

High-dimensional Distribution Learning

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Mathematical Introduction to Machine Learning

Peking University, Fall 2023

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Example: Generate natural images



Figure 1: images generated by BigGAN (Brock et al., 2018)

Example: Style transfer

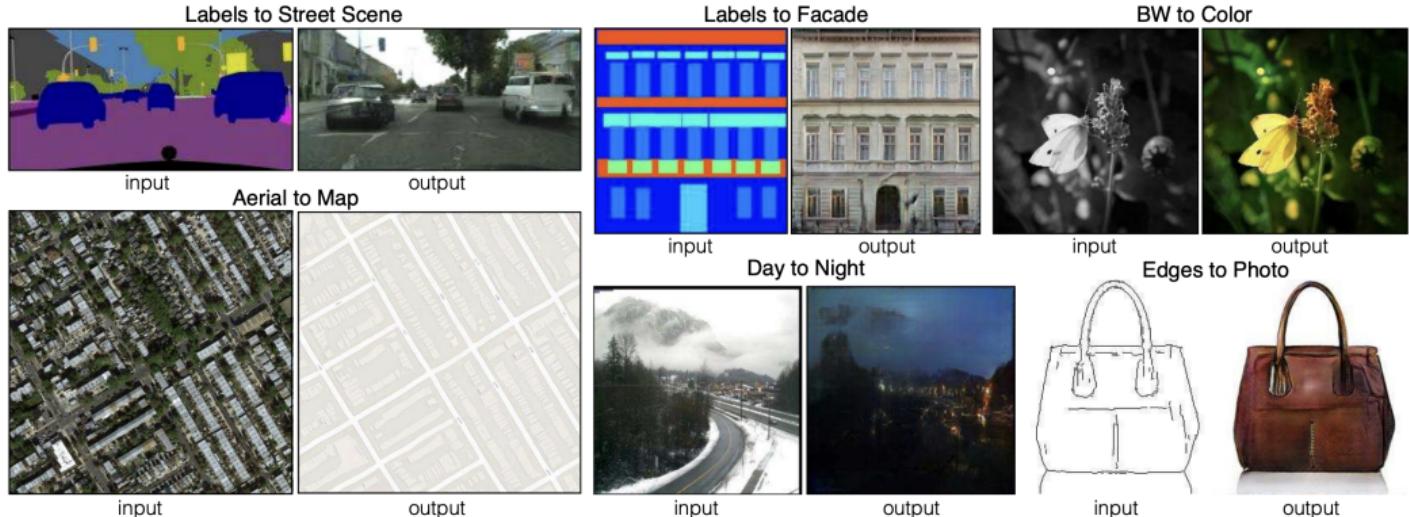


Figure 2: Style transfers with pix2pix ([Isola, et. al., 2017](#))

Example: Generate images from text description

Try this <https://huggingface.co/spaces/stabilityai/stable-diffusion>.



Example: Generate images from text description



Figure 3: Generated by <https://beta.dreamstudio.ai> with the prompt “Great wall in mountains, stars, Vincent van Gogh”.

Distribution Learning

- **General goal:** Given $\{x_i\}_{i=1}^n$ drawn from unknown ρ^* , estimate ρ^* using these samples.
- **Task:**
 - Estimate the likelihood (classical).
 - Draw new samples
- **Approaches:** density estimation and generative model.

Mathematical problem: How to model/parameterize a distribution?

History

- Gaussian mixture model, histogram estimator, and kernel density estimator. All these models take the following basis-expansion form:

$$\hat{f}_h(x; a, \mu) = \sum_{i=1}^m a_i k_h(x, \mu_i),$$

with $\sum_{j=1}^m a_j = 1$ and $a_j \geq 0, \forall j = 1, \dots, m$.

- In modern ML tasks, ρ^* is a high-dimensional distribution, e.g., the distribution of human faces.



- Classical linear methods all suffer from the curse of dimensionality in approximating ρ^* .

How do we represent distribution?

- Represent and learn distributions through functions.

Energy-based models

Density function: Let $V_\theta : \mathcal{X} \mapsto \mathbb{R}$ be a parametric potential energy function. Then, the Gibbs distribution:

$$p_\theta(x) = \frac{e^{-V_\theta(x)}}{\int e^{-V_\theta(x)} dx} = e^{-V_\theta(x)}/Z_\theta.$$

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- Learning a distribution is reduced to learn a energy function V_θ . Hence, It is often referred as an energy-based model
(<http://yann.lecun.com/exdb/publis/pdf/lecun-06.pdf>).
- $Z_\theta = \int e^{-V_\theta(x)} dx$ is the called *partition function*. We usually are unable to evaluate the density $p_\theta(x)$ since Z_θ is hard to compute.
- We can sample p_θ with MCMC sampler but this might be not efficient.

Transform-based models

Pushforward distribution: Let $Z \sim Q$ be a simple distribution, e.g., $Q = \mathcal{N}(0, I_D)$ and $Q = \text{Unif}([0, 1]^D)$. Let $G : \mathbb{R}^D \mapsto \mathbb{R}^d$ be a transform (also called **generator**). Then, the distribution P is generated through the transform G :

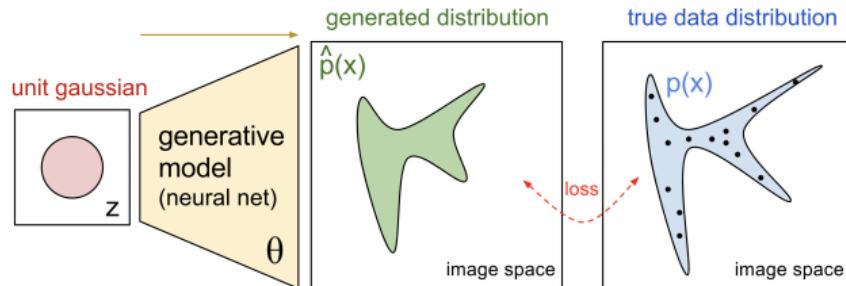
$$P = \text{Law}(X), \quad X = G_\theta(Z), \quad Z \sim Q.$$

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- In this modeling, the complex distribution P is generated from a simple distribution Q . Learning P is reduced to learn a generator G .



- We can use neural networks to parameterize G .

Transform-based models (Cont'd)

- One often choose $D \ll d$. In such a case, P is a singular distribution without a density function. In particular, P concentrates on a D -dimensional sub-manifold in \mathbb{R}^d :

$$\text{Supp}(P) = \text{Range}(G).$$

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 - Draw z_1, \dots, z_n independently from Q .
 - Then, $\{x_i = G(z_i)\}_{i=1}^n$ are IID samples from P .

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 - Then, $\{x_i = G(z_i)\}_{i=1}^n$ are IID samples from P .
- Computing expectation:

$$\mathbb{E}_{X \sim P}[f(X)] = \mathbb{E}_{Z \sim Q}[f(G(Z))] \approx \frac{1}{n} \sum_{i=1}^n f(G(z_i)).$$

The density of transform-based models

- By abuse of notation, let $Q(\cdot)$ denote the density function of Q . When $d = D$, X has the following density function:

$$P(x) = Q(G^{-1}(x)) |\det(\nabla G^{-1}(x))|.$$

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- A simple derivation. Let h be a test function. Then,

$$\begin{aligned} \int h(x)p(x) dx &= \int h(G(z))q(z) dz \quad (\text{definition of push-forward distribution}) \\ &= \int h(y)q(G^{-1}(y)) \frac{dz}{dy} dy \quad (\text{change of variable}) \\ &= \int h(y)q(G^{-1}(y)) |\det \nabla G^{-1}(y)| dy. \end{aligned}$$

Hence, $p(x) = q(G^{-1}(x)) |\det \nabla G^{-1}(x)|$.

- This case is useful when we would like to estimate likelihoods.

How can we construct G such that

- The $G^{-1}(x)$ and $\det \nabla G^{-1}(x)$ can be computed **efficiently**.

The flow-based models provide a principled approach to design this kind of G !

Flow-based models

Suppose $f_w : \mathbb{R}^d \mapsto \mathbb{R}^d$ be a simple invertible map. Flow-based models construct complex transforms through a “flow” of simple transform f_w by

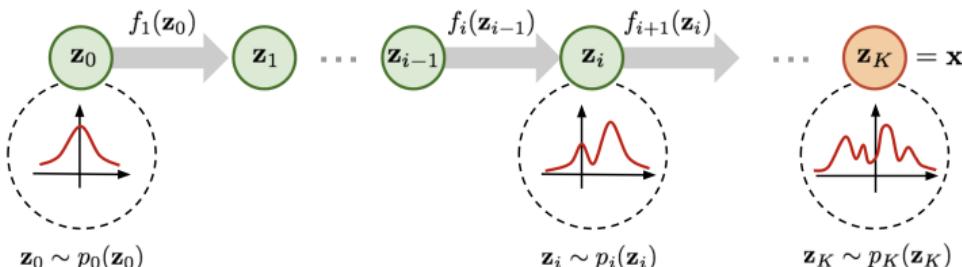
$$G_\theta = f_{w_K} \circ f_{w_{K-1}} \circ \cdots \circ f_{w_1} : \mathbb{R}^d \mapsto \mathbb{R}^d,$$

where $\theta = (w_1, \dots, w_K)$. It can be rewritten as

$$z_0 = z$$

$$z_t = f_{w_t}(z_{t-1}), \quad t = 1, \dots, K$$

$$G_\theta(z) = z_K$$



Flow-based models (Cont'd)

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- Note that $|\det \nabla G_\theta^{-1}(x)| = 1/|\det \nabla G_\theta(z)|$ and

$$\det \nabla G_\theta(z) = \left(\det \frac{dz_L}{dz_{L-1}} \right) \left(\det \frac{dz_L}{dz_{L-1}} \right) \cdots \left(\det \frac{dz_1}{dz_0} \right).$$

Hence,

$$\log |\det \nabla_z G_\theta(z)| = \sum_{t=0}^{L-1} \log |\nabla f_{w_t}(z_{t-1})|$$

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- Note that the computation cost of $\det \nabla f_w(z)$ can be as slow as $O(d^3)$. Hence we need to design f_w such that its inverse and the determinant of Jacobian can be efficiently computed.

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In the literature, there are many choices:

- Normalizing flow (Tabak & Vanden-Eijnden, 2010)
- **NICE**: nonlinear independent components estimation (Dinh et al., 2014)
- **Real-NVP**: real-valued Non-volume preserving (Dinh et al., 2017)
- Masked autoregressive flow (Papamakarios et al., 2017)
- Inverse autoregressive flow (Kingma et al., 2016)
- **Continuous normalizing flow (CNF)** (Chen et al., 2019).

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We will only cover details of NICE and reva-NVP, whose designing principle is to ensure:

∇f_w is **lower triangular**.

In this case, the computational cost is $O(d)$.

NICE

Decompose z into two disjoint subsets: $z = (z_{1:s}, z_{s+1:d})$. Then, NICE proposes the following **additive coupling transform** $x = f(z)$:

$$\begin{aligned}x_{1:s} &= z_{1:s} \\x_{s+1:d} &= z_{s+1:d} + v(z_{1:s})\end{aligned}$$

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- We do not need to compute the determinant of Jacobian for NICE. Great!! But this restricts the expressive power.

Real-NVP

Real-NVP adds scaling factors to NICE:

$$\begin{aligned}x_{1:s} &= z_{1:s} \\x_{s+1:d} &= z_{s+1:d} \odot e^{u(z_{1:s})} + v(z_{1:s}),\end{aligned}$$

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- Real-NVP is not volume-preserving.

Remarks

- Note that the additive coupling transform leaves part of its input unchanged. To fix this issue, we need to exchange the role of two subsets for different steps.

The choice of loss function

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- Different from supervised learning, choosing $L(\cdot, \cdot)$ is highly non-trivial. **There are no such thing called fitting error at the i -th sample.**
- There are many variants of norm, divergence, distance for comparing two distributions:
 - P_{θ} may not have a density function, e.g., the transform-based models.
 - Computing the density of P_{θ} may be intractable or expensive, e.g., the energy-based models.

- Designing loss functions

What is a practical loss function?

- Consider the L^p distance:

$$\int |P_\theta(x) - \hat{P}_n(x)|^p dx.$$

- The total variation:

$$TV(P_\theta, \hat{P}_n).$$

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We are unable to evaluate these losses since we only have samples x_1, \dots, x_n from ρ^* .

A practical choice of metric must be an expectation in \hat{P}_n ; otherwise, the metric is not computable.

Strong form

- Strong form: Need P_θ to have a density function.

$$\begin{aligned} KL(\hat{P}_n || P_\theta) &= \int \log \frac{\hat{P}_n(x)}{P_\theta(x)} d\hat{P}_n(x) \\ &= \text{constant} - \mathbb{E}_{\hat{P}_n} [\log P_\theta(x)] \\ &= \text{constant} - \frac{1}{n} \sum_{i=1}^n \log P_\theta(x_i) \end{aligned} \tag{3}$$

- It is equivalent to maximizing the likelihood.
- In fact, (3) is the only practical density-based loss (homework).

Weak form

Weak Form: View P as a linear functional over certain function classes.

$$L(P, P') = \sup_{f \in \mathcal{F}} \mathbb{E}_P[f] - \mathbb{E}_{P'}[f] \quad (4)$$

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Intuitively speaking, weak metrics measure the differences of two distributions by comparing their “generalized” moments .

- $\mathcal{F} = \{x, x^2, x^3, \dots\} \rightarrow$ the classic moment methods.
- $\mathcal{F} = \{\|f\|_{L^\infty} \leq 1\} \rightarrow$ the total variation norm.
- $\mathcal{F} = \{\|f\|_{\text{Lip}} \leq 1\} \rightarrow$ the 1-Wasserstein metric.
- $\mathcal{F} = \text{unit ball in RKHS space} \rightarrow$ the maximum mean discrepancy distance.
- $\mathcal{F} = \text{neural networks (with certain constraints)} \rightarrow$ the neural distance.

The models

Loss functions:

- Strong: log-likelihood

$$\min_P -\mathbb{E}_{P^*} [\log P(x)].$$

- Weak: dual norm

$$\min_P \max_{f \in \mathcal{F}} \mathbb{E}_P[f] - \mathbb{E}_{P^*}[f].$$

Representations:

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Combinations: Different combinations lead to different models.

- Weak metric + generator = GAN (Generative adversarial network):
- Strong metric: Variational autoencoder (VAE), normalizing flow, diffusion-based generative model, autoregressive models, etc.

Generative adversarial network (GAN)

Rename the test function as the discriminator D .

- Weak formulation of Jensen-Shannon divergence:

$$\begin{aligned} JS(P, P') &= \frac{1}{2} D_{KL}(P \parallel \frac{P + P'}{2}) + \frac{1}{2} D_{KL}(P' \parallel \frac{P + P'}{2}) \\ &= \sup_q (\mathbb{E}_P[\log q(x)] + \mathbb{E}_{P'}[\log(1 - q(x))]) \end{aligned}$$

where the supremum is taken with all measurable functions $q : \mathbb{R}^d \mapsto [0, 1]$.

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- Neural network formulation:

$$L(P, P') = \sup_D (\mathbb{E}_P[\log(1 - D(x))] + \mathbb{E}_{P'}[\log D(x)]) ,$$

where $D : \mathbb{R}^d \mapsto (0, 1)$ is a neural network. It is essentially a binary classifier.

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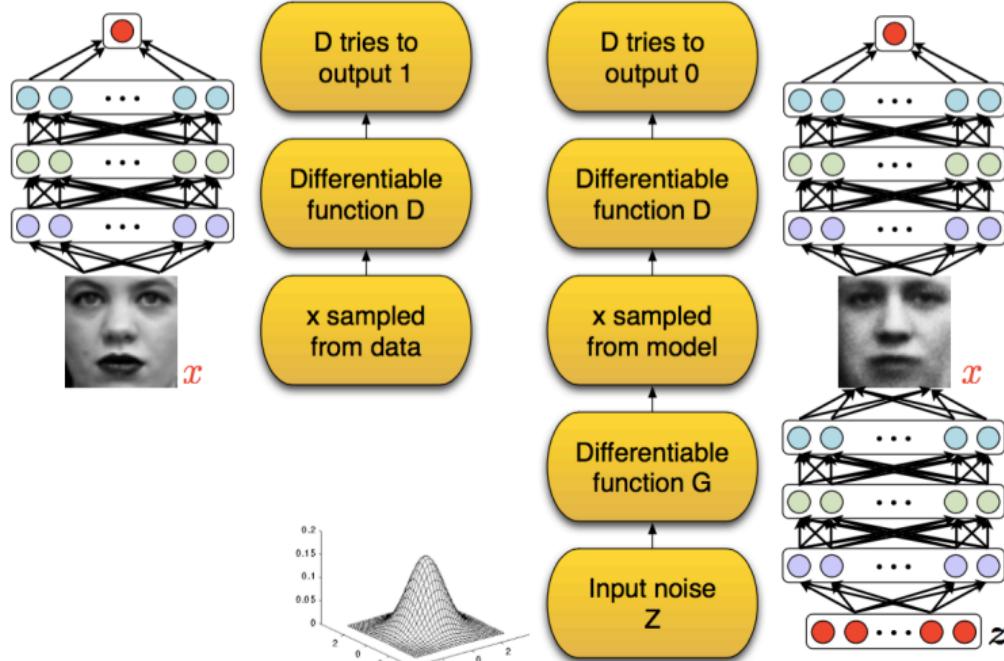
- In total, the problem becomes a minimax problem:

$$\min_G \max_D \left(\mathbb{E}_{z \sim Q}[\log(1 - D(G(z)))] + \frac{1}{n} \sum_{i=1}^n \log D(x_i) \right).$$

GAN: The original game motivation

A game between the generator and discriminator:

- Discriminator: Distinguish the fake and real data.
- Generator: generate fake data $G(z)$ such that $\{G(z)\}_z$ are undistinguishable with the real data $\{x_i\}_i$.



Wasserstein GAN

Choose test functions as constraint neural networks.

$$\min_{\theta_1 \in U} \max_{\theta_2} \mathbb{E}_z [f_{\theta_1}(G_{\theta_2}(z))] - \frac{1}{n} \sum_{i=1}^n f_{\theta_1}(x_i) \quad (5)$$

- Both f_{θ_1} and G_{θ_2} are neural networks.
- In the original Wasserstein GAN, $U = \{\theta : \max_i |\theta_i| \leq \delta\}$ with the δ tuned for each problems.
- There are many other choices of U , such as gradient penalty, spectral normalization, etc.

Evaluate our models

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Weak metrics:

- Human judgement.
- Wasserstein W_2 metric: Computation suffers from the curse of dimensionality.
- Frechet inception distance: Approximating W_2 with only means and covariances.

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Weak metrics:

- Human judgement.
- Wasserstein W_2 metric: Computation suffers from the curse of dimensionality.
- Frechet inception distance: Approximating W_2 with only means and covariances.

Strong metrics:

- Log-likelihood.
- Inception score: Let $C(x)$ be an ImageNet classifier. If $C(x)$ has small entropy on x , then the classifier is confident about the label of x . This implies that x looks like an image (at least for $C(x)$).

Training procedure

- Strong form:

$$\min_{\theta} - \sum_i \log p_{\theta}(x_i)$$

Train with SGD/ADAM.

- Weak form:

$$\min_{\theta_2} \max_{\theta_1} \mathbb{E}_{x \sim \hat{P}_n} [D(x; \theta_1)] - \mathbb{E}_z [D(G(z; \theta_2); \theta_1)]$$

This is not a standard optimization but a minimax problem.

Solve the minimax problem

$$\min_{\theta_2} \max_{\theta_1} \mathbb{E}_{x \sim \hat{P}_n} [D(x; \theta_1)] - \mathbb{E}_z [D(G(z; \theta_2); \theta_1)]$$

Each step $(\theta_1(t), \theta_2(t)) \mapsto (\theta_1(t+1), \theta_2(t+1))$ updates as follows.

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- **Maximization-step:** Let $\theta_1(t, 0) = \theta_1(t)$.

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- **Maximization-step:** Let $\theta_1(t, 0) = \theta_1(t)$.
 - For $k = 1, \dots, m$, randomly sample $z_{1,k}, \dots, z_{B,k}$ and update the generator as follows

$$\theta_1(t, k) = \theta_1(t, k-1) + \eta_1 \nabla_{\theta_1} \left(\frac{1}{B_1} \sum_i D(x_i; \theta_1(t)) - \frac{1}{B_2} \sum_j D(G(z_j; \theta_2(t)); \theta_1(t, k-1)) \right)$$

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Solve the minimax problem

$$\min_{\theta_2} \max_{\theta_1} \mathbb{E}_{x \sim \hat{P}_n} [D(x; \theta_1)] - \mathbb{E}_z [D(G(z; \theta_2); \theta_1)]$$

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- Return $\theta_1(t+1) = \theta_1(t, m)$.
- **Minimization-step:** Update the discriminator:

$$\theta_2(t+1) = \theta_2(t) - \eta_2 \nabla_{\theta_2} \left(\frac{1}{B} \sum_j D(G(z_j; \theta_2(t, k)); \theta_1(t)) \right),$$

where $\{x_i\}$ and $\{z_j\}$ are the minibatch samples.

Issues

- **The training of weak models is very unstable**, in particular when the maximization step is updated only a few steps—a choice preferred in practice.
Moreover, we do not have a good criterion to monitor the training progress since the weak norm cannot be estimated in a reasonable way.

Issues

- **The training of weak models is very unstable**, in particular when the maximization step is updated only a few steps—a choice preferred in practice.
Moreover, we do not have a good criterion to monitor the training progress since the weak norm cannot be estimated in a reasonable way.
- **Mode collapse**: Are there metrics that can detect the mode collapse?



Figure 4: Left: Images from [Zhao et al., 2017] Energy-based GAN

Summary

Distribution learning: Normalizing flow, GAN, etc.

- Representation:
 - Energy-based models
 - Transform-based models: flow-based models (NICE, real-NVP, etc.)
- Loss designing:
 - Strong form: MLE/KL-divergence;
 - Weak form: The choice of test functions.
- Evaluation: Weak and strong metrics.

There are many important issues (in particular of the training) uncovered in this lecture.

Diffusion Model

Supplementary Wasserstein metric

- Define a distance between two sets of points $\{\mathbf{x}_i\}_{i=1}^n$ and $\{\mathbf{y}_j\}_{j=1}^n$:

$$\min_{\pi \in S_n} \sqrt{\frac{1}{n} \sum_{i=1}^n \|\mathbf{x}_i - \mathbf{y}_{\pi(i)}\|^2}$$

- Generalize to probability measures P and Q : the matching becomes a joint distribution $\pi(\mathbf{x}, \mathbf{y})$

$$\Pi(P, Q) := \{\pi \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d), \pi_{\mathbf{x}} = P, \pi_{\mathbf{y}} = Q\}$$

Define the Wasserstein metric W_p

$$W_p(P, Q) := \min_{\pi \in \Pi(P, Q)} (\mathbb{E}_{\pi(\mathbf{x}, \mathbf{y})} [\|\mathbf{x} - \mathbf{y}\|^p])^{1/p}$$

- For W_1 , we have the Kantorovich-Rubinstein theorem:

$$W_1(P, Q) = \sup_{\|f\|_{Lip} \leq 1} \mathbb{E}_P[f] - \mathbb{E}_Q[f]$$

Duality holds for W_n in general, but the formula for W_1 is simplest.