

# Should penalized least squares regression be interpreted as Maximum A Posteriori estimation?

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## Abstract

Penalized least squares regression is often used for signal denoising and inverse problems, and is commonly interpreted in a Bayesian framework as a Maximum A Posteriori (MAP) estimator, the penalty function being the negative logarithm of the prior. For example, the widely used quadratic program (with an  $\ell^1$  penalty) associated to the LASSO / Basis Pursuit Denoising is very often considered as the MAP under a Laplacian prior. The objective of this paper is to highlight the fact that, while this is *one* possible Bayesian interpretation, there can be other equally acceptable Bayesian interpretations. Therefore, solving a penalized least squares regression problem with penalty  $\varphi(x)$  should not necessarily be interpreted as assuming a prior  $C \cdot \exp(-\varphi(x))$  and using the MAP estimator. In particular, we show that for *any* prior  $p_X(x)$ , the conditional mean can be interpreted as a MAP with some prior  $C \cdot \exp(-\varphi(x))$ . Vice-versa, for *certain* penalties  $\varphi(x)$ , the solution of the penalized least squares problem is indeed the *conditional mean*, with a certain prior  $p_X(x)$ . In general we have  $p_X(x) \neq C \cdot \exp(-\varphi(x))$ .

**EDICS:** SAS-STAT

## I. INTRODUCTION

Consider the problem of estimating an unknown signal  $x \in \mathbb{R}^n$  from a noisy observation  $y = x + b$ , also known as *denoising*. Given an arbitrary noisy observation  $y$  the goal is to estimate the noiseless

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signal  $x$ : in practice, designing a denoising scheme amounts to choosing a function  $\psi : \mathbb{R}^n \rightarrow \mathbb{R}^n$  which provides estimates of the form  $\hat{x} = \psi(y)$ . However, unless we specify further what we mean by "noise" and "signal", denoising is a completely ill-posed problem since any pair  $x, b$  such that  $y = x + b$  can be replaced by  $x' = x + z, b' = b - z$ . Practical denoising schemes hence have to rely on various types of prior information on  $x$  and  $b$  to design an appropriate denoising function  $\psi$ .

### A. Bayesian estimation

A standard statistical approach to the denoising problem consists in assuming that  $x$  and  $b$  are drawn independently at random from known *prior* probability distributions  $P_X$  and  $P_B$ . Under this *model*, given a cost function  $\mathcal{C}(\hat{x}, x)$  that measures the quality of an estimator  $\hat{x}$  in comparison to the true quantity to estimate  $x$ , the Bayes estimator is defined as an estimator  $\psi$  with minimum expected cost:

$$\arg \min_{\psi} \mathbb{E} \{ \mathcal{C}(\psi(X + B), X) \}.$$

For a quadratic cost function  $\mathcal{C}(\hat{x}, x) := \|\hat{x} - x\|_2^2$  the Bayes estimator is the conditional mean [5]

$$\psi_{\star}(y) := \mathbb{E}(X|Y = y). \quad (\text{I.1})$$

Even though this estimator is "optimal" in the above defined sense, its computation involves a high-dimensional integral and cannot generally be done explicitly. In practice, Monte-Carlo simulations can be used to approximate the integral.

Often more amenable to efficient numerical optimization is the popular Maximum A Posteriori (MAP) criterion, which exploits Bayes rule

$$\begin{aligned} \psi_{MAP}(y) &:= \arg \max_x p(x|y) = \arg \max_x p(y|x)p(x) \\ &= \arg \min_x \{ -\log p_B(y - x) - \log p_X(x) \}. \end{aligned}$$

For white Gaussian noise  $b$ , since  $p_B(b) \propto \exp(-\|b\|_2^2/2)$ , the MAP under the prior  $p_X$  can be expressed as

$$\arg \min_x \frac{1}{2} \|y - x\|_2^2 + [-\log p_X(x)]. \quad (\text{I.2})$$

### B. Regularization

Optimization problems of the type (I.2) have also been often considered in signal processing without explicit reference to probabilities or priors, under the generic form

$$\arg \min_x \frac{1}{2} \|y - x\|_2^2 + \varphi(x). \quad (\text{I.3})$$

The deterministic objective is to achieve a tradeoff between the data-fidelity term  $\|y-x\|_2^2$  and the penalty term  $\varphi(x)$ , which promotes solutions with certain properties. In particular, when the function  $\varphi$  is non-smooth at the origin, such as  $\varphi(x) = |x|^p, 0 < p \leq 1$ , the optimum of the criterion (I.3) is known to have few nonzero entries. Regularization with such penalty functions is at the basis of *shrinkage* techniques [3] for signal denoising. More recently, these approaches have become a very popular mean of promoting *sparse* solutions to under-determined or ill-conditioned linear inverse problems  $y = \mathbf{A}x + b$ , and are now a key tool for compressed sensing [4].

### C. Plurality of Bayesian interpretations of regularization

Given the identity of the optimization problems (I.2) and (I.3) when<sup>1</sup>  $p_X(x) \propto \exp(-\varphi(x))$ , the regularization problem (I.3) is often interpreted as "solving the MAP under the prior  $C \cdot \exp(-\varphi(x))$  (and white Gaussian noise)". In particular, when  $\varphi(x) = \|x\|_1$ , a possible interpretation of (I.3) is MAP denoising under a Laplacian prior on  $x$  and white Gaussian noise.

The main objective of this paper is to highlight the fact that while the MAP with prior  $C \cdot \exp(-\varphi(x))$  is *one* Bayesian interpretation of the estimator (I.3), *there can be other Bayesian interpretations*. We focus on white Gaussian denoising, and we show that for *any* prior  $p_X(x)$ , the conditional mean can be interpreted as a MAP with some prior  $C \cdot \exp(-\varphi(x))$ . Vice-versa, for certain functions  $\varphi$ , the estimator (I.3) can equally be interpreted as the *conditional mean*, with a prior  $p_X(x)$ . In general we do not have  $p_X(x) \propto \exp(-\varphi(x))$ .

## II. MAIN RESULTS

From now on we focus on Gaussian denoising:  $B \in \mathbb{R}^n$  is a centered normal Gaussian variable with law  $\mathcal{N}(0, \mathbf{I}_n)$  and probability density function (pdf)  $p_B(b) \propto \exp(-\|b\|_2^2/2)$ . We let  $X \in \mathbb{R}^n$  be a random variable independent of  $B$ , with law  $P_X$  and pdf<sup>2</sup>  $p_X(x)$  and  $Y = X + B$  be the noisy observation.

In this setting the conditional mean is (see Appendix A)

$$\psi_\star(y) = y + \frac{1}{p_Y(y)} \left[ \frac{\partial}{\partial y_i} p_Y(y) \right]_{i=1}^n = y + \nabla \log p_Y(y) \quad (\text{II.1})$$

where  $p_Y := p_X \star p_B$  is the pdf<sup>3</sup> of the noisy observation  $y$ .

<sup>1</sup>The notation  $f(x) \propto g(x)$  means  $f(x) = C \cdot g(x)$  for all  $x$ , where  $C \neq 0$  is some constant independent of  $x$ .

<sup>2</sup>For simplicity we consider random variables which admit a pdf.

<sup>3</sup>The pdf  $p_Y$  is sometimes referred to as the *evidence* of the observation.

Next we study whether  $\psi_*$  can also be written as the optimum of an optimization problem of the MAP type (I.3), with an appropriate choice of  $\varphi$ . Namely, we investigate when  $\psi_*$  can be identified with the *proximity operator* [2] of a function  $\varphi$ , where we recall the definition

$$\text{prox}_\varphi(y) := \arg \min_{z \in \mathbb{R}^n} \left\{ \frac{1}{2} \|y - z\|_2^2 + \varphi(z) \right\}. \quad (\text{II.2})$$

For smooth  $\varphi$  we have the implicit characterization [2]

$$\text{prox}_\varphi(y) := y - \nabla \varphi[\text{prox}_\varphi(y)], \quad \forall y \in \mathbb{R}^n. \quad (\text{II.3})$$

Comparing with (II.3), we see that if  $\psi_* = \text{prox}_\varphi$  then

$$\nabla \varphi[\psi_*(y)] = -\nabla \log p_Y(y), \quad \forall y \in \mathbb{R}^n. \quad (\text{II.4})$$

Since  $\psi_*$  is *one-to-one* from  $\mathbb{R}^n$  to  $\text{Im}\psi_*$  (see Corollary A.2 in Appendix B), the relation (II.4) characterizes the functions  $\varphi$  such that  $\psi_* = \text{prox}_\varphi$ , leading to our theorem.

**Theorem II.1.** *Consider  $Y = X + B$  where  $B \sim \mathcal{N}(0, \mathbf{I}_n)$  and  $X \sim P_X$  are independent.*

- 1) *The conditional mean  $\psi_*(\cdot)$  is one-to-one and  $C^\infty$  from  $\mathbb{R}^n$  onto  $\text{Im}\psi_*$ . Its reciprocal  $\psi_*^{-1}(\cdot) : \text{Im}\psi_* \rightarrow \mathbb{R}^n$  is also  $C^\infty$ .*
- 2) *We have  $\psi_* = \text{prox}_{\varphi_*}$  where  $\varphi_* : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$  is defined by:*

$$\begin{aligned} \varphi_*(x) &:= -\frac{1}{2} \|\nabla \log p_Y(\psi_*^{-1}(x))\|_2^2 - \log p_Y[\psi_*^{-1}(x)], \\ &\quad \text{for } x \in \text{Im}\psi_{CM}; \\ \varphi_*(x) &:= +\infty, \\ &\quad \text{for } x \notin \text{Im}\psi_*. \end{aligned} \quad (\text{II.5})$$

- 3) *If  $\tilde{\varphi}$  satisfies  $\psi_* = \text{prox}_{\tilde{\varphi}}$  then there is a constant  $c \in \mathbb{R}$  such that  $\tilde{\varphi}(x) = \varphi_*(x) + c$  for all  $x \in \text{Im}\psi_*$ .*
- 4) *For every  $y \in \mathbb{R}^n$ , the value  $\psi_*(y) = \text{prox}_{\varphi_*}(y)$  is the unique local minimum of the function  $\frac{1}{2} \|y - x\|^2 + \varphi_*(x)$ .*

*The conditional mean with prior  $p_X$  and white Gaussian noise is therefore also the MAP with prior  $C \cdot \exp(-\varphi_*(x))$  and white Gaussian noise.*

**Remark II.2.** Even though the function  $x \mapsto \frac{1}{2} \|y - x\|^2 + \varphi_*(x)$  admits a unique local minimum for any  $y$ , the function  $\varphi_*$  defined in (II.5) can be nonconvex, as shown with the following single variable example ( $n = 1$ ). A function  $\psi : \mathbb{R} \rightarrow \mathbb{R}$  can be written  $\psi = \text{prox}_\varphi$  with  $\varphi$  a proper lower semi-continuous function from  $\mathbb{R}$  to  $\mathbb{R}$  if, and only if, the function  $\psi$  is non-expansive and increasing [2]. Here, in the

case  $n = 1$ ,  $\psi_*$  is increasing (cf Lemma A.1 in Appendix B), but for certain priors  $p_X$  it is expansive (see Remark A.3 in Appendix B): its derivative exceeds one at some point. Since the associated  $\varphi_*$  is  $C^\infty$ , it is proper and continuous, hence it cannot be convex.

*Remark II.3.* Caution is in order when interpreting  $\psi_*$  as "the MAP estimator with prior  $\exp(-\varphi_*(x))$ ". This only makes sense if the function  $x \mapsto \exp(-\varphi_*(x))$  is integrable, although in the opposite case some authors refer to the MAP with a "non-informative prior".

### III. DISCUSSION

For Gaussian priors  $X \sim \mathcal{N}(0, \Sigma)$ , the conditional mean is the Wiener filter, which is also the MAP and the minimum mean square linear estimator [5], so  $\varphi_*(x) = -\log p_X(x)$ .

However, the MAP and the conditional mean are not generically equivalent, so there are choices of  $p_X$  (non Gaussian) for which we *do not* have the identity  $\varphi_*(x) = -\log p_X(x)$ . Indeed, observe that for any prior  $p_X(x)$ , the penalty function  $\varphi_*(x)$  defined in Theorem II.1 has the following properties:

- the function  $\varphi_* : \text{Im}\psi_* \rightarrow \mathbb{R}$  is  $C^\infty$ ;
- for any  $y$ , the function  $x \mapsto \frac{1}{2}\|y - x\|_2^2 + \varphi_*(x)$  admits a unique local minimum.

Therefore, the identity  $\varphi_*(x) = -\log p_X(x)$  cannot be satisfied if  $-\log p_X(x)$  fails to satisfy one of these properties.

For example, generalized Gaussian priors  $p_X(x) \propto \exp(-\alpha\|x\|_p^p)$  with  $0 < p \leq 1$  are *not smooth* at  $x = 0$ , hence not in  $C^\infty$ : for such priors we cannot even have the identity  $\varphi_*(x) = a - b \log p_X(x)$  for any  $a, b \in \mathbb{R}$ .

One may also wonder whether a reciprocal to Theorem II.1 is possible. Given a penalty function  $\varphi(x)$ , one can always define  $\psi(y) = \text{prox}_\varphi(y)$ , and define  $q(y) = \psi(y) - y$ . However, the main difficulty is to understand when one can write  $q(y) = \nabla(p_X \star p_B)(y)$  for some pdf  $p_X$ . This is not always possible, for example if  $\varphi(x)$  is not sufficiently smooth.

### IV. CONCLUSION AND PERSPECTIVES

We proved that the conditional mean estimator for Gaussian denoising can always be written as a MAP (and that the MAP estimator with certain penalty functions can be interpreted as a conditional mean). These results, in conjunction with Nikolova's highlighting of model distortions brought by MAP estimation [6], indicate that one should be cautious when interpreting penalized least squares regression scheme in terms of priors:

- If the data follows a prior  $C \cdot \exp(-\varphi(x))$  and if we choose the MAP as a criterion for estimating it, then the resulting denoising scheme takes the form of penalized least squares regression with penalty  $\varphi(x)$ . However, this MAP estimator may have poor denoising performance for this type of data [6].
- In practice, the choice of penalized least squares regression with penalty  $\varphi(x)$  is seldomly associated to the *belief* that the data follows the prior  $C \cdot \exp(-\varphi(x))$ . Instead, it rather stems from the *need* for numerical efficiency and the *empirical observation* that it achieves good denoising performance for the considered class of data.

Given an arbitrary penalty  $\varphi(x)$ , it remains an open problem to understand for which priors  $p_X(x)$  we obtain "good" denoising performance of penalized least squares regression (for example: performance comparable to the conditional mean).

One can imagine concrete applications of the results presented here for certain priors: in general the conditional mean  $\psi_*(y)$  is *a priori* expressed as an intractable high-dimensional integral; however, if the penalty function  $\varphi_*(x)$  admits a simple expression amenable to efficient numerical optimization (e.g., convex optimization), then the conditional mean can be computed efficiently. Developing such approaches requires a more in depth understanding of the properties of penalty functions  $\varphi_*(x)$  obtained through Theorem II.1. Of particular interest would be the construction of explicit examples where  $\varphi_*(x)$  is "simple" while  $p_Y$  involves an intractable integral.

Another interesting perspective is to obtain alternate statistical interpretations of a larger class of penalized least squares regression estimators (e.g., with non-smooth  $\varphi(x)$  such as those leading to sparse estimates). As remarked above, the lack of smoothness makes it impossible to interpret such estimators in terms of a conditional mean, however one may seek interpretations that leave the strict Bayesian framework: for example, one may wish to obtain an interpretation as the optimum of a hybrid Bayesian cost function

$$\min_{\psi} \{\mathbb{E}\mathcal{C}(\psi(X + B), X) + \mathbf{K}(\psi)\}$$

where the term  $\mathbf{K}(\cdot)$  forces the function  $\psi$  to be in some function class. Eventually, one may also wish to extend these results to ill-posed linear inverse problems of the type  $y = \mathbf{A}x + b$ , and to deal with non-Gaussian noise.

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## APPENDIX

### A. Proof of the identity (II.1)

If  $\psi$  minimizes the expected square loss, then by the orthogonality relation [5], for any function  $\delta : y \mapsto \delta(y)$  we must have  $\mathbb{E}\langle \psi(Y) - X, \delta(Y) \rangle = 0$ . Hence we obtain the condition

$$\forall \delta, \quad \mathbb{E}\langle \psi(Y) - Y, \delta(Y) \rangle = -\mathbb{E}\langle B, \delta(Y) \rangle.$$

Since  $Y = X + B$  has the pdf  $p_Y = p_X \star p_B$ , we thus require that for any  $\delta$

$$\int p_Y(y) \langle \psi(y) - y, \delta(y) \rangle dy = -\mathbb{E}\langle B, \delta(Y) \rangle.$$

Using argument similare to those involved in Stein's risk estimator [7], [1], the right hand side above can be rewritten as follows:

$$\begin{aligned} -\mathbb{E}\langle B, \delta(X + B) \rangle &= -\mathbb{E}_X \int p_B(b) \langle b, \delta(X + b) \rangle db \\ &= +\mathbb{E}_X \int \langle \nabla p_B(b), \delta(X + b) \rangle db \\ &= \iint p_X(x) \sum_{i=1}^n \frac{\partial}{\partial b_i} p_B(b) \cdot \delta_i(x + b) dx db \\ &\stackrel{(a)}{=} \sum_{i=1}^n \iint p_X(x) \frac{\partial}{\partial b_i} p_B(y - x) \cdot \delta_i(y) dx dy \\ &= \sum_{i=1}^n \int (p_X \star \frac{\partial}{\partial b_i} p_B)(y) \cdot \delta_i(y) dy \\ &= \int \sum_{i=1}^n \frac{\partial}{\partial b_i} (p_X \star p_B)(y) \cdot \delta_i(y) dy \\ &= \int \langle \nabla p_Y(y), \delta(y) \rangle dy. \end{aligned}$$

In (a) we used the change of variable  $y = x + b$ . We finally obtain the condition: for all  $y$ ,  $p_Y(y)[\psi(y) - y] = \nabla p_Y(y)$ . It is easy to check that  $p_Y(y)$  cannot vanish, hence this eventually reads  $\psi(y) - y = \frac{1}{p_Y(y)} \nabla p_Y(y) = \nabla \log p_Y(y)$ .

### B. Other technical lemmata

We begin by proving that  $\psi_\star$  is always one-to-one.

**Lemma A.1.** Denote  $\psi_\star(y) = (\psi_\star^i(y))_{i=1}^n$  where  $\psi_\star^i(\cdot) : \mathbb{R}^n \rightarrow \mathbb{R}$  is scalar valued. The  $n \times n$  Jacobian matrix  $J[\psi_\star](y) := \left[ \frac{\partial}{\partial y_j} \psi_\star^i(y) \right]_{ij}$  is symmetric positive definite:

$$\langle v, J[\psi_\star](y) \cdot v \rangle > 0, \quad \forall y \in \mathbb{R}^n, v \neq 0.$$

and satisfies the identity

$$J[\psi_\star](y) = \left[ \delta_{ij} + \frac{\partial^2}{\partial y_i \partial y_j} \log p_Y(y) \right]_{ij} = \mathbf{I} + \nabla^2 \log p_Y(y).$$

*Proof:* For simplicity, we do the proof in the single variable case ( $n = 1$ ). The extension to higher dimension follows the same steps and poses no special difficulty. We indicate the main differences when needed. Since  $\psi_\star(y) := y + p'_Y(y)/p_Y(y)$  we have  $\psi'(y) = (p_Y^2(y) + p_Y''(y)p_Y(y) - [p_Y'(y)]^2) / p_Y^2(y)$ . Since  $n = 1$ , what we need to prove is  $\psi'(y) > 0$  for all  $y$ , or equivalently

$$p_Y^2(y) + p_Y''(y)p_Y(y) - [p_Y'(y)]^2 > 0, \quad \forall y.$$

Since  $p_Y = p_X \star p_B$ ,  $p'_Y = p_X \star p'_B$ ,  $p''_Y = p_X \star p''_B$  and  $p_B(b) \propto \cdot e^{-b^2/2}$ , we have

$$\begin{aligned} p'_B(b) &\propto e^{-b^2/2} \cdot (-b), \\ p''_B(b) &\propto e^{-b^2/2} \cdot (b^2 - 1) \end{aligned}$$

therefore  $p_Y^2(y) + p_Y''(y)p_Y(y) - [p_Y'(y)]^2$  is proportional to

$$\begin{aligned} &\iint p_X(y-b)p_X(y-b') \cdot e^{-(b^2+b'^2)/2} \\ &\cdot \left( 1 + \frac{b^2-1}{2} + \frac{b'^2-1}{2} - bb' \right) dbdb' \\ &= \iint p_X(y-b)p_X(y-b') \\ &\cdot e^{-(b^2+b'^2)/2} \cdot \frac{(b-b')^2}{2} dbdb' \geq 0 \end{aligned} \tag{A.1}$$

where we used the non-negativity of the integrand<sup>4</sup>. With the change of variable  $x = y - b$ ,  $x' = y - b'$ , we conclude that  $\psi'(y) \geq 0$  with equality only if the function  $(x, x') \mapsto p_X(x)p_X(x')$  is identically zero on  $\mathbb{R}^2 \setminus \{(x, x), x \in \mathbb{R}\}$ . This implies  $p_X(x) = 0$  for all  $x$ , which is impossible since  $p_X$  is a proper pdf. ■

<sup>4</sup>For  $n > 1$  the scalar factor  $(b - b')^2$  in (A.1) becomes  $\langle b - b', v \rangle^2$ .

**Corollary A.2.** *The function  $y \mapsto \psi_*(y)$  is one-to-one from  $\mathbb{R}^n$  to  $\text{Im}\psi_*$ : for any pair  $y, y' \in \mathbb{R}^n$ , if  $\psi_*(y) = \psi_*(y')$  then  $y = y'$ . Moreover, it is  $C^\infty$  and its reciprocal is  $C^\infty$ .*

*Proof:* We let the reader check that  $p_Y$  cannot vanish and is  $C^\infty$ , hence  $\psi_*$  is  $C^\infty$ . To prove that  $\psi_*$  is one-to-one, we proceed by contradiction, assuming that  $\psi_*(y) = \psi_*(y')$  while  $y' \neq y$ . We define  $v := (y' - y)/\|y' - y\|_2$  and the function  $f : t \mapsto f(t) := \langle v, \psi_*(y + tv) \rangle \in \mathbb{R}$ . We have  $f(0) = f(\|y' - y\|_2)$ , and  $f$  is smooth, hence its derivative must vanish for some  $0 < t < \|y' - y\|_2$ . However by Lemma A.1 the derivative is  $f'(t) = \langle v, J[\psi_*](y + tv) \cdot v \rangle > 0$  which yields a contradiction. ■

*Remark A.3.* The computations done in the proof of Lemma A.1 indicate that for certain choices of the prior  $p_X$  we can ensure that  $\psi_*$  is *not* a non-expansive function. We will show it in the single variable case, and similar examples can be built in higher dimensions. By definition, a function  $f : \mathbb{R} \rightarrow \mathbb{R}$  is non-expansive if  $|f(y') - f(y)| \leq |y' - y|$  for all  $y, y'$ . If  $f$  is differentiable and non-expansive we must have  $|f'(y)| \leq 1$  for all  $y$ . We prove below that if  $p_X$  is symmetric ( $\forall x, p_X(-x) = p_X(x)$ ) and if from some  $\varepsilon > 0$  we have  $p_X(x) = 0$  for  $|x| \leq 1 + \varepsilon$ , then  $\psi'_*(0) > (1 + \varepsilon)^2$ .

*Proof:* It can be checked using the computations done in the proof of Lemma A.1 that

$$\psi'_*(0) = \frac{\iint p_X(-b)p_X(-b') \cdot e^{-(b^2+b'^2)/2} \cdot \frac{(b-b')^2}{2} dbdb'}{\iint p_X(-b)p_X(-b') \cdot e^{-(b^2+b'^2)/2} dbdb'} > 0.$$

Since  $p_X$  is symmetric, easy manipulations show

$$\begin{aligned} \psi'_*(0) &= \frac{\iint p_X(b)p_X(b') \cdot e^{-(b^2+b'^2)/2} \cdot \frac{b^2+b'^2}{2} dbdb'}{\iint p_X(b)p_X(b') \cdot e^{-(b^2+b'^2)/2} dbdb'} \\ &= \frac{\iint p_X(b)p_X(b') \cdot e^{-(b^2+b'^2)/2} \cdot b^2 dbdb'}{\iint p_X(b)p_X(b') \cdot e^{-(b^2+b'^2)/2} dbdb'} \end{aligned}$$

Since  $p_X(x) = 0$  for  $|x| \leq 1 + \varepsilon$  we obtain  $\psi'_*(0) \geq (1 + \varepsilon)^2$ . ■

### C. Proof of Theorem II.1

The fact that  $\psi_*$  is one-to-one and  $C^\infty$  with  $C^\infty$  reciprocal function was proved in Corollary A.2. We now wish to check that the proximity operator of  $\varphi_*$  defined by (II.5) is indeed  $\psi_*$ . The definition of  $\varphi_*(x)$  for  $x \notin \text{Im}\psi_*$  ensures that  $\text{prox}_{\varphi_*}$  takes its values in  $\text{Im}\psi_*$ . We let the reader check that a consequence of Lemma A.1 is that the set  $\text{Im}\psi_*$  is open. The key point will be to check that there is a *unique* local minimum of  $x \mapsto \frac{1}{2}\|y - x\|_2^2 + \varphi_*(x)$ , which is exactly at  $\psi_*(y)$ . This will imply in

particular that the global minimum  $\text{prox}_{\varphi_*}(y)$  is equal to  $\psi_*(y)$ . Denoting  $x$  any local minimum, and  $u$  such that  $\psi_*(u) = x$ ,  $u$  must be a local minimum of

$$\begin{aligned} \frac{1}{2}\|y - \psi_*(u)\|_2^2 + \varphi_*[\psi_*(u)] &= \frac{1}{2}\|\psi_*(u) - y\|_2^2 \\ &\quad - \frac{1}{2}\|\nabla q(u)\|_2^2 - q(u) \end{aligned}$$

(where for the sake of brevity we denoted  $q(y) = \nabla \log p_Y(y)$ ) hence it must satisfy the stationary point equation

$$J[\psi_*](u) \cdot [\psi_*(u) - y] - \nabla^2 q(u) \cdot \nabla q(u) - \nabla q(u) = 0.$$

Using the relation  $J[\psi_*](u) = 1 + \nabla^2 q(u) > 0$  (Lemma A.1) this becomes

$$J[\psi_*](u) \cdot [\psi_*(u) - y - \nabla q(u)] = 0$$

hence  $\psi_*(u) = y + \nabla q(u)$ . Since  $\psi_*(u) = u + \nabla q(u)$  we conclude that  $u = y$ , and therefore  $x = \psi_*(u) = \psi_*(y)$ .

To conclude, assume the function  $\tilde{\varphi} : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$  satisfies  $\psi_* = \text{prox}_{\tilde{\varphi}}$ . By (II.4) we must have for all  $y$ :  $\nabla \tilde{\varphi}[\psi_*(y)] = -\nabla \log p_Y(y) = \nabla \varphi_*[\psi_*(y)]$ . In other words, for any  $x \in \text{Im} \psi_*$ ,  $\nabla(\tilde{\varphi} - \varphi_*)(x) = 0$ . Since  $\psi_*$  is a one-to-one mapping of  $\mathbb{R}^n$  onto  $\text{Im} \psi_*$ , the set  $\text{Im} \psi_*$  is connected hence there must be a constant  $C \in \mathbb{R}$  such that for all  $x \in \text{Im} \psi_*$ ,  $\tilde{\varphi}(x) = \varphi_*(x) + C$ .

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