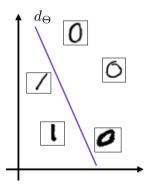
OPTIMISATION METHODS FOR COMPUTATIONAL IMAGING

Chapter 3 - Variational approaches in supervised learning

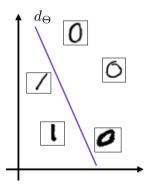
Nelly Pustelnik - ENS Lyon Audrey Repetti - Heriot-Watt University

Journées SMAI-MODE 2022 – Limoges

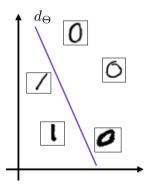
- ▶ Database: $\mathcal{S} = \left\{ (\mathbf{u}_{\ell}, \mathbf{c}_{\ell}) \in \mathcal{H} \times \mathcal{G} \mid \ell \in \{1, \dots, L\} \right\}$ e.g. $\mathbf{u}_{\ell} \in \underbrace{\mathbb{R}^{N}}_{\mathcal{H}}$ image and $\mathbf{c}_{\ell} \in \underbrace{\{-1, 1\}}_{\mathcal{G}}$ classe
- ▶ Goal: Learn a prediction function $d_{\Theta} \colon \mathcal{H} \to \mathcal{G}$



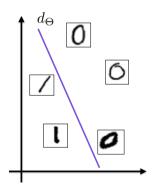
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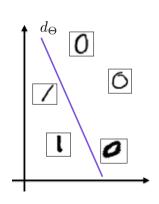
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- ▶ Typical choices for \mathcal{H} :
 - $ightharpoonup \mathcal{H} = \mathbb{R}^N$ for image of size $N = N_1 \times N_2$;
 - $ightharpoonup \mathcal{H} = \mathbb{R}^{N imes M}$ for multivariate images with N samples and M components;

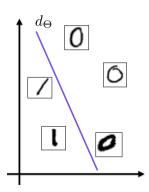


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- ▶ Typical choices for \mathcal{G} :
 - \triangleright $\mathcal{G} = \{-1, +1\}$ for binary classification;
 - $ightharpoonup \mathcal{G} = \{1, \dots, K\}$ for multiclass classification;
 - $ightharpoonup \mathcal{G} = \mathbb{R}$ for regression;
 - $ightharpoonup \mathcal{G} = \mathbb{R}^K$ for multivariate regression;



Example: Supervised learning

▶ Database: $S = \{(u_{\ell}, c_{\ell}) \in \mathcal{H} \times \mathcal{G} \mid \ell \in \{1, \dots, L\}\}$



Example: Supervised learning

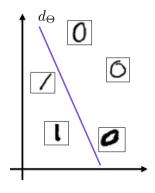
▶ Database: $S = \{(u_{\ell}, c_{\ell}) \in \mathcal{H} \times \mathcal{G} \mid \ell \in \{1, \dots, L\}\}$

examples:
$$u_\ell = 1$$
 and $z_\ell = 2$
$$u_\ell = 8$$
 and $z_\ell = 9$

- $\varphi(\mathbf{u})\colon \mathbb{R}^N \to \mathbb{R}^M$: mapping from the input space onto an arbitrary feature space with M>N
 - ⇒ linearization

examples: convolution networks.

scattering coefficients.



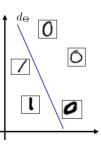
Objective

▶ The predictor relies on K different discriminating functions $D_{\theta^{(k)}} : \mathbb{R}^N \to \mathbb{R}$:

$$\boxed{ \begin{aligned} & \mathsf{D}_{\theta^{(k)}}(\mathbf{u}) = (\mathbf{w}^{(k)})^{\top} \varphi(\mathbf{u}) + b^{(k)} & \text{where} & \theta_k = \{\mathbf{w}^{(k)}, b^{(k)}\} \end{aligned}} \\ \text{with } \phi(\mathbf{u}) = [\varphi(\mathbf{u})^{\top} \mathbf{1}]^{\top} \text{ and } \Theta = [\underbrace{(\mathbf{w}^{(1)})^{\top}, b^{(1)}}_{q(1)}, \dots, \underbrace{(\mathbf{w}^{(K)})^{\top}, b^{(K)}}_{q(K)}]^{\top} }_{q(K)} \end{aligned}}$$

► The predictor selects the class that best matches an observation

$$d_{\Theta}(\mathbf{u}) = \arg \max_{1 \le k \le K} D_{\theta^{(k)}}(\mathbf{u})$$



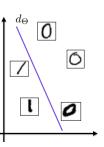
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$$\boxed{ \begin{aligned} & \mathsf{D}_{\theta^{(k)}}(\mathbf{u}) = (\mathbf{w}^{(k)})^\top \varphi(\mathbf{u}) + b^{(k)} & \Leftrightarrow & D_k(\mathbf{u}) = (\theta^{(k)})^\top \phi(\mathbf{u}) \end{aligned} }$$
 with $\phi(\mathbf{u}) = [\varphi(\mathbf{u})^\top 1]^\top$ and $\Theta = [\underbrace{(\mathbf{w}^{(1)})^\top, b^{(1)}}_{(K)}, \dots, \underbrace{(\mathbf{w}^{(K)})^\top, b^{(K)}}_{(K)}]^\top }_{(K)}$

► The predictor selects the class that best matches an observation

$$d_{\Theta}(\mathbf{u}) = \arg \max_{1 \le k \le K} D_{\theta^{(k)}}(\mathbf{u})$$



Objective

▶ Objective of the learning stage: estimate Θ to correctly predict the input-output pair $(u_{\ell}, c_{\ell}) \in \mathcal{S}$ for every $\ell \in \{1, \dots, L\}$,

$$d_{\Theta}(\mathbf{u}) = \arg\max_{1 \leqslant k \leqslant K} D_{\theta^{(k)}}(\mathbf{u}): \qquad \mathbf{c}_{\ell} = \argmax_{1 \leqslant k \leqslant K} (\theta^{(k)})^{\top} \phi(\mathbf{u}_{\ell})$$

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$$\begin{split} d_{\Theta}(\mathbf{u}) &= \arg \max_{1 \leqslant k \leqslant K} D_{\theta^{(k)}}(\mathbf{u}): \qquad \mathbf{c}_{\ell} = \arg \max_{1 \leqslant k \leqslant K} \left(\theta^{(k)}\right)^{\top} \phi(\mathbf{u}_{\ell}) \\ &\Leftrightarrow \quad \max_{k \neq \mathbf{c}_{\ell}} \left(\theta^{(k)} - \theta^{(\mathbf{c}_{\ell})}\right)^{\top} \phi(\mathbf{u}_{\ell}) < 0 \end{split}$$

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 [relax the strict ineqality]
$$\Leftrightarrow \quad \max_{k\neq \mathbf{c}_{\ell}} (\theta^{(k)} - \theta^{(\mathbf{c}_{\ell})})^{\top} \phi(\mathbf{u}_{\ell}) \leqslant -\mu_{\ell} \end{split}$$

with $\mu_{\ell} > 0$

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with $\mu_{\ell} > 0$ and $\zeta_{\ell} \geqslant 0$.

Multiclass SVM

$$\begin{aligned} & \underset{(\Theta,\xi) \in \mathbb{R}^{(M+1)K} \times \mathbb{R}^L}{\text{minimise}} & & \sum_{k=1}^K \|\theta^{(k)}\|_2^2 + \lambda \sum_{\ell=1}^L \xi^{(\ell)} \quad \text{subj. to} \\ & & & \begin{cases} (\forall \ell \in \{1,...,L\}) & \max_{k \neq c_\ell} \ (\theta^{(k)} - \theta^{(c_\ell)})^\top \phi(\mathbf{u}_\ell) \leqslant \xi_\ell - \mu_\ell, \\ (\forall \ell \in \{1,...,L\}) & & \xi_\ell \geqslant 0, \end{cases} \end{aligned}$$

or equivalently

$$\underset{\Theta \in \mathbb{R}^{(M+1)K}}{\text{minimize}} \sum_{k=1}^{K} \|\theta^{(k)}\|_{2}^{2} + \lambda \sum_{\ell=1}^{L} \max \left\{0, \mu_{\ell} + \max_{k \neq c_{\ell}} \left(\theta^{(k)} - \theta^{(c_{\ell})}\right)^{\top} \phi(u_{\ell})\right\}.$$

Alternative to standard SVM data-term

$$h(\Theta) = \sum_{\ell=1}^{L} \max \left\{ 0, \mu_{\ell} + \max_{k \neq c_{\ell}} \left(\theta^{(k)} - \theta^{(c_{\ell})} \right)^{\top} \phi(\mathbf{u}_{\ell}) \right\}.$$

- ► Multiclass SVM [Blondel et al.] $h(\Theta) = \sum_{\ell=1}^{L} \sum_{k \neq c_{\ell}} \left(\max \left\{ 0, \mu_{\ell} + (\theta^{(k)} \theta^{(c_{\ell})})^{\top} \phi(\mathbf{u}_{\ell}) \right\} \right)^{2}$
- ► Multinomial logistic regression [Krishnapuram et al.] $h(\Theta) = \sum_{\ell=1}^{L} \log \left(1 + \sum_{k \neq c_{\ell}} \exp \left\{ \mu_{\ell} + (\theta^{(k)} \theta^{(c_{\ell})})^{\top} \phi(\mathbf{u}_{\ell}) \right\} \right)$
- "one-vs-all" strategy binary SVM [Laporte et al.] with \widetilde{c}_ℓ being equal to 1 if $c_\ell = k$, and -1 otherwise $h(\Theta) = \sum_{\ell=1}^L \left(\max\left\{0, \mu_\ell + \widetilde{c}_\ell \; (\theta^{(k)})^\top \phi(\mathbf{u}_\ell)^\top \right\} \right)^2$

- ▶ Database: $S = \{(u_{\ell}, c_{\ell}) \in \mathcal{H} \times \mathcal{G} \mid \ell \in \{1, ..., L\}\}$
- ▶ Goal: Learn a prediction function $d_{\Theta} \colon \mathcal{H} \to \mathcal{G}$
- Learning procedure relies on a minimization problem:

minimise
$$\underbrace{\frac{1}{L} \sum_{\ell=1}^{L} F(\mathbf{c}_{\ell}, d_{\Theta}(\mathbf{u}_{\ell}))}_{\text{Data-term}} + \lambda \underbrace{R(\Theta)}_{\text{Prior}}$$

Example: Supervised learning

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► Linear predictor: $d_{\Theta}(u) = \Theta^{\top}u$

$$\begin{array}{ll} \odot \ \mbox{Ridge regression:} & \min \limits_{\Theta \in \mathcal{H}} & \frac{1}{L} \sum_{\ell=1}^{L} (c_{\ell} - \Theta^{\top} \mathbf{u}_{\ell})^{2} + \lambda \|\Theta\|_{2}^{2} \\ \odot \ \mbox{Logistic classification:} & \min \limits_{\Theta \in \mathcal{H}} & \frac{1}{L} \sum_{\ell=1}^{L} \log \Big(1 + e^{-c_{\ell} \Theta^{\top} \mathbf{u}_{\ell}} \Big) + \lambda \|\Theta\|_{2}^{2} \\ \end{array}$$

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- ► Linear predictor: $d_{\Theta}(u) = \Theta^{\top}u$
 - \Rightarrow can be extended to $d_{\Theta}(u) = \Theta^{\top} \phi(u)$ (e.g. ϕ scattering transform)
 - \odot Ridge regression: $\underset{\Theta \in \mathcal{H}}{\operatorname{minimise}} \quad \frac{1}{L} \sum_{\ell=1}^{L} (\mathbf{c}_{\ell} \Theta^{\top} \mathbf{u}_{\ell})^{2} + \lambda \|\Theta\|_{2}^{2}$
 - $\odot \text{ Logistic classification:} \quad \underset{\Theta \in \mathcal{H}}{\text{minimise}} \quad \tfrac{1}{L} \sum_{\ell=1}^L \log \Bigl(1 + e^{-c_\ell \Theta^\top u_\ell} \Bigr) + \lambda \|\Theta\|_2^2$

- ▶ Database: $S = \{(\mathbf{u}_{\ell}, \mathbf{c}_{\ell}) \in \mathcal{H} \times \mathcal{G} \mid \ell \in \{1, \dots, L\}\}$
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► Linear predictor:
$$d_{\Theta}(\mathbf{u}) = \Theta^{\top}\mathbf{u}$$

- ⊙ Sparse regression:
- $\begin{aligned} & \underset{\Theta \in \mathcal{H}}{\text{minimise}} & & \frac{1}{L} \sum_{\ell=1}^{L} (c_{\ell} \Theta^{\top} u_{\ell})^{2} + \lambda \|\Theta\|_{1} \\ & \underset{\Theta \in \mathcal{H}}{\text{minimise}} & & \frac{1}{L} \sum_{\ell=1}^{L} \log \Big(1 + e^{-c_{\ell} \Theta^{\top} u_{\ell}} \Big) + \lambda \|\Theta\|_{1} \end{aligned}$ • Sparse logistic classification:
- $\underset{\Theta \in \mathcal{H}}{\text{minimise}} \ \ \frac{1}{L} \sum_{\ell=1}^{L} \max \left(0, 1 c_{\ell} \Theta^{\top} u_{\ell}\right) + \lambda \|\Theta\|_{2}^{2}$ SVM classification:

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$$\underset{\Theta}{\text{minimise}} \ \underbrace{\frac{1}{L} \sum_{\ell=1}^{L} F(\mathbf{c}_{\ell}, d_{\Theta}(\mathbf{u}_{\ell}))}_{\text{Data-term}} \ + \ \lambda \underbrace{R(\Theta)}_{\text{Prior}}$$

- ► Linear predictor: $d_{\Theta}(\mathbf{u}) = \Theta^{\mathsf{T}}\mathbf{u}$ \Rightarrow Convex non-smooth problems
 - \odot Sparse regression: $\min_{\Theta \in \mathcal{H}} \frac{1}{L} \sum_{\ell=1}^{L} (c_{\ell} \Theta^{\top} u_{\ell})^2 + \lambda \|\Theta\|_1$
 - \odot Sparse logistic classification: $\min_{\Theta \in \mathcal{U}} \frac{1}{L} \sum_{\ell=1}^{L} \log \left(1 + e^{-c_{\ell} \Theta^{\top} u_{\ell}}\right) + \lambda \|\Theta\|_{1}$
 - \odot SVM classification: $\min_{\Theta \in \mathcal{H}} \frac{1}{L} \sum_{\ell=1}^{L} \max \left(0, 1 c_{\ell} \Theta^{\top} u_{\ell}\right) + \lambda \|\Theta\|_{2}^{2}$

Experiment 2

MNIST database

- $\bigstar N = 28 \times 28$
- ◆ K = 10
- ♦ 60000 training images
- ♦ 10000 test images

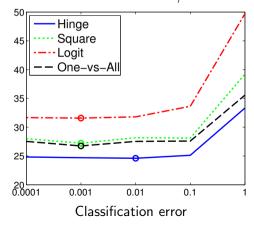
Scattering convolution network [Bruna & Mallat, 2013]

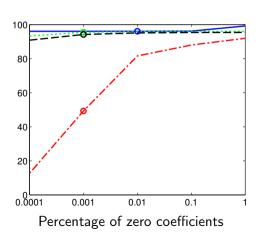
- ♦ 2 wavelet layers
- ♦ 4 scales DWT
- **♦** Feature mapping: ϕ : $\mathbb{R}^{28 \times 28} \mapsto \mathbb{R}^{14 \times 14 \times 81}$

SMAI-MODE 10/12

Experiment 2

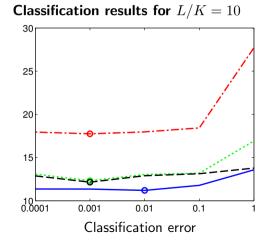
Classification results for L/K=3

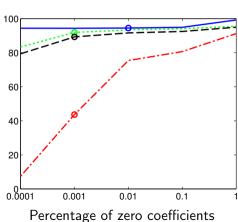




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Experiment 2





SMAI-MODE 11/12

Example: Supervised learning

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► Neural network predictor:

$$d_{\Theta}(\mathbf{u}) = \eta^{[K]}(W^{[K]}\eta^{[K-1]}(W^{[K-1]}\dots\eta^{[2]}(W^{[2]}\eta^{[1]}(W^{[1]}u))\dots))$$

- \odot Linear operators: $W^{[1]}, W^{[2]}, \ldots, W^{[K]}$
- \odot Activation functions: $\eta^{[1]}, \eta^{[2]}, \ldots, \eta^{[K]}$

SMAI-MODE 11/12

Example: Supervised learning

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► Neural network predictor: ⇒ Non-convex problems

$$d_{\Theta}(\mathbf{u}) = \eta^{[K]}(W^{[K]}\eta^{[K-1]}(W^{[K-1]}\dots\eta^{[2]}(W^{[2]}\eta^{[1]}(W^{[1]}u))\dots))$$

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Proximal algorithms

General objective function

Find
$$\widehat{y} \in \operatorname*{Argmin}_{y \in \mathcal{H}} \sum_{j=1}^{J} f_j(H_j y)$$

where H_j linear operator from \mathcal{H} to \mathcal{G}_j and $(f_j)_{1 \leq j \leq J}$ belong to the class of convex functions, l.s.c., and proper from \mathcal{G}_j to $]-\infty,+\infty]$.

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► Numerous proximal algorithms

Bauschke-Combettes, 2017

- Forward-Backward
- Douglas-Rachford
- ADMM
- Primal-dual ...



Number of articles per year on Google scholar containing "proximal algorithms" since 1997.