# Generative models

how they work and how to train them

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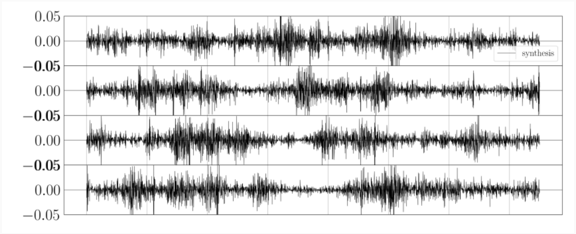
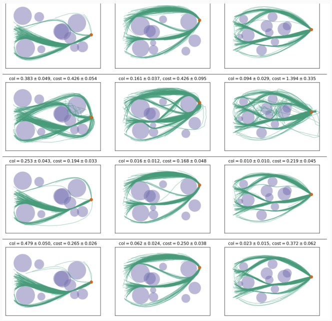
## Intro: Generative Modelling

## $x_*^1, \ldots, x_*^n$: dataset drawn from an unknown distribution $\rho_*$ ("target")





The two goals of generative modelling:

1. Generate ‘new’ samples from $\rho_*$ (direct problem)
2. Find a ‘good’ estimator $\hat{\rho}_*$ for $\rho_*$ (inverse problem)

**Examples of generative models**: EBMs, GANs, VAEs, Normalizing Flows, Neural ODEs, Noise Contrastive Estimation, Diffusions, Flow matching, Consistency models

## Energy-Based Models

## Defining EBMs

$U_\theta : \mathbb{R}^d \to \mathbb{R}_+ =$ parametrized family of functions ("model energies")

Definition of the model densities:

$$\rho_\theta(x) = \frac{e^{-U_\theta(x)}}{Z_\theta} \qquad\qquad Z_\theta = \int e^{-U_\theta(x)} dx.$$

## Defining EBMs

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Examples:

- $U_\theta(x) = \langle x, \theta x \rangle$ with $\theta$ a square matrix: centered Gaussian distributions
- $U_\theta(x) = |x - \theta|$: family of Laplace distributions
- $U_\theta(x)$ = a complicated neural network with parameters $\theta$: deep EBMs

## Training an EBM

The goal is to find the optimal $\theta_*$ achieving the best 'fit' between the model $\rho_\theta$ and the true unknown density $\rho_*$.

$$\theta_* \in \arg\min \mathrm{dist}(\rho_*, \rho_\theta)$$

**Q:** how do we choose the distance?

## Using an EBM

Once $U_{\theta_*}$ has been trained, new synthetic samples are obtained by sampling from the distribution

$$\hat{\rho}_* = \rho_{\theta_*} = \frac{e^{-U_{\theta_*}}}{Z_{\theta_*}}.$$

This step typically needs MCMC methods such as Langevin:

$$X_{\tau+1} = X_\tau - \eta \nabla_x U_{\theta_*}(X_\tau) + \sqrt{\eta}\xi_\tau \qquad \xi_\tau \sim \mathcal{N}(0, I)$$

This is called “implicit generation” [Du and Mordatch 19].

## Advantages of EBMs

- **Simplicity.** Only one neural network $U_\theta$
  $\rightarrow$ *VAEs and GANs require at least two!*
- **Flexibility.** We can exploit the tradeoff between quality and cost
  $\rightarrow$ *impossible with feed-forward generators such as GANs or NFs*
- **Compositionality.** Combining different EBMs is as simple
  $\rightarrow$ *just add the energies*
- **Reusability.** Can be used to help various other tasks
  $\rightarrow$ *inpainting, importance sampling, OOD detection...*

## Choosing the right loss for EBM learning

**Kullback-Leibler divergence $\leftrightarrow$ max-likelihood**

$$\begin{aligned}\mathrm{dist}(\rho_\theta, \rho_*) &= \mathbb{E}_{X\sim\rho_*} \log \rho_*(X)) - \log \rho_\theta(X) \\ &\approx \mathrm{cst} - \frac{1}{n} \sum \log \rho_\theta(x_i^*)\end{aligned}$$

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**Fisher divergence**

$$\begin{aligned}\mathrm{dist}(\rho_\theta, \rho_*) &= \mathbb{E}_{X\sim\rho_*} |\nabla \log \rho_*(X) - \nabla \log \rho_\theta(X)|^2 \\ &\approx \frac{1}{n}\sum |\nabla \log \rho_*(x_i^*) - \nabla \log \rho_\theta(x_i^*)|^2\end{aligned}$$

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**Other losses?**

Bregman, NCE loss, etc.

## Training procedures
## I: max-likelihood

## Gradient ascent on Energy-Based Models

Goal: maximize $L(\theta) = \mathbb{E}_*[\log \rho_\theta] = -\mathbb{E}_*[U_\theta + \log Z_\theta]$

$$\nabla_\theta L(\theta) = -\mathbb{E}_*[U_\theta] - \nabla \log Z_\theta$$

Computation of $\nabla_\theta \log Z_\theta$:

$$\frac{\nabla_\theta Z_\theta}{Z_\theta} = \int -\nabla_\theta U_\theta(x) e^{-U_\theta(x)} \frac{1}{Z_\theta} dx = -\mathbb{E}_\theta[\nabla_\theta U_\theta]$$

**Gradient of the log-likelihood**

$$\nabla_\theta L(\theta) = \mathbb{E}_\theta[\nabla_\theta U_\theta] - \mathbb{E}_*[\nabla_\theta U_\theta]$$

Gradient ascent with stepsize $\eta > 0$ :

$$\theta_{t+1} - \theta_t = \eta \times \left(\mathbb{E}_{\theta_t}[\nabla_\theta U_{\theta_t}] - \mathbb{E}_*[\nabla_\theta U_{\theta_t}]\right)$$

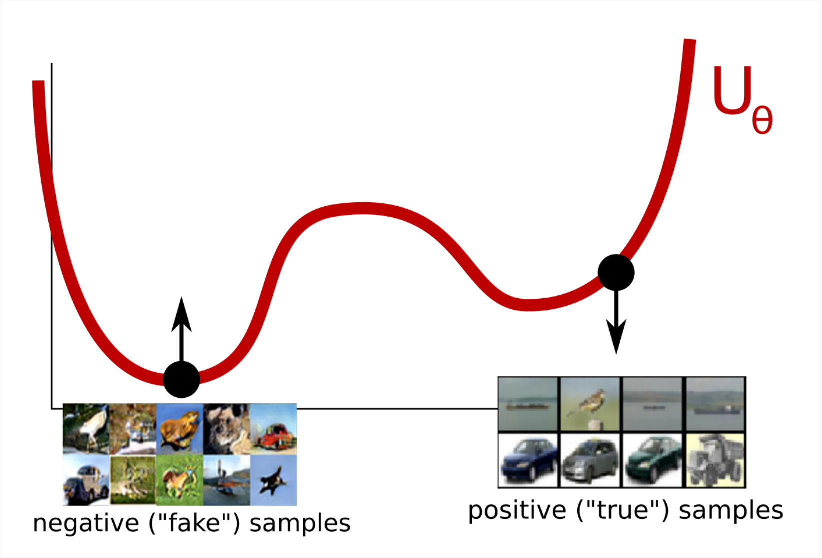
$$\nabla_\theta L(\theta) = \nabla_\theta \left(\mathbb{E}_\theta[U_\theta(X)] - \mathbb{E}_*[U_\theta(X)]\right)$$

$\mathbb{E}_*[U_\theta]$
$x_i^* =$ "positive samples"
from $\rho_*$
$\approx \frac{1}{n}\sum_i U_{\theta_t}(x_*^i)$

$\mathbb{E}_{\theta_t}[U_\theta]$
$y_i =$ "negative samples"
from $\rho_{\theta_t}$
$\approx \frac{1}{n}\sum_i U_{\theta_t}(y_i)$

**"contrastive learning" :**

- pull down the energy of positive samples, $\mathbb{E}_*[U_\theta]$
- pull up the energy of negative samples, $\mathbb{E}_{\theta_t}[U_\theta]$


$U_\theta$
negative ("fake") samples
positive ("true") samples

## MCMC sampling is too costly

**Q:** at each gradient step, how do we get the negative samples for computing $\mathbb{E}_\theta[U_\theta]$?

**A:** using MCMC/Langevin methods...

At step $t$, initialize $X_0^i$ ("walkers"), then for $\tau = 0, \dots, T_{mix}$,

$$X_{\tau+1}^i = X_\tau^i - \eta \nabla_x U_\theta(X_\tau^i) + \sqrt{2\eta}\xi_\tau$$

and estimate

$$\mathbb{E}_{\theta_t}[U_{\theta_t}] \approx \frac{1}{N_{walkers}} \sum_{i=1}^{N_{walkers}} U_{\theta_t}(X_{T_{mix}}^i).$$

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If $T_{mix}$ is large, this is too costly.

Each gradient ascent step will consume $T_{mix}$ MCMC sampling steps for each of the $N_{walkers}$ chains!

## Contrastive Divergence with $k$ steps (CD-$k$), [Hinton 2005]

- don't let the chain reach $T_{mix}$ steps. Use only $k$ steps ($k = 1$).
- initialize each chain directly at the training points $\{x_*^i\}$.

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[Hyvarinen 2007]
in the limit of small noise $\eta \to 0$, CD-1 = score matching.

[Yair and Michaeli 20] CD-1 is an adversarial game

[Agoritsas et al 23] Effect of non-convergent sampling

## Persistent Contrastive Divergence (PCD), [Tieleman 2008]

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Practically: maintain a set of *walkers* $X_t^i$. At step $t+1$,
1) approximate $\mathbb{E}_{\theta_t}[U_{\theta_t}] \approx \frac{1}{n}\sum_{i=1}^{N} U_{\theta_t}(X_t^i)$,
2) compute $\theta_{t+1}$ using the approximation,
3) move the walkers with $X_{t+1} = X_t - \eta \nabla U_{\theta_{t+1}}(X_t) + \sqrt{2\eta}\xi$

$\Rightarrow$ leads to mode collapse.

## Replay buffer techniques [Du and Mordatch 2019]

- don't let the chain reach $T_{mix}$ steps. Use only $k$ steps ($k = 1$).
- ~~Initialize each chain directly at the training points $\{x_*^i\}$.~~
- ~~initialize each chain directly where the previous chain ended.~~
- initialize, sometimes from the past, sometimes from pure noise

$+$ many other tricks.

## Training procedures
## II: alternative losses

a Noise Contrastive methods

b GANs

c Score Matching

d Denoising score matching

## a. Noise Contrastive Estimation [Gutmann & Hyvarinen 2010]

Let $\mu$ be a known density and $y_i \sim \mu$ be iid.

**Idea**: train a binary classifier with logistic regression to distinguish between `true` samples $x_i^*$ and `fake` samples $y_i$.

**Bayes' rule** gives the optimal classifier $D_{\mathrm{opt}}$:

$$D_{\mathrm{opt}}(x) = \mathbb{P}(\texttt{true} \mid x) = \frac{p(x \mid \texttt{true})}{p(x \mid \texttt{fake}) + p(x \mid \texttt{true})}$$

$$= \frac{\rho_*(x)}{\rho_*(x) + \mu(x)}$$

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Goal: maximize $R(\theta) = \sum_{i=1}^n \log D_\theta(x_i^*) + \log(1 - D_\theta(y_i))$.

Set $D_\theta(x) = F_\theta(x)/(F_\theta(x) + \mu(x))$ with $F_\theta(x) = e^{-U_\theta(x) + c_\theta}$.

If $D_{\theta_*} \approx D_{\mathrm{opt}}$ then $F_{\theta_*} \approx \rho_*$

The normalization $\int e^{-U_\theta + c_\theta} = 1$ is automatic!

## b. Limitations of NCE and GANs

- if $\mu$ is too close to $\rho_*$ then training the classifier is too difficult
- if $\mu$ is too different to $\rho_*$ then classifying is too easy, there are near-optimal classifiers very different than the optimal one

**the GAN idea**

$\Rightarrow$ also train a "fake sample generator", say $\mu_\beta$, instead of using always the same fixed generator $\mu$

GAN objective: $\min_\theta \max_\beta \mathbb{E}_*[\log D_\theta] + \mathbb{E}_{\mu_\beta}[\log(1 - D_\theta)]$

Min-Max problems are hard.

## c. Score Matching [Hyvarinen 2005]

Goal: minimize $SM(\theta) = \mathbb{E}_*[|\nabla \log \rho_\theta - \nabla \log \rho_*|^2]$.

Hyvarinen 2005

$$SM(\theta) = \mathrm{cst} + \mathbb{E}_*[|\nabla \log \rho_\theta|^2 + 2\Delta \log \rho_\theta].$$

- Parametrize the score $\nabla \log \rho_\theta$ with a neural network $s_\theta$
- Minimize $\mathbb{E}_*[|s_\theta|^2 + 2\nabla_x \cdot (s_\theta)]$ using gradient descent

Problem 1: for $\nabla_\theta SM(\theta)$ we need to compute "double derivatives" like

$$\nabla_\theta \nabla_x \cdot s_\theta(x).$$

Problem 2: inferring $\log \rho$ from $s_\theta \approx \nabla \log \rho_\theta$ ?

**Proof of Hyvarinen's identity:** it's just an integration by parts.

For $p, q$ two smooth densities with fast decay at $\infty$,

$$\begin{aligned}
\mathbb{E}_p[|\nabla \log p - \nabla \log q|^2] &= \int p|\nabla \log p - \nabla \log q|^2 \\
&= \int p|\nabla p/p - \nabla q/q|^2 \\
&= c_p + \int p|\nabla/q|^2 - 2\int \nabla p \cdot \nabla \log q \\
&= c_p + \int p|\nabla \log q|^2 + 2\int p\nabla \cdot \nabla \log q \\
&= c_p + \mathbb{E}_p[|\nabla \log q|^2 + 2\Delta \log q]
\end{aligned}$$

## d. Denoising Score Matching [Vincent 2009]

Let us corrupt the original samples with noise:

$$y_i^* = x_i^* + \epsilon_i \qquad \epsilon_i \sim \mathcal{N}(0, \sigma^2)$$

distribution of $y_i^* = \rho_* * \mathcal{N}$.

Vincent 2009

$$SM(\theta) = \mathrm{cst} + \mathbb{E}_{X \sim \rho_*, \varepsilon \sim g}[|\nabla \log g(\varepsilon) - \nabla \log \rho_\theta(X + \varepsilon)|^2].$$

- Parametrize the score of the noisy distribution with $s_\theta$ (NN)
- Minimize $\mathbb{E}[|\epsilon/\sigma - s_\theta(X + \epsilon)|^2]$
- $\Rightarrow$ no double derivatives!

## Limitations

1) In the presence of high energy barriers, SM methods and variants cannot learn the relative weights of the modes and/or lead to mode collapse.

2) The score $s_{\theta_*} \approx \nabla \log \rho_*$ does not give direct access to the density!

3) Results were good... but not as good as GANs

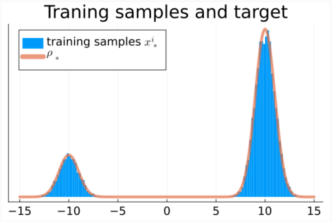
## Training procedures III: some insights from toy models

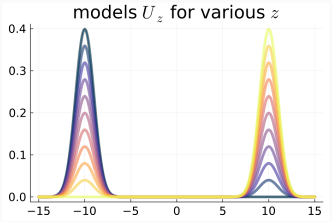
**Model: all gaussian mixtures with modes $a = -10, b = 10$:**

$$U_z(x) = -\log\left(e^{-|x-a|^2/2} + e^{-z}e^{-|x-b|^2/2}\right)$$

$$Z_z = (1 + e^{-z})\sqrt{2\pi}$$

$$\rho_z(x) = \frac{e^{-|x-a|^2/2} + e^{-z}e^{-|x-b|^2/2}}{(1 + e^{-z})\sqrt{2\pi}}$$





Target: $\rho_* = \rho_{z_*}$ for some $z_*$ with $q_* = \frac{e^{-z_*}}{1+e^{-z_*}} \approx 0.8$.

## Useful approximations

$$\nabla_x U_z(x) = \frac{(x-a)e^{-(x-a)^2/2} + e^{-z}(x-b)e^{-(x-b)^2/2}}{e^{-(x-a)^2/2} + e^{-z}e^{-(x-b)^2/2}}$$

$$\approx (x-a)1_{x \text{ close to } a} + (x-b)1_{x \text{ close to } b}$$

---

$$\nabla_z U_z(x) = e^{-z}e^{-(x-b)^2/2}/U_z(x) \approx 1_{x \text{ is close to } b}$$

---

$$\forall z, w \qquad \mathbb{E}_w[\nabla_z U_z] \approx \mathbb{P}_w(\text{ mode } b) = \frac{e^{-w}}{1+e^{-w}}$$

Gradient flow (continuous version of the discrete gradient descent):

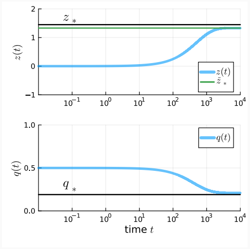
$$\dot{z}(t) = -\nabla_z \, \mathrm{loss}(\rho_*, \rho_{z(t)})$$

where $\mathrm{loss}$ is one of the various objectives above.

## Success of max-likelihood

$$\begin{aligned}\dot{z}(t) &= \mathbb{E}_{z(t)}[\nabla_z U_{z(t)}] - \mathbb{E}_{z_*}[\nabla_z U_{z(t)}] \\ &\approx \frac{e^{-z(t)}}{1+e^{-z(t)}} - \frac{e^{-z_*}}{1+e^{-z_*}}.\end{aligned}$$

Clearly this system converges towards its unique FP $z(t) = z_*$.



## Failure of score matching

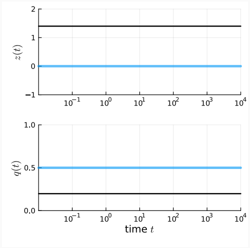
$$\dot{z}(t) = -\nabla_z SM(z) = \nabla_z \mathbb{E}_{z_*}[|\nabla \log \rho_{z(t)} - \nabla \log \rho_{z_*}|^2]$$

Remember that

$$\nabla \log \rho_z(x) \approx (x-a)1_{x \text{ close to } a} + (x-b)1_{x \text{ close to } b}$$

$\Rightarrow \nabla \log \rho_z(x)$ does not depend on $z$, hence $\nabla_z SM(z) \approx 0$.

This leads to the "no learning" phenomenon $\dot{z}(t) \approx 0$



## Mode collapse in PCD

Here the negative samples are generated using

$$dX_t = -\nabla_x U_{z(t)}(X_t)dt + \sqrt{2}dB_t$$

Remember that

$$\nabla_x U_z(x) \approx (x-a)1_{x \text{ close to } a} + (x-b)1_{x \text{ close to } b}$$

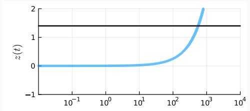
$X_t$ close to $b \Rightarrow dX_t \approx -(X_t - b)dt + \sqrt{2}dB_t$: Ornstein-Uhlenbeck
$X_t$ close to $a \Rightarrow dX_t \approx -(X_t - a)dt + \sqrt{2}dB_t$: Ornstein-Uhlenbeck

*There is no transfer of walkers between modes a and b!*

The distribution of $X_t$ does not change and is equal to $\rho_{z(0)}$:

$$\dot{z}(t) \approx \frac{e^{-z(0)}}{1+e^{-z(0)}} - \frac{e^{-z_*}}{1+e^{-z_*}} = \mathrm{cst}$$

This leads to mode collapse, $z(t) \to \pm\infty$.



Thanks for the invitation!

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## Some references (with links)

How to train your EBMs (Song & Kingma)

Score Matching (Hyvarinen)

Denoising score matching (Vincent)

Noise contrastive estimation (Gutman and Hyvarinen)

Conditional NCE (Ma and Collins)

Improved CD (Du et al.)

Implicit generation (Du et al.)

Reduce, Reuse, Recycle (Du et al.)

Efficient training of EBMs (Carbone et al.)

From SM to diffusion models (Song and Ermon)