Deep approaches to semi-supervised learning

Anders Boesen Lindbo Larsen

Department of Applied Mathematics and Computer Science Technical University of Denmark

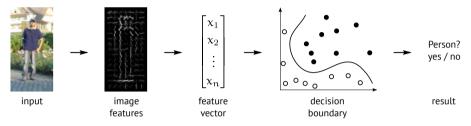


Outline

- Deep learning introduction
- Unsupervised pretraining with autoencoders
- Ladder networks (semi-supervised autoencoders)
- Generative adversarial networks
- Scaling up autoencoders to complex data distributions (images)

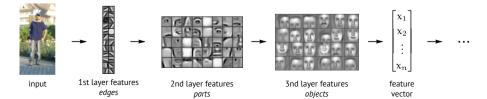
'Shallow' computer vision

Hand-engineer a *clever* representation of the input image.

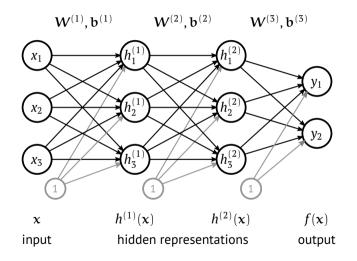


Deep feature learning

Learn a hierarchical representation of the input.



Neural networks 101



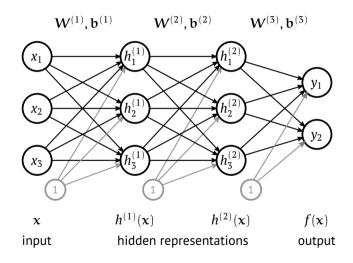
Hidden units are calculated from

$$h^{(0)}(\mathbf{x}) = \mathbf{x}$$

$$h^{(i)}(\mathbf{x}) = \sigma \left(\mathbf{W}^{(i)} h^{(i-1)}(\mathbf{x}) + \mathbf{b}^{(i)} \right)$$

$$\sigma(\mathbf{x}) = \frac{1}{1 + \exp(-\mathbf{x})}$$

Neural networks 101



Given a training sample (x, y), and a loss function \mathcal{L} , e.g.

$$\mathcal{L}(f(\mathbf{x}),\mathbf{y}) = \|f(\mathbf{x}) - \mathbf{y}\|_2^2$$

the network parameters are optimized using *back-propagation*.

Learn to solve the given task from data.

 $\mathbf{y} = f(\mathbf{x}; \mathbf{\theta})$

- x: Input (e.g. image).
- y: Output (e.g. *bird*, *cat*, *dog*).
- *f*: Neural network.
- θ: Network parameters.

Learn to solve the given task from data.

 $\mathbf{y} = f(\mathbf{x}; \mathbf{\theta})$

- x: Input (e.g. image).
- y: Output (e.g. *bird*, *cat*, *dog*).
- *f*: Neural network.
- θ: Network parameters.

Learn θ from from pairs x, y using gradient descent wrt. a chosen loss function.

$$\mathcal{L}(\mathbf{y}, f(\mathbf{x}; \mathbf{\theta}))$$

Learn to solve the given task from data.

 $\mathbf{y} = f(\mathbf{x}; \mathbf{\theta})$

- x: Input (e.g. image).
- y: Output (e.g. *bird*, *cat*, *dog*).
- *f*: Neural network.
- θ: Network parameters.

Learn θ from from pairs x, y using gradient descent wrt. a chosen loss function.

$$\mathcal{L}(\mathbf{y}, f(\mathbf{x}; \mathbf{\theta}))$$

Hierarchical function decomposition allows us to learn distributed representations of our input.

$$f(\mathbf{x}; \mathbf{\theta}) = f^{(n)} \left(\dots f^{(1)} \left(\mathbf{x}; \mathbf{\theta}^{(1)} \right) \dots; \mathbf{\theta}^{(n)} \right)$$

The good

- Powerful function approximation.
- Local optima not problematic with high-dimensional parameters.
- Feature disentangling.

The bad

- Computationally intensive.
- Can easily overfit.
- Require lots of data.

The ugly

- Finding a good architecture (layer types, layer ordering).
- Hyperparameter tuning (layer sizes, learning rate, weight initialization).

Beyond supervised models

- By construction, neural networks lend themselves to supervised learning.
- How do we leverage the power of neural networks in the unlabeled case?
- How do we combine network functions to form a semi-supervised model handling both unlabeled and labeled data?

Unsupervised pretraining

Vincent, P., Larochelle, H., Lajoie, I., et al. [2010]. "Stacked denoising autoencoders: Learning useful representations in a deep network with a local denoising criterion". In: *Journal of Machine Learning Research* 11.Dec, pp. 3371–3408.

Hinton, G. E. and Salakhutdinov, R. R. [2006]. "Reducing the dimensionality of data with neural networks". In: *Science* 313.5786, pp. 504–507.

ldea

- Learn features in an unsupervised manner.
- Transfer learned features to a supervised model.
- Hope that the pretrained features alleviate overfitting.

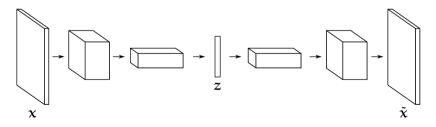
ldea

- Learn features in an unsupervised manner.
- Transfer learned features to a supervised model.
- Hope that the pretrained features alleviate overfitting.

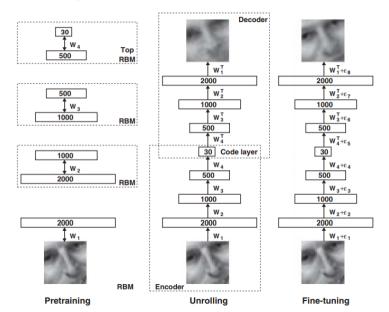
Note: Today, supervised training of neural networks has improved such that pretraining rarely is beneficial.

Autoencoders

- Learn an encoder-decoder architecture to reconstruct a dataset sample x as \tilde{x} .
- Train using a chosen loss function, e.g. $\mathcal{L}\left(\mathbf{x}, \tilde{\mathbf{x}}\right) = \|\mathbf{x} \tilde{\mathbf{x}}\|^2$.
- Bottleneck representation *z* forces encoder to *disentangle* input.

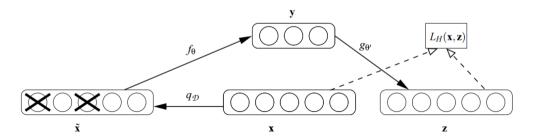


Layer-wise pretraining scheme

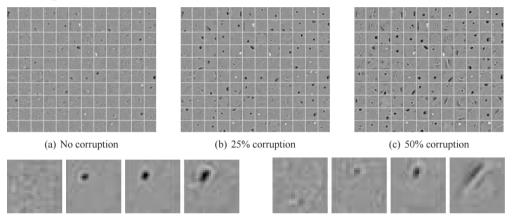


Denoising autoencoders

- Corrupt input to make higher level representations more robust.
- Very similar to dropout.
 - Prevents co-adaptation of features.
 - Effective regularizer.
 - Model averaging.



Denoising autoencoders, filters



(e) Neuron B (0%, 10%, 20%, 50% corruption)

(d) Neuron A (0%, 10%, 20%, 50% corruption)

Denoising autoencoders, results

Data Set	SVM _{rbf}	DBN-1	SAE-3	DBN-3	SDAE-3 (v)
MNIST	1.40±0.23	1.21 ±0.21	$1.40{\pm}0.23$	1.24±0.22	1.28±0.22 (25%)
basic	3.03 ±0.15	$3.94{\pm}0.17$	3.46 ± 0.16	$3.11{\scriptstyle \pm 0.15}$	2.84 ±0.15 (10%)
rot	$11.11{\pm}0.28$	$14.69{\scriptstyle\pm0.31}$	$10.30{\scriptstyle \pm 0.27}$	$10.30{\scriptstyle \pm 0.27}$	9.53±0.26 (25%)
bg-rand	$14.58{\scriptstyle\pm0.31}$	$9.80{\pm}0.26$	$11.28{\scriptstyle\pm0.28}$	6.73±0.22	10.30±0.27 (40%)
bg-img	$22.61{\scriptstyle\pm0.37}$	$16.15{\scriptstyle\pm0.32}$	$23.00{\scriptstyle\pm0.37}$	$16.31{\pm}0.32$	16.68±0.33 (25%)
bg-img-rot	$55.18{\scriptstyle\pm0.44}$	$52.21{\scriptstyle\pm0.44}$	$51.93{\scriptstyle \pm 0.44}$	$47.39{\scriptstyle\pm0.44}$	43.76 ±0.43 (25%)
rect	2.15 ±0.13	$4.71{\scriptstyle\pm0.19}$	$2.41{\scriptstyle\pm0.13}$	$2.60{\pm}0.14$	1.99 ±0.12 (10%)
rect-img	$24.04{\scriptstyle\pm0.37}$	$23.69{\scriptstyle\pm0.37}$	$24.05{\scriptstyle\pm0.37}$	$22.50{\scriptstyle\pm0.37}$	21.59 ±0.36 (25%)
convex	$19.13{\scriptstyle\pm0.34}$	$19.92{\scriptstyle\pm0.35}$	$18.41{\pm}0.34$	$18.63{\scriptstyle\pm0.34}$	19.06 ±0.34 (10%)
tzanetakis	$14.41{\scriptstyle\pm2.18}$	$18.07{\pm}1.31$	16.15 ± 1.95	$18.38{\scriptstyle\pm1.64}$	16.02 ±1.04(0.05)

Semi-supervised learning with Ladder networks

Rasmus, A., Berglund, M., Honkala, M., et al. [2015]. "Semi-supervised Learning with Ladder Networks". In: *Advances in Neural Information Processing Systems 28*. Ed. by C. Cortes, N. D. Lawrence, D. D. Lee, et al. Curran Associates, Inc., pp. 3546–3554.

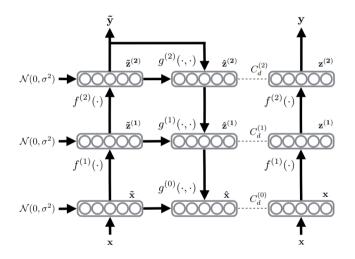
Mohammad, P., Linxi, F., Philemon, B., et al. [2016]. "Deconstructing the Ladder Network Architecture". In: *Proceedings of the 33rd International Conference on Machine Learning (ICML)*.

ldea

- Combine a discriminative network with the encoder network of an autoencoder.
- Perform layerwise denoising (lateral connection).
- Ingenious architecture engineering.
 - Gaussian noise after batch normalization.
 - Squared-error denoising criterion after batch normalization.

Ladder architecture

- Encode *x* both with and without noise.
- Decode by combining lateral and downward signal.
- Layer-wise reconstruction error with clean encoding as target.
- Cross-entropy error for labeled examples.



Results, MNIST

Table 1: A collection of previously reported MNIST test errors in the permutation invariant setting followed by the results with the Ladder network. * = SVM. Standard deviation in parentheses.

Test error % with # of used labels	100	1000	All
Semi-sup. Embedding (Weston et al., 2012)	16.86	5.73	1.5
Transductive SVM (from Weston et al., 2012)	16.81	5.38	1.40*
MTC (Rifai <i>et al.</i> , 2011)	12.03	3.64	0.81
Pseudo-label (Lee, 2013)	10.49	3.46	
AtlasRBF (Pitelis et al., 2014)	$8.10 (\pm 0.95)$	3.68 (± 0.12)	1.31
DGN (Kingma <i>et al.</i> , 2014)	$3.33 (\pm 0.14)$	$2.40 (\pm 0.02)$	0.96
DBM, Dropout (Srivastava et al., 2014)			0.79
Adversarial (Goodfellow et al., 2015)			0.78
Virtual Adversarial (Miyato et al., 2015)	2.12	1.32	$0.64~(\pm 0.03)$
Baseline: MLP, BN, Gaussian noise	$21.74 (\pm 1.77)$	$5.70 (\pm 0.20)$	$0.80 (\pm 0.03)$
Γ -model (Ladder with only top-level cost)	$3.06 (\pm 1.44)$	$1.53~(\pm 0.10)$	$0.78~(\pm 0.03)$
Ladder, only bottom-level cost	$1.09 (\pm 0.32)$	$0.90 (\pm 0.05)$	$0.59 (\pm 0.03)$
Ladder, full	$1.06 (\pm 0.37)$	0.84 (± 0.08)	$0.57 (\pm 0.02)$

Variational autoencoders

Later this week!

Generative adversarial networks

Goodfellow, I., Pouget-Abadie, J., Mirza, M., et al. [2014]. "Generative Adversarial Nets". In: *Advances in Neural Information Processing Systems 27*. Ed. by Z. Ghahramani, M. Welling, C. Cortes, et al. Curran Associates, Inc., pp. 2672–2680.

Salimans, T., Goodfellow, I. J., Zaremba, W., et al. [2016]. "Improved Techniques for Training GANs". In: *CoRR* abs/1606.03498.

Radford, A., Metz, L., and Chintala, S. [2016]. "Unsupervised representation learning with deep convolutional generative adversarial networks". In: *Proceedings of the International Conference on Learning Representations*.

Idea

- Learn to generate samples that imitate real data samples.
- Discriminator network: learn to tell generated samples from real dataset samples (binary classification).
- · Generator network: learn to fool the discriminator.

Setup

 $\mathbf{x} \sim p_{\mathsf{data}()}$, Dataset sample $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$, Noisy variable

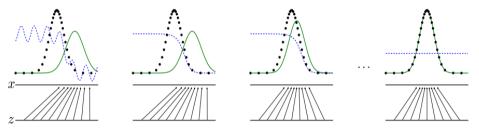
 $Dis(\cdot)$, Discriminator network $Gen(\cdot)$, Generator network

Training objective:

$$\min_{\text{Gen}} \max_{\text{Dis}} \mathbb{E}_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x})} \left[\log \text{Dis}(\mathbf{x}) \right] + \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} \left[\log(1 - \text{Dis}(\text{Gen}(\mathbf{z}))) \right]$$

GAN example

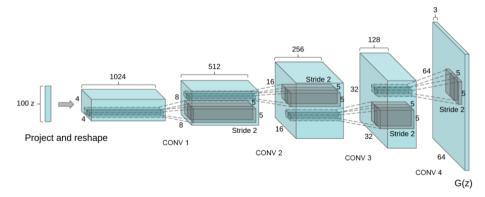
Near-convergence behavior on 1D data.



- Black dotted line: Data distribution, $p_{\mathsf{data}}(x) \sim \mathcal{N}(\cdot)$
- Green line: Generative distribution, Gen(x)
- Blue dashed line: Discriminative distribution
- *x*, black line: data space
- *z*, black line: *z*-space, $p_z(z) \sim \mathsf{Uniform}(\cdot)$

Convolutional decoder architecture

When generating images, the generator network dilutes high-dimensionsional features in exchange for increased resolution.



Semi-supervised GAN discriminator

For classification: Discriminator predicts K + 1 classes where the extra class represents the generated sample.

$$\begin{split} L &= -\mathbb{E}_{\boldsymbol{x}, y \sim p_{\text{data}}(\boldsymbol{x}, y)} [\log p_{\text{model}}(y | \boldsymbol{x})] - \mathbb{E}_{\boldsymbol{x} \sim G} [\log p_{\text{model}}(y = K + 1 | \boldsymbol{x})] \\ &= L_{\text{supervised}} + L_{\text{unsupervised}}, \text{ where} \\ L_{\text{supervised}} &= -\mathbb{E}_{\boldsymbol{x}, y \sim p_{\text{data}}(\boldsymbol{x}, y)} \log p_{\text{model}}(y | \boldsymbol{x}, y < K + 1) \\ L_{\text{unsupervised}} &= -\{\mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})} \log[1 - p_{\text{model}}(y = K + 1 | \boldsymbol{x})] + \mathbb{E}_{\boldsymbol{x} \sim G} \log[p_{\text{model}}(y = K + 1 | \boldsymbol{x})]\}, \end{split}$$

Semi-supervised GAN discriminator

For classification: Discriminator predicts K + 1 classes where the extra class represents the generated sample.

$$\begin{split} L &= -\mathbb{E}_{\boldsymbol{x}, y \sim p_{\text{data}}(\boldsymbol{x}, y)} [\log p_{\text{model}}(y|\boldsymbol{x})] - \mathbb{E}_{\boldsymbol{x} \sim G} [\log p_{\text{model}}(y = K + 1|\boldsymbol{x})] \\ &= L_{\text{supervised}} + L_{\text{unsupervised}}, \text{ where} \\ L_{\text{supervised}} &= -\mathbb{E}_{\boldsymbol{x}, y \sim p_{\text{data}}(\boldsymbol{x}, y)} \log p_{\text{model}}(y|\boldsymbol{x}, y < K + 1) \\ L_{\text{unsupervised}} &= -\{\mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})} \log [1 - p_{\text{model}}(y = K + 1|\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{x} \sim G} \log [p_{\text{model}}(y = K + 1|\boldsymbol{x})]\}, \end{split}$$

Model	Test error rate for			
	a given number of labeled samples			
	1000	2000	4000	8000
Ladder network [24]			$20.40 {\pm} 0.47$	
CatGAN [14]			$19.58 {\pm} 0.46$	
Our model	$21.83 {\pm} 2.01$	$19.61 {\pm} 2.09$	$18.63 {\pm} 2.32$	17.72 ± 1.82
Ensemble of 10 of our models	$19.22 {\pm} 0.54$	$17.25 {\pm} 0.66$	$15.59 {\pm} 0.47$	$14.87 {\pm} 0.89$

Semi-supervised GAN discriminator

For classification: Discriminator predicts K + 1 classes where the extra class represents the generated sample.

$egin{array}{lll} L = -\mathbb{E}_{m{x},y\sim p} \ = L_{ ext{supervised}} \end{array}$			$_{\text{lodel}}(y = K + 1 z)$	$\boldsymbol{r})]$
$L_{ ext{supervised}} = -\mathbb{E}_{oldsymbol{x},y\sim p}$		- m		
$L_{ ext{unsupervised}} = - \{ \mathbb{E}_{oldsymbol{x} \sim p_{ ext{d}}} \}$		· · · · · · · · · · · · · · · · · · ·	$\mathcal{E}_{\boldsymbol{x}\sim G}\log[p_{\mathrm{model}}]$	$y = K + 1 \boldsymbol{x})]\},$
Model	7) - <u>S</u> (m 🔣 S		r rate for	
	- C C A M		f labeled samples	
			4000	8000
Ladder network [24]			$20.40 {\pm} 0.47$	
CatGAN [14]			$19.58 {\pm} 0.46$	
Our model			$18.63 {\pm} 2.32$	17.72 ± 1.82
Ensemble of 10 of our models	$19.22 {\pm} 0.54$	$17.25 {\pm} 0.66$	$15.59 {\pm} 0.47$	$14.87 {\pm} 0.89$

Autoencoding beyond pixels using a learned similarity measure

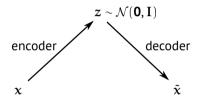
Larsen, A. B. L., Sønderby, S. K., Larochelle, H., et al. [2016]. "Autoencoding beyond pixels using a learned similarity metric". In: *Proceedings of the 33rd International Conference on Machine Learning (ICML)*.

ldea

- Element-wise loss function $\mathcal{L}(\mathbf{x}, \tilde{\mathbf{x}}) = \|\mathbf{x} \tilde{\mathbf{x}}\|^2$ is unsuitable for natural images.
- Why not try convnet features as a basis for measuring image similarity?
- Let's use features from a *generative adversarial network* to remain unsupervised.

Our building blocks

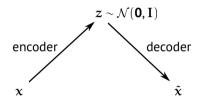
Variational autoencoder



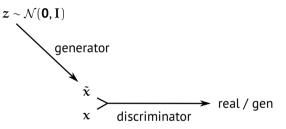
- Good for MNIST-style data.
- Doesn't scale to natural images because of element-wise similarity measures.

Our building blocks

Variational autoencoder



Generative adversarial network

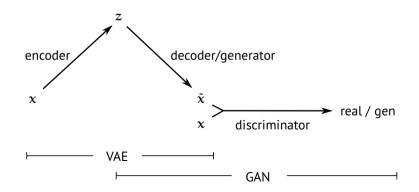


- Good for MNIST-style data.
- Doesn't scale to natural images because of element-wise similarity measures.

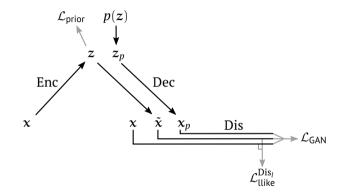
- Capable of generating natural looking images.
- No inference network.

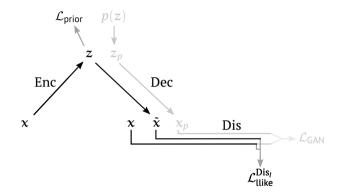
Combining VAEs with GANs

- Collapse the VAE decoder and the GAN generator into one network.
- Move the reconstruction error up in the discriminator network.
- Train both VAE and GAN simultaneously from scratch.



Implementation details



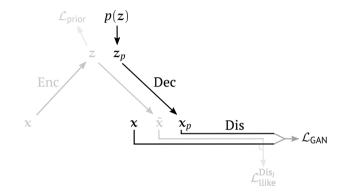


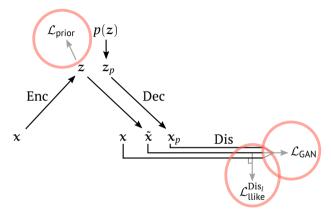
Pixel-based observation model:

 $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mathbf{x} \mid \tilde{\mathbf{x}}, \mathbf{I})$

Feature-based observation model:

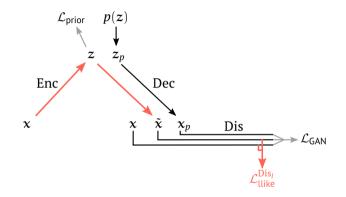
$$p(\text{Dis}_l(\mathbf{x}) \mid \mathbf{z}) =$$



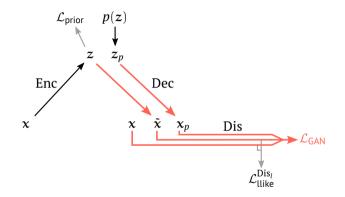


Training objective:

$$\mathcal{L} = \underbrace{\mathcal{L}_{\mathsf{prior}} + \mathcal{L}_{\mathsf{llike}}^{\mathrm{Dis}_l}}_{\mathcal{L}_{\mathsf{VAE}}} + \mathcal{L}_{\mathsf{GAN}}$$



Update only encoder/decoder networks wrt. reconstruction error.



Update only decoder/discriminator networks wrt. adversarial loss.

Experiments

Mainly using 64×64 images from the CelebA dataset. [Liu et al. 2015]



Models

- VAE Plain variational autoencoder with pixel-wise image similarity.
- VAE_{Dis}, VAE with feature-wise similarities from a pretrained GAN.
- VAE/GAN Our hybrid method.
- GAN Plain generative adversarial network.

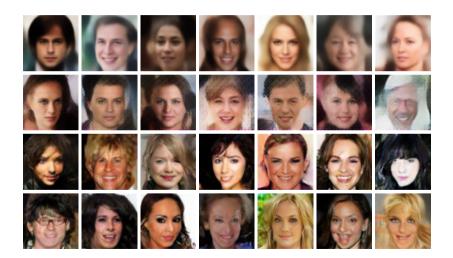
Samples

VAE

 $\mathsf{VAE}_{\mathrm{Dis}_l}$

VAE/GAN

GAN



Reconstructions

Input

VAE

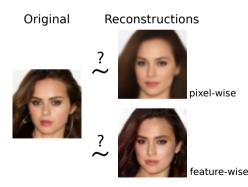
 $\mathsf{VAE}_{\mathrm{Dis}_l}$

VAE/GAN



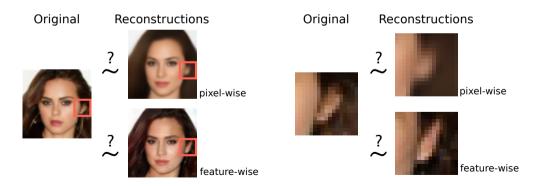
What is a good image reconstruction?

- Human visual perception is not pixel-perfect.
- Should we require perfect pixels from our model?



What is a good image reconstruction?

- Human visual perception is not pixel-perfect.
- · Should we require perfect pixels from our model?
- Arguably, semantic concepts are more important than pixels.



Visual attribute vectors

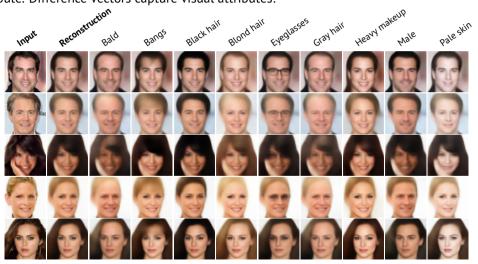
After unsupervised training, we calculate the mean z difference for images with/without an attribute. Difference vectors capture visual attributes:



VAE/GAN

Visual attribute vectors

After unsupervised training, we calculate the mean z difference for images with/without an attribute. Difference vectors capture visual attributes:



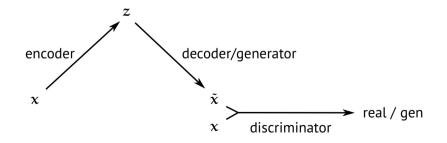
Interpolations in latent space

I sent my adviser into latent space and sampled a few visual attribute vectors:



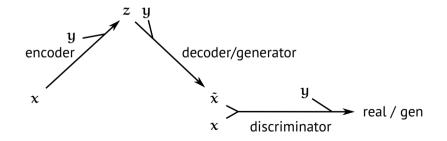
Quantitative results: Recognizability of generated attributes

Idea: Learn a conditional model p(x | y, z) where y are visual attributes. Generate images from sampled z and attribute queries y.



Quantitative results: Recognizability of generated attributes

Idea: Learn a conditional model p(x | y, z) where y are visual attributes. Generate images from sampled z and attribute queries y.



Ouantitative results: Recognizability of generated attributes

Idea: Learn a conditional model $p(\mathbf{x} | \mathbf{y}, \mathbf{z})$ where \mathbf{y} are visual attributes. Generate images from sampled z and attribute queries \mathbf{u} .



Prominent attributes: White. Mouth Closed, Male, Curly Hair, Eyes Open, Pale Skin, Frowning, Pointy Nose, Teeth Not Visible



VAE

GAN



Ouerv

VAE

GAN



Prominent attributes: White, Male, Curly Hair, Frowning, Pointy Nose, Eyeglasses, Narrow Eves. Teeth Not Visible. Senior



Quantitative results: Recognizability of generated attributes

Idea: Learn a conditional model p(x | y, z) where y are visual attributes. Generate images from sampled z and attribute queries y.

Evaluation: Attribute prediction error from a separately trained regressor convnet.

Model	Cosine similarity (best of 10)	Mean squared error
LFW test set	0.9193	14.1987
VAE	0.9030	$\textbf{27.59} \pm \textbf{1.42}$
GAN	0.8892	$\textbf{27.89} \pm \textbf{3.07}$
VAE/GAN	0.9114	$\textbf{22.39} \pm \textbf{1.16}$

Final words

Take-home messages

- You can learn useful structures from fragile error signals.
- Good disentangled representations can make the discriminative task easier.

Thanks