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NYU | COURANT INSTITUTE OF MATHEMATICAL SCIENCES

MATHEMATICS OF DEEP LEARNING

JOAN BRUNA , CIMS + CDS, NYU, SPRING'18

Lecture 1: The Curse of Dimensionality

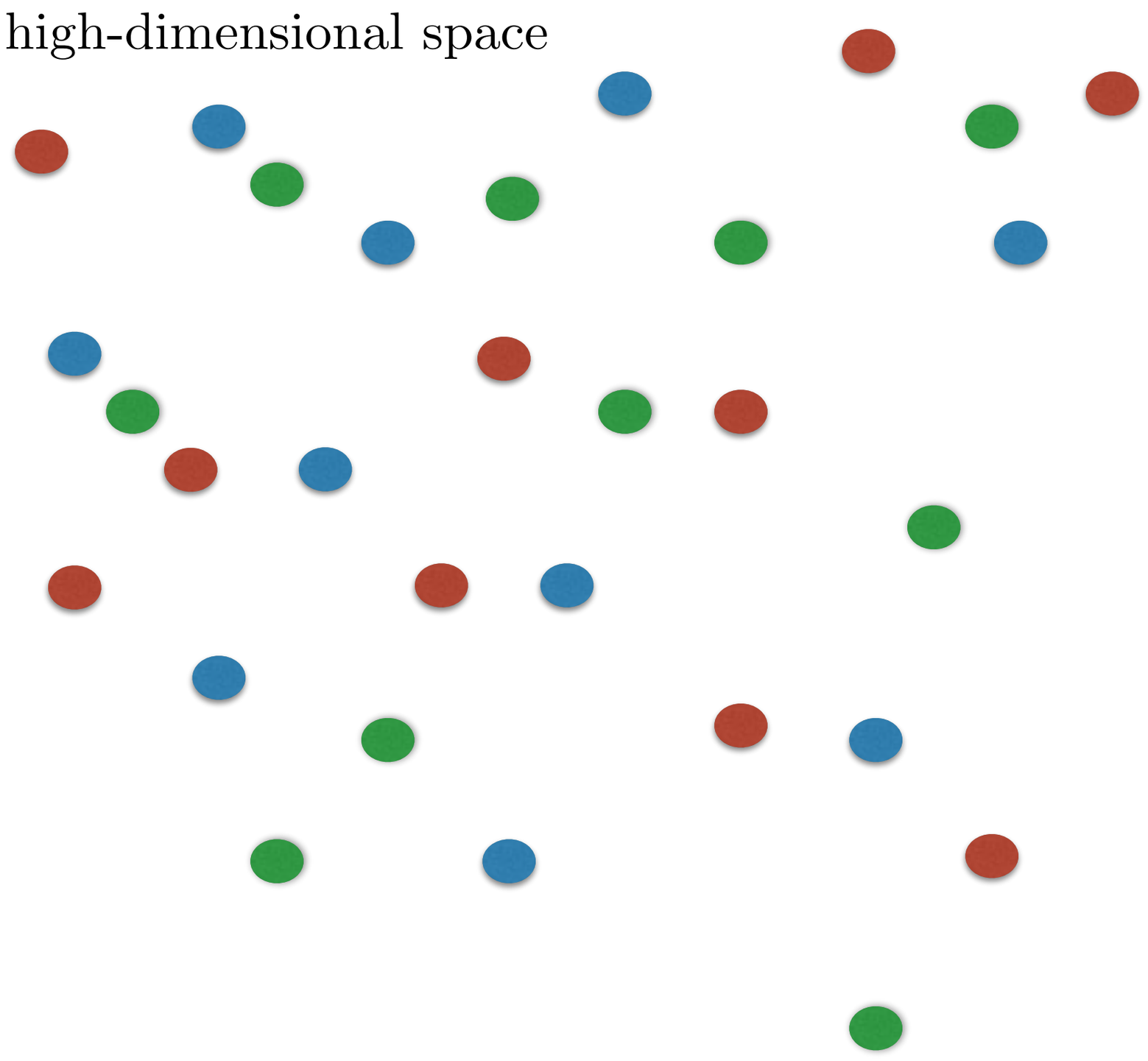
COURSE OVERVIEW

- Part I: Geometry of Data

- Part II: Geometry of Optimization and Generalization.

- Parallel Curricula [Optional, TA: Cinjon Resnik]
  - Focus on RL

PART I: GEOMETRY OF DATA



PART I: GEOMETRY OF DATA

high-dimensional space

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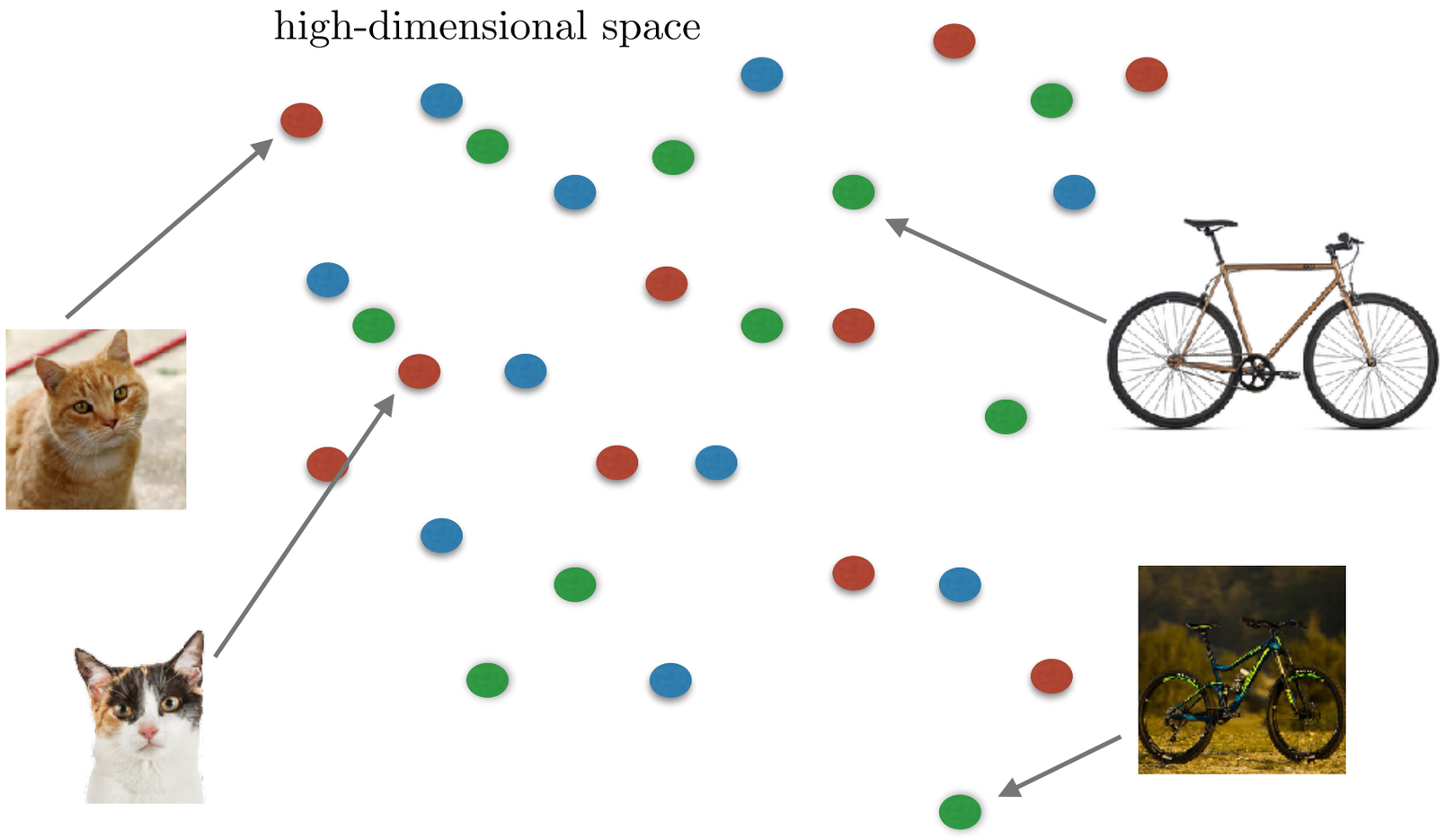

- Learning can be seen as a high-dimensional interpolation problem: estimate unknown function $f : \mathcal{X} \subseteq \mathbb{R}^d \to \mathcal{Y}$ given its values on n training points

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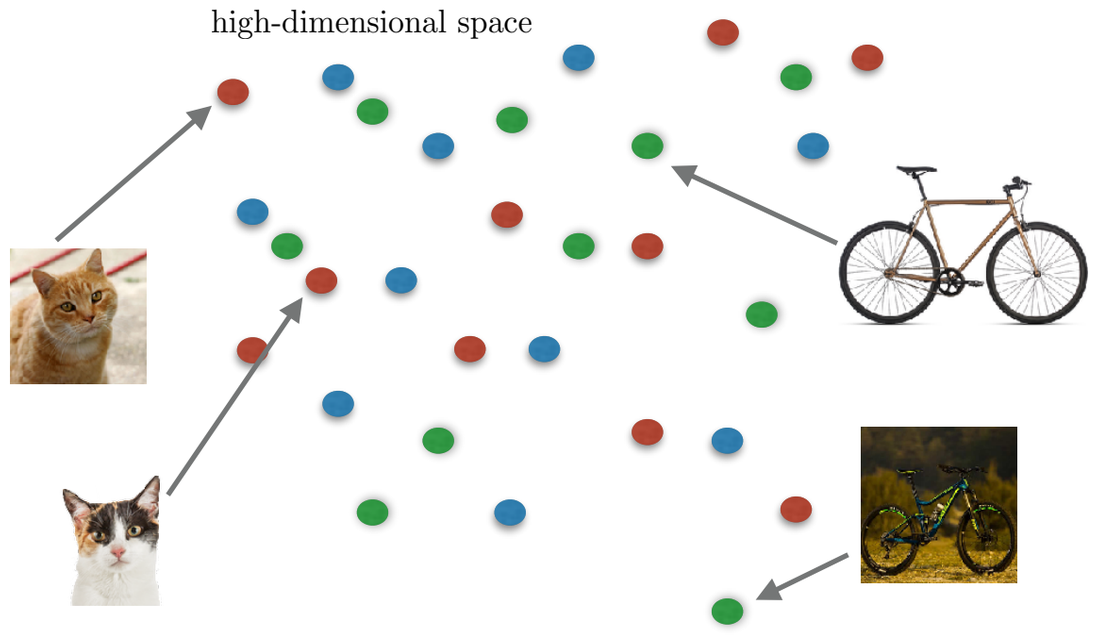

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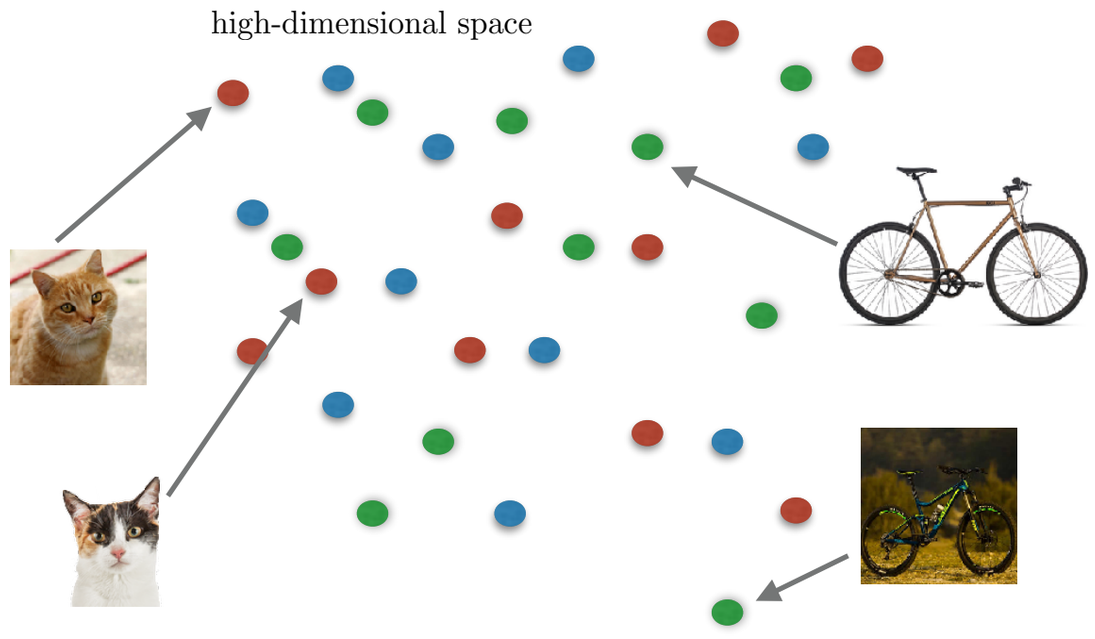

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- This problem is ill-defined without assumptions on *f*.
  - ***Which assumptions?***

PART I: GEOMETRY OF DATA

- Regularity of f is defined relative to a distance in $\mathcal{X}$ and $\mathcal{Y}$.
- E.g., f is Lipschitz with respect to distances $d_{\mathcal{X}}, d_{\mathcal{Y}}$ if

$$\exists\ C\ s.t\ \forall\ x, x'\ ,\ d_{\mathcal{Y}}(f(x), f(x')) \leq C d_{\mathcal{X}}(x, x')\ .$$

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- Take standard Euclidean metric and assume real outputs:

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- How many points $N(\epsilon)$ do we need to observe to guarantee that $|\hat{f}(x) - f(x)| \leq \epsilon$?

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$$|\hat{f}(x) - f(x)| \leq \epsilon\ ?$$

- This is equivalent to finding an "ϵ-covering" of the data. If we simply assume compactness (e.g. finite energy), then $N(\epsilon) \simeq \epsilon^{-d}$.

PART I: GEOMETRY OF DATA

- This is an instance of the curse of dimensionality
  - more on that in today's lecture.
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- Thus, we need further regularity priors on the class of functions (=tasks) we are interested in.
- In typical deep learning applications, input space $\mathcal{X}$ is
  - Images / Videos: $\mathcal{X} = L^2(\Omega)$, $\Omega =$ Grid of 2d, 3d pixels.
  - Time-series: $\mathcal{X} = L^2(\mathbb{R})$
  - Text: $\mathcal{X} =$ sequences over discrete alphabet.
- Are there distances in $\mathcal{X}$ that encode regularity of typical tasks f ?

PART I: GEOMETRY OF DATA

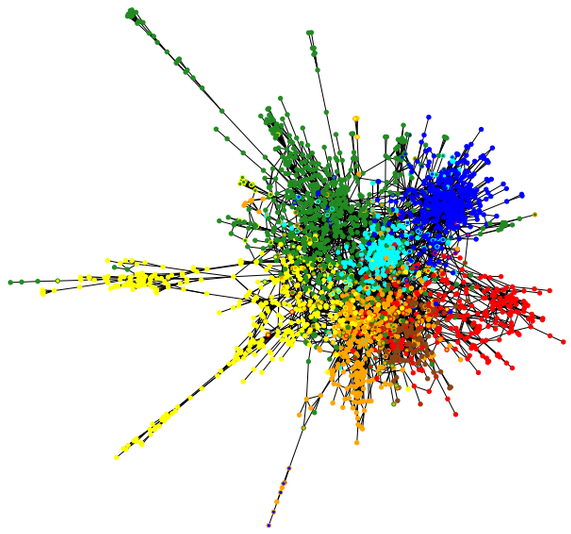
- We will introduce the notion of geometric stability
- In a vector space, not a lot of operations defined (only linear operations in fact).
- In a functional space, we can exploit much more structure
  - for instance, we can consider changes of variable given by geometric transformations (eg translation, rotations).

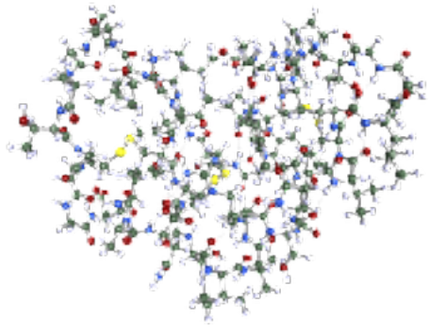
  - it turns out these are really meaningful in many machine learning contexts.

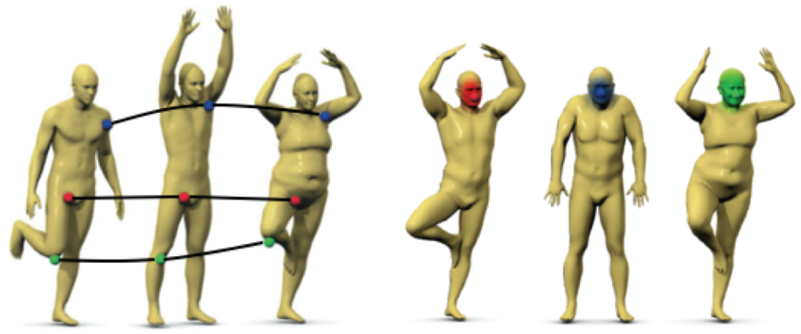
PART I: GEOMETRY OF DATA

- How to properly define geometric stability?
- How to exploit it with appropriate representations?
  - As it turns out, CNNs are one possibility.
- Supervised and unsupervised learning under geometric stability.

- How to generalize the notion of geometric stability to more general domains?
  - Non-Euclidean geometry
  - Graphs.
  - Applications







Correspondence Similarity

PART II: GEOMETRY OF OPTIMIZATION AND GENERALIZATION

- Essentially all deep learning models are trained with some form of Stochastic Gradient Descent.
- Convergence properties of SGD and its variants (momentum, adam, adagrad,etc.)
  - Can we learn something about SGD by studying continuous time optimization?
  - Langevin Dynamics, Fokker-Plank, Stochastic Differential Equations.

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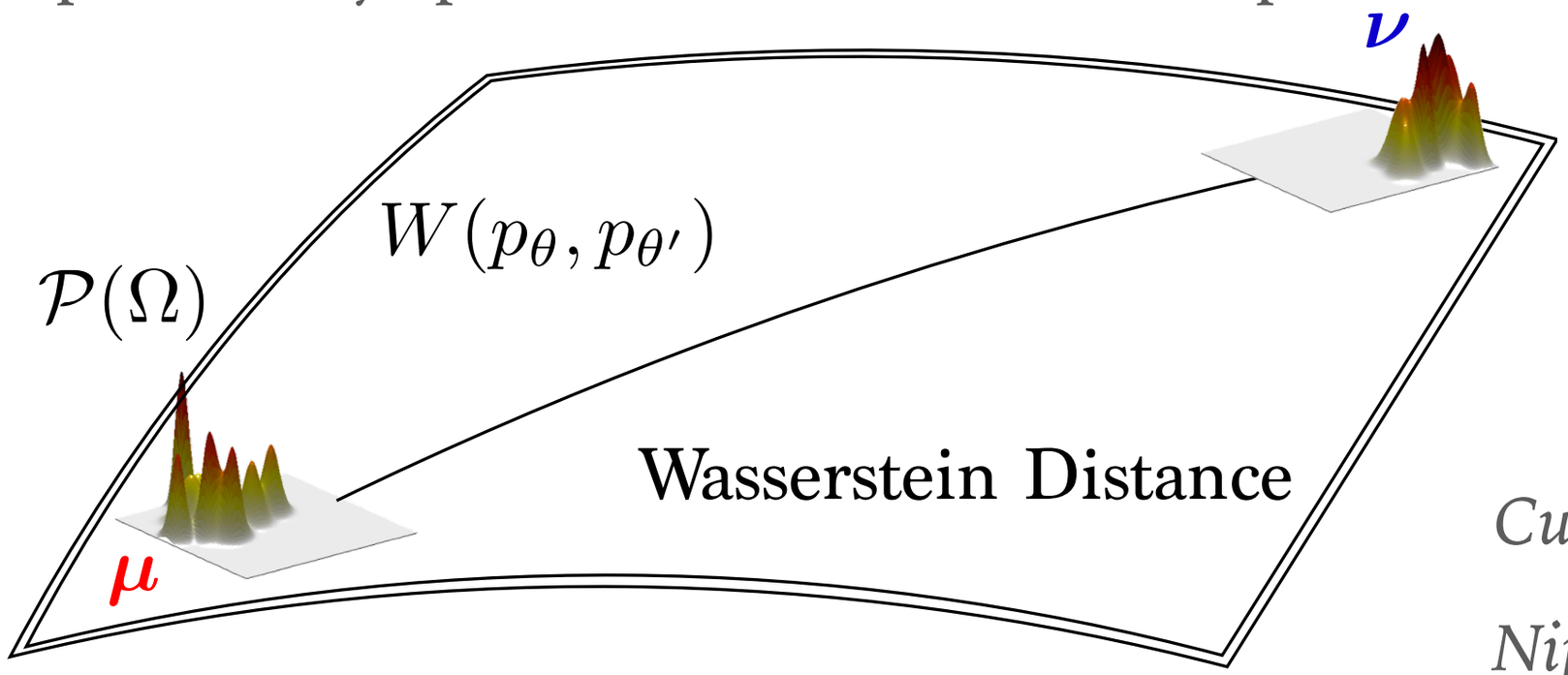
  - Langevin Dynamics, Fokker-Plank, Stochastic Differential Equations.
- Gradients belong to tangent spaces.
  - In Euclidean spaces, we assimilate the tangent space at each point with the space itself.
  - What is the “right” space where to think about optimization/learning?

PART II: GEOMETRY OF OPTIMIZATION AND GENERALIZATION

- Overview of Information Geometry [Amari, Rao, Kullback]
  - Describes the manifold of probability measure using Fisher metric.
- Reproducing Kernel Hilbert Spaces (RKHS).
  - Enable convex optimization machinery.
- Optimal Transport and Generalization
  - Studies probability spaces defined over metric spaces.

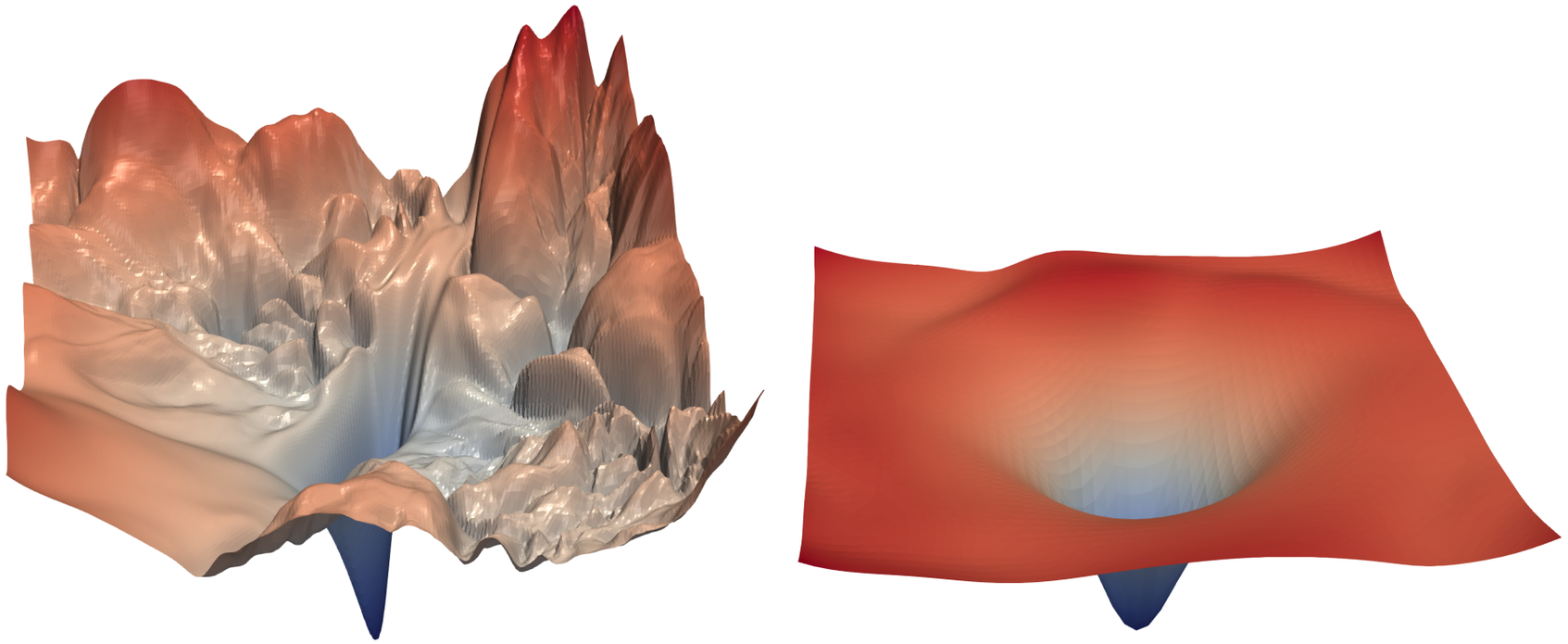


Cuturi & Solomon

Nips'17 OT

PART II: GEOMETRY OF OPTIMIZATION AND GENERALIZATION

- Optimization Landscape of neural networks.



(a) without skip connections

(b) with skip connections

[Li et al.'17]

- Full of poor local minima?
- Role of overparametrisation/architecture?
- Is this a problem in terms of generalization?

PARALLEL CURRICULA

- **Optional.**
- Led by Cinjon Resnik.
- Fridays 11am-12:30pm WWH 101
- *Mission*: "Understand the impactful papers in Machine Learning by going back to their roots, building the tree of dependencies, and envisioning where the leaves will grow."

- We will start with a curriculum targeted to AlphaGo [Deepmind, Nature'16].

LOGISTICS

- Course website:

  https://joanbruna.github.io/MathsDL-spring18/

- Office Hours: Tuesdays, 9-11am. Office 612 60 5th ave.

GRADING

- Midterm project checkpoint [25%]
  - Abstract Proposal detailing the specific topic.
  - Due: March 9th.
- Class Participation [25%]
- Final Project [50%]
- Parallel Curricula [+ 25% bonus]

FINAL PROJECT

- In-depth survey article about a selected topic.
- By groups of {1,2} people.
- Project due May 1st, based on feedback from Proposal.
- Similar in depth as:
  - BAIR Research blog. [baseline]
  - Off the convex path/argmin [happy]
  - Distill.pub [enthusiastic]
- At the end of the semester, projects will be integrated into course website.
  - Best projects will be encouraged to submit to Distill!

LECTURE 1: THE CURSE OF DIMENSIONALITY IN ML

- Statistical Curses
  - In Supervised Learning.
  - In Unsupervised Learning.
  - Remarkable exception: Principal Component Analysis.
- Learning Curses
  - Gradient-free curses?
  - Gradient-descent failures.
- Conclusion: Learning without Priors?

WHAT IS THE CURSE OF DIMENSIONALITY?

- It refers generally to the intrinsic statistical/computational drama arising when a quantity of interest scales exponentially with the input dimensionality.
  - so, always watch out for dimensions in the exponents!
  - Equivalently, this reflects a bound that depends roughly on the number of “distinct” instances of the problem.

- We will see some examples to familiarize ourselves with it.

PRELIMINARIES: RATE OF CONVERGENCE/ RATE OF APPROXIMATION

- Rates in statistics: As a function of number of (iid) observations, how fast does the estimator approach the desired quantity? in which sense we measure convergence?

- Rates in optimization: How fast does my algorithm converge to a designated solution?

- Rates in approximation theory: approximation error as a function of number of basis elements.

EMPIRICAL RISK MINIMIZATION: SUPERVISED LEARNING SETUP

- Data distribution:
  $(X, Y) \sim \mathcal{D}$, $X \in \mathbb{R}^d$, $Y = \pm 1$ (binary classification).
- Loss $\ell(y, f(x))$ (mean-square, hinge, logistic).
- Hypothesis class: Function space $\mathcal{F} = \{f : \mathcal{X} \to \mathbb{R}\}$.

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- Population and Empirical Risk:
  $\widehat{\mathcal{D}}$ = empirical distribution from n iid samples.

$$\mathcal{R}(f) = \mathbb{E}_{\mathcal{D}}[\ell(Y, f(X))] \ .$$

$$\widehat{\mathcal{R}}(f) = \mathbb{E}_{\widehat{\mathcal{D}}}[\ell(Y, f(X))] = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(x_i)) \ ,$$

- Empirical Risk Minimization:

$$\hat{f}_\delta = \arg \min_{f \in \mathcal{F}; \|f\|_{\mathcal{F}} \leq \delta} \widehat{\mathcal{R}}(f) \ .$$

SUPERVISED LEARNING

- "Fundamental Theorem of ML":

$$\mathcal{R}(f) = \underbrace{\widehat{\mathcal{R}}(f)}_{\text{empirical loss}} + \underbrace{[\mathcal{R}(f) - \widehat{\mathcal{R}}(f)]}_{\text{generalization gap}}$$

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- More precisely, suppose we have approximately solved the ERM: $f_\delta \; s.t \; \mathcal{R}(f_\delta) \leq \epsilon + \inf_{\|f\|_{\mathcal{F}} \leq \delta} \mathcal{R}(f)$.
- Then [Shalev-Shwartz, Ben-David'14]:

$$\mathcal{R}(\hat{f}_\delta) - \inf_{f \in \mathcal{F}} \mathcal{R}(f) \leq \underbrace{\left[\inf_{\|f\|_{\mathcal{F}} \leq \delta} \mathcal{R}(f) - \inf_{f \in \mathcal{F}} \mathcal{R}(f)\right]}_{\text{approximation}} + 2 \underbrace{\sup_{\|f\|_{\mathcal{F}} \leq \delta} \left|\widehat{\mathcal{R}}(f) - \mathcal{R}(f)\right|}_{\text{statistical}} + \epsilon \; .$$

- Approximation error decreases by making $\mathcal{F}$ larger, but statistical error increases.

CURSES IN EMPIRICAL RISK MINIMIZATION

- Consider two extremes.
- No prior structure: $\mathcal{F} =$ Lipschitz continuous functions.
  [von Luxburg, Bousquet'04, Bach'17]

$$|\mathcal{R}(f) - \hat{R}(f)| \simeq n^{-\frac{1}{d+3}} \log n \ .$$

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- Less structure: $\mathcal{F} =$ One-layer ReLU networks with regularization:
  [Bach'17]

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k: size of hidden layer.

- Sample complexity to reach generalization gap ϵ?

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$$\Omega(\epsilon^{-d}) \text{ vs } \Omega(d/\epsilon^2)!$$

UNSUPERVISED LEARNING

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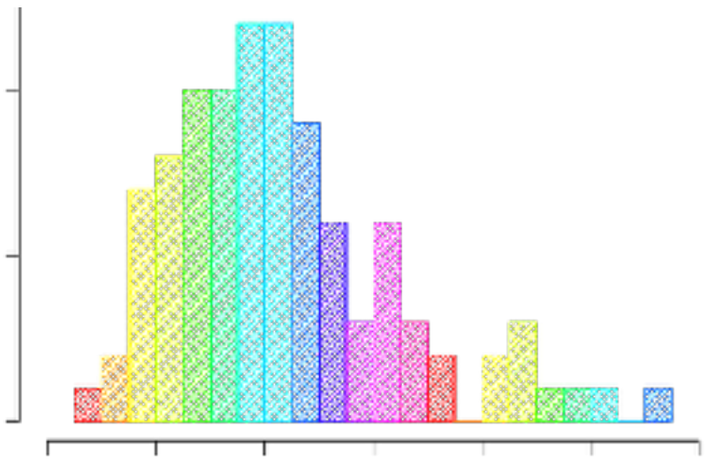

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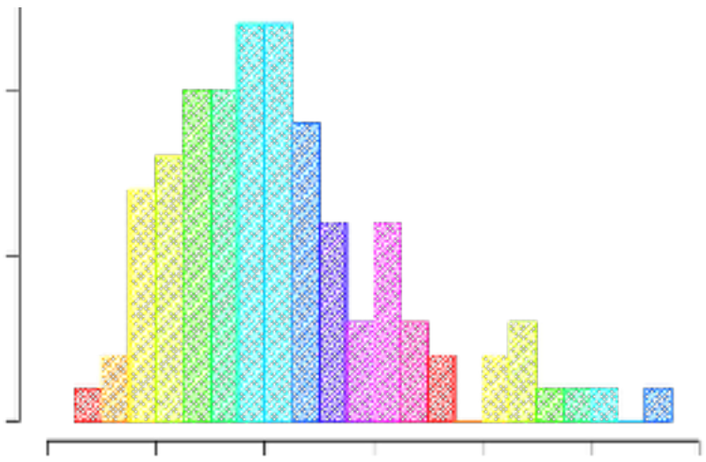

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$$\sup_{x \in \mathbb{R}^d} |\hat{p}_\sigma(x) - p(x)| \lesssim \sigma^\alpha + \sqrt{\frac{\log n}{n\sigma^d}}$$.[Tsybakov'08, Jiang'17]

(assuming p is α-Holder continuous).

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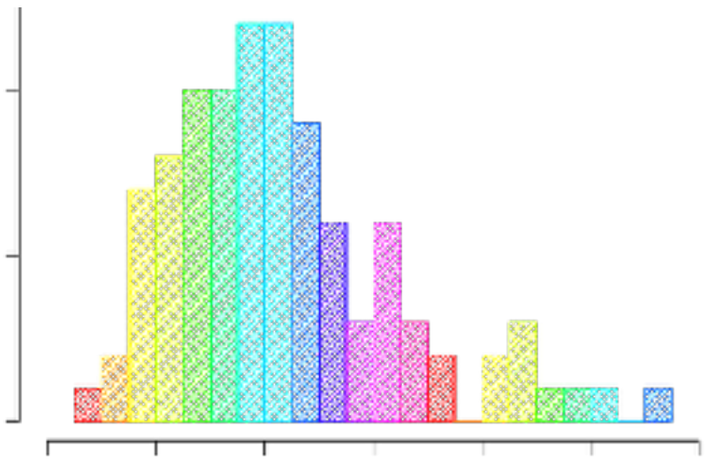

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- Leads to a rate

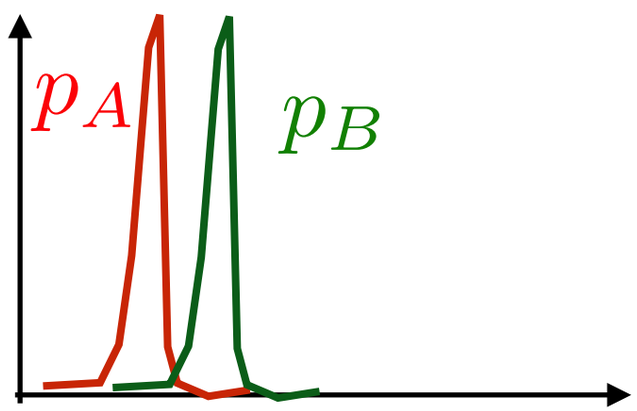
$$|\hat{p} - p|_\infty \simeq n^{-\alpha/(2\alpha+d)}$$

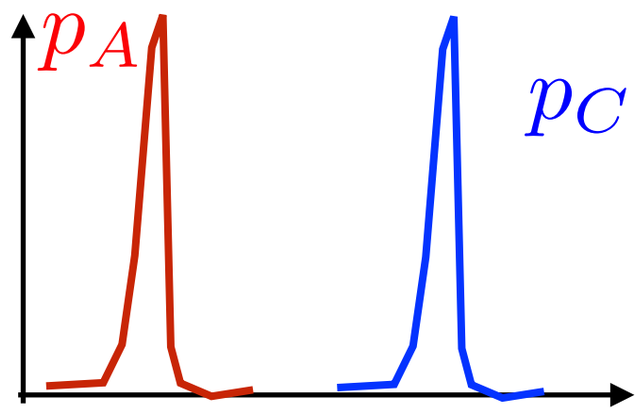
UNSUPERVISED LEARNING USING OPTIMAL TRANSPORT

- Perhaps issue with metric? TV, MSE all produce similar rates.
- Recently, interest in doing unsupervised learning with *transportation distances*.
- Do they also suffer from curse of dimensionality?

OPTIMAL TRANSPORT (SNEAK PREVIEW)

- Consider two measures μ, ν defined on a *metric* space Ω.





$$\mathrm{MSE}(p_A, p_B) \approx \mathrm{MSE}(p_A, p_C) = O(1)$$

- Can we find a distance between measures that takes the metric structure of Ω into account?

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- Consider $\Pi(\mu,\nu) = \{P \in \mathcal{P}(\Omega \times \Omega)\,;\, \forall\ A, B \subset \Omega,$
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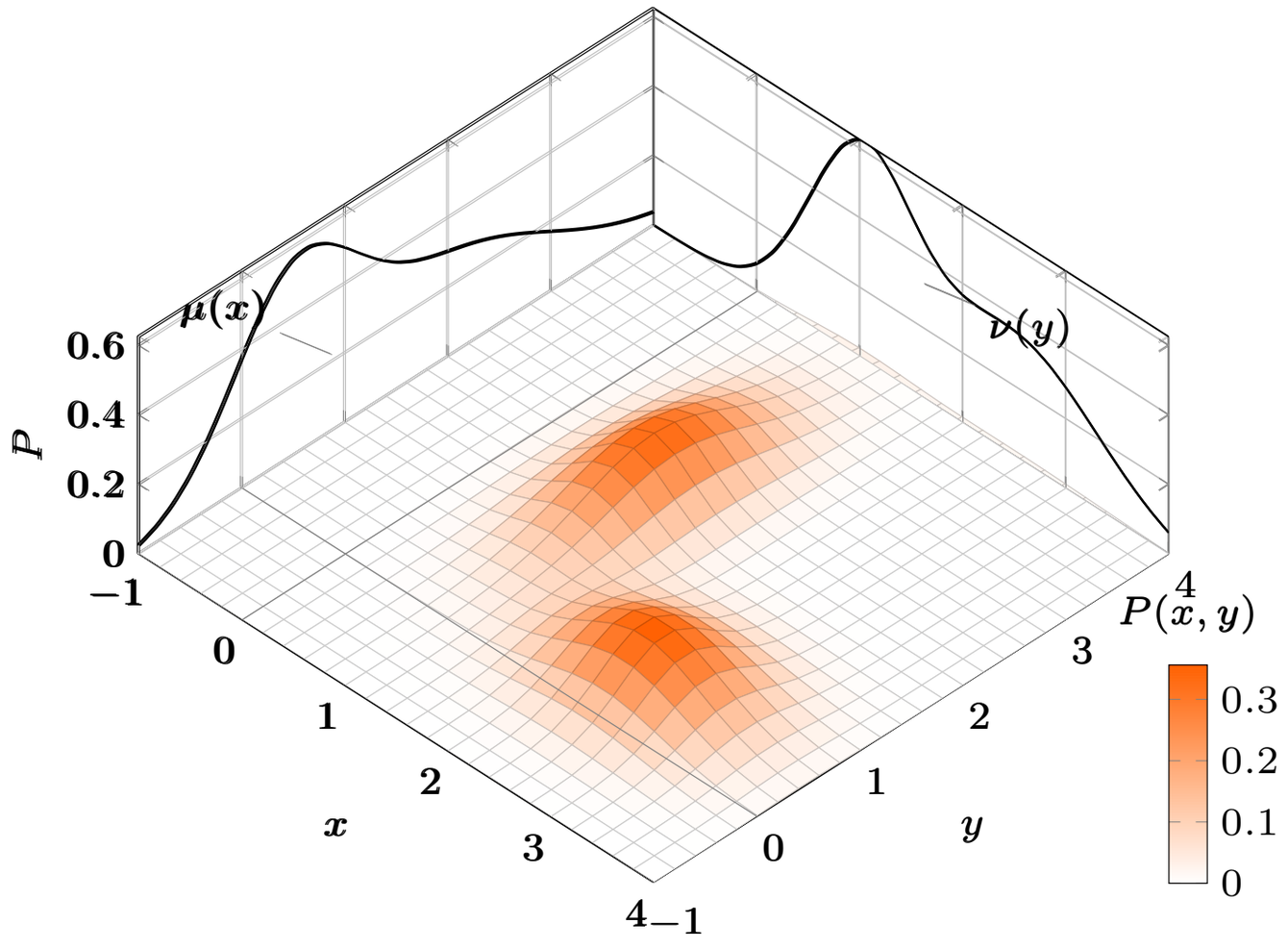

[from NIPS'17 OT tutorial, Cuturi & Solomon]

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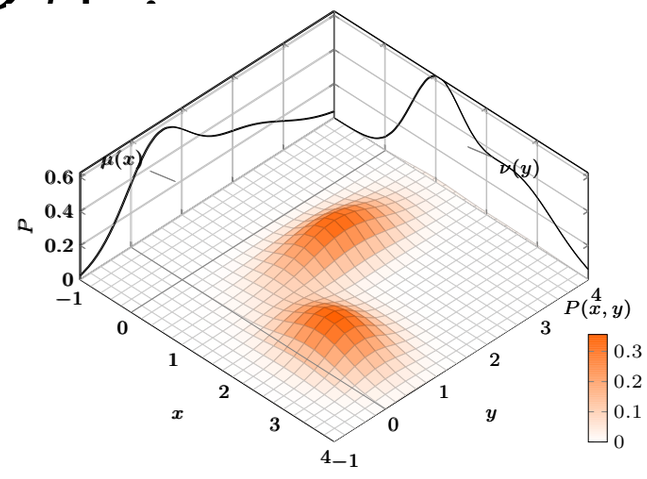

- The *p-Wasserstein* distance $(p \geq 1)$ is

$$W_p^p(\mu,\nu) = \inf_{P \in \Pi(\mu,\nu)} \mathbb{E}_{(X,Y)\sim P}\, \mathrm{dist}_\Omega(X,Y)$$

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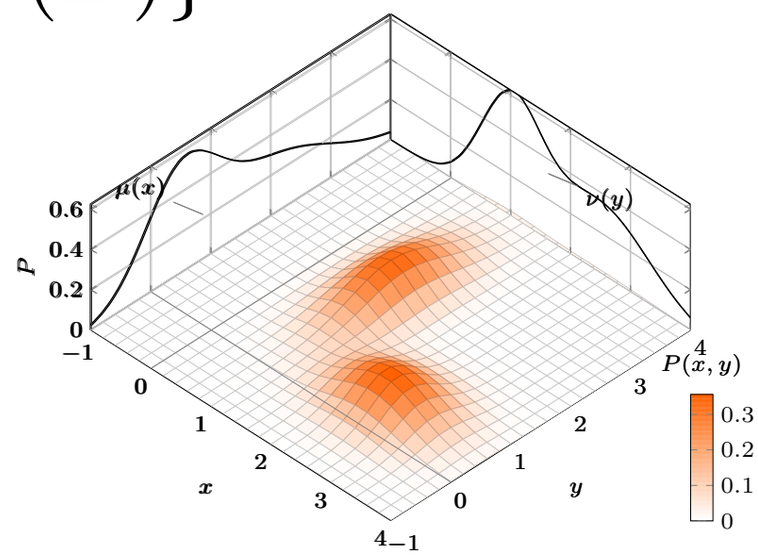

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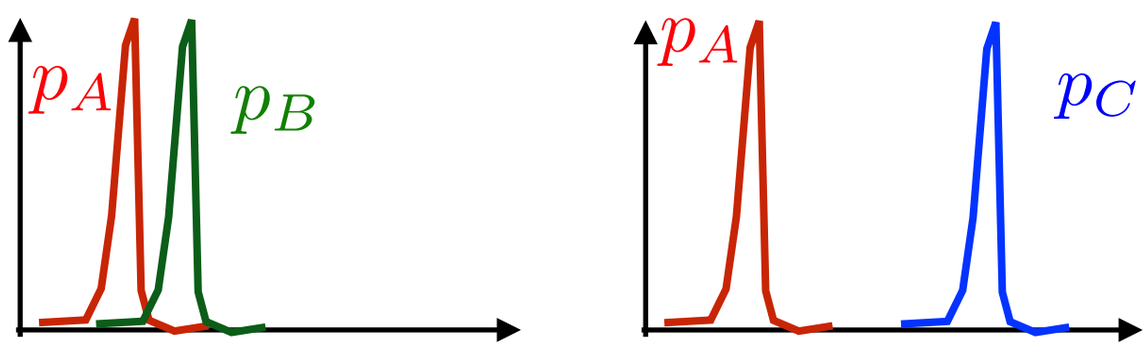
- When $p=1$, it admits a dual formulation.



$$W(p_A, p_B) \ll W(p_A, p_C)$$

OPTIMAL TRANSPORT IN MACHINE LEARNING

- Given "true" measure μ and a model $\nu(\theta), \mu, \nu(\theta) \in \mathcal{P}(\Omega)$, we would like to find parameters θ such that

$$\inf_{\theta} W(\mu, \nu(\theta))$$

- But instead of μ , we only have access to empirical measure

$$\hat{\mu}_n = \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i} \ , \ x_i \text{ iid} \sim \mu \ .$$

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- Again, we face a "bias-variance" tradeoff:

$$W(\mu, \nu(\theta)) \leq \underbrace{W(\mu, \hat{\mu}_n)}_{\text{statistical error}} + \underbrace{W(\hat{\mu}_n, \nu(\theta))}_{\text{approximation error}} \ .$$

OPTIMAL TRANSPORT IN MACHINE LEARNING

- Bad news [Dudley'68]: If μ is absolutely continuous wrt Lebesgue measure on $\mathbb{R}^d$, then

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- Lesson: ambient dimension is not necessarily the driving force behind the curse of dimensionality.
- Possible alternative: Energy-distances [Sejdinovic et al'12].
- How often can this be assumed in practice?

COVARIANCE ESTIMATION AND PCA

- Principal Component Analysis: ubiquitous data analysis tool for dimensionality reduction, data exploration, etc.
- Given $\mu \in \mathcal{P}(\mathbb{R}^d)$ with finite energy ($\mathbb{E}_{X\sim\mu}\|X\|^2 < \infty$), it consists in the spectral decomposition of its covariance operator:

$$\Sigma = \mathbb{E}_{X\sim\mu}(X - \mathbb{E}X)(X - \mathbb{E}X)^\top \in \mathbb{R}^{d\times d} \ .$$

$$\Sigma = U\Lambda U^\top \ , \ U^\top U = \mathbf{I}, \Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_d) \ .$$

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- Empirical covariance operator: $\Sigma, \widehat{\Sigma}_n \succeq 0$.

$$\widehat{\Sigma}_n = \mathbb{E}_{X\sim\hat{\mu}_n}(X - \mathbb{E}X)(X - \mathbb{E}X)^\top = \frac{1}{n}\sum_{i=1}^{n}(x_i - \overline{x})(x_i - \overline{x})^\top \ .$$

ESTIMATING THE PRINCIPAL COMPONENTS

- How good is this estimator? Is it cursed?

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Theorem [Vershynin]: For distributions with bounded order-q moment, the empirical covariance satisfies

$$\|\widehat{\Sigma}_n - \Sigma\| \lesssim O(\log\log n)^2 \left(\frac{n}{d}\right)^{1/2-2/q}.$$

- It follows that for a desired approximation $\|\widehat{\Sigma}_n - \Sigma\| \leq \epsilon$ we need $O((\log\log d)^\alpha d) \simeq O(d)$ samples. $\left(\frac{1}{\alpha} + \frac{1}{q} = \frac{1}{4}\right)$

- Lesson: Covariance estimation is legit in high dimensions!

CURSES IN OPTIMIZATION

- The curse of dimensionality not only manifests itself in statistics.
- In complexity theory, it captures EXPTIME/EXPSPACE problems.

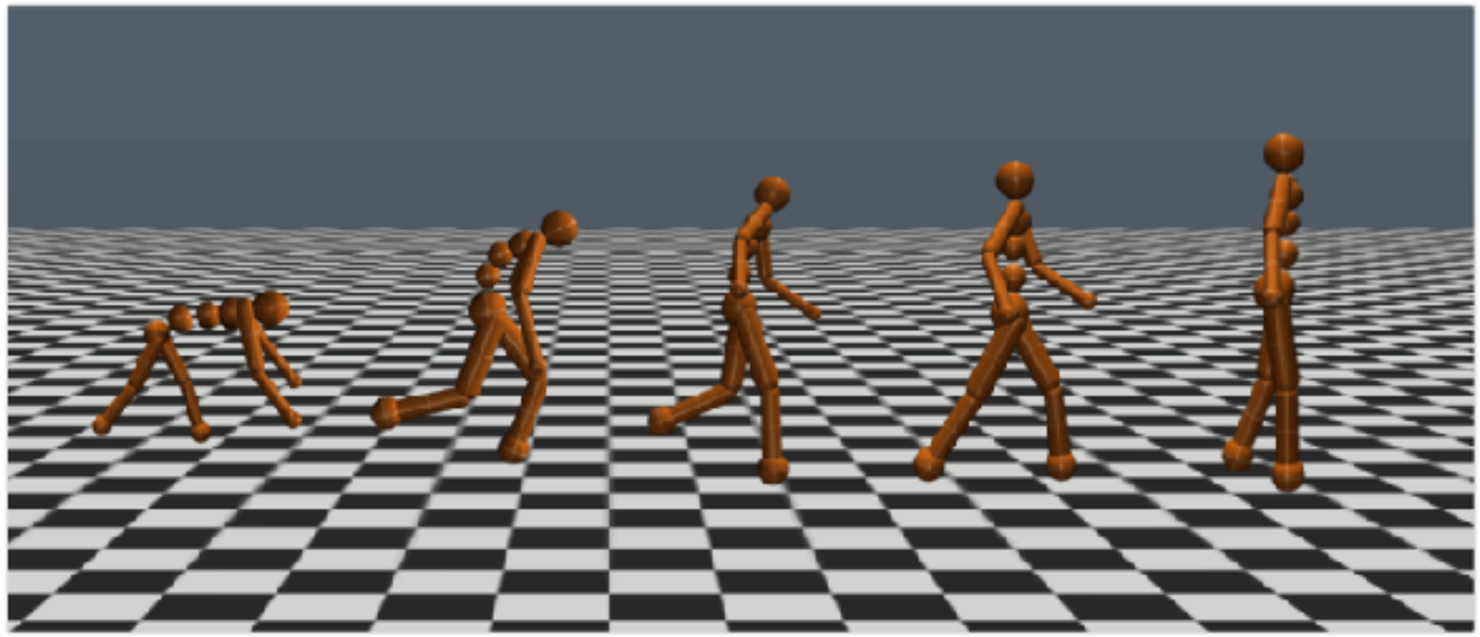
- How does it affect our ability to *learn*, ie optimize an objective function?

GRADIENT-FREE OPTIMIZATION

Welcoming the Era of Deep Neuroevolution

By Kenneth O. Stanley & Jeff Clune

December 18, 2017



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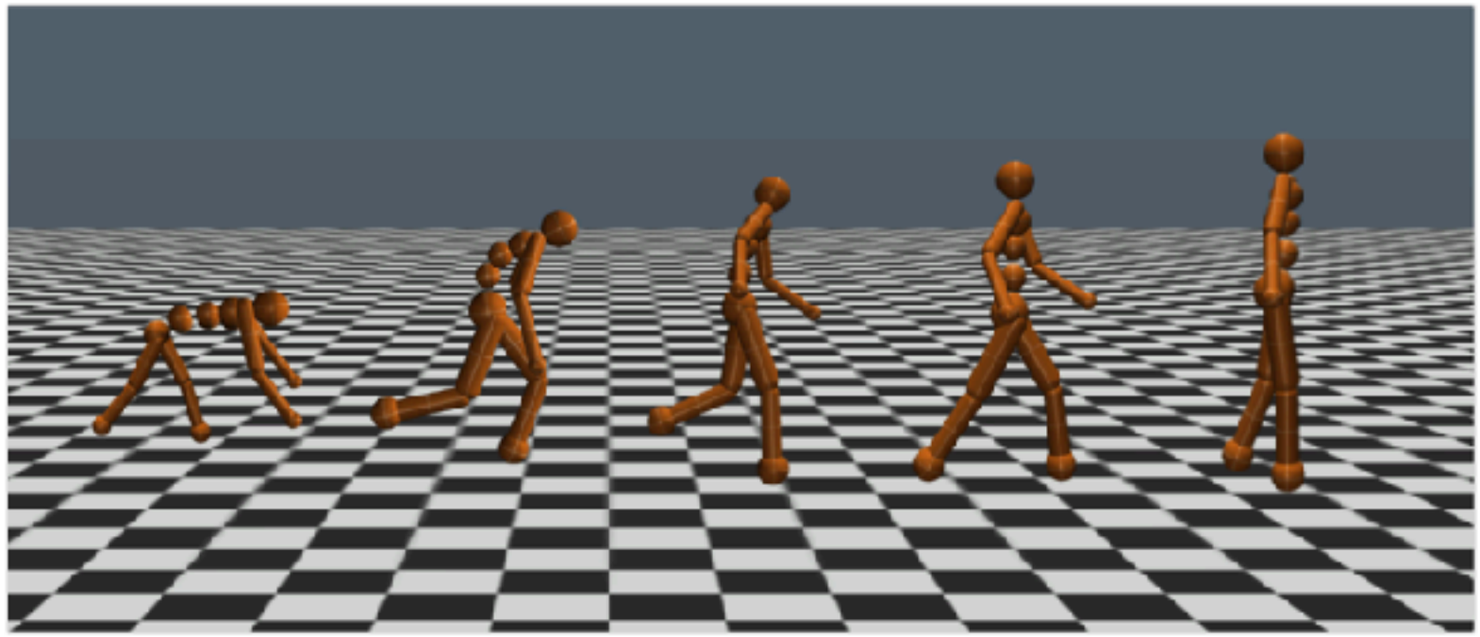

- What is *Neuroevolution*? $(F : \mathbb{R}^d \to \mathbb{R})$
- It is an iterative optimization scheme of the form

$$x_{t+1} = x_t + \frac{\alpha}{2\sigma}[F(x_t + \sigma\beta_t) - F(x_t - \sigma\beta_t)]\beta_t \ , \ \beta_t \sim \mathcal{N}(0, I) \ .$$

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- If σ is small, then the update approximates a (random) directional derivative:

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- Thus

$$\mathbb{E}_{\beta_t} \left\{ \frac{1}{2\sigma}[F(x_t + \sigma\beta_t) - F(x_t - \sigma\beta_t)]\beta_t \right\} \to \mathbb{E}\left\{ \langle \nabla F(x_t), \beta_t \rangle \beta_t \right\} = \nabla F(x_t) \ .$$

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- We are doing a stochastic (gradient-free) approximation of the gradient.

- What is the price to pay of not using gradient information?

GRADIENT-FREE IS NOT TOTALLY CURSED...

- It turns out [Nesterov, Spokoiny'10] that
  - Using directional derivatives $(\sigma \to 0)$ requires at most $O(d)$ times more iterations than standard sub gradient method.
  - Using finite-differences, we require $O(d^2)$ times more iterations in general.

- ... but in many DL tasks, $d \sim 10^8$!
- That said, such methods can be vastly parallelized.

CURSE OF GRADIENT DESCENT

- Consider a supervised learning setting where labels $y = h(x)$ are generated according to some hypothesis $h \in \mathcal{H}$.
- Gradient descent learning attempts to minimize

$$\min_{\theta} \mathcal{L}_h(\theta) = \mathbb{E}_x\{\ell(\Phi_\theta(x), h(x))\}$$

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  using gradient information $\nabla_\theta \mathcal{L}_h(\theta)$.
- Consider the variance of that gradient wrt the hypothesis class:

$$\mathrm{Var}(\mathcal{H}, \mathcal{L}, \theta) = \mathbb{E}_h \left\| \nabla \mathcal{L}_h(\theta) - \mathbb{E}_{h'} \nabla \mathcal{L}_{h'}(\theta) \right\|^2$$

- It measures how much information gradient conveys on target function $h \in \mathcal{H}$.

CURSE OF GRADIENT DESCENT

- Theorem [Shalev-Shwartz et al.'17]: If
  - $\mathcal{H}$ consists of real functions $\mathbb{E}_x\|h(x)\|^2 \leq 1$, such that $\mathbb{E}_x\{h(x)h'(x)\} = 0$ for $h \neq h' \in \mathcal{H}$.
  - $\Phi_\theta(x)$ satisfies $\mathbb{E}_x\{\|\nabla_\theta \Phi_\theta(x)\|^2\} \leq G(\theta)^2$ for some scalar $G(\theta)$.
  - ℓ is either square loss or binary classification Lipschitz loss.

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  Then $\mathrm{Var}(\mathcal{H}, \mathcal{L}, \theta) \leq \frac{G(\theta)^2}{|\mathcal{H}|}$.
- When learning from a large collection of uncorrelated functions, sensitivity of the gradient to the target function decreases linearly with $|\mathcal{H}|$.
- How does that relate to dimensionality of the problem?

CURSE OF GRADIENT DESCENT

- Let's illustrate it with the example of learning *parity functions*:

$$\mathcal{H} = \{x \mapsto (-1)^{\langle x, v \rangle} \; ; \; x, v \in \{0,1\}^d\} \; .$$

  - $|\mathcal{H}| = 2^d$, and
  - $\mathbb{E}_x\{h(x)h'(x)\} = \mathbb{E}_x\{(-1)^{\langle x, v+v' \rangle} = \prod_{v_i \neq v'_i} \mathbb{E}_{x_i}(-1)^{x_i} = \delta(v - v') \; .$
- It follows that $\mathrm{Var}(\mathcal{H}, \mathcal{L}, \theta) \leq \frac{G(\theta)^2}{2^d}$.
- By Chebyshev inequality, the gradient at any point θ will concentrate independently of v.
- This is regardless of which class of predictors.
- Hard to learn with gradient descent, but easy by solving a linear system! (albeit in $\mathbb{Z}_2$).