Artificial Intelligence Unsupervised Learning and Causation

LÉON BOTTOU

FACEBOOK AI RESEARCH & NEW YORK UNIVERSITY

Facebook AI Research

- Mission: advancing the field of machine intelligence.
- Open research: we publish papers, we
- More than a hundred permanents and growing.
- New York, Menlo Park, Paris, Montreal, Seattle, …

https://research.fb.com/category/facebook-ai-research-fair/

https://github.com/facebookresearch

Summary

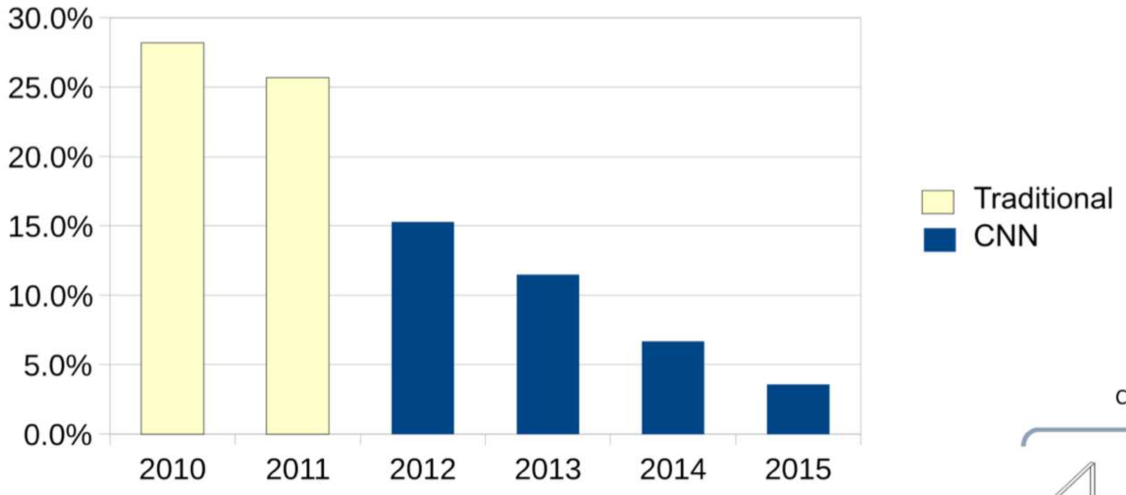
1. What works in AI?
2. What does not work?
3. A detective guesswork?
4. Causation hints
5. Causal direction
6. Causation and unsupervised learning
7. Wasserstein GANs
8. The geometry of weak Integral Probability Metrics

Conclusion

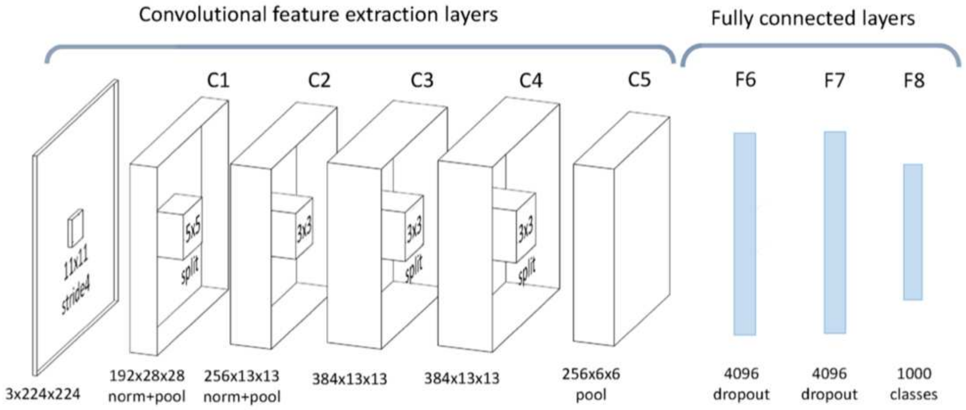
1- What works in AI?

WHY ARE PEOPLE SO EXCITED?

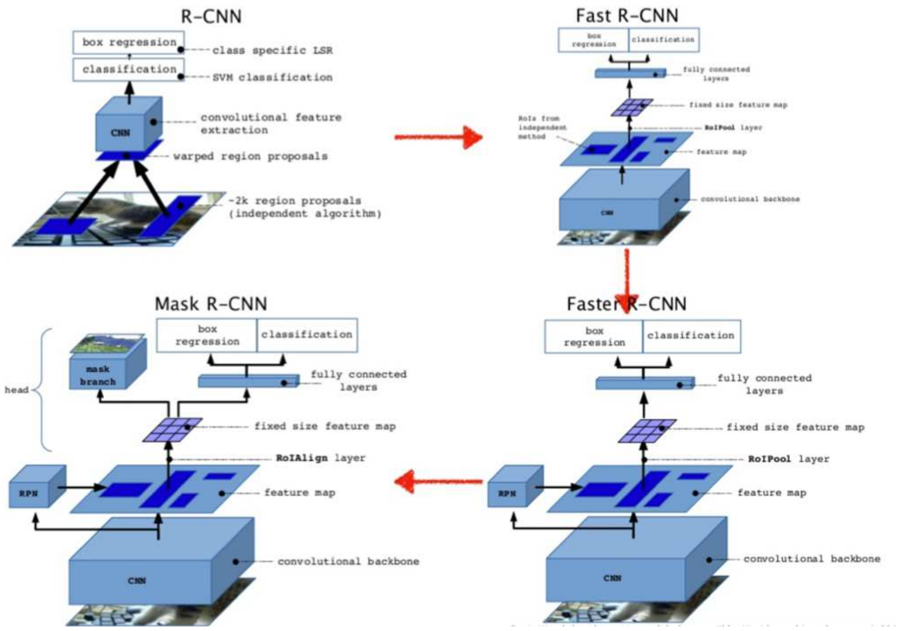
Object recognition in images



Top5 error rate of the annual winner of the ImageNet image classification challenge. CNNs break through in 2012.

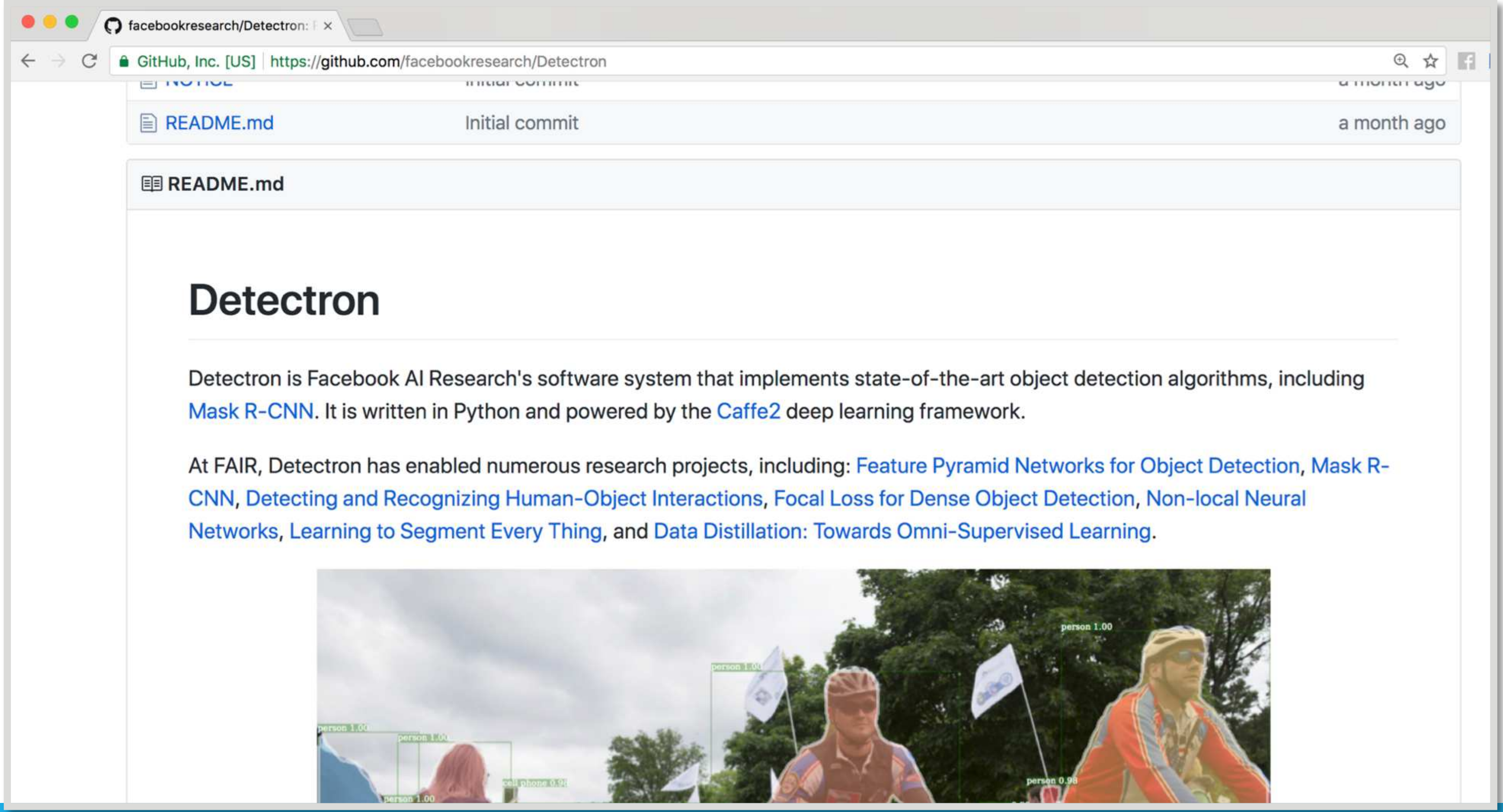


Object recognition in images



Such systems are really being used on a large scale.

Object recognition in images



facebookresearch/Detectron: F ×
GitHub, Inc. [US] | https://github.com/facebookresearch/Detectron
person 1.00
person 1.00
person 1.00
person 1.00
cell phone 0.96
person 1.00
person 0.98

NOTICE Initial commit a month ago

README.md Initial commit a month ago

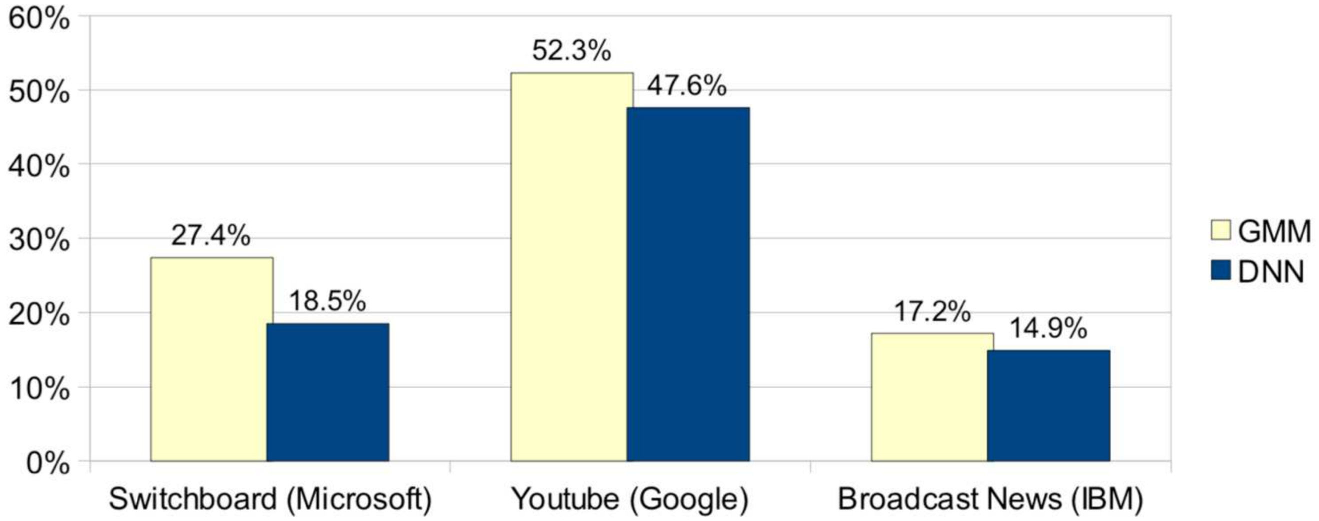
README.md

Detectron

Detectron is Facebook AI Research's software system that implements state-of-the-art object detection algorithms, including Mask R-CNN. It is written in Python and powered by the Caffe2 deep learning framework.

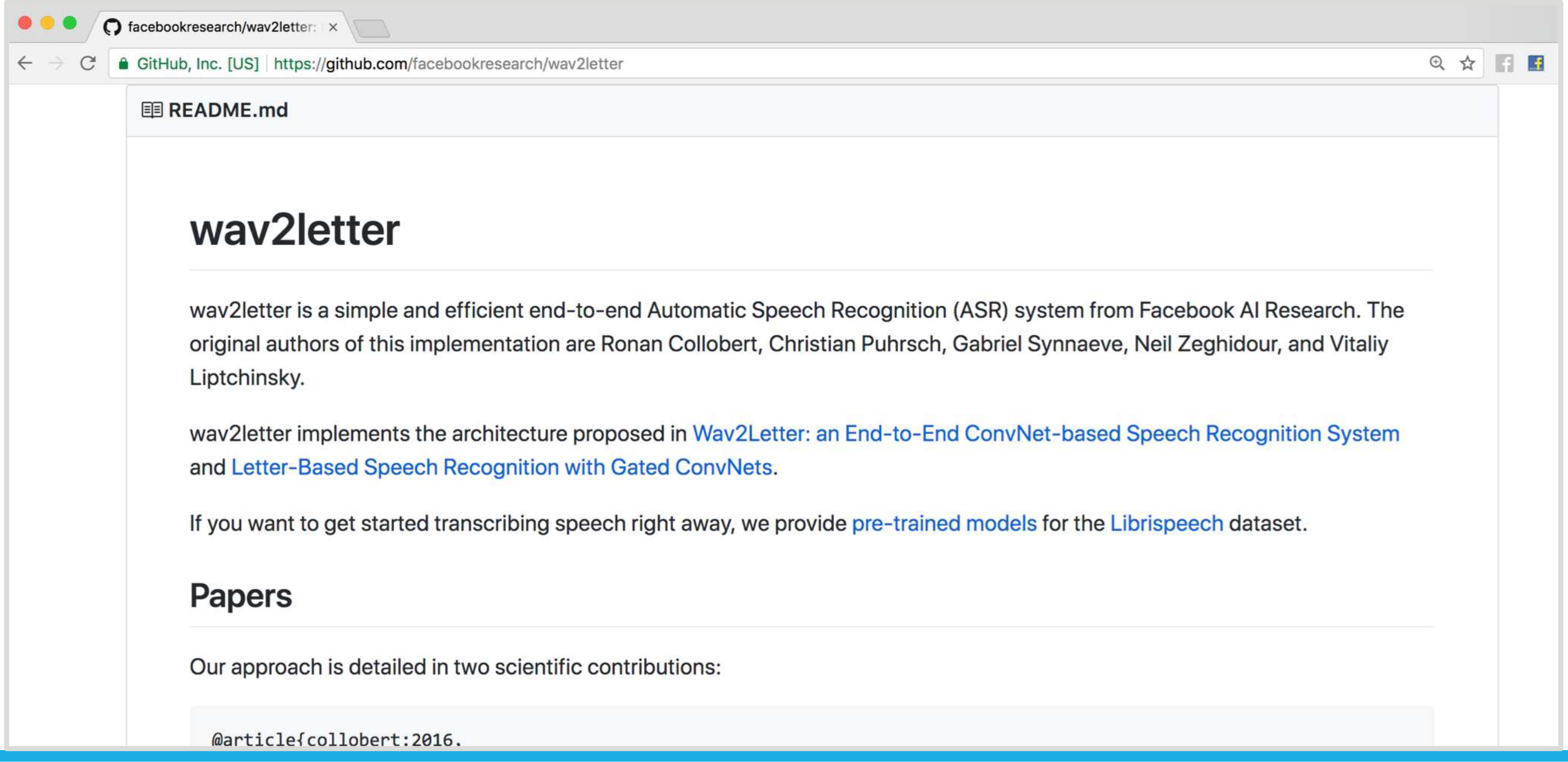
At FAIR, Detectron has enabled numerous research projects, including: Feature Pyramid Networks for Object Detection, Mask R-CNN, Detecting and Recognizing Human-Object Interactions, Focal Loss for Dense Object Detection, Non-local Neural Networks, Learning to Segment Every Thing, and Data Distillation: Towards Omni-Supervised Learning.

Speech recognition



Comparison (2012) of the word error rates achieved by traditional GMMs and DNNs, reported by three different research groups on three different benchmark.

Speech recognition



facebookresearch/wav2letter
GitHub, Inc. [US] | https://github.com/facebookresearch/wav2letter

README.md

wav2letter

wav2letter is a simple and efficient end-to-end Automatic Speech Recognition (ASR) system from Facebook AI Research. The original authors of this implementation are Ronan Collobert, Christian Puhrsch, Gabriel Synnaeve, Neil Zeghidour, and Vitaliy Liptchinsky.

wav2letter implements the architecture proposed in Wav2Letter: an End-to-End ConvNet-based Speech Recognition System and Letter-Based Speech Recognition with Gated ConvNets.

If you want to get started transcribing speech right away, we provide pre-trained models for the Librispeech dataset.

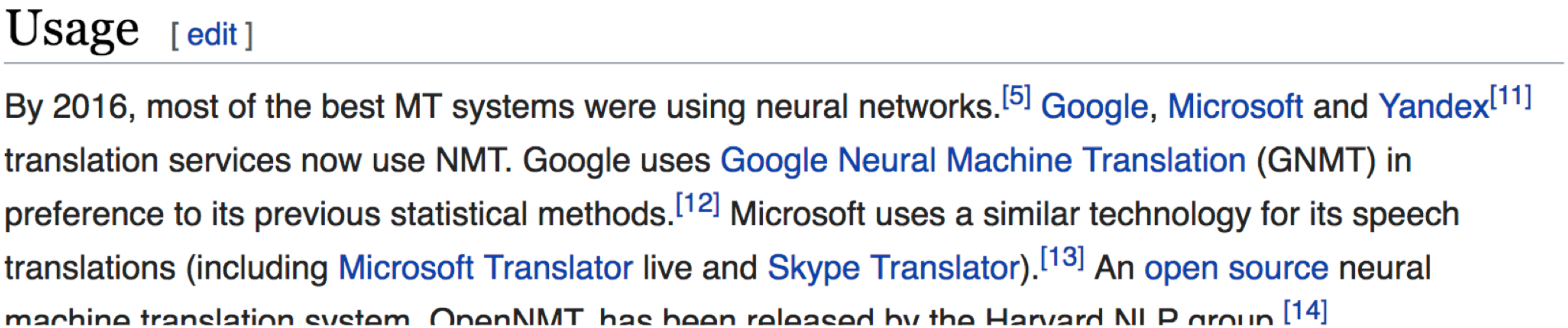
Papers

Our approach is detailed in two scientific contributions:

```
@article{collobert:2016,
```

Machine translation

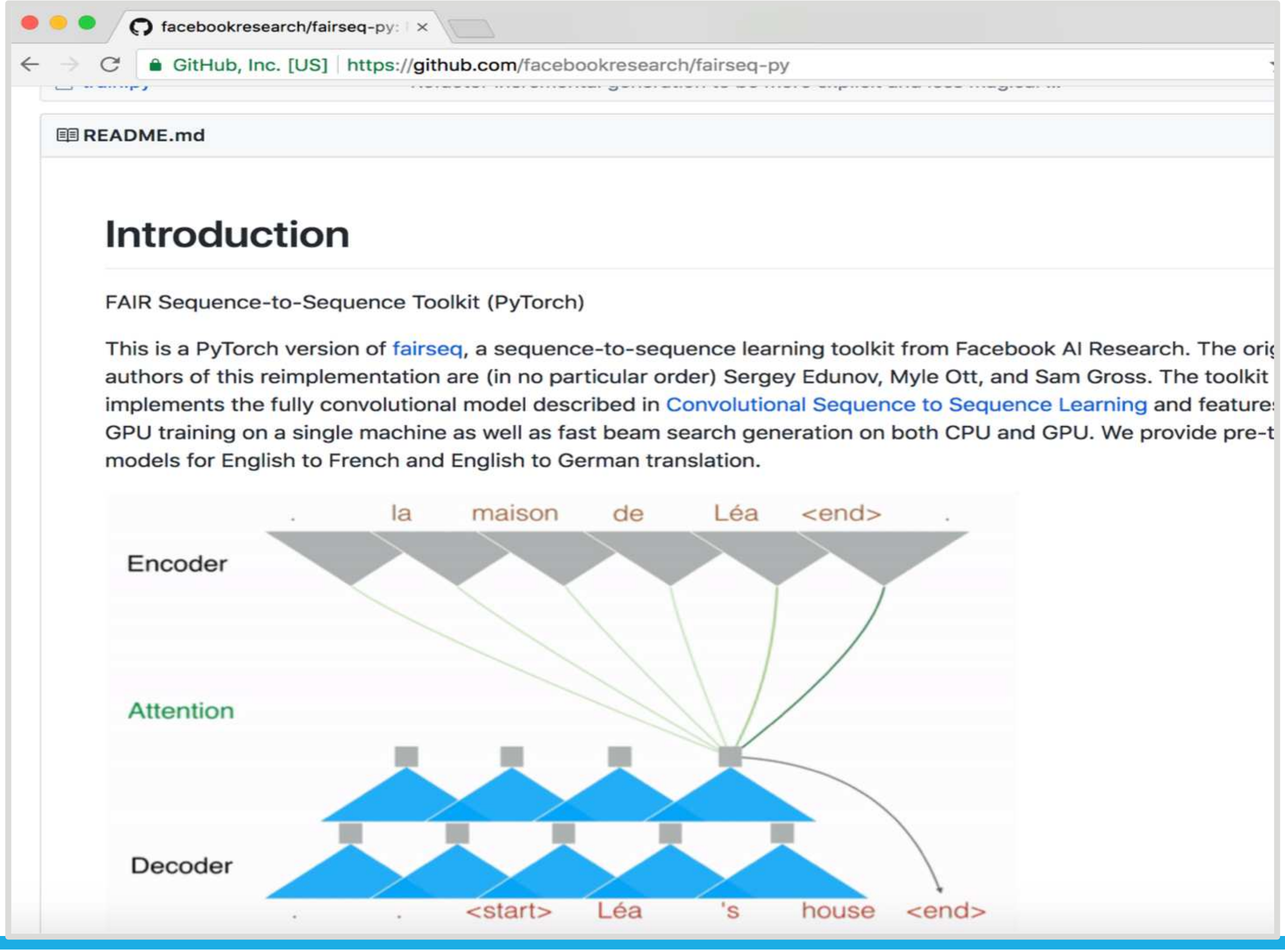
Although it is far from perfect (more on this later), Wikipedia says:



Usage [edit]

By 2016, most of the best MT systems were using neural networks.[5] Google, Microsoft and Yandex[11] translation services now use NMT. Google uses Google Neural Machine Translation (GNMT) in preference to its previous statistical methods.[12] Microsoft uses a similar technology for its speech translations (including Microsoft Translator live and Skype Translator).[13] An open source neural machine translation system, OpenNMT, has been released by the Harvard NLP group.[14]

Machine translation



facebookresearch/fairseq-py:
GitHub, Inc. [US] | https://github.com/facebookresearch/fairseq-py
README.md

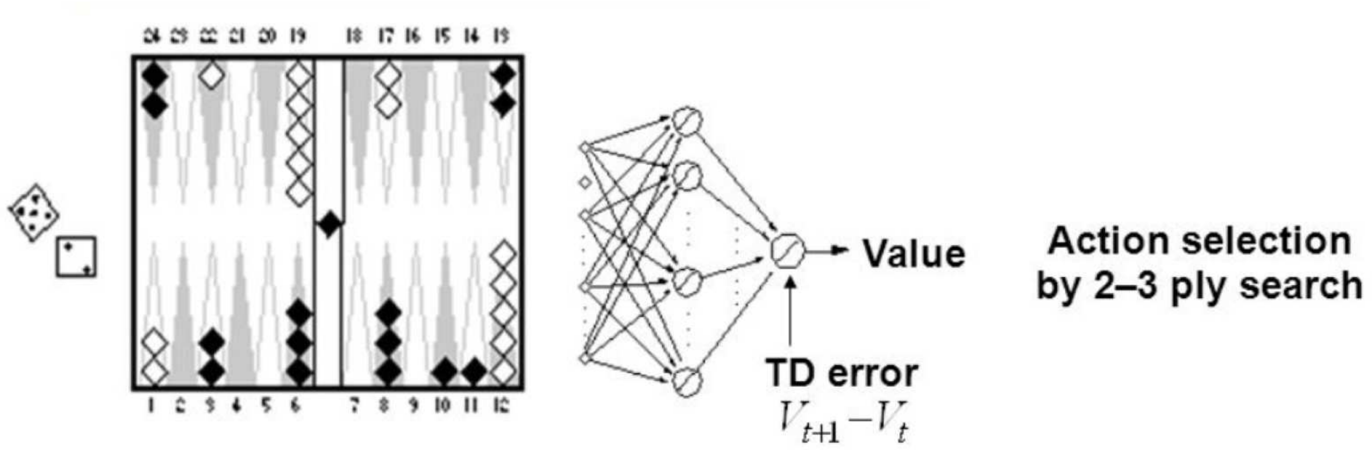
Introduction

FAIR Sequence-to-Sequence Toolkit (PyTorch)

This is a PyTorch version of fairseq, a sequence-to-sequence learning toolkit from Facebook AI Research. The orig authors of this reimplementation are (in no particular order) Sergey Edunov, Myle Ott, and Sam Gross. The toolkit implements the fully convolutional model described in Convolutional Sequence to Sequence Learning and feature GPU training on a single machine as well as fast beam search generation on both CPU and GPU. We provide pre-t models for English to French and English to German translation.

Reinforcement learning in games

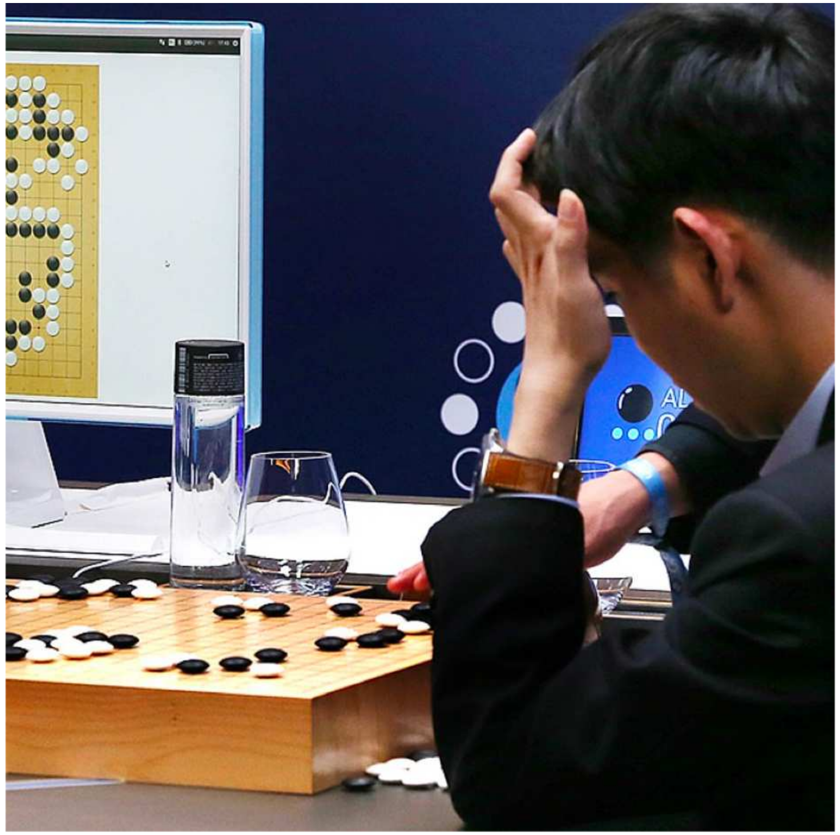
- TD-Gammon (Tesauro, 1992-1995)



  - Trained by self play.
  - Arguably the best backgammon player in the world.

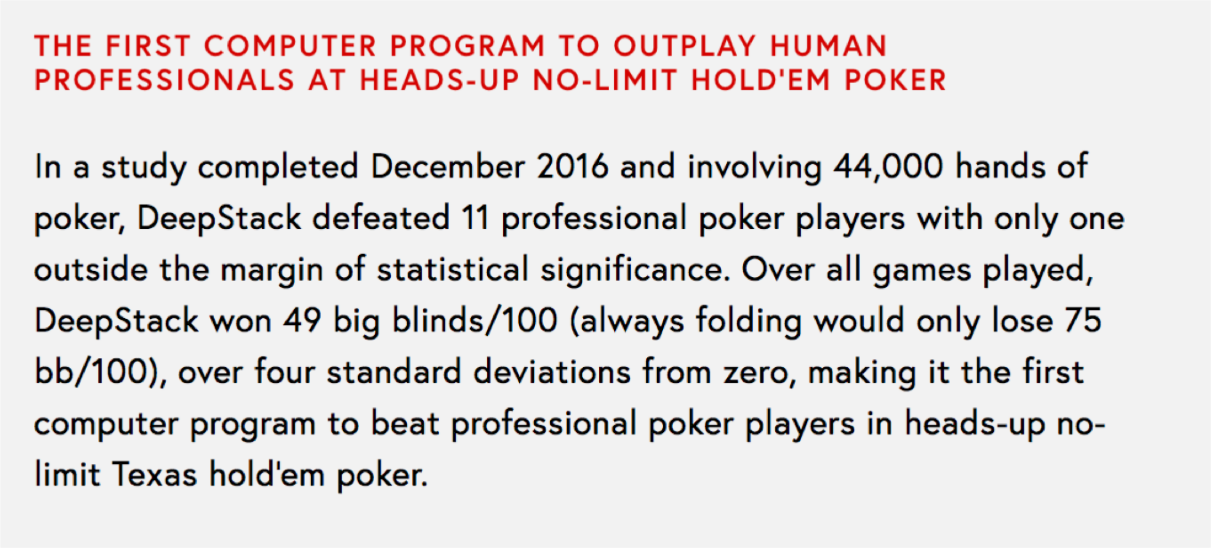
Reinforcement learning in games

- AlphaGo (Deepmind)
  - Trained with self-play.
  - Arguably the best Go player in the world.
  - Go is more complex than backgammon.
  - Go still is a full information game.
  - Go games can be simulated at high speed (unlike self-driving cars.)



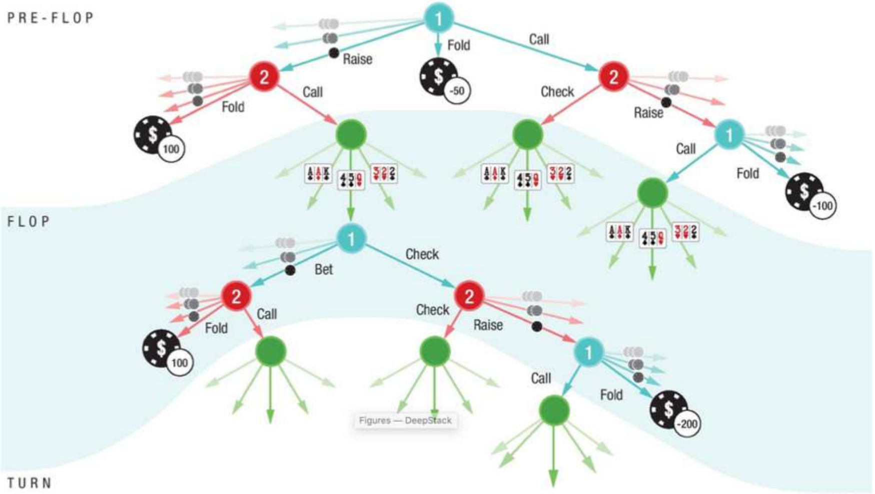
Reinforcement learning in games

- DeepStack (Moravčík et al., 2017)



THE FIRST COMPUTER PROGRAM TO OUTPLAY HUMAN PROFESSIONALS AT HEADS-UP NO-LIMIT HOLD'EM POKER

In a study completed December 2016 and involving 44,000 hands of poker, DeepStack defeated 11 professional poker players with only one outside the margin of statistical significance. Over all games played, DeepStack won 49 big blinds/100 (always folding would only lose 75 bb/100), over four standard deviations from zero, making it the first computer program to beat professional poker players in heads-up no-limit Texas hold'em poker.



- No longer a full information game.
- Still can be simulated at high speed.

2- What doesnt work?

WHY ARE PEOPLE TOO EXCITED?

Training demands too much data

- Locating and recognizing objects in images

  after training on more images than a human can see.

- Translating natural languages (somehow)

  after training on more bi-text than a human can read.

Supervised learning

- Playing Atari games

  after playing more games than any teenager can endure.

- Playing Go (famously)

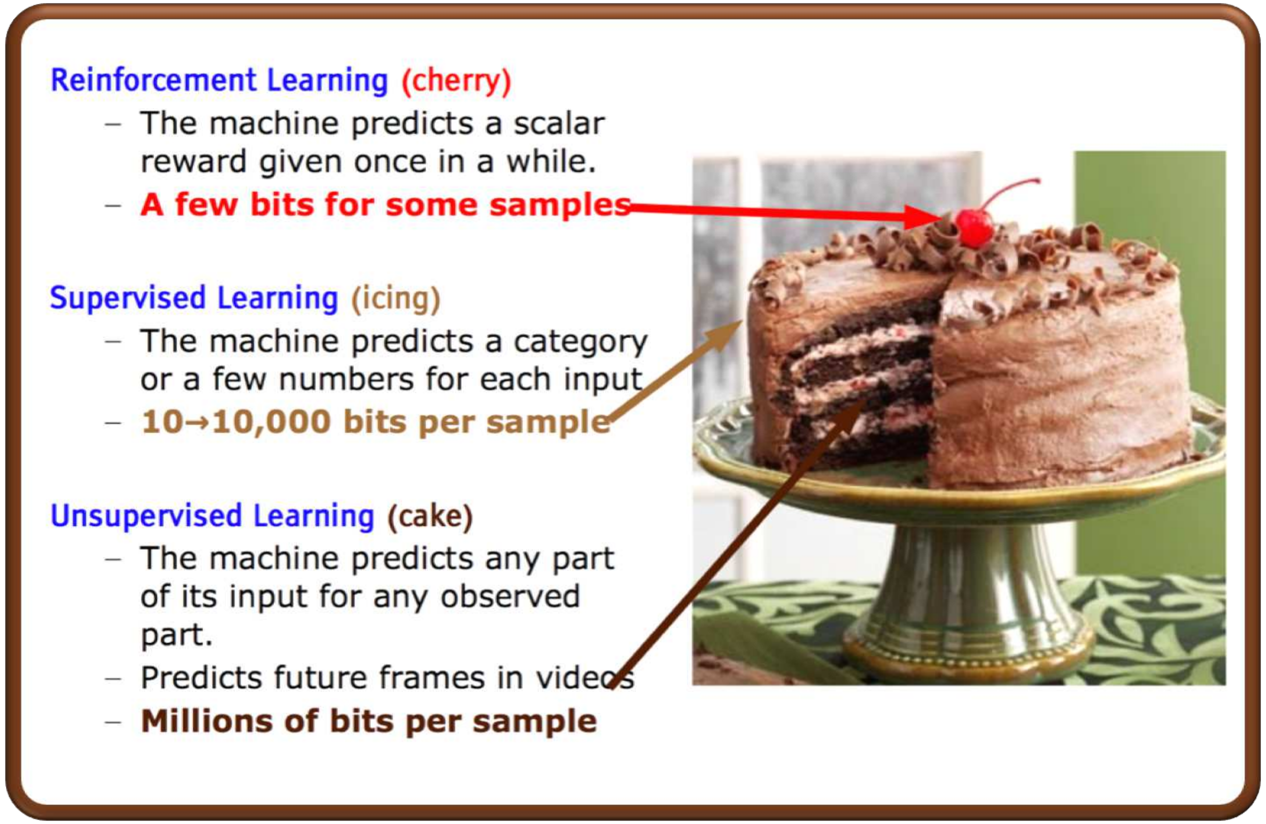
  after playing more grandmaster level games than mankind.

Reinforcement learning

Training demands too much data

- Yann LeCun’s chocolate cake

  - In reinforcement learning, the learning algorithm focuses on the reward signal.
  - In supervised learning, the learning algorithm focuses on the manually annotated class labels.
  - But there may be a lot of signal in the patterns themselves.



Reinforcement Learning (cherry)

- The machine predicts a scalar reward given once in a while.
- **A few bits for some samples**

Supervised Learning (icing)

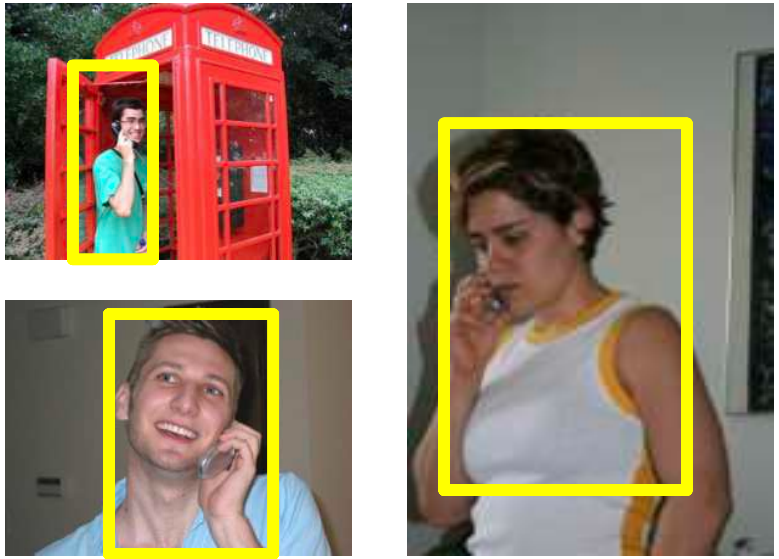
- The machine predicts a category or a few numbers for each input
- **10→10,000 bits per sample**

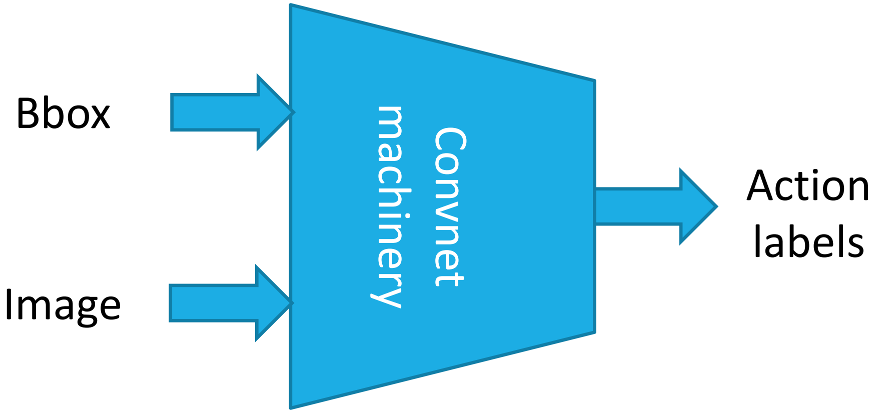
Unsupervised Learning (cake)

- The machine predicts any part of its input for any observed part.
- Predicts future frames in videos
- **Millions of bits per sample**

The statistical problem is only a proxy

Example: detection of the action “*giving a phone call*”

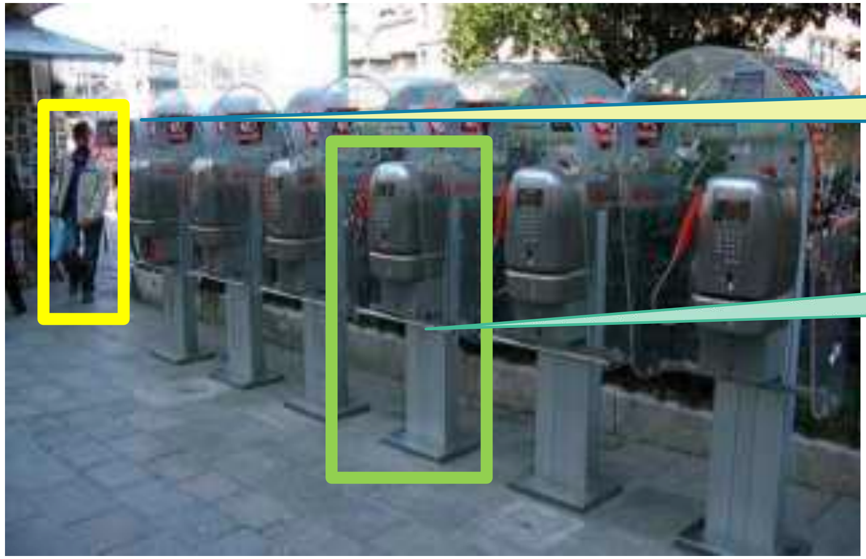




(Oquab et al., CVPR 2014)
~70% correct (SOTA)

The statistical problem is only a proxy

Example: detection of the action “*giving a phone call*”

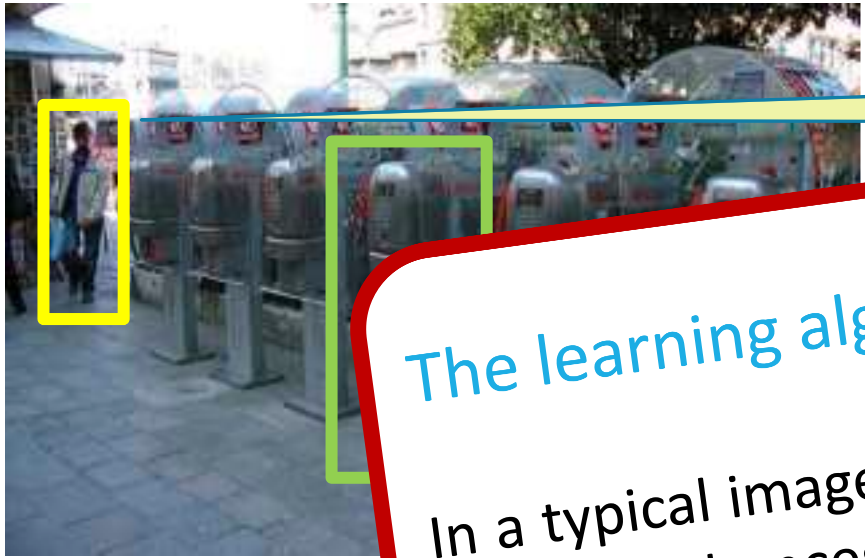


Not giving a phone call.

Giving a phone call ????

The statistical problem is only a proxy

Example: detection of the action “*giving a phone call*”



Not giving a phone call

The learning algorithm is statistically correct!

In a typical image dataset, when an image shows a person near a phone, chances are that the person is giving a phone call.

The statistical problem is only a proxy

- Strong statistical biases in large datasets often mask the semantics
- Another example: Visual Question Answering

What color is the jacket?
-Red and blue.
-Yellow.
-Black.
-Orange.

How many cars are parked?
-Four.
-Three.
-Five.
-Six.

What event is this?
-A wedding.
-Graduation.
-A funeral.
-A picnic.

When is this scene taking place?
-Day time.
-Night time.
-Evening.
-Morning.

No need to see the image!

What is covering the ground?
- Snow
- Candies
- Grass
- Refuse

Structure does not help our systems

- Structure in computer vision
  - Scenes are made of objects, objects are made of parts,
  - Objects interacts through their parts, …
- Structure in natural language
  - Sentences have a recursive grammatical structure,
  - This structure is associated to meaning.

Structure allows us to reason.
This is an important component of our human experience.

Structure does not help our systems

"Adding structural knowledge to machine learning systems should improve the performance!"

- This does not go very far in practice
  - Earlier techniques in computer vision used to recognize objects from their parts, only to be outperformed by convolutional neural networks.
  - For many natural language processing tasks such as document classification, sentiment analysis,* or text tagging, smartly using bags of bigrams give state-of-the-art performance. Their order does not seem to matter!
  - Earlier techniques in machine translation used to leverage the grammatical structure of the sentences, only to be displaced by neural models that only use the sequence of words.

*See for instance (Scheible & Schütze, 2013) https://arxiv.org/abs/1301.2811

Structure does not help our systems

"Adding structural knowledge to machine learning systems should improve the performance!"

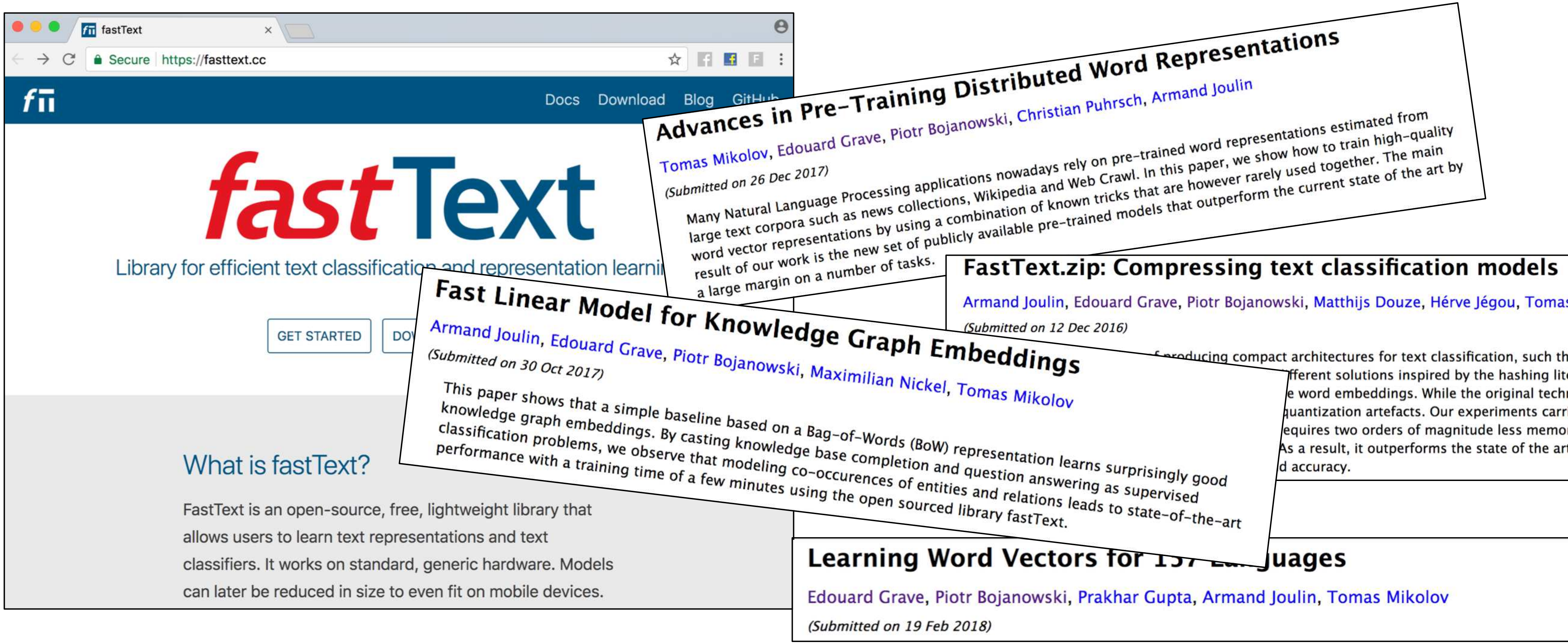
- This does not go very far in practice
  - Earlier techniques in co only to be outperf
  - For many natural la ent analysis,* or text tagging, sma Their order does no
  - Earlier techniques in d to leverage the grammatical structure of the sentences, only to be displaced by neural models that only use the sequence of words.

"Every time I fire a linguist, the performance of the speech recognizer goes up"

Attributed to F. Jelinek, around 1988.

*See for instance (Scheible & Schütze, 2013) https://arxiv.org/abs/1301.2811

The FastText story



fastText

Library for efficient text classification and representation learni

What is fastText?

FastText is an open-source, free, lightweight library that allows users to learn text representations and text classifiers. It works on standard, generic hardware. Models can later be reduced in size to even fit on mobile devices.

Advances in Pre-Training Distributed Word Representations

Tomas Mikolov, Edouard Grave, Piotr Bojanowski, Christian Puhrsch, Armand Joulin

(Submitted on 26 Dec 2017)

Many Natural Language Processing applications nowadays rely on pre-trained word representations estimated from large text corpora such as news collections, Wikipedia and Web Crawl. In this paper, we show how to train high-quality word vector representations by using a combination of known tricks that are however rarely used together. The main result of our work is the new set of publicly available pre-trained models that outperform the current state of the art by a large margin on a number of tasks.

FastText.zip: Compressing text classification models

Armand Joulin, Edouard Grave, Piotr Bojanowski, Matthijs Douze, Hérve Jégou, Tomas

(Submitted on 12 Dec 2016)

f producing compact architectures for text classification, such th
fferent solutions inspired by the hashing lit
e word embeddings. While the original techn
quantization artefacts. Our experiments carr
equires two orders of magnitude less memo
As a result, it outperforms the state of the ar
d accuracy.

Fast Linear Model for Knowledge Graph Embeddings

Armand Joulin, Edouard Grave, Piotr Bojanowski, Maximilian Nickel, Tomas Mikolov

(Submitted on 30 Oct 2017)

This paper shows that a simple baseline based on a Bag-of-Words (BoW) representation learns surprisingly good knowledge graph embeddings. By casting knowledge base completion and question answering as supervised classification problems, we observe that modeling co-occurences of entities and relations leads to state-of-the-art performance with a training time of a few minutes using the open sourced library fastText.

Learning Word Vectors for 157 Languages

Edouard Grave, Piotr Bojanowski, Prakhar Gupta, Armand Joulin, Tomas Mikolov

(Submitted on 19 Feb 2018)

What is structure for, exactly?

- This may not be a problem with structure,
  but a problem with our benchmarking methods.

We usually report an average performance measured on a testing set.

- The average performance emphasizes understanding frequent sentences …

  “ How do you do? ”

- … and places little weight on understanding rarer sentences.

  “ The bank was about to close when the four masked men showed up. ”

What is structure for, exactly?

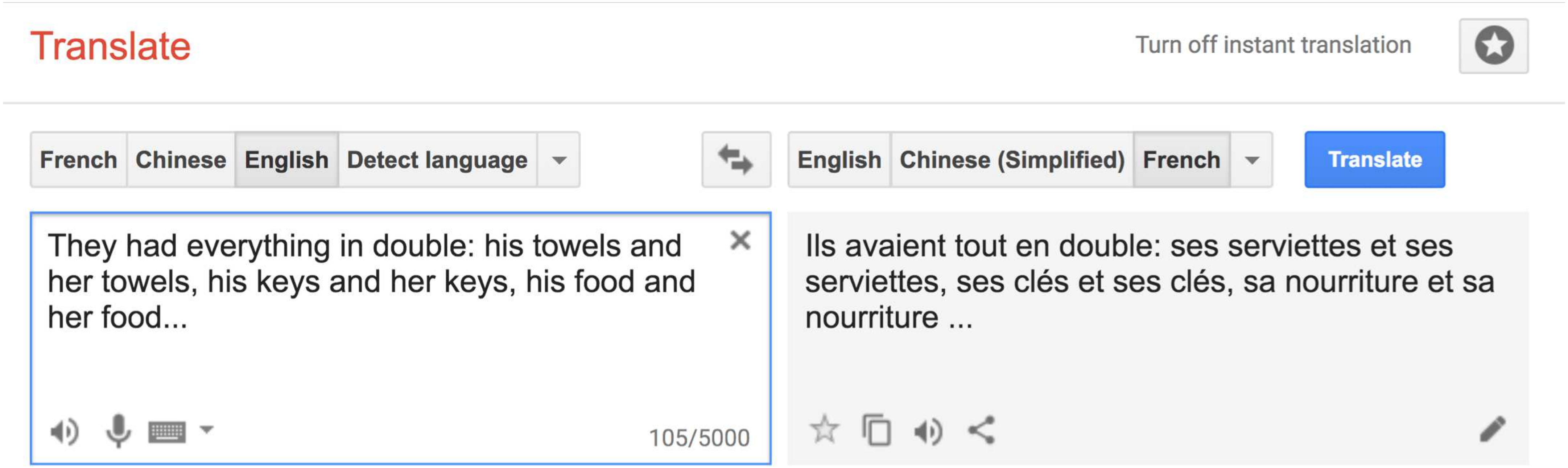
What is the purpose of the grammatical structure of language

- to help describing the distribution of existing sentences?
- to help constructing new sentences that describe new situations?

Observed / Frequent

Potential / Rare

Statistics ≠ Semantics



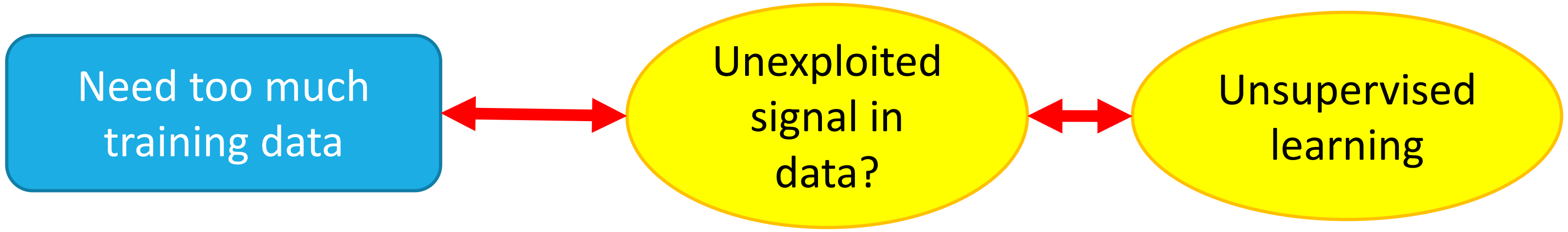
They had everything in double: his towels and her towels, his keys and her keys, his food and her food...

Ils avaient tout en double: ses serviettes et ses serviettes, ses clés et ses clés, sa nourriture et sa nourriture ...

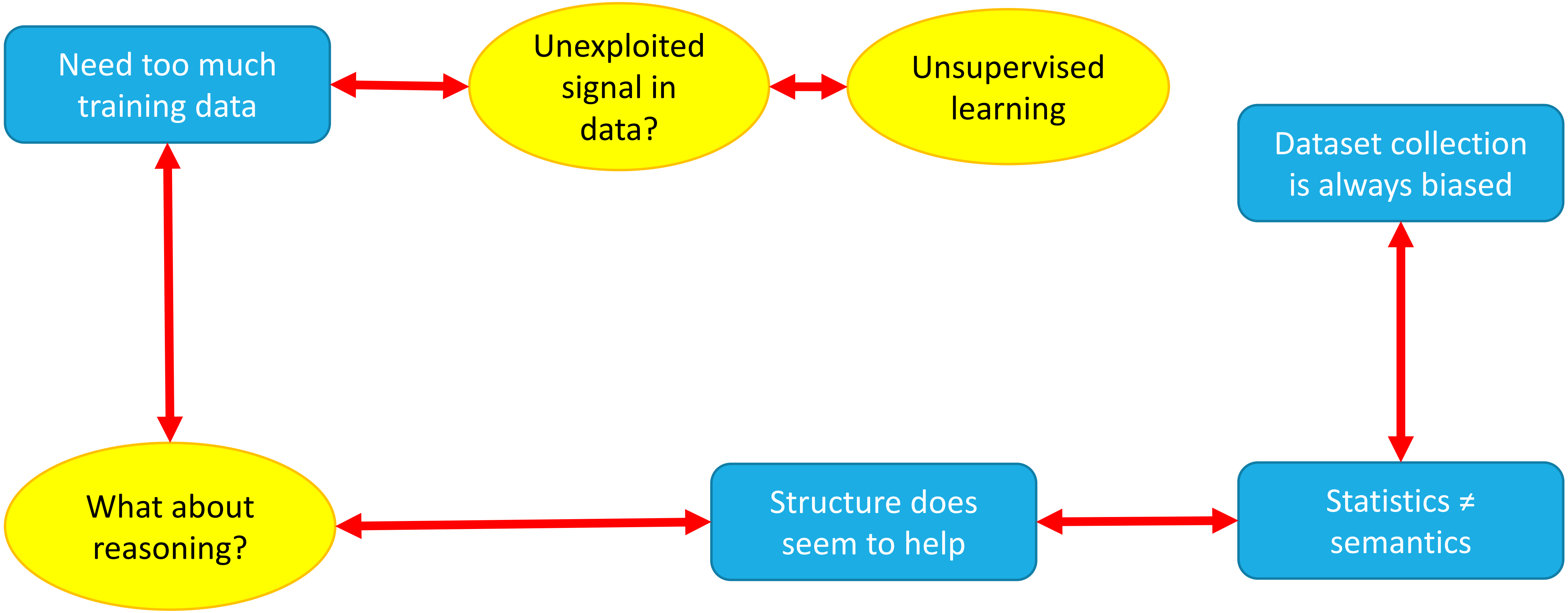
(Example from D. Hofdstader, 2018.)

3- Detective guesswork

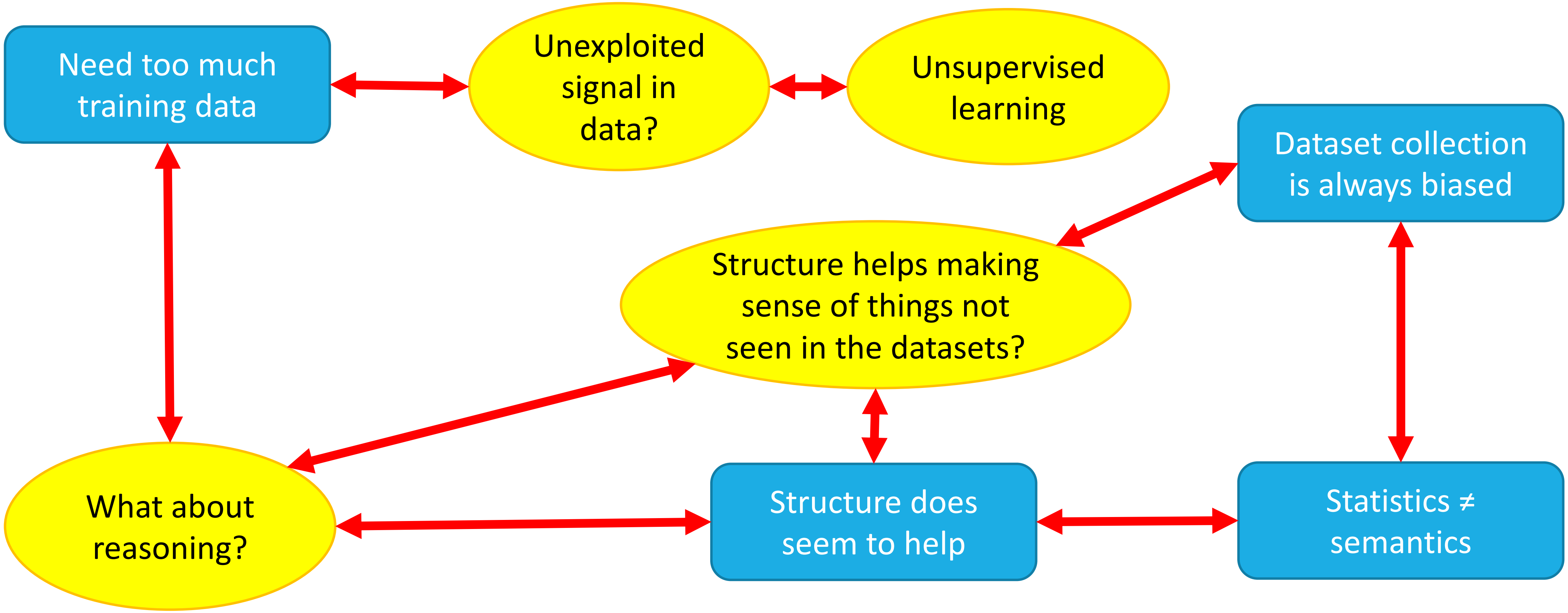
The pinboard (1)



The pinboard (2)


Need too much training data
Unexploited signal in data?
Unsupervised learning
Dataset collection is always biased
What about reasoning?
Structure does seem to help
Statistics ≠ semantics

The pinboard (3)



Need too much training data

Unexploited signal in data?

Unsupervised learning

Dataset collection is always biased

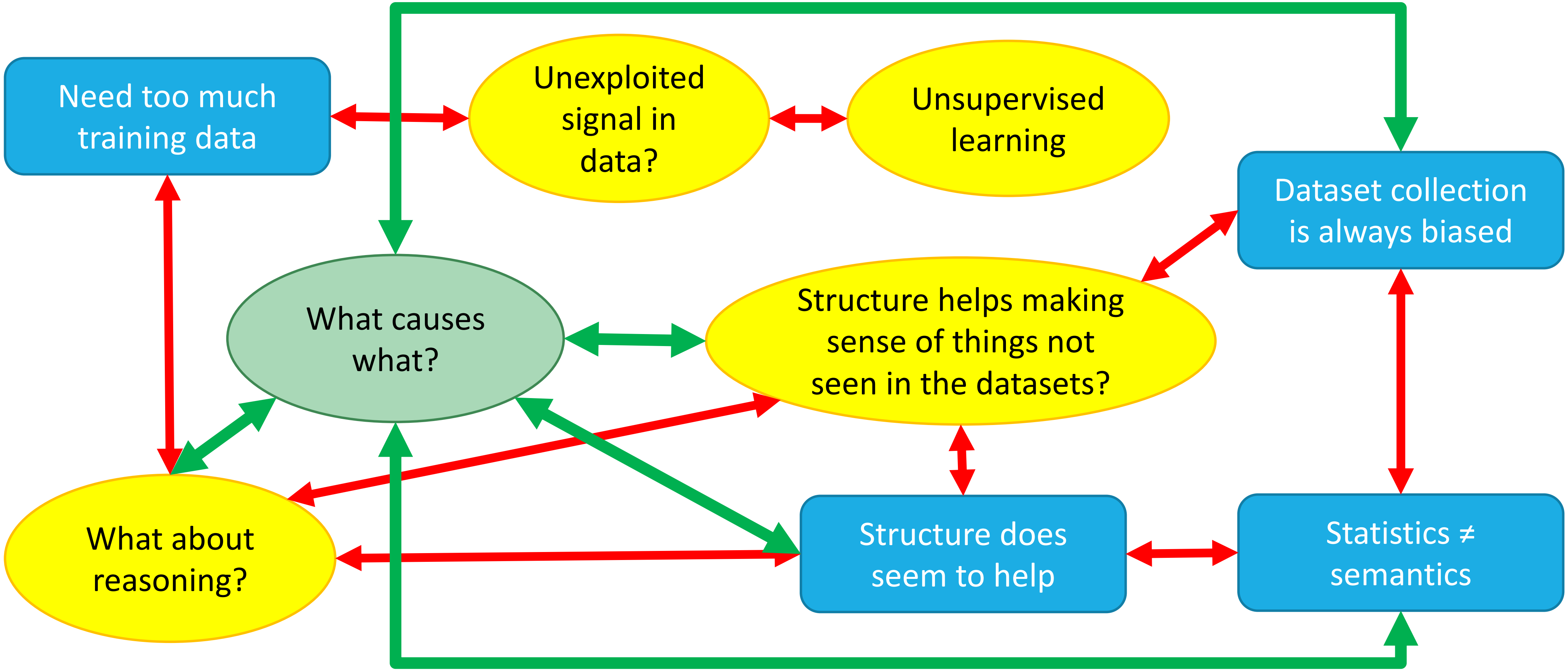
Structure helps making sense of things not seen in the datasets?

What about reasoning?

Structure does seem to help

Statistics ≠ semantics

Causation



Need too much training data

Unexploited signal in data?

Unsupervised learning

Dataset collection is always biased

What causes what?

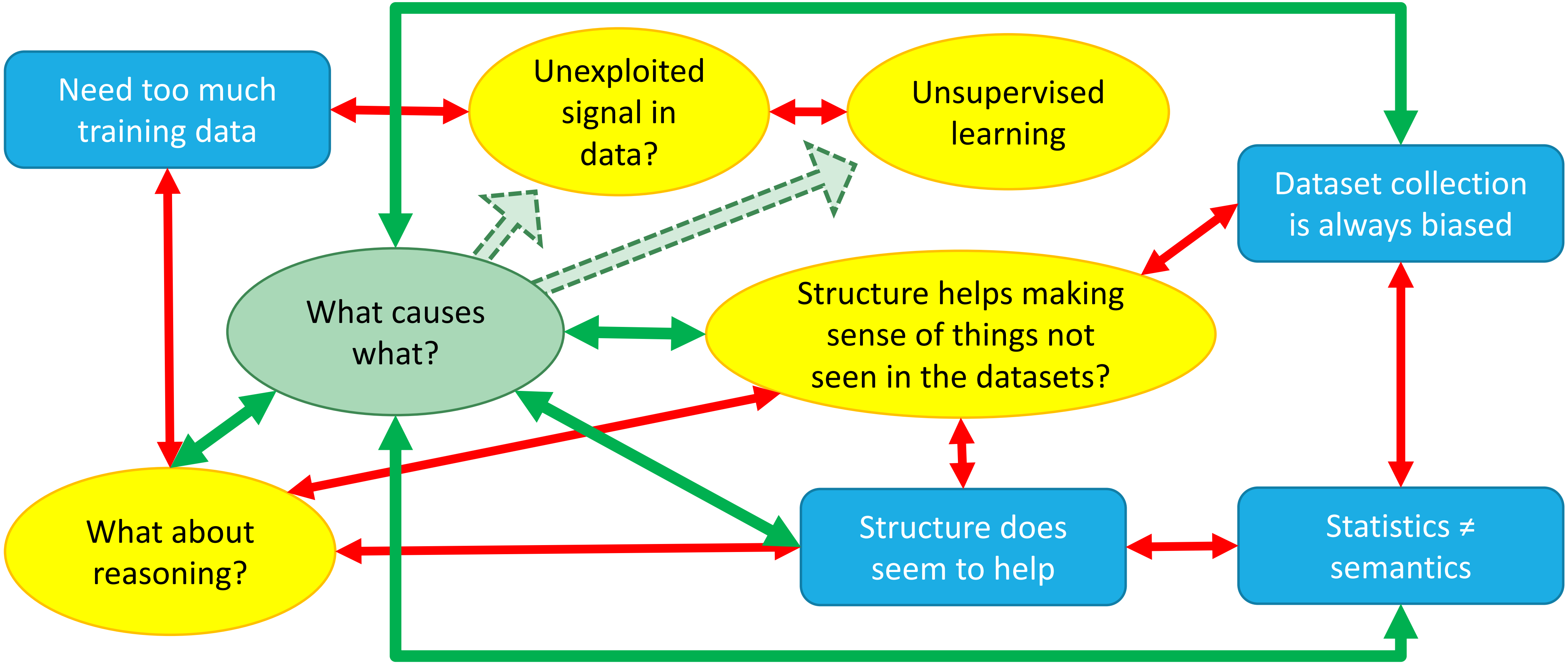
Structure helps making sense of things not seen in the datasets?

What about reasoning?

Structure does seem to help

Statistics ≠ semantics

What about these arrows?



Need too much training data

Unexploited signal in data?

Unsupervised learning

Dataset collection is always biased

What causes what?

Structure helps making sense of things not seen in the datasets?

What about reasoning?

Structure does seem to help

Statistics ≠ semantics

4- Causation hints

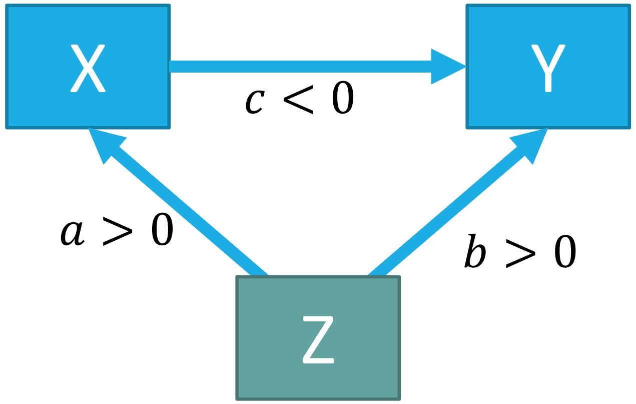
(LOPEZ-PAZ, NISHIHARA, CHINTALA, SCHÖLKOPF, & BOTTOU - CVPR17)

Causal information in the data distribution?

Causation ≠ Correlations

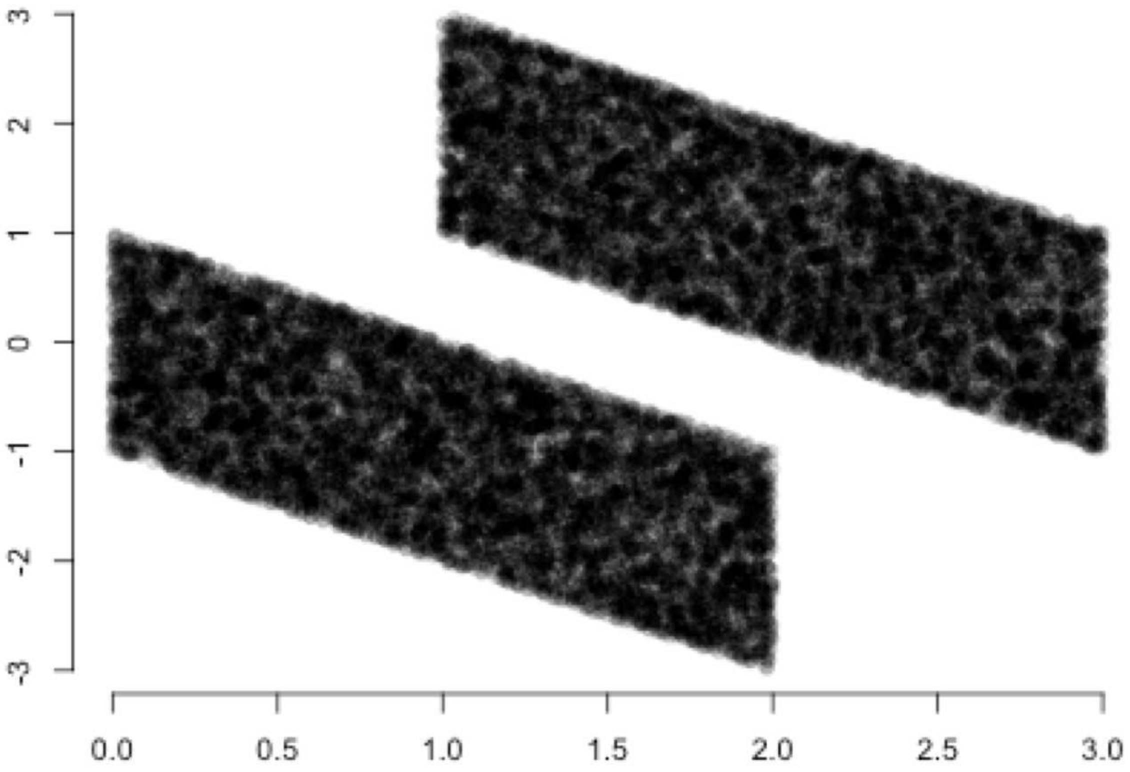
Simpson confounding

$X = aZ + \mathcal{U}(-s_1, s_1)$ $\quad$ $Y = bZ + cX + \mathcal{U}(-s_2, s_2)$

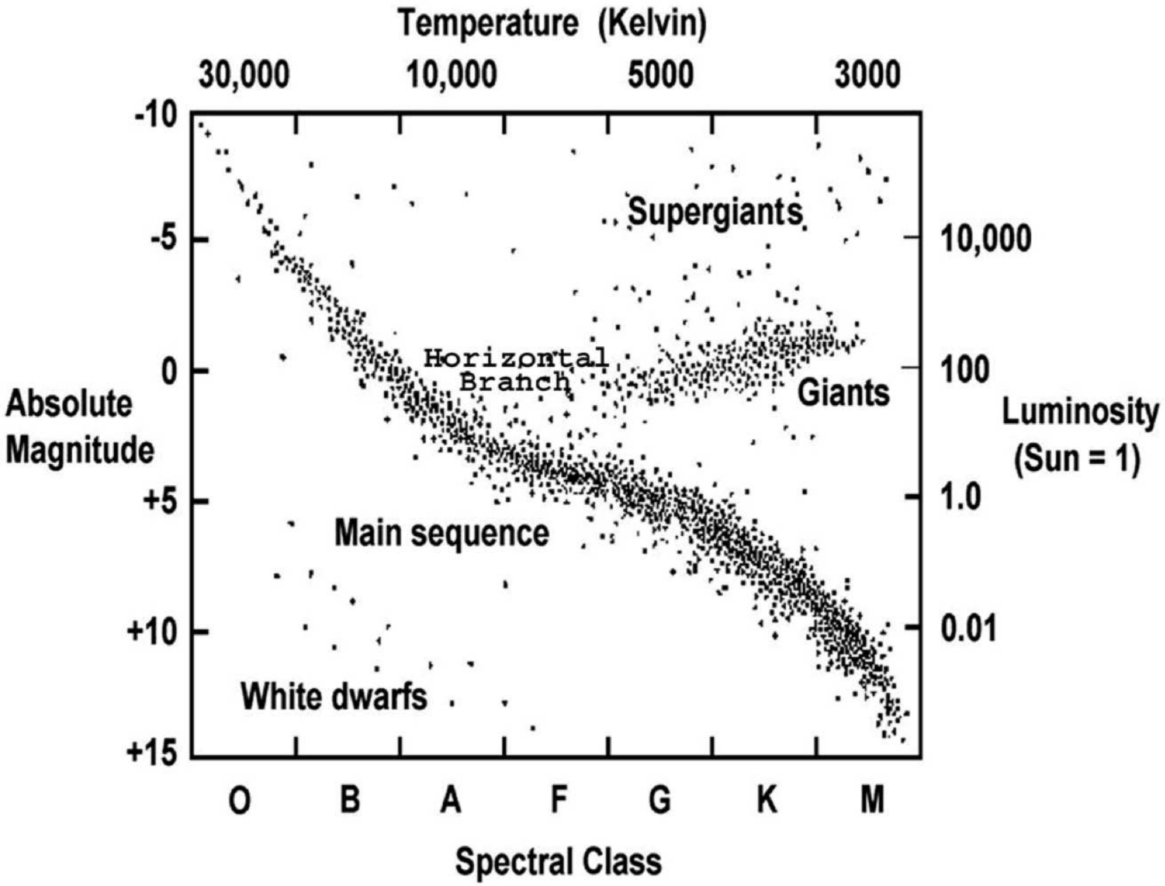


$Z \sim \text{Bernoulli}, p = \frac{1}{2}$

Causal footprints in the XY-scatterplot!



More scatterplots



The Hertzsprung–Russell diagram shows the relationship between the stars' absolute magnitudes or luminosities versus their stellar classifications or effective temperatures.

Scientists clearly draw causal conclusions from a scatterplot, even when interventions are impossible.

Causal information in the data distribution?

- Observation can lead to causal intuitions.
- We can then apply the scientific method.

How to build an unsupervised learning machine that gets causal intuitions?

5- Causal direction

(LOPEZ-PAZ, NISHIHARA, CHINTALA, SCHÖLKOPF, & BOTTOU - CVPR17)

Causal problems with two variables

Given two observed variables X, Y

I. Either X causes Y,

II. or Y causes X,

III. or X and Y have unobserved common causes,

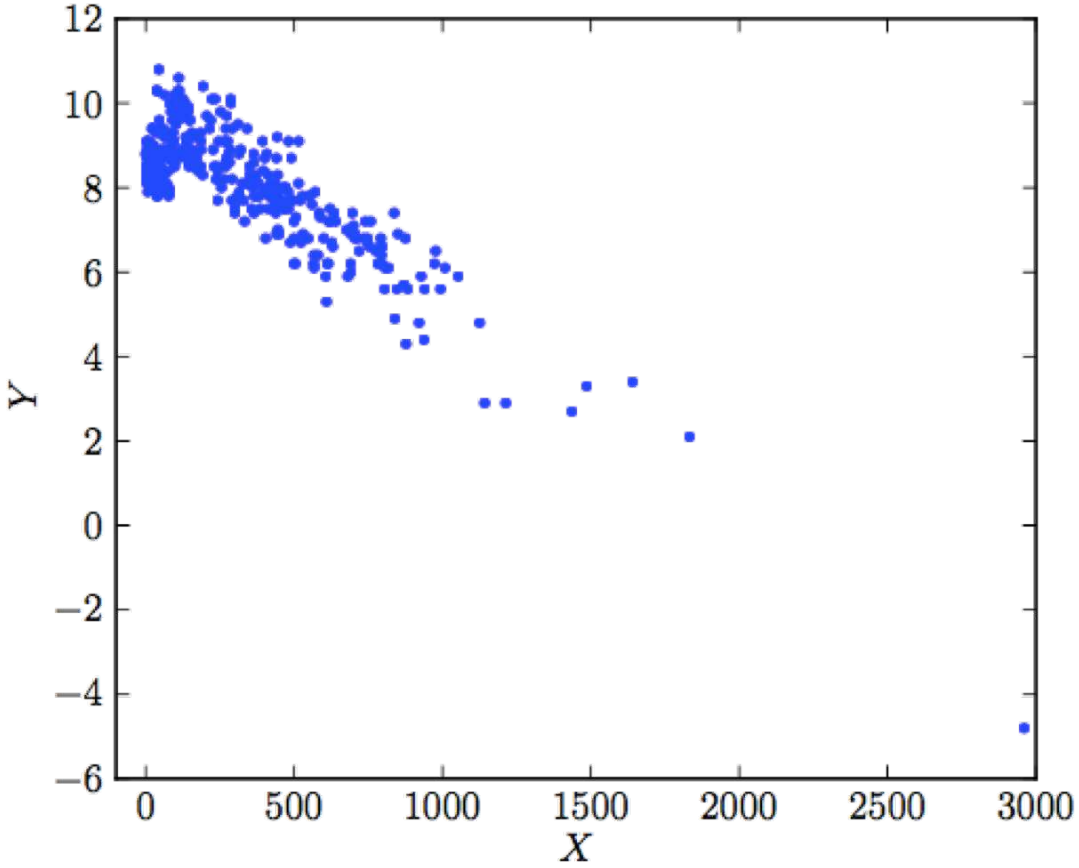
IV. or X and Y are independent.

Reichenbach

potentially confounding

Let’s focus on causal direction detection (I and II)

How does causal direction look like?



In this scatter plot

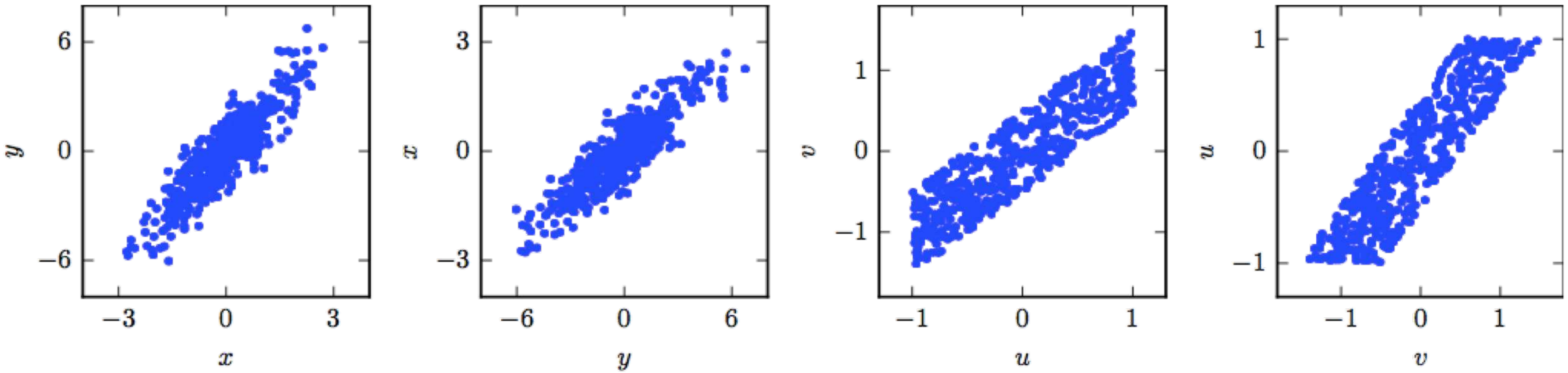
- X is altitude.
- Y is average temperature.

Does the scatter plot reveal whether

- X causes Y
- or Y causes X ?

Footprint example 1 – additive noise

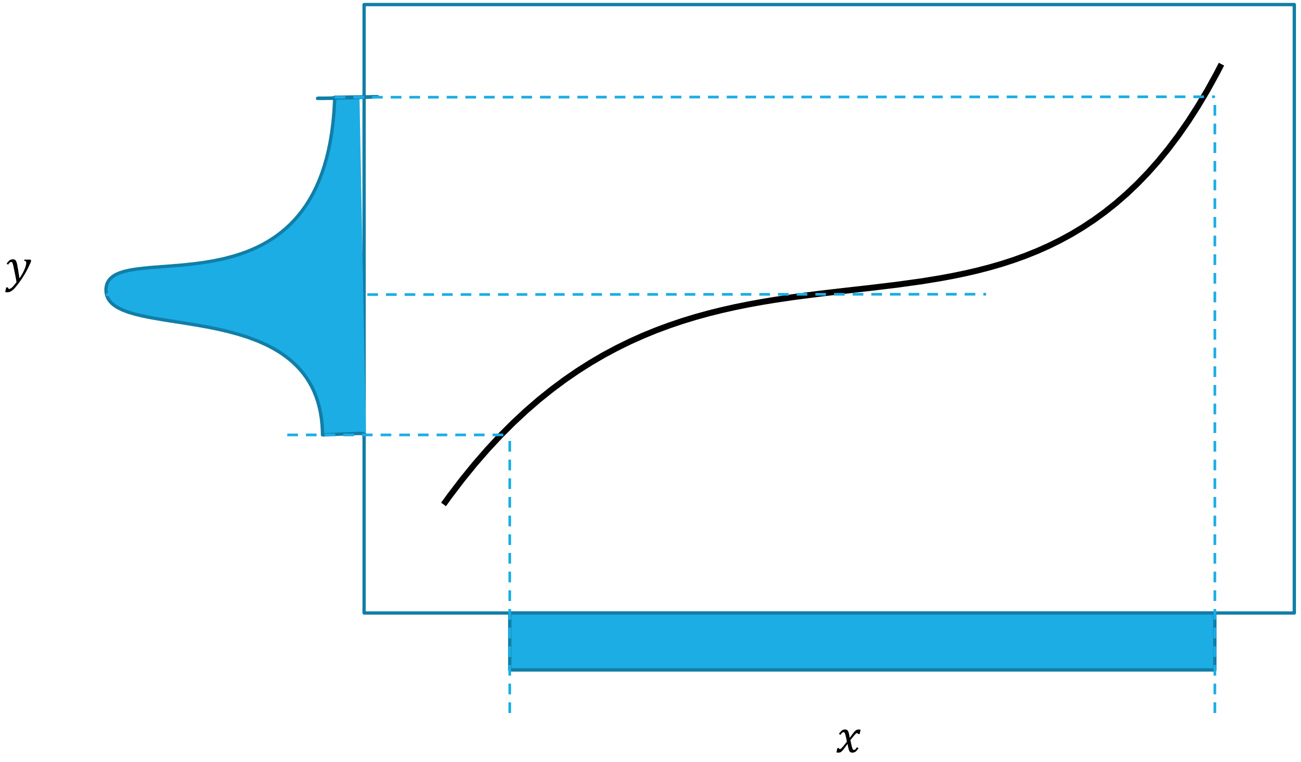
$Y = \alpha\, X + \beta + Noise$



Sometimes the high moments (the corners) reveal something.

(PETERS ET AL., 14)

Footprint example 2 -- coincidences



(JANZING ET AL., 2011)

From scatterplot to causation direction

Detecting causation direction at scale

- We could build a long list of causal footprint examples, then decide which example is most appropriate for a given scatterplot, etc.
- Or we can construct a classifier...

(Lopez-Paz, et al., 2015)

Featurizing a scatterplot

High moments?

- $F_{rs} = \frac{1}{m} \sum_{j=1}^{m} x_j^r y_j^s$ for well chosen r and s.

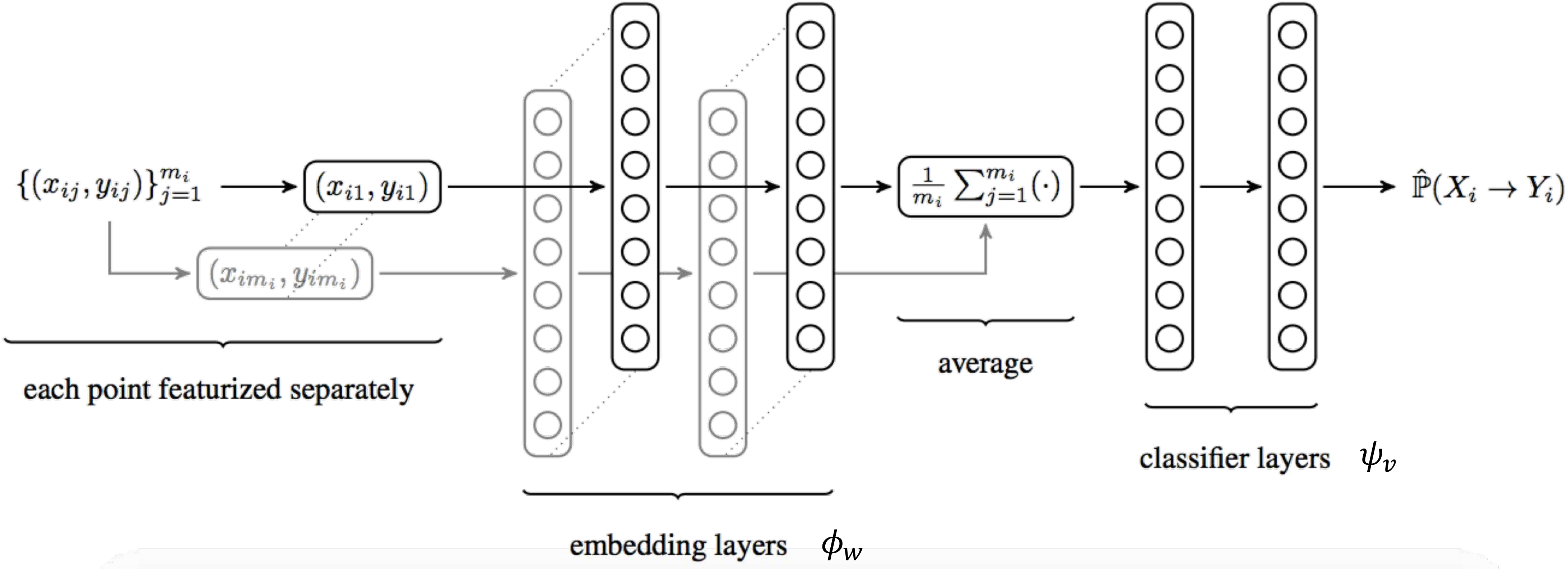
Reproducing Kernel Hilbert space?

- $F = \frac{1}{m} \sum_{j=1}^{\infty ?} \phi(x_j,\ y_j) \in \mathcal{H}_K$ with $\langle \phi(.), \phi(.) \rangle_K = K(.,.)$

Learning the features and the classifier

- $F_w = \frac{1}{m} \sum_{j=1}^{m} \phi_w(x_j,\ y_j)$

Neural Causation Classifier


$\{(x_{ij}, y_{ij})\}_{j=1}^{m_i}$
(x_{i1}, y_{i1})
(x_{im_i}, y_{im_i})
$\frac{1}{m_i}\sum_{j=1}^{m_i}(\cdot)$
$\hat{\mathbb{P}}(X_i \to Y_i)$
each point featurized separately
embedding layers ϕ_w
average
classifier layers ψ_v

Training NCC

We do not have access to large causal direction datasets

But we can generate artificial scatterplots.

$$Y = f(X) + v(X)\varepsilon$$

Step 1 - draw distribution on X

- Draw $k \sim \mathcal{U}\{1,2,3,4,5\}$ $\quad \mathrm{r, s} \sim \mathcal{U}[0,5]$
- Take a mixture of k Gaussians with $\mu \sim \mathcal{N}(0, r)$ and $\sigma \sim \mathcal{N}(0, s)$

Training NCC

Step 2 - draw mechanism f

- Cubic spline with random number of random knots…

Step 3 - draw noise

- Noise ε is Gaussian with random variance $\sim\mathcal{U}[0,5]$
- Function $v(X)$ is another cubic spline with random knots.

Step 4 – generate causal scatter plot $X \rightarrow Y$

- Draw x_j, ε_j then compute $y_j = f(x_j) + v(x_j)\varepsilon_j$
- Rescale x_j, y_j to enforce marginal mean 0 and sdev 1

Training NCC

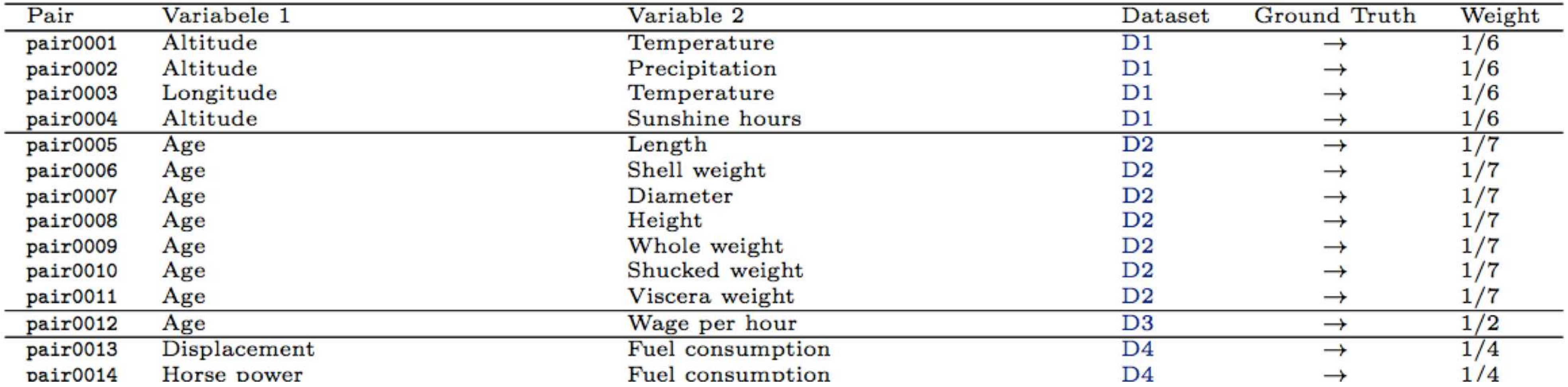
Step 6 – Generate training examples

- Scatterplot $\{(x_j, y_j)\}$ is associated with target label 1
- Scatterplot $\{(y_j, x_j)\}$ is associated with target label 0

Repeat 100000 to generate a training set.
Train the neural network classifier with the usual bag of tricks.
(dropout regularization, rmsprop, cross-validation, etc.)

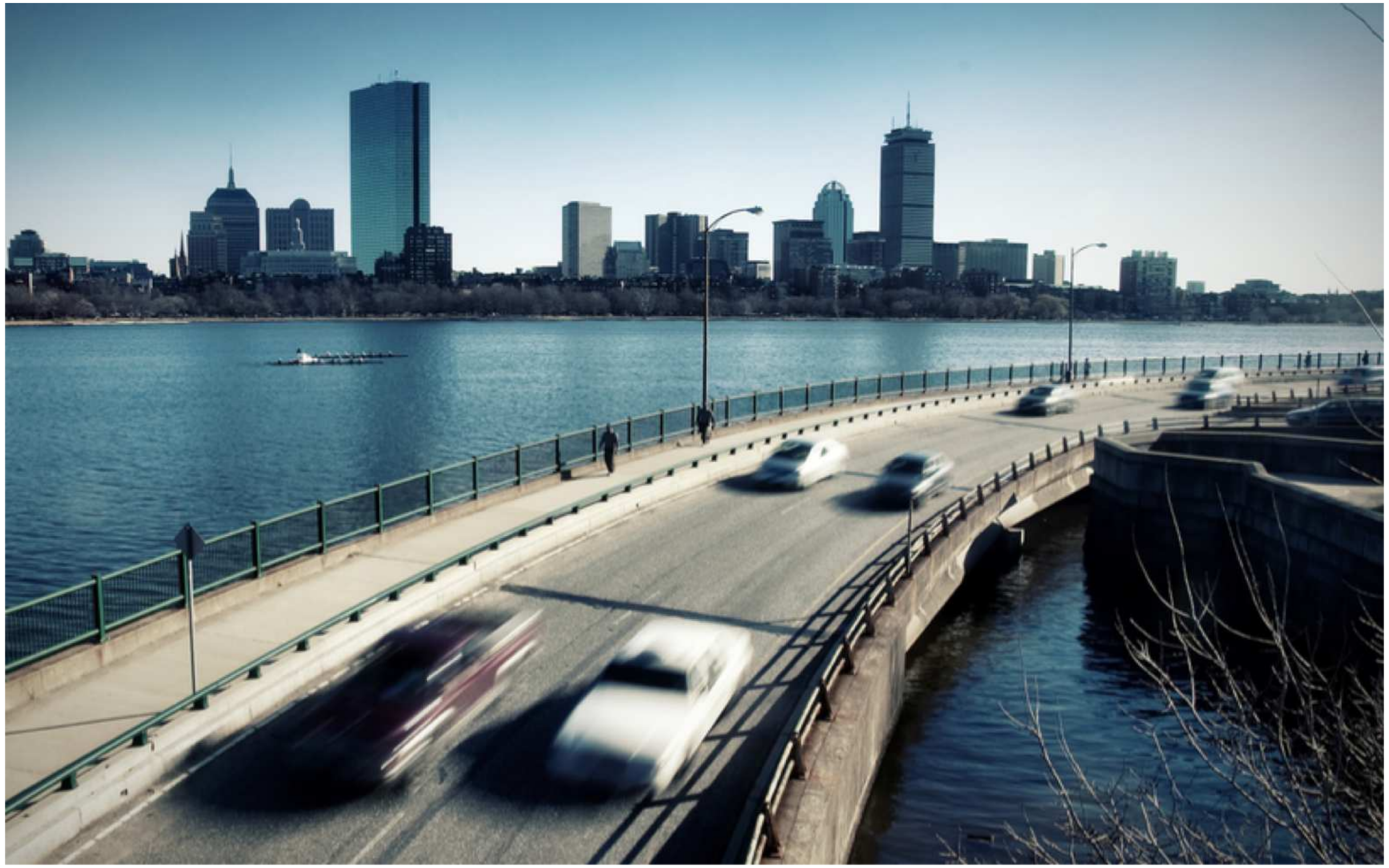
Sanity check

- After training on artificial data, NCC achieves state-of-the-art [79%] performance on the *Tübingen cause-effect dataset”,* which contains 100 cause-effect pairs (https://webdav.tuebingen.mpg.de/cause-effect)



Pair	Variabele 1	Variable 2	Dataset	Ground Truth	Weight
pair0001	Altitude	Temperature	D1	→	1/6
pair0002	Altitude	Precipitation	D1	→	1/6
pair0003	Longitude	Temperature	D1	→	1/6
pair0004	Altitude	Sunshine hours	D1	→	1/6
pair0005	Age	Length	D2	→	1/7
pair0006	Age	Shell weight	D2	→	1/7
pair0007	Age	Diameter	D2	→	1/7
pair0008	Age	Height	D2	→	1/7
pair0009	Age	Whole weight	D2	→	1/7
pair0010	Age	Shucked weight	D2	→	1/7
pair0011	Age	Viscera weight	D2	→	1/7
pair0012	Age	Wage per hour	D3	→	1/2
pair0013	Displacement	Fuel consumption	D4	→	1/4
pair0014	Horse power	Fuel consumption	D4	→	1/4

Counterfactual on images



Asymmetric relation

- How would this image would have looked like if one had removed the cars?
- How would this image would have looked like if one had removed the bridge?

Can we use image datasets to identify the *causal dispositions* of object categories?

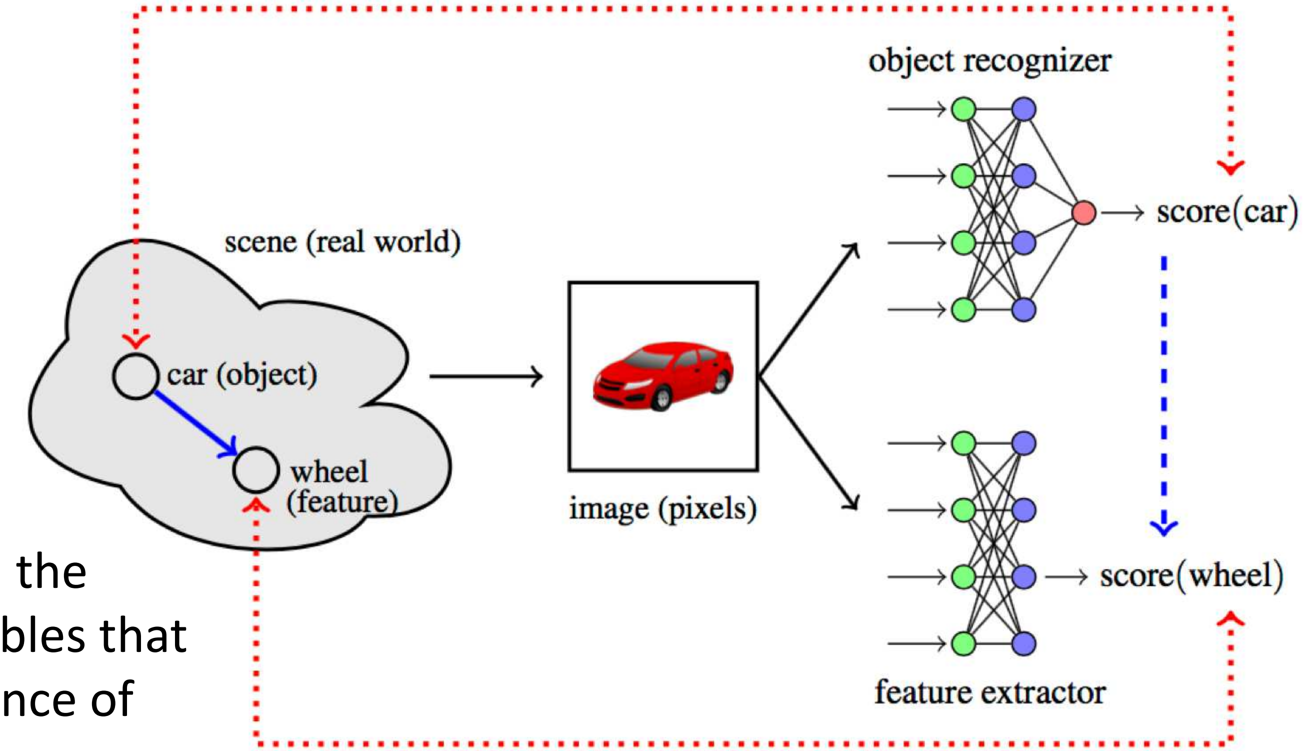
How to validate a result?

Causal and anti-causal features

For each object category, we can also define two sets of scene features

- The causal features are those that cause the presence of the object of interest. *If the object of interest had not been present in the image, these feature would still have appeared*.
- The anticausal features are those that are caused by the presence of the object of interest. *If the object of interest had not been present in the image, these feature would not have appeared*.

Proxy variables & shadow footprints



Assume there is
a causal footprint in the distribution of variables that represent the presence of an object or a feature

We apply NCC to these scores reveals to find out which features are causal or anticausal for each object category

Same pre-trained NCC for all categories!

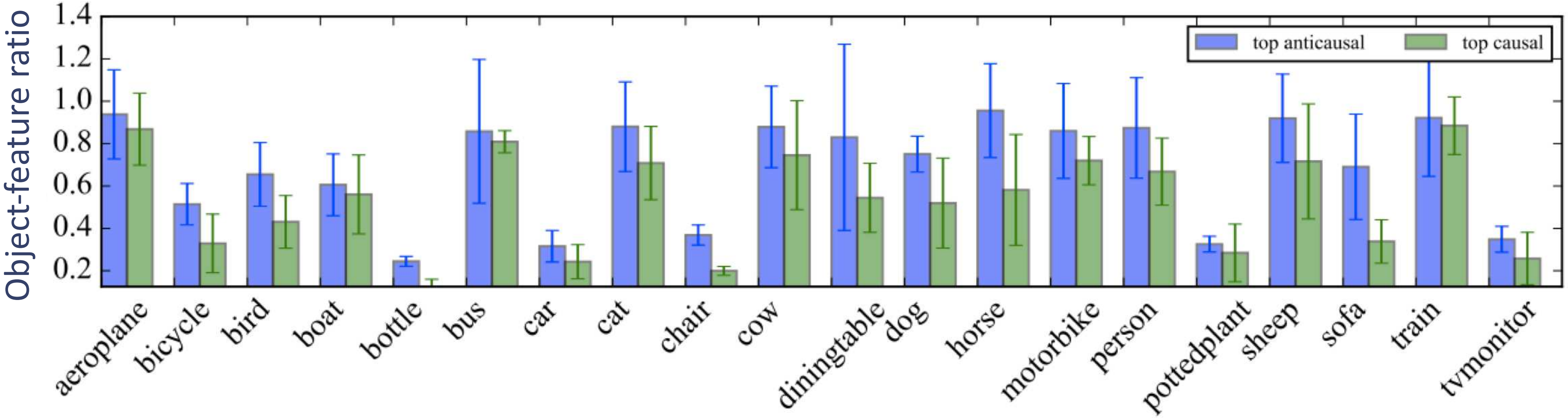
Object features and context features

In computer vision, one is often interested in another distinction

- The object features "belong" to the object and are most often activated inside the object bounding box.
  Example: car wheels, person eyes, etc.
- The context features are those most often activated outside the bounding box.
  Example: road under a car, car shadow

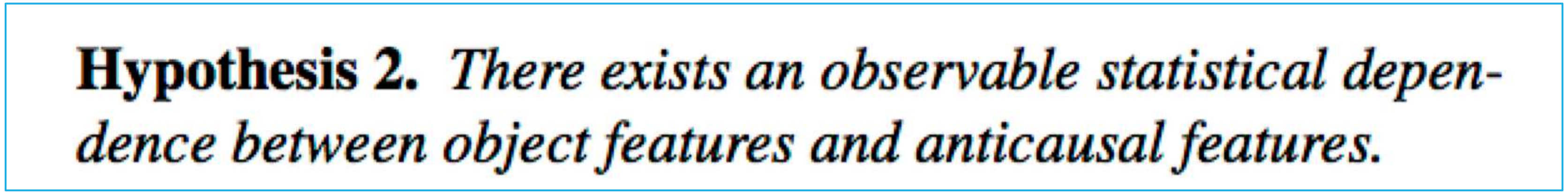
Background story
"bags of visual words"

Results



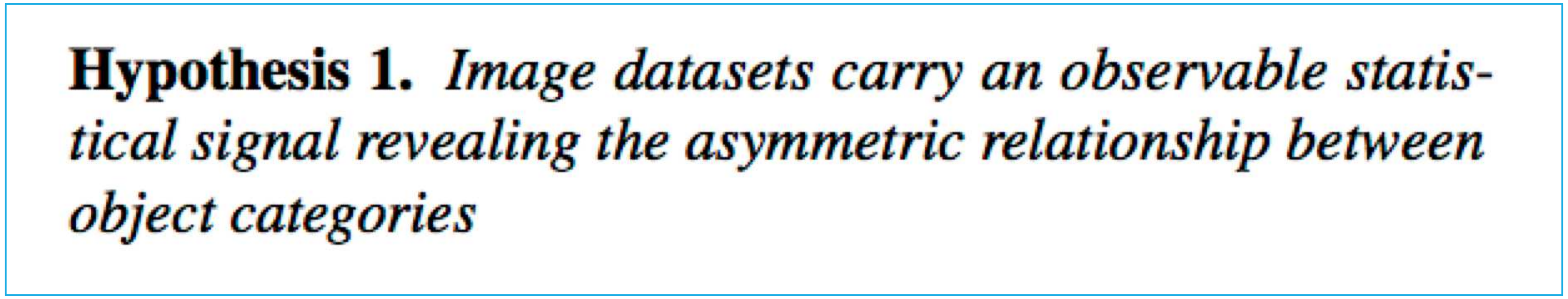
- Top anticausal features have higher object scores for all twenty categories.
- The probability that this happens for all 20 classes out of chance is $2^{-20} \approx 10^{-6}$.

Hypotheses



Hypothesis 2. *There exists an observable statistical dependence between object features and anticausal features.*

⇒



Hypothesis 1. *Image datasets carry an observable statistical signal revealing the asymmetric relationship between object categories*

More information

- The effect disappears completely if we replace NCC by the correlation coefficient (or its absolute value) between the feature and the category.
- The effect appears to be robust to many details of the experiment such as the precise composition of the NCC data, the precise computation of object/context scores, the methods we use to determine a continuous proxy for the categories, etc.

6- Causation and unsupervised learning

(WITH MARTIN ARJOVSKY, DAVID LOPEZ-PAZ AND MAXIME OQUAB)

The mythical unsupervised learning

What is inside the cake?

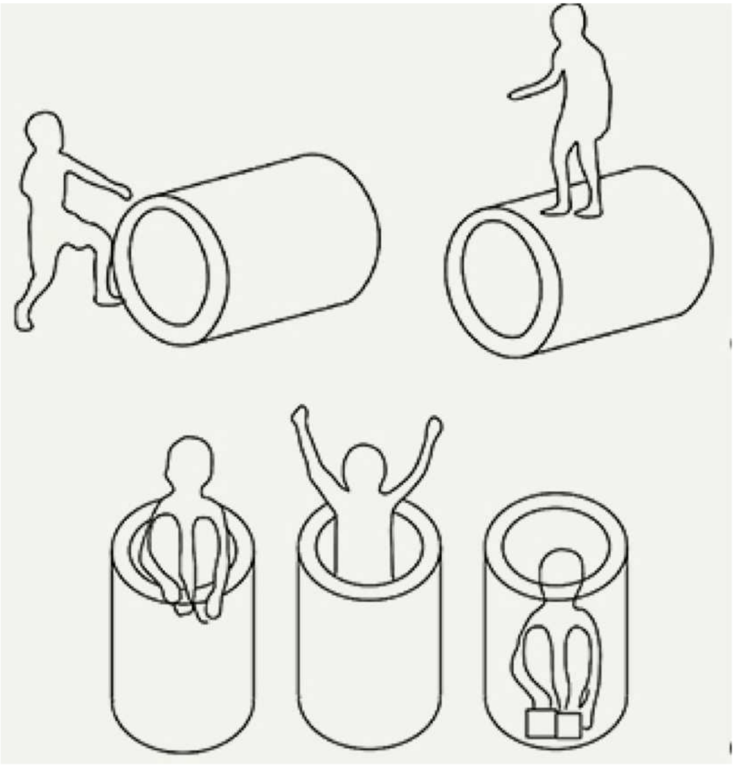
- Yann says "predictive modeling"
  and speaks about multimodal distributions.

  "when the pen falls, you do not know exactly where it will fall, but you know that the floor will stop it."

- Without labels, everything is in $P(X)$.
  Statisticians say "density estimation".

  See (Hastie et al., 2009) chapter 14.

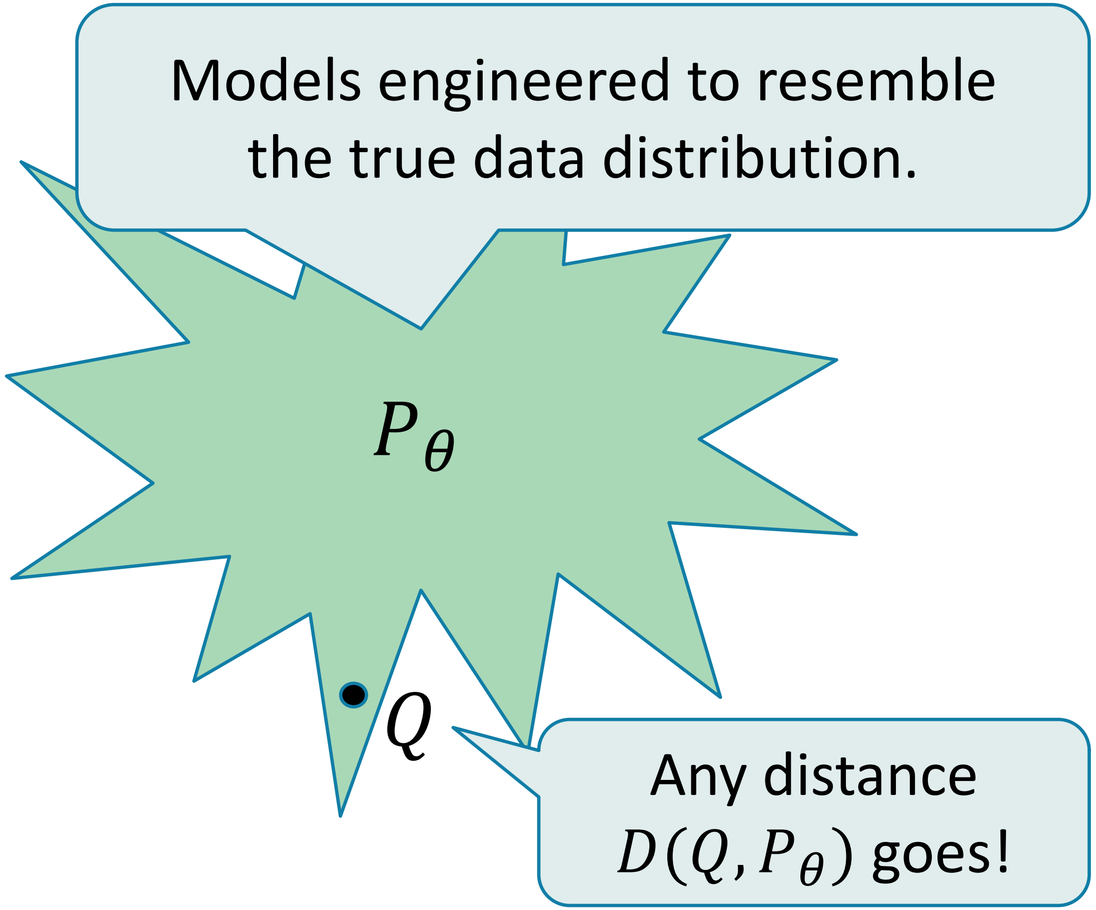
The mythical unsupervised learning



What is inside the cake?

- What about "discovering affordances"?
  - what can I do with a new toy?
  - what can others do with it?
  - what will be the result?
- This entails "discovering causal mechanisms"
  - whoever knows the distribution can reproduce what was demonstrated in the training data.
  - whoever knows the causal mechanism can play with the new toy in new ways.

Traditional unsupervised learning



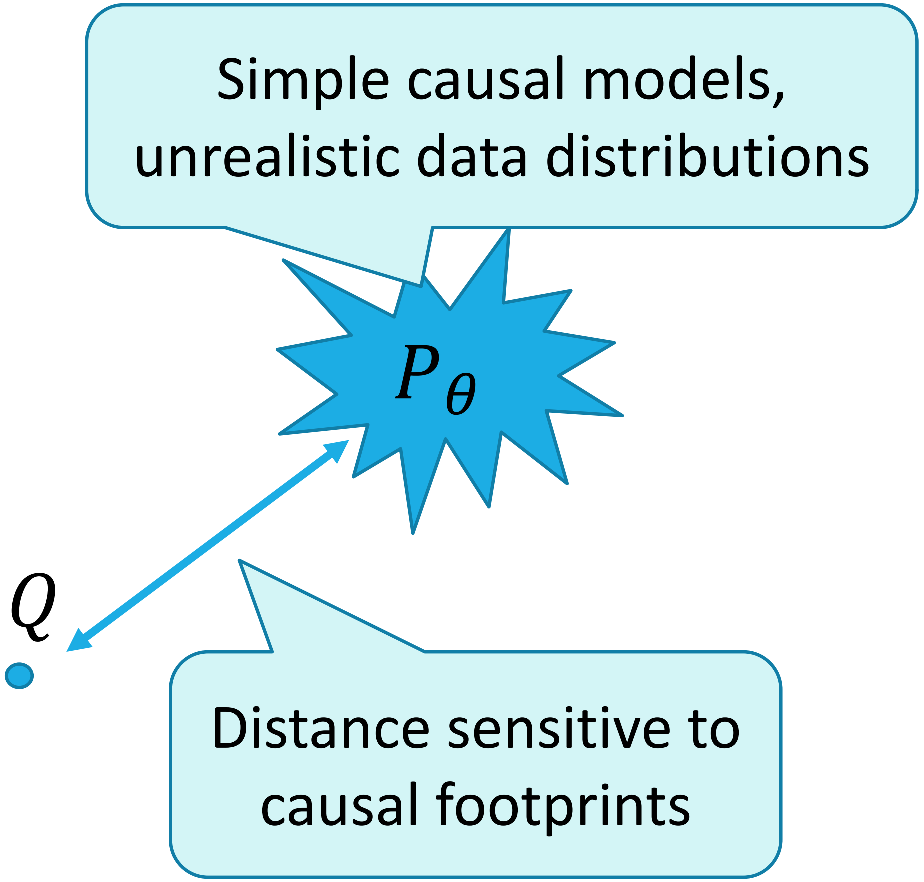
Models engineered to resemble the true data distribution.

Any distance $D(Q, P_\theta)$ goes!

- Most systems train θ using the Maximum Likelihood Principle.
- If any observation has likelihood zero, the likelihood of the whole data set is zero, and its maximization is meaningless.
- Therefore one must model everything.
- This is why the models are highly engineered to resemble the true distribution enough.
- Complex models.

Simple models for a complex world

Alternative approach



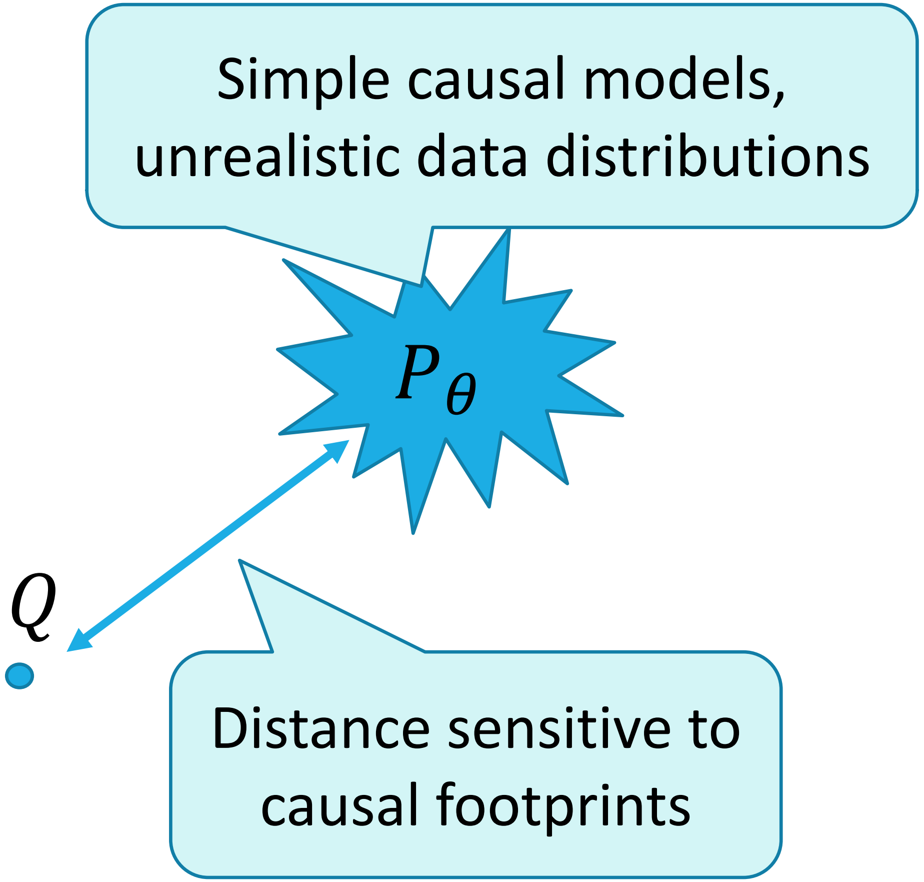
Simple causal models, unrealistic data distributions

Distance sensitive to causal footprints

- When Q is far from the optimal P_θ, optimizing different distances $D(Q, P_\theta)$ yields different solutions.

- Minimizing a distance $D(Q, P_\theta)$ sensitive to causation hints will select a model P_θ that possesses the same hints as the target distribution Q,
- … and hopefully reveal causal phenomena.

Alternative approach


Simple causal models, unrealistic data distributions
P_θ
Q
Distance sensitive to causal footprints

- When Q is far from the optimal P_θ, optimizing different distances $D(Q, P_\theta)$ yields different solutions.

- Minimizing a di
  sensitiv
  pefully reveal causal
  henomena.

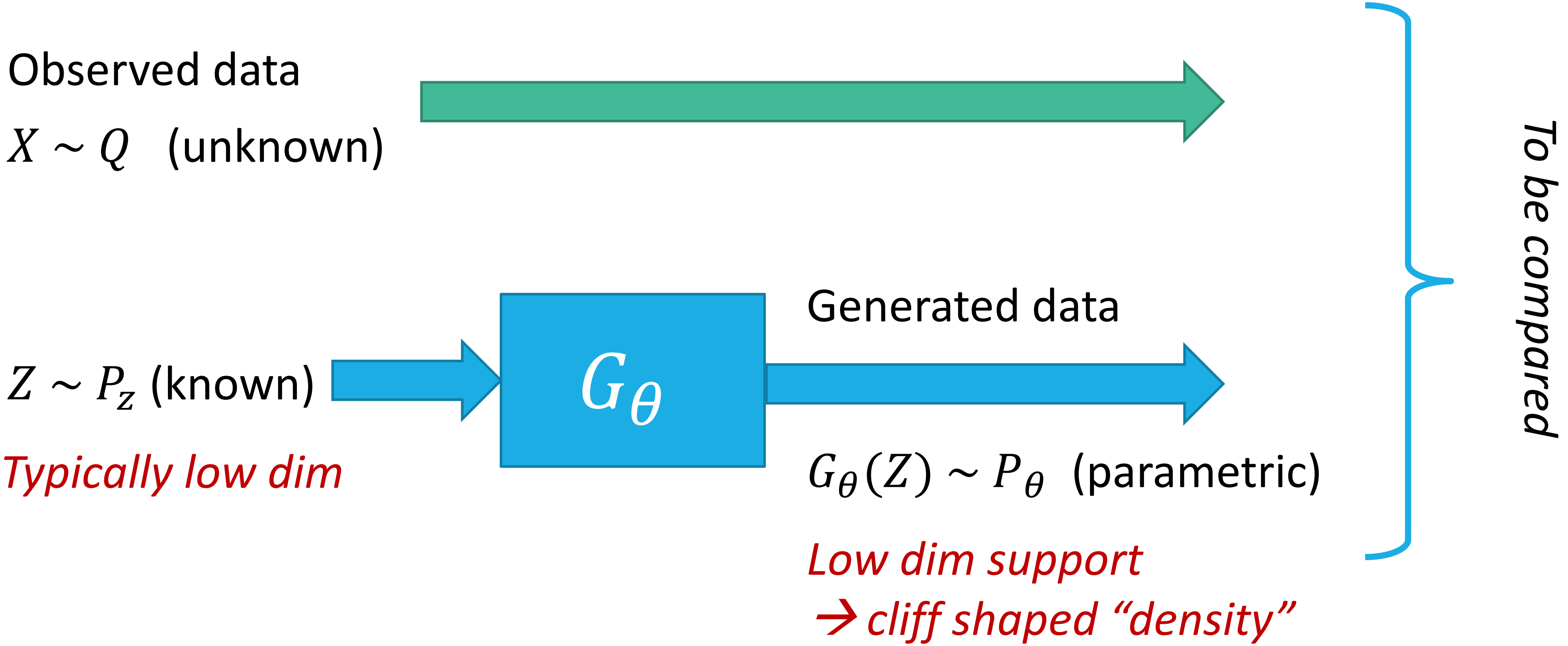
How to construct such a distance?

Distances

How to construct such a distance?

- We do not know how to construct a distance that is sensitive to causal hints.
- Let’s start by looking at the known probabilistic distances.
- Implicit distribution models are amenable to many distances.
- The popular generative adversarial networks are a good example of implicit modeling.

Implicit modeling



Observed data

$X \sim Q$ (unknown)

$Z \sim P_z$ (known)

Typically low dim

Generated data

$G_\theta(Z) \sim P_\theta$ (parametric)

Low dim support

→ cliff shaped "density"

To be compared

Comparing distributions

- The *Total Variation* (TV) distance

$$\delta(\mathbb{P}_r, \mathbb{P}_g) = \sup_{A \in \Sigma} |\mathbb{P}_r(A) - \mathbb{P}_g(A)| \ .$$

- The *Kullback-Leibler* (KL) divergence

$$KL(\mathbb{P}_r \| \mathbb{P}_g) = \int \log\left(\frac{P_r(x)}{P_g(x)}\right) P_r(x) d\mu(x) \ ,$$

VAE

requires densities, asymmetric, possibly infinite

Comparing distributions

- The *Jensen-Shannon* (JS) divergence

$$JS(\mathbb{P}_r, \mathbb{P}_g) = KL(\mathbb{P}_r \| \mathbb{P}_m) + KL(\mathbb{P}_g \| \mathbb{P}_m) \ ,$$

symmetric, does not require densities, $0 \leq JS \leq \log(2)$

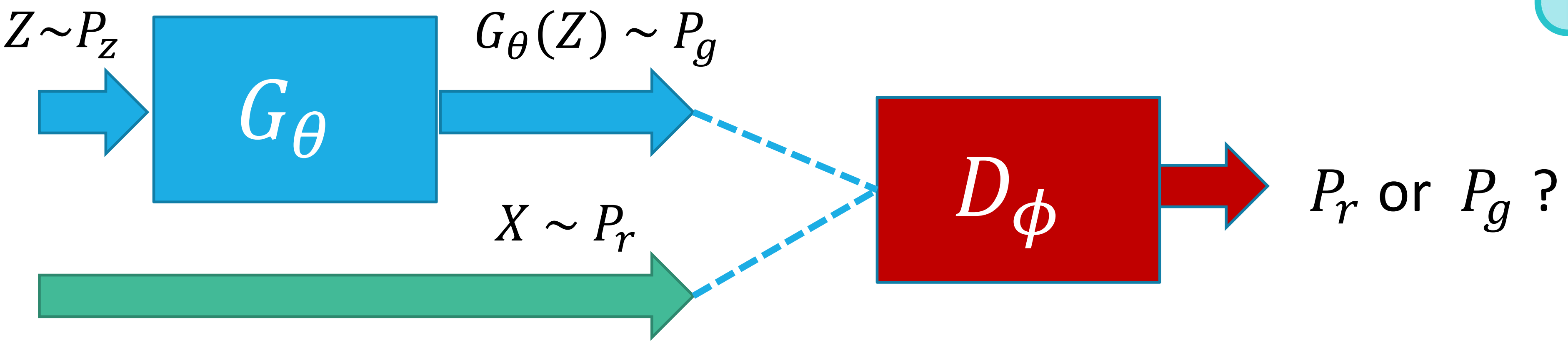
- The *Earth-Mover* (EM) distance or Wasserstein-1

$$W(\mathbb{P}_r, \mathbb{P}_g) = \inf_{\gamma \in \Pi(\mathbb{P}_r, \mathbb{P}_g)} \mathbb{E}_{(x,y)\sim\gamma}\big[\, \|x - y\| \,\big] \ ,$$

always defined, involves metric on underlying space.

Generative adversarial network

GAN



Discriminator maximizes and generator minimizes

$$L(\phi, \theta) = \mathbb{E}_{x \sim \mathbb{P}_r}[\log D_\phi(x)] + \mathbb{E}_{z \sim p_Z}[\log(1 - D_\phi(g_\theta(z)))]$$

Findings (work in progress)

1. We should prefer topologically weak distances
2. Optimizing a Wasserstein-like distance makes GANS work more reliably.
3. There are other topologically weak distances with better statistical properties and better optimization algorithms than the Wasserstein distance. But these distances also impose strict geometry constraints that may
   a. make it harder to minimize the nonconvex landscape,
   b. be incompatible with the idea of a distance sensitive to causal hints.

- (1) (2) : (Arkovsky et al., "Wasserstein GANS", ICML 2017)
- (3a) : (Bottou et al., "Geometrical Insights for Implicit Generative Modeling", ArXiV:1712.07822, 2017)

Findings (work in progress)

1. We should prefer topologically weak distances
2. Optimizing a Wasserstein-like distance makes GANS work more reliably.
3. There are other topologically weak distances with better statistical properties and better optimization algorithms than the Wasserstein distance. But these distances also impose strict geometry constraints that may
   a. make it harder to minimize the nonconvex landscape,
   b. be incompatible with the idea of a distance sensitive to causal hints.

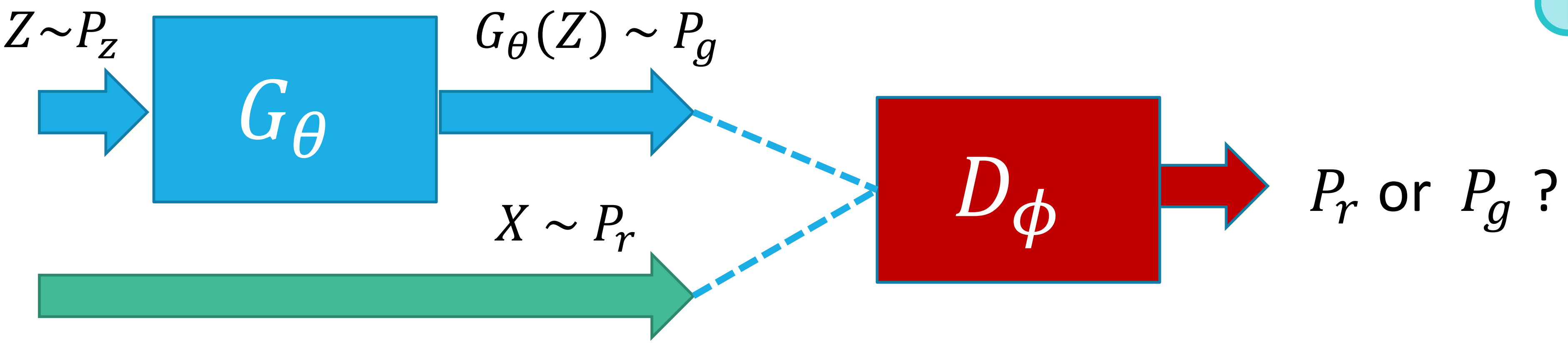
- (1) (2) : (Arkovsky et al., "Wasserstein GANS", ICML 2017)
- (3a) : (Bottou et al., "Geometrical Insights for Implicit Generative Modeling", ArXiV:1712.07822, 2017)

7- Wasserstein GANs

(ARJOVSKY, CHINTALA, BOTTOU, 2017)

Generative adversarial network

GAN



Discriminator maximizes and generator minimizes

$$L(\phi,\theta) = \mathbb{E}_{x\sim\mathbb{P}_r}[\log D_\phi(x)] + \mathbb{E}_{z\sim p_Z}[\log(1 - D_\phi(g_\theta(z)))]$$

Generative adversarial network

Discriminator maximizes and generator minimizes

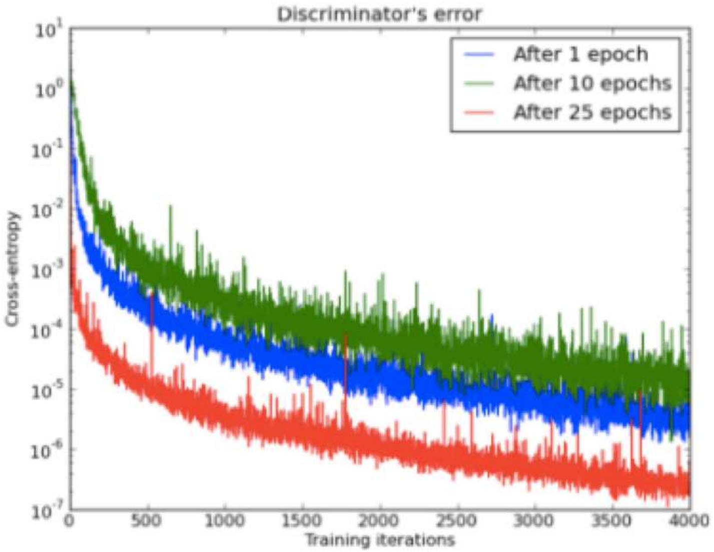
$$L(\phi, \theta) = \mathbb{E}_{x \sim \mathbb{P}_r}[\log D_\phi(x)] + \mathbb{E}_{z \sim p_Z}[\log(1 - D_\phi(g_\theta(z)))]$$

Nasty saddle point problem

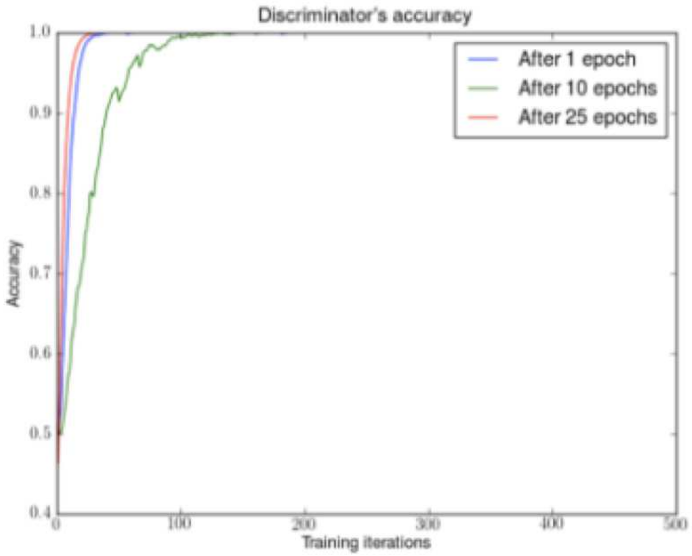
- Keeping the discriminator optimal :
  $\min_\theta L(\phi^*(\theta), \theta)$ minimizes $JS(P_r, P_g)$
- Keeping the generator optimal
  $\max_\phi L(\phi, \theta^*(\phi))$ yields garbage

Problem with GAN training

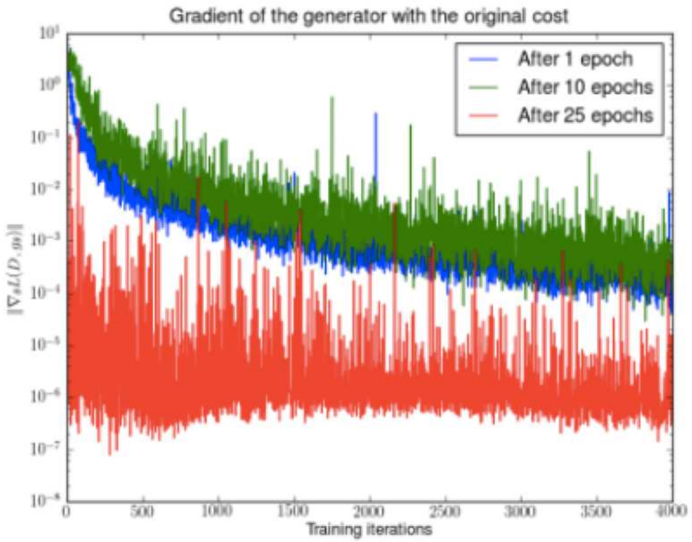
If one trains the discriminator thoroughly, the generator receives no gradient…



Discriminator's error



Discriminator's accuracy



Gradient of the generator with the original cost

Alternate GAN training

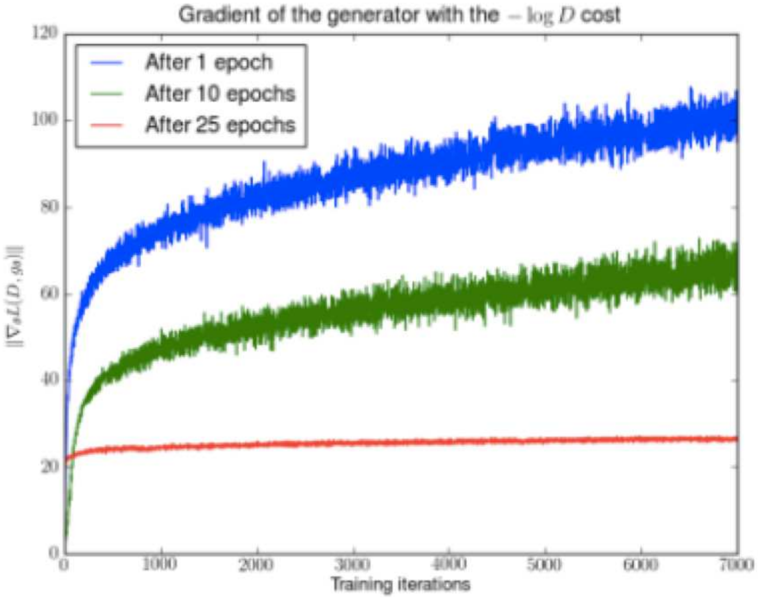
Alternate update that has less vanishing gradients

$$\Delta\theta \propto \mathbb{E}_{z\sim p_Z}[\nabla_\theta \log(D_\phi(g_\theta(z)))]$$

Under optimality optimizes

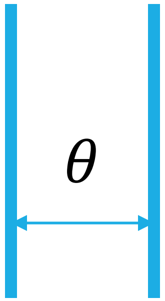
$$KL(\mathbb{P}_\theta \| \mathbb{P}_r) - 2JSD(\mathbb{P}_r \| \mathbb{P}_\theta)$$

Problems: JSD with the wrong sign, reverse KL has high mode dropping. Still unstable when D is good.



Distributions with low dimensional support

Let P_0 and P_θ be two uniform distributions supported by parallel line segments separated by distance θ.



Continuous in θ

- $W(\mathbb{P}_0, \mathbb{P}_\theta) = |\theta|,$
- $JS(\mathbb{P}_0, \mathbb{P}_\theta) = \begin{cases} \log 2 & \text{if } \theta \neq 0 \text{ ,} \\ 0 & \text{if } \theta = 0 \text{ ,} \end{cases}$
- $KL(\mathbb{P}_\theta \| \mathbb{P}_0) = KL(\mathbb{P}_0 \| \mathbb{P}_\theta) = \begin{cases} +\infty & \text{if } \theta \neq 0 \text{ ,} \\ 0 & \text{if } \theta = 0 \text{ ,} \end{cases}$
- and $\delta(\mathbb{P}_0, \mathbb{P}_\theta) = \begin{cases} 1 & \text{if } \theta \neq 0 \text{ ,} \\ 0 & \text{if } \theta = 0 \text{ .} \end{cases}$

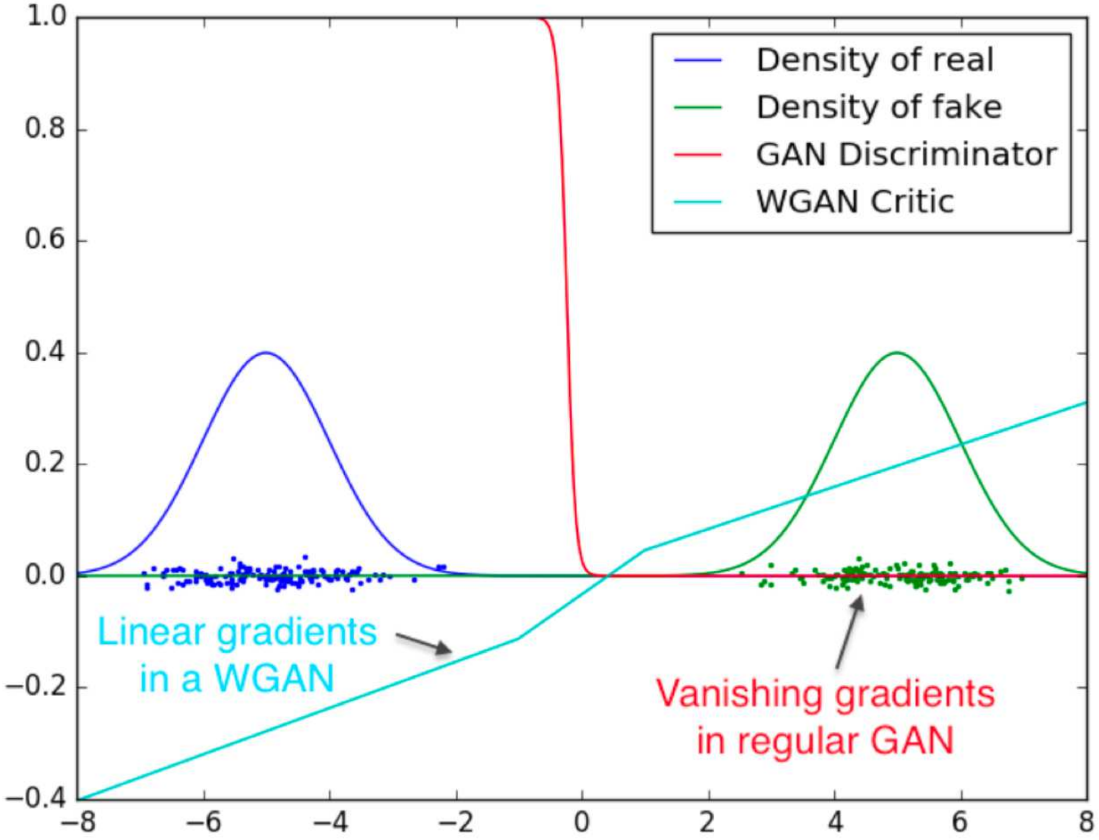
Optimizing a Wasserstein(ish) distance

Wasserstein-1 has a simple dual formulation (Kantorovich)

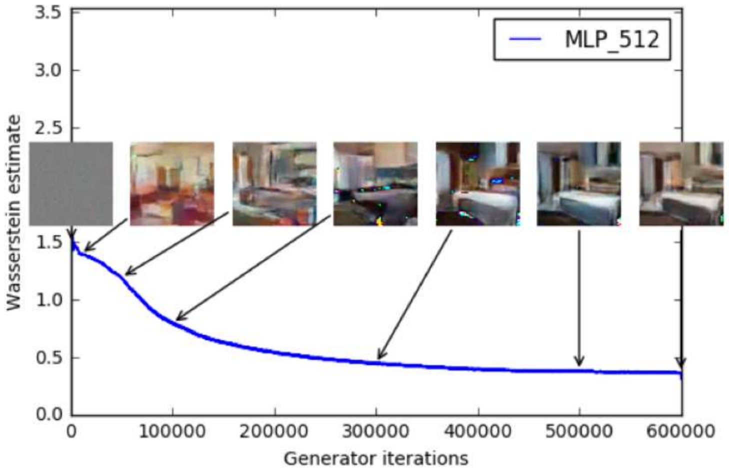
$$W(\mathbb{P}_r, \mathbb{P}_\theta) = \max_{\|f\|_L \leq 1} \mathbb{E}_{x \sim \mathbb{P}_r}[f(x)] - \mathbb{E}_{x \sim \mathbb{P}_\theta}[f(x)]$$

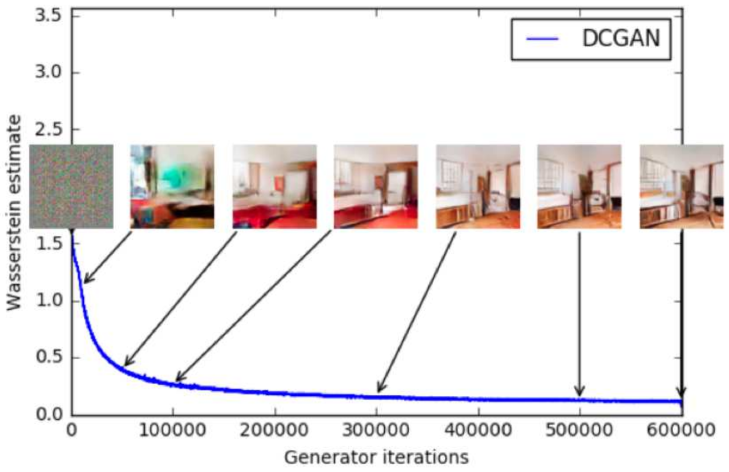
- Parametrize $f(x)$, for instance with a neural network.
- Enforce Lipschitz constraint, for instance by aggressively clipping the weights.
- Maintain $f(x)$ well trained, and train $G_\theta(z)$ by back-prop through $f(x)$.
- No vanishing gradients!

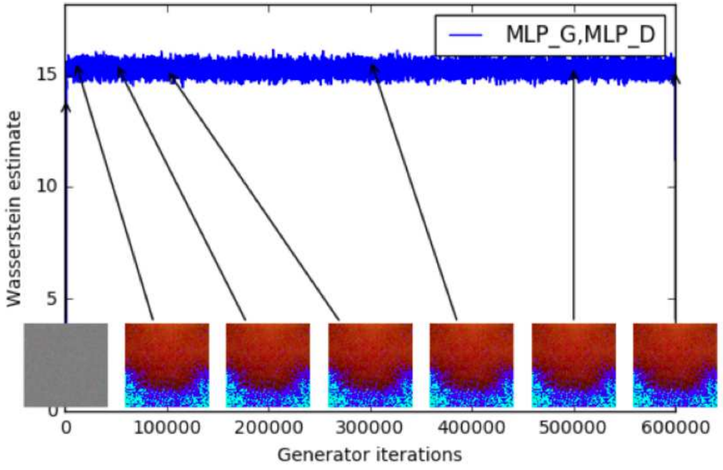
No vanishing gradients



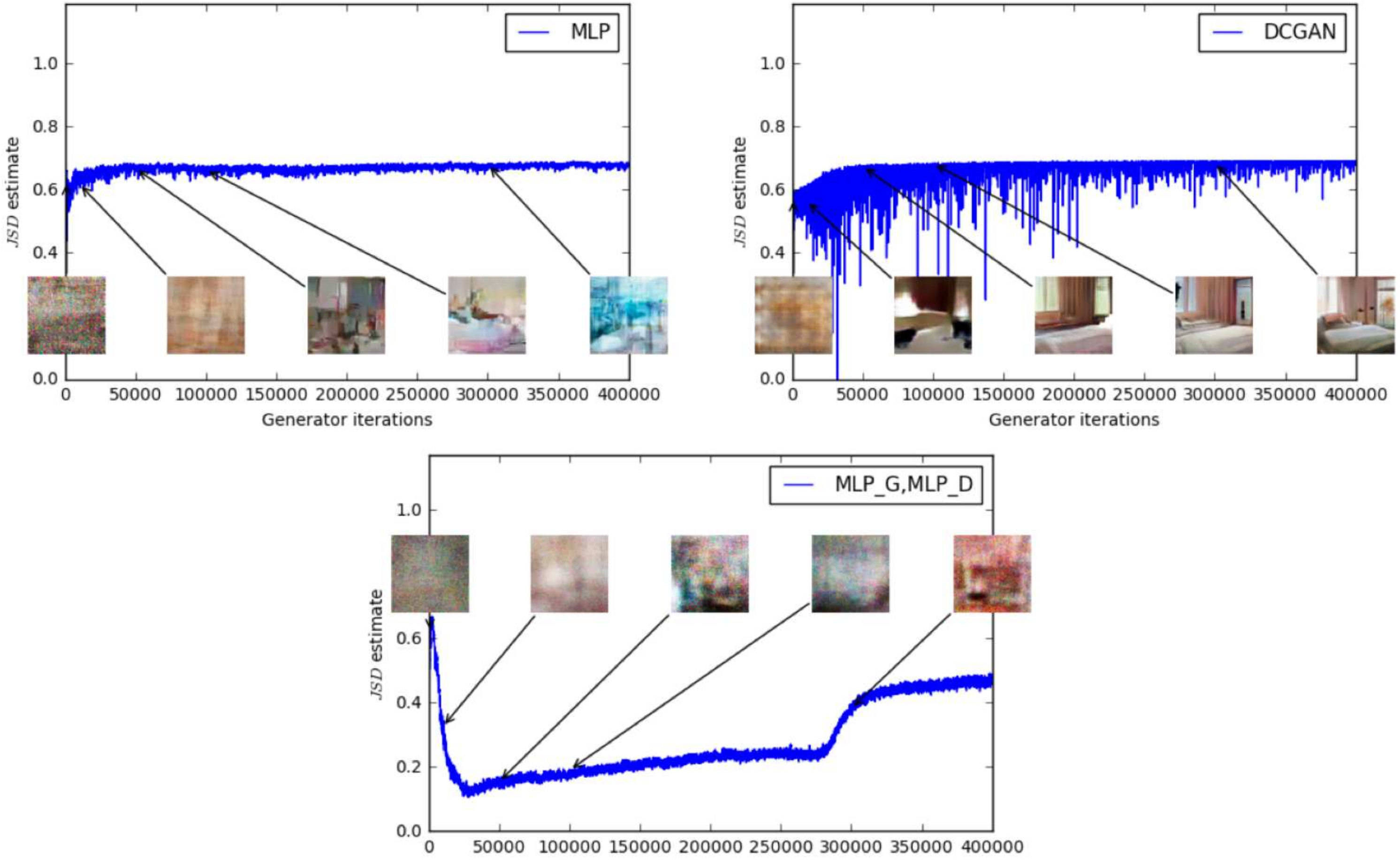
WGAN loss correlates with sample quality







Normal GAN loss does not correlate with sample quality



WGAN is less sensitive to modeling choices

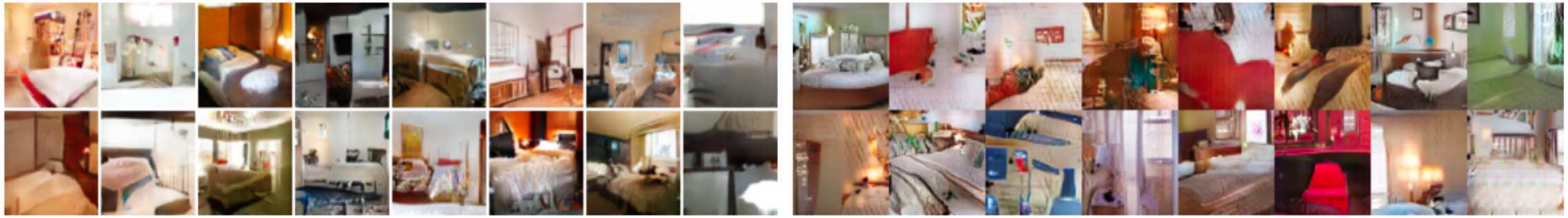


Figure 5: Algorithms trained with a DCGAN generator. Left: WGAN algorithm. Right: standard GAN formulation. Both algorithms produce high quality samples.

WGAN is less sensitive to modeling choices

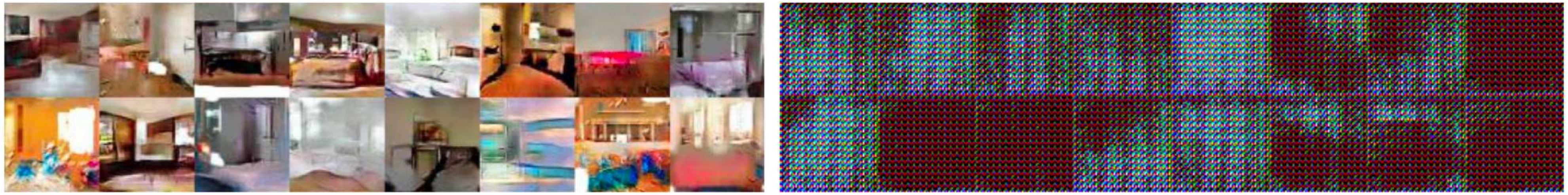


Figure 6: Algorithms trained with a generator without batch normalization and constant number of filters at every layer (as opposed to duplicating them every time as in [18]). Aside from taking out batch normalization, the number of parameters is therefore reduced by a bit more than an order of magnitude. Left: WGAN algorithm. Right: standard GAN formulation. As we can see the standard GAN failed to learn while the WGAN still was able to produce samples.

WGAN is less sensitive to modeling choices

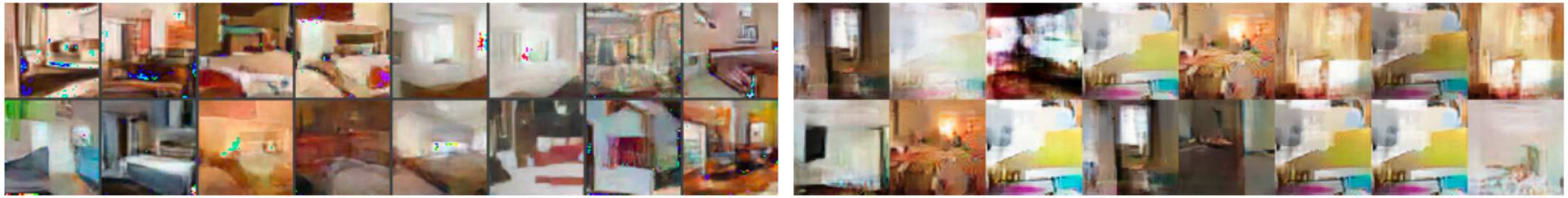
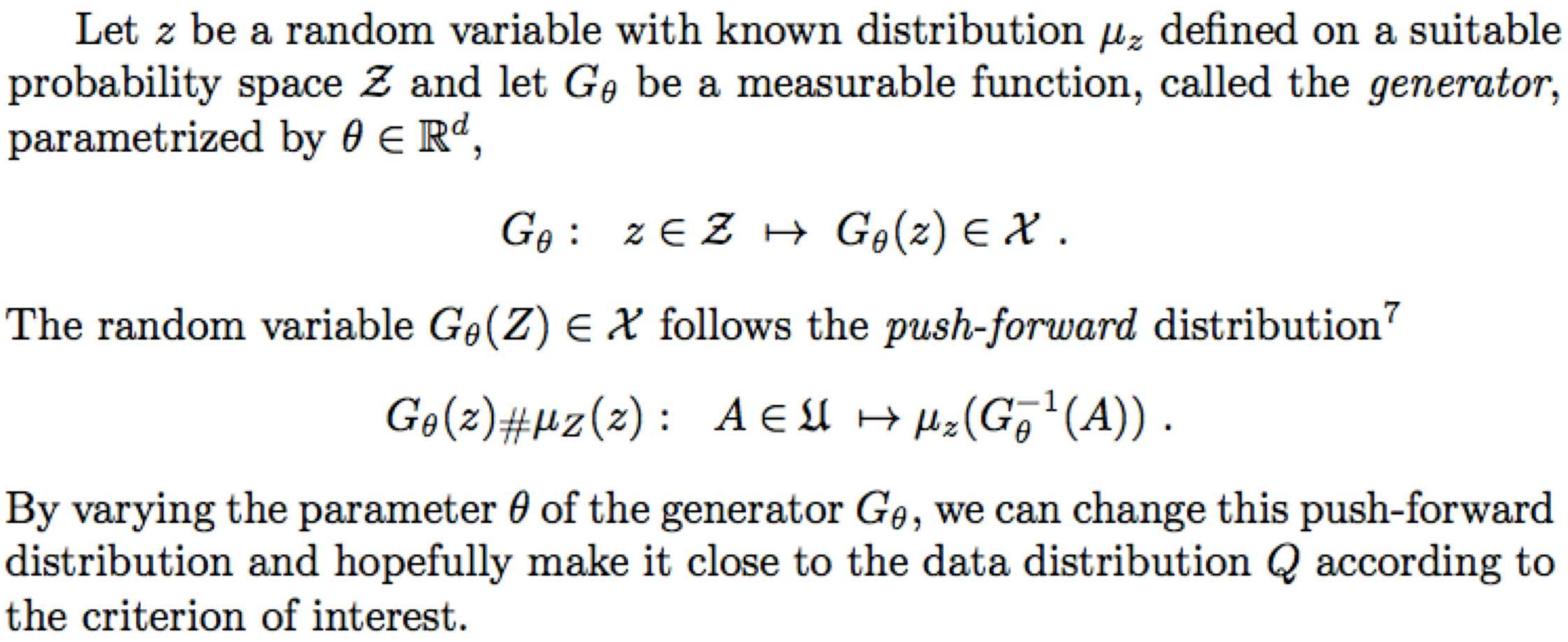


Figure 7: Algorithms trained with an MLP generator with 4 layers and 512 units with ReLU nonlinearities. The number of parameters is similar to that of a DCGAN, but it lacks a strong inductive bias for image generation. Left: WGAN algorithm. Right: standard GAN formulation. The WGAN method still was able to produce samples, lower quality than the DCGAN, and of higher quality than the MLP of the standard GAN. Note the significant degree of mode collapse in the GAN MLP.

8- The geometry of weak Integral Probability Metrics

Implicit modeling



Let z be a random variable with known distribution μ_z defined on a suitable probability space $\mathcal{Z}$ and let G_θ be a measurable function, called the *generator*, parametrized by $\theta \in \mathbb{R}^d$,

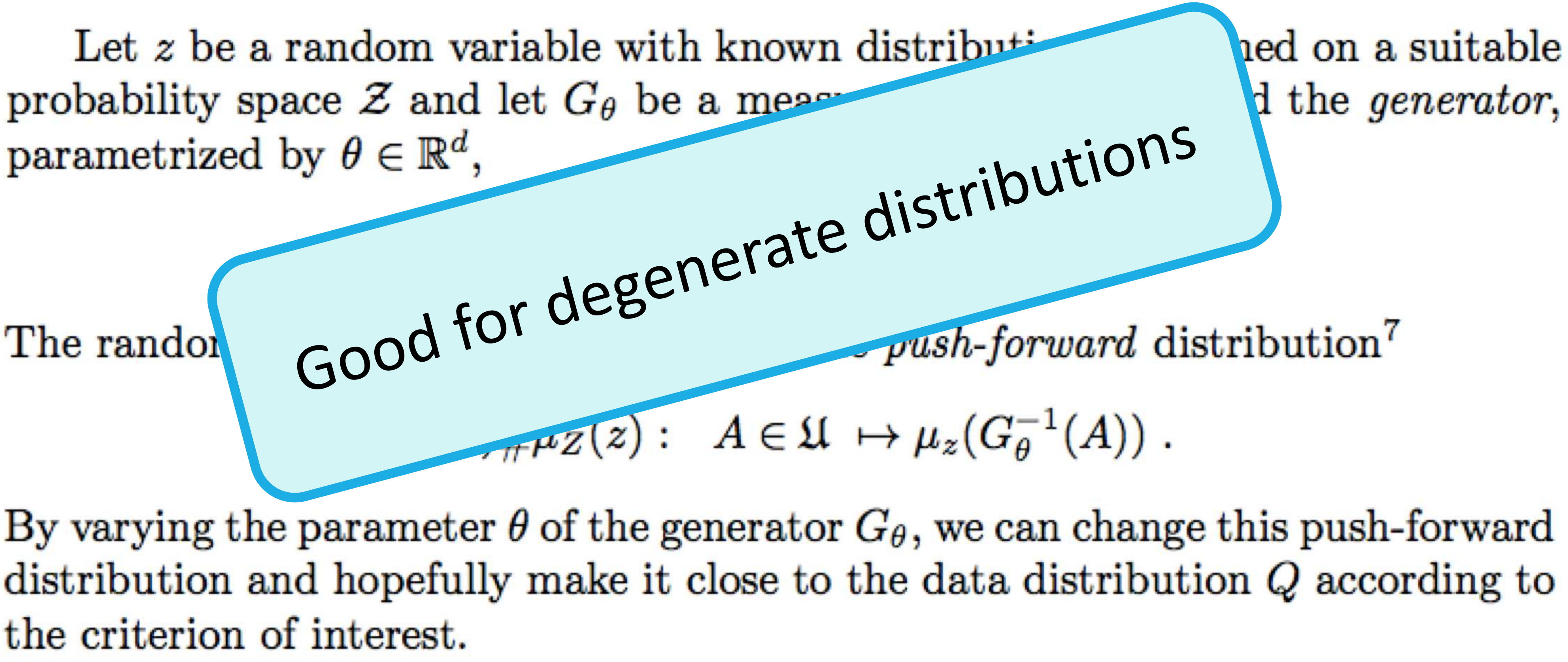
$$G_\theta : \quad z \in \mathcal{Z} \ \mapsto \ G_\theta(z) \in \mathcal{X} \ .$$

The random variable $G_\theta(Z) \in \mathcal{X}$ follows the *push-forward* distribution[7]

$$G_\theta(z)_{\#}\mu_Z(z) : \quad A \in \mathfrak{U} \ \mapsto \mu_z(G_\theta^{-1}(A)) \ .$$

By varying the parameter θ of the generator G_θ, we can change this push-forward distribution and hopefully make it close to the data distribution Q according to the criterion of interest.

Implicit modeling



Let z be a random variable with known distributi ned on a suitable probability space $\mathcal{Z}$ and let G_θ be a meas d the *generator*, parametrized by $\theta \in \mathbb{R}^d$,

The rando *push-forward* distribution[7]

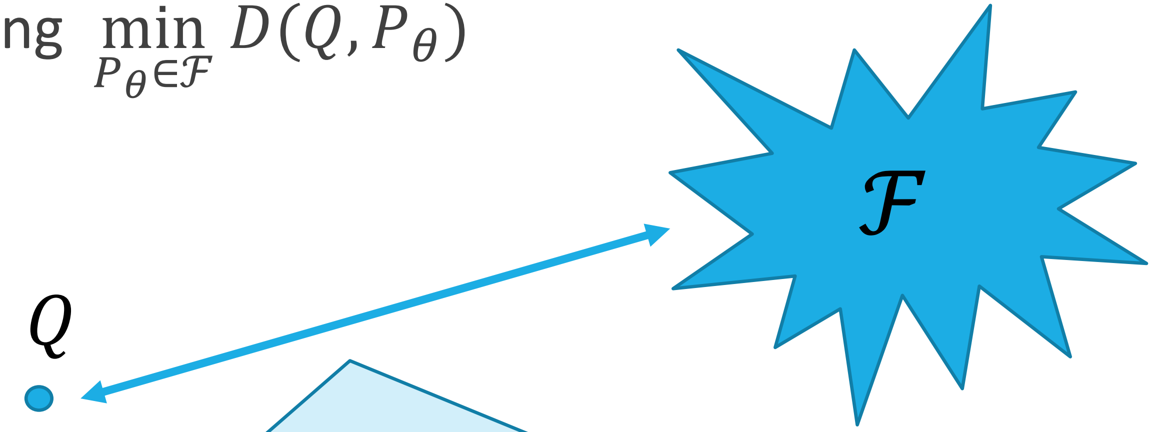
$$_{\#}\mu_Z(z): \quad A \in \mathfrak{U} \mapsto \mu_z(G_\theta^{-1}(A)) \; .$$

By varying the parameter θ of the generator G_θ, we can change this push-forward distribution and hopefully make it close to the data distribution Q according to the criterion of interest.

Good for degenerate distributions

Learning

- Let Q be the training data distribution (the complex world)
- Let $P_\theta \in \mathcal{F}$ be the (implicit) parametric models (the simple models)
- Learn by minimizing $\min_{P_\theta \in \mathcal{F}} D(Q, P_\theta)$



When Q is far from $\mathcal{F}$, the choice of a distance matters!

Probability comparison criteria for implicit models

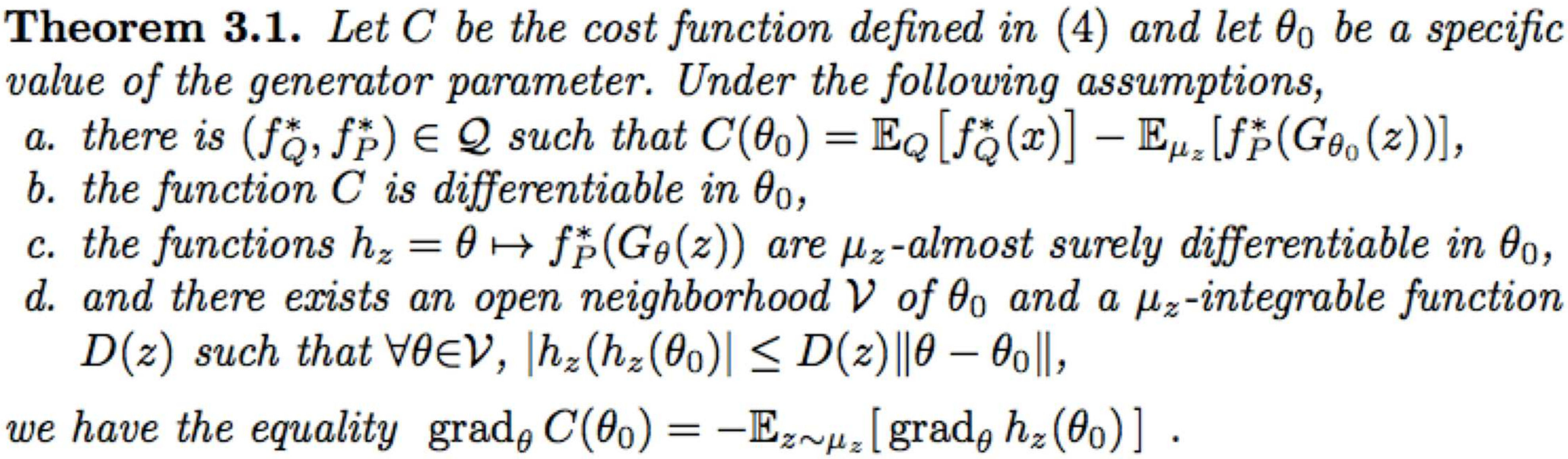
$$D(Q,P) = \sup_{(f_Q,f_P)\in\mathcal{Q}} \mathbb{E}_Q[f_Q(x)] - \mathbb{E}_P[f_P(x)]$$

Gives a broad family of probability distances

by changing the set of pairs $\left(f_Q, f_P\right)$ considered in the supremum.

$$\min_{\theta}\left\{ C(\theta) \overset{\Delta}{=} \max_{(f_Q,f_P)\in\mathcal{Q}} \mathbb{E}_{x\sim Q}[f_Q(x)] - \mathbb{E}_{z\sim\mu_z}[f_P(G_\theta(z))] \right\} . \tag{4}$$

Envelope theorem



Theorem 3.1. *Let C be the cost function defined in (4) and let θ_0 be a specific value of the generator parameter. Under the following assumptions,*

a. *there is $(f_Q^*, f_P^*) \in \mathcal{Q}$ such that $C(\theta_0) = \mathbb{E}_Q\left[f_Q^*(x)\right] - \mathbb{E}_{\mu_z}[f_P^*(G_{\theta_0}(z))]$,*

b. *the function C is differentiable in θ_0,*

c. *the functions $h_z = \theta \mapsto f_P^*(G_\theta(z))$ are μ_z-almost surely differentiable in θ_0,*

d. *and there exists an open neighborhood $\mathcal{V}$ of θ_0 and a μ_z-integrable function $D(z)$ such that $\forall\theta{\in}\mathcal{V}$, $|h_z(h_z(\theta_0)| \leq D(z)\|\theta - \theta_0\|$,*

we have the equality $\operatorname{grad}_\theta C(\theta_0) = -\mathbb{E}_{z\sim\mu_z}[\operatorname{grad}_\theta h_z(\theta_0)]$.

(Arjovsky et al., ICML 2017)

Algorithmic ideas

The ideal world

- After optimizing $\left(f_Q, f_P\right)$ we can get unbiased estimates of the gradient of $C(\theta)$.
- Such gradient estimates can be used for stochastic gradient descent on θ.

The real world

- We cannot really optimize $\left(f_Q, f_P\right)$ -- too slow, too hard, not enough data…
- In practice interleave (many) stochastic ascent steps on $\left(f_Q, f_P\right)$
  and (relatively few) stochastic descent steps on θ.
- This can be slow and tricky. Lots of room for improvement. Search for “xxxGAN”.

Algorithmic ideas

The ideal world

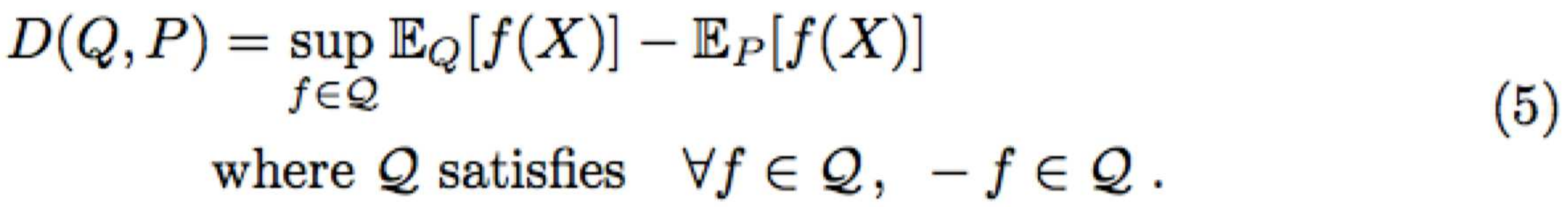
- After optimizing $\left(f_Q, f_P\right)$ we can get unbia $C(\theta)$.
- Such gradient estimates

The real w

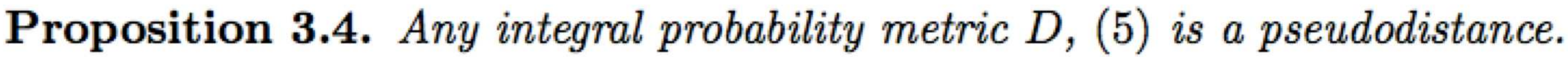
- We cannot rea ow, too hard, not enough data…
- In practice inter ny) stochastic ascent steps on $\left(f_Q, f_P\right)$ and (relatively few) stochastic descent steps on θ.
- This can be slow and tricky. Lots of room for improvement. Search for "xxxGAN".

Lets assume that this works.
What about the distances?

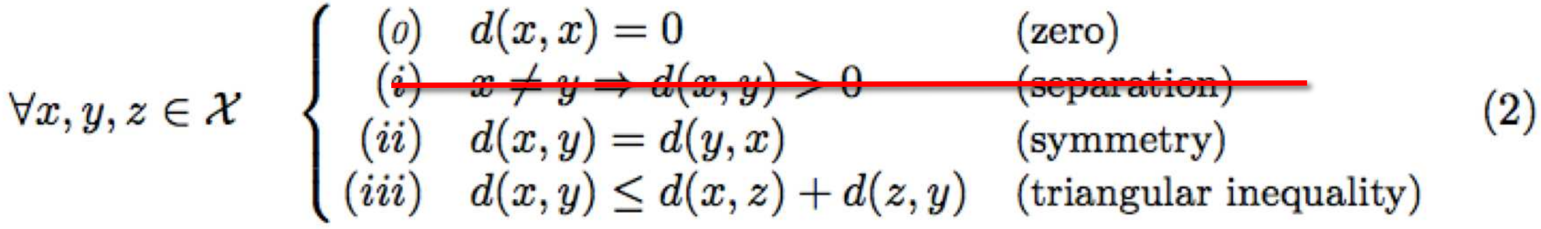
Integral Probability Metrics (IPM)



$$D(Q,P) = \sup_{f \in \mathcal{Q}} \mathbb{E}_Q[f(X)] - \mathbb{E}_P[f(X)] \qquad \text{where } \mathcal{Q} \text{ satisfies } \quad \forall f \in \mathcal{Q}, \; -f \in \mathcal{Q}\,. \tag{5}$$



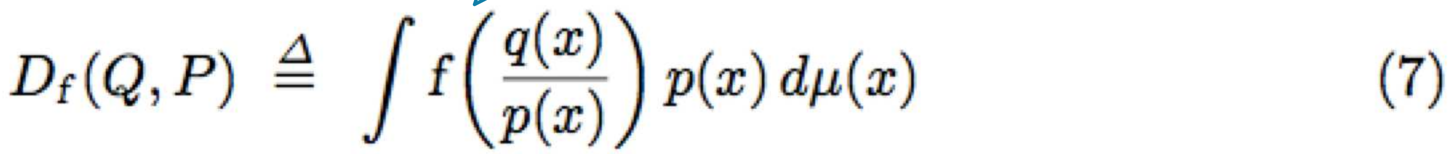
Proposition 3.4. *Any integral probability metric D, (5) is a pseudodistance.*



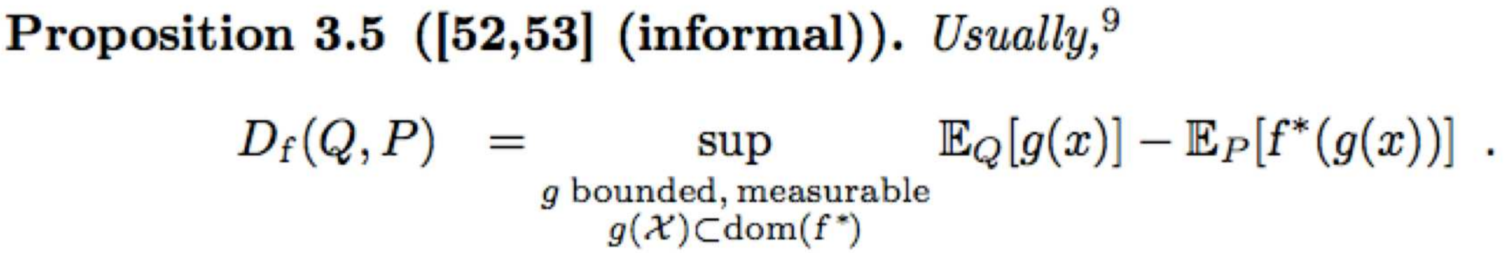
$$\forall x, y, z \in \mathcal{X} \quad \left\{ \begin{array}{rll} (o) & d(x,x) = 0 & \text{(zero)} \\ \cancel{(i)} & \cancel{x \neq y \Rightarrow d(x,y) > 0} & \cancel{\text{(separation)}} \\ (ii) & d(x,y) = d(y,x) & \text{(symmetry)} \\ (iii) & d(x,y) \leq d(x,z) + d(z,y) & \text{(triangular inequality)} \end{array} \right. \tag{2}$$

f-divergences

With f convex such that f(1)=0

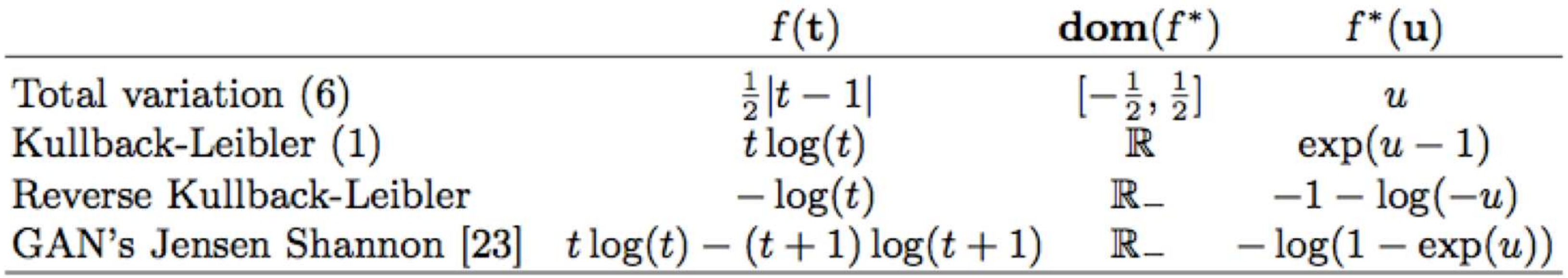


$$D_f(Q,P) \triangleq \int f\left(\frac{q(x)}{p(x)}\right) p(x)\, d\mu(x) \tag{7}$$



Proposition 3.5 ([52,53] (informal)). *Usually,*[9]

$$D_f(Q,P) = \sup_{\substack{g \text{ bounded, measurable} \\ g(\mathcal{X}) \subset \mathrm{dom}(f^*)}} \mathbb{E}_Q[g(x)] - \mathbb{E}_P[f^*(g(x))] \; .$$



	$f(\mathbf{t})$	$\mathbf{dom}(f^*)$	$f^*(\mathbf{u})$
Total variation (6)	$\frac{1}{2}\|t-1\|$	$[-\frac{1}{2}, \frac{1}{2}]$	u
Kullback-Leibler (1)	$t\log(t)$	$\mathbb{R}$	$\exp(u-1)$
Reverse Kullback-Leibler	$-\log(t)$	$\mathbb{R}_-$	$-1-\log(-u)$
GAN's Jensen Shannon [23]	$t\log(t)-(t+1)\log(t+1)$	$\mathbb{R}_-$	$-\log(1-\exp(u))$

(Nguyen et al., IEEE Trans Inf Theory 2010) (Nowozin et al., NIPS 2016)

Wasserstein distances

$$\forall Q, P \in \mathcal{P}_{\mathcal{X}}^{p} \qquad W_p(Q,P)^p \triangleq \inf_{\pi \in \Pi(Q,P)} \mathbb{E}_{(x,y)\sim\pi}[\,d(x,y)^p\,] \;, \qquad (8)$$

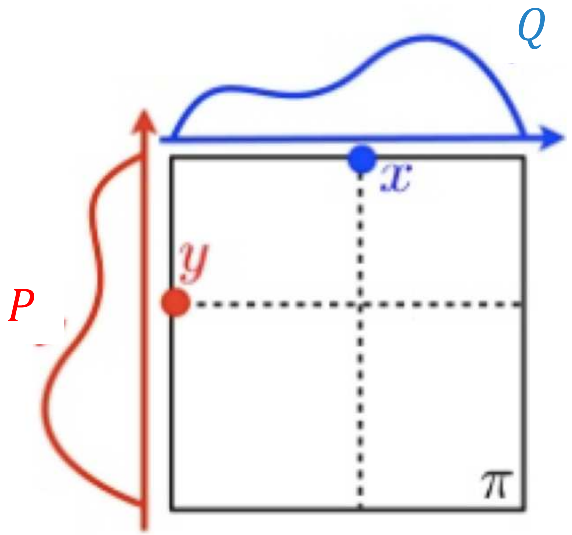


Image stolen from Gabriel Peyré slides:
"An introduction to Optimal Transport"

See also Cedric Villani
"Optimal Transport Old and New" (2009)

Wasserstein distances

Kantorovich duality

$$\forall Q, P \in \mathcal{P}_{\mathcal{X}}^{p} \qquad W_p(Q,P)^p = \sup_{(f_Q, f_P) \in \mathcal{Q}_c} \mathbb{E}_Q[f_Q(x)] - \mathbb{E}_P[f_P(x)] \ , \qquad (13)$$

$$\forall Q, P \in \mathcal{P}_{\mathcal{X}}^{1} \qquad W_1(Q,P) = \sup_{f \in \mathrm{Lip1}} \mathbb{E}_Q[f(x)] - \mathbb{E}_P[f(x)] \ . \qquad (14)$$

IPM!

Energy distance - Euclidean case

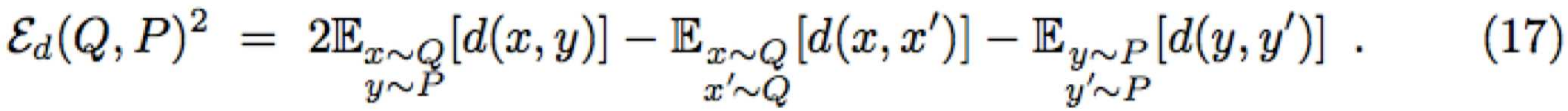
$$\mathcal{E}(Q,P)^2 \triangleq 2\mathbb{E}_{\substack{x\sim Q\\ y\sim P}}[\|x-y\|] - \mathbb{E}_{\substack{x\sim Q\\ x'\sim Q}}[\|x-x'\|] - \mathbb{E}_{\substack{y\sim P\\ y'\sim P}}[\|y-y'\|] \ , \qquad (15)$$

This seems weird but it turns out that:

$$\mathcal{E}(Q,P)^2 = \frac{1}{c_d}\int_{\mathbb{R}^d} \frac{|\hat{q}(t)-\hat{p}(t)|^2}{\|t\|^{d+1}}dt \quad \text{with} \quad c_d = \frac{\pi^{\frac{d+1}{2}}}{\Gamma(\frac{d+1}{2})} \ . \qquad (16)$$

(Szekely 2002, Szekely & Rizzo 2013)

Energy distance – Generalized

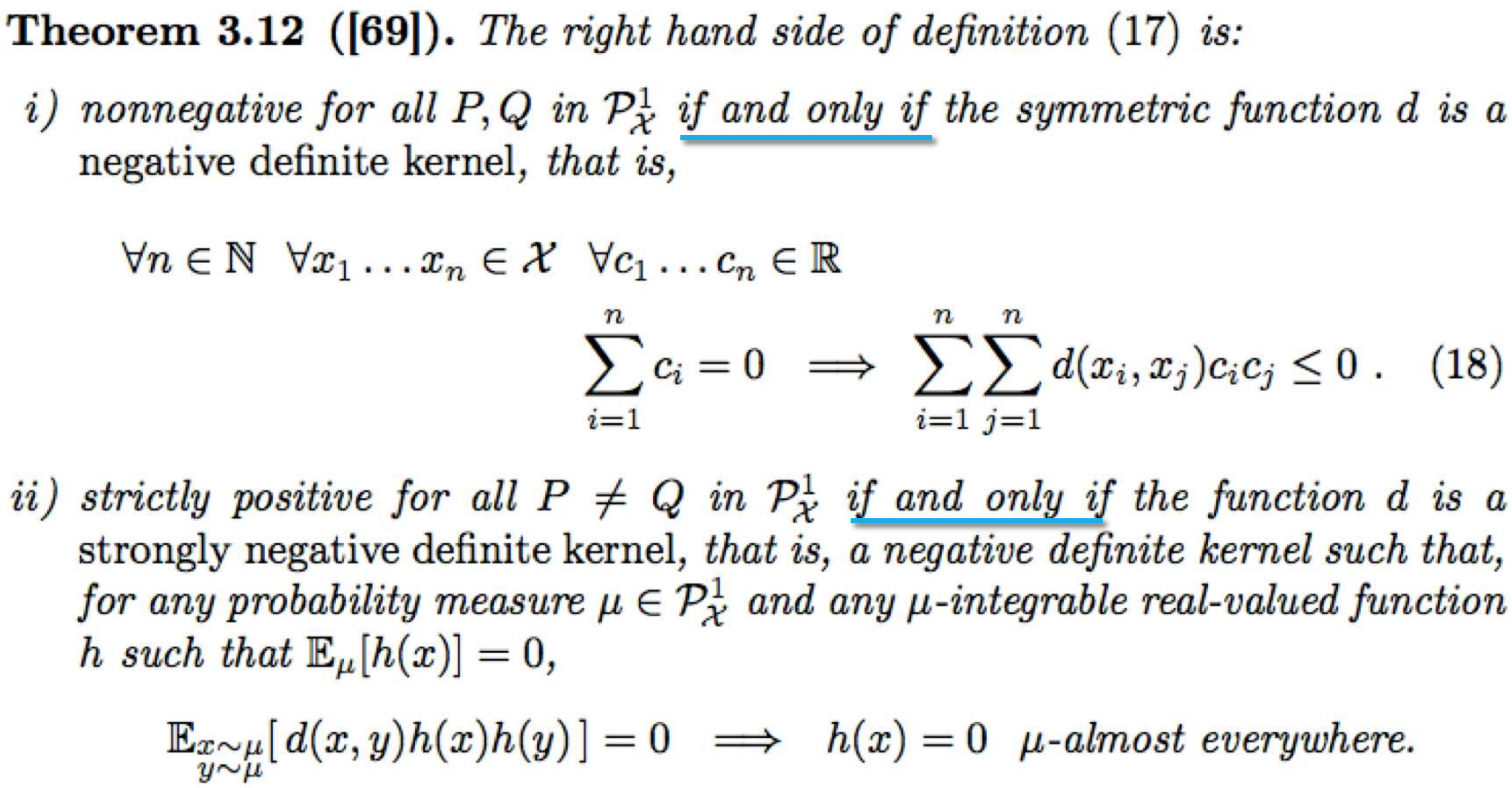


$$\mathcal{E}_d(Q,P)^2 \;=\; 2\mathbb{E}_{\substack{x\sim Q\\ y\sim P}}[d(x,y)] - \mathbb{E}_{\substack{x\sim Q\\ x'\sim Q}}[d(x,x')] - \mathbb{E}_{\substack{y\sim P\\ y'\sim P}}[d(y,y')]\ . \qquad (17)$$

Is this positive?
Is this a distance?

(Szekely 2002, Szekely & Rizzo 2013)

Energy distance – Generalized



Theorem 3.12 **([69]).** *The right hand side of definition* (17) *is:*

i) nonnegative for all P, Q *in* $\mathcal{P}^1_{\mathcal{X}}$ *if and only if the symmetric function* d *is a* negative definite kernel, *that is,*

$$\forall n \in \mathbb{N} \quad \forall x_1 \dots x_n \in \mathcal{X} \quad \forall c_1 \dots c_n \in \mathbb{R}$$

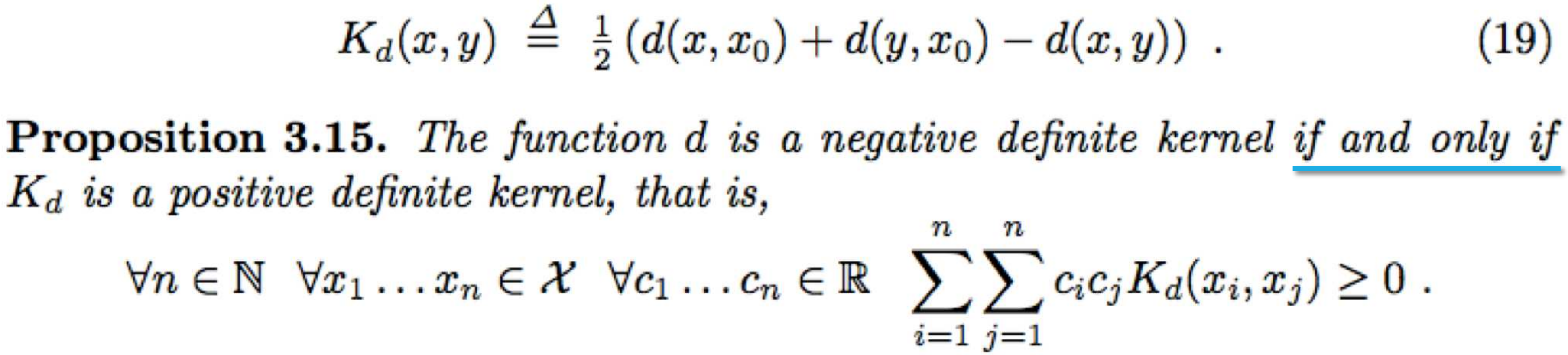
$$\sum_{i=1}^{n} c_i = 0 \implies \sum_{i=1}^{n}\sum_{j=1}^{n} d(x_i, x_j) c_i c_j \leq 0 \,. \qquad (18)$$

ii) strictly positive for all $P \neq Q$ *in* $\mathcal{P}^1_{\mathcal{X}}$ *if and only if the function* d *is a* strongly negative definite kernel, *that is, a negative definite kernel such that, for any probability measure* $\mu \in \mathcal{P}^1_{\mathcal{X}}$ *and any* μ*-integrable real-valued function* h *such that* $\mathbb{E}_\mu[h(x)] = 0$,

$$\mathbb{E}_{\substack{x\sim\mu \\ y\sim\mu}}[\, d(x,y)h(x)h(y)\,] = 0 \implies h(x) = 0 \quad \mu\text{-almost everywhere.}$$

(Zinger & al, 1989)

Energy distance – Surprise

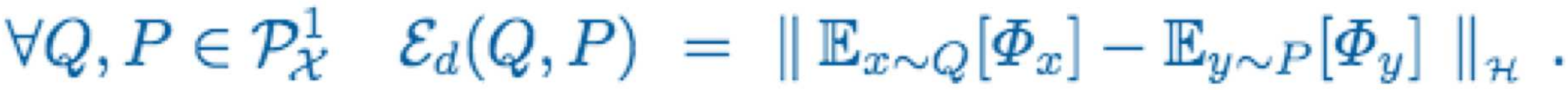


$$K_d(x,y) \stackrel{\Delta}{=} \tfrac{1}{2}\left(d(x,x_0)+d(y,x_0)-d(x,y)\right) \;. \qquad (19)$$

Proposition 3.15. *The function d is a negative definite kernel if and only if K_d is a positive definite kernel, that is,*

$$\forall n\in\mathbb{N} \;\; \forall x_1\ldots x_n\in\mathcal{X} \;\; \forall c_1\ldots c_n\in\mathbb{R} \quad \sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j K_d(x_i,x_j)\geq 0 \;.$$

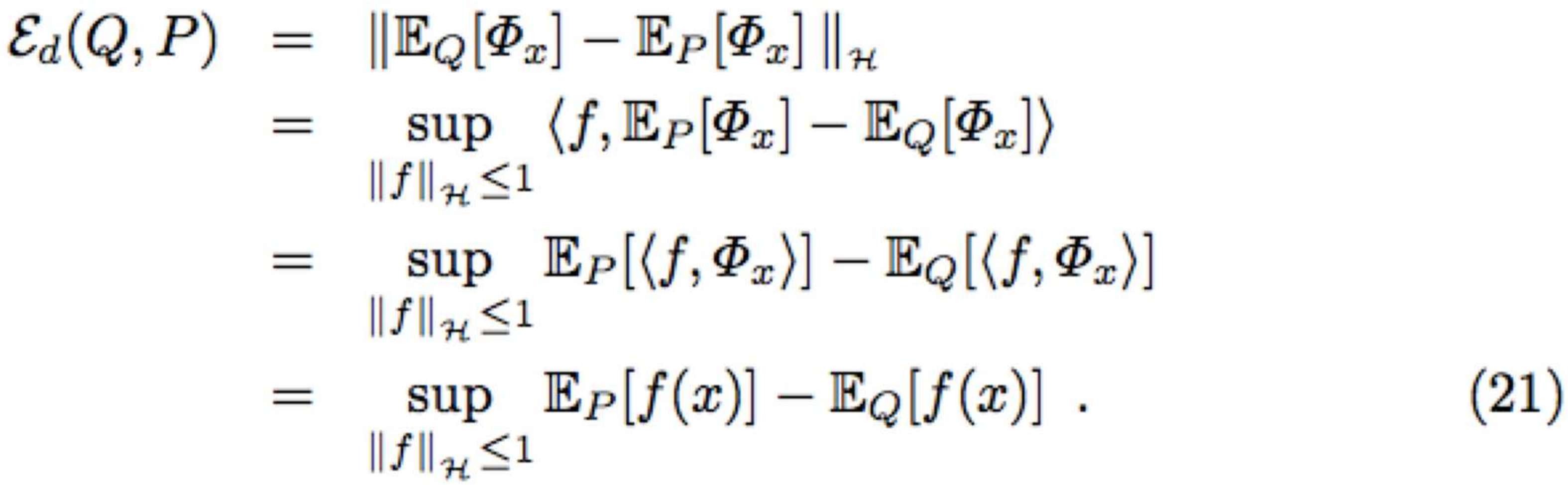
Then, thanks to RKHS theory…



$$\forall Q,P\in\mathcal{P}^1_{\mathcal{X}} \quad \mathcal{E}_d(Q,P) \;=\; \|\, \mathbb{E}_{x\sim Q}[\Phi_x] - \mathbb{E}_{y\sim P}[\Phi_y] \,\|_{\mathcal{H}} \;.$$

(Sejdinovic et al, 2013) (Rachev et al., 2013)

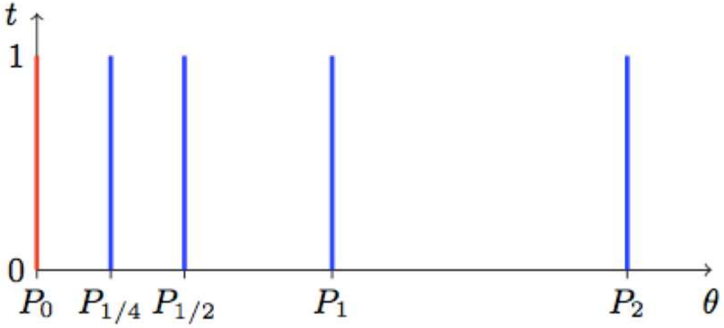
Energy distance
= Maximum Mean Discrepancy (MMD)



$$\begin{aligned}\mathcal{E}_d(Q,P) &= \|\mathbb{E}_Q[\Phi_x] - \mathbb{E}_P[\Phi_x]\|_{\mathcal{H}} \\ &= \sup_{\|f\|_{\mathcal{H}}\leq 1} \langle f, \mathbb{E}_P[\Phi_x] - \mathbb{E}_Q[\Phi_x]\rangle \\ &= \sup_{\|f\|_{\mathcal{H}}\leq 1} \mathbb{E}_P[\langle f, \Phi_x\rangle] - \mathbb{E}_Q[\langle f, \Phi_x\rangle] \\ &= \sup_{\|f\|_{\mathcal{H}}\leq 1} \mathbb{E}_P[f(x)] - \mathbb{E}_Q[f(x)] \ . \qquad (21)\end{aligned}$$

(Gretton et al., 2012)

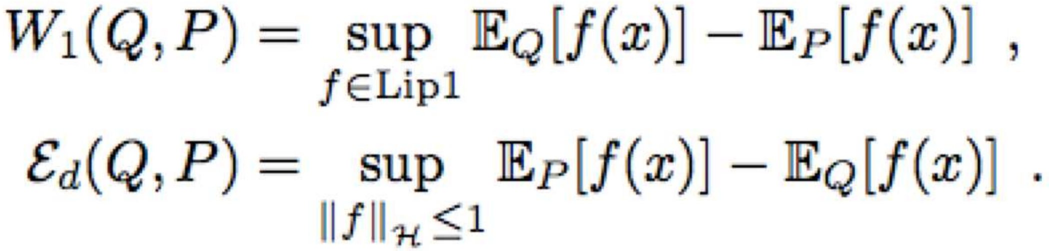
Strong topology vs weak topology



- $W(\mathbb{P}_0, \mathbb{P}_\theta) = |\theta|$,
- $JS(\mathbb{P}_0, \mathbb{P}_\theta) = \begin{cases} \log 2 & \text{if } \theta \neq 0\,, \\ 0 & \text{if } \theta = 0\,, \end{cases}$
- $KL(\mathbb{P}_\theta \| \mathbb{P}_0) = KL(\mathbb{P}_0 \| \mathbb{P}_\theta) = \begin{cases} +\infty & \text{if } \theta \neq 0\,, \\ 0 & \text{if } \theta = 0\,, \end{cases}$
- and $\delta(\mathbb{P}_0, \mathbb{P}_\theta) = \begin{cases} 1 & \text{if } \theta \neq 0\,, \\ 0 & \text{if } \theta = 0\,. \end{cases}$

(Arjovsky et al., ICML 2017)

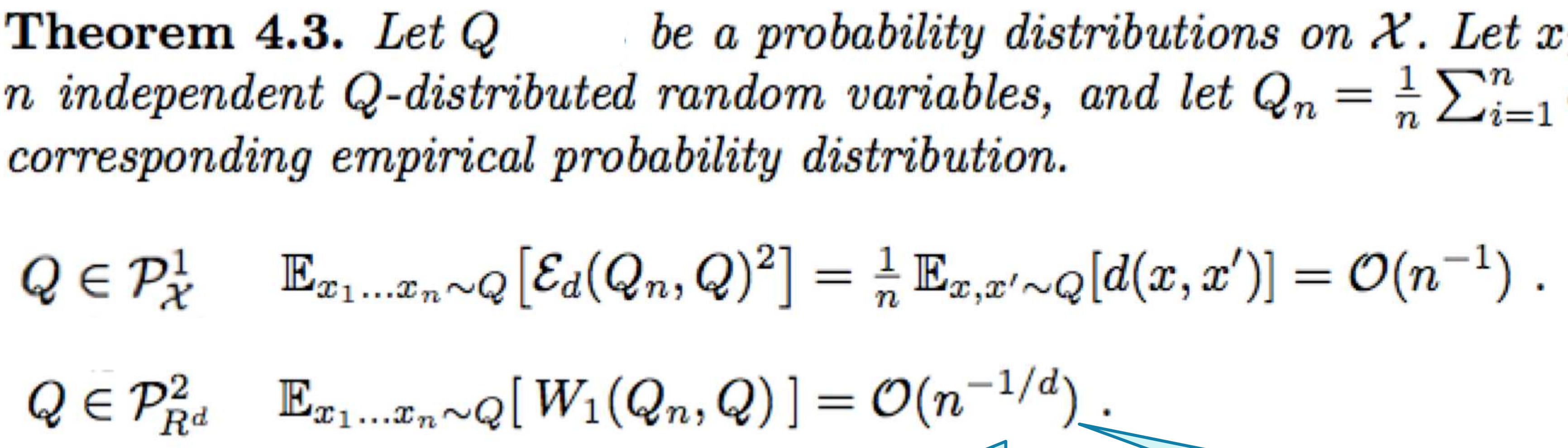
How different are WD and MMD?



$$W_1(Q,P) = \sup_{f \in \mathrm{Lip1}} \mathbb{E}_Q[f(x)] - \mathbb{E}_P[f(x)] \ ,$$

$$\mathcal{E}_d(Q,P) = \sup_{\|f\|_{\mathcal{H}} \leq 1} \mathbb{E}_P[f(x)] - \mathbb{E}_Q[f(x)] \ .$$

How different are WD and MMD?



Theorem 4.3. *Let Q be a probability distributions on $\mathcal{X}$. Let $x_1 \ldots x_n$ be n independent Q-distributed random variables, and let $Q_n = \frac{1}{n}\sum_{i=1}^{n}\delta_{x_i}$ be the corresponding empirical probability distribution.*

$$Q \in \mathcal{P}^1_{\mathcal{X}} \qquad \mathbb{E}_{x_1 \ldots x_n \sim Q}\left[\mathcal{E}_d(Q_n, Q)^2\right] = \frac{1}{n}\mathbb{E}_{x,x' \sim Q}[d(x,x')] = \mathcal{O}(n^{-1}) \ .$$

$$Q \in \mathcal{P}^2_{R^d} \qquad \mathbb{E}_{x_1 \ldots x_n \sim Q}[\, W_1(Q_n, Q)\,] = \mathcal{O}(n^{-1/d}) \ .$$

This is reached (Sanjeev's sphere)

Wasserstein seem hopeless

How different are WD and MMD?

Things look different in practice

- ED/MMD training of low dim implicit models works nicely.
- ED/MMD training of high dim implicit models often gets stuck.
- whereas "WD" training of the same high dim implicit models can give results.

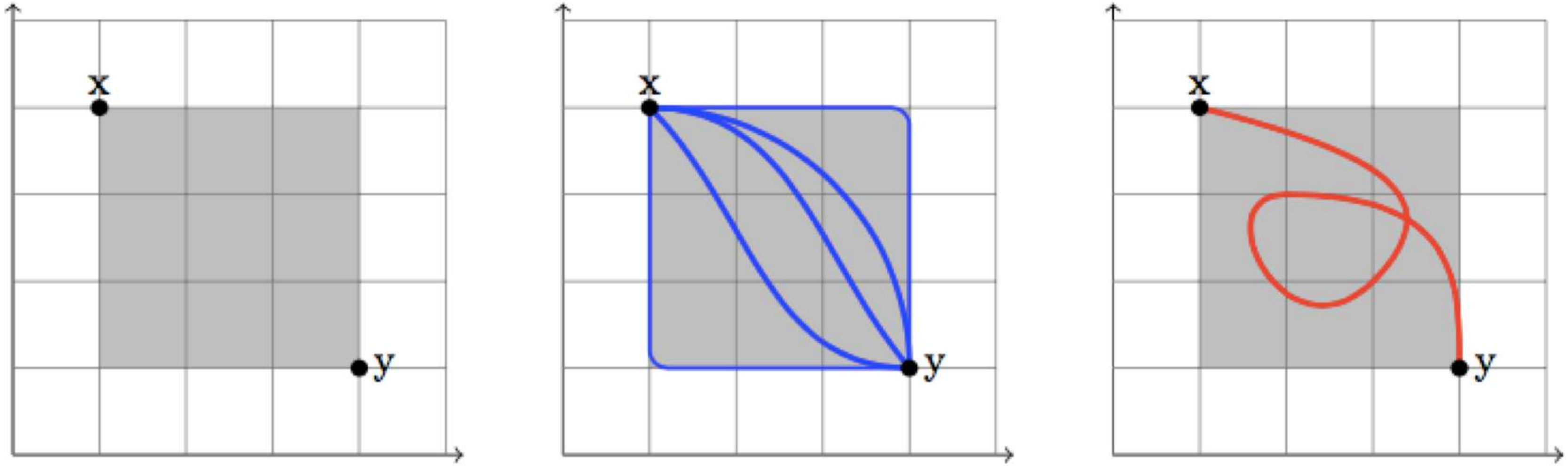
WD-like.

Just the opposite of what one would expect !

3– Geodesic geometry for probability measures

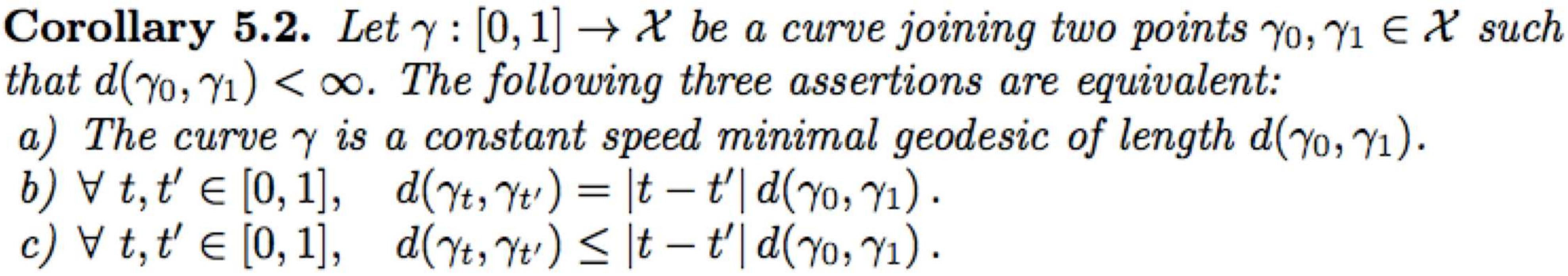
Minimal geodesics

Theorem 5.1. *Let $\gamma : [a,b] \to \mathcal{X}$ be a curve joining two points γ_a, γ_b such that $d(\gamma_a, \gamma_b) < \infty$. This curve is a minimal geodesic of length $d(\gamma_a, \gamma_b)$ if and only if* $\forall\ a \le t \le t' \le b, \quad d(\gamma_a, \gamma_t) + d(\gamma_t, \gamma_{t'}) + d(\gamma_{t'}, \gamma_b) = d(\gamma_a, \gamma_b)\,.$



$\mathbb{R}^2$ equipped with the L_1 distance.

Constant speed reparametrization



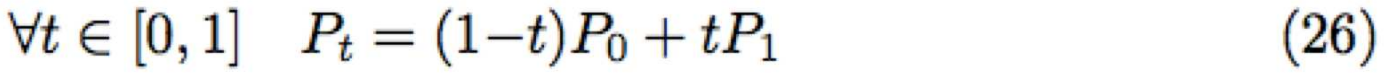
Corollary 5.2. *Let $\gamma : [0,1] \to \mathcal{X}$ be a curve joining two points $\gamma_0, \gamma_1 \in \mathcal{X}$ such that $d(\gamma_0, \gamma_1) < \infty$. The following three assertions are equivalent:*

a) The curve γ is a constant speed minimal geodesic of length $d(\gamma_0, \gamma_1)$.

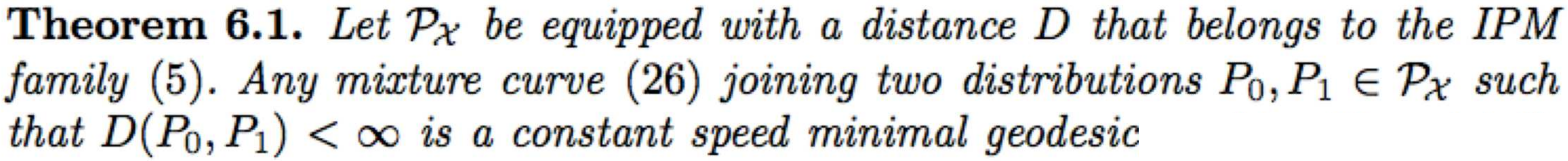
b) $\forall\ t, t' \in [0,1], \quad d(\gamma_t, \gamma_{t'}) = |t - t'|\, d(\gamma_0, \gamma_1)$.

c) $\forall\ t, t' \in [0,1], \quad d(\gamma_t, \gamma_{t'}) \leq |t - t'|\, d(\gamma_0, \gamma_1)$.

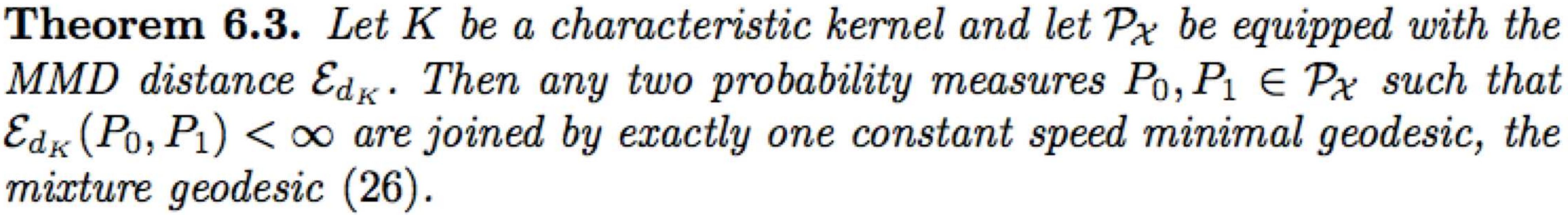
Mixture geodesics



$$\forall t \in [0,1] \quad P_t = (1-t)P_0 + tP_1 \qquad (26)$$

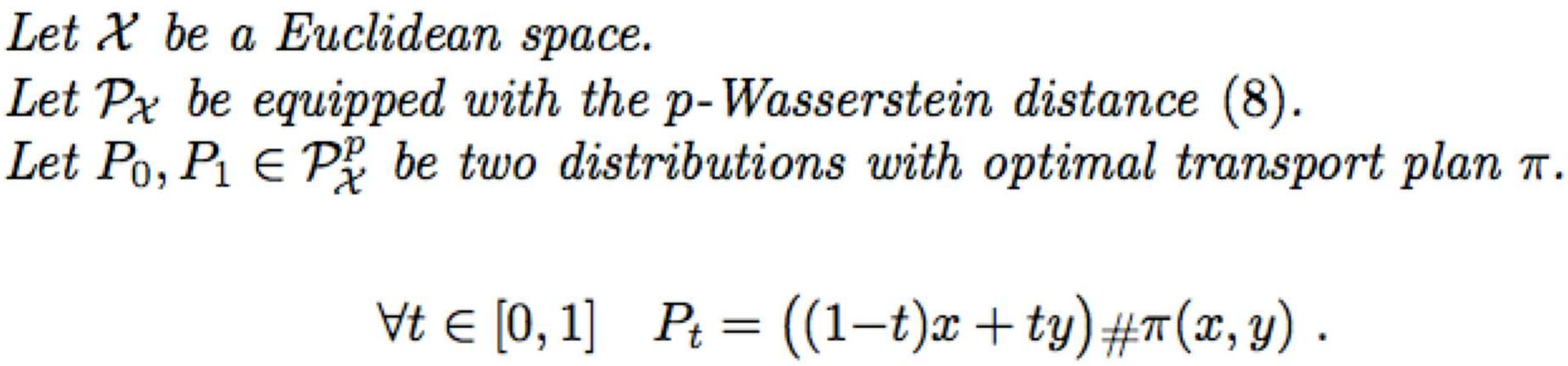


Theorem 6.1. *Let $\mathcal{P}_\mathcal{X}$ be equipped with a distance D that belongs to the IPM family* (5)*. Any mixture curve* (26) *joining two distributions $P_0, P_1 \in \mathcal{P}_\mathcal{X}$ such that $D(P_0, P_1) < \infty$ is a constant speed minimal geodesic*



Theorem 6.3. *Let K be a characteristic kernel and let $\mathcal{P}_\mathcal{X}$ be equipped with the MMD distance $\mathcal{E}_{d_K}$. Then any two probability measures $P_0, P_1 \in \mathcal{P}_\mathcal{X}$ such that $\mathcal{E}_{d_K}(P_0, P_1) < \infty$ are joined by exactly one constant speed minimal geodesic, the mixture geodesic* (26).

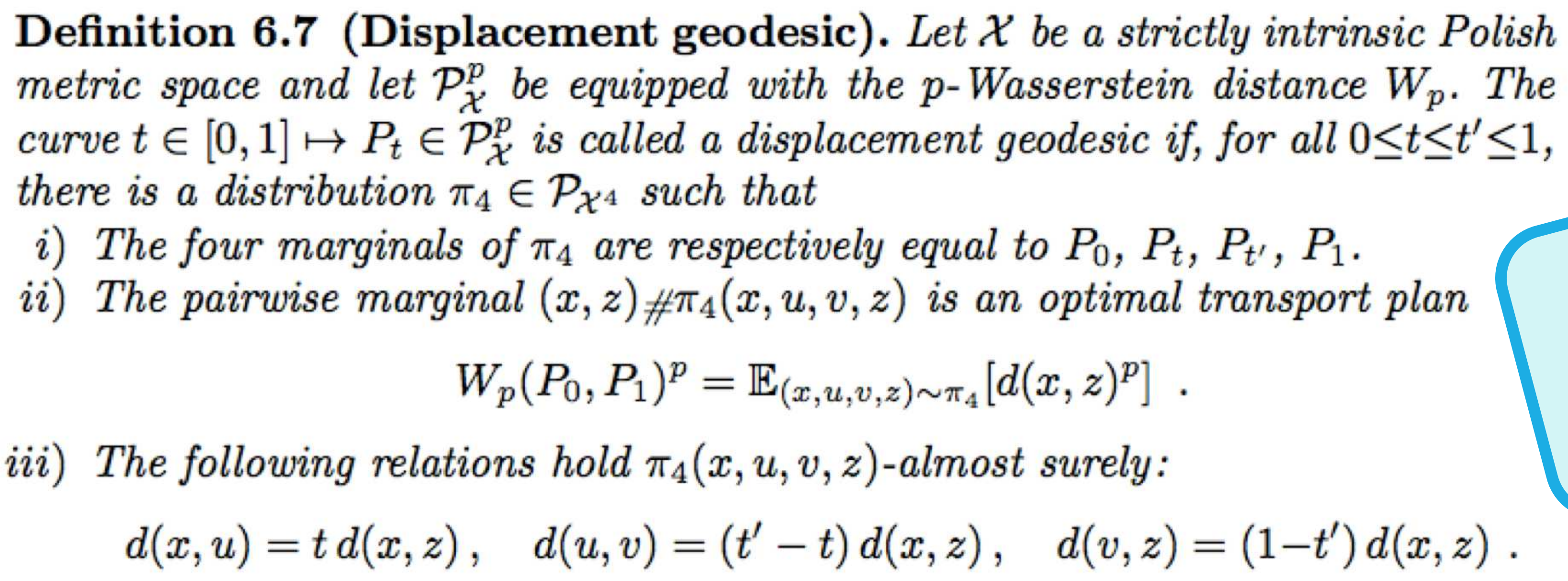
Displacement geodesics (Euclidean)



Let $\mathcal{X}$ be a Euclidean space.
Let $\mathcal{P}_{\mathcal{X}}$ be equipped with the p-Wasserstein distance (8).
Let $P_0, P_1 \in \mathcal{P}_{\mathcal{X}}^p$ be two distributions with optimal transport plan π.

$$\forall t \in [0,1] \quad P_t = \big((1-t)x + ty\big)_{\#}\pi(x,y) \ .$$

Displacement geodesics (General)



Definition 6.7 (Displacement geodesic). *Let $\mathcal{X}$ be a strictly intrinsic Polish metric space and let $\mathcal{P}^p_{\mathcal{X}}$ be equipped with the p-Wasserstein distance W_p. The curve $t \in [0,1] \mapsto P_t \in \mathcal{P}^p_{\mathcal{X}}$ is called a displacement geodesic if, for all $0 \leq t \leq t' \leq 1$, there is a distribution $\pi_4 \in \mathcal{P}_{\mathcal{X}^4}$ such that*

i) The four marginals of π_4 are respectively equal to P_0, P_t, $P_{t'}$, P_1.

ii) The pairwise marginal $(x,z)\#\pi_4(x,u,v,z)$ is an optimal transport plan

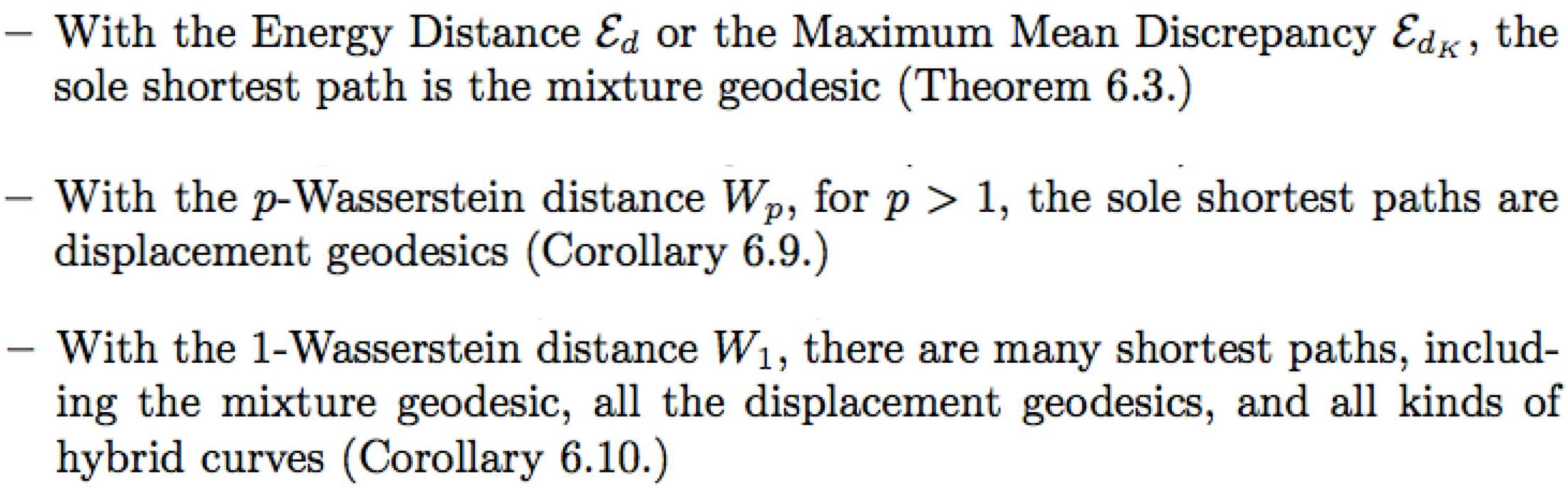
$$W_p(P_0,P_1)^p = \mathbb{E}_{(x,u,v,z)\sim\pi_4}[d(x,z)^p] \ .$$

iii) The following relations hold $\pi_4(x,u,v,z)$-almost surely:

$$d(x,u) = t\,d(x,z)\,, \quad d(u,v) = (t'-t)\,d(x,z)\,, \quad d(v,z) = (1-t')\,d(x,z)\ .$$

Essentially the same thing

The geodesics of WD and MMD

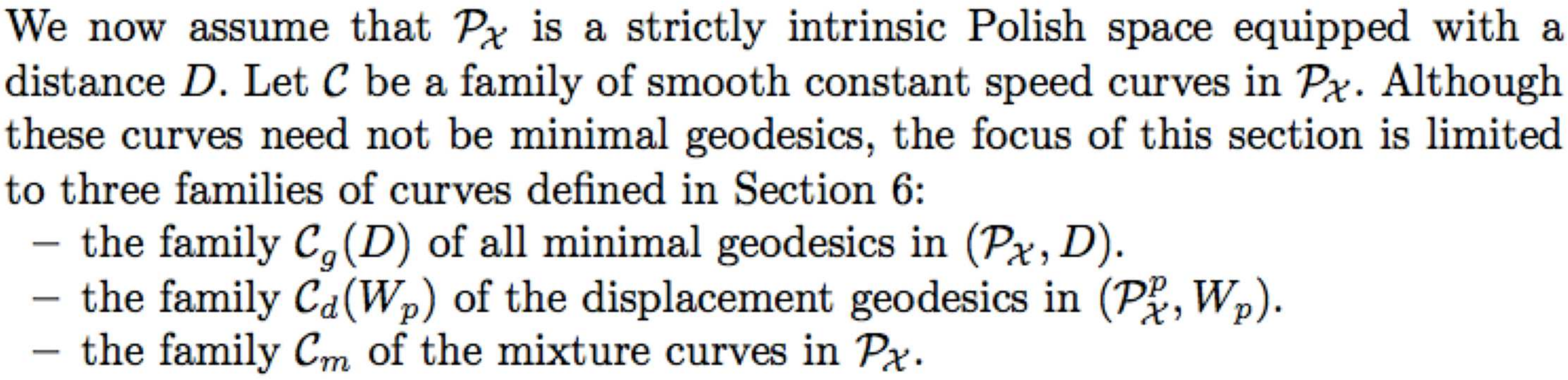


– With the Energy Distance $\mathcal{E}_d$ or the Maximum Mean Discrepancy $\mathcal{E}_{d_K}$, the sole shortest path is the mixture geodesic (Theorem 6.3.)

– With the p-Wasserstein distance W_p, for $p > 1$, the sole shortest paths are displacement geodesics (Corollary 6.9.)

– With the 1-Wasserstein distance W_1, there are many shortest paths, including the mixture geodesic, all the displacement geodesics, and all kinds of hybrid curves (Corollary 6.10.)

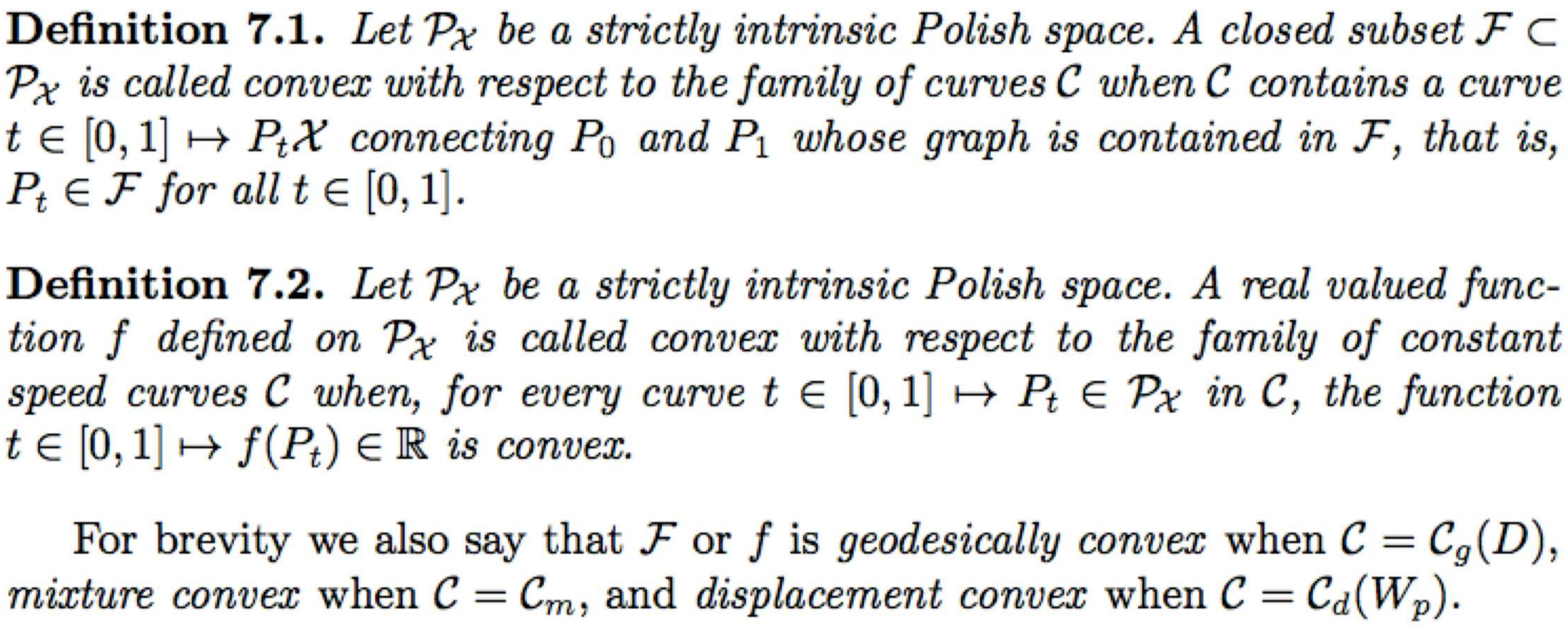
Families of curves



We now assume that $\mathcal{P}_{\mathcal{X}}$ is a strictly intrinsic Polish space equipped with a distance D. Let $\mathcal{C}$ be a family of smooth constant speed curves in $\mathcal{P}_{\mathcal{X}}$. Although these curves need not be minimal geodesics, the focus of this section is limited to three families of curves defined in Section 6:

- the family $\mathcal{C}_g(D)$ of all minimal geodesics in $(\mathcal{P}_{\mathcal{X}}, D)$.
- the family $\mathcal{C}_d(W_p)$ of the displacement geodesics in $(\mathcal{P}^p_{\mathcal{X}}, W_p)$.
- the family $\mathcal{C}_m$ of the mixture curves in $\mathcal{P}_{\mathcal{X}}$.

Convexity w.r.t. a family of curves

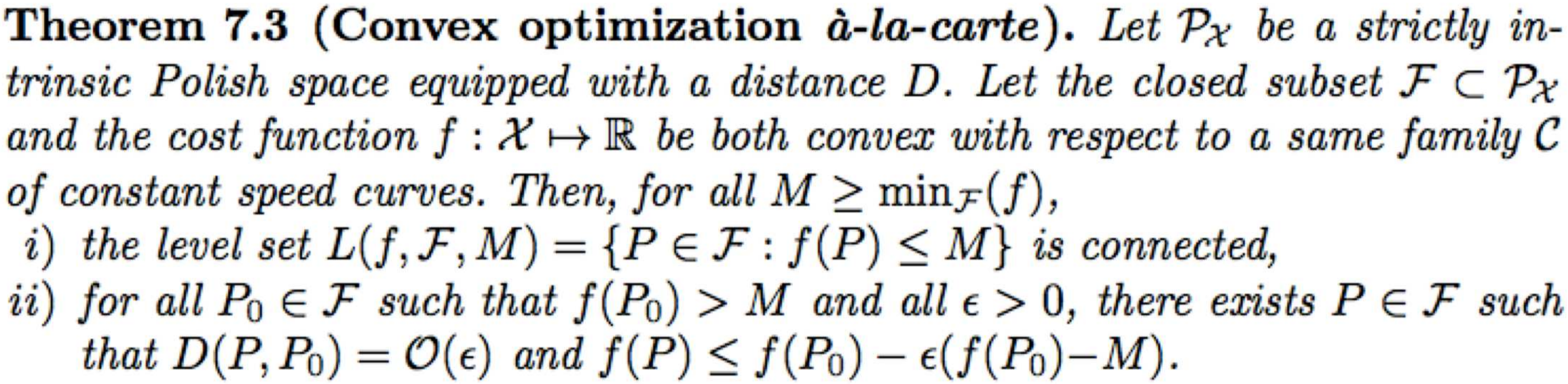


Definition 7.1. *Let $\mathcal{P}_\mathcal{X}$ be a strictly intrinsic Polish space. A closed subset $\mathcal{F} \subset \mathcal{P}_\mathcal{X}$ is called convex with respect to the family of curves $\mathcal{C}$ when $\mathcal{C}$ contains a curve $t \in [0,1] \mapsto P_t\mathcal{X}$ connecting P_0 and P_1 whose graph is contained in $\mathcal{F}$, that is, $P_t \in \mathcal{F}$ for all $t \in [0,1]$.*

Definition 7.2. *Let $\mathcal{P}_\mathcal{X}$ be a strictly intrinsic Polish space. A real valued function f defined on $\mathcal{P}_\mathcal{X}$ is called convex with respect to the family of constant speed curves $\mathcal{C}$ when, for every curve $t \in [0,1] \mapsto P_t \in \mathcal{P}_\mathcal{X}$ in $\mathcal{C}$, the function $t \in [0,1] \mapsto f(P_t) \in \mathbb{R}$ is convex.*

For brevity we also say that $\mathcal{F}$ or f is *geodesically convex* when $\mathcal{C} = \mathcal{C}_g(D)$, *mixture convex* when $\mathcal{C} = \mathcal{C}_m$, and *displacement convex* when $\mathcal{C} = \mathcal{C}_d(W_p)$.

Convex optimization à-la-carte



Theorem 7.3 (Convex optimization *à-la-carte*). *Let $\mathcal{P}_\mathcal{X}$ be a strictly intrinsic Polish space equipped with a distance D. Let the closed subset $\mathcal{F} \subset \mathcal{P}_\mathcal{X}$ and the cost function $f : \mathcal{X} \mapsto \mathbb{R}$ be both convex with respect to a same family $\mathcal{C}$ of constant speed curves. Then, for all $M \geq \min_\mathcal{F}(f)$,*

i) the level set $L(f, \mathcal{F}, M) = \{P \in \mathcal{F} : f(P) \leq M\}$ is connected,

ii) for all $P_0 \in \mathcal{F}$ such that $f(P_0) > M$ and all $\epsilon > 0$, there exists $P \in \mathcal{F}$ such that $D(P, P_0) = \mathcal{O}(\epsilon)$ and $f(P) \leq f(P_0) - \epsilon(f(P_0) - M)$.

A descent algorithm will find the global minimum.

Even with a nonconvex parametrization of $P_\theta \in \mathcal{F}$.

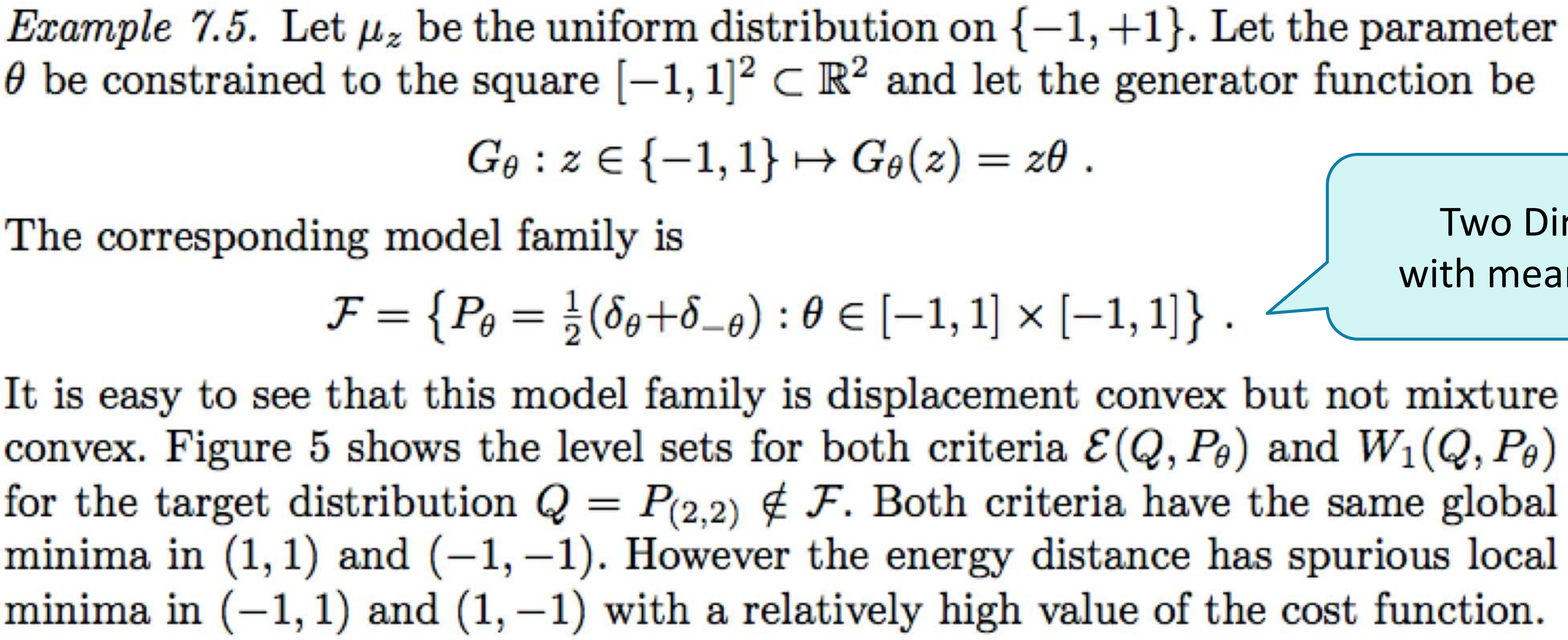
The convexity of implicit model families

Short story

- An implicit model family cannot be mixture convex while having a nice smooth generator $G_\theta(z)$.
- It is relatively easy to make implicit model families that are displacement convex.

Explain!

How things can go wrong



Example 7.5. Let μ_z be the uniform distribution on $\{-1,+1\}$. Let the parameter θ be constrained to the square $[-1,1]^2 \subset \mathbb{R}^2$ and let the generator function be

$$G_\theta : z \in \{-1,1\} \mapsto G_\theta(z) = z\theta \ .$$

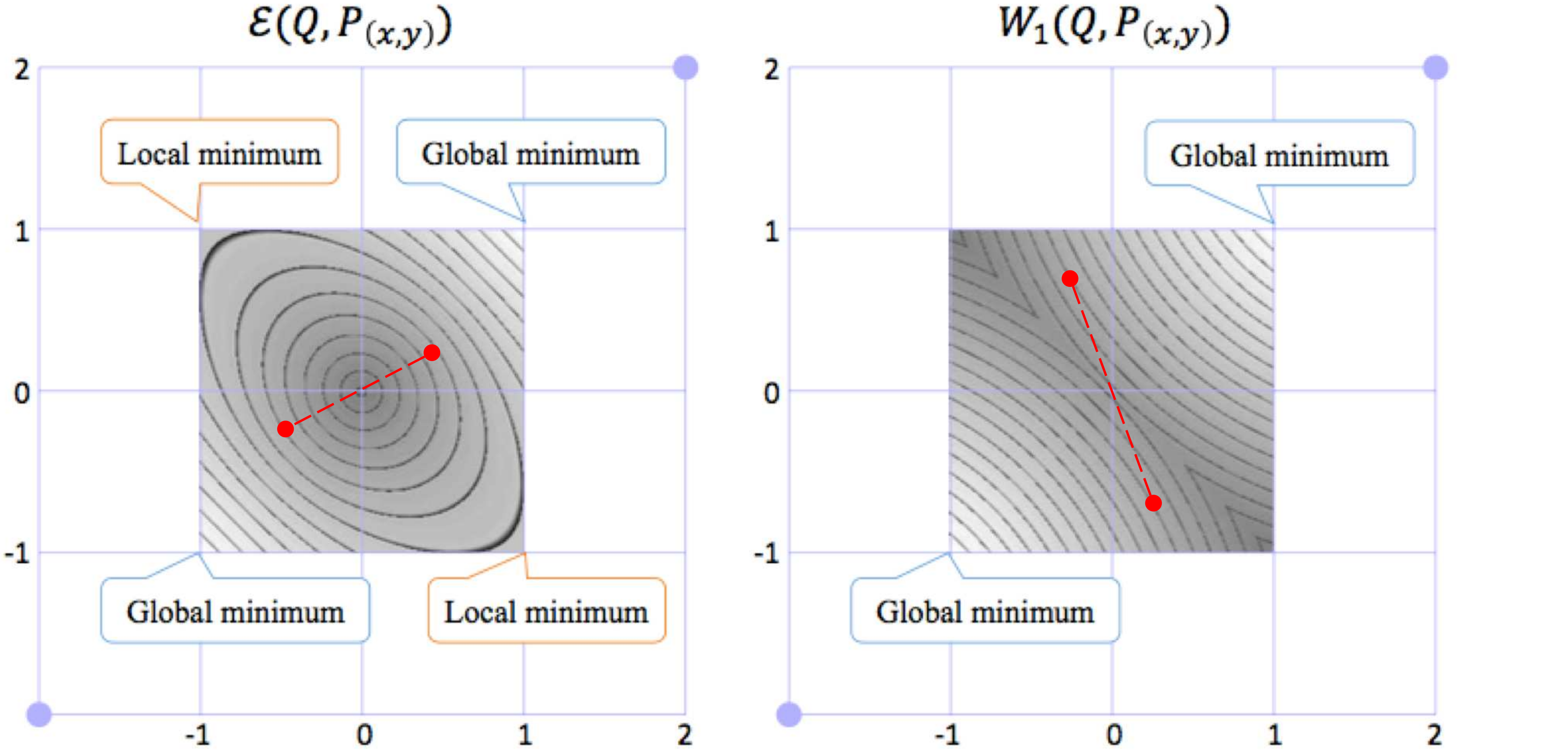
The corresponding model family is

$$\mathcal{F} = \left\{ P_\theta = \tfrac{1}{2}(\delta_\theta + \delta_{-\theta}) : \theta \in [-1,1] \times [-1,1] \right\} \ .$$

It is easy to see that this model family is displacement convex but not mixture convex. Figure 5 shows the level sets for both criteria $\mathcal{E}(Q, P_\theta)$ and $W_1(Q, P_\theta)$ for the target distribution $Q = P_{(2,2)} \notin \mathcal{F}$. Both criteria have the same global minima in $(1,1)$ and $(-1,-1)$. However the energy distance has spurious local minima in $(-1,1)$ and $(1,-1)$ with a relatively high value of the cost function.

Two Dirac distributions with mean zero in a square.

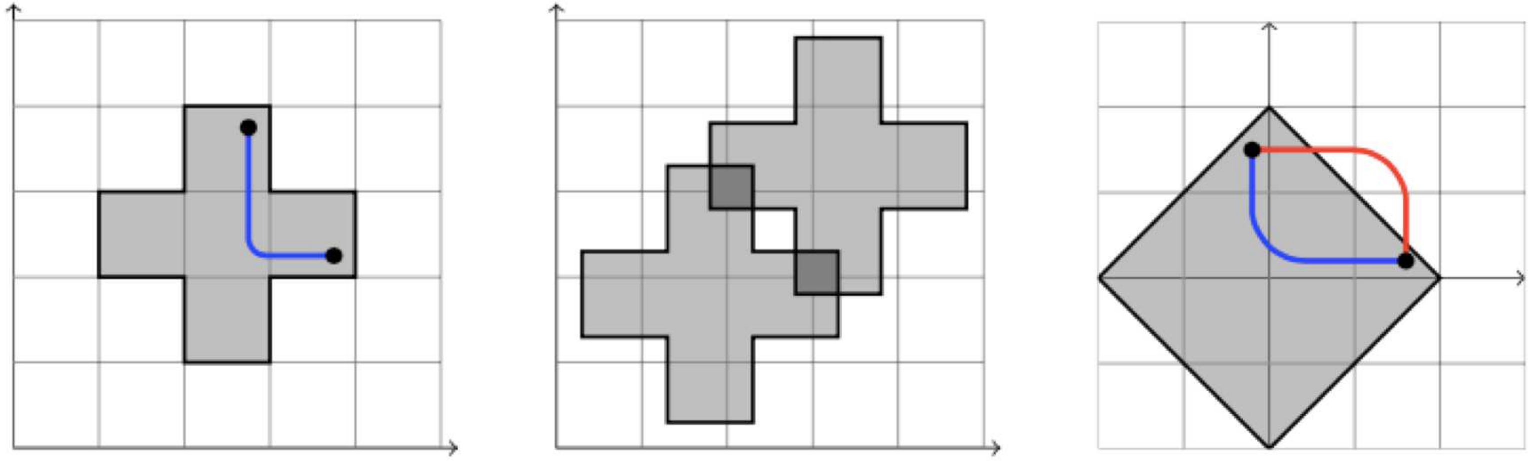
How things can go wrong



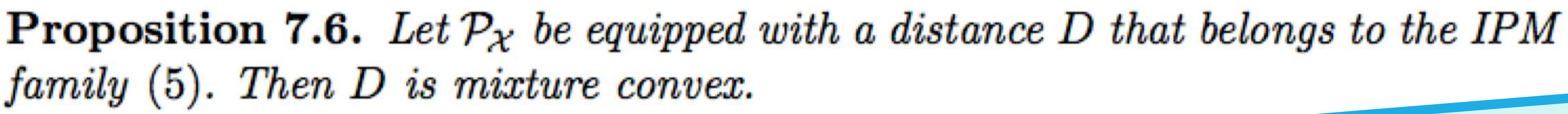
The convexity of distance functions

- Learn by minimizing $\min_{P_\theta \in \mathcal{F}} D(Q, P_\theta)$

When is $D(Q, P_\theta)$ geodesically convex?



Mixture-convexity

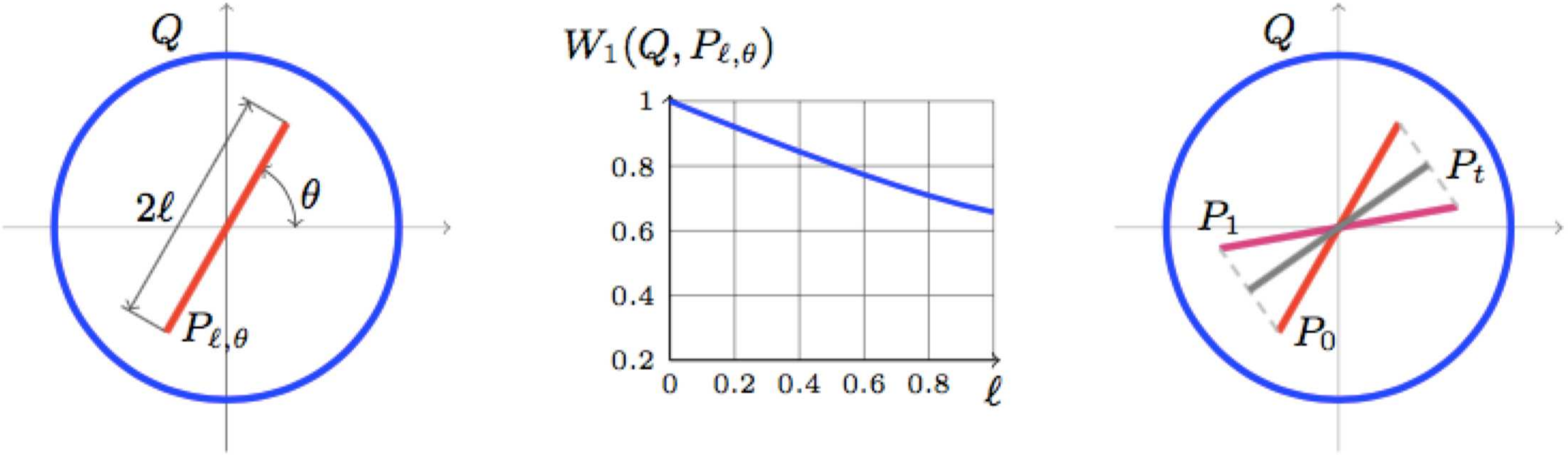


Proposition 7.6. *Let $\mathcal{P}_{\mathcal{X}}$ be equipped with a distance D that belongs to the IPM family* (5). *Then D is mixture convex.*

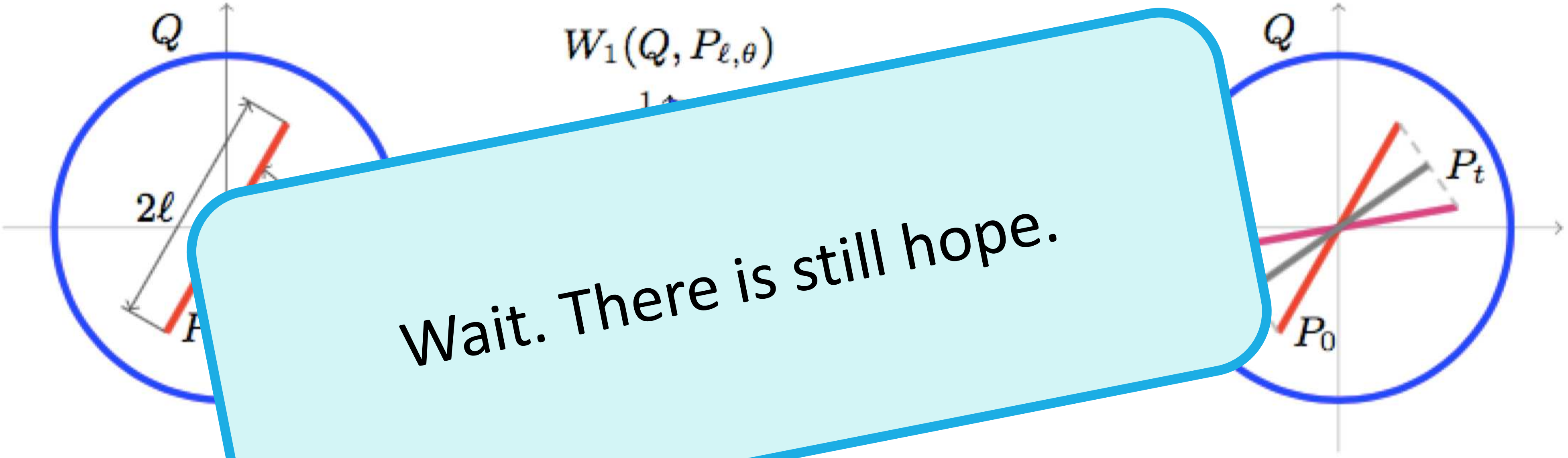
Therefore

- $\mathcal{E}_d(Q, P)$ is mixture convex and geodesically convex.
- $W_1(Q, P)$ is mixture convex

The Wasserstein distance is not displacement convex

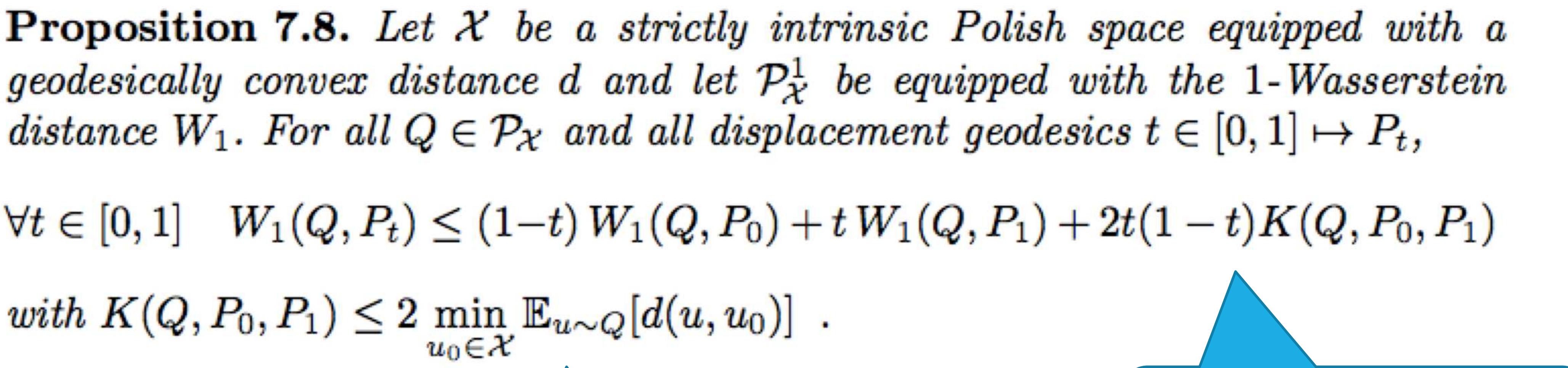


The Wasserstein distance is not displacement convex



Wait. There is still hope.

Almost convexity



Proposition 7.8. *Let $\mathcal{X}$ be a strictly intrinsic Polish space equipped with a geodesically convex distance d and let $\mathcal{P}^1_{\mathcal{X}}$ be equipped with the 1-Wasserstein distance W_1. For all $Q \in \mathcal{P}_{\mathcal{X}}$ and all displacement geodesics $t \in [0,1] \mapsto P_t$,*

$$\forall t \in [0,1] \quad W_1(Q,P_t) \leq (1-t)\,W_1(Q,P_0) + t\,W_1(Q,P_1) + 2t(1-t)K(Q,P_0,P_1)$$

with $K(Q,P_0,P_1) \leq 2 \min_{u_0 \in \mathcal{X}} \mathbb{E}_{u \sim Q}[d(u,u_0)]$.

BOUND THE CONVEXITY VIOLATION

GROSS BOUND

Almost convexity

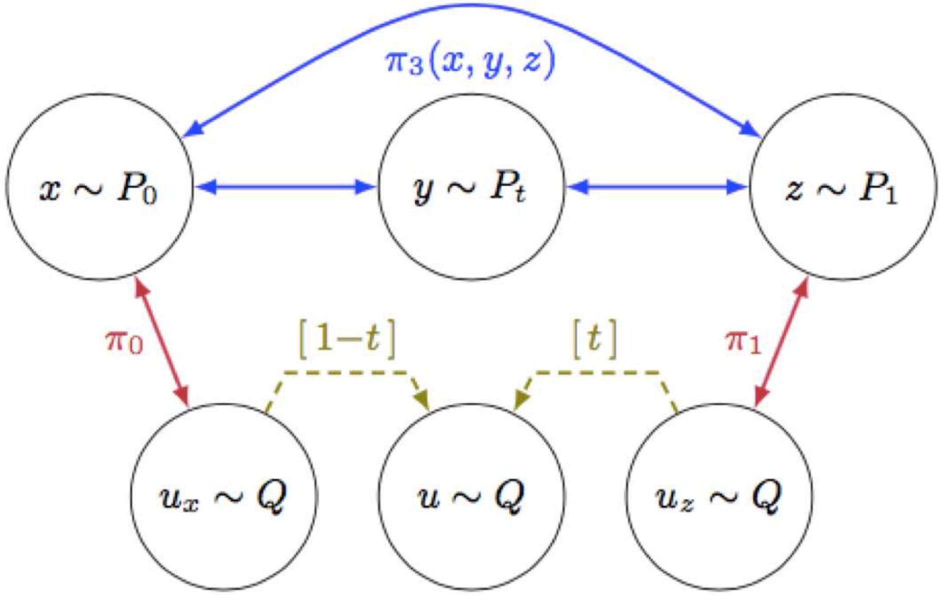
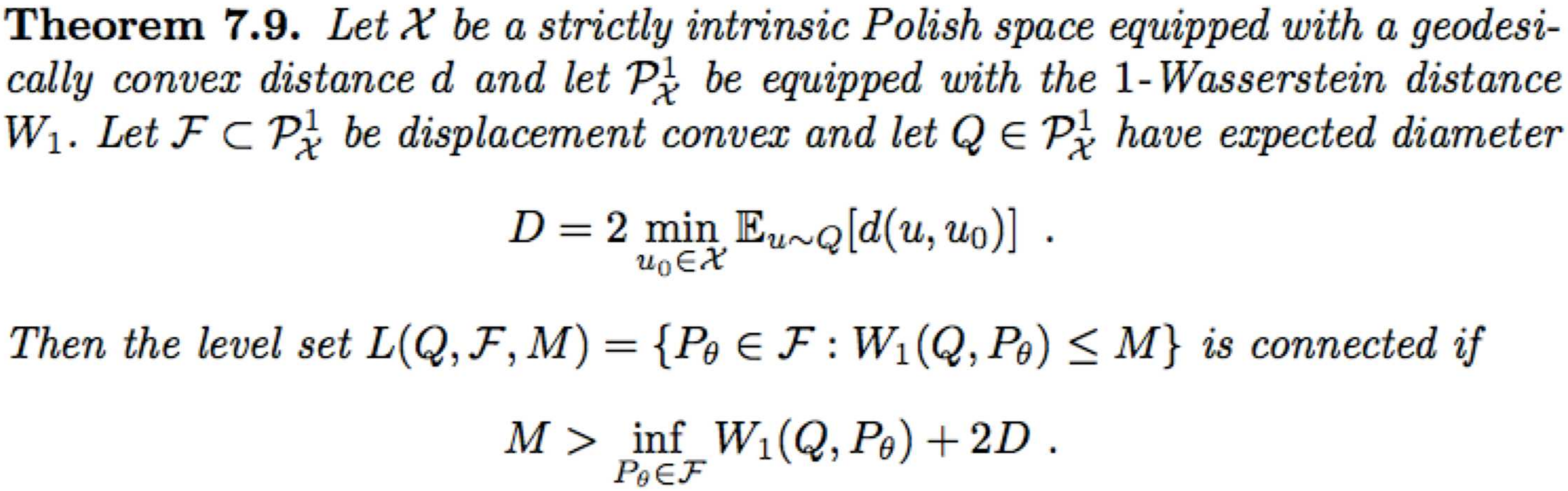


Fig. 8. The construction of $\pi \in \mathcal{P}_{\mathcal{X}^6}$ in the proof of Proposition 7.8.

Descent works until it gets too close



Theorem 7.9. *Let $\mathcal{X}$ be a strictly intrinsic Polish space equipped with a geodesically convex distance d and let $\mathcal{P}^1_{\mathcal{X}}$ be equipped with the 1-Wasserstein distance W_1. Let $\mathcal{F} \subset \mathcal{P}^1_{\mathcal{X}}$ be displacement convex and let $Q \in \mathcal{P}^1_{\mathcal{X}}$ have expected diameter*

$$D = 2 \min_{u_0 \in \mathcal{X}} \mathbb{E}_{u \sim Q}[d(u, u_0)] \ .$$

Then the level set $L(Q, \mathcal{F}, M) = \{P_\theta \in \mathcal{F} : W_1(Q, P_\theta) \leq M\}$ is connected if

$$M > \inf_{P_\theta \in \mathcal{F}} W_1(Q, P_\theta) + 2D \ .$$

Related works

Many authors went for this kind of results

- Amari – Information geometry
- Freeman & Bruna, 2017 – connectivity of level sets in relu networks
- Aufflinger & Ben Arous 2013 – random functions on the sphere
- More?

Critical difference

All these work look at the intrinsic geometry of a family of models.
We look at the geometry of the entire family of probability measures,
then introduce convexity concepts for the parametrized families of interest.

Conclusion

Recapitulation

- Economically meaningful technological successes
  have triggered a new wave of hope (and hype) about Artificial Intelligence.
- Statistics ≠ semantics
  $\Longrightarrow$ machine learning alone cannot crack AI
  $\Longrightarrow$ we need a couple conceptual breakthroughs.

→ Causation seems to plays an central role (detective guesswork.)

→ Even static image datasets contains hints about causal relations (experimental results.)

→ Using the right probability distances could help (some theoretical and experimental results.)