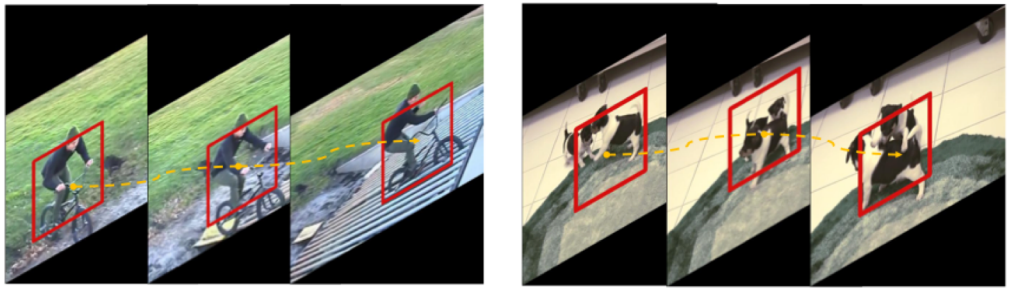
Unsupervised Learning of Visual Representations using Videos, Wang & Gupta 2015

Idea: Object Tracking in Videos

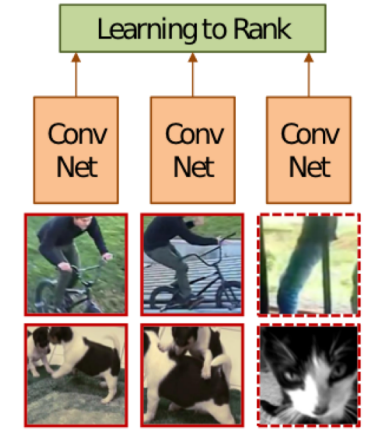


[Wang & Gupta 2015]

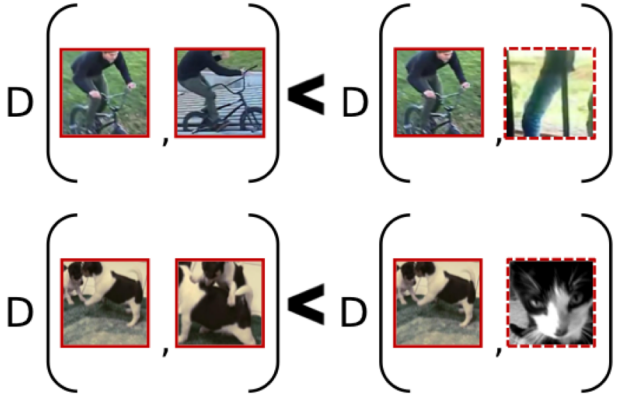
Approach



(a) Unsupervised Tracking in Videos



(b) Siamese-triplet Network



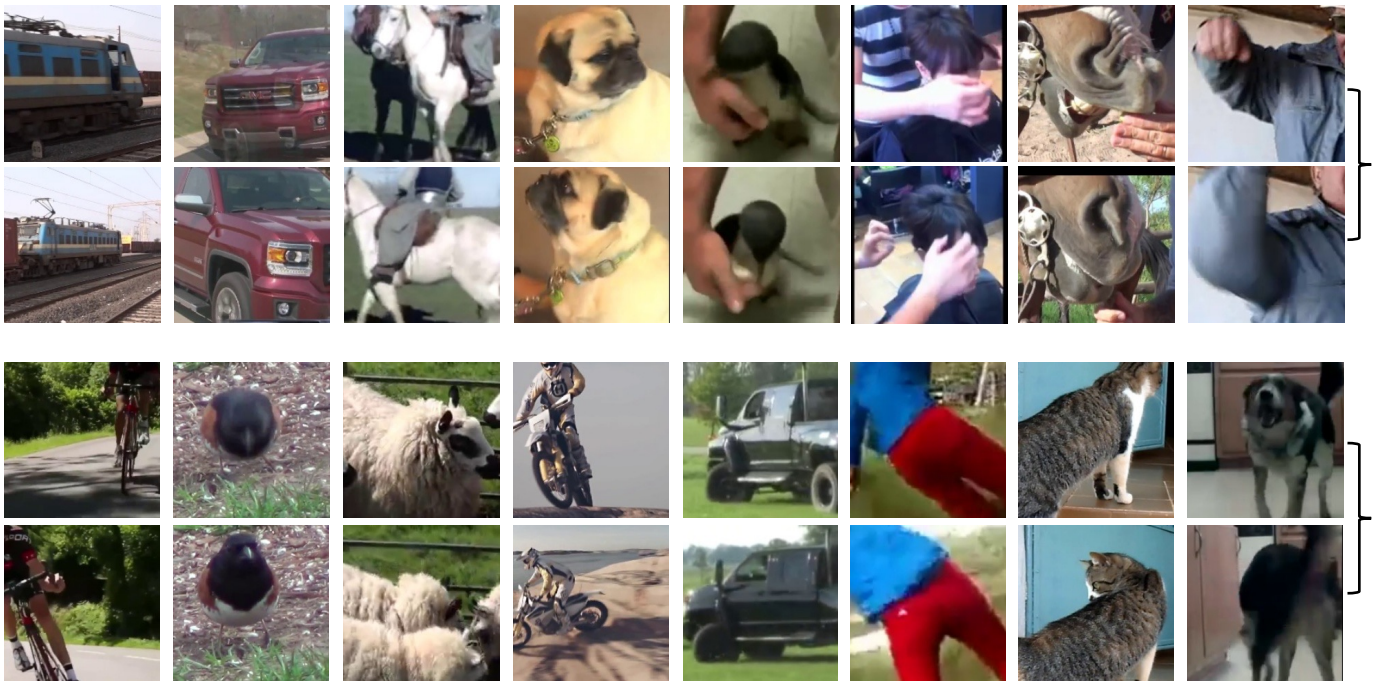
(c) Ranking Objective

- Use object tracking in videos
- Classify if patches belong to the same track or not

[Wang & Gupta 2015]

Patch Mining In Videos

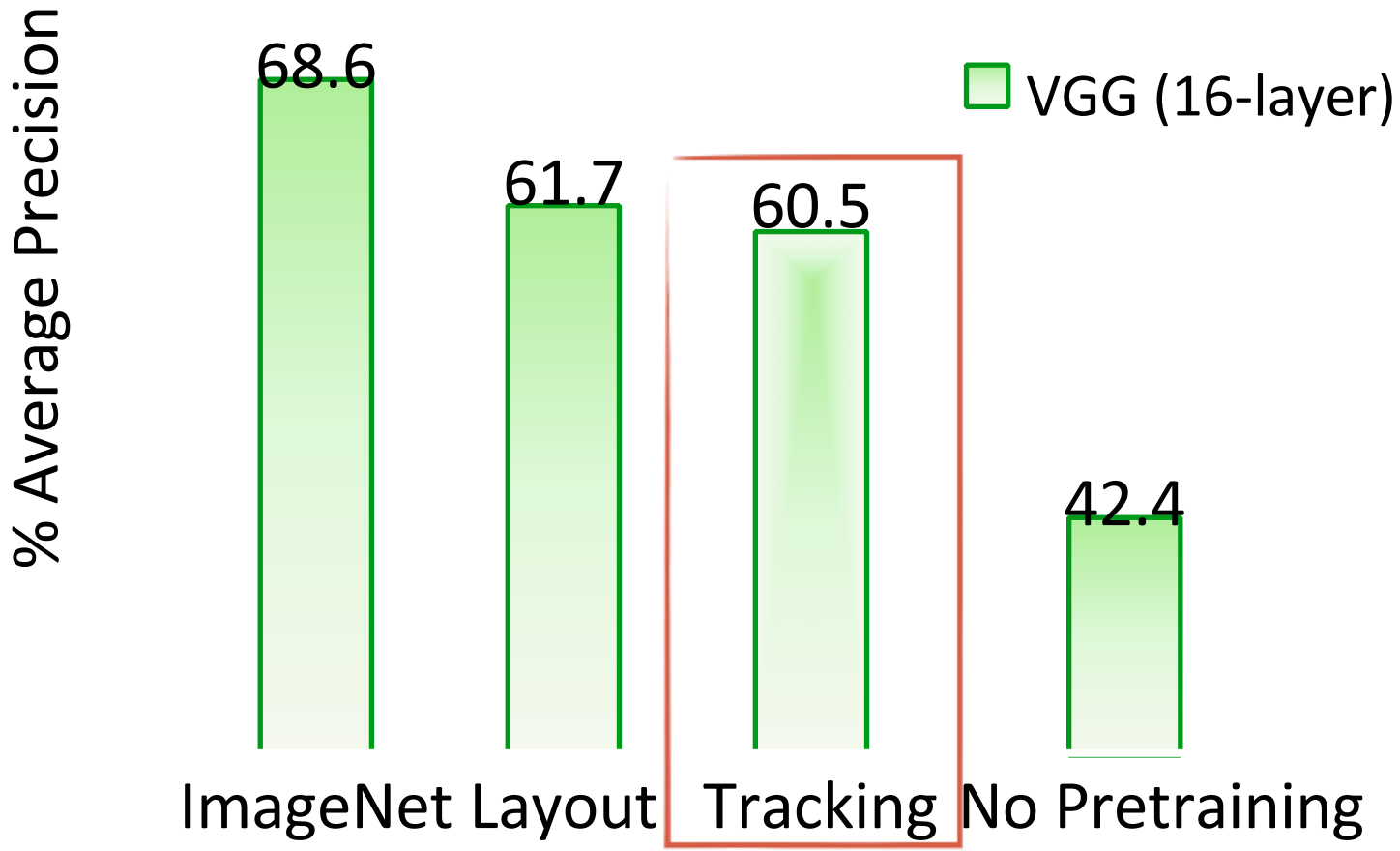
- Track 8M patches in 100K videos from YouTube.
- Use off-the-shelf tracking algorithms with no learning.



[Wang & Gupta 2015]

VOC 2007 Detection Performance

(pretraining for R-CNN)



[Wang & Gupta 2015]

Leveraging Temporal Video Structure

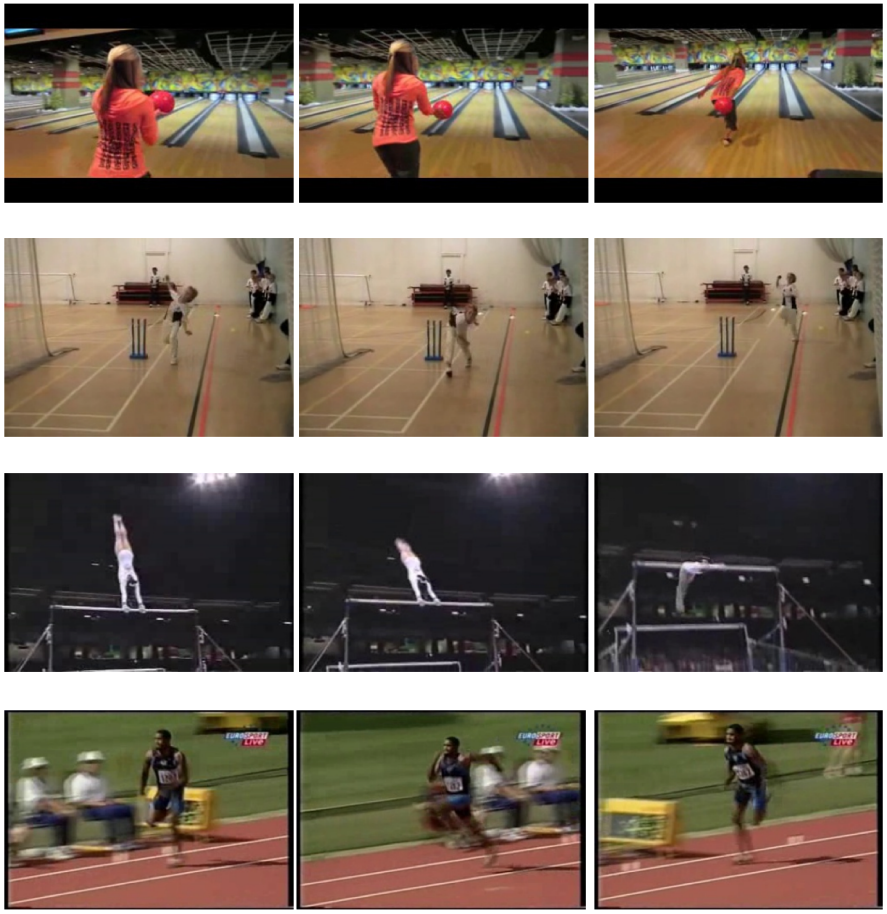
[Shuffle and learn: unsupervised learning using temporal order verification, Misra et al. ECCV 2016]

- Videos have temporal structure

- Can we use this to learn an image representation?

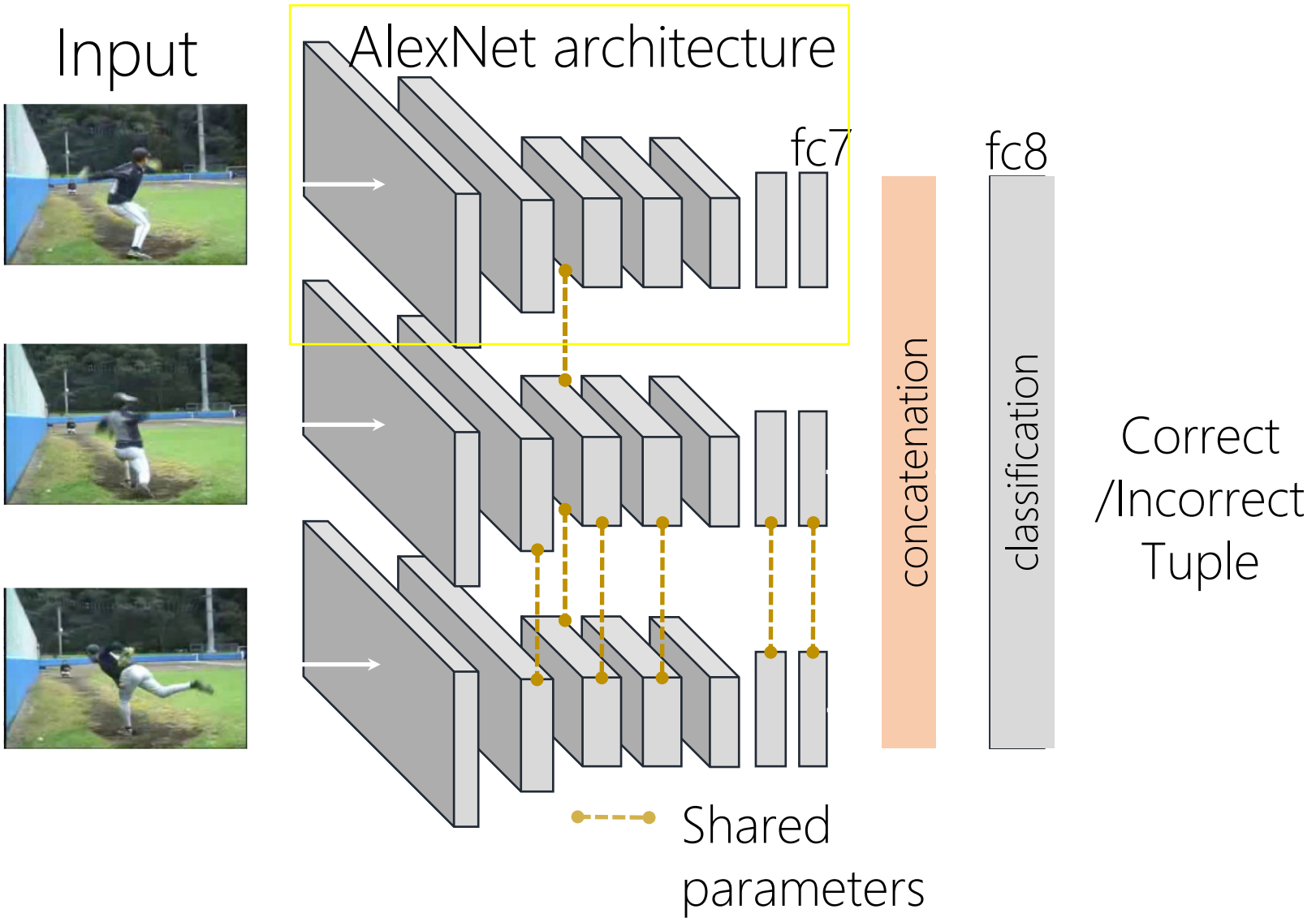



Positive



Negative

[Misra et al. ECCV 2016]



[Misra et al. ECCV 2016]

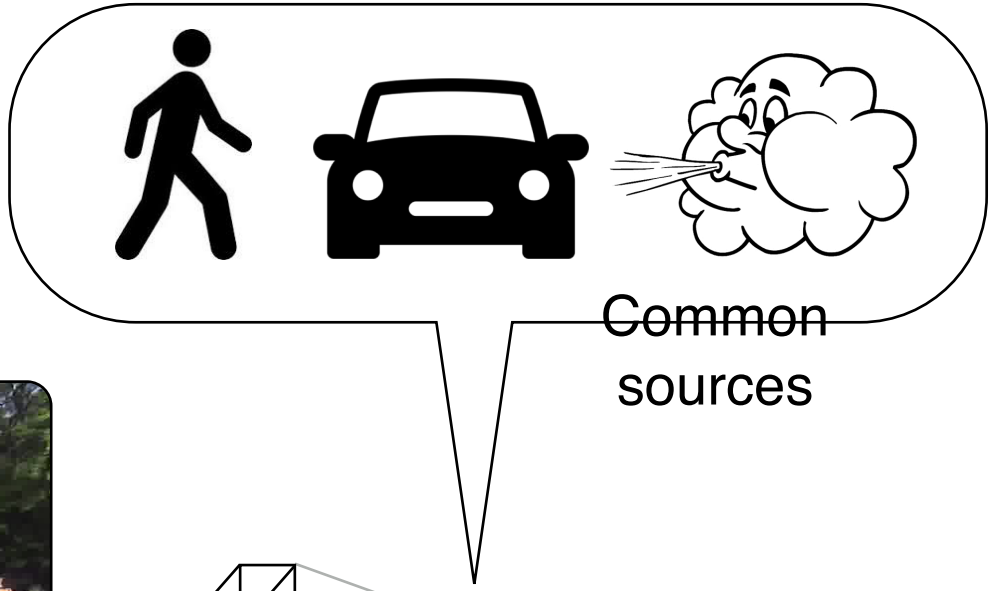
Results: Finetune on Action Recognition

Dataset	Initialization	Mean Classification Accuracy
UCF101	Random	38.6
	Ours	50.2
	ImageNet pre-trained	**67.1**
HMDB51	Random	13.3
	Ours	18.1
	UCF101 pre-trained	15.2
	ImageNet pre-trained	**28.5**

[Misra et al. ECCV 2016]

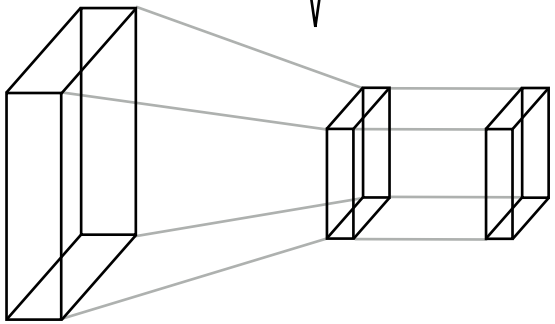
Visual + Audio

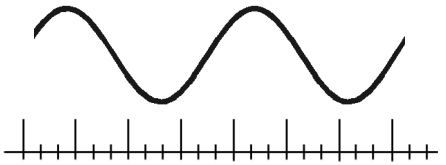
[Ambient Sound Provides Supervision for Visual Learning,
[Owens et al. (2016)]



Common sources

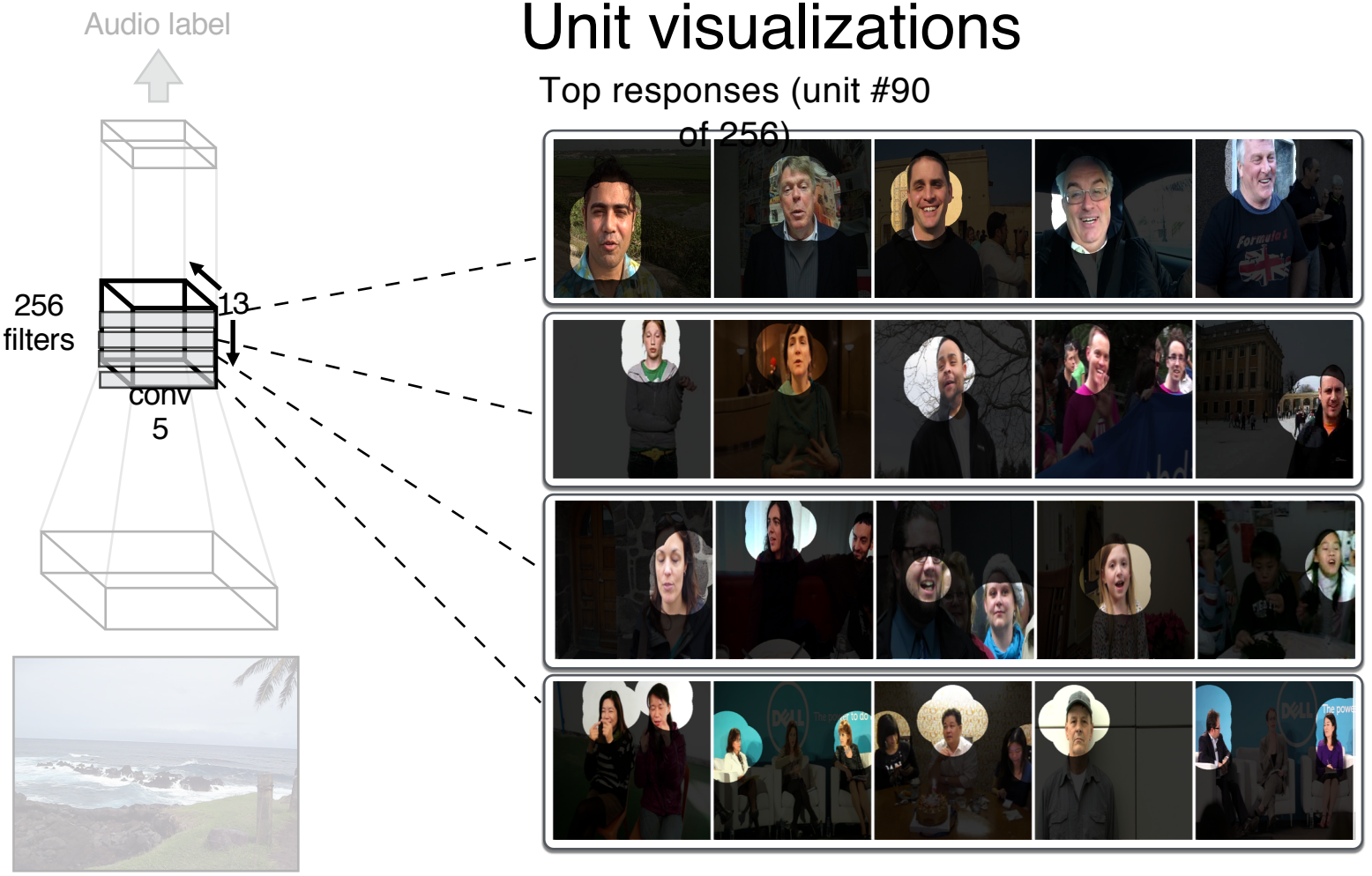
Image



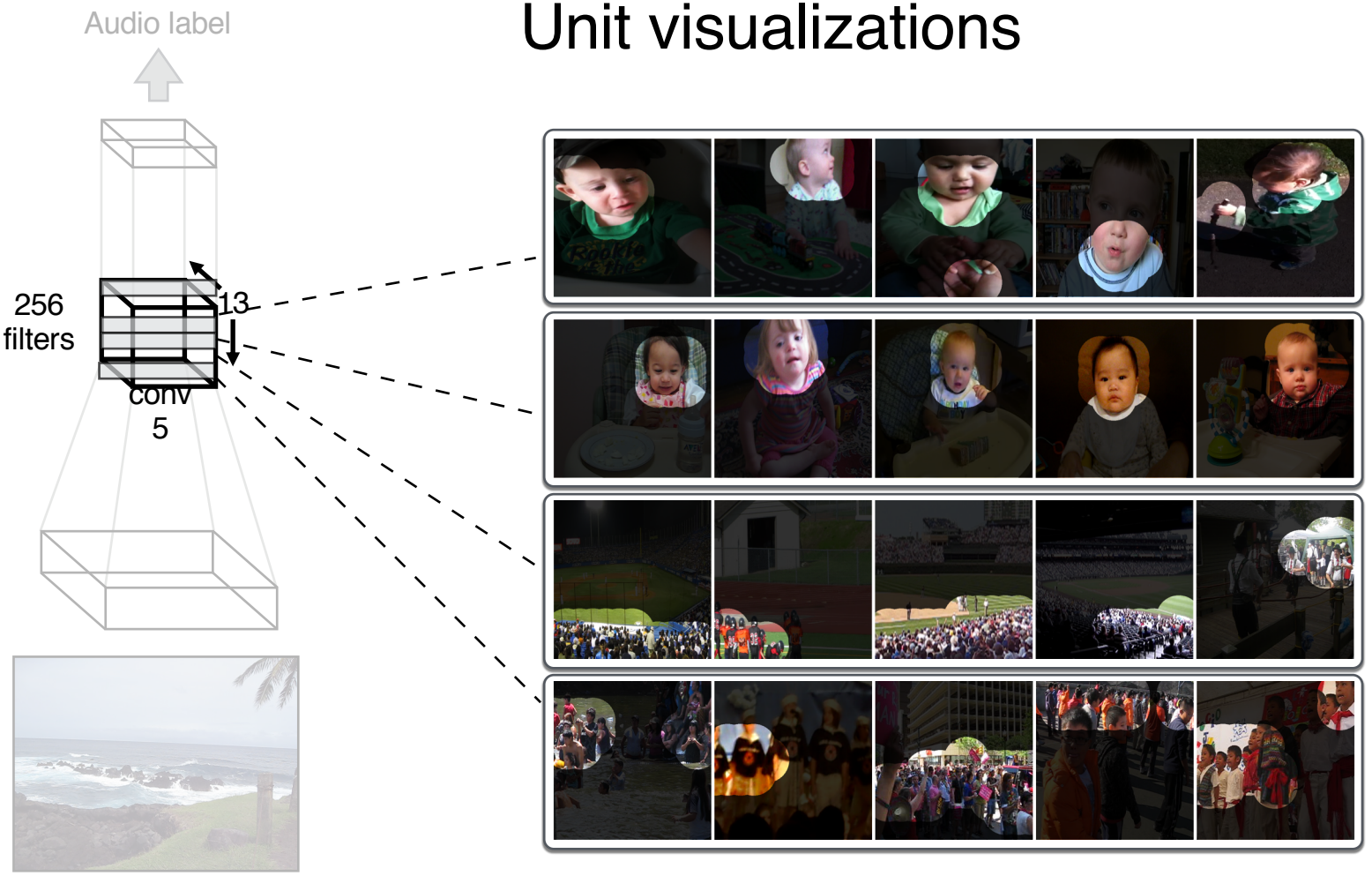


Audio

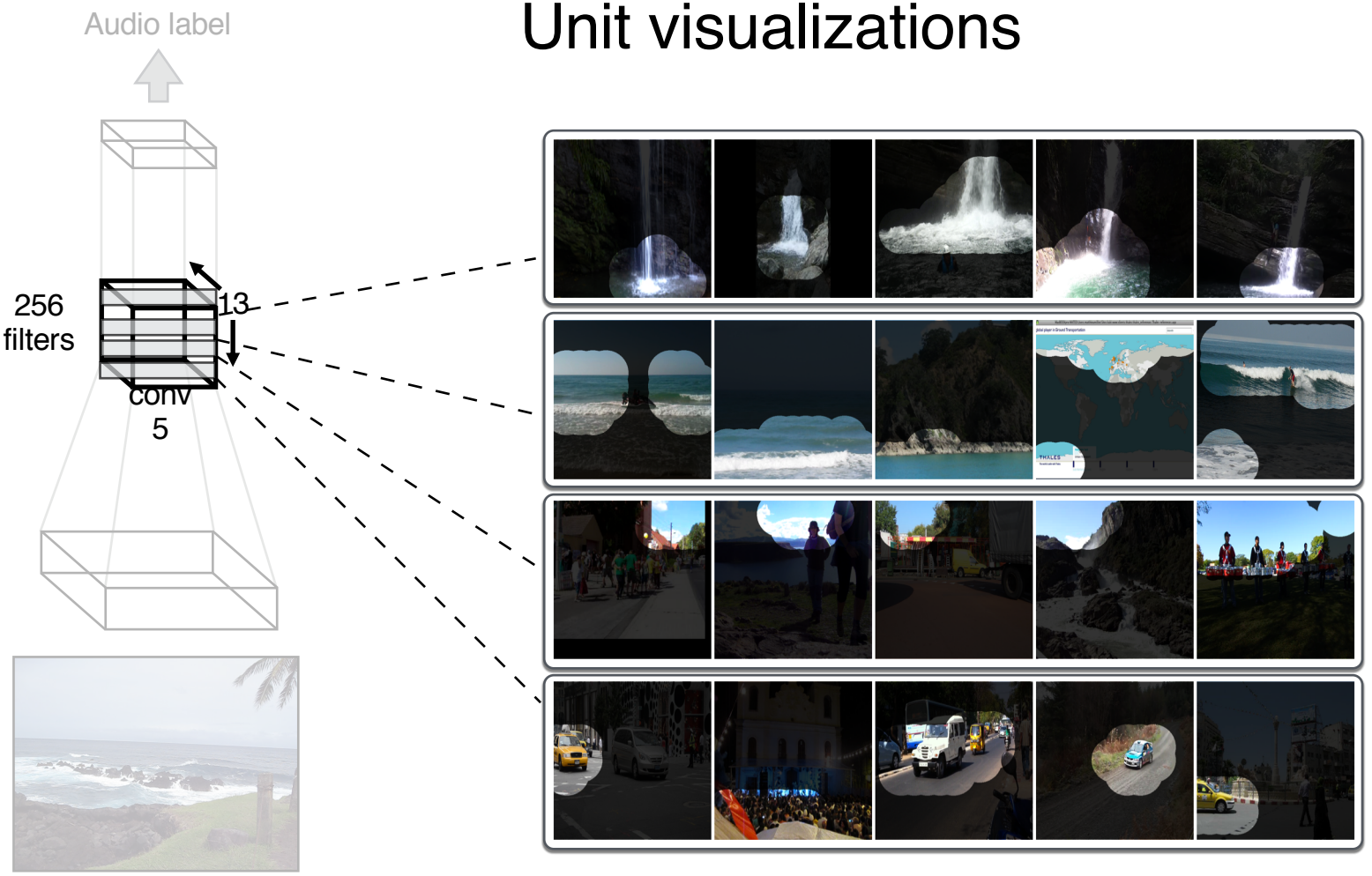
Unit visualizations



Unit visualizations



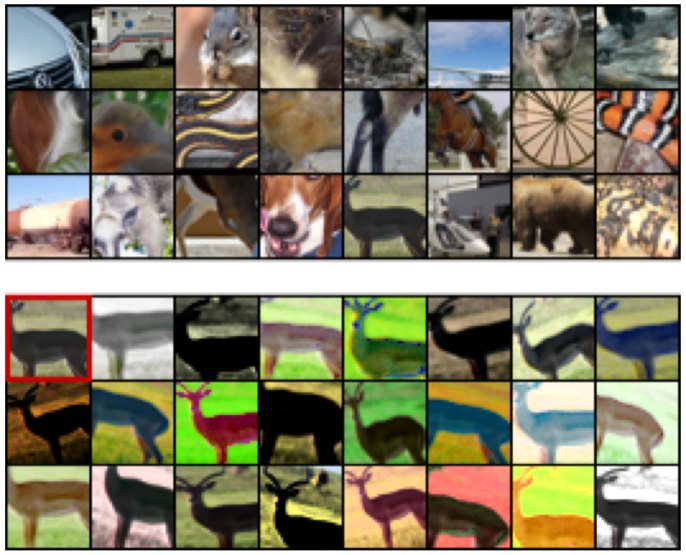
Unit visualizations



Main issue with all these methods

- All these models rely on expert knowledge
- Need to define y(x) for each new domain
- Not clear how to select a y(x) that is a good target to learn all-purpose features

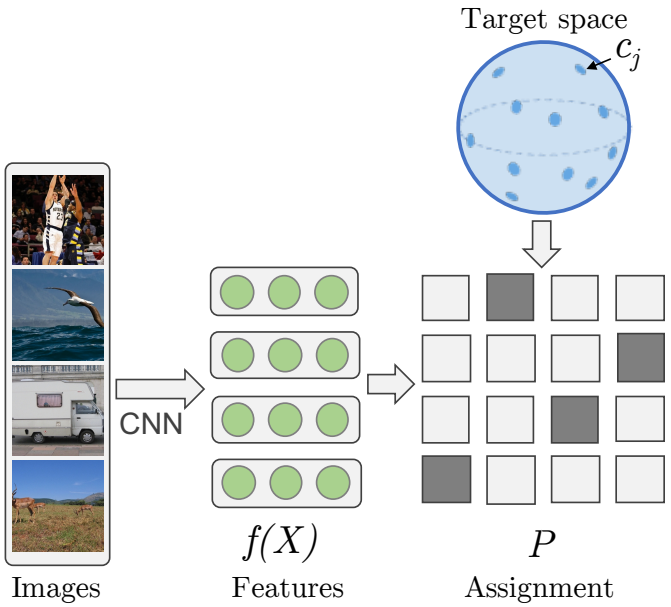
[Dosovitskiy et al. ICLR 2014]



- 1 class = single image + its transformations
- Learn to classify each "class"
- Domain knowledge about appropriate transformations
- does not scale

Unsupervised Learning by Predicting Noise

[Bojanowski & Joulin, ICML 2017]



- Inspired by Dosovitskiy et al.
- Learn mapping from images to a sphere
- Fix targets on sphere
- Simultaneously:
  - Learn the mapping
  - Optimize the assignment between images and targets

Deep Discriminative Clustering

- We are given a set of n images

$$\{x_1, \ldots, x_n\}$$

- We want to learn a visual features f without using labels

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \min_{y_i} \ell(f_\theta(x_i), y_i)$$

$$\min_{\theta} \min_{Y} \frac{1}{2n} \|f_\theta(X) - Y\|_F^2$$

- We use the L2 loss

[Bojanowski & Joulin, ICML 2017]

Label Collapse Problem

- Optimization over Y would lead to a collapse
- Repulsive costs are tricky to use
- Can impose constraints on Y but hard to optimize

[Bojanowski & Joulin, ICML 2017]

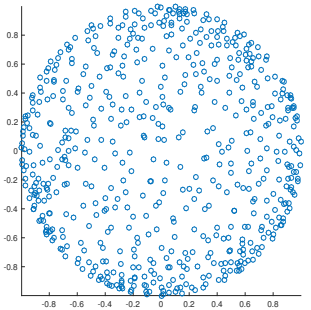
Fixing the Target Representation

- Instead, we fix the target representation
- Allow a reassignment between targets and images

$$Y = PC \qquad \mathcal{P} = \{P \in \{0,1\}^{n \times k} \mid P\mathbf{1} = \mathbf{1}, P^\top \mathbf{1} = \mathbf{1}\}$$

- Targets C are **uniformly sampled on the sphere**

$$\min_\theta \min_{P \in \mathcal{P}} \frac{1}{2n} \|f_\theta(X) - PC\|_F^2$$



- Final objective function

[Bojanowski & Joulin, ICML 2017]

Optimization

- We minimize our cost function in an on-line fashion
- We use the following algorithm:

Require: T batches of images, $\lambda_0 > 0$
  for $t = \{1, \ldots, T\}$ **do**
    Obtain batch b and representations r
    Compute $f_\theta(X_b)$
    Compute P^* by minimizing w.r.t. P
    Compute $\nabla_\theta L(\theta)$ using P^*
    Update $\theta \leftarrow \theta - \lambda_t \nabla_\theta L(\theta)$
  end for

[Bojanowski & Joulin, ICML 2017]

Optimizing the Permutation Matrix

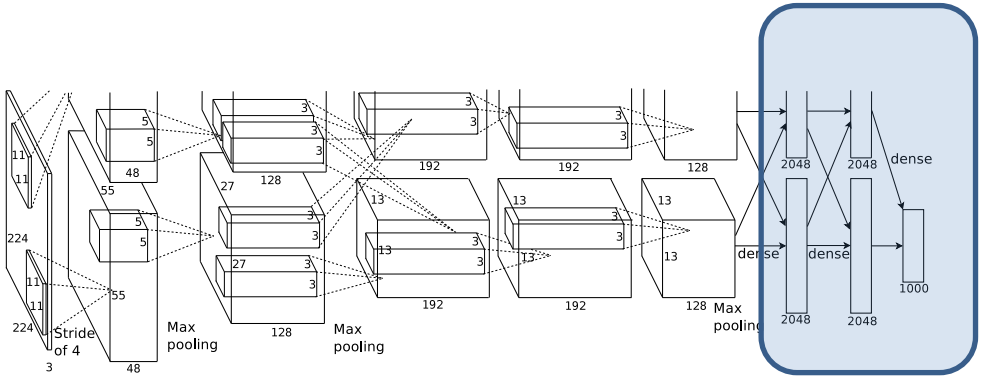
- At theta fixed, the permutation is obtained by solving

$$\max_{P \in \mathcal{P}} \operatorname{Tr}\left(P C f_\theta(X)^\top\right).$$

- Which is a linear program on the set of permutation matrices $\mathcal{O}(nb^2)$
- We can use the Hungarian algorithm

[Bojanowski & Joulin, ICML 2017]

Experimental Setup



- AlexNet architecture
- Learn unsupervised features on ImageNet training set
- Retrain a classifier on top for a target transfer task, i.e. PASCAL VOC Classification / Detection

[Bojanowski & Joulin, ICML 2017]

Baselines

- Self supervised models
  - Wang & Gupta – Temporal coherence in videos
  - Doersch et al. – Predict context patches
  - Zhang et al. – Predict color
  - Norouzi & Favaro – Solve jigsaw puzzles

- Unsupervised model
  - GAN
  - Auto-encoder
  - BI-GAN (Donahue et al.)

[Bojanowski & Joulin, ICML 2017]

Pascal VOC - results

	Classification		Detection
Trained layers	fc6-8	all	all
ImageNet labels	78.9	79.9	56.8
Agrawal et al.	31.0	54.2	43.9
Pathak et al.	34.6	56.5	44.5
Wang & Gupta	55.6	63.1	47.4
Doersch et al.	55.1	65.3	51.1
Zhang et al.	61.5	65.6	46.9
Autoencoder	16.0	53.8	41.9
GAN	40.5	56.4	-
BiGAN	52.3	60.1	46.9
NAT	56.7	65.3	49.4

- compare favorably to SOTA
- Poor performance of AE / GAN

[Bojanowski & Joulin, ICML 2017]

Nearest Neighbor Queries

[Bojanowski & Joulin, ICML 2017]

Bojanowski & Joulin Summary

- Simple unsupervised approach
- No domain expert knowledge
- Scales to **very large** datasets
- Close to supervised pipeline
- SOTA performance (at the time) amongst unsupervised methods

Summary

- Power of DL comes from ability to learn good representations
- Wide range of Unsupervised / Self-Supervised methods that devise "free" supervisory signals which can be used to learn representations via DL
- Unsolved problem:
  - Should be domain agnostic
  - Should be (nearly) as good as supervised methods