Statistical Optimal Transport

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Overview

1. **Chapter 1** - Optimal Transport
2. **Chapter 2** - Estimation of Wasserstein distances
3. **Chapter 3** - Estimation of transport maps
   - Problem formulation
   - Naïve approach and limitations
   - The semidual problem
   - A special case: affine transport maps
   - Stability of the semidual problem
   - Obtaining the slow rate
   - One - shot localization
   - Obtaining the fast rate

Recall

Theorem (Fundamental theorem of OT)

Let $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, $X \sim \mu$ and assume that μ has a density. TFAE:

1. $\bar{\gamma} \in \Gamma_{\mu,\nu}$ is an optimal coupling for W_2^2.
2. There exists a convex function φ such that $(X, \nabla\varphi(X)) \sim \bar{\gamma}$.
3. (Kantorovich duality)

$$\int \|x-y\|^2 \, d\bar{\gamma}(x,y) = \sup_{f \in L^1(\mu), g \in L^1(\nu)} \left(\int f \, d\mu + \int g \, d\nu \right),$$

where $f(x) + g(y) \leq \|x-y\|^2$.

Recall

Semidual formulation

If $\nabla\varphi$ is the optimal transport map, then φ solves

$$\min_{\phi} \mathcal{S}(\phi) := \int \phi \, d\mu + \int \phi^* \, d\nu$$

Problem Formulation

- **Given:**
  - Samples $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} \mu$
  - Samples $Y_1, \ldots, Y_n \overset{\text{i.i.d.}}{\sim} \nu$
- **Goal:** Estimate the optimal transport map T from μ to ν.
- **Performance Measure:**

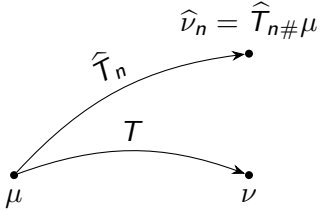
$$\int \|\widehat{T}_n(x) - T(x)\|^2 \, \mu(dx)$$

Relation to Wasserstein Distance

- **Integrated L^2 Error Controls Wasserstein Distance:**

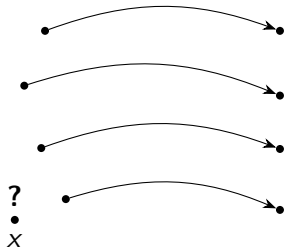
$$W_2^2(\widehat{\nu}_n, \nu) \leq \int \| \widehat{T}_n(x) - T(x) \|^2 \, \mu(dx)$$

- **Illustration:**



Naïve Approach and Limitations

- **Naïve Approach:** Compute optimal coupling between empirical measures μ_n and ν_n.
- **Issue:** Resulting map $\widehat{T}_n$ is only defined on sample points $\{X_i\}$.
- **Challenge:** Extending $\widehat{T}_n$ to all of $\mathbb{R}^d$ is non-trivial.



Interpolate?

Naïve Approach and Limitations - cont.

- **Setting:** Assume $d = 1$. $X_{(1)} < \cdots < X_{(n)}, Y_{(1)} < \cdots < Y_{(n)}$ - samples in sorted order.

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- **One nearest neighbour estimator:** Given $x \in [0, 1]$, let $X_{(i)}$ denote the largest sample from μ such that $X_{(i)} \leq x$. Set $\widehat{T}_n(x) := Y_{(i)}$ (if no such $X_{(i)}$ exists, then output $\widehat{T}_n(x) := 0$).

Naïve Approach and Limitations - cont.

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(Pointwise) Fast rate for 1NN estimator

Assume μ and ν have densities supported on $[0, 1]$, bounded away from 0 and ∞. For $x \in [0, 1]$,

$$\mathbb{E}|\widehat{T}_n(x) - T(x)|^2 \lesssim \frac{1}{n}$$

where T is the true optimal transport map $F_\nu^\dagger \circ F_\mu$ from μ to ν.

- **Sketch of proof:**
- The argument can be extended to show fast rate for the integrated error $\mathbb{E}\|\widehat{T}_n - T\|^2_{L^2(\mu)}$
- **Higher dimensions:** See **"Plugin Estimation of Smooth Optimal Transport Maps"** by Manole, Balakrishnan, Niles-Weed and Wasserman, 2021. (Slightly different definition using Voronoi cells)

Naïve Approach and Limitations - cont.

Rate of 1NN estimator [**MBNWW'21, Proposition 15**]

Let $\mu, \nu \in \mathcal{P}_{ac}([0,1]^d)$ admit densities p, q (respectively) such that $\gamma^{-1} \leq p \leq \gamma$ over $[0,1]^d$, for some $\gamma > 0$. Also, assume that the optimal transport plan is $\frac{1}{\lambda}-$strongly convex and $\lambda-$smooth then

$$\mathbb{E}\left\| \widehat{T}_n^{1\mathrm{NN}} - T \right\|^2_{L_2^2(P)} \lesssim_\lambda (\log n)^2 \begin{cases} n^{-1}, & d \leq 3 \\ n^{-1}(\log n)^2, & d = 4 \\ n^{-2/d}, & d \geq 5. \end{cases}$$

Naïve Approach and Limitations - cont.

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CURSE OF DIMENSIONALITY

Alternative Estimation Strategy

- **Semidual Formulation:**
  - Offers a principled way to estimate T over $\mathbb{R}^d$.
- **Advantages:**
  - Incorporates additional assumptions (e.g., smoothness).
  - Dimension-free fast rates

The Semidual Problem

- **Semidual Functional:**

$$\mathcal{S}(\phi) = \int \phi \, d\mu + \int \phi^* \, d\nu$$

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- **Optimal Transport Map:**
  - $T = \nabla\varphi$, where φ minimizes $\mathcal{S}(\phi)$ among all $\phi \in \mathcal{F}$, a subclass of convex $\mu-$ae differentiable functions in $L_1(\mu)$.
  - Smoothness assumptions on $\mathcal{F}$ necessary to derive rates.
  - In applications, we generally know $\mathcal{F}$ beforehand.

Estimation via the Semidual

- **Empirical Semidual Functional:**

$$\widehat{\varphi} = \arg\min_{\phi \in \mathcal{F}} \mathcal{S}_n(\phi)$$

where

$$\mathcal{S}_n(\phi) = \int \phi \, d\mu_n + \int \phi^* \, d\nu_n$$

- **Estimator:** $\widehat{T}_n = \nabla \widehat{\varphi}$.

Recall (Gaussian OT)

Problem

Let $m_i \in \mathbb{R}^d$ and Σ_i be positive definite $d \times d$ matrices and let $\mu_i := \mathcal{N}(m_i, \Sigma_i)$, $i = 1, 2$. Assume further that Σ_1 and Σ_2 commute. We consider the (W_2^2)-OT problem from μ_1 to μ_2.

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1. $T_{\#}(\mu_1) = \mu_2$;
2. T is the gradient of a convex function on $\mathbb{R}^d$.

Recall (Gaussian OT - cont.)

The naive choice

$$T(x) = \Sigma_2^{1/2}\Sigma_1^{-1/2}(x - m_1) + m_2.$$

works if Σ_1 and Σ_2 commute. With this choice, we obtain

$$W_2^2(\mu_1, \mu_2) = \|m_1 - m_2\|^2 + \|\Sigma_1^{1/2} - \Sigma_2^{1/2}\|_{\mathrm{HS}}^2.$$

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Remark: This only gives an upper bound if Σ_1 and Σ_2 don't commute.

A Special Case: Affine Transport Maps

- **Scenario:**
  - $\mu = \mathcal{N}(0, I)$ is known, and we obtain samples from $\nu = (\nabla\varphi)_{\#}\mu$ for some $\varphi \in \mathcal{F}$, the class of all convex quadratic functions $x \mapsto \frac{1}{2}x^\top Ax + b^\top x$ with $A \succeq 0$.

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- **Estimator:**
  - $\nu = \mathcal{N}(b, A^2)$ and $\nabla\varphi = Ax + b = Cov(\nu)^{1/2}x + Mean(\mu)$
  - Use sample mean $\widehat{m}$ and covariance $\widehat{\Sigma}$.

$$\widehat{T}_n(x) = \widehat{\Sigma}^{1/2}x + \widehat{m}$$

Affine Transport Maps - cont.

Proposition

Let $\mathcal{F}$ be the set of all convex quadratic functions on $\mathbb{R}^d$. Let $\mu = \mathcal{N}(0, I)$, and write ν_n for an empirical measure consisting of i.i.d. samples from a probability measure ν. If

$$\hat{\varphi} = \arg\min_{\varphi \in \mathcal{F}} \left\{ \int \varphi \, d\mu + \int \varphi^* \, d\nu_n \right\},$$

then

$$\nabla \hat{\varphi}(x) = \hat{\Sigma}^{1/2} x + \hat{m},$$

where $\hat{m}$ and $\hat{\Sigma}$ are the mean and covariance of ν_n, respectively.

Sketch of proof

By definition, $\hat{\varphi} = \frac{1}{2} x^\top \hat{A} x + \hat{b}^\top x$, where $(\hat{A}, \hat{b})$ solve

$$\min_{A \succeq 0,\, b \in \mathbb{R}^d} \left[\int \left(\frac{1}{2} x^\top A x + b^\top x \right) \mu(dx) + \int \left(\frac{1}{2} y^\top A y + b^\top y \right)^* \nu_n(dy) \right].$$

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- $\left(\frac{1}{2} y^\top A y + b^\top y \right)^* = \frac{1}{2} (y - b)^\top A^{-1} (y - b)$
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- $\left(\frac{1}{2} y^\top A y + b^\top y\right)^* = \frac{1}{2} (y - b)^\top A^{-1} (y - b)$
- Can replace ν_n by $\mathcal{N}(\hat{m}, \hat{\Sigma})$
- The convex function $\hat{\varphi} = \frac{1}{2} x^\top \hat{\Sigma} x + \hat{m}^\top x$ which solves the **semidual** problem for Gaussian OT lies in $\mathcal{F}$.

Fast rate for Gaussian OT (Sketch)

Let $\hat{A} = \hat{\Sigma}$ and $\hat{b} = \hat{m}$.

- **Simplification:**

$$\begin{aligned}
\mathbb{E}_x \left[\| T(x) - \hat{T}(x) \|^2 \right] &= \mathbb{E}_x \left[\| (A - \hat{A})x + (b - \hat{b}) \|^2 \right] \\
&= \mathbb{E}_x \left[x^\top (A - \hat{A})^\top (A - \hat{A}) x \right] + \| b - \hat{b} \|^2 \\
&= \operatorname{trace} \left((A - \hat{A})^\top (A - \hat{A}) \right) + \| b - \hat{b} \|^2 \\
&= \| A - \hat{A} \|_{\mathrm{HS}}^2 + \| b - \hat{b} \|^2 .
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&= \|A-\hat{A}\|_{\mathrm{HS}}^2 + \|b-\hat{b}\|^2.
\end{aligned}$$

$$\mathbb{E}\left[\mathbb{E}_x\left[\|T(x) - \hat{T}(x)\|^2\right]\right] = \mathbb{E}\left[\|A-\hat{A}\|_{\mathrm{HS}}^2\right] + \mathbb{E}\left[\|b-\hat{b}\|^2\right].$$

Fast Rate for Gaussian OT (Sketch) - cont.

- **Rate for mean:**

$$\hat{b} \sim \mathcal{N}\left(b, \frac{A^2}{n}\right) \implies \mathbb{E}\left[\|b - \hat{b}\|^2\right] = \frac{1}{n}\,\mathrm{trace}(A^2)$$

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- **Rate for covariance term:**

$$\mathbb{E}\|A - \hat{A}\|_{\mathrm{HS}}^2 \sim \mathbb{E}\left\|\frac{1}{2}A^{-1}\left(\hat{\Sigma}^{\frac{1}{2}} - \Sigma^{\frac{1}{2}}\right)\right\|_{\mathrm{HS}}^2$$

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As $n \times \hat{\Sigma} \sim W_p(A^2, n-1)$, letting $\Sigma = A^2$, and $\Delta = \hat{\Sigma}^{\frac{1}{2}} - \Sigma^{\frac{1}{2}}$ we have

$$\frac{1}{4}\mathbb{E}\operatorname{trace}\left(\Sigma^{-1}\Delta\Delta^\top\right) \sim \frac{1}{4}\operatorname{tr}\left(\Sigma^{-1} \cdot \frac{1}{n-1}\left(\Sigma \circ \Sigma + \Sigma \otimes \Sigma\right)\right)$$

Slow rate for the semidual estimator

Hence, for the Gaussian OT, we get a rate of $\Theta_d\left(\frac{1}{n}\right)$.

Can we generalize this?

Look at **"Concentration bounds for linear Monge mapping estimation and optimal transport domain adaptation"** by Flamary, Lounici and Ferrari, 2020, for extension to subGaussian case and different sample sizes.

Slow rate for the semidual estimator

What about other distributions?

Slow rate for the semidual estimator

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Theorem 2

Assume $\mathcal{F}$ is "nice". The semidual estimator $\hat{\varphi}$ satisfies the bound

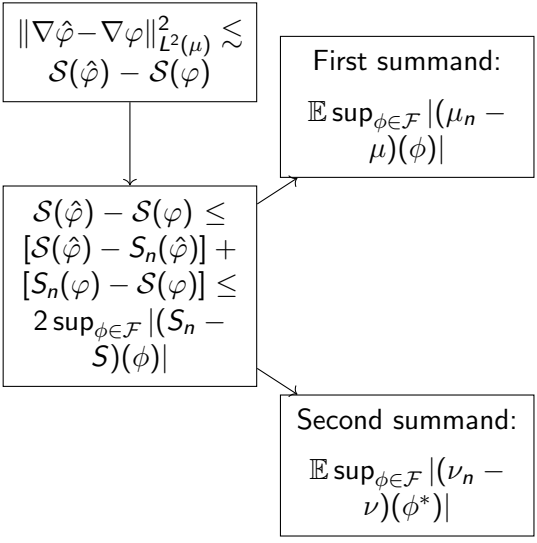
$$\mathbb{E}\|\nabla\hat{\varphi} - \nabla\varphi\|^2_{L_2(\mu)} \lesssim n^{-1/2}.$$

Slow rate for the semidual estimator - cont.

$$\|\nabla\hat{\varphi}-\nabla\varphi\|^2_{L^2(\mu)} \lesssim \mathcal{S}(\hat{\varphi}) - \mathcal{S}(\varphi)$$

$$\mathcal{S}(\hat{\varphi}) - \mathcal{S}(\varphi) \leq [\mathcal{S}(\hat{\varphi}) - S_n(\hat{\varphi})] + [S_n(\varphi) - \mathcal{S}(\varphi)] \leq 2\sup_{\phi\in\mathcal{F}} |(S_n - \mathcal{S})(\phi)|$$

Slow rate for the semidual estimator - cont.



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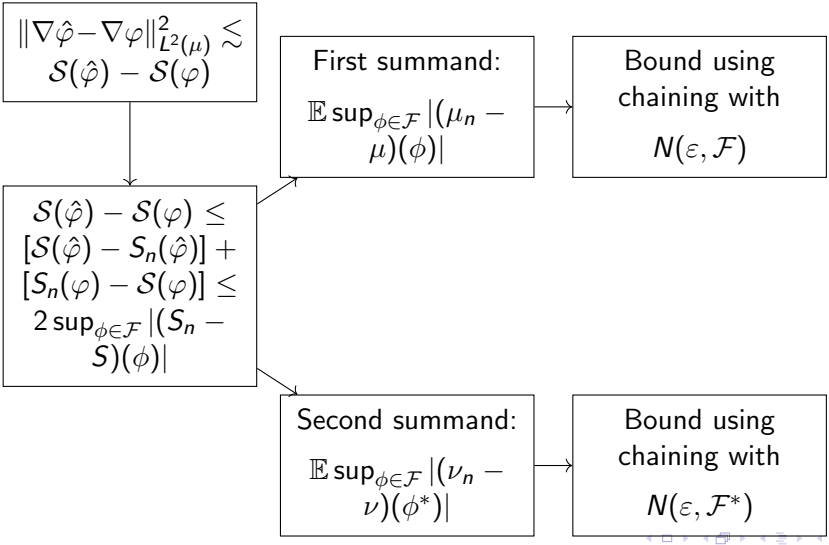

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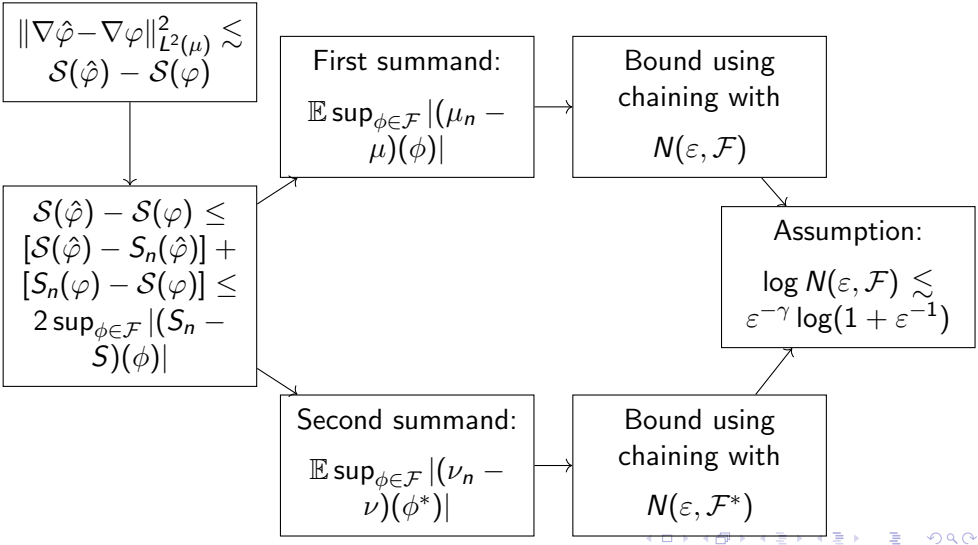

Next time:

Obtaining the slow rate

Recap

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- **Semidual Estimator:** $\widehat{T}_n = \nabla\widehat{\varphi}$.
- **Example of Gaussian OT:** $\widehat{T}_n = \hat{\Sigma}^{1/2}x + \hat{m}$
- **Slow rate:** $\mathbb{E}\|\nabla\hat{\varphi} - \nabla\varphi\|^2_{L_2(\mu)} \lesssim n^{-1/2}$

Stability of the Semidual Problem

Theorem 1 (Stability):

If ϕ is strongly convex and smooth, satisfying $\frac{1}{2}I \preceq \nabla^2\phi(x) \preceq 2I$ for $\|x\| < 1$, then

$$\frac{1}{4}\|\nabla\phi - \nabla\varphi\|^2_{L^2(\mu)} \leq \mathcal{S}(\phi) - \mathcal{S}(\varphi) \leq \|\nabla\phi - \nabla\varphi\|^2_{L^2(\mu)}.$$

Stability of the Semidual Problem - Proof

We will use, without proof, the following results from convex analysis (vide **Appendix 9** of **Statistical Optimal Transport** by Chewi, Niles-Weed, Rigollet):

- For $\alpha > 0$, ϕ is $\alpha-$strongly convex iff ϕ^* is $\frac{1}{\alpha}-$smooth.
- $\nabla\phi$ is a diffeomorphism with inverse $\nabla\phi^*$
- $\phi(x) + \phi^*(\nabla\phi(x)) = \langle x, \nabla\phi(x)\rangle$

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Easy to see for $\phi(x) = \frac{1}{2}\langle x, Ax\rangle + \langle b, x\rangle + c$

Stability of the Semidual Problem - Proof

- **Pushforward:**

$$\begin{aligned}\mathcal{S}(\phi) &= \int \phi(x)\,\mu(dx) + \int \phi^*(y)\,\nu(dy) \\ &= \int \left(\phi(x) + \phi^*(\nabla\varphi(x))\right)\mu(dx).\end{aligned}$$

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- **Strong convexity of ϕ^*:**

$$\begin{aligned}\phi^*(\nabla\varphi(x)) \geq & \phi^*(\nabla\phi(x)) + \langle \nabla\phi^*(\nabla\phi(x)), \nabla\varphi(x) - \nabla\phi(x)\rangle \\ & + \frac{1}{4}\|\nabla\varphi(x) - \nabla\phi(x)\|^2,\end{aligned}$$

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- **Using properties outlined earlier:**

$$\begin{aligned}\phi(x) + \phi^*(\nabla\varphi(x)) &\geq \langle x, \nabla\varphi(x)\rangle + \frac{1}{4}\|\nabla\varphi(x) - \nabla\phi(x)\|^2 \\ &= \varphi(x) + \varphi^*(\nabla\varphi(x)) + \frac{1}{4}\|\nabla\varphi(x) - \nabla\phi(x)\|^2\end{aligned}$$

Stability of the Semidual Problem - Proof

$$\implies \mathcal{S}(\phi) \geq \mathcal{S}(\varphi) + \frac{1}{4}\|\nabla\varphi - \nabla\phi\|^2_{L^2(\mu)}.$$

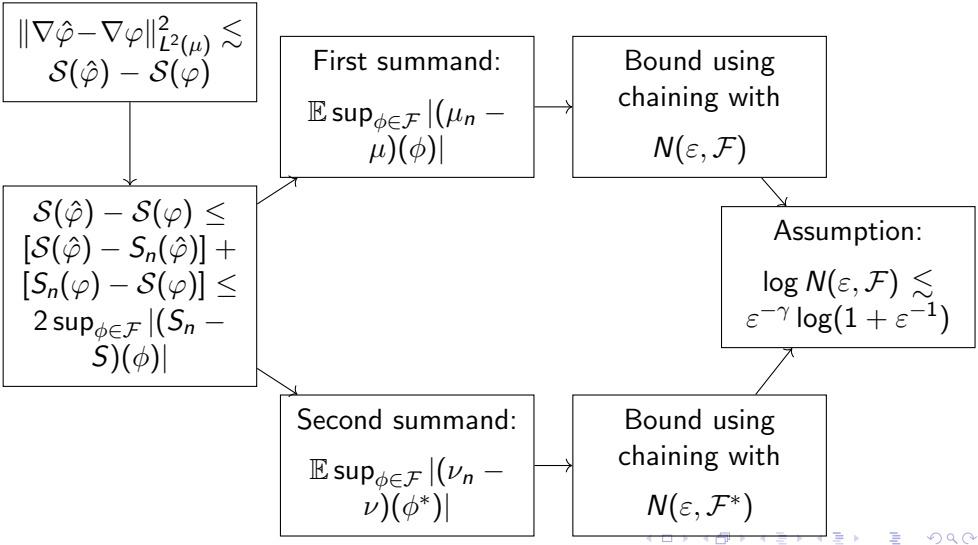
Stability of the Semidual Problem - Proof

$$\implies \mathcal{S}(\phi) \geq \mathcal{S}(\varphi) + \frac{1}{4}\|\nabla\varphi - \nabla\phi\|^2_{L^2(\mu)}.$$

- **Now using smoothness:** Similarly, the other direction follows by upper bounding $S(\phi)$ using the smoothness of ϕ^*

$$\mathcal{S}(\phi) \leq \mathcal{S}(\varphi) + \|\nabla\varphi - \nabla\phi\|^2_{L^2(\mu)}.$$

Obtaining the slow rate - cont.



Obtaining the slow rate - cont.

Chaining bound **[vH14, Theorem 5.31]**

If $\mathcal{F}$ is a set of real-valued functions on Ω such that $\|f\|_{L^\infty(\Omega)} \leq R$ for all $f \in \mathcal{F}$, then

$$\mathbb{E} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \{f(X_i) - \mathbb{E} f(X_i)\} \lesssim \inf_{\tau > 0} \left\{ \tau + \frac{1}{\sqrt{n}} \int_{\tau}^{R} \sqrt{\log N(\varepsilon, \mathcal{F})}\, \mathrm{d}\varepsilon \right\}.$$

Obtaining the slow rate - cont.

So far, we have

$$\mathbb{E}\|\nabla\hat{\varphi} - \nabla\varphi\|^2_{L^2(\mu)} \lesssim \mathbb{E}\sup_{\phi\in\mathcal{F}}|(\mu_n - \mu)(\phi)| + \mathbb{E}\sup_{\phi\in\mathcal{F}}|(\nu_n - \nu)(\phi^*)|.$$

- **Assumption:** there exists a positive constant R such that $\|\phi\|_{L^\infty(\Omega)} \leq R$ for all $\phi \in \mathcal{F}$.

Obtaining the slow rate - cont.

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$$\mathbb{E}\sup_{\phi\in\mathcal{F}}|(\mu_n - \mu)(\phi)| \lesssim \frac{1}{\sqrt{n}}\int_0^R \sqrt{\log N(\varepsilon, \mathcal{F})}\,\mathrm{d}\varepsilon.$$

Obtaining the slow rate - cont.

Assumption for Covering Numbers

For simplicity, we focus on the case where the class of functions is small enough that the covering numbers satisfy

$$\log N(\varepsilon, \mathcal{F}) \lesssim \varepsilon^{-\gamma} \log(1 + \varepsilon^{-1}), \quad \gamma \in [0, 1) \tag{3.5}$$

Obtaining the slow rate - cont.

Example (Lipschitz in the parameter)

Assume that $\mathcal{F} = \{\phi_\theta\}_{\theta \in \Theta}$, where $\Theta \subset \mathbb{R}^M$ is bounded, and the potentials satisfy $\|\phi_\theta - \phi_{\theta'}\|_{L^\infty(\Omega)} \lesssim \|\theta - \theta'\|$. Then there exists a positive constant C such that the covering numbers of $\mathcal{F}$ satisfy $\log \mathcal{N}(\varepsilon, \mathcal{F}) = 0$ if $\varepsilon \geq C$ and

$$\log \mathcal{N}(\varepsilon, \mathcal{F}) \lesssim \log(1 + \varepsilon^{-1})$$

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Obtaining the slow rate - cont.

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otherwise.

For instance, convex quadratic functions are Lipschitz in the parameter (A, b), provided we restrict to $\Omega = B_1(0)$

Obtaining the slow rate - cont.

Sketch of Proof:

- Say, $\mathcal{F} \subseteq B_R(0)$ for some $R > 0$.
- For any $\delta > 0$, there exists $\theta_1, \ldots, \theta_N$ with $N \leq (1 + 2R\delta^{-1})^M$ such that $\bigcup_{i=1}^{N} B_\delta(\theta_i) \supset \Theta$.

  (For instance, take a δ packing of Θ. The balls $B_{\frac{\delta}{2}}(\theta_i)$ then are all disjoint and lie inside $B_{R+\frac{\delta}{2}}(0)$. This bounds N by volumetric computation.)

Obtaining the slow rate - cont.

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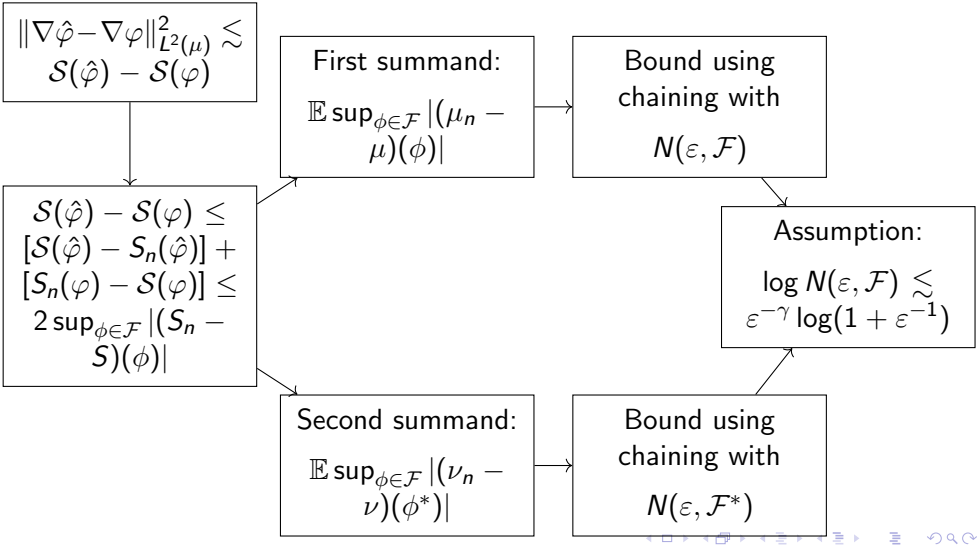
- $\phi_{\theta_1}, \ldots, \phi_{\theta_N}$ is an $O(\delta)$-cover of $\mathcal{F}$.
- Taking $\delta = c\varepsilon$ for a sufficiently small positive constant c yields the claim.

Obtaining the slow rate - cont.



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- **Bounding the Covering Number:**

$$\frac{1}{\sqrt{n}} \int_0^R \sqrt{\log N(\varepsilon, \mathcal{F})}\, \mathrm{d}\varepsilon \lesssim \frac{1}{\sqrt{n}} \int_0^R \varepsilon^{-\gamma/2} \sqrt{\log(1 + \varepsilon^{-1})}\, \mathrm{d}\varepsilon \lesssim n^{-1/2},$$

- **Conjugation is a contraction:**

$$|\phi^*(y) - \psi^*(y)| = \left| \sup_{x \in \Omega} \{\langle x, y \rangle - \phi(x)\} - \sup_{x' \in \Omega} \{\langle x', y \rangle - \psi(x')\} \right|$$

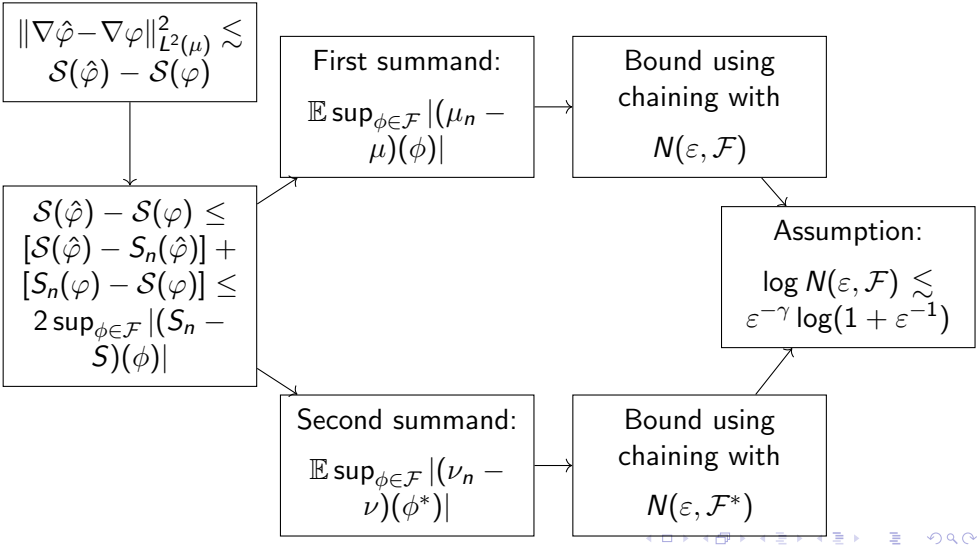
$$\leq \sup_{x \in \Omega} |\phi(x) - \psi(x)| = \|\phi - \psi\|_{L^\infty(\Omega)}.$$

- For any $\varepsilon > 0$,

$$N(\varepsilon, \mathcal{F}^*) \leq N(\varepsilon, \mathcal{F}).$$

- Bound as before

Obtaining the slow rate - cont.



Obtaining the slow rate - cont.

Theorem 2 (Slow rate for semi-dual estimator)

Adopt the assumption for covering numbers. Further, assume that

- The supports of μ and ν lie in $\Omega = B_1(0)$.
- The set $\mathcal{F}$ is bounded in L^∞ on Ω, i.e., $\sup_{\phi \in \mathcal{F}} \|\phi\|_{L^\infty(\Omega)} \leq R$ for some $R > 0$.
- The potentials satisfy $\phi(0) = 0$ and $\phi(x) = +\infty$ if $x \notin \Omega$.
- The potentials are lower-semicontinuous, smooth, and strongly convex on Ω: $\frac{1}{2} I \preceq \nabla^2 \phi(x) \preceq 2I$ if $\|x\| < 1$.

Then the semidual estimator $\hat{\varphi}$ satisfies the bound

$$\mathbb{E}\|\nabla \hat{\varphi} - \nabla \varphi\|^2_{L_2(\mu)} \lesssim_{R,\gamma} n^{-1/2}$$

One-shot Localization

The Localization Argument

Define

$$\varphi_\varepsilon = (1-\lambda)\varphi + \lambda\hat{\varphi}, \quad \lambda = \frac{\varepsilon}{\varepsilon + \|\nabla\hat{\varphi} - \nabla\varphi\|_{L^2(\mu)}}.$$

Then,

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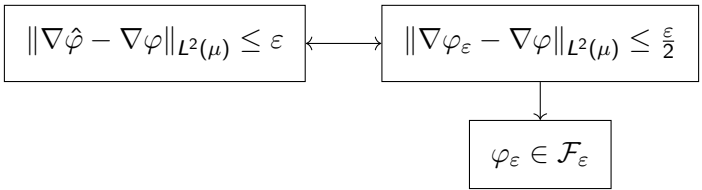


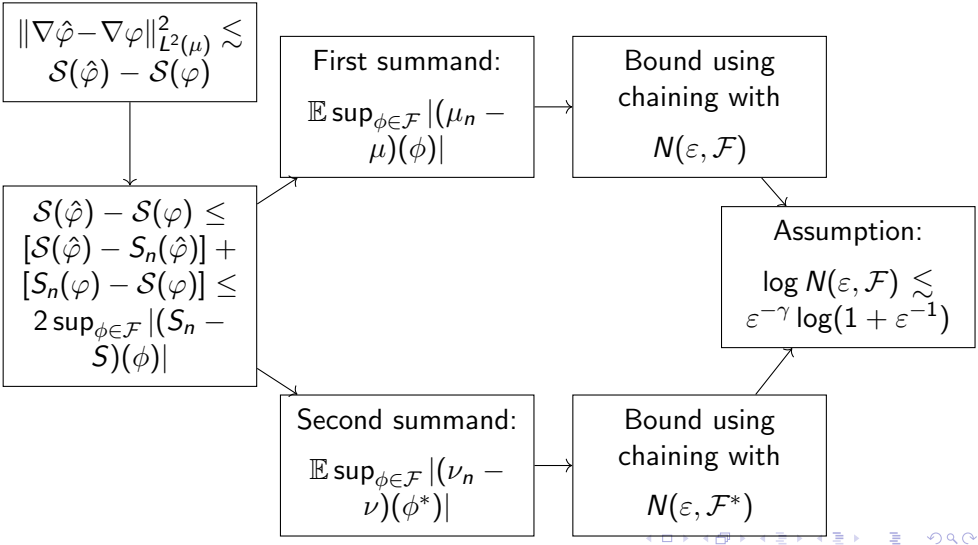
Fast rate for the semidual estimator

Theorem 2

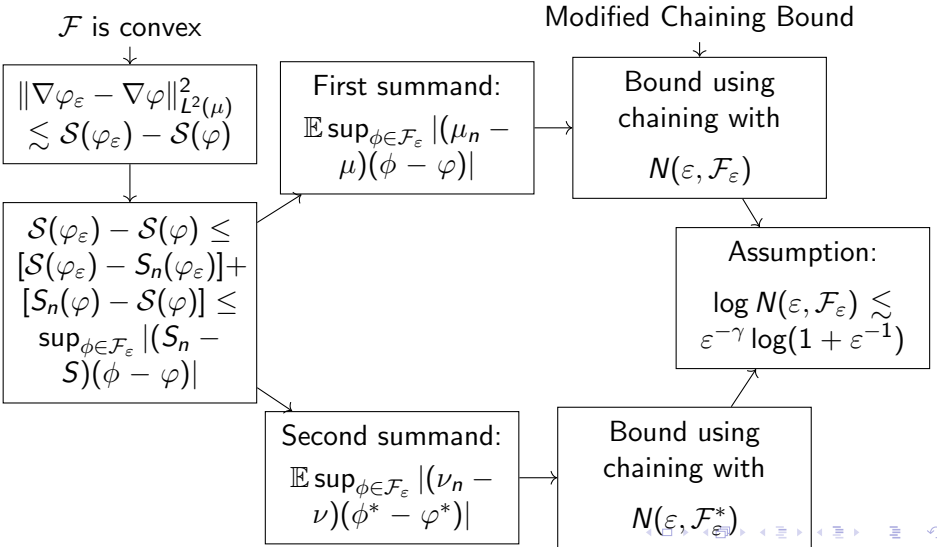
Assume $\mathcal{F}$ and μ are "nice". The semidual estimator $\hat{\varphi}$ satisfies the bound

$$\mathbb{E}\|\nabla\hat{\varphi} - \nabla\varphi\|^2_{L_2(\mu)} \lesssim \left(\frac{\log n}{n}\right)^{\frac{2}{2+\gamma}}.$$

Looking back : Obtaining the slow rate



Obtaining the fast rate - cont.



Obtaining the fast rate

Next time:

Modified Chaining Bound

Questions from last day

1. Motivating the 1-NN construction
2. Proof of pointwise fast rate
3. The restricted class $\mathcal{F}$
4. The γ in covering number bounds
5. Adaptive estimators

Motivating 1-NN

- **Setting:** Optimal Transport (OT) between counting measures on $\{x_1, x_2, x_3\}$ and $\{y_1, y_2, y_3\}$, where $x_1 < x_2 < x_3$ and $y_1 < y_2 < y_3$.

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- **Equivalent Question:**

$$\min_{\sigma} \sum_i (x_i - y_{\sigma(i)})^2 = \sum_i x_i^2 + \sum_i y_i^2 - 2 \max_{\sigma} \sum_i x_i y_{\sigma(i)}$$

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- **Local changes:** (Cyclical monotonicity type argument)
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  $\sigma = Id$ is the optimum.

Motivating 1-NN - cont.

The Rearrangement Inequality

Given $x_1 < x_2 \ldots < x_n$ and $y_1 < y_2 \ldots < y_n$, we have

$$\sum x_i y_i > \sum x_i y_{\sigma(i)} > \sum x_i y_{n+1-i}$$

Motivating 1-NN - cont.

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OT for the counting measure

Given $x_1 < x_2 \ldots < x_n$ and $y_1 < y_2 \ldots < y_n$, the optimal transport map between the counting measures on them is the **Id (minimizes the quadratic cost)** and the most suboptimal transport map is $\mathbf{i} \mapsto \mathbf{n} + \mathbf{1} - \mathbf{i}$ **(maximizes the quadratic cost)**.

Motivating the 1-NN - cont.

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Motivating the 1-NN - cont.

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  But if f is decreasing, it is the most suboptimal transport map.

  So, in the case of $Y = -X$, the 1-NN estimator is not trying to estimate $-Id$.

Proof of the pointwise fast rate

(Pointwise) Fast rate for 1NN estimator

Assume μ and ν have densities supported on $[0,1]$, bounded away from 0 and ∞. For $x \in [0,1]$,

$$\mathbb{E}|\widehat{T}_n(x) - T(x)|^2 \lesssim \frac{1}{n}$$

where T is the true optimal transport map $F_\nu^\dagger \circ F_\mu$ from μ to ν.

Proof of the pointwise fast rate - cont.

- Let $N_x := \sum_{i=1}^n \mathbf{1}\{X_i \le x\}$ and $N'_y := \sum_{i=1}^n \mathbf{1}\{Y_i \le y\}$. Argue that

$$\mathbb{E}\|\hat{T}(x) - T(x)\|^2 \le \int_0^A \mathbb{P}\left(N_x \ge N'_{T(x)+t}\right) 2t dt + \int_0^A \mathbb{P}\left(N_x \le N'_{T(x)-t}\right) 2t dt$$

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  We used: $\mathbb{P}(X \le x) \le \mathbb{P}(T(X) \le T(x))$, as T must be increasing.
- Using the Dvoretzky–Kiefer–Wolfowitz inequality, argue that the finite n probability and the limiting probability are close.

The restricted class $\mathcal{F}$

- We got the slow rate $\frac{1}{\sqrt{n}}$ and will derive the fast rate $\left(\frac{\log n}{n}\right)^{\frac{2}{2+\gamma}}$ under very general regularity conditions on $\mathcal{F}$ (lower-semicontinuity, smoothness, strong convexity, a.s. boundedness).
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- **Situation 1:** We know the functional form of the measures μ and ν are able to derive the functional form of $\varphi \in \mathcal{F}$.

  Look at **"Optimal transport map estimation in general function spaces"** by Divol, Niles-Weed, Pooladian, 2024.

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Approx. by large parametric classes **[DNWP24, Theorem 3]**

Consider μ and $\mathcal{F}$ that satisfy regularity assumptions as before. Assume that φ is both "smooth" and "strongly convex". Let $(\mathcal{F}_j)_j$ be an approximating family of the class of potentials that is "smooth". Then, for J such that $2^J \asymp n^{1/(2s+d-4)}$, it holds that

$$\mathbb{E}\|\nabla\hat{\varphi}_{\mathcal{F}_J} - \nabla\varphi\|^2_{L^2(\mu)} \lesssim_{\log n} n^{-\frac{2(s-1)}{2s+d-4}}.$$

Here, d is approximately linear in the metric entropy of $\mathcal{F}$ and s is approximately the infimum of the quantity $\frac{-1}{j}\log_2\|\nabla\varphi - \nabla\varphi_j\|$

The γ in covering number bounds

- **In the book:** $\gamma \in [0, 1)$
- Let $u = \log(x^{-1}) = -\log x$. Then:

$$
\begin{aligned}
I &= \int_0^A x^{-\frac{\gamma}{2}} \sqrt{\log(1 + x^{-1})}\, dx \\
&= \int_{\log(A^{-1})}^{\infty} e^{\frac{\gamma}{2} u} \sqrt{\log(1 + e^{u})} \cdot e^{-u}\, du \\
&= \int_{\log(A^{-1})}^{\infty} e^{-\left(1 - \frac{\gamma}{2}\right) u} \sqrt{\log(1 + e^{u})}\, du.
\end{aligned}
$$

  Diverges for $\gamma \geq 2$

- **"Large" function classes:** Lipschitz functions in dimensions ≥ 2

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Adaptive Estimators

- **Semidual estimator is not adaptive:** The rates in our estimator depend on nuisance parameters like R and γ of the function class $\mathcal{F}$ itself.
- **An adaptive estimator:** Wait for chapter 4, and then read:

  "Entropic estimation of optimal transport map" by Pooladian, Niles-Weed, 2024.

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- **Problem formulation :** Given samples from μ and $\nu = T_{\#}\mu$, (T - optimal transport with quadratic costs), estimate T.

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- **Slow rate:** $\mathbb{E}\|\nabla \hat{\varphi} - \nabla \varphi\|^2_{L_2(\mu)} \lesssim n^{-1/2}$
- **Issue:** Minimizing over the entire class $\mathcal{F}$.

  A priori no control over $\|\nabla \phi - \nabla \varphi\|_{L^2(\mu)}$ for $\phi \in \mathcal{F}$

Recap - cont.

- **Localised class:** $\mathcal{F}_\varepsilon = \{\phi \in \mathcal{F} \mid \|\nabla\phi - \nabla\varphi\|_{L^2(\mu)} \leq \varepsilon\}$

Recap - cont.

- **Localised class:** $\mathcal{F}_\varepsilon = \{\phi \in \mathcal{F} \mid \|\nabla\phi - \nabla\varphi\|_{L^2(\mu)} \leq \varepsilon\}$
- **Localised estimator:**

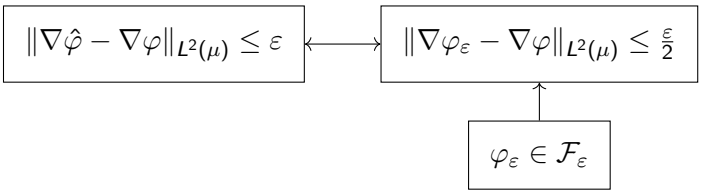
$$\varphi_\varepsilon = (1-\lambda)\varphi + \lambda\hat{\varphi}, \quad \lambda = \frac{\varepsilon}{\varepsilon + \|\nabla\hat{\varphi} - \nabla\varphi\|_{L^2(\mu)}}.$$

Recap - cont.

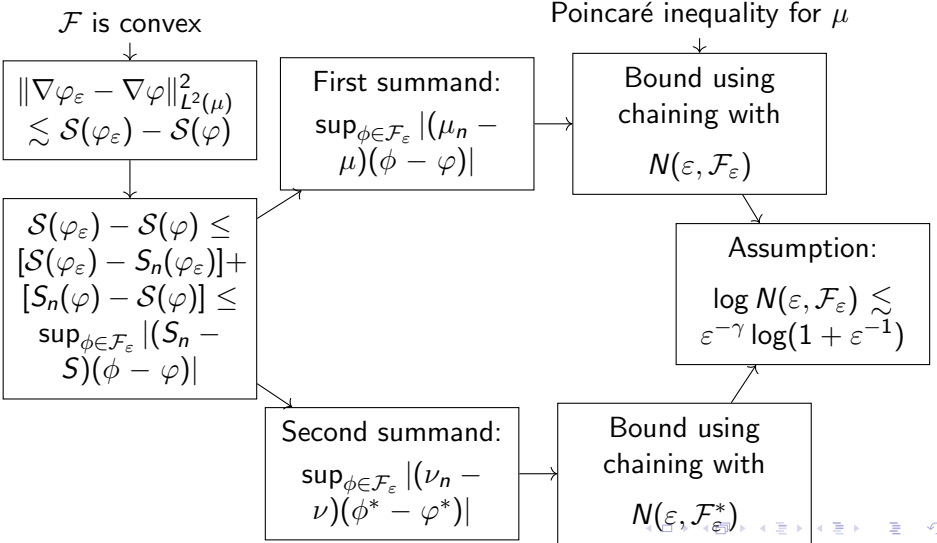
- **Localised class:** $\mathcal{F}_\varepsilon = \{\phi \in \mathcal{F} \mid \|\nabla\phi - \nabla\varphi\|_{L^2(\mu)} \leq \varepsilon\}$
- **Localised estimator:**

$$\varphi_\varepsilon = (1-\lambda)\varphi + \lambda\hat{\varphi}, \quad \lambda = \frac{\varepsilon}{\varepsilon + \|\nabla\hat{\varphi} - \nabla\varphi\|_{L^2(\mu)}}.$$

- **Justification:**



Obtaining the fast rate - cont.



Obtaining the fast rate - cont.

Modified Chaining Bound **[vdVW23, Theorem 2.14.21]**

Let P be a probability measure on a set $\Omega \subseteq \mathbb{R}^d$. Let $X_1, \ldots, X_n \overset{\text{i.i.d.}}{\sim} P$. If $\mathcal{F}$ is a set of real-valued functions such that $\|f\|_{L^2(P)} \leq \sigma$ and $\|f\|_{L^\infty(\Omega)} \leq R$ for all $f \in \mathcal{F}$, then

$$\mathbb{E} \sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} \{f(X_i) - \mathbb{E}f(X_i)\} \lesssim \frac{1}{\sqrt{n}} \int_0^\sigma \sqrt{\log N(\epsilon, \mathcal{F})}\, d\epsilon + \frac{1}{n} \int_0^R \log N(\epsilon, \mathcal{F})\, d\epsilon.$$

Obtaining the fast rate - cont.

Poincare inequality $\implies$ L^2 bound

In addition to previous assumptions, suppose μ satisfies a Poincaré inequality. Then

$$\|\phi - \varphi - \mu(\phi - \varphi)\|_{L^2(\mu)} \lesssim \varepsilon$$

$$\|\phi^* - \varphi^* - \nu(\phi^* - \varphi^*)\|_{L^2(\nu)} \lesssim \varepsilon$$

for all $\phi \in \mathcal{F}_\varepsilon$.

Obtaining the fast rate - cont.

- **Poincaré Inequality $\implies$ L^2 Bound for μ:**

$$\|\phi - \varphi - \mu(\phi - \varphi)\|^2_{L^2(\mu)} \leq C\|\nabla(\phi - \varphi)\|^2_{L^2(\mu)} \lesssim \varepsilon^2.$$

Obtaining the fast rate - cont.

- **Poincaré Inequality $\implies$ L^2 Bound for μ:**

$$\|\phi - \varphi - \mu(\phi - \varphi)\|^2_{L^2(\mu)} \leq C\|\nabla(\phi - \varphi)\|^2_{L^2(\mu)} \lesssim \varepsilon^2.$$

- **Poincaré Inequality $\implies$ L^2 Bound for ν:**

$$\|\phi^* - \varphi^* - \nu(\phi^* - \varphi^*)\|^2_{L^2(\nu)} \leq C\|\nabla(\phi^* - \varphi^*)\|^2_{L^2(\nu)} \lesssim \varepsilon^2.$$

Obtaining the fast rate - cont.

- **Poincaré Inequality $\implies$ L^2 Bound for μ:**

$$\|\phi - \varphi - \mu(\phi - \varphi)\|^2_{L^2(\mu)} \leq C\|\nabla(\phi - \varphi)\|^2_{L^2(\mu)} \lesssim \varepsilon^2.$$

- **Poincaré Inequality $\implies$ L^2 Bound for ν:**

$$\|\phi^* - \varphi^* - \nu(\phi^* - \varphi^*)\|^2_{L^2(\nu)} \leq C\|\nabla(\phi^* - \varphi^*)\|^2_{L^2(\nu)} \lesssim \varepsilon^2.$$

- But we haven't proved (i) a Poincaré inequality for ν (ii) a bound for $\|\nabla(\phi^* - \varphi^*)\|^2_{L^2(\nu)}$

Obtaining the fast rate - cont.

- **Poincaré Inequality ν:** The Poincaré inequality for μ implies that for any $f \in L^2(\nu)$,

$$\int \left(f - \int f \, d\nu \right)^2 d\nu = \int \left(f \circ \nabla\varphi - \int f \circ \nabla\varphi \, d\mu \right)^2 d\mu$$

$$\leq C \int \|\nabla(f \circ \nabla\varphi)\|^2 d\mu \leq 4C \int \|\nabla f(\nabla\varphi(x))\|^2 d\mu \leq 4C \int \|\nabla f\|^2 d\nu$$

Obtaining the fast rate - cont.

- **Poincaré Inequality ν:** The Poincaré inequality for μ implies that for any $f \in L^2(\nu)$,

$$\int \left(f - \int f \, d\nu \right)^2 d\nu = \int \left(f \circ \nabla\varphi - \int f \circ \nabla\varphi \, d\mu \right)^2 d\mu$$

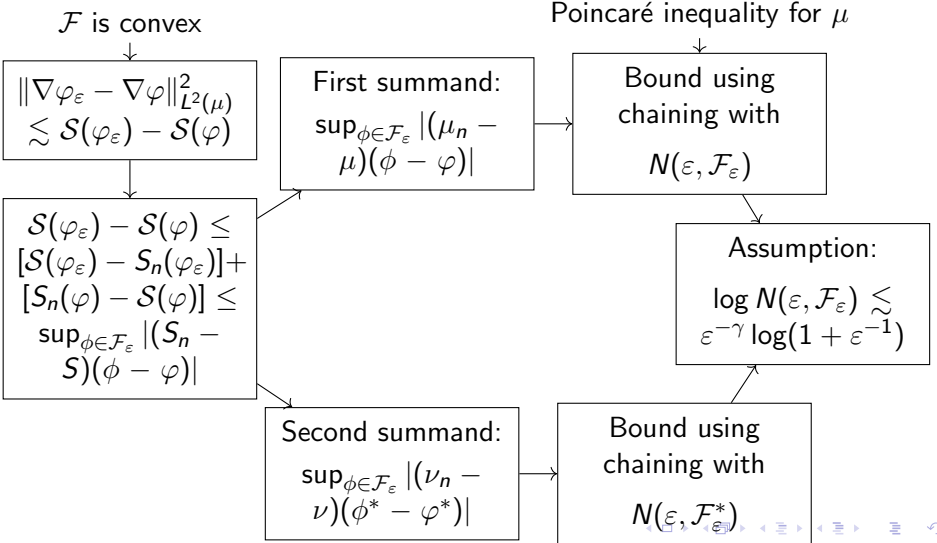
$$\leq C \int \|\nabla(f \circ \nabla\varphi)\|^2 d\mu \leq 4C \int \|\nabla f(\nabla\varphi(x))\|^2 d\mu \leq 4C \int \|\nabla f\|^2 d\nu$$

- **Duality Implies Bound for $\|\nabla(\phi^* - \varphi^*)\|^2_{L^2(\nu)}$:** Define T such that $T(\phi^*) = S(\phi)$. Then, for φ^* is the minimizer of T. The stability result for T implies that

$$\frac{1}{4}\|\nabla\phi^* - \nabla\varphi^*\|^2_{L^2(\nu)} \leq \mathcal{T}(\phi^*) - \mathcal{T}(\varphi^*) = \mathcal{S}(\phi) - \mathcal{S}(\varphi) \leq \|\nabla\phi - \nabla\varphi\|^2_{L^2(\mu)}.$$

Therefore, $\|\nabla\phi^* - \nabla\varphi^*\|^2_{L^2(\nu)} \lesssim \varepsilon^2$ for all $\phi \in \mathcal{F}_\varepsilon$.

Obtaining the fast rate - cont.



Obtaining the fast rate - cont.

Theorem 3 (Fast rate for semi-dual estimator)

Adopt the assumption for covering numbers. Further, assume that

- The supports of μ and ν lie in $\Omega = B_1(0)$.
- $\sup_{\phi \in \mathcal{F}} \|\phi\|_{L^\infty(\Omega)} \leq R$ for some $R > 0$.
- The potentials satisfy $\phi(0) = 0$ and $\phi(x) = +\infty$ if $x \notin \Omega$.
- The potentials are lower-semicontinuous, smooth, and strongly convex on Ω: $\frac{1}{2} I \preceq \nabla^2 \phi(x) \preceq 2I$ if $\|x\| < 1$.
- $\mathcal{F}$ is convex.
- μ satisfies a Poincaré inequality.

Then the semidual estimator $\hat{\varphi}$ satisfies the bound

$$\mathbb{E}\|\nabla\hat{\varphi} - \nabla\varphi\|^2_{L^2(\mu)} \lesssim_{R,\gamma} \left(\frac{\log n}{n}\right)^{\frac{2}{2+\gamma}}$$

Questions from last day

1. Approximation by large parametric class
2. How does the rate depend on the parameters of the Neural Network?

The restricted class $\mathcal{F}$

Approx. by large parametric classes **[DNWP24, Theorem 3]**

Consider μ and $\mathcal{F}$ that satisfy regularity assumptions as before. Assume that φ is both "smooth" and "strongly convex". Let $(\mathcal{F}_j)_j$ be an approximating family of the class of potentials that is "smooth". Then, for J such that $2^J \asymp n^{1/(2s+d-4)}$, it holds that

$$\mathbb{E}\|\nabla\hat{\varphi}_{\mathcal{F}_J} - \nabla\varphi\|^2_{L^2(\mu)} \lesssim_{\log n} n^{-\frac{2(s-1)}{2s+d-4}}.$$

Here, d is approximately linear in the **log of the metric entropy** of $\mathcal{F}$ and s is approximately the infimum of the quantity $\frac{-1}{j}\log_2\|\nabla\varphi - \nabla\varphi_j\|$.

The restricted class $\mathcal{F}$

The dimension d

For every $\tau > 0$ the ball B_τ centered at φ (resp. the ball B_τ^* centered at φ^*) of radius τ in $\mathcal{F}$ for the pseudo-norm $g \mapsto \|\nabla g\|_{L^2(P)}$ (resp. in $\mathcal{F}^*$ for the pseudo-norm $g^* \mapsto \|\nabla g^*\|_{L^2(Q)}$) satisfies for all $0 < \epsilon < \tau$,

$$\log \mathcal{N}(\epsilon, B_\tau, L^2(P)) \lesssim_{\log_+(1/\epsilon), \log_+(1/\tau)} \left(\frac{\epsilon}{\tau}\right)^{-d}$$

$$\log \mathcal{N}(\epsilon, B_\tau^*, L^2(Q)) \lesssim_{\log_+(1/\epsilon), \log_+(1/\tau)} \left(\frac{\epsilon}{\tau}\right)^{-d}$$

The restricted class $\mathcal{F}$

The dimension d

For every $\tau > 0$ the ball B_τ centered at φ (resp. the ball B_τ^* centered at φ^*) of radius τ in $\mathcal{F}$ for the pseudo-norm $g \mapsto \|\nabla g\|_{L^2(P)}$ (resp. in $\mathcal{F}^*$ for the pseudo-norm $g^* \mapsto \|\nabla g^*\|_{L^2(Q)}$) satisfies for all $0 < \epsilon < \tau$,

$$\log \mathcal{N}(\epsilon, B_\tau, L^2(P)) \lesssim_{\log_+(1/\epsilon), \log_+(1/\tau)} \left(\frac{\epsilon}{\tau}\right)^{-d}$$

$$\log \mathcal{N}(\epsilon, B_\tau^*, L^2(Q)) \lesssim_{\log_+(1/\epsilon), \log_+(1/\tau)} \left(\frac{\epsilon}{\tau}\right)^{-d}$$

What about **s** ?

Questions from last day

1. Approximation by large parametric class
2. How does the rate depend on the parameters of the Neural Network?

The restricted class $\mathcal{F}$ - cont.

Example (ReQU Neural Networks)

Assume regularity conditions as before. Further, suppose $\mathcal{F} \subseteq \mathcal{C}_L^s([0,1]^d)$ for some $L \geq 0$ and $s > 2$. There exists a family $\mathcal{F}_j$ of ReQU neural networks with

- **Depth (Number of Layers):** $D_j = O\big(\log d + \lfloor s \rfloor + \log\log L\big)$.
- **Width (Number of Neurons per Layer):** $W_j = O\big(d(2^j + \lfloor s \rfloor)^d\big)$
- **Total Number of Parameters:** $N_j = O\big((ds + d^2 + \log\log L)(2^j + \lfloor s \rfloor)^d\big)$.

which approximates $\mathcal{F}$ well in Hölder norm. We then modify the family of potentials to be equal to $+\infty$ outside $B(0, 2R)$. Then for a certain choice of J

$$\mathbb{E}\|\nabla\widehat{\varphi}_{\tilde{\mathcal{F}}_J} - \nabla\varphi_0\|_{L^2(P)}^2 \lesssim_{\log n} n^{-\frac{2(s-1)}{2s+d-4}}.$$

Next time:

Entropic Optimal Transport