Decision Making and Inference Under Model Misspecification

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Goal:

Goals: a) Introduce optimal transport methods popular applications and properties, then b) use these results for robust peformance analysis and finally c) also show how optimal transport applied to statistical estimation.

Agenda

- Day 1: Introduction to Optimal Transport (Primals and Duals)

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- Day 2: Distributionally robust performance analysis and optimization.

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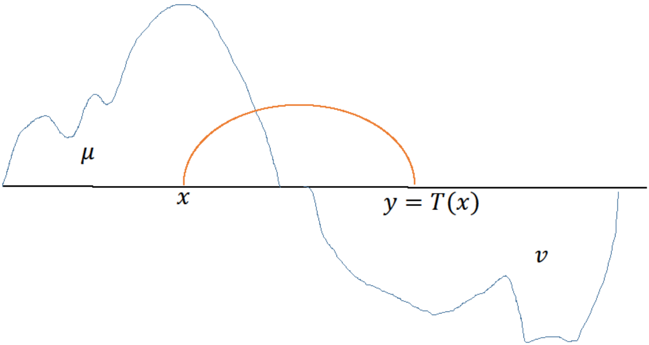
- Day 2: Distributionally robust performance analysis and optimization.
- Day 3: Statistical properties of estimators.

Monge-Kantorovich Problem & Duality
(see e.g. C. Villani's 2008 textbook)

Monge Problem

- What's the cheapest way to transport a pile of sand to cover a sinkhole?



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- where $c\left(x,y\right)\geq 0$ is the cost of transporting x to y.
- $T\left(X\right)\sim v$ means $T\left(X\right)$ follows distribution $v\left(\cdot\right)$.
- Problem is highly non-linear, not much progress for about 160 yrs!

Kantorovich Relaxation: Primal Problem

- Let $\Pi(\mu, v)$ be the class of joint distributions π of random variables (X, Y) such that

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- Linear programming (infinite dimensional):

$$\begin{aligned} D_c(\mu, v) \quad : \quad &= \min_{\pi(dx,dy)\geq 0} \int_{\mathcal{X}\times\mathcal{Y}} c(x, y)\, \pi(dx, dy) \\ & \int_{\mathcal{Y}} \pi(dx, dy) = \mu(dx), \int_{\mathcal{X}} \pi(dx, dy) = v(dy). \end{aligned}$$

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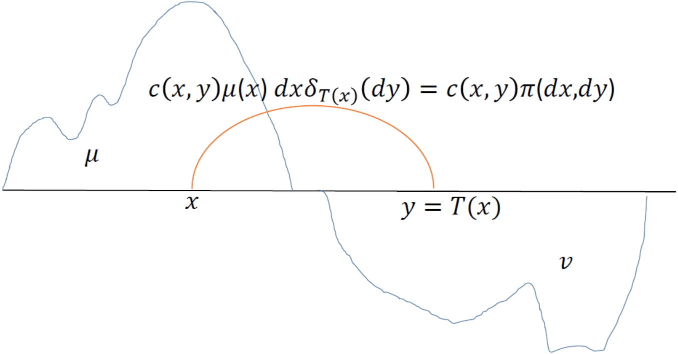
- If $c(x, y) = d(x, y)$ (d-metric) then $D_c(\mu, v)$ is a metric <– We'll check this later (this is Wasserstein distance).

Illustration of Optimal Transport Costs

- Monge's solution would take the form

$$\pi^* (dx, dy) = \delta_{\{T(x)\}} (dy) \, \mu (dx) \, .$$



Warm up exercise to practice primal interpretation...

Warm up exercise: Check that $D_c(\cdot)$ is a metric if $c(x,y) = d(x,y)$ where $d(\cdot)$ is a metric.

i) $D_d(\mu, v) = D_d(v, \mu)$

ii) $D_d(\mu, v) \geq 0$ and $D_d(\mu, v) = 0$ if and only if $\mu = v$.

iii) $D_d(\mu, w) \leq D_d(\mu, v) + D_d(v, w)$.

Kantorovich Relaxation: Primal Problem

- Keep in mind primal:

$$D_c(\mu, v) \quad := \min_{\pi(dx,dy)\geq 0} \int_{\mathcal{X}\times\mathcal{Y}} d(x,y)\, \pi(dx,dy)$$

$$\int_{\mathcal{Y}} \pi(dx,dy) = \mu(dx), \int_{\mathcal{X}} \pi(dx,dy) = v(dy).$$

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- Primal always has a solution (if c is lower semicontinuous) $->$ easy to see if $\mathcal{Y}$ and $\mathcal{X}$ are compact.
- If $D_d(\mu, v) = 0$, then $E_{\pi^*}(d(X,Y)) = 0$, then $X = Y$-π^* a.s. so $\mu(A) = \pi(X \in A) = \pi(Y \in A) = v(A)$.

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- Now verify triangle inequality

$$D_d(\mu, w) \leq D_d(\mu, v) + D_d(v, w).$$

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- Pick X, Y, Z so that $X \sim \mu$, $Y \sim v$ and $Z \sim w$. Sample $Y \sim v$ and then $X|Y = y$ from the optimal coupling solving $D_d(\mu, v)$. Also, sample $Z|Y = y$ using optimal coupling for computing $D_d(v, w)$.

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- Previous construction gives a coupling for X and Z, which is not necessarily optimal for computing $D_d(\mu, w)$.

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- Previous construction gives a coupling for X and Z, which is not necessarily optimal for computing $D_d(\mu, w)$.
- On the other hand, $d(X, Z) \leq d(X, Y) + d(Y, Z)$ because $d(\cdot)$ is a metric.
- Thus $D_d(\mu, w) \leq E(d(X, Z)) \leq D_d(\mu, v) + D_d(v, w)$.

Towards the Dual Problem

It is always natural to study the dual of a linear programming problem...

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- Primal:

$$\min_{\pi(dx,dy)\geq 0} \int_{\mathcal{X}\times\mathcal{Y}} d\left(x,y\right)\pi\left(dx,dy\right)$$

$$\int_{\mathcal{Y}} \pi\left(dx,dy\right) = \mu\left(dx\right), \int_{\mathcal{X}} \pi\left(dx,dy\right) = v\left(dy\right).$$

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- Dual:

$$\sup_{\alpha,\beta} \int_{\mathcal{X}} \alpha\left(x\right)\mu\left(dx\right) + \int_{\mathcal{Y}} \beta\left(y\right)v\left(dy\right)$$

$$\alpha\left(x\right) + \beta\left(y\right) \leq c\left(x,y\right) \;\; \forall\left(x,y\right) \in \mathcal{X}\times\mathcal{Y}.$$

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- Here α and β can be taken continuous

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- Now comes Victoria, who has a business...
- Vicky promises to transport on behalf of Martin and Henry the whole amount.

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- Existence of dual optimizers: $c(x, y) \leq a(x) + b(y)$ so $E_\mu a(X) < \infty$, $E_\mu b(Y) < \infty$.

Proof Technique: Sketch of Strong Duality

- Suppose $\mathcal{X}$ and $\mathcal{Y}$ compact

$$\inf_{\pi \geq 0} \sup_{\alpha,\beta} \left\{ \int_{\mathcal{X}\times\mathcal{Y}} c\left(x,y\right) \pi\left(dx,dy\right) \right.$$
$$- \int_{\mathcal{X}\times\mathcal{Y}} \alpha\left(x\right) \pi\left(dx,dy\right) + \int_{\mathcal{X}} \alpha\left(x\right) \mu\left(dx\right)$$
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- Swap sup and inf using **Sion's min-max theorem** by a compactness argument and conclude.

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\end{aligned}
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- Swap sup and inf using **Sion's min-max theorem** by a compactness argument and conclude.
- *Some amount of work to extend to general Polish spaces.*

Application of Optimal Transport in Economics

Economic Interpretations & Some Closed Form Solutions
(see e.g. A. Galichon's 2016 textbook & McCann 2013 notes).

Applications in Labor Markets

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- Companies want to *minimize* total production cost

$$\int \alpha(x)\,\mu(x)\,dx + \int \beta(y)\,v(y)\,dy$$

- Letting a central planner organize the Labor market.

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- Over assignments $\pi(\cdot)$ which satisfy market clearing

$$\int_{\mathcal{Y}} \pi(dx, dy) = \mu(dx), \int_{\mathcal{X}} \pi(dx, dy) = v(dy).$$

Solving for Optimal Transport Coupling

- **Suppose that** $\Psi(x,y) = xy$, $\mu(x) = I(x \in [0,1])$, $v(y) = e^{-y} I(y > 0)$.

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- Solve primal by sampling: Let $\{X_i^n\}_{i=1}^n$ and $\{Y_i^n\}_{i=1}^n$ both i.i.d. from μ and v, respectively.

$$F_{\mu_n}(x) = \frac{1}{n} \sum_{i=1}^n I(X_i^n \leq x), \; F_{v_n}(y) = \frac{1}{n} \sum_{j=1}^n I\left(Y_j^n \leq y\right)$$

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- Consider

$$\max_{\pi\left(x_i^n, x_j^n\right) \geq 0} \sum_{i,j} \Psi\left(x_i^n, y_j^n\right) \pi\left(x_i^n, y_j^n\right)$$

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- **Clearly, simply sort and match is the solution!**

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- Think of $Y_j^n = -\log\left(1 - U_j^n\right) = F_v^{-1}\left(U_j^n\right)$ for U_j^ns i.i.d. uniform$(0, 1)$.

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- The j-th order statistic $X_{(j)}^n$ is matched to $Y_{(j)}^n$.
- As $n \to \infty$, $X_{(nt)}^n \to t$, so $Y_{(nt)}^n \to -\log(1-t)$.
- Thus, the optimal coupling as $n \to \infty$ is $X = U$ and $Y = -\log(1-U)$ (comonotonic coupling).
- In general, the optimal coupling is $X = F_\mu^{-1}(U)$ and $Y = F_v^{-1}(U)$.

Identities for Wasserstein Distances

- Comonotonic coupling is the solution if $\partial^2_{x,y}\Psi(x,y) \geq 0$ - supermodularity:

$$\Psi\left(x \vee x', y \vee y'\right) + \Psi\left(x \wedge x', y \wedge y'\right) \geq \Psi(x,y) + \Psi\left(x', y'\right)$$

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- **Corollary:** Suppose $c(x,y) = |x-y|$ then $X = F_\mu^{-1}(U)$ and $Y = F_v^{-1}(U)$ thus

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Identities for Wasserstein Distances

- Comonotonic coupling is the solution if $\partial^2_{x,y}\Psi(x,y) \geq 0$ - supermodularity:

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- Similar identities are common for Wasserstein distances...

Interesting Insight on Salary Effects

- In equilibrium, by the envelope theorem

$$\begin{aligned}\dot{\beta}^*(y) &= \frac{d}{dy}\sup_x\left[\Psi(x,y)-\alpha^*(x)\right]=\frac{\partial}{\partial y}\Psi(x_y,y)=x_y\\ \dot{\alpha}^*(x) &= \frac{\partial}{\partial x}\Psi(x,y_x)=y_x=F_v^{-1}\left(F_\mu(x)\right).\end{aligned}$$

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\end{aligned}$$

- We also know that $y = -\log(1-x)$, or $x = 1-\exp(-y)$

$$\begin{aligned}
\beta^*(y) &= y+\exp(-y)-1+\beta^*(0). \\
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- What if $\Psi(x,y)\rightarrow\Psi(x,y)+f(x)$? (i.e. productivity changes).

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- What if $\Psi(x,y) \to \Psi(x,y) + f(x)$? (i.e. productivity changes).
- *Answer: salaries increase if* $f(\cdot)$ is increasing.

Additional properties of Optimal Transport Solutions:
Kantorovich-Rubinstein Duality and Wasserstein GAN.

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- Note that given β, we should pick

$$\alpha(x) = \beta^{d}(x) := \inf_{y}\{\beta(y) + d(x, y)\},$$

similarly once $\alpha(\cdot)$ is chosen, we could improve by picking

$$\beta^{dd}(y) = \sup_{x}\{\beta^{d}(x) - d(x, y)\}.$$

Transforms are Lipschitz

- Moreover, observe that $\beta^d(\cdot)$ is 1-Lipschitz

$$\begin{aligned}
\beta^d(x) &= \inf_y \{\beta(y) + d(x,y)\} \text{ <- recall def} \\
\beta^d(x) - \beta^d(x') &= \beta(y_x) + d(x, y_x) \\
&\quad -\beta(y_{x'}) - d(x, y_{x'}) \\
&\leq d(x, y_{x'}) - d(x, y_{x'}) \leq d(x, x').
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- Same argument is true for $\beta^{dd}(y)$.

The Transform of a Lipschitz Function is the Function Itself

- Moreover,
$$\beta^d(x) := \inf_y \{\beta(y) + d(x,y)\} \leq \beta(x)$$
and if β is 1-Lipschitz (meaning $|\beta(x) - \beta(y)| \leq d(x,y)$) then
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\beta^d(x) - \beta(x) &= \inf_y \{d(x,y) + \beta(y) - \beta(x)\} \\
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- Consequently, if β is 1-Lipschitz $\beta = \beta^{d}$... So, the dual can be simplified.

Back to Wasserstein Distances

- Original Dual:

$$\max E_{\mu}\alpha\left(X\right)-E_{v}\beta\left(Y\right)$$
$$s.t.\ \alpha\left(x\right)-\beta\left(y\right)\leq d\left(x,y\right)\ \ \forall\ \ x,y\in\mathcal{S}\ .$$

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- This is the basis for so-called Wasserstein GAN (Generative Adversarial Networks) – popular in artificial intelligence.

- Have you even thought about how to generate a "face" at random? (https://github.com/hindupuravinash/the-gan-zoo).

A Quick Discussion on Wasserstein GAN

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$$\min_{\theta < \text{NN parameter}} D_d \left(v_\theta, \mu_n \right),$$

where μ_n represents the empirical measure of images.

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- Use another Neural Network to parameterize α (i.e. a 1-Lip function).
- Apply automatic differentiation to compute gradients & run stochastic gradient descent.

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- So, in the end the dual is simplified to

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- Similarly, given y, if and only if $x \in \partial\alpha^*(y)$.
- But by Rademacher's theorem $\alpha(\cdot)$ is differentiable almost everywhere. So, given $X \sim \mu$, $Y = \nabla\alpha(X)$.

Optimal Transport with Quadratic Costs

- Consequently, this establishes Brennier's Theorem: If $c(x,y) = \|x-y\|_2^2/2$ then the optimal coupling

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  (by complementary slackness).

- Therefore $\nabla\bar{\alpha}(x) \in \partial\alpha(x)$ and by Rademacher $\nabla\bar{\alpha} = \nabla\alpha$ almost surely.

Optimal Transport with Quadratic Costs

- Example: Suppose that $X \sim N(0, I)$ and $Y \sim N(0, \Sigma)$ we want to transport X into Y optimally using the cost $c(x, y) = \|x - y\|_2^2 / 2$.

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- **So, we must have that $A \cdot A = \Sigma$, the solution is that A is the polar factorization of Σ.**
- *From here it is easy to derive what the general optimal transport map is between two Gaussians (try this as an exercise).*

Illustration of Optimal Transport in Image Analysis

- Santambrogio (2010)'s illustration

The discussion is based on

B. & Murthy (2016)

https://arxiv.org/abs/1604.01446.

https://pubsonline.informs.org/doi/abs/10.1287/moor.2018.0936?journalCod

A Distributionally Robust Performance Analysis

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for a complex model P_{true}.

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- Model P_{true} might be unknown or too difficult to work with.
- So, we introduce a proxy P_0 which provides a good trade-off between tractability and model fidelity (e.g. Brownian motion for random walk approximations).

A Distributionally Robust Performance Analysis

- For $f(\cdot)$ upper semicontinuous with $E_{P_0}|f(X)| < \infty$

$$\begin{aligned} &\sup E_P(f(Y)) \\ &D_c(P, P_0) \leq \delta , \end{aligned}$$

X takes values on a Polish space and $c(\cdot)$ is lower semi-continuous.

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X takes values on a Polish space and $c(\cdot)$ is lower semi-continuous.

- Also an infinite dimensional linear program

$$\sup \int_{\mathcal{X}\times\mathcal{Y}} f(y)\,\pi(dx, dy)$$
$$s.t. \int_{\mathcal{X}\times\mathcal{Y}} c(x, y)\,\pi(dx, dy) \leq \delta$$
$$\int_{\mathcal{Y}} \pi(dx, dy) = P_0(dx).$$

A Distributionally Robust Performance Analysis

- Formal duality:

$$
\begin{aligned}
Dual &= \inf_{\lambda \geq 0, \alpha} \left\{ \lambda \delta + \int \alpha(x) P_0(dx) \right\} \\
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- *We refer to this as RoPA Duality in this talk.*
- Let us consider an important case first: $f(y) = I(y \in A)$ & $c(x, x) = 0$.

A Distributionally Robust Performance Analysis

- So, if $f(y) = I(y \in A)$ and $c_A(X) = \inf\{y \in A : c(x,y)\}$, then

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- If $c_A(X)$ is continuous under P_0 & $E_0(c_A(X)) \geq \delta$, then

$$\delta = E_0 \left[c_A(X) I \left(c_A(X) \leq 1/\lambda_*\right) \right].$$

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- **Problem:** Model (P_{true}) may be complex, intractable or simply unknown...

A Distributionally Robust Risk Analysis Formulation

- **Our solution:** Estimate u_T by solving

$$\sup_{D_c(P_0,P)\leq\delta} P_{true}\left(R\left(t\right)\in B \text{ for some } t\in\left[0,T\right]\right),$$

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Connections to Distributionally Robust Optimization

- Standard choices based on divergence (such as Kullback-Leibler) - Hansen & Sargent (2016)

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- **Optimal transport is a natural option!**

Application 1: Back to Classical Risk Problem

- Suppose that

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c(x,y) &= d_J(x(\cdot), y(\cdot)) = \text{Skorokhod } J_1 \text{ metric.} \\
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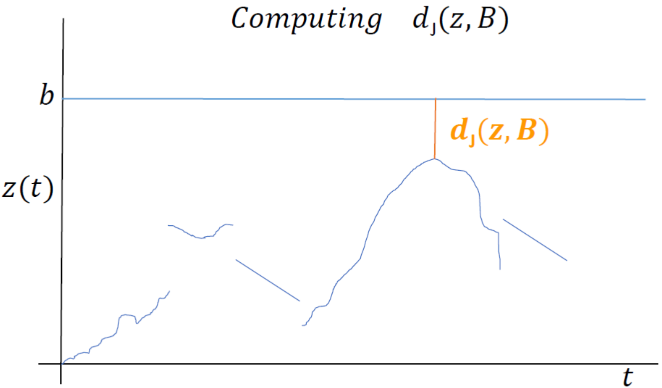
- **Let $P_0(\cdot)$ be the Wiener measure want to compute**

$$
\sup_{D_c(P_0,P)\leq\delta} P(Z \in B_b).
$$

Application 1: Computing Distance to Bankruptcy



- **So:** $\{c_{B_b}(Z) \leq 1/\lambda_*\} = \{\sup_{t\in[0,1]} Z(t) \geq b - 1/\lambda^*\}$, and

$$\sup_{D_c(P_0,P)\leq\delta} P(Z \in B_b) = P_0\left(\sup_{t\in[0,1]} Z(t) \geq b - 1/\lambda^*\right).$$

Application 1: Computing Uncertainty Size

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- We discuss choosing δ non-parametrically momentarily.

Application 1: Illustration of Coupling

- Given arrivals and claim sizes let $Z(t) = m_2^{-1/2} \sum_{k=1}^{N(t)} (X_k - m_1)$

Algorithm 1 To embed the process $(Z(t) : t \geq 0)$ in Brownian motion $(B(t) : t \geq 0)$
Given: Brownian motion $B(t)$, moment m_1 and independent realizations of claim sizes $X_1, X_2, \ldots$

Initialize $\tau_0 := 0$ and $\Psi_0 := 0$. For $j \geq 1$, recursively define,

$$\tau_{j+1} := \inf\left\{ s \geq \tau_j : \sup_{\tau_j \leq r \leq s} B_r - B_s = X_{j+1} \right\}, \text{ and } \Psi_j := \Psi_{j-1} + X_j.$$

Define the auxiliary processes

$$\tilde{S}(t) := \sum_{j>0} \sup_{\tau_j \leq s \leq t} B(s) \mathbf{1}(\tau_j \leq t < \tau_{j+1}) \text{ and } \tilde{N}(t) := \sum_{j \geq 0} \Psi_j \mathbf{1}(\tau_j \leq t < \tau_{j+1}).$$

Let $A(t) := \tilde{N}(t) + \tilde{S}(t)$, and identify the time change $\sigma(t) := \inf\{s : A(s) = m_1 t\}$. Next, take the time changed version $Z(t) := \tilde{S}(\sigma(t))$.

Replace $Z(t)$ by $-Z(t)$ and $B(t)$ by $-B(t)$.

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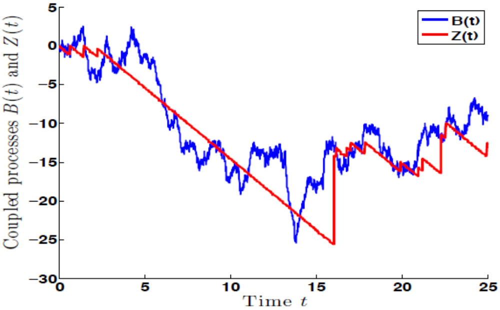
- See also Fomivoch, Gonzalez-Cazares, Ivanovs (2021).

FIGURE 4. A coupled path output by Algorithm 1



Application 1: Numerical Example

- Assume Poisson arrivals.
- *Pareto claim sizes with index* **2.2** – $\left(P\left(V > t\right) = 1/\left(1+t\right)^{2.2}\right)$.
- Cost $c\left(x,y\right) = d_J\left(x,y\right)^2$ <– note power of 2.
- Used Algorithm 1 to calibrate (estimating means and variances from data).

b	$\frac{P_0(\text{Ruin})}{P_{true}(\text{Ruin})}$	$\frac{P^*_{robust}(\text{Ruin})}{P_{true}(\text{Ruin})}$
100	1.07×10^{-1}	12.28
150	2.52×10^{-4}	10.65
200	5.35×10^{-8}	10.80
250	1.15×10^{-12}	10.98

- See also Birghila, Aigner, Engelke (2021)

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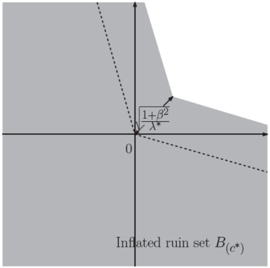

(b)Computation of worst-case ruin using the baseline measure

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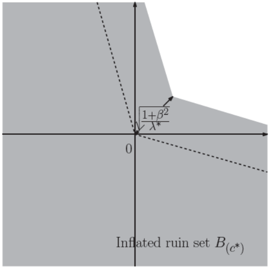

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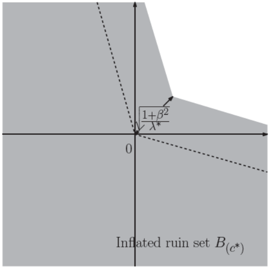

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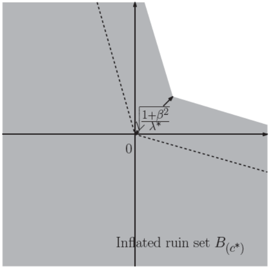

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- See also Engelke and Ivanovs (2017).

A Bit of Background on Online Advertising

Background: (Very) Simplified version of Demand Side Platforms (DSPs)

User requests publisher's page (say NYT) → Exchange bids to DSPs on behalf of publishers → DSPs send bids to Exchange on behalf of advertisers

Goal of DSP: Maximize revenue on behalf of advertisers

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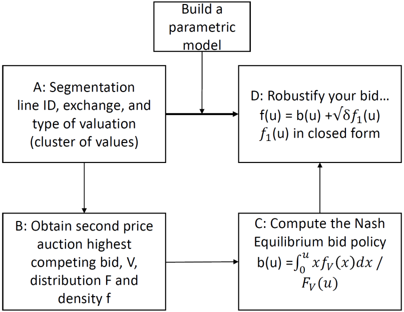
- Now, first price auction exchanges have become popular.
- How to transfer information from second-price exchanges into first-price exchanges?

Transfer Information and Mitigation of Model Error

Summary of blue print

A –> B –> C –> D



Notations

- U_i = (dlls/1000) value of the item in auction i *if we win*. We write $U_i = u_i$ when value is given.
- b_i = (dlls/1000) is what we bid in the i-th auction (cost in 1st price auction).
- V_i = (dlls/1000) is the highest competing bid in the i-th auction.
- f_{V_i} = the probability density function of V_i.
- F_{V_i} = the cumulative distribution function of V_i.

Model and Performance Measure

- A Simplified Model:

$$\max_{\{b_1,\ldots,b_n\}} \frac{1}{n} \sum_{i=1}^{n} (u_i - b_i)\, P\left(V_i \leq b_i \middle| U_i = u_i\right),$$

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- *Also assume conditional independence.*

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- Setting the derivative with respect to b equal to zero yields

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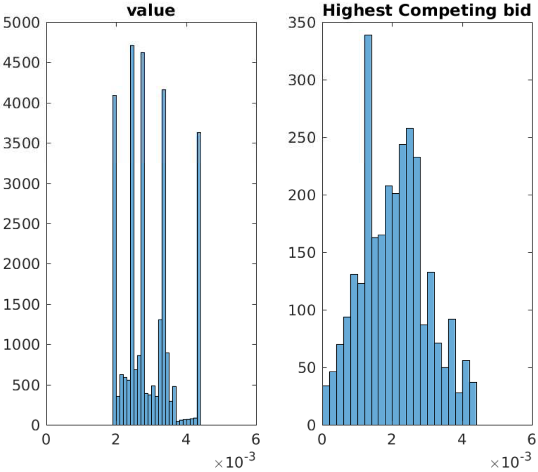
- We go back to this in part II)...

Inducing Homogeneity and Conditional Independence



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- It turns out that

$$\begin{aligned} D(F,G) &= \min\{E(|X-Y|) \text{ over all joint distributions} \\ &\quad \text{such that } X \text{ has CDF } F \text{ and } Y \text{ has CDF } G\}. \end{aligned}$$

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- Let $\lambda = \lambda_b \geq 0$ be a Lagrange multiplier, the "worst case distribution" is
$$\begin{aligned} V^* &= V \cdot I(V > b) + b \cdot I(b - \lambda < V \leq b) \\ &\quad + V \cdot I(V \leq b - \lambda) \, . \end{aligned}$$

Quantifying Model Mispecifications

- We now want
$$\max_b \min_{D(F,F_V)\leq\delta} (u-b)\,F(b)\,.$$
- If we write $\bar{F}(x) = 1 - F(x) = P(V > x)$, then the inner minimization is equivalent to
$$\max_{D(F,F_V)\leq\delta} \bar{F}(b) = \max_{D(F,F_V)\leq\delta} P_F(V > b) = P_F(V > b - \lambda_b)\,.$$
- Let $\lambda = \lambda_b \geq 0$ be a Lagrange multiplier, the "worst case distribution" is
$$\begin{aligned} V^* &= V \cdot I(V > b) + b \cdot I(b - \lambda < V \leq b) \\ &\quad + V \cdot I(V \leq b - \lambda)\,. \end{aligned}$$
- Intuitively: re-arrange V as cheaply as possible to produce V^* so that $V^* > b$ happens (λ computed to satisfy cost constraint).

Quantifying Model Mispecifications

- Conclusion: We are trying to find the (Nash Equilibrium) policy $b^*(u) = f(u)$ so

$$\begin{aligned} & \max_b \min_{D(F, F_{\bar{V}}) \leq \delta} (u-b) F_{\bar{V}}\left(f^{-1}(b)\right) \\ = \quad & \max_b (u-b) F_{\bar{V}}\left(f^{-1}(b) - \lambda_{f^{-1}(b)}\right). \end{aligned}$$

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- Optimizing over $b(\cdot)$ we obtain

$$b(u) = \frac{\int_0^u x f_{\bar{V}}(x-\lambda_x)\left(1-\dot{\lambda}(x)\right) dx}{F_{\bar{V}}(u-\lambda_u)},$$

with

$$\int_{u-\lambda_u}^{u} (u-v) f_{\bar{V}}(v)\, dv = \delta.$$

Approximate Distributionally Robust Equilibrium Bidding Policies

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- While the previous equations can be solved numerically, they may be a bit cumbersome to implement.
- So, we provide an asymptotic expansion as $\delta \rightarrow 0$.
- This leads to a bidding strategy of the form

$$b_\delta (u) = b_0 (u) + \delta^{1/2} b_1 (u) + O(\delta),$$

where

$$b_0 (u) = E(\bar{V} | \bar{V} \leq u) = \int_0^u x f_{\bar{V}}(x)\, dx / F_{\bar{V}}(x)$$

and

$$b_1 (u) = \frac{\sqrt{2}}{F_{\bar{V}}(u)} \left(\int_0^u \sqrt{f_{\bar{V}}(x)} dx - \frac{f_{\bar{V}}(u)}{F_{\bar{V}}(u)} \int_0^u F_{\bar{V}}(x)\, dx \right).$$

Example

- Example 3: Back to logistic model

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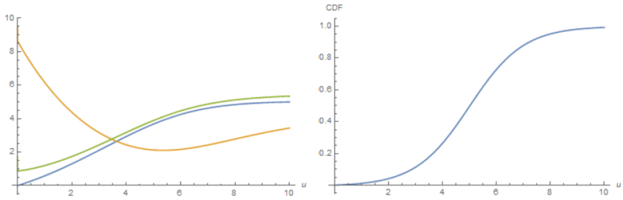
- $P\left(\bar{V} \leq x\right) = \left(1 + \exp\left(-xc\right)\right) / \left(1 + \exp\left(a - xc\right)\right)$ for $a \in R$, $c > 0$.

Example

- Example 3: Back to logistic model
- $P\left(\bar{V} \leq x\right) = \left(1 + \exp\left(-xc\right)\right) / \left(1 + \exp\left(a - xc\right)\right)$ for $a \in R$, $c > 0$.
- $a = 5$, $c = 1$ and $\delta = .01$ (figures in \$/1000)

We show the bidding policy and CDF for $a = 5, c = 1, \delta = 0.01$ in the following plot.



(a) Bidding policy (b) CDF of V

Our Goal

So, now we want to add a player optimizing a decision and play the game:

$$\min_{\theta} \max_{D(P,P_n)\leq\delta} E\left(l\left(X,\theta\right)\right).$$

Based on: Robust Wasserstein Profile Inference (B., Murthy & Kang '16)
https://arxiv.org/abs/1610.05627
https://www.cambridge.org/core/journals/journal-of-applied-probability/article/abs/robust-wasserstein-profile-inference-and-applications-to-machine-learning

- Consider estimating $\beta_* \in R^m$ in linear regression

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where $\{(Y_i, X_i)\}_{i=1}^n$ are data points.

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- Optimal Least Squares approach consists in estimating β_* via

$$\min_{\beta} E_{P_n}\left[\left(Y - \beta^T X\right)^2\right] = \min_{\beta} \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - \beta^T X_i\right)^2$$

Distributionally Robust Optimization in Machine Learning

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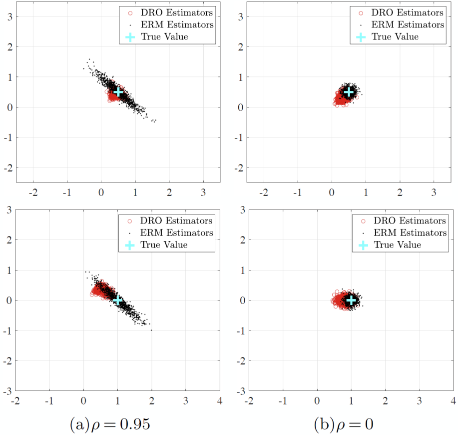
- Apply the distributionally robust estimator based on optimal transport.

Applying Distributionally Robust Optimization in Linear Regression

Estimation of θ_* with DRO (○) and without DRO (∘)



Connection to Sqrt-Lasso

Theorem (B., Kang, Murthy (2016)) Suppose that

$$c\left((x,y),(x',y')\right) = \begin{cases} \|x - x'\|_q^2 & \text{if } \quad y = y' \\ \infty & \text{if } \quad y \neq y' \end{cases}.$$

Then, if $1/p + 1/q = 1$

$$\max_{P:D_c(P,P_n)\leq\delta} E_P^{1/2}\left(\left(Y - \beta^T X\right)^2\right) = E_{P_n}^{1/2}\left[\left(Y - \beta^T X\right)^2\right] + \sqrt{\delta}\,\|\beta\|_p.$$

Remark 1: This is sqrt-Lasso (Belloni et al. (2011)).

Logistic Regression

- Classical classification model:

$$
\begin{aligned}
P\left(Y=1|X\right) &= \frac{\exp\left(\beta^{T}X\right)}{1+\exp\left(\beta^{T}X\right)} = \frac{1}{\exp\left(-\beta^{T}X\right)+1} \\
P\left(Y=-1|X\right) &= \frac{1}{1+\exp\left(\beta^{T}X\right)}
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P(Y=-1|X) &= \frac{1}{1+\exp\left(\beta^T X\right)}
\end{aligned}
$$

- The likelihood of (y, x) is:

$$
-\log\left(1+\exp\left(-y\beta^T x\right)\right)
$$

Logistic Regression

- Therefore, given $\{(y_i, x_i)\}_{i=1}^n$ maximum likelihood is equivalent to

$$\max_{\beta} -\sum_{i=1}^{n} \log\left(1 + \exp\left(-y_i \beta^T x_i\right)\right).$$

Logistic Regression

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$$\max_\beta - \sum_{i=1}^n \log\left(1+\exp\left(-y_i\beta^T x_i\right)\right).$$

- Also equivalent to

$$\begin{aligned} & \min_\beta E_{P_n}\left[\log\left(1+\exp\left(-Y\beta^T X\right)\right)\right] \\ = \quad & \min_\beta \frac{1}{n}\sum_{i=1}^n \log\left(1+\exp\left(-y_i\beta^T x_i\right)\right). \end{aligned}$$

Regularized Logistic Regression

Theorem (B., Kang, Murthy (2016)) Suppose that

$$c\left((x,y),(x',y')\right) = \begin{cases} \|x-x'\|_q & \text{if } \quad y = y' \\ \infty & \text{if } \quad y \neq y' \end{cases}.$$

Then,

$$\sup_{P:\ \mathcal{D}_c(P,P_n)\leq\delta} E_P\left[\log(1+e^{-Y\beta^T X})\right] = E_{P_n}\left[\log(1+e^{-Y\beta^T X})\right] + \delta\,\|\beta\|_p\,.$$

Remark 1: First studied via an approximation in Esfahani and Kuhn (2015).

Theorem (B., Kang, Murthy (2016)) Suppose that

$$c\left((x,y),(x',y')\right) = \begin{cases} \|x - x'\|_q & \text{if} \quad y = y' \\ \infty & \text{if} \quad y \neq y' \end{cases}.$$

Then,

$$\sup_{P:\ \mathcal{D}_c(P,P_n)\leq\delta} E_P[\left(1 - Y\beta^T X\right)^+]$$
$$= E_{P_n}\left[\left(1 - Y\beta^T X\right)^+\right] + \delta\,\|\beta\|_p .$$

Unification and Extensions of Regularized Estimators

- Distributionally Robust Optimization using Optimal Transport recovers many other estimators...

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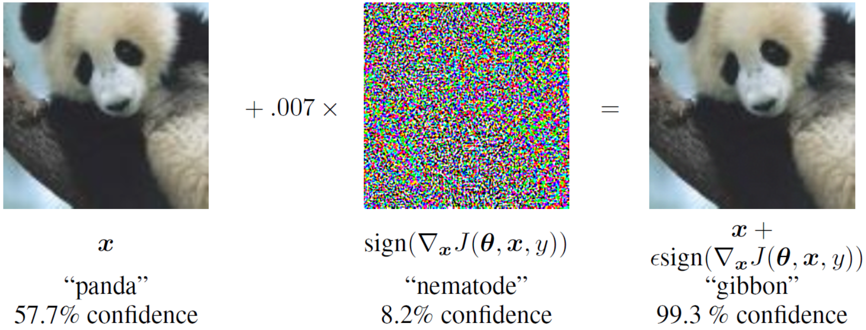
- See the excellent tutorials by Kuhn et al (2019) and Rahimian & Mehrotra (2019).
- Other areas in which optimal transport arises in machine learning

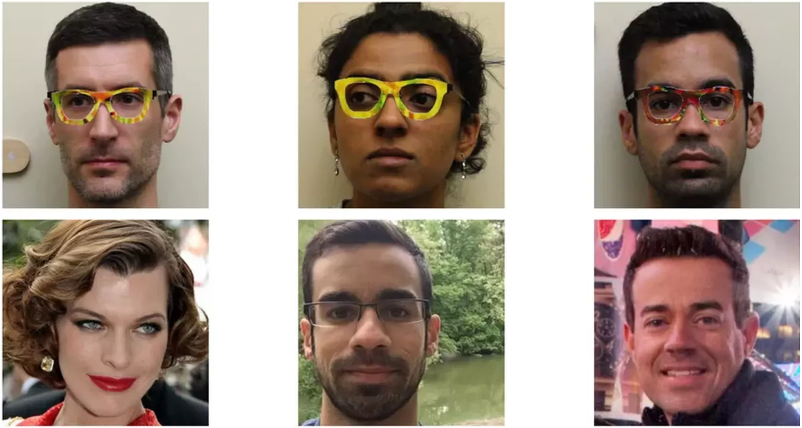
Deep Neural Networks: Adversarial Attacks

- Szegedy, Zaremba, Sutskever, Bruna, Erhan, Goodfellow, and Fergus (2014).



Deep Neural Networks: Adversarial Attacks

- Sharif, Bhagavatula, Bauer, and Reiter (2016)



Deep Neural Networks: Adversarial Attacks

- Picture from the BBC

Chinese man caught by facial recognition at pop concert

13 April 2018


GETTY IMAGES

Chinese police have used facial recognition technology to locate and arrest a man who was among a crowd of 60,000 concert goers.

How Regularization and Dual Norms Arise?

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- Recall RoPA Duality: Pick $c\left((x,y),(x',y')\right) = \left\|(x,y)-(x',y')\right\|_q^2$

$$\max_{P:D_c(P,P_n)\leq\delta} E_P\left(\left((X,Y)\cdot(\beta,1)\right)^2\right)$$

$$= \min_{\lambda\geq 0}\left\{\lambda\delta + E_{P_n}\sup_{(x',y')}\left[\left((x',y')\cdot(\beta,1)\right)^2 - \lambda\left\|(X,Y)-(x',y')\right\|_q^2\right.\right.$$

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- Let's focus on the inside E_{P_n}...

How Regularization and Dual Norms Arise?

- Let $\Delta = (X, Y) - (x', y')$

$$
\begin{aligned}
& \sup_{(x',y')} \left[\left((x', y') \cdot (\beta, 1) \right)^2 - \lambda \left\| (X, Y) - (x', y') \right\|_q^2 \right] \\
= & \sup_{\Delta} \left[((X, Y) \cdot (\beta, 1) - \Delta \cdot (\beta, 1))^2 - \lambda \left\| \Delta \right\|_q^2 \right] \\
= & \sup_{\left\| \Delta \right\|_q} \left[(|(X, Y) \cdot (\beta, 1)| + \left\| \Delta \right\|_q \left\| (\beta, 1) \right\|_p)^2 - \lambda \left\| \Delta \right\|_q^2 \right]
\end{aligned}
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= & \sup_{\Delta} \left[((X, Y) \cdot (\beta, 1) - \Delta \cdot (\beta, 1))^2 - \lambda \left\| \Delta \right\|_q^2 \right] \\
= & \sup_{\left\| \Delta \right\|_q} \left[(\left| (X, Y) \cdot (\beta, 1) \right| + \left\| \Delta \right\|_q \left\| (\beta, 1) \right\|_p)^2 - \lambda \left\| \Delta \right\|_q^2 \right]
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- Last equality uses $z \to z^2$ is symmetric around origin and $|a \cdot b| \leq \|a\|_p \|b\|_q$.

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\end{aligned}
$$

- Last equality uses $z \to z^2$ is symmetric around origin and $|a \cdot b| \leq \|a\|_p \|b\|_q$.
- Note problem is now one-dimensional (easily computable).

- Use RoPA: with $c\left(\left(x,y\right),\left(x',y'\right)\right)=\left\|x-x'\right\|_{q}I\left(y=y'\right)+\infty I\left(y\neq y'\right)$

$$
\begin{aligned}
&\sup_{P:\ \mathcal{D}_c(P,P_n)\leq\delta} E_P\left[\left(1-Y\beta^T X\right)^+\right] \\
&= \min_{\lambda\geq 0}\left[\lambda\delta+E_{P_n}\left\{\max_{x}\left(\left(1-Y\beta^T x\right)^+-\lambda\left\|x-X\right\|_q\right)\right\}\right] \\
&= \min_{\lambda\geq 0}\left[\lambda\delta+E_{P_n}\left\{\max_{\Delta}\left(\left(1-Y\beta^T X-Y\beta^T\Delta\right)^+-\lambda\left\|\Delta\right\|_q\right)\right\}\right] \\
&= \min_{\lambda\geq 0}\left[\lambda\delta+E_{P_n}\left\{\max_{\Delta}\left(\left(1-Y\beta^T X+\left\|\beta\right\|_p\left\|\Delta\right\|_q\right)^+-\lambda\left\|\Delta\right\|_q\right)\right\}\right. \\
&= \min_{\lambda\geq\left\|\beta\right\|_p}\left[\lambda\delta+E_{P_n}\left\{\max_{\left\|\Delta\right\|_q}\left(\left(1-Y\beta^T X+\left\|\beta\right\|_p\left\|\Delta\right\|_q\right)^+-\lambda\left\|\Delta\right\|_q\right.\right.\right. \\
&= \min_{\lambda\geq\left\|\beta\right\|_p}\left[\lambda\delta+E_{P_n}\left(1-Y\beta^T X\right)^+\right]=\lambda\left\|\beta\right\|_p+E_{P_n}\left(1-Y\beta^T X\right)
\end{aligned}
$$

Explaining the Adversarial Attacks of Neural Networks

- So, in general
$c\left(\left(x,y\right),\left(x',y'\right)\right)=\left\|x-x'\right\|_q I\left(y=y'\right)+\infty I\left(y\neq y'\right)$

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&= \min_{\lambda\geq 0}\left[\lambda\delta+E_{P_n}\left\{\max_\Delta\left(l\left(\theta,Y,X+\Delta\right)-\lambda\left\|\Delta\right\|_q\right)\right\}\right] \\
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\end{aligned}$$

- If $\delta\approx 0$, then λ is large, so inner maximization

$$\begin{aligned}
&\max_{\Delta}\left(l\left(\theta,Y,X+\Delta/\lambda\right)-\left\|\Delta\right\|_q\right)\\
\approx\ & l\left(\theta,Y,X\right)+\left\|l_x\left(\theta,Y,X\right)\right\|_p\left\|\Delta\right\|_q/\lambda-\left\|\Delta\right\|_q
\end{aligned}$$

Summary

- The worst case perturbation is given by Δ such that

$$l_x(\theta, Y, X) \cdot \Delta/\lambda = \|l_x(\theta, Y, X)\|_p \|\Delta\|_q /\lambda,$$

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- So, $\delta \approx 0$ means perturbing by

$$\epsilon \cdot sign(l_x(\theta, Y, X))$$

  for $\epsilon > 0$.
- This explains the nature of the panda example given earlier.

Can We Defend Against Attacks?

- Naturally, it makes sense then to train networks using

$$
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& \min_{\theta} \max_{D(P,P_n)\leq\delta} E_P\left(l\left(\theta, Y, X\right)\right) \\
= \quad & \min_{\theta}\{\lambda\delta + E_{P_n} \max_{x}[l\left(\theta, Y, x\right) - \lambda\left\|x - X\right\|_q].
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- This will automatically protect against attacks.
- This is an active area of research currently.
- But there may be many possible attacks.

On Role of Transport Cost...

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- Suppose that $\|x - x'\|_A^2 = (x - x')\, A\, (x - x)$ with A positive definite (Mahalanobis distance).

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- *Intuition: Think of A diagonal, encoding inverse variability of X_is...*

On Role of Transport Cost...

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Connections to Statistical Analysis

Based on:

Robust Wasserstein Profile Inference (B., Murthy & Kang '16)

https://arxiv.org/abs/1610.05627

Highlight: How to choose size of uncertainty?

Towards an Optimal Choice of Uncertainty Size

- How to choose uncertainty size in a data-driven way?

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- Use left hand side to define a statistical principle to choose δ.
- Important: Optimizing δ is equivalent to optimizing regularization!

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- The analysis of this object is extensively studied in the theory of Empirical Processes.
- Unfortunately, it turns out that typically $D\left(P_{true}, P_n\right) = O\left(n^{-1/d}\right)$ (Dudley '68) for $d > 2$.

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- So, instead, we'll focus on an optimal (in some sense to be explained) approach.

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- It is natural to say that

$$\Lambda_\delta(n) = \{\bar{\beta}(P) : P \in \mathcal{U}_\delta(n)\}$$

are *plausible estimates* of β_*.

Optimal Choice of Uncertainty Size

- Given a confidence level $1-\alpha$ we advocate choosing δ via

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- In simple words: Find the smallest δ so that β_* is plausible with confidence level $1-\alpha$.

The Robust Wasserstein Profile Function

- The value $\bar{\beta}(P)$ is characterized by

$$E_P\left(\nabla_\beta\left(Y-\beta^T X\right)^2\right)=2E_P\left(\left(Y-\beta^T X\right)X\right)=0.$$

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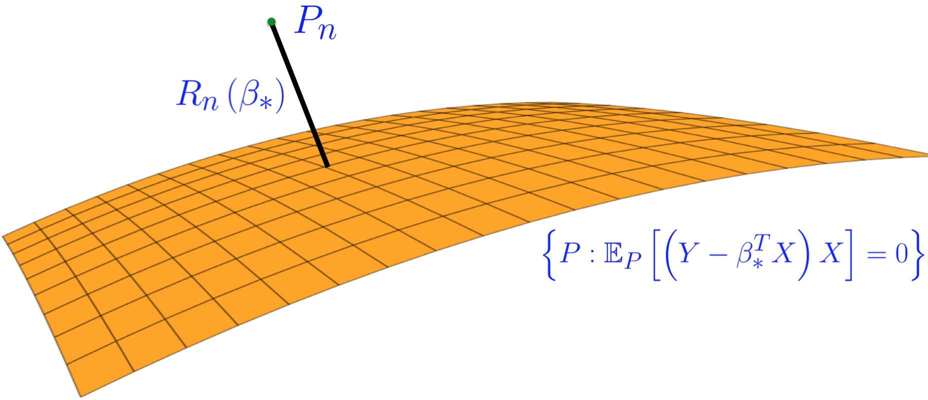
- **So δ is $1-\alpha$ quantile of $R_n(\beta_*)$!**

The Robust Wasserstein Profile Function



Computing Optimal Regularization Parameter

Theorem (B., Murthy, Kang (2016)) *Suppose that* $\{(Y_i, X_i)\}_{i=1}^n$ *is an i.i.d. sample with finite variance, with*

$$c\left((x,y),(x',y')\right) = \begin{cases} \|x - x'\|_q^2 & \text{if} \quad y = y' \\ \infty & \text{if} \quad y \neq y' \end{cases},$$

then

$$nR_n(\beta_*) \Rightarrow L_1,$$

where L_1 *is explicitly and*

$$L_1 \overset{D}{\leq} L_2 := \frac{E[e^2]}{E[e^2] - (E|e|)^2} \|N(0, Cov\,(X))\|_q^2.$$

Remark: We recover same order of regularization (but L_1 gives the optimal constant!)

Discussion on Optimal Uncertainty Size

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- We characterize the asymptotic constant (not only order) in optimal regularization:
$$P\left(L_1 \leq \eta_{1-\alpha}\right) = 1 - \alpha.$$
- $R_n\left(\beta_*\right)$ is inspired by Empirical Likelihood – Owen (1988).

A Toy Example Illustrating Proof Techniques

- Consider

$$\min_{\beta} \max_{P:\mathcal{D}_c(P,P_n)\leq\delta} E\left[(Y-\beta)^2\right]$$

with $c(y,y') = (y-y')^{\rho}$ and define

$$\begin{aligned} R_n(\beta) &= \min_{\pi(dy,du)\geq 0} \int (y-u)^{\rho}\, \pi(dy,du) : \\ & \int_{u\in\mathbb{R}} \pi(dy,du) = \frac{1}{n}\delta_{\{Y_i\}}(dy) \;\; \forall i, \\ & 2\int\int (u-\beta)\, \pi(dy,du) = 0. \end{aligned}$$

A Toy Example Illustrating Proof Techniques

- Dual linear programming problem: Plug in $\beta = \beta_*$

$$
\begin{aligned}
R_n(\beta_*) &= \sup_{\lambda \in \mathbb{R}} \left\{ -\frac{1}{n} \sum_{i=1}^{n} \sup_{u \in \mathbb{R}} \left\{ \lambda(u - \beta_*) - |Y_i - u|^{\rho} \right\} \right\} \\
&= \sup_{\lambda \in \mathbb{R}} \left\{ \begin{array}{c} -\frac{\lambda}{n} \sum_{i=1}^{n} (Y_i - \beta_*) \\ -\frac{1}{n} \sum_{i=1}^{n} \sup_{u \in \mathbb{R}} \left\{ \lambda(u - Y_i) - |Y_i - u|^{\rho} \right\} \end{array} \right\} \\
&= \sup_{\lambda} \left\{ -\frac{\lambda}{n} \sum_{i=1}^{n} (Y_i - \beta_*) - (\rho - 1) \left| \frac{\lambda}{\rho} \right|^{\frac{\rho}{\rho-1}} \right\} \\
&= \left| \frac{1}{n} \sum_{i=1}^{n} (Y_i - \beta_*) \right|^{\rho} = \frac{1}{n^{1/2}} \left| N(0, \sigma^2) \right|^{\rho}.
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- Optimal complexity algorithms for continuous problems is still an open problem.

Discussion: Some Open Problems

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- Computational methods: Typical approach is entropic regularization (new methods currently developed in the machine learning literature).

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- OT can be used for statistical inference using RWP function.