

# QUALITY AND DIVERSITY IN GENERATIVE MODELS THROUGH THE LENS OF $f$ -DIVERGENCES

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UNIVERSITÉ PARIS UMR 7243

 **MILES**  
Machine Intelligence and Learning Systems

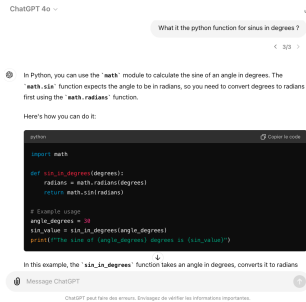


# GENERATIVE MODELS

## CONTEXT

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

### Text Generation



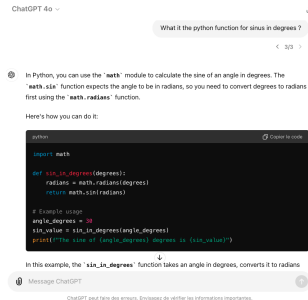
eg: Code Completion

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Text Generation



eg: Code Completion

Image/Video Generation

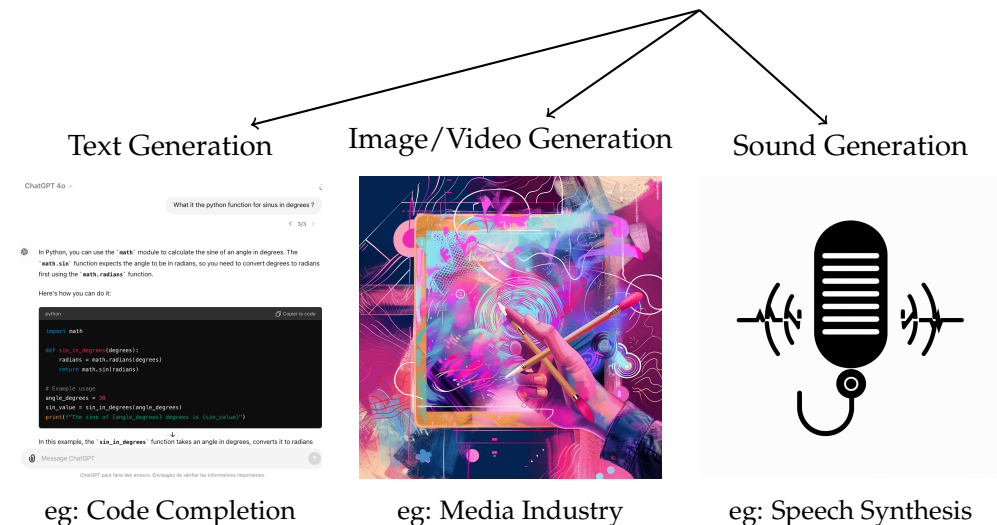


eg: Media Industry

# GENERATIVE MODELS

## CONTEXT

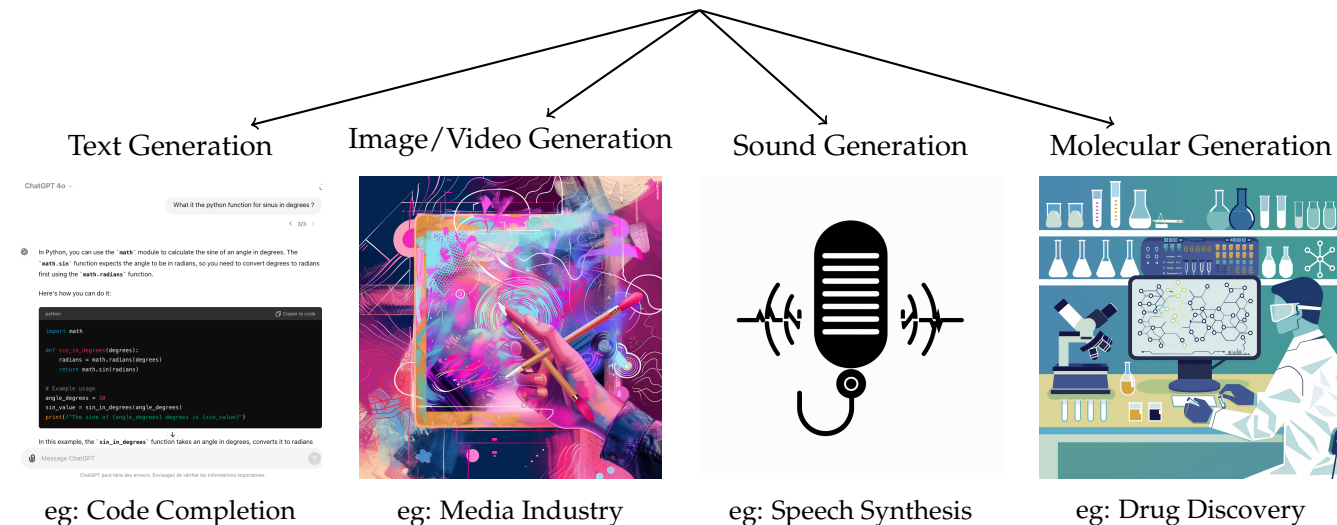
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# THE VARIOUS PERFORMANCES OF GENERATIVE MODELS

## 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.*

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# 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. **Optimizing:** 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?

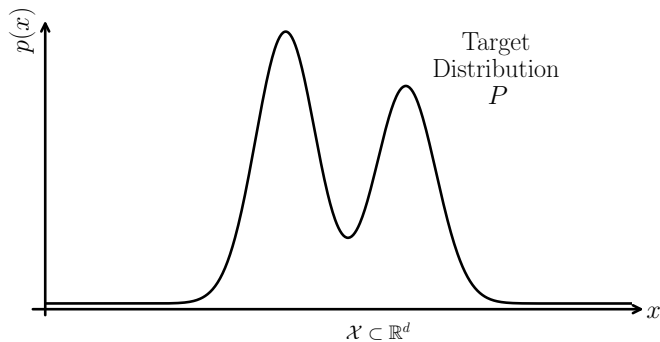
## SECTION 1: EVALUATING

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



# GENERATIVE MODELS

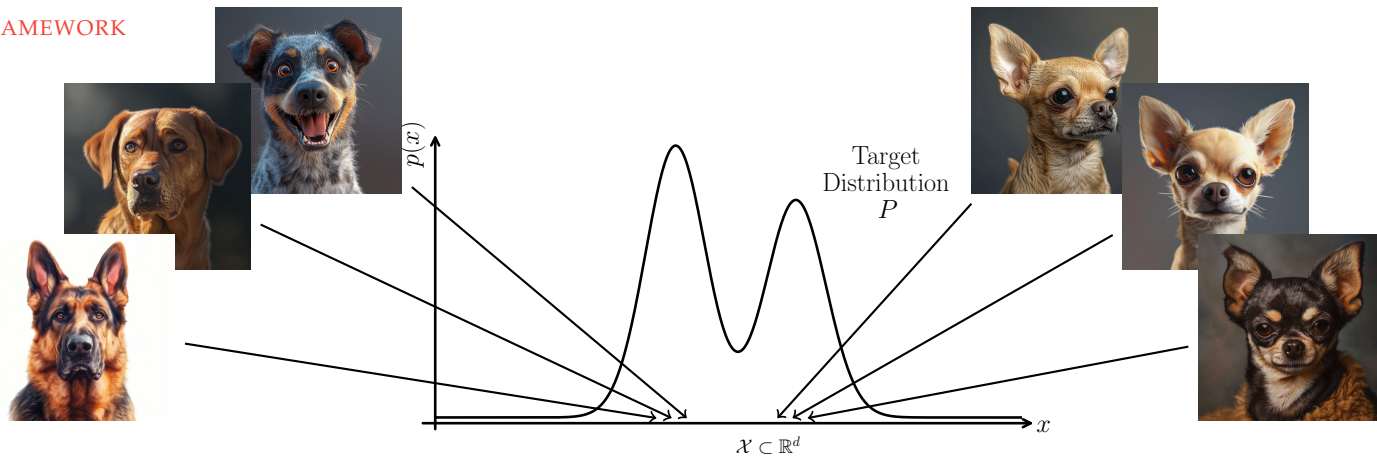
## FRAMEWORK



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

# GENERATIVE MODELS

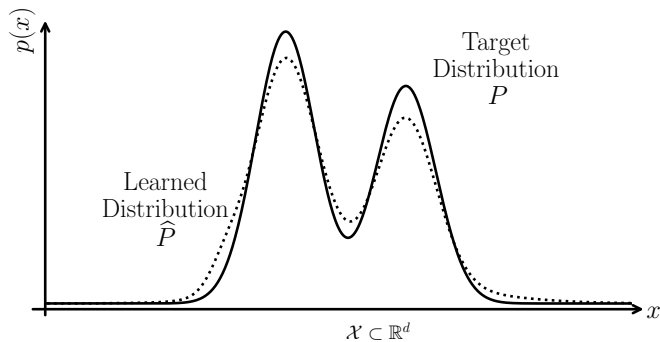
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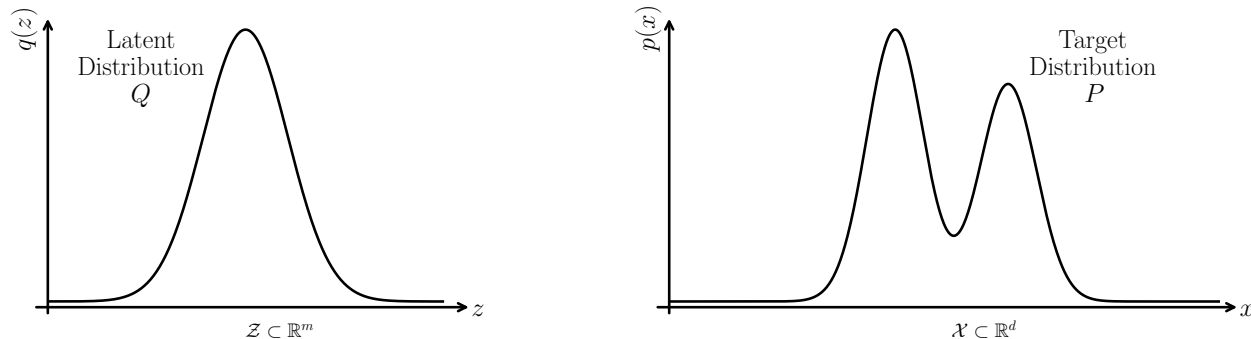
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- **Goal:** Learn a *parameterized distribution*  $\hat{P}$  that approximate  $P$ :

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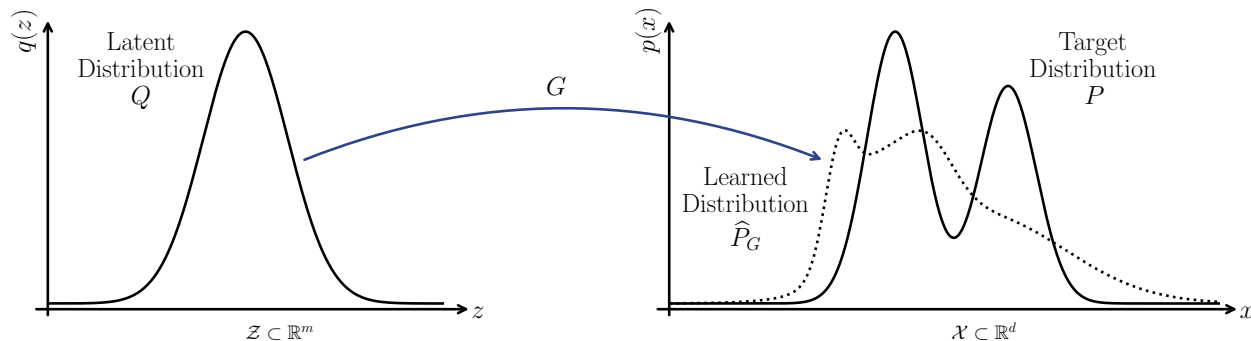
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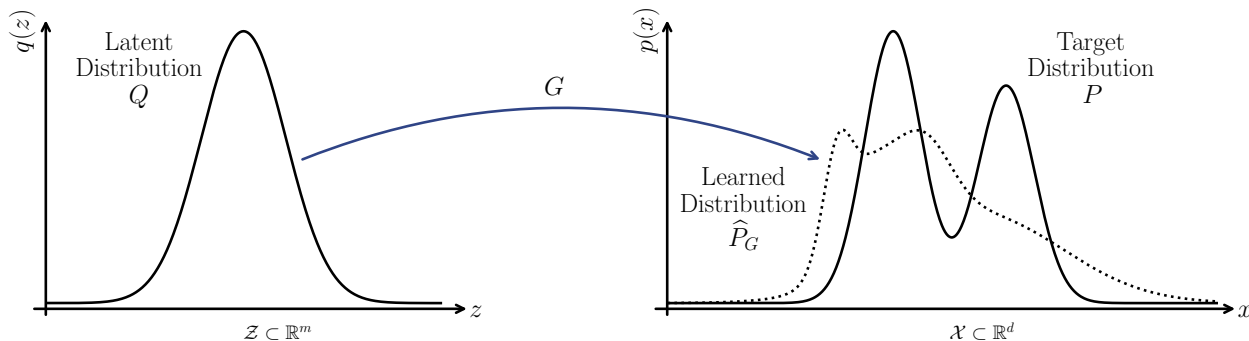
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  2. Take a *generator model*  $G$  represented by a neural network. Take  $\hat{P}_G = G\#Q$ .

# GENERATIVE MODELS

## FRAMEWORK

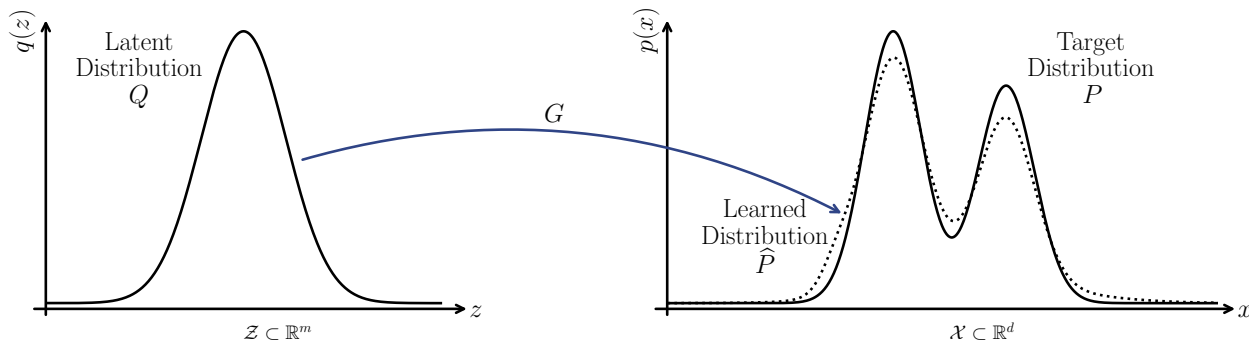


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  3. Compute  $G^{\text{opt}}$  that minimize a *dissimilarity measure*  $D$  between  $P$  and  $\hat{P}_G$ :

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

# GENERATIVE MODELS

## FRAMEWORK



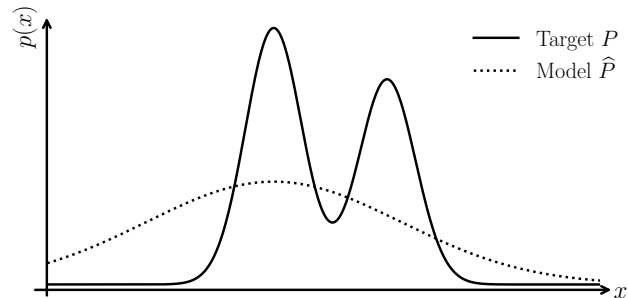
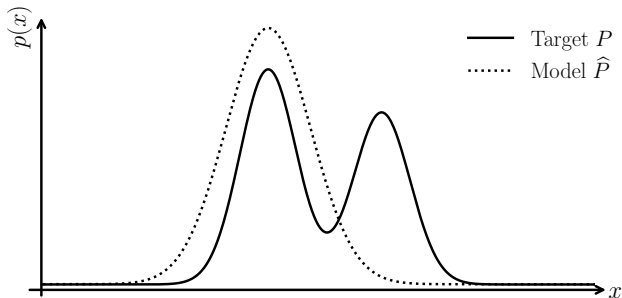
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# GENERATIVE MODELS

## IN PRACTICE

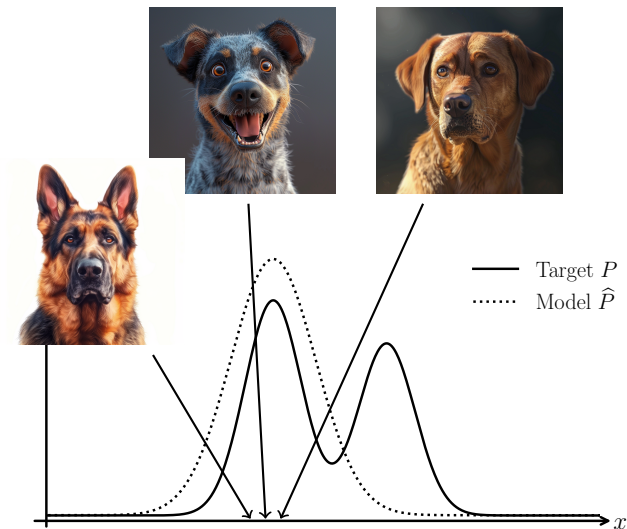
$$\hat{P} \neq P$$



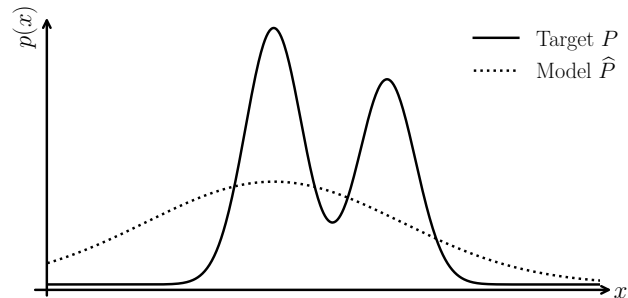


# GENERATIVE MODELS

## IN PRACTICE



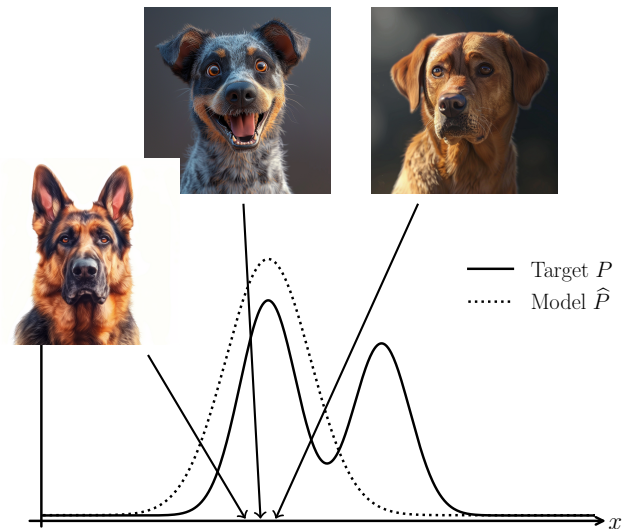
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Low Diversity

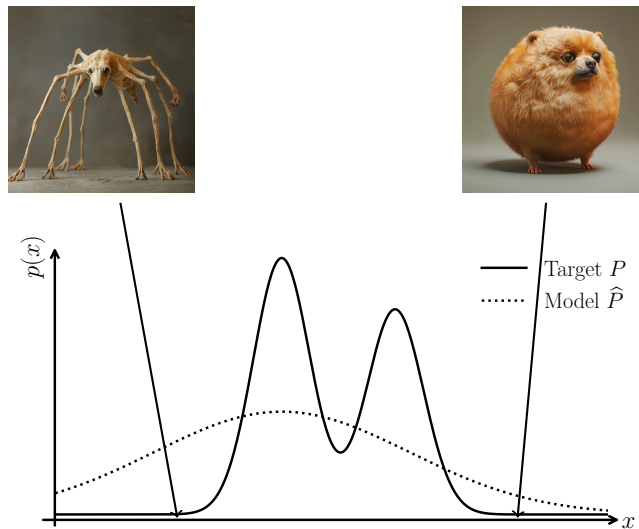
# GENERATIVE MODELS

## IN PRACTICE



Low Diversity

$$\hat{P} \neq P$$



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

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Precision

=

What proportion of **generated** samples are **realistic**?

# PRECISION AND RECALL FOR GENERATIVE MODELS

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Quality



Precision

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Diversity



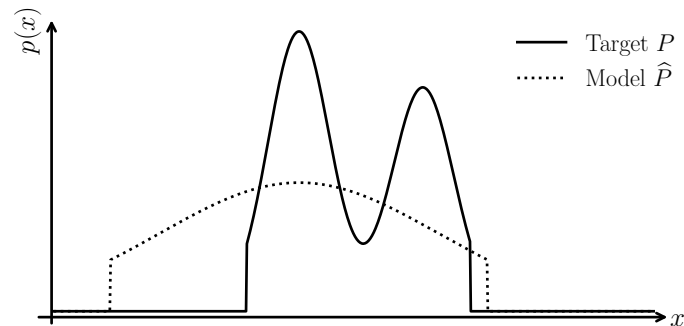
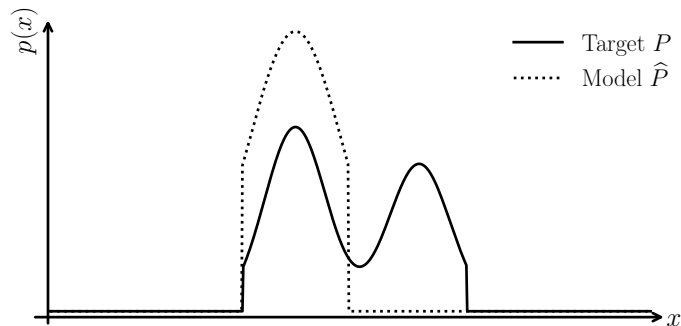
Recall

=

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 2.1 (Support-Based Precision and Recall - Kynkäänniemi et al. [8].)

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

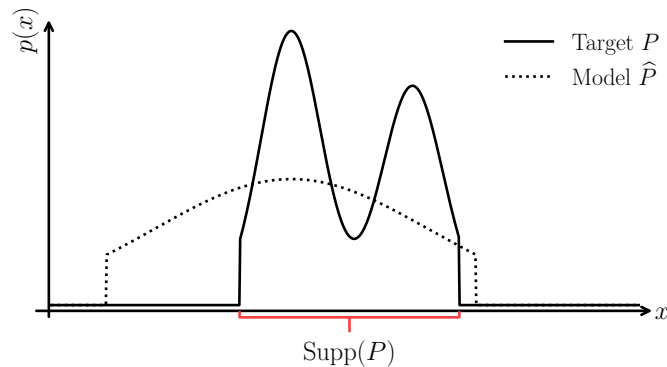
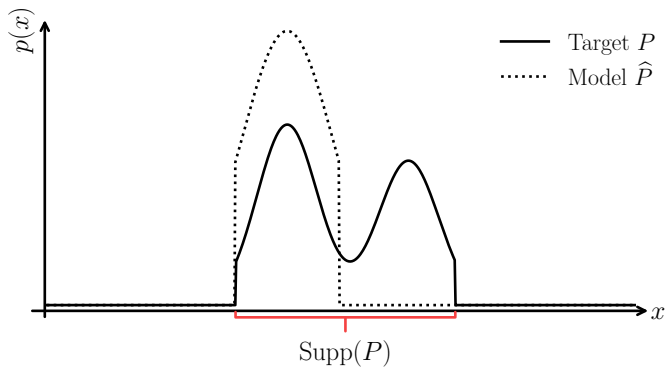
$$\bar{\alpha} := \hat{P}(\text{Supp}(P)) \quad \text{and} \quad \bar{\beta} := P(\text{Supp}(\hat{P})). \quad (1)$$

# 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:

$$\bar{\alpha} = \hat{P}(\text{Supp}(P)).$$



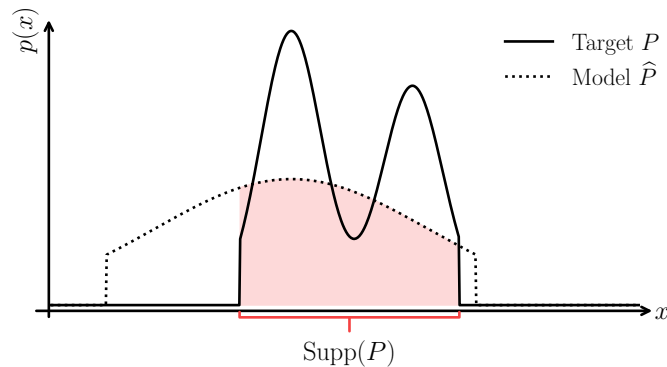
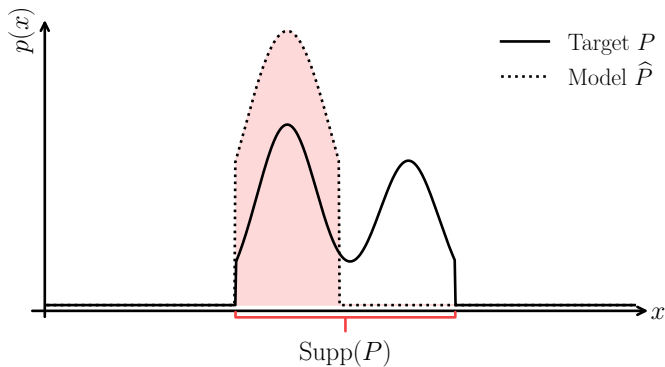


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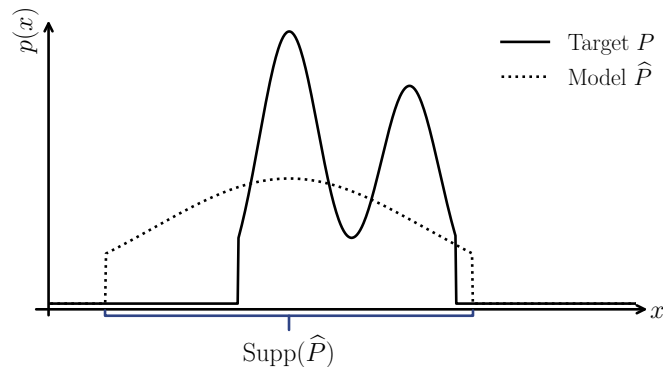
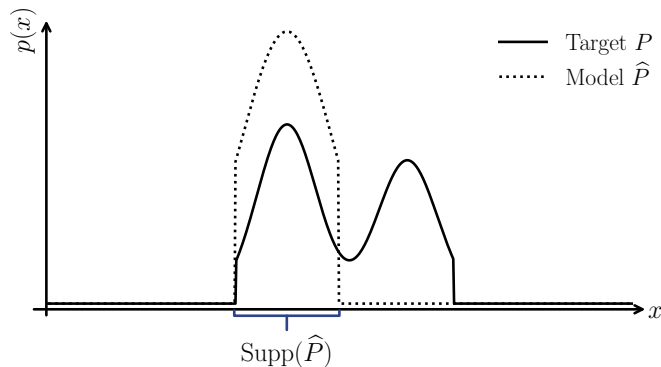


# PRECISION AND RECALL FOR GENERATIVE MODELS

## FOR FINITE SUPPORT

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

$$\bar{\beta} = P(\text{Supp}(\hat{P})).$$

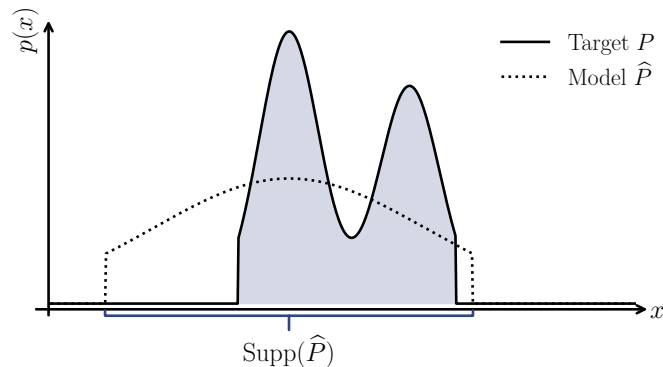
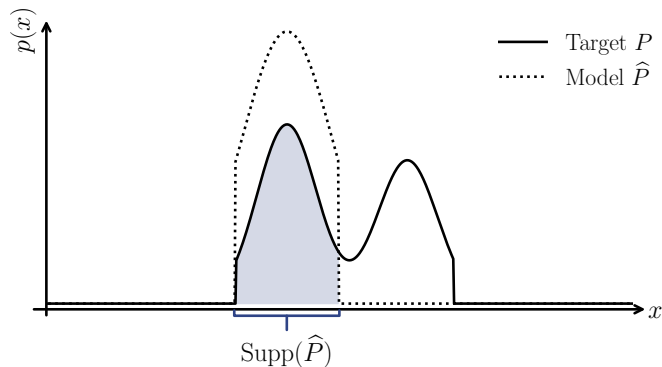


# PRECISION AND RECALL FOR GENERATIVE MODELS

## FOR FINITE SUPPORT

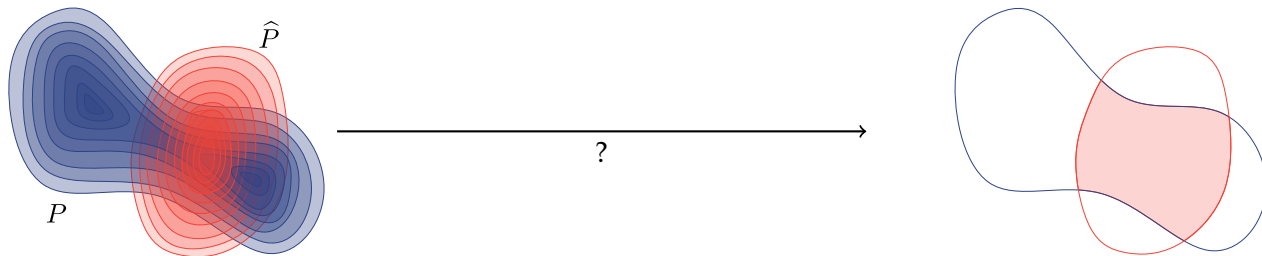
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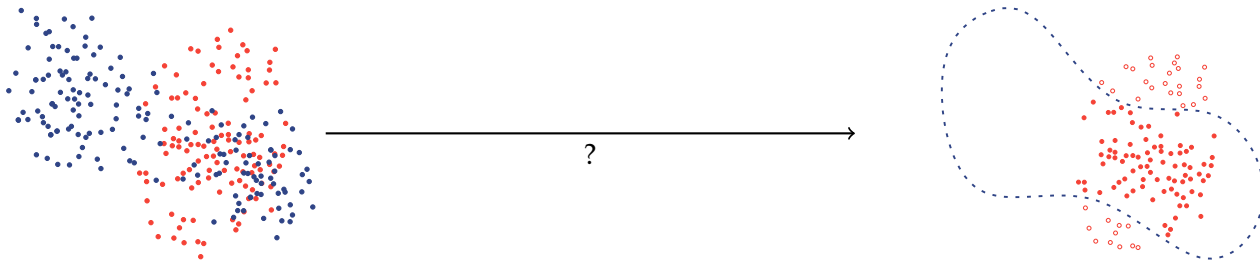
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## ESTIMATING THE PRECISION AND RECALL



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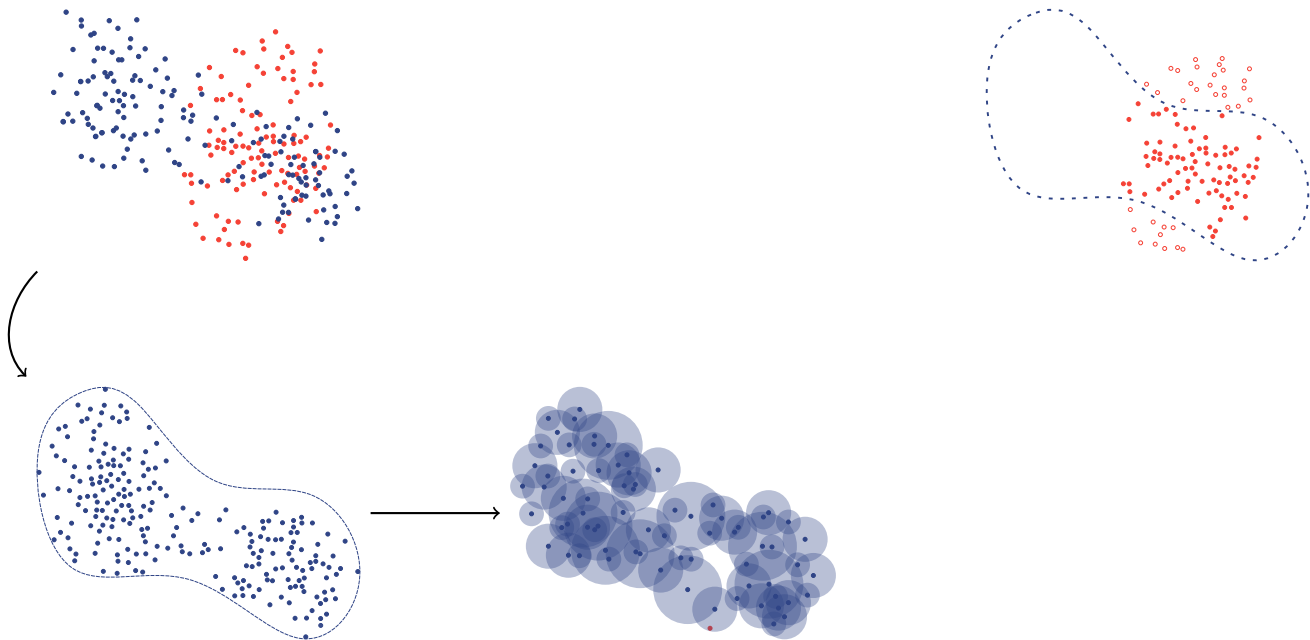
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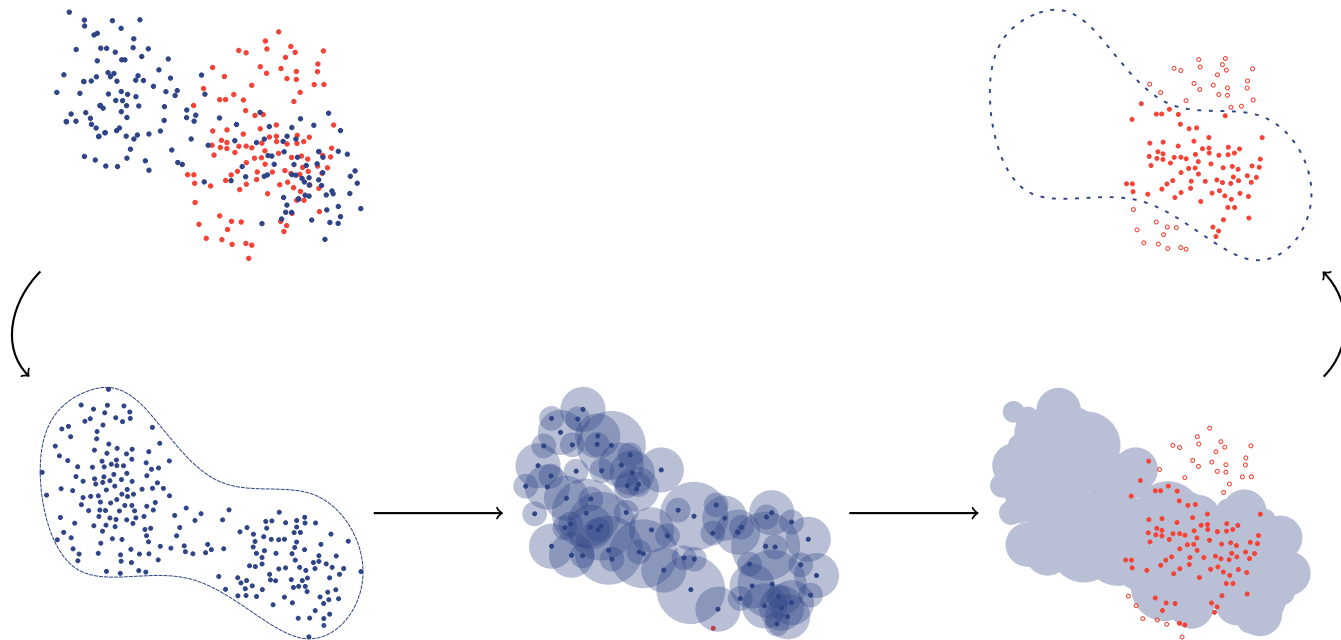
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## ESTIMATING THE PRECISION AND RECALL





# PRECISION AND RECALL FOR GENERATIVE MODELS

## IN PRACTICE

MNIST Dataset [14]



# PRECISION AND RECALL FOR GENERATIVE MODELS

## IN PRACTICE

Low Precision    High Recall



Precision: 0.54    Recall: 0.91

MNIST Dataset [14]



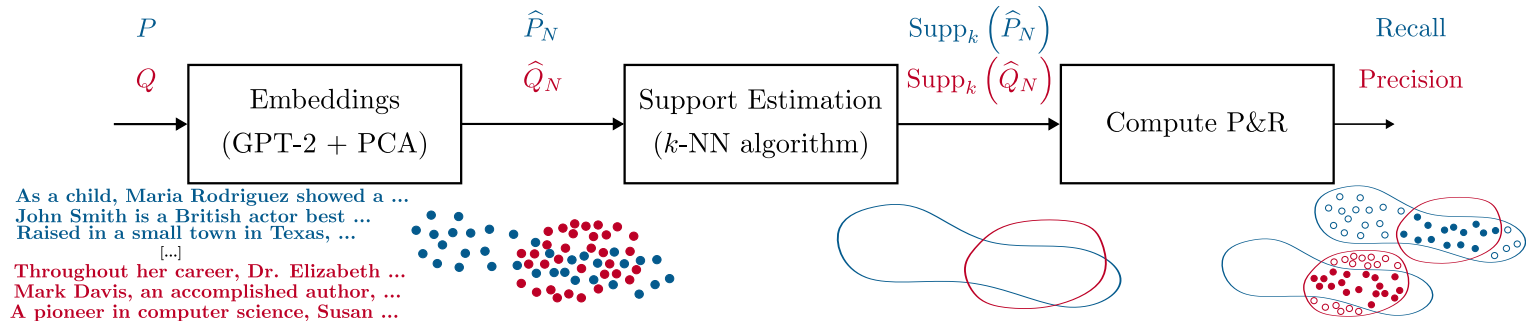
High Precision    Low Recall



Precision: 0.80    Recall: 0.70

# PRECISION AND RECALL FOR GENERATIVE MODELS

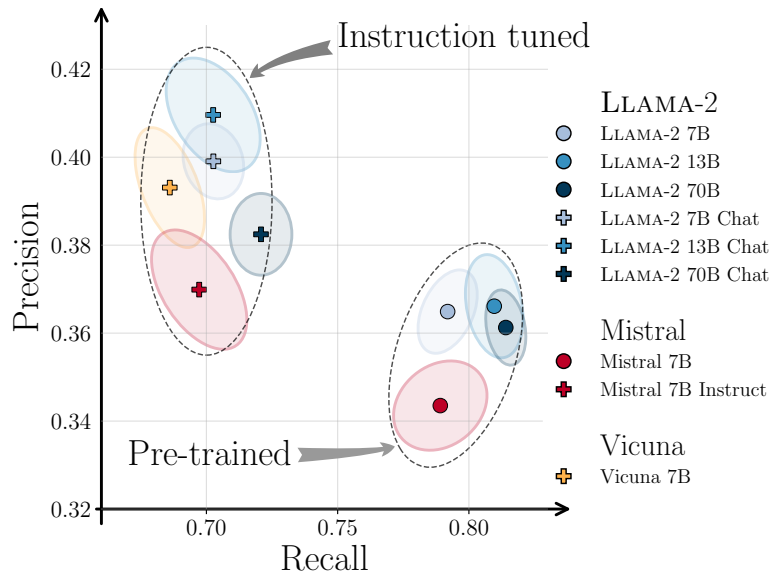
## FOR LLMs



# PRECISION AND RECALL FOR GENERATIVE MODELS

## FOR LLMs

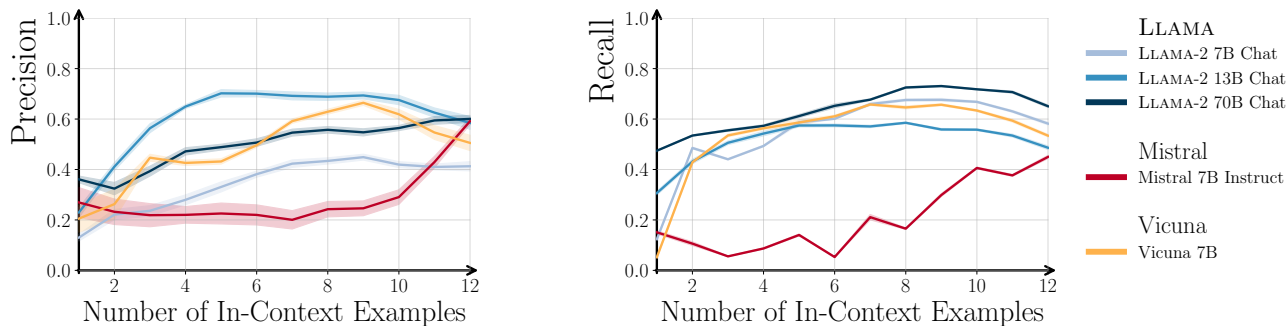
On open-ended generation, the quality and diversity of LLMs can be evaluated using Precision and Recall for instance on Webtext: Bronnec et al. [3]



# PRECISION AND RECALL FOR GENERATIVE MODELS

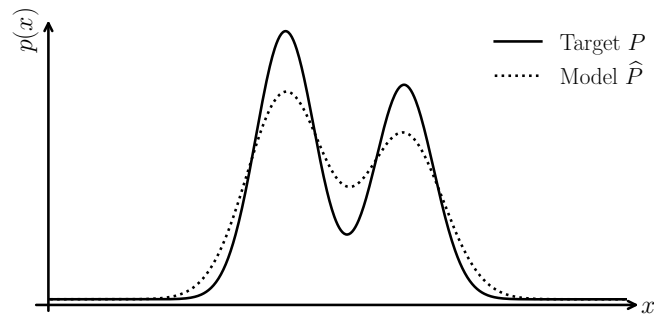
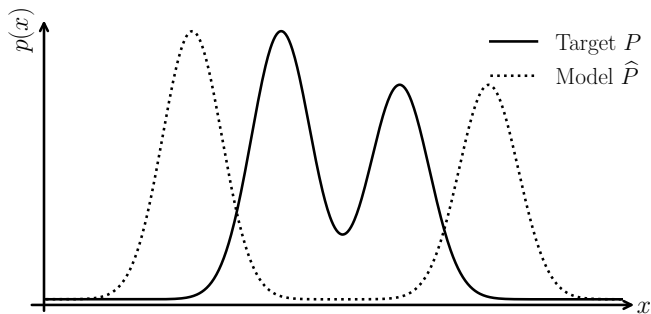
## FOR LLMs

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:



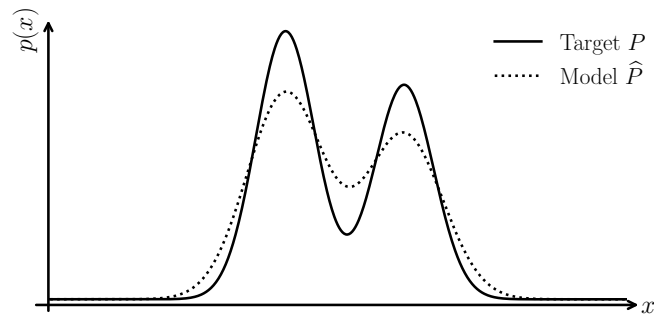
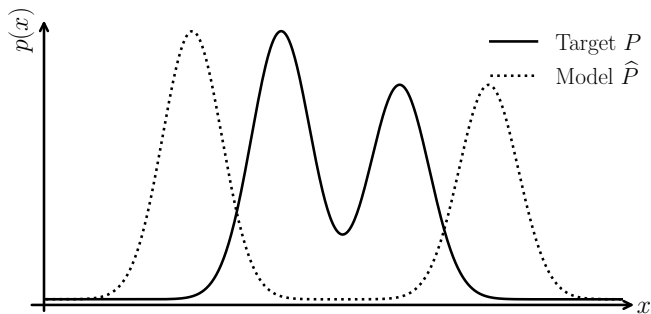
# PRECISION AND RECALL FOR GENERATIVE MODELS

FOR INFINITE SUPPORT



# PRECISION AND RECALL FOR GENERATIVE MODELS

FOR INFINITE SUPPORT



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

## PR-CURVE FOR GENERATIVE MODELS

### DEFINITION

#### Definition 2.2 (PR-Curve for Generative Models - Sajjadi et al. [11], Simon et al. [12])

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

$$\text{PRD}(P, \hat{P}) = \{(\alpha_\lambda, \beta_\lambda) \mid \lambda \in [0, \infty]\} \quad (2)$$

with:

$$\alpha_\lambda = \int_{\mathcal{X}} \min(\lambda p(\mathbf{x}), \hat{p}(\mathbf{x})) \, \mathrm{d}\mu(\mathbf{x}) \quad \text{and} \quad \beta_\lambda = \int_{\mathcal{X}} \min(p(\mathbf{x}), \hat{p}(\mathbf{x})/\lambda) \, \mathrm{d}\mu(\mathbf{x}). \quad (3)$$

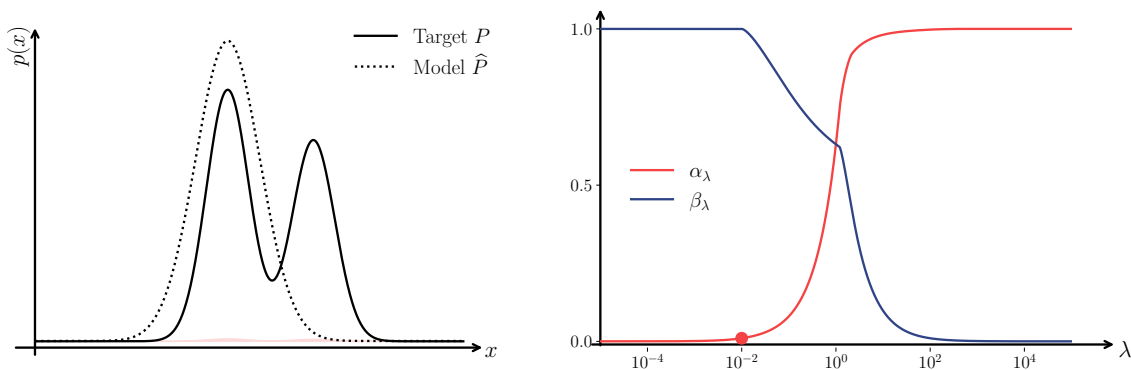


## PR-CURVE FOR GENERATIVE MODELS

### DEFINITION

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

$$\alpha_\lambda = \int_{\mathcal{X}} \min(\lambda p(x), \hat{p}(x)) \, d\mu(x) \quad (4)$$

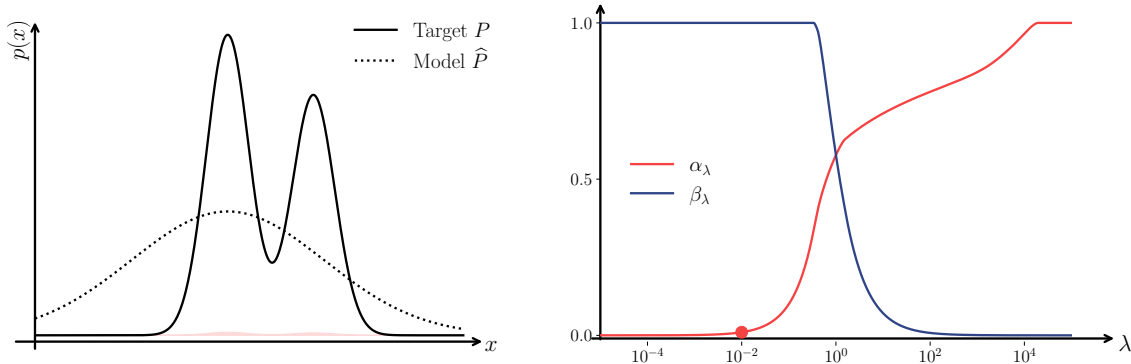


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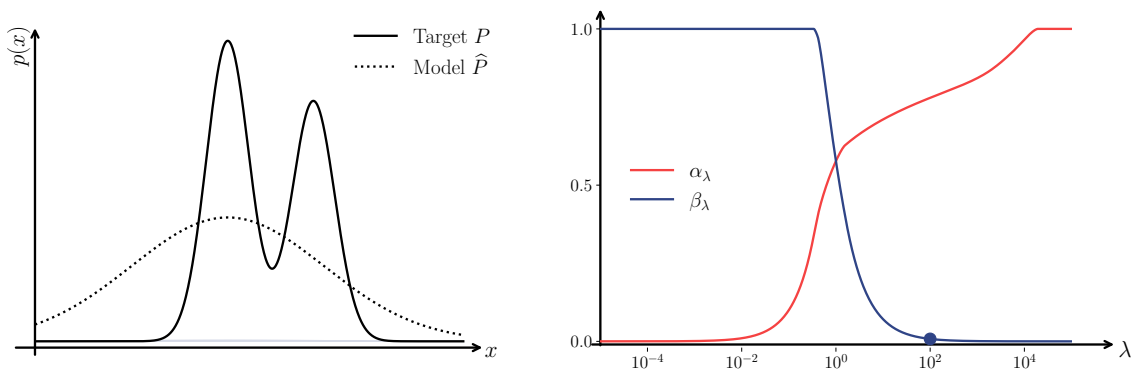


## PR-CURVE FOR GENERATIVE MODELS

### DEFINITION

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

$$\beta_\lambda = \int_{\mathcal{X}} \min(p(x), \hat{p}(x)/\lambda) d\mu(x) \quad (5)$$

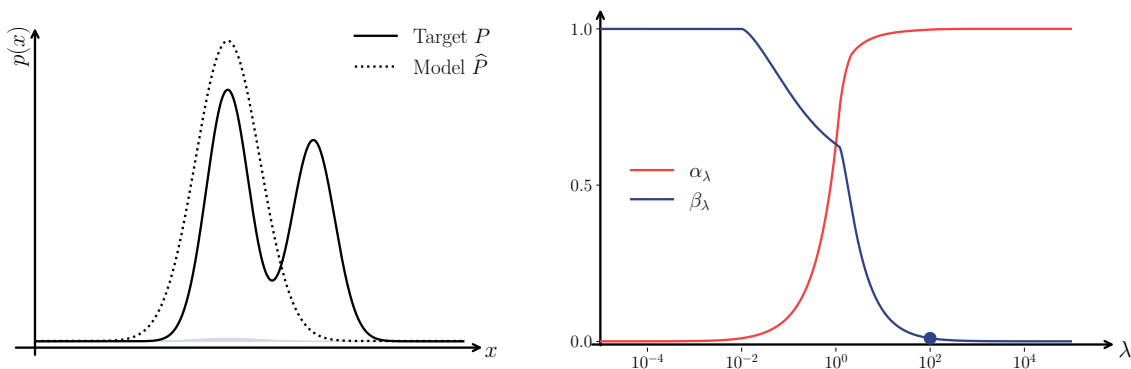


## PR-CURVE FOR GENERATIVE MODELS

### DEFINITION

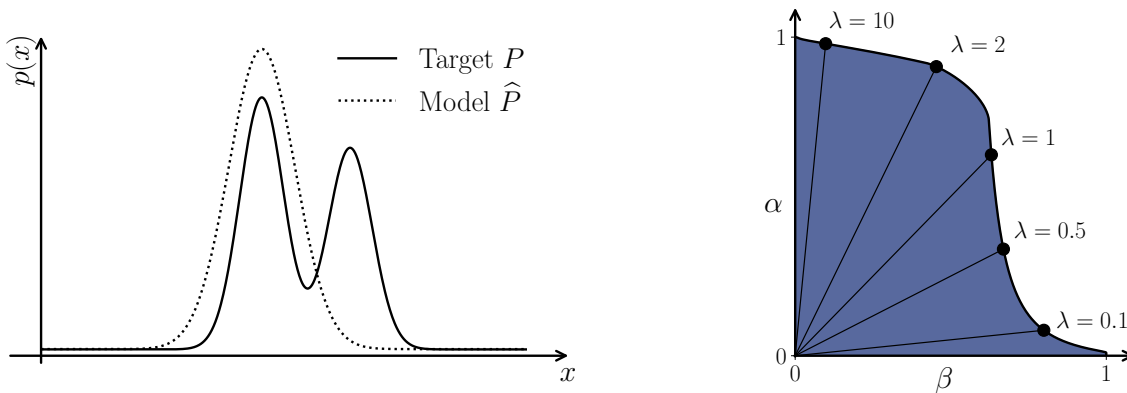
For the Recall,  $p$  is compared to  $\hat{p}/\lambda$  for different threshold  $\lambda \in [0, +\infty]$ :

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# PR-CURVE FOR GENERATIVE MODELS

## EXAMPLES



**Figure.** Learning distribution with **low recall** and **high precision**.

# PR-CURVE FOR GENERATIVE MODELS

## EXAMPLES

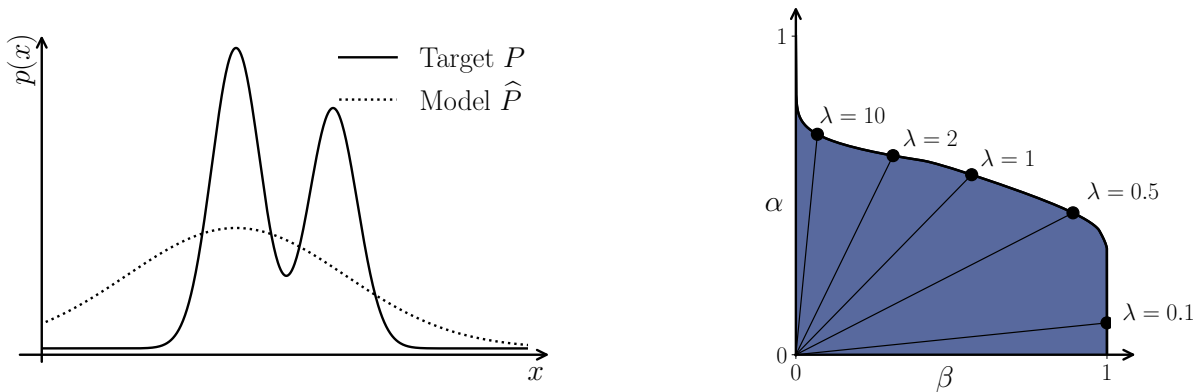
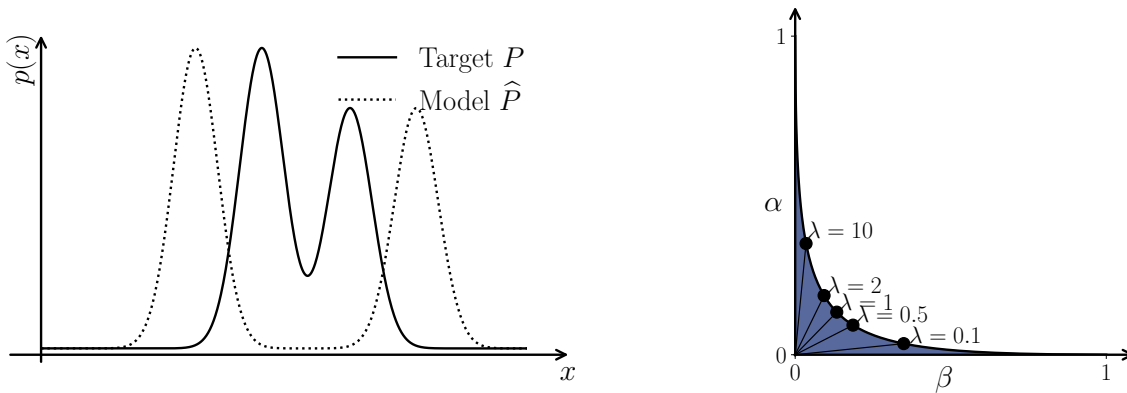


Figure. Learning distribution with high recall and low precision.

# PR-CURVE FOR GENERATIVE MODELS

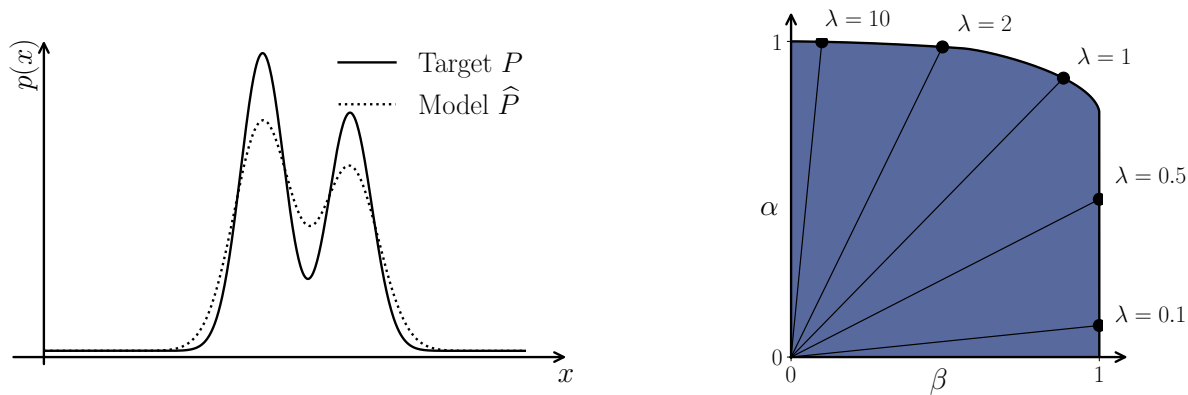
## EXAMPLES



**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:

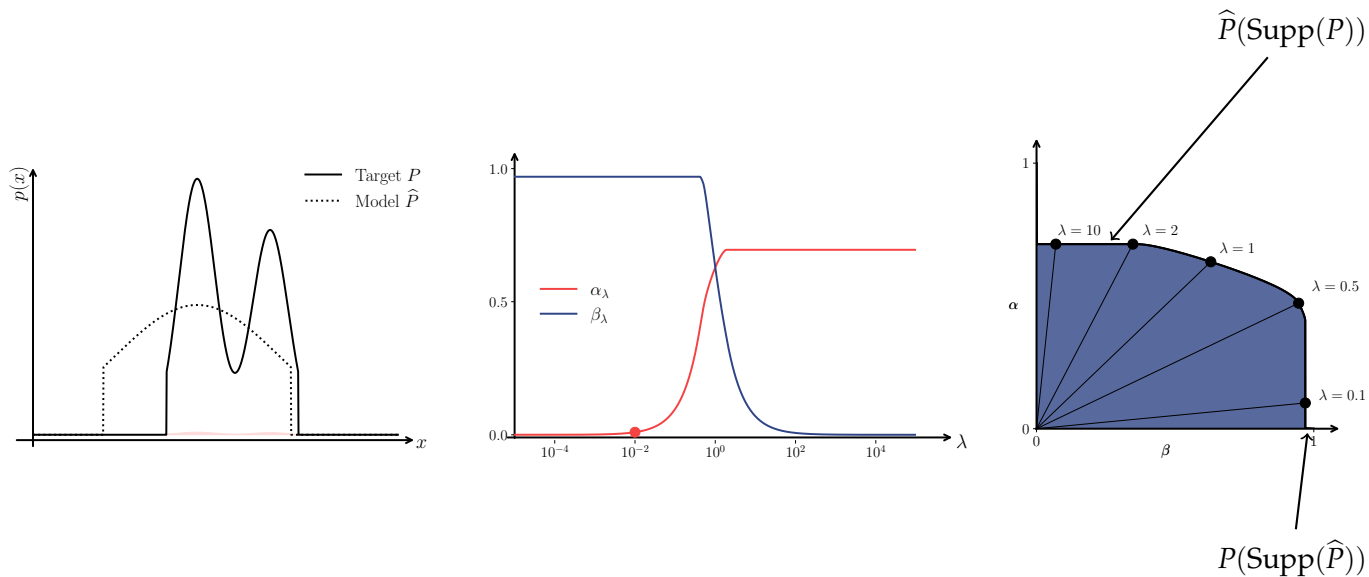
### Theorem 2.3 (Support-based and PR-Curves - Siry et al. [13])

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

$$\bar{\alpha} = \max_{\lambda} \alpha_{\lambda} = \alpha_{\infty} \quad \text{and} \quad \bar{\beta} = \max_{\lambda} \beta_{\lambda} = \beta_0. \quad (6)$$

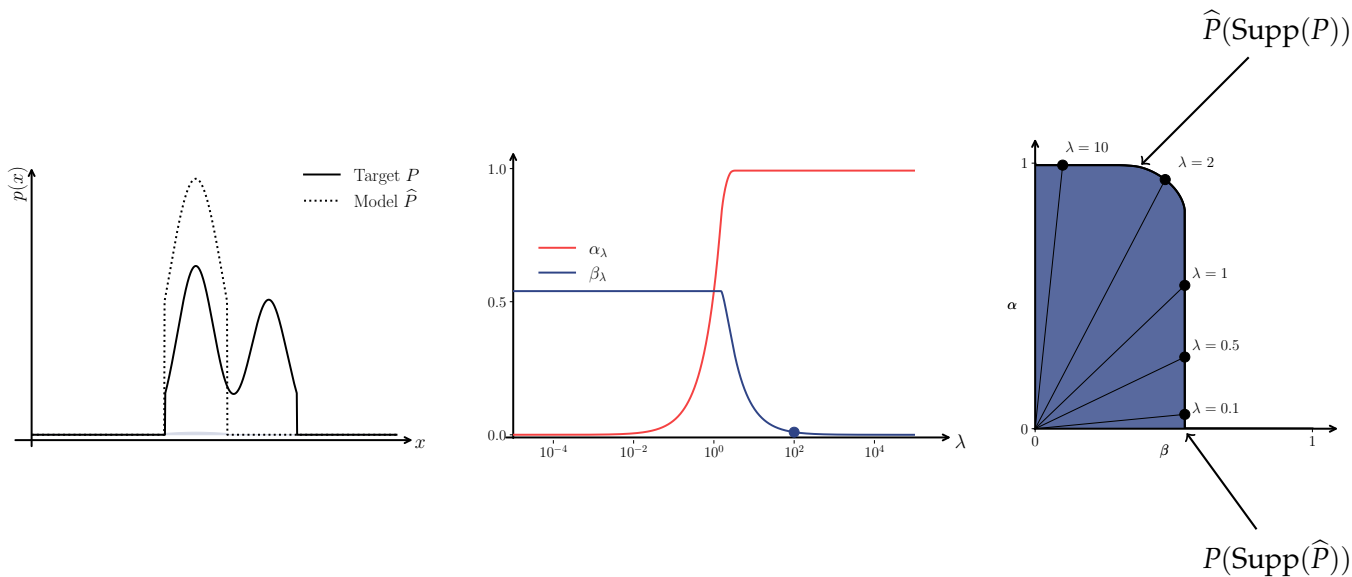
# PR-CURVE AND SUPPORT-BASED PRECISION AND RECALL

## RELATION



# PR-CURVE AND SUPPORT-BASED PRECISION AND RECALL

## RELATION



# PR-CURVE FOR GENERATIVE MODELS

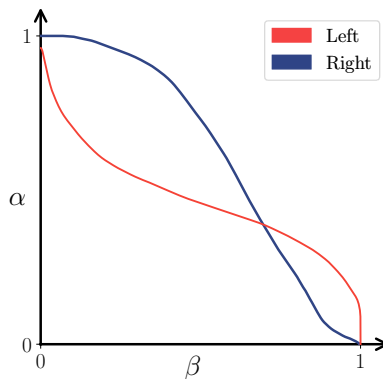
## IN PRACTICE

Low Precision    High Recall



Precision: 0.54    Recall: 0.91

PR-Curves



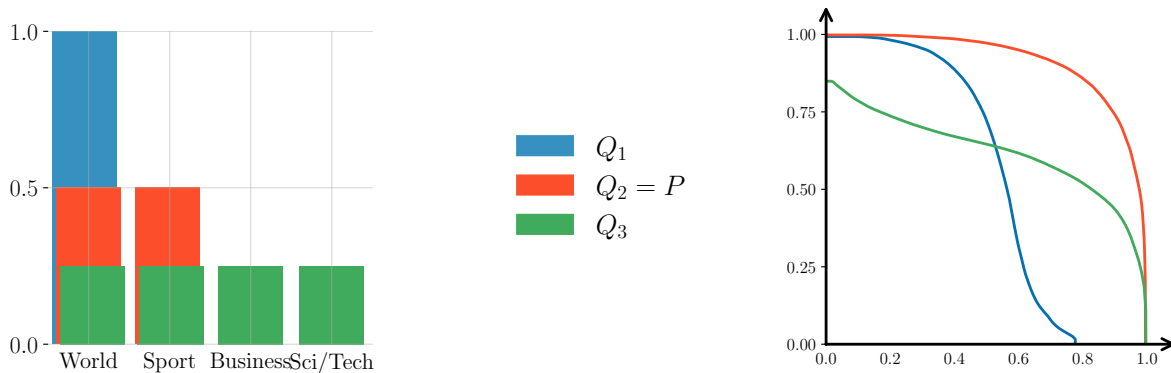
High Precision    Low Recall



Precision: 0.80    Recall: 0.70

# PR-CURVE FOR GENERATIVE MODELS

IN NLP



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

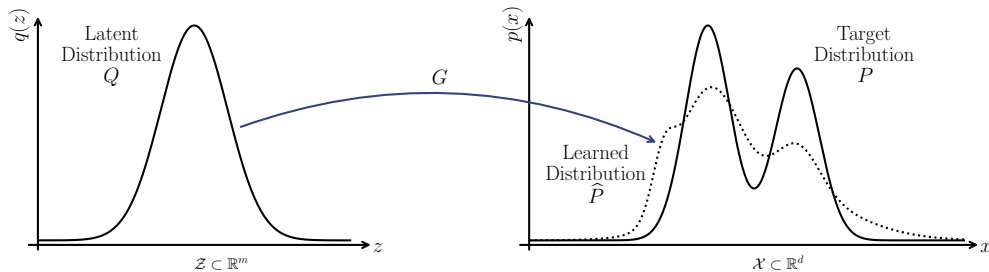
## SECTION 2: OPTIMIZING

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

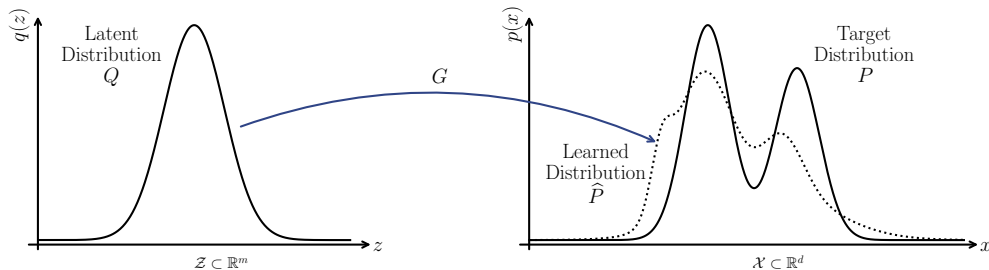
# TUNING PRECISION AND RECALL IN GENERATIVE MODELS

## TRUNCATION

Hard Truncation  
Karras et al. [6]



Soft Truncation  
Kingma and Dhariwal [7]

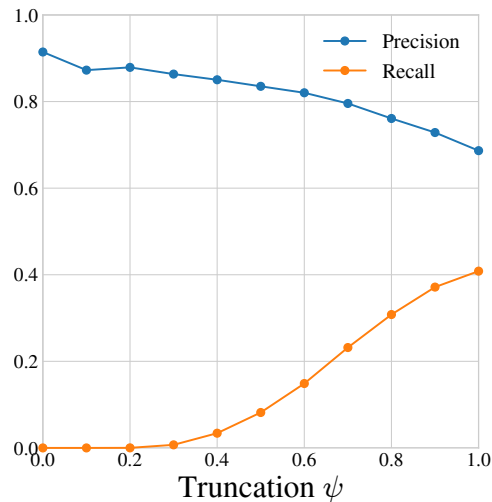


## SECTION 2: OPTIMIZING

### HARD TRUNCATION



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

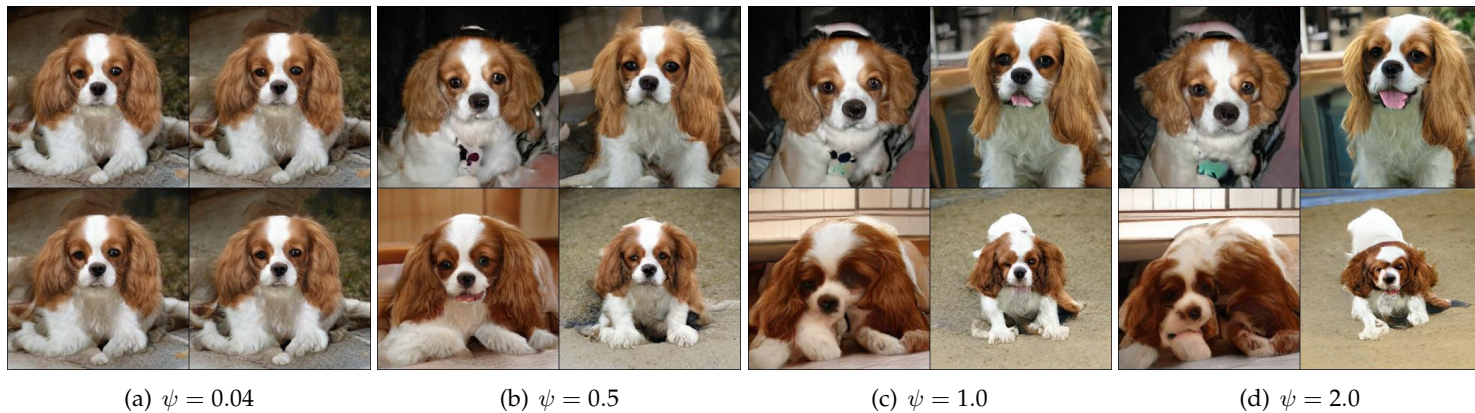


**Figure.** Source: [8]



## SECTION 2: OPTIMIZING

### SOFT TRUNCATION



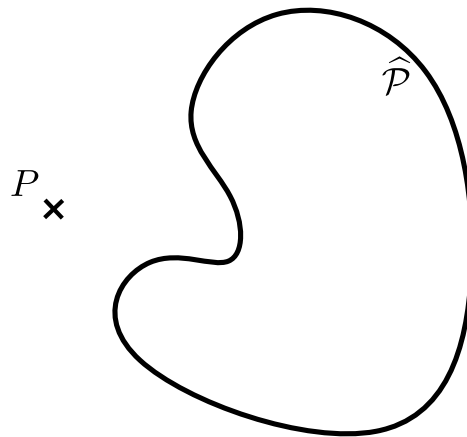
**Figure.** Soft-Truncation on BigGAN. Source:[2].

# TRAINING A GENERATIVE MODEL

## IN GENERAL

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

$$\min_G D(P, \hat{P}_G) \quad (6)$$



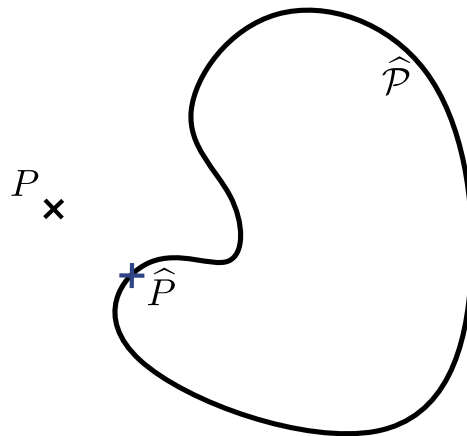
Distribution Space

# 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  $\hat{P}$ :

$$\min_G \mathcal{D}_f(P \parallel \hat{P}_G) \quad (6)$$



Distribution Space

## $f$ -DIVERGENCES

### DEFINITION

#### Definition 3.1 ( $f$ -divergences)

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

$$\mathcal{D}_f(P \parallel \hat{P}) = \int_{\mathcal{X}} \hat{p}(\mathbf{x}) f\left(\frac{p(\mathbf{x})}{\hat{p}(\mathbf{x})}\right) \mathrm{d}\mu(\mathbf{x}). \quad (7)$$

## $f$ -DIVERGENCES

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$$\mathcal{D}_f(P \parallel \hat{P}) = \int_{\mathcal{X}} \hat{p}(\mathbf{x}) f\left(\frac{p(\mathbf{x})}{\hat{p}(\mathbf{x})}\right) \mathrm{d}\mu(\mathbf{x}). \quad (7)$$

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

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$f$ -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  $\mathcal{X} \rightarrow \mathbb{R}$ .

# ESTIMATING $f$ -DIVERGENCES

## DUAL VARIATIONAL FORM

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- ▶  $\mathcal{T}$  be the set of all measurable functions  $\mathcal{X} \rightarrow \mathbb{R}$ .

### Theorem 3.2 (Dual variational form of an $f$ -divergence- Nguyen et al. [9])

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

$$\mathcal{D}_f(P \parallel \hat{P}) = \sup_{T \in \mathcal{T}} (\mathbb{E}_{\mathbf{x} \sim P} [T(\mathbf{x})] - \mathbb{E}_{\mathbf{x} \sim \hat{P}} [f^*(T(\mathbf{x}))]). \quad (8)$$

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:

$$\min_G \max_T \underbrace{\mathbb{E}_{\mathbf{x} \sim P} [T(\mathbf{x})] - \mathbb{E}_{\mathbf{x} \sim \hat{P}_G} [f^*(T(\mathbf{x}))]}_{\mathcal{D}_{f,T}^{\text{dual}}} \quad (9)$$

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

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# TRAINING A GENERATIVE MODEL WITH $f$ -DIVERGENCES

## USING THE DUAL VARIATIONAL FORM

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

$$\min_G \max_T \mathbb{E}_{\mathbf{x} \sim P} [\log(D(\mathbf{x}))] - \mathbb{E}_{\mathbf{x} \sim \hat{P}_G} [f^*(\log(D(\mathbf{x})))] \quad (9)$$

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

# TRAINING A GENERATIVE MODEL WITH $f$ -DIVERGENCES

## USING THE DUAL VARIATIONAL FORM

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

$$\min_G \max_T \mathbb{E}_{\mathbf{x} \sim P} [\log (D(\mathbf{x}))] + \mathbb{E}_{\mathbf{x} \sim \hat{P}_G} [\log (1 - D(\mathbf{x}))] \quad (9)$$

- ▶ The discriminator  $T$  is trained *to estimate* the divergence.
- ▶ The generator  $G$  is trained *to minimize* the divergence.
- ▶ With  $T(\mathbf{x}) = \log(D(\mathbf{x}))$  with  $D(\mathbf{x}) \in [0, 1]$ .
- ▶  $f^*(t) = f_{\text{JS}}^*(t) = -\log(1 - \exp(t))$  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:

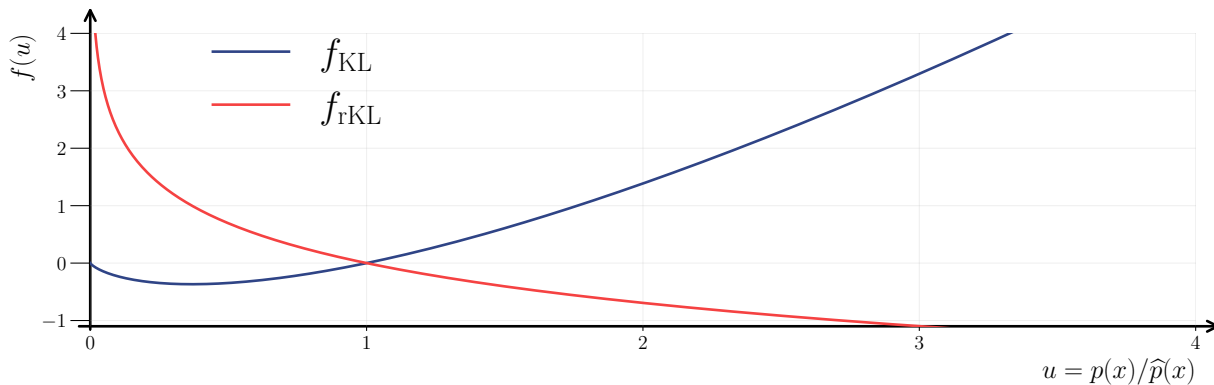
$$\min_G \max_T \underbrace{\mathbb{E}_{\mathbf{x} \sim P} [T(\mathbf{x})] - \mathbb{E}_{\mathbf{x} \sim \hat{P}_G} [f^*(T(\mathbf{x}))]}_{\mathcal{D}_{f,T}^{\text{dual}}} \quad (9)$$

- ▶ The discriminator  $T$  is trained *to estimate* the divergence.
- ▶ The generator  $G$  is trained *to minimize* the divergence.
- ▶ Generative Adversarial Networks [4] for *the Jensen-Shannon divergence*.
- ▶ Extended to other  $f$ -divergences by Nowozin et al. [10].
- ▶ Extend to other generative models such as Normalizing Flows by Grover et al. [5].

## EFFECT OF THE $f$ -DIVERGENCE ON THE LEARNED DISTRIBUTION

All  $f$ -divergences are not equal:

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

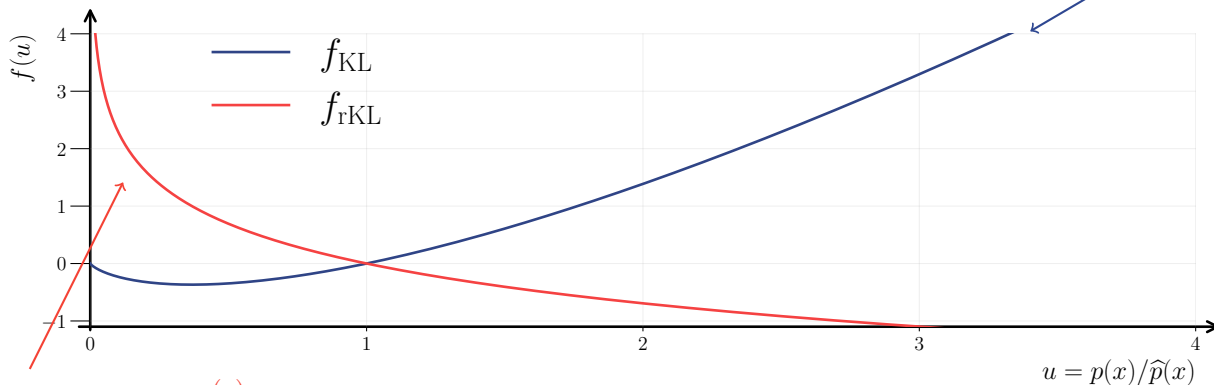


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$$\mathcal{D}_f(P\|\hat{P}) = \mathbb{E}_{x \sim \hat{P}} \left[ f \left( \frac{p(x)}{\hat{p}(x)} \right) \right]$$

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



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

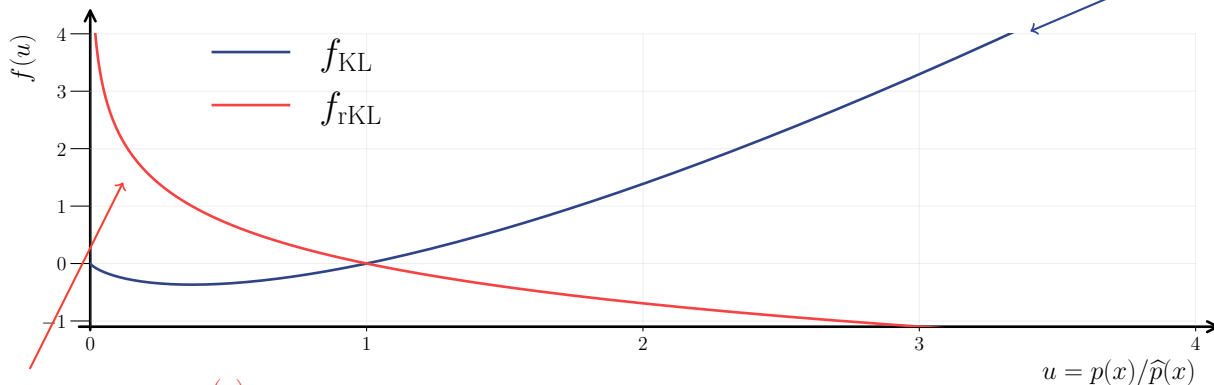


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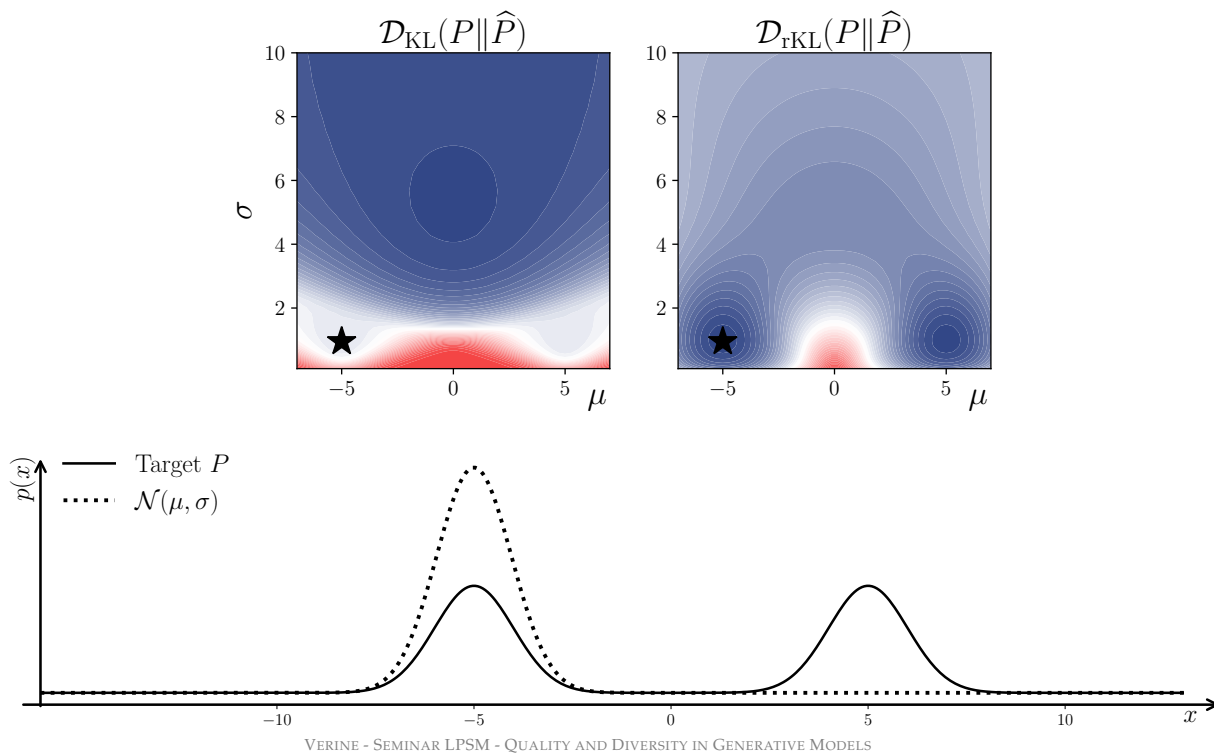
$$\mathcal{D}_f(P||\hat{P}) = \mathbb{E}_{x \sim \hat{P}} \left[ f \left( \frac{p(x)}{\hat{p}(x)} \right) \right]$$

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

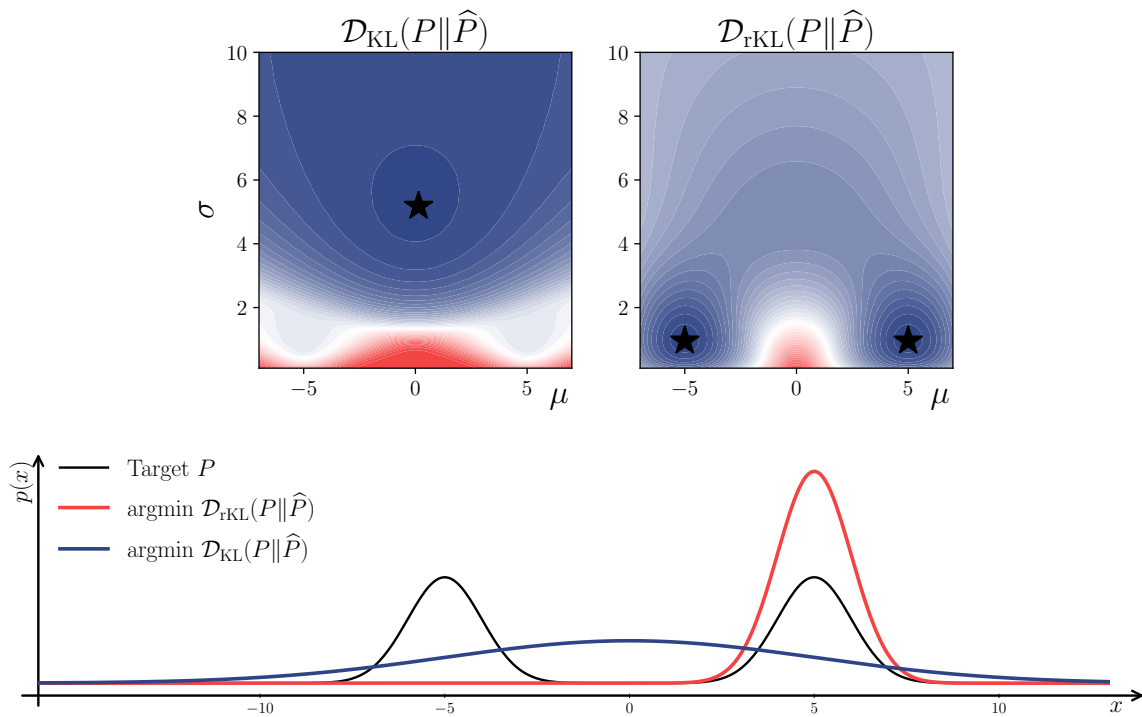


Penalizing low values of  $\frac{p(x)}{\hat{p}(x)}$   
Favors high precision

## EXAMPLES OF $f$ -DIVERGENCE MINIMIZATION



## EXAMPLES OF $f$ -DIVERGENCE MINIMIZATION



## SECTION 2: OPTIMIZING

### CONTRIBUTIONS

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

- ▶ What is the relation between the Precision-Recall curve and  $f$ -divergences?
- ▶ Can we optimize a point on the Precision-Recall curve using  $f$ -divergences?

## SECTION 2: OPTIMIZING CONTRIBUTIONS

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

- ▶ What is the relation between the Precision-Recall curve and  $f$ -divergences?
- ▶ Can we optimize a point on the Precision-Recall curve using  $f$ -divergences?

#### List of contributions:

- ▶ We show that the PR-Divergence is an  $f$ -divergence.
- ▶ We show that any  $f$ -divergence can be written as a weighted average PR-Divergences.
- ▶ We propose an algorithm to optimize the PR-Divergence.

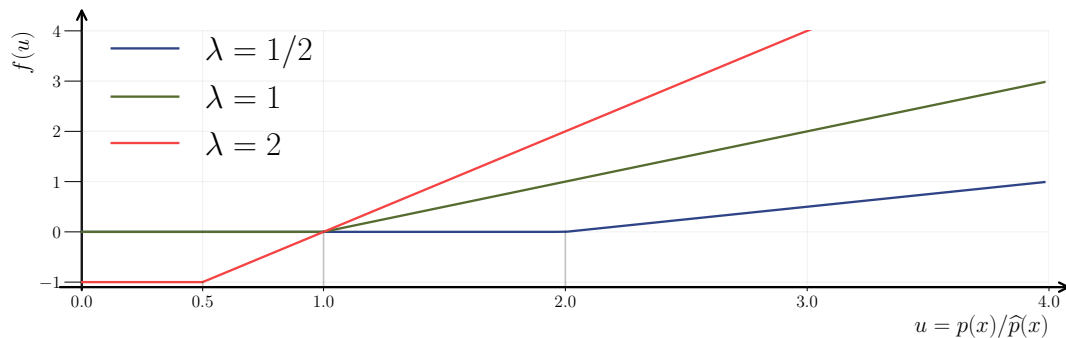
# PRECISION-RECALL DIVERGENCE

## DEFINITION

### Definition 3.3 (PR-Divergence generator function $f_\lambda$ )

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

$$f_\lambda(u) = \begin{cases} \max(\lambda u, 1) - \max(\lambda, 1) & \text{for } \lambda \in [0, +\infty[, \\ \mathbb{1}_{\{u=0\}} & \text{for } \lambda = +\infty. \end{cases} \quad (10)$$



# PRECISION-RECALL DIVERGENCE

## PROPERTIES

### Proposition 3.4 (PR-Divergence)

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

$$\mathcal{D}_{\lambda\text{-PR}}(P \parallel \hat{P}) = \int_{\mathcal{X}} \hat{p}(x) f_{\lambda} \left( \frac{p(x)}{\hat{p}(x)} \right) d\mu(x) \quad (11)$$

belongs to the class of  $f$ -divergences.

# PRECISION-RECALL DIVERGENCE

## LINKING THE PR-DIVERGENCE TO THE PR-CURVE

### Theorem 3.5 (PR-Curves as a function of $\mathcal{D}_{\lambda\text{-PR}}$ )

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

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

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



# PRECISION-RECALL DIVERGENCE

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

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

A direct consequence of Theorem 3.5:

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

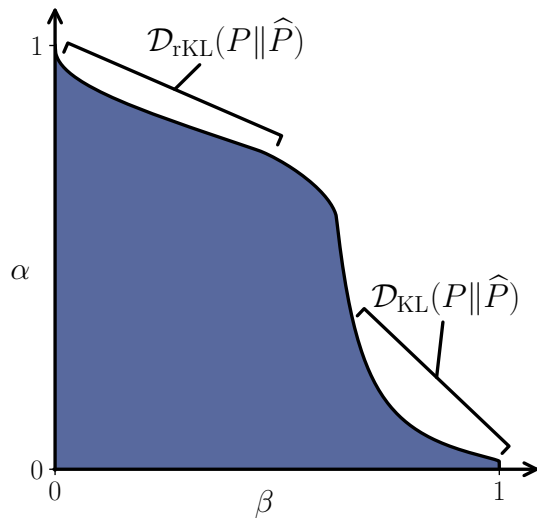
# EXPLAINING QUALITY/DIVERSITY

## CONNECTION BETWEEN PR-DIVERGENCE AND $f$ -DIVERGENCES

### Theorem 3.6 ( $f$ -divergences as a weighted average of PR-Divergences)

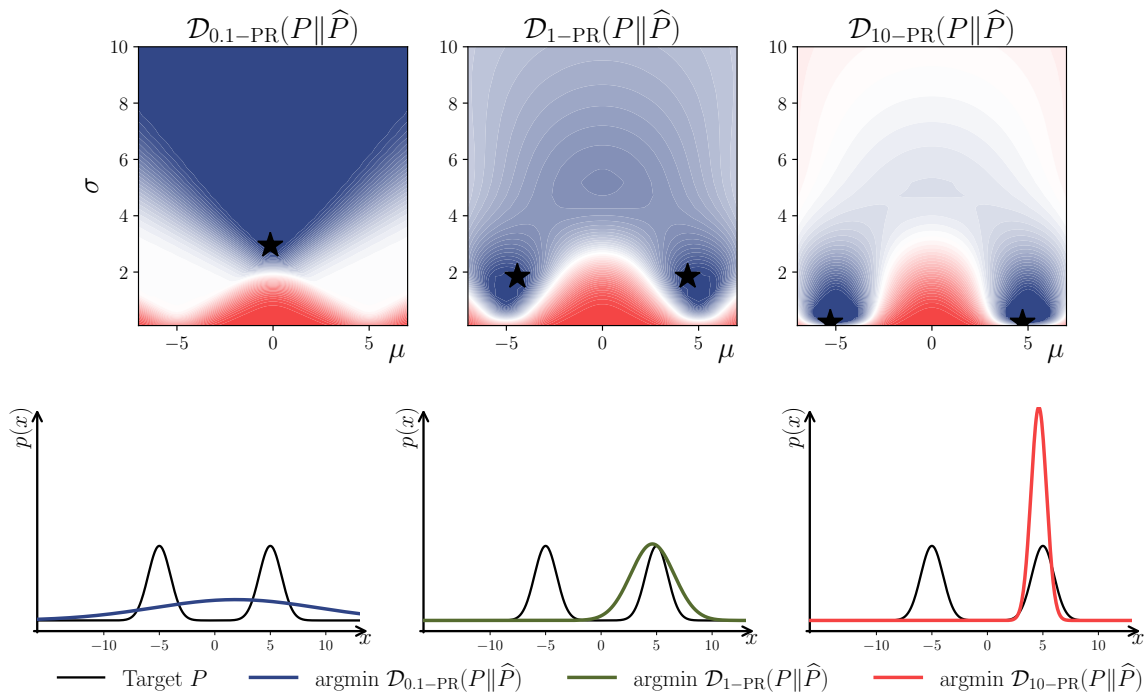
For any  $P, \hat{P} \in \mathcal{P}(\mathcal{X})$  supported on all  $\mathcal{X}$  and any  $\lambda \in [0, +\infty]$ , then:

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



# OPTIMIZING THE PR-DIVERGENCE

## EXAMPLES



# OPTIMIZING THE PR-DIVERGENCE

## EXAMPLES

# OPTIMIZING THE PR-DIVERGENCE

## IN PRACTICE

If we train a model to minimize the PR-Divergence, we can use the dual variational form:

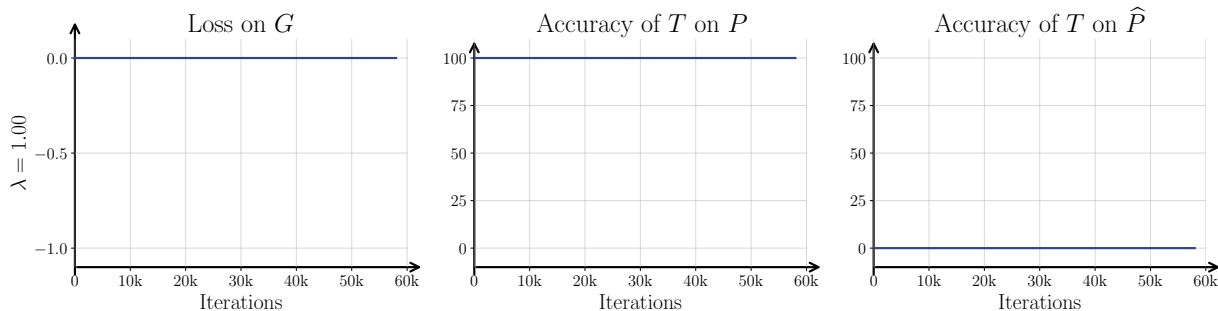
$$\min_G \max_T \mathbb{E}_{\mathbf{x} \sim P} [T(\mathbf{x})] - \mathbb{E}_{\mathbf{x} \sim \hat{P}_G} [f_\lambda^*(T(\mathbf{x}))]. \quad (12)$$

# OPTIMIZING THE PR-DIVERGENCE

## IN PRACTICE

If we train a model to minimize the PR-Divergence, we can use the dual variational form:

$$\min_G \max_T \mathbb{E}_{\mathbf{x} \sim P} [T(\mathbf{x})] - \mathbb{E}_{\mathbf{x} \sim \hat{P}_G} [f_\lambda^*(T(\mathbf{x}))]. \quad (12)$$



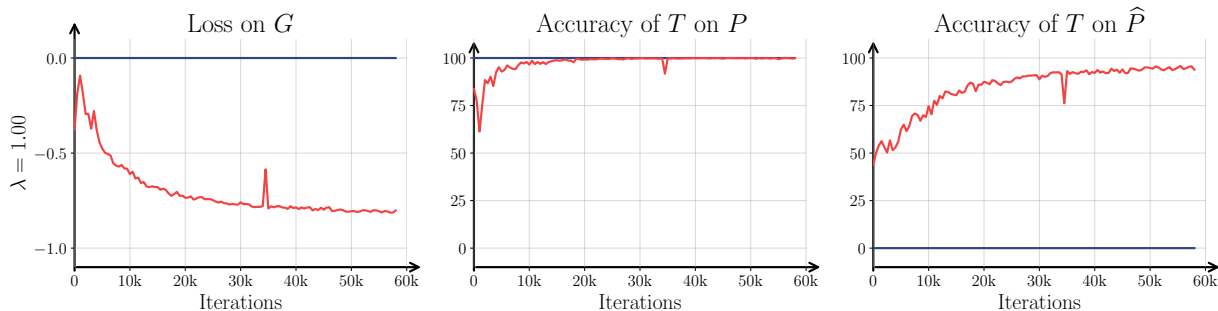
The naive approach *fails* to optimize the PR-Divergence.

# OPTIMIZING THE PR-DIVERGENCE

## IN PRACTICE

If we train a model to minimize the PR-Divergence, we can use the dual variational form:

$$\min_G \max_T \mathbb{E}_{\mathbf{x} \sim P} [T(\mathbf{x})] - \mathbb{E}_{\mathbf{x} \sim \hat{P}_G} [f_{\lambda}^*(T(\mathbf{x}))]. \quad (12)$$



We propose *a new approach* to optimize the PR-Divergence.

# OPTIMIZING THE PR-DIVERGENCE

## OUR APPROACH

We choose an auxiliary function  $g$  to train  $T_g$  is trained to estimate the  $f$ -divergence  $\mathcal{D}_g$ :

$$\max_T \mathbb{E}_{\mathbf{x} \sim P} [T(\mathbf{x})] - \mathbb{E}_{\mathbf{x} \sim \hat{P}} [g^*(T(\mathbf{x}))] \quad (13)$$



## OPTIMIZING THE PR-DIVERGENCE

### OUR APPROACH

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$$\max_T \mathbb{E}_{\mathbf{x} \sim P} [T(\mathbf{x})] - \mathbb{E}_{\mathbf{x} \sim \hat{P}} [g^*(T(\mathbf{x}))] \quad (13)$$

At optimality, we have:

$$\nabla g^*(T_g^{\text{opt}}(\mathbf{x})) = \frac{p(\mathbf{x})}{\hat{p}(\mathbf{x})}. \quad (14)$$

# OPTIMIZING THE PR-DIVERGENCE

## OUR APPROACH

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At optimality, we have:

$$\nabla g^*(T_g^{\text{opt}}(\mathbf{x})) = \frac{p(\mathbf{x})}{\hat{p}(\mathbf{x})}. \quad (14)$$

Any  $f$ -divergence can be computed using the primal estimation as follows using  $T_g$ :

$$\mathcal{D}_f(P \parallel \hat{P}) = \mathbb{E}_{\mathbf{x} \sim \hat{P}} \left[ f \left( \frac{p(\mathbf{x})}{\hat{p}(\mathbf{x})} \right) \right] = \mathbb{E}_{\mathbf{x} \sim \hat{P}} \left[ f \left( \nabla g^*(T_g^{\text{opt}}(\mathbf{x})) \right) \right]. \quad (15)$$

# OPTIMIZING THE PR-DIVERGENCE

## OUR APPROACH

## CONVERGENCE OF THE PROPOSED APPROACH

### BOUNDING THE ESTIMATION ERROR

#### Theorem 3.7 (Bound on the estimation of an $f$ -divergence using an auxiliary $g$ -divergence)

Let  $f, g : \mathbb{R}^+ \rightarrow \mathbb{R}$  be such that  $g$  is  $\mu$ -strongly convex,  $f$  is  $\sigma$ -Lipschitz, and  $\mathcal{D}_f, \mathcal{D}_g$  be  $f$ -divergences. For any discriminator  $T : \mathcal{X} \rightarrow \text{dom}(g^*)$ , let  $r(\mathbf{x}) = \nabla g^*(T(\mathbf{x}))$ . Then:

$$\mathcal{D}_g(P \parallel \hat{P}) - \mathcal{D}_{g,T}^{\text{dual}} \leq \epsilon \implies \left| \mathcal{D}_f(P \parallel \hat{P}) - \mathcal{D}_{f,T}^{\text{primal}}(P \parallel \hat{P}) \right| \leq \sigma \sqrt{\frac{2\epsilon}{\mu}}. \quad (16)$$

## CONVERGENCE OF THE PROPOSED APPROACH

### BOUNDING THE ESTIMATION ERROR

#### Theorem 3.7 (Bound on the estimation of an $f$ -divergence using an auxiliary $g$ -divergence)

Let  $f, g : \mathbb{R}^+ \rightarrow \mathbb{R}$  be such that  $g$  is  $\mu$ -strongly convex,  $f$  is  $\sigma$ -Lipschitz, and  $\mathcal{D}_f, \mathcal{D}_g$  be  $f$ -divergences. For any discriminator  $T : \mathcal{X} \rightarrow \text{dom}(g^*)$ , let  $r(x) = \nabla g^*(T(x))$ . Then:

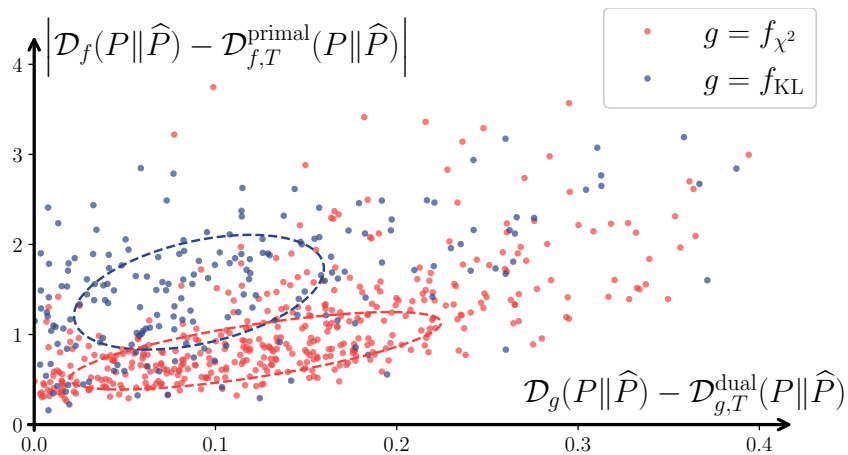
$$\mathcal{D}_g(P \parallel \hat{P}) - \mathcal{D}_{g,T}^{\text{dual}} \leq \epsilon \implies \left| \mathcal{D}_f(P \parallel \hat{P}) - \mathcal{D}_{f,T}^{\text{primal}}(P \parallel \hat{P}) \right| \leq \sigma \sqrt{\frac{2\epsilon}{\mu}}. \quad (16)$$

The smaller the error on  $T$  is,

the smaller the error on estimating  
 $\mathcal{D}_f$  using  $T$  is.

# CONVERGENCE OF THE PROPOSED APPROACH

## 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

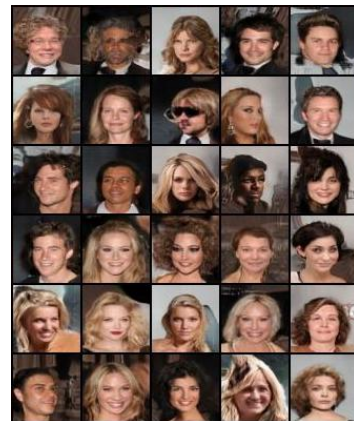
## TRAINING GANs

| Model            |         | CIFAR-10 $32 \times 32$ |              |              | CelebA $64 \times 64$ |              |              |
|------------------|---------|-------------------------|--------------|--------------|-----------------------|--------------|--------------|
|                  |         | FID                     | P            | R            | FID                   | P            | R            |
| Baseline         | Big-GAN | 13.37                   | 86.51        | 65.66        | 9.16                  | 78.41        | <b>51.42</b> |
| $\lambda = 0.05$ |         | 13.29                   | 81.10        | 70.63        | -                     | -            | -            |
| $\lambda = 0.1$  |         | <b>11.62</b>            | 81.78        | <b>74.58</b> | -                     | -            | -            |
| $\lambda = 0.2$  |         | 13.36                   | 84.85        | 65.13        | 8.79                  | 83.37        | 44.07        |
| $\lambda = 0.5$  |         | 14.50                   | 83.27        | 68.23        | <b>6.03</b>           | 77.60        | <b>55.98</b> |
| $\lambda = 1.0$  |         | 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                 | <b>83.96</b> | 25.81        |
| $\lambda = 10.0$ |         | 39.69                   | 84.11        | 39.29        | -                     | -            | -            |
| $\lambda = 20.0$ |         | 67.03                   | <b>90.03</b> | 21.81        | -                     | -            | -            |

When  $\lambda$  increases,  $\left\{ \begin{array}{l} \text{Precision} \uparrow \\ \text{Recall} \downarrow \end{array} \right.$



$\lambda = 0.1$



$\lambda = 10$



## OPTIMIZING THE PR-DIVERGENCE WITH OUR APPROACH

### FINE-TUNING GANS

| Model             | ImageNet $128 \times 128$ |              |              | FFHQ $256 \times 256$ |              |              |
|-------------------|---------------------------|--------------|--------------|-----------------------|--------------|--------------|
|                   | FID                       | P            | R            | FID                   | P            | R            |
| Baseline BigGAN   | 9.83                      | 28.04        | 41.21        | 41.41                 | 65.57        | <b>10.17</b> |
| 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 $\psi = 2.0$ | <b>9.69</b>               | 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        | <b>42.38</b> | <b>35.24</b>          | 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                     | <b>30.87</b> | 28.38        | 38.16                 | <b>84.31</b> | 8.52         |

When  $\lambda$  increases,  $\left\{ \begin{array}{l} \text{Precision} \uparrow \\ \text{Recall} \downarrow \end{array} \right.$  with better performances than truncation.

## SECTION 3: IMPROVING

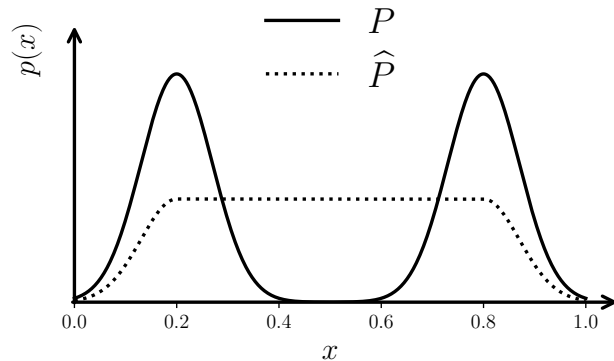
**Improving:**  
How can we improve the  
quality and diversity of a  
pre-trained generative models?

# SAMPLING FROM A GENERATIVE MODEL

## GENERAL SETTING

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

- ▶ Sample  $z \sim Q$ .
- ▶ Compute  $x = G(z)$ .



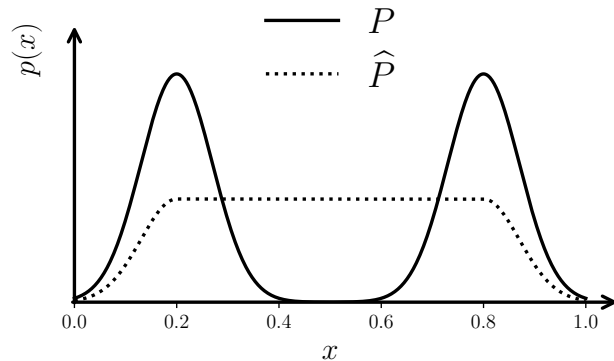
# SAMPLING FROM A GENERATIVE MODEL

## GENERAL SETTING

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

- ▶ Sample  $z \sim Q$ .
- ▶ Compute  $x = G(z)$ .

$$P \neq \hat{P}$$



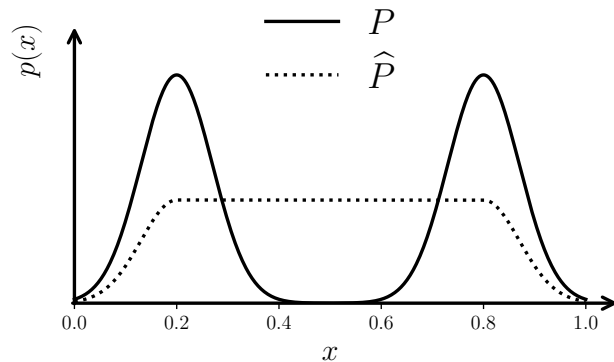
# SAMPLING FROM A GENERATIVE MODEL

## GENERAL SETTING

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

- ▶ Sample  $z \sim Q$ .
- ▶ Compute  $x = G(z)$ .

We have an estimation of  $\frac{p(x)}{\hat{p}(x)}$ .



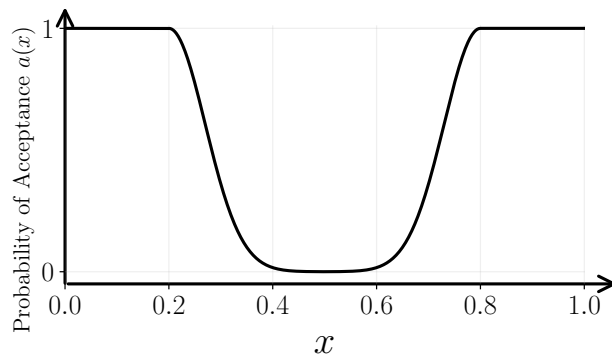
# SAMPLING FROM A GENERATIVE MODEL

## REJECTION SAMPLING

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

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

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



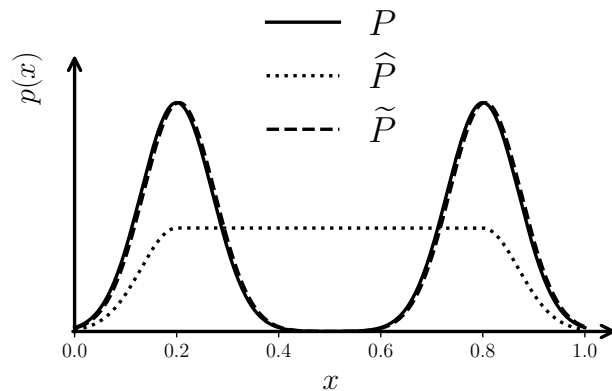
# SAMPLING FROM A GENERATIVE MODEL

## REJECTION SAMPLING

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

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

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



# SAMPLING FROM A GENERATIVE MODEL

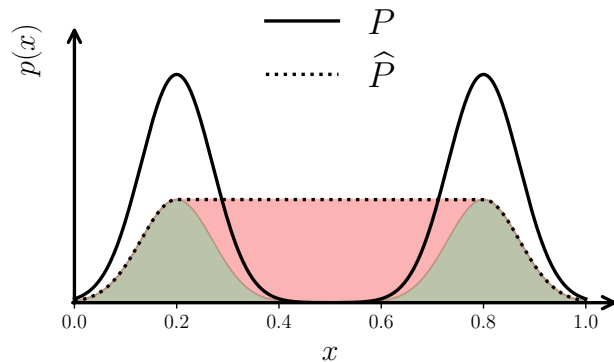
## REJECTION SAMPLING

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

- ▶ Sample  $z \sim Q$ .
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- ▶ Accept  $x$  with probability  $a(x)$ .

The acceptance rate is :

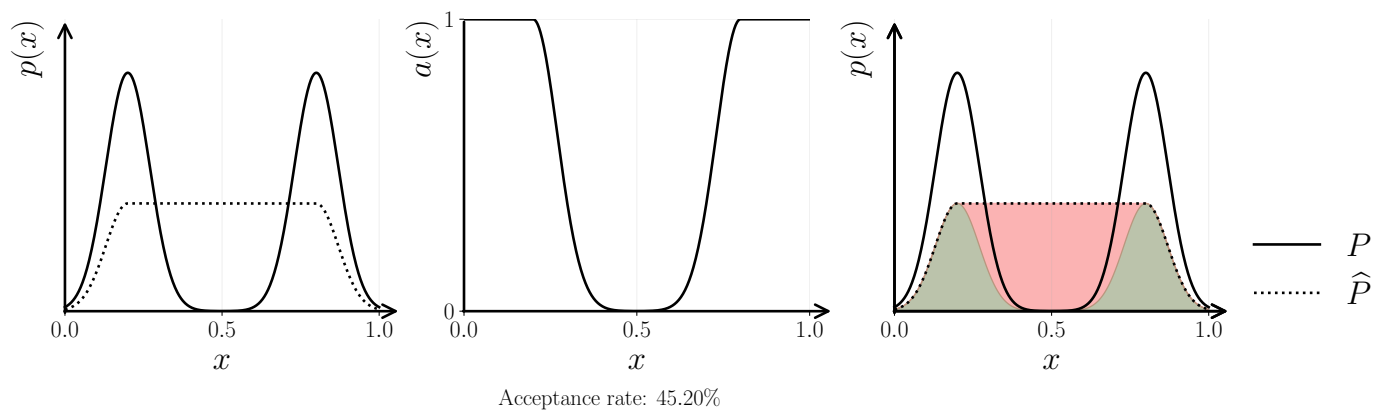
$$\mathbb{E}_{\hat{P}}[a(x)] .$$





# SAMPLING FROM A GENERATIVE MODEL

## REJECTION SAMPLING IN HIGH DIMENSION



# BUDGETED REJECTION SAMPLING

## TUNING THE ACCEPTANCE RATE

### Definition 4.1 (Discriminator Rejection Sampling (DRS) - Azadi et al. [1])

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

$$a_{\text{DRS}}(\mathbf{x}) = \frac{r(\mathbf{x})}{r(\mathbf{x}) (1 - e^\gamma) + Me^\gamma}.$$

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

# BUDGETED REJECTION SAMPLING

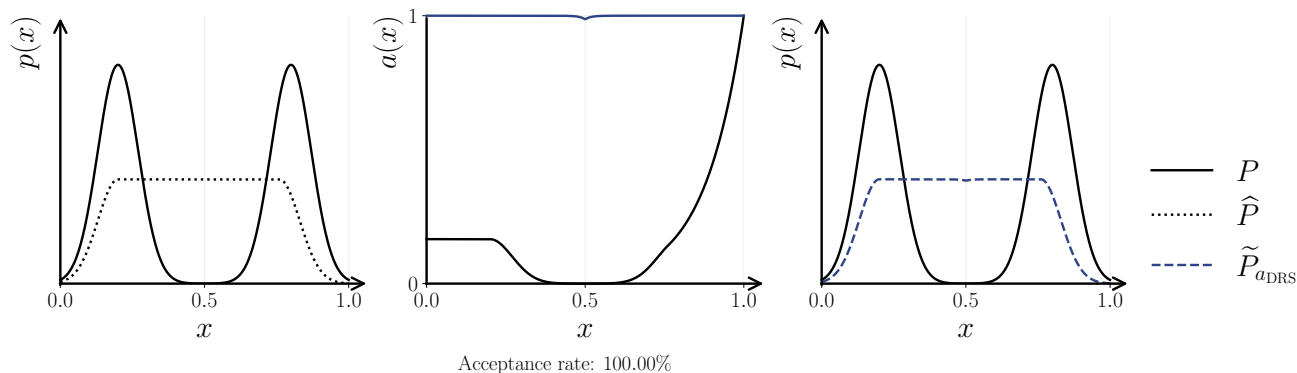
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## SECTION 3: IMPROVING CONTRIBUTIONS

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

- ▶ How can we apply Rejection Sampling with a limited budget?
- ▶ How does it improve Precision and Recall?

## SECTION 3: IMPROVING CONTRIBUTIONS

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

- ▶ How can we apply Rejection Sampling with a limited budget?
- ▶ How does it improve Precision and Recall?

#### **List of contributions:**

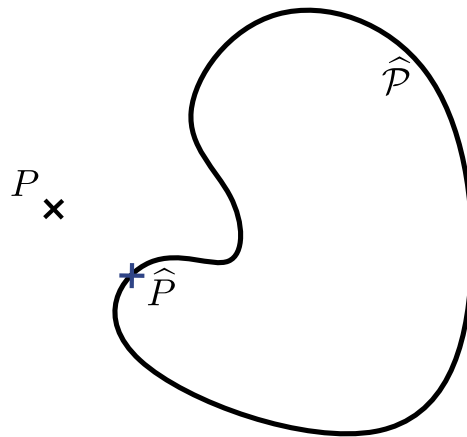
- ▶ We introduce the Optimal Budgeted Rejection Sampling (OBRS).
- ▶ We show how OBRS improves the Precision the learned distribution.
- ▶ We show that training a generative model with OBRS improves the Recall.

# OPTIMAL BUDGETED REJECTION SAMPLING

## DEFINITION

Traditionally, the goal is:

$$\min_G \mathcal{D}_f(P \parallel \hat{P}_G)$$



Distribution Space

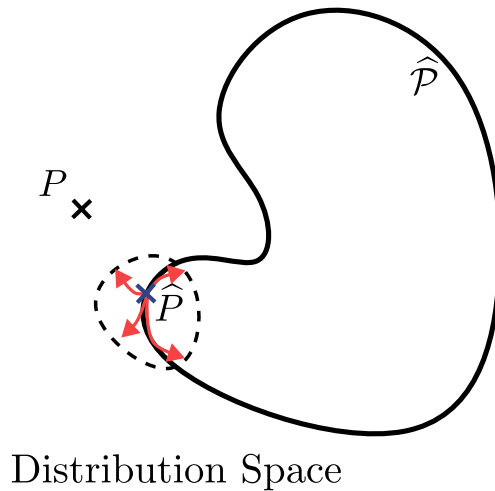
# OPTIMAL BUDGETED REJECTION SAMPLING

## DEFINITION

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

$$\min_a \mathcal{D}_f(P \| \tilde{P}_a)$$

s.t. the acceptance rate is greater than  $1/K$ .

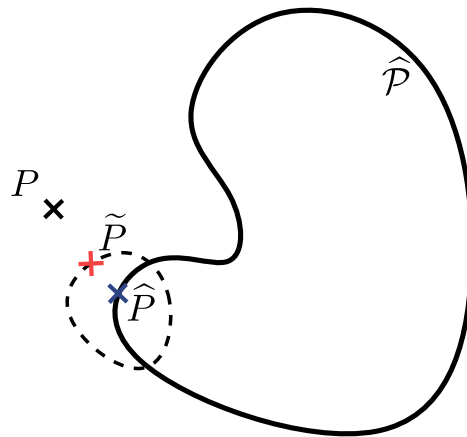


# OPTIMAL BUDGETED REJECTION SAMPLING

## DEFINITION

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

$$\begin{aligned} \min_a \quad & \mathcal{D}_f(P \| \tilde{P}_a) \\ \text{s.t.} \quad & \begin{cases} \mathbb{E}_{\hat{P}}[a(\mathbf{x})] \geq 1/K, \\ \forall \mathbf{x} \in \mathcal{X}, 0 \leq a(\mathbf{x}) \leq 1. \end{cases} \end{aligned} \quad (17)$$



Distribution Space



# OPTIMAL BUDGETED REJECTION SAMPLING

## DEFINITION

### Theorem 4.2 (Optimal Acceptance Function)

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

$$a_{\text{OBRS}}(\mathbf{x}) = \min \left( \frac{p(\mathbf{x})}{\hat{p}(\mathbf{x})} \frac{c_K}{M}, 1 \right), \quad (18)$$

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

# OPTIMAL BUDGETED REJECTION SAMPLING

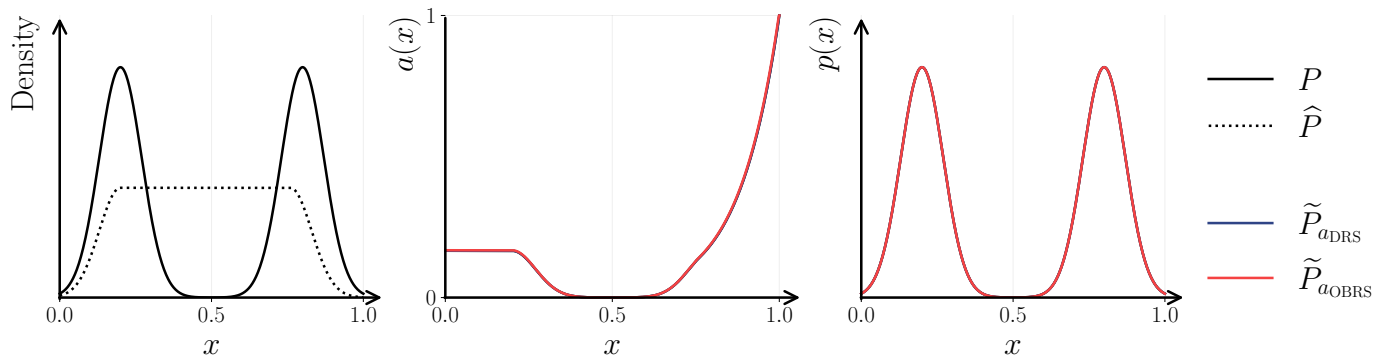
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Acceptance rate: 7.91%

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

Does not depend on  $f$ .

Same acceptance function to improve  
Precision and Recall.

# IMPROVING PRECISION AND RECALL

## EFFECT OF THE OBRS

### Proposition 4.3 (Precision and Recall Improvement)

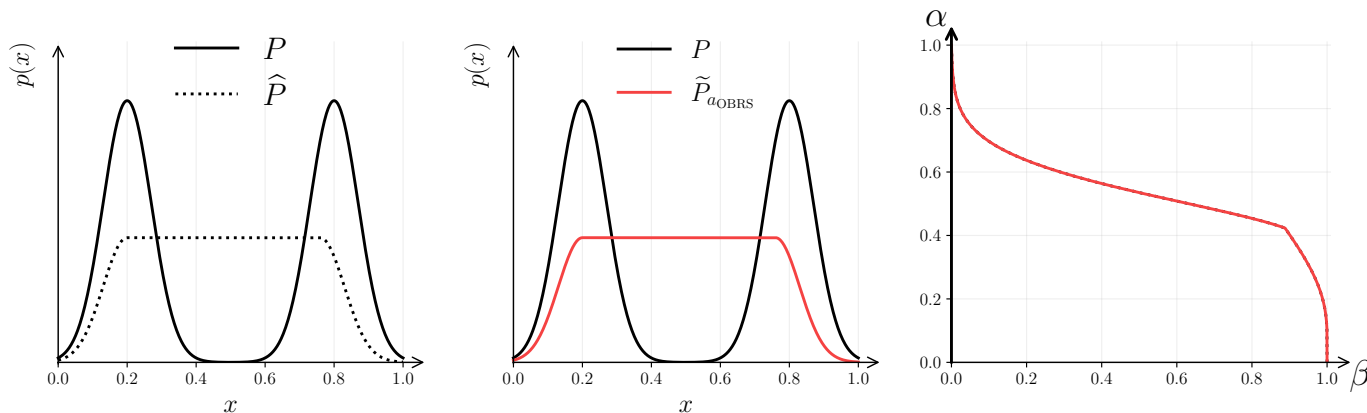
Let  $K \leq M$  be the budget for the OBRS. For any  $(\alpha, \beta) \in \text{PRD}(P, \hat{P})$  we have  $(\alpha', \beta) \in \text{PRD}(P, \tilde{P}_{a_{\text{OBRS}}})$  with  $\alpha' = \min \{1, K\alpha\}$ .

# IMPROVING PRECISION AND RECALL

## EFFECT OF THE OBRS

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



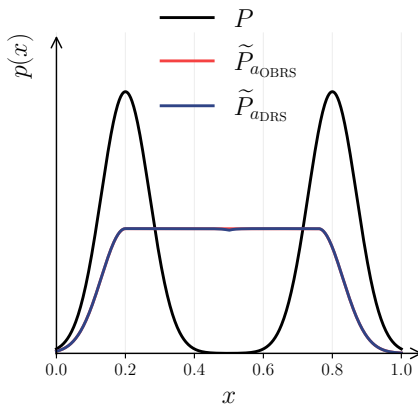
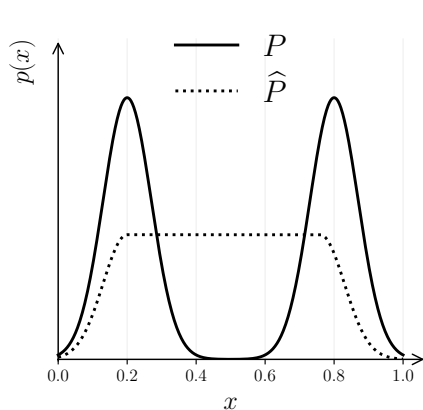
Acceptance rate: 100.00%

# IMPROVING PRECISION AND RECALL

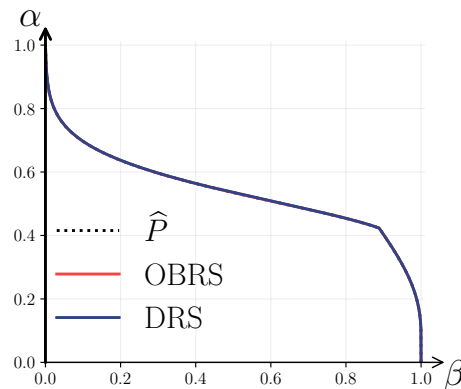
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Acceptance rate: 100.00%

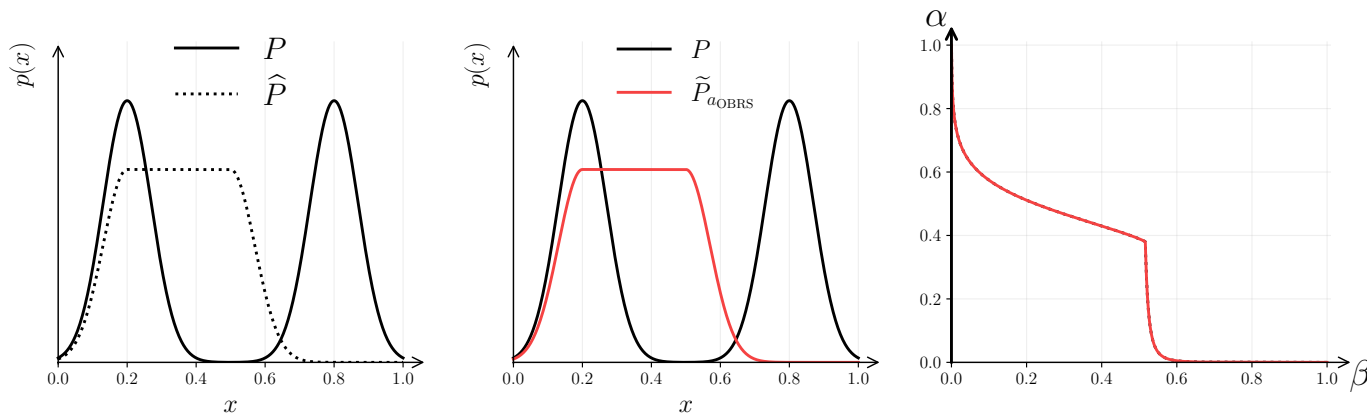


# IMPROVING PRECISION AND RECALL

## EFFECT OF THE OBRS

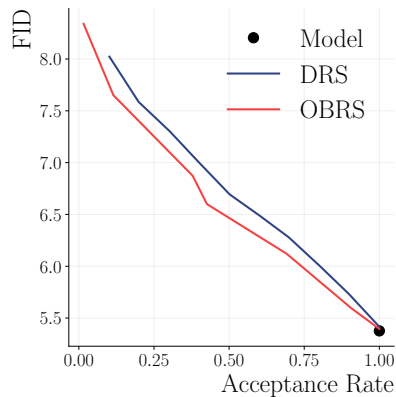
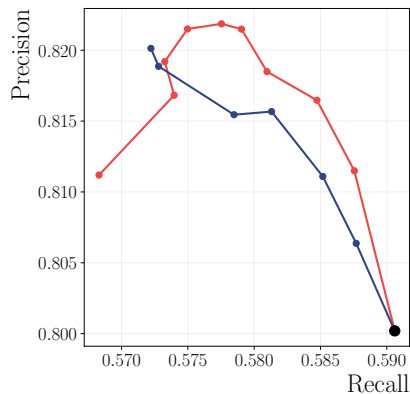
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Acceptance rate: 100.00%

## IMPROVING PRECISION AND RECALL IN PRACTICE



| 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 |

GAN on CelebA

Diffusion Model on  
CIFAR-10



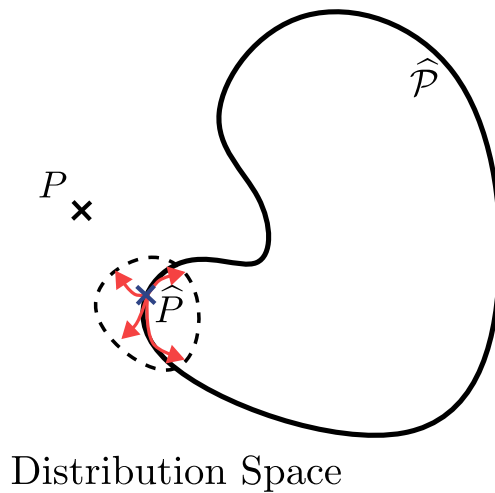
# TRAINING GENERATIVE MODELS WITH OBRS

## OBJECTIVE

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

$$\min_a \mathcal{D}_f(P \| \tilde{P}_a)$$

s.t. the acceptance rate is greater than  $1/K$ .



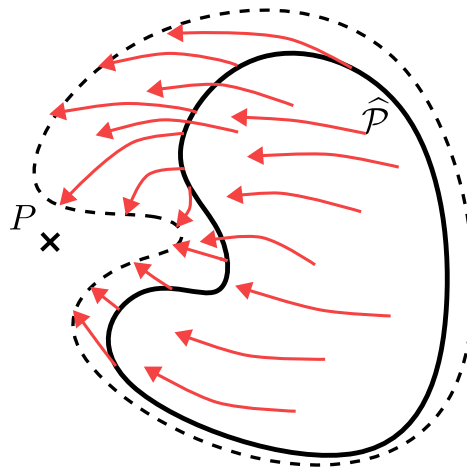
# TRAINING GENERATIVE MODELS WITH OBRS

## OBJECTIVE

We can train  $G$  to optimize:

$$\min_G \min_a \mathcal{D}_f(P \| \tilde{P}_{a,G})$$

s.t. the acceptance rate is greater than  $1/K$ .



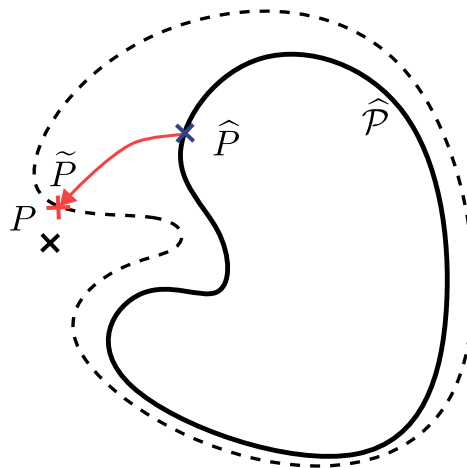
Distribution Space

# TRAINING GENERATIVE MODELS WITH OBRs

## OBJECTIVE

We can train  $G$  to optimize:

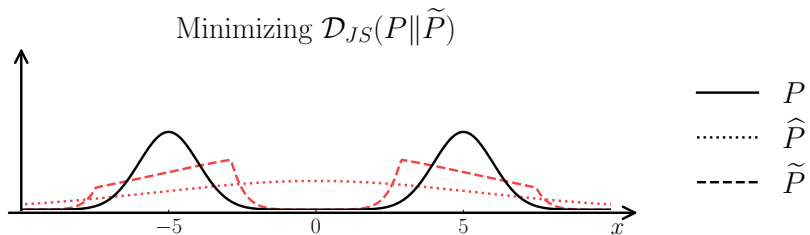
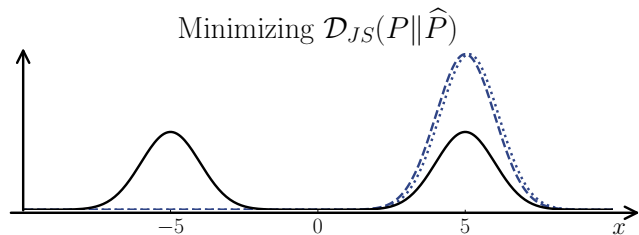
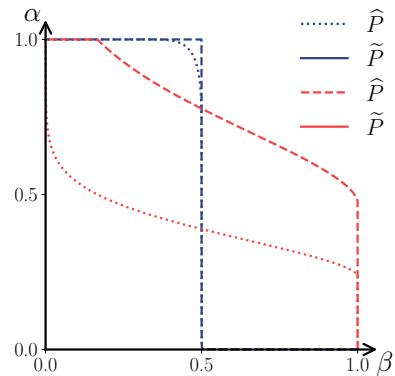
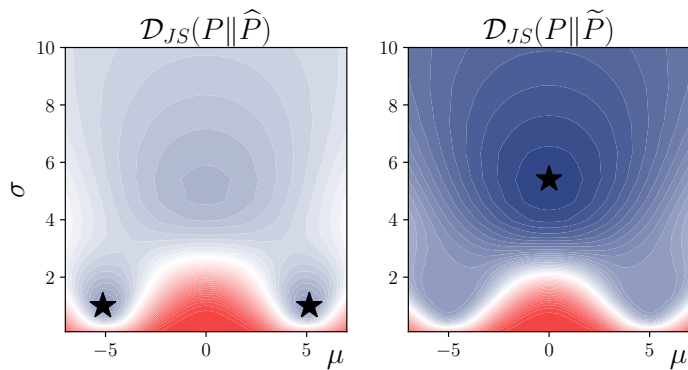
$$\begin{aligned} \min_G \min_a \mathcal{D}_f(P \| \tilde{P}_{a,G}) \\ \text{s.t.} \quad \text{the acceptance rate is greater than } 1/K. \end{aligned}$$



Distribution Space

# TRAINING WITH OBRS

## EXAMPLE



# TRAINING WITH OBRS

## IN PRACTICE

| Dataset                      | Method     | FID          | P            | R            |
|------------------------------|------------|--------------|--------------|--------------|
| CelebA<br>$64 \times 64$     | Hinge Loss | 9.33         | <b>80.23</b> | 57.78        |
|                              | Tw/OBRS    | <b>3.74</b>  | 74.40        | <b>65.15</b> |
| ImageNet<br>$128 \times 128$ | Hinge Loss | 12.18        | <b>27.75</b> | 34.33        |
|                              | Tw/OBRS    | <b>11.65</b> | 26.84        | <b>46.16</b> |

Training with OBRS increases the Recall.

# CONCLUSION

## AND PERSPECTIVES

- ▶ Quality and diversity are two important aspects of generative models.
- ▶ Generally at odds with each other, but can be balanced.
- ▶ The trade-off must be optimized.

# CONCLUSION

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### Optimizing the trade-off

- ▶ Connecting PR-Curves and  $f$ -divergences
  - Focusing on the AUC
  - Building a symmetric PR-Divergence
- ▶ Minimizing the PR-Divergence
  - Apply the method to Diffusion Models
  - Investigate other training strategies

# CONCLUSION

## AND PERSPECTIVES

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### Improving the quality and diversity

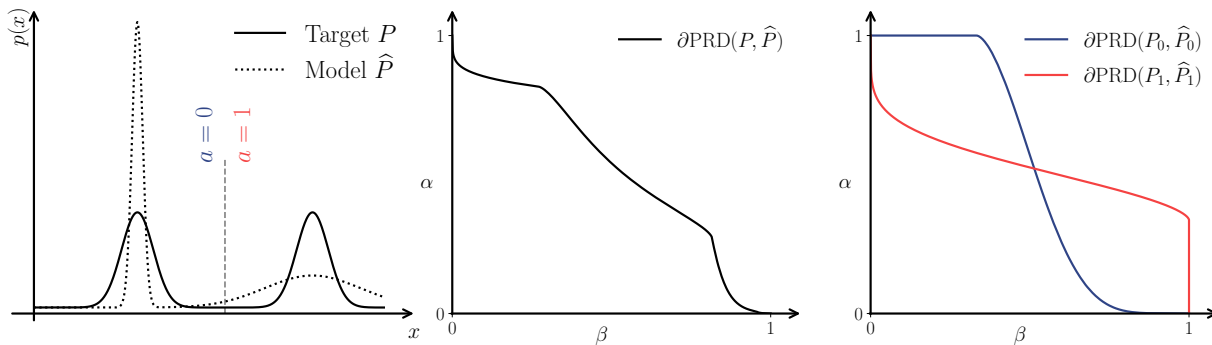
- ▶ Optimal Budgeted Rejection Sampling
  - Investigate the density ratio estimation error
  - Apply the method during denoising in Diffusion Models
- ▶ Training to improve diversity
  - Build formal proofs



# BROADER PERSPECTIVES

## FAIRNESS IN GENERATIVE MODELS

There are no metrics to distinguish between *fair* and *unfair* generations in terms of Precision and Recall.



## CONCLUSION

# Questions

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### **Temporary page!**

L<sup>A</sup>T<sub>E</sub>X was unable to guess the total number of pages correctly. As there was some unprocessed data that should have been added to the final page this extra page has been added to receive it.

If you rerun the document (without altering it) this surplus page will go away, because L<sup>A</sup>T<sub>E</sub>X now knows how many pages to expect for this document.