Kernelized Wasserstein Natural Gradient

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Outline

- General problem and Motivation
- Wasserstein Natural Gradient
- Kernelized Wasserstein Natural Gradient
- Experiments

Motivation: General problem

Given a model ρ_θ of the form:

$$X \sim \rho_\theta \iff X = h_\theta(Z), \qquad Z \sim \nu$$

Consider the learning problem:

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Image

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First order methods

Large scale models $\Rightarrow$ SGD

$$\theta_{t+1} = \theta_t - \gamma \widehat{\nabla \mathcal{L}}(\rho_{\theta_t})$$

First order methods

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Euclidean gradient

First order methods

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- Fast training (using autodiff and GPUs)
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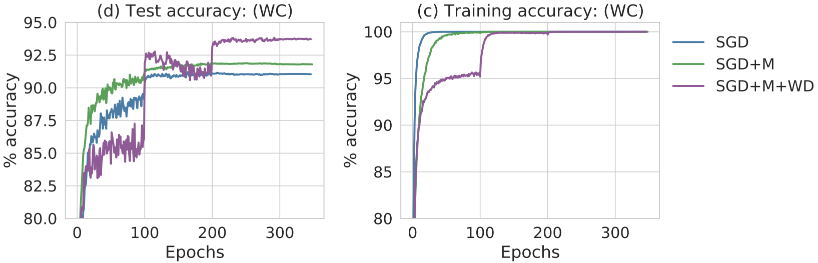
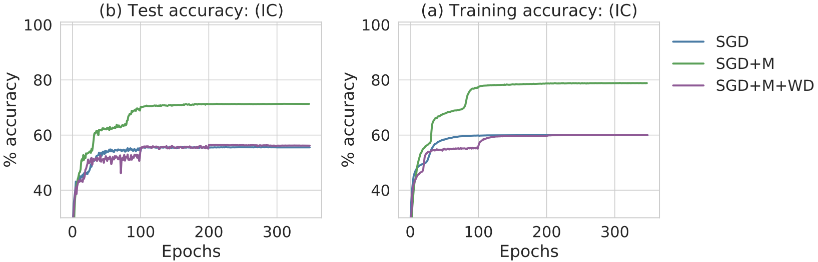


First order methods: Challenges

Large scale models $\Rightarrow$ SGD

$$\theta_{t+1} = \theta_t - \gamma \widehat{\nabla \mathcal{L}}(\rho_{\theta_t})$$

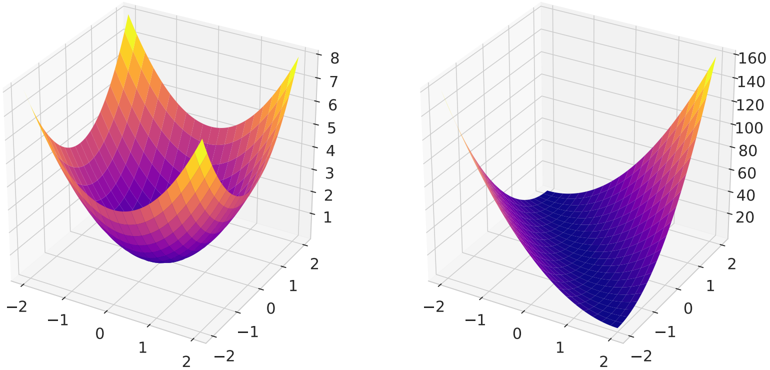
- Sensitive to parametrization
- Can fail miserably when the problem is ill-conditioned



Ill-conditioned problem

Definition (Ill-conditioned problem)

A problem $\min_\theta \mathcal{L}(\rho_\theta)$ is ill-conditioned if the hessian $H\mathcal{L}(\rho_\theta)$ at a local optimum θ^* has a high condition number: $\kappa := \frac{\lambda_{max}}{\lambda_{min}}$



Second order methods

Ill-conditioned problem $\Rightarrow$ Second order methods!!

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Preconditioner

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Euclidean gradient

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- When the density of ρ_θ is available ...
- Can choose $\hat{G}(\theta_t)$ as an estimator of the fisher information matrix:

$$G_F(\theta_t) = \int \nabla \rho_{\theta_t}(x) \nabla \rho_{\theta_t}(x)^\top \rho_\theta(x) \, \mathrm{d}x$$

$$\nabla^F \mathcal{L}(\rho_\theta) := G_F(\theta_t)^{-1} \nabla \mathcal{L}(\rho_{\theta_t})$$

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- $\nabla^F \mathcal{L}(\rho_\theta)$ called the *Fisher Natural gradient*.

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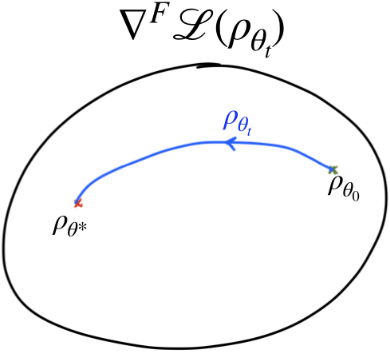
- Robust to parametrization.

Second order methods: Robustness to parametrization



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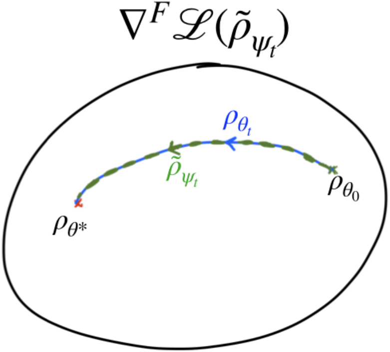

Second order methods: Robustness to parametrization

Fisher Natural gradient descent: $\theta_{t+1} = \theta_t - \gamma \nabla^F \mathcal{L}(\rho_{\theta_t})$

- Have a change of variables $\psi = \Psi(\theta)$ and write $\tilde{\rho}_\psi = \rho_\theta$.

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- Have a change of variables $\psi = \Psi(\theta)$ and write $\tilde{\rho}_\psi = \rho_\theta$.
- Continuous-time limit of the Fisher natural gradient:

$$\dot{\theta}_t = -\nabla^F \mathcal{L}(\rho_{\theta_t}), \quad \theta_0$$
$$\dot{\psi}_t = -\nabla^F \mathcal{L}(\tilde{\rho}_{\psi_t}), \quad \psi_0 = \Psi(\theta_0)$$

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Second order methods: Robustness to parametrization

Fisher Natural gradient descent: $\theta_{t+1} = \theta_t - \gamma \nabla^F \mathcal{L}(\rho_{\theta_t})$

- Have a change of variables $\psi = \Psi(\theta)$ and write $\tilde{\rho}_\psi = \rho_\theta$.
- Continuous-time limit of the Fisher natural gradient:

$$\begin{aligned}\dot{\theta}_t &= -\nabla^F \mathcal{L}(\rho_{\theta_t}), \quad \theta_0 \\ \dot{\psi}_t &= -\nabla^F \mathcal{L}(\tilde{\rho}_{\psi_t}), \quad \psi_0 = \Psi(\theta_0)\end{aligned}$$

- Robustness to parametrization $\Rightarrow \psi_t = \Psi(\theta_t)$
- Doesn't hold for the euclidean gradient in general!

Second order methods: Challenges

Fisher Natural gradient descent: $\theta_{t+1} = \theta_t - \gamma \hat{G}_F(\theta_t)^{-1} \widehat{\nabla \mathcal{L}}(\rho_{\theta_t})$

[1] [Grosse and Martens, 2016, George et al., 2018]

Second order methods: Challenges

Fisher Natural gradient descent: $\theta_{t+1} = \theta_t - \gamma \hat{G}_F(\theta_t)^{-1} \widehat{\nabla \mathcal{L}}(\rho_{\theta_t})$

- Computational: Expensive to store and invert $\hat{G}_F(\theta)$ at every iteration .
- Prior works proposed cheap approximations of $\hat{G}_F(\theta)$ [1].
- Requires to know the density ρ_θ.

[1] [Grosse and Martens, 2016, George et al., 2018]

Contributions

A second order method based on the Wasserstein natural gradient which is:

- Robust to parametrization
- Doesn't require access to the density of the model
- Trades-off between accuracy and computational cost
- Comes with convergence rates.

General recipe for natural gradients

1. Choose a distance/divergence d defined on the model ρ_θ:

$$\min_u \nabla \mathcal{L}(\rho_{\theta_t})^\top u + d(\rho_{\theta_t+u}, \rho_{\theta_t})$$

2. Second order expansion of d at ρ_θ:

$$d(\rho_{\theta_t+u}, \rho_{\theta_t}) \simeq \frac{1}{2} u^\top G(\theta_t) u$$

3. Solve:

$$\min_u \nabla \mathcal{L}(\rho_{\theta_t})^\top u + \frac{1}{2} u^\top G(\theta_t) u$$

Recipe for Fisher natural gradients

1. Choose the *KL* as a divergence

$$\min_u \nabla\mathcal{L}(\rho_{\theta_t})^\top u + KL(\rho_{\theta_t+u}|\rho_{\theta_t})$$

2. Second order expansion of *KL* at ρ_θ:

$$KL(\rho_{\theta_t+u}, \rho_{\theta_t}) \simeq \frac{1}{2}u^\top G_F(\theta_t)u$$

3. Solve:

$$\min_u \nabla\mathcal{L}(\rho_{\theta_t})^\top u + \frac{1}{2}u^\top G_F(\theta_t)u$$

Wasserstein Natural Gradient: Step 1

1. Choose $d(\rho_\theta, \rho_{\theta+u}) = \frac{1}{2} W_2^2(\rho_\theta, \rho_{\theta+u})$

$$\min_u \nabla \mathcal{L}(\rho_{\theta_t})^\top u + \frac{1}{2\lambda} W_2^2(\rho_{\theta_t+u}, \rho_{\theta_t})$$

- Well defined even when ρ_θ doesn't admit a density

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$$W_2^2(\delta_{\theta_1}, \delta_{\theta_2}) = \|\theta_1 - \theta_2\|^2$$

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- W_2 has a nice geometric interpretation:

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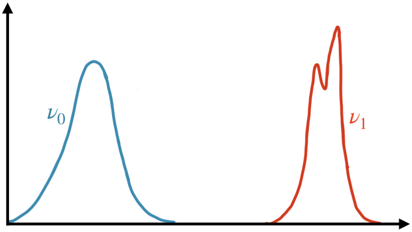

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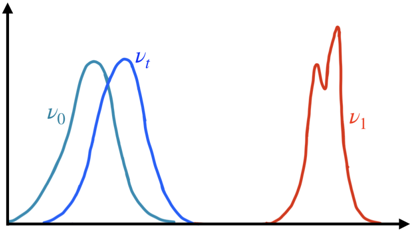

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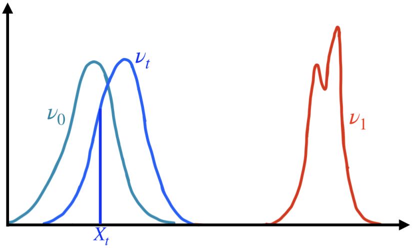

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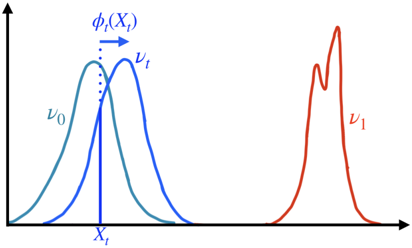

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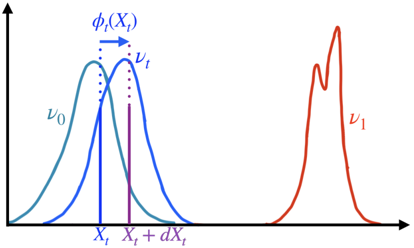

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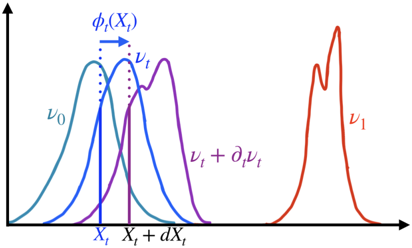

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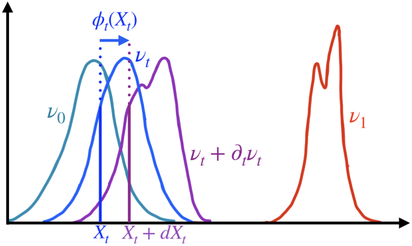
Continuity equation: $\partial_t \nu_t + div(\nu_t \phi_t) = 0$

Boundary conditions: $\nu_0 = p, \quad \nu_1 = q$



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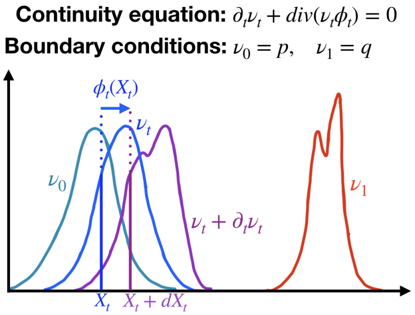

Benamou-Brenier formula[2]: $W_2^2(p, q) := \inf_{(\nu_t, \phi_t)} \int_0^1 \int \|\phi_t(x)\|^2 \, \mathrm{d}\nu_t(x)$

[2] [Benamou and Brenier, 2000]

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Wasserstein Natural Gradient: Step 2

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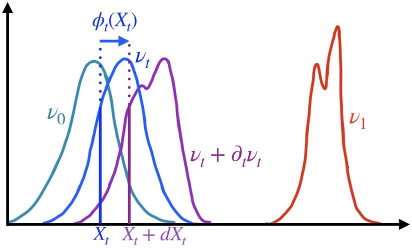

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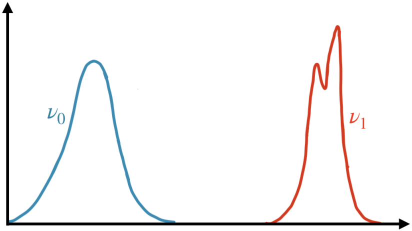

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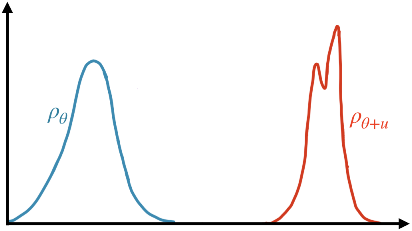

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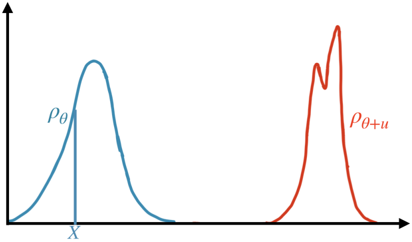

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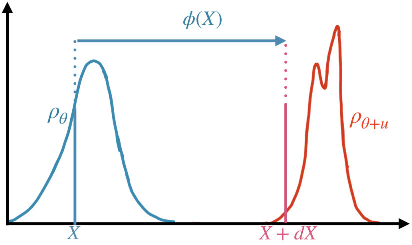

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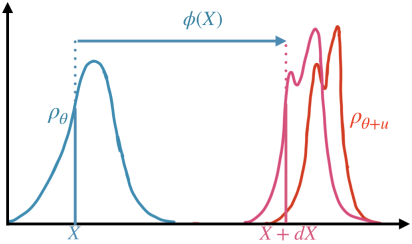

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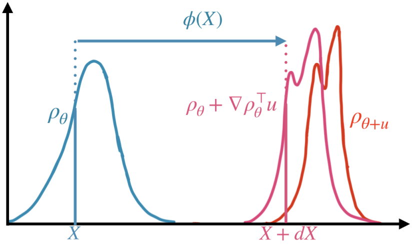

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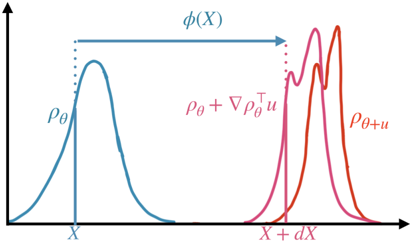
Elliptic equation: $\nabla \rho_\theta^\top u + div(\rho_\theta \phi) = 0$



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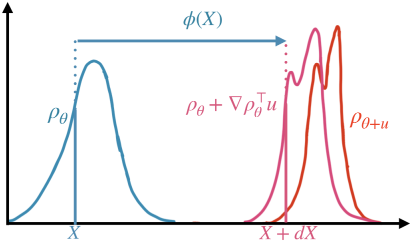
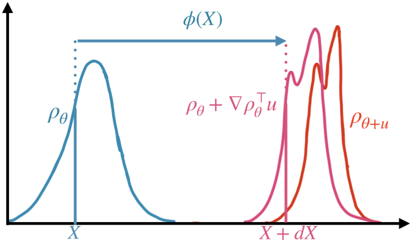


$$\frac{1}{2}W_2^2(\rho_\theta, \rho_{\theta+u}) \simeq \inf_\phi \int \|\phi(x)\|^2 \,\mathrm{d}\rho_\theta(x)$$

Wasserstein Natural Gradient: Step 2

2. Taylor expansion of $\frac{1}{2}W_2^2(\rho_\theta, \rho_{\theta+u})$

Elliptic equation: $\nabla\rho_\theta^\top u + div(\rho_\theta\phi) = 0$



$$W_2^2(\rho_\theta, \rho_{\theta+u}) \simeq \int \|\phi(x)\|^2 \, \mathrm{d}\rho_\theta(x)$$

ϕ constrained to be 'almost' a gradient of a real valued function.

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Wasserstein Natural Gradient: Step 2

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Variational expression for elliptic equations:

$$\nabla\rho_\theta^\top u + div(\rho_\theta \phi) = 0$$

$$\Updownarrow$$

$$\phi \in \arg \sup_{f \in C_c^\infty(\Omega)} \nabla\rho_\theta(f)^\top u - \frac{1}{2}\mathbb{E}_{\rho_\theta}[\|\nabla f(x)\|^2]$$

Wasserstein Natural Gradient: Step 2

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General recipe for natural gradients

1. Choose a distance/divergence d defined on the model ρ_θ:

$$\min_u \nabla \mathcal{L}(\rho_{\theta_t})^\top u + d(\rho_{\theta_t+u}, \rho_{\theta_t})$$

2. Second order expansion of d at ρ_θ:

$$d(\rho_{\theta_t+u}, \rho_{\theta_t}) \simeq \frac{1}{2} u^\top G(\theta_t) u$$

3. Solve:

$$\min_u \nabla \mathcal{L}(\rho_{\theta_t})^\top u + \frac{1}{2} u^\top G(\theta_t) u$$

Wasserstein Natural Gradient: Step 3

3. Solve:

$$\min_{u} \nabla \mathcal{L}(\rho_\theta)^\top u + \sup_{f \in C_c^\infty(\Omega)} \nabla \rho_\theta(f)^\top u - \frac{1}{2}\mathbb{E}_{\rho_\theta}[\|\nabla_x f(x)\|^2]$$

Wasserstein Natural Gradient: Step 3

3. Solve:

$$\min_{u} \sup_{f \in C_c^\infty(\Omega)} \left(\nabla \mathcal{L}(\rho_\theta) + \nabla \rho_\theta(f)\right)^\top u - \frac{1}{2}\mathbb{E}_{\rho_\theta}[\|\nabla_x f(x)\|^2]$$

Wasserstein Natural Gradient: Step 3

3. Solve:

$$\min_{u} \sup_{f \in C_c^\infty(\Omega)} (\overbrace{\nabla \mathcal{L}(\rho_\theta) + \nabla \rho_\theta(f)}^{\mathcal{U}_\theta(f)})^\top u - \frac{1}{2}\mathbb{E}_{\rho_\theta}[\|\nabla_x f(x)\|^2]$$

Wasserstein Natural Gradient: Step 3

3. Solve:

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Kernelized Wasserstein Natural Gradient

$$\min_{u} \sup_{f \in C_c^\infty(\Omega)} \mathcal{U}_\theta(f)^\top u - \frac{1}{2}\mathbb{E}_{\rho_\theta}[\|\nabla_x f(x)\|^2]$$

[3] [Mroueh et al., 2019]

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- Replace $C_c^\infty(\Omega)$ by a nicer space: an RKHS $\mathcal{H}$[3].

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$$\min_{u} \sup_{f \in \mathcal{H}} \mathcal{U}_\theta(f)^\top u - \frac{1}{2}\mathbb{E}_{\rho_\theta}[\|\nabla_x f(x)\|^2] + \frac{1}{2}(\epsilon \|u\|^2 - \lambda \|f\|_{\mathcal{H}}^2)$$

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- Regularization terms $\Rightarrow$ Ensure strong convexity/concavity
- Minimax Theorem[5] $\Rightarrow$ Exchange order of min and sup.
- Optimal descent direction u^* given by:

$$u^* = -\frac{1}{\epsilon}\mathcal{U}_\theta(f^*)$$

$$f^* = \arg\min_{f \in \mathcal{H}} \mathbb{E}_{\rho_\theta}[\|\nabla_x f(x)\|^2] + \frac{1}{\epsilon}\|\mathcal{U}_\theta(f)\|^2 + \lambda \|f\|^2_{\mathcal{H}}$$

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KWNG: Sample based version

Have some i.i.d. samples $(Z_n)_{1 \leq n \leq N}$ from ν and $X_n = h_\theta(Z_n)$:

$$\hat{u}^* = -\frac{1}{\epsilon}\widehat{\mathcal{U}}_\theta(\hat{f}^*),$$

$$\hat{f}^* = \arg\min_{f \in \mathcal{H}} \frac{1}{N}\sum_{n=1}^{N} \|\nabla_x f(X_n)\|^2 + \frac{1}{\epsilon}\|\widehat{\mathcal{U}}_\theta(f)\|^2 + \lambda\|f\|_{\mathcal{H}}^2$$

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- Representer theorem $\Rightarrow$ Optimal solution $\hat{f}^*$ of the form:

$$\hat{f}^* = \sum_{n=1}^{N}\sum_{i=1}^{d} \beta_{n,i}\partial_i k(X_n, .)$$

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- $\beta_{n,i}$ obtained by solving a linear system of size Nd!!

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- Nystrom projections [6] $\Rightarrow$ Reduce computational cost:

$$\hat{f}_M^* = \sum_{m=1}^{M} \alpha_m \partial_{i_m} k(\widetilde{X}_m, .)$$

[6] [Rudi et al., 2015, Sutherland et al., 2017]

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Randomly sampled from $\{1, ..., d\}$

M sub-samples from $(X_i)_{1\leq i\leq N}$

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KWNG: Sample based version

After some further calculations:

$$\widehat{\nabla^W \mathcal{L}(\theta)} = \frac{1}{\epsilon}\left(I - T^\top (TT^\top + \lambda \epsilon K + \epsilon CC^\top)^\dagger T \right) \widehat{\nabla \mathcal{L}(\theta)}$$

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$$C_{m,(n,i)} = \frac{1}{\sqrt{N}} \partial_{i_m} \partial_{i+d} k(\widetilde{X}_m, X_n)$$

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After some further calculations:

$$K_{m,m'} = \partial_{i_m}\partial_{i_{m'}+d} k(\widetilde{X}_m, \widetilde{X}_{m'})$$

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$$C_{m,(n,i)} = \frac{1}{\sqrt{N}}\partial_{i_m}\partial_{i+d}k(\widetilde{X}_m, X_n)$$

$T := \nabla\tau(\theta)$ with $\tau(\theta)_m = \frac{1}{N}\sum_{n=1}^{N}\partial_{i_m}k(\widetilde{X}_m, h_\theta(Z_n))$

Theory: Consistency and convergence rates

Theorem

Let δ be such that $0 \leq \delta \leq 1$. Under smoothness assumptions on the model characterized by some constant $c \geq 0$, for N large enough, $M \sim (dN^{\frac{2+c}{4+c}}\log(N))$, $\lambda \sim N^{\frac{1}{2b+1}}$ and $\epsilon \lesssim N^{-\frac{1}{4+c}}$, it holds with probability at least $1-\delta$ that:

$$\|\widehat{\nabla^W \mathcal{L}(\theta)} - \nabla^W \mathcal{L}(\theta)\|^2 = \mathcal{O}\Big(N^{-\frac{2}{4+c}}\Big).$$

KWNG: Ridgeless version

Additional structure when $\lambda = 0$:

$$\widehat{\nabla^{W}\mathcal{L}(\theta)} = \frac{1}{\epsilon}\left(I - T^{\top}(TT^{\top} + \epsilon CC^{\top})^{\dagger} T\right)\widehat{\nabla\mathcal{L}(\theta)}$$

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$$T_m = \frac{1}{N} \sum_{n=1}^{N} \nabla_\theta \partial_{i_m} k(Y_m, h_\theta(Z_n))$$

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$$\widehat{\nabla^W \mathcal{L}(\theta)} = \frac{1}{\epsilon}\left(I - T^\top (TT^\top + \epsilon CC^\top)^\dagger T\right)\widehat{\nabla \mathcal{L}(\theta)}$$

$$T = CB, \qquad B_n = \nabla_\theta h_\theta(Z_n)$$

KWNG: Ridgeless version

Additional structure when $\lambda = 0$:

$$\widehat{\nabla^W \mathcal{L}(\theta)} = \frac{1}{\epsilon}\left(I - B^\top C^\top (CBB^\top C^\top + \epsilon CC^\top)^\dagger CB\right)\widehat{\nabla \mathcal{L}(\theta)}$$

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where $CC^\top = USU^\top$

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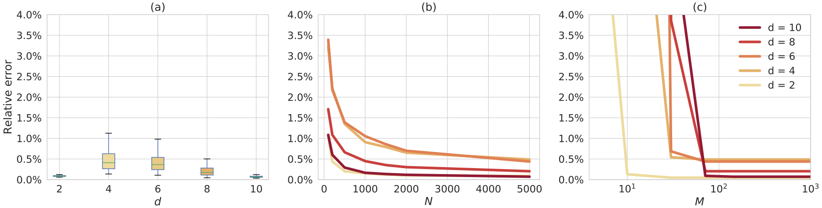
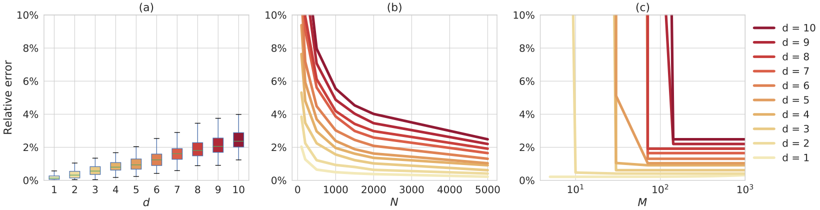
Experimental evaluation: Synthetic models

Hyper-spheres: $X = a + rZ, \qquad Z \sim \mathbb{S}_d$



Experimental evaluation: Synthetic models

$$\text{Gaussians: } X = a + rZ, \qquad Z \sim \mathcal{N}(0, I)$$



Experimental evaluation: Sensitivity to the choice of the kernel

- Gaussian kernel $k(x, y) = \exp(-\frac{\|x-y\|^2}{\sigma})$

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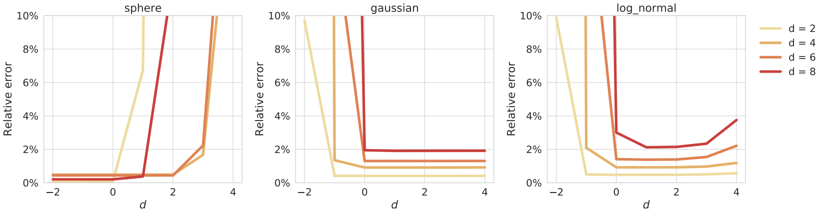

Experimental evaluation: Optimization trajectory

- Gaussian model for ρ_θ
- Loss functional $\mathcal{L}(\rho_\theta) = W_2^2(\rho_\theta, \rho_{\theta^*})$.

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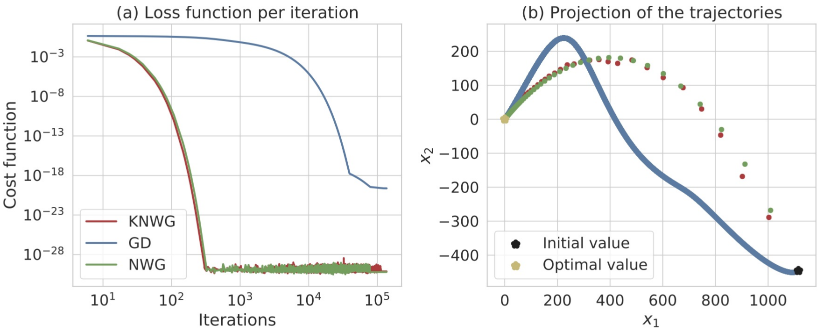

Experimental evaluation: Classification task

Well-conditioned problem:

$$\min_{\theta} \mathcal{L}(\rho_\theta) := \int \ell(h_\theta(Z), Y) \, \mathrm{d}\nu(Z, Y)$$

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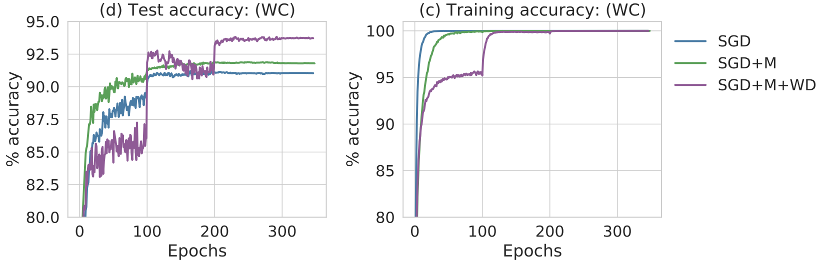

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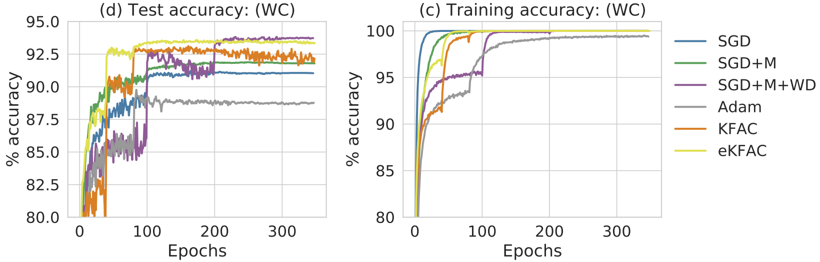

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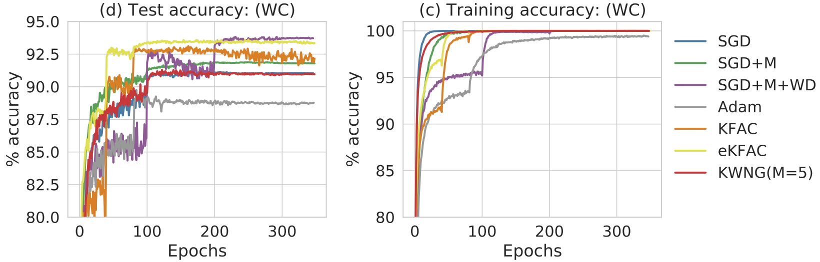

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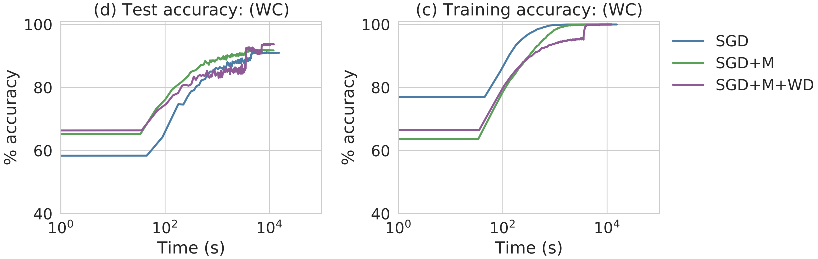

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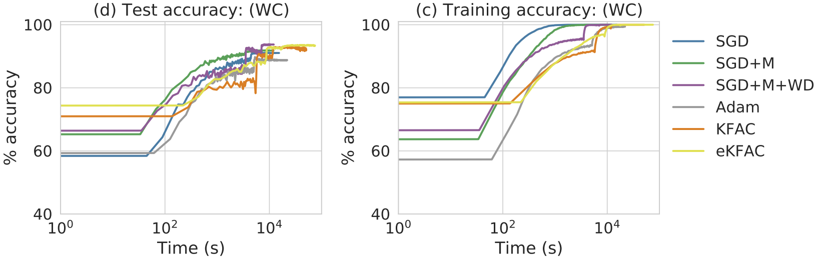

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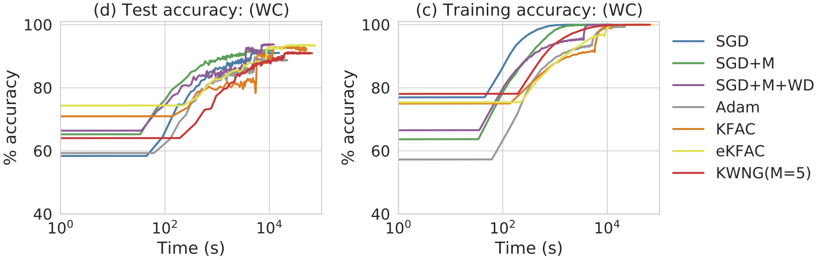

Experimental evaluation: Classification task

Ill-conditioned problem:

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U is a diagonal matrix with $\kappa = 10^7$

Experimental evaluation: Classification task

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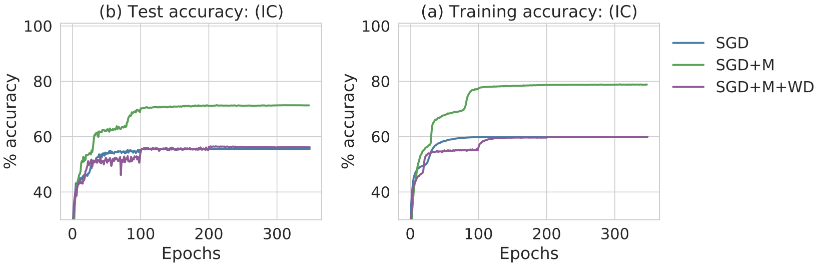
$$\min_{\theta} \mathcal{L}(\rho_\theta) := \int \ell(Uh_\theta(Z), Y)\, \mathrm{d}\nu(Z, Y)$$

U is a diagonal matrix with $\kappa = 10^7$

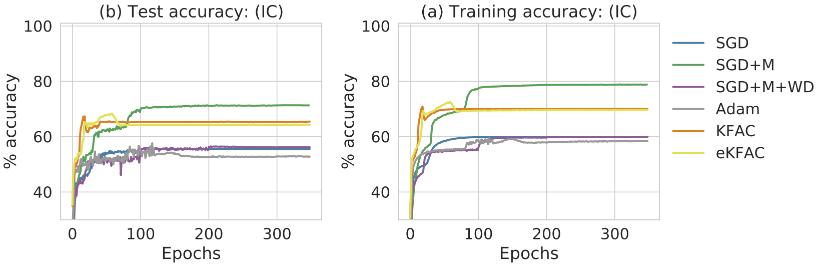


Experimental evaluation: Classification task

Ill-conditioned problem:

$$\min_{\theta} \mathcal{L}(\rho_\theta) := \int \ell(Uh_\theta(Z), Y) \, \mathrm{d}\nu(Z, Y)$$

U is a diagonal matrix with $\kappa = 10^7$



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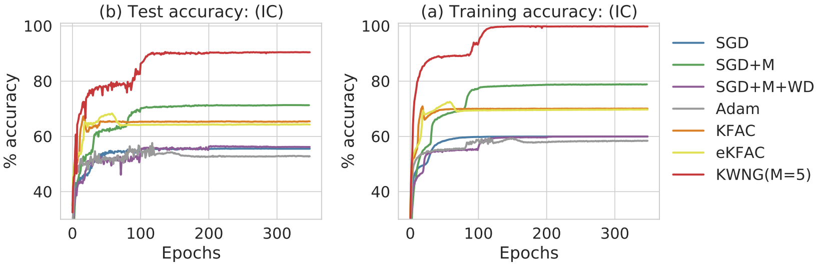

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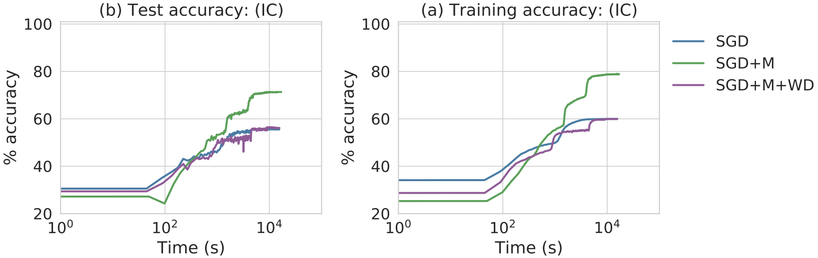

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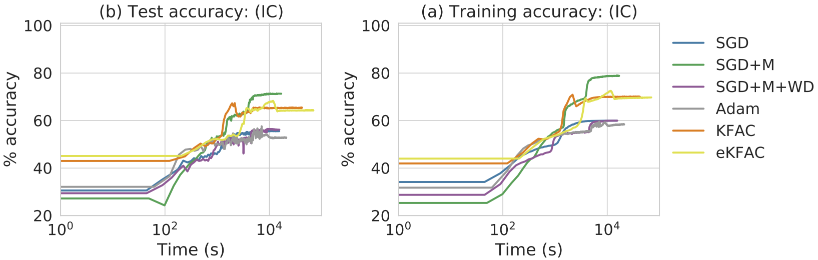

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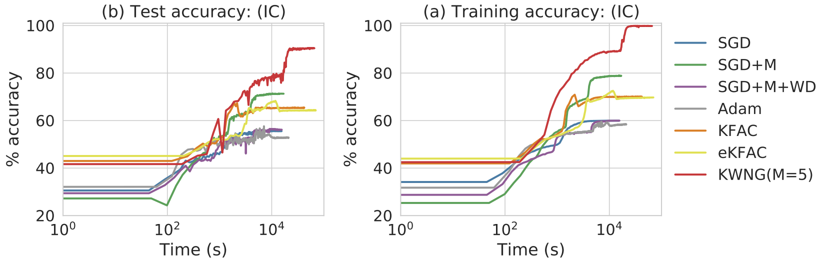


Conclusion

Summary of contributions

- Proposed to use the Wasserstein natural gradient for ill-conditioned problems
- A new algorithm to estimate the Wasserstein natural gradient
- Convergence rate: trade-off between computational complexity and statistical accuracy

Future work:

- Consistency result for the ridgeless version [7]
- Potential application in RL (implicit policy for RL [8])

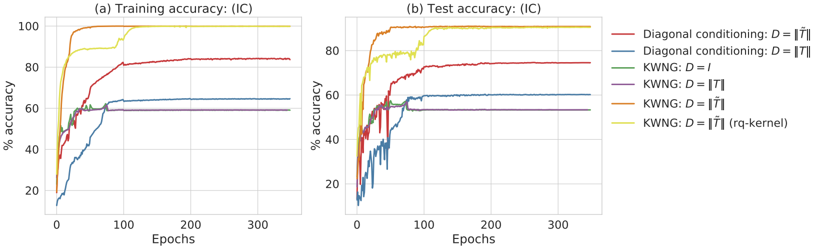
[7] [Liang et al., 2017]

[8] [Tang and Agrawal, 2019]

Thank you !

Ablation study

- Choice of the damping matrix $D(\theta)$
- Choice of the kernel (gaussian vs rational quadratic)



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