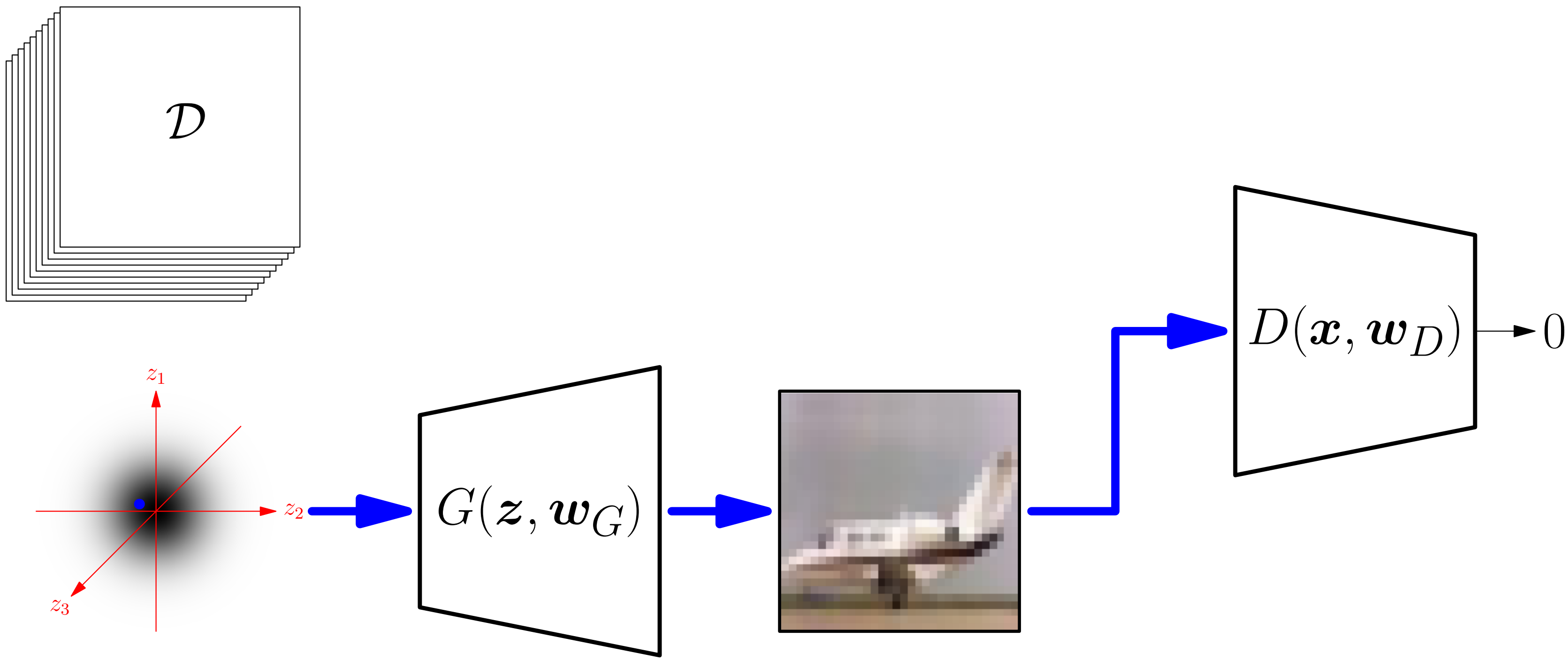
Advanced Machine Learning

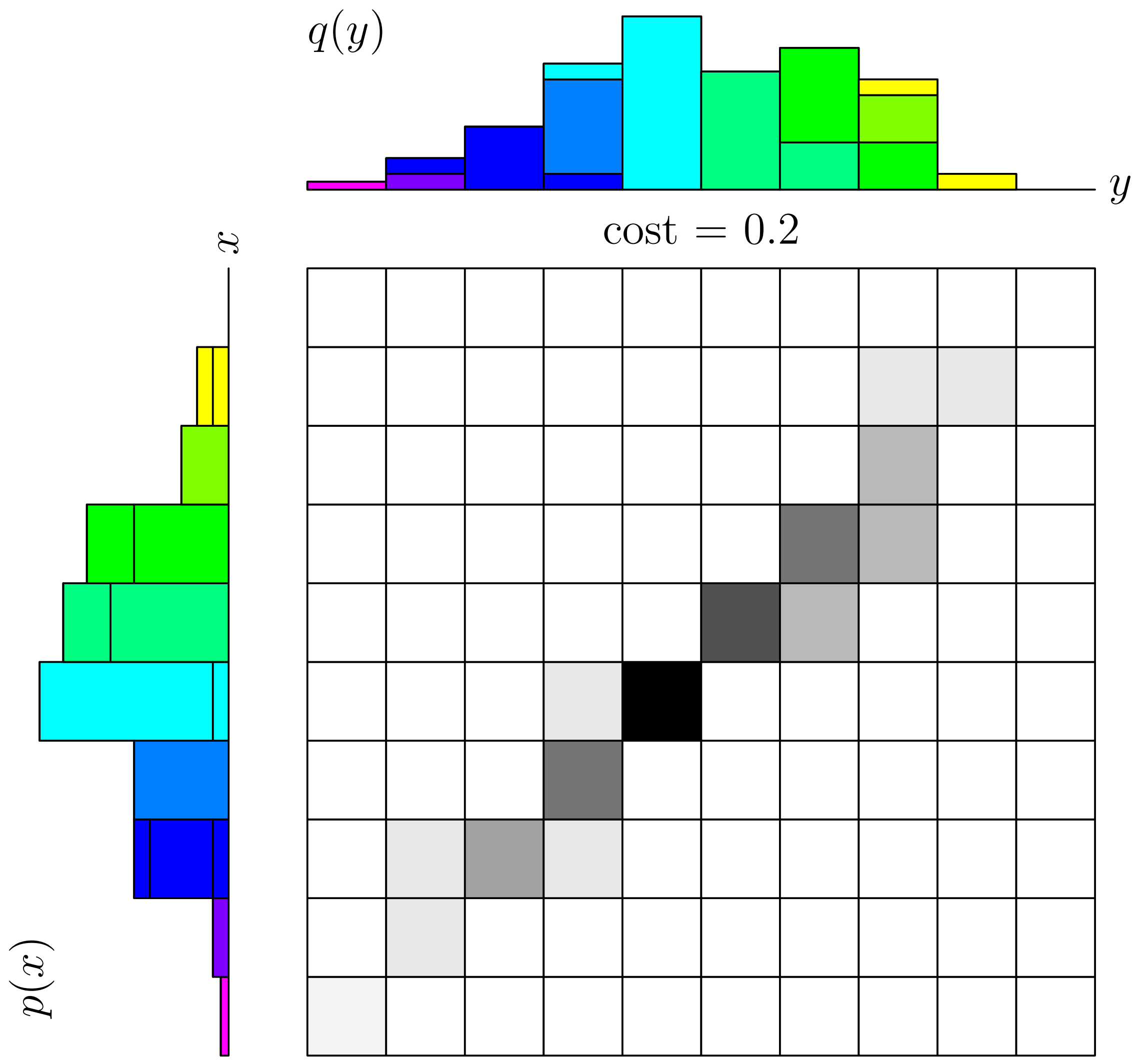
Wasserstein GANs



GANs, Wasserstein distance, Duality, WGANs

Outline

1. **GANs**
2. Wasserstein Distance
3. Wasserstein GANs



Generative Adversarial Networks

- One of the applications of Deep Learning that has most excited the public are **Generative Adversarial Networks** or GANs
- Their aim is to generate new random samples from the same distribution as some training set, $\mathcal{D}$
- Their number of real world applications are

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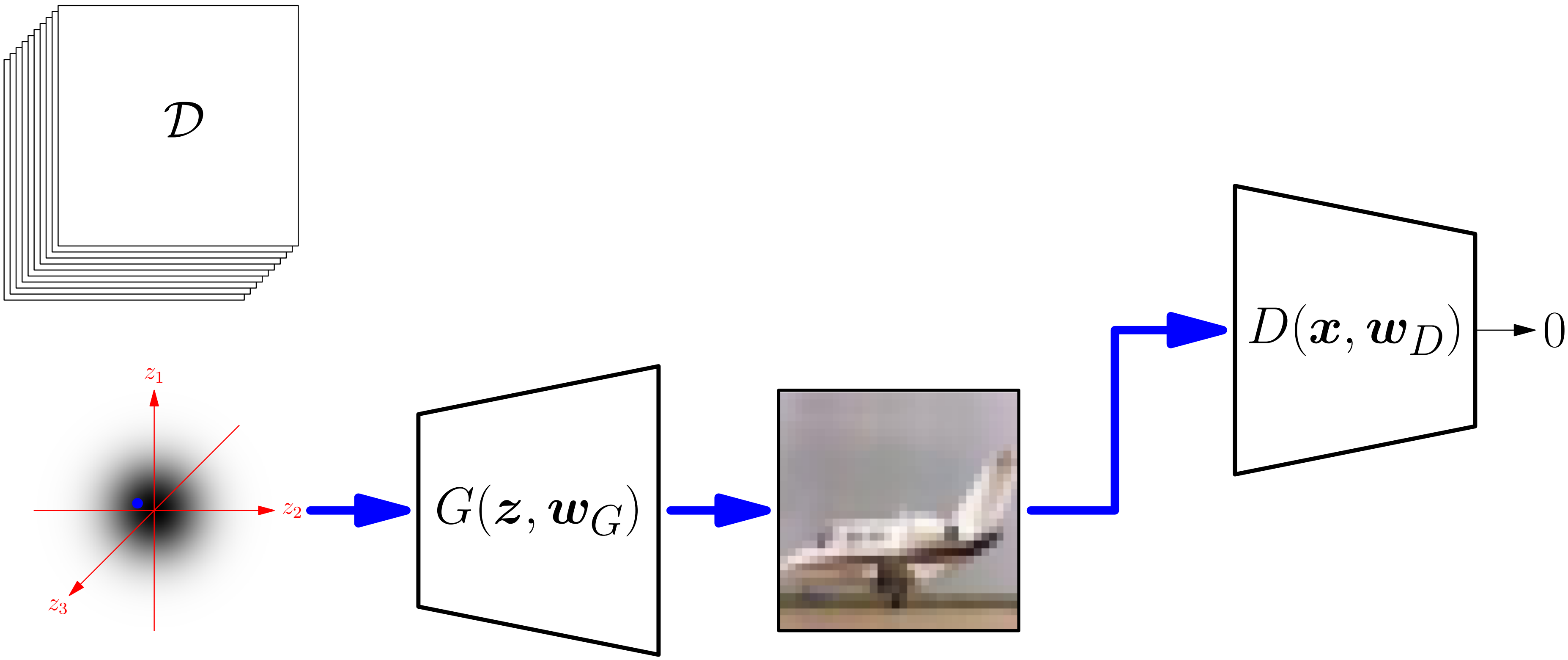
- *Out of date warning:* someone invented diffusion models

How GANs Work



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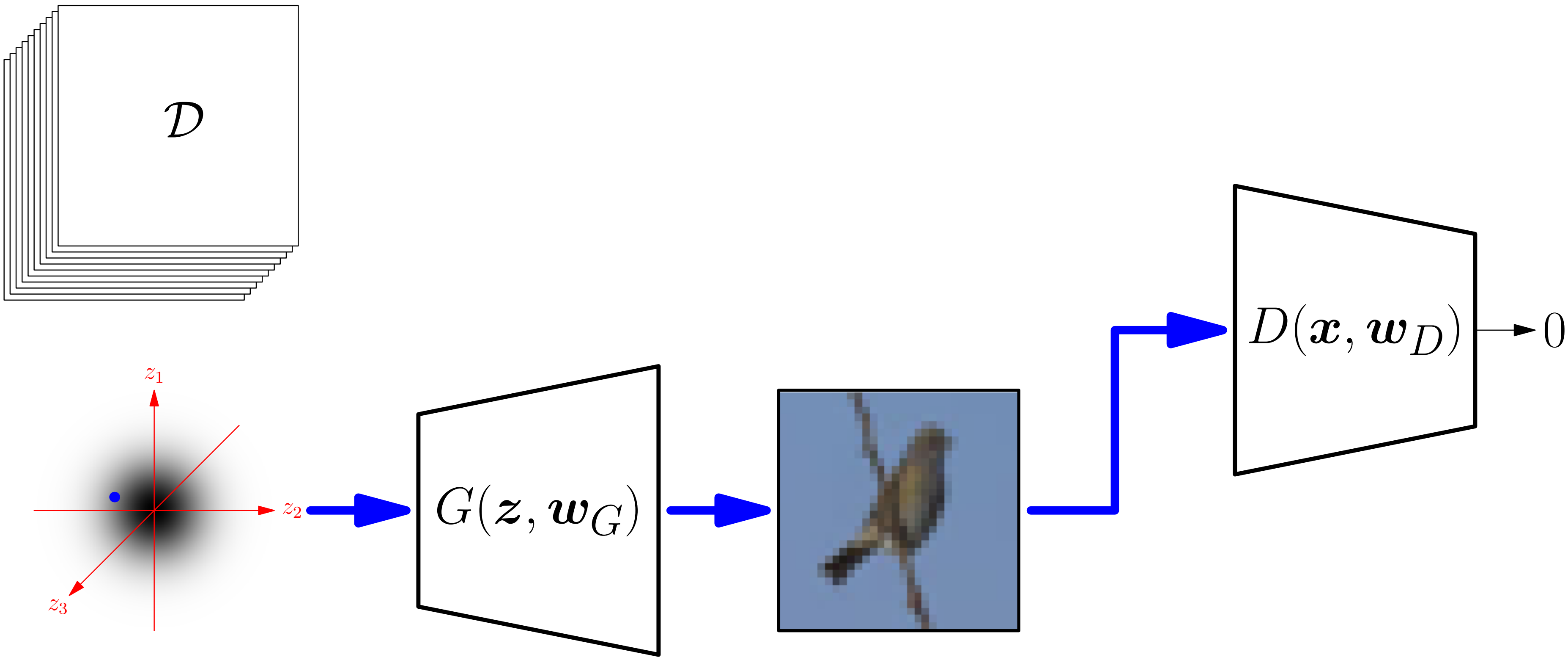

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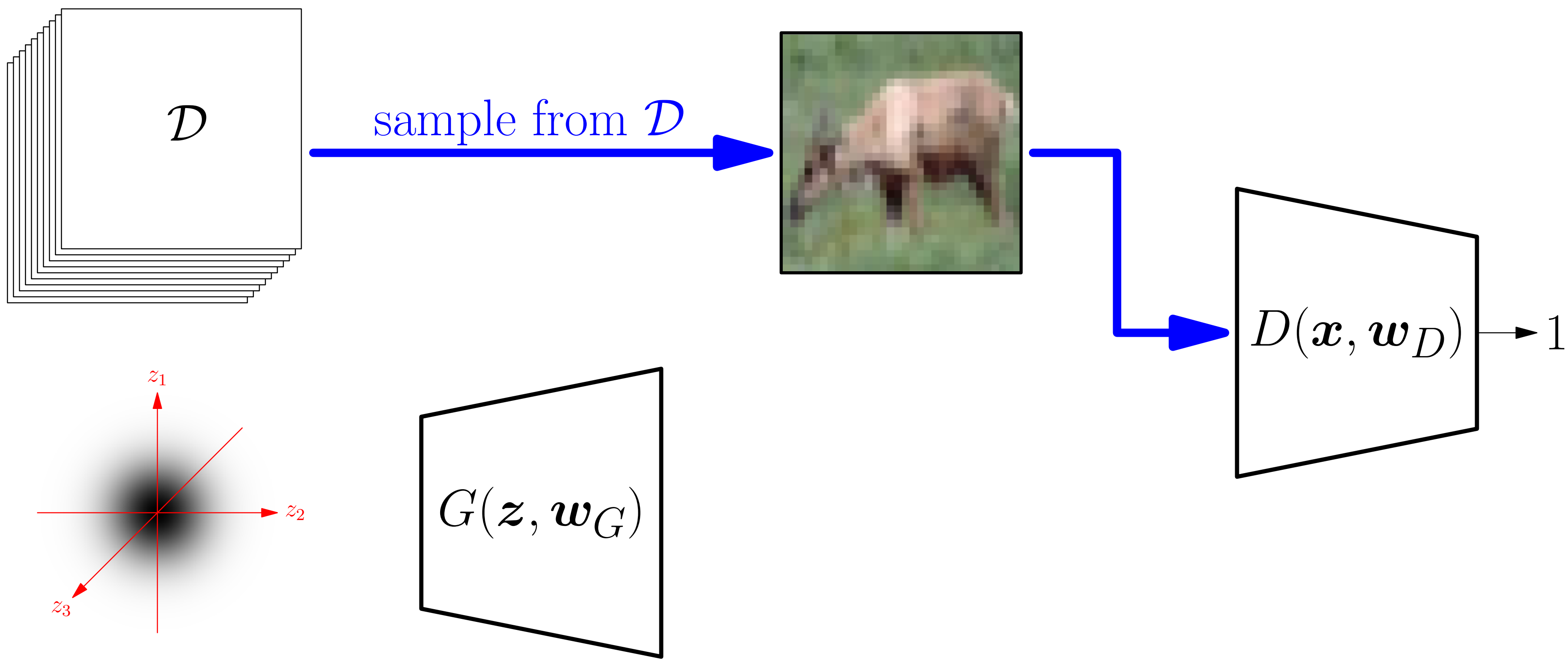

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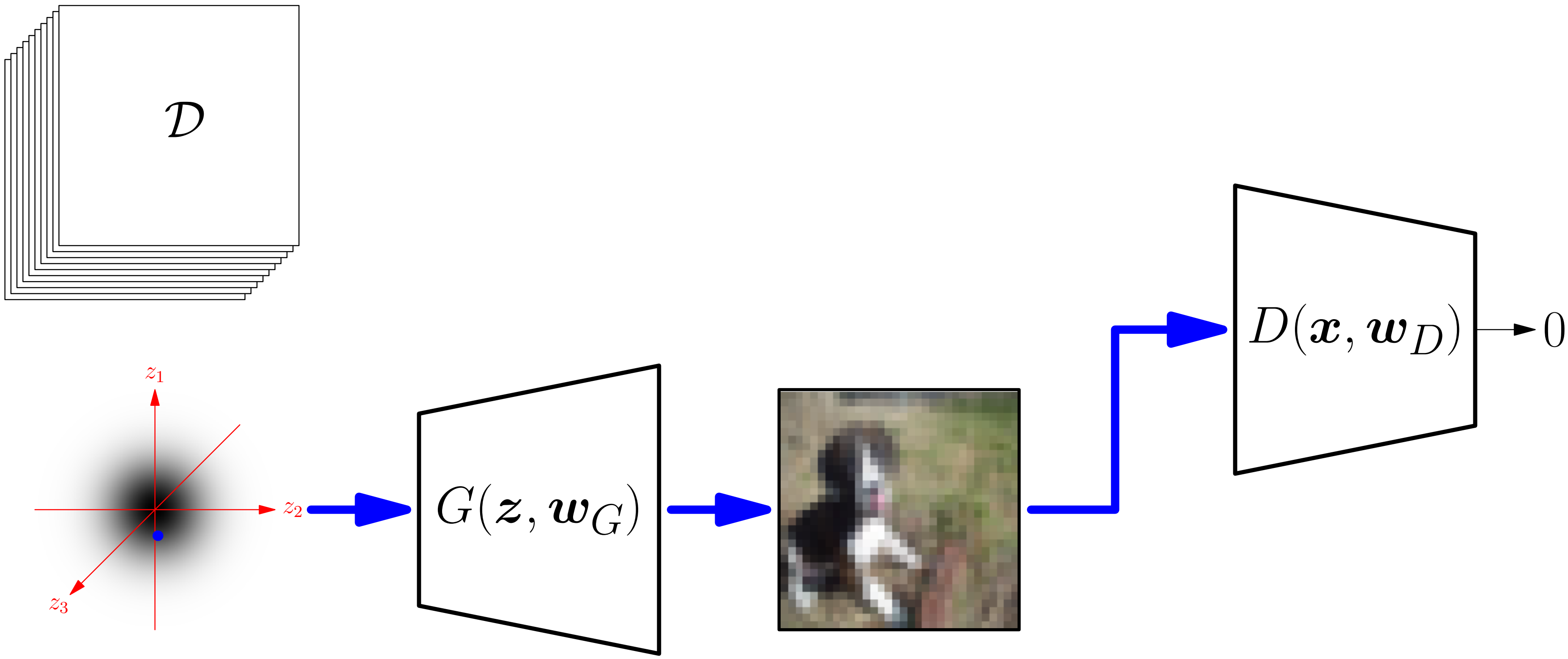

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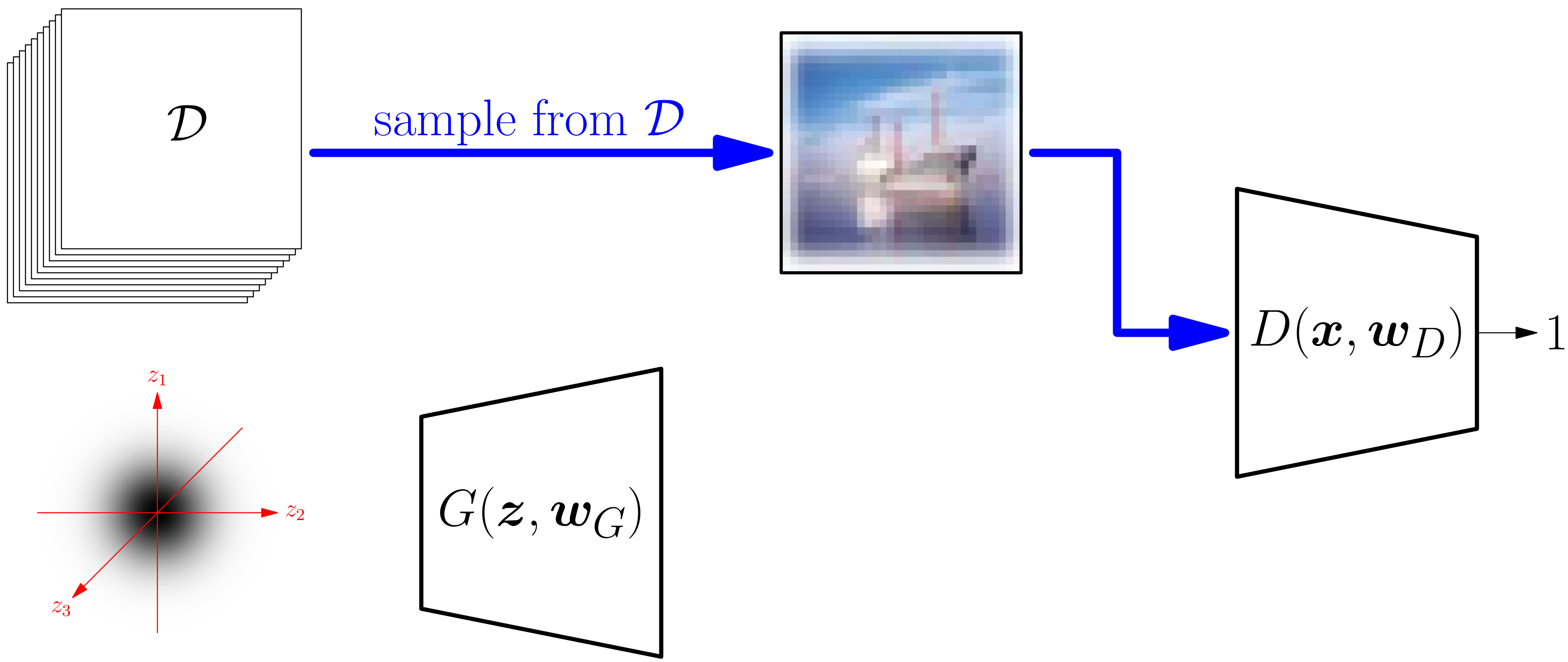

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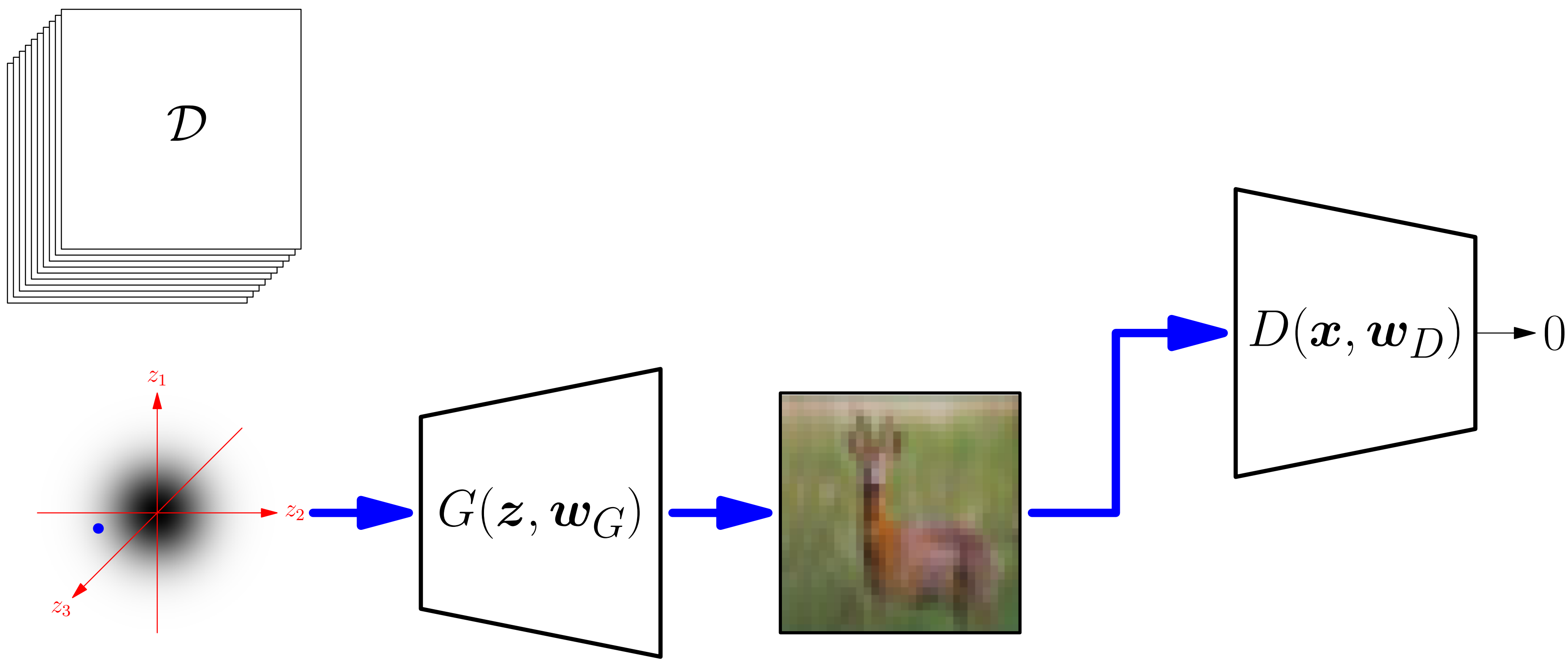

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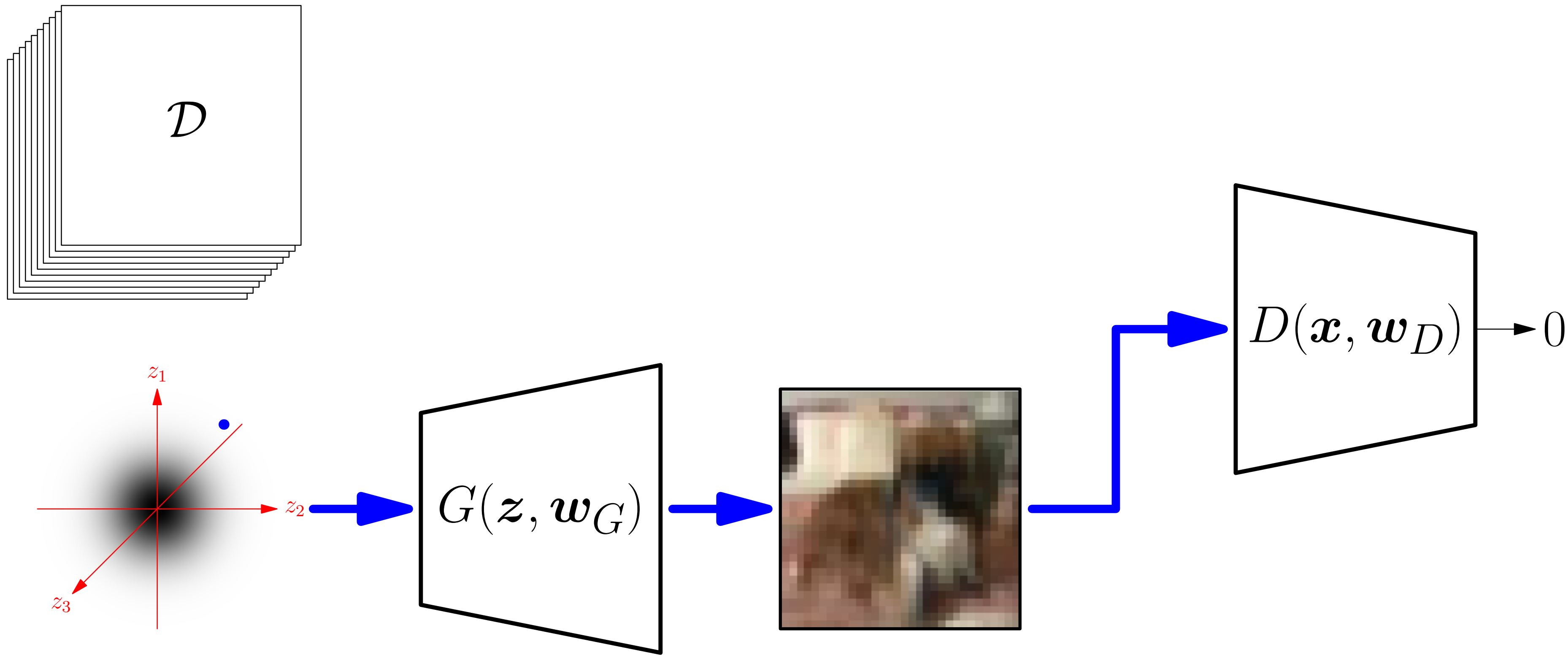

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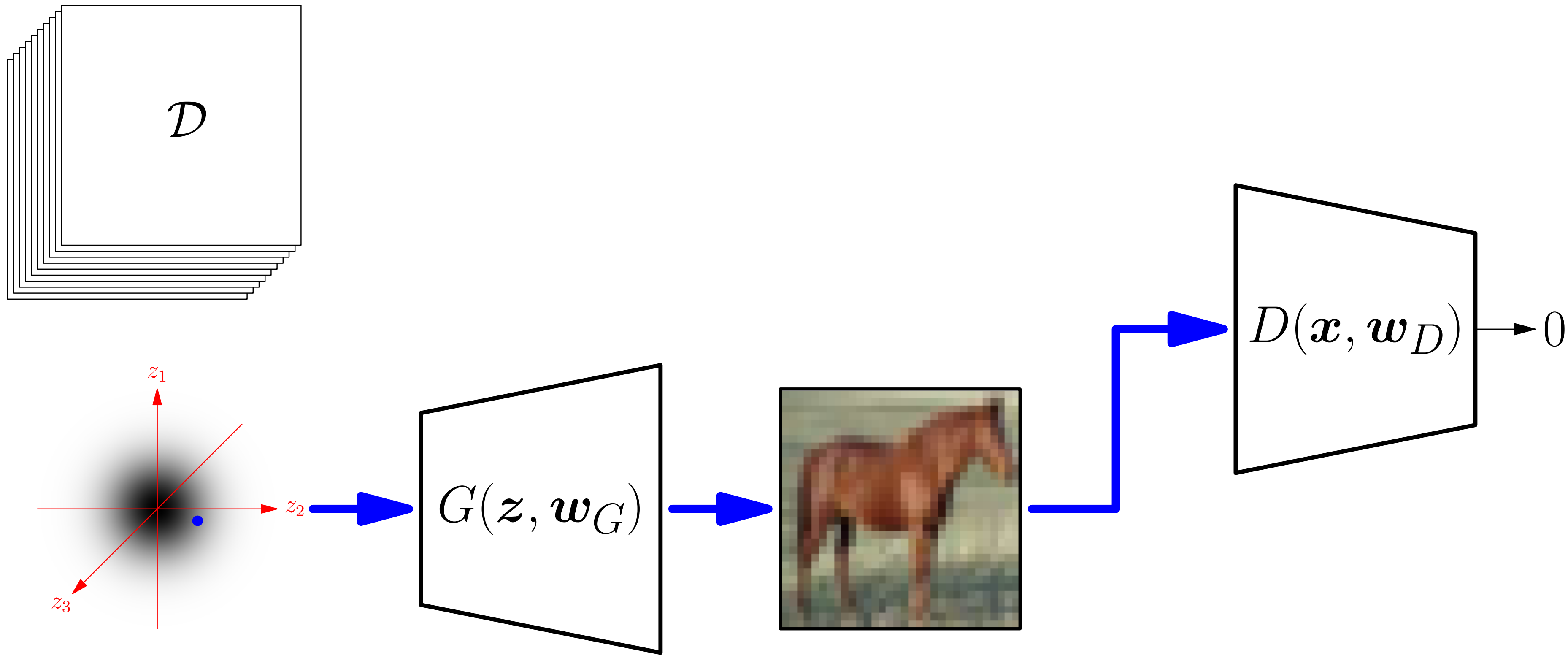

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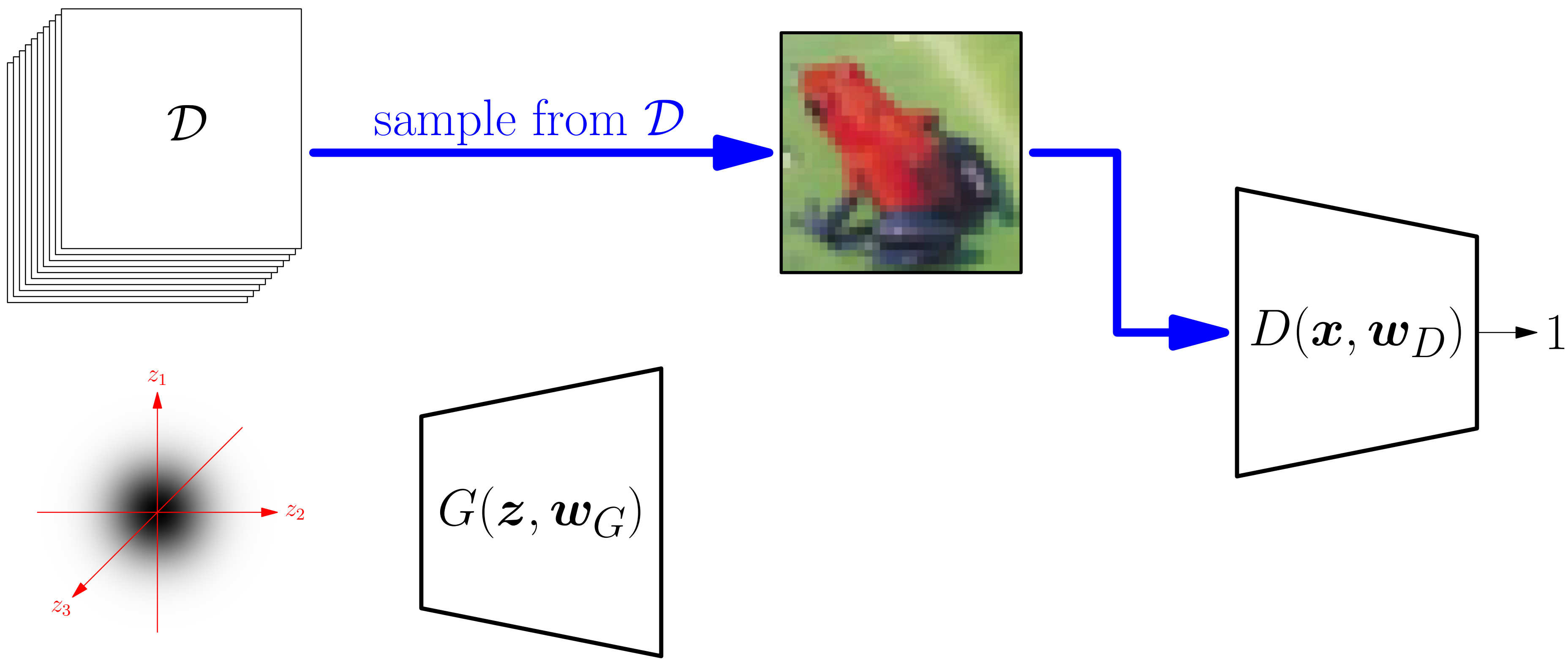

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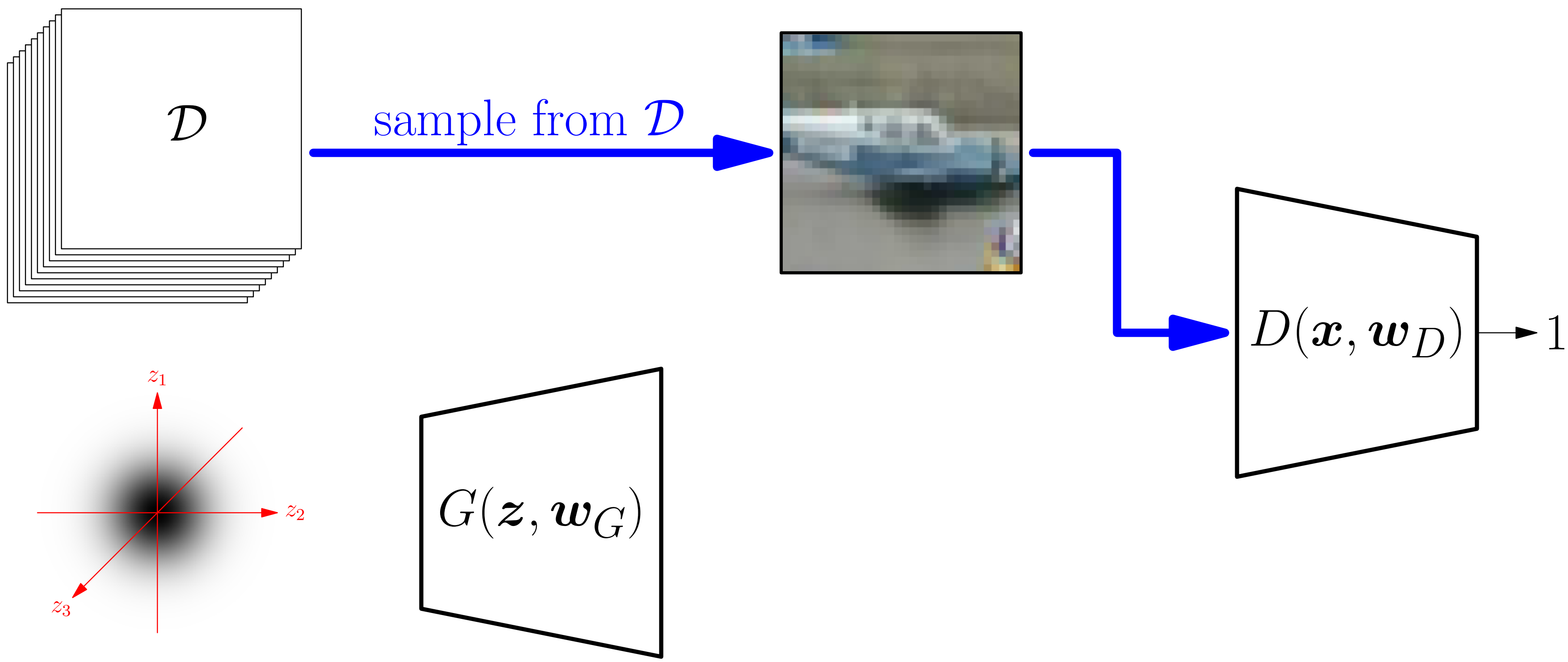

Training GANs

- The loss of the generator depends on its ability to trick the discriminator
- The loss of the discriminator depends on its ability not to be tricked
- We try to train the two networks simultaneously
- We hope that over time the generator produces better and better fakes

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Problems of GANs

- GANs are notoriously difficult to train
- The generator and discriminator training can decouple
- Often the discriminator becomes too good at correctly identifying the generated images
- Then there can be little gradient information to help the generator as every small change in parameters doesn't significantly change the discriminator decision
- To try to solve this problem we first make a seemly unconnected diversion

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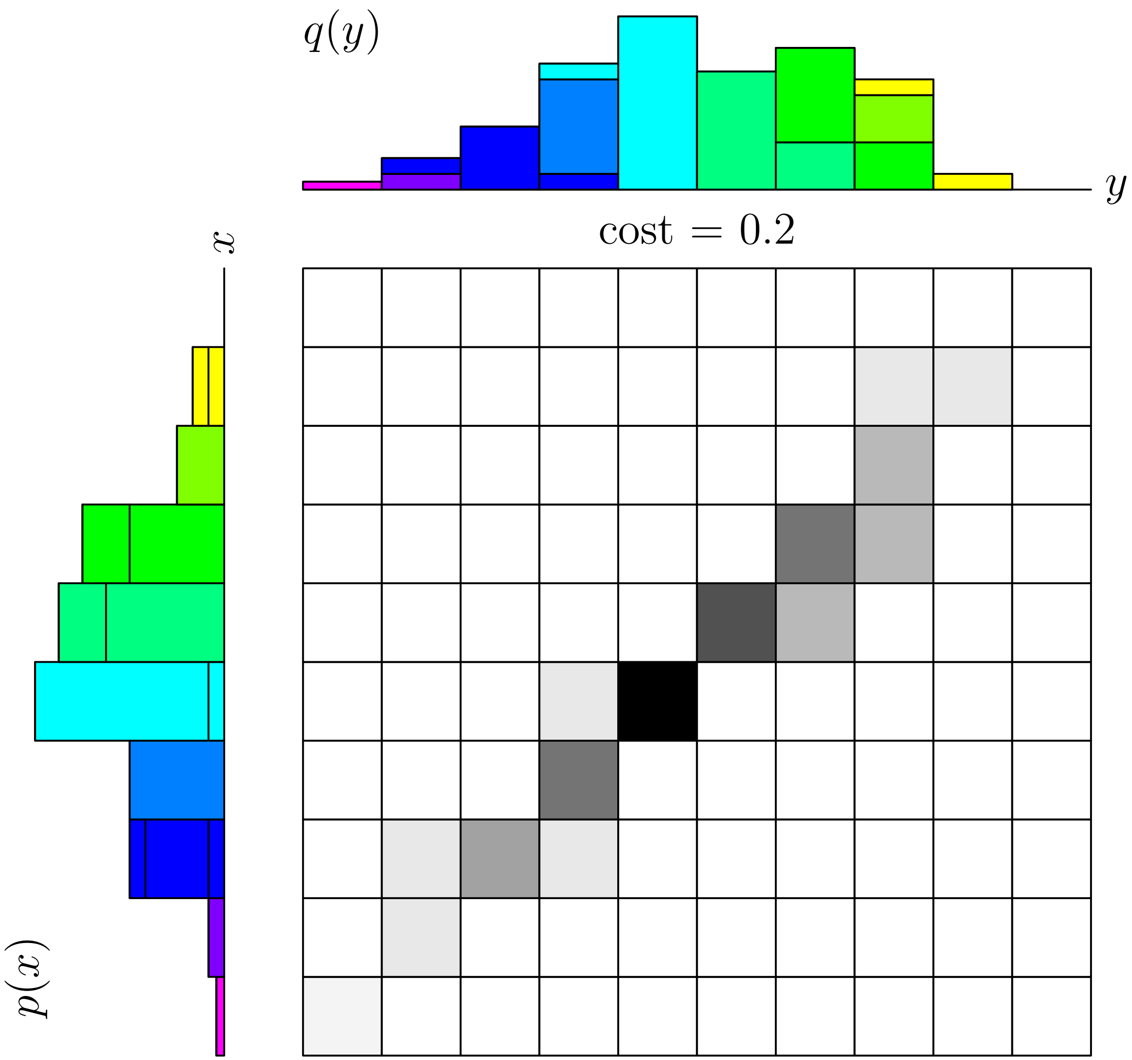

Measuring Distances Between Distributions

- In many machine learning tasks we want to minimise the distance between two probability distributions
- This requires that we can measure distances between probability distributions
- One prominent measure is the Kullback-Leibler or KL divergence

$$\mathrm{KL}(p\|q) = \int p(\boldsymbol{x}) \log\left(\frac{p(\boldsymbol{x})}{q(\boldsymbol{y})}\right) \mathrm{d}\boldsymbol{x}$$

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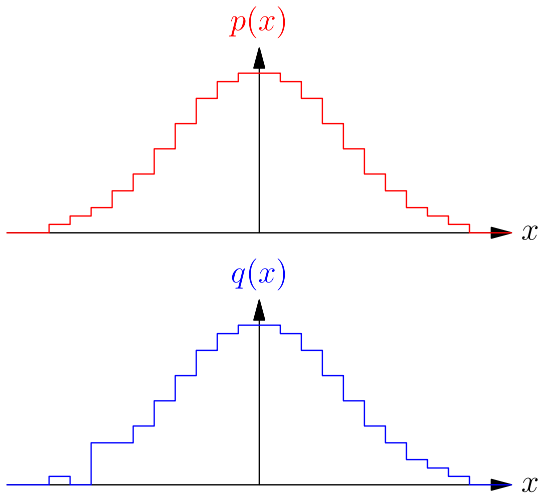
Trouble with KL

- KL-divergences are non-negative quantities that are minimised when the two probability distributions are the same
- They are not distances (they aren't symmetric and they don't satisfy the triangular inequality)
- We don't really care about this, but what we do care about is that if $q(\boldsymbol{x}) = 0$ when $p(\boldsymbol{x}) \neq 0$ then $\log\left(\frac{p(\boldsymbol{x})}{q(\boldsymbol{y})}\right)$ diverges



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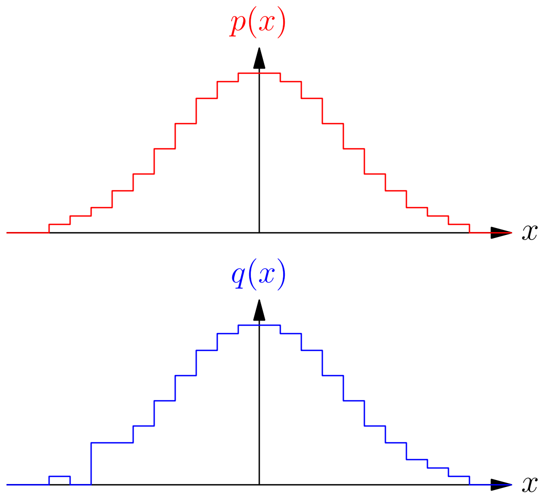

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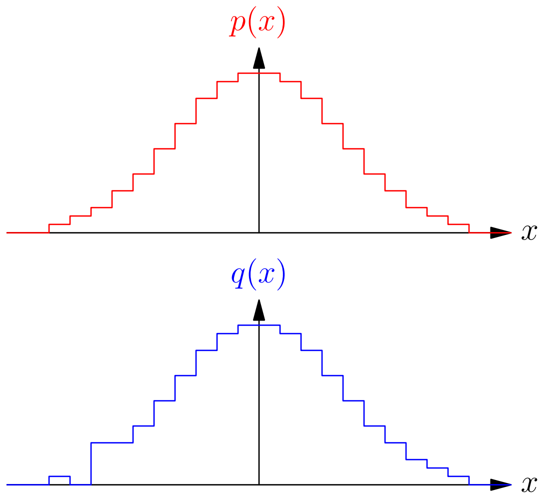

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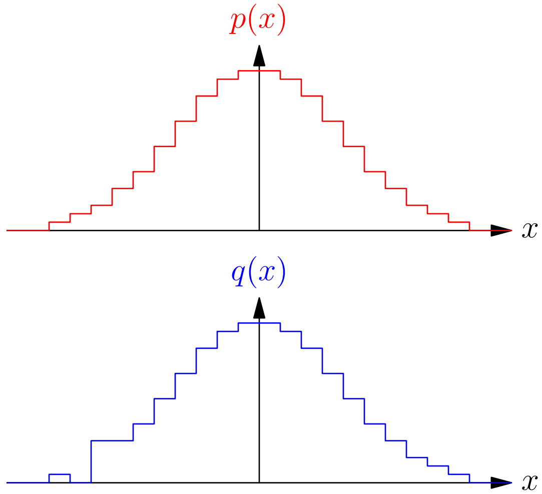

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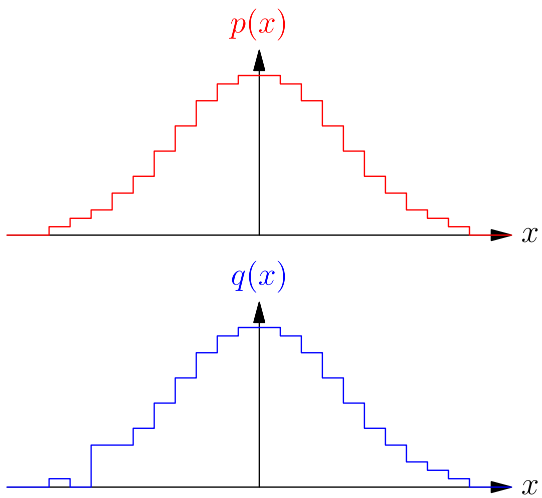
Wasserstein Distance

- A more benign measure of the differences between two probability functions is the **Wasserstein** or **Earth Moving** distance

- This is a true distance, but more importantly for us it measure distance in a very natural way so that distributions that are close has a small Wasserstein distance



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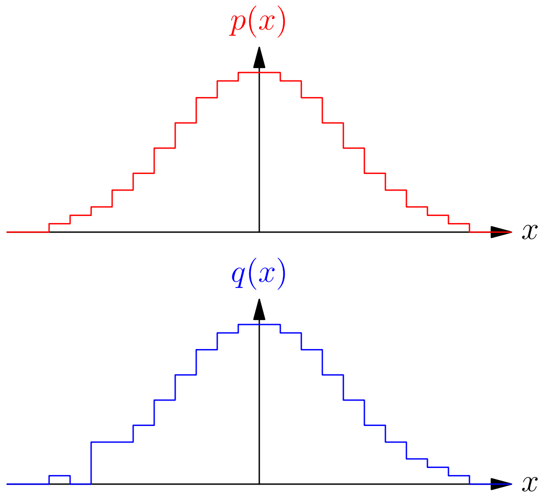

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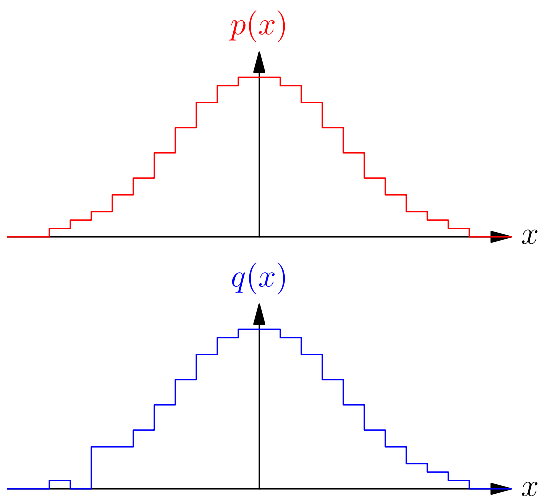

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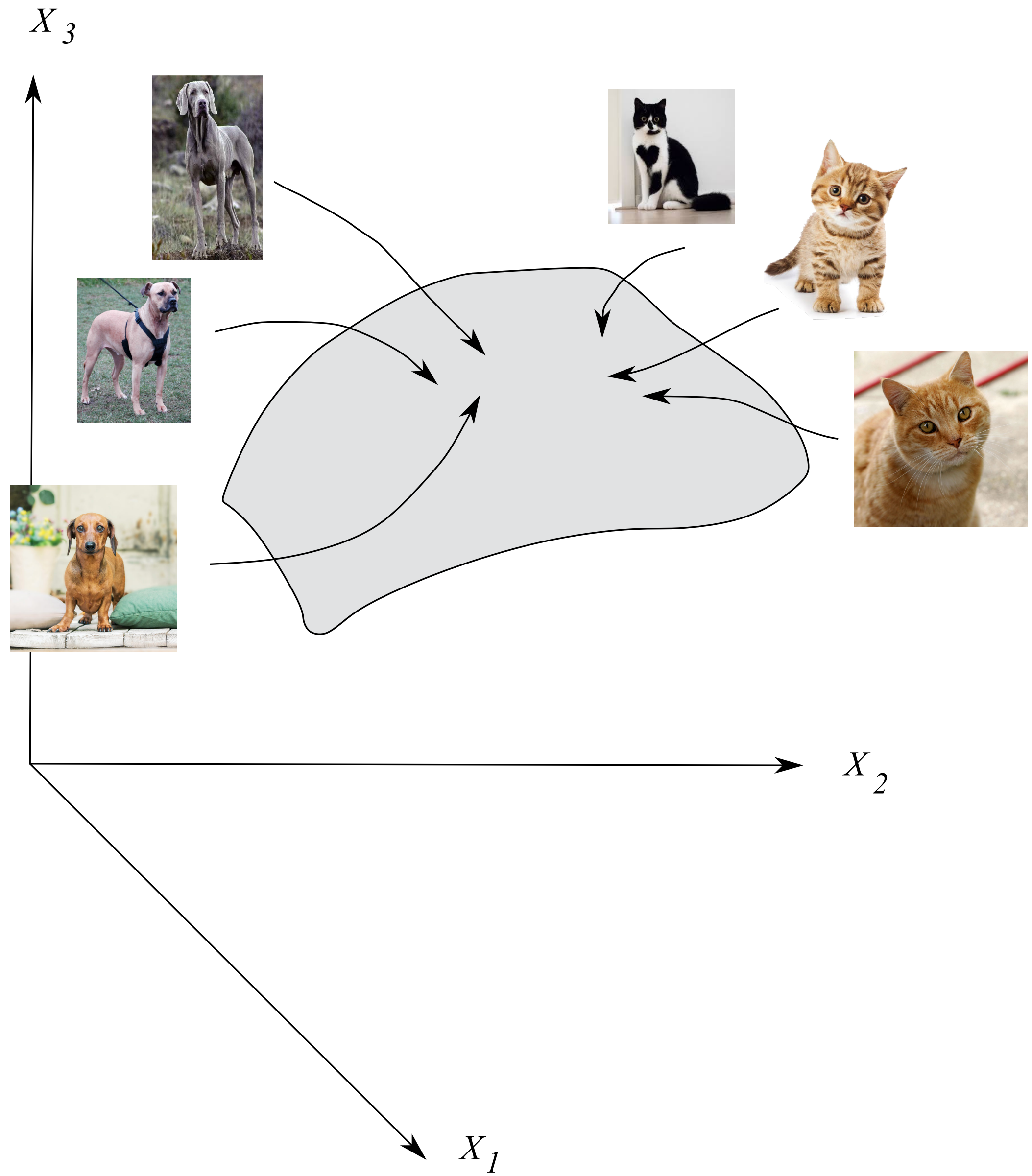
High Probability Manifold



Transportion Policy

- But how do we formalise the Wasserstein distance?
- A good place to start is to define a transportation policy $\gamma(\boldsymbol{x}, \boldsymbol{y})$ with

$$\int \gamma(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{y} = p(\boldsymbol{x}) \qquad \int \gamma(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{x} = q(\boldsymbol{y})$$

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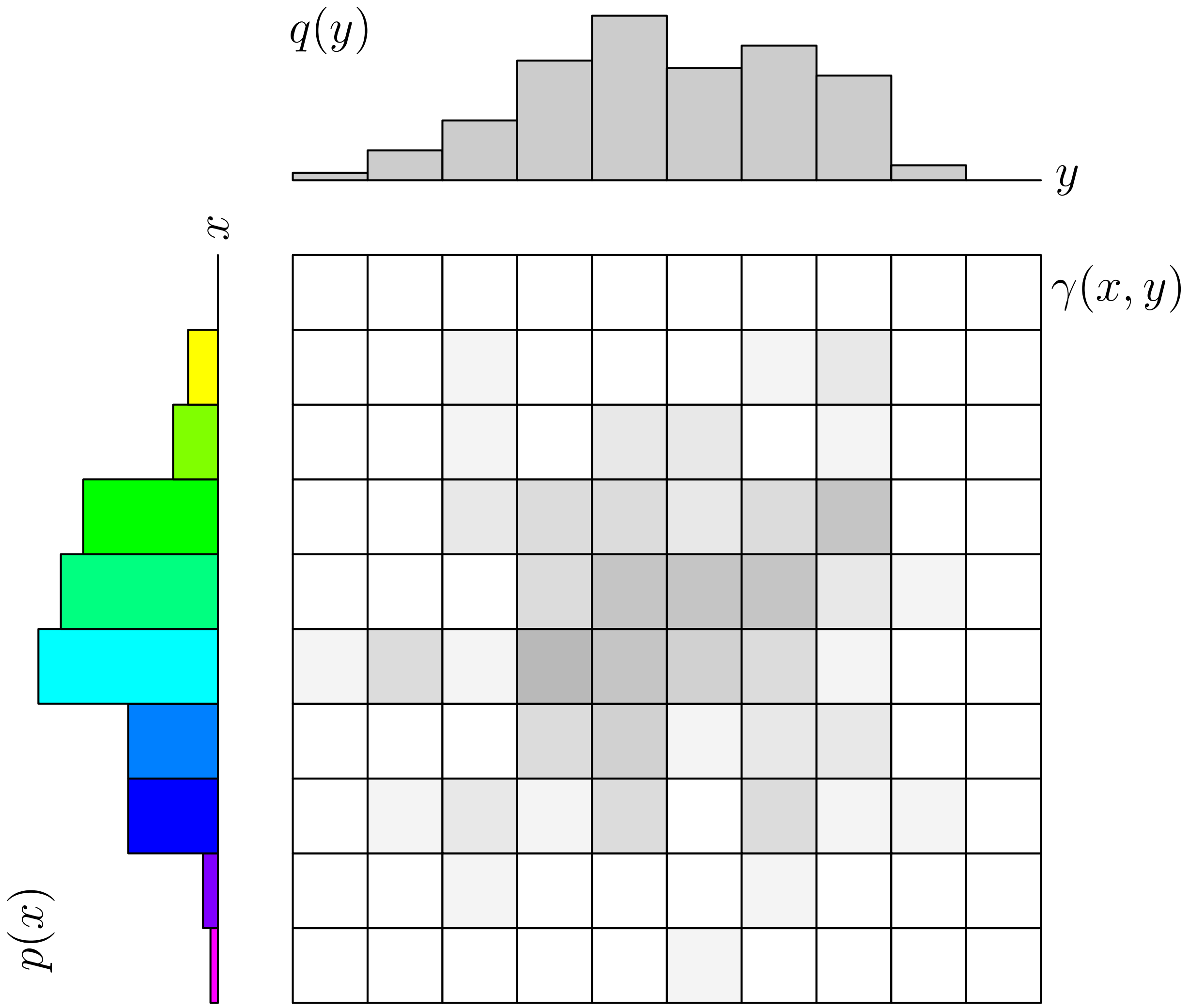

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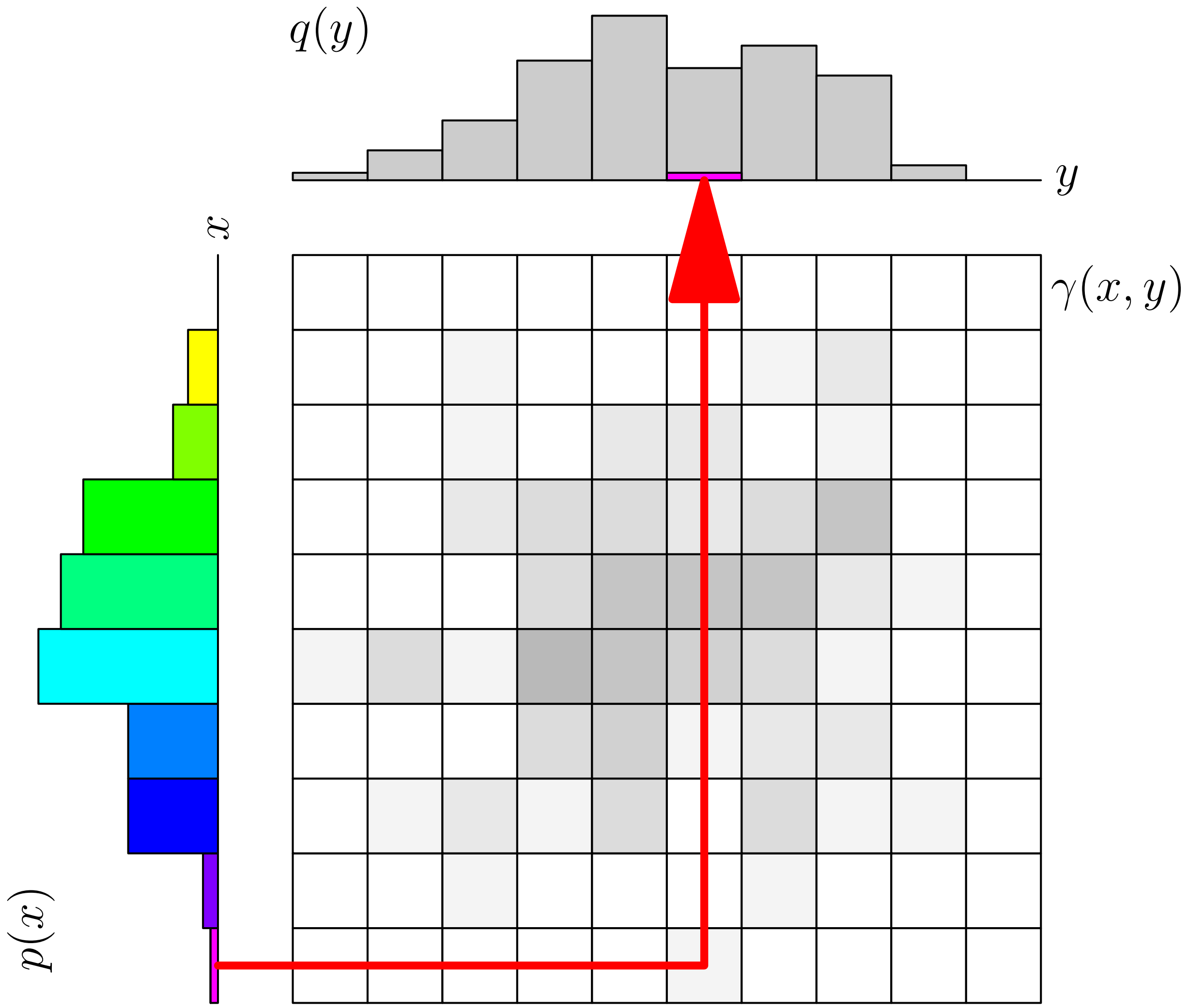

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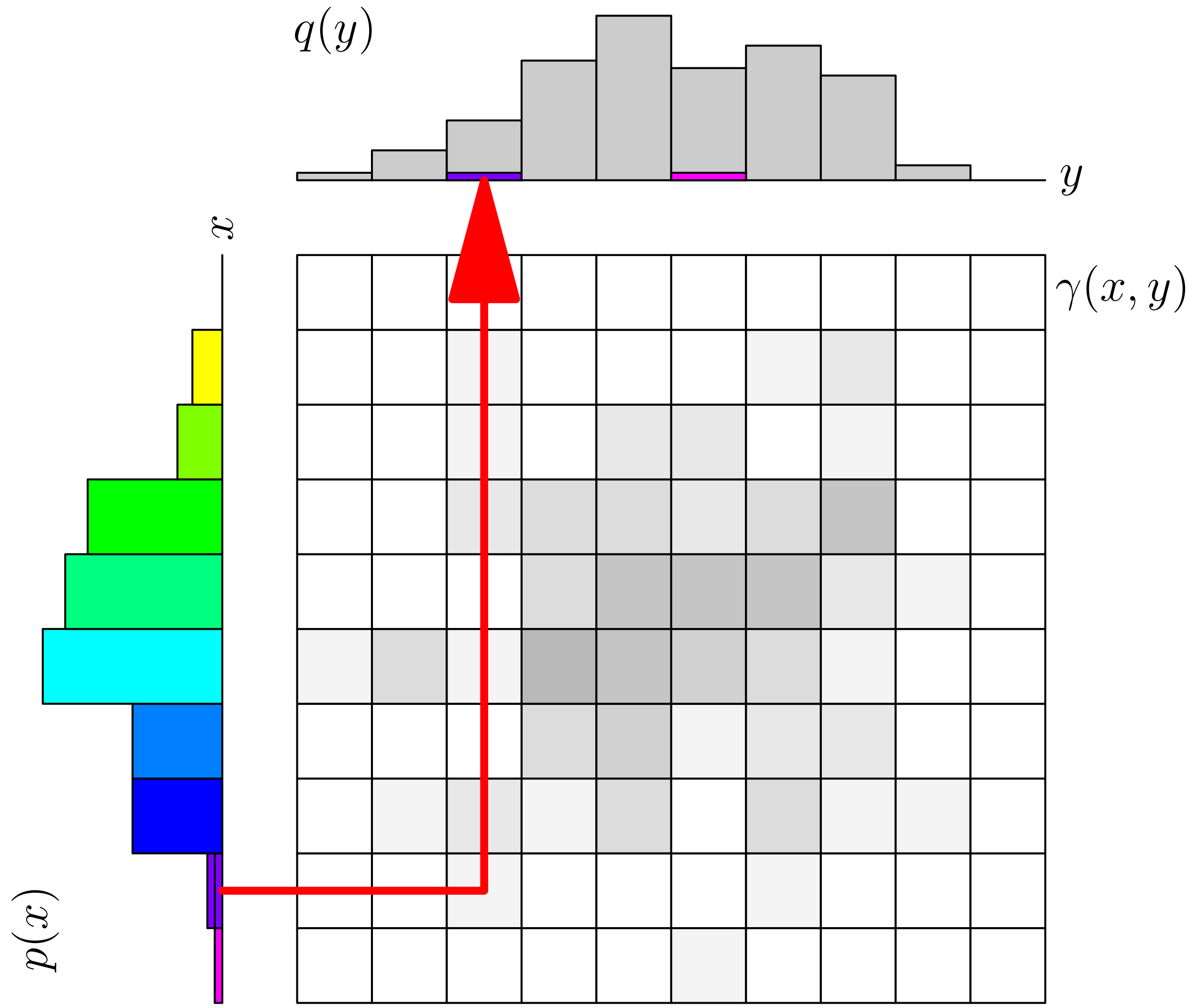

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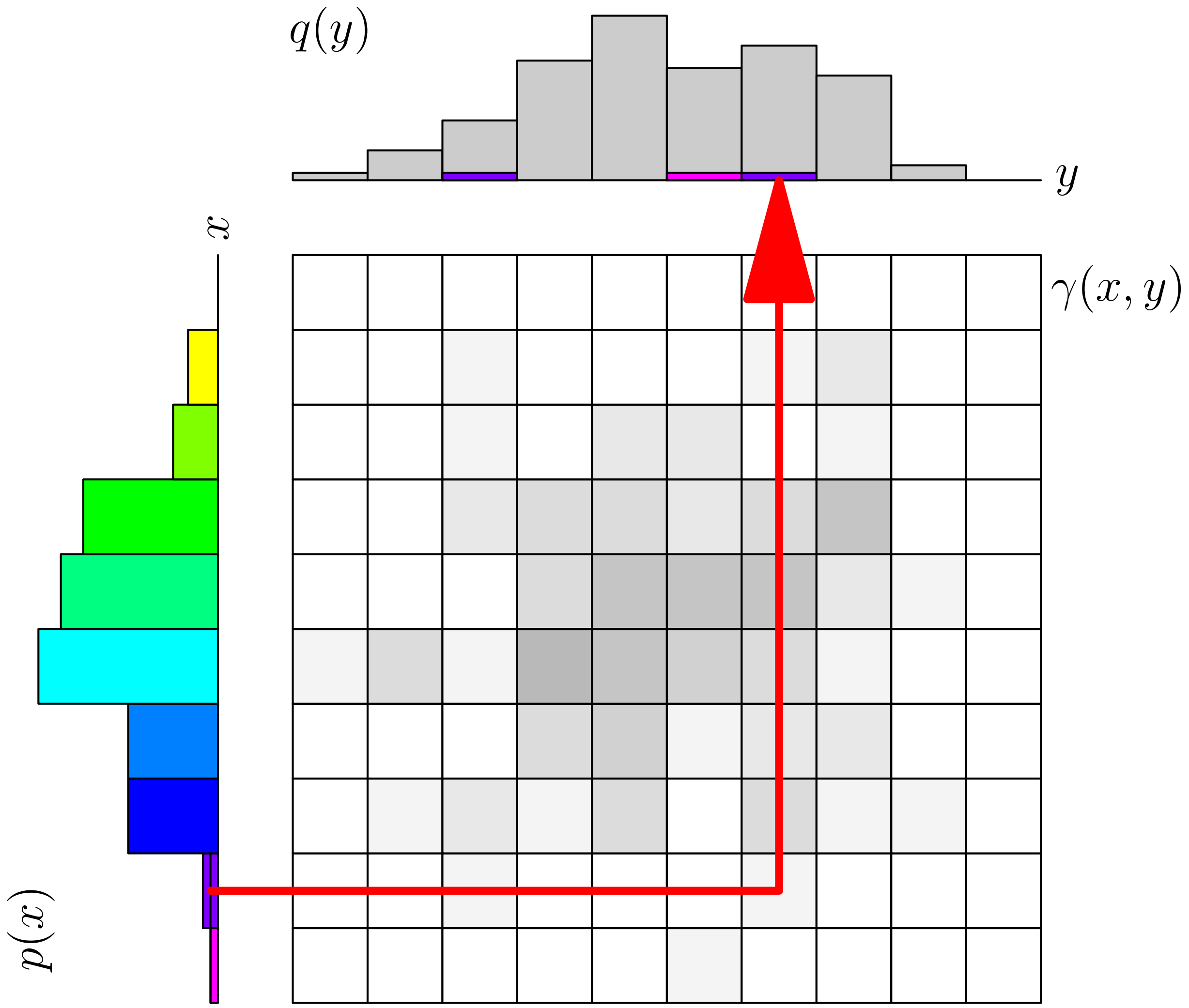

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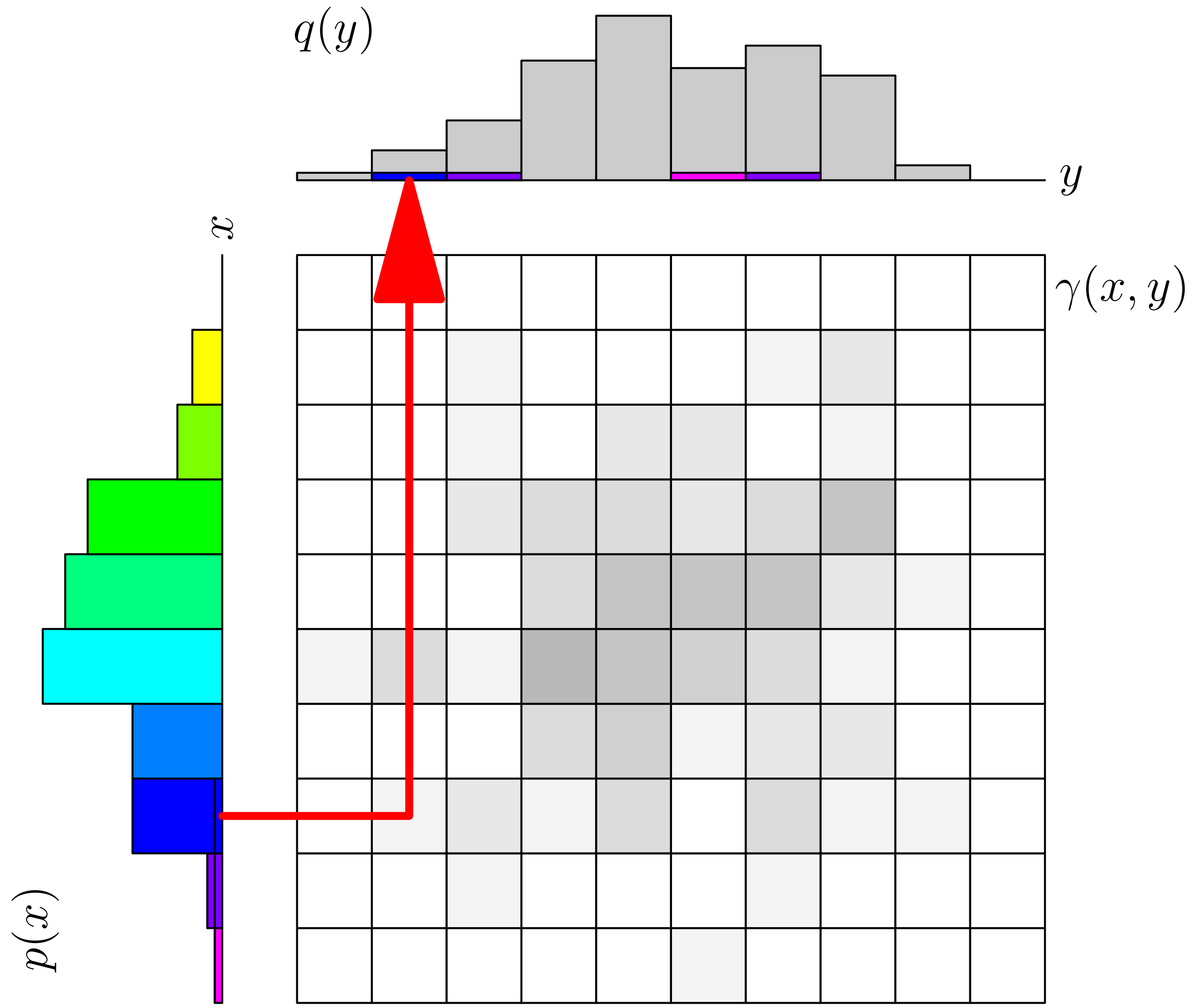

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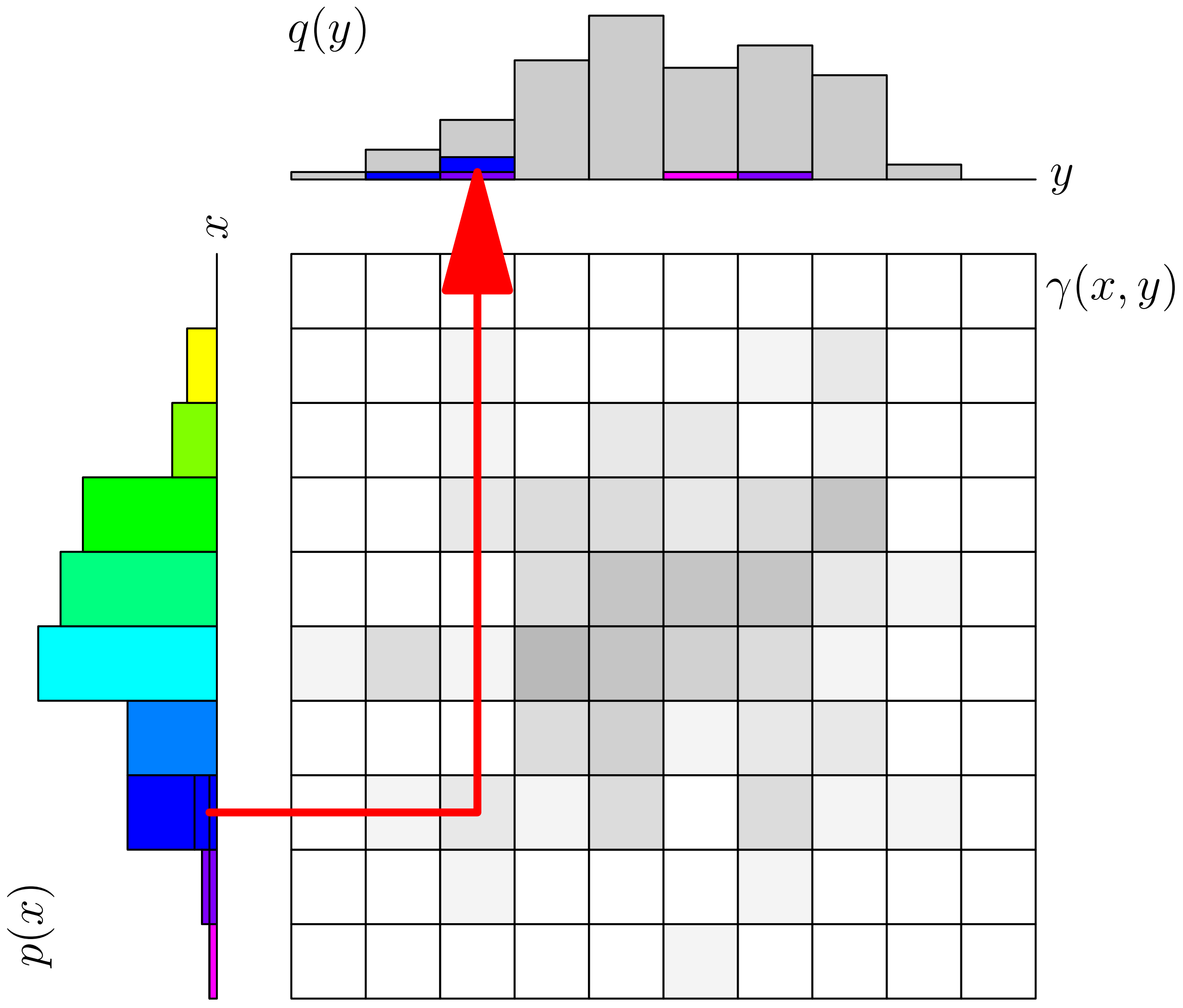

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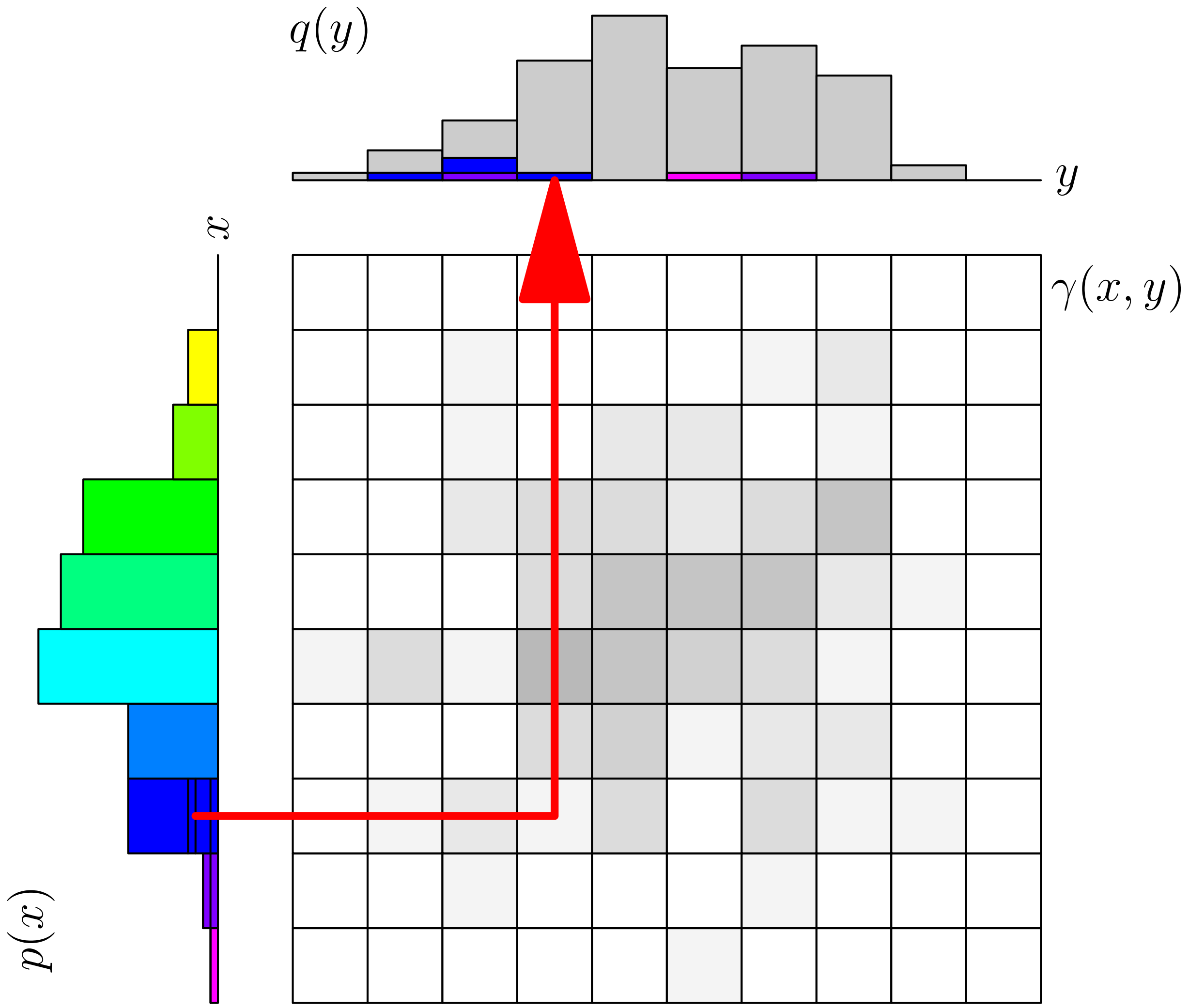

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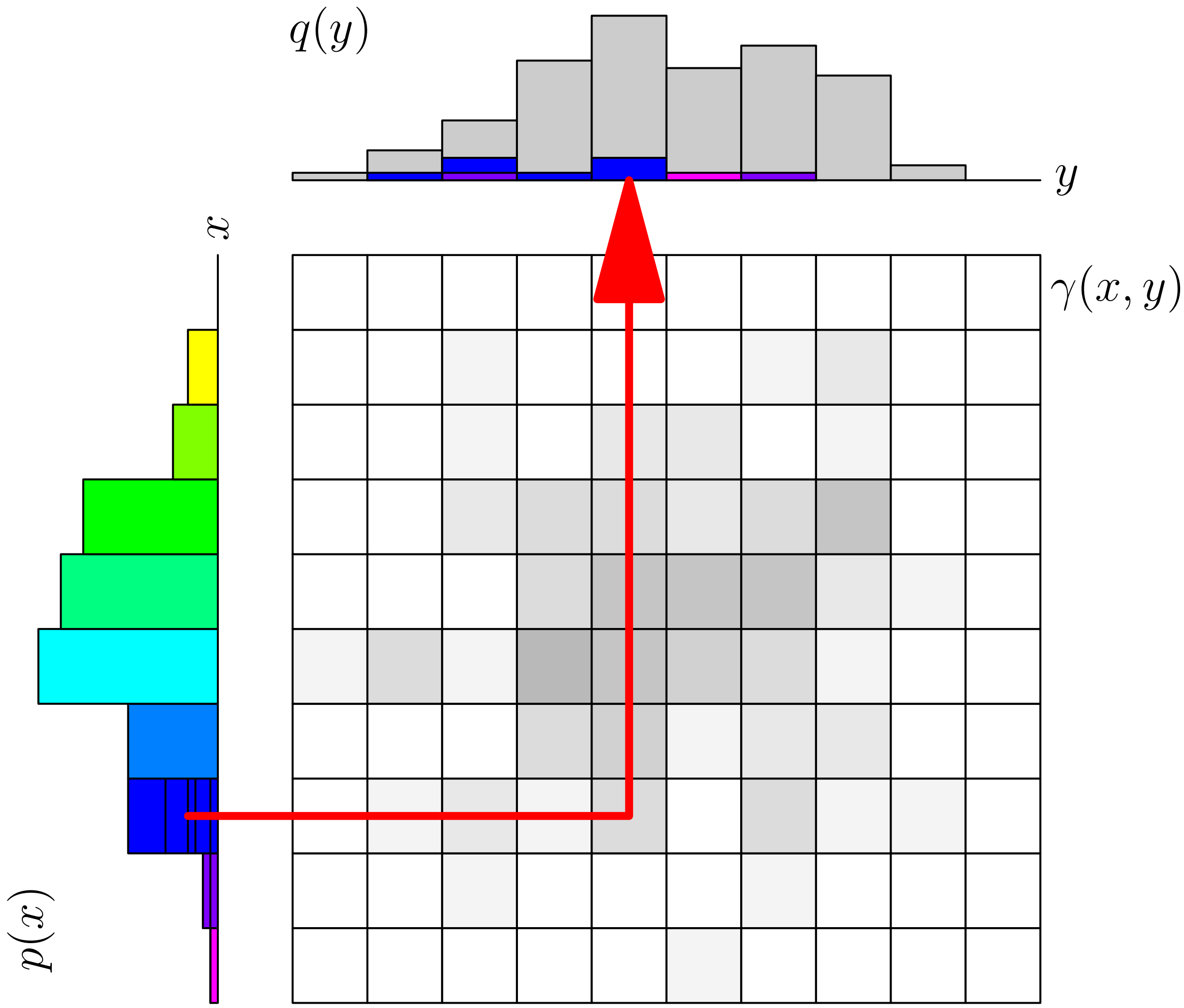

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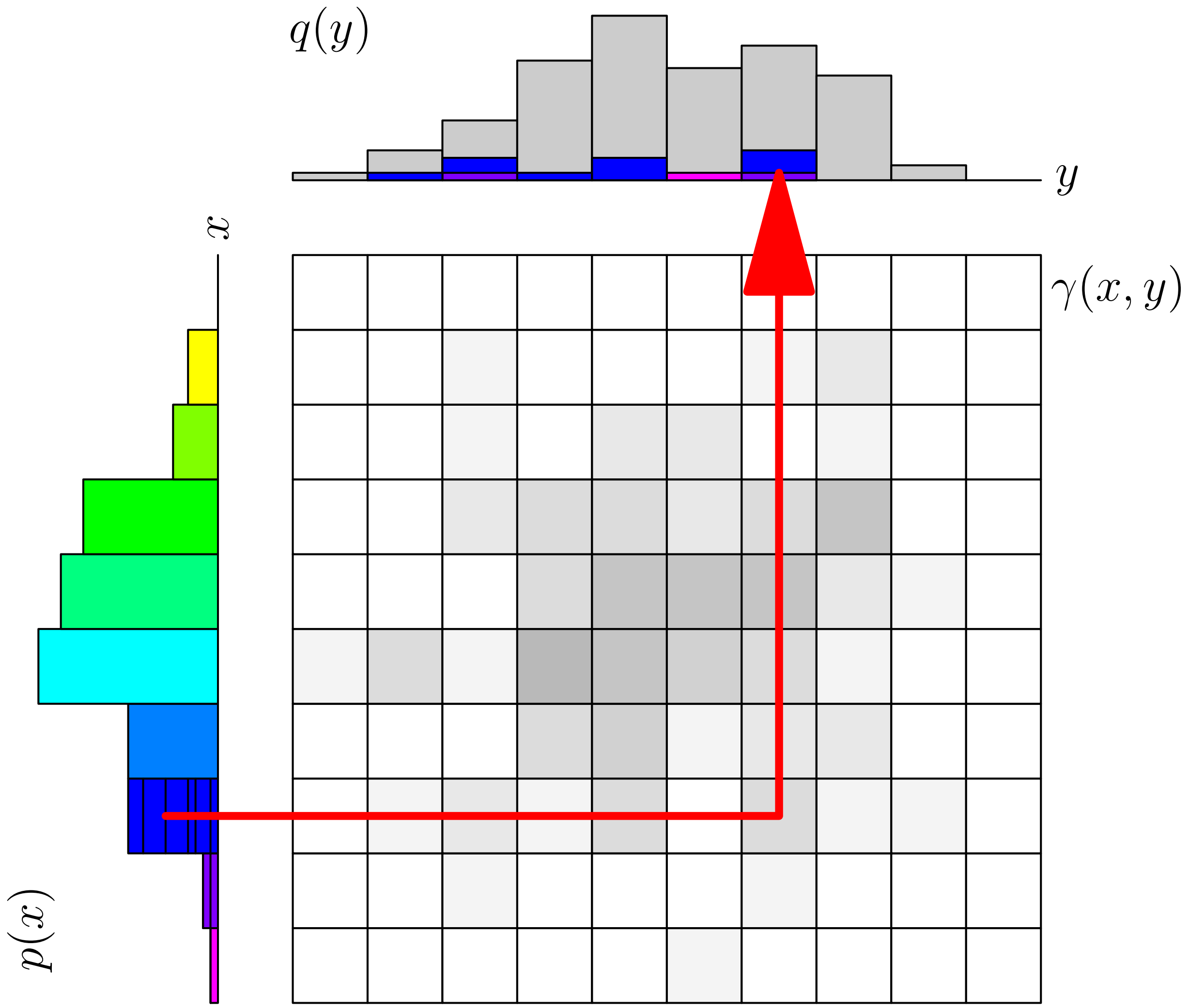

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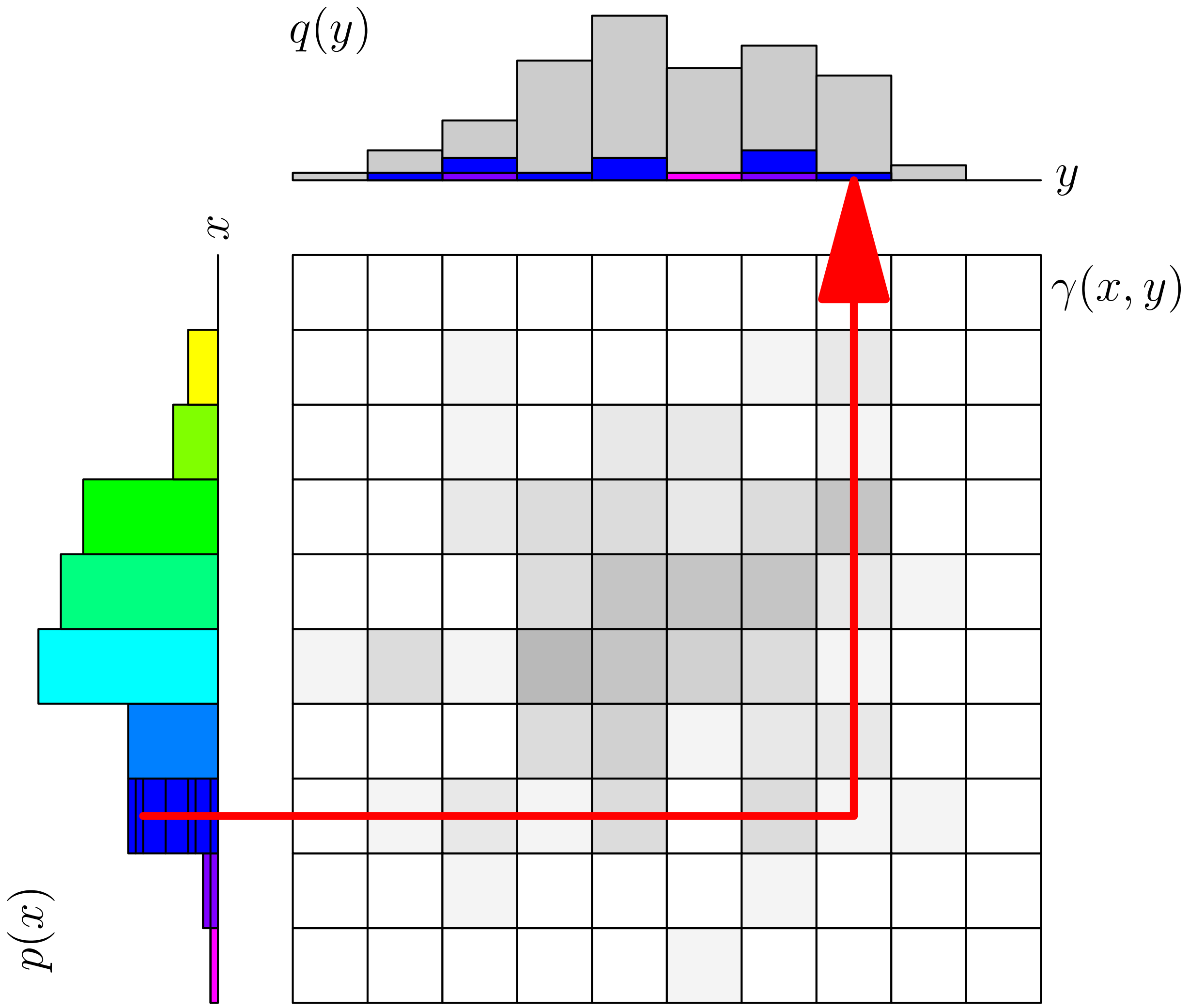

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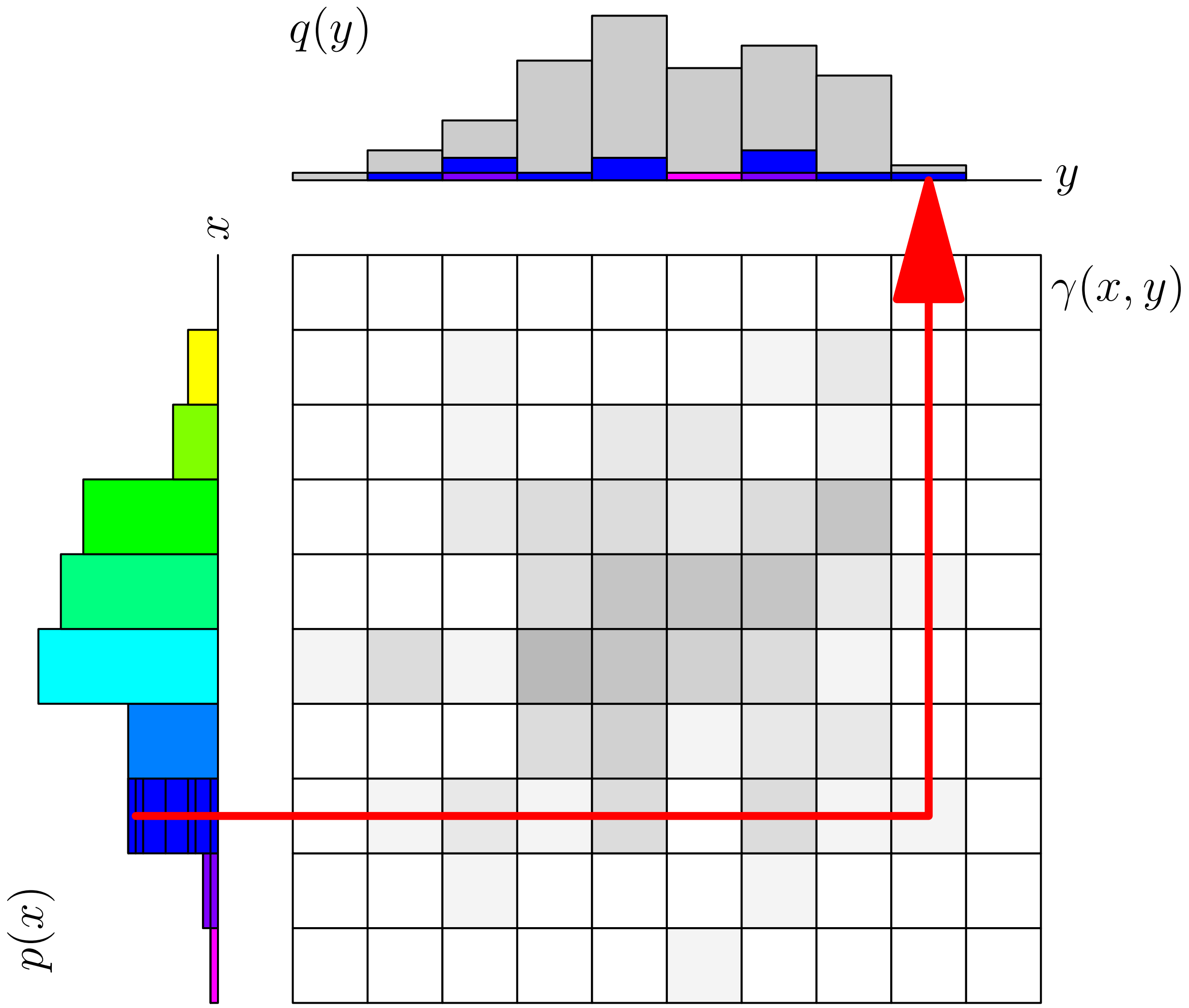

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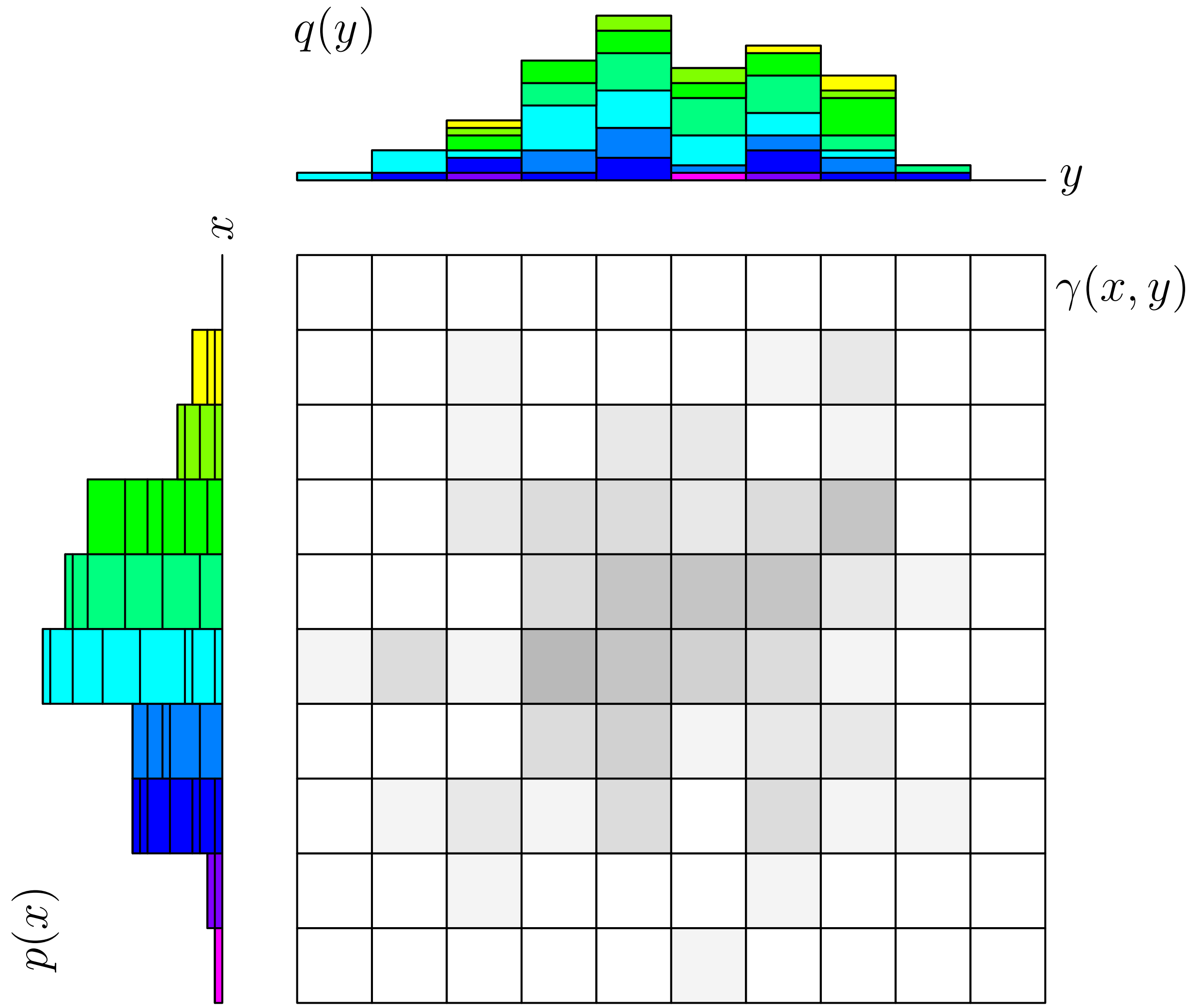

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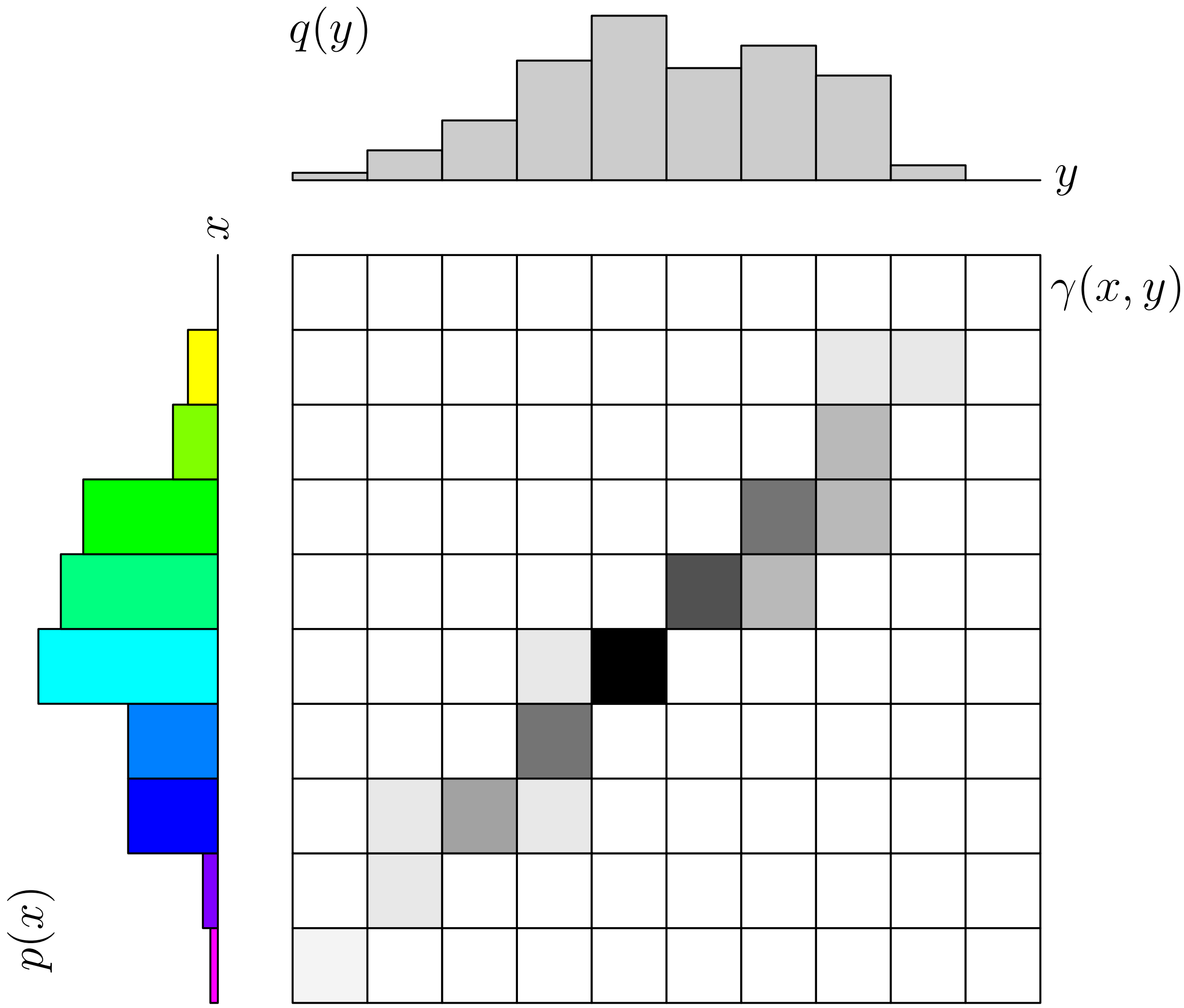

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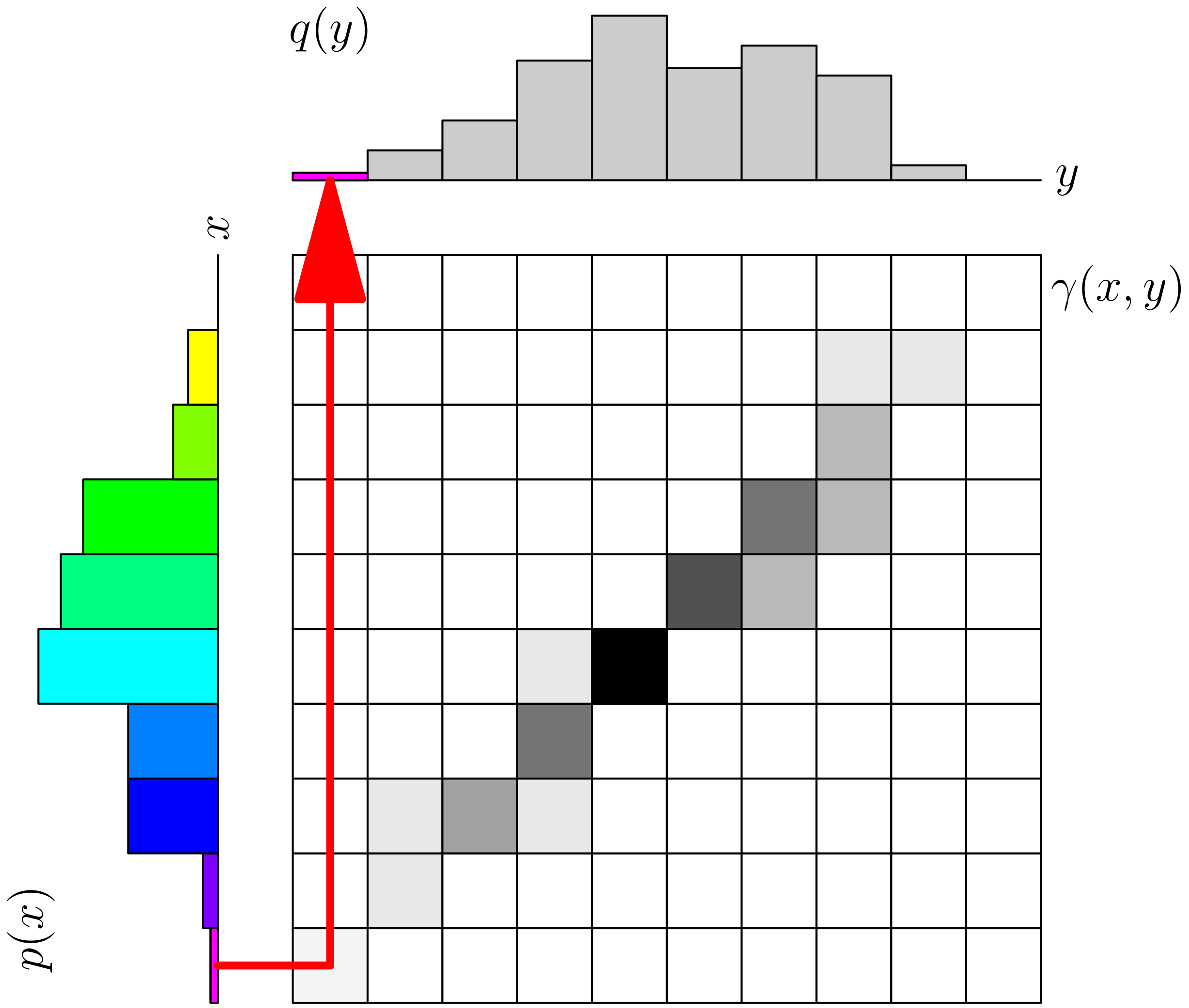

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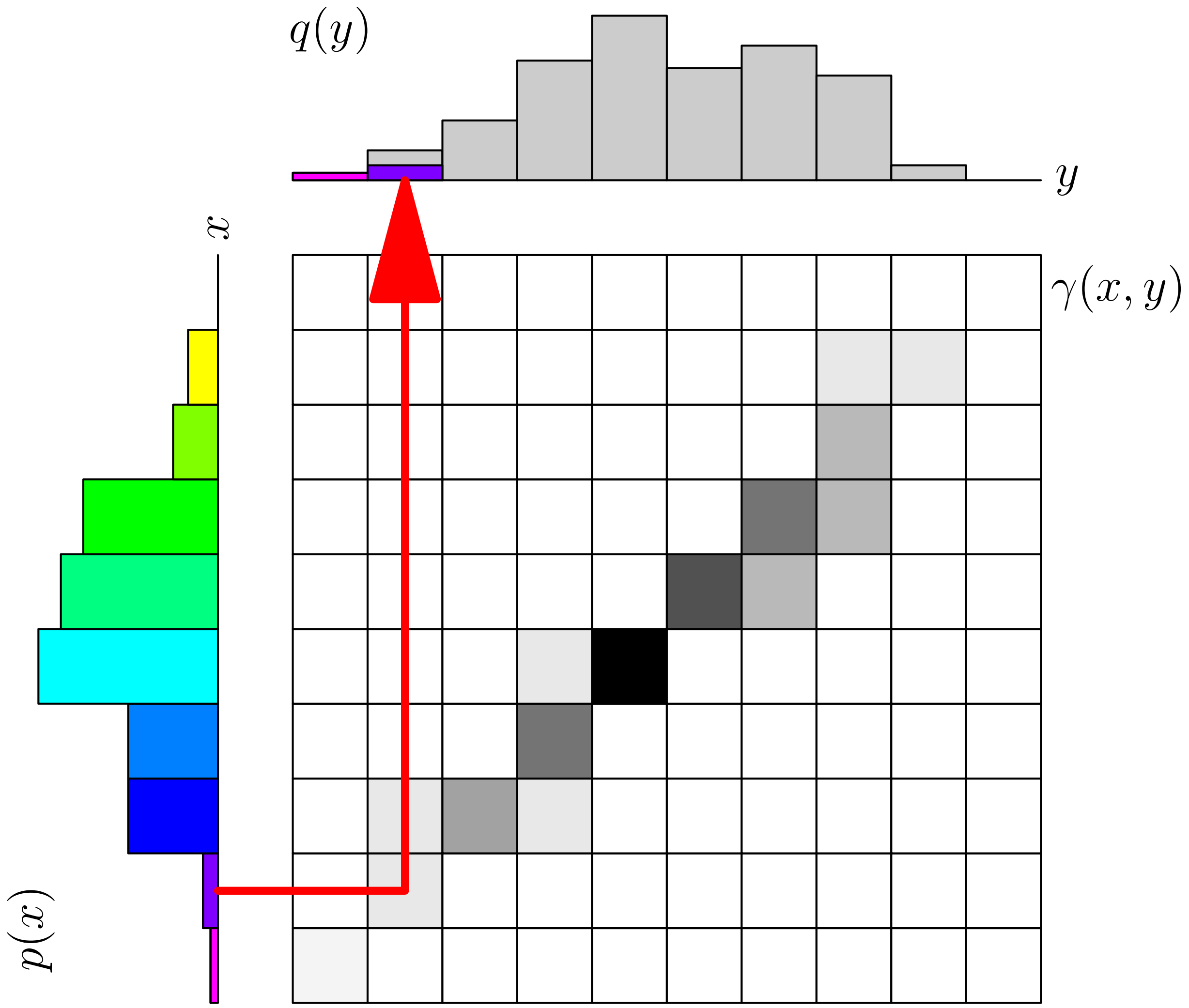

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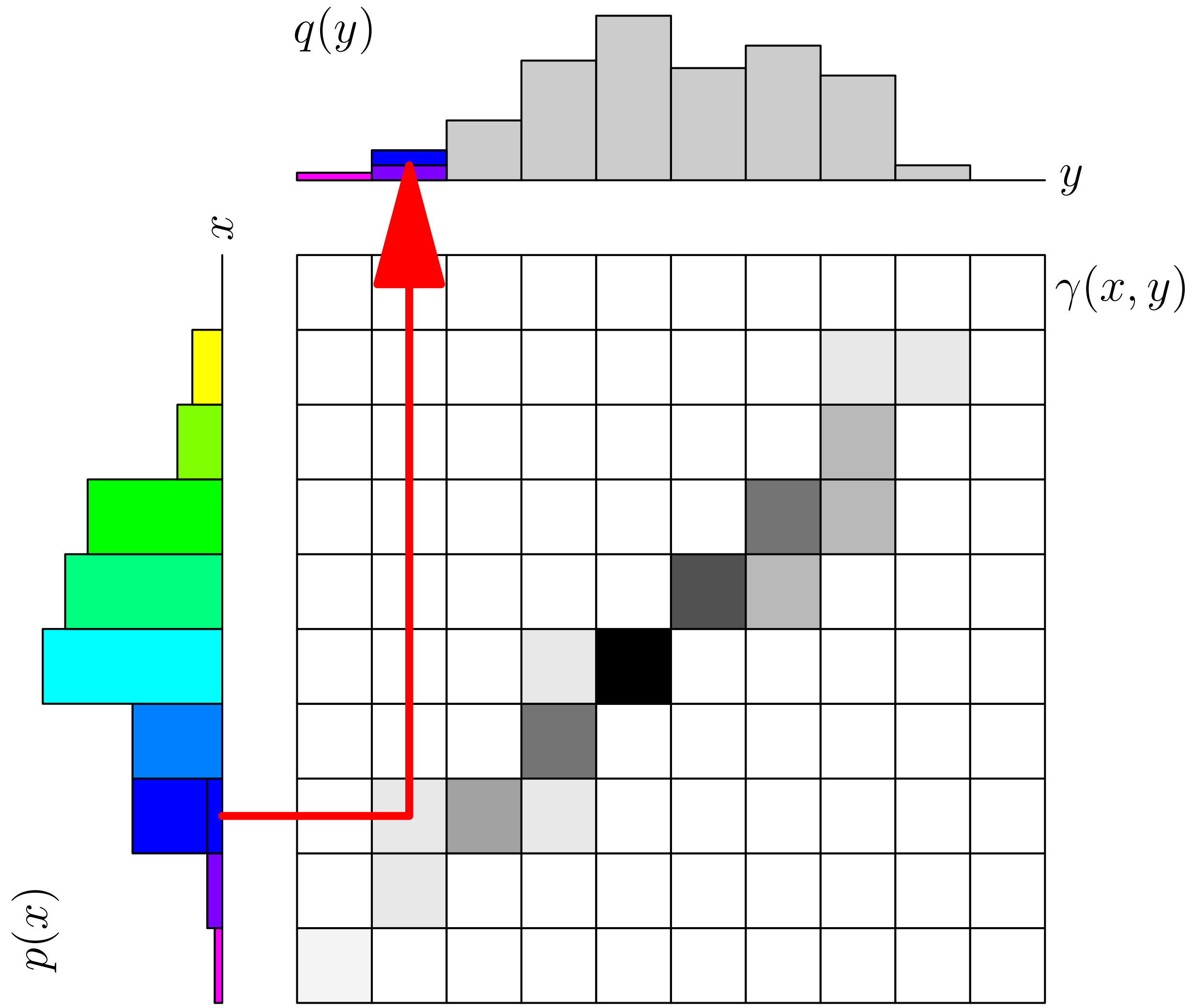

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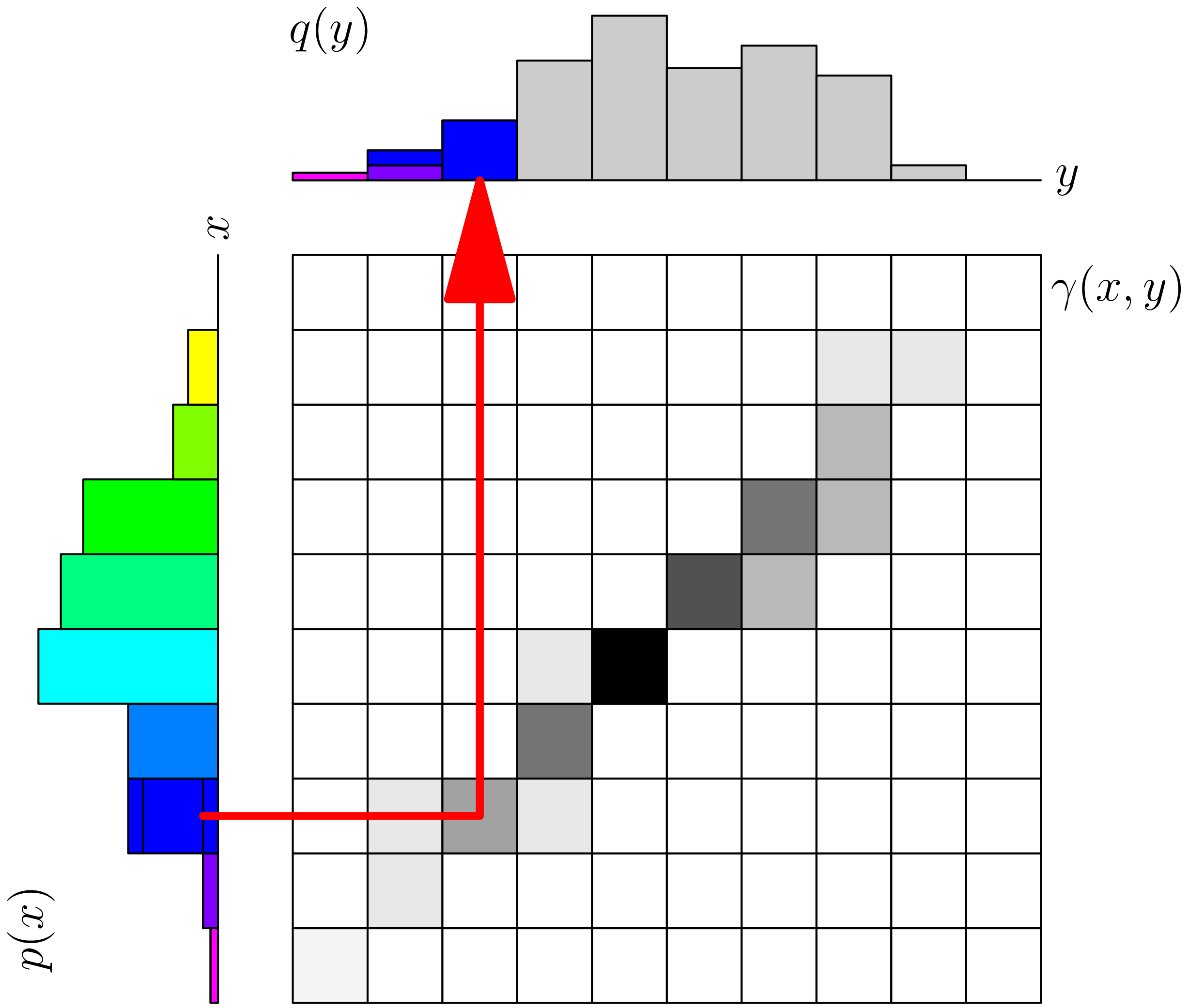

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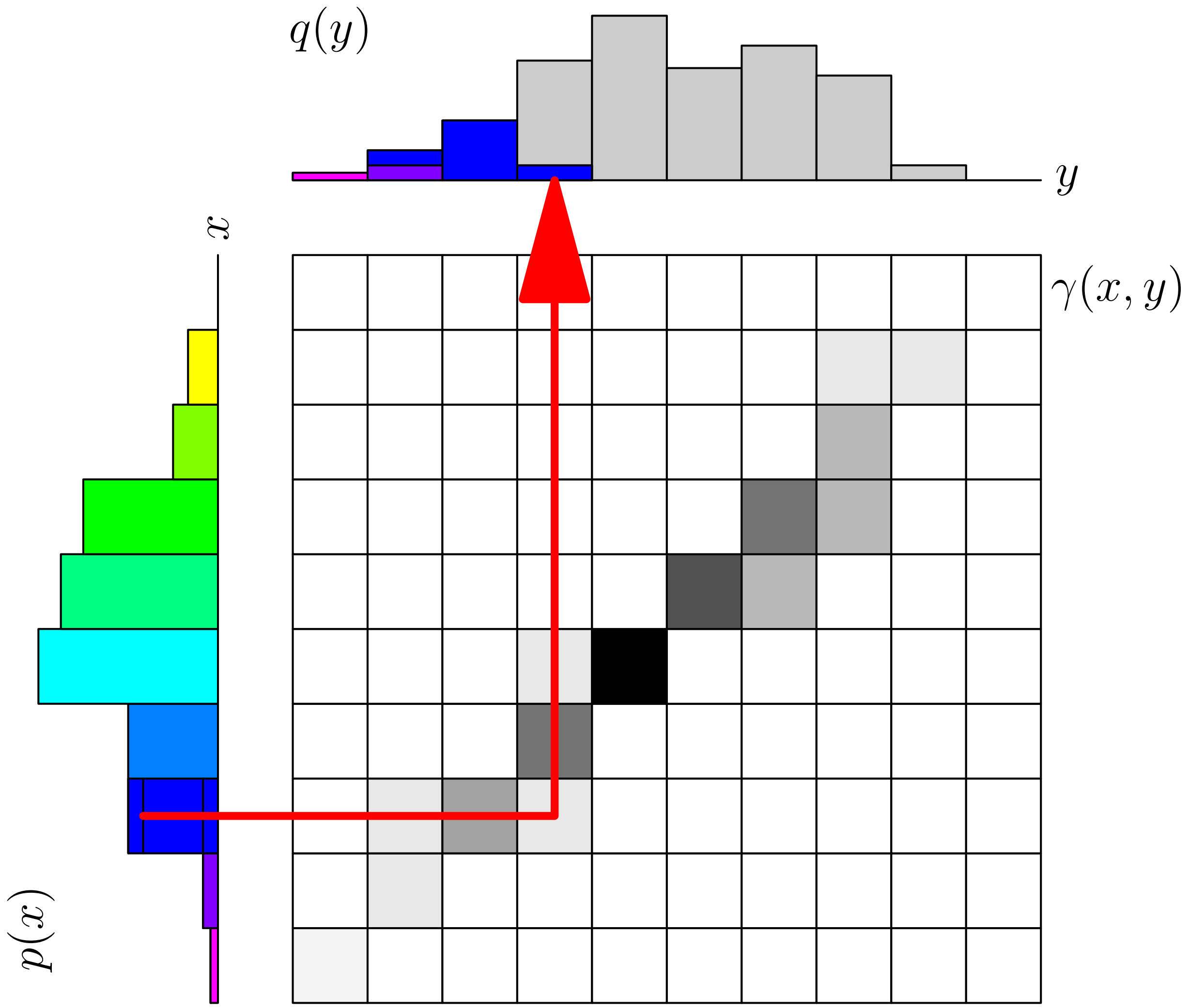

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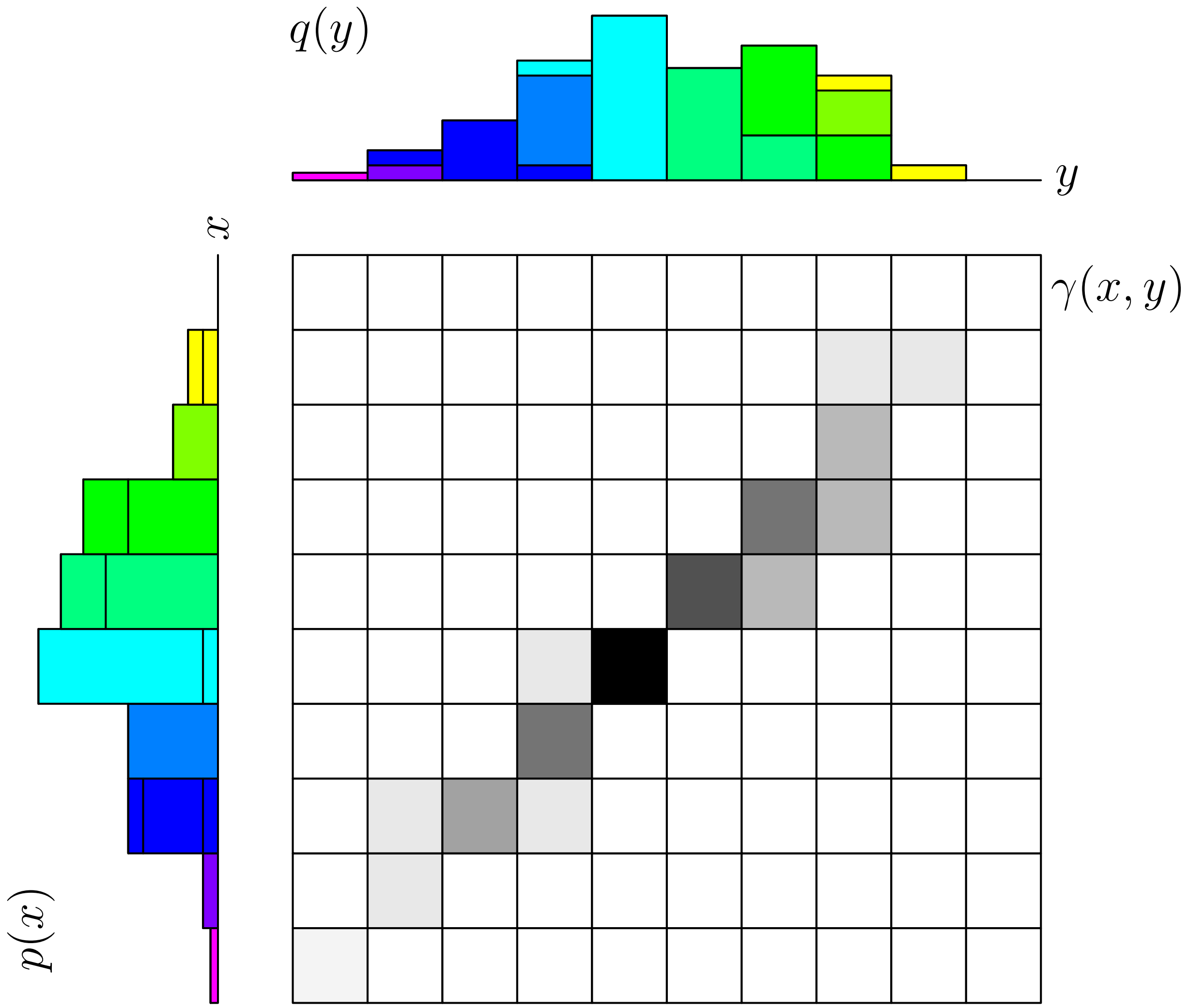

The Cost of Transport

- We want to choose the transportation policy that minimises the amount of probability mass we need to move
- Let $d(\boldsymbol{x},\boldsymbol{y}) = \|\boldsymbol{x}-\boldsymbol{y}\|$ be a distance measure then the cost of a transportation policy is

$$C(\gamma) = \int\int d(\boldsymbol{x},\boldsymbol{y})\gamma(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y}$$

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$$C(\gamma) = \int\int d(\boldsymbol{x}, \boldsymbol{y}) \gamma(\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}\boldsymbol{x} \mathrm{d}\boldsymbol{y} = \mathbb{E}_{\gamma}[d(\boldsymbol{x}, \boldsymbol{y})]$$

  where we interpret $\gamma(\boldsymbol{x}, \boldsymbol{y})$ as a probability distribution

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- We want to choose the transportation policy that minimises the amount of probability mass we need to move
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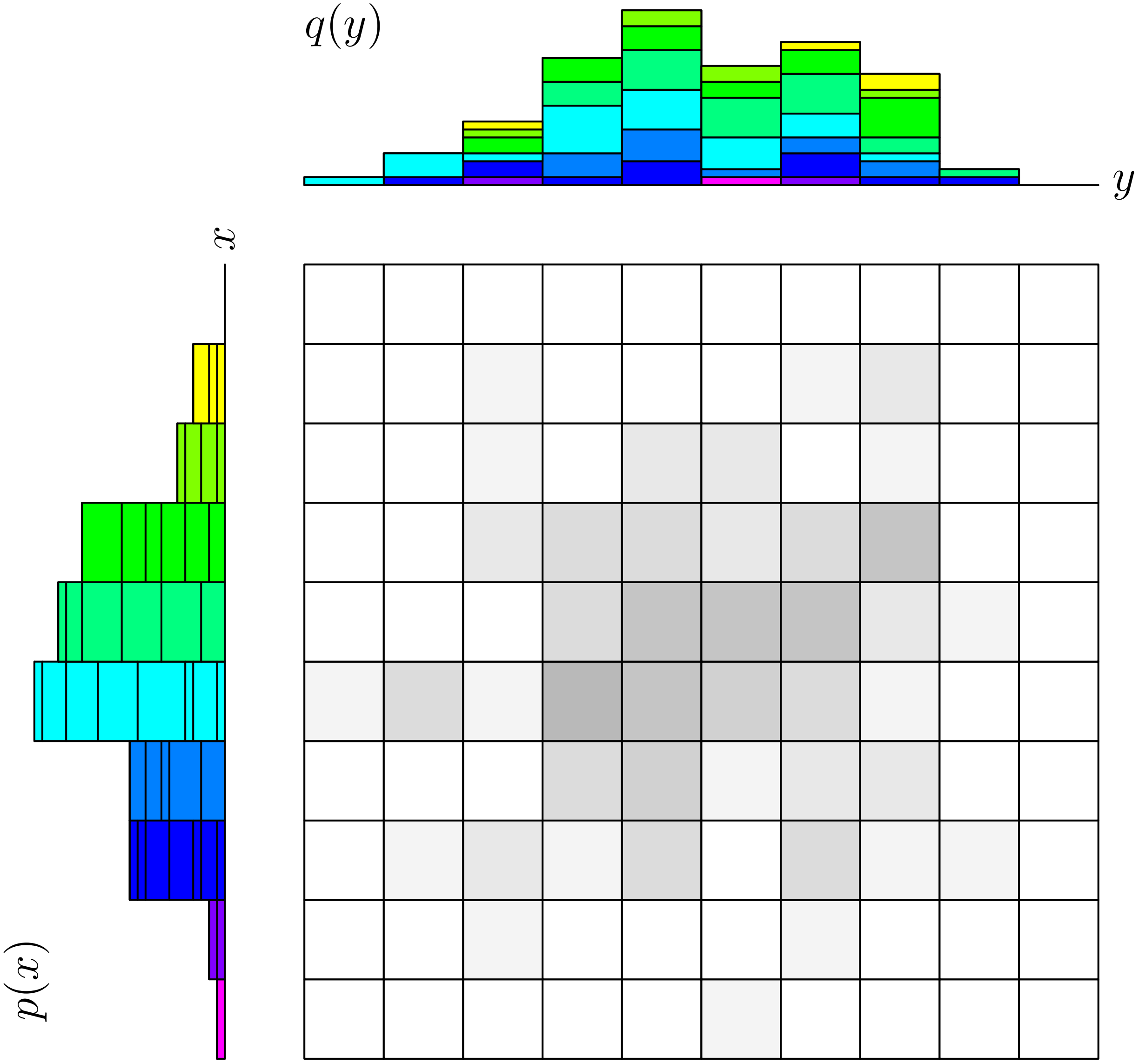
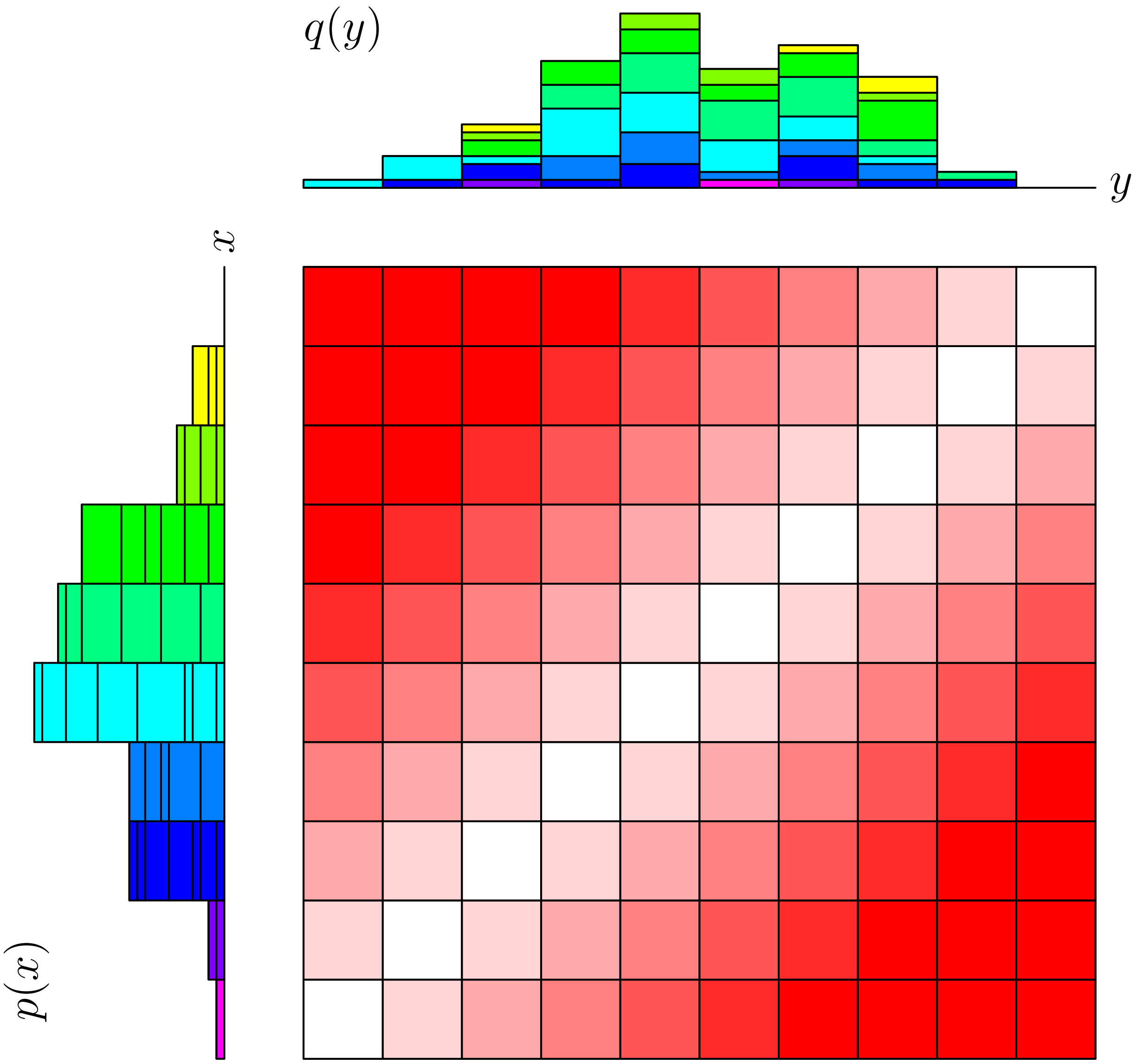
$$C(\gamma) = \int\int d(\boldsymbol{x},\boldsymbol{y})\gamma(\boldsymbol{x},\boldsymbol{y})\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} = \mathbb{E}_{\gamma}[d(\boldsymbol{x},\boldsymbol{y})]$$

  where we interpret $\gamma(\boldsymbol{x},\boldsymbol{y})$ as a probability distribution
- Usually we take $d(\boldsymbol{x},\boldsymbol{y})$ to be the Euclidean distance, but we can choose any distance

Transportation Cost



Transportation Cost



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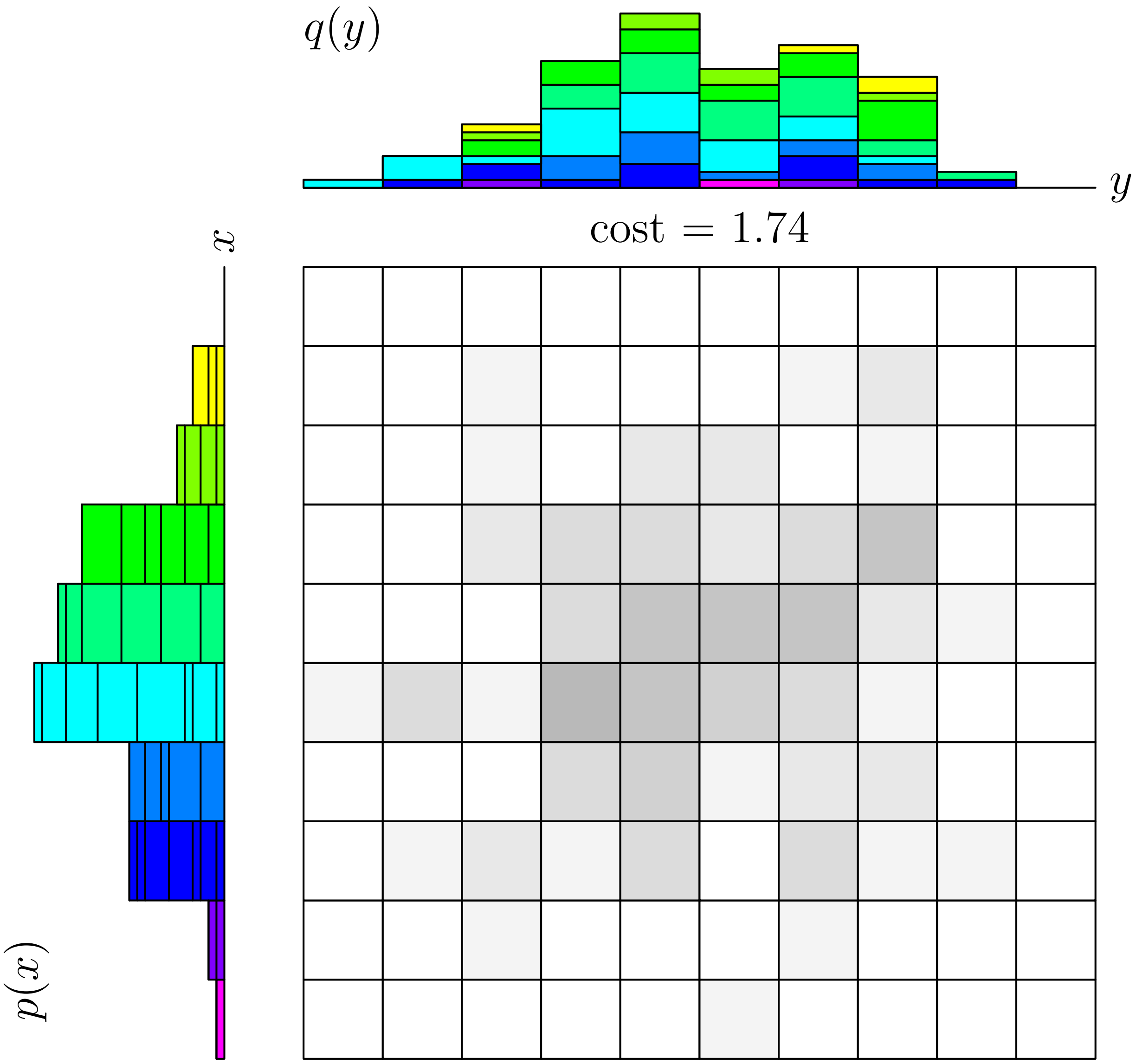

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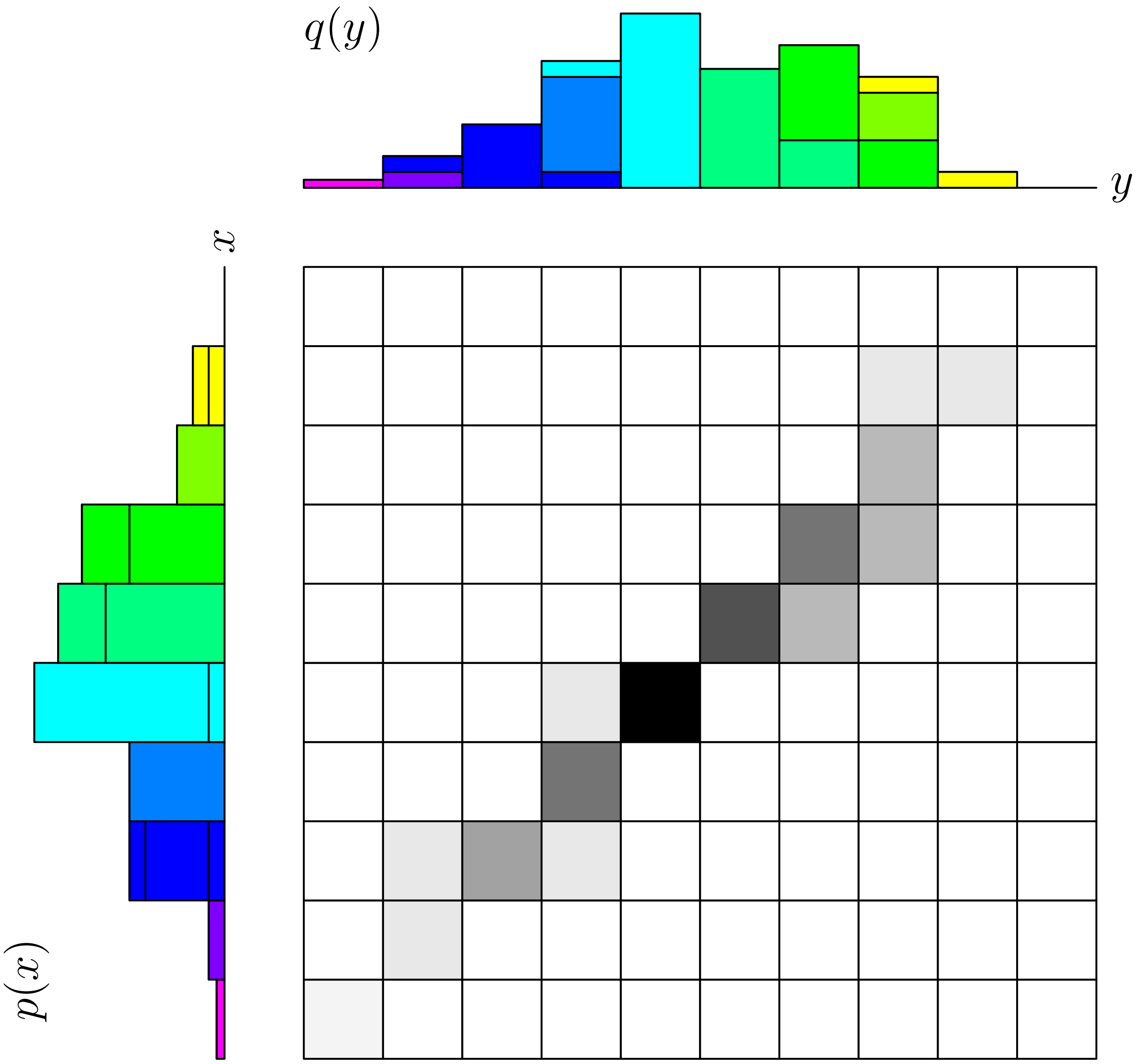

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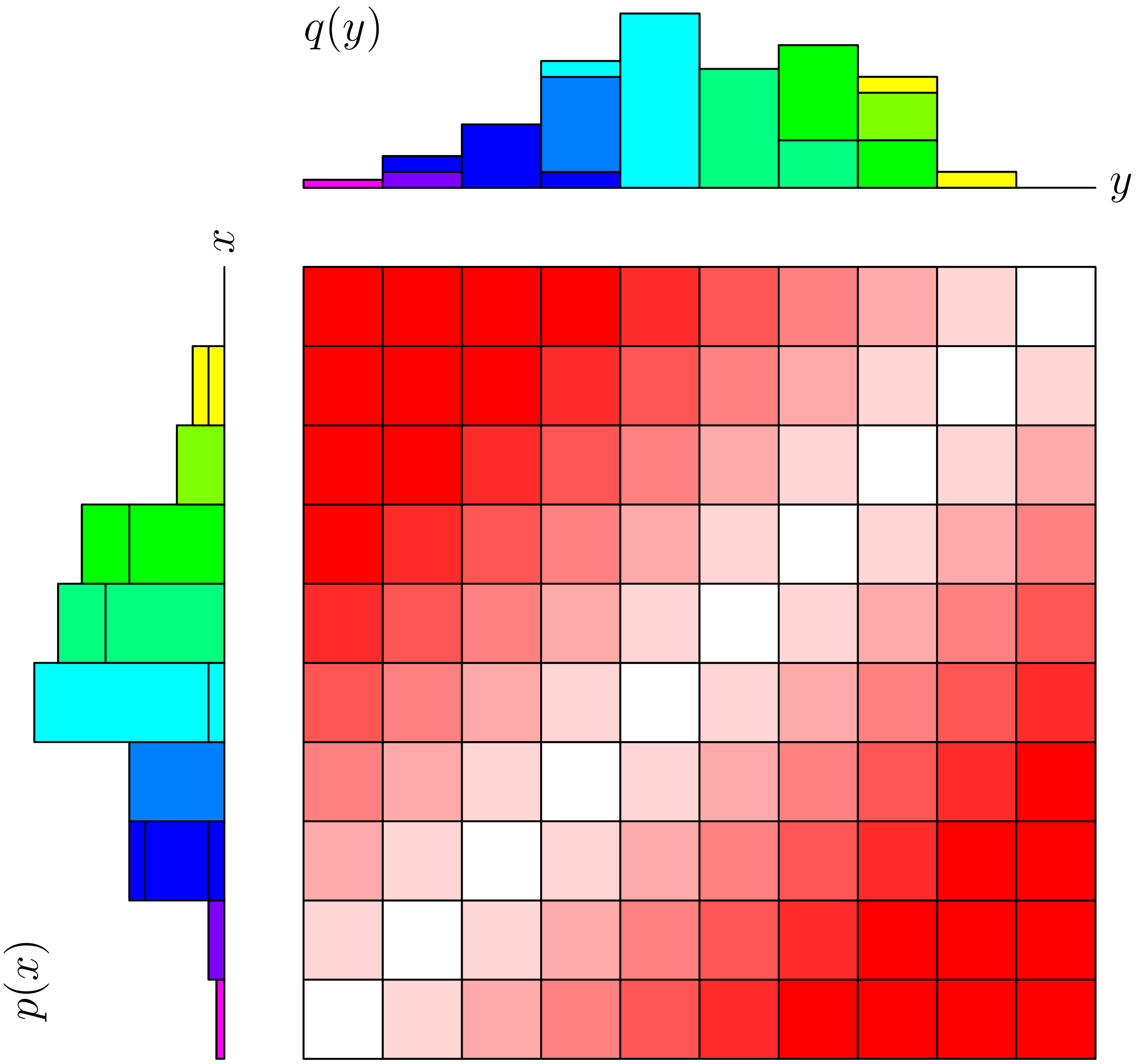

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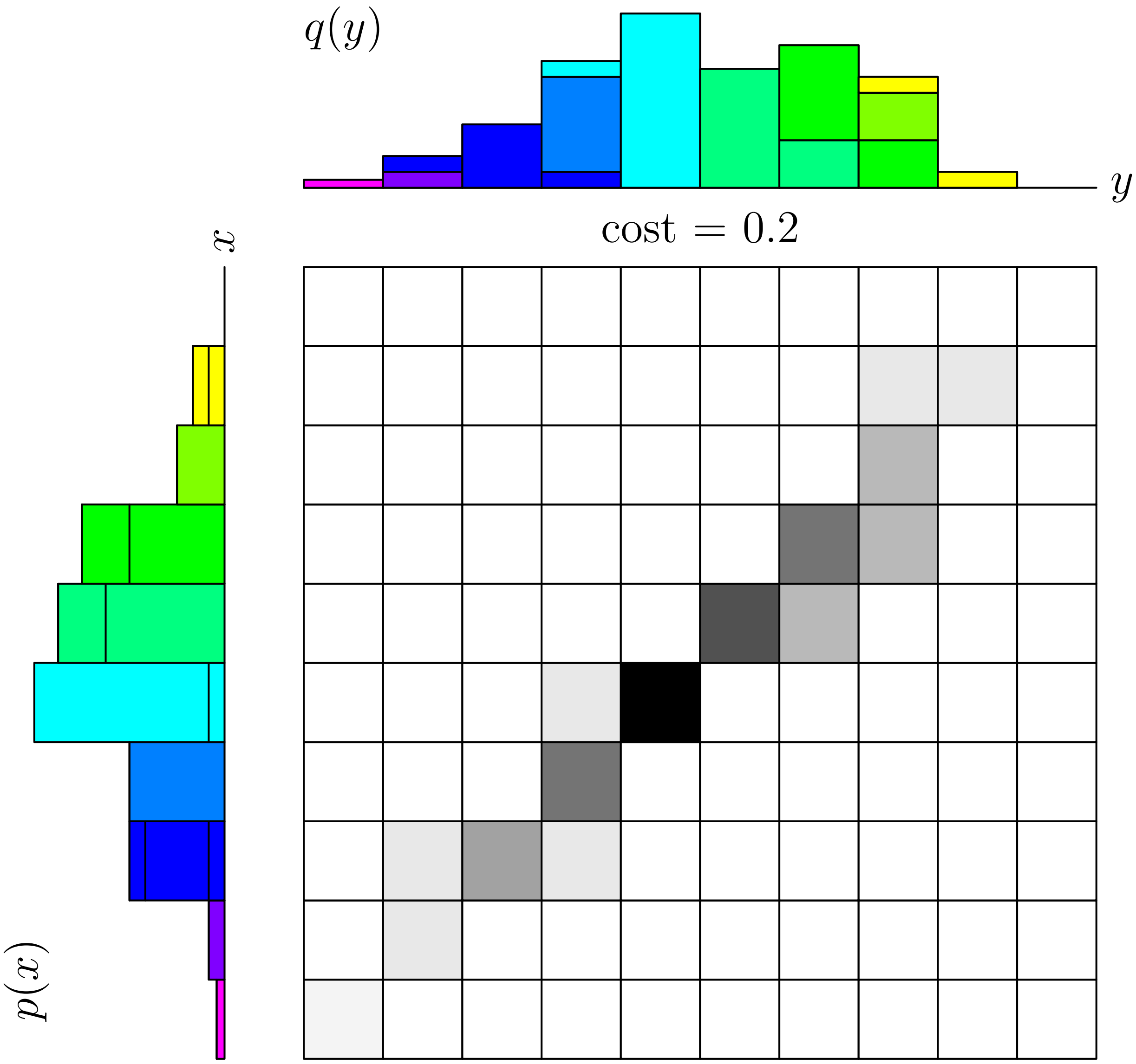

The Wasserstein Distance

- The Wasserstein distance $W(p,q)$ between two probability distributions is defined as

$$W(p,q) = \min_{\gamma \in \Lambda(p,q)} \mathbb{E}_\gamma[d(\boldsymbol{x},\boldsymbol{y})]$$

- Where $\Lambda(p,q)$ is the set of joint distributions $\gamma(\boldsymbol{x},\boldsymbol{y})$ such that

$$\int \gamma(\boldsymbol{x},\boldsymbol{y}) \mathrm{d}\boldsymbol{y} = p(\boldsymbol{x}) \qquad \int \gamma(\boldsymbol{x},\boldsymbol{y}) \mathrm{d}\boldsymbol{x} = q(\boldsymbol{y})$$

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Computing the Wasserstein Distance

- To compute the Wasserstein distance we have to solve a minimisation task!
- This looks nasty, but it is a (continuous) linear programmming problem
- Suppose p and q were discrete distribution (i.e. $\boldsymbol{x}$ and $\boldsymbol{y}$ only take discrete points)
- Then we could treat each value of $\gamma(\boldsymbol{x}, \boldsymbol{y})$ as an element of a vector $\boldsymbol{\gamma}$ and each value of $d(\boldsymbol{x}, \boldsymbol{y})$ as an element of a vector $\boldsymbol{D}$
- Our objective is to choose $\boldsymbol{\gamma}$ to minimise $\boldsymbol{D}^{\mathsf{T}}\boldsymbol{\gamma}$

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Constraints

$$\sum_j \gamma(\boldsymbol{x}_i, \boldsymbol{y}_j) = p(\boldsymbol{x}_i) \qquad \sum_i \gamma(\boldsymbol{x}_i, \boldsymbol{y}_j) = q(\boldsymbol{y}_j)$$

$$\mathbf{A}\,\boldsymbol{\gamma} = \boldsymbol{P}$$

$$\left(\begin{array}{cccc:cccc:cccc:cccc}
1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 & \cdots & \cdots & \cdots & \cdots & 0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & 1 & 1 & \cdots & 1 & \cdots & \cdots & \cdots & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & \cdots & \cdots & \cdots & 1 & 1 & \cdots & 1 \\
\hdashline
1 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & \cdots & \cdots & \cdots & \cdots & 1 & 0 & \cdots & 0 \\
0 & 1 & \cdots & 0 & 0 & 1 & \cdots & 0 & \cdots & \cdots & \cdots & \cdots & 0 & 1 & \cdots & 0 \\
\vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots \\
0 & 0 & \cdots & 1 & 0 & 0 & \cdots & 1 & \cdots & \cdots & \cdots & \cdots & 0 & 0 & \cdots & 1
\end{array}\right)
\left(\begin{array}{c}
\gamma(x_1,\, y_1) \\ \gamma(x_2,\, y_1) \\ \vdots \\ \gamma(x_n,\, y_1) \\ \hdashline
\gamma(x_1,\, y_2) \\ \gamma(x_2,\, y_2) \\ \vdots \\ \gamma(x_n,\, y_2) \\ \hdashline
\vdots \\ \vdots \\ \vdots \\ \vdots \\ \hdashline
\gamma(x_1,\, y_n) \\ \gamma(x_2,\, y_n) \\ \vdots \\ \gamma(x_n,\, y_n)
\end{array}\right)
=
\left(\begin{array}{c}
q(y_1) \\ q(y_2) \\ \vdots \\ q(y_n) \\ \hdashline p(x_1) \\ p(x_2) \\ \vdots \\ p(x_n)
\end{array}\right)$$

Lagrange Formulation

- For discrete distributions

$$\min_{\boldsymbol{\gamma}} \boldsymbol{D}^{\mathsf{T}}\gamma$$

$$\text{subject to} \quad \boldsymbol{A}\boldsymbol{\gamma} = \boldsymbol{P}, \quad \boldsymbol{\gamma} \geq 0$$

- Writing the Lagrangian

$$\mathcal{L}(\boldsymbol{\gamma}, \boldsymbol{\alpha}) = \boldsymbol{D}^{\mathsf{T}}\gamma - \boldsymbol{\alpha}^{\mathsf{T}}\left(\mathbf{A}^{\mathsf{T}}\gamma - \boldsymbol{P}\right)$$

where $\boldsymbol{\alpha}$ is a vector of Lagrange multipliers

- The solution to the discrete optimisation problem is given by

$$\min_{\boldsymbol{\gamma}} \max_{\boldsymbol{\alpha}} \mathcal{L}(\boldsymbol{\gamma}, \boldsymbol{\alpha})$$

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- We can rearrange

$$\begin{aligned}\mathcal{L}(\boldsymbol{\gamma},\boldsymbol{\alpha}) &= \boldsymbol{D}^{\mathsf{T}}\boldsymbol{\gamma} - \boldsymbol{\alpha}^{\mathsf{T}}(\mathbf{A}\boldsymbol{\gamma} - \boldsymbol{P}) \\ &= \boldsymbol{P}^{\mathsf{T}}\boldsymbol{\alpha} - \boldsymbol{\gamma}^{\mathsf{T}}\big(\mathbf{A}^{\mathsf{T}}\boldsymbol{\alpha} - \boldsymbol{D}\big)\end{aligned}$$

- We note that $\boldsymbol{\gamma} \geq 0$ so the dual problem is to find a vector $\boldsymbol{\alpha}$ that maximises $\boldsymbol{P}^{\mathsf{T}}\boldsymbol{\alpha}$ subject to the constraints $\mathbf{A}^{\mathsf{T}}\boldsymbol{\alpha} \leq \boldsymbol{D}$

- Although the vector form allows us to make connections with our earlier discussion of linear programming, it is a little difficult to interpret

Dual Form

- We can rearrange

$$\begin{aligned}\mathcal{L}(\gamma, \boldsymbol{\alpha}) &= \boldsymbol{D}^{\mathsf{T}}\gamma - \boldsymbol{\alpha}^{\mathsf{T}}(\mathbf{A}\gamma - \boldsymbol{P}) \\ &= \boldsymbol{P}^{\mathsf{T}}\boldsymbol{\alpha} - \gamma^{\mathsf{T}}\left(\mathbf{A}^{\mathsf{T}}\boldsymbol{\alpha} - \boldsymbol{D}\right)\end{aligned}$$

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Explicit Form

- We can write a Lagrangian for the original problem

$$\mathcal{L} = \sum_{i,j} d(\boldsymbol{x}_i, \boldsymbol{y}_i)\gamma(\boldsymbol{x}_i, \boldsymbol{y}_j) - \sum_i \alpha(\boldsymbol{x}_i) \left(\sum_j \gamma(\boldsymbol{x}_i, \boldsymbol{y}_j) - p(\boldsymbol{x}_i) \right)$$
$$- \sum_j \beta(\boldsymbol{y}_j) \left(\sum_i \gamma(\boldsymbol{x}_i, \boldsymbol{y}_j) - q(\boldsymbol{y}_j) \right)$$

subject to $\gamma(\boldsymbol{x}_i, \boldsymbol{y}_j) \geq 0$

- Rearranging

$$\mathcal{L} = \sum_i \alpha(\boldsymbol{x}_i) p(\boldsymbol{x}_i) + \sum_j \beta(\boldsymbol{y}_j) q(\boldsymbol{y}_j) - \sum_{i,j} \gamma(\boldsymbol{x}_i, \boldsymbol{y}_j) \big(\alpha(\boldsymbol{x}_i) + \beta(\boldsymbol{y}_j) - d(\boldsymbol{x}_i, \boldsymbol{y}_{\boldsymbol{i}})\big)$$

- This is eqivalent to maximising $\sum_i \alpha(\boldsymbol{x}_i) p(\boldsymbol{x}_i) + \sum_j \beta(\boldsymbol{y}_j) q(\boldsymbol{y}_j)$, subject to

$$\forall i, j \quad \alpha(\boldsymbol{x}_i) + \beta(\boldsymbol{y}_j) \leq d(\boldsymbol{x}_i, \boldsymbol{y}_{\boldsymbol{j}})$$

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subject to $\gamma(\boldsymbol{x}_i, \boldsymbol{y}_j) \geq 0$ where $\alpha(\boldsymbol{x}_i)$ and $\beta(\boldsymbol{y}_j)$ are Lagrange multipliers (they are components of $\boldsymbol{\alpha}$)

- Rearranging

$$\mathcal{L} = \sum_i \alpha(\boldsymbol{x}_i)p(\boldsymbol{x}_i) + \sum_j \beta(\boldsymbol{y}_j)q(\boldsymbol{y}_j) - \sum_{i,j} \gamma(\boldsymbol{x}_i, \boldsymbol{y}_j)\big(\alpha(\boldsymbol{x}_i) + \beta(\boldsymbol{y}_j) - d(\boldsymbol{x}_i, \boldsymbol{y}_{\boldsymbol{i}})\big)$$

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Continuous Form

- We can write a Lagrangian for the continuous problem

$$\mathcal{L} = \iint d(\boldsymbol{x},\boldsymbol{y})\,\gamma(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}\boldsymbol{y} - \int \alpha(\boldsymbol{x}) \left(\int \gamma(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{y} - p(\boldsymbol{x}) \right) \mathrm{d}\boldsymbol{x} \\ - \int \beta(\boldsymbol{y}) \left(\int \gamma(\boldsymbol{x},\boldsymbol{y})\,\mathrm{d}\boldsymbol{x} - q(\boldsymbol{y}) \right) \mathrm{d}\boldsymbol{y}$$

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Dual Form Constraint

- We note that $\alpha(\boldsymbol{x}) + \beta(\boldsymbol{y}) \leq d(\boldsymbol{x},\boldsymbol{y})$ for all $\boldsymbol{x}$ and $\boldsymbol{y}$
- This has to be true when $\boldsymbol{x} = \boldsymbol{y}$ so that

$$\alpha(\boldsymbol{x}) + \beta(\boldsymbol{x}) \leq d(\boldsymbol{x},\boldsymbol{x}) = 0$$

- So $\beta(\boldsymbol{x}) = -\alpha(\boldsymbol{x}) - \epsilon(\boldsymbol{x})$ where $\epsilon(\boldsymbol{x}) \geq 0$
- But want to maximise

$$\int \alpha(\boldsymbol{x}) p(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} + \int \beta(\boldsymbol{y}) q(\boldsymbol{y}) \mathrm{d}\boldsymbol{y} = \int \alpha(\boldsymbol{x}) \left(p(\boldsymbol{x}) - q(\boldsymbol{x})\right) \mathrm{d}\boldsymbol{x} - \int q(\boldsymbol{x}) \epsilon(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}$$

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Dual Form Constraint

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- Thus the dual problem is to find a function $\alpha(\boldsymbol{x})$—or a vector of functions $(\alpha(\boldsymbol{x}_i)|i)$—that maximises

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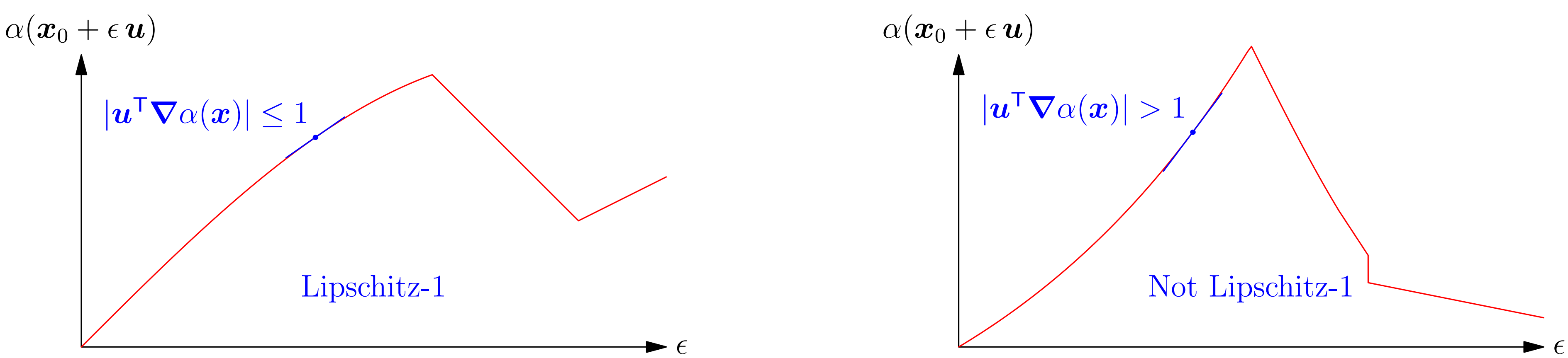
Lipschitz-1 Functions

- We note for a Lipschitz-1 function and any unit vector $\boldsymbol{u}$

$$\boldsymbol{u}^{\mathsf{T}}\boldsymbol{\nabla}\alpha(\boldsymbol{x}) = \lim_{\epsilon \to 0} \frac{\alpha(\boldsymbol{x}) - \alpha(\boldsymbol{x} + \epsilon\,\boldsymbol{u})}{\epsilon}$$

- That is, at every point the gradient in all directions must be less than 1



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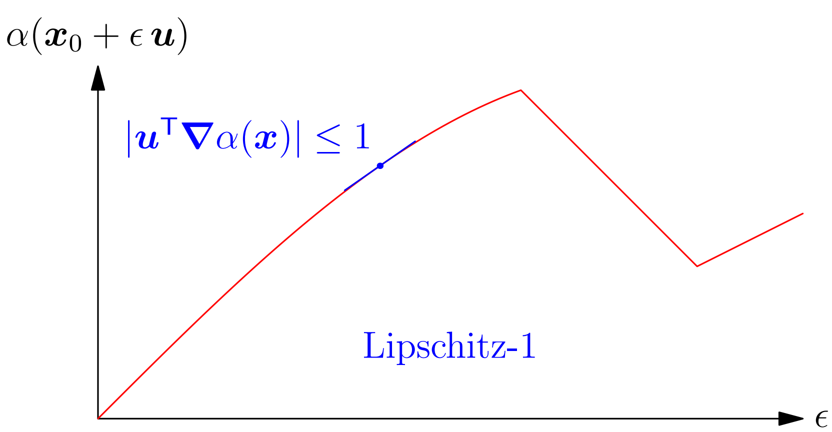

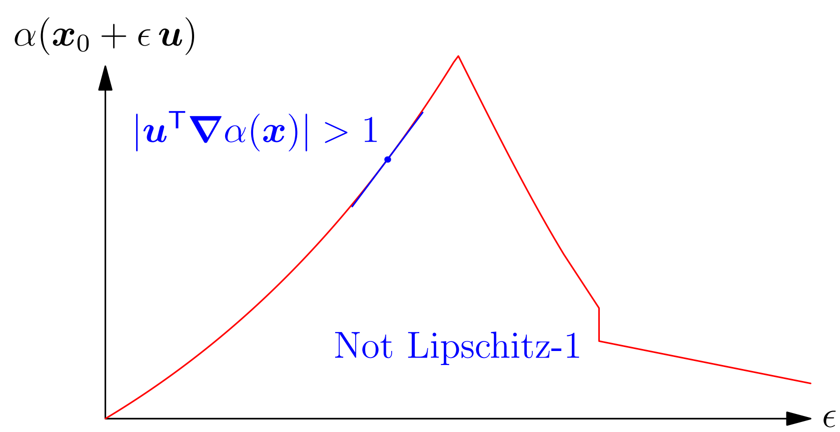

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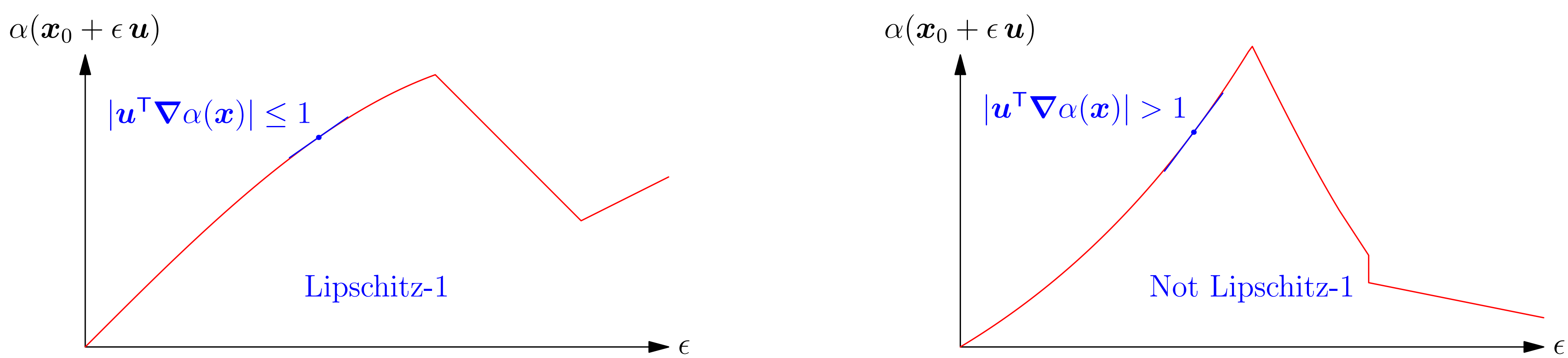

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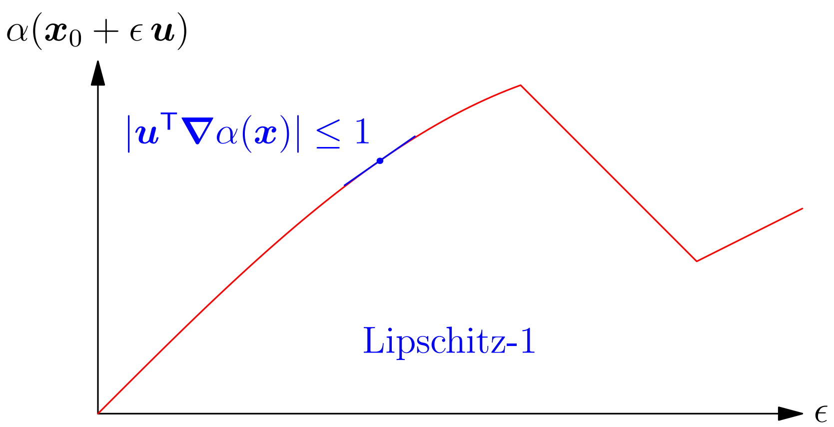

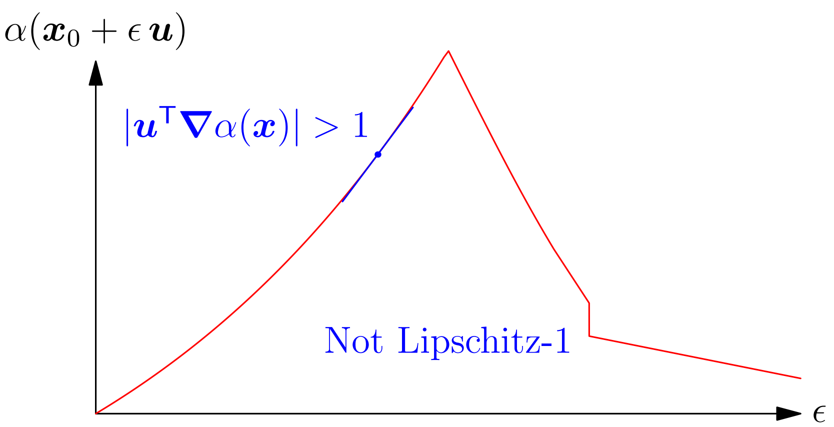

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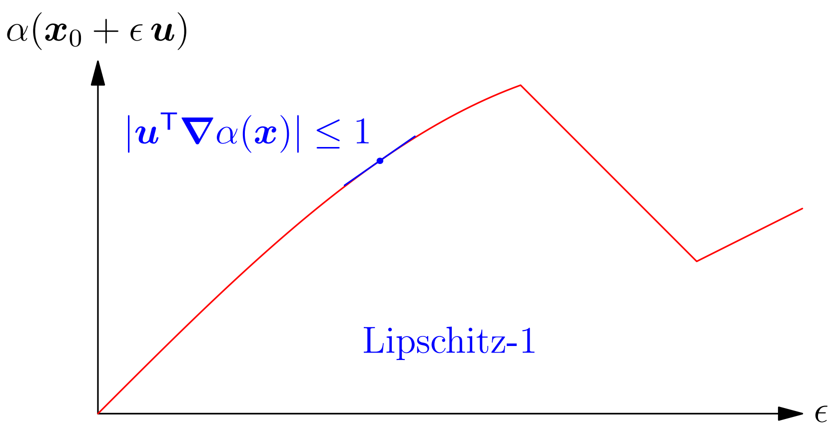

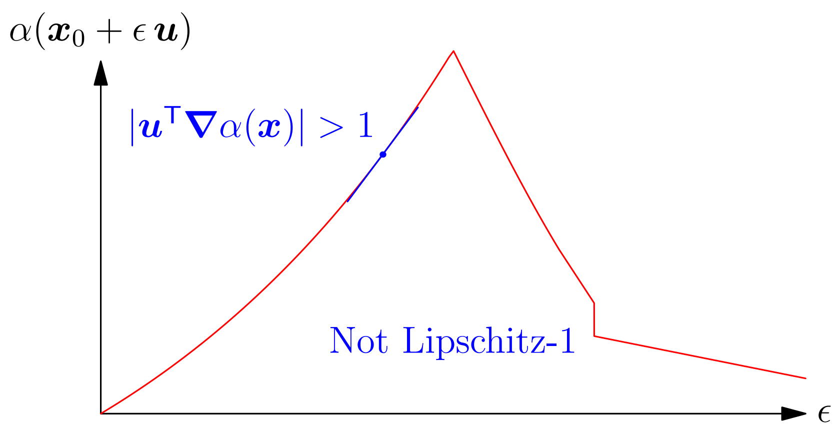

Calculating the Wasserstein Distance

- To recall the big picture we want to compute the Wasserstein distance

$$W(p,q) = \min_{\gamma \in \Lambda(p,q)} \mathbb{E}_\gamma[d(\boldsymbol{x},\boldsymbol{y})]$$

- For high dimensional objects $\gamma(\boldsymbol{x},\boldsymbol{y})$ would be a huge object to approximate

- Instead we can compute the Wasserstein distance in the dual formulation

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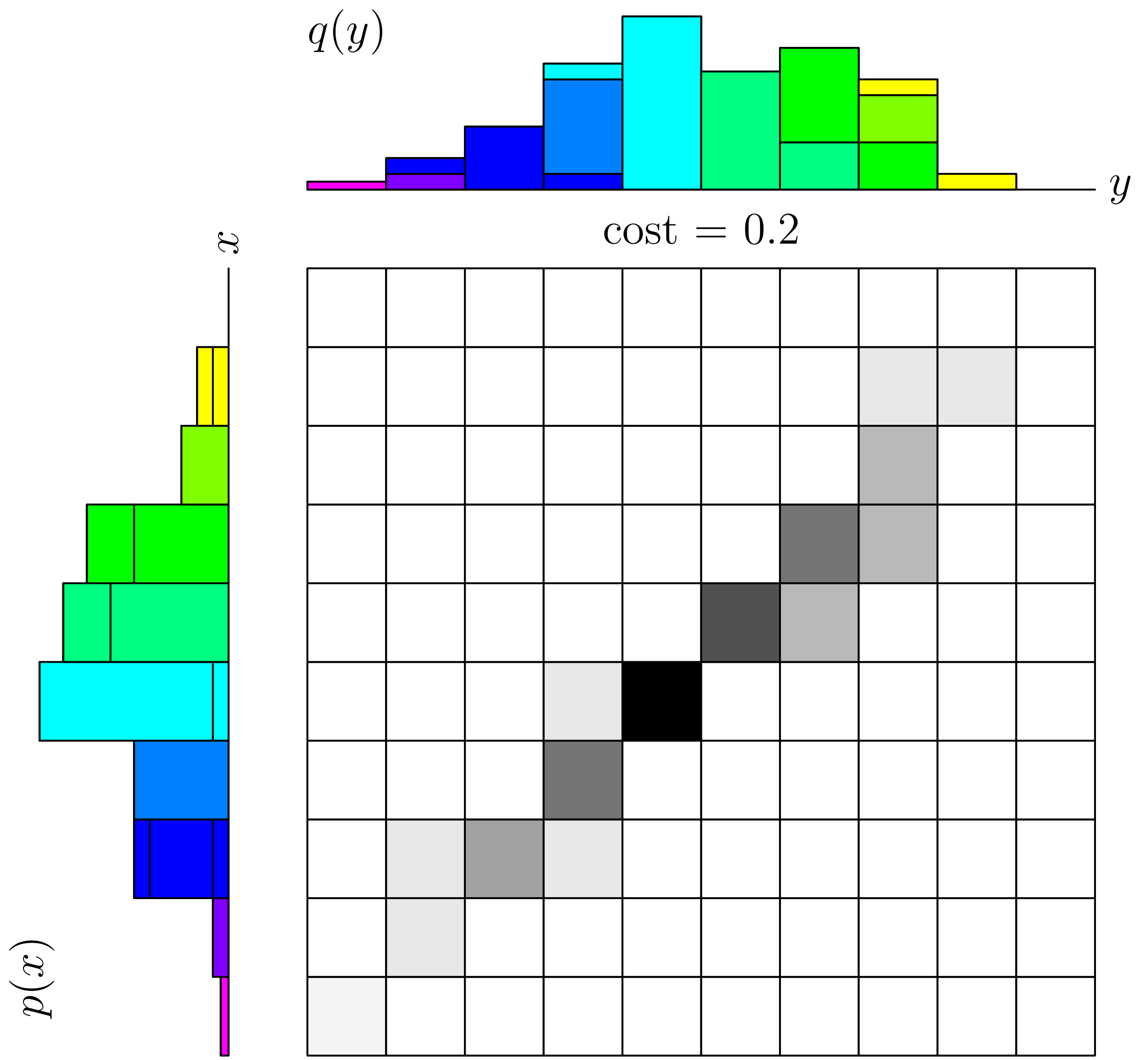
Outline

1. GANs
2. Wasserstein Distance
3. **Wasserstein GANs**



Back to GANs

- What has this got do with GANs?
- Suppose we want to minimise the distance between the distribution $p(\boldsymbol{x})$ of real images (of which $\mathcal{D}$ are samples) and the distribution $q(\boldsymbol{x})$ of images drawn from a generator
- We can use a normal GAN generator, $G(\boldsymbol{z}, \boldsymbol{w}_G)$, that generates an image when given a random variable $\boldsymbol{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- To do this we choose the weights, $\boldsymbol{w}_G$ of the generator to minimise

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$$\mathbb{E}_p[\alpha(\boldsymbol{x})] \approx \frac{1}{|\mathcal{B}|}\sum_{\boldsymbol{x}\in\mathcal{B}}\alpha(\boldsymbol{x}), \qquad \mathbb{E}_q[\alpha(\boldsymbol{x})] \approx \frac{1}{n}\sum_{i=1}^{n}\alpha(G(\boldsymbol{z}_i, \boldsymbol{w}_G))$$

- where $\mathcal{B} \subset \mathcal{D}$ is a minibatch of true images and $\boldsymbol{z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

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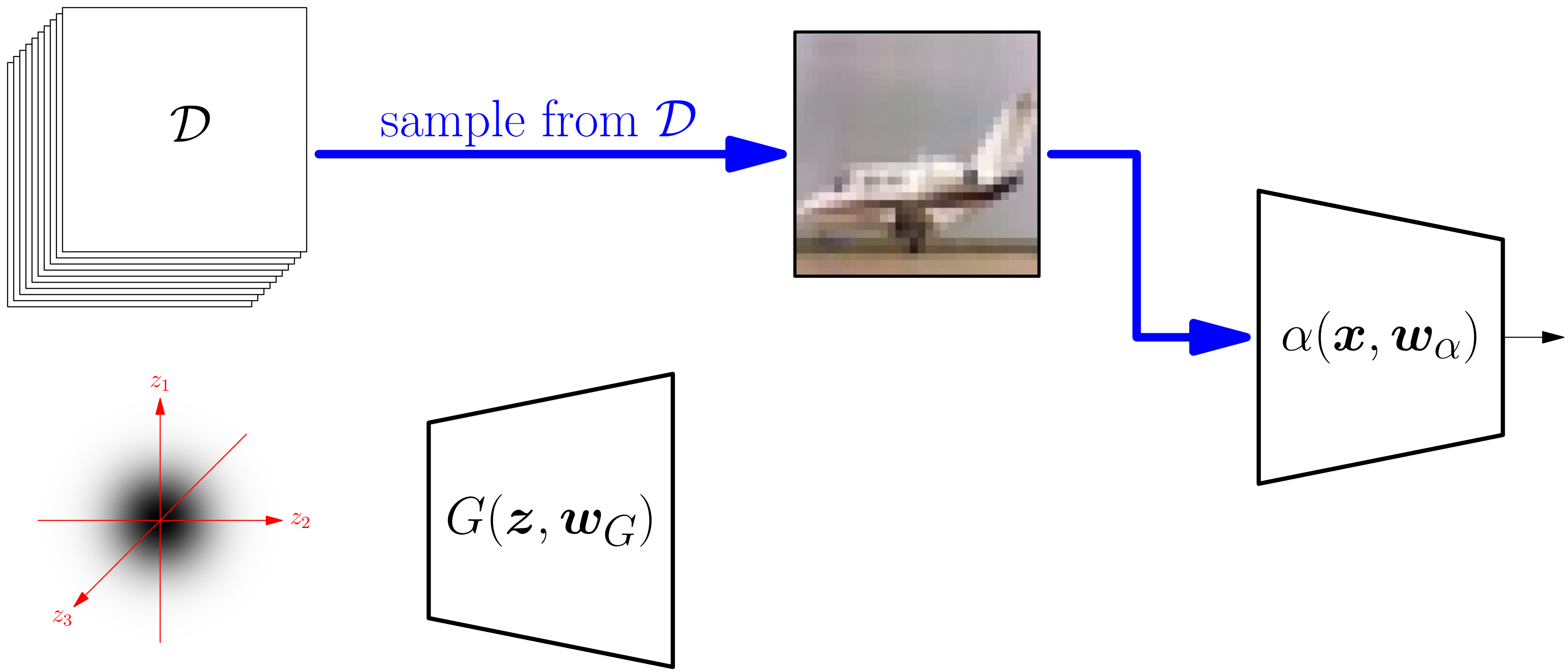

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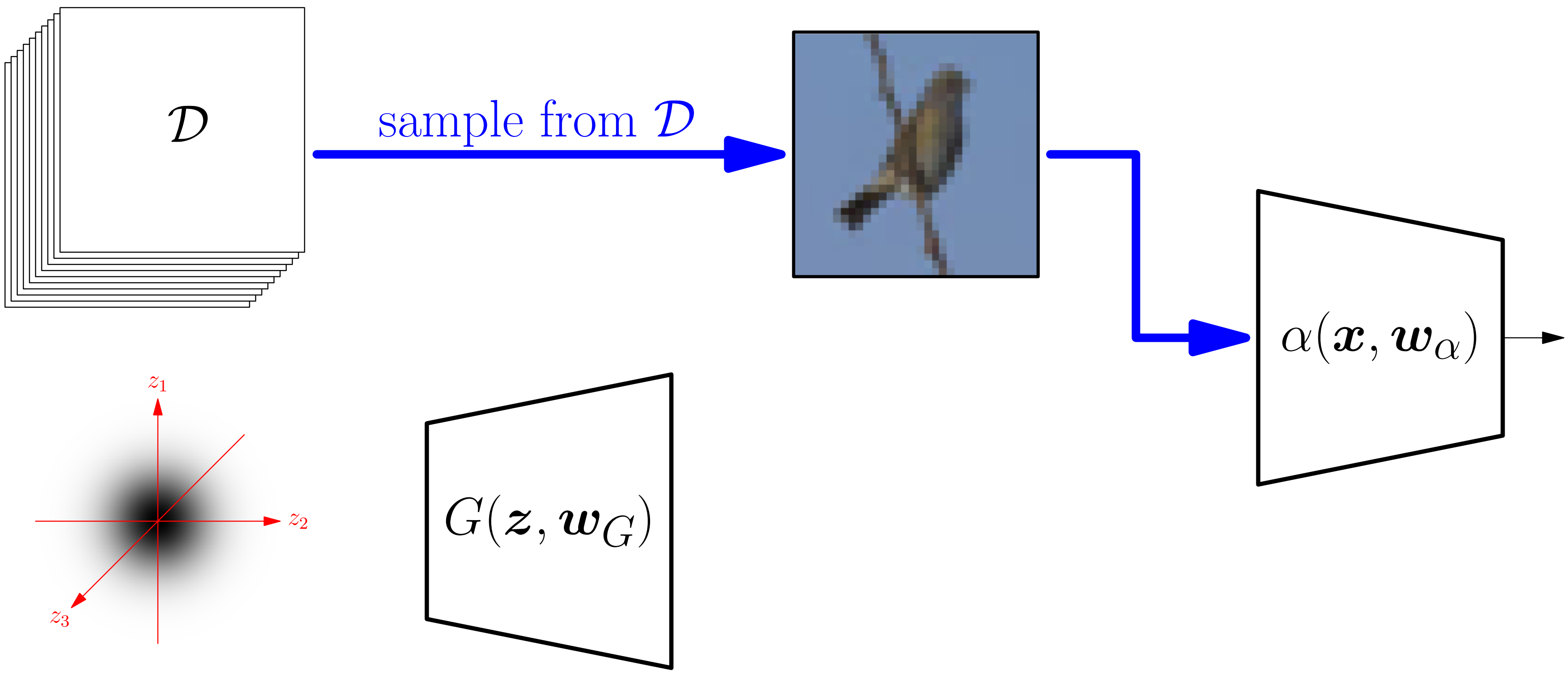

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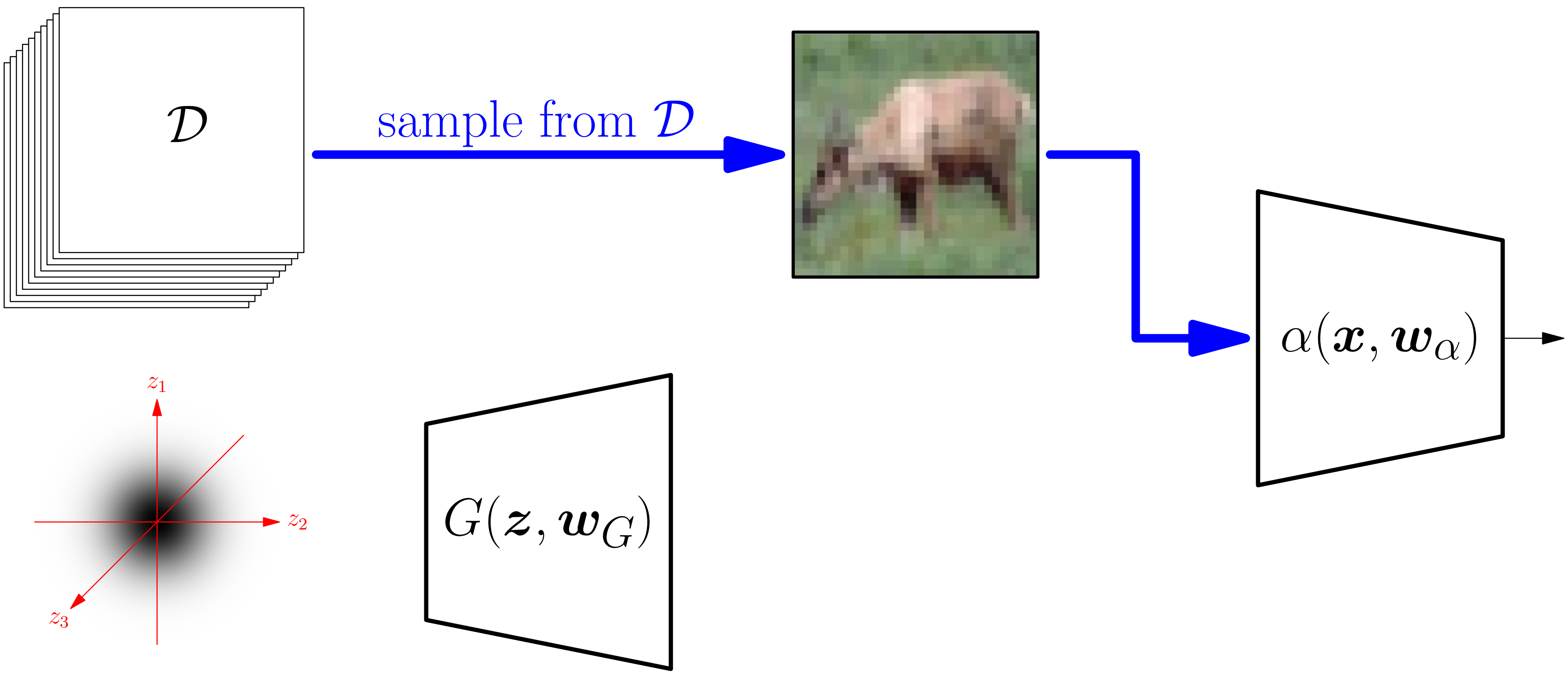

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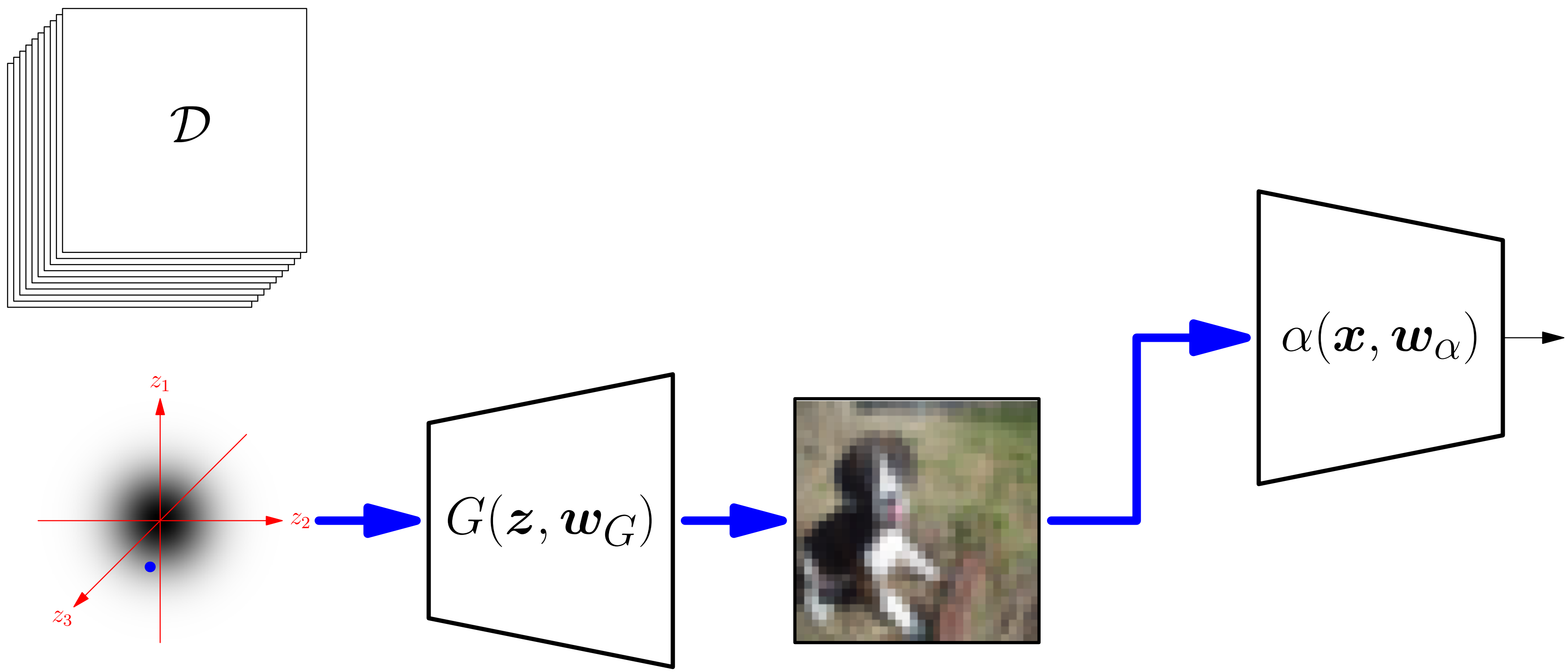

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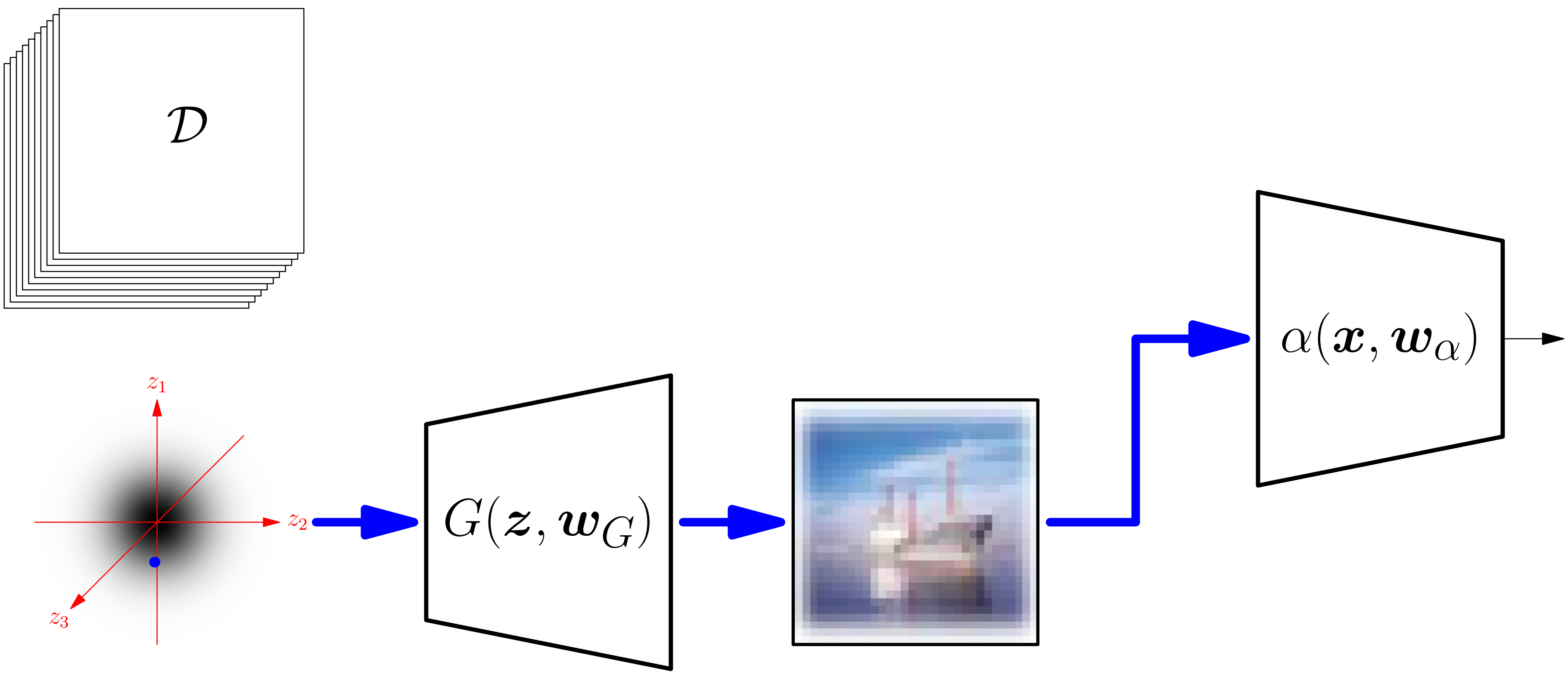

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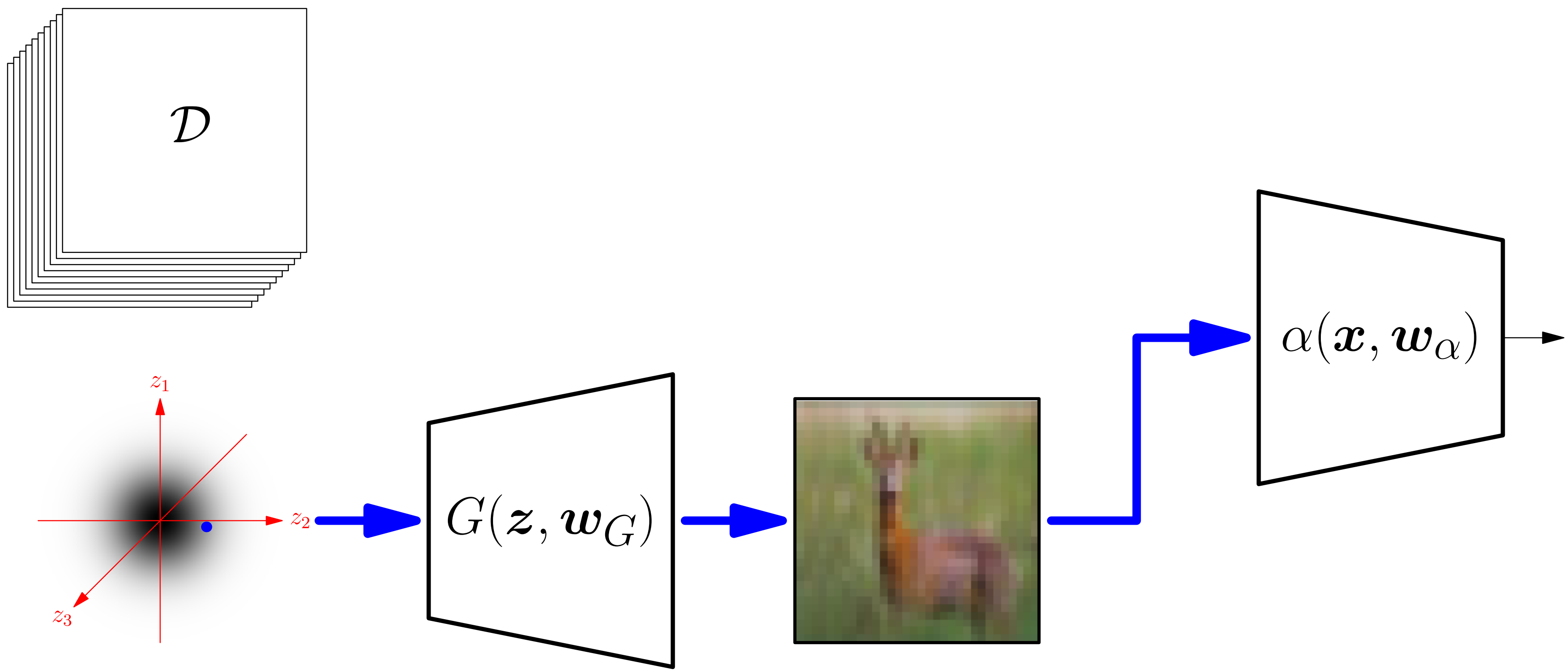

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- By trying to minimise the Wasserstein distance between the distribution of a generator and a true distribution we arrive at optimising two adversarial networks just like a GAN
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