Exponentially Weighted Aggregate with the Laplace Prior

Joint work with Edwin Grappin and Quentin Paris

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Estimation of sparse vectors and matrices

Problem formulation

Regression model and prediction

- **Regression model:** we observe n feature-label pairs $(\boldsymbol{X}_i, Y_i) \in \mathbb{R}^p \times \mathbb{R}$ such that

$$Y_i = \boldsymbol{X}_i^\top \boldsymbol{\beta}^* + \xi_i \quad \Leftrightarrow \quad \boldsymbol{Y} = \mathbf{X}\boldsymbol{\beta}^* + \boldsymbol{\xi}$$

  with $\boldsymbol{\xi} = [\xi_1, \ldots, \xi_n] \sim \mathcal{N}_n(\mathbf{0}, \sigma^2 \mathbf{I}_n)$.

- **Regression vector:** The p-dimensional vector $\boldsymbol{\beta}^*$ is unknown.
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- **Prediction loss:** The quality of an estimator $\widehat{\beta}_n$ is measured by

$$\ell_n(\widehat{\boldsymbol{\beta}}_n, \boldsymbol{\beta}^*) = \frac{1}{n}\|\mathbf{X}(\widehat{\boldsymbol{\beta}}_n - \boldsymbol{\beta}^*)\|_2^2 = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{X}_i^\top \widehat{\boldsymbol{\beta}}_n - \boldsymbol{X}_i^\top \boldsymbol{\beta}^*)^2.$$

- **Curse of dimensionality:** OLS behaves poorly if $n \ll p$.

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Sparsity, approximate sparsity and mis-specification

- **s-sparsity:** When p is large, to make consistent estimation of $\boldsymbol{\beta}^*$ feasible, we assume that

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- **δ-approximate s-sparsity:** for some $\bar{\boldsymbol{\beta}} \in \mathbb{R}^p$,

$$\|\bar{\boldsymbol{\beta}}\|_0 \leq s \quad \text{and} \quad \|\bar{\boldsymbol{\beta}} - \boldsymbol{\beta}^*\|_1 \leq \delta.$$

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- **Mis-specification:** $\boldsymbol{\beta}^*$ is neither sparse nor approximately sparse, but there is an approximately sparse vector $\bar{\boldsymbol{\beta}}$ with a small prediction error $\ell_n(\bar{\boldsymbol{\beta}}, \boldsymbol{\beta}^*)$.

  This $\bar{\boldsymbol{\beta}}$ is the (δ-approximately s-sparse) oracle.
  Can we mimic the oracle ?

Low-rank, approximate low-rank and mis-specification

- The role of sparsity in matrix estimation problems is most often played by the low rank assumption (sparsity of the spectrum).
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Lasso, Bayesian Lasso and EWA

Estimating sparse vectors by the lasso

- **Regression model, prediction loss:** $n \times p$ matrix $\mathbf{X}$ and $\boldsymbol{Y} \in \mathbb{R}^p$ such that

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- **Lasso [Tibshirani 96]:** ℓ_1 penalized least squares

$$\widehat{\boldsymbol{\beta}}^{\mathrm{L}} \in \operatorname*{arg\,min}_{\boldsymbol{\beta} \in \mathbb{R}^p} \left\{ {}^1\!/_{2n} \|\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 + \lambda \|\boldsymbol{\beta}\|_1 . \right\}$$

- Fast computation by LARS or convex programming.

Prediction accuracy of the lasso

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- **Oracle inequality** [Koltchinskii, Lounici and Tsybakov 2011; D., Hebiri and Lederer 2017]: if $\lambda \geq \sqrt{({}^2\!/_n) \log(p/\alpha)}$ then with probability $\geq 1 - \alpha$

$$\ell_n(\widehat{\boldsymbol{\beta}}^{\mathrm{L}}, \boldsymbol{\beta}^*) \leq \ell_n(\bar{\boldsymbol{\beta}}, \boldsymbol{\beta}^*) + \min_J \left\{ 4\lambda \|\bar{\boldsymbol{\beta}}_{J^c}\|_1 + ({}^3\!/_\kappa)\lambda^2 |J| \right\}.$$

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- **Fast rate:** For getting the fast rate $({}^s\!/_n) \log(p)$, we do need the restricted eigenvalue (RE) condition $\kappa > 0$ [Bickel, Ritov, Tsybakov (2009), D., Hebiri and Lederer 2017].

Estimating sparse vectors by the Bayesian lasso

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- **Posterior** density is then

$$\widehat{\pi}_n(\boldsymbol{\beta}) \propto \exp\Big\{ - (1/2\sigma^2) \|\boldsymbol{Y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 - (n\lambda/\sigma^2) \|\boldsymbol{\beta}\|_1 \Big\}.$$

- **Bayesian lasso** [Park and Casella 2008]: posterior mean

$$\widehat{\boldsymbol{\beta}}^{\mathrm{BL}} = \int \boldsymbol{\beta}\, \widehat{\pi}_n(d\boldsymbol{\beta}).$$

- **Remark:** the MAP coincides with the lasso.

Properties of the Bayesian lasso

- **Pros**
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  - No matter the λ, $\widehat{\boldsymbol{\beta}}^{\mathrm{BL}}$ does not converge at the optimal rate [Castillo, Schmidt-Hieber and van der Vaart 2015], $\forall C > 0$

$$\widehat{\pi}_n\left(\left\{\boldsymbol{\beta} : \ell_n(\boldsymbol{\beta}, \boldsymbol{\beta}^*) \leq \frac{Cs\log p}{n}\right\}\right) \xrightarrow[n\to\infty]{} 0, \qquad \text{a.s.}$$

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One solution is to change the prior (spike-and-slab) but then the computation becomes NP-hard.

EWA and PAC-Bayes approach

- **Pseudo-posterior:** for some prior π_0, define

$$\widehat{\pi}_{n,\tau} \in \arg\min_{p(\cdot)} \left\{ \int_{\mathbb{R}^p} \frac{1}{2n} \|\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta}\|_2^2 \, p(d\boldsymbol{\beta}) + \tau \mathcal{K}(p\|\pi_0) \right\},$$

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- **Explicit form:**

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- **Exponentially weighted aggregate (EWA):**

$$\widehat{\boldsymbol{\beta}}_{\tau}^{\mathrm{EWA}} = \int_{\mathbb{R}^p} \boldsymbol{\beta} \, \widehat{\pi}_{n,\tau}(d\boldsymbol{\beta}).$$

- If $\tau = \sigma^2/n$, then the EWA coincides with the Bayes estimator.

EWA and the Laplace prior

- One can used a scaled Laplace prior in the EWA.
- The resulting (suitably re-parameterized) pseudo-posterior is

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- This estimator interpolates the lasso and the Bayesian lasso:
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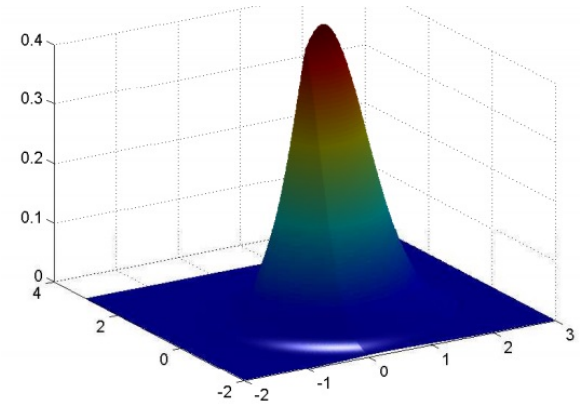
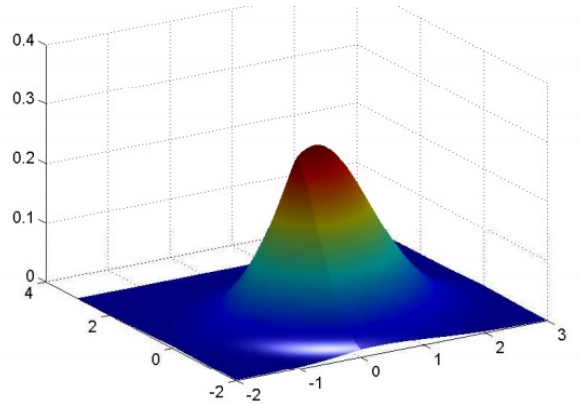
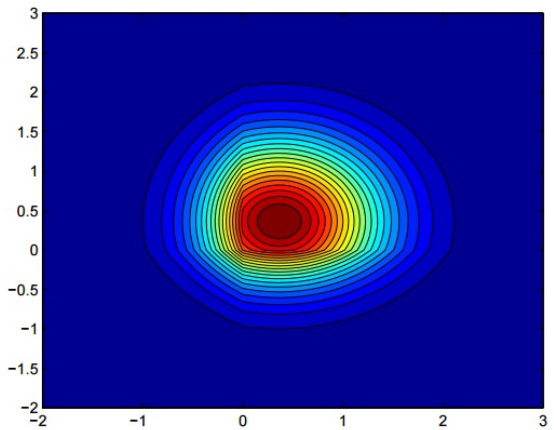
- **Questions:**
  - Is the EWA suitable for prediction under the sparsity scenario? If it is, what is the range of temperature τ providing good prediction accuracy?
  - How do the statistical properties of the EWA compare with those of the lasso?

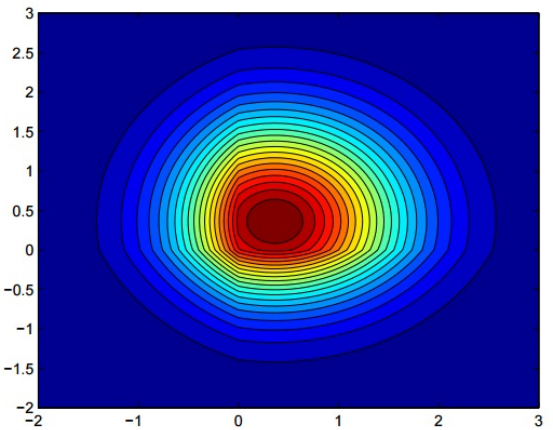
EWA and the Laplace prior







$\tau = 0.5$



$\tau = 0.8$

Main results

Oracle inequality for the EWA

Theorem 1

Assume that $\boldsymbol{\xi} \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_n)$ and that $\max_{j \in [p]} {}^1\!/_n \|\boldsymbol{x}^j\|_2^2 \leq 1$. Suppose, in addition, that $\lambda \geq 2\sigma\sqrt{({}^2\!/_n)\log(p/\alpha)}$, for some $\alpha \in (0,1)$. Then, with probability at least $1-\alpha$,

$$\ell_n(\widehat{\boldsymbol{\beta}}_\tau^{\mathrm{EWA}}, \boldsymbol{\beta}^*) \leq \min_{J \subset [p]} \left\{ \ell_n(\bar{\boldsymbol{\beta}}, \boldsymbol{\beta}^*) + 4\lambda \|\bar{\boldsymbol{\beta}}_{J^c}\|_1 + \frac{9\lambda^2 |J|}{4\kappa} \right\} + 2p\tau. \quad (1)$$

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Remarks

1. This is a sharp OI, since the leading constant is 1.
2. This risk bound extends the risk bounds available for the lasso [D., Hebiri and Lederer 2017] to the EWA.
3. The last term in the above risk bound, $2p\tau$, reflects the influence of the temperature τ; if $\tau = \sigma^2/(pn)$ this term is negligible.

Pseudo-posetrior concentration

Theorem 2

Assume that $\boldsymbol{\xi} \sim \mathcal{N}(0, \sigma^2 \mathbf{I}_n)$ and that $\max_{j \in [p]} {}^1\!/_n \|\boldsymbol{x}^j\|_2^2 \leq 1$. Assume that $\lambda \geq 2\sigma\sqrt{({}^2\!/_n)\log({}^p\!/_\alpha)}$. Then, with probability at least $1-\alpha$ on data, the pseudo-posterior $\widehat{\pi}_{n,\tau}$ with the Laplace prior puts at least a weight $1 - 2e^{-\sqrt{p}/16}$ on the set

$$\left\{ \boldsymbol{\beta} : \ell_n(\boldsymbol{\beta}, \boldsymbol{\beta}^*) \leq \min_{J \subset [p]} \left(\ell_n(\bar{\boldsymbol{\beta}}, \boldsymbol{\beta}^*) + 4\lambda \|\bar{\boldsymbol{\beta}}_{J^c}\|_1 + \frac{9\lambda^2 |J|}{2\kappa} \right) + 8p\tau \right\}.$$

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Remarks

1. A random sample from $\widehat{\pi}_{n,\tau}$ is almost as good as the pseudo-posterior mean.
2. It might be easier to sample from $\widehat{\pi}_{n,\tau}$ rather than to compute the pseudo-posterior mean.
3. The method is sparsity-adaptive.

Main idea of the proof of Theorem 1

- Let $V_n(\boldsymbol{\beta})$ be the penalized log-likelihood.
- The lasso estimator and the EWA are

$$\widehat{\boldsymbol{\beta}}^{\mathrm{L}} \in \arg\min_{\boldsymbol{\beta}} V_n(\boldsymbol{\beta}), \qquad \widehat{\boldsymbol{\beta}}_{\tau}^{\mathrm{EWA}} = \frac{1}{C} \int_{\mathbb{R}^p} \boldsymbol{\beta} \, \exp\{-V_n(\boldsymbol{\beta})/\tau\} \, d\boldsymbol{\beta}.$$

- **Known:** the proof of the OI for the lasso builds on

$$\nabla V_n(\widehat{\boldsymbol{\beta}}^{\mathrm{L}}) = \mathbf{0} \qquad [\text{rigorously } \mathbf{0} \in \partial V_n(\widehat{\boldsymbol{\beta}}^{\mathrm{L}})].$$

- **New:** the analogue of the above condition is:

$$\int_{\mathbb{R}^p} \nabla V_n(\boldsymbol{\beta}) \, \widehat{\pi}_n(\boldsymbol{\beta}) \, d\boldsymbol{\beta} = C \int_{\mathbb{R}^p} \nabla \big[\widehat{\pi}_n(\boldsymbol{\beta})\big] \, d\boldsymbol{\beta} = \mathbf{0}.$$

- Additionally, for every $j \in [p]$, $\displaystyle\int_{\mathbb{R}^p} \nabla \big[\beta_j \widehat{\pi}_n(\boldsymbol{\beta})\big] \, d\boldsymbol{\beta} = \mathbf{0}$.

Main ingredient of the proof of Theorem 2

Magic theorem [Bobkov and Madiman 2011]

Let $\widehat{\pi}_n(\boldsymbol{u}) \propto \exp(-V_n(\boldsymbol{u})/\tau)$ be a log-concave probability density[a] and let $\boldsymbol{\beta}$ be a random vector drawn from $\widehat{\pi}_n$. Then, for any $t > 0$, the inequality

$$V_n(\boldsymbol{\beta}) \le \int_{\mathbb{R}^p} V_n(\boldsymbol{u})\, \widehat{\pi}_n(\boldsymbol{u})\, \mathrm{d}\boldsymbol{u} + \sqrt{p}\tau t$$

holds with probability at least $1 - 2e^{-t/16}$.

[a] This means that V_n is a convex function.

Lasso versus EWA

- Both are computable in polynomial time, but the lasso computation is faster.
- Theoretical guarantees for the lasso and the EWA are equally good, provided that the temperature τ is small.
- The EWA is less sensitive to the variations in the data.
  - The SURE for the lasso [Tibshirani and Taylor, 2012] is given by

$$\widehat{R}^{\mathrm{L}}(\lambda) = \frac{1}{n}\|\boldsymbol{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}^{\mathrm{L}}(\lambda)\|_2^2 - \sigma^2 + \frac{2\sigma^2}{n}\mathsf{rank}(\mathbf{X}_{\mathcal{A}(\lambda)}),$$

    where $\mathcal{A}(\lambda) = \{j \in [p] : \beta_j^{\mathrm{L}}(\lambda) \neq 0\}$.
    This function is even not continuous.
  - The SURE for the EWA is

$$\widehat{R}^{\mathrm{EWA}}(\lambda) = \frac{1}{n}\|\boldsymbol{y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_{\tau}^{\mathrm{EWA}}(\lambda)\|_2^2 - \sigma^2 + \frac{2\sigma^2}{n^2\tau}\mathbf{Var}_{\widehat{\pi}_n(\lambda)}[\mathbf{X}\boldsymbol{\beta}].$$

OI for the EWA in the matrix trace regression

Recall that the ℓ_1-norm $\|\beta\|_1$ is replaced by the nuclear norm $\|\mathbf{B}\|_1$.

Let us define $\upsilon_{\mathbf{X}} = \left\| \frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i \mathbf{X}_i^\top \right\|^{1/2} \bigvee \left\| \frac{1}{n} \sum_{i=1}^{n} \mathbf{X}_i^\top \mathbf{X}_i \right\|^{1/2}$.

Theorem 3

Assume that $\lambda \geq 2\sigma\upsilon_{\mathbf{X}}\{2/n \log((m_1+m_2)/\alpha)\}^{1/2}$, for some $\alpha \in (0,1)$. Then, with probability at least $1-\alpha$, the matrix $\widehat{\mathbf{B}}^{\mathrm{EWA}}$ satisfies

$$\ell_n(\widehat{\mathbf{B}}^{\mathrm{EWA}}, \mathbf{B}^*) \leq \min_J \left\{ \ell_n(\bar{\mathbf{B}}, \mathbf{B}^*) + 4\lambda \|\mathcal{P}_{J^c}(\bar{\mathbf{B}})\|_1 + \frac{9\lambda^2 |J|}{4\kappa} \right\} + 2m_1 m_2 \tau,$$

where the min is over all subsets $J \subset [\mathrm{rank}(\bar{\mathbf{B}})]$.

We have a similar result on pseudo-posterior concentration.

Summary and outlook

- We have obtained nonasymptotic risk bounds for the EWA with Laplace prior, both in vector- and matrix-regression models.
- If the temperature $\tau \leq \sigma^2/(np)$, then the EWA is as good as the lasso.
- The pseudo-posterior has nice concentration properties.
- This can be extended to random design, but more technical and additional terms appear.
- Current/future work:
  - Computational complexity of drawing from $\widehat{\pi}_{n,\tau}$.
  - Assessing the sensitivity of the EWA as compared to the lasso.


thank you
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спасибо
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kop khun krap
go raibh maith agat
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terima kasih
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dakujem
takk
taiku
tapadh leat
мерси
감사합니다
ありがとう
ευχαριστώ
sagolun
hvala
mauruuru
dank je
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Баярлалаа
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mèsi
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diolch
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shukriya
xièxie
najis tuke
kam sah hamnida
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