



Technische
Universität
Braunschweig

Quadratically regularized optimal transport

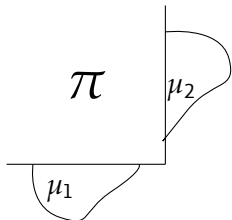
Dirk Lorenz joint with Christoph Brauer, Christian Clason, Paul Manns, Christian Meyer, and Benedikt Wirth, February 7, 2019

Variational methods and optimization in imaging, IHP Paris

Optimal transport of measures

- μ_i mass distributions on compact $\Omega_i \subset \mathbb{R}^{d_i}$ (Radon measures)
- $\|\mu\|_{\mathfrak{M}} = \sup\{\int f \, d\mu : f \in C, \|f\|_{\infty} \leq 1\}$

Kantorovich [1941]: Find a *transport plan* $\pi \in \mathfrak{M}(\Omega_1 \times \Omega_2)$ with marginals μ_1 and μ_2 :



$\pi(x, y)$ indicates how much mass is transported from x to y .

Optimal:

$$\inf_{\pi} \int_{\Omega_1 \times \Omega_2} c(x, y) \, d\pi(x, y),$$

$$\text{s.t. } P_1\pi = \mu_1, P_2\pi = \mu_2$$

- Numerous applications in imaging and machine learning (color transfer, generative models, image interpolation,...)
[Computational Optimal Transport, Peyré, Cuturi 2019]

- **Regularization and duality**

- Entropic regularization

- Quadratic regularization

- Algorithms

- Illustration

Regularization

- Transport plan in general singular measure [Brenier 1987],
- General regularization for π to be in a function space

$$\inf_{\pi} \int_{\Omega_1 \times \Omega_2} c \, d\pi + \frac{\gamma}{2} R(\pi) \quad \text{subject to} \quad \begin{aligned} \int_{\Omega_2} \pi(x_1, x_2) \, dx_2 &= \mu_1(x_1), \\ \int_{\Omega_1} \pi(x_1, x_2) \, dx_1 &= \mu_2(x_2), \\ \pi(x_1, x_2) &\geq 0 \end{aligned}$$

- $R : X \rightarrow \mathbb{R} \cup \{\infty\}$ for some suitable function space X

Formal dual

- Primal problem

$$\inf_{\pi} \int_{\Omega_1 \times \Omega_2} c \, d\pi + \frac{\gamma}{2} R(\pi) \quad \text{subject to} \quad \int_{\Omega_2} \pi(x_1, x_2) \, dx_2 = \mu_1(x_1),$$
$$\int_{\Omega_1} \pi(x_1, x_2) \, dx_1 = \mu_2(x_2),$$
$$\pi(x_1, x_2) \geq 0$$

- Formally computing the dual problem: Formal KKT conditions

$$\gamma \partial R(\pi)(x_1, x_2) + c(x_1, x_2) - \alpha_1(x_1) - \alpha_2(x_2) - \rho(x_1, x_2) \ni 0,$$
$$\rho(x_1, x_2) \geq 0, \quad \rho(x_1, x_2) \pi(x_1, x_2) = 0, \quad \pi(x_1, x_2) \geq 0,$$

$$\int_{\Omega_2} \pi(x_1, x_2) \, dx_2 = \mu_1(x_1),$$
$$\int_{\Omega_1} \pi(x_1, x_2) \, dx_1 = \mu_2(x_2),$$

Formal dual

- Leads to formal dual:

$$\inf_{\alpha_1, \alpha_2} R^*((\alpha_1 \oplus \alpha_2 - c)_+) - \int \alpha_1 d\mu_1 - \int \alpha_2 d\mu_2$$

with convex conjugate R^* , α_i some functions on Ω_i and

$$\alpha_1 \oplus \alpha_2(x_1, x_2) = \alpha_1(x_1) + \alpha_2(x_2).$$

- Notably, a smaller optimization problem...
- Existence of solutions of dual problem?

- Regularization and duality
- **Entropic regularization**
- Quadratic regularization
- Algorithms
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Entropic regularization

- Use entropy

$$R(\pi) = \begin{cases} \int_{\Omega_1 \times \Omega_2} \pi(x_1, x_2) \log(\pi(x_1, x_2)) \, d(x_1, x_2) & \pi \geq 0 \\ \infty & \text{else} \end{cases}$$

- Analysis in the set of Borel measures with densities [Carlier et al., 2017] and [Chizat et al. 2018]

Entropically regularized discrete optimal transport

- Entropic regularization of optimal transport

$$\min_{\pi} \sum_{i,j} c_{ij} \pi_{ij} - \gamma \pi_{ij} (\log(\pi_{ij}) - 1)$$

subject to marginals (row and column sums)

- Lagrange multipliers $\alpha, \beta \in \mathbb{R}^N$ for the constraints give optimality system

$$c_{ij} + \gamma \log(\pi_{ij}) + \alpha_j + \beta_i = 0$$

Solved by

$$\pi_{ij} = \exp(-\frac{c_{ij}}{\gamma}) \exp(-\frac{\alpha_j}{\gamma}) \exp(-\frac{\beta_i}{\gamma})$$

- Matrix form:

$$\pi = \text{diag}(\exp(-\alpha/\gamma)) M \text{diag}(\exp(-\beta/\gamma)), \quad M_{ij} = \exp(-c_{ij}/\gamma)$$

Sinkhorn-Knopp iteration for regularized discrete optimal transport

- Find $\alpha, \beta \in \mathbb{R}^N$, such that

$$\pi = \text{diag}(\exp(-\alpha/\gamma)) M \text{diag}(\exp(-\beta/\gamma))$$

- Set $p_j = \exp(-\alpha_j/\gamma)$, $q_i = \exp(-\beta_i/\gamma)$ and iterate

$$p^{k+1} = \frac{u}{Mq^k}, \quad q^{k+1} = \frac{v}{M^T p^{k+1}}$$

“Alternatingly scale rows and columns to correct sums”

- Application of Sinkhorn-Knopp for optimal transport [Cuturi 2013]

Analysis in the Orlicz space $L \log L$

Theorem

An optimal transport plan π^ exists if and only if $\mu_i \in L \log L(\Omega_i)$.*

- $f \in L \log L$, if $\int |f| \log(|f|)_+ dx < \infty$
- $L \log L$ is a Banach function space - in fact an Orlicz space
- Equipped with Luxemburg norm

$$\|f\|_{L^\phi} = \inf\{\lambda > 0 \mid \int_{\Omega} \phi\left(\frac{|f|}{\lambda}\right) dx \leq 1\}.$$

with $\phi(t) = t \log(t)_+$.

Strong duality

Theorem

If c continuous and $\exp(-c/\gamma)$ integrable, then

$$\sup_{\alpha_i \in C(\Omega_i)} \int_{\Omega_1} \alpha_1 d\mu_1 + \int_{\Omega_2} \alpha_2 d\mu_2 - \gamma \int_{\Omega_1 \times \Omega_2} \exp \left[\frac{-c + \alpha_1 \oplus \alpha_2}{\gamma} \right] d(x_1, x_2)$$

is the predual of the entropically regularized OT problem and strong duality holds. If the supremum is finite, the primal problem has a minimizer.

Proof: Slater's condition and pointwise conjugation.

- Primal minimizers π^* are unique (by strict convexity), lie in $L \log L$ and $\text{supp } \pi^* = \text{supp } \mu_1 \times \text{supp } \mu_2$
- Unclear: Dual existence? (coercivity unclear) What do optimality conditions mean if there is no dual existence?

Dual existence for entropic regularization

- In a nutshell: Substitute

$$u_i = \begin{cases} e^{\alpha_i/\gamma} & \alpha \leq 0 \\ \frac{\alpha_i}{\gamma} + 1 & \text{else} \end{cases}$$

and observe that dual problem equals

$$\inf_{u_1, u_2 \geq 0} \int \Phi(u_1) \Phi(u_2) \exp(-c/\gamma) - \int \Psi(u_1) \mu_1 - \int \Psi(u_2) \mu_2$$

with

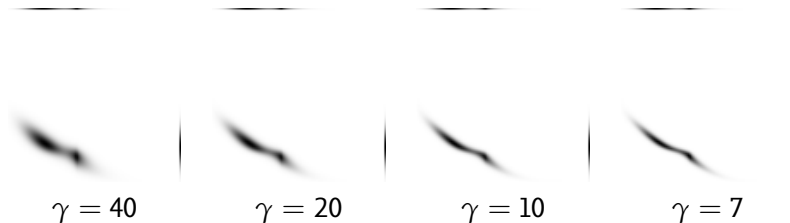
$$\Phi(s) = \begin{cases} s & 0 \leq s \leq 1 \\ e^{s-1} & s > 1 \end{cases}, \quad \Psi(s) = \log(\Phi(s)) = \begin{cases} \log(s) & 0 \leq s \leq 1 \\ s-1 & s > 1 \end{cases}$$

- Show coercivity and lower semi-continuity in $L_{\exp} \times L_{\exp}$ and get
- **Theorem:** The dual problem admits a solution $u_i \in L_{\exp}$ (and hence, optimal Lagrange multipliers α_i exist).

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Why a different regularization?

- Entropic regularization gives simple characterization of minimizers and extremely simple algorithm
- Existence theory quite cumbersome, takes place in non-reflexive Orlicz-space
- Plain Sinkhorn algorithm gets unstable for small regularization γ
- Transport plans always have full support



What about working in L^2 ?

Quadratic regularization

$$\inf_{\pi} \int_{\Omega_1 \times \Omega_2} c \, d\pi + \frac{\gamma}{2} \|\pi\|_2^2 \quad \text{subject to} \quad \begin{aligned} \int_{\Omega_2} \pi(x_1, x_2) \, dx_2 &= \mu_1(x_1), \\ \int_{\Omega_1} \pi(x_1, x_2) \, dx_1 &= \mu_2(x_2), \\ \pi(x_1, x_2) &\geq 0 \end{aligned}$$

- **Lemma:** Has a solution iff $\mu_i \in L^2(\Omega_i)$, $\mu_i \geq 0$ and same integral.
- Γ convergence for $\gamma \rightarrow 0$ in L^2 (strongly)
- Appeared in the discrete case in [Blondel, Seguy, Rolet 2018], [Essid, Solomon 2018],

Formal optimality

Quadratic

$$\pi^*$$

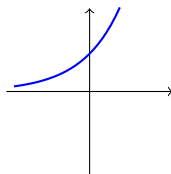
$$\mu_1$$

Entropic

$$= e^{\frac{\alpha_1(x_1) + \alpha_2(x_2) - c(x_1, x_2)}{\gamma}}$$

$$= \int_{\Omega_2} e^{\frac{\alpha_2(x_2) - c(x_1, x_2)}{\gamma}} dx_2 e^{\alpha_1(x_1)}$$

$\exp(x)$



$$(e^{\alpha_1} \otimes e^{\alpha_2})(x_1, x_2) = e^{\alpha_1(x_1)} e^{\alpha_2(x_2)}$$

Formal optimality

Quadratic

$$\pi^* = \frac{(\alpha_1(x_1) + \alpha_2(x_2) - c(x_1, x_2))_+}{\gamma}$$

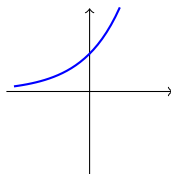
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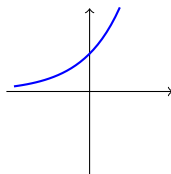
$$\mu_1 = \int_{\Omega_2} \frac{(\alpha_1(x_1) + \alpha_2(x_2) - c(x_1, x_2))_+}{\gamma} dx_2$$

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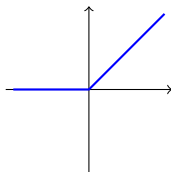
Formal optimality

Quadratic

$$\pi^* = \frac{(\alpha_1(x_1) + \alpha_2(x_2) - c(x_1, x_2))_+}{\gamma}$$

$$\mu_1 = \int_{\Omega_2} \frac{(\alpha_1(x_1) + \alpha_2(x_2) - c(x_1, x_2))_+}{\gamma} dx_2$$

$$(x)_+ = \max(x, 0)$$

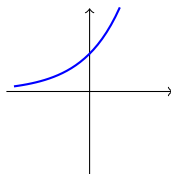


Entropic

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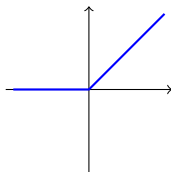
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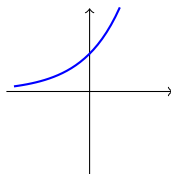
$$(\alpha_1 \oplus \alpha_2)(x_1, x_2) = \alpha_1(x_1) + \alpha_2(x_2)$$

Entropic

$$= e^{\frac{\alpha_1(x_1) + \alpha_2(x_2) - c(x_1, x_2)}{\gamma}}$$

$$= \int_{\Omega_2} e^{\frac{\alpha_2(x_2) - c(x_1, x_2)}{\gamma}} dx_2 e^{\alpha_1(x_1)}$$

$$\exp(x)$$



$$(e^{\alpha_1} \otimes e^{\alpha_2})(x_1, x_2) = e^{\alpha_1(x_1)} e^{\alpha_2(x_2)}$$

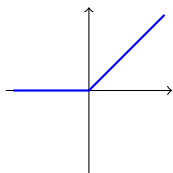
Formal optimality

Quadratic

$$\pi^* = \frac{(\alpha_1(x_1) + \alpha_2(x_2) - c(x_1, x_2))_+}{\gamma}$$

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$$(x)_+ = \max(x, 0)$$



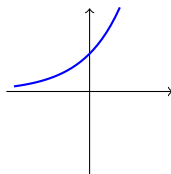
$$(\alpha_1 \oplus \alpha_2)(x_1, x_2) = \alpha_1(x_1) + \alpha_2(x_2)$$

Entropic

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$$= \int_{\Omega_2} e^{\frac{\alpha_2(x_2) - c(x_1, x_2)}{\gamma}} dx_2 e^{\alpha_1(x_1)}$$

$$\exp(x)$$



$$(e^{\alpha_1} \otimes e^{\alpha_2})(x_1, x_2) = e^{\alpha_1(x_1)} e^{\alpha_2(x_2)}$$

\rightsquigarrow sparser π^* , but nonsmooth, non-separable optimality; dual existence?

Dual problem

- **Lemma:** The dual for the quadratically regularized problem is

$$\inf_{\alpha_i \in L^2(\Omega_i)} \left[\frac{1}{2} \|(\alpha_1 \oplus \alpha_2 - c)_+\|_2^2 - \gamma \langle \mu_1, \alpha_1 \rangle - \gamma \langle \mu_2, \alpha_2 \rangle =: \Phi(\alpha_1, \alpha_2) \right].$$

Dual problem

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- Existence of Lagrange multipliers need:
 1. No duality gap
 2. Dual existence

Dual problem

- **Lemma:** The dual for the quadratically regularized problem is

$$\inf_{\alpha_i \in L^2(\Omega_i)} \left[\frac{1}{2} \|(\alpha_1 \oplus \alpha_2 - c)_+\|_2^2 - \gamma \langle \mu_1, \alpha_1 \rangle - \gamma \langle \mu_2, \alpha_2 \rangle =: \Phi(\alpha_1, \alpha_2) \right].$$

- Existence of Lagrange multipliers need:

1. No duality gap
2. Dual existence

- Dual existence?

! No coercivity in $L^2 \times L^2$ since negative entries only controlled by inner products, i.e. only by L^1 -norm

Dual existence – strategy

- Assumptions: cost function $c \geq \underline{c} > -\infty$ continuous, marginals μ_i continuous and $\mu_i \geq \delta > 0$ with same integral.
- Strategy to prove dual existence:
 1. Show that minimizers α_1, α_2^* exist in $L^1(\Omega_1) \times L^1(\Omega_2)$
 2. Show that these are actually in L^2
 3. Conclude that they still solve the dual problem

Dual existence, step 1

- Observe that $\Phi(\alpha_1, \alpha_2) = G(\alpha_1 \oplus \alpha_2 - c) + C$ with

$$G(w) = \int_{\Omega} (w_+)^2 - w\mu \, dx, \quad \Omega = \Omega_1 \times \Omega_2, \quad \mu = \gamma\mu_1 \otimes \mu_2$$

- G coercive in the norm $\|w\|_{L^1+L^2} = \inf_{w=u+v} (\|u\|_{L^2} + \|v\|_{L^1})$
- Fact 1:** For minimizing sequence w^n : $(w^n)_+$ bounded in $L^2(\Omega)$, $(w^n)_-$ bounded in $L^1(\Omega)$.
- Lemma:** If $w^n \in L^2$ and $w^n \rightharpoonup^* w^*$ in \mathfrak{M} , $G(w^n)$ bounded, then $G(w^*) \leq \liminf G(w^n)$ and $(w^*)_+ \in L^2$.
- Proof:** Use result by Fonseca/Leoni on weak* lsc functionals on L^1 , to show $w^*_+ \in L^1$ and structure of G to upgrade to $w^*_+ \in L^2$.
- Note that w^*_- may still be a measure!

Dual existence – more lemmas

- **Lemma:** Let $\alpha_i \in \mathfrak{M}(\Omega_i)$ with Lebesgue decompositions, $\alpha_i = f_i + \eta_i$ satisfying $f_i \ll \lambda$ and $\eta_i \perp \lambda$ for $i \in \{1, 2\}$. Then,

$$(\alpha_1 \oplus \alpha_2 - c)_+ = (f_1 \oplus f_2 - c + (\eta_1)_+ \oplus (\eta_2)_+)_+.$$

\rightsquigarrow Consequence: Dropping negative singular part does decrease objective, so minimizer has no negative singular part

- **Proposition:** Dual solution α_1^*, α_2^* exist in L^1 .

Proof: Combine all previous results to show existence in \mathfrak{M} and then upgrade to L^1

- **Theorem:** Dual solutions actually in L^2 .

Proof: Clear for positive part. For negative part show that they are even bounded.

Optimality conditions

- **Lemma:** No duality gap
- **Theorem:** Primal $\pi^* \in L^2(\Omega)$ is optimal iff there exist $\alpha_i^* \in L^2(\Omega_i)$ such that

$$\begin{aligned}\pi^* - \frac{1}{\gamma} (\alpha_1^* \oplus \alpha_2^* - c)_+ &= 0 && \lambda\text{-a.e. in } \Omega, \\ \int_{\Omega_2} (\alpha_1^* \oplus \alpha_2^* - c)_+ \, dx_2 &= \gamma\mu_1 && \lambda_1\text{-a.e. in } \Omega_1, \\ \int_{\Omega_1} (\alpha_1^* \oplus \alpha_2^* - c)_+ \, dx_1 &= \gamma\mu_2 && \lambda_2\text{-a.e. in } \Omega_2.\end{aligned}$$

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Discrete optimality system

- Discrete optimality system: Optimal $\pi = \frac{1}{\gamma} (\alpha \oplus \beta - c)_+$ fulfills

$$\sum_{i=1}^M (\alpha_i + \beta_j - c_{ij})_+ = \gamma \mu_j^+, j = 1, \dots, N$$

$$\sum_{j=1}^N (\alpha_i + \beta_j - c_{ij})_+ = \gamma \mu_i^-, i = 1, \dots, M$$

with $\mu^+ \in \mathbb{R}^N$, $\mu^- \in \mathbb{R}^M$, $\pi \in \mathbb{R}^{M \times N}$

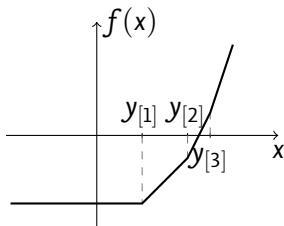
- Each of the first N equations does only depend on one β_j (last M only on one α_i): Use nonlinear Gauß-Seidel
- Non-smooth but Lipschitz-continuous optimality system: Use semismooth Newton method

Gauß-Seidel

- Each equation $\sum_{i=1}^M (\alpha_i \oplus \beta_j - c_{ij})_+ = \gamma \mu_j^+$ of the form:
For vector y find real variable x such that

$$f(x) = \sum_j (x - y_j)_+ - b = 0$$

- Sort $y_{[1]} \leq y_{[2]} \leq \dots$:



Simple search or semismooth Newton...

Semismooth Newton

- Solve $F(\alpha, \beta) = 0$ with $F : \mathbb{R}^{M+N} \rightarrow \mathbb{R}^{M+N}$

$$F(\alpha, \beta) = \begin{pmatrix} F_1(\alpha, \beta) \\ F_2(\alpha, \beta) \end{pmatrix} = \begin{pmatrix} (\sum_{j=1}^N (\alpha_i \oplus \beta_j - c_{ij})_+ - \gamma \mu_i^-)_{i=1, \dots, M} \\ (\sum_{i=1}^M (\alpha_i \oplus \beta_j - c_{ij})_+ - \gamma \mu_j^+)_{j=1, \dots, N} \end{pmatrix}$$

- Newton matrix

$$G = \begin{pmatrix} \text{diag}(\sigma \mathbf{1}_N) & \sigma \\ \sigma^T & \text{diag}(\sigma^T \mathbf{1}_M) \end{pmatrix}, \quad \sigma_{ij} = \begin{cases} 1 & \alpha_i + \beta_j - c_{ij} \geq 0 \\ 0 & \text{otherwise.} \end{cases}$$

- Newton iteration

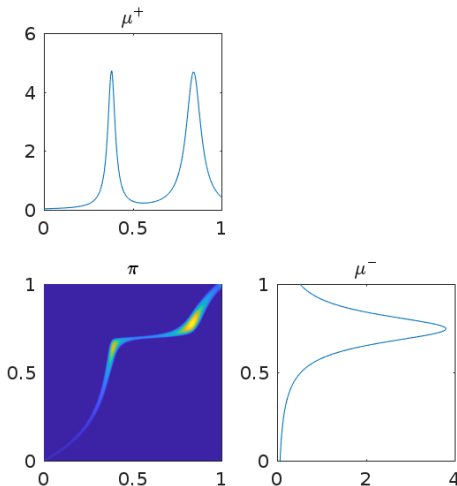
$$\begin{pmatrix} \alpha^{k+1} \\ \beta^{k+1} \end{pmatrix} = \begin{pmatrix} \alpha^k \\ \beta^k \end{pmatrix} - \begin{pmatrix} \delta \alpha^k \\ \delta \beta^k \end{pmatrix} \quad \text{where} \quad F(\alpha^k, \beta^k) = G \begin{pmatrix} \delta \alpha^k \\ \delta \beta^k \end{pmatrix}.$$

(plus slight regularization and Armijo line-search if necessary)

- Regularization and duality
- Entropic regularization
- Quadratic regularization
- Algorithms
- **Illustration**

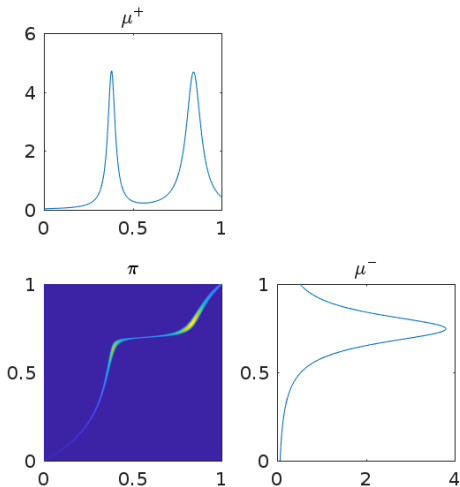
Γ -convergence of quadratic regularization

$$\gamma = 10$$



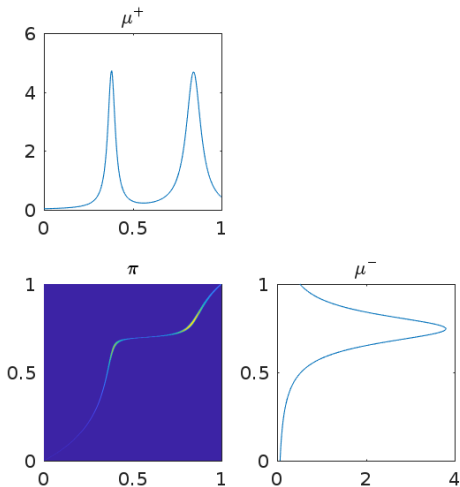
Γ -convergence of quadratic regularization

$$\gamma = 1$$



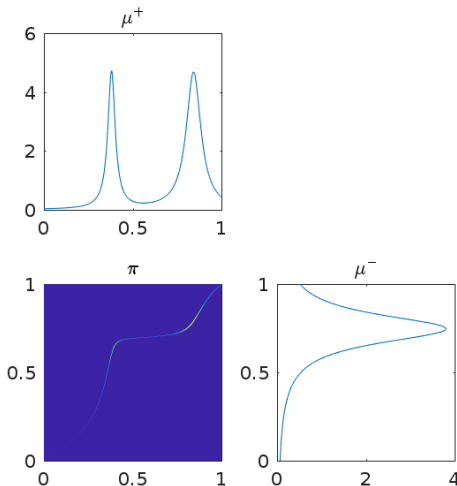
Γ -convergence of quadratic regularization

$$\gamma = 0.1$$

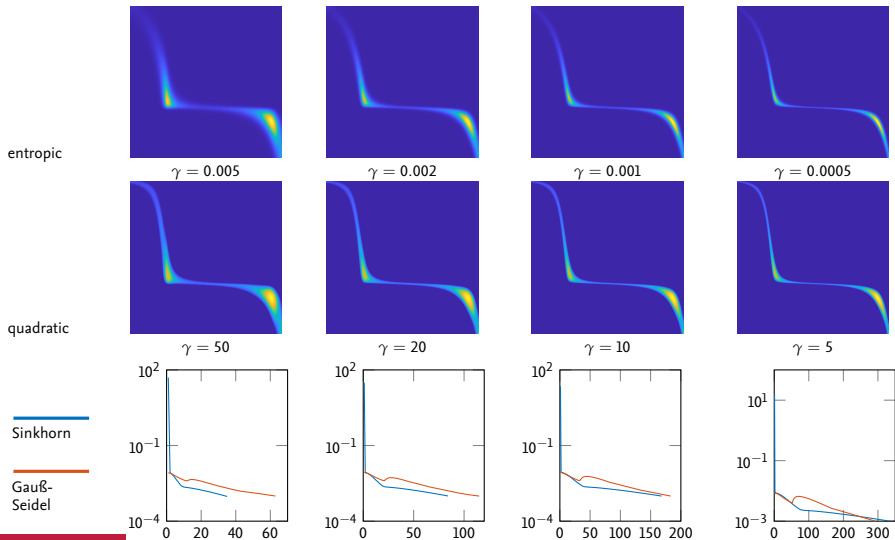


Γ -convergence of quadratic regularization

$$\gamma = 0.01$$



Comparison of quadratic and entropic regularization



Mesh independence

- Consider continuous marginals μ^\pm on $[0, 1]$
- Discretize everything piecewise constant

$$\pi(x, y) := \sum_{i,j=0}^{N-1} \pi_{ij} \chi_{(\frac{i}{N}, \frac{i+1}{N}) \times (\frac{j}{N}, \frac{j+1}{N})}(x, y),$$

$$c(x, y) := \sum_{i,j=0}^{N-1} c_{ij} \chi_{(\frac{i}{N}, \frac{i+1}{N}) \times (\frac{j}{N}, \frac{j+1}{N})}(x, y),$$

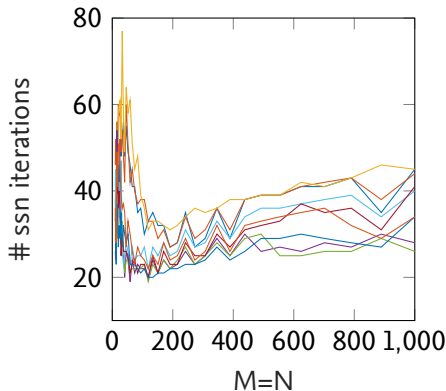
$$\mu^\pm(x) := \sum_{i=0}^{N-1} \mu_i^\pm \chi_{(\frac{i}{N}, \frac{i+1}{N})}(x),$$

$$\alpha^{1/2}(x) := \sum_{i=0}^{N-1} \alpha_i^{1/2} \chi_{(\frac{i}{N}, \frac{i+1}{N})}(x),$$

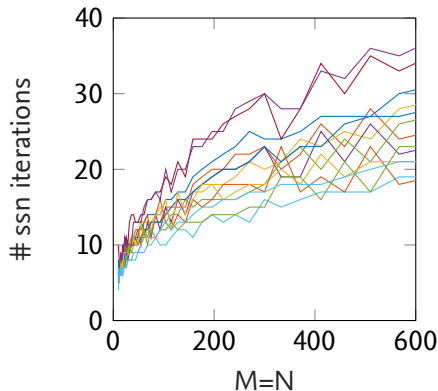
- Compute c_{ij} and μ_i^\pm by exact integrals

Mesh independence - ssn

$\gamma = 0.001$, tolerance 10^{-8}

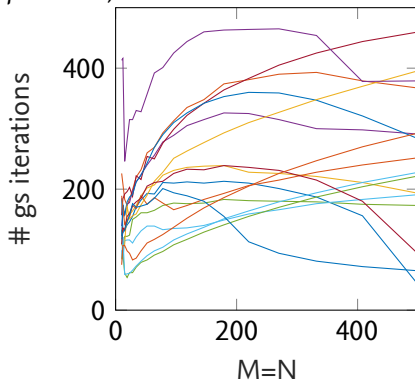


$\gamma = 1/N$, tolerance 10^{-8}

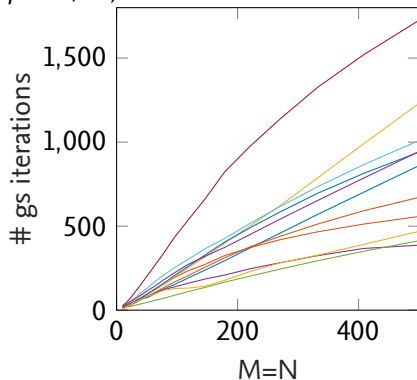


Mesh independence - gs

$\gamma = 0.01$, tolerance 10^{-3}



$\gamma = 1/N$, tolerance 10^{-3}



- **Regularization and duality**
- **Entropic regularization**
- **Quadratic regularization**
- **Algorithms**
- **Illustration**