6.874 Deep Learning in the Life Sciences

Lecture 6

Generative Models: GANs, VAEs, Learning Representations

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Slides Credit: Ben Lengerich, Relja Arandjelovic, Fei-Fei Li, Justin Johnson, Serena Yeung

Interpretable Deep Learning

1. Intro to Interpretability

1a. Interpretability definition: Convert implicit NN information to human-interpretable information

1b. Motivation: Verify model works as intended; debug classifier; make discoveries; Right to explanation

1c. Ante-hoc (train interpretable model) vs. **Post-hoc** (interpret complex model; degree of "locality")

2. Interpreting Deep Neural Networks

2a. Interpreting Models (macroscopic, understand internals) vs. **decisions** (microscopic, practical applications)

2b. Interpreting Models: Weight visualization, Surrogate model, Activation maximization, Example-based

2c. Interpreting Decisions:

- Example-based
- Attribution Methods: why are gradients noisy?
- Gradient-based Attribution: SmoothGrad, Interior Gradient
- Backprop-based Attribution: Deconvolution, Guided Backpropagation

3. Evaluating Attribution Methods

3a. Qualitative: Coherence: Attributions should highlight discriminative features / objects of interest

3b. Qualitative: Class Sensitivity: Attributions should be sensitive to class labels

3c. Quantitative: Sensitivity: Removing feature with high attribution ➔ large decrease in class probability

3d. Quantitative: ROAR & KAR. Low class prob cuz image unseen ➔ remove pixels, retrain, measure acc. drop

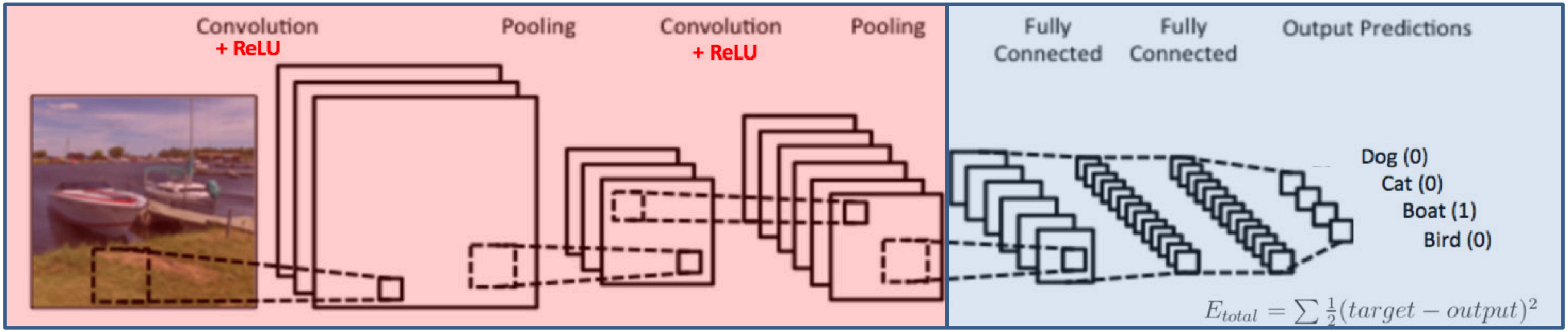
Slides by Beomsu Kim, KAIST

Previously

- We’ve seen ways to model X->Y for a fixed dataset
- But that’s not what the world looks like:
  - No Y
  - Limited samples
  - Many related datasets
  - Changes over time
- Can we learn the rules which govern how the real world varies?

Learning Representations

Key idea: **Representation** learning



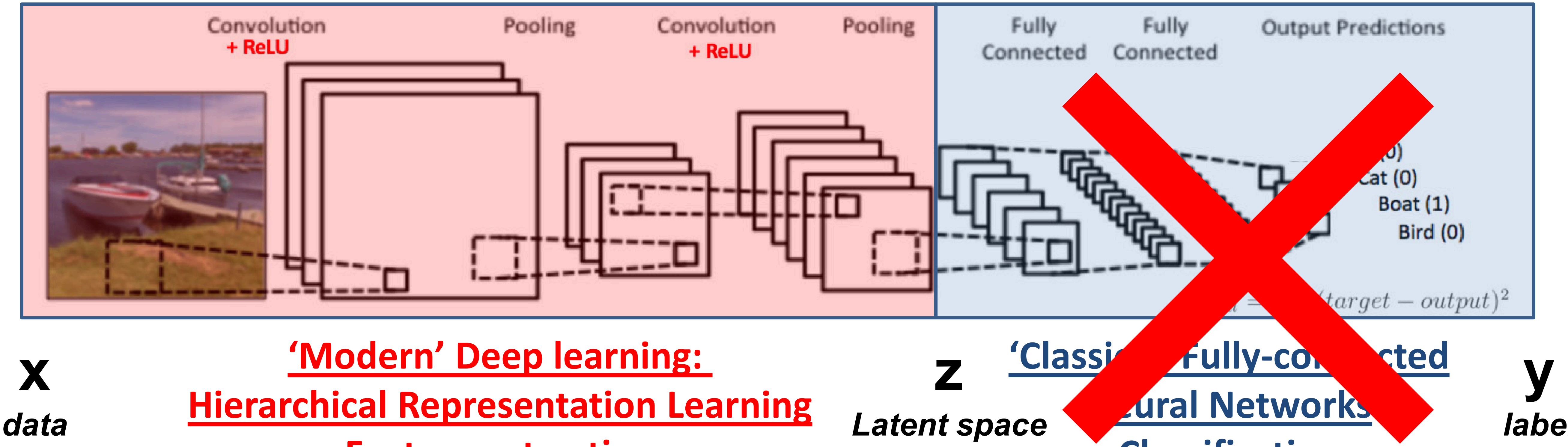
‘Modern’ Deep learning:
Hierarchical Representation Learning
Feature extraction

‘Classical’ Fully-connected
Neural Networks
Classification

In deep learning, the two tasks are **coupled**:

- the classification task “drives” the feature extraction
- Extremely powerful and general paradigm
  - ➔ **Be creative**! The field is still at its infancy!
  - ➔ New application domains (e.g. beyond images) can have **structure** that current architectures **do not capture/exploit**
  - ➔ Genomics/biology/neuroscience can help drive development of **new architectures**

Representation learning **without annotations**?



x
data

‘Modern’ Deep learning:
Hierarchical Representation Learning
Feature extraction

z
Latent space representation

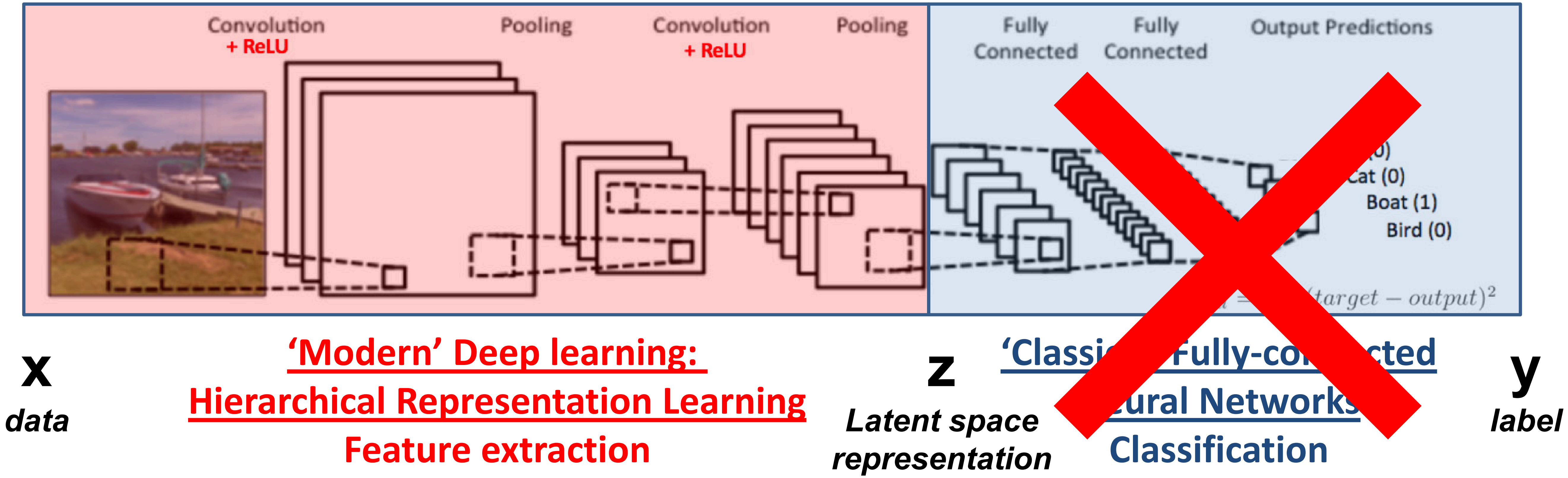
‘Classical’ Fully-connected
Neural Networks
Classification

y
label

Many ideas are possible (and yours could be even better!):

1. Predict the future: RNNs, Video
2. Pretext tasks: predict self, before/after, missing patch, correct rotation, colorization, up-sampling, multimodal
3. Compression: Autoencoder (predict self, through clamp), representation **z**
4. Capture parameter distribution (variance): Variational Auto-Encoders
5. Make latent space parameters z meaningful, orthogonal, explicit, tuneable
6. Train using a second network: GANs - Improve quality of output images
7. The Sky is the Limit

Representation learning **without annotations**?



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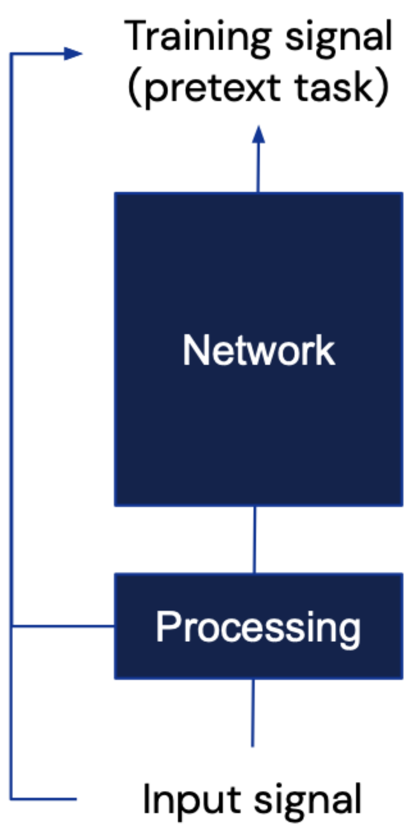
Pretext Tasks

A tour of pretext tasks

Self-supervised learning

- **Goal:** Learn good representations
- **Means:** Construct a pretext task
  - Don't care about the pretext task itself
  - Only important it enables learning



Don't care

Useful behaviour emerges

Often distorts/hides parts of the signal

Rough pretext task classification

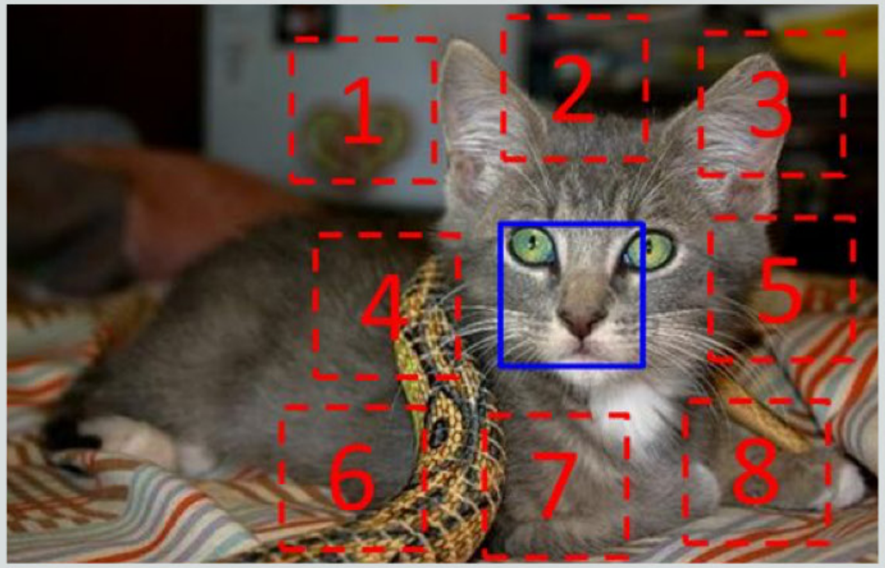
- Inferring structure
- Transformation prediction
- Reconstruction
- Exploiting time
- Multimodal
- Instance classification

Disclaimer

- Rough classification of tasks, some fit multiple categories
- Trying to cover many but inevitably missing many works
- Often have to pick one of multiple concurrent similar methods
- If A comes before B in this presentation, it doesn't mean A did it first

Slide Credit: Relja Arandjelovic

Inferring structure



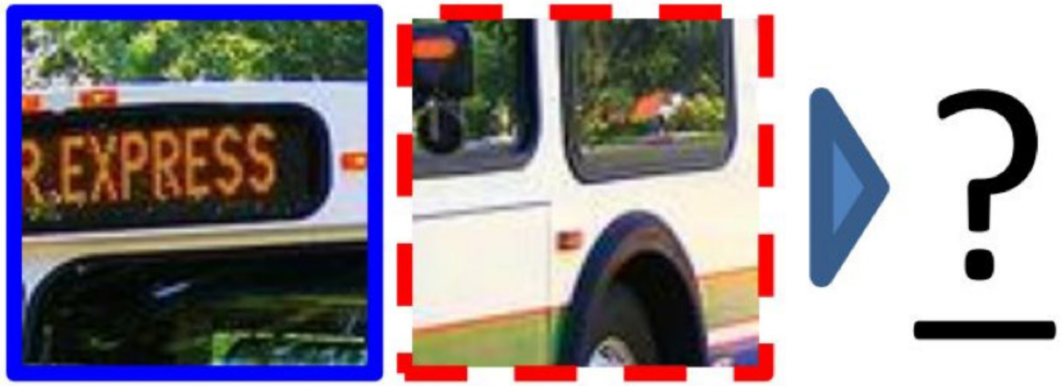
Slide Credit: Relja Arandjelovic

["Unsupervised visual representation learning by context prediction", Doersh et al. 15]

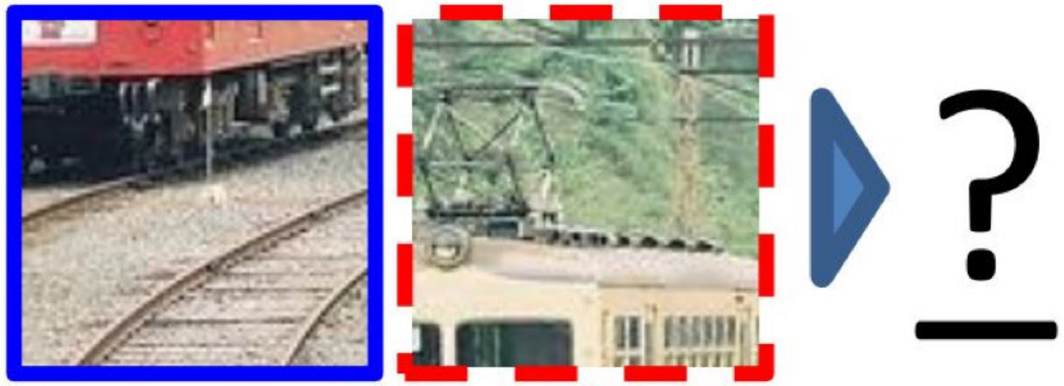
Context prediction

Can you guess the spatial configuration for the two pairs of patches?

Question 1:



Question 2:

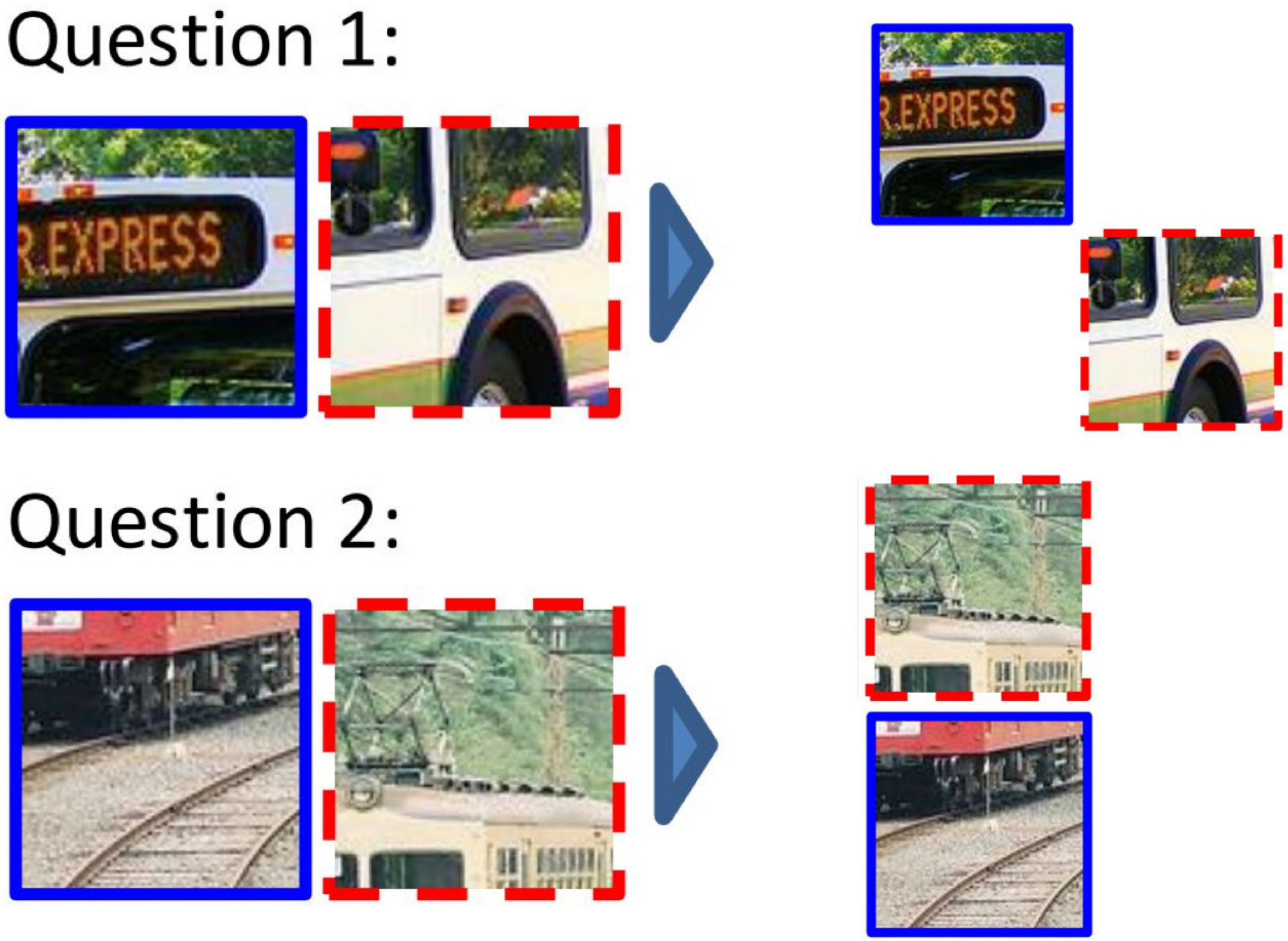


Slide Credit: Relja Arandjelovic

["Unsupervised visual representation learning by context prediction", Doersh et al. 15]

Context prediction

Can you guess the spatial configuration for the two pairs of patches? Much easier if you recognize the object!



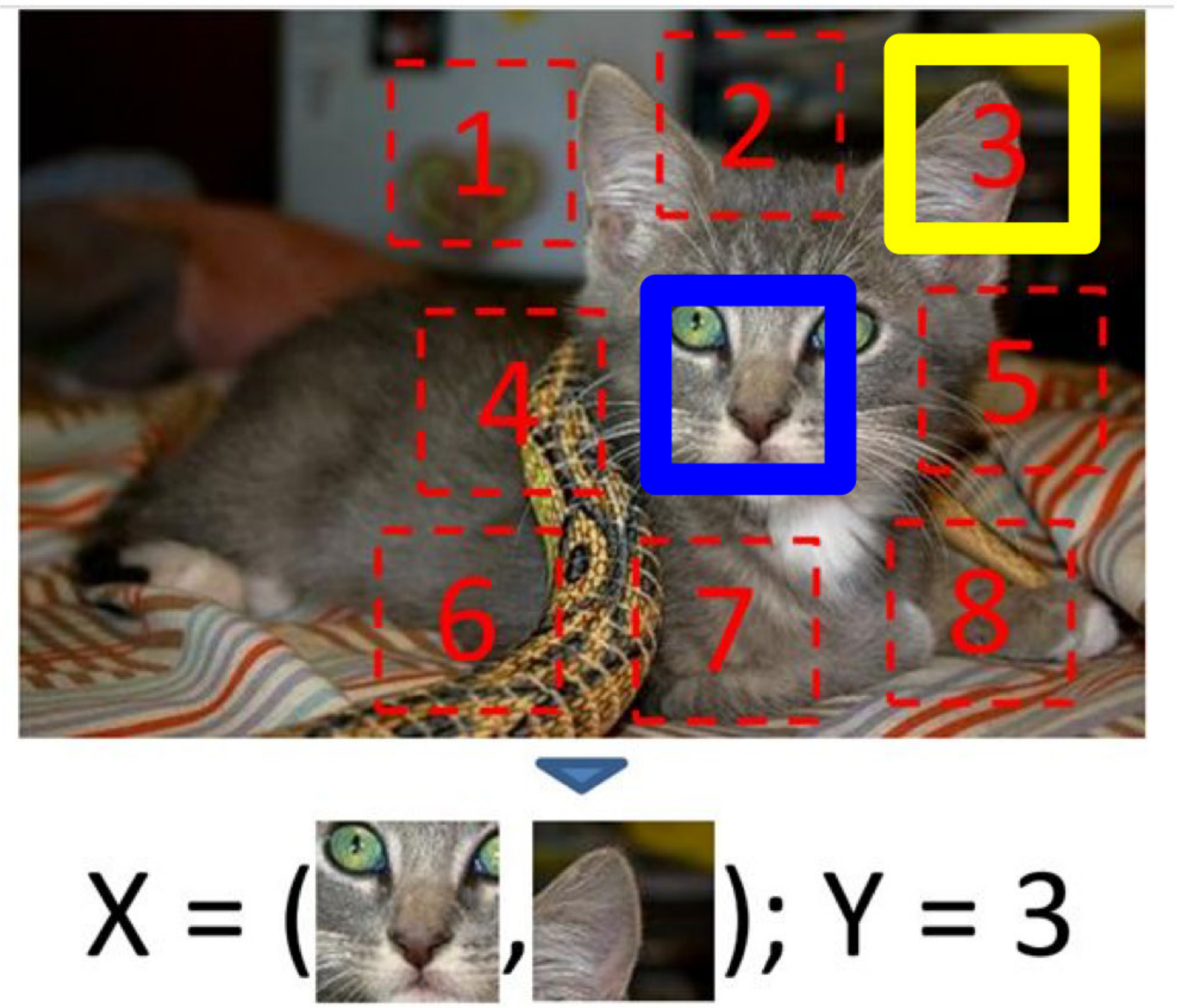
Intuition

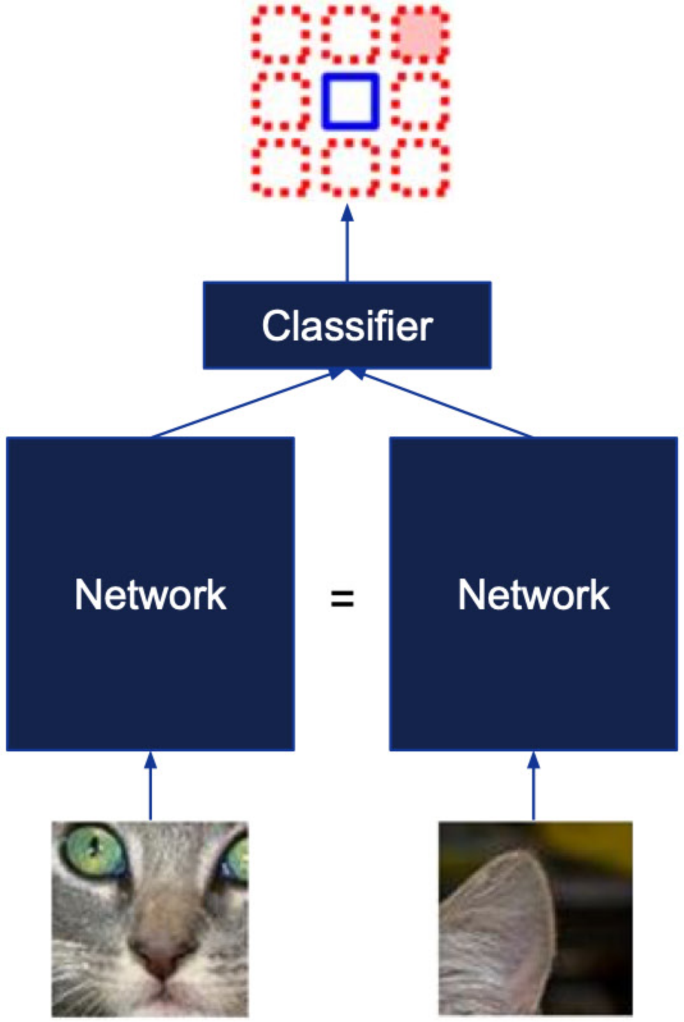
- The network should learn to recognize object parts and their spatial relations

Slide Credit: Relja Arandjelovic

["Unsupervised visual representation learning by context prediction", Doersh et al. 15]

Context prediction





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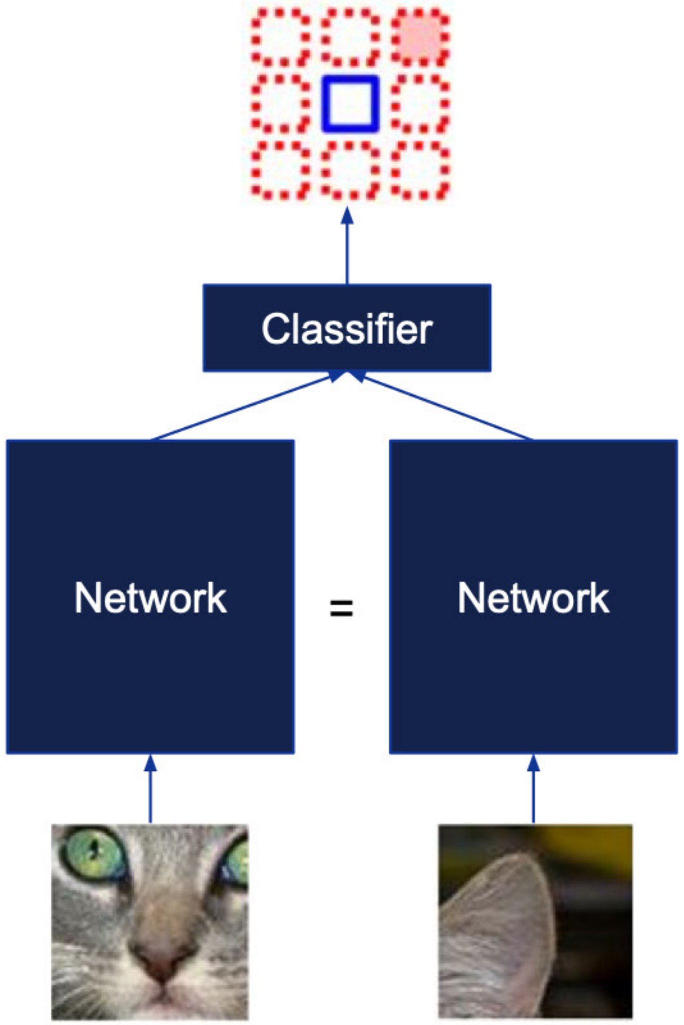


Pros

- (arguably) The first self-supervised method
- Intuitive task that should enable learning about object parts

Cons

- Assumes training images are photographed with canonical orientations (and canonical orientations exist)
- Training on patches, but trying to learn image representations
- Networks can "cheat" so special care is needed [discussed later]
  - Further gap between train and eval
- Not fine-grained enough due to no negatives from other images
  - e.g. no reason to distinguish cat from dog eyes
- Small output space - 8 cases (positions) to distinguish?

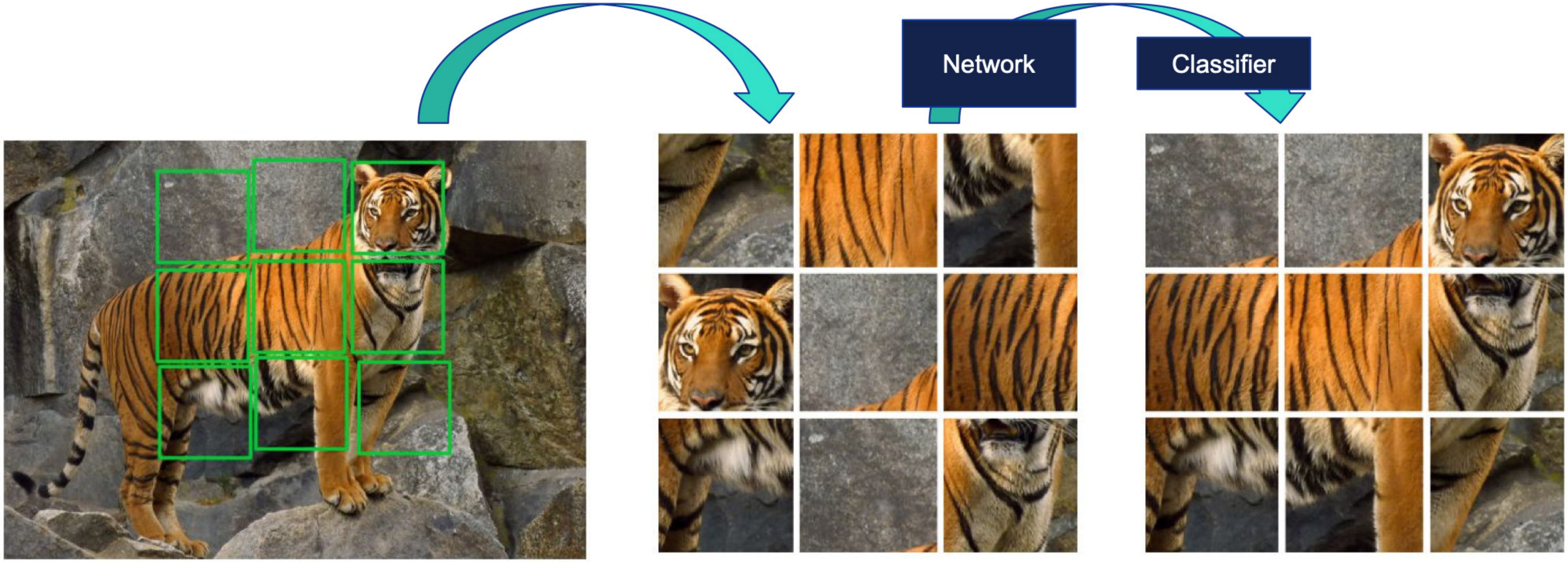
Slide Credit: Relja Arandjelovic

["Unsupervised learning of visual representations by solving jigsaw puzzles", Noroozi et al. 17]

Jigsaw puzzles

Divide image into patches and permute them

Predict the permutation



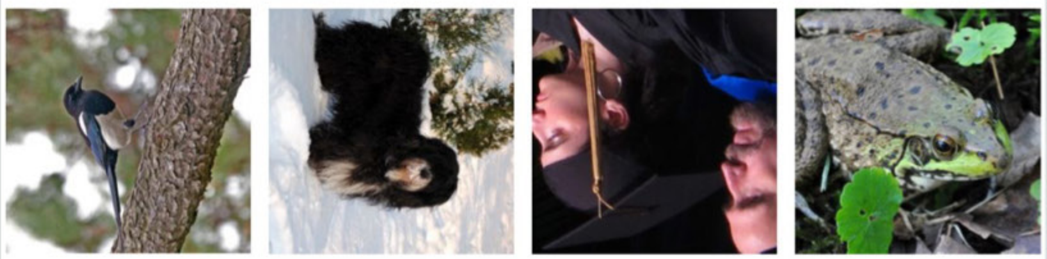
Network

Classifier

Pros & Cons: Same as for context prediction apart from being harder

Slide Credit: Relja Arandjelovic

Transformation prediction



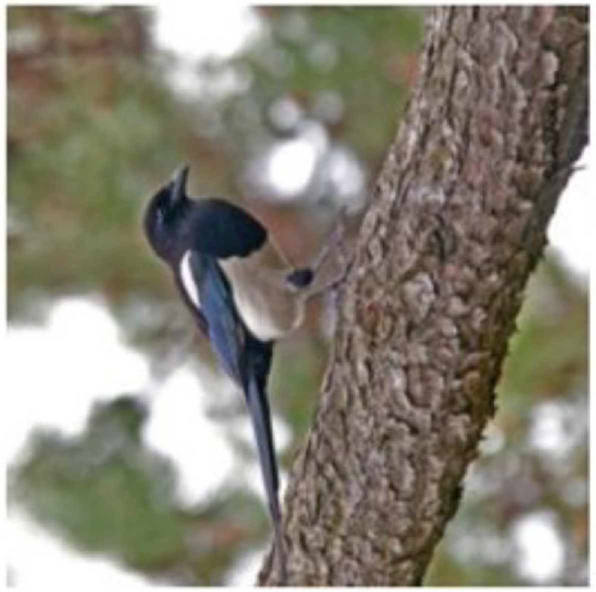
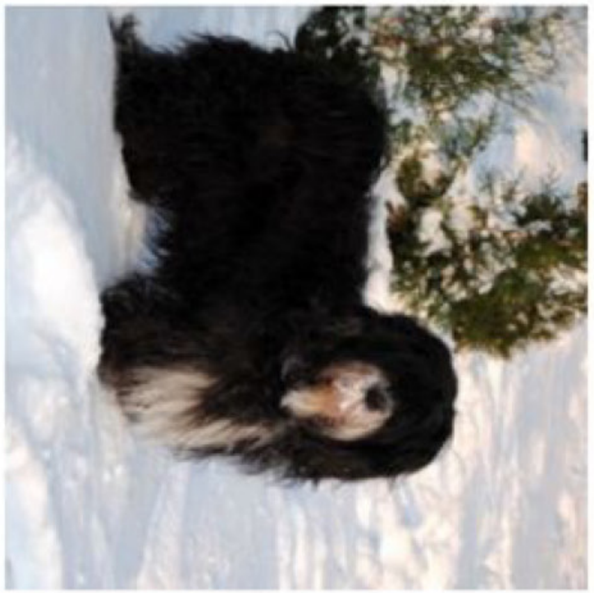
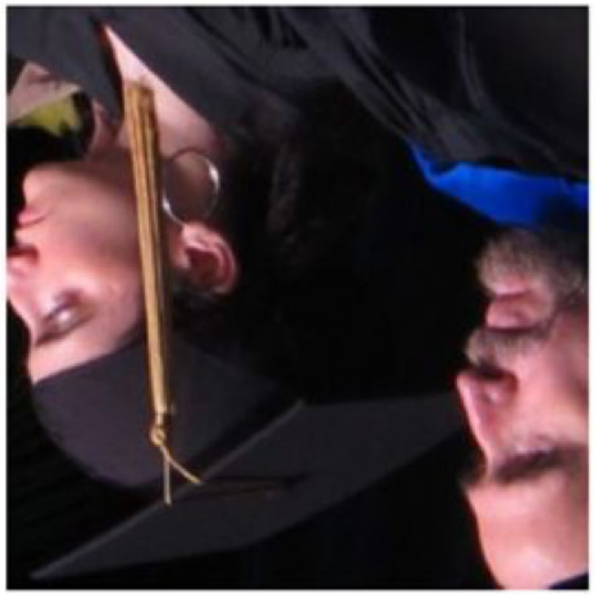
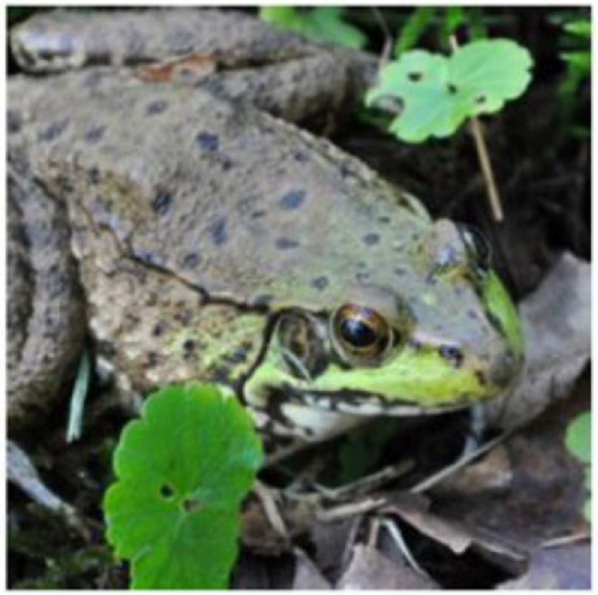
90° rotation 270° rotation 180° rotation 0° rotation

Slide Credit: Relja Arandjelovic

["Unsupervised representation learning by predicting image rotations", Gidaris et al. 18]

Rotation prediction

Can you guess how much rotated is applied?

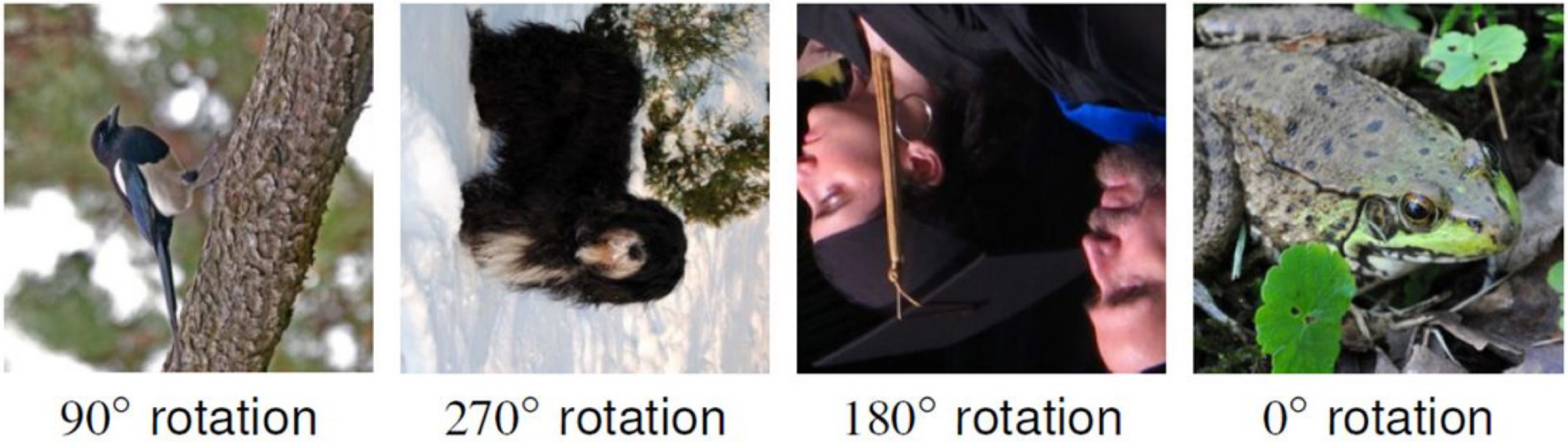





Slide Credit: Relja Arandjelovic

["Unsupervised representation learning by predicting image rotations", Gidaris et al. 18]

Rotation prediction

Can you guess how much rotated is applied? Much easier if you recognize the content!



90° rotation 270° rotation 180° rotation 0° rotation

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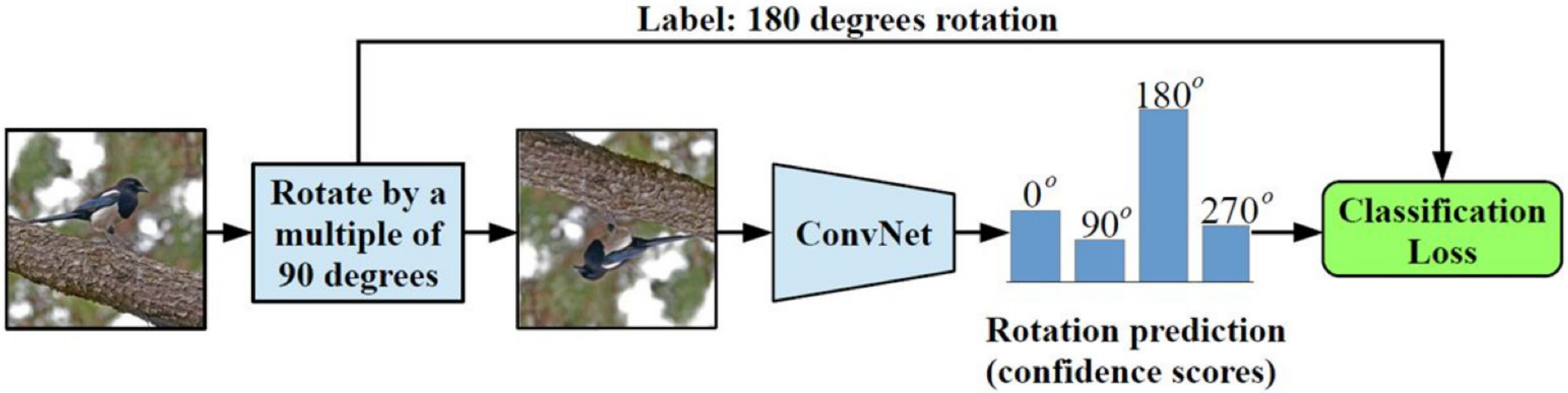
Rotation prediction


Label: 180 degrees rotation
Rotate by a multiple of 90 degrees
ConvNet
0^o
90^o
180^o
270^o
Classification Loss
Rotation prediction (confidence scores)

Pros

- Very simple to implement and use, while being quite effective

Cons

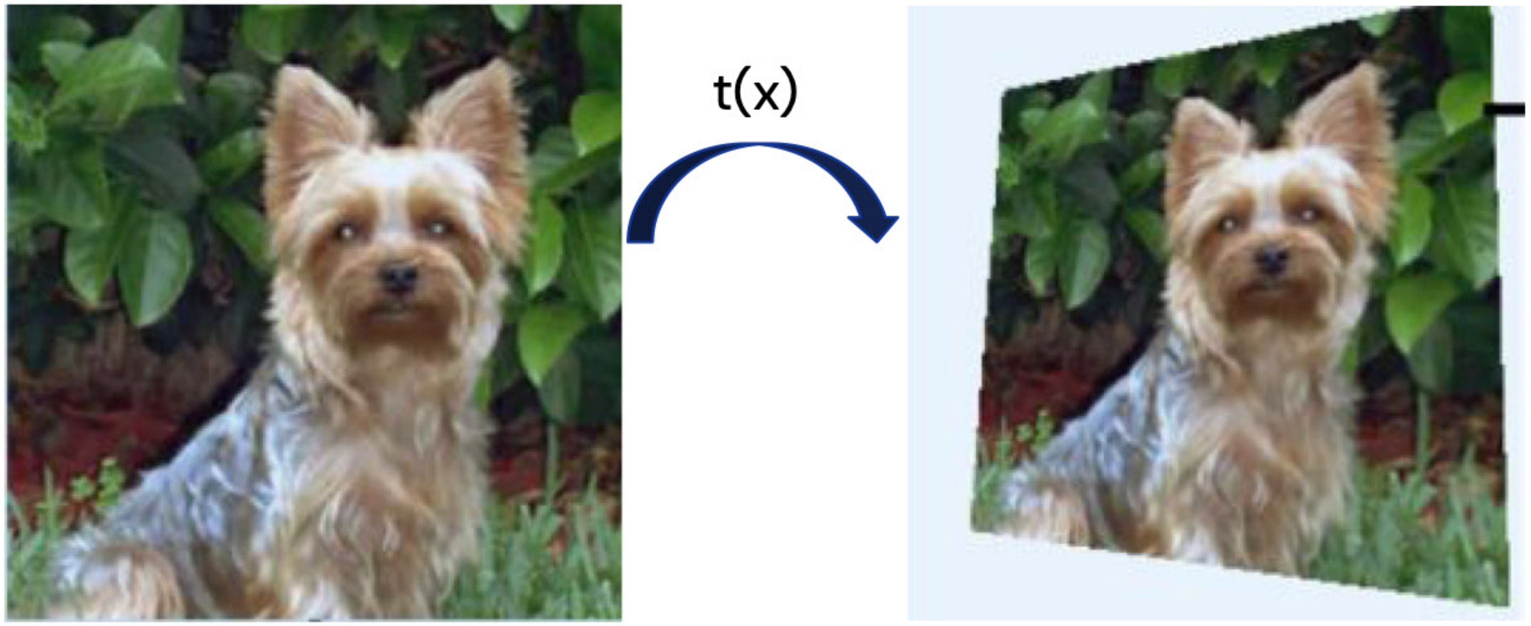
- Assumes training images are photographed with canonical orientations (and canonical orientations exist)
- Train-eval gap: no rotated images at eval
- Not fine-grained enough due to no negatives from other images
  - e.g. no reason to distinguish cat from dog
- Small output space - 4 cases (rotations) to distinguish [not trivial to increase; see later]
- Some domains are trivial e.g. StreetView ⇒ just recognize sky

Slide Credit: Relja Arandjelovic

["AET vs. AED: Unsupervised representation learning by auto-encoding transformations rather than data", Zhang et al. 19]

Relative transformation prediction

Estimate the transformation between two images. Requires good features



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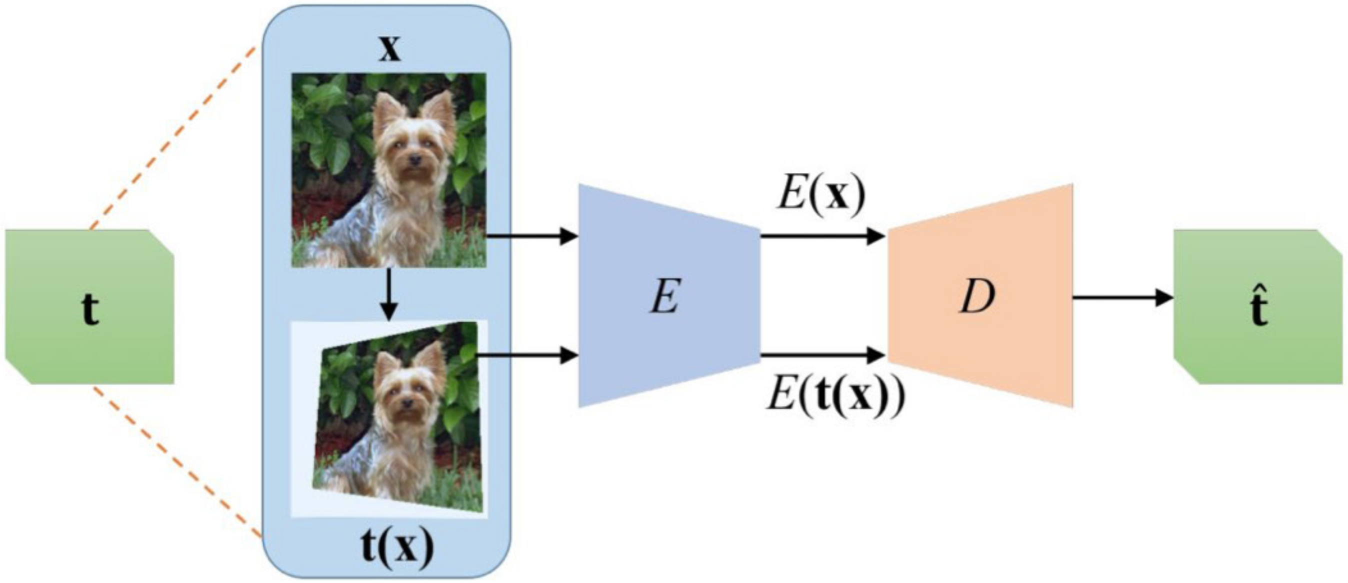
Relative transformation prediction



Pros

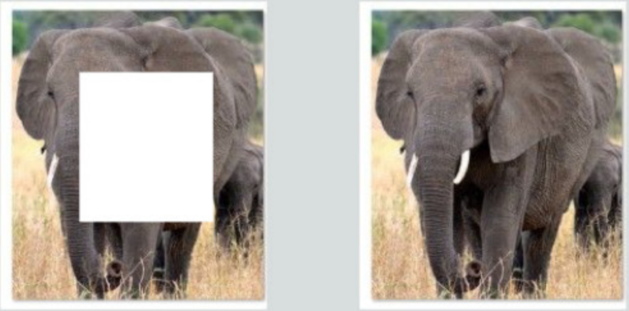
- In line with classical computer vision, e.g. SIFT was developed for matching

Cons

- Train-eval gap: no transformed images at eval
- Not fine-grained enough due to no negatives from other images
  - e.g. no reason to distinguish cat from dog
- Questionable importance of semantics vs low-level features (assuming we want semantics)
  - Features are potentially not invariant to transformations

Slide Credit: Relja Arandjelovic

Reconstruction



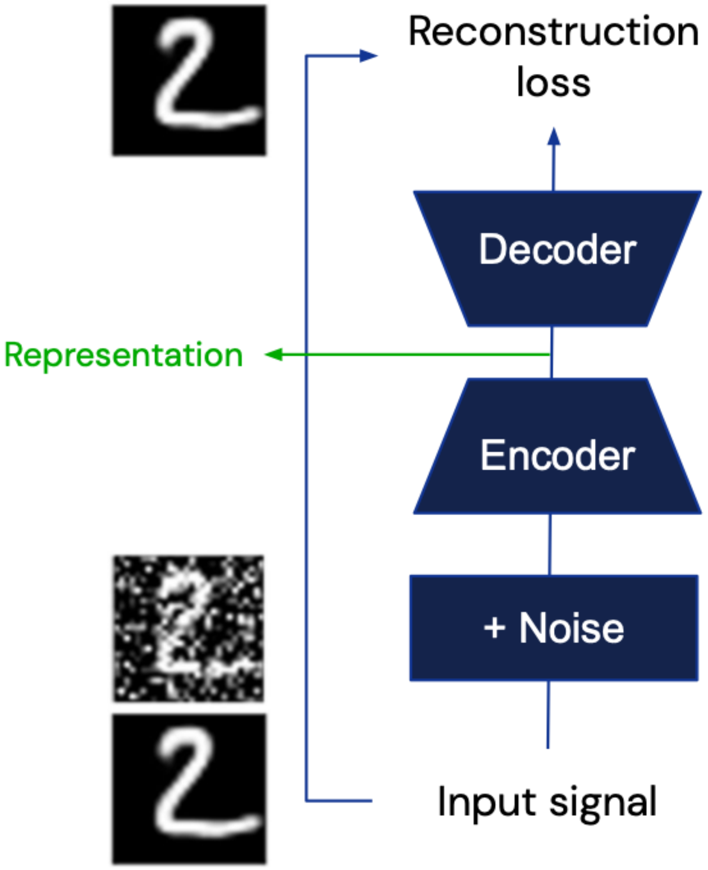
Slide Credit: Relja Arandjelovic

["Extracting and composing robust features with denoising autoencoders", Vincent et al. 08]

Denoising autoencoders

What is the noise and what is the signal?

Recognizing the digit helps!



Reconstruction loss

Decoder

Representation

Encoder

+ Noise

Input signal

Pros

- Simple classical method
- Apart from representations, we get a denoiser for free

Cons

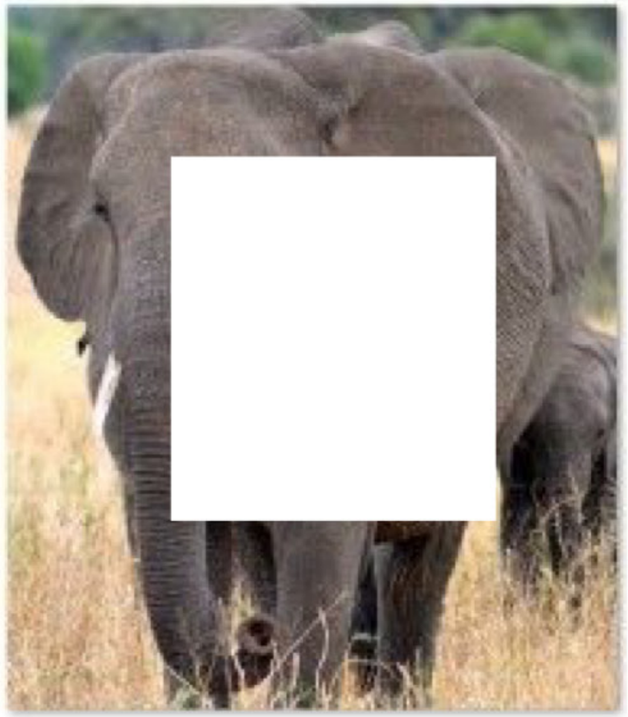
- Train-eval gap: training on noisy data
- Too easy, no need for semantics - low level cues are sufficient

Slide Credit: Relja Arandjelovic

["Context encoders: Feature learning by inpainting", Pathak et al. 16]

Context encoders

What goes in the middle?

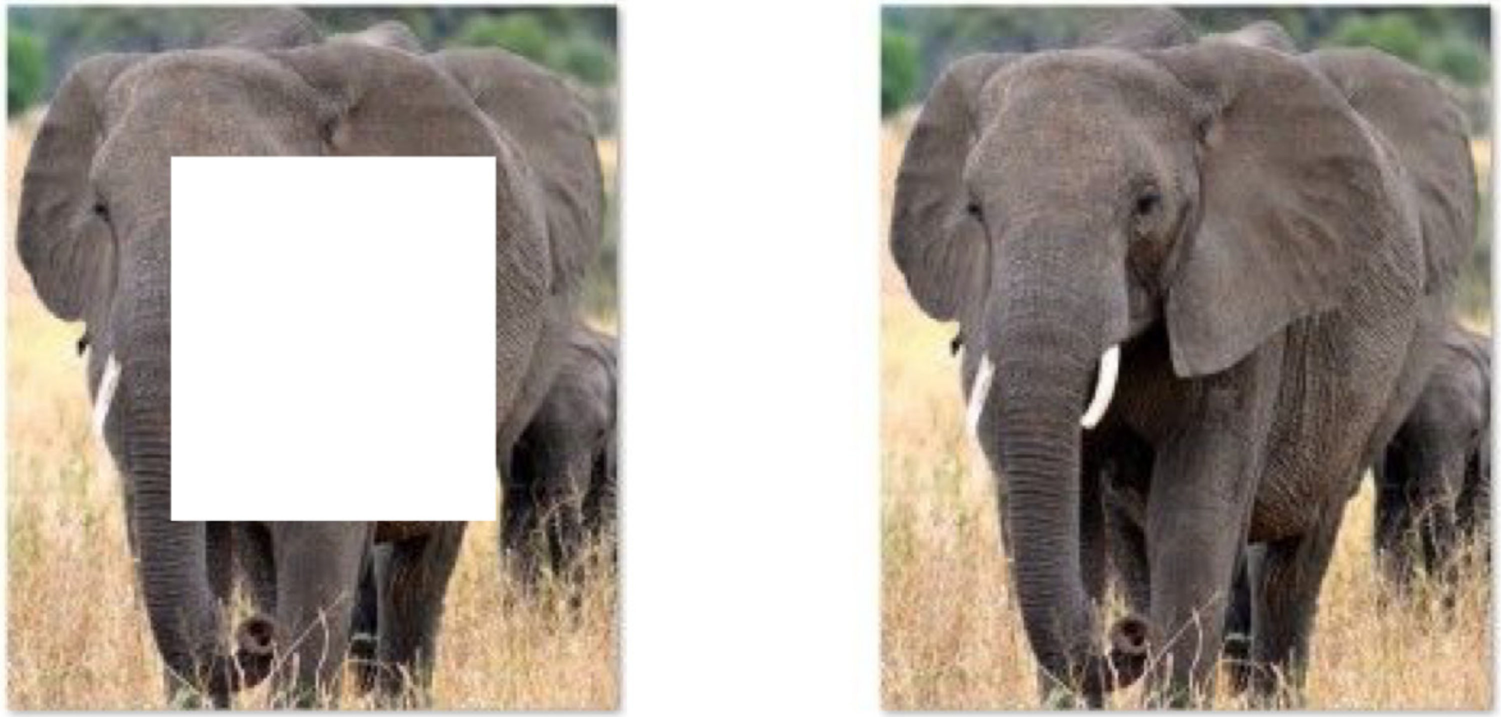


Slide Credit: Relja Arandjelovic

["Context encoders: Feature learning by inpainting", Pathak et al. 16]

Context encoders

What goes in the middle? Much easier if you recognize the objects!



Natural language processing (e.g. word2vec, BERT)

All [MASK] have tusks. ⇒ All elephants have tusks.

["Distributed representations of words and phrases and their compositionality", Mikolov et al. 13]
["BERT: Pre-training of deep bidirectional transformers for language understanding", Devlin et al. 18]

Slide Credit: Relja Arandjelovic

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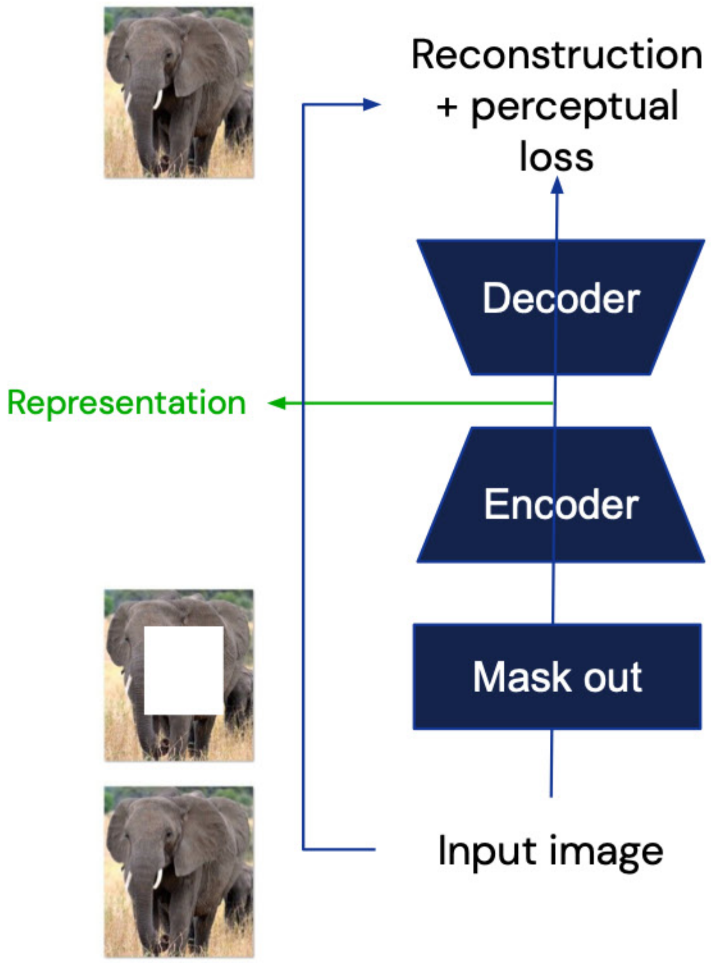
Context encoders



Pros

- Requires preservation of fine-grained information

Cons

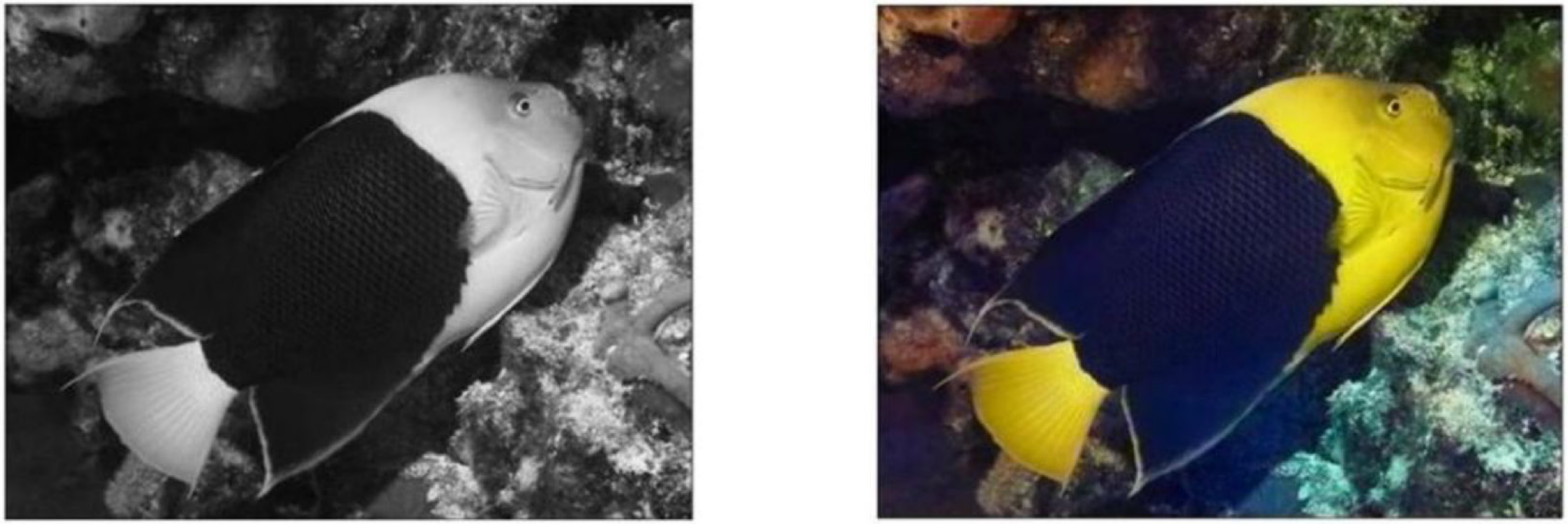
- Train-eval gap: no masking at eval
- Reconstruction is too hard and ambiguous
- Lots of effort spent on "useless" details: exact colour, good boundary, etc

Slide Credit: Relja Arandjelovic

["Colorful image colorization", Zhang et al. 16]

Colorization

What is the colour of every pixel? Hard if you don't recognize the object!



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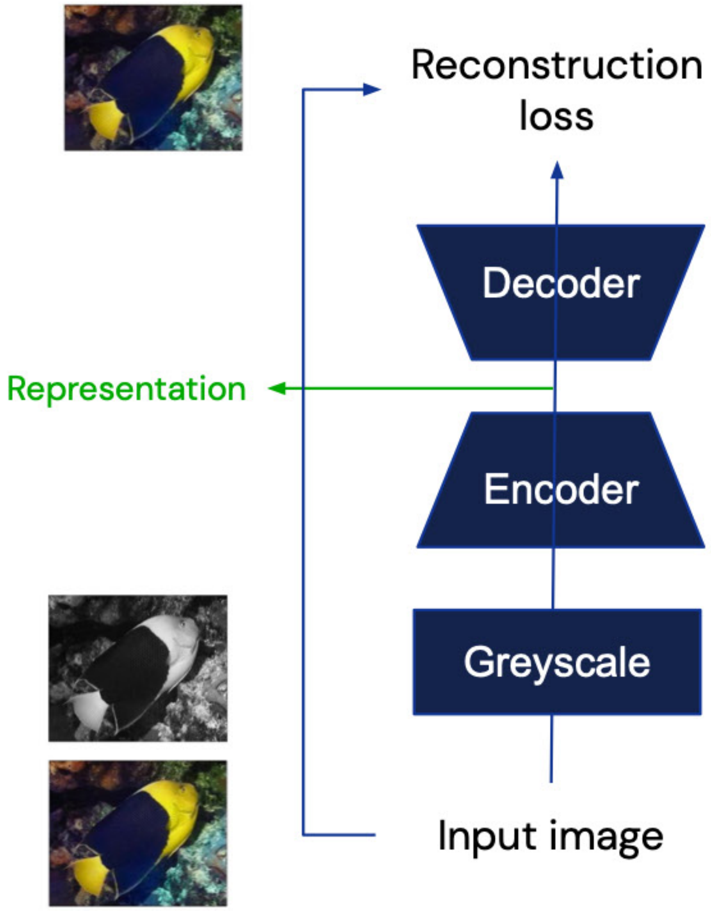
Context encoders



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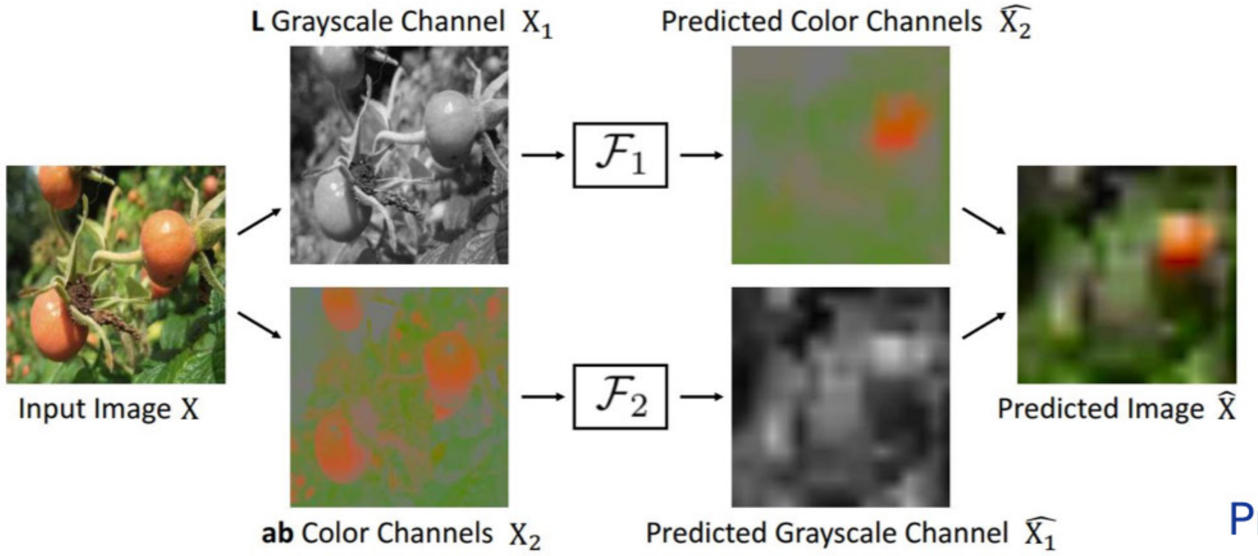
- Reconstruction is too hard and ambiguous
- Lots of effort spent on "useless" details: exact colour, good boundary, etc
- Forced to evaluate on greyscale images, losing information

Slide Credit: Relja Arandjelovic

["Split-brain autoencoders: Unsupervised learning by cross-channel prediction", Zhang et al. 17]

Context encoders ⇒ Split-brain encoders


L Grayscale Channel X_1
Predicted Color Channels $\widehat{X_2}$
$\mathcal{F}_1$
Input Image X
Predicted Image $\hat{X}$
$\mathcal{F}_2$
ab Color Channels X_2
Predicted Grayscale Channel $\widehat{X_1}$

Pros

- Requires preservation of fine-grained information

Cons

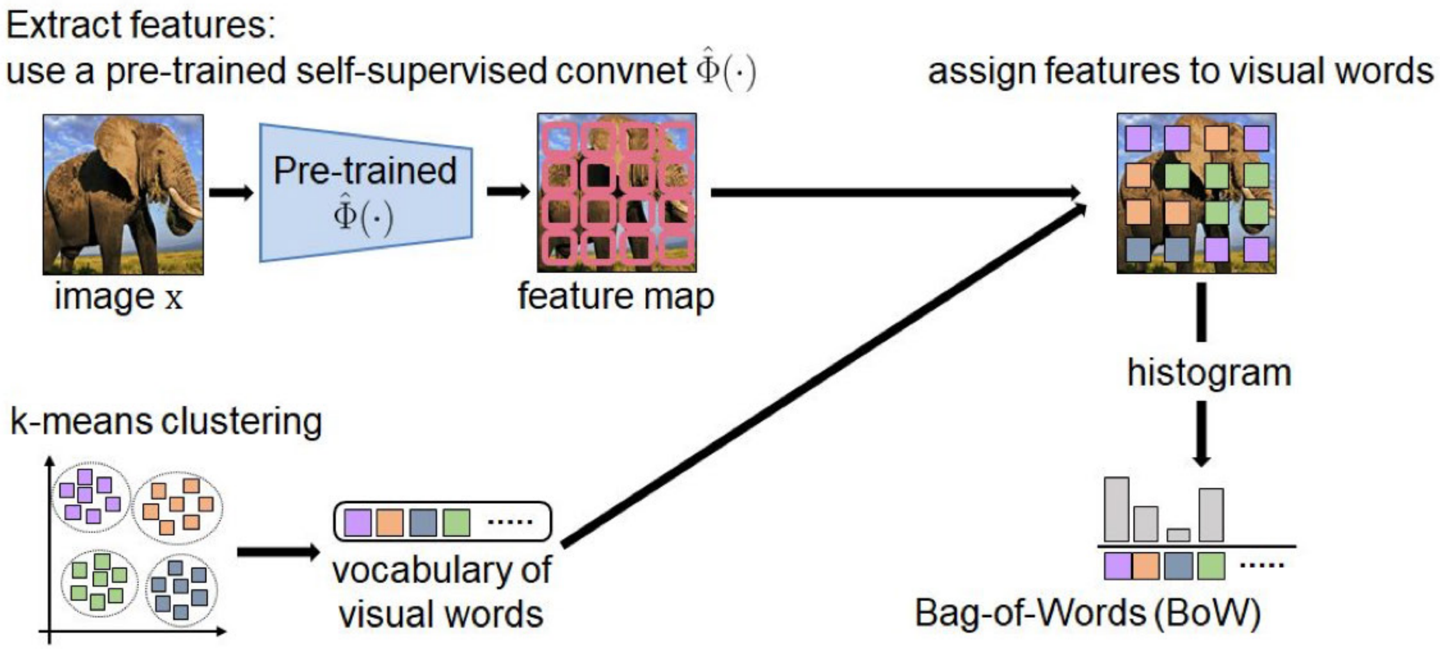
- Reconstruction is too hard and ambiguous
- Lots of effort spent on "useless" details: exact colour, good boundary, etc
- ~~Forced to evaluate on greyscale images, losing information~~
- Processes different chunks of the input independently

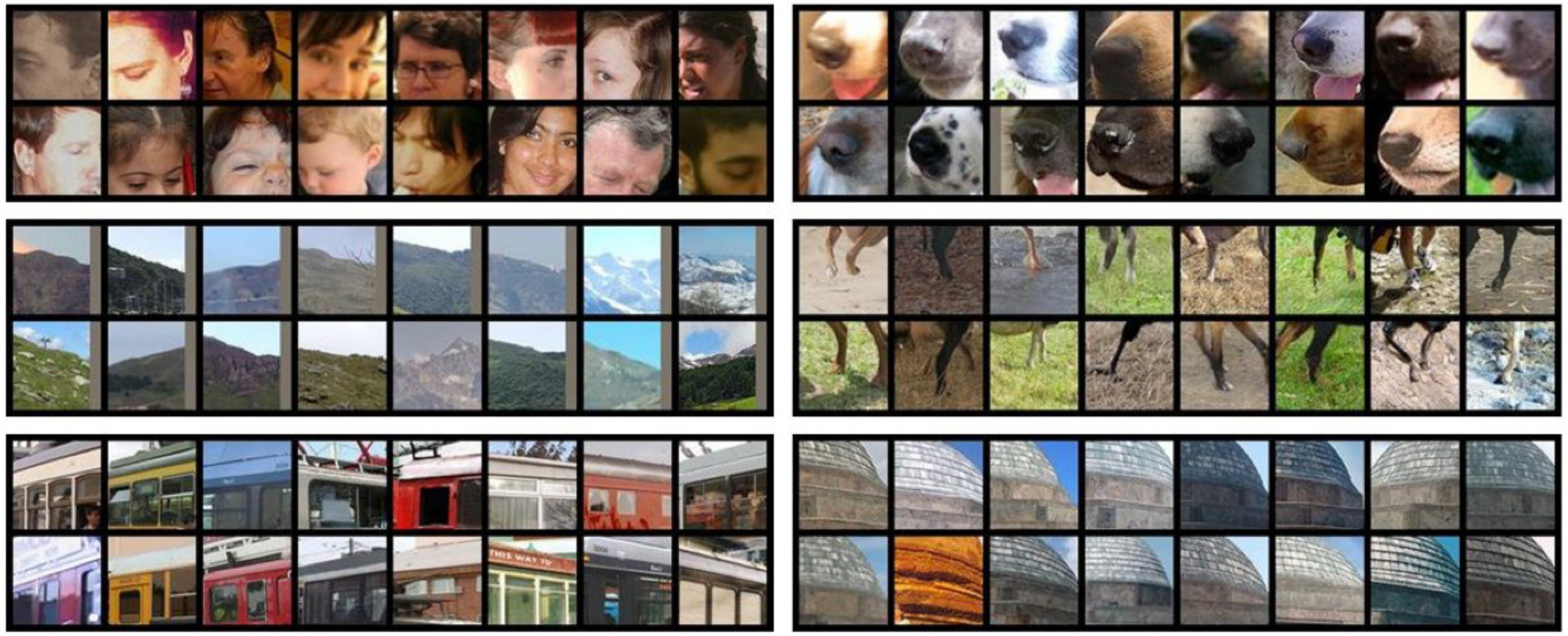
Slide Credit: Relja Arandjelovic

["Learning representations by predicting bags of visual words", Gidaris et al. 20]

Predicting bag-of-words

Bag-of-words reminder



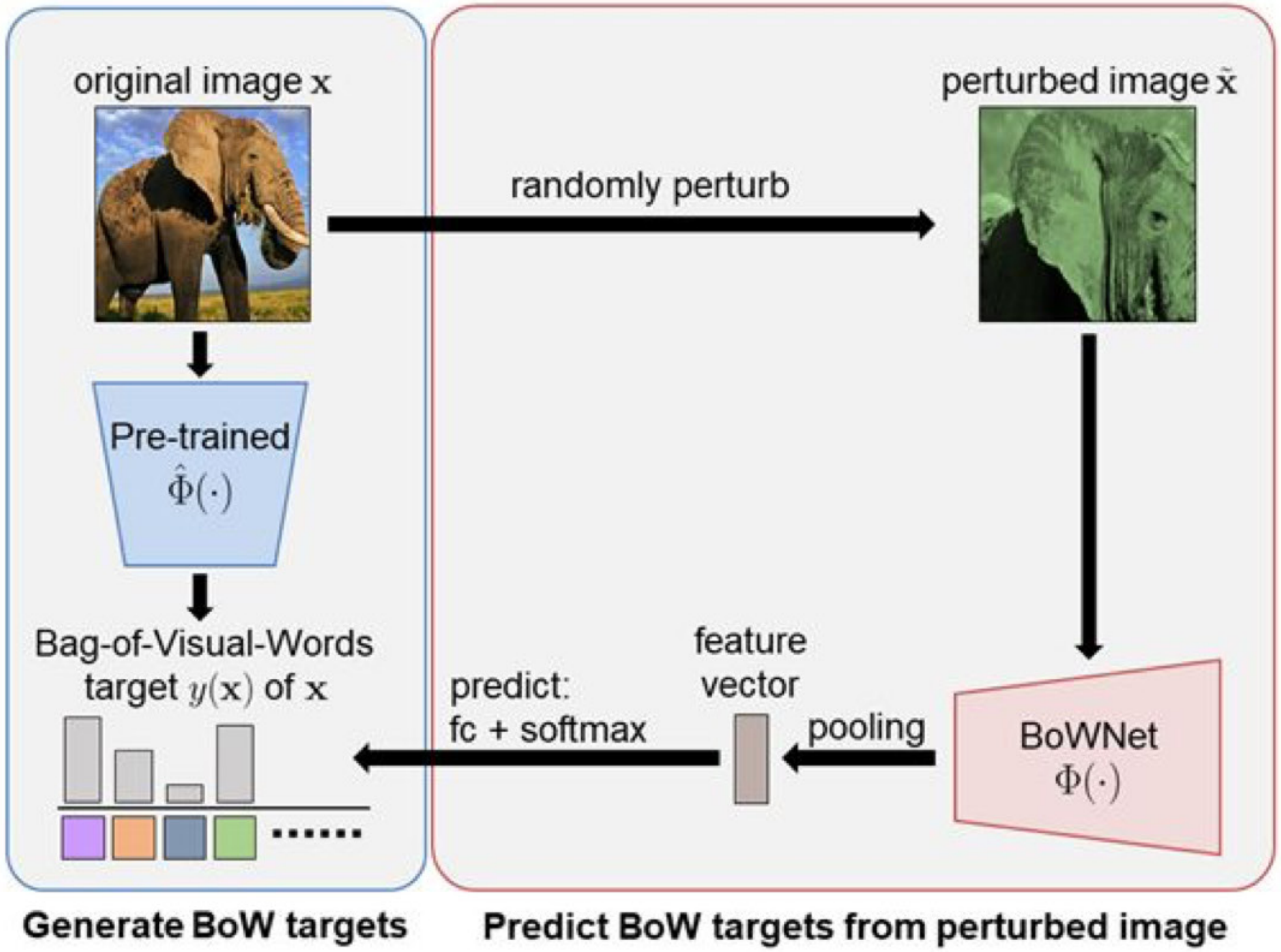


- Loses low-level details
- Encodes mid/high-level concepts

Slide Credit: Relja Arandjelovic

["Learning representations by predicting bags of visual words", Gidaris et al. 20]

Predicting bag-of-words

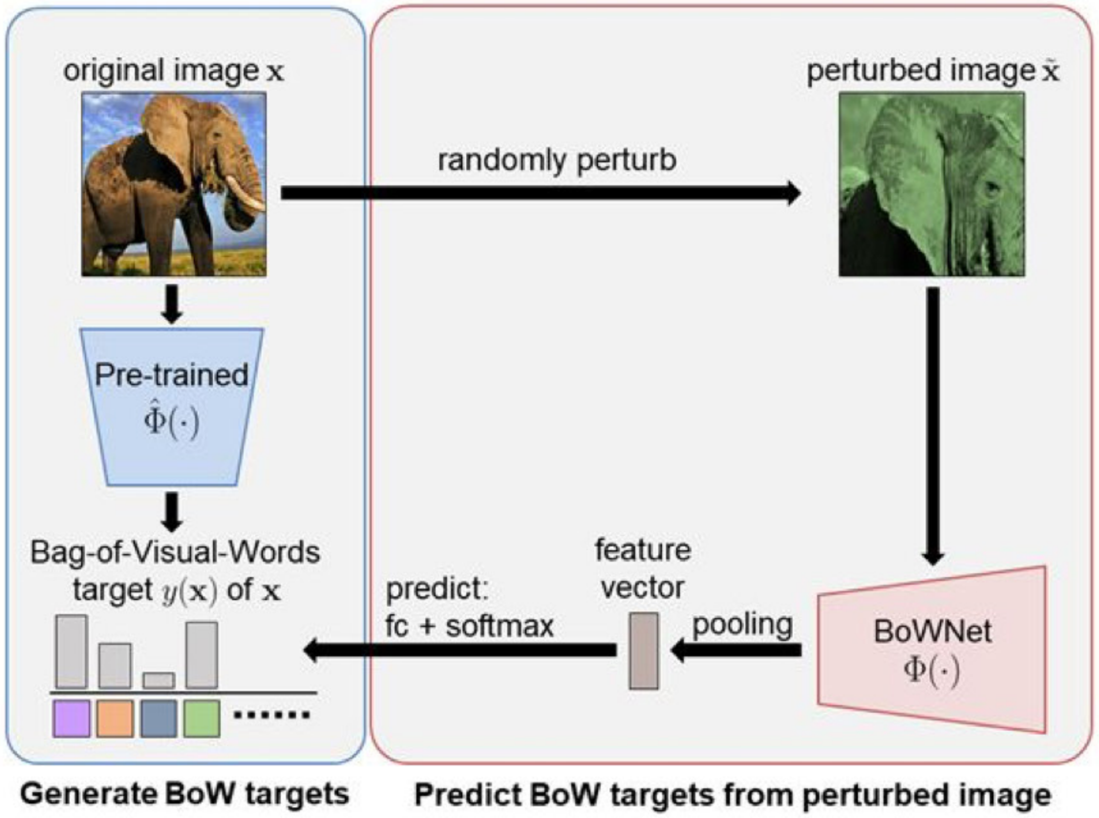


Inspired by NLP: targets = discrete concepts (words)

Slide Credit: Relja Arandjelovic

["Learning representations by predicting bags of visual words", Gidaris et al. 20]

Predicting bag-of-words



Pros

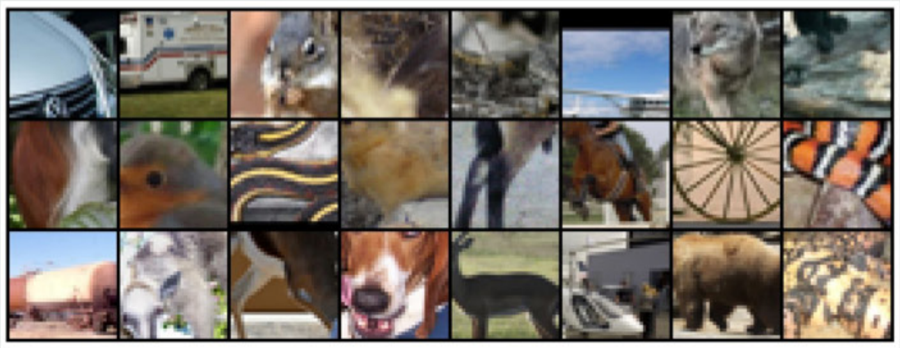
- Representations are invariant to desired transformations
- Learn contextual reasoning skills
  - Infer words of missing image regions

Cons

- Requires bootstrapping from another network
  - e.g. hard to learn more fine-grained features
- Pitfalls of BoW
  - (partial) loss of spatial information
  - SpatialBoW not improving

Slide Credit: Relja Arandjelovic

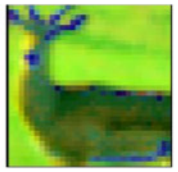
Instance classification

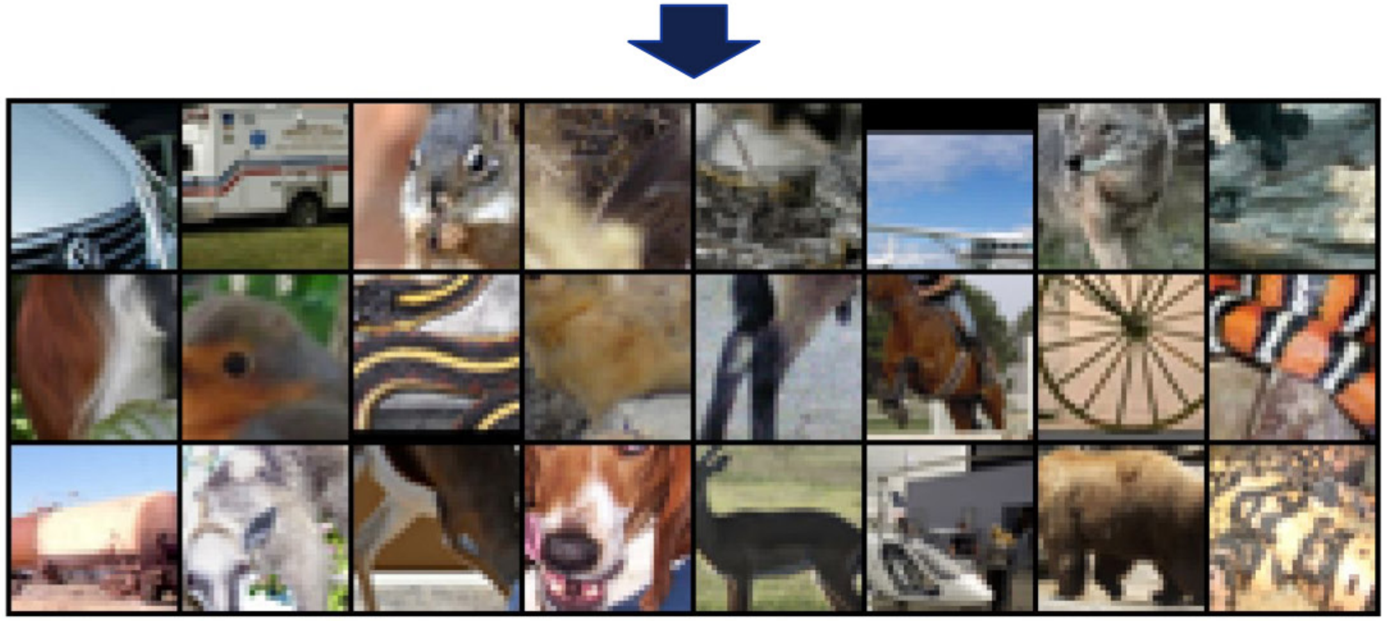


Slide Credit: Relja Arandjelovic

["Discriminative unsupervised feature learning with exemplar convolutional neural networks", Dosovitskiy et al. 14]

Exemplar ConvNets

This  is a distorted crop extracted from an image, which of these crops has the same source image?



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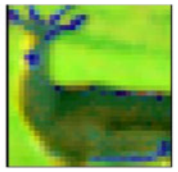
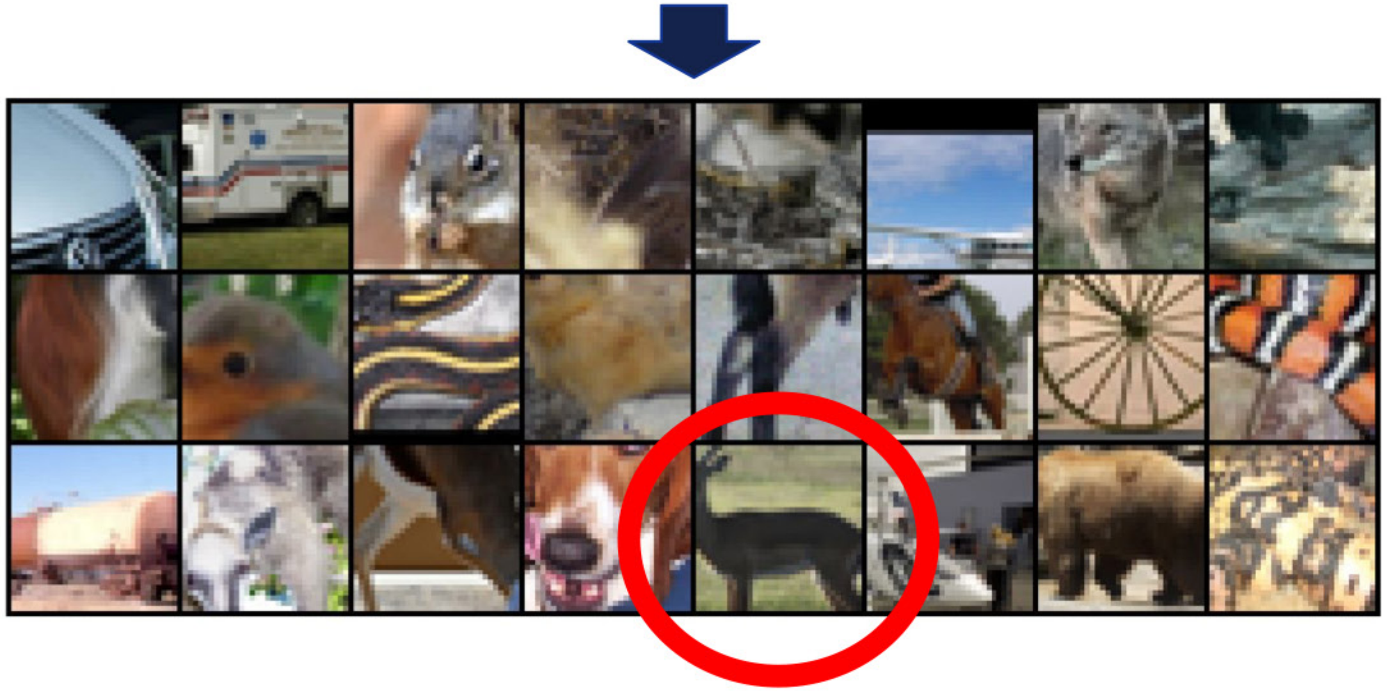
Exemplar ConvNets

This  is a distorted crop extracted from an image, which of these crops has the same source image?

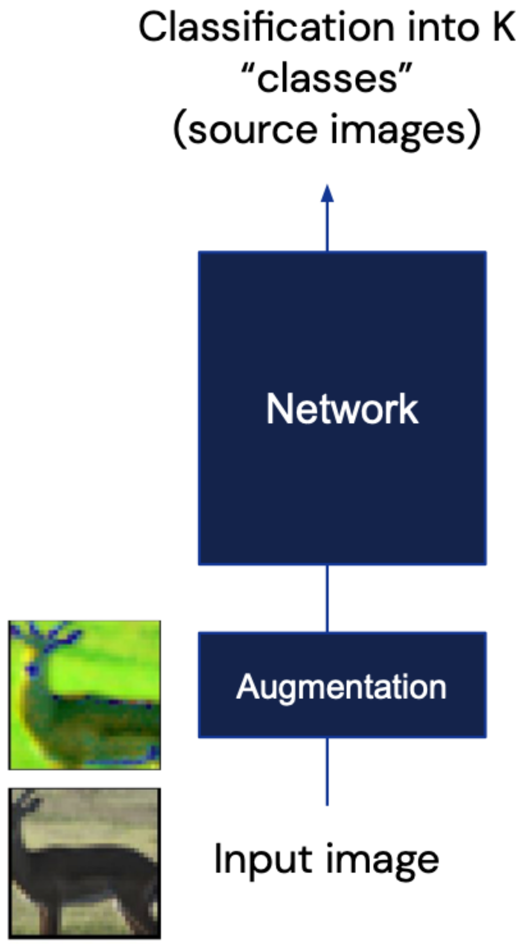


Easy if robust to the desired transformations (geometry and colour)

Slide Credit: Relja Arandjelovic

["Discriminative unsupervised feature learning with exemplar convolutional neural networks", Dosovitskiy et al. 14]

Exemplar ConvNets



Pros

- Representations are invariant to desired transformations
- Requires preservation of fine-grained information

Cons

- Choosing the augmentations is important
- Exemplar based: images of the same class or instance are negatives
  - Nothing prevents it from focusing on the background
- Original formulation is not scalable (number of "classes" = dataset size)

Slide Credit: Relja Arandjelovic

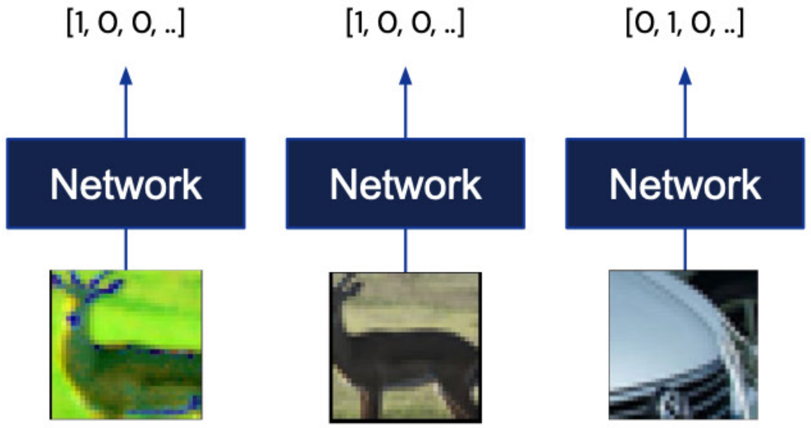
["Representation Learning with Contrastive Predictive Coding", van den Oord et al. 18]

Exemplar ConvNets via metric learning

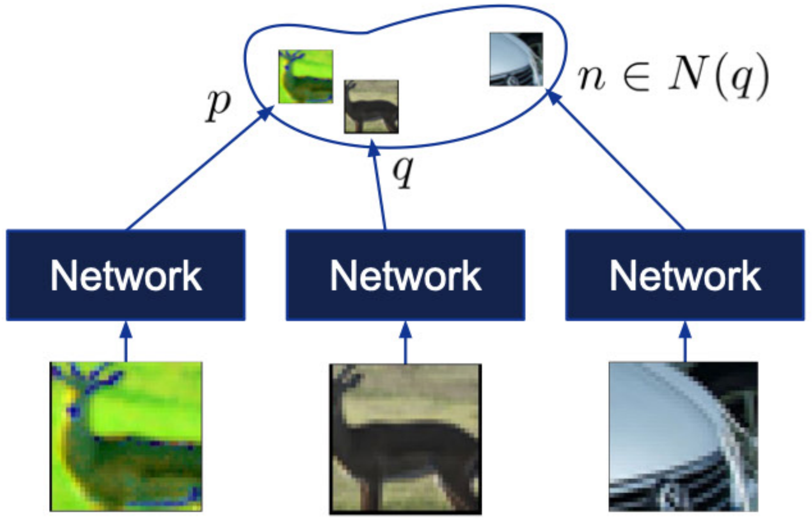
Exemplar ConvNets are not scalable (number of "classes" = number of training images)

- Reformulate in terms of metric learning
- Traditional losses such as contrastive or triplet ["Multi-task self-supervised visual learning", Doersch and Zisserman 17], ["HowTo100M: Learning a text-video embedding by watching hundred million narrated video clips", Miech et al. 19]
- Recently popular: InfoNCE ["Representation Learning with Contrastive Predictive Coding", van den Oord et al. 18]
    - Used by many recent methods: CPC, AMDIM, SimCLR, MoCo, ..

Classification



Metric learning



Slide Credit: Relja Arandjelovic

["Representation Learning with Contrastive Predictive Coding", van den Oord et al. 18]

Noise Contrastive Estimation

InfoNCE loss (a specific popular version)

- For **q**uery, **p**ositive and **n**egative:

$$-\log \frac{\exp(q^T p)}{\exp(q^T p) + \sum_{n\in N(q)} \exp(q^T n)}$$

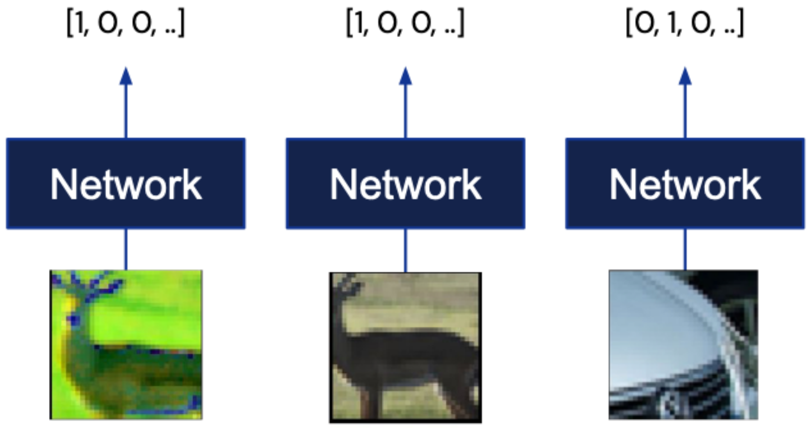
- Like a ranking loss: (q,p) should be close, (q,n) should be far
- An implementation

$$logits = [q^T p, q^T n_1, q^T n_2, ..] = q^T [p, n_1, n_2, ..]$$
$$labels = [1, 0, 0, ..]$$
$$InfoNCE = cross\_entropy(softmax(logits), labels)$$

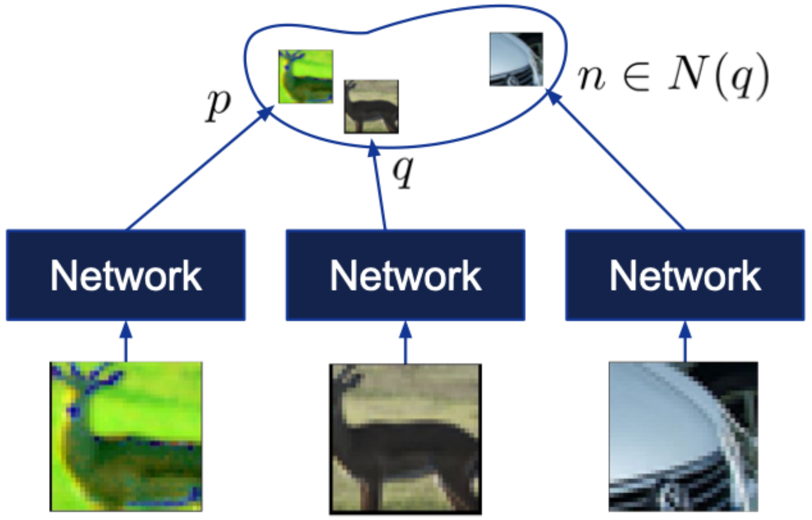
- Squint and see classification loss
  - Replace $[p, n_1, n_2, ..]$ with $[w_p, w_{n_1}, w_{n_2}, ..]$
  - Like classification with weight=exemplars

- More details and perspectives in the next part

Classification



Metric learning



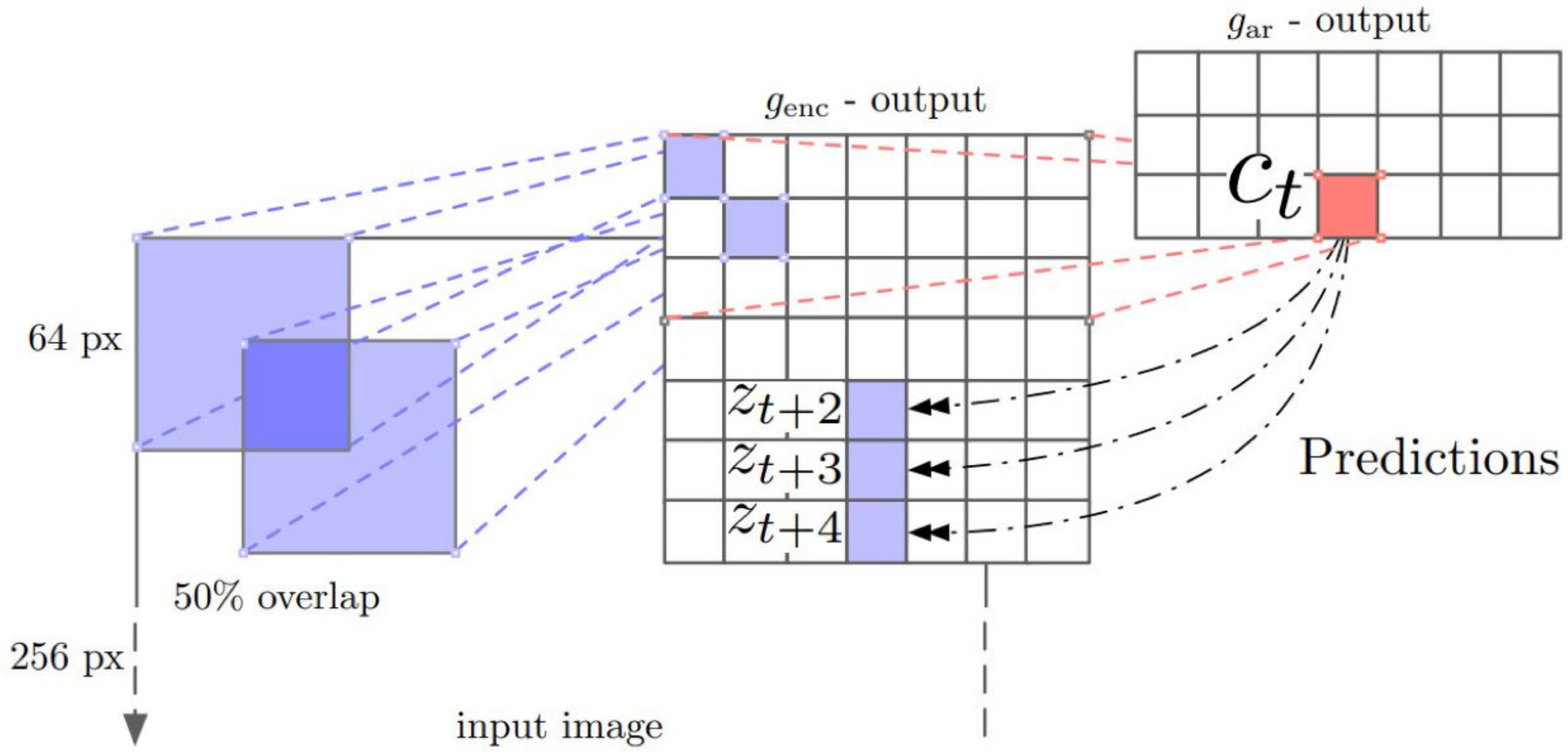
Slide Credit: Relja Arandjelovic

["Representation Learning with Contrastive Predictive Coding", van den Oord et al. 18]
["Data-efficient image recognition with contrastive prediction coding", Hénaff et al. 19]

Contrastive predictive coding (CPC)

Roughly: Context Prediction + Exemplar ConvNets

- From a patch, predict representations of other patches below it
- Use InfoNCE loss to contrast the (predictions, correct, negatives)
  - Negatives: other patches from the same image and other images



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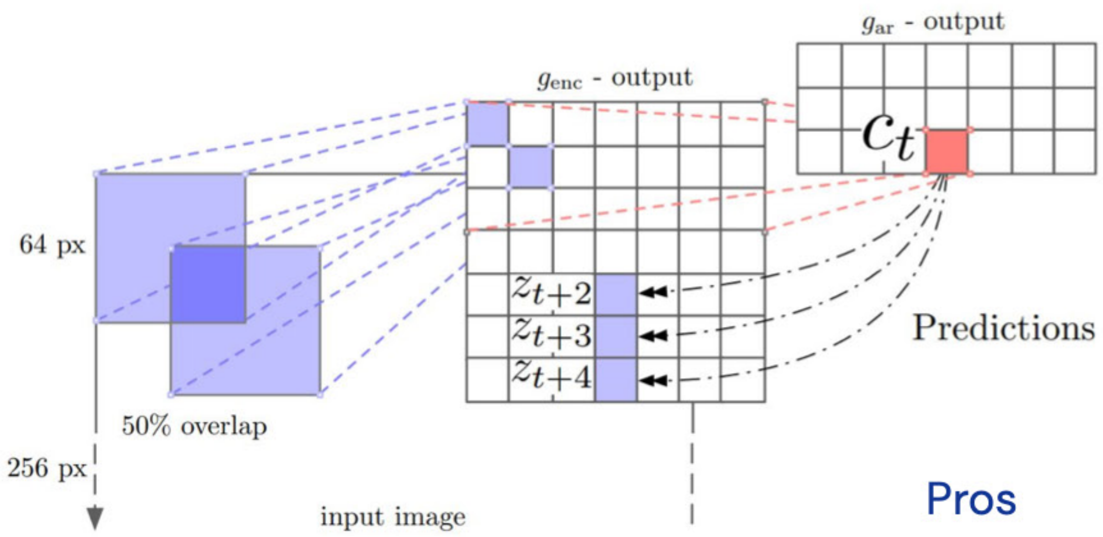
Contrastive predictive coding (CPC)



Pros

- Generic framework easily applied to images, video, audio, NLP, ..
- Exemplar: Requires preservation of fine-grained information
- Context prediction: Should enable learning about object parts

Cons

- Exemplar based: images of the same class or instance are negatives
- Train-eval gap: training on patches, evaluating on images
- Assumes training images are photographed with canonical orientations (and canonical orientations exist)
- Somewhat slow training due to dividing into patches

Slide Credit: Relja Arandjelovic

Exploiting time

Slide Credit: Relja Arandjelovic

["Learning features by watching objects move", Pathak et al. 16]

Watching objects move

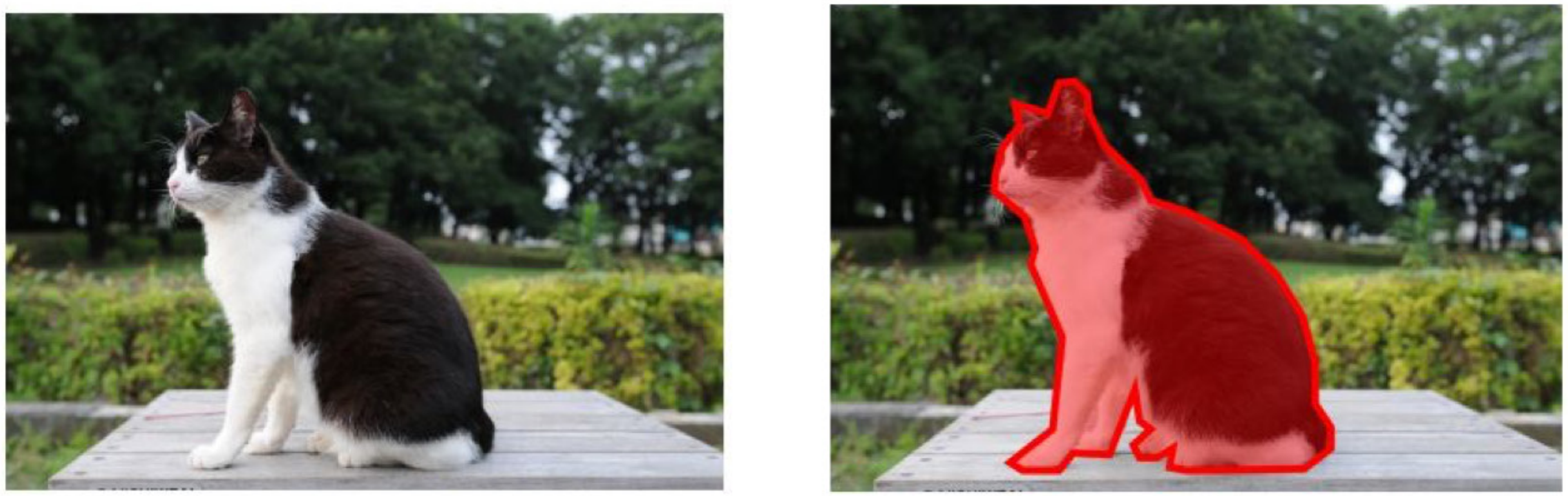
Which pixels will move?

Slide Credit: Relja Arandjelovic

["Learning features by watching objects move", Pathak et al. 16]

Watching objects move

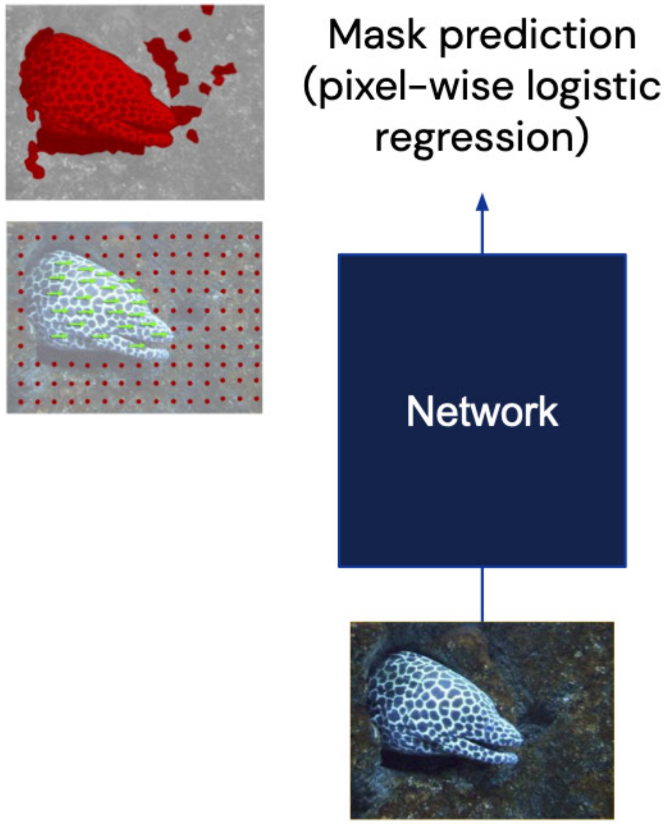
Which pixels will move? Easy if we can segment objects!



Slide Credit: Relja Arandjelovic

["Learning features by watching objects move", Pathak et al. 16]

Watching objects move



Pros

- Emerging behaviour: segmentation
- No train-eval gap

Cons

- "Blind spots": stationary objects
- Potential focus on large salient objects
- Depends on an external motion segmentation algorithm
- Cannot be extended to temporal nets (pretext task would be trivial)

Slide Credit: Relja Arandjelovic

["Tracking emerges by colorizing videos", Vondrick et al. 18]

Tracking by colorization

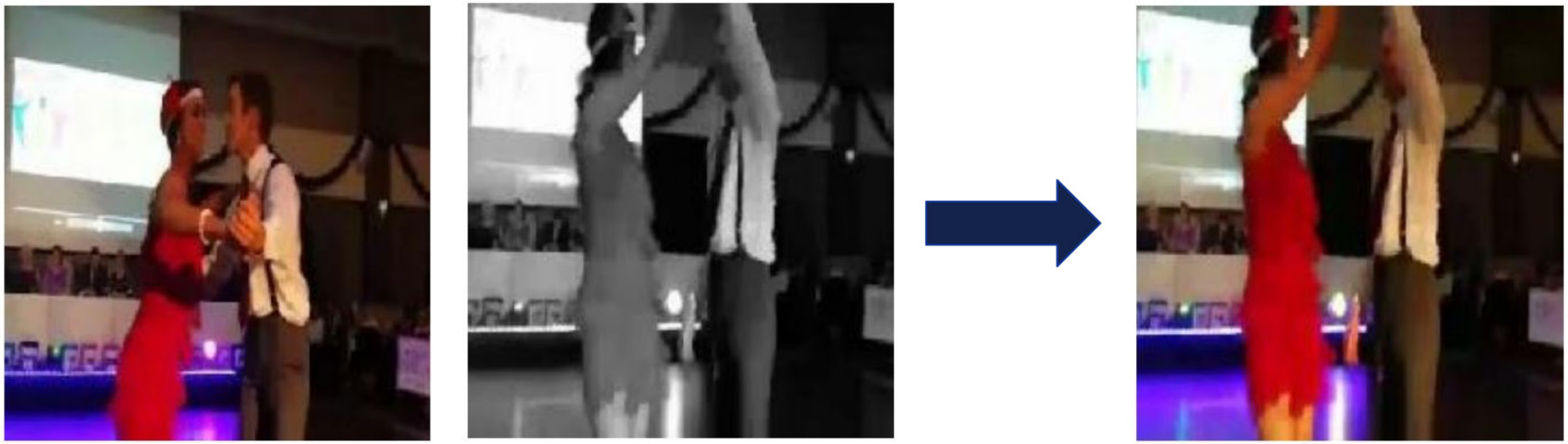
Given an earlier frame, colourize the new one.

Slide Credit: Relja Arandjelovic

["Tracking emerges by colorizing videos", Vondrick et al. 18]

Tracking by colorization

Given an earlier frame, colourize the new one. Easy if everything can be tracked!



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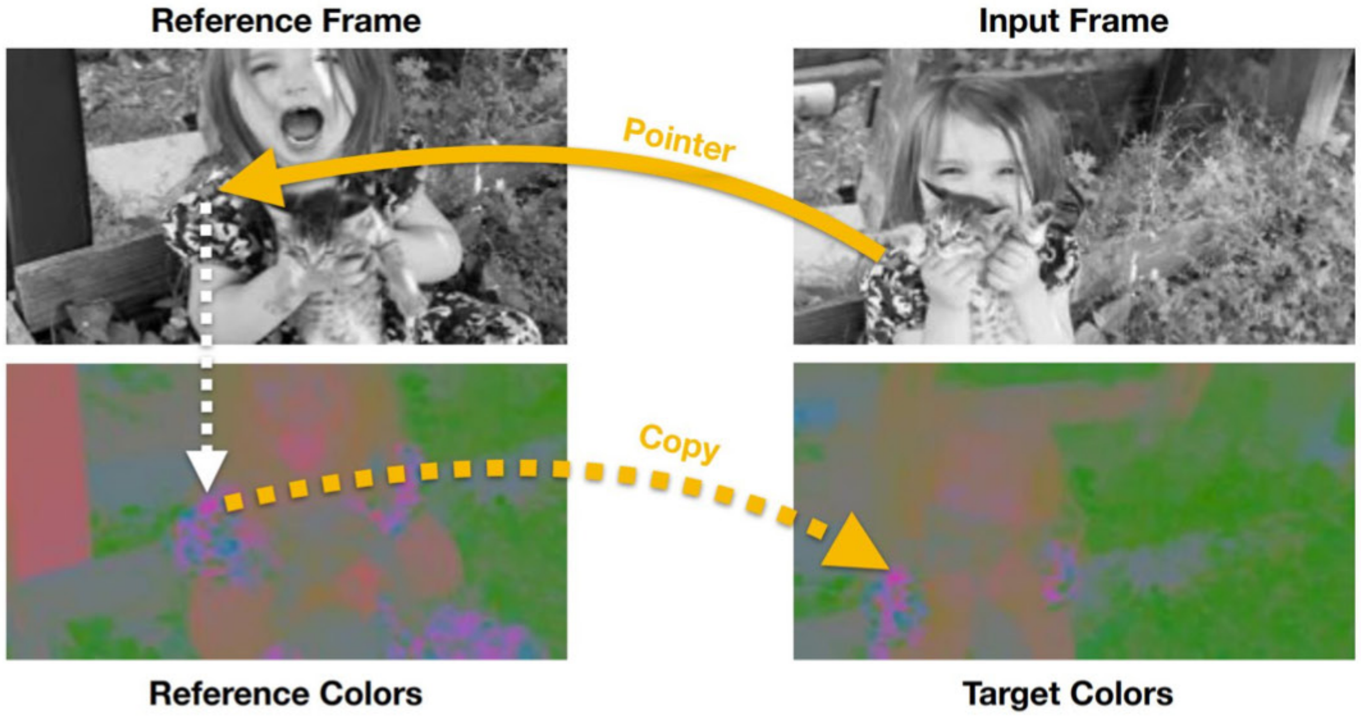
Tracking by colorization



Pros

- Emerging behaviour: tracking, matching, optical flow, segmentation

Cons

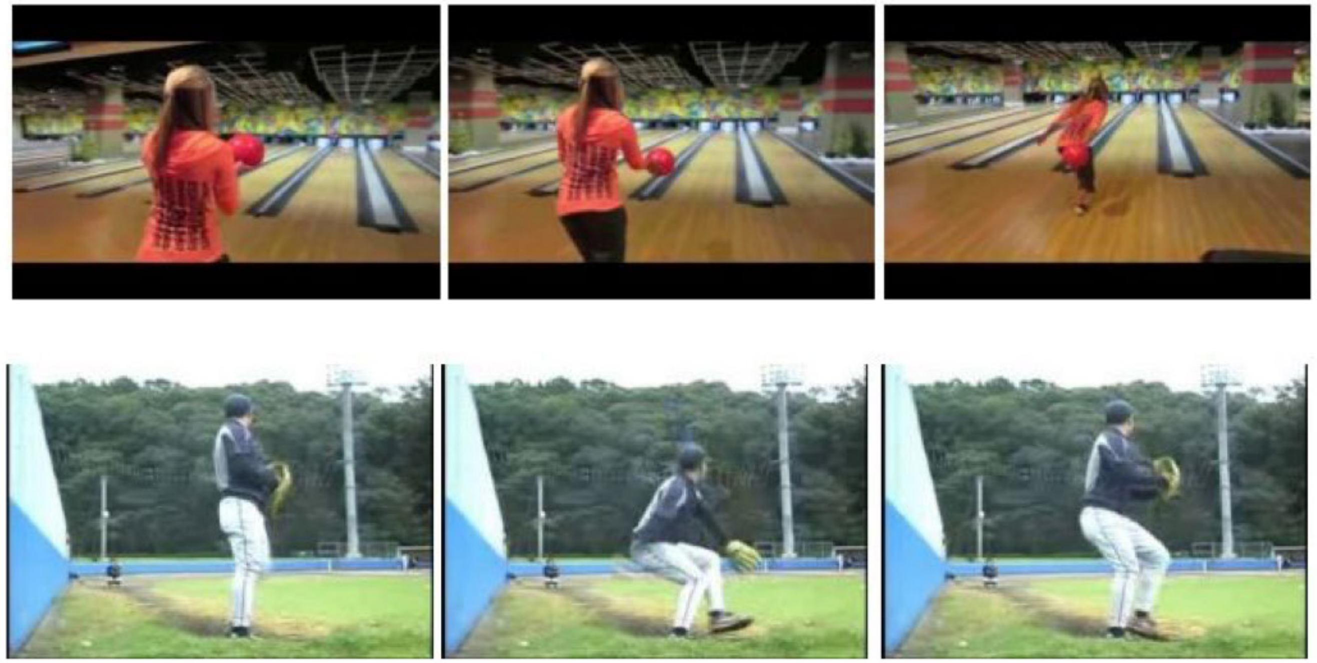
- Low level cues are effective – less emphasis on semantics
- Forced to evaluate on greyscale frames, losing information

Slide Credit: Relja Arandjelovic

["Shuffle and learn: Unsupervised learning using temporal order verification", Misra et al. 16]

Temporal ordering

Is this sequence of frames correctly ordered?

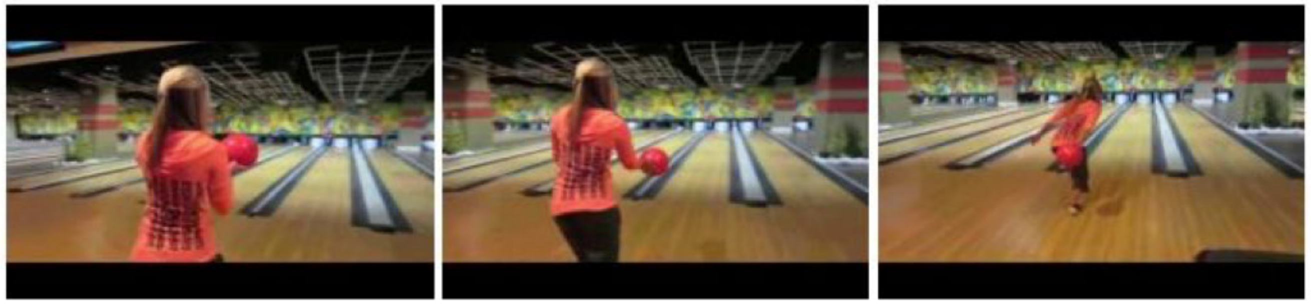


Slide Credit: Relja Arandjelovic

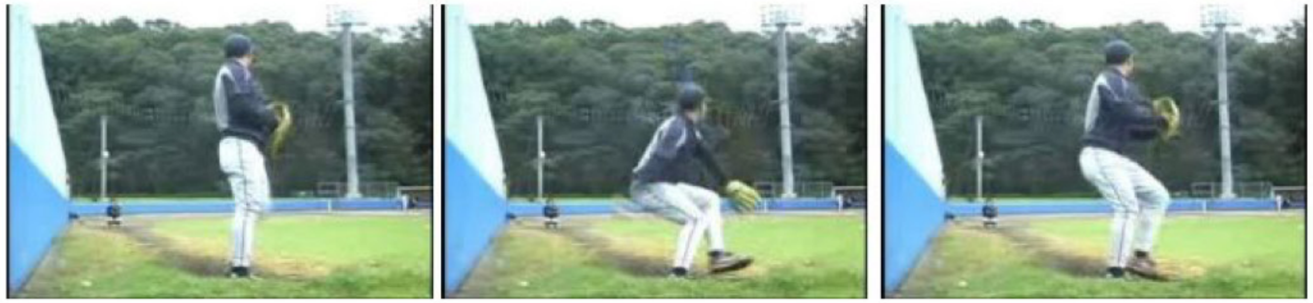
["Shuffle and learn: Unsupervised learning using temporal order verification", Misra et al. 16]

Temporal ordering

Is this sequence of frames correctly ordered? Easy if we recognize the action and human pose!



✓



✗

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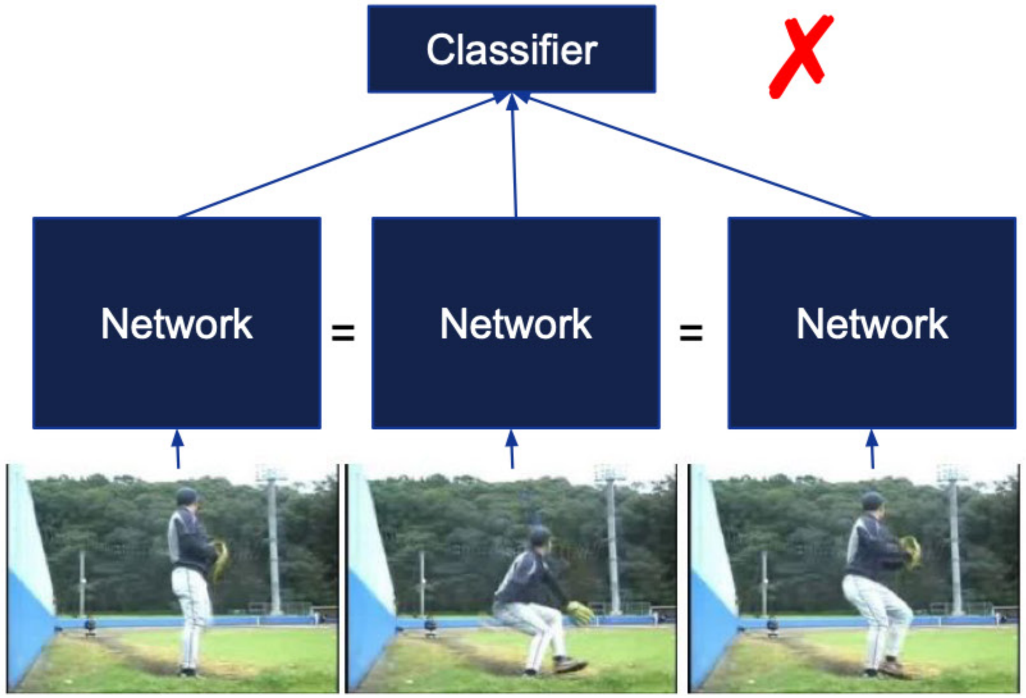
Temporal ordering



Pros

- No train-eval gap
- Learns to recognize human pose

Cons

- Mostly focuses on human pose - not always sufficient
- Questionable if it can be extended to temporal nets (potentially task becomes too easy)

Extensions

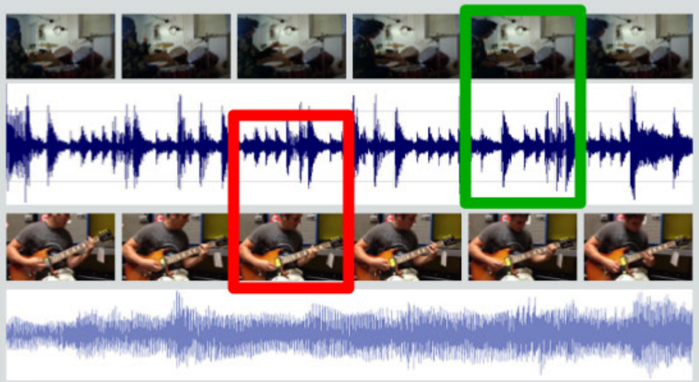
- N frames with one randomly placed - find it

  ["Self-supervised video representation learning with odd-one-out networks", Fernando et al. 16]
- Ranking loss: embeddings should be similar for frames close in time and dissimilar for far away frames

  ["Time-contrastive networks: Self-supervised learning from video", Sermanet et al. 17]

Slide Credit: Relja Arandjelovic

Multimodal

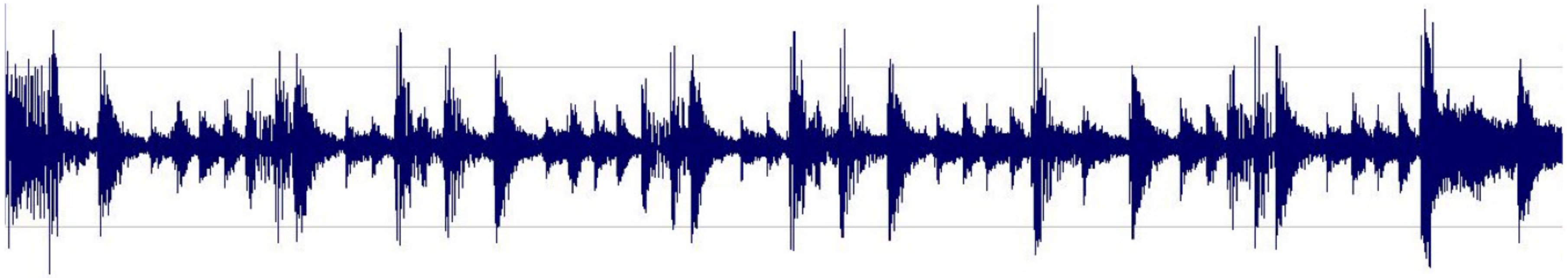


Slide Credit: Relja Arandjelovic

["Look, Listen and Learn", Arandjelović et al. 17]

Audio-visual correspondence

Does the sound go with the image?



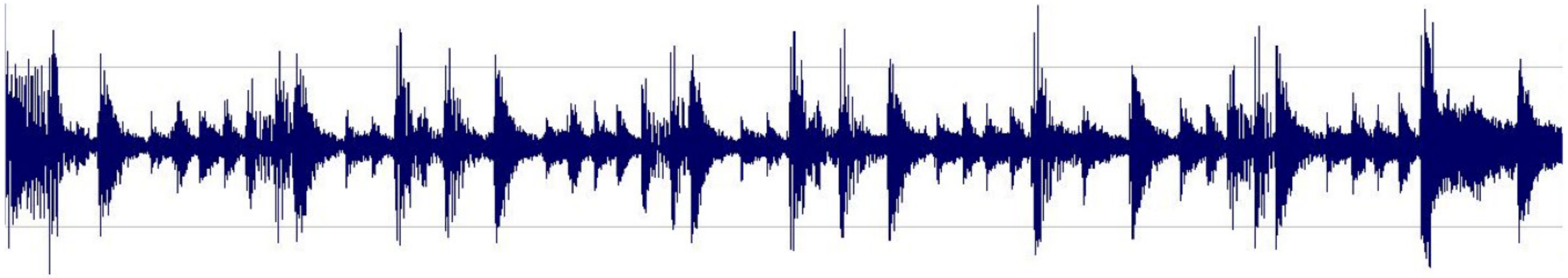
Slide Credit: Relja Arandjelovic

["Look, Listen and Learn", Arandjelović et al. 17]

Audio-visual correspondence

Does the sound go with the image? Easy if we recognize what is happening in both the frame and the audio

✗



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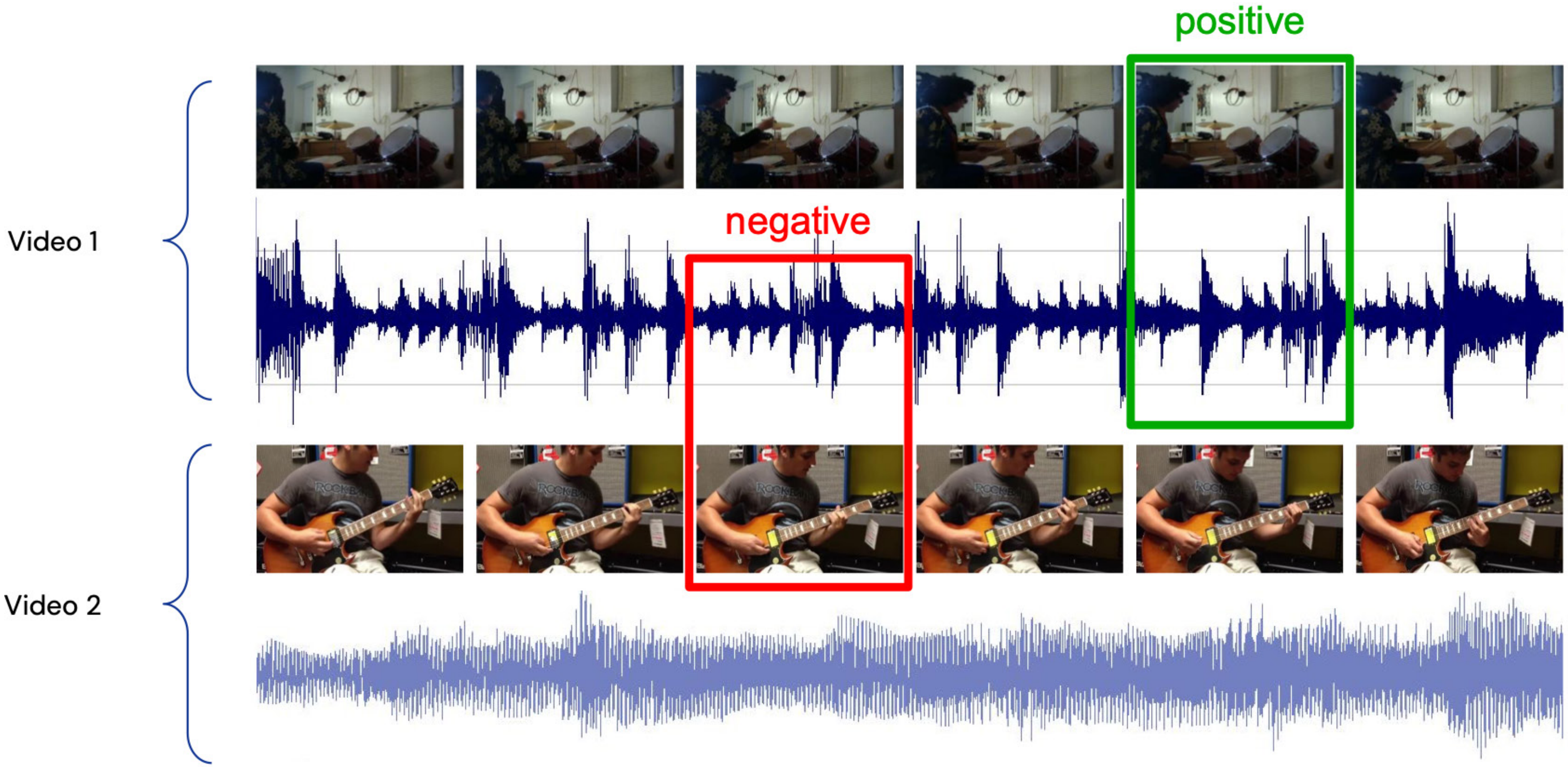

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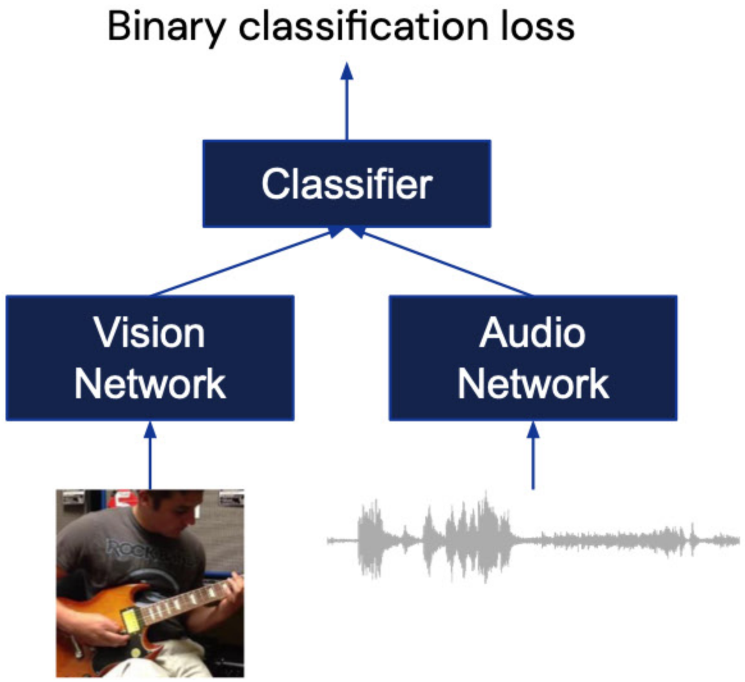


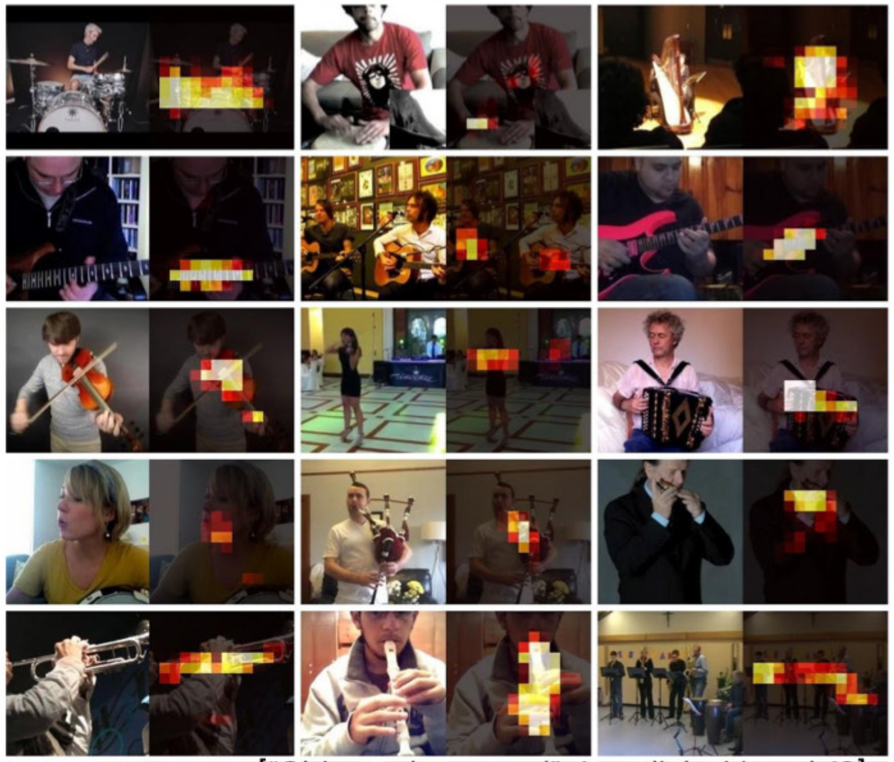
Binary classification loss

Classifier

Vision Network

Audio Network

[“Look, Listen and Learn”, Arandjelović et al. 17]



[“Objects that sound”, Arandjelović et al. 18]

Pros

- Natural different views of the training data, no need for augmentations
- No train-eval gap
- Representations in both modalities for free

Cons

- “Blind spots”: not everything makes a sound
- Exemplar based: videos of the same class or instance are negatives
- Small output space – two cases (corresponds or not)
  - Can be improved by contrastive approaches

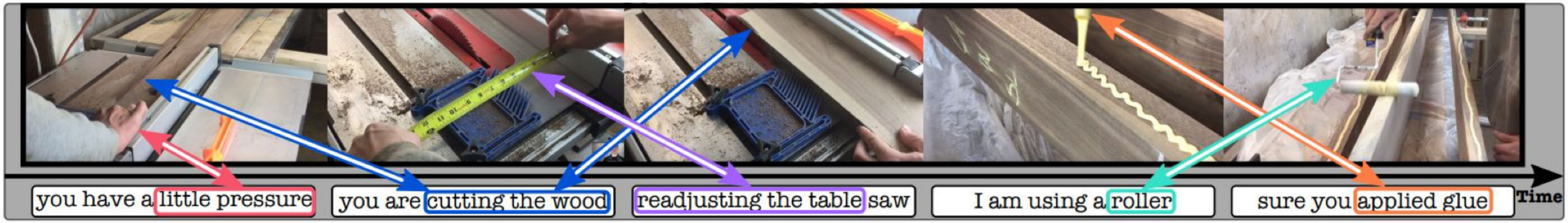
Slide Credit: Relja Arandjelovic

["End-to-end learning of visual representations from uncurated instructional videos", Miech et al. 19]

Leveraging narration

Does the narration go with the video?

(Text obtained from automatic speech recognition)



Slide Credit: Relja Arandjelovic

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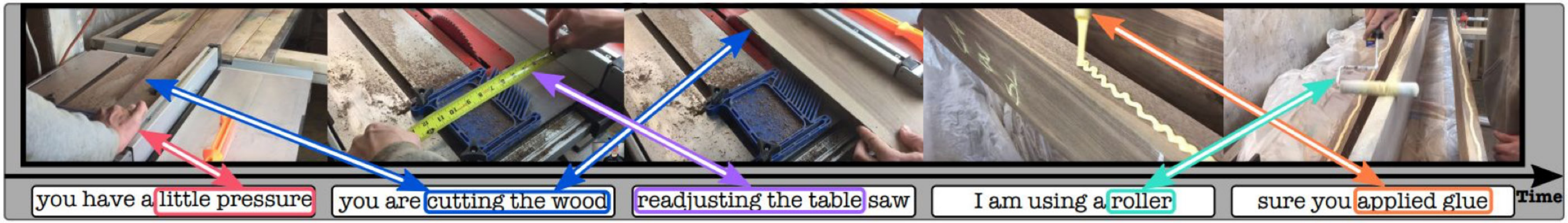
Leveraging narration

Does the narration go with the video? Easy if we recognize what is happening in the video and narrations

(Text obtained from automatic speech recognition)



Complication compared to the audio-visual case:

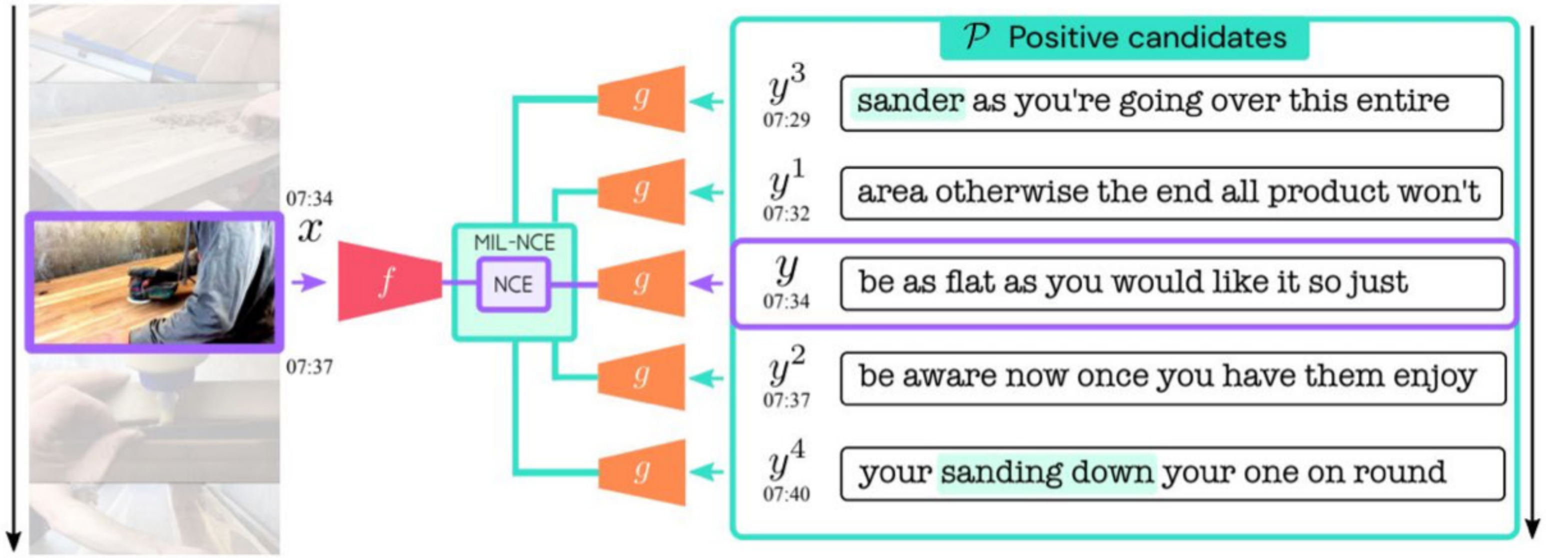
- Narration and visual content are less aligned

Slide Credit: Relja Arandjelovic

["End-to-end learning of visual representations from uncurated instructional videos", Miech et al. 19]

Leveraging narration

Multiple instance learning extension of the NCE loss


$\mathcal{P}$ Positive candidates
07:34
x
07:37
f
MIL-NCE
NCE
g
y^3 07:29
sander as you're going over this entire
y^1 07:32
area otherwise the end all product won't
y 07:34
be as flat as you would like it so just
y^2 07:37
be aware now once you have them enjoy
y^4 07:40
your sanding down your one on round

Pros

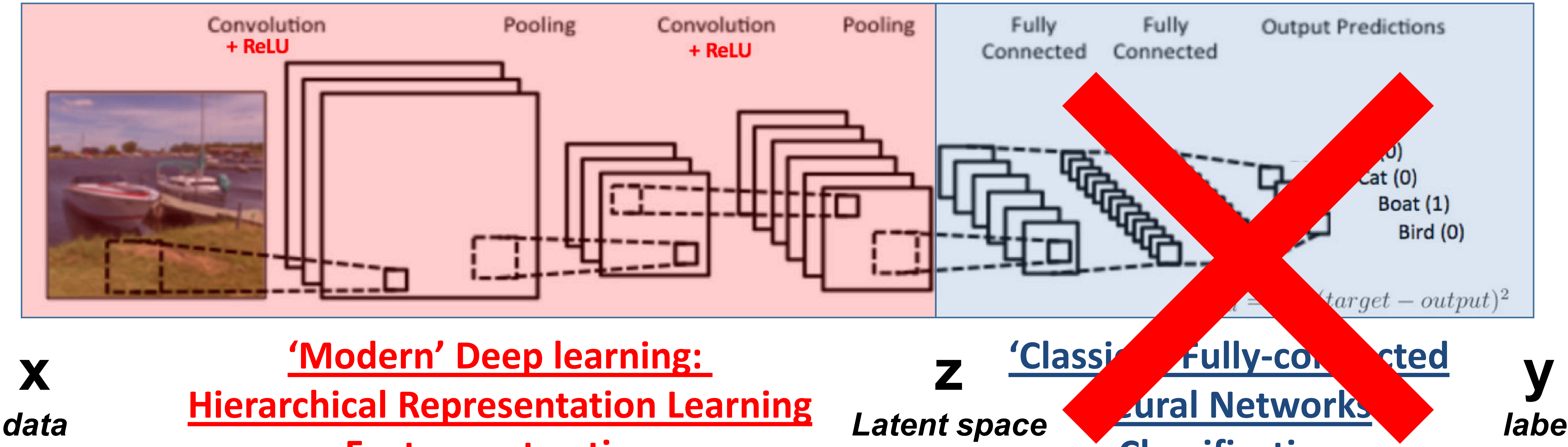
- Natural different views of the training data, no need for augmentations
- No train-eval gap
- Representations in both modalities for free

Cons

- "Blind spots": not everything is mentioned in narrations
- Exemplar based: videos of the same class or instance are negatives
- Assumes a single language, potentially non-trivial to extend to more

Slide Credit: Relja Arandjelovic

Representation learning **without annotations**?



x
data

'Modern' Deep learning:
Hierarchical Representation Learning
Feature extraction

z
Latent space representation

'Classic' Fully-connected
Neural Networks
Classification

y
label

Many ideas are possible (and yours could be even better!):

1. Predict the future: RNNs, Video
2. Compression: Autoencoder (predict self, through clamp), representation **z**
3. Pretext tasks: predict self, before/after, missing patch, correct rotation, colorization, up-sampling, multimodal
4. Capture parameter distribution (variance): Variational Auto-Encoders
5. Make latent space parameters z meaningful, orthogonal, explicit, tuneable
6. Train using a second network: GANs - Improve quality of output images
7. The Sky is the Limit

Auto-Encoders

Some background first: Autoencoders

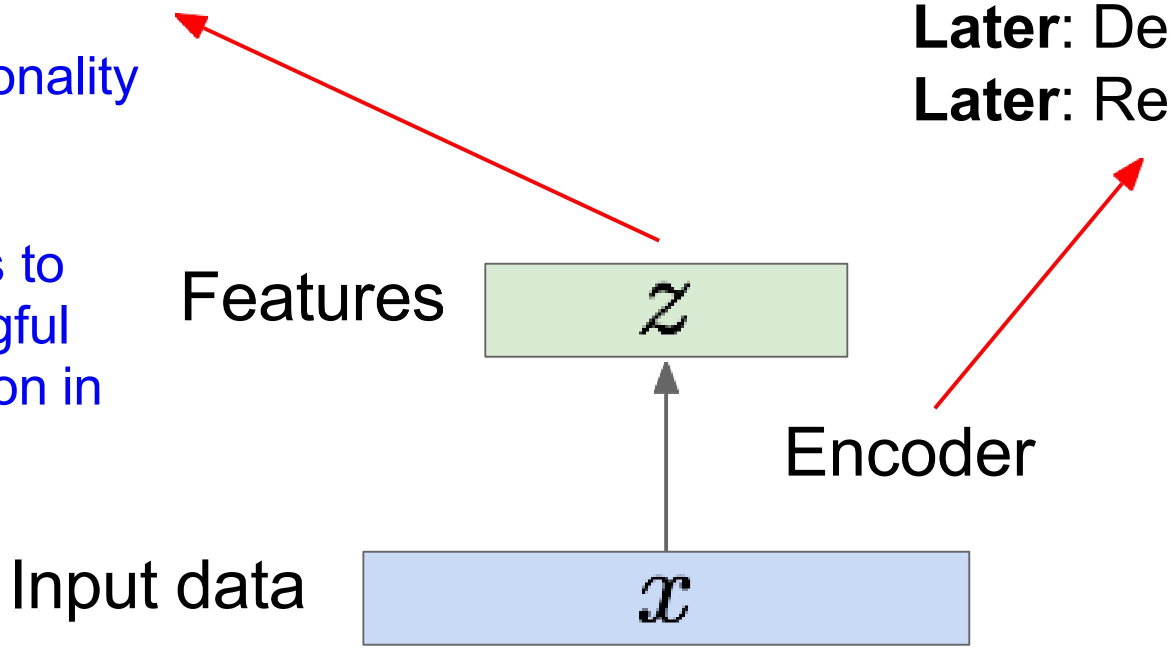
Unsupervised approach for learning a lower-dimensional feature representation from unlabeled training data

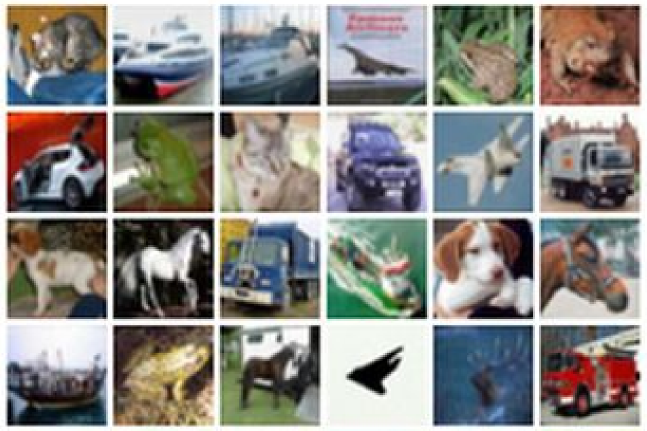
z usually smaller than **x** (dimensionality reduction)

Q: Why dimensionality reduction?

A: Want features to capture meaningful factors of variation in data

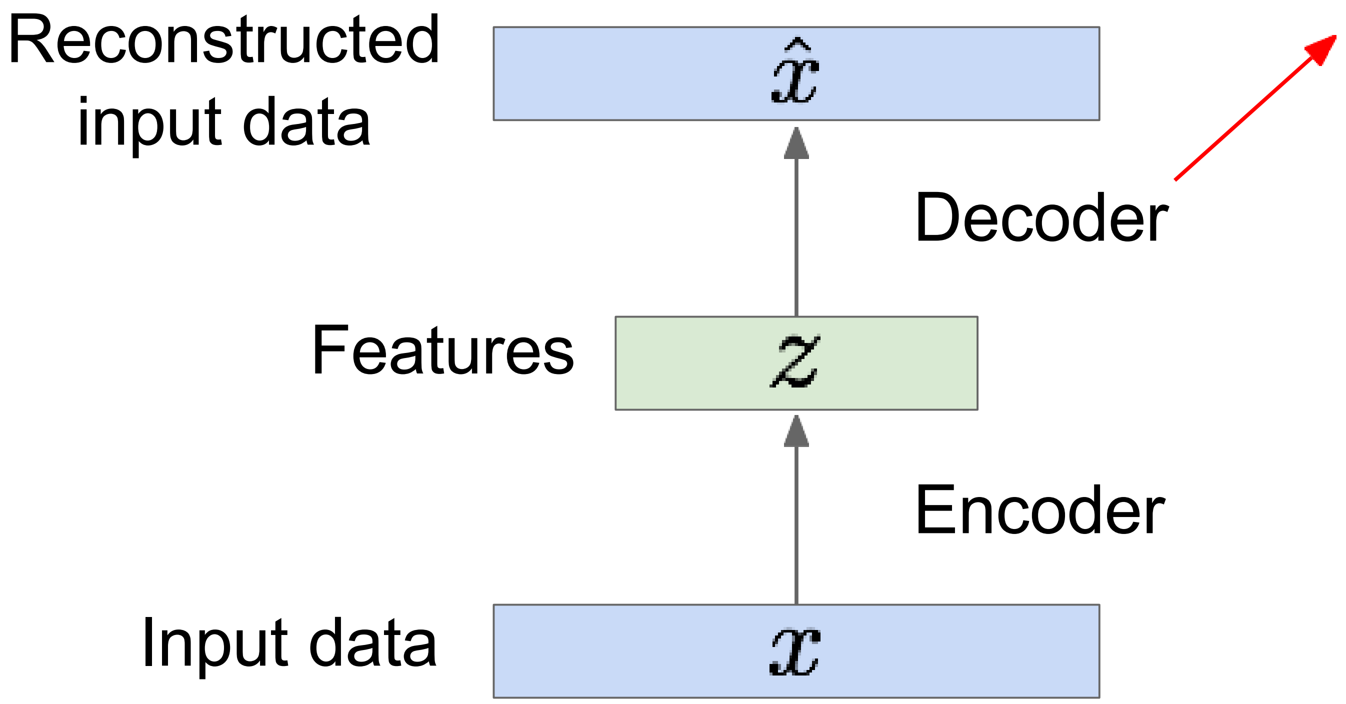
Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN



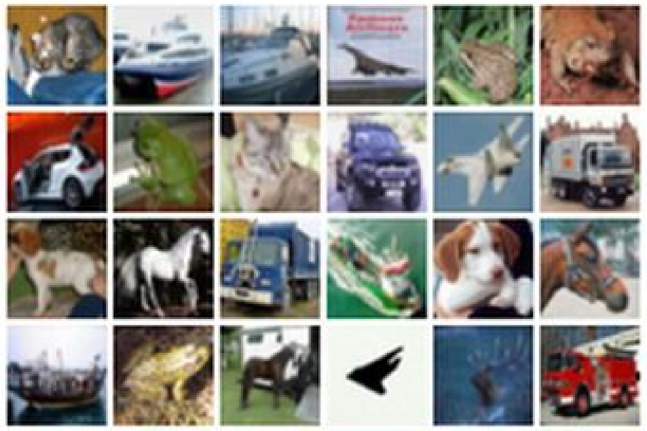


Some background first: Autoencoders

How to learn this feature representation?
Train such that features can be used to reconstruct original data
"Autoencoding" - encoding itself



Originally: Linear + nonlinearity (sigmoid)
Later: Deep, fully-connected
Later: ReLU CNN (upconv)



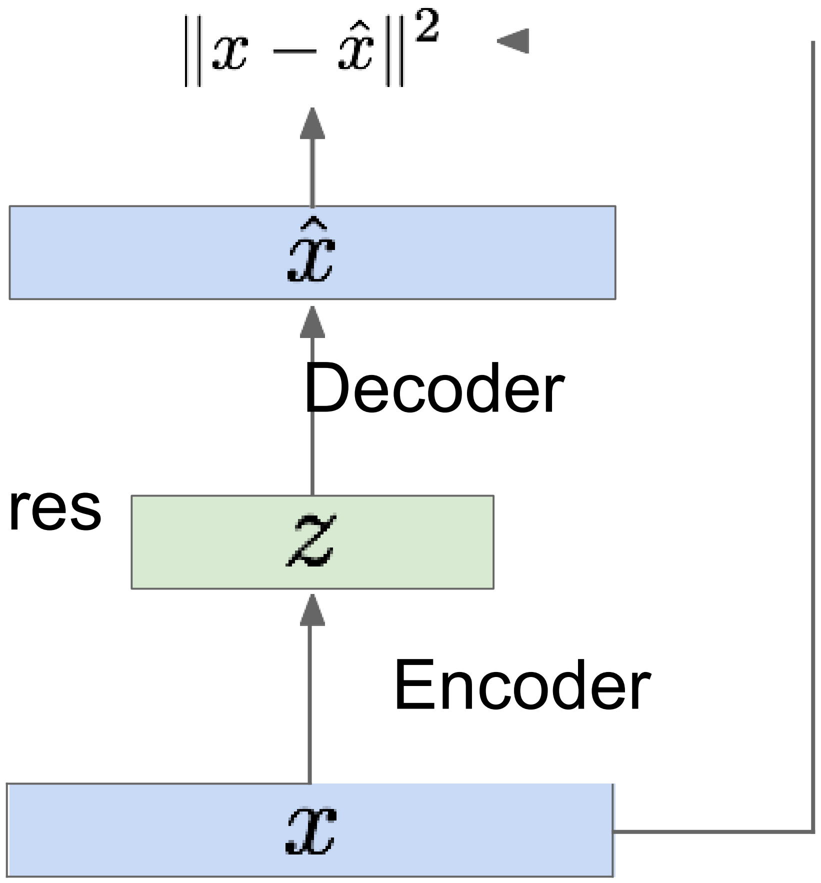
Some background first: Autoencoders

Train such that features can be used to reconstruct original data

Doesn't use labels!

L2 Loss function:

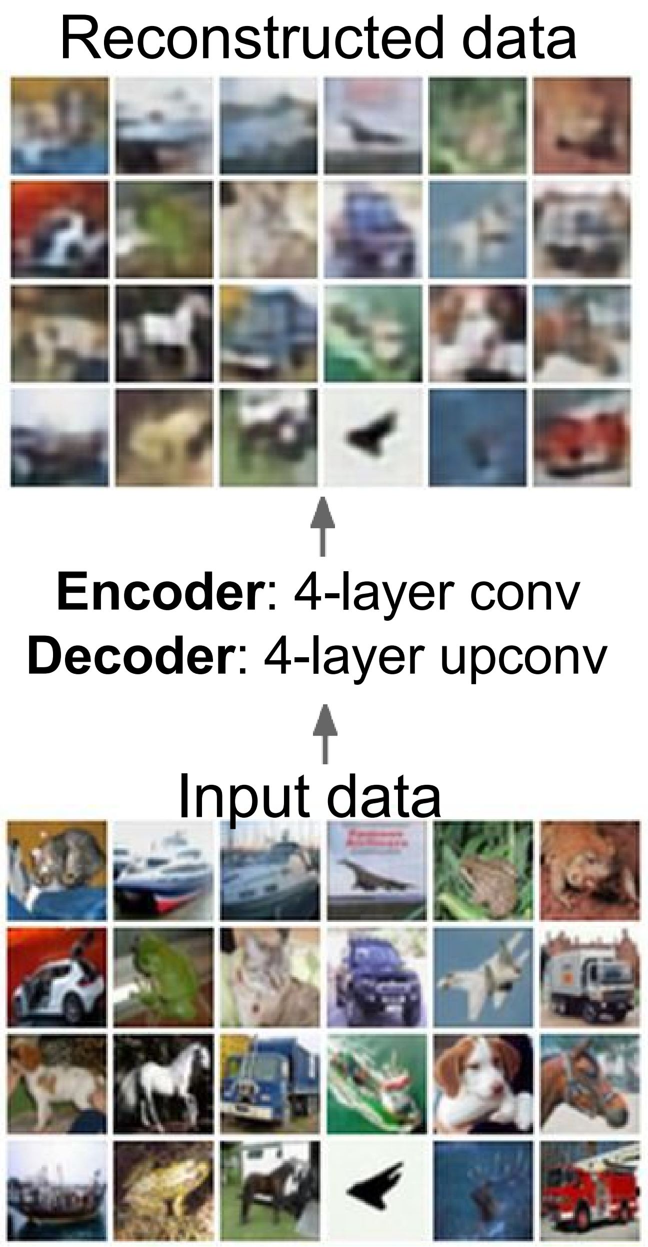
$$\|x - \hat{x}\|^2$$



Reconstructed input data

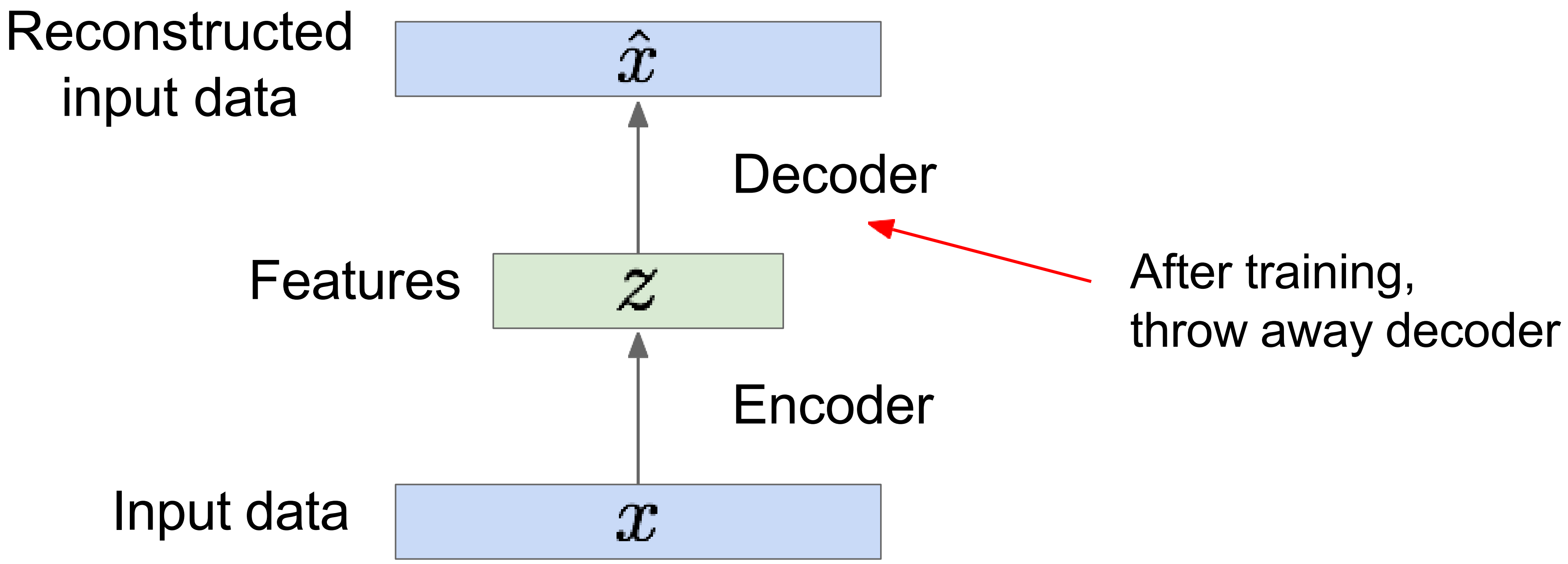
Featu res

Input data



Encoder: 4-layer conv
Decoder: 4-layer upconv

Some background first: Autoencoders



Reconstructed input data

$\hat{x}$

Decoder

Features

z

Encoder

Input data

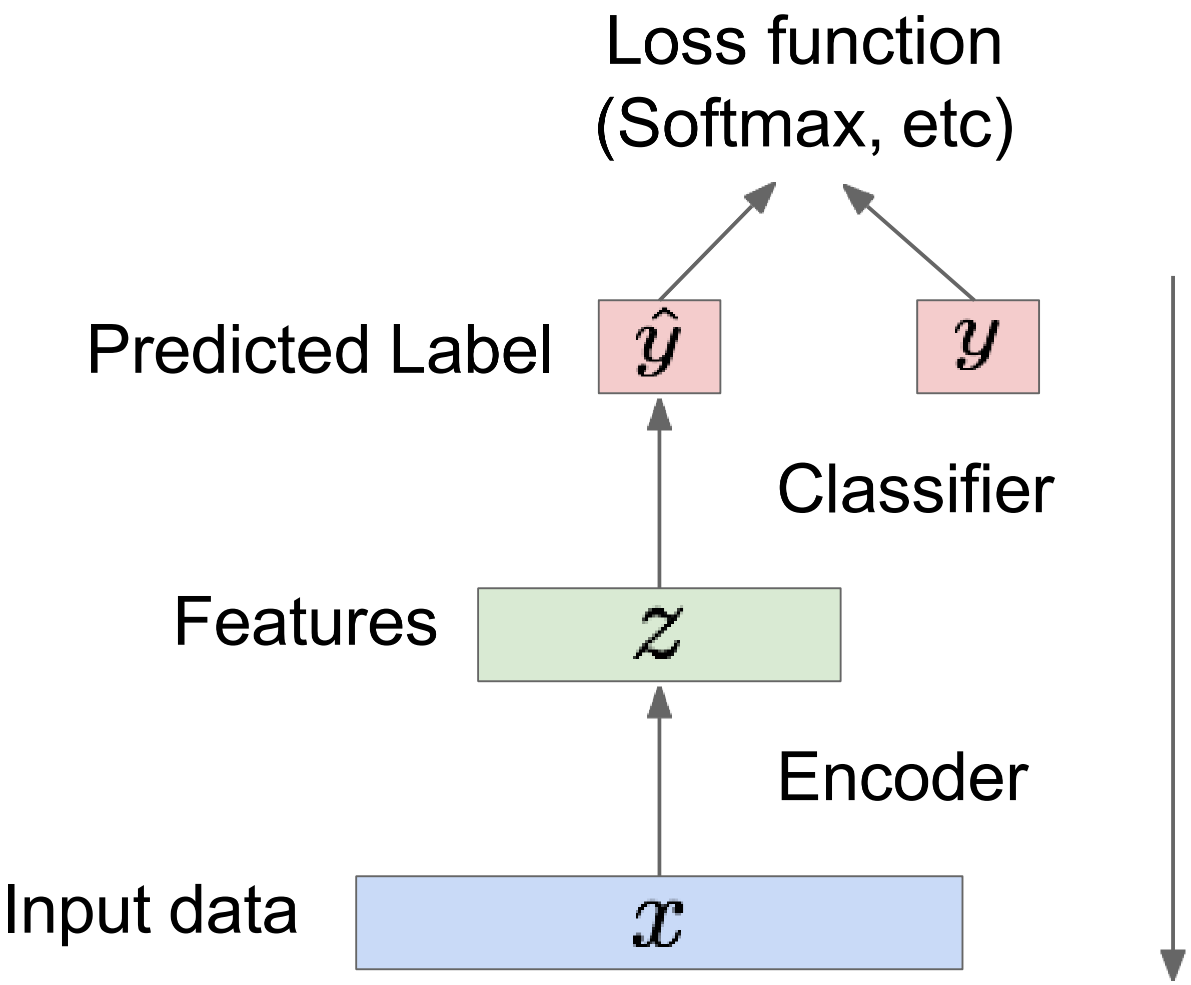
x

After training, throw away decoder

Slides: Fei-Fei Li, Justin Johnson, Serena Yeung

Some background first: Autoencoders

Encoder can be used to initialize a **supervised** model



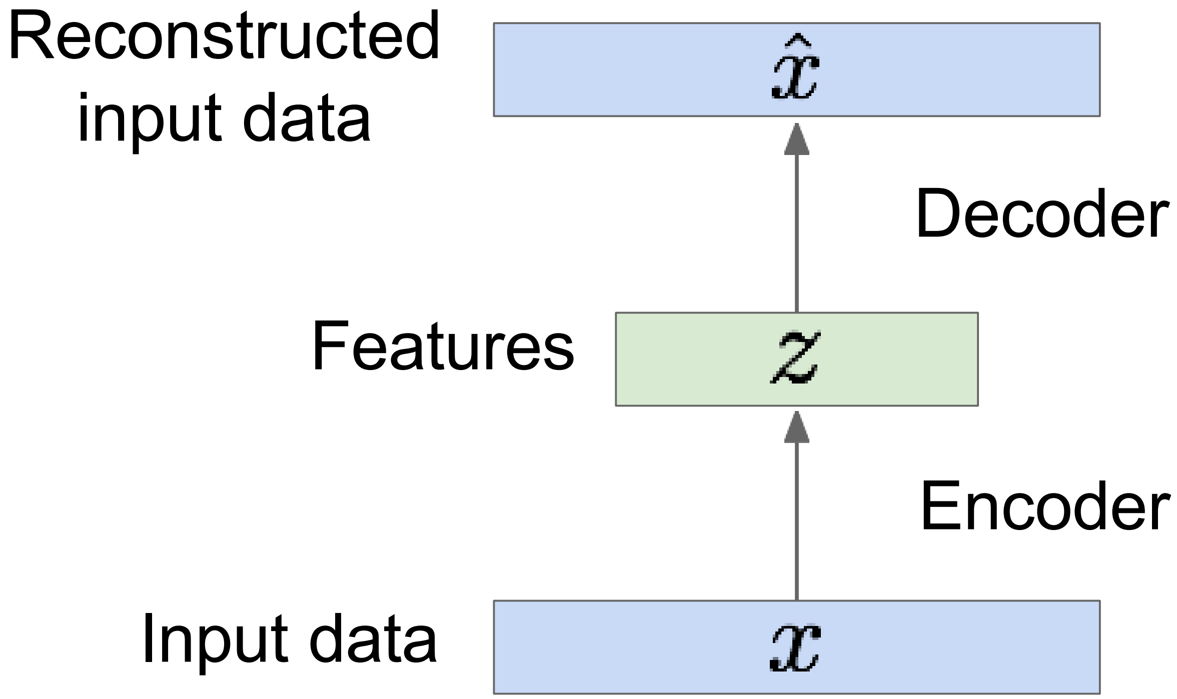
Fine-tune encoder jointly with classifier

bird plane

dog deer truck

Train for final task (sometimes with small data)

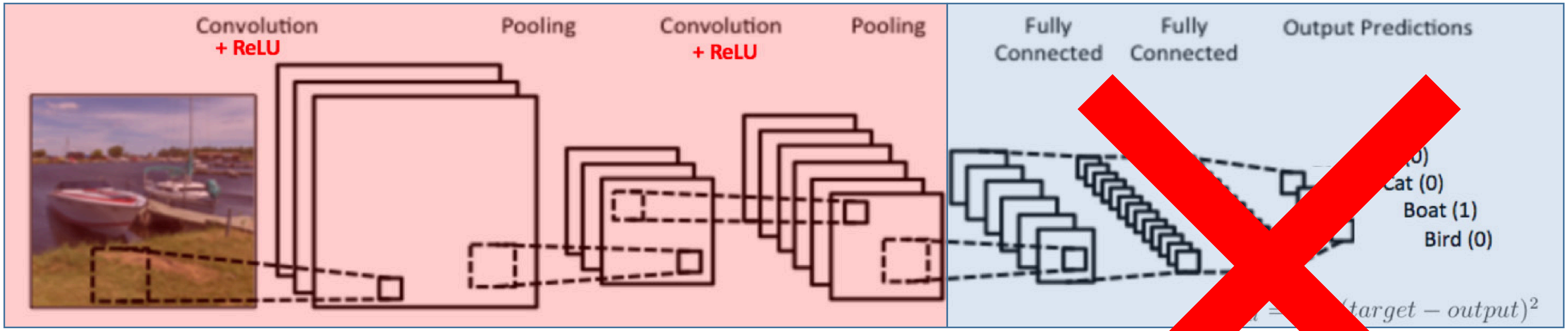
Some background first: Autoencoders



Autoencoders can reconstruct data, and can learn features to initialize a supervised model

Features capture factors of variation in training data. Can we generate new images from an autoencoder?

Representation learning **without annotations**?



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Variational AutoEncoders (VAEs)

Variational Autoencoders

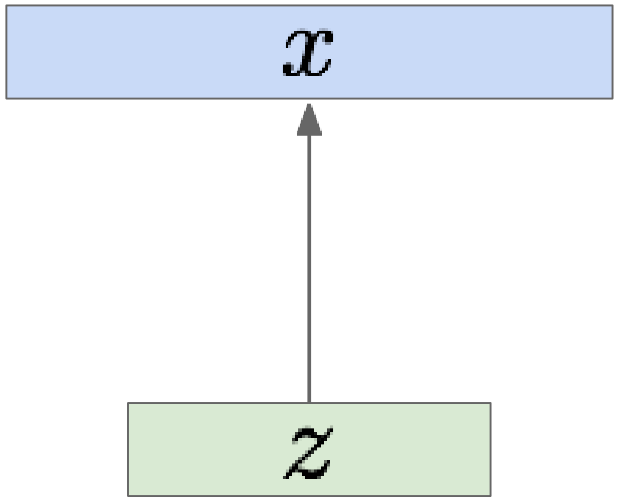
Probabilistic spin on autoencoders - will let us sample from the model to generate data!

Assume training data $\{x^{(i)}\}_{i=1}^{N}$ is generated from underlying unobserved (latent) representation **z**

Intuition (remember from autoencoders!): **x** is an image, **z** is latent factors used to generate **x:** attributes, orientation, etc.

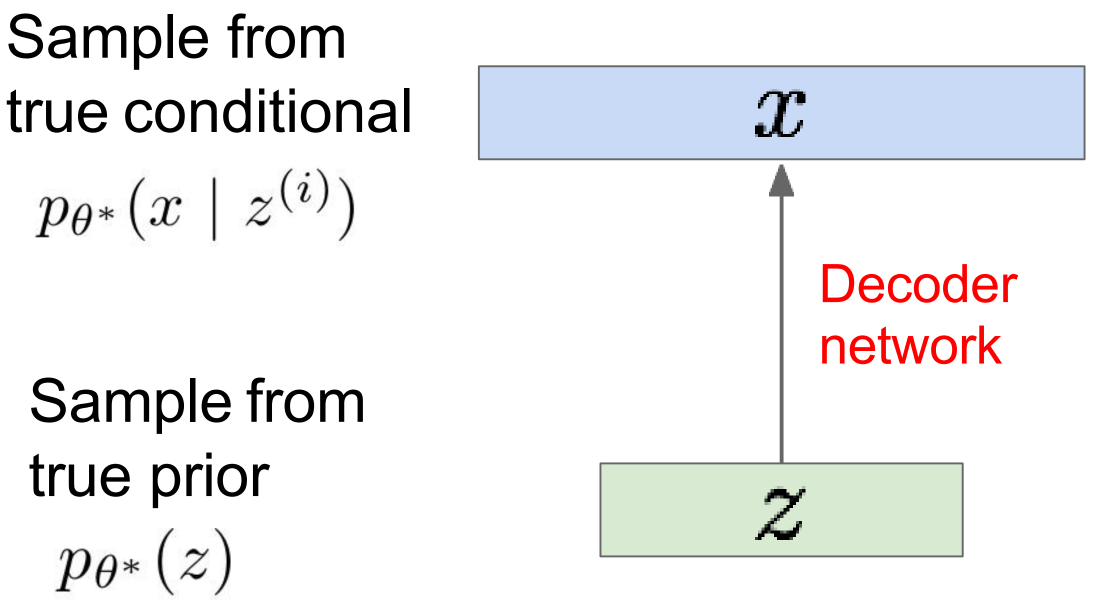
Sample from true conditional $p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior $p_{\theta^*}(z)$



Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders



Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

Decoder network

Sample from true prior

$p_{\theta^*}(z)$

We want to estimate the true parameters θ^* of this generative model.

How should we represent this model?

Choose prior p(z) to be simple, e.g. Gaussian.

Conditional p(x|z) is complex (generates image) => represent with neural network

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

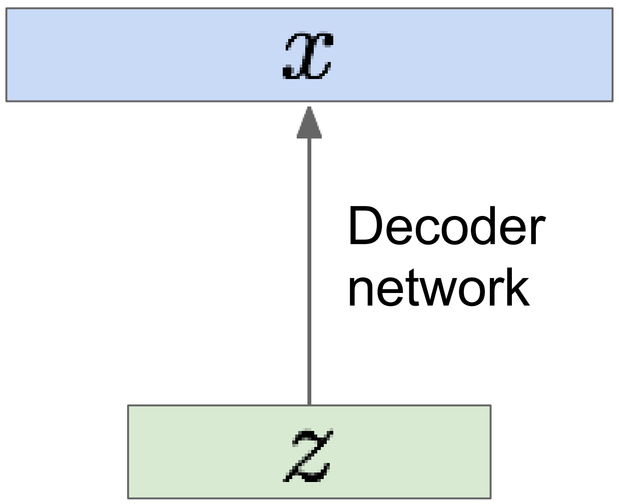
Variational Autoencoders

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

$p_{\theta^*}(z)$



We want to estimate the true parameters θ^* of this generative model.

How to train the model?

Remember strategy for training generative models from FVBNs. Learn model parameters to maximize likelihood of training data

$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Now with latent z

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

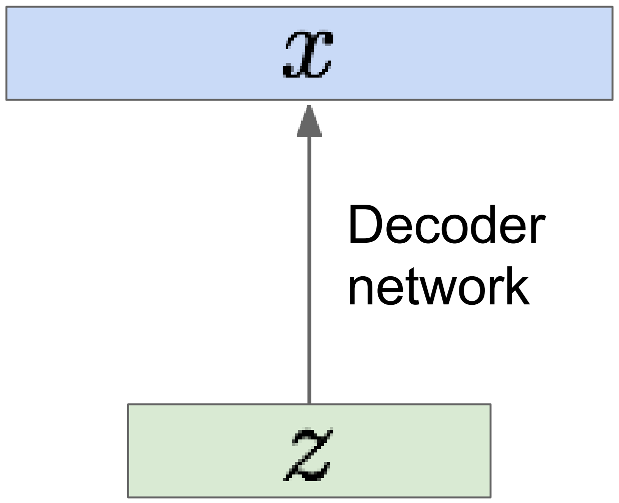
Variational Autoencoders

Sample from true conditional

$p_{\theta^*}(x \mid z^{(i)})$

Sample from true prior

$p_{\theta^*}(z)$



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$$p_\theta(x) = \int p_\theta(z) p_\theta(x|z) dz$$

Q: What is the problem with this?

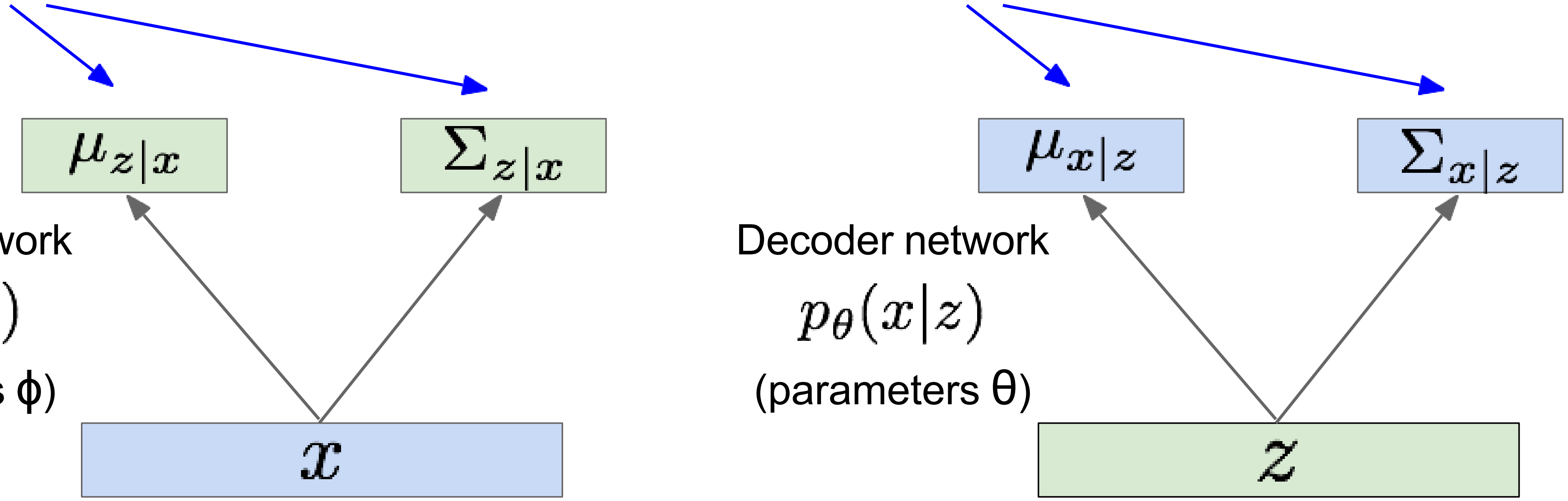
Intractable!

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic Mean and (diagonal) covariance of **z | x**

Mean and (diagonal) covariance of **x | z**



Encoder network

$q_\phi(z|x)$

(parameters ϕ)

Decoder network

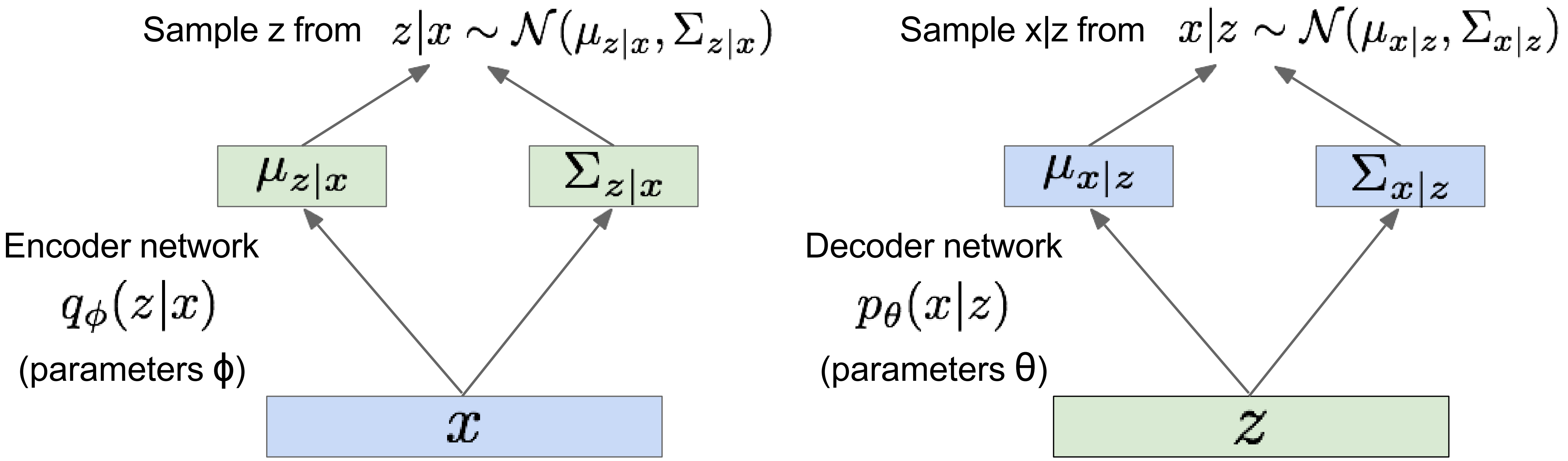
$p_\theta(x|z)$

(parameters θ)

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

Since we're modeling probabilistic generation of data, encoder and decoder networks are probabilistic



Sample z from $z|x \sim \mathcal{N}(\mu_{z|x}, \Sigma_{z|x})$

Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$

Encoder network

$q_\phi(z|x)$

(parameters ϕ)

Decoder network

$p_\theta(x|z)$

(parameters θ)

Kingma and Welling, "Auto-Encoding Variational Bayes", ICLR 2014

Variational Autoencoders

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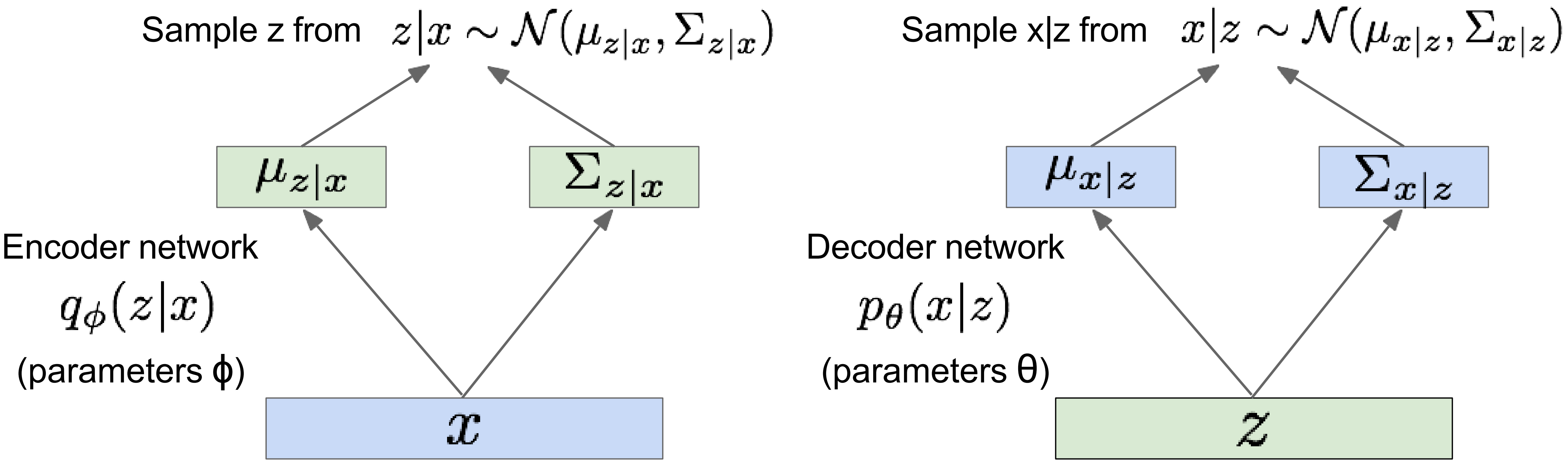


Sample z from $z|x \sim \mathcal{N}(\mu_{z|x}, \Sigma_{z|x})$

$\mu_{z|x}$ $\Sigma_{z|x}$

Encoder network

$q_\phi(z|x)$

(parameters ϕ)

x

Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$

$\mu_{x|z}$ $\Sigma_{x|z}$

Decoder network

$p_\theta(x|z)$

(parameters θ)

z

Encoder and decoder networks also called “recognition”/“inference” and “generation” networks

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders

Now equipped with our encoder and decoder networks, let’s work out the (log) data likelihood:

$$
\begin{aligned}
\log p_\theta(x^{(i)}) &= \mathbf{E}_{z \sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \qquad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z) p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \qquad (\text{Bayes' Rule}) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z) p_\theta(z)}{p_\theta(z \mid x^{(i)})} \frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \qquad (\text{Multiply by constant}) \\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \qquad (\text{Logarithms}) \\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z)) + D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))
\end{aligned}
$$

The expectation wrt. z (using encoder network) let us write nice KL terms

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$
\begin{aligned}
\log p_\theta(x^{(i)}) &= \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \qquad (p_\theta(x^{(i)}) \text{ Does not depend on } z)\\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \qquad (\text{Bayes' Rule})\\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \qquad (\text{Multiply by constant})\\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \qquad (\text{Logarithms})\\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z)) + D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))
\end{aligned}
$$

We want to maximize the data likelihood

Decoder network gives $p_\theta(x|z)$, can compute estimate of this term through sampling. (Sampling differentiable through reparam. trick, see paper.)

This KL term (between Gaussians for encoder and z prior) has nice closed-form solution!

$p_\theta(z|x)$ intractable (saw earlier), can't compute this KL term :(But we know KL divergence always >= 0.

Variational Autoencoders

Now equipped with our encoder and decoder networks, let’s work out the (log) data likelihood:

$$
\begin{aligned}
\log p_\theta(x^{(i)}) &= \mathbf{E}_{z\sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \qquad (p_\theta(x^{(i)}) \text{ Does not depend on } z) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \qquad (\text{Bayes' Rule}) \\
&= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \qquad (\text{Multiply by constant}) \\
&= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \qquad (\text{Logarithms}) \\
&= \boxed{\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\boxed{\geq 0}}
\end{aligned}
$$

We want to maximize the data likelihood

Tractable lower bound which we can take gradient of and optimize! ($p_\theta(x|z)$ differentiable, KL term differentiable)

Variational Autoencoders

Now equipped with our encoder and decoder networks, let's work out the (log) data likelihood:

$$\log p_\theta(x^{(i)}) = \mathbf{E}_{z \sim q_\phi(z|x^{(i)})}\left[\log p_\theta(x^{(i)})\right] \quad (p_\theta(x^{(i)}) \text{ Does not depend on } z)$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Bayes' Rule)}$$

$$= \mathbf{E}_z\left[\log \frac{p_\theta(x^{(i)} \mid z)p_\theta(z)}{p_\theta(z \mid x^{(i)})} \frac{q_\phi(z \mid x^{(i)})}{q_\phi(z \mid x^{(i)})}\right] \quad \text{(Multiply by constant)}$$

$$= \mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z)}\right] + \mathbf{E}_z\left[\log \frac{q_\phi(z \mid x^{(i)})}{p_\theta(z \mid x^{(i)})}\right] \quad \text{(Logarithms)}$$

$$= \underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)}, \theta, \phi)} + \underbrace{D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z \mid x^{(i)}))}_{\geq 0}$$

Reconstruct the input data

Make approximate posterior distribution close to prior

$$\boxed{\log p_\theta(x^{(i)}) \geq \mathcal{L}(x^{(i)}, \theta, \phi)}$$

Variational lower bound ("ELBO")

$$\boxed{\theta^*, \phi^* = \arg\max_{\theta,\phi} \sum_{i=1}^{N} \mathcal{L}(x^{(i)}, \theta, \phi)}$$

Training: Maximize lower bound

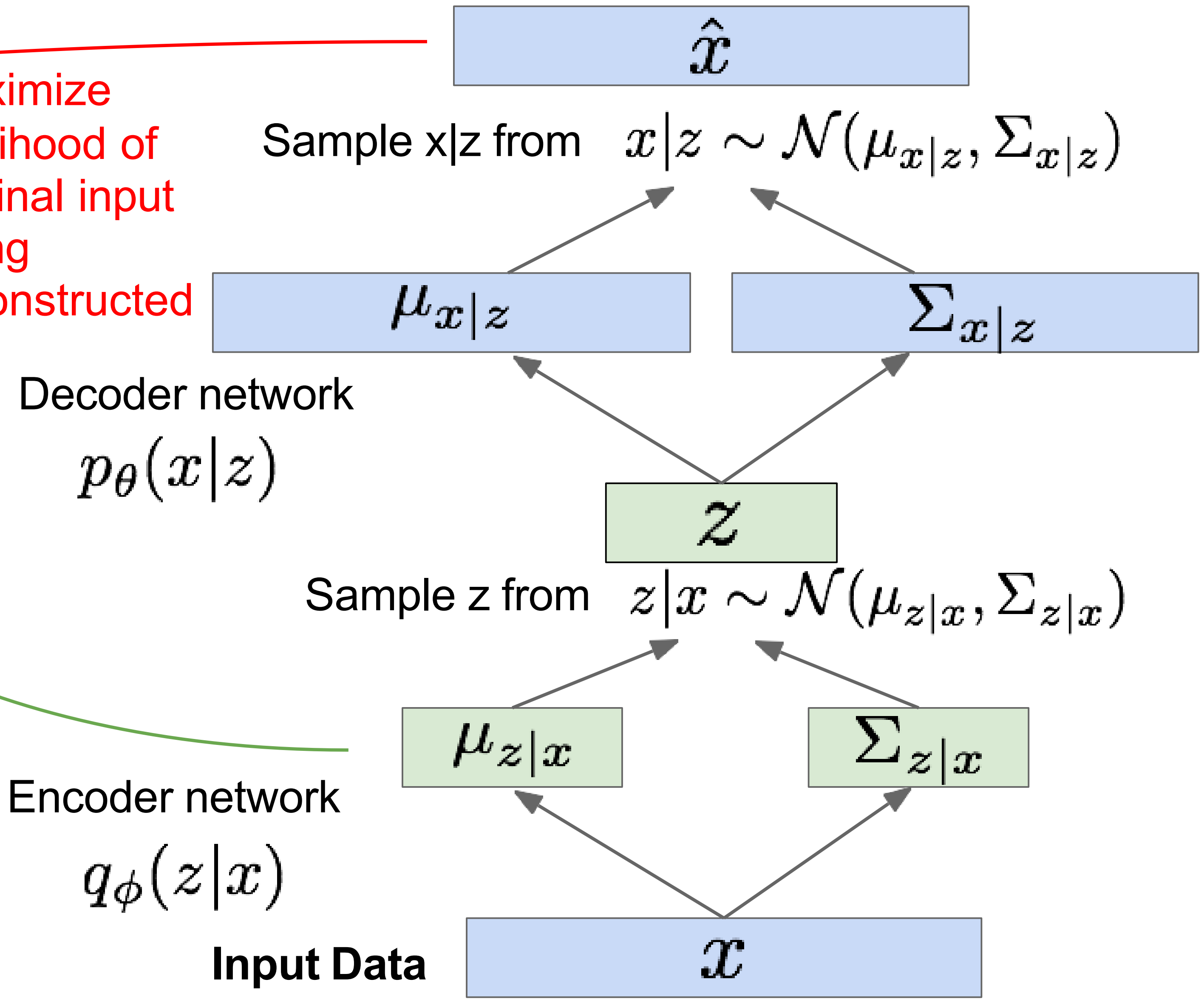
Variational Autoencoders

Putting it all together: maximizing the likelihood lower bound

$$\underbrace{\mathbf{E}_z\left[\log p_\theta(x^{(i)} \mid z)\right] - D_{KL}(q_\phi(z \mid x^{(i)}) \,||\, p_\theta(z))}_{\mathcal{L}(x^{(i)},\theta,\phi)}$$

Maximize likelihood of original input being reconstructed

Make approximate posterior distribution close to prior

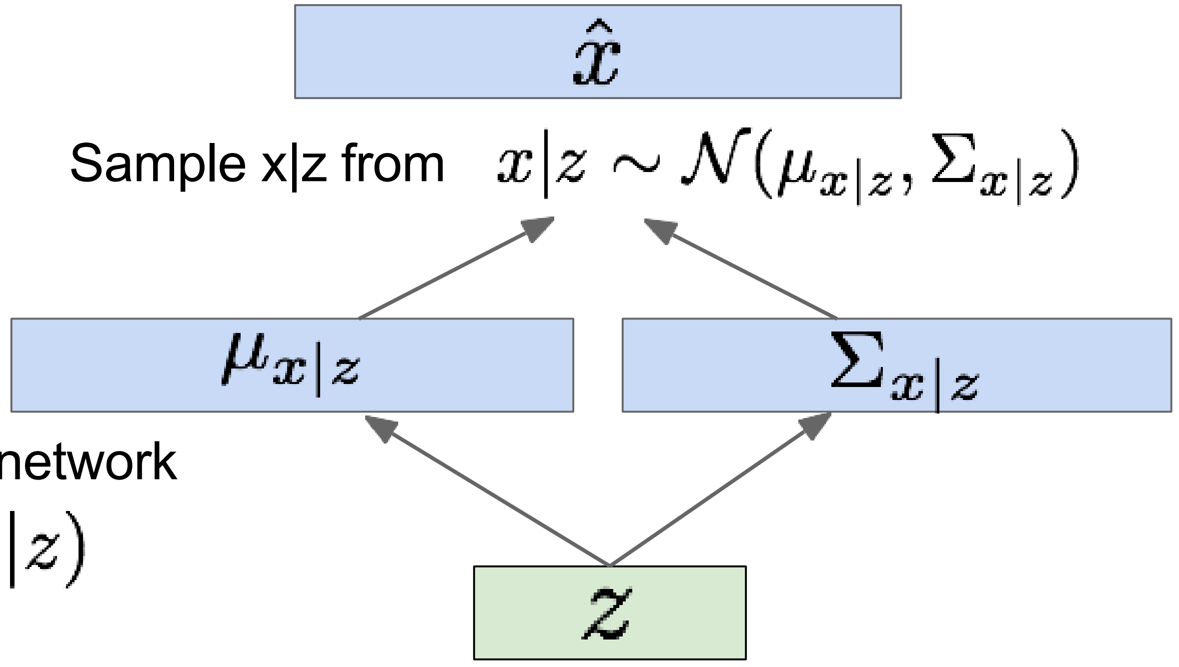


For every minibatch of input data: compute this forward pass, and then backprop!

Slides: Fei-Fei Li, Justin Johnson, Serena Yeung

Variational Autoencoders: Generating Data!

Use decoder network. Now sample z from prior!



Sample x|z from $x|z \sim \mathcal{N}(\mu_{x|z}, \Sigma_{x|z})$

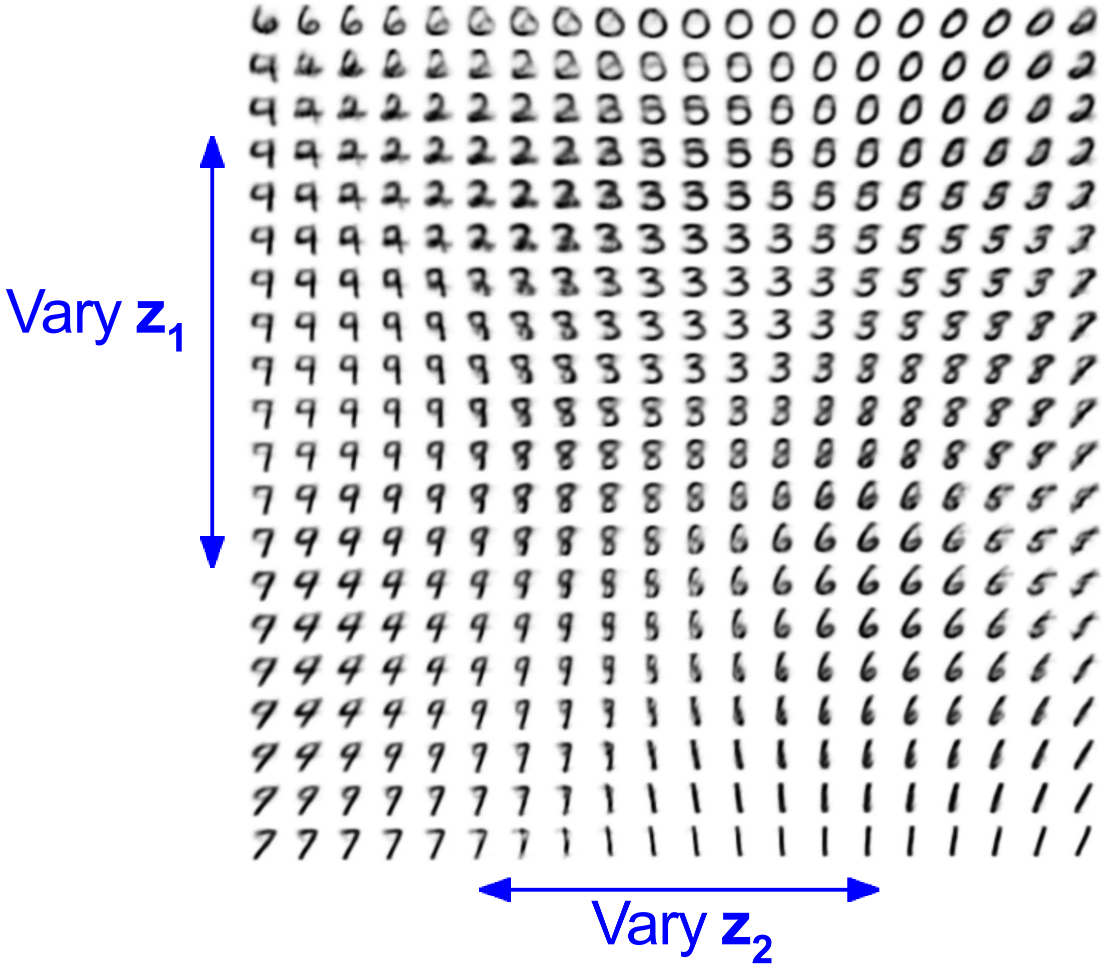
Decoder network

$p_\theta(x|z)$

Sample z from $z \sim \mathcal{N}(0, I)$

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Data manifold for 2-d **z**



Variational Autoencoders: Generating Data!

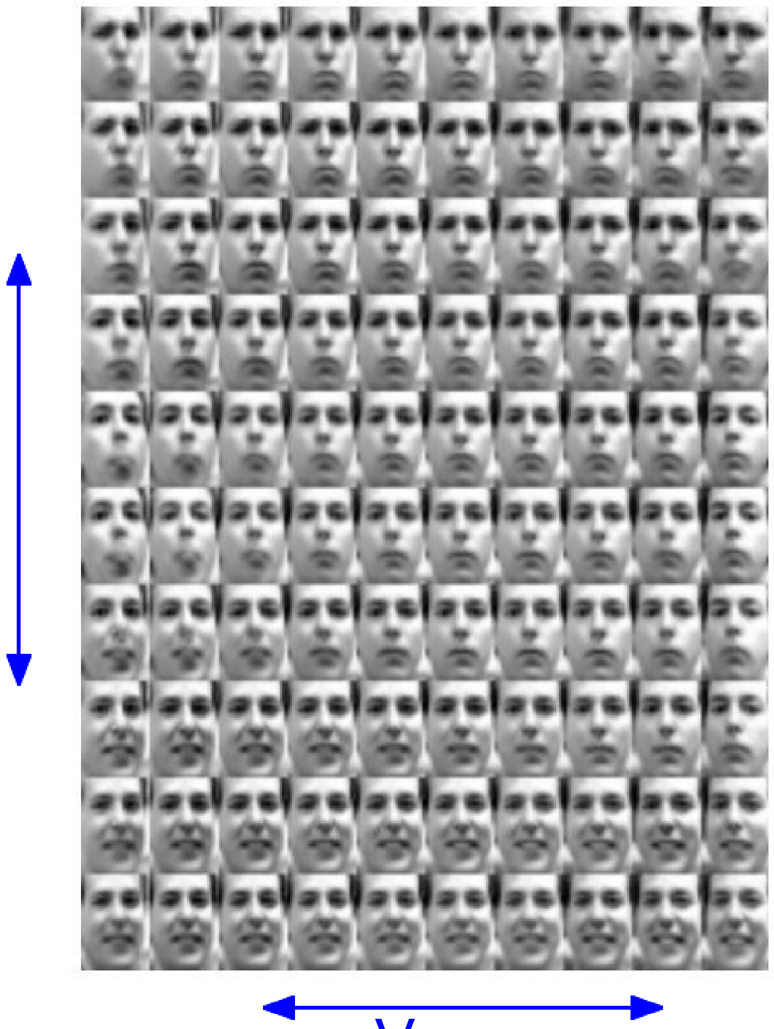
Diagonal prior on **z** => independent latent variables

Different dimensions of **z** encode interpretable factors of variation

Also good feature representation that can be computed using $q_\phi(z|x)$!

Degree of smile

Vary $\mathbf{z}_1$

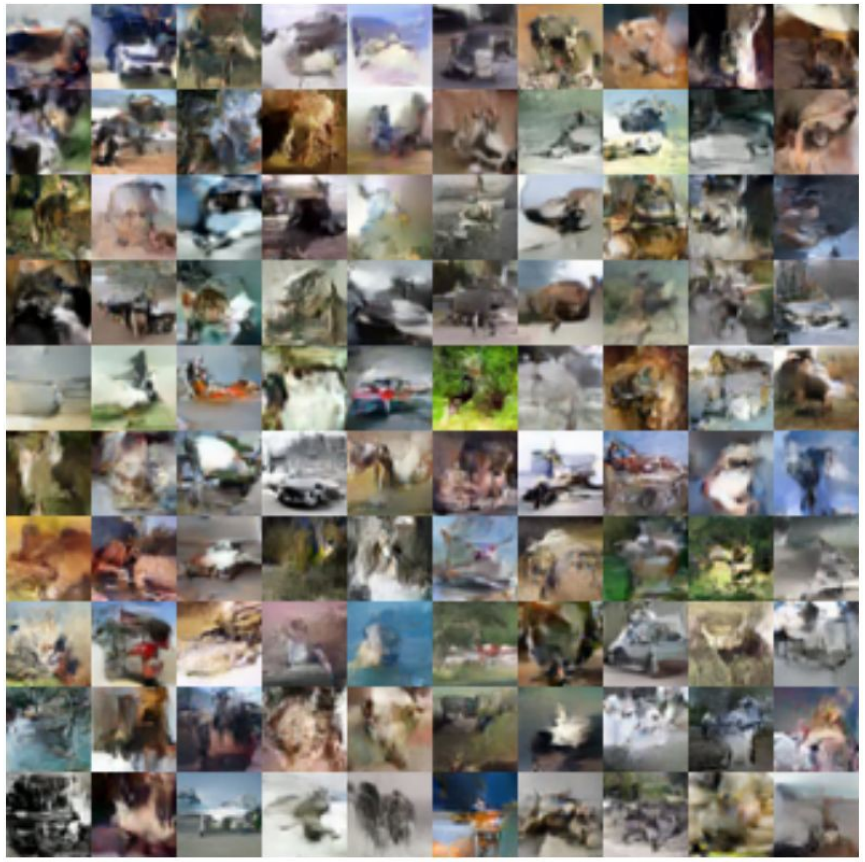


Vary $\mathbf{z}_2$

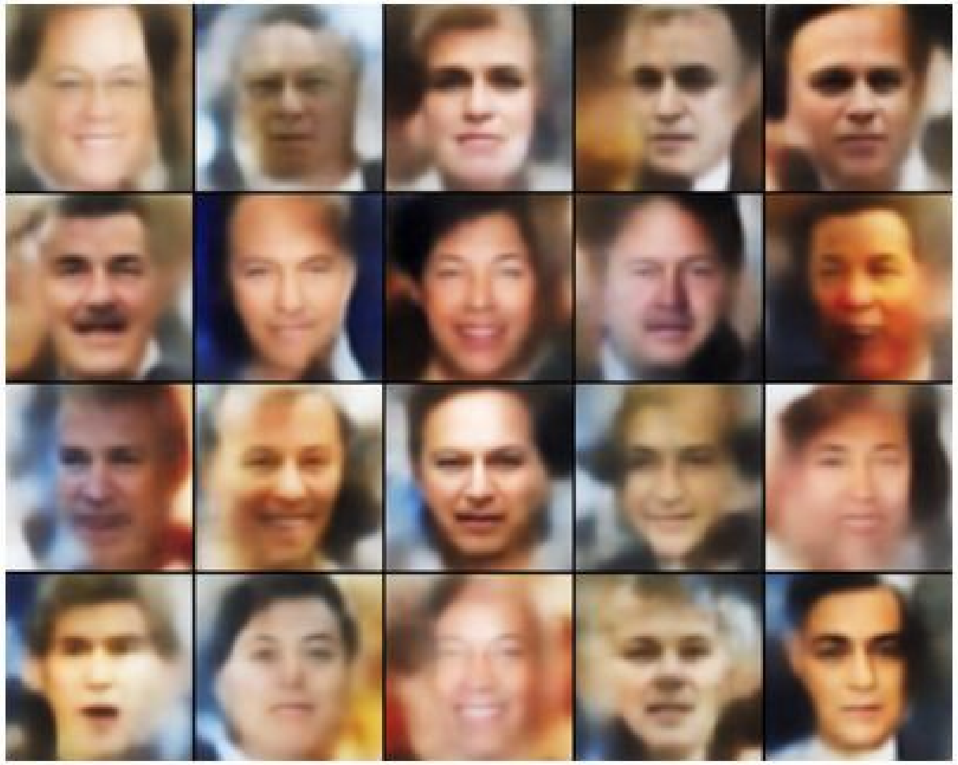
Head pose

Kingma and Welling, “Auto-Encoding Variational Bayes”, ICLR 2014

Variational Autoencoders: Generating Data!



32x32 CIFAR-10



Labeled Faces in the Wild

Figures copyright (L) Dirk Kingma et al. 2016; (R) Anders Larsen et al. 2017. Reproduced with permission.

Variational Autoencoders

Probabilistic spin to traditional autoencoders => allows generating data
Defines an intractable density => derive and optimize a (variational) lower bound

Pros:

- Principled approach to generative models
- Allows inference of q(z|x), can be useful feature representation for other tasks

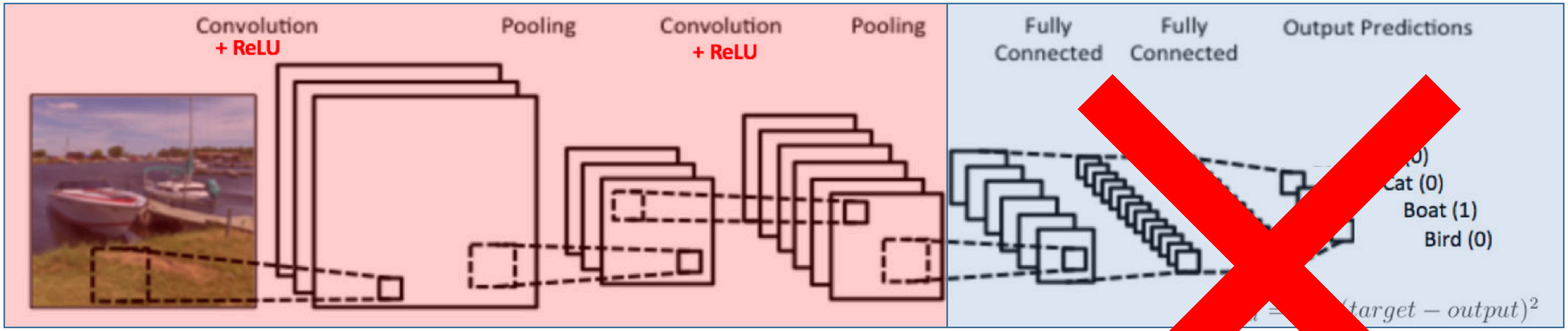
Cons:

- Maximizes lower bound of likelihood: okay, but not as good evaluation as PixelRNN/PixelCNN
- Samples blurrier and lower quality compared to state-of-the-art (GANs)

Active areas of research:

- More flexible approximations, e.g. richer approximate posterior instead of diagonal Gaussian, e.g., Gaussian Mixture Models (GMMs)
- Incorporating structure in latent variables, e.g., Categorical Distributions

Representation learning **without annotations**?



x *data*

‘Modern’ Deep learning:
Hierarchical Representation Learning
Feature extraction

z *Latent space representation*

‘Classic’ Fully-connected Neural Networks
Classification

y *label*

Many ideas are possible (and yours could be even better!):

1. Predict the future: RNNs, Video
2. Compression: Autoencoder (predict self, through clamp), representation **z**
3. Pretext tasks: predict self, before/after, missing patch, correct rotation, colorization, up-sampling, multimodal
4. Capture parameter distribution (variance): Variational Auto-Encoders
5. Make latent space parameters z meaningful, orthogonal, explicit, tuneable
6. Train using a second network: GANs - Improve quality of output images
7. The Sky is the Limit

GANs:
Generative Adversarial Networks

Generative Adversarial Networks

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

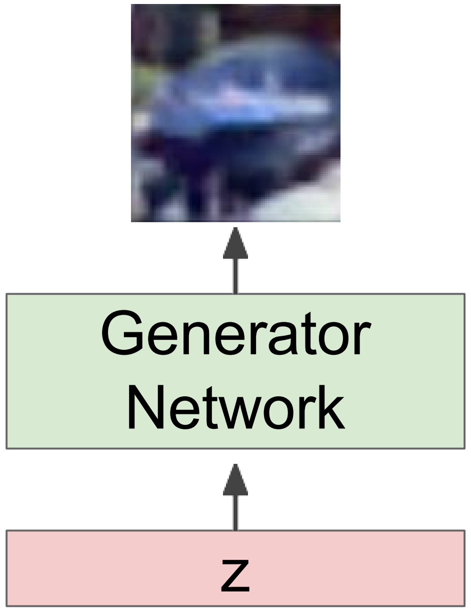
Problem: Want to sample from complex, high-dimensional training distribution. No direct way to do this!

Solution: Sample from a simple distribution, e.g. random noise. Learn transformation to training distribution.

Q: What can we use to represent this complex transformation?

A: A neural network!

Output: Sample from training distribution

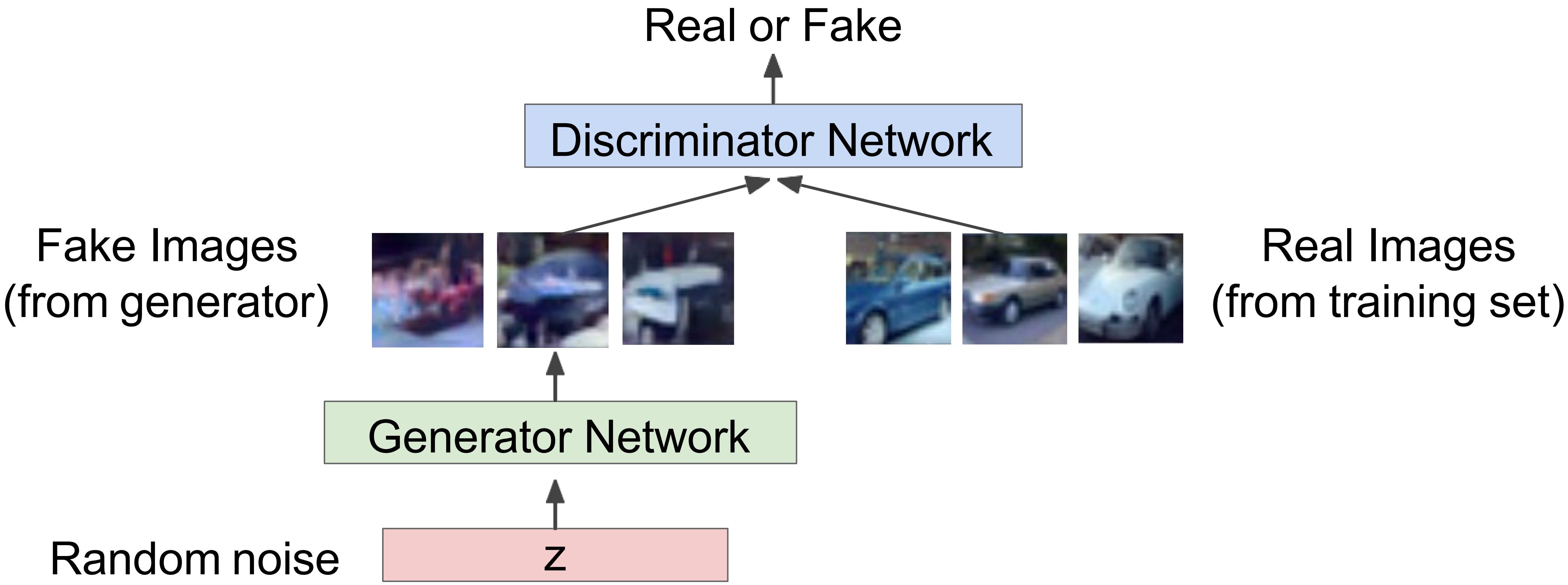


Input: Random noise

Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images



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Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images

Train jointly in **minimax game**

Minimax objective function:

Discriminator outputs likelihood in (0,1) of real image

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log \underbrace{D_{\theta_d}(x)}_{\substack{\text{Discriminator output} \\ \text{for real data x}}} + \mathbb{E}_{z \sim p(z)} \log(1 - \underbrace{D_{\theta_d}(G_{\theta_g}(z))}_{\substack{\text{Discriminator output for} \\ \text{generated fake data G(z)}}}) \right]$$

- Discriminator (θ_d) wants to **maximize objective** such that D(x) is close to 1 (real) and D(G(z)) is close to 0 (fake)
- Generator (θ_g) wants to **minimize objective** such that D(G(z)) is close to 1 (discriminator is fooled into thinking generated G(z) is real)

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

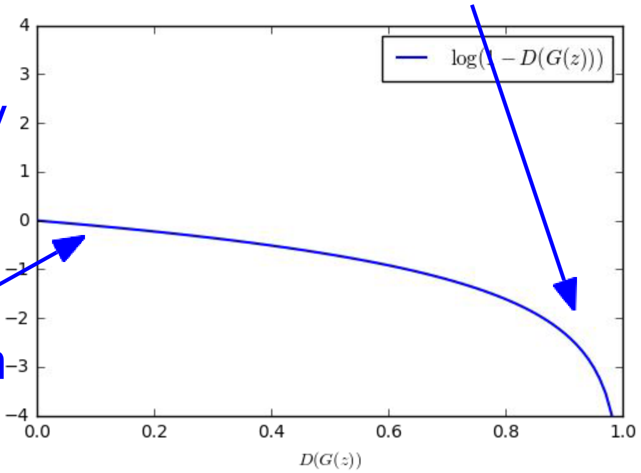
1. **Gradient ascent** on discriminator

$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Gradient descent** on generator

$$\min_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z)))$$

In practice, optimizing this generator objective does not work well!



Gradient signal dominated by region where sample is already good

When sample is likely fake, want to learn from it to improve generator. But gradient in this region is relatively flat!

Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Minimax objective function:

$$\min_{\theta_g} \max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

Alternate between:

1. **Gradient ascent** on discriminator

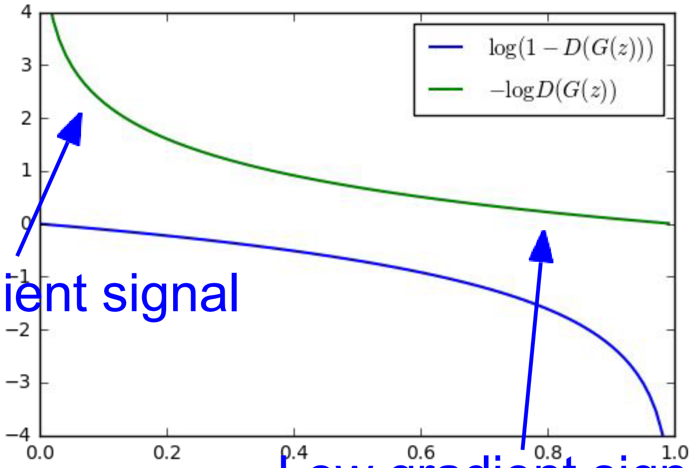
$$\max_{\theta_d} \left[\mathbb{E}_{x \sim p_{data}} \log D_{\theta_d}(x) + \mathbb{E}_{z \sim p(z)} \log(1 - D_{\theta_d}(G_{\theta_g}(z))) \right]$$

2. **Instead: Gradient ascent** on generator, different objective

$$\max_{\theta_g} \mathbb{E}_{z \sim p(z)} \log(D_{\theta_d}(G_{\theta_g}(z)))$$

Instead of minimizing likelihood of discriminator being correct, now maximize likelihood of discriminator being wrong.
Same objective of fooling discriminator, but now higher gradient signal for bad samples => works much better! Standard in practice.

Aside: Jointly training two networks is challenging, can be unstable. Choosing objectives with better loss landscapes helps training, is an active area of research.



High gradient signal

Low gradient signal

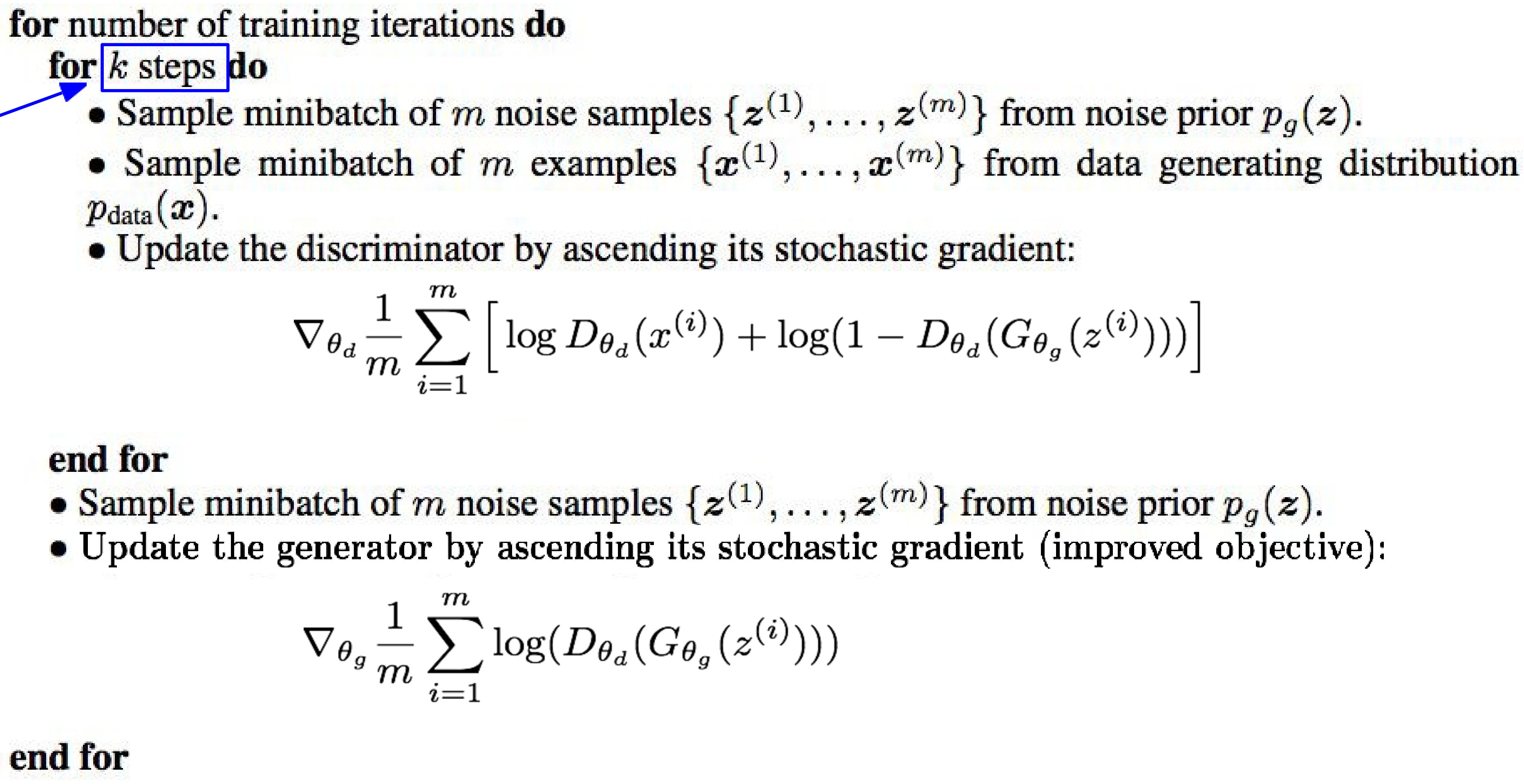
Training GANs: Two-player game

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Putting it together: GAN training algorithm

Some find k=1 more stable, others use k > 1, no best rule.

Recent work (e.g. Wasserstein GAN) alleviates this problem, better stability!

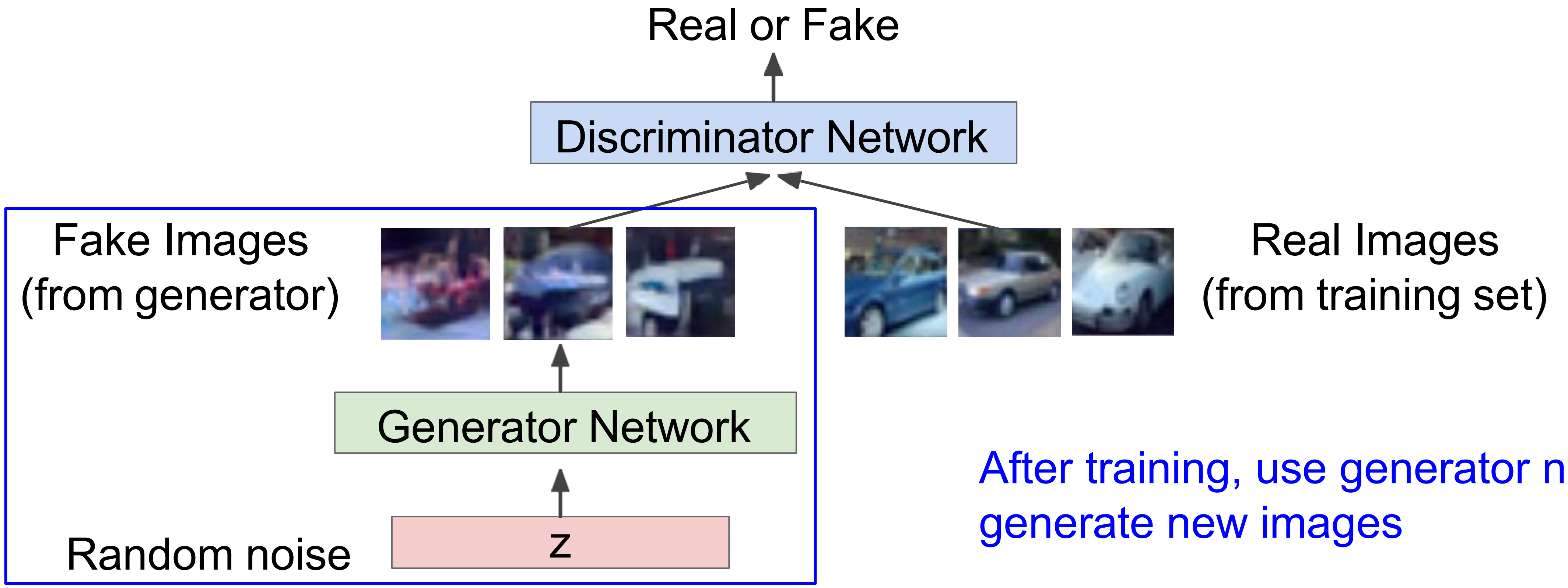


```
for number of training iterations do
    for $\boxed{k \text{ steps}}$ do
        • Sample minibatch of $m$ noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
        • Sample minibatch of $m$ examples $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ from data generating distribution $p_{\text{data}}(\boldsymbol{x})$.
        • Update the discriminator by ascending its stochastic gradient:
            $\nabla_{\theta_d} \frac{1}{m} \sum_{i=1}^{m} \left[ \log D_{\theta_d}(x^{(i)}) + \log(1 - D_{\theta_d}(G_{\theta_g}(z^{(i)}))) \right]$
    end for
    • Sample minibatch of $m$ noise samples $\{\boldsymbol{z}^{(1)}, \dots, \boldsymbol{z}^{(m)}\}$ from noise prior $p_g(\boldsymbol{z})$.
    • Update the generator by ascending its stochastic gradient (improved objective):
        $\nabla_{\theta_g} \frac{1}{m} \sum_{i=1}^{m} \log(D_{\theta_d}(G_{\theta_g}(z^{(i)})))$
end for
```

Training GANs: Two-player game

Ian Goodfellow et al., "Generative Adversarial Nets", NIPS 2014

Generator network: try to fool the discriminator by generating real-looking images
Discriminator network: try to distinguish between real and fake images



After training, use generator network to generate new images

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Mean Squared Error Can Ignore Small but Task-Relevant Features

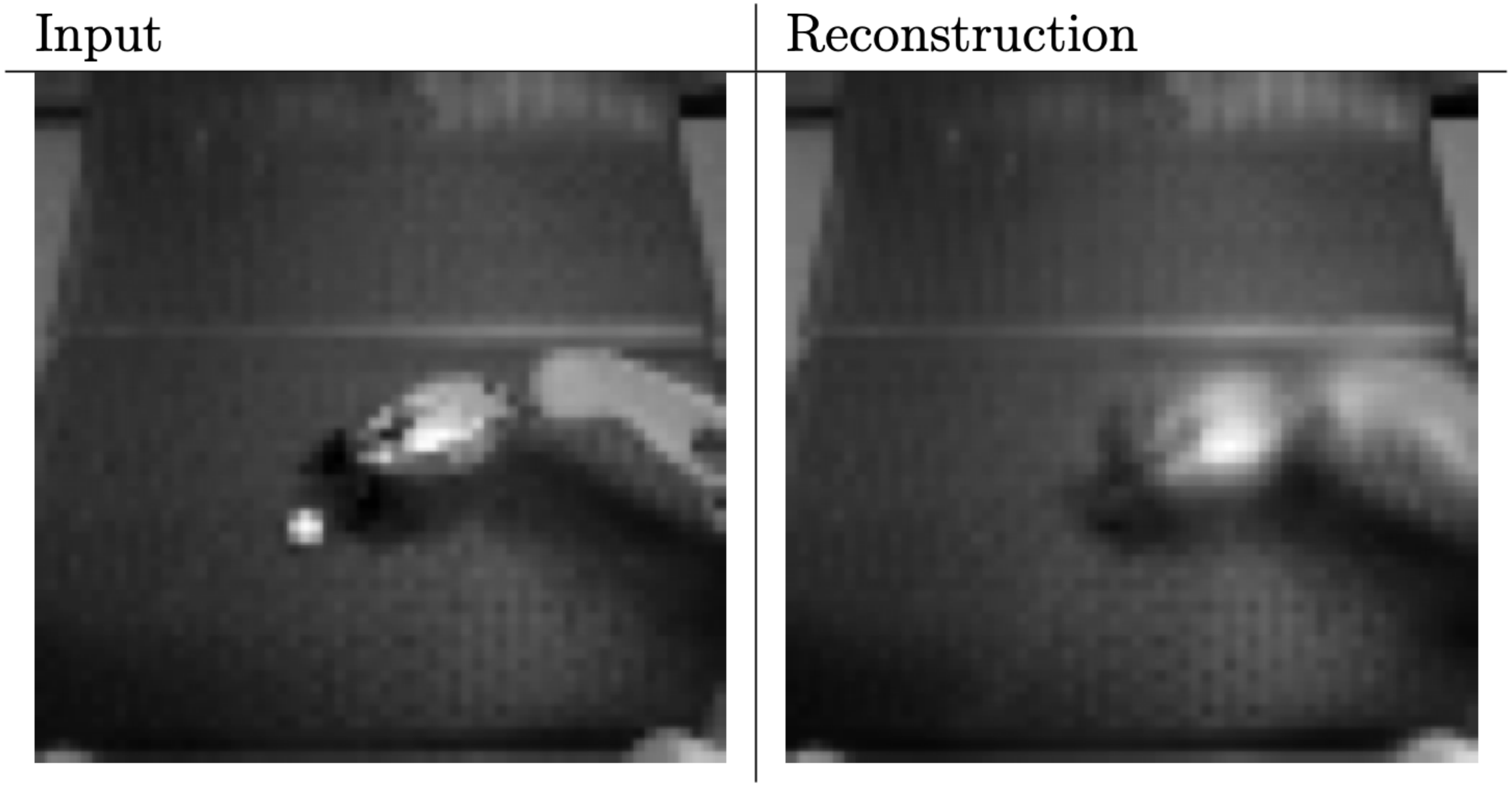


Figure 15.5

The ping pong ball vanishes because it is not large enough to significantly affect the mean squared error

Slide Credit: Ian Goodfellow

(Goodfellow 2017)

Adversarial Losses Preserve Any Features with Highly Structured Patterns

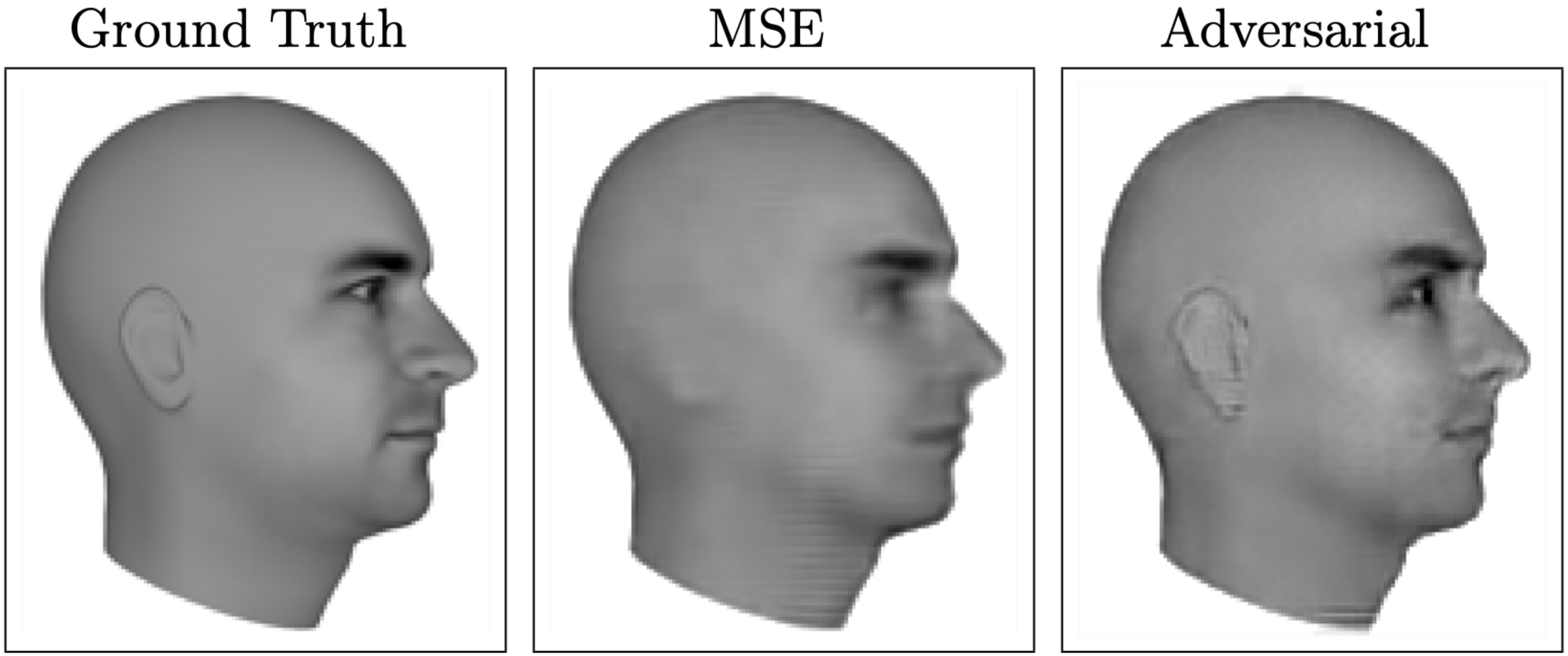


Figure 15.6

Mean squared error loses the ear because it causes a small change in few pixels. Adversarial loss preserves the ear because it is easy to notice its absence.

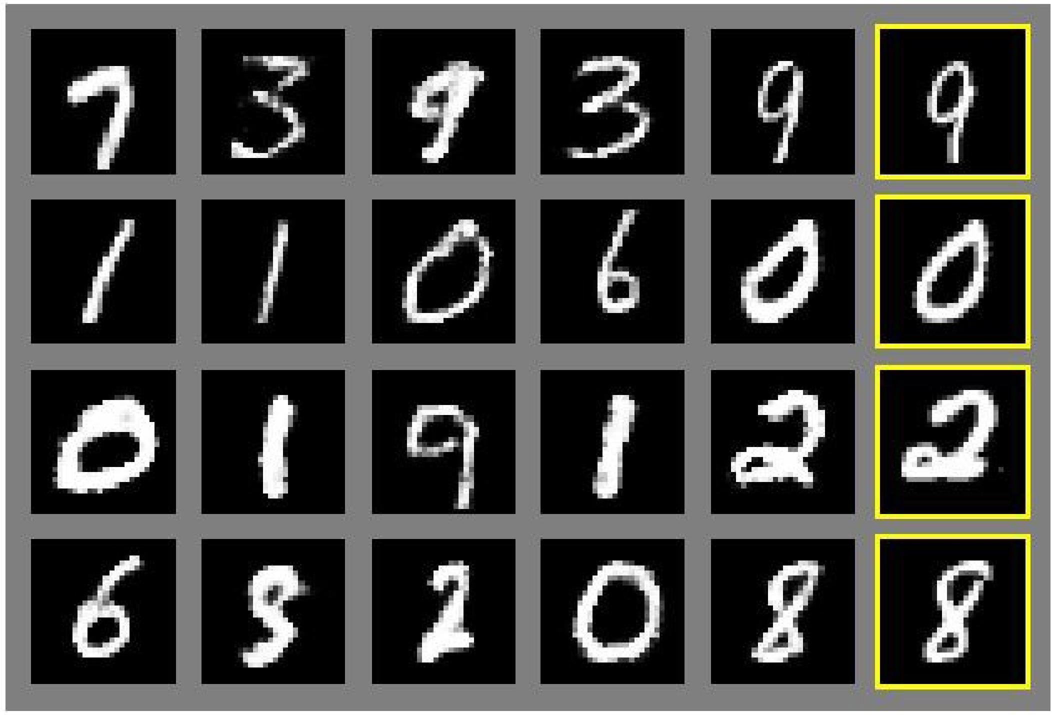
Slide Credit: Ian Goodfellow

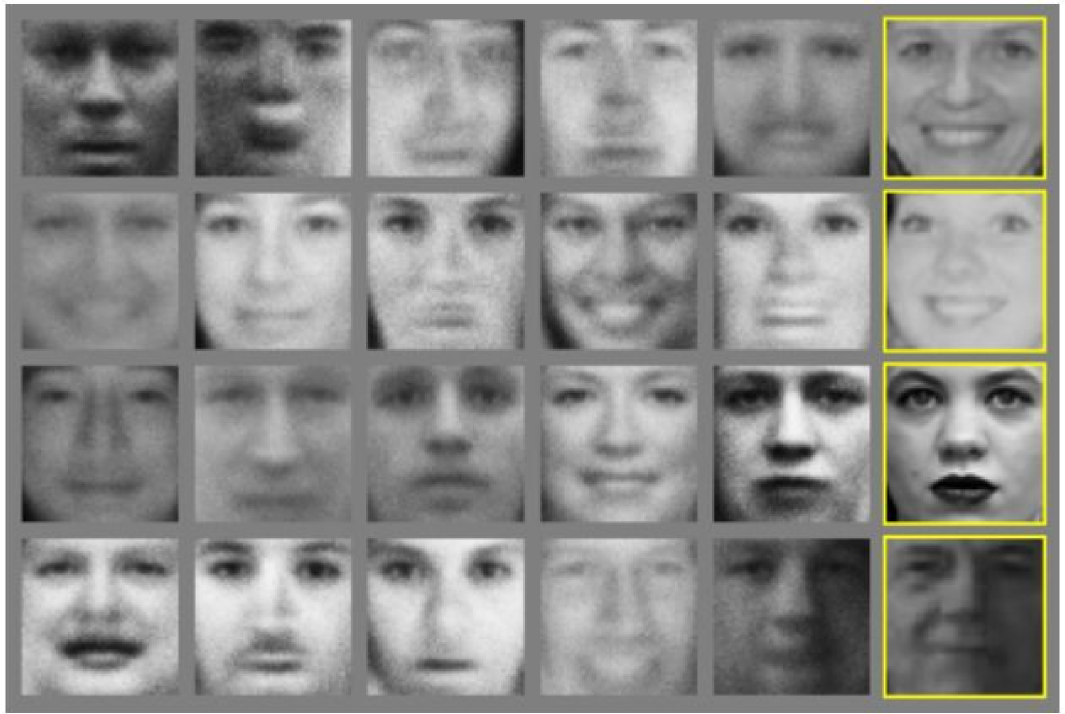
(Goodfellow 2017)

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generative Adversarial Nets

Generated samples





Nearest neighbor from training set

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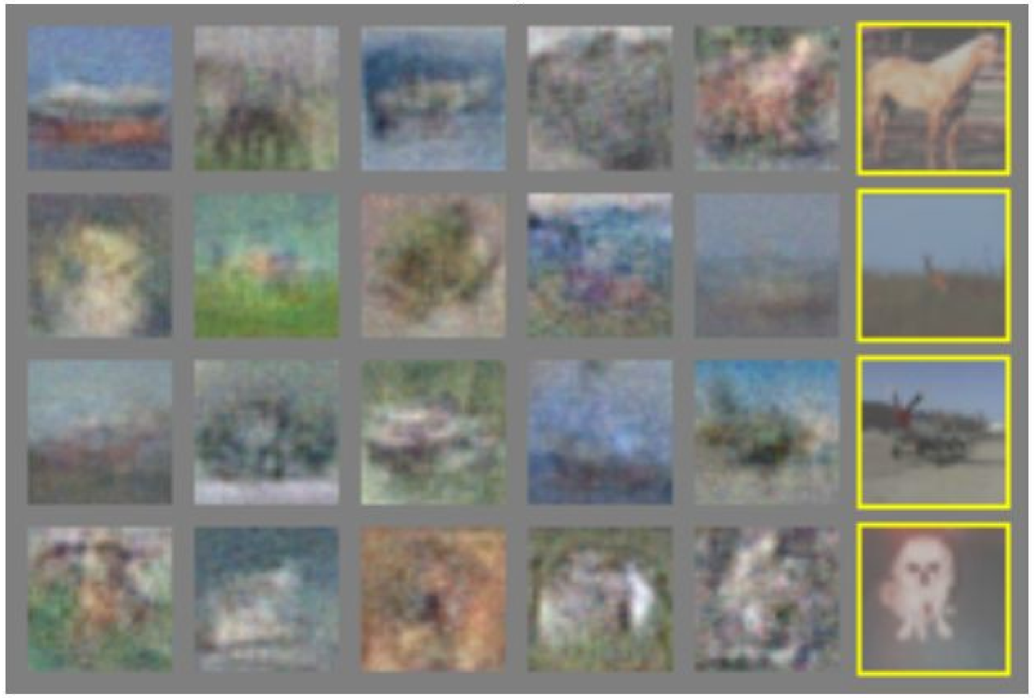
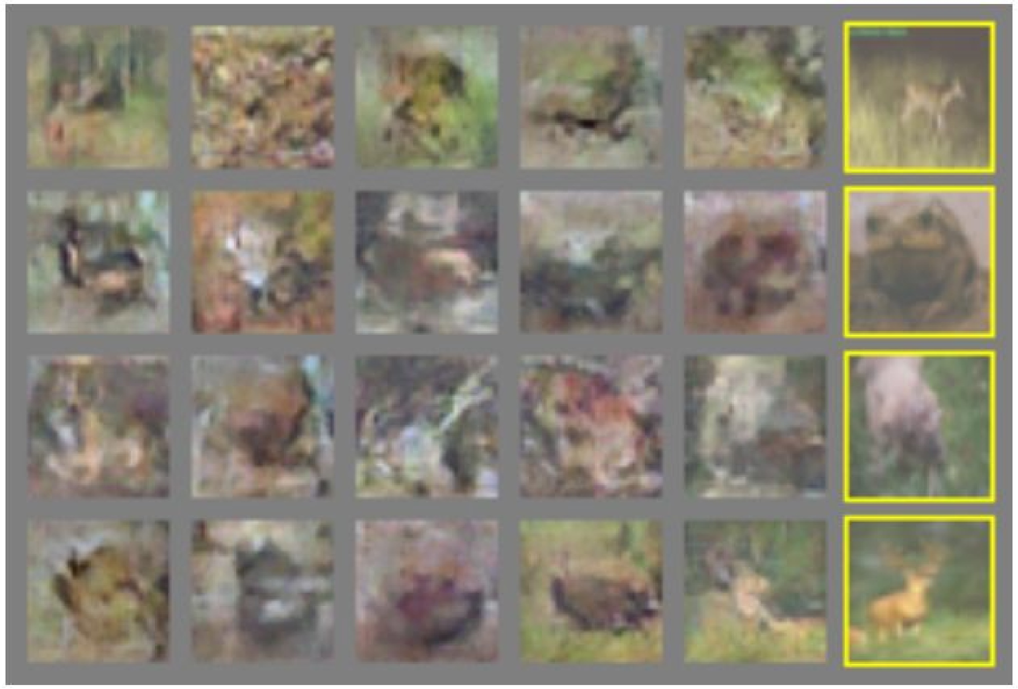
Generative Adversarial Nets

Ian Goodfellow et al., “Generative Adversarial Nets”, NIPS 2014

Generated samples (CIFAR-10)





Nearest neighbor from training set

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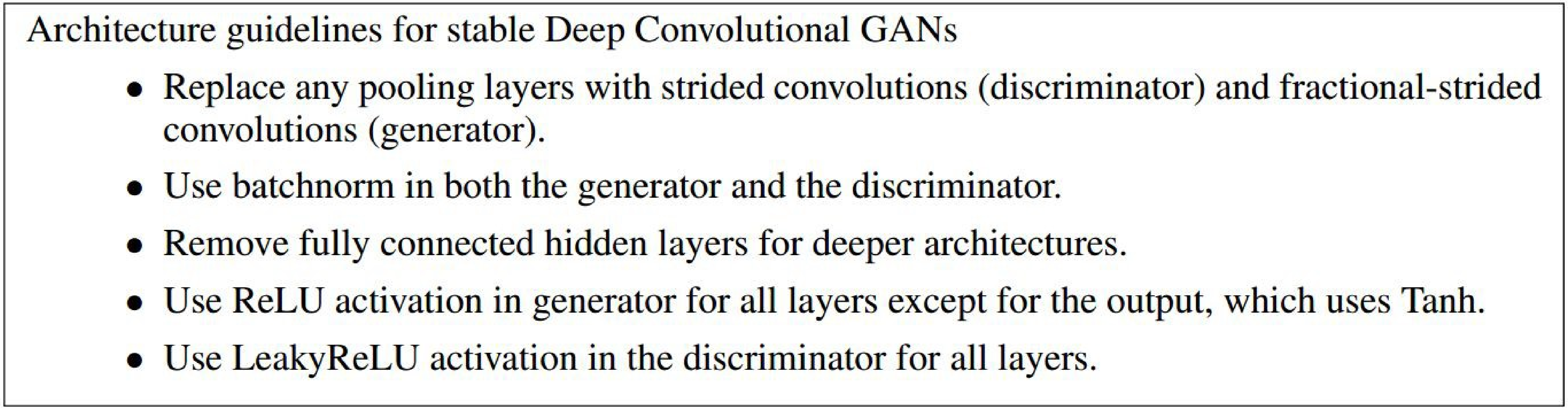
GANs + CNNs: Convolutional Architectures for Generative Adversarial Networks

Generative Adversarial Nets: Convolutional Architectures

Generator is an upsampling network with fractionally-strided convolutions
Discriminator is a convolutional network

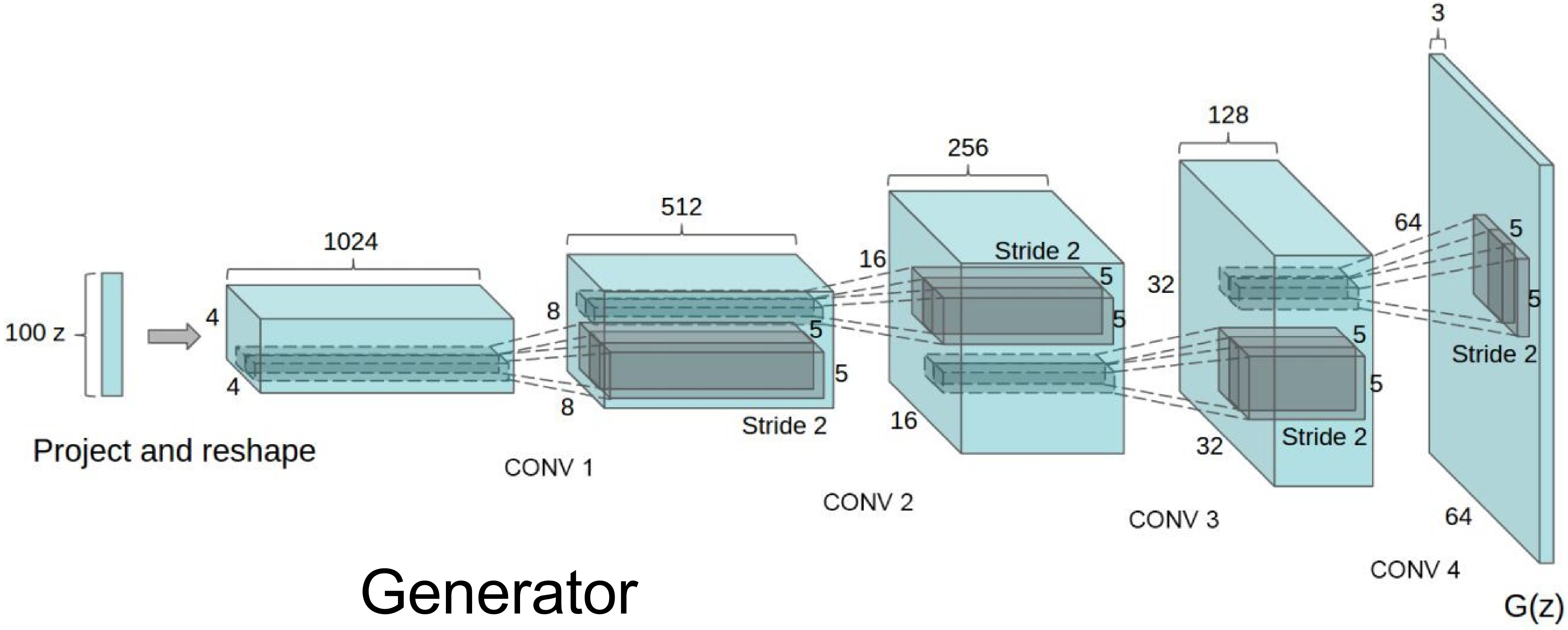


Architecture guidelines for stable Deep Convolutional GANs

- Replace any pooling layers with strided convolutions (discriminator) and fractional-strided convolutions (generator).
- Use batchnorm in both the generator and the discriminator.
- Remove fully connected hidden layers for deeper architectures.
- Use ReLU activation in generator for all layers except for the output, which uses Tanh.
- Use LeakyReLU activation in the discriminator for all layers.

Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

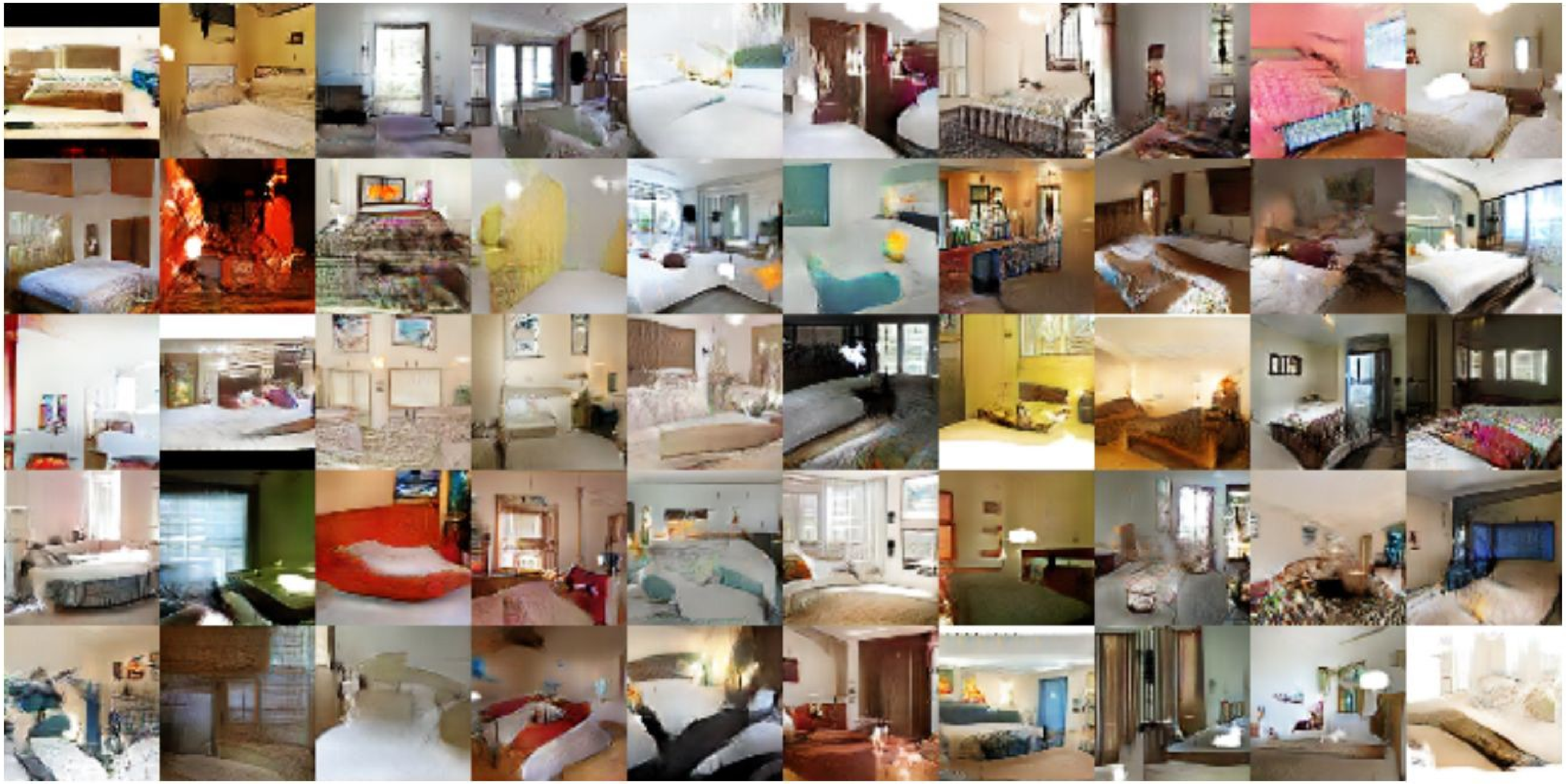


Generator

Radford et al, “Unsupervised Representation Learning with Deep Convolutional Generative Adversarial Networks”, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

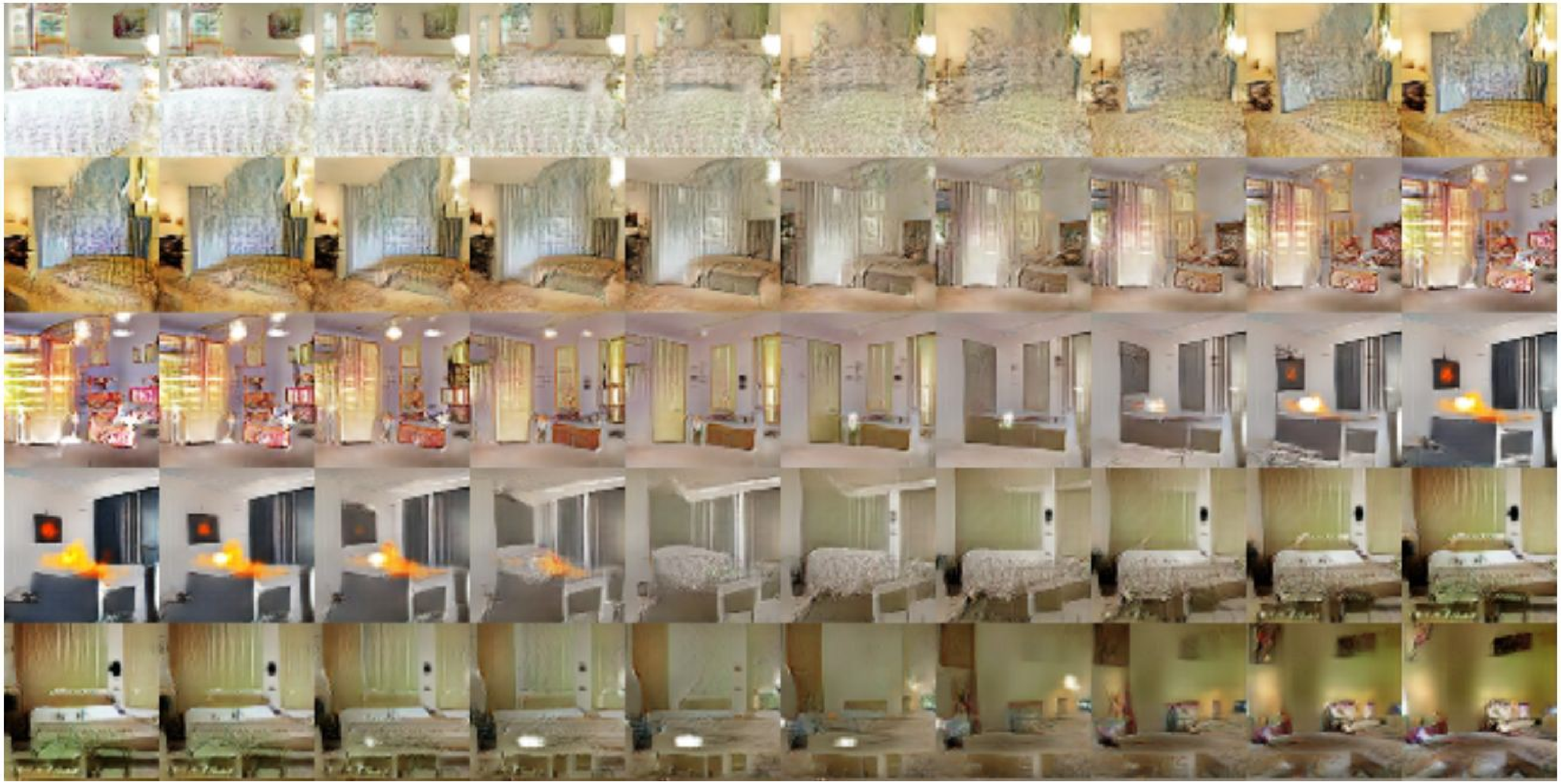
Samples from the model look much better!



Radford et al, ICLR 2016

Generative Adversarial Nets: Convolutional Architectures

Interpolating between random points in laten space



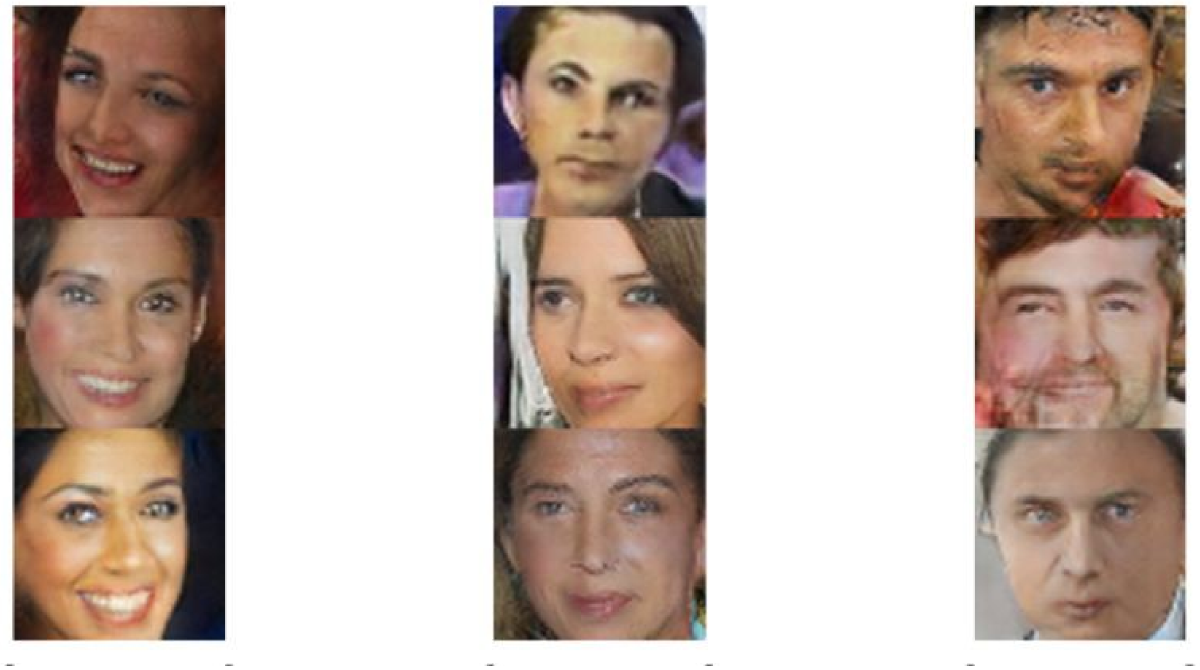
Radford et al, ICLR 2016

Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016

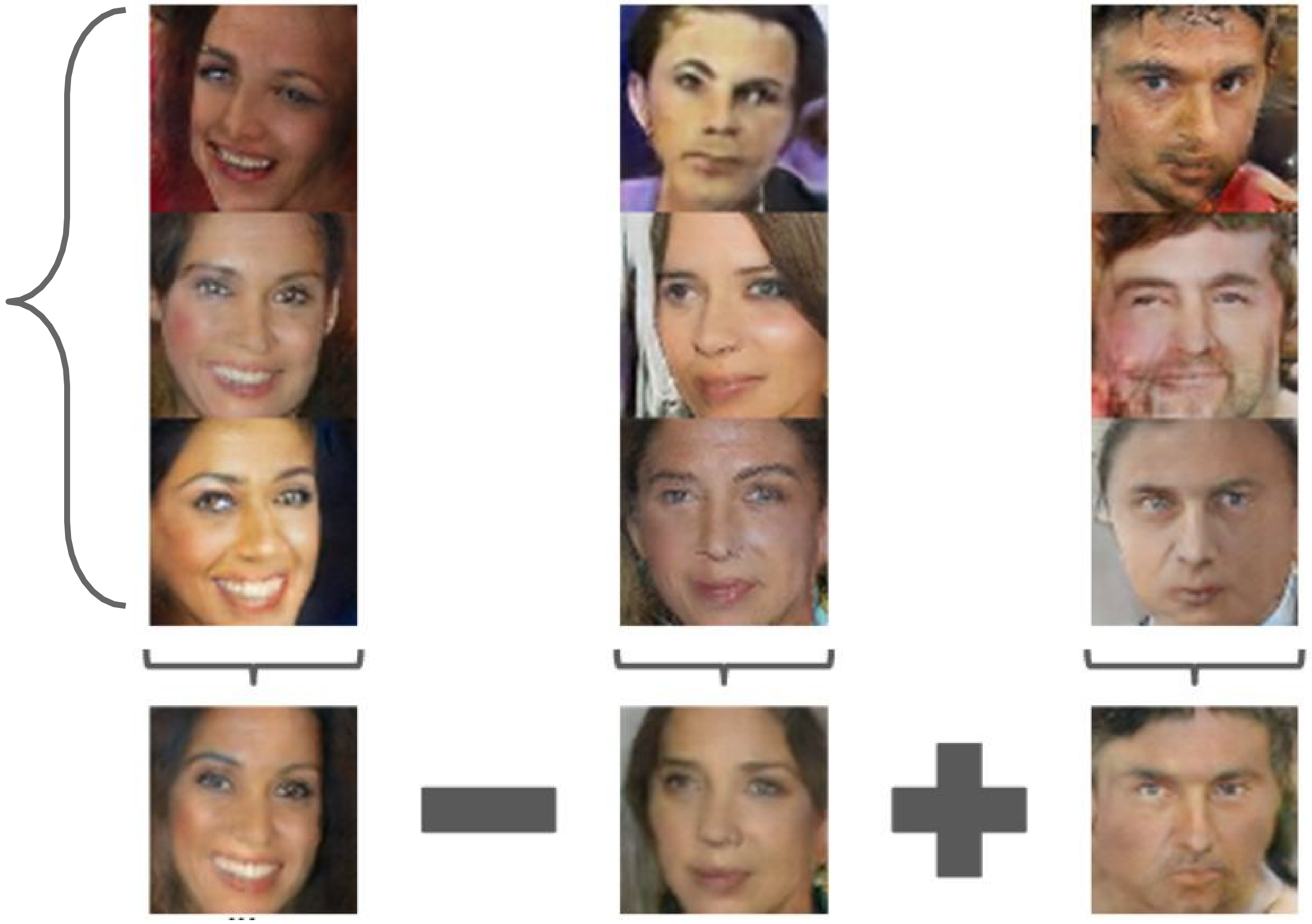
Smiling woman Neutral woman Neutral man

Samples from the model



Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016



Smiling woman Neutral woman Neutral man

Samples from the model

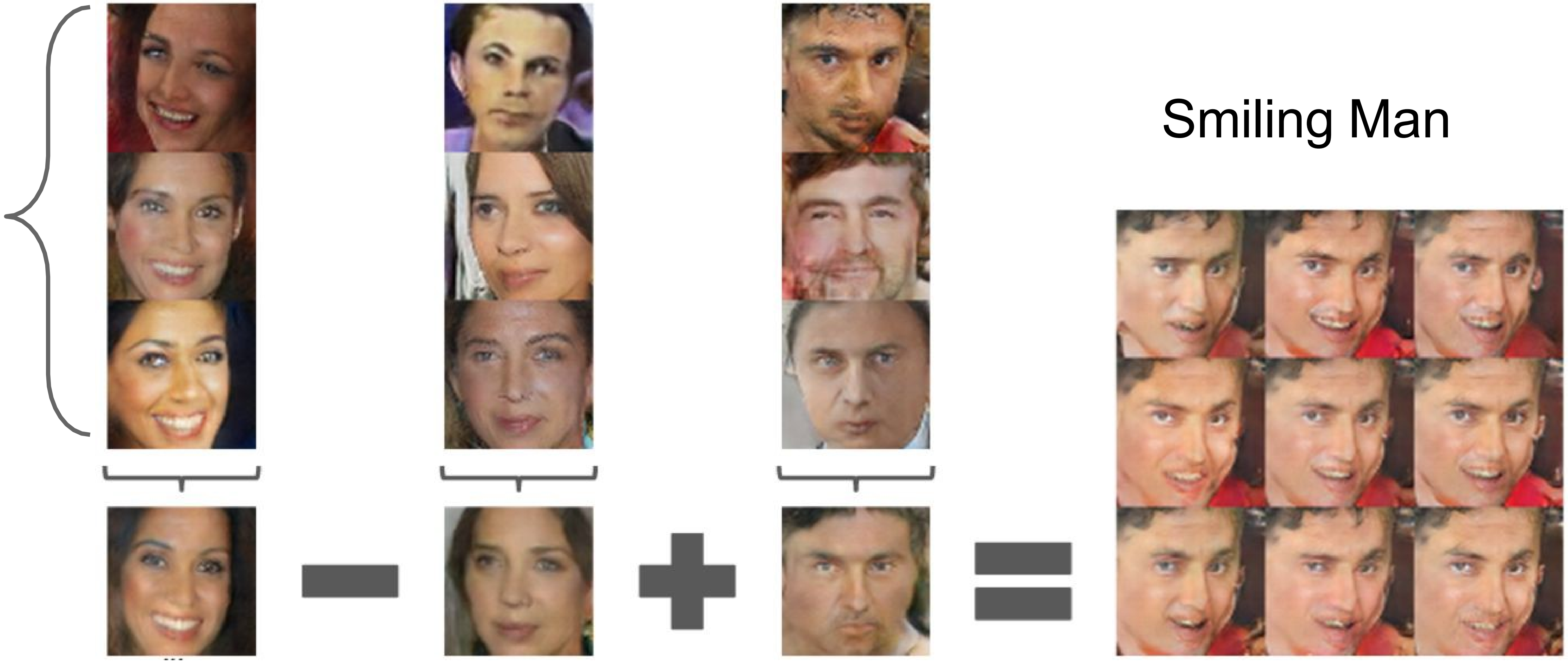
Average Z vectors, do arithmetic

Generative Adversarial Nets: Interpretable Vector Math

Radford et al, ICLR 2016

Smiling woman   Neutral woman   Neutral man

Samples from the model

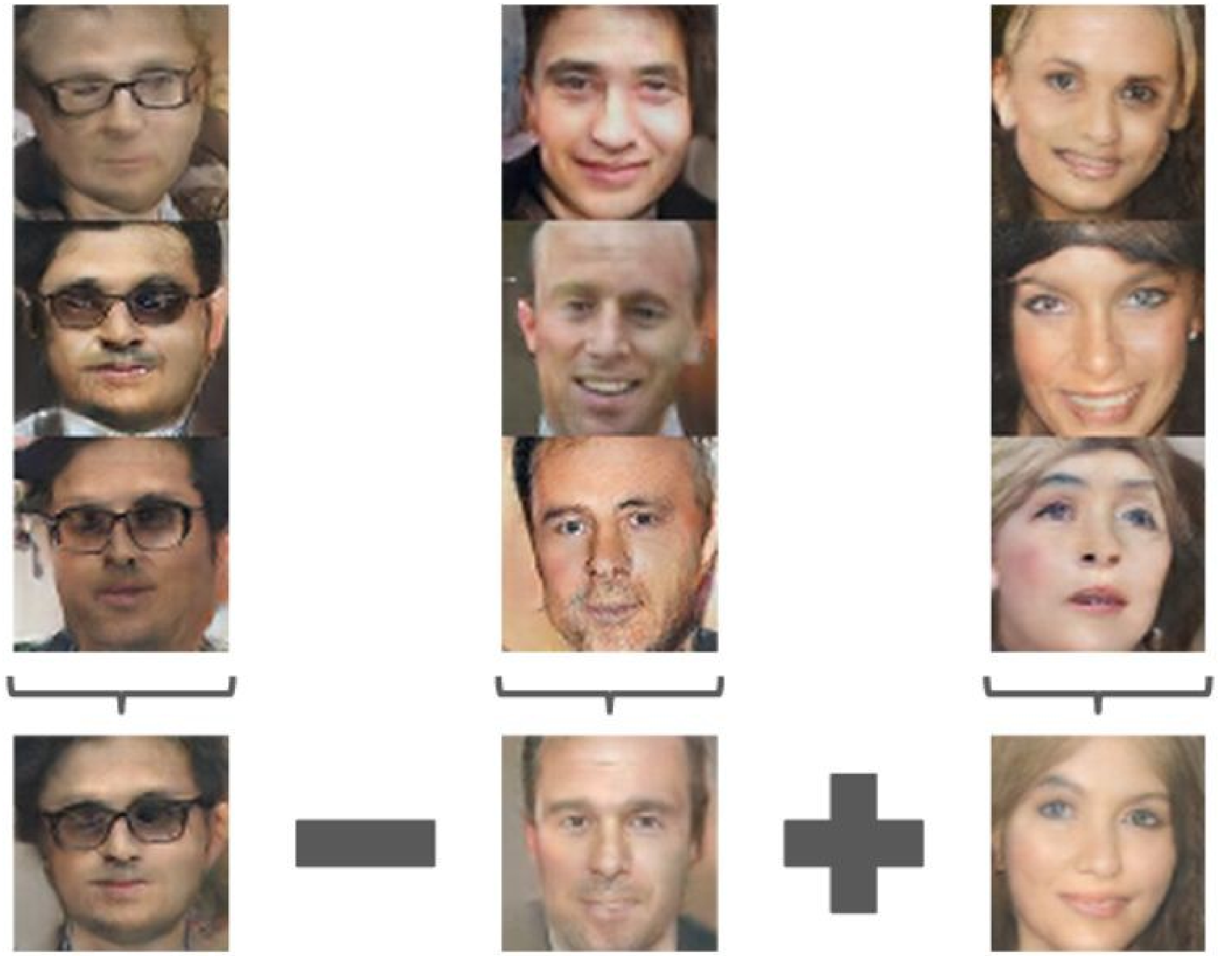


Smiling Man

Average Z vectors, do arithmetic

Generative Adversarial Nets: Interpretable Vector Math

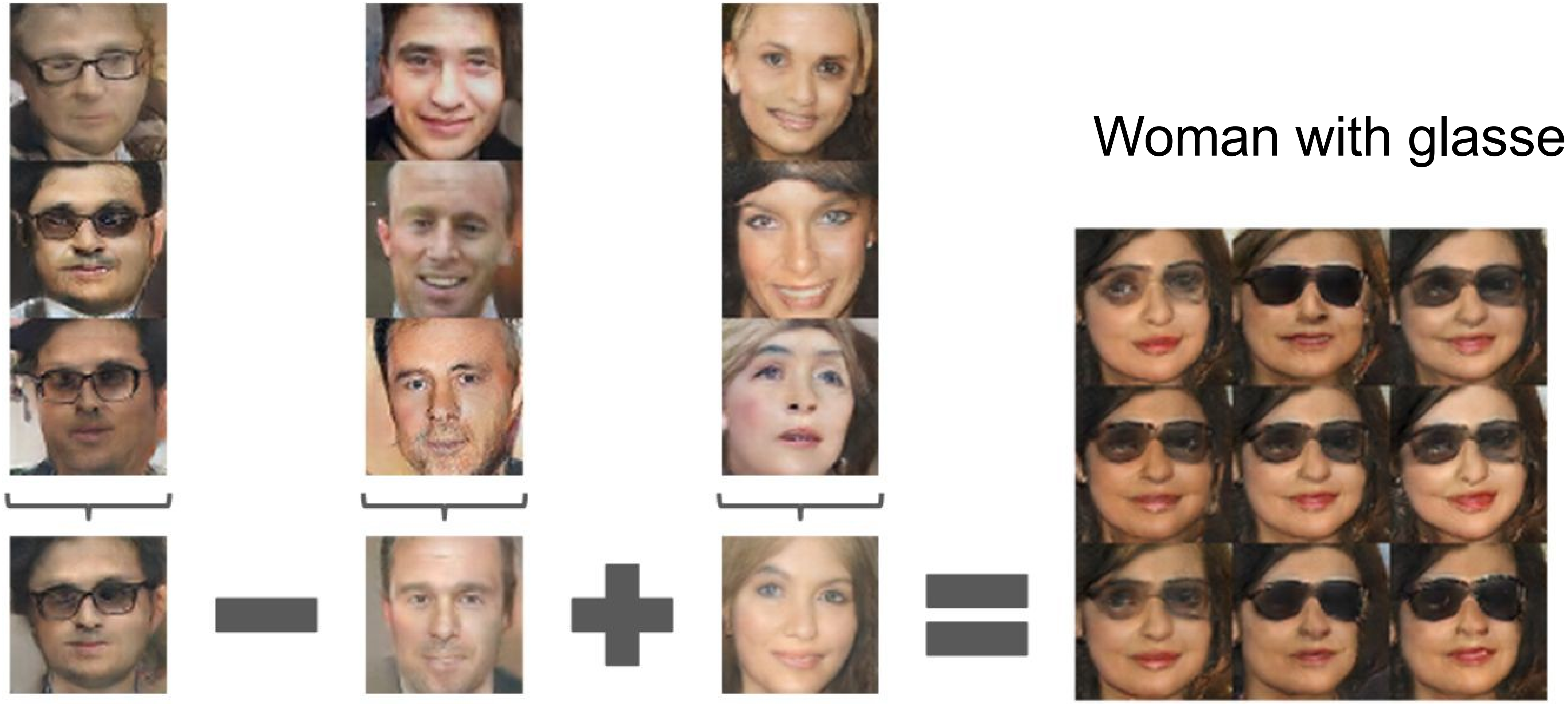
Glasses man No glasses man No glasses woman



Radford et al,
ICLR 2016

Generative Adversarial Nets: Interpretable Vector Math

Radford et al,
ICLR 2016



Glasses man

No glasses man

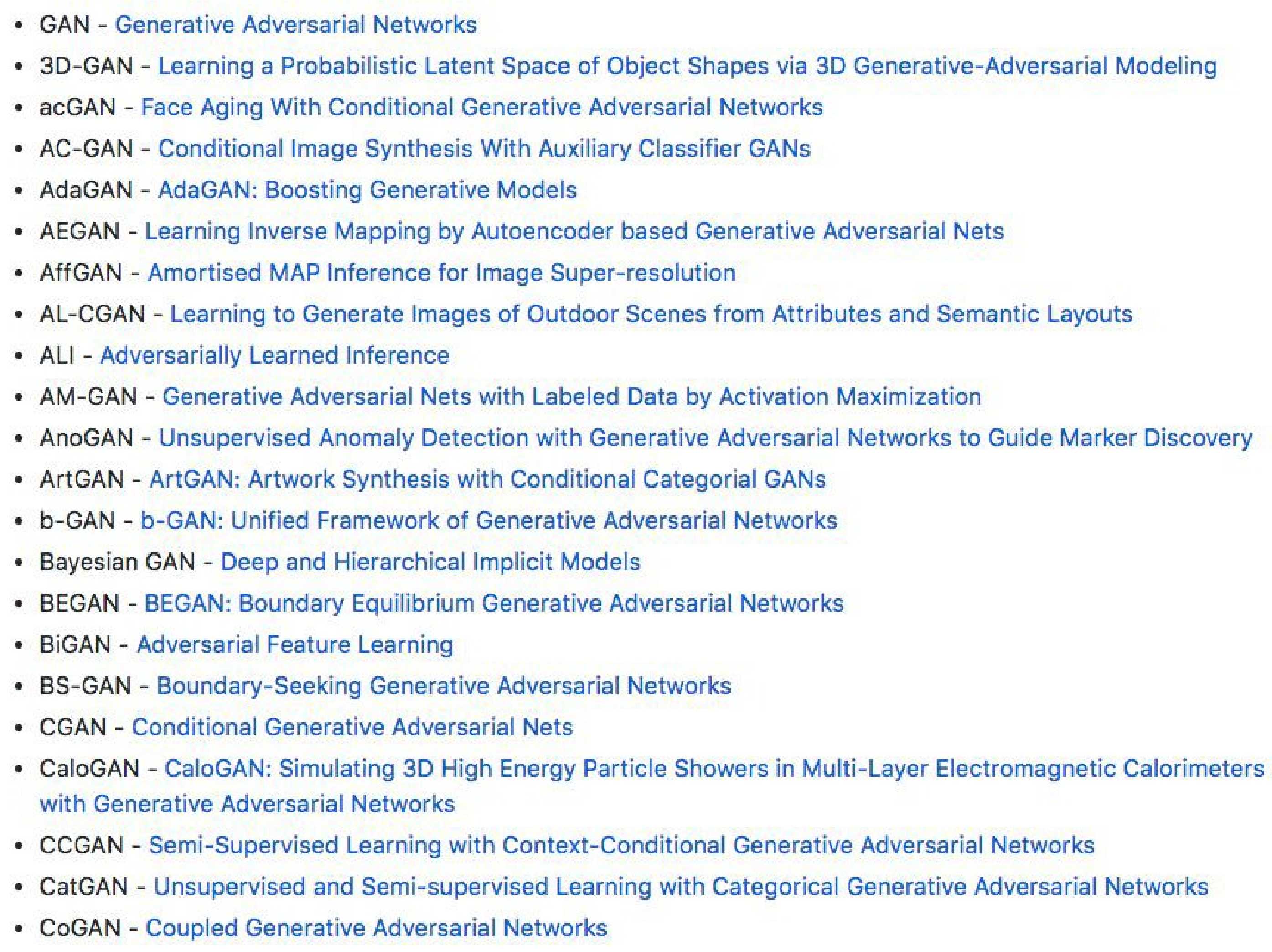
No glasses woman

Woman with glasses

Next-Generation GANs

2017: Explosion of GANs

“The GAN Zoo”



- GAN - Generative Adversarial Networks
- 3D-GAN - Learning a Probabilistic Latent Space of Object Shapes via 3D Generative-Adversarial Modeling
- acGAN - Face Aging With Conditional Generative Adversarial Networks
- AC-GAN - Conditional Image Synthesis With Auxiliary Classifier GANs
- AdaGAN - AdaGAN: Boosting Generative Models
- AEGAN - Learning Inverse Mapping by Autoencoder based Generative Adversarial Nets
- AffGAN - Amortised MAP Inference for Image Super-resolution
- AL-CGAN - Learning to Generate Images of Outdoor Scenes from Attributes and Semantic Layouts
- ALI - Adversarially Learned Inference
- AM-GAN - Generative Adversarial Nets with Labeled Data by Activation Maximization
- AnoGAN - Unsupervised Anomaly Detection with Generative Adversarial Networks to Guide Marker Discovery
- ArtGAN - ArtGAN: Artwork Synthesis with Conditional Categorial GANs
- b-GAN - b-GAN: Unified Framework of Generative Adversarial Networks
- Bayesian GAN - Deep and Hierarchical Implicit Models
- BEGAN - BEGAN: Boundary Equilibrium Generative Adversarial Networks
- BiGAN - Adversarial Feature Learning
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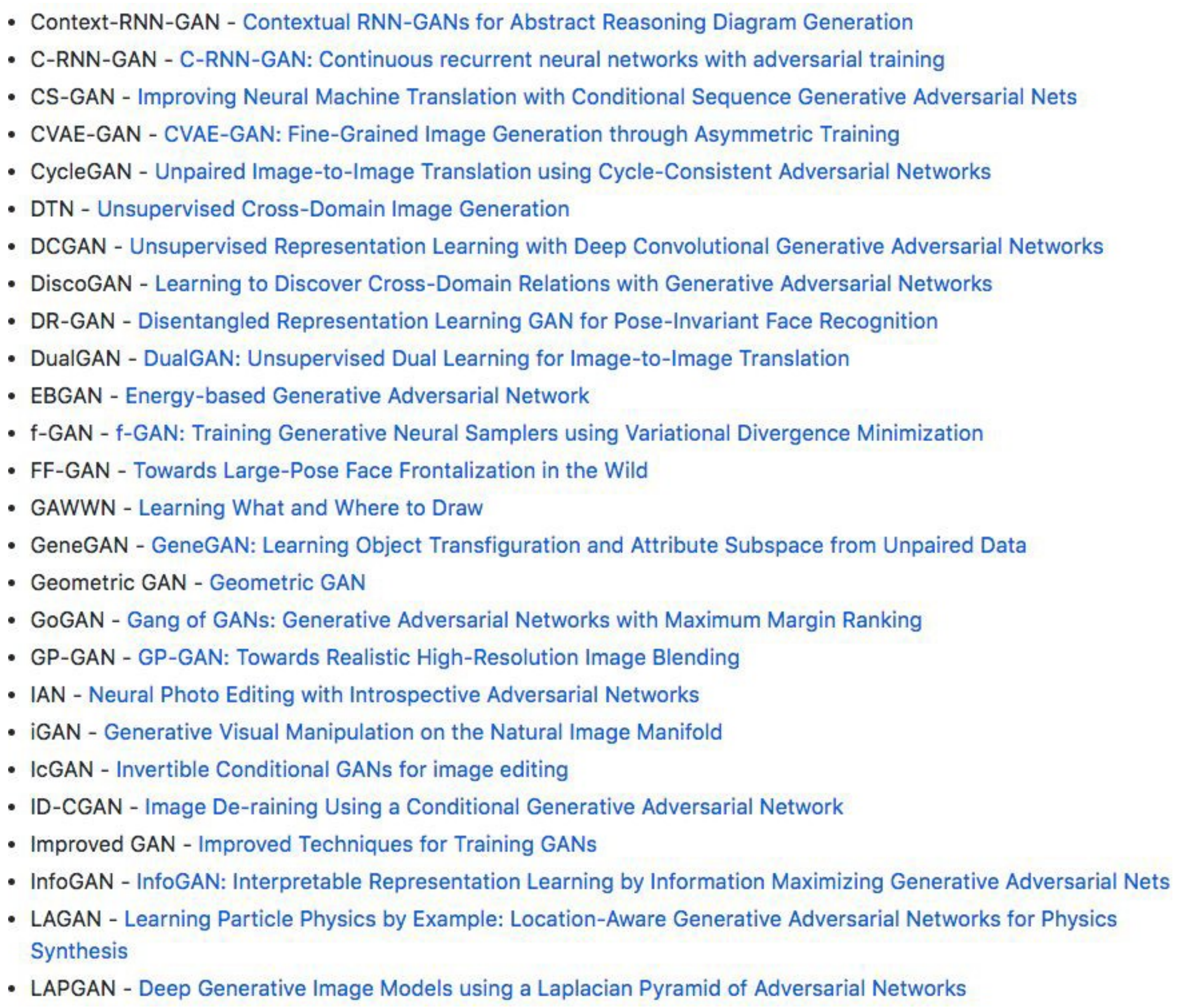
- CaloGAN - CaloGAN: Simulating 3D High Energy Particle Showers in Multi-Layer Electromagnetic Calorimeters with Generative Adversarial Networks
- CCGAN - Semi-Supervised Learning with Context-Conditional Generative Adversarial Networks
- CatGAN - Unsupervised and Semi-supervised Learning with Categorical Generative Adversarial Networks
- CoGAN - Coupled Generative Adversarial Networks



- Context-RNN-GAN - Contextual RNN-GANs for Abstract Reasoning Diagram Generation
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- CS-GAN - Improving Neural Machine Translation with Conditional Sequence Generative Adversarial Nets
- CVAE-GAN - CVAE-GAN: Fine-Grained Image Generation through Asymmetric Training
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- DTN - Unsupervised Cross-Domain Image Generation
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- DiscoGAN - Learning to Discover Cross-Domain Relations with Generative Adversarial Networks
- DR-GAN - Disentangled Representation Learning GAN for Pose-Invariant Face Recognition
- DualGAN - DualGAN: Unsupervised Dual Learning for Image-to-Image Translation
- EBGAN - Energy-based Generative Adversarial Network
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- FF-GAN - Towards Large-Pose Face Frontalization in the Wild
- GAWWN - Learning What and Where to Draw
- GeneGAN - GeneGAN: Learning Object Transfiguration and Attribute Subspace from Unpaired Data
- Geometric GAN - Geometric GAN
- GoGAN - Gang of GANs: Generative Adversarial Networks with Maximum Margin Ranking
- GP-GAN - GP-GAN: Towards Realistic High-Resolution Image Blending
- IAN - Neural Photo Editing with Introspective Adversarial Networks
- iGAN - Generative Visual Manipulation on the Natural Image Manifold
- IcGAN - Invertible Conditional GANs for image editing
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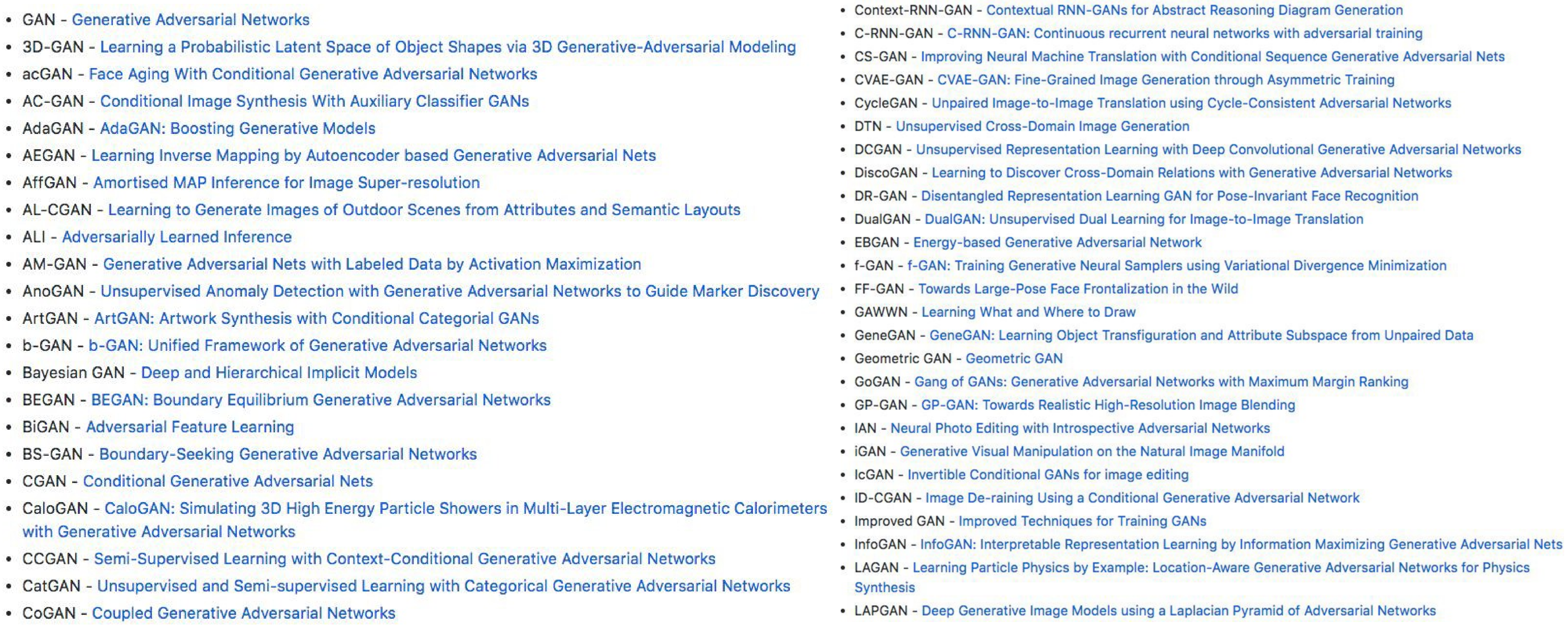
- InfoGAN - InfoGAN: Interpretable Representation Learning by Information Maximizing Generative Adversarial Nets
- LAGAN - Learning Particle Physics by Example: Location-Aware Generative Adversarial Networks for Physics Synthesis
- LAPGAN - Deep Generative Image Models using a Laplacian Pyramid of Adversarial Networks

https://github.com/hindupuravinash/the-gan-zoo

2017: Explosion of GANs

See also: https://github.com/soumith/ganhacks for tips and tricks for trainings GANs

“The GAN Zoo”



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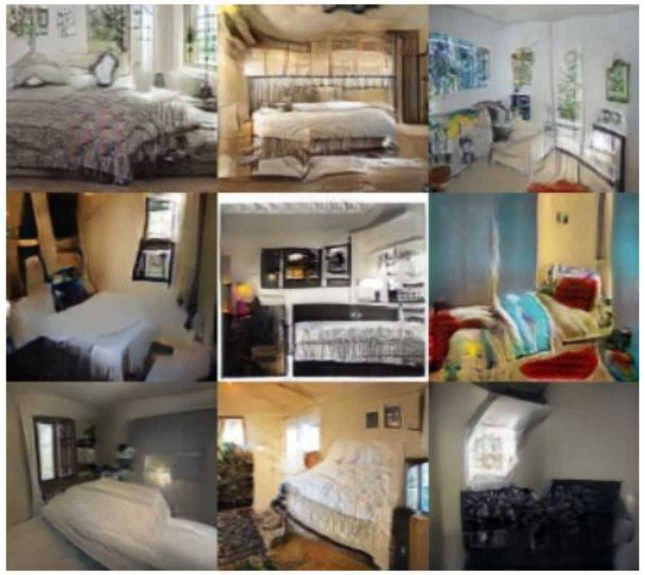
https://github.com/hindupuravinash/the-gan-zoo

2017: Explosion of GANs

Better training and generation



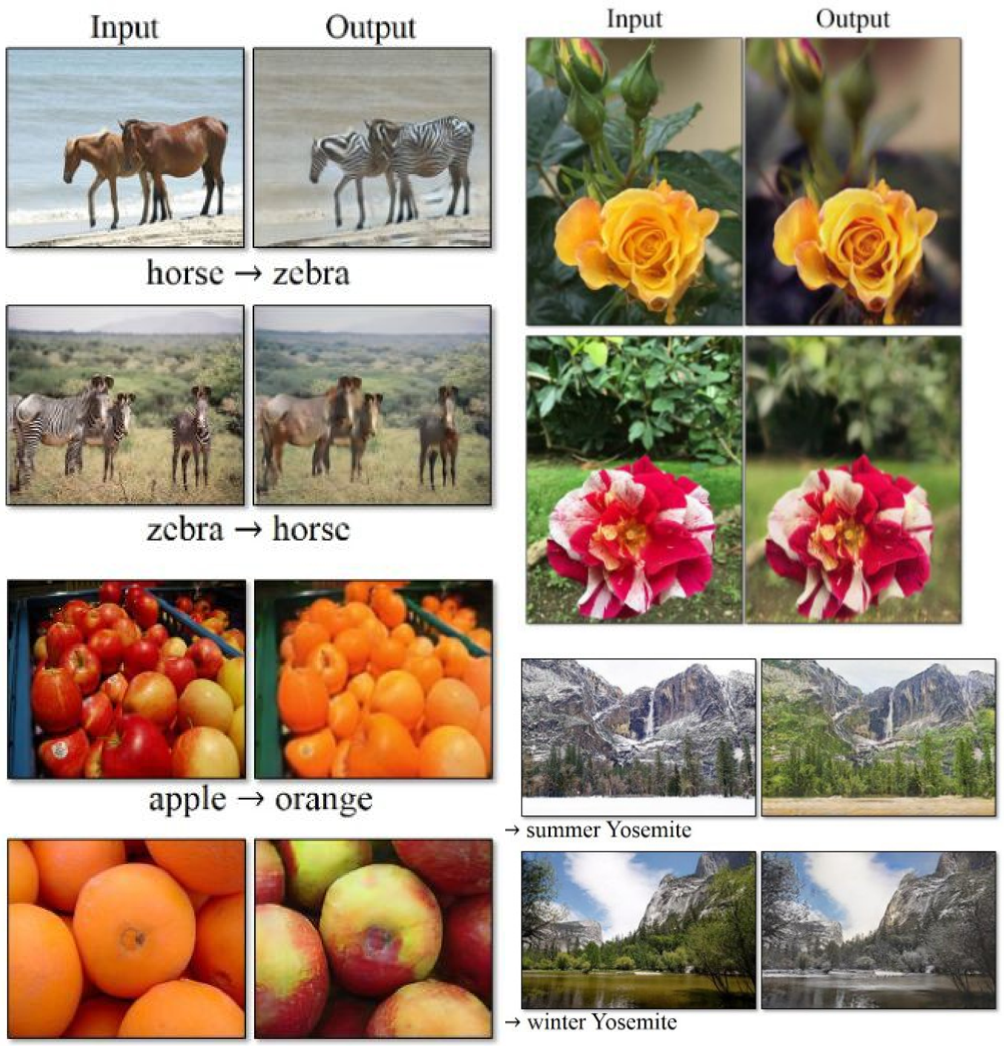
LSGAN, Zhu 2017.

Wasserstein GAN,
Arjovsky 2017.
Improved Wasserstein
GAN, Gulrajani 2017.

Progressive GAN, Karras 2018.

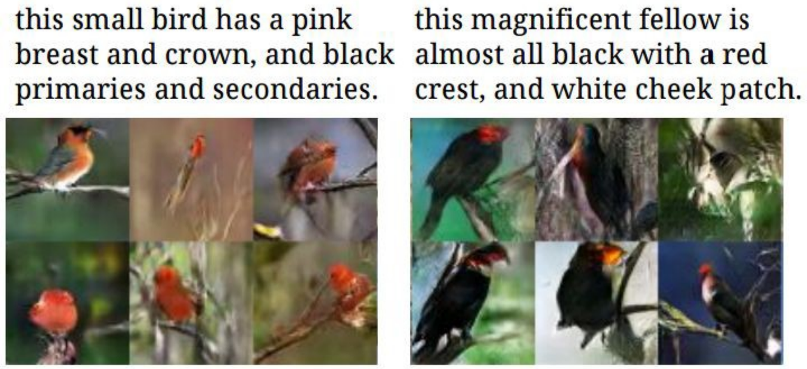
2017: Explosion of GANs

Source->Target domain transfer



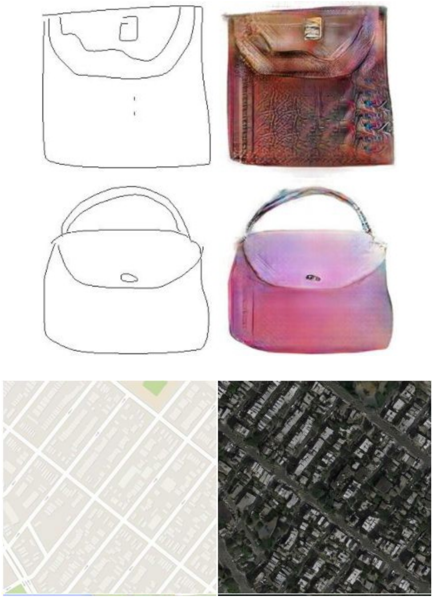
CycleGAN. Zhu et al. 2017.

Text -> Image Synthesis


this small bird has a pink breast and crown, and black primaries and secondaries.
this magnificent fellow is almost all black with a red crest, and white cheek patch.

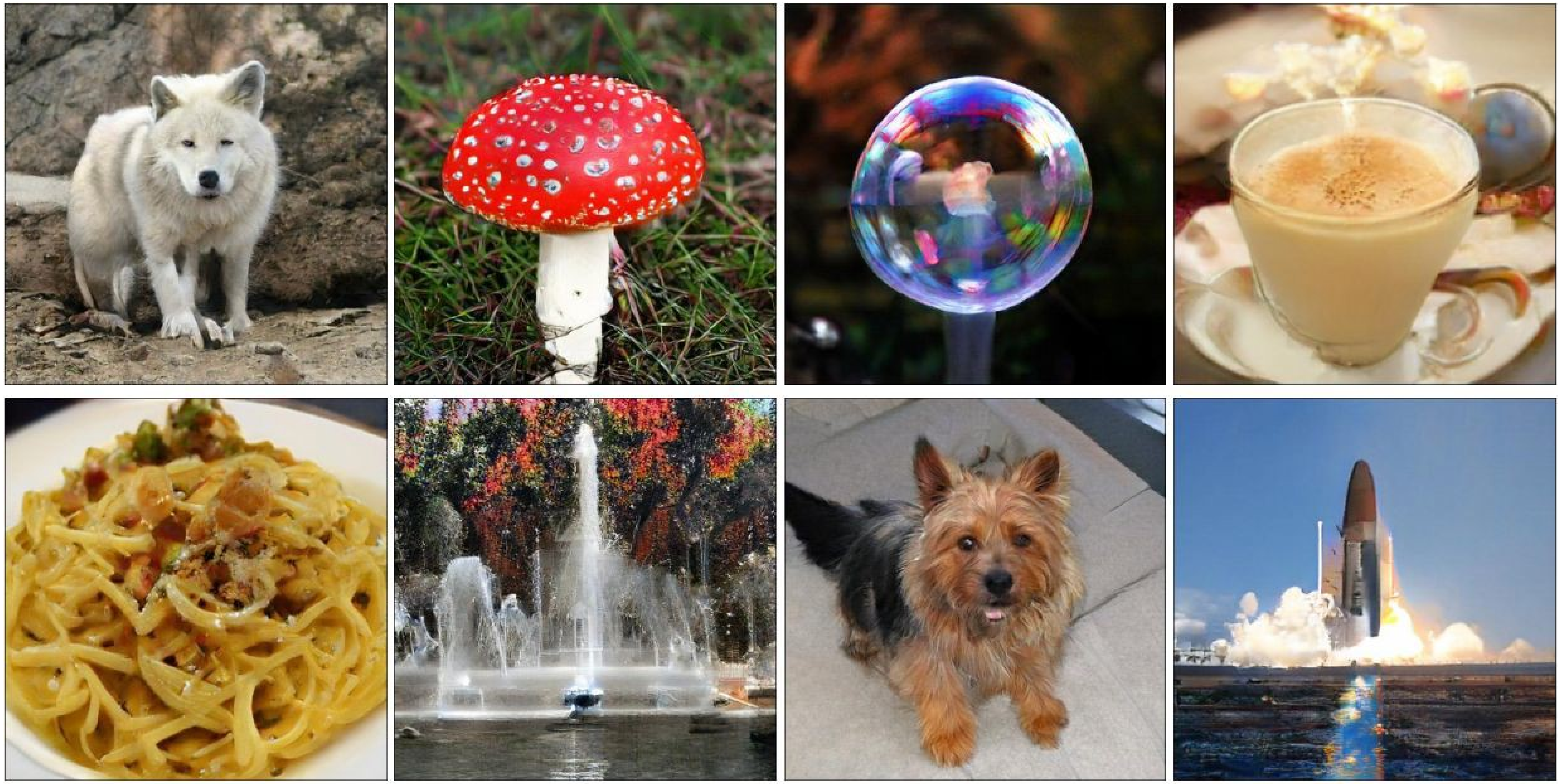
Reed et al. 2017.

Many GAN applications



Pix2pix. Isola 2017. Many examples at https://phillipi.github.io/pix2pix/

2019: BigGAN



Brock et al., 2019

Style GANs

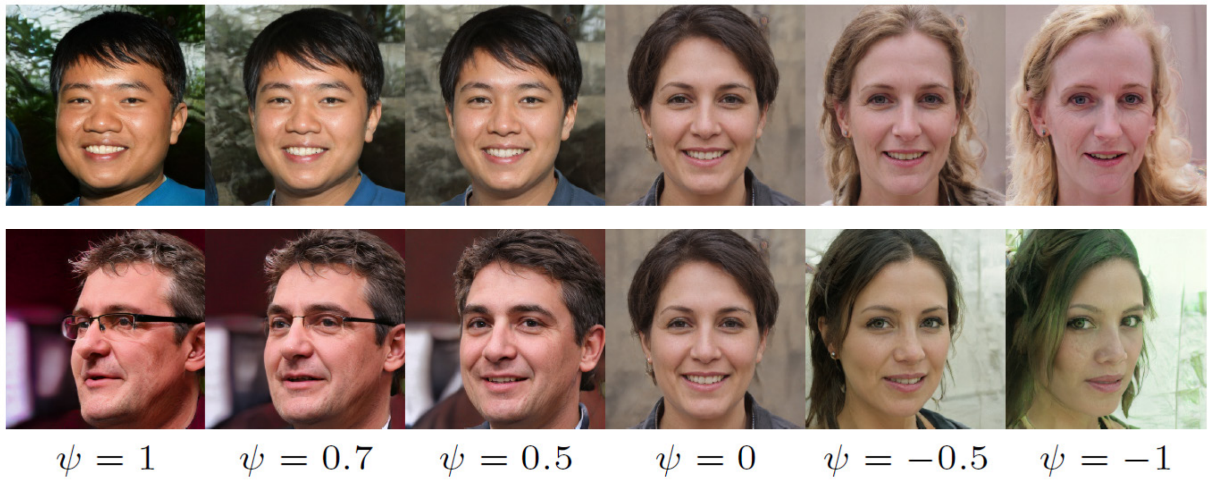
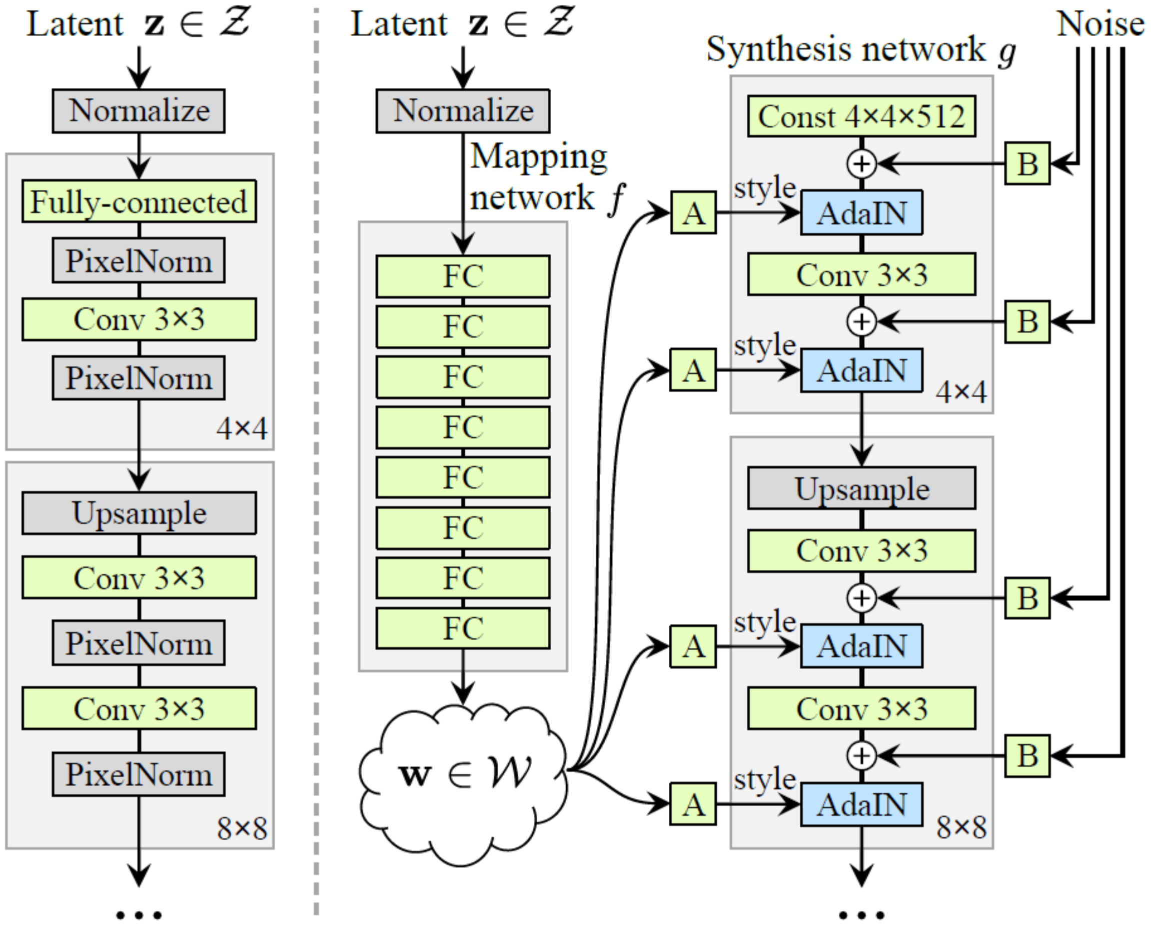


Figure 8. The effect of truncation trick as a function of style scale ψ. When we fade $\psi \to 0$, all faces converge to the "mean" face of FFHQ. This face is similar for all trained networks, and the interpolation towards it never seems to cause artifacts. By applying negative scaling to styles, we get the corresponding opposite or "anti-face". It is interesting that various high-level attributes often flip between the opposites, including viewpoint, glasses, age, coloring, hair length, and often gender.



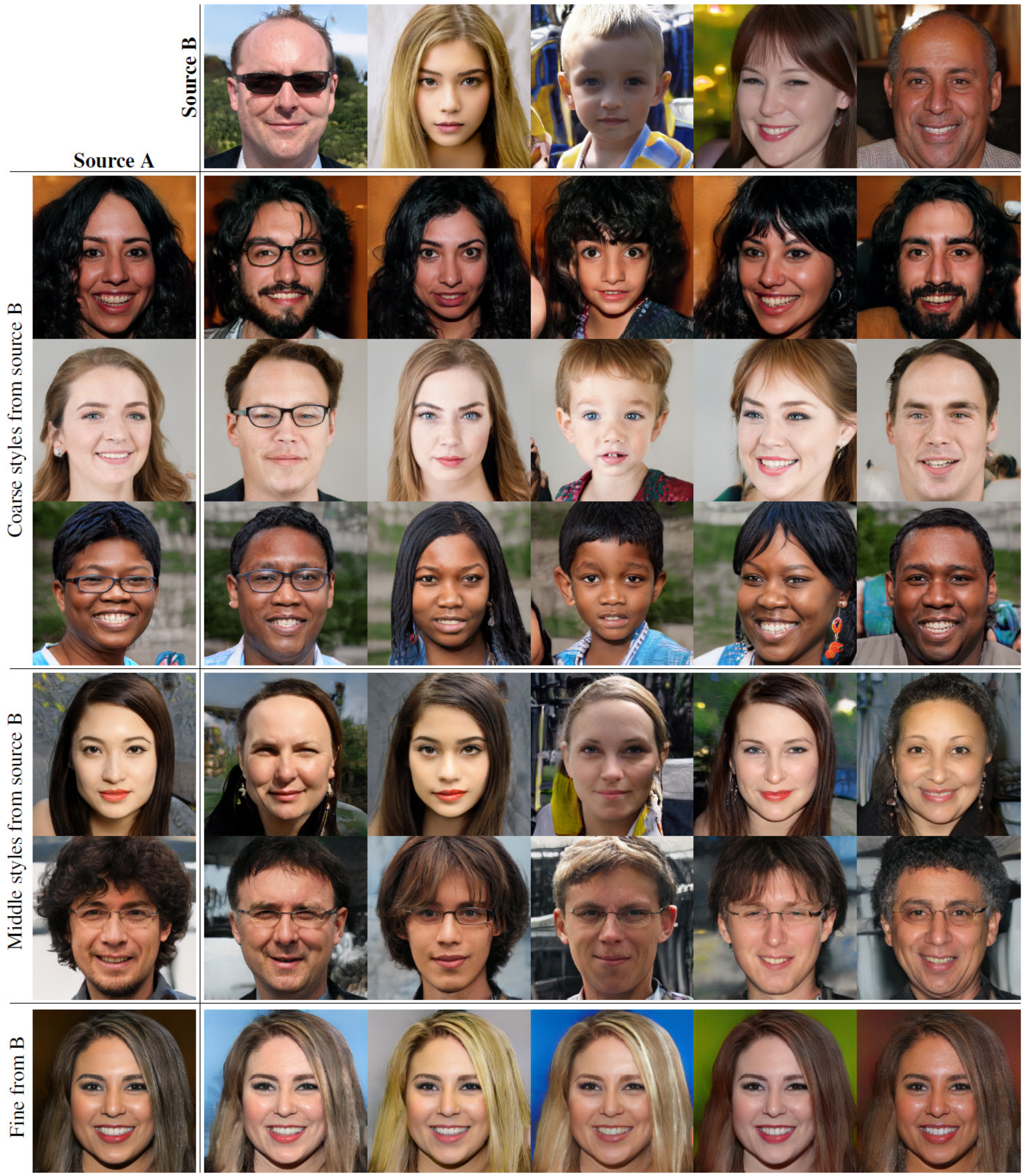
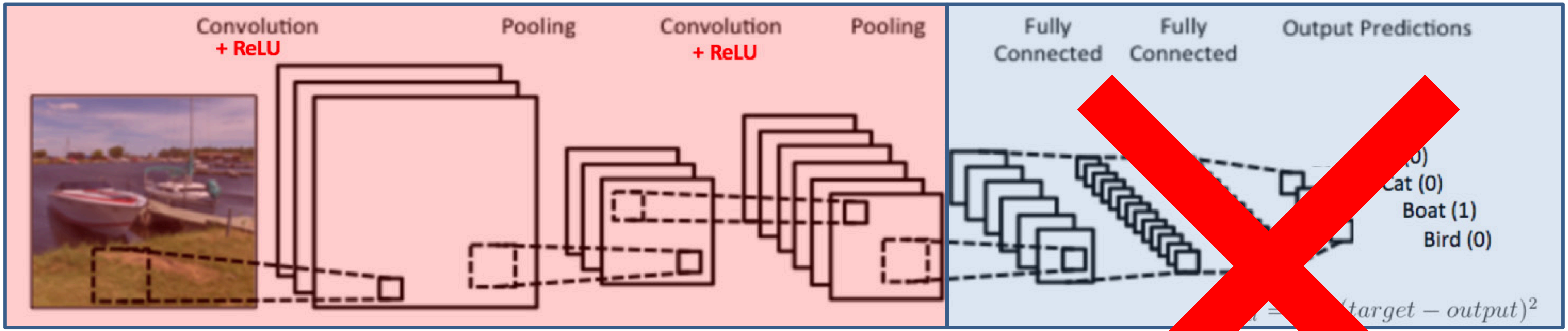


Figure 3. Two sets of images were generated from their respective latent codes (sources A and B); the rest of the images were generated by copying a specified subset of styles from source B and taking the rest from source A. Copying the styles corresponding to coarse spatial resolutions (4^2 – 8^2) brings high-level aspects such as pose, general hair style, face shape, and eyeglasses from source B, while all colors (eyes, hair, lighting) and finer facial features resemble A. If we instead copy the styles of middle resolutions (16^2 – 32^2) from B, we inherit smaller scale facial features, hair style, eyes open/closed from B, while the pose, general face shape, and eyeglasses from A are preserved. Finally, copying the fine styles (64^2 – 1024^2) from B brings mainly the color scheme and microstructure.

Representation learning **without annotations**?



x
data

<u>‘Modern’ Deep learning:</u>
<u>Hierarchical Representation Learning</u>
Feature extraction

z
Latent space representation

<u>‘Classical’ Fully-connected</u>
<u>Neural Networks</u>
Classification

y
label

<u>Many ideas are possible (and yours could be even better!):</u>

1. Predict the future: RNNs, Video
2. Compression: Autoencoder (predict self, through clamp), representation **z**
3. Pretext tasks: predict self, before/after, missing patch, correct rotation, colorization, up-sampling, multimodal
4. Capture parameter distribution (variance): Variational Auto-Encoders
5. Make latent space parameters z meaningful, orthogonal, explicit, tuneable
6. Train using a second network: GANs - Improve quality of output images
7. The Sky is the Limit

Taxonomy of Generative Models

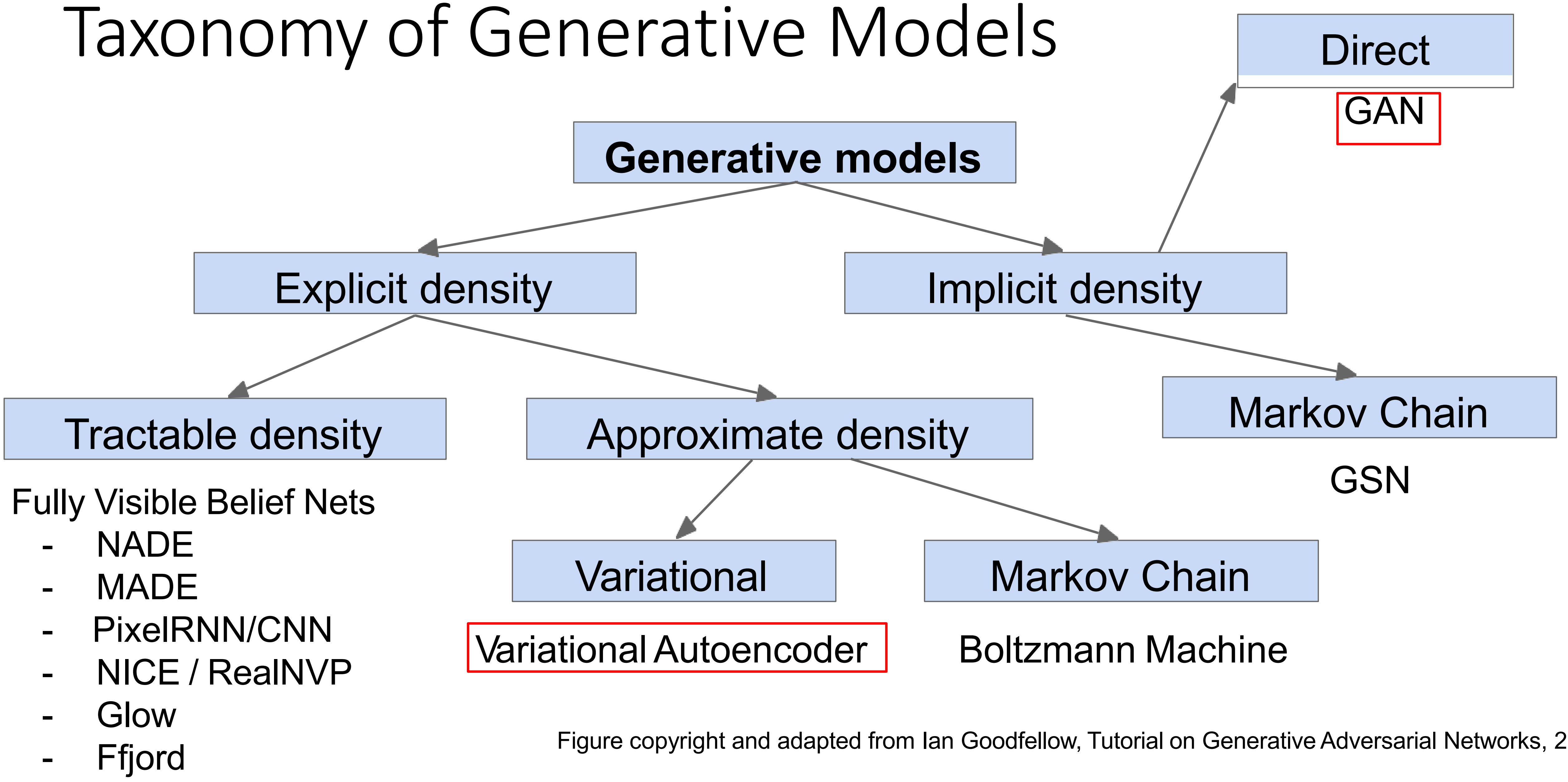


Figure copyright and adapted from Ian Goodfellow, Tutorial on Generative Adversarial Networks, 2017.

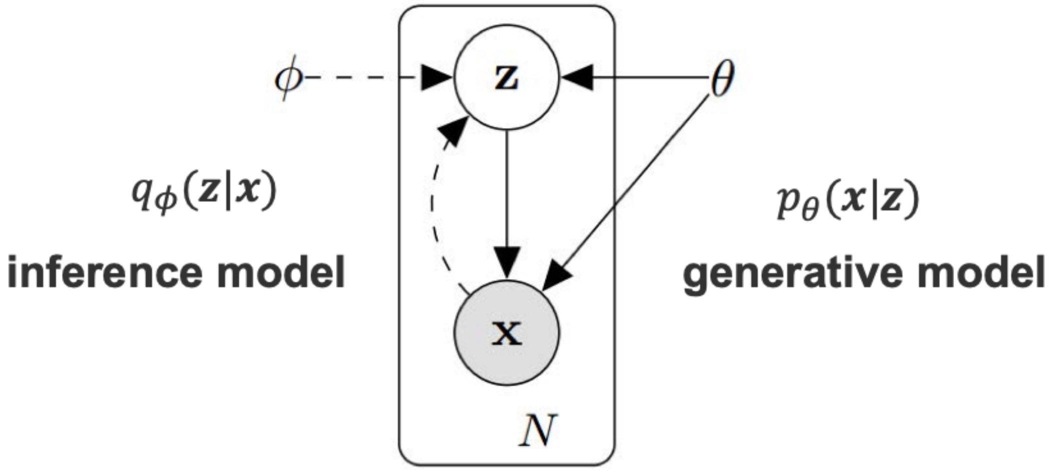
GANs ⇔ VAEs

Let’s look at VAE and GAN more closely…

From Eric Xing’s slides for CMU 10-708
Based on “On Unifying Deep Generative Models”

Variational Autoencoders (VAEs)

- [Kingma & Welling, 2014]
- Use variational inference with an inference model
  - Enjoy similar applicability with wake-sleep algorithm
- Generative model $p_\theta(\boldsymbol{x}|\boldsymbol{z})$, and prior $p(\boldsymbol{z})$
  - Joint distribution $p_\theta(\boldsymbol{x},\boldsymbol{z}) = p_\theta(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})$
- Inference model $q_\phi(\boldsymbol{z}|\boldsymbol{x})$



$q_\phi(\boldsymbol{z}|\boldsymbol{x})$

inference model

$p_\theta(\boldsymbol{x}|\boldsymbol{z})$

generative model

Figure courtesy: Kingma & Welling, 2014

Generative Adversarial Nets (GANs)

- [Goodfellow et al., 2014]
- Generative model $\boldsymbol{x} = G_\theta(\boldsymbol{z}), \quad \boldsymbol{z} \sim p(\boldsymbol{z})$
  - Map noise variable $\boldsymbol{z}$ to data space $\boldsymbol{x}$
  - Define an implicit distribution over $\boldsymbol{x}$: $p_{g_\theta}(\boldsymbol{x})$
    - a stochastic process to simulate data $\boldsymbol{x}$
    - Intractable to evaluate likelihood
- Discriminator $D_\phi(\boldsymbol{x})$
  - Output the probability that $\boldsymbol{x}$ came from the data rather than the generator
- No explicit inference model
- No obvious connection to previous models with inference networks like VAEs
  - We will build formal connections between GANs and VAEs later

A unified view of deep generative models

- Literatures have viewed these DGM approaches as distinct model training paradigms
  - GANs: achieve an equilibrium between generator and discriminator
  - VAEs: maximize lower bound of the data likelihood

- Let's study a new formulation for DGMs
  - Connects GANs, VAEs, and other variants, under a unified view
  - Links them back to inference and learning of Graphical Models, and the wake-sleep heuristic that approximates this
  - Provides a tool to analyze many GAN-/VAE-based algorithms
  - Encourages mutual exchange of ideas from each individual class of models

Generative Adversarial Nets (GANs):

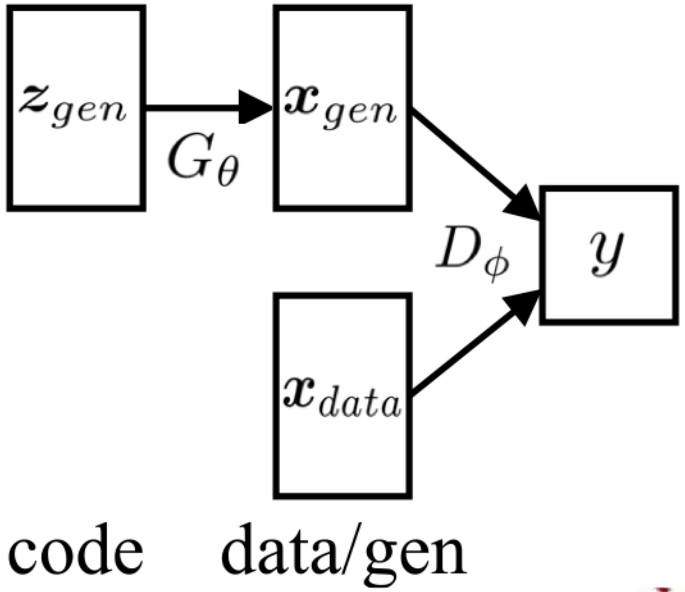
- Implicit distribution over $\boldsymbol{x} \sim p_\theta(\boldsymbol{x}|y)$

$$p_\theta(\boldsymbol{x}|y) = \begin{cases} p_{g_\theta}(\boldsymbol{x}) & y = 0 \\ p_{data}(\boldsymbol{x}) & y = 1. \end{cases}$$

(distribution of generated images)

(distribution of real images)

- $\boldsymbol{x} \sim p_{g_\theta}(\boldsymbol{x}) \Leftrightarrow \boldsymbol{x} = G_\theta(\boldsymbol{z}),\ \boldsymbol{z} \sim p(\boldsymbol{z}|y=0)$
- $\boldsymbol{x} \sim p_{data}(\boldsymbol{x})$
  - the code space of $\boldsymbol{z}$ is degenerated
  - sample directly from data



A new formulation

- Rewrite GAN objectives in the ”variational-EM” format
- Recap: conventional formulation:

$$\max_{\boldsymbol{\phi}} \mathcal{L}_\phi = \mathbb{E}_{\boldsymbol{x}=G_\theta(\boldsymbol{z}),\boldsymbol{z}\sim p(\boldsymbol{z}|y=0)}\left[\log(1-D_\phi(\boldsymbol{x}))\right] + \mathbb{E}_{\boldsymbol{x}\sim p_{data}(\boldsymbol{x})}\left[\log D_\phi(\boldsymbol{x})\right]$$

$$\max_{\boldsymbol{\theta}} \mathcal{L}_\theta = \mathbb{E}_{\boldsymbol{x}=G_\theta(\boldsymbol{z}),\boldsymbol{z}\sim p(\boldsymbol{z}|y=0)}\left[\log D_\phi(\boldsymbol{x})\right] + \mathbb{E}_{\boldsymbol{x}\sim p_{data}(\boldsymbol{x})}\left[\log(1-D_\phi(\boldsymbol{x}))\right]$$

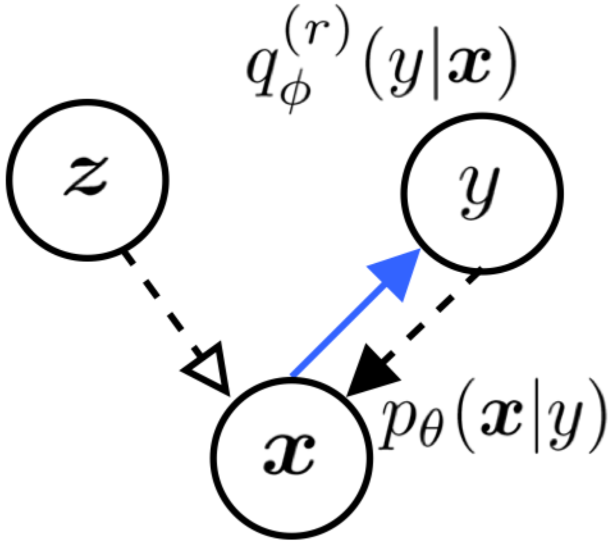
$$= \mathbb{E}_{\boldsymbol{x}=G_\theta(\boldsymbol{z}),\boldsymbol{z}\sim p(\boldsymbol{z}|y=0)}\left[\log D_\phi(\boldsymbol{x})\right]$$

- Rewrite in the new form
  - Implicit distribution over $\boldsymbol{x} \sim p_\theta(\boldsymbol{x}|y)$

$$\boldsymbol{x} = G_\theta(\boldsymbol{z}),\ \boldsymbol{z} \sim p(\boldsymbol{z}|y)$$

  - Discriminator distribution $q_\phi(y|\boldsymbol{x})$

$$q_\phi^r(y|\boldsymbol{x}) = q_\phi(1-y|\boldsymbol{x}) \quad \text{(reverse)}$$


$q_\phi^{(r)}(y|\boldsymbol{x})$
$\boldsymbol{z}$
y
$\boldsymbol{x}$
$p_\theta(\boldsymbol{x}|y)$

$$\max_{\boldsymbol{\phi}} \mathcal{L}_\phi = \mathbb{E}_{p_\theta(\boldsymbol{x}|y)p(y)}\left[\log q_\phi(y|\boldsymbol{x})\right]$$

$$\max_{\boldsymbol{\theta}} \mathcal{L}_\theta = \mathbb{E}_{p_\theta(\boldsymbol{x}|y)p(y)}\left[\log q_\phi^r(y|\boldsymbol{x})\right]$$

GANs vs. Variational EM

Variational EM

- Objectives

$$\max_{\phi} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}} = \mathbb{E}_{q_{\boldsymbol{\phi}}(z|x)}[\log p_{\boldsymbol{\theta}}(x|z)] + KL\left(q_{\phi}(z|x)||p(z)\right)$$

$$\max_{\theta} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}} = \mathbb{E}_{q_{\boldsymbol{\phi}}(z|x)}[\log p_{\boldsymbol{\theta}}(x|z)] + KL\left(q_{\phi}(z|x)||p(z)\right)$$

  - Single objective for both θ and ϕ
  - Extra prior regularization by $p(z)$
- The reconstruction term: maximize the conditional log-likelihood of x with the generative distribution $p_{\theta}(x|z)$ conditioning on the latent code z inferred by $q_{\phi}(z|x)$

- $p_{\theta}(x|z)$ is the generative model
- $q_{\phi}(z|x)$ is the inference model

GAN

- Objectives

$$\max_{\boldsymbol{\phi}} \mathcal{L}_{\phi} = \mathbb{E}_{p_{\theta}(\boldsymbol{x}|y)p(y)}\left[\log q_{\phi}(y|\boldsymbol{x})\right]$$

$$\max_{\boldsymbol{\theta}} \mathcal{L}_{\theta} = \mathbb{E}_{p_{\theta}(\boldsymbol{x}|y)p(y)}\left[\log q_{\phi}^{r}(y|\boldsymbol{x})\right]$$

  - Two objectives
  - Have global optimal state in the game theoretic view
- The objectives: maximize the conditional log-likelihood of y (or $1 - y$) with the distribution $q_{\phi}(y|x)$ conditioning on data/generation x inferred by $p_{\theta}(x|y)$

- Interpret $q_{\phi}(y|x)$ as the generative model
- Interpret $p_{\theta}(x|y)$ as the inference model

GANs vs. Variational EM

- **Interpret x as latent variables**
- **Interpret generation of x as performing inference over latent**

In VEM, we minimize the following:

$$F(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = -\log p(\boldsymbol{x}) + KL\left(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})\right)$$

→ KL (inference model | posterior)

Variational EM

- Objectives

$$\max_{\phi} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}} = \mathbb{E}_{q_{\phi}(z|x)}[\log p_{\theta}(x|z)] + KL\left(q_{\phi}(z|x)||p(z)\right)$$
$$\max_{\theta} \mathcal{L}_{\boldsymbol{\phi},\boldsymbol{\theta}} = \mathbb{E}_{q_{\phi}(z|x)}[\log p_{\theta}(x|z)] + KL\left(q_{\phi}(z|x)||p(z)\right)$$

  - Single objective for both θ and ϕ
  - Extra prior regularization by $p(z)$
- The reconstruction term: maximize the conditional log-likelihood of x with the generative distribution $p_{\theta}(x|z)$ conditioning on the latent code z inferred by $q_{\phi}(z|x)$
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GAN

- Objectives

$$\max_{\boldsymbol{\phi}} \mathcal{L}_{\phi} = \mathbb{E}_{p_{\theta}(\boldsymbol{x}|y)p(y)}\left[\log q_{\phi}(y|\boldsymbol{x})\right]$$
$$\max_{\boldsymbol{\theta}} \mathcal{L}_{\theta} = \mathbb{E}_{p_{\theta}(\boldsymbol{x}|y)p(y)}\left[\log q^{r}_{\phi}(y|\boldsymbol{x})\right]$$

  - Two objectives
  - Have global optimal state in the game theoretic view
- The objectives: maximize the conditional log-likelihood of y (or $1-y$) with the distribution $q_{\phi}(y|x)$ conditioning on data/generation x inferred by $p_{\theta}(x|y)$
- Interpret $q_{\phi}(y|x)$ as the generative model
- Interpret $p_{\theta}(x|y)$ as the inference model

GANs: minimizing KLD

- As in Variational EM, we can further rewrite in the form of minimizing KLD to reveal more insights into the optimization problem
- For each optimization step of $p_{\theta}(\boldsymbol{x}|y)$ at point $(\theta = \theta_0, \phi = \phi_0)$, let
  - $p(y)$: uniform prior distribution
  - $p_{\theta=\theta_0}(\boldsymbol{x}) = \mathrm{E}_{p(y)}\left[p_{\theta=\theta_0}(\boldsymbol{x}|y)\right]$
  - $q^r(\boldsymbol{x}|y) \propto q^r_{\phi=\phi_0}(y|\boldsymbol{x})p_{\theta=\theta_0}(\boldsymbol{x})$
- *Lemma 1*: The updates of $\boldsymbol{\theta}$ at $\boldsymbol{\theta}_0$ have

$$\nabla_\theta \Big[-\mathbb{E}_{p_\theta(\boldsymbol{x}|y)p(y)} \left[\log q^r_{\phi=\phi_0}(y|\boldsymbol{x})\right] \Big] \Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0} =$$

$$\nabla_\theta \Big[\mathbb{E}_{p(y)} \left[\mathit{KL}\left(p_\theta(\boldsymbol{x}|y) \| q^r(\boldsymbol{x}|y)\right)\right] - \mathit{JSD}\left(p_\theta(\boldsymbol{x}|y=0) \| p_\theta(\boldsymbol{x}|y=1)\right) \Big] \Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0},$$

  - KL: KL divergence
  - JSD: Jensen-shannon divergence

GANs: minimizing KLD

- *Lemma 1*: The updates of $\boldsymbol{\theta}$ at $\boldsymbol{\theta}_0$ have

$$\nabla_\theta \Big[-\mathbb{E}_{p_\theta(\boldsymbol{x}|y)p(y)} \big[\log q^r_{\phi=\phi_0}(y|\boldsymbol{x})\big] \Big] \Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0} =$$

$$\nabla_\theta \Big[\mathbb{E}_{p(y)} \big[\mathrm{KL}\left(p_\theta(\boldsymbol{x}|y) \| q^r(\boldsymbol{x}|y)\right)\big] - \mathrm{JSD}\left(p_\theta(\boldsymbol{x}|y=0) \| p_\theta(\boldsymbol{x}|y=1)\right)\Big] \Big|_{\boldsymbol{\theta}=\boldsymbol{\theta}_0}$$

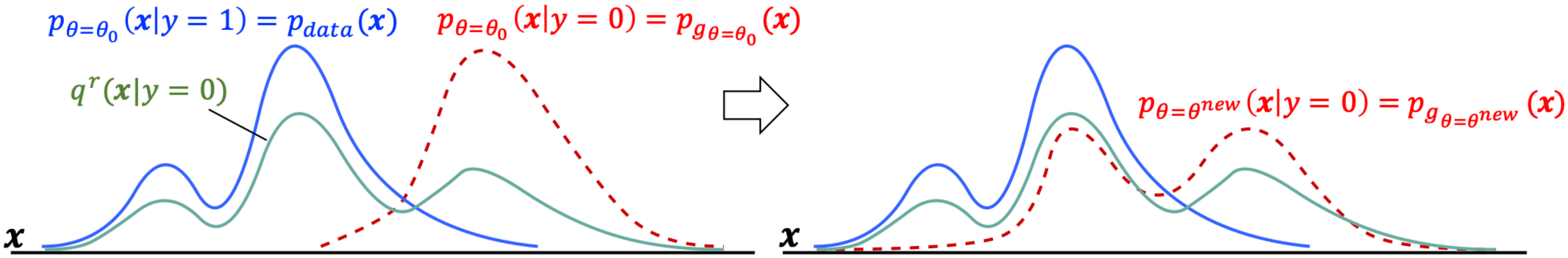
- Connection to variational inference
  - See $\boldsymbol{x}$ as latent variables, y as visible
  - $p_{\theta=\theta_0}(\boldsymbol{x})$: prior distribution
  - $q^r(\boldsymbol{x}|y) \propto q^r_{\phi=\phi_0}(y|\boldsymbol{x}) p_{\theta=\theta_0}(\boldsymbol{x})$: posterior distribution
  - $p_\theta(\boldsymbol{x}|y)$: variational distribution
    - Amortized inference: updates model parameter $\boldsymbol{\theta}$
- Suggests relations to VAEs, as we will explore shortly

In VEM, we minimize the following:

$$F(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = -\log p(\boldsymbol{x}) + KL\left(q_{\boldsymbol{\phi}}(\boldsymbol{z}|\boldsymbol{x}) \mid\mid p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})\right)$$

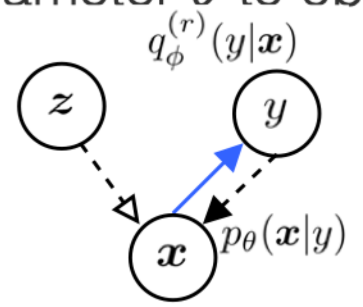
→ KL (inference model | posterior)

GANs: minimizing KLD

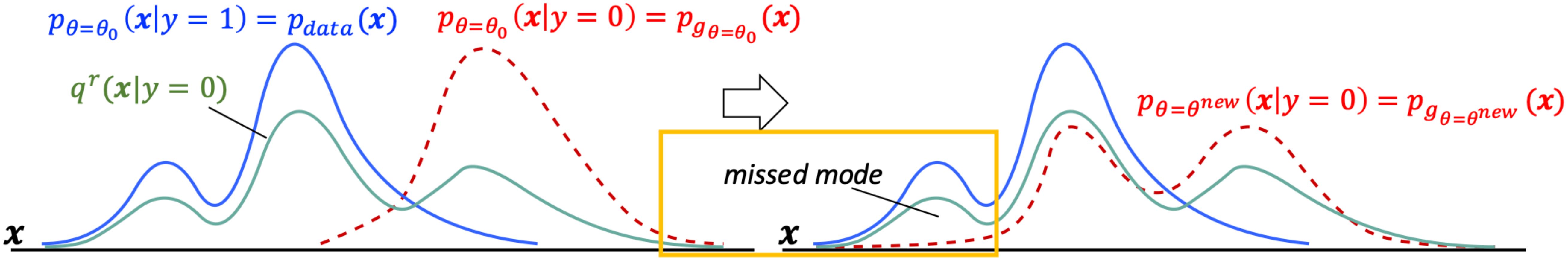


- Minimizing the KLD drives $p_{g_\theta}(\boldsymbol{x})$ to $p_{data}(\boldsymbol{x})$
  - By definition: $p_{\theta=\theta_0}(\boldsymbol{x}) = \mathrm{E}_{p(y)}[p_{\theta=\theta_0}(\boldsymbol{x}|y)] = \left(p_{g_{\theta=\theta_0}}(\boldsymbol{x}) + p_{data}(\boldsymbol{x})\right)/\,2$
  - $\mathrm{KL}\big(p_\theta(x|y=1)||q^r(x|y=1)\big) = \mathrm{KL}\big(p_{data}(x)||q^r(x|y=1)\big)$: constant, no free parameters
  - $\mathrm{KL}\big(p_\theta(x|y=0)||q^r(x|y=0)\big) = \mathrm{KL}\left(p_{g_\theta}(x)||q^r(x|y=0)\right)$: parameter $\boldsymbol{\theta}$ to optimize
    - $q^r(\boldsymbol{x}|y=0) \propto q^r_{\phi=\phi_0}(y=0|\boldsymbol{x})p_{\theta=\theta_0}(\boldsymbol{x})$
      - seen as a mixture of $p_{g_{\theta=\theta_0}}(\boldsymbol{x})$ and $p_{data}(\boldsymbol{x})$
      - mixing weights induced from $q^r_{\phi=\phi_0}(y=0|\boldsymbol{x})$
    - Drives $p_{g_\theta}(\boldsymbol{x}|y)$ to mixture of $p_{g_{\theta=\theta_0}}(\boldsymbol{x})$ and $p_{data}(\boldsymbol{x})$

      $\Rightarrow$ Drives $p_{g_\theta}(\boldsymbol{x})$ to $p_{data}(\boldsymbol{x})$


$q_\phi^{(r)}(y|\boldsymbol{x})$
$\boldsymbol{z}$
y
$\boldsymbol{x}$
$p_\theta(\boldsymbol{x}|y)$

GANs: minimizing KLD



- Missing mode phenomena of GANs
  - Asymmetry of KLD
    - Concentrates $p_\theta(\boldsymbol{x}|y=0)$ to large modes of $q^r(\boldsymbol{x}|y)$

      $\Rightarrow p_{g_\theta}(\boldsymbol{x})$ misses modes of $p_{data}(\boldsymbol{x})$
  - Symmetry of JSD
    - Does not affect the behavior of mode missing

$$\mathrm{KL}\left(p_{g_\theta}(x) || q^r(x|y=0)\right)$$
$$= \int p_{g_\theta}(x) \log \frac{p_{g_\theta}(x)}{q^r(x|y=0)} dx$$

- **Large positive contribution to the KLD in the regions of x space where $q^r(x|y=0)$ is small, unless $p_{g_\theta}(x)$ is also small**
- **$\Rightarrow p_{g_\theta}(x)$ tends to avoid regions where $q^r(x|y=0)$ is small**

Recap: conventional formulation of VAEs

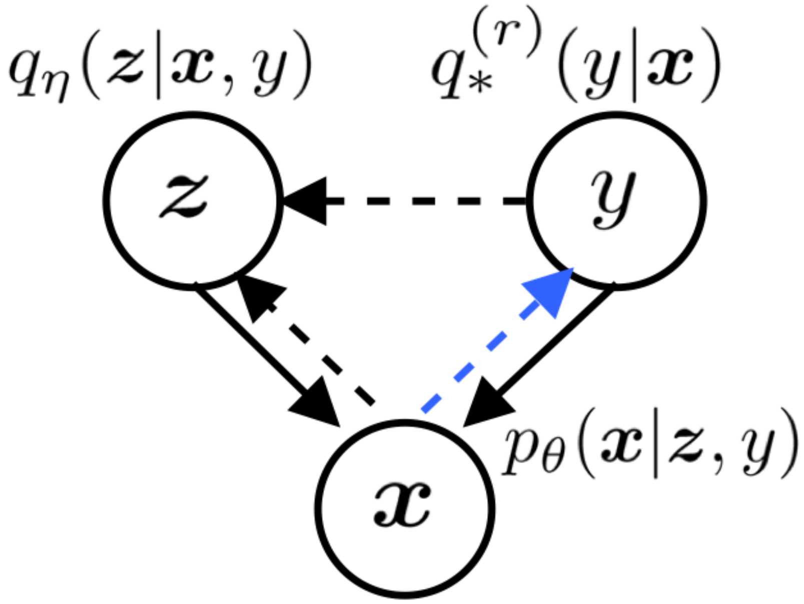
- Objective:

$$\max_{\boldsymbol{\theta},\boldsymbol{\eta}} \mathcal{L}_{\theta,\eta}^{\text{vae}} = \mathbb{E}_{p_{data}(\boldsymbol{x})} \left[\mathbb{E}_{\tilde{q}_\eta(\boldsymbol{z}|\boldsymbol{x})} \left[\log \tilde{p}_\theta(\boldsymbol{x}|\boldsymbol{z}) \right] - \text{KL}(\tilde{q}_\eta(\boldsymbol{z}|\boldsymbol{x}) \| \tilde{p}(\boldsymbol{z})) \right]$$

  - $\tilde{p}(\boldsymbol{z})$: prior over $\boldsymbol{z}$
  - $\tilde{p}_\theta(\boldsymbol{x}|\boldsymbol{z})$: generative model
  - $\tilde{q}_\eta(\boldsymbol{z}|\boldsymbol{x})$: inference model
  - Only uses real examples from $p_{data}(\boldsymbol{x})$, lacks adversarial mechanism

- To align with GANs, let's introduce the real/fake indicator y and adversarial discriminator

VAEs: new formulation



$q_\eta(\boldsymbol{z}|\boldsymbol{x}, y)$
$q_*^{(r)}(y|\boldsymbol{x})$
$\boldsymbol{z}$
y
$\boldsymbol{x}$
$p_\theta(\boldsymbol{x}|\boldsymbol{z}, y)$

- Assume a *perfect* discriminator $q_*(y|\boldsymbol{x})$
  - $q_*(y=1|\boldsymbol{x}) = 1$ if $\boldsymbol{x}$ is real examples
  - $q_*(y=0|\boldsymbol{x}) = 1$ if $\boldsymbol{x}$ is generated samples
  - $q_*^r(y|\boldsymbol{x}) := q_*(1-y|\boldsymbol{x})$
- Generative distribution

$$p_\theta(\boldsymbol{x}|\boldsymbol{z}, y) = \begin{cases} p_\theta(\boldsymbol{x}|\boldsymbol{z}) & y = 0 \\ p_{data}(\boldsymbol{x}) & y = 1. \end{cases}$$

- Let $p_\theta(\boldsymbol{z}, y|\boldsymbol{x}) \propto p_\theta(\boldsymbol{x}|\boldsymbol{z}, y)p(\boldsymbol{z}|y)p(y)$
- *Lemma 2*

$$\begin{aligned} \mathcal{L}^{vae}_{\theta,\eta} &= 2 \cdot \mathbb{E}_{p_{\theta_0}(\boldsymbol{x})} \left[\mathbb{E}_{q_\eta(\boldsymbol{z}|\boldsymbol{x},y)q_*^r(y|\boldsymbol{x})} \left[\log p_\theta(\boldsymbol{x}|\boldsymbol{z}, y) \right] - KL(q_\eta(\boldsymbol{z}|\boldsymbol{x}, y)q_*^r(y|\boldsymbol{x}) \| p(\boldsymbol{z}|y)p(y)) \right] \\ &= 2 \cdot \mathbb{E}_{p_{\theta_0}(\boldsymbol{x})} \left[-KL\left(q_\eta(\boldsymbol{z}|\boldsymbol{x}, y)q_*^r(y|\boldsymbol{x}) \| p_\theta(\boldsymbol{z}, y|\boldsymbol{x}) \right) \right]. \end{aligned}$$

$p_\theta(\mathbf{z}, y|\mathbf{x}) \propto p_\theta(\mathbf{x}|\mathbf{z}, y)p(\mathbf{z}|y)p(y)$

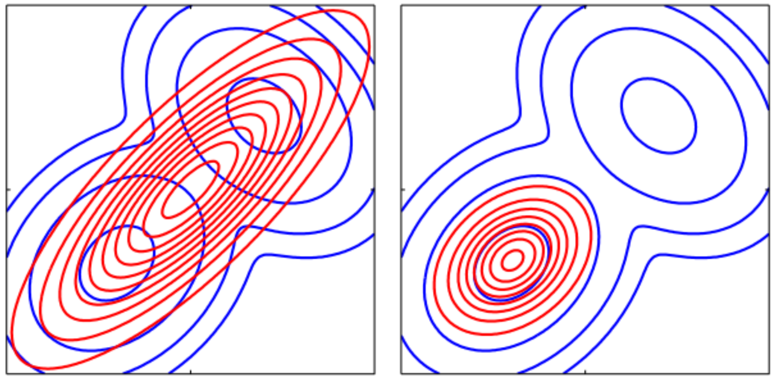
GANs vs VAEs side by side

	GANs (InfoGAN)	VAEs
Generative distribution	$p_\theta(\boldsymbol{x}\|y) = \begin{cases} p_{g_\theta}(\boldsymbol{x}) & y = 0 \\ p_{data}(\boldsymbol{x}) & y = 1. \end{cases}$	$p_\theta(\boldsymbol{x}\|\boldsymbol{z}, y) = \begin{cases} p_\theta(\boldsymbol{x}\|\boldsymbol{z}) & y = 0 \\ p_{data}(\boldsymbol{x}) & y = 1. \end{cases}$
Discriminator distribution	$q_\phi(y\|\boldsymbol{x})$	$q_*(y\|\boldsymbol{x})$, perfect, degenerated
$\boldsymbol{z}$-inference model	$q_\eta(\mathbf{z}\|\boldsymbol{x}, y)$ of InfoGAN	$q_\eta(\mathbf{z}\|\boldsymbol{x}, y)$
KLD to minimize	$\min_\theta \mathrm{KL}\ (p_\theta(\boldsymbol{x}\|y) \ \|\| \ q^r(\boldsymbol{x}\|\mathbf{z}, y))$ $\sim \min_\theta \mathrm{KL}(P_\theta \ \|\| \ Q)$	$\min_\theta \mathrm{KL}\left(q_\eta(\mathbf{z}\|\boldsymbol{x}, y)q_*^r(y\|\boldsymbol{x}) \ \|\| \ p_\theta(\mathbf{z}, y\|\boldsymbol{x})\right)$ $\sim \min_\theta \mathrm{KL}(Q \ \|\| \ P_\theta)$

GANs vs VAEs side by side

	GANs (InfoGAN)	VAEs
KLD to minimize	$\min_\theta \text{KL}\left(p_\theta(\boldsymbol{x} \mid y) \Vert q^r(\boldsymbol{x} \mid \boldsymbol{z}, y)\right)$ $\sim \min_\theta \text{KL}(P_\theta \Vert Q)$	$\min_\theta \text{KL}(q_\eta(\boldsymbol{z} \mid \boldsymbol{x}, y) q_*^r(y \mid \boldsymbol{x}) \Vert p_\theta(\boldsymbol{z}, y \mid \boldsymbol{x}))$ $\sim\min_\theta \text{KL}(Q \Vert P_\theta)$

- Asymmetry of KLDs inspires combination of GANs and VAEs
  - GANs: $\min_\theta \text{KL}(P_\theta||Q)$ tends to missing mode
  - VAEs: $\min_\theta \text{KL}(Q||P_\theta)$ tends to cover regions with small values of p_{data}



Mode covering **Mode missing**

[Figure courtesy: PRML]

Discriminative vs. Generative: Blurring the Distinction

Generative vs. Discriminative Classifiers

Training classifiers involves estimating f: X → Y, or P(Y|X)

Generative classifiers:

- Assume some functional form for P(X|Y), P(X)
- Estimate parameters of P(X|Y), P(X) directly from training data
- Use Bayes rule to calculate $P(Y|X= x_i)$

Discriminative classifiers:

1. Assume some functional form for P(Y|X)

2. Estimate parameters of P(Y|X) directly from training data

Slide Credit: Tom Mitchell

- Consider learning f: X → Y, where
  - X is a vector of real-valued features, < X_1 X_n >
  - Y is boolean
  - assume all X_i are conditionally independent given Y
  - model $P(X_i \mid Y = y_k)$ as Gaussian $N(\mu_{ik},\sigma)$
  - model P(Y) as binomial (p)

- What does that imply about the form of P(Y|X)?

$$P(Y = 1|X =< x_1, ...x_n >) = \frac{1}{1 + exp(w_0 + \sum_i w_i x_i)}$$

Slide Credit: Tom Mitchell

Logistic regression

- Logistic regression represents the probability of category *i* using a linear function of the input variables:

$$P(Y=i|X=x)=g(w_{i0}+w_{i1}x_1+\ldots+w_{id}x_d)$$

where for *i<k*

$$g(z_i)=\frac{e^{z_i}}{1+\sum_{j=1}^{K-1}e^{z_j}}$$

and for *k*

$$g(z_k)=\frac{1}{1+\sum_{j=1}^{K-1}e^{z_j}}$$

Slide Credit: Tom Mitchell

Generative-Discriminative Pairs

Example: assume Y boolean, X = <X_1, X_2, …, X_n>, where x_i are boolean, perhaps dependent on Y, conditionally independent given Y

Generative model: naïve Bayes:

$$\widehat{p}(x_i = 1|y = b) = \frac{s\{x_i = 1, y = b\} + l}{s\{y = b\} + 2l}$$

s indicates size of set.

l is smoothing parameter

$$\widehat{p}(y = b) = \frac{s\{y = b\}}{\sum_j s\{y = j\}}$$

Classify new example *x* based on ratio

$$\frac{\widehat{p}(y = T|x)}{\widehat{p}(y = F|x)} = \frac{\widehat{p}(y = T) \prod_{i=1}^{n} \widehat{p}(x_i|y = T)}{\widehat{p}(y = F) \prod_{i=1}^{n} \widehat{p}(x_i|y = F)}$$

Equivalently, based on sign of log of this ratio

Slide Credit: Tom Mitchell

Generative-Discriminative Pairs

Example: assume Y boolean, X = <x_1, x_2, …, x_n>, where x_i are boolean, perhaps dependent on Y, conditionally independent given Y

Generative model: naïve Bayes:

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$$\widehat{p}(y = b) = \frac{s\{y = b\}}{\sum_j s\{y = j\}}$$

Classify new example *x* based on ratio

$$\frac{\widehat{p}(y = T|x)}{\widehat{p}(y = F|x)} = \frac{\widehat{p}(y = T)\prod_{i=1}^{n} \widehat{p}(x_i|y = T)}{\widehat{p}(y = F)\prod_{i=1}^{n} \widehat{p}(x_i|y = F)}$$

Discriminative model: logistic regression

$$\widehat{p}(y = T|x; \beta, \theta) = 1/(1 + exp(-\sum_{i=1}^{n} \beta_i x_i - \theta))$$

Note both learn linear decision surface over X in this case

What is the difference asymptotically?

Notation: let $\epsilon(h_{A,m})$ denote error of hypothesis learned via algorithm A, from *m* examples

- If assumed model correct (e.g., naïve Bayes model), and finite number of parameters, then

$$\epsilon(h_{Dis,\infty}) = \epsilon(h_{Gen,\infty})$$

- If assumed model incorrect

$$\epsilon(h_{Dis,\infty}) \leq \epsilon(h_{Gen,\infty})$$

Note assumed discriminative model can be correct even when generative model incorrect, but not vice versa

Slide Credit: Tom Mitchell

Some experiments from UCI data sets

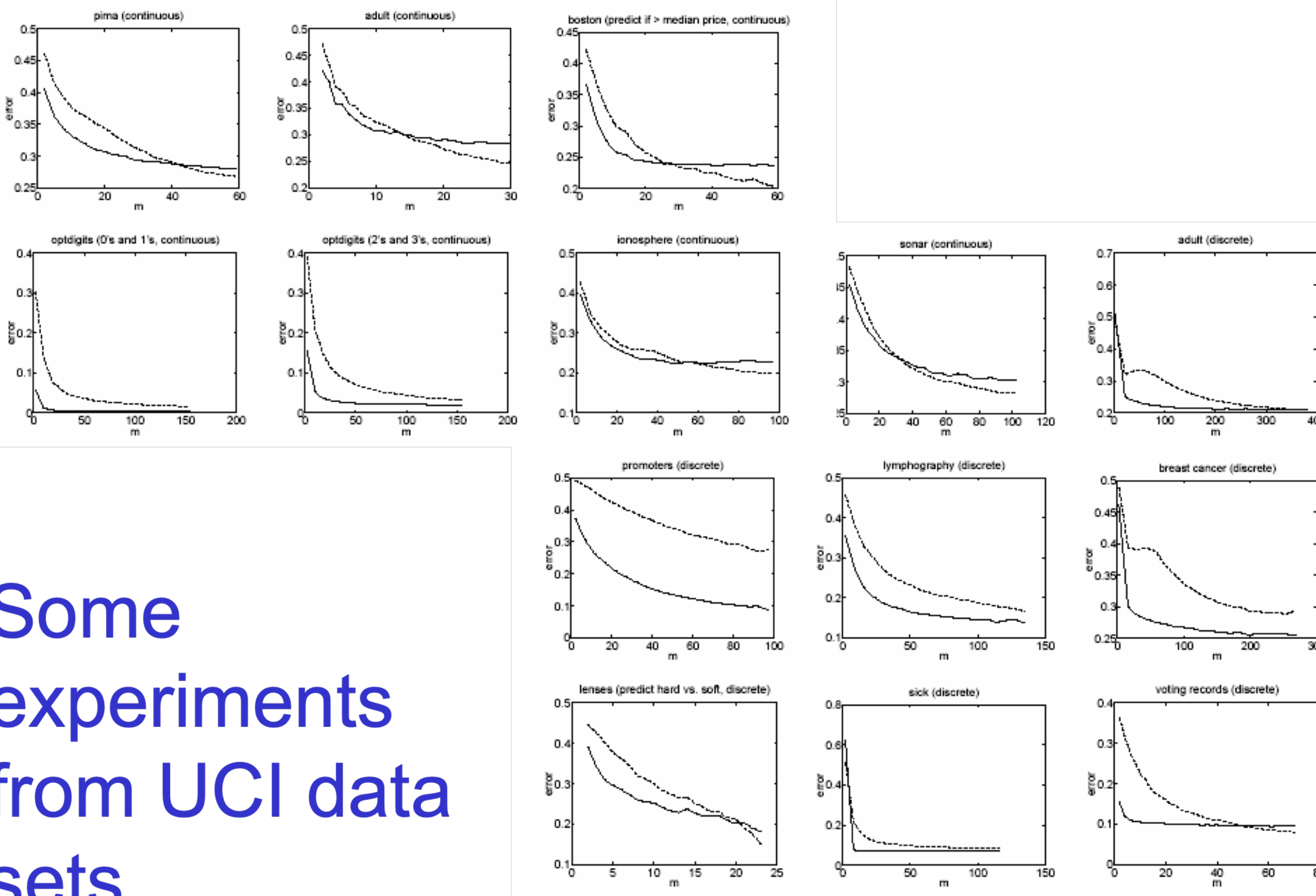

Figure 1: Results of 15 experiments on datasets from the UCI Machine Learnin repository. Plots are of generalization error vs. m (averaged over 1000 randor train/test splits). Dashed line is logistic regression; solid line is naive Bayes.