Evaluating and tuning precision and recall for Generative Models

Data Science Lab

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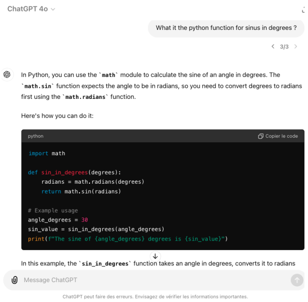
Generative Models
Context

In the past few years, generative models have made significant progress in various domains of application.

Text Generation



eg: Code Completion

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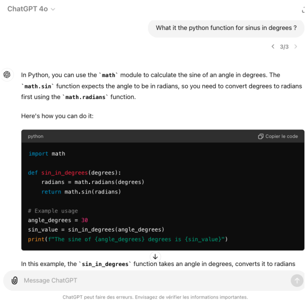
Image/Video Generation



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eg: Media Industry

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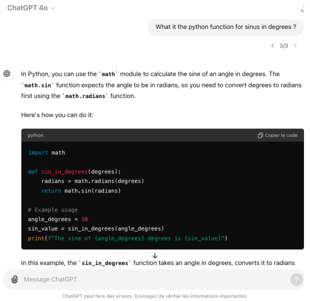

eg: Code Completion

Image/Video Generation

eg: Media Industry

Sound Generation

eg: Speech Synthesis

Generative Models

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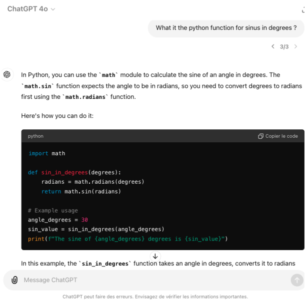

eg: Code Completion

Image/Video Generation

eg: Media Industry

Sound Generation

eg: Speech Synthesis

Molecular Generation

eg: Drug Discovery

The various performances of Generative Models
Motivation

As the generation becomes better, the evaluation becomes more challenging.

DALL·E 2 (2023)

?

Midjourney v5 (2023)

Prompt: *A dog playing with a child.*

THE VARIOUS PERFORMANCES OF GENERATIVE MODELS
MOTIVATION

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DALL·E 2 (2023)

$\neq$

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Prompt: *A dog playing with a child.*

The various performances of Generative Models
Traditional Metrics

Two metrics are often used to evaluate generative models:

- Inception Score (IS) [24]
- Fréchet Inception Distance (FID) [15]

Question : Can they separately evaluate quality and diversity of generative models?

Assume that we have a pre-trained classifier Inception-v3:

Definition 1.1 (Inception Score)

Let denote $\mathbb{P}(Y|\boldsymbol{x})$ be the conditional class distribution of an image $\boldsymbol{x}$ given by the Inception-v3 model and $\mathbb{P}(Y)$ the class distribution in dataset sampled from P. The Inception Score is defined as:

$$\mathrm{IS}(\widehat{P}) = \exp\left(\mathbb{E}_{\boldsymbol{x}\sim\widehat{P}}\left[\mathcal{D}_{\mathrm{KL}}(\mathbb{P}(Y|\boldsymbol{x})\|\mathbb{P}(Y))\right]\right)$$

where $\mathcal{D}_{\mathrm{KL}}$ is the Kullback-Leibler divergence.

With H being the entropy function, IS can be reformulated as:

$$\log\left(\mathrm{IS}(\widehat{P})\right) = H\left(\mathbb{E}_{\boldsymbol{x}\sim\widehat{P}}\left[\mathbb{P}(Y|\boldsymbol{x})\right]\right) - \mathbb{E}_{\boldsymbol{x}\sim\widehat{P}}\left[H\left(\mathbb{P}(Y|\boldsymbol{x})\right)\right].$$

Traditional Metrics

Inception Score

$$\log\left(\mathrm{IS}(\widehat{P})\right) = H\left(\mathbb{E}_{\boldsymbol{x}\sim\widehat{P}}\left[\mathbb{P}(Y|\boldsymbol{x})\right]\right) - \mathbb{E}_{\boldsymbol{x}\sim\widehat{P}}\left[H\left(\mathbb{P}(Y|\boldsymbol{x})\right)\right].$$

Inception Score is maximized :

- if for every $\boldsymbol{x} \sim \widehat{P}$, $H_Y\left(\mathbb{P}(Y|\boldsymbol{x})\right)$ is minimized. This suggests that the classification model is highly confident in predicting a singular label per image, which implies that the images are clearly recognizable and of high quality.
- if the entropy of $\mathbb{E}_{\boldsymbol{x}\sim\widehat{P}}\left[\mathbb{P}(Y|\boldsymbol{x})\right]$ is maximized. The label predictions must be uniformly distributed over all possible labels. This indicates that the generative model generates heterogeneous labels, thereby ensuring diversity.

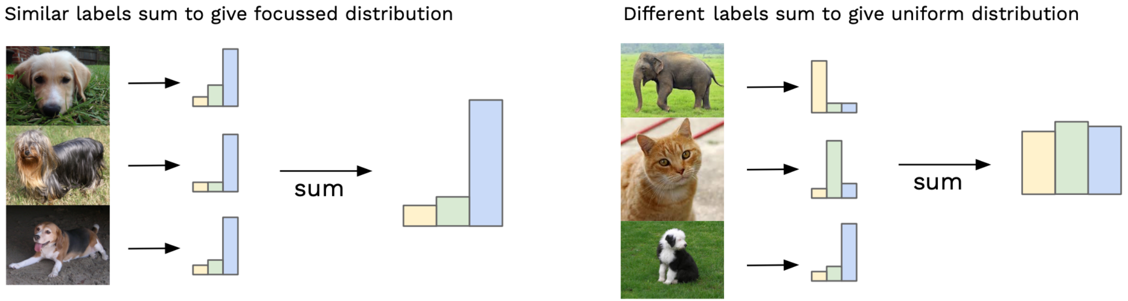


Figure. Source: medium.com

Traditional Metrics

IS falls short

However, in practical applications, the Inception Score has revealed several shortcomings [11, 6, 3, 23]:

- The IS is not sensitive to measuring intraclass diversity. In particular, if the model generates only one high-quality image per class, the IS will be high.
- The IS does not directly measure the realism of individual images. If the images are peripherally saturating, noisy, or distorted, and if the classification confidence is high, they are evaluated as realistic.
- The IS is biased toward the classes represented in ImageNet, since the Inception-v3 model is trained on this dataset. For instance, if the goal is to evaluate models that generate faces such as the CelebA dataset, IS will favor models generating faces with glasses, sunglasses, or cowboy hat, since these attributes are ImageNet classes.
- IS is not necessarily optimal when the generated images are identical to the dataset. Since it does not directly compare the generated distribution with the true data distribution, Barratt and Sharma [3] shows that IS(P) is not always optimal.

Traditional Metrics
Fréchet Inception Distance

The Fréchet Inception Distance (FID) compares the statistics of generated samples to real samples based on the features extracted using the output of the last pooling layer of Inception-v3, which is in dimension 2048, we denote it $\phi : \mathbb{R}^d \to \mathbb{R}^m$. We take two sets of samples $\{\boldsymbol{x}_1^{\text{real}}, \ldots, \boldsymbol{x}_N^{\text{real}}\}$ drawn from both P and $\{\boldsymbol{x}_1^{\text{fake}}, \ldots, \boldsymbol{x}_N^{\text{fake}}\}$ drawn from $\widehat{P}$. We consider the empirical mean and covariance of the latent representation of the samples:

$$\boldsymbol{\mu} = \frac{1}{N}\sum_{i=1}^{N} \phi(\boldsymbol{x}_i^{\text{real}}) \quad \text{and} \quad \boldsymbol{\Sigma} = \frac{1}{N-1}\sum_{i=1}^{N} \left(\phi(\boldsymbol{x}_i^{\text{real}}) - \boldsymbol{\mu}\right)\left(\phi(\boldsymbol{x}_i^{\text{real}}) - \boldsymbol{\mu}\right)^\top,$$

$$\hat{\boldsymbol{\mu}} = \frac{1}{N}\sum_{i=1}^{N} \phi(\boldsymbol{x}_i^{\text{fake}}) \quad \text{and} \quad \widehat{\boldsymbol{\Sigma}} = \frac{1}{N-1}\sum_{i=1}^{N} \left(\phi(\boldsymbol{x}_i^{\text{fake}}) - \hat{\boldsymbol{\mu}}\right)\left(\phi(\boldsymbol{x}_i^{\text{fake}}) - \hat{\boldsymbol{\mu}}\right)^\top$$

Definition 1.2 (Fréchet Inception Distance)

The Fréchet Inception Distance is defined as the Wasserstein-2 distance between two multivariate Gaussians $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ and $\mathcal{N}(\hat{\boldsymbol{\mu}}, \widehat{\boldsymbol{\Sigma}})$:

$$\text{FID} = \|\boldsymbol{\mu} - \hat{\boldsymbol{\mu}}\|^2 + \text{Tr}\left(\boldsymbol{\Sigma} + \widehat{\boldsymbol{\Sigma}} - 2(\boldsymbol{\Sigma}\widehat{\boldsymbol{\Sigma}})^{1/2}\right)$$

Traditional Metrics

FID falls short

FID is still the most widely used metric to evaluate generative models, but it has several limitations [15, 6, 10]:

- The FID compares statistical summaries (mean and covariance) of the latent distributions of Inception, a discriminative model. Therefore, it may not capture all aspects of image quality, such as texture and local structure, that are perceptible to humans.
- FID assumes that the latent representations follow a Gaussian distribution, which may not hold true in practice. This assumption can lead to inaccurate assessments of the similarity between real and generated data distributions.
- FID does not distinguish between different types of error in image generation. For example, it treats a noisy object the same as a completely wrong object being generated, which may not align with human judgment.
- Similarly to IS, FID accounts for both quality and diversity, but without a clear trade-off.

Traditional Metrics

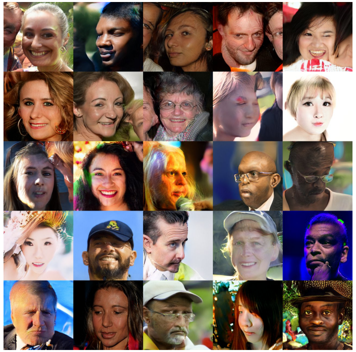
FID falls short

For example, Kynkäänniemi et al. [19] highlights the limitations of FID with samples drawn from StyleGAN:

(a) Set A - FID= 91.7

(b) Set B - FID= 16.9

(c) Set C - FID= 4.5



(d) Set D - FID= 16.7

Outline

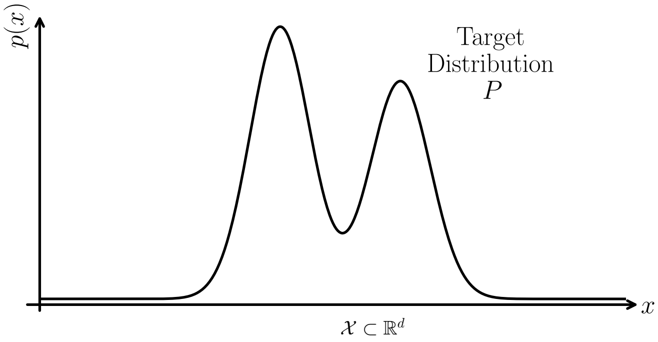
In this presentation, we discuss on evaluating, optimizing and improving quality and diversity of generative models:

1. **Evaluating:** How can we assess quality and diversity independently in Generative Models?
2. **Tuning:** Can we optimize a specific trade-off between quality and diversity?
3. **Improving:** How can we improve the quality and diversity of a pre-trained generative models?

Evaluating:
How can we assess quality and diversity independtly in Generative Models?

Generative Models

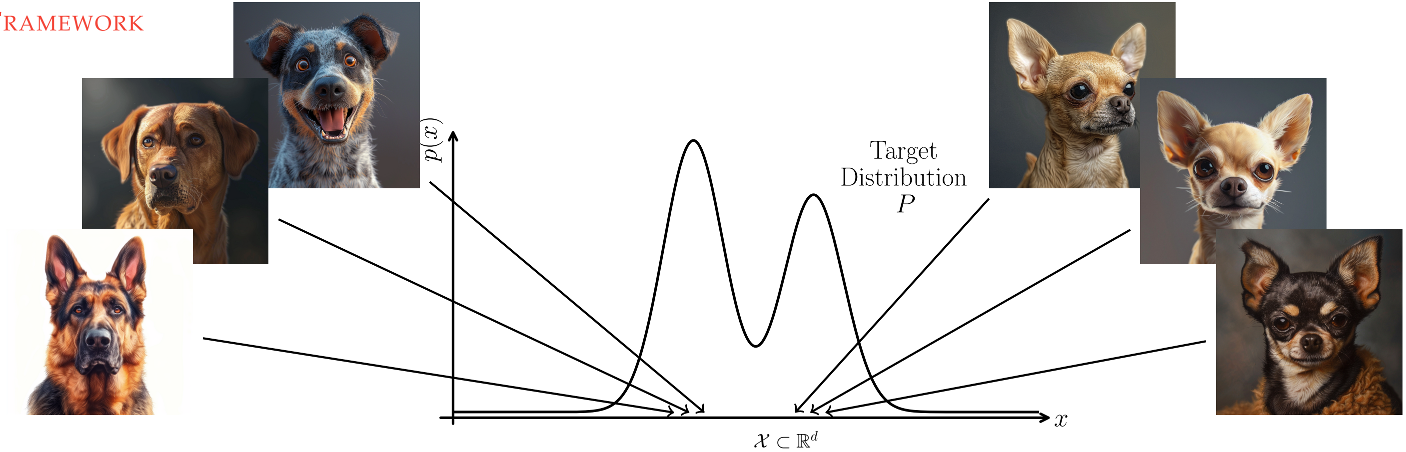
Framework



- Assumption: There is an unknown *target distribution* P in $\mathcal{X} \subset \mathbb{R}^d$.

Generative Models

Framework



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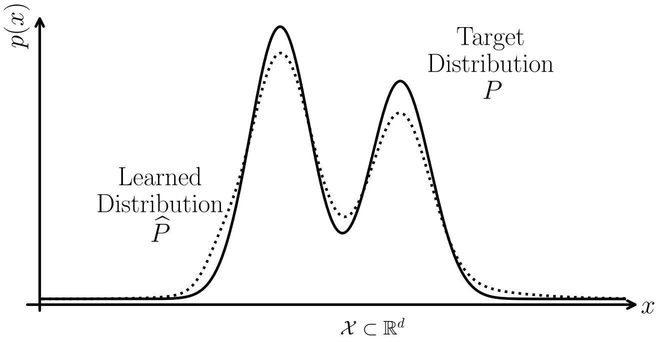
Generative Models
Framework



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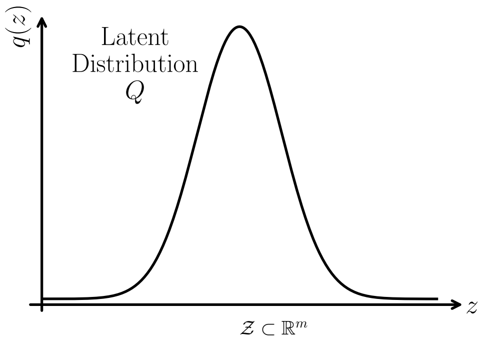
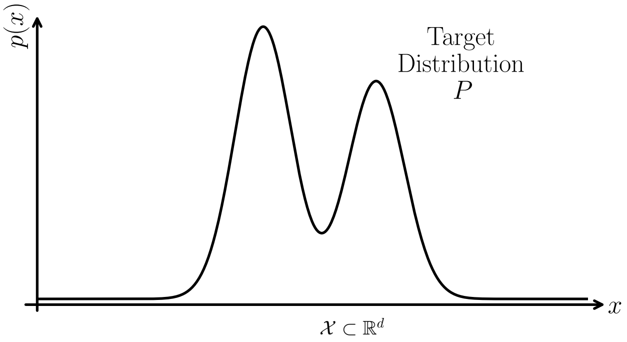
- Goal: Learn a *parameterized distribution* $\widehat{P}$ that approximate P:

Generative Models

Framework





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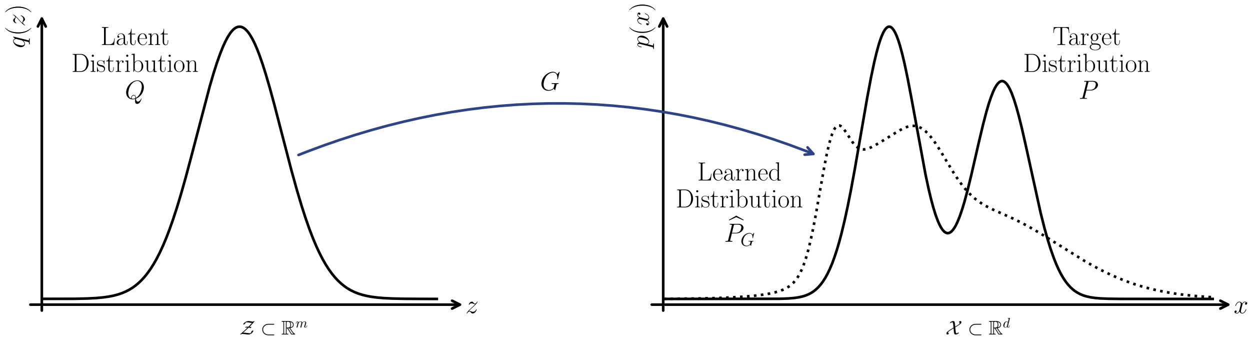
GENERATIVE MODELS
FRAMEWORK



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  2. Take *a generator model* G represented by a neural network. Take $\widehat{P}_G = G\#Q$.

Generative Models

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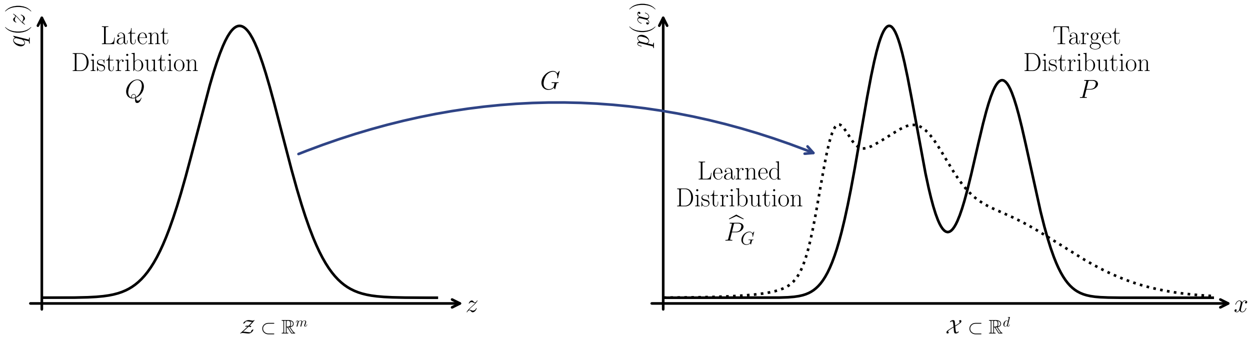

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  3. Compute G^{opt} that minimize *a dissimilarity measure* D between P and $\widehat{P}_G$:

$$G^{\text{opt}} = \underset{G}{\text{argmin}}\, D(P, \widehat{P}_G)$$

Generative Models

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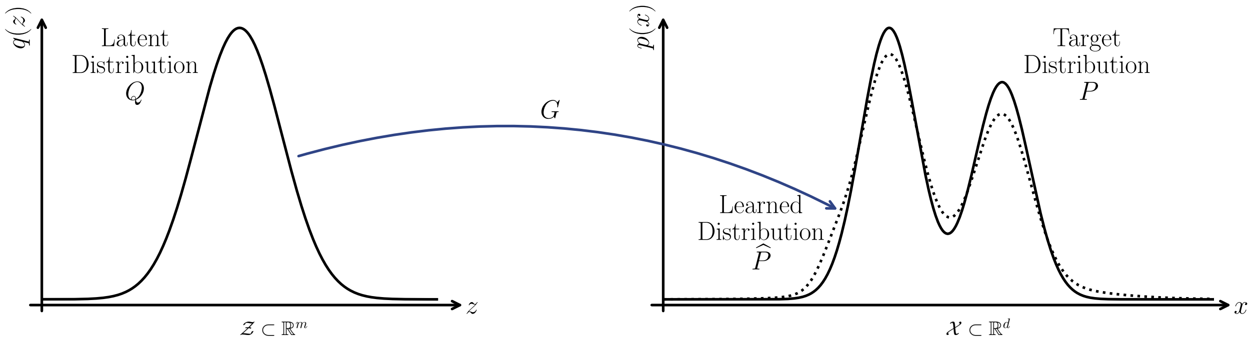

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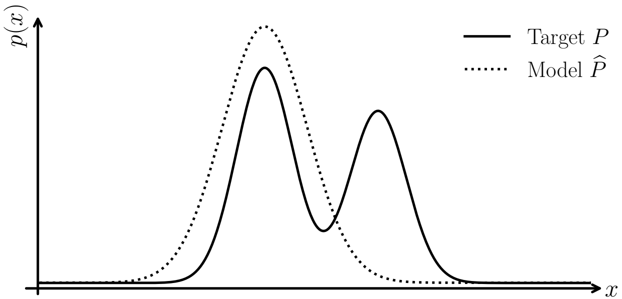
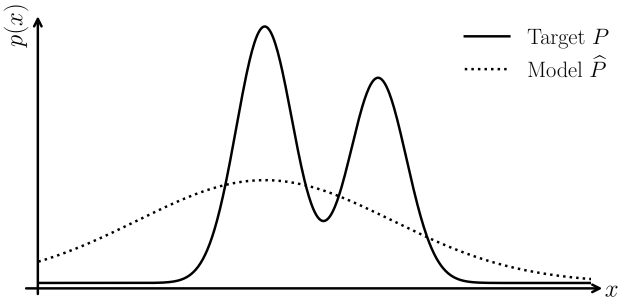
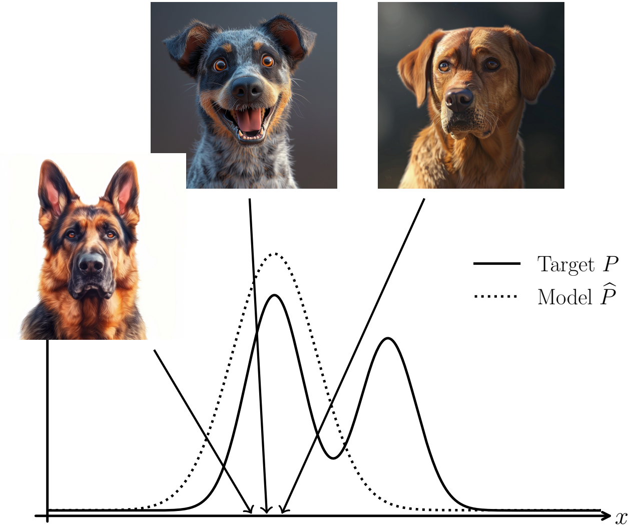
Generative Models
In Practice

$$\widehat{P} \neq P$$







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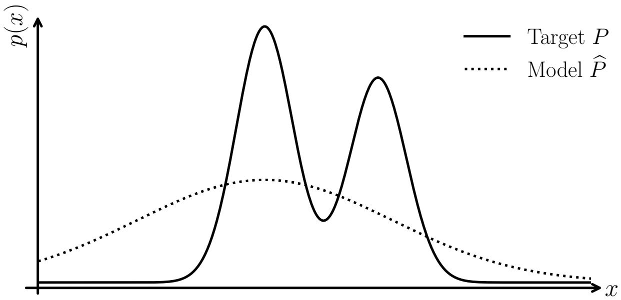
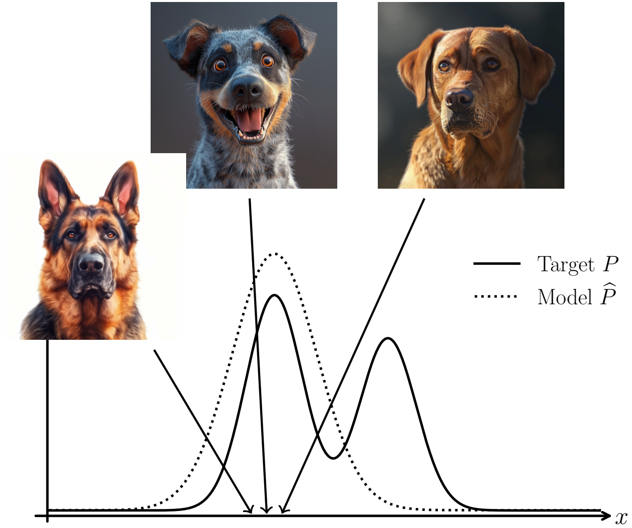
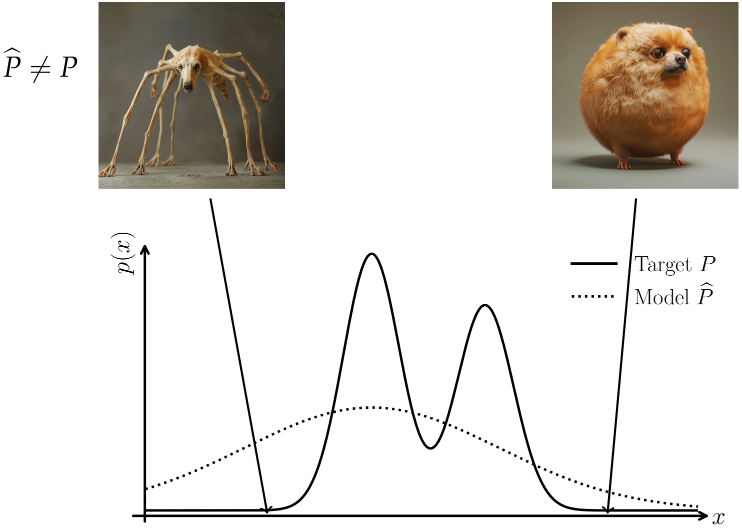


Low Diversity

Generative Models

In Practice





Low Diversity

Low Quality

Precision and Recall for Generative Models

Metrics to evaluate quality and diversity

To assess models, we use the notion of Precision and Recall, inspired from Information Retrieval:

Quality Diversity

Precision and Recall for Generative Models

Metrics to evaluate quality and diversity

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Quality

Diversity

$\downarrow$

Precision

$=$

What proportion of generated samples are realistic?

Precision and Recall for Generative Models

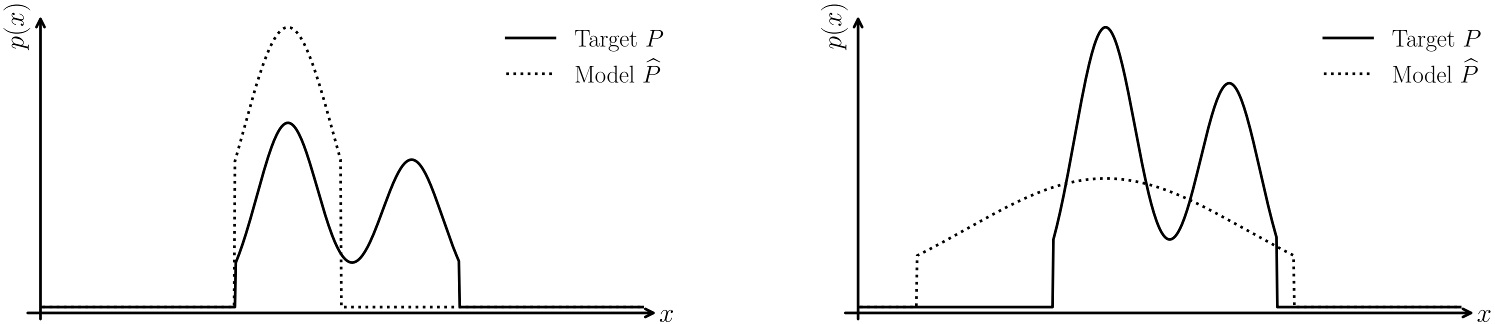
Metrics to evaluate quality and diversity

To assess models, we use the notion of Precision and Recall, inspired from Information Retrieval:

Quality	Diversity
$\downarrow$	$\downarrow$
Precision	Recall
=	=
What proportion of generated samples are realistic?	What proportion of real samples can be generated?

Precision and Recall for Generative Models

For finite support



Precision and Recall for Generative Models

For finite support

Definition 1.3 (Support-Based Precision and Recall - [19].)

For any distributions $P \in \mathcal{P}(\mathcal{X})$ and $\widehat{P} \in \mathcal{P}(\mathcal{X})$, we say that the distribution P has precision $\bar{\alpha}$ at recall $\bar{\beta}$ with respect to $\widehat{P}$ if

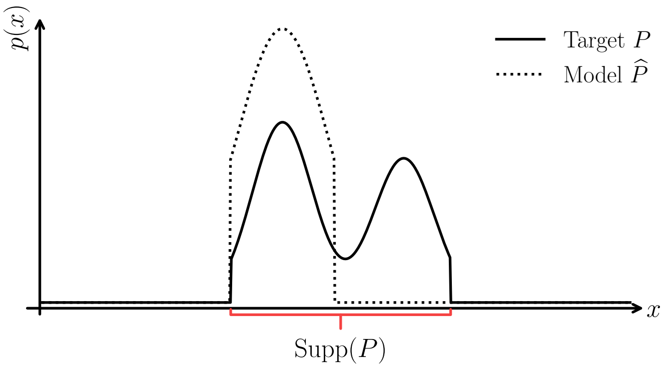
$$\bar{\alpha} := \widehat{P}(\mathrm{Supp}(P)) \quad \textit{and} \quad \bar{\beta} := P(\mathrm{Supp}(\widehat{P})).$$

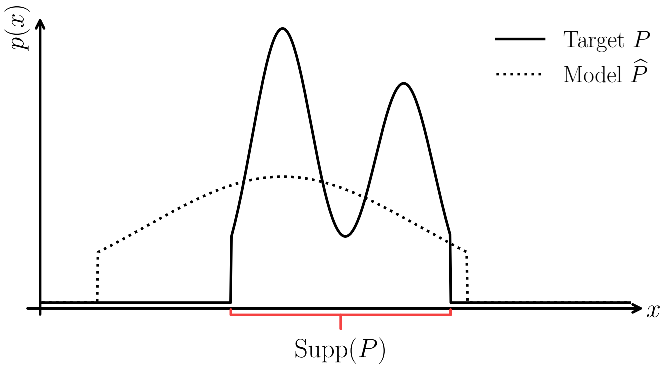
Precision and Recall for Generative Models

For finite support

Precision for finite support is the proportion of generated data that lies on the support of the real data:

$$\bar{\alpha} = \widehat{P}(\mathrm{Supp}(P)).$$





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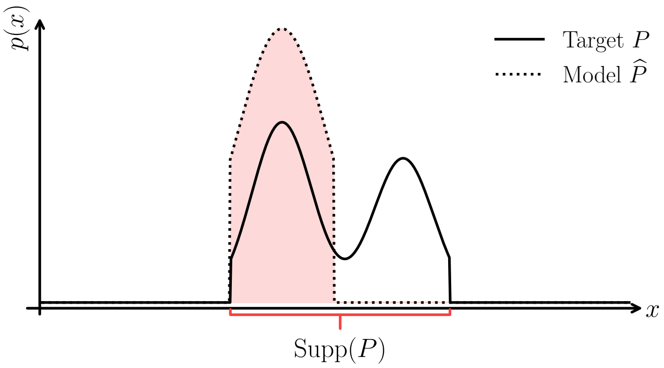
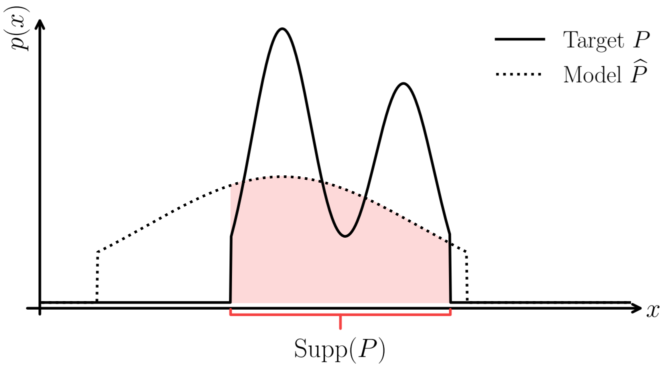
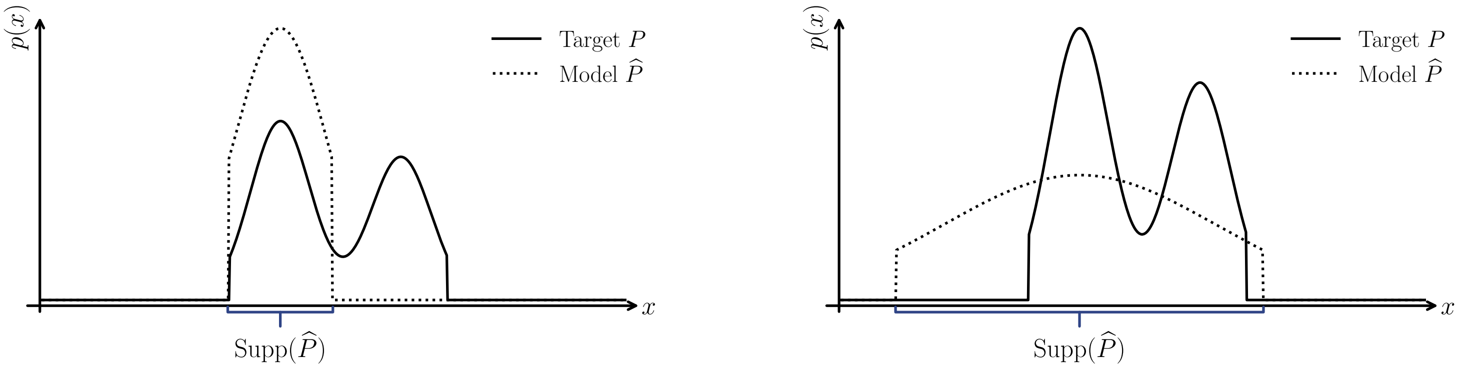




Precision and Recall for Generative Models
For finite support

Recall for finite support is the proportion of the support of the real data that is covered by the generated data:

$$\bar{\beta} = P(\mathrm{Supp}(\widehat{P})).$$



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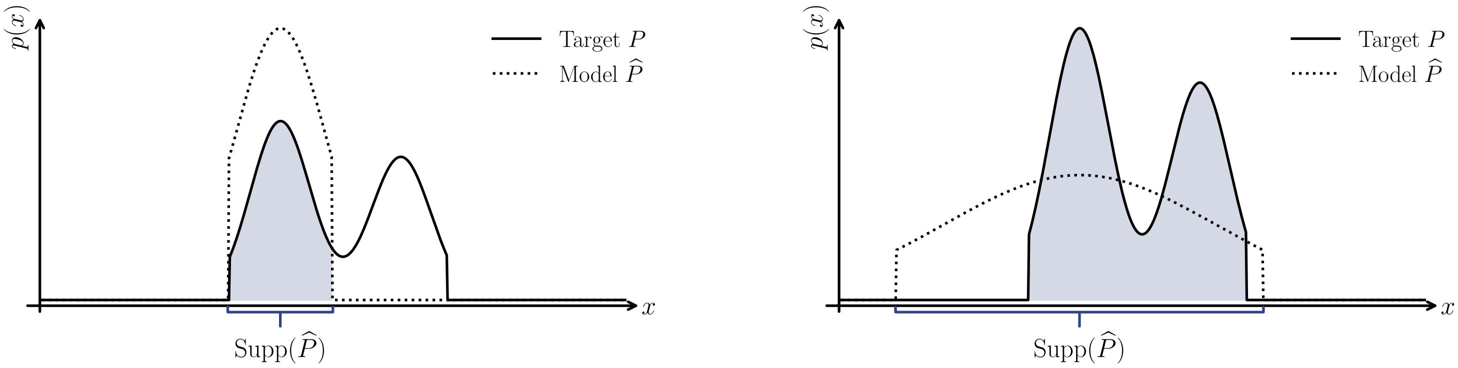
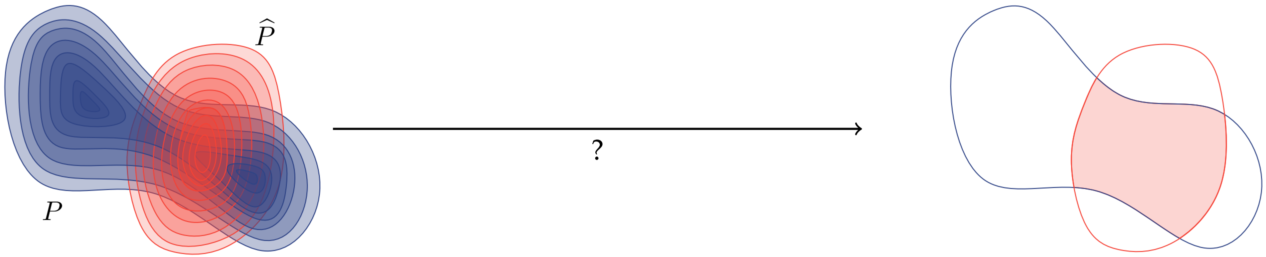


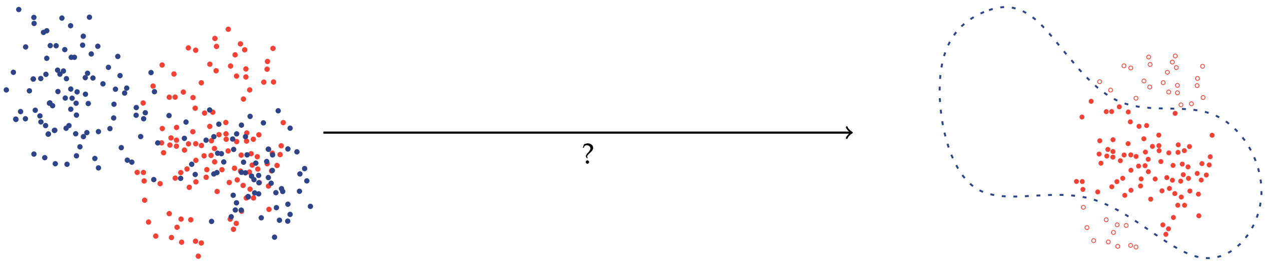
Precision and Recall for Generative Models

Estimating the Precision and Recall



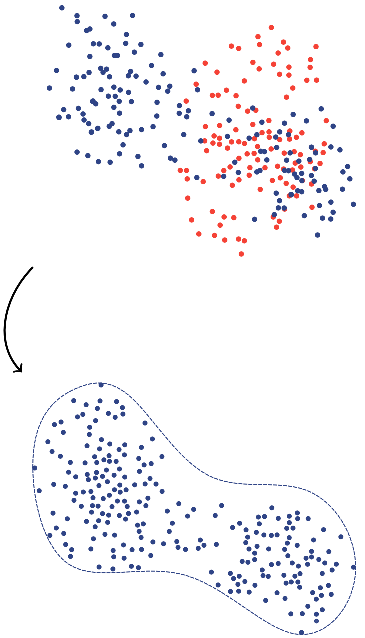
Precision and Recall for Generative Models

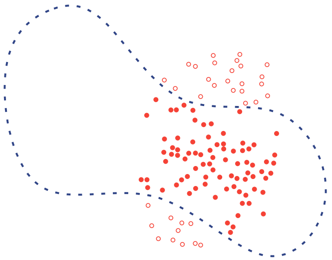
Estimating the Precision and Recall



Precision and Recall for Generative Models

Estimating the Precision and Recall





Precision and Recall for Generative Models

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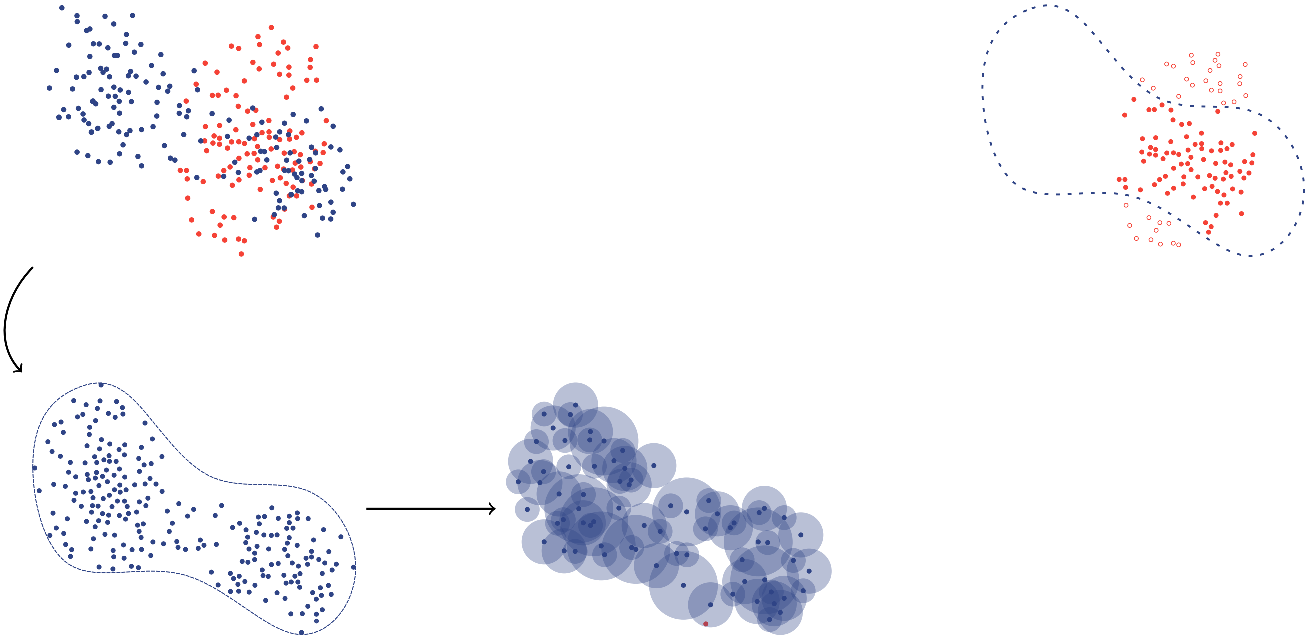
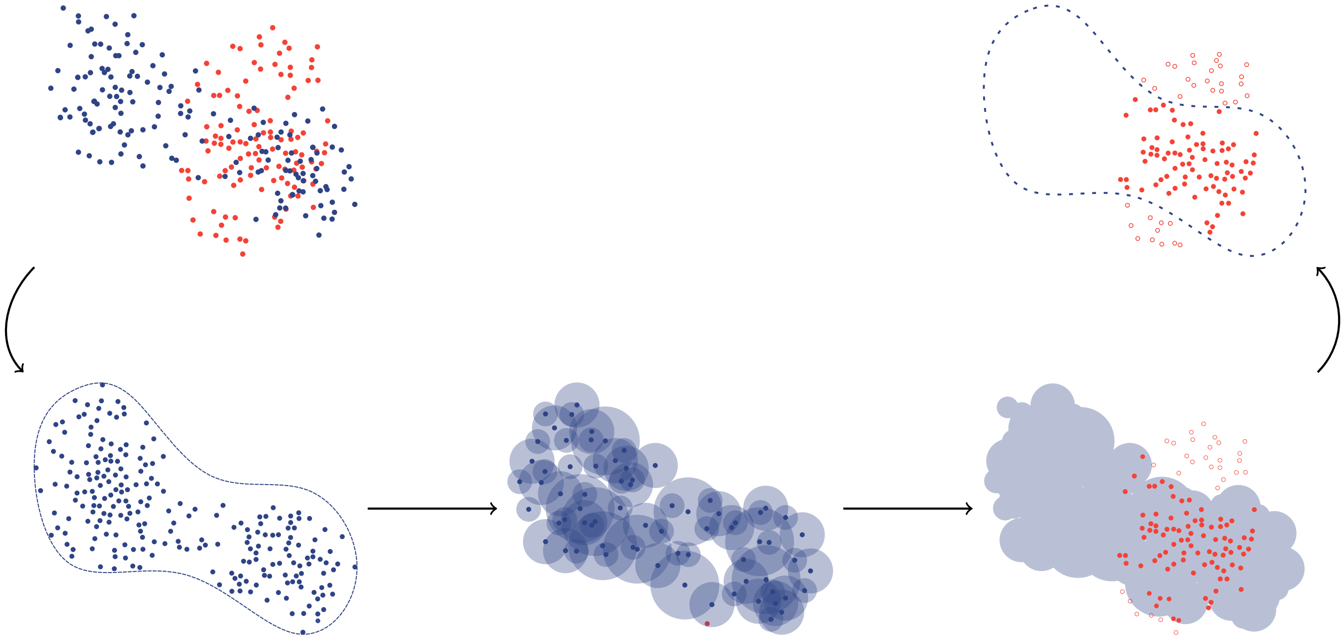


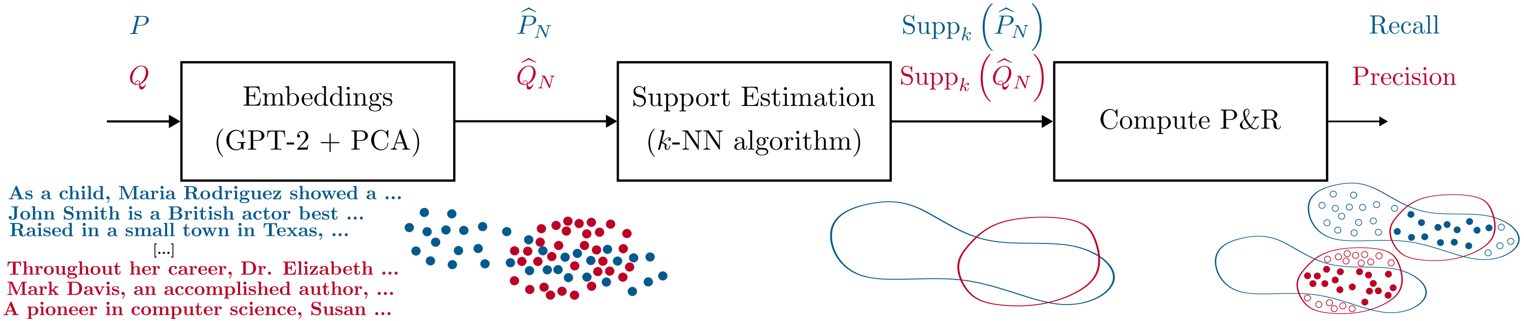
Precision and Recall for Generative Models

Estimating the Precision and Recall



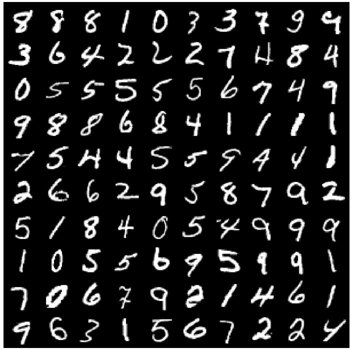
Precision and Recall for Generative Models

For LLMs



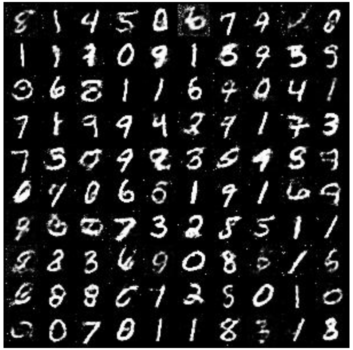
Precision and Recall for Generative Models
In Practice

MNIST Dataset [32]



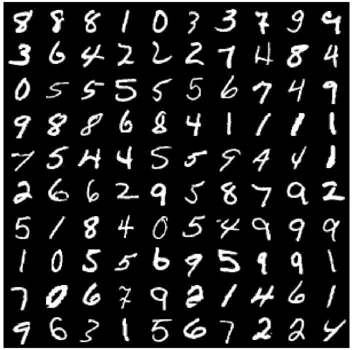
Precision and Recall for Generative Models
In Practice

Low Precision High Recall



Precision: 0.54 Recall: 0.91

MNIST Dataset [32]

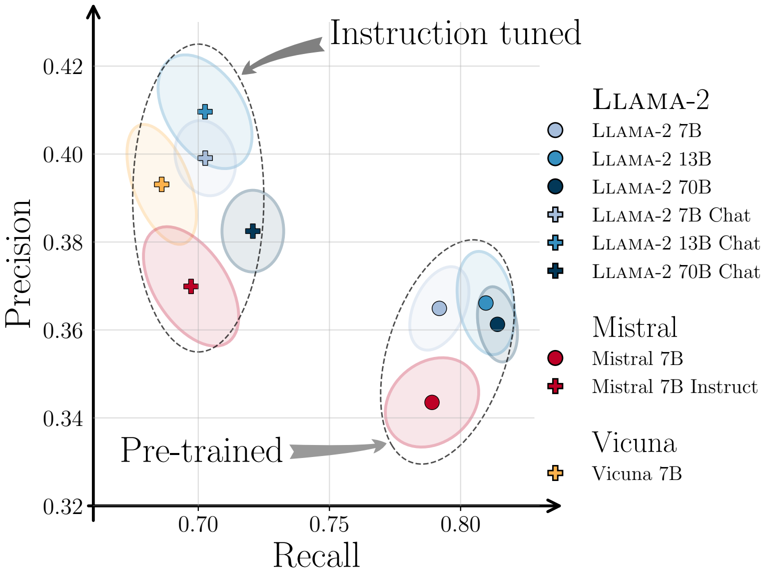


High Precision Low Recall

Precision: 0.80 Recall: 0.70

Precision and Recall for Generative Models
For LLMs

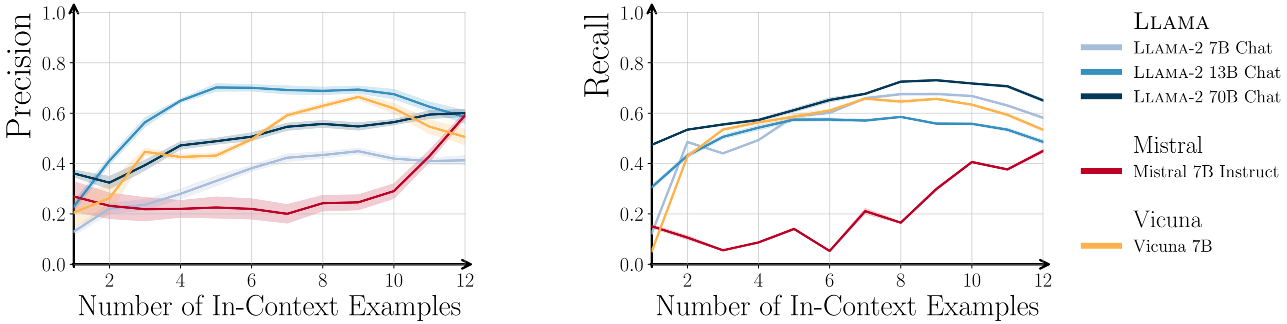
On open-ended generation, the quality and diversity of LLMs can also be evaluated using Precision and Recall: Bronnec et al. [8]



Precision and Recall for Generative Models

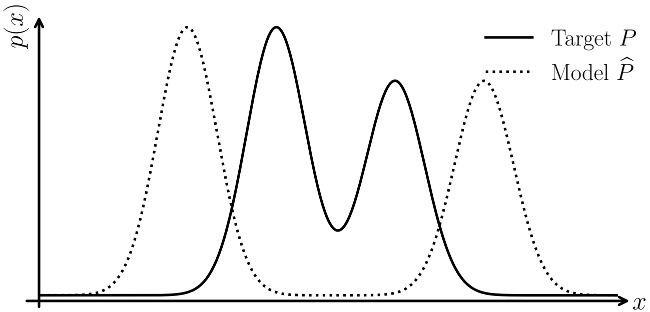
For LLMs

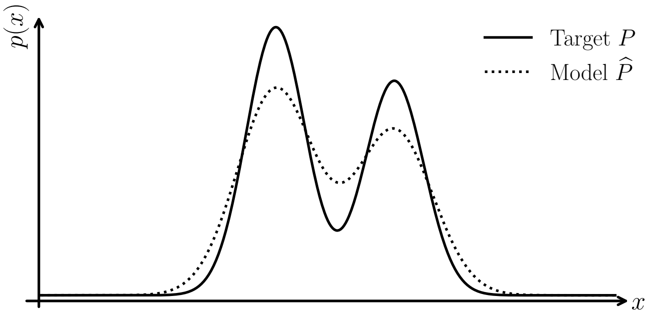
We can also evaluate the quality and diversity of LLMs on Chatbot open-ended generation. We can for instance check the impact of In-Context examples on the quality and diversity of the generated text. For instance on Wikipedia Biographies generation:



Precision and Recall for Generative Models

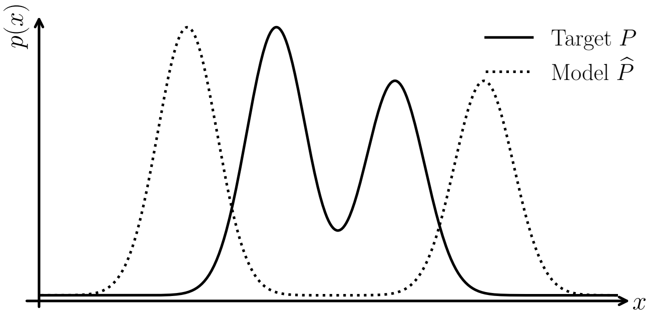
For inifinite support

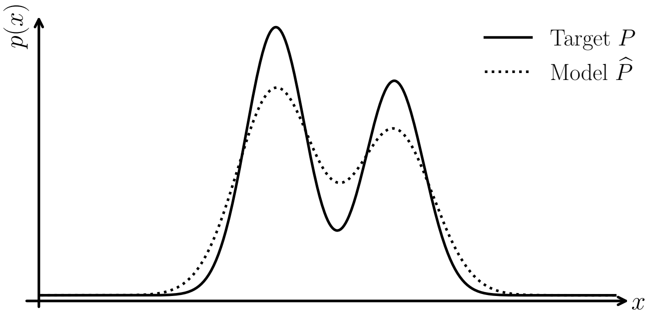




Precision and Recall for Generative Models

For inifinite support





Both distributions have **perfect** Precision *and* Recall.

PR-Curve for Generative Models
Definition

Definition 1.4 (PR-Curve for Generative Models - Sajjadi et al. [23], Simon et al. [25])

Let $P, \widehat{P} \in \mathcal{P}(\mathcal{X})$ *be two distributions such that* $P, \widehat{P} \ll \mu$. *The PR-Curve is the set* $\mathrm{PRD}(P, \widehat{P})$ *defined as:*

$$\mathrm{PRD}(P, \widehat{P}) = \{(\alpha_\lambda, \beta_\lambda) \mid \lambda \in [0, \infty]\}$$

with:

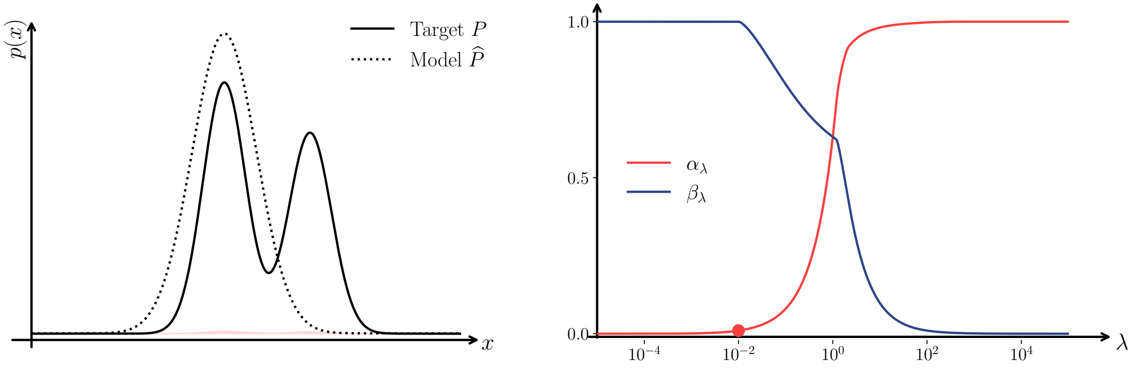
$$\alpha_\lambda = \int_{\mathcal{X}} \min\left(\lambda p(\boldsymbol{x}), \widehat{p}(\boldsymbol{x})\right) \mathrm{d}\mu(\boldsymbol{x}) \quad \textit{and} \quad \beta_\lambda = \int_{\mathcal{X}} \min\left(p(\boldsymbol{x}), \widehat{p}(\boldsymbol{x})/\lambda\right) \mathrm{d}\mu(\boldsymbol{x}).$$

PR-Curve for Generative Models

Definition

For the Precision, λp is compared to $\widehat{p}$ for different threshold $\lambda \in [0, +\infty]$:

$$\alpha_\lambda = \int_{\mathcal{X}} \min\left(\lambda p(\boldsymbol{x}), \widehat{p}(\boldsymbol{x})\right) \mathrm{d}\mu(\boldsymbol{x}) \tag{1}$$



PR-Curve for Generative Models
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For the Precision, λp is compared to $\widehat{p}$ for different threshold $\lambda \in [0, +\infty]$:

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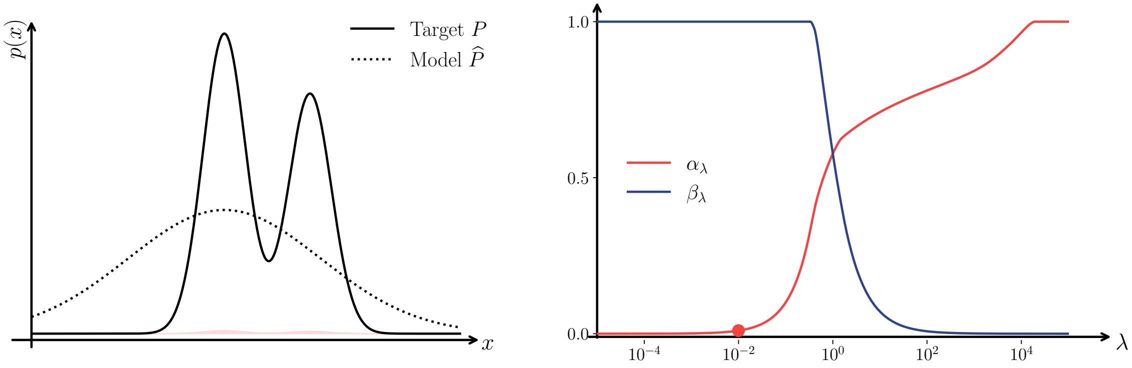
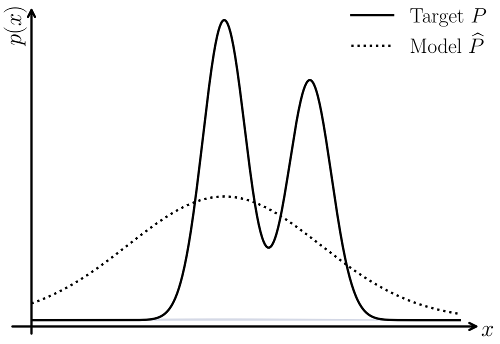
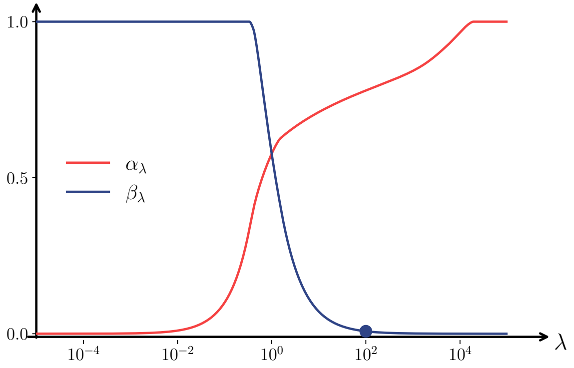


PR-Curve for Generative Models
Definition

For the Recall, p is compared to $\widehat{p}/\lambda$ for different threshold $\lambda \in [0, +\infty]$:

$$\beta_\lambda = \int_{\mathcal{X}} \min\left(p(\boldsymbol{x}), \widehat{p}(\boldsymbol{x})/\lambda\right) \mathrm{d}\mu(\boldsymbol{x}) \tag{2}$$

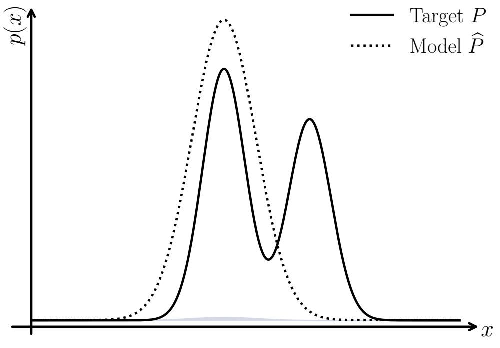


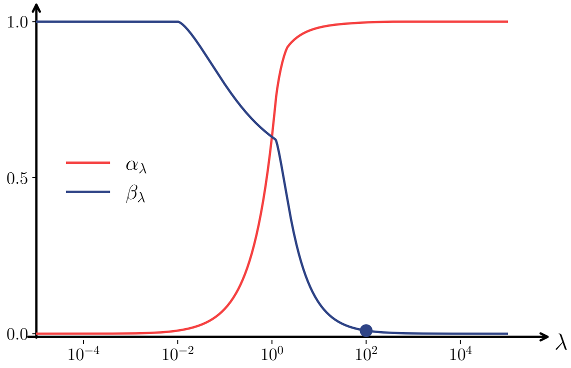


PR-Curve for Generative Models
Definition

For the Recall, p is compared to $\widehat{p}/\lambda$ for different threshold $\lambda \in [0, +\infty]$:

$$\beta_\lambda = \int_{\mathcal{X}} \min\left(p(\boldsymbol{x}), \widehat{p}(\boldsymbol{x})/\lambda\right) \mathrm{d}\mu(\boldsymbol{x}) \tag{2}$$





PR-Curve for Generative Models

Examples

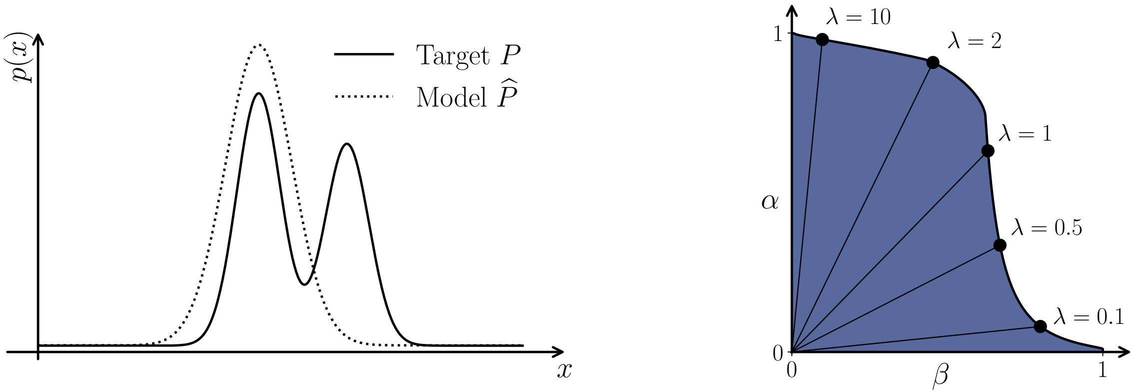
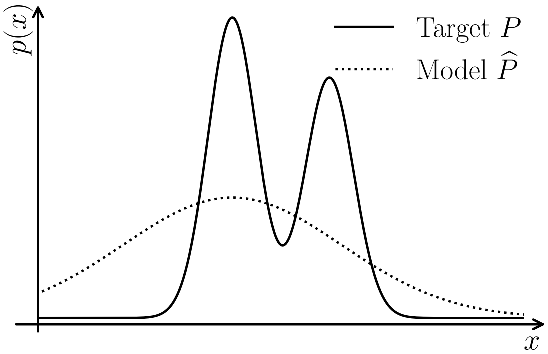


Figure. Learning distribution with low recall and high precision.

PR-Curve for Generative Models
Examples



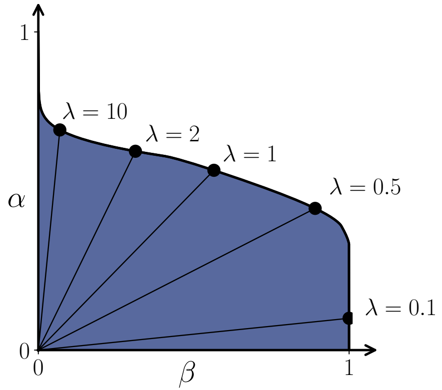


Figure. Learning distribution with high recall and low precision.

PR-Curve for Generative Models

Examples

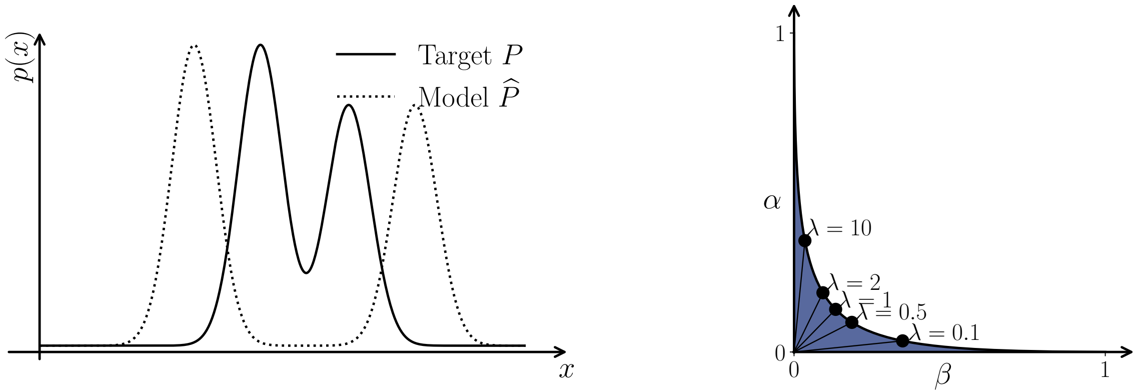


Figure. Learning distribution with low recall and low precision.

PR-Curve for Generative Models

Examples

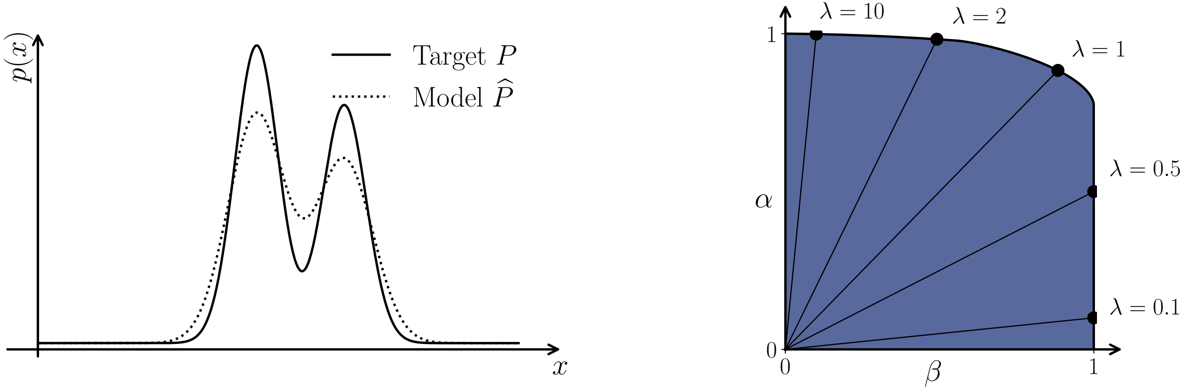


Figure. Learning distribution with high recall and high precision.

PR-Curve and Support-Based Precision and Recall

Relation

The PR-Curve is a generalization of the Precision and Recall for finite support:

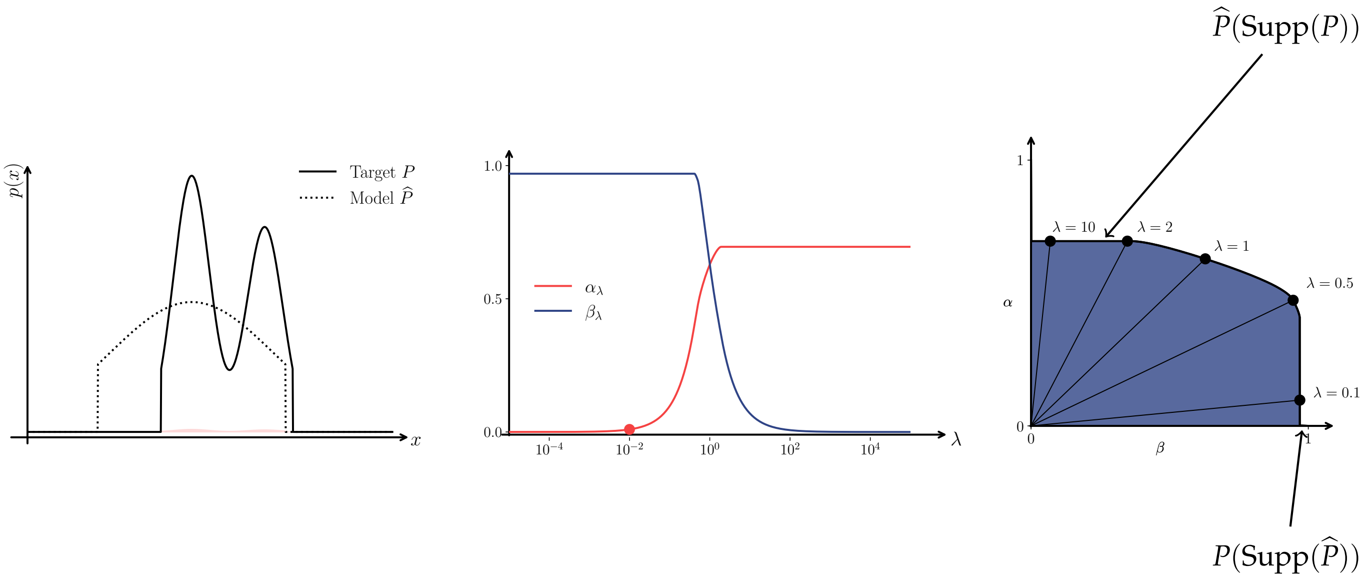
Theorem 1.5 (Support-based and PR-Curves - Siry et al. [26])

Let $P, \widehat{P} \in \mathcal{P}(\mathcal{X})$ be two distributions. Then, the support-based Precision and Recall $(\bar{\alpha}, \bar{\beta})$ are related to the PR-Curve values $\mathrm{PRD}(P, \widehat{P})$ for $\lambda = 0$ and $\lambda = \infty$:

$$\bar{\alpha} = \max_{\lambda} \alpha_{\lambda} = \alpha_{\infty} \quad \textit{and} \quad \bar{\beta} = \max_{\lambda} \beta_{\lambda} = \beta_{0}.$$

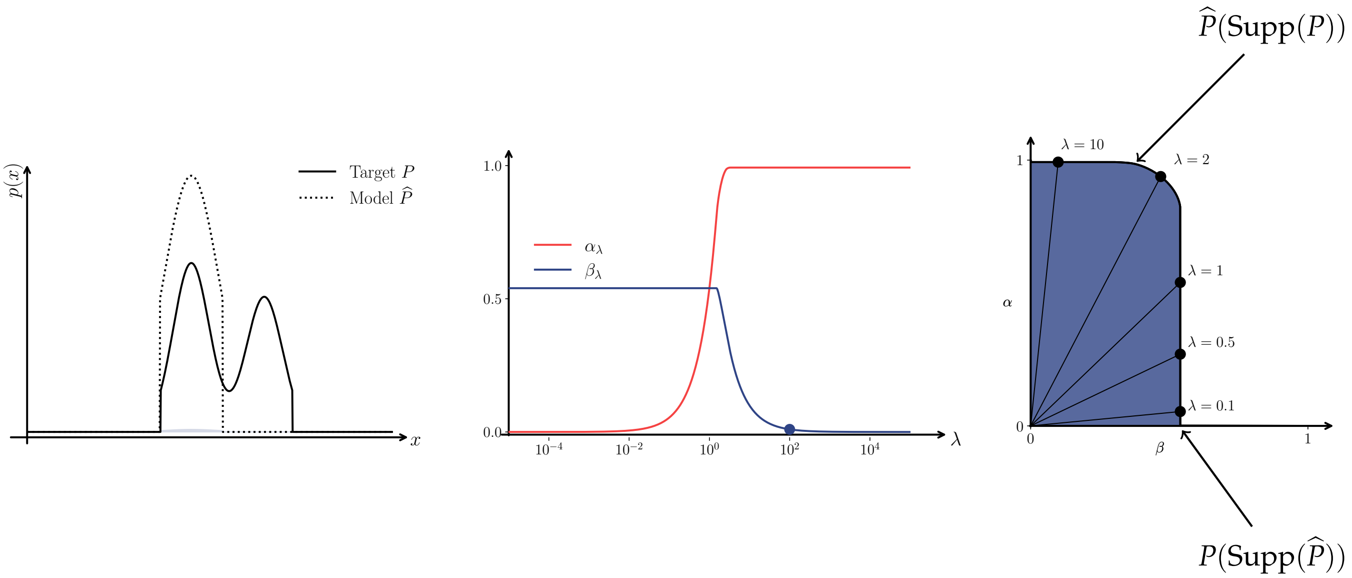
PR-Curve and Support-Based Precision and Recall

Relation



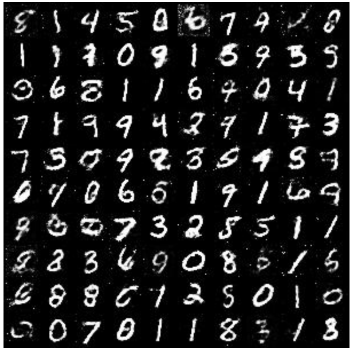
PR-Curve and Support-Based Precision and Recall

Relation



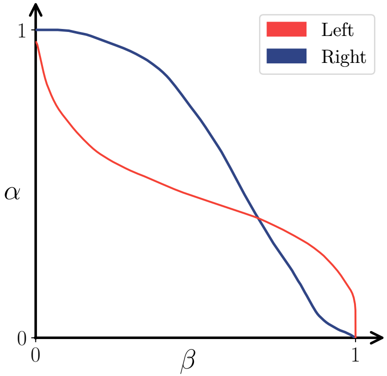
PR-Curve for Generative Models
In Practice

Low Precision High Recall



Precision: 0.54 Recall: 0.91

PR-Curves



High Precision Low Recall

Precision: 0.80 Recall: 0.70

PR-Curve for Generative Models
In NLP

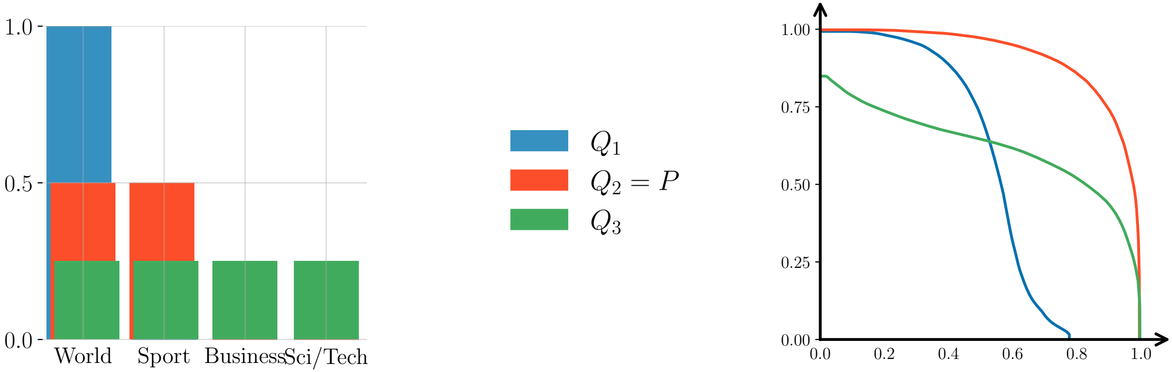


Figure. PR-Curve for distributions journal articles: AG News.

On the Platform

Metrics used to evaluate your models are:

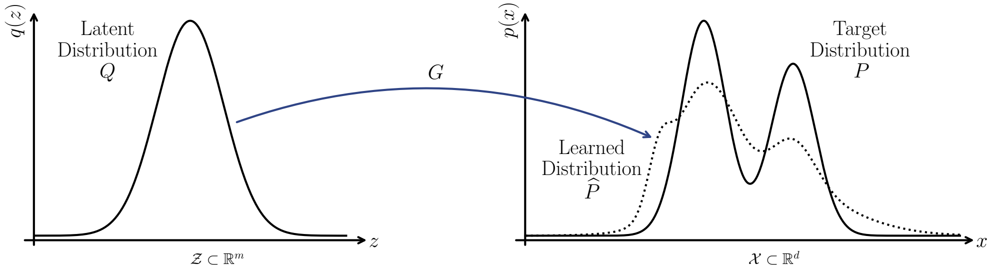
- FID
- Precision (for finite support)
- Recall (for finite support)
- (Obviously) the visual inspection of the generated samples.

Tuning:
How can we tune a model to
a specific trade-off between
Precision and Recall?

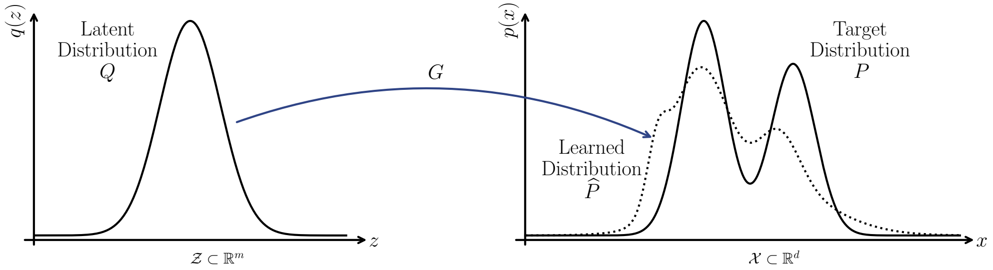
Tuning Precision and Recall in Generative Models

Truncation

Hard Trunctation
Karras et al. [17]



Soft Trunctation
Kingma and Dhariwal [18]



Tuning Precision and Recall in Generative Models

Hard Truncation

Figure. From left to right: $\psi = 0.0$, $\psi = 0.3$ $\psi = 0.7$ $\psi = 1.0$.

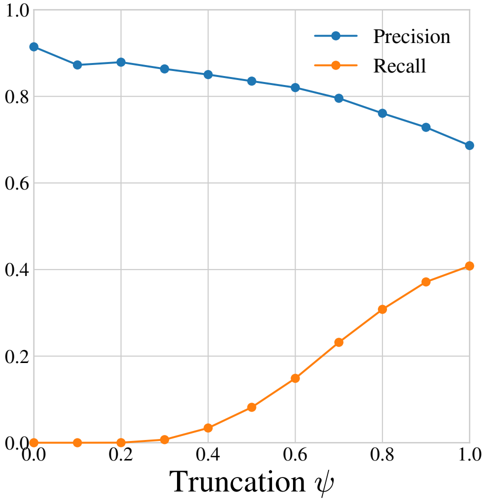


Figure. Source: [19]

Tuning Precision and Recall in Generative Models

Soft Truncation

(a) $\psi = 0.04$ (b) $\psi = 0.5$ (c) $\psi = 1.0$ (d) $\psi = 2.0$

Figure. Soft-Truncation on BigGAN. Source:[7].

Tuning Precision and Recall in Generative Models

Temperature scaling

In LLMs, we can tune the temperature. Let's assume that the model is outputting a categorical distribution with probability $\widehat{P}(x_l|\boldsymbol{x}_{<i})$ for a token x_l with a given context $\boldsymbol{x}_{<i}$. We can tune the temperature $t > 0$ as follows:

$$\widehat{P}^t(x_l|\boldsymbol{x}_{<i}) = \frac{\widehat{P}(x_l|\boldsymbol{x}_{<i})^{1/t}}{\sum_{x_i \in \mathcal{V}^L} \widehat{P}(x_i|\boldsymbol{x}_{<i})^{1/t}}.$$

Tuning Precision and Recall in Generative Models

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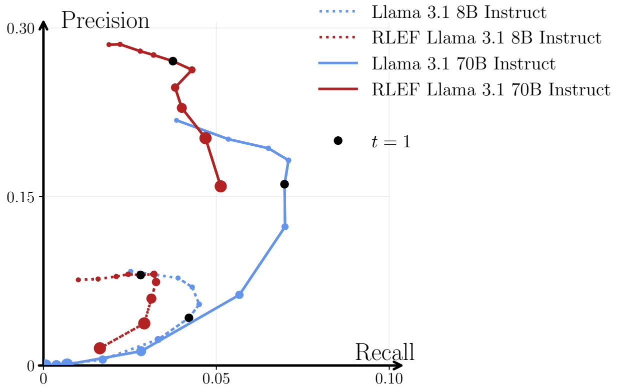


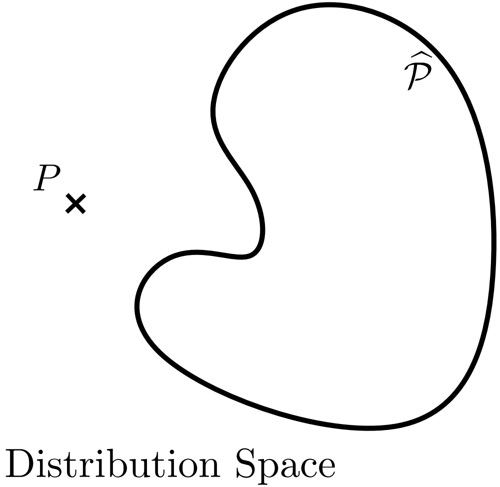
Figure. Effect on the PR-Curve for different temperatures for Coda Llama 2. Source: Verine et al. [30].

Training a Generative Model

in general

Traditionally, the goal is to minimize *a dissimilarity measure* between the target distribution P and the learned distribution $\widehat{P}$:

$$\min_G \; D(P, \widehat{P}_G) \tag{3}$$

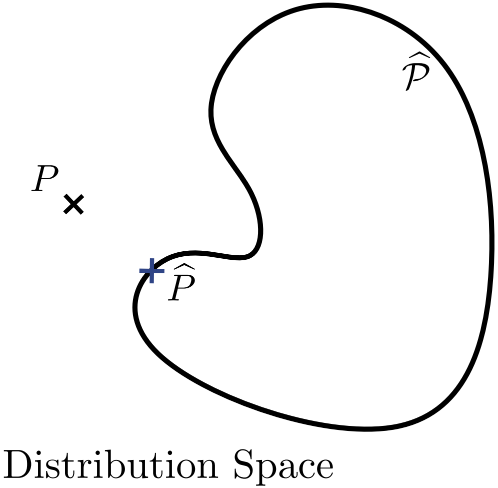


Training a Generative Model

with f-divergences

Traditionally, the goal is to minimize *an f-divergence* between the target distribution P and the learned distribution $\widehat{P}$:

$$\min_{G} \; \mathcal{D}_f(P \| \widehat{P}_G) \tag{3}$$



Definition 2.1 (f-divergences)

For any two probability distributions P and $\widehat{P}$ in $\mathcal{P}(\mathcal{X})$ such that $P, \widehat{P} \ll \mu$. Let p and $\widehat{p}$ be the Radon-Nikodym densities of P and $\widehat{P}$ with respect to μ, respectively. Let f be any convex lower semi-continuous function $f : [0, \infty] \to]-\infty, +\infty]$ such that $f(1) = 0$, the f-divergence between P and $\widehat{P}$ is

$$\mathcal{D}_f(P \| \widehat{P}) = \int_{\mathcal{X}} \widehat{p}(\boldsymbol{x}) f\left(\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}\right) \mathrm{d}\mu(\boldsymbol{x}). \tag{4}$$

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Usual divergences are f-divergences:

- Kullback-Leibler (KL),
- Reverse Kullback-Leibler (rKL),
- Jensen-Shannon (JS),
- Total Variation (TV),
- $\alpha-$divergences.

Estimating f-divergences

Dual variational form

f-divergences are *hardly tractable* in practice. However, they can be approximated by a dual approximation.

Estimating f-divergences

Dual variational form

f-divergences are *hardly tractable* in practice. However, they can be approximated by a dual approximation.

- $f^*(t) = \sup_{u \in \mathbb{R}} \{tu - f(u)\}$ be *the Fenchel conjugate* of f.
- $\mathcal{T}$ be the set of all measurable functions $\mathcal{X} \to \mathbb{R}$.

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- $f^*(t) = \sup_{u \in \mathbb{R}} \{tu - f(u)\}$ be *the Fenchel conjugate* of f.
- $\mathcal{T}$ be the set of all measurable functions $\mathcal{X} \to \mathbb{R}$.

Theorem 2.2 (Dual variational form of an f-divergence- Nguyen et al. [20])

Let $P, \widehat{P} \in \mathcal{P}(\mathcal{X})$ two distributions such that P is absolutely continuous with respect to $\widehat{P}$ and f a suitable generator function. The f-divergence between P and $\widehat{P}$ admits a dual variational form:

$$\mathcal{D}_f(P \| \widehat{P}) = \sup_{T \in \mathcal{T}} \left(\mathbb{E}_{\boldsymbol{x} \sim P}\left[T(\boldsymbol{x})\right] - \mathbb{E}_{\boldsymbol{x} \sim \widehat{P}}\left[f^*(T(\boldsymbol{x}))\right] \right). \tag{5}$$

We use $T^{\text{opt}} \in \mathcal{T}$ to denote the function that achieves the supremum.

Training a Generative Model with f-divergences

Using the dual variational form

By doing so, we can rewrite the optimization problem as:

$$\min_{G} \max_{T} \underbrace{\mathbb{E}_{\boldsymbol{x}\sim P}\left[T(\boldsymbol{x})\right] - \mathbb{E}_{\boldsymbol{x}\sim \widehat{P}_G}\left[f^*(T(\boldsymbol{x}))\right]}_{\mathcal{D}_{f,T}^{\text{dual}}} \tag{6}$$

Training a Generative Model with f-divergences

Using the dual variational form

By doing so, we can rewrite the optimization problem as:

$$\min_{G} \max_{T} \underbrace{\mathbb{E}_{\boldsymbol{x} \sim P}\left[T(\boldsymbol{x})\right] - \mathbb{E}_{\boldsymbol{x} \sim \widehat{P}_G}\left[f^*(T(\boldsymbol{x}))\right]}_{\mathcal{D}^{\text{dual}}_{f,T}} \tag{6}$$

- The discriminator T is trained *to estimate* the divergence.
- The generator G is trained *to minimize* the divergence.

Training a Generative Model with f-divergences

Using the dual variational form

By doing so, we can rewrite the optimization problem as:

$$\min_G \max_T \underbrace{\mathbb{E}_{\boldsymbol{x}\sim P}\left[T(\boldsymbol{x})\right] - \mathbb{E}_{\boldsymbol{x}\sim \widehat{P}_G}\left[f^*(T(\boldsymbol{x}))\right]}_{\mathcal{D}^{\text{dual}}_{f,T}} \tag{6}$$

- The discriminator T is trained *to estimate* the divergence.
- The generator G is trained *to minimize* the divergence.

Training a Generative Model with f-divergences

Using the dual variational form

By doing so, we can rewrite the optimization problem as:

$$\min_G \max_T \; \mathbb{E}_{\boldsymbol{x}\sim P}\left[\log\left(D(\boldsymbol{x})\right)\right] - \mathbb{E}_{\boldsymbol{x}\sim\widehat{P}_G}\left[f^*\left(\log(D(\boldsymbol{x}))\right)\right] \tag{6}$$

- The discriminator T is trained *to estimate* the divergence.
- The generator G is trained *to minimize* the divergence.
- With $T(\boldsymbol{x}) = \log(D(\boldsymbol{x}))$ with $D(\boldsymbol{x}) \in [0, 1]$.

Training a Generative Model with f-divergences

Using the dual variational form

By doing so, we can rewrite the optimization problem as:

$$\min_{G} \max_{T} \; \mathbb{E}_{\boldsymbol{x}\sim P}\left[\log\left(D(\boldsymbol{x})\right)\right] + \mathbb{E}_{\boldsymbol{x}\sim \widehat{P}_G}\left[\log\left(1 - D(\boldsymbol{x})\right)\right] \tag{6}$$

- The discriminator T is trained *to estimate* the divergence.
- The generator G is trained *to minimize* the divergence.
- With $T(\boldsymbol{x}) = \log(D(\boldsymbol{x}))$ with $D(\boldsymbol{x}) \in [0, 1]$.
- $f^*(t) = f^*_{\mathrm{JS}}(t) = -\log(1 - \exp(t))$ for the Jensen-Shannon divergence.

We recover the original GAN framework.

Training a Generative Model with f-divergences

Using the dual variational form

By doing so, we can rewrite the optimization problem as:

$$\min_G \max_T \underbrace{\mathbb{E}_{\boldsymbol{x}\sim P}\left[T(\boldsymbol{x})\right] - \mathbb{E}_{\boldsymbol{x}\sim \widehat{P}_G}\left[f^*(T(\boldsymbol{x}))\right]}_{\mathcal{D}_{f,T}^{\text{dual}}} \tag{6}$$

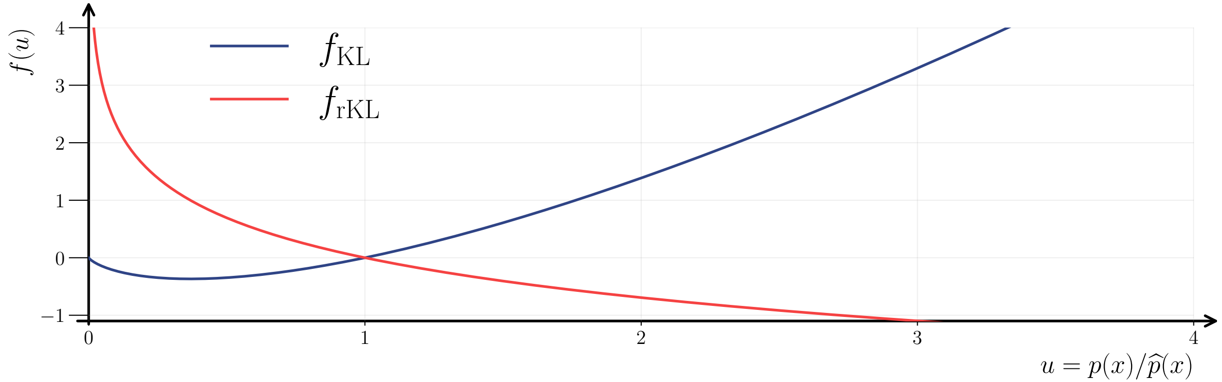
- The discriminator T is trained *to estimate* the divergence.
- The generator G is trained *to minimize* the divergence.

- Generative Adversarial Networks [12] for *the Jensen-Shannon divergence*.
- Extended to other f-divergences by Nowozin et al. [21].
- Extend to other generative models such as Normalizing Flows by Grover et al. [13].

Effect of the f-divergence on the learned distribution

All f-divergences are not equal:

$$\mathcal{D}_f(P \| \widehat{P}) = \mathbb{E}_{\boldsymbol{x} \sim \widehat{P}} \left[f \left(\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})} \right) \right]$$

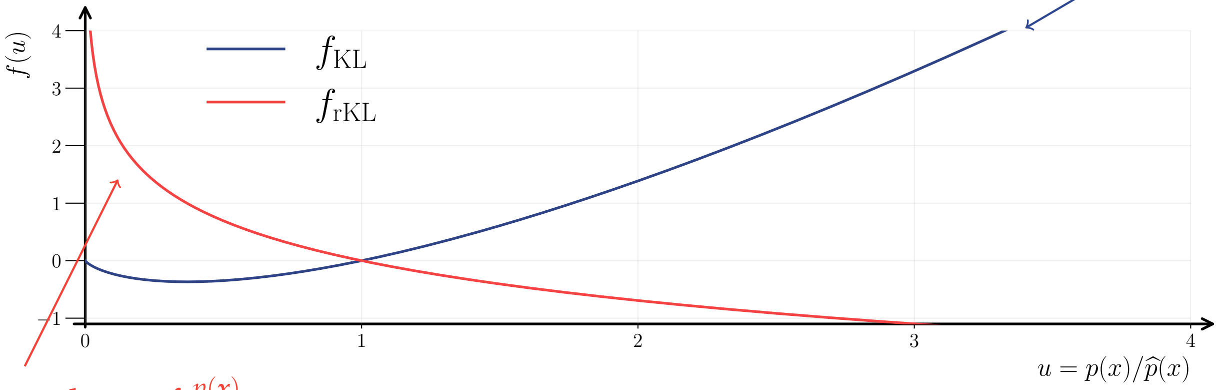


Effect of the f-divergence on the learned distribution

All f-divergences are not equal:

$$\mathcal{D}_f(P\|\widehat{P}) = \mathbb{E}_{\boldsymbol{x}\sim\widehat{P}}\left[f\left(\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}\right)\right]$$

Penalizing high values of $\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}$



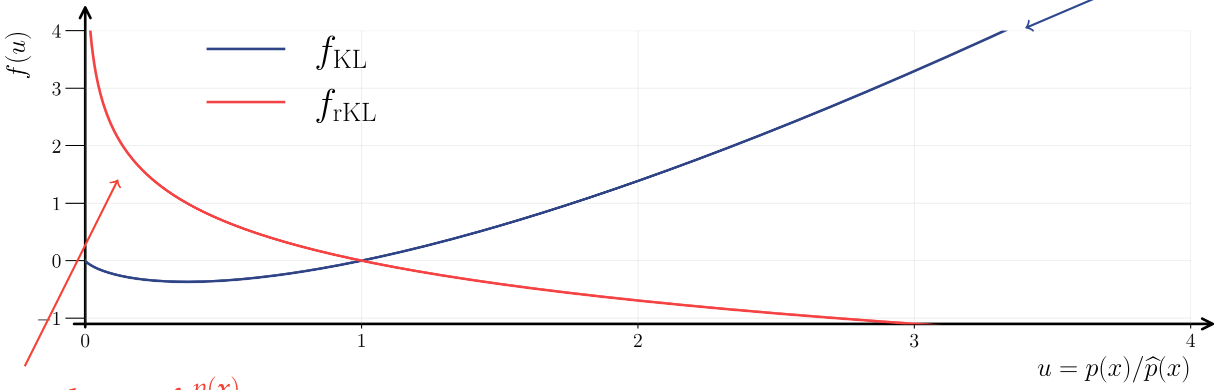
Penalizing low values of $\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}$

EFFECT OF THE f-DIVERGENCE ON THE LEARNED DISTRIBUTION

All f-divergences are not equal:

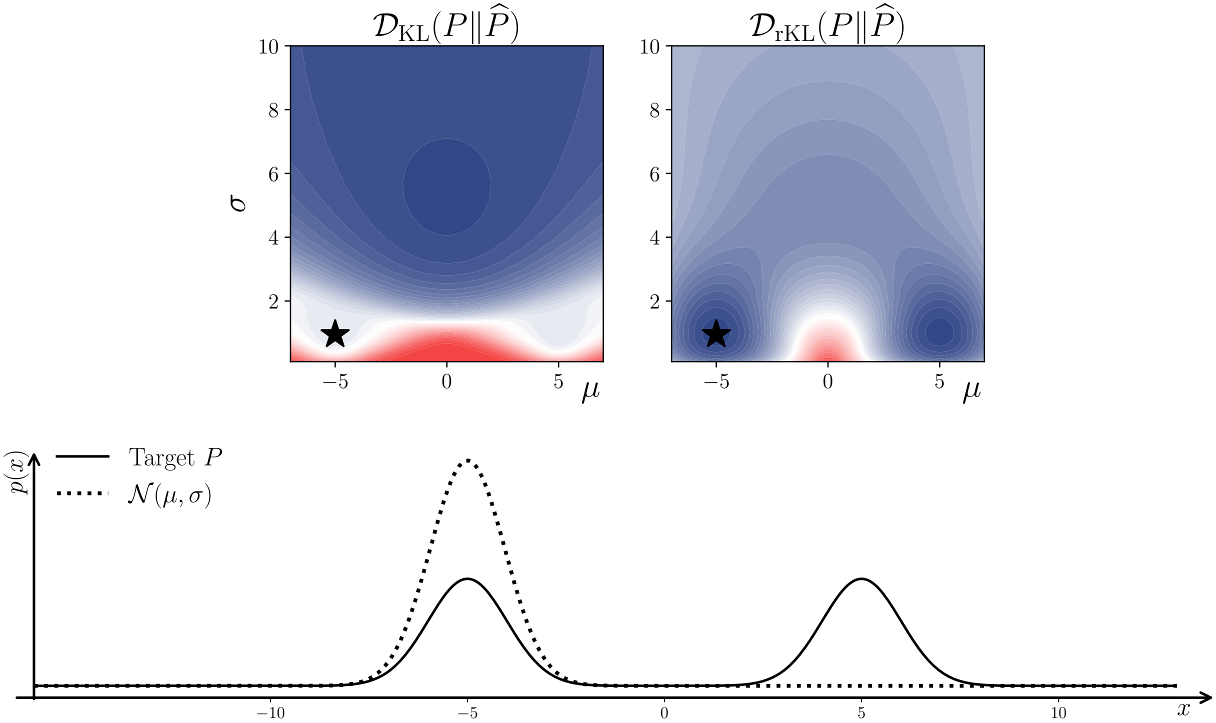
$$\mathcal{D}_f(P\|\widehat{P}) = \mathbb{E}_{\boldsymbol{x}\sim\widehat{P}}\left[f\left(\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}\right)\right]$$

Penalizing high values of $\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}$
Favors high recall

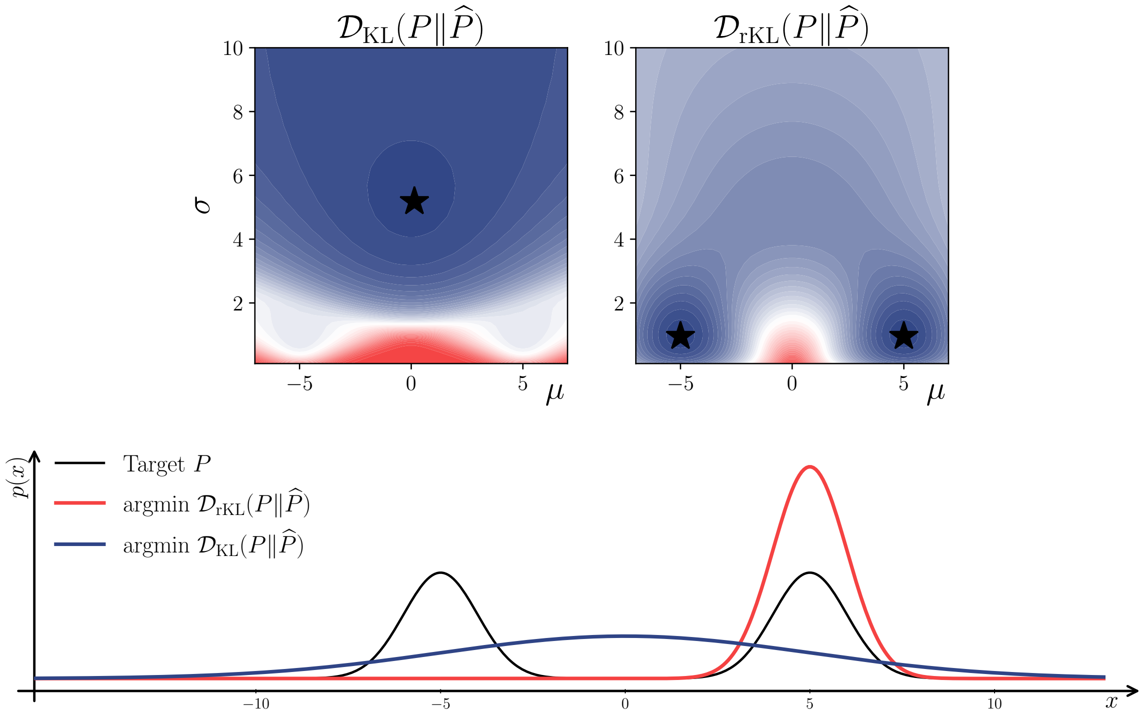


Penalizing low values of $\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}$
Favors high precision

Examples of f-divergence minimization



Examples of f-divergence minimization



Can we optimize a specific trade-off between Precision and Recall?

Can we optimize a specific trade-off between Precision and Recall?

- What is the relation between the Precision-Recall curve and f-divergences?

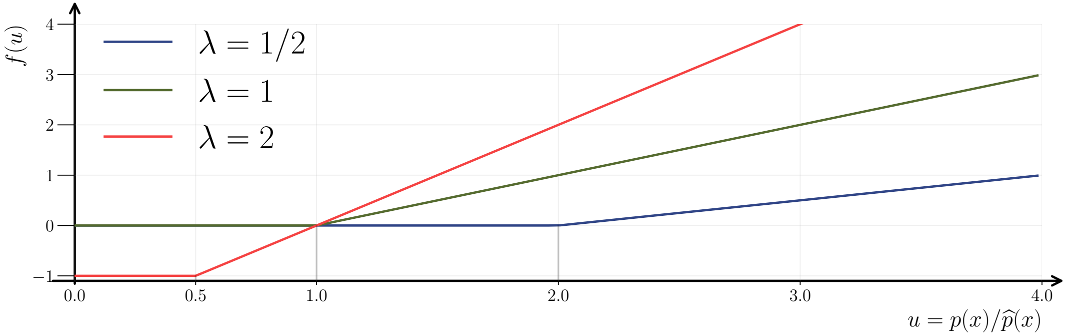
Precision-Recall Divergence

Definition

Definition 2.3 (PR-Divergence generator function f_λ)

Given a trade-off parameter $\lambda \in [0, +\infty]$, *we define the generator function* $f_\lambda : [0, +\infty] \to]-\infty, +\infty]$ *given by*

$$f_\lambda(u) = \begin{cases} \max(\lambda u, 1) - \max(\lambda, 1) & \text{for } \lambda \in [0, +\infty[, \\ \mathbb{1}_{\{u=0\}} & \text{for } \lambda = +\infty. \end{cases} \tag{7}$$



Proposition 2.4 (PR-Divergence)

For any distributions $P, \widehat{P} \in \mathcal{P}(\mathcal{X})$ such that $P, \widehat{P} \ll \mu$, then for any $\lambda \in [0, +\infty]$ the PR-Divergence defined as

$$\mathcal{D}_{\lambda\text{-PR}}(P \| \widehat{P}) = \int_{\mathcal{X}} \widehat{p}(\boldsymbol{x}) f_{\lambda}\left(\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}\right) \mathrm{d}\mu(\boldsymbol{x}) \tag{8}$$

belongs to the class of f-divergences.

Precision-Recall Divergence

Linking the PR-Divergence to the PR-Curve

Theorem 2.5 (PR-Curves as a function of $\mathcal{D}_{\lambda\text{-PR}}$)

Given $P, \widehat{P} \in \mathcal{P}(\mathcal{X})$ such that $P, \widehat{P} \ll \mu$ and $\lambda \in [0, +\infty]$, the PR-Curve $\partial\mathrm{PRD}$ is related to the PR-Divergence $\mathcal{D}_{\lambda\text{-PR}}(P\|\widehat{P})$ as follows.

$$\alpha_\lambda(P\|\widehat{P}) = \min(1, \lambda) - \mathcal{D}_{\lambda\text{-PR}}(P\|\widehat{P}).$$

$$\beta_\lambda(P\|\widehat{P}) = \min(1, \lambda) - \mathcal{D}_{\lambda\text{-PR}}(\widehat{P}\|P).$$

Theorem 2.5 (PR-Curves as a function of $\mathcal{D}_{\lambda\text{-PR}}$)

Given $P, \widehat{P} \in \mathcal{P}(\mathcal{X})$ such that $P, \widehat{P} \ll \mu$ and $\lambda \in [0, +\infty]$, the PR-Curve $\partial\mathrm{PRD}$ is related to the PR-Divergence $\mathcal{D}_{\lambda\text{-PR}}(P\|\widehat{P})$ as follows.

$$\alpha_\lambda(P\|\widehat{P}) = \min(1, \lambda) - \mathcal{D}_{\lambda\text{-PR}}(P\|\widehat{P}).$$

$$\beta_\lambda(P\|\widehat{P}) = \min(1, \lambda) - \mathcal{D}_{\lambda\text{-PR}}(\widehat{P}\|P).$$

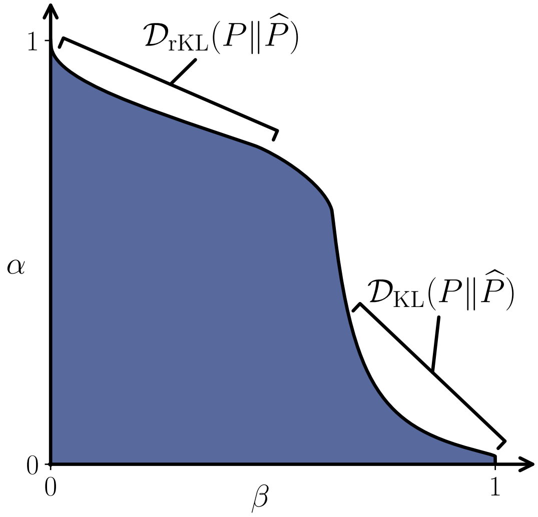
A direct consequence of Theorem 2.5:

$$\operatorname*{argmin}_{\widehat{P}\in\mathcal{P}(\mathcal{X})} \mathcal{D}_{\lambda\text{-PR}}(P\|\widehat{P}) = \operatorname*{argmax}_{\widehat{P}\in\mathcal{P}(\mathcal{X})} \alpha_\lambda(P\|\widehat{P}).$$

Theorem 2.6 (f-divergences as a weighted average of PR-Divergences)

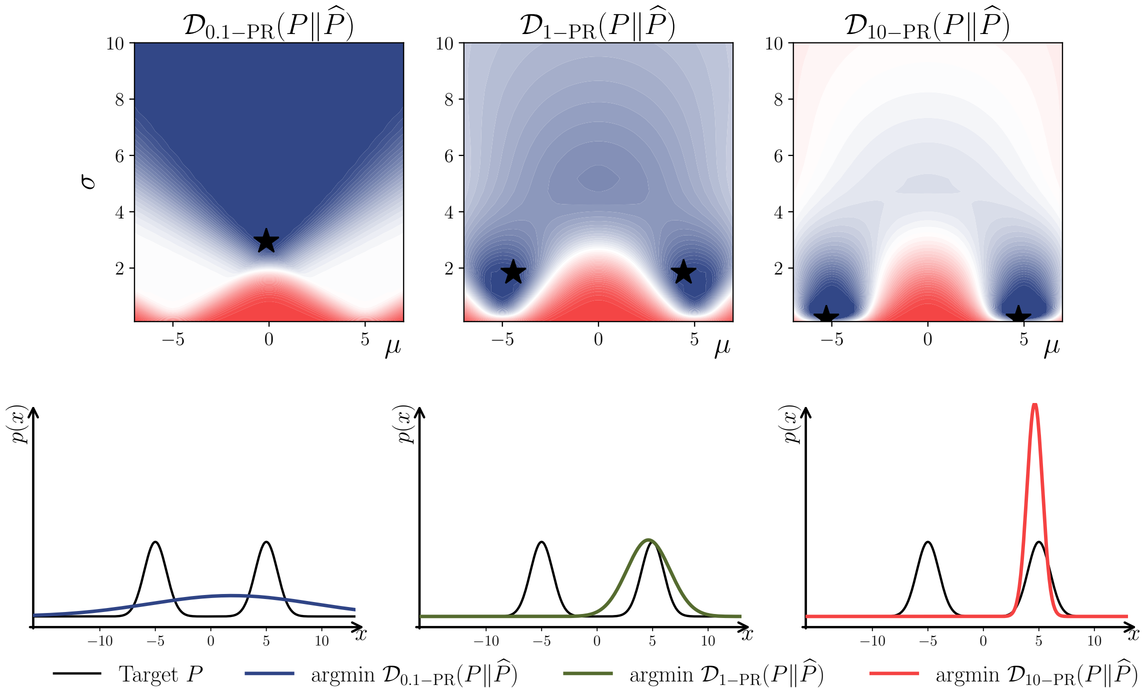
For any $P, \widehat{P} \in \mathcal{P}(\mathcal{X})$ supported on all $\mathcal{X}$ and any $\lambda \in [0, +\infty]$, then:

$$\mathcal{D}_f(P\|\widehat{P}) = \int_0^{\infty} \frac{1}{\lambda^3} f''\left(\frac{1}{\lambda}\right) \mathcal{D}_{\lambda\text{-PR}}(P\|\widehat{P}) \mathrm{d}\lambda,$$



Optimizing the PR-Divergence

Examples

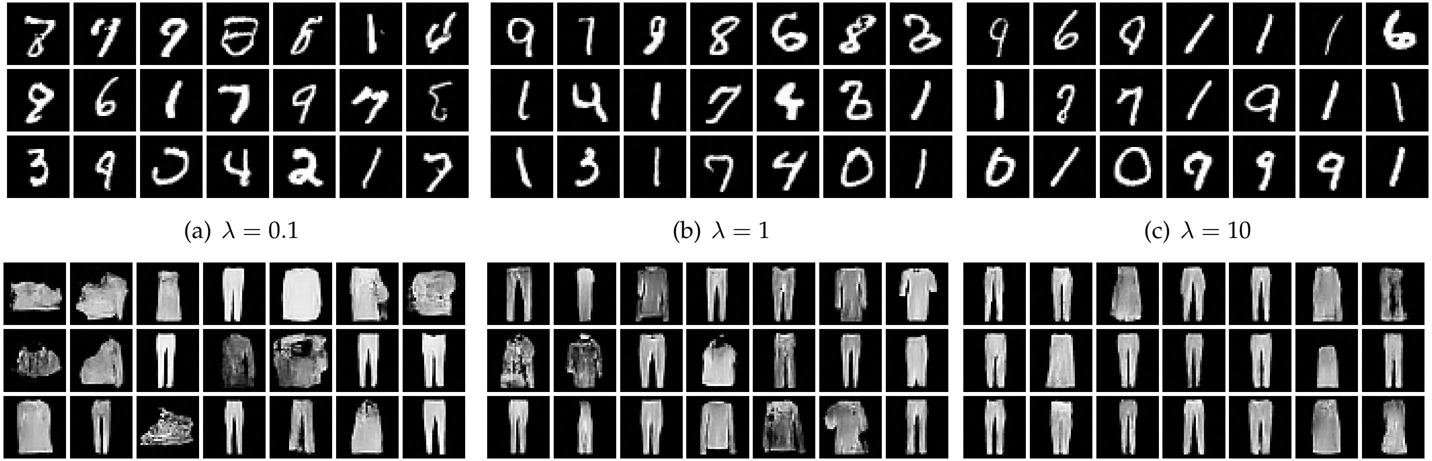


Optimizing the PR-Divergence

Examples

Optimizing the PR-Divergence with our approach

In Practice



(a) $\lambda = 0.1$ (b) $\lambda = 1$ (c) $\lambda = 10$

(d) $\lambda = 0.1$ (e) $\lambda = 1$ (f) $\lambda = 10$

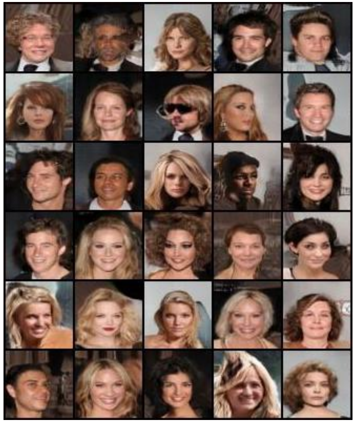
Optimizing the PR-Divergence with our approach

Training GANs

Model	CIFAR-10 32 × 32			CelebA 64 × 64		
	FID	P	R	FID	P	R
Baseline Big-GAN	13.37	86.51	65.66	9.16	78.41	**51.42**
$\lambda = 0.05$	13.29	81.10	70.63	-	-	-
$\lambda = 0.1$	**11.62**	81.78	**74.58**	-	-	-
$\lambda = 0.2$	13.36	84.85	65.13	8.79	83.37	44.07
$\lambda = 0.5$	14.50	83.27	68.23	**6.03**	77.60	**55.98**
$\lambda = 1.0$	14.03	83.04	69.35	13.07	81.70	36.85
$\lambda = 2.0$	16.94	84.93	59.79	14.23	82.98	32.87
$\lambda = 5.0$	32.54	83.39	56.94	22.45	**83.96**	25.81
$\lambda = 10.0$	39.69	84.11	39.29	-	-	-
$\lambda = 20.0$	67.03	**90.03**	21.81	-	-	-

$$\text{When } \lambda \text{ increases, } \begin{cases} \text{Precision} \uparrow \\ \text{Recall} \downarrow \end{cases}$$

$\lambda = 0.1$



$\lambda = 10$

Optimizing the PR-Divergence with our approach

Fine-Tuning GANs

Model	ImageNet 128 × 128			FFHQ 256 × 256		
	FID	P	R	FID	P	R
Baseline BigGAN	9.83	28.04	41.21	41.41	65.57	**10.17**
Soft $\psi = 0.7$	11.39	23.04	31.13	56.43	76.59	4.87
Soft $\psi = 0.5$	15.49	20.20	19.83	82.05	84.48	1.58
Hard $\psi = 2.0$	**9.69**	25.83	39.89	43.32	68.84	8.66
Hard $\psi = 1.0$	12.12	21.86	35.42	56.19	76.44	4.76
Hard $\psi = 0.5$	15.21	21.13	29.55	71.32	80.99	4.84
$\lambda = 0.2$	9.92	26.69	42.04	35.66	78.70	9.45
$\lambda = 0.5$	10.82	26.83	**42.38**	**35.24**	78.41	9.66
$\lambda = 1.0$	20.42	29.72	28.21	35.91	78.95	8.32
$\lambda = 2.0$	20.21	30.27	30.49	36.33	81.10	8.69
$\lambda = 5.0$	20.76	**30.87**	28.38	38.16	**84.31**	8.52

When λ increases, $\begin{cases} \text{Precision} \uparrow \\ \text{Recall} \downarrow \end{cases}$ with better performances than truncation.

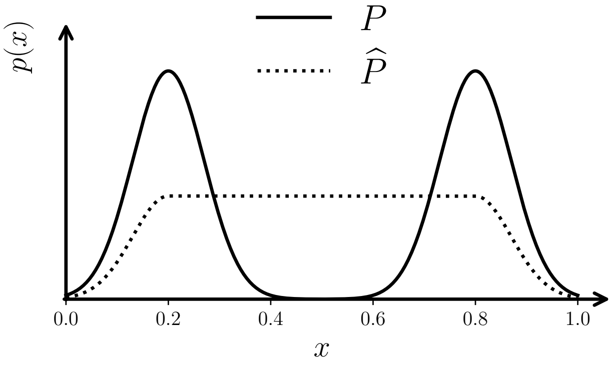
Improving:
How can we improve the quality and diversity of a pre-trained generative models?

Sampling from a generative model

General Setting

To sample a point from the learned distribution $\widehat{P}$:

- Sample $\boldsymbol{z} \sim Q$.
- Compute $\boldsymbol{x} = G(\boldsymbol{z})$.



Sampling from a generative model
General Setting

To sample a point from the learned distribution $\widehat{P}$:
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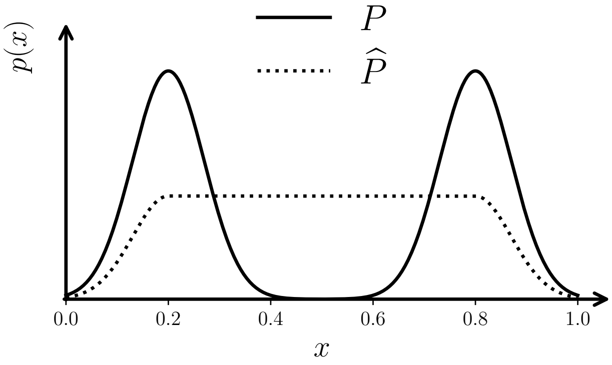
- Compute $\boldsymbol{x} = G(\boldsymbol{z})$.

$$P \neq \widehat{P}$$

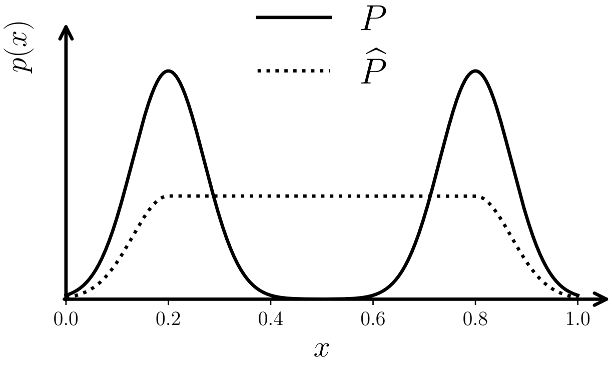


Sampling from a generative model
General Setting

To sample a point from the learned distribution $\widehat{P}$:

- Sample $\boldsymbol{z} \sim Q$.
- Compute $\boldsymbol{x} = G(\boldsymbol{z})$.

We have an estimation of $\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}$ using $\nabla f^*(T(\boldsymbol{x}))$.



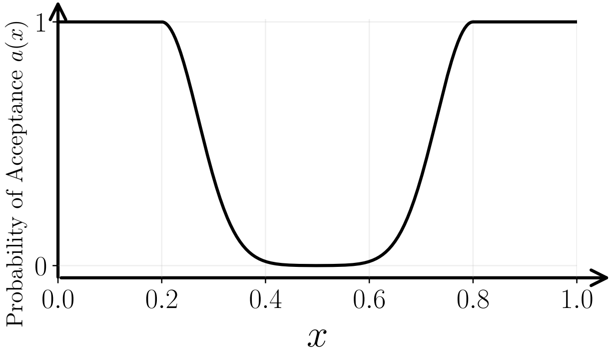
Sampling from a generative model

Rejection Sampling

To sample a point from the refined distribution $\widetilde{P}$:

- Sample $\boldsymbol{z} \sim Q$.
- Compute $\boldsymbol{x} = G(\boldsymbol{z})$.
- Accept $\boldsymbol{x}$ with probability $a(\boldsymbol{x})$.

Using $\frac{p(\boldsymbol{x})}{\widetilde{p}(\boldsymbol{x})}$ in $a(\boldsymbol{x})$ allows sampling from P.



Sampling from a generative model

Rejection Sampling

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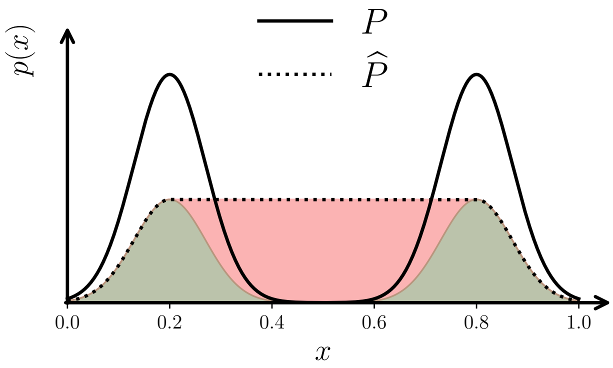


The acceptance rate is :

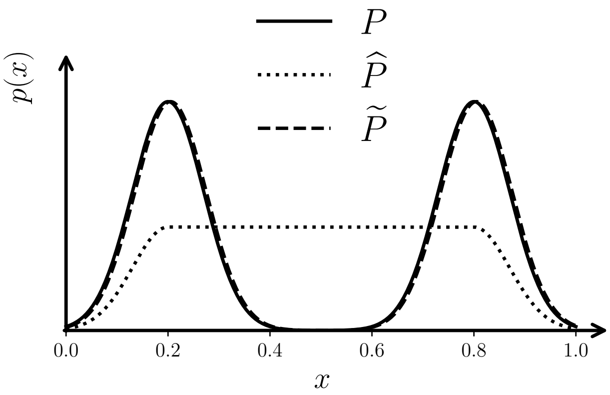
$$\mathbb{E}_{\widehat{P}}\left[a(\boldsymbol{x})\right].$$

Sampling from a generative model
Rejection Sampling

To sample a point from the refined distribution $\widetilde{P}$:

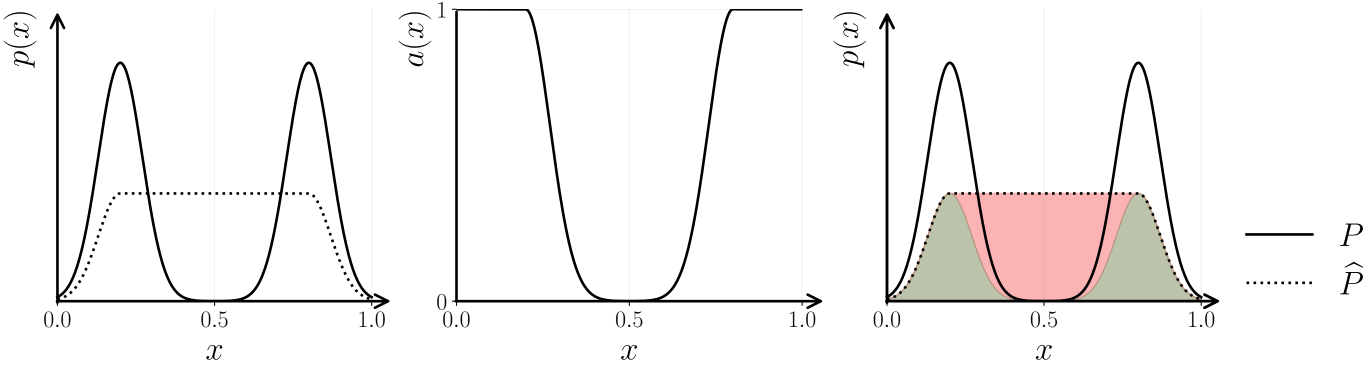
- Sample $\boldsymbol{z} \sim Q$.
- Compute $\boldsymbol{x} = G(\boldsymbol{z})$.
- Accept $\boldsymbol{x}$ with probability $a(\boldsymbol{x})$.

It defines a new distribution $\widetilde{P}$.



Sampling from a generative model

Rejection Sampling in high dimension



Acceptance rate: 45.20%

Definition 3.1 (Discriminator Rejection Sampling (DRS) - Azadi et al. [2])

Let $\gamma \in \mathbb{R}$, the acceptance probability is:

$$a_{\mathrm{DRS}}(\boldsymbol{x}) = \frac{r(\boldsymbol{x})}{r(\boldsymbol{x})\left(1 - e^{\gamma}\right) + Me^{\gamma}}.$$

If $\gamma < 0$, then the acceptance rate increases.

Budgeted Rejection Sampling

Tuning the acceptance rate

Definition 3.1 (Discriminator Rejection Sampling (DRS) - Azadi et al. [2])

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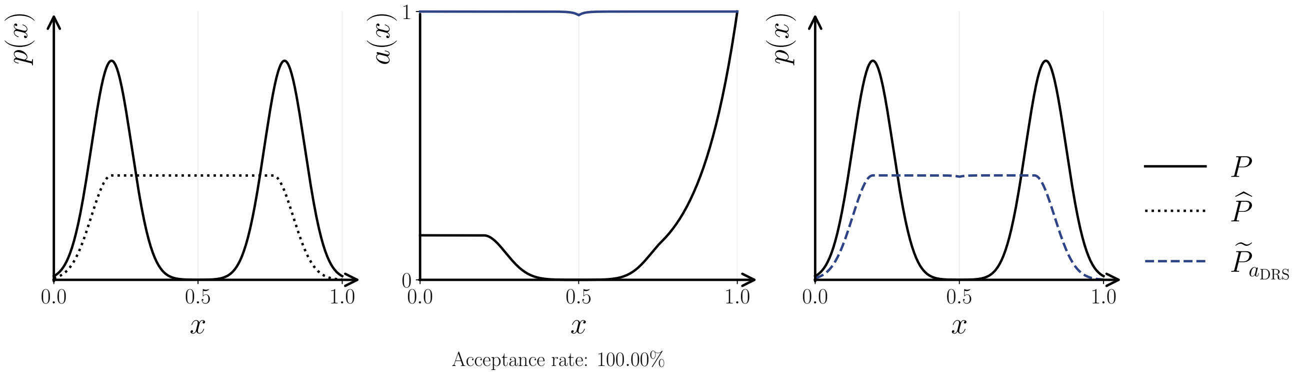
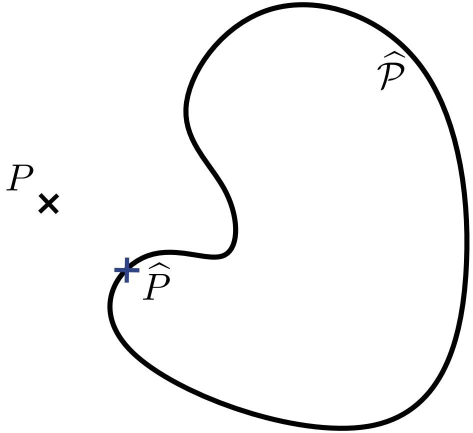


Optimal Budgeted Rejection Sampling
Definition

Traditionally, the goal is:

$$\min_{G} \quad \mathcal{D}_f(P \| \widehat{P}_G)$$

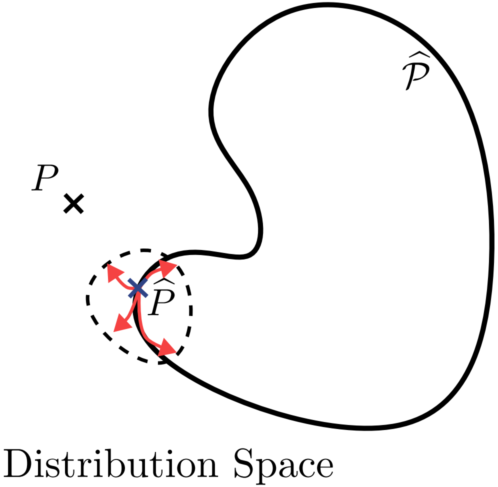


Optimal Budgeted Rejection Sampling
Definition

Traditionally, the goal is:

$$\min_{G} \quad \mathcal{D}_f(P \| \widehat{P}_G)$$

An acceptance function $a(\boldsymbol{x})$ such that the acceptance rate is greater than $1/K$ defines a refined distribution $\widetilde{P}_a$ in a convex set that contains $\widehat{P}_G$.

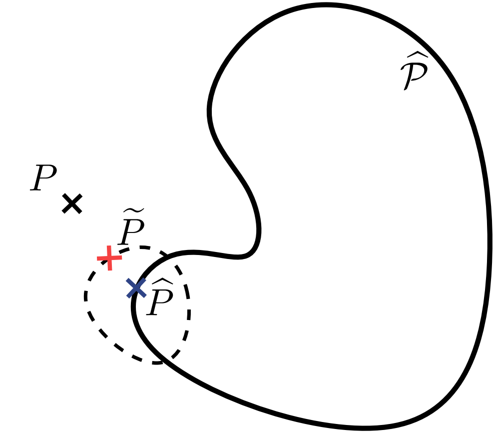


Optimal Budgeted Rejection Sampling

Definition

With a given $\widehat{P}_G$, our goal is:

$$\begin{aligned} \min_{a} \quad & \mathcal{D}_f(P \| \widetilde{P}_a) \\ \text{s.t.} \; & \begin{cases} \mathbb{E}_{\widehat{P}}\left[a(\boldsymbol{x})\right] \geq 1/K, \\ \forall \boldsymbol{x} \in \mathcal{X},\, 0 \leq a(\boldsymbol{x}) \leq 1. \end{cases} \end{aligned} \tag{9}$$



Optimal Budgeted Rejection Sampling

Definition

Theorem 3.2 (Optimal Acceptance Function)

For a sampling budget $K \geq 1$ and finite $\mathcal{X}$, the solution is,

$$a_{\mathrm{OBRS}}(\boldsymbol{x}) = \min\left(\frac{p(\boldsymbol{x})}{\widehat{p}(\boldsymbol{x})}\frac{c_K}{M}, 1\right), \tag{10}$$

where $c_K \geq 1$ is such that $\mathbb{E}_{\boldsymbol{x}\sim\widehat{p}}[a_{\mathrm{OBRS}}(\boldsymbol{x})] = 1/K$.

Optimal Budgeted Rejection Sampling

Definition

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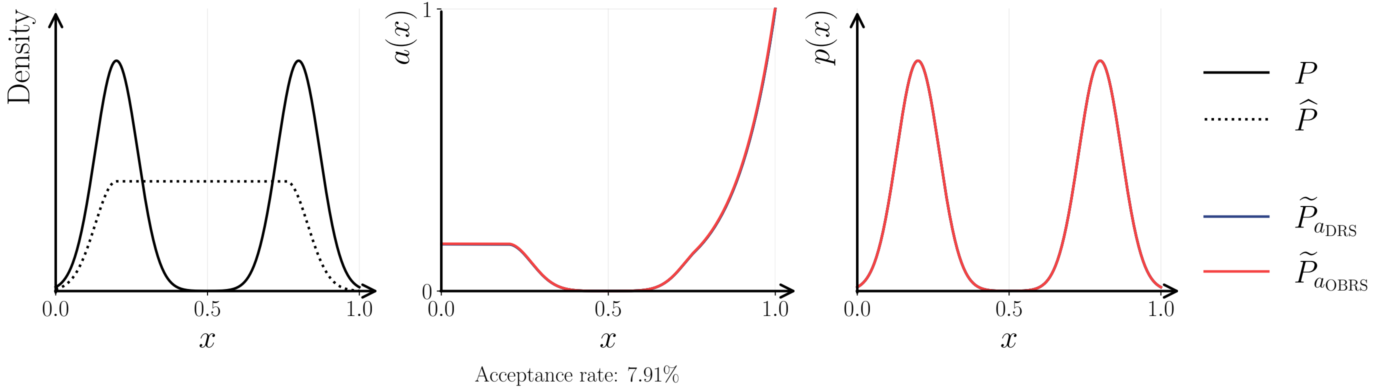

Improving Precision and Recall

Effect of the OBRS

Proposition 3.3 (Precision and Recall Improvement)

Let $K \leq M$ be the budget for the OBRS. For any $(\alpha, \beta) \in \mathrm{PRD}(P, \widehat{P})$ we have $(\alpha', \beta) \in \mathrm{PRD}(P, \widetilde{P}_{a_{\mathrm{OBRS}}})$ with $\alpha' = \min\{1, K\alpha\}$.

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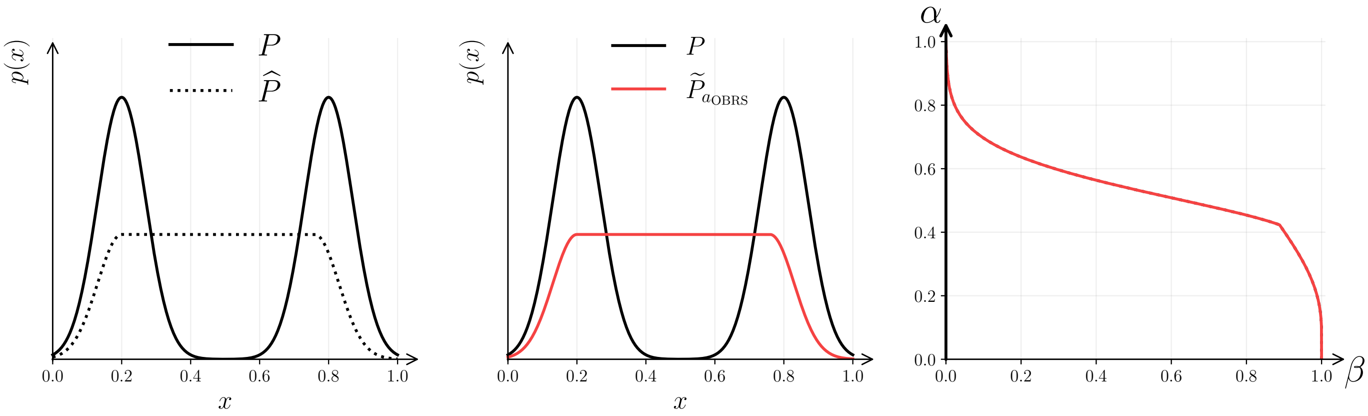

Acceptance rate: 100.00%

Improving Precision and Recall

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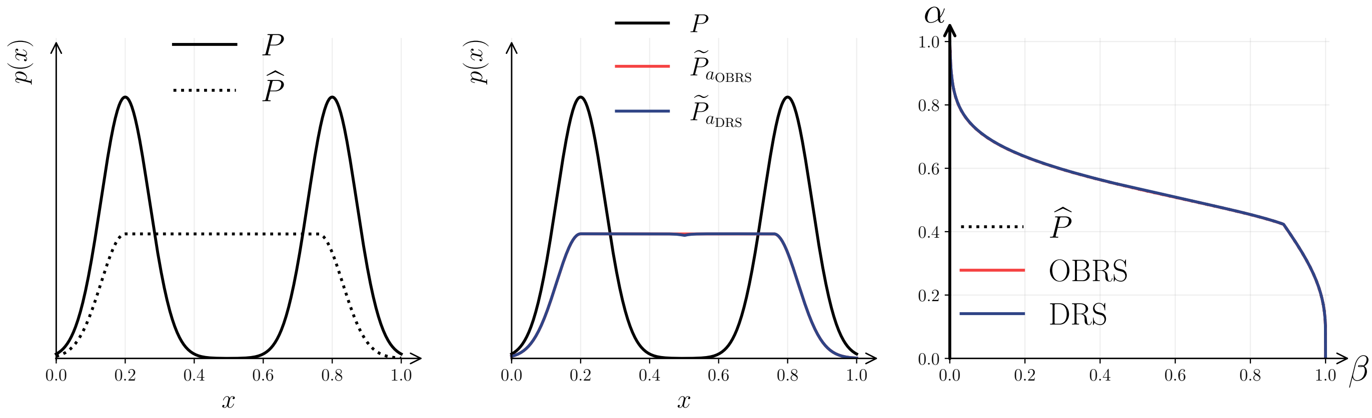

Acceptance rate: 100.00%

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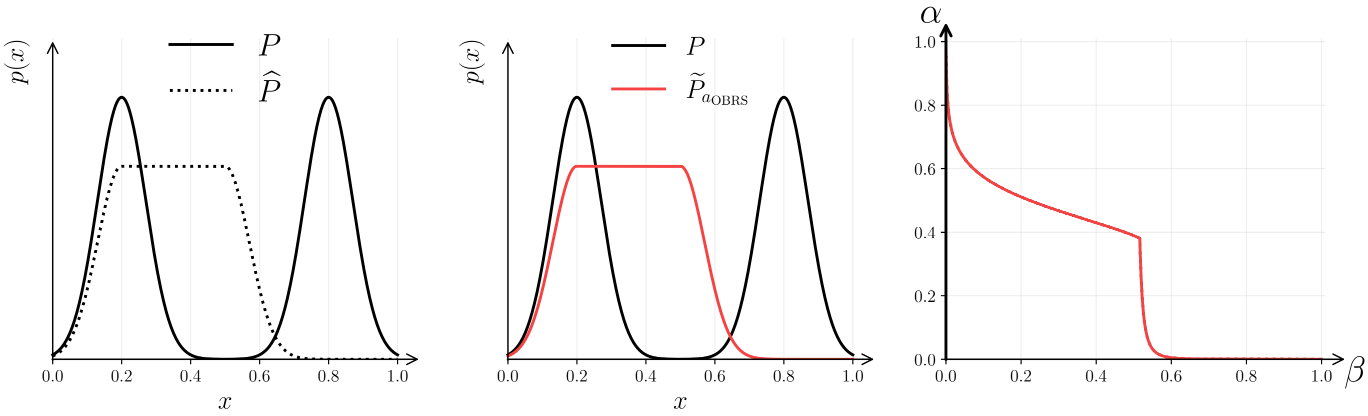
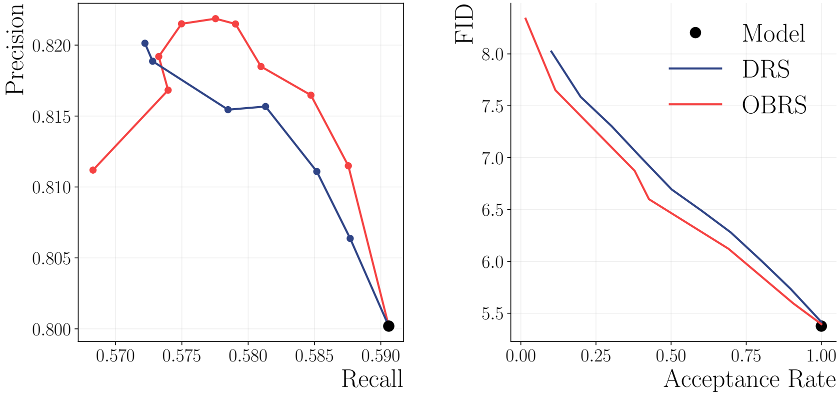


Acceptance rate: 100.00%



GAN on CelebA

1/K	FID	P	R
0.25	1.57	78.48	86.73
0.50	1.58	78.23	86.05
0.75	1.77	77.94	86.54
1	1.97	77.91	86.62

Diffusion Model on CIFAR-10

Other Methods to improve Precision and Recall
Boosting

Boosting Generative models:

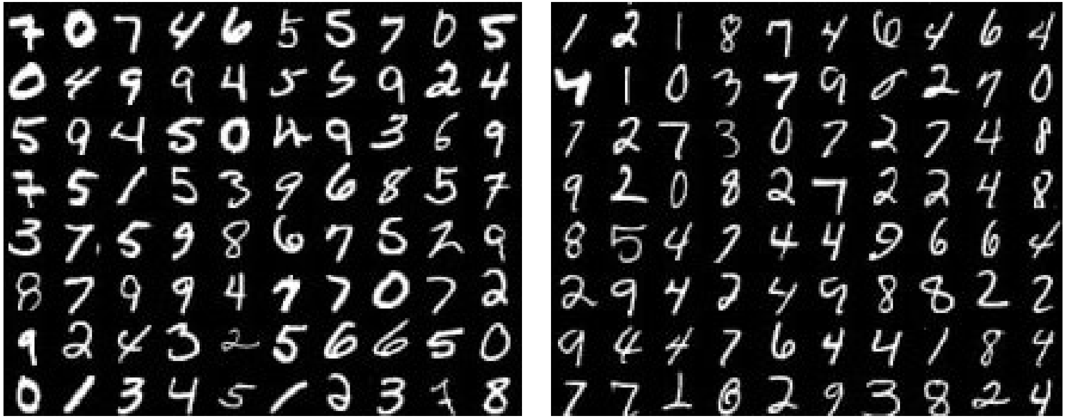


Figure. Left: Samples from the dataset given high weights by the discriminator. Right: Samples from the dataset given low weights by the discriminator. The next model will focus on the sample on the right. Source: Tolstikhin et al. [28]

- Tolstikhin et al. [28]
- Grover and Ermon [14]

Other Methods to improve Precision and Recall
Gradient Ascent

Using the discriminator as a classifier and perform a gradient descent:

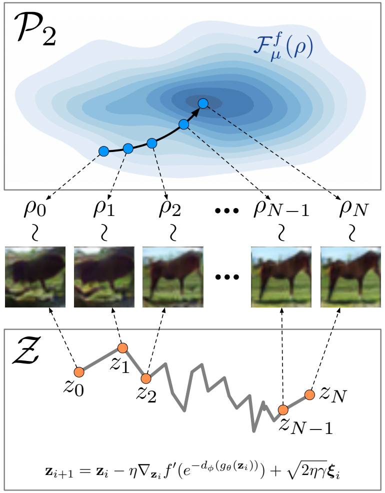


Figure. Source: Ansari et al. [1]

- Ansari et al. [1]
- Tanaka [27]
- Che et al. [9]

Other Methods to improve Precision and Recall

Gaussian Mixtures

Training a Gaussian Mixture $\mathcal{N}(\mu_k, \sigma I)$ in the latent space:

(a) $\sigma = 0.1$ (b) $\sigma = 1$ (c) $\sigma = 2$ (d) Precision and Recall

Figure. Source: Ben-Yosef and Weinshall [4]

- Ben-Yosef and Weinshall [4]
- Pandeva and Schubert [22]
- Alternative idea: Use Expectation-Maximization Bishop [5]

Recap

References to evaluate generative models:

- FID: Heusel et al. [15]
- PR-Curves: Sajjadi et al. [23]
- Support based metrics: Kynkäänniemi et al. [19]

Methods to tune precision and recall:

- Truncation: Karras et al. [17], Kingma and Dhariwal [18]
- f-GAN: Nowozin et al. [21]
- PR-GAN: Verine et al. [31]

Recap

Methods to improve precision and recall:

- Rejecting samples: Azadi et al. [2], Verine et al. [31], Turner et al. [29], Tanaka [27]
- Boosting: Tolstikhin et al. [28], Grover and Ermon [14]
- Gradient Ascent: Ansari et al. [1], Tanaka [27], Che et al. [9]
- Latent Space Reshaping: Ben-Yosef and Weinshall [4], Pandeva and Schubert [22], Issenhuth et al. [16]
- EM in the latent space: Bishop [5]

Conclusion

Thanks !

How to SLURM ?

Data Science Lab

Constant Bourdrez

PhD Student,
Centre des Données, ENS-PSL

October 29, 2025

What is SLURM?

- Open-source workload manager for high-performance clusters.
- Schedules and queues jobs; matches jobs to available nodes.
- Allocates requested resources (CPU, GPU, memory) reliably.
- Provides monitoring and accounting tools (e.g., `squeue`, `sacct`).

Traditional Slurm Workflow

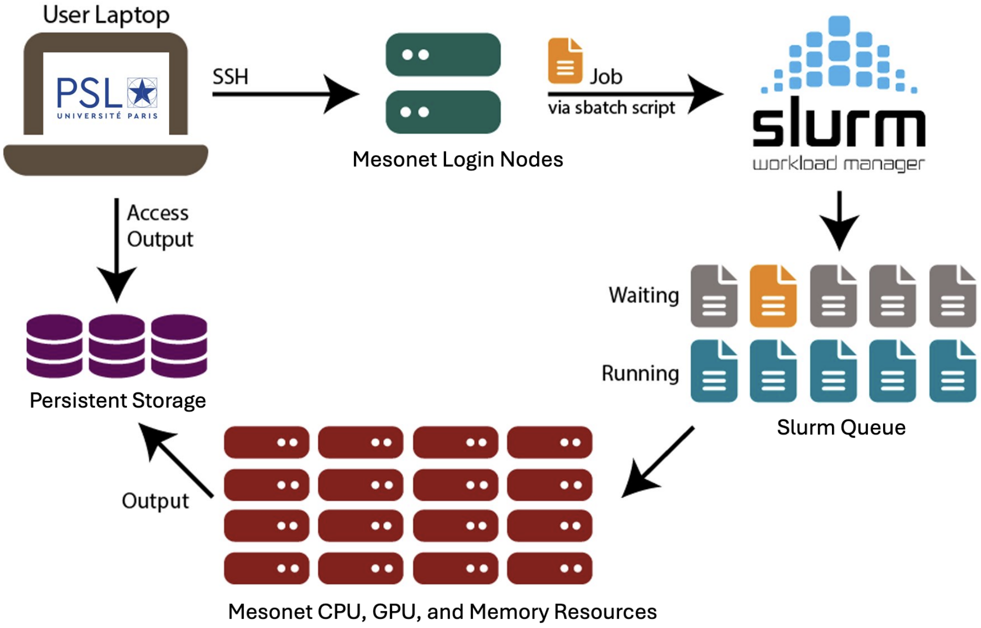
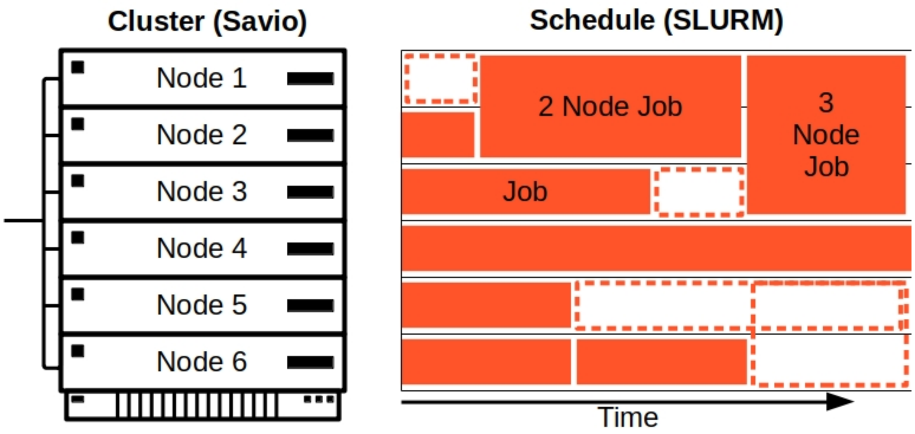


Figure. Typical SLURM job submission and execution workflow.

Slurm Backfill

- Jobs at the top of the queue have highest priority.
- Slurm can run lower-priority jobs **without delaying higher-priority jobs**.
- Helps smaller jobs run and prevents large jobs from blocking the system.
- Especially useful for multi-node job scheduling.



Submitting a SLURM job

```bash
name="GAN_TRAINING"
outdir="outputs"

echo "Launching job $name"

sbatch <<EOT
#!/bin/bash
#SBATCH -p mesonet
#SBATCH -N 1
#SBATCH -c 28
#SBATCH --gres=gpu:${n_gpu}
#SBATCH --time=00:20:00
#SBATCH --mem=256G
#SBATCH --account=m25146
#SBATCH --job-name=${name}
#SBATCH --cpus-per-task=4
#SBATCH --output=$outdir/path.txt

source activate venv/bin/activate
python my_program.py
EOT
```

Basic Commands

Submit a job:

```
sbatch myscript.sh
```

```
chmod +x myscript.sh
./myscript.sh
```

Check your jobs:

```
squeue -u $USER
```

Cancel a job:

```
scancel JOB_ID
```

Generating an SSH Key for MesoNET

Step 1: Generate a new SSH key

```
ssh-keygen -t ed25519 -C "your_email@example.com"
```

- Press Enter to accept the default file location. (.ssh/id_ed25519)
- Enter a passphrase if you want extra security (optional).

Step 2: Copy the public key

```
cat .ssh/id_ed25519.pub
```

This prints your public key in the terminal.

Step 3: Add your key to MesoNET

1. Log in to your MesoNET account.
2. Go to the **SSH Keys** section and paste the public key you copied from the terminal.
3. Save your changes.

Connecting to Juliet (MesoNET)

Prerequisites:

- A valid **MesoNET account**
- An **SSH key** associated with your account

Connect via SSH:

```
ssh username@juliet.mesonet.fr
```

Replace `username` with your MesoNET ID. **Optional SSH configuration:**

```
Host juliet
  Hostname juliet.mesonet.fr
  User username
  IdentityFile [PathToYourSSHKey]
  IdentitiesOnly yes
```

Replace `username` and `[PathToYourSSHKey]` with your information.

Thanks !

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