Introduction to Adsorption-Based Generative Models

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Generative models like GANs and diffusion models have been pivotal in advancing AI-generated content. This article introduces a new approach based on adsorption thermodynamics, aiming to address some inherent limitations of these models.

Generative Adversarial Networks (GANs)

GANs are a popular type of generative model composed of two neural networks: a generator and a discriminator. They work in tandem to produce realistic data. However, GANs face challenges such as mode collapse, where the generator produces a limited variety of outputs, and instability during training, requiring extensive tuning of hyperparameters (ar5iv) (Stanford Applied Physics).

Diffusion Models

Diffusion models, inspired by non-equilibrium thermodynamics, gradually add noise to data in a forward process and then learn to reverse this process to reconstruct the original data. These models, though capable of producing high-quality outputs, are computationally intensive and slow due to the need for numerous iterative steps in both forward and backward processes (ar5iv) (Stanford Applied Physics).

Adsorption Model

To overcome the limitations of GANs and diffusion models, we propose the Adsorption Model. This model leverages adsorption thermodynamics to manage phase transitions and symmetry breaking, aiming to streamline the generative process and reduce computational demands. By focusing on the principles of adsorption, it promises a more efficient and faster approach to generating data compared to traditional diffusion models.

In an adsorption process, we assume we have a bulk phase from which molecules diffuse and attach to the surface of a porous media. This exchange is spontaneous since it will reduce the Gibbs free energy to the minimum. The chemical potential of the bulk phase and adsorbed phase are equal to each other. From the first law of thermodynamics for a closed system where no work is applied to the system, for an isothermal system one can write the conservation of energy as follows

$$T\Delta S = \Delta U \quad (1)$$

Where T is the temperature, S is entropy and U is the enthalpy of the system. From Boltzmann definition for entropy (equistate probability for all ensembles)

$$S = k_B log W \quad (2)$$

Where k_B is the boltzmann constant and W is the number of configurations of the system. At equilibrium molecules exchange between the bulk phase and the adsorbed phase. Figure 1 shows an example of such a state. Assuming we have single site density in the bulk phase and monolayer adsorption on the surface one can write

Energy exchange when a molecule leaves bulk to get adsorbed on the surface

$$S_1 = k_B log(W_0((1 - x_b)x_a) \quad (3a)$$

$$U_1 = z_b E_a x_b \quad (3b)$$

Energy exchange when a molecule leaves adsorbed phase to occupy a site in the bulk phase

$$S_2 = k_B log(W_0((1 - x_a)x_b) \quad (4a)$$

$$U_2 = E_s + z_a E_a x \quad (4b)$$

Where W_0 is the number of background configurations. x_a and x_b are the probability that adsorbate or bulk sites are occupied. The probability in in the range $(0, 1)$. E_s is the surface-adsorbate interaction energy, E_a is the adsorbate-adsorbate interaction energy. z_a and z_b are the coordination number in the bulk and adsorbed phase. Typically the coordination number is taken as 4 in two dimensional and 6 in three-dimensional systems. As shown by Ising model, if the coordination number is less than or equal to 2, the model can't detect the phase split events (spontaneous symmetry breaking). In our model, the bulk phase is three dimensional, and the monolayer adsorbed phase is a two dimensional structure.

Plugging in equations 3 and 4 in equation 1 we can write the energy conservation as

$$k_B T log\left(\frac{(1-x_a)x_b}{(1-x_b)x_a}\right) = E_s + E_a(z_a x_a - z_b x_b) \quad (5)$$

we can normalize the energy terms by dividing them by $k_B T$, then we have

$$log\left(\frac{(1-x_a)x_b}{(1-x_b)x_a}\right) = \varepsilon_s + \varepsilon_a(z_a x_a - z_b x_b) \quad (6)$$

In equation 6, the only unknown is x_a, adsorbate density (probability). Coordination numbers are geometrical and considered design parameters. Surface energy and adsorbate energy, i.e. ε_s and ε_a are parameters. Bulk density, x_b is also a parameter but it is treated differently. The model is evaluated for multiple values of bulk densities and for each the adsorbate density is calculated. Overall adsorption is calculated from the equation

$$\Gamma = C(x_a - x_b)$$

Where C is the monolayer capacity and Γ is the total adsorption. Figure 1 shows the schematic of adsorption-desorption exchanges when the system is at equilibrium. Two forces prefer the molecules to stay on the surface, the surface interactions, and the lateral interactions. On the other hand in the bulk phases the lateral interaction prefers the molecules to stay in the bulk phase. As show by equation 6 these internal energy changes cancel out with changes in the entropy of the system during these molecular exchanges.

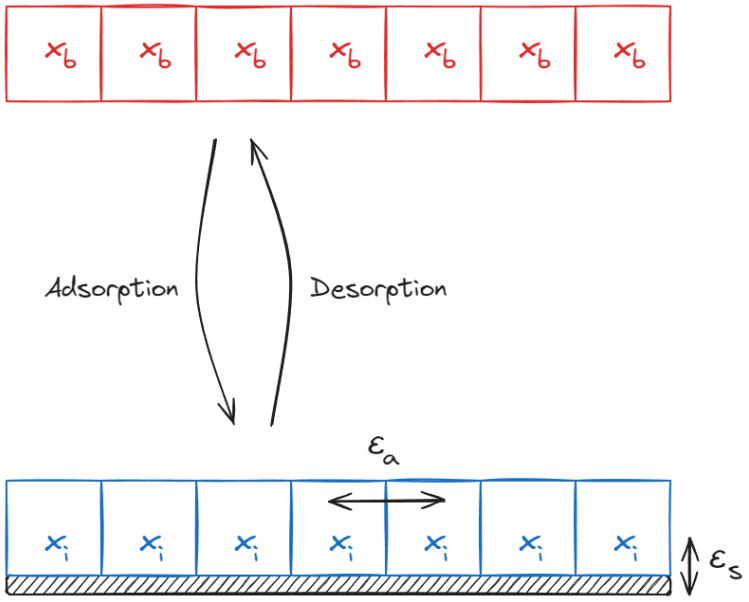

Figure 1: Adsorption equilibrium state between the bulk phase (x_b) and the adsorbed phase (x_a).

Figure 2 shows an example of adsorption hysteresis. In the presence of strong lateral forces, we witness adsorption-desorption hysteresis. Adsorption hysteresis refers to the phenomenon where the adsorption and desorption isotherms of a material do not coincide. This typically occurs in porous materials where the adsorption process involves the filling of pores, and the desorption process involves the emptying of these pores, which happens at different relative

pressures. This hysteresis loop indicates a path dependency, meaning the state of the system depends on its history, particularly the process of adsorption or desorption.

Spontaneous symmetry breaking involves a system that, under normal conditions, exhibits a certain symmetry, but under specific conditions (such as low temperature or phase transitions), it adopts a ground state that breaks this symmetry. In the context of adsorption hysteresis, the system of adsorbed molecules on a porous material surface can initially be considered to have symmetrical potential energy with respect to adsorption and desorption. However, due to interactions and energy barriers within the pores, the process breaks this symmetry, resulting in different paths for adsorption and desorption.

The hysteresis loop in adsorption is a manifestation of the energy barriers and the metastable states that the system can occupy, illustrating that the energy landscape is not symmetric. Once the adsorption starts, the system follows a different path compared to the desorption path, showing a kind of broken symmetry. This break in symmetry is spontaneous because it arises naturally from the dynamics of the adsorption and desorption processes without any external symmetry-breaking fields.

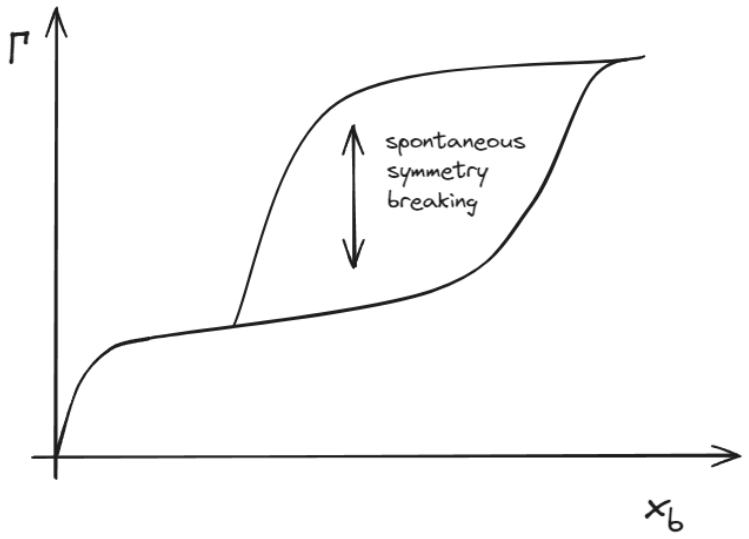

Figure 2: Shape of an adsorption isotherm when phase transition (spontaneous symmetry breaking) happens, which produces adsorption hysteresis. Depending on the sta

Adsorption based Generative model

Given the theoretical discussion we had in the previous section, we can use this to design a new generative architecture. In this work I discuss an architecture for image generation, even though the model can be extended for other modalities with appropriate tweeks.

Imagine we want to generate an image from a text input. Without losing generality we assume the image is monochromatic and the color of each pixel is in the range of $(0,\ 1)$. Figure 3 shows an example of a stack of adsorption layers. Assume we want to generate an image of dimensions 5 by 8. The figure shows the pixels of each image. To produce an image from text input, we start with a random noise at layer 1 and layer by layer we improve the image quality. The transition from one layer to the second layer is modeled as an adsorption process, where two layers are at thermodynamic equilibrium with each other. The difference between this model and the physical adsorption model is that, in the case of physical adsorption, we assumed single site probability for the bulk phase and single site probability for the adsorbate density. However, for image generation we treat each pixel as an independent site (degree of freedom) which is in coordination with other pixels.

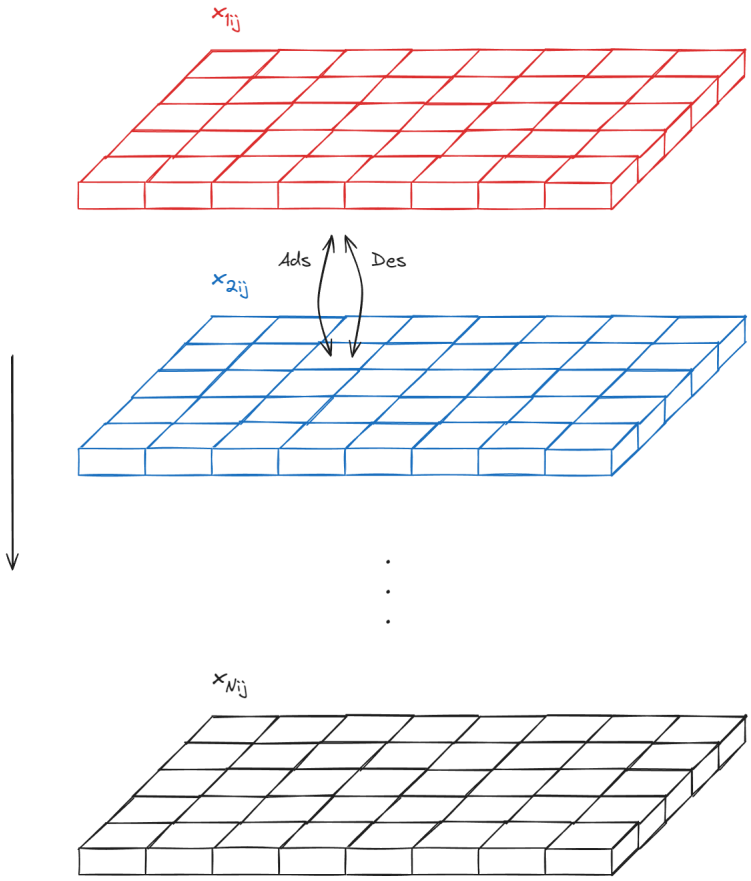

Figure 3: Schematic of layer by layer adsorption, in adsorption based generic model

In this algorithm the parameters to learn are the energy parameters, ε_s and ε_a which scale linearly with the pixel dimension (context window). The algorithm needs to learn how to transformer pixels from step i to step $i + 1$. For that, the model needs to solve the system of equations (6) for all of the pixels. At each step, the adsorption model utilizes the U-Net architecture.