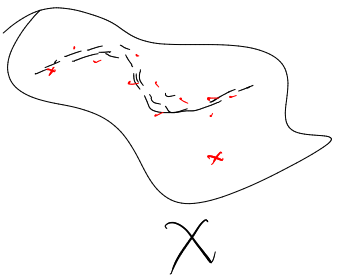
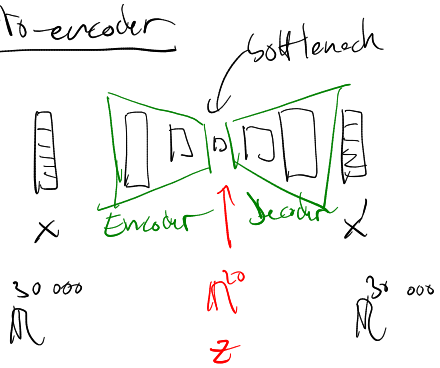
Generative models

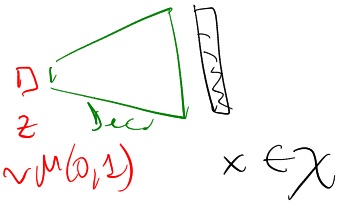


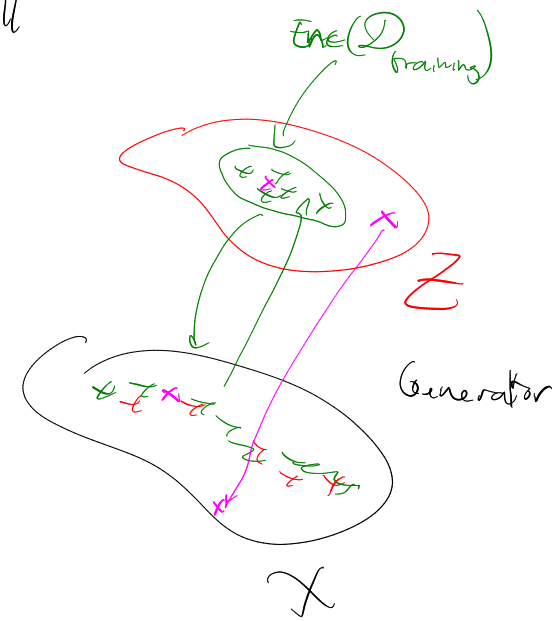
$\mathcal{X}$

Auto-encoder

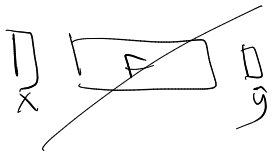


Loss: $\|x' - x\|$

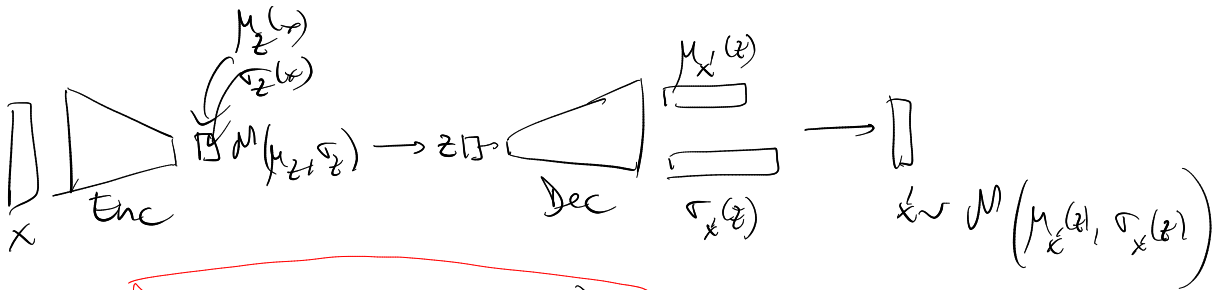




Variational Auto-encoder (VAE)



parametrized family of distributions $\Rightarrow$ stochastic network

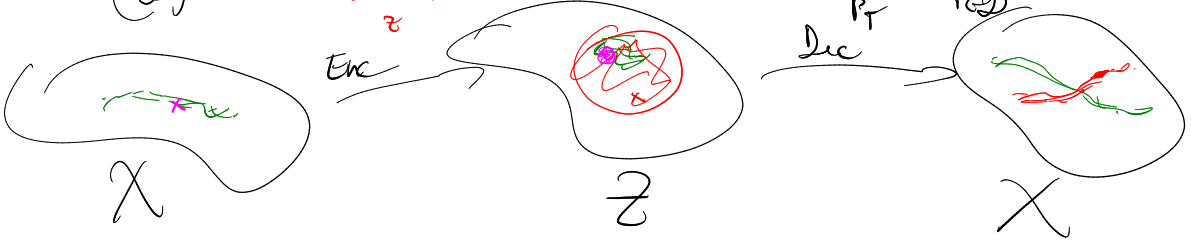


Training criterion: $KL(P_{Target} \| P_{Generated})$ $\rightarrow$ ELBO $\rightarrow$ Monte Carlo approximation

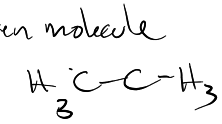
$\int p_T \rightarrow \sum_{i \in D}$

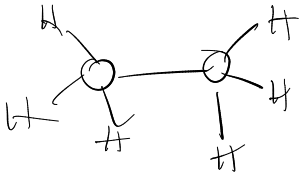
(D) $\quad$ $Dec(\mathcal{N}(0,1))$

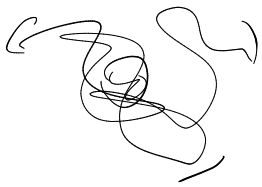
Generation: sample $z \sim \mathcal{N}(0,1)$



ex (not common) given molecule







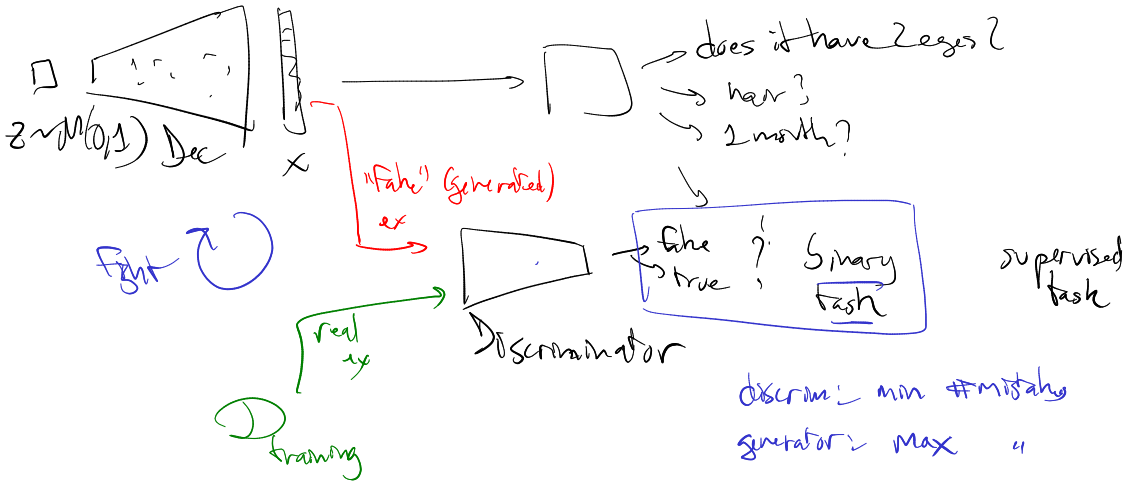
distribution of all 3D conformations

- target distribution: Boltzmann distribution

$$p(c) \propto e^{-\beta E(c)}$$

usual ex:  → empirically estimate $p(x)$

Adversarial setting: { GAN: Generative Adversarial Networks; DANN: Domain-Adversarial NN



discrim: min #mistakes

generator: max "

→ Linked to Kolmogorov test

Extension: Wasserstein GAN (WGAN)

Optimal transport

Kantorovich-Rubinstein duality

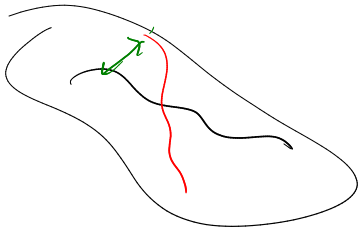
$$OT(P_G, P_T) = \sup_{f,\ \|f\| \le 1 \text{ Lipschitz}} \mathbb{E}_{x \sim P_G}[f(x)] - \mathbb{E}_{x \sim P_T}[f(x)]$$

(P_G: generated, P_T: target)

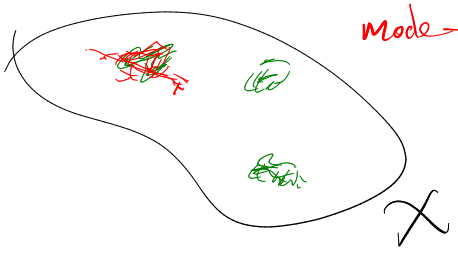
"weight-clipping"

∇-penalty

$$+\left(\|\nabla_x f\| - 1\right)^2$$

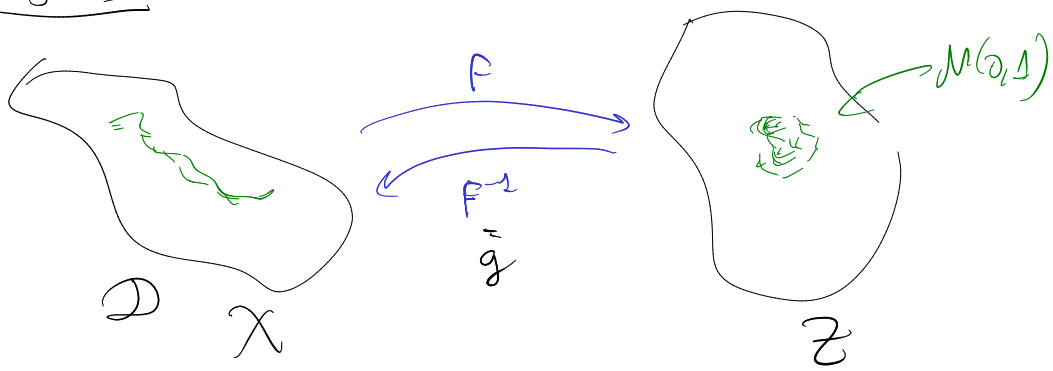


Issue:



mode-drop: no feedback about parts of P_{target} not sampled

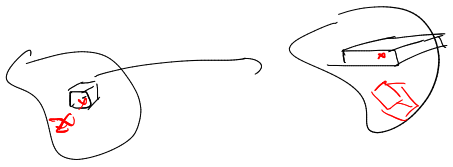
Normalizing flows



- find f s.t. $f(\mathcal{D}) \simeq \mathcal{N}(0,1)$
- f: invertible

$\Rightarrow$ generate by computing $f^{-1}(z \sim \mathcal{N}(0,1))$

$g: \mathcal{Z} \to \mathcal{X}$



Jacobian:

$$\frac{dg}{dx} = J_{(x)}$$

$z \sim p(z)$ $\quad p(x=g(z))$

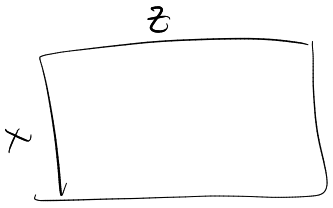
$= p(z) \,/\, \det \frac{dg}{dx}$

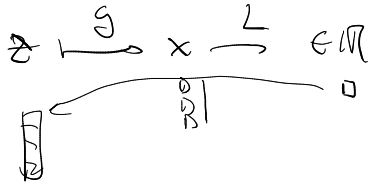
optimize $KL(P_{Target} \,||\, P_{Generated})$

$F(x)$

$$\uparrow \quad -\log p_6(x) = -\log p_M(z) + \log \det J_{(x)}$$

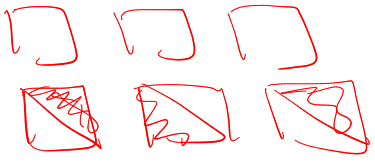
J:





$J = \frac{dg}{dx}$:

$$= \frac{df_L}{df_{L-1}} \times \frac{df_{L-1}}{df_{L-2}} \cdots \frac{df_1}{dx}$$



$$\det J = \prod_l \det \frac{df_l}{df_{l-1}}$$