Advanced Topics in Machine Learning (deep generative modelling)

Lecture 6: Representation learning and evaluation

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Outline of Lecture 6

Representations and evaluation:

- Review of generative model families
  - Conditional models
- Representation learning
  - Representations from deep networks
  - Probing representations
- Evaluation of generative models
  - Likelihood-based evaluation
  - Sample-based evaluation

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Discriminative modelling is a special case of conditional modelling where the conditioning variable is the input and the output is a label (or class).

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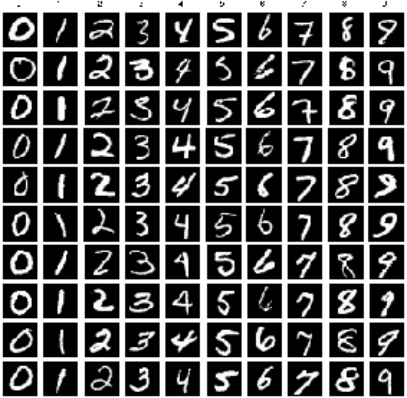

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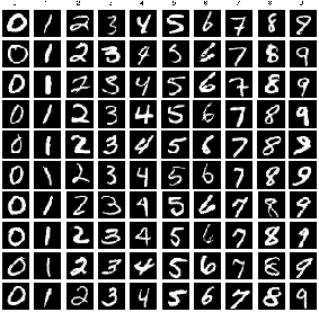
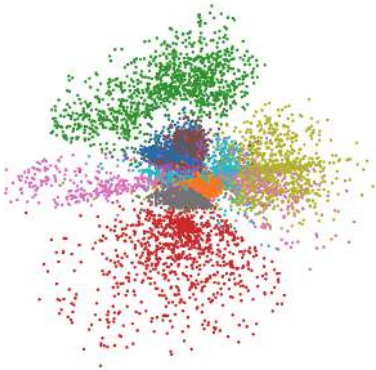
Encodings from generative models

Recall: latent variables 'encode' the cdata



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



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These representations are generally not identifiable and emerge only as a side effect of data modelling:

- No way to know which of many possible representations we get
- Compose with invertible transformations to get other representations that are equally good

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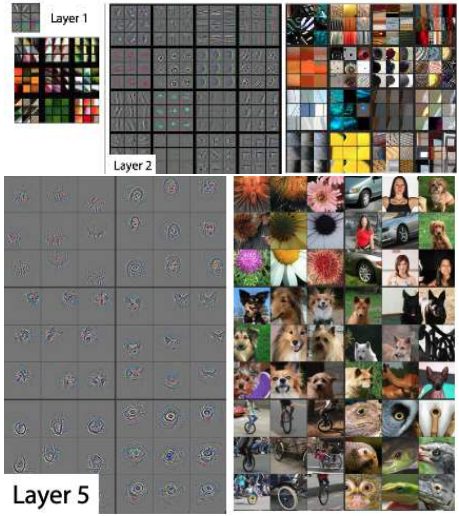

[Zeiler and Fergus, 2014]

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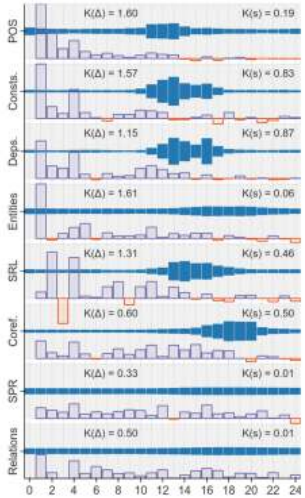
- In 'large' language models, the hidden units correspond to a variety of linguistic features



[Tenney et al., 2019]

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  - Masked language models are a special case of this
  - Related to diffusion modelling (in two weeks)

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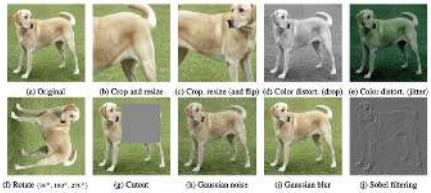
  - Take a **batch** of data points $\{x_1, \ldots, x_n\}$
  - Apply a random transformation, to which the representation should be invariant, to get $\{\tilde{x}_1, \ldots, \tilde{x}_n\}$
  - Somehow enforce that $f_\theta(x_i)$ is close to $f_\theta(\tilde{x}_i)$ but far from the $f_\theta(x_j)$ for $j \neq i$



[Chen et al., SimCLR, 2020]

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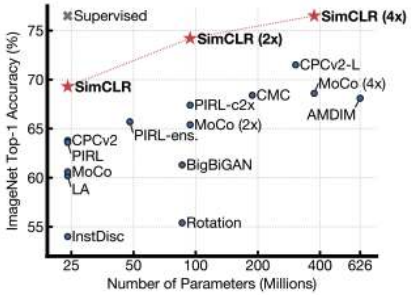

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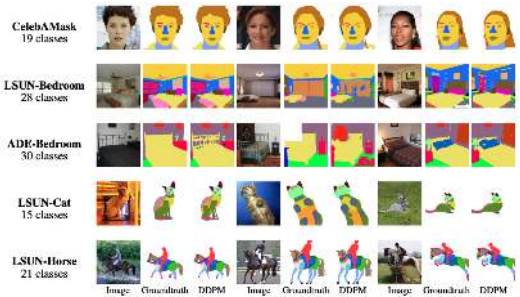

[Baranchuk et al., 2022]

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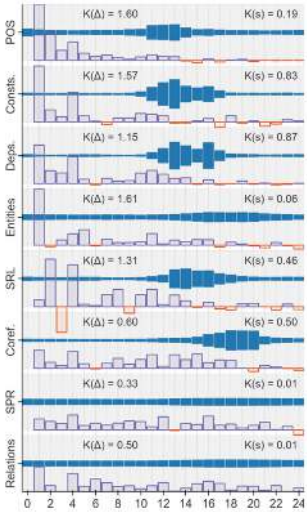

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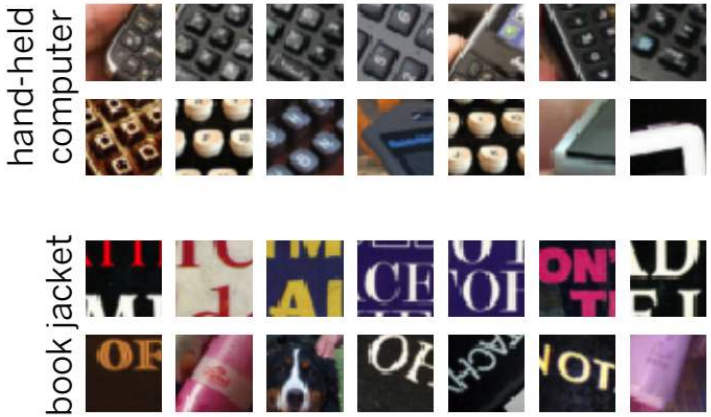

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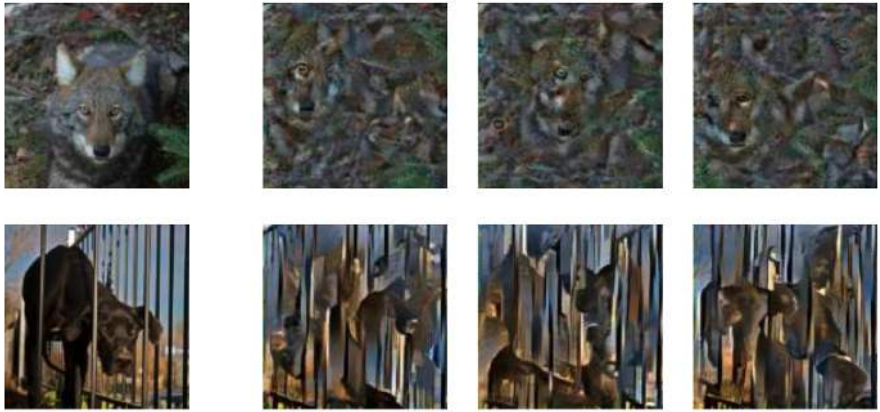

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- Very large models may contain 'circuits' responsible for approximate execution of simple symbolic routines (copying, memory, . . .)
  - Controversial: you can find a circuit for anything if you look hard enough. . .

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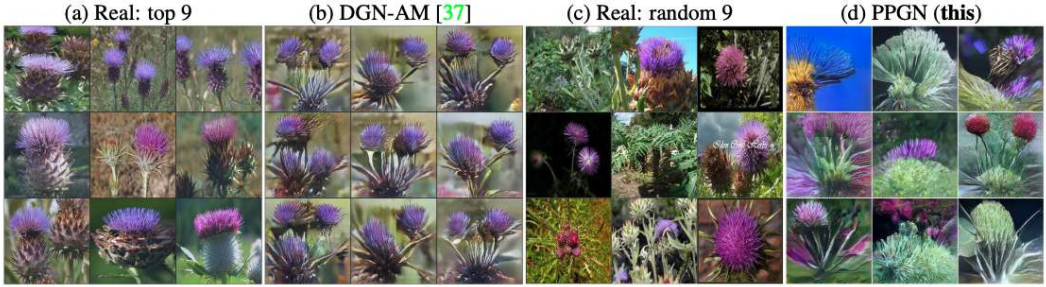

[Nguyen et al., 'Plug & Play Generative Networks', 2017]

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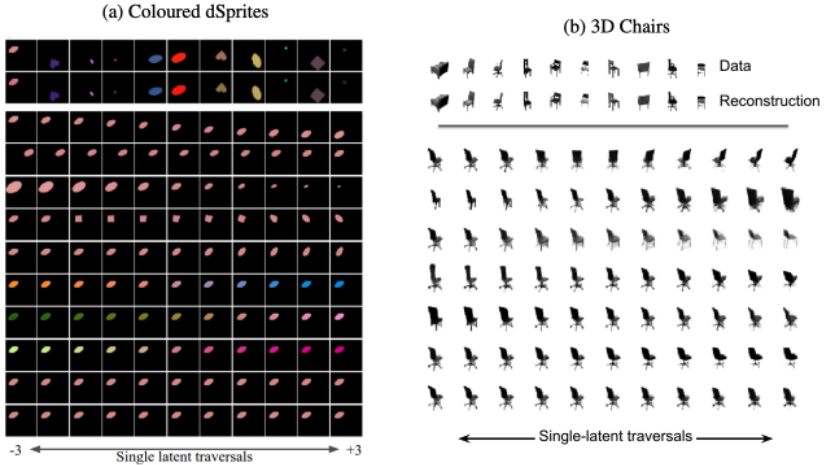

[Burgess et al., Understanding disentangling in β-VAE, 2018]

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  - Changing the sentiment of a text while keeping the content
- **Disentanglement:** different dimensions of the representation correspond to different properties of the data, can be independently controlled
  - In principle, should allow **compositionality** of representations $\rightsquigarrow$ **systematic generalisation**
  - Active area of research (but somewhat lacking in clear definitions and metrics)

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- Often reported in 'bits per dimension': $\mathrm{BPD} = \frac{\mathrm{NLL}}{d \log 2}$ for data in $\mathbb{R}^d$
  - Best BPDs for MNIST are ~ 1 (note $\log_2 256 = 8$ for a uniform distribution over 8-bit pixel values),
  - Best bits per character for character-level language modelling: ~ 1 bit per character (note $\log_2 27 \approx 4.8$ bpc for a uniform distribution)

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- In some domains, considered to be 'saturated' (no longer meaningfully distinguishes between models)

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- Compute a divergence between the **empirical** distributions $\frac{1}{n}\sum_{i=1}^{n} \delta_{x_i}$ and $\frac{1}{m}\sum_{j=1}^{m} \delta_{\tilde{x}_j}$

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Often, first map to a representation space, that is, compare $\{f(x_1), \ldots, f(x_n)\}$ to $\{f(\tilde{x}_1), \ldots, f(\tilde{x}_m)\}$ for some pretrained representation f

Sample-based evaluation

Compare samples from the model to *samples* from the data distribution

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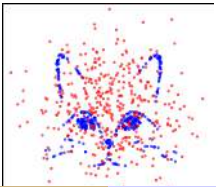
- What divergence should be used?



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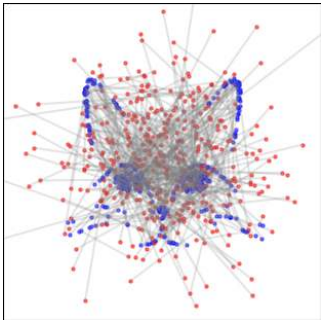

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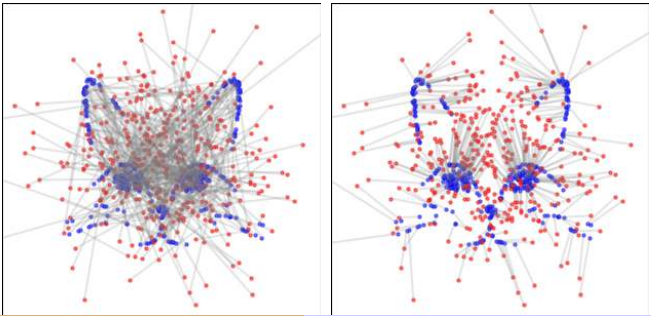

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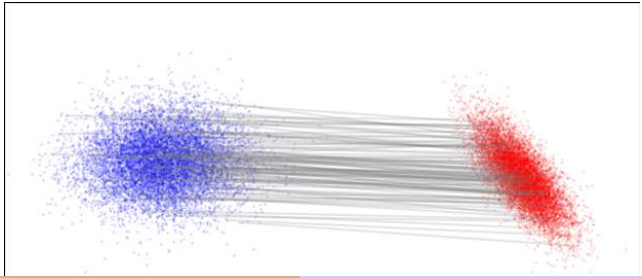

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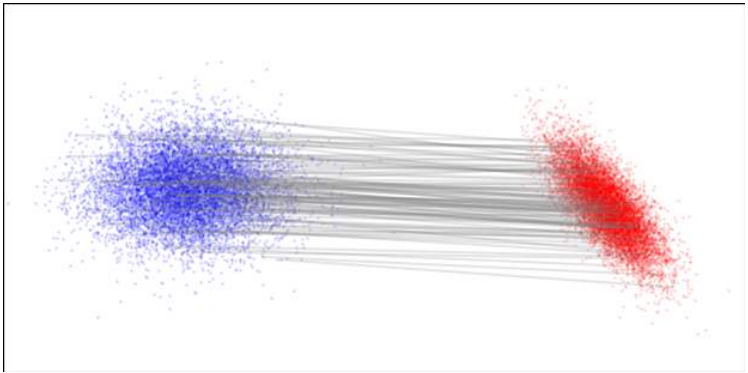
- Can also be defined for densities or different numbers of samples
- Many generalisations and rich mathematical theory, connections throughout ML
  - Replace the squared distance with some other cost function
  - Add entropy regularisation ($\rightsquigarrow$ **Sinkhorn distance**)
  - Connections with diffusion modelling, GANs, optimisation (see [Peyré, 'Optimal and Diffusion Transports in Machine Learning'] for interesting examples)

Fréchet Inception Distance

The Wasserstein distance between two Gaussian distributions has a closed-form solution:

$$\mathcal{W}_2^2(\mathcal{N}(\mu_1, \Sigma_1), \mathcal{N}(\mu_2, \Sigma_2)) = \|\mu_1 - \mu_2\|^2 + \mathrm{Tr}\left(\Sigma_1 + \Sigma_2 - 2\left(\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2}\right)^{1/2}\right)$$



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- FID is the Wasserstein distance between these two Gaussians

Fréchet Inception Distance

CIFAR-10

Model	NFE↓	FID↓
BigGAN [3]	1	14.73
TransGAN [87]	1	9.26
ViTGAN [42]	1	6.66
DDGAN [94]	4	3.75
Diffusion StyleGAN2 [90]	1	3.19
StyleGAN2 + ADA [30]	1	2.42
StyleGAN3-R + ADA [32, 25]	1	10.83
DDPM [20]	1000	3.21
DDIM [76]	50	4.67
VE [78, 33]	35	3.11
VP [78, 33]	35	2.48
Ours—Config E	1	1.96

ImageNet (64×64)

Model	NFE↓	FID↓
BigGAN-deep [3]	1	4.06
DDPM [20]	250	11.0
DDIM [76]	50	13.7
ADM [7]	§250	2.91
EDM [33]	79	2.23
CT [79]	2	11.1
CD [79]	3	4.32
iCT-deep [77]	2	2.77
DMD [96]	1	2.62
Ours—Config E	1	2.09

from [Huang et al., 'The GAN is Dead; Long Live the GAN!', 2025]

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- Various metrics intended to better capture quality, diversity, and novelty, *e.g.*, feature likelihood divergence (FLD)
- For images: LPIPS (not a distributional distance, but a distance between individual samples, correlated with human judgement)

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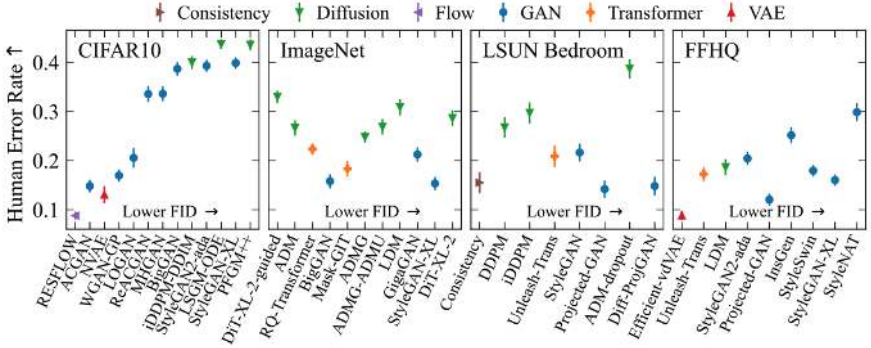

[Stein et al., 'Exposing flaws of generative model evaluation metrics. . . ', 2023]

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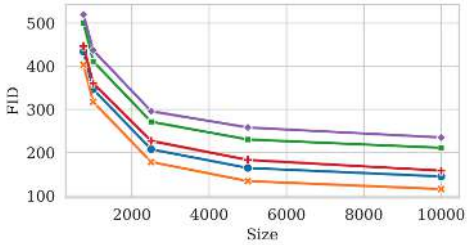

[Jiralerspong et al., 'Feature Likelihood Divergence...', 2023]

Conclusion and looking ahead

- Representation learning is a side effect of generative model training
- Evaluation of generative models requires selecting a metric that is appropriate for the model and the domain and reflection on the features whose distribution is being compared
- Likelihood-based metrics not always appropriate, especially for very high-dimensional data where deep features are more important than low-level details
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- Sample-based metrics can be more correlated with human judgement, but are often noisy and rely on a good choice of representation
- Next time: a different view on evaluating 'generative AI'