The surface Laplacian technique in EEG: Theory and methods

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This paper reviews the method of surface Laplacian differentiation to study EEG. We focus on topics that are helpful in the literature, and discuss the problem of computational performance, which is particularly important in the context of EEG sphenoid data sets that can be very large. Along this line, the matrix representation of the surface Laplacian operator is carefully discussed and some figures are given illustrating the advantages of this approach. In the final remarks, we briefly sketch a possible way to incorporate finite-size electrodes into Laplacian estimates that could guide further developments.

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1. Introduction

The surface Laplacian (SL) technique is a powerful method to study EEG. It emerged from the seminal works of Nicholson (1973), Freeman and Nicholson (1975), Nicholson and Freeman (1975), and Hjorth (1975). These were followed by efforts to develop better computational methods (see Gevins (1988, 1989); Gevins et al. (1990); Perrin et al. (1989); Law et al. (1993a); Yao (2002); Carvalhaes and Suppes (2011)) as well as attempts to combine the SL with other methods (Kayser and Tenke, 2006a, 2006b, Carvalhaes et al., 2009), making the technique increasingly popular among EEG researchers. For instance, modern applications include studies on generators of event-related potentials (Kayser and Tenke, 2006a, 2006b), quantitative EEG (Tenke et al., 2011), spectral coherence (Srinivasan et al., 2007; Winter et al., 2007), event-related synchronization/desynchronization (Del Percio et al., 2007), phase-lock synchronization (Doesburg et al., 2008), estimation of cortical connectivity (Astolfi et al., 2007), high-frequency EEG (Fitzgibbon et al., 2013), and brain–computer interface (Lu et al., 2013), just to mention a few.

The motivation for using the SL is grounded on Ohm's law, which establishes a local relationship between the SL of scalp potentials and the underlying flow of electric current caused by brain activity (see Appendix in Carvalhaes et al. (2014)). Presumably, this local relation should improve spatial resolution, reflecting electrical activity from a more restricted cortical area than what is observed in conventional topography.

In contrast to other high-resolution techniques, such as cortical surface imaging (Nunez et al., 1994; Yao, 1996; Yao et al., 2001), the SL has the advantage of not requiring a volume conductor model of the head or a detailed specification of neural sources, but objections to it may arise due to a combination of factors. First, there is a noticeable difficulty in understanding the technique in-depth (Nunez and Westdorp, 1994). While EEG potentials can be physically understood in terms of current flow or in analogy with the gravitational potential, interpreting the SL operation seems much less intuitive, as it involves the application of a second-order partial differential operator to a scalar potential distribution. Second, it appears surprising to many that one can obtain a reference-independent quantity from a signal which is seen to have been contaminated by a reference in its very origin (Nunez and Srinivasan, 2006), ch 7. Third, it is not possible to guarantee that the theoretical advantages associated to the use of the Laplacian differentiation will be preserved in the practical world of imperfect measurements and finite samples. In fact, reliable estimates of the Laplacian derivation are technically challenging, and computational methods to perform this task are still a subject of research.

The literature dedicated to provide theoretical explanations about the SL technique is scarce (see Nunez and Srinivasan (2006); Tenke and Kayser (2012)). There are still some gaps that, if filled, can help comprehension and permit a more intuitive view of it. It is the intention...
of this paper to contribute to this matter. For this purpose, Section 2 provides physical insights on the SL technique that are seldom discussed, but that are at the heart of some issues of interest to the EEG researcher. Section 3 focuses on the computational aspects, providing a comprehensive review of selected methods and their advantages and limitations. In Section 3.5 we present the method of estimating the SL derivation by means of a matrix transformation, and Section 3.6 focuses on the regularization problem of smoothing splines that significantly affects SL estimates.

2. An overview of the physics of EEG

Here we discuss the main theoretical ideas behind the use of the SL to introduce concepts from the physics of EEG that are often unfamiliar to the EEG researcher, and that have direct relevance to the SL technique. We do not attempt to reproduce the main arguments about the relationship between the SL and the dura-surface potential, nor with the Current Source Density (CSD), which are found, for example, in Nunez and Srinivasan (2006). Instead we focus on the more fundamental aspects that are often overlooked.

2.1. Physical interpretation of the SL

To better understand the physical meaning of the SL, we start with the volume Laplacian, or simply Laplacian, and its relationship to the quasi-static electric field and potential. Here our treatment is standard, and can be found in any standard textbook such as Jackson (1999) or Schey (2004). Our discussion focuses only on aspects that are directly relevant to EEG.

The scalp EEG always refers to the potential with respect to some reference electrode, but from a physics point of view the electric field is more fundamental than the potential. To see this, let us recall that the field has a measurable effect: for a particle of charge $q$, the field $E(r)$ at the position $r$ is operationally defined by the ratio between the electric force $F_q$ acting on the charge at $r$ and the value of $q$. Here we use the standard notation of representing scalar quantities in italics (i.e. $\rho \rightarrow \hat{\rho}$ for the electric charge and $E$ for the electric field, and we also use the symbol $\equiv$ for an equality that arises from a definition. From this, the field measures the force per unit of charge, i.e., $E$ (as a function of the position $r$) is given by

$$E(r) = \frac{1}{q} F_q(r).$$

For simplicity we ignore any temporal dependence of $E$, but our results are the same, for all practical purposes, in the typical range of frequencies involved in the brain electrical activity (Jackson, 1999; Nunez and Srinivasan, 2006).

Electric fields generated by point charges are described by Coulomb’s Law. A consequence of this law is that $E$ is a conservative field, i.e., the line integral

$$V_{AB} = - \int_{r_A}^{r_B} E(r) \cdot dr$$

between two points $r_A$ and $r_B$ is independent of the path along which it is computed. The value $V_{AB}$ has an important physical meaning; it corresponds to the work per unit of charge necessary to be done on a charged particle when it goes through the field $E$ from position $r_A$ to $r_B$ at a constant speed. Thus, $V_{AB}$ is not only measurable, but of practical use. But also of importance is that the path-independence of $V_{AB}$ implies the existence of a function $V(r)$ such that

$$V_{AB} = V(r_B) - V(r_A).$$

This function is called the electric potential of the field $E$.

One important relationship between $E$ and $V(r)$ is given by the gradient operator. The gradient of $V(r)$, denoted $\nabla V(r)$, is defined, in Cartesian coordinates, as

$$\nabla V(r) = \frac{\partial V(r)}{\partial x} \hat{i} + \frac{\partial V(r)}{\partial y} \hat{j} + \frac{\partial V(r)}{\partial z} \hat{k},$$

where $\hat{i}, \hat{j},$ and $\hat{k}$ are the orthonormal basis vectors. The gradient is the spatial derivative of $V$ at $r$, and it forms a vector field with the following properties. For a unitary vector $\hat{u}$, $\nabla V(r) \cdot \hat{u}$ gives the rate of change of the function $V$ at point $r$ in the direction $\hat{u}$. Thus, $\nabla V(r)$ at $r$ is a vector, pointing at the direction where the function $V$ changes the most, whose magnitude is the rate of change. In other words, the direction perpendicular to $\nabla V(r)$ points at the direction of the isopotential lines. From this, it is possible to prove that the function $V(r)$ relates to the field by the expression

$$E(r) = -\nabla V(r),$$

i.e., the field is the negative gradient of the potential.

It is easy to see that $V(r)$ is not uniquely defined, as any function $V'(r)$ given by

$$V'(r) = V(r) - V_0,$$

where $V_0$ is an arbitrary constant, also gives the same differences of potential $V_{AB}$ between $r_A$ and $r_B$, and therefore the same gradient (for instance, when we take the limit of $\Delta r \rightarrow r_A - r_B$ very small). As an example, let us consider the electric field from a point particle with charge $q$ situated at position $r_0$, which is given by

$$E(r) = \frac{q}{4\pi \epsilon_0} \frac{r - r_0}{(r - r_0)^3}.$$  

It is easy to show that a potential satisfying Eq. (2) is given by

$$V(r) = - \frac{q}{4\pi \epsilon_0} \frac{1}{|r - r_0|}.$$  

For another potential $V'(r) = - \frac{q}{4\pi \epsilon_0} \frac{1}{|r - r_0|} + V_0$, we see at once that its gradient is exactly the same as for $V(r)$, since $V_0$ would disappear in derivative in Eq. (4). However, the potential (7) is often given in textbooks, as it corresponds to a reference in a point infinitely distant from $r_0$ (i.e. $V \rightarrow 0$ when $|r| \rightarrow \infty$).

In a volume conductor, such as the brain, the electric field is related to the current density $j$ by

$$E(r) = \rho j(r),$$

where $\rho = 1/\sigma$ is the resistivity, given by the inverse of the conductivity $\sigma$. Eq. (8) is sometimes referred to as the vector form of Ohm’s Law. In a medium with resistivity $\rho$, a map of the potential function may be used to compute $E(r)$ and, via Eq. (8), estimate current sources. Though we are interested in the SL, for completeness we examine the meaning of the Laplacian, which comes from Gauss’s Law. In its differential form Gauss’s Law is written as

$$\text{Div}(E) = 4\pi \rho_0.$$  

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1 Here, for simplicity, we are ignoring the fact that $\rho$ may depend of both on position and time $\rho = \rho(r, t)$. Furthermore, when the media is anisotropic, $E(r)$ is not necessarily in the same direction as $j(r)$, and $\rho$ needs to be a rank-two tensor. However, at the scalp, Eq. (8) is an excellent approximation to EEG, as the $\rho$ is approximately isotropic in the tangential direction (Rush and Driscoll, 1968; Nicholson and Freeman, 1975; Wolters et al., 2006; Petrov, 2012).
where \( \rho_{Q} \) is the charge density. Here \( \text{Div}(\mathbf{E}) \) is the divergence of the electric field \( \mathbf{E} \), a linear differential operator acting on \( \mathbf{E} \), which in Cartesian coordinates, where the electric field is represented by \( \mathbf{E} = E_x \hat{x} + E_y \hat{y} + E_z \hat{z} \), takes the form
\[
\text{Div}(\mathbf{E}) = \frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z}.
\]

The divergence of \( \mathbf{E} \) can be interpreted as a local measure of the difference between how much field (technically, its flux) gets into an infinitesimal volume surrounding the point where it is computed and how much of this field gets out. If the divergence is zero, the same amount of field that gets in also gets out; if the divergence is negative, more field gets in than out (sink); and if the divergence is positive, more field gets out than comes in (source). For this reason, the divergence of \( \mathbf{E} \) is a measure of sources and sinks of the field. Thus, Gauss’s law has the interpretation that electric charges are sources of an electric field: if there are no electric charges, the divergence of the field is zero.

Now, from Eq. (5) we have at once that
\[
\text{Div}(\mathbf{E}) = -\text{Div}(\nabla V).
\]

The divergence of the gradient, \( \text{Div}(\nabla V) \), is defined as the Laplacian of \( V \), denoted by \( \nabla^2 V \) or \( \Delta V \). The Laplacian does not have an interpretation that is as straightforward as the ones for the divergence or the gradient. Its meaning is related to the mean value of the potential around the point where it is computed. For example, imagine that \( \nabla^2 V \) is positive at some point \( r \) where \( V \) has a local minimum (first derivative is zero). Such positive value means that for any small area surrounding \( r \), most of the values of \( V \) are greater than \( V(r) \). So, we can interpret \( \nabla^2 V \) as measuring the relative mean value of the potential around the point. We can also think of the Laplacian of \( V \) as simply the divergence of \( \mathbf{E} \). Thus, from Eq. (10) and Eq. (9) it follows that the Laplacian of the potential is proportional to the electric field sources, i.e.,
\[
\nabla^2 V = -4\pi \rho_{Q}.
\]

The above discussion showed the connection between \( \mathbf{E} \) and \( V \). However, it did not take into account some characteristics of the EEG. First, the EEG is measured over the scalp, which is a curved surface. Second, such measurements are often not directly of the field, but are differences of potential associated to currents flowing in the circuit formed between two electrodes, the measuring device, and the current flow density in the head. In the head, such currents define a vector field consisting of currents from the brain, dura surface, bone, and scalp. This current density is proportional at each point to the electric field. But outside of the head, the EEG measuring apparatus closes the circuit and measures the small current associated with such system (Metting van Rijn et al., 1990, 1991). Finally, because such measurements are on the scalp, they happen where there is a significant change in conductivity (interface scalp/air). All of those points have some consequence for the interpretations of the field and Laplacian.

Starting with the Laplacian, the most common assumption is that sources of interest are inside the skull, and that there are no sources in the scalp itself (Nunez and Srinivasan, 2006). But if we start with this assumption, we have that, from Eq. (9),
\[
\nabla^2 V = 0.
\]

Using the expression for the Laplacian in Cartesian coordinates, we have
\[
\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0.
\]

Let us now choose the coordinate system such that the scalp is on the plane \( x, y \) (for small areas, this is a good approximation). Then we can rewrite Eq. (13) as
\[
\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = \frac{\partial E}{\partial z}.
\]

The left hand side of Eq. (15) is defined as the SL of \( V \),
\[
\text{SL}_V(V) = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2},
\]

and Eq. (15) shows that \( \text{SL}_V(V) \) is related to how abruptly the normal component of the current changes in the direction perpendicular to the surface. Thus, if \( \text{SL}_V(V) \) is nonzero, conceptually, in the absence of sources, the current change in this direction means a fanning out of the current lines. In the case of the scalp, this means that a nonzero \( \text{SL}_V(V) \) corresponds to diverging (with respect to the radial direction) current lines under the scalp, which is associated to the presence of a source of currents inside the skull. Thus, the SL has a direct relationship to currents under the scalp, and it can be shown that it is related to electrical activities on the dura surface (Nunez and Srinivasan, 2006).

2.2. Properties of the SL

With an interpretation of the SL in terms of currents and fields, we now turn to some of its properties, starting with its reference-free property. This may seem puzzling, as in most cases the SL is computed from the scalp potential, which is itself a reference-dependent quantity. To illustrate this issue, let us examine a simple example from geometry. Imagine two events whose locations are given by the points \( P \) and \( Q \).

This, of course, is an approximation, given that in some EEG setups, the electrodes can chemically generate currents. The discussion of currents generated by the scalp–electrode interface is beyond the scope of this paper (see Metting van Rijn et al. (1990, 1991); Huigen et al. (2002); Chi et al. (2010)).

It may be argued that Eq. (12) may not be well-defined on the surface of the scalp because of its discontinuous boundary conditions. First of all, it is important to point out that the Laplacian is related through the right hand side of Eq. (12) to a physically measurable quantity, and therefore always defined at a point. Second, the ill-defined character of the Laplacian comes from oversimplified mathematical models of the boundary conditions, and can be eliminated by simply taking the lateral derivative at the interface. For instance, for the equations below, such as Eq. (13), if we think about the direction \( z \) as perpendicular to the scalp, with increasing values as we leave the scalp, then we can think of the term involving a derivative with respect to \( z \) as defined as the left derivative (outward bound).

Finally, from a practical point of view, such points where the derivatives are not well defined consist of a set of measure zero, and therefore of little practical importance (see Carvalhaes et al. (2014), for details).
From an observer O (Fig. 1), P and Q’s positions are the (reference-dependent) vectors $r_P$ and $r_Q$. This dependency on reference can be seen by the fact that another observer $O'$ describes such positions by the vectors $r'_P$ and $r'_Q$, which are clearly different from $r_P$ and $r_Q$. Thus, the geometrical meaning of, say, the length of the position vector $r_P$, is not only related to the event, but to a combination of such event and an arbitrary choice of reference system, making this quantity reference dependent. However, there are many geometrical reference-free quantities that can be constructed from the reference-dependent positions $r_P$ and $r_Q$. For example, the vector connecting $P$ and $Q$ is reference-free, since it is given by $r = r_P - r_Q = r'_P - r'_Q$. Notice that $r$ has the feature of depending only on characteristics of the system of interest, $P$ and $Q$. Another reference-free quantity is the distance $d$ between $P$ and $Q$, defined by $d^2 = r^2 = (r_P - r_Q) \cdot (r_P - r_Q)$. Thus, from reference-dependent geometrical quantities it is possible to obtain reference-free ones.

For the EEG, the reference-free property is not unrelated to the fact that the SL has physical meaning, whereas the scalp potential does not\(^9\). For instance, in a medium where the electric conductivity $\sigma$ is non-zero, such as in the brain, skull, or scalp, the field relates to a (local) current by

$$E = \rho j,$$

where $\rho = 1/\sigma$ is the resistivity and $j$ is the electric current density. The electric potential, on the other hand, is not operationally defined; instead, the difference of potential between two points is. For instance, as seen above, in most EEG experiments what is measured is the current between two electrodes, which is proportional to the difference of potential between them. In practice, the potential differences are estimated by the insertion of a circuit in parallel with the electrodes, such that currents $I$ in this circuit can be measured (Nunez and Srinivasan, 2006) as a proxy for the difference of potential; the effect of such measurement is minimized by designing a high impedance measuring circuit (Mettler, van Rijn et al., 1990, 1991). So, if we define a potential $V(r)$, the value of it tells us nothing about measurable quantities in $r$, what is measurable is the potential difference between two observation points,

$$\Delta V = V(r') - V(r).$$

In other words, from a physical point of view it is nonsensical to say that the potential at a point $P$ is $V(r_P)$; however, it makes sense to say that the electric field at $P$ is $E(r_P)$. From the electric field we can obtain the Laplacian, given by $\nabla^2 E$. Thus, the Laplacian is simply the divergence of $E$, and as such is nonzero where there are sinks or sources of electric field.

In practice, directly measuring the scalp field or SL is technically very difficult. However, the usual measurements of differences of potential on the scalp is technically (fairly) easy. It is therefore common to use

\(^9\) Furthermore, this property is connected to claims that the EEG topography is not affected by changes in the reference electrode, which corresponds to the statement that differences of potential between two points across the topography are invariant with respect to the reference.

\(^{10}\) We also acknowledge the work of Freeman and Nicholson (1975), who employed a discretization scheme to approximate the Laplacian of extra-cellular potentials in CSD analysis.
depicts the construction used here. In it, each electrode occupies an individual node of a regular grid specified by the discrete variables \( i \) and \( j \), in replacement to the continuous variables \( x \) and \( y \) used before. Two major assumptions are made. First, the scalp surface is locally approximately flat, and second the measuring electrodes are equidistant, forming a square grid of size \( h \). The first assumption leads to the following differential form in Cartesian coordinates (see also Section 2.1)

\[
\text{Lap}(V) = \frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2}.
\]  

(18)

With the second assumption we approximate \( \text{Lap}(V) \) at a central node \((i,j)\) by Abramowitz and Stegun (1964), 25.3.30

\[
\text{Lap}(V)_{(i,j)} \approx \frac{V_{(i-1,j)} + V_{(i+1,j)} + V_{(i,j-1)} + V_{(i,j+1)} - 4V_{(i,j)}}{h^2}.
\]  

(19)

The mathematics behind this approximation is nontrivial and for completeness we include it in Appendix A.

As expected from Section 2.2, this approximation is reference-free. To see this, replace \( V \) with \( V - V_{\text{ref}} \) at each node (including the central node) and note that the common reference \( V_{\text{ref}} \) is canceled. The right hand side of Eq. (19) can be interpreted as a change in reference to the average over the four nearest neighbors of node \((i,j)\). If the reference electrode is located on the scalp we can reconstruct the Laplacian at this location, where \( V = 0 \), by computing

\[
\text{Lap}(V)_{\text{ref}} \approx \frac{V_{(i-1,j)} + V_{(i+1,j)} + V_{(i,j-1)} + V_{(i,j+1)}}{h^2}.
\]  

(20)

The multiplicative factor \( 1/h^2 \) in Eqs. (19) and (20) ensures the correct physical unit of \( \text{Lap}(V) \), which is Volt per centimeter square \((V/cm^2)\), but in many situations this is ignored, as originally done in Hjorth (1975).

Approximation (19) is usually referred to as Hjorth’s approximation. A limitation of Hjorth’s approximation is that it applies only to electrodes located at a central node, thus not accounting for estimates along the border of the electrode grid. For border electrodes, Hjorth suggested a less accurate approximation using just three electrodes aligned along the border. In an effort to account for estimations at all electrode sites, we developed the scheme in Fig. 3. For instance, estimates along the left border, where \( j = 1 \), are given by

\[
\text{Lap}(V)_{(i,1)} \approx \frac{V_{(i-1,1)} + V_{(i+1,1)} - 2V_{(i,2)} + V_{(i,3)} - V_{(i,1)}}{h^2}.
\]  

(21)

and at the upper-left corner

\[
\text{Lap}(V)_{(1,1)} \approx \frac{-2V_{(1,2)} + V_{(1,3)} - 2V_{(2,1)} + V_{(3,1)} + 2V_{(1,1)}}{h^2}.
\]  

(22)
Our calculations are shown in Appendix A. As it occurs with approximation (19), these expressions average the potential with weights that sum to zero, thus canceling the reference potential.

The procedure described in Appendix A can be used to obtain approximations combining more than five electrodes. However, increasing complexity does not result necessarily into more accurate estimates. Approximations for unevenly-spaced electrodes can also be derived, but we will not address this here (cf. Tenke et al. (1998)).

Finite difference provides a measure of accuracy in terms of the discretization parameter \( h \). As explained in Appendix A, approximation (19) is said to be accurate to the second-order of \( h \), shorthand \( O(h^2) \), while for peripheral electrodes the five-point approximations (21) and (22) are accurate to \( O(h) \). The higher the order, the more accurate is the approximation (Abramowitz and Stegun, 1964). Therefore, in principle, making \( h \) small by using high-density electrode arrays should reduce discretization error and improve estimates. Moreover, a small \( h \) is also useful to reduce error due to the unrealistic geometry of the plane scalp model, which is more salient over sparse electrode sites. In the absence of an appropriate measure for regulation, high-density arrays can also help reduce influence of non-local activities from unrelated sources. But exceptions are expected to occur. In fact, all this reasoning was based on the assumption of a point electrode, which is not restricted to the planar scalp model. In this case, the Laplacian differentiation (19), these expressions average the potential with weights that equalize the partial derivatives (cf. Wahba (1990), for details). The parameter \( \lambda \) is thereby chosen to be such that the solution to the problem of smoothing \( M = (m + 2/3) \) and \( M < N \). In addition, \( m \) must be greater than 2 for the SL differentiation to be well-defined. The functions \( \nu_1, \ldots, \nu_M \) are linearly independent polynomials in three variables of degree less than \( m \) (cf. Carvalhaes and Suppes (2011), for computational details).

Using matrix notation we can express the unknowns \( c_i \)'s and \( d_i \)'s as the solution to the linear system (Duchon, 1977; Meinguet, 1979; Wahba, 1990; Green and Silverman, 1994; Eubank, 1999)

\[
\mathbf{K}^{+} = \mathbf{Q}^{-1}_{N} \left( \mathbf{K} + \mathbf{N} \mathbf{A} \mathbf{I} \right) \left( \mathbf{T}^{T} \mathbf{d} \right) = \left( \mathbf{v} \right)
\]

where \( \mathbf{k} = (c_1, \ldots, c_N)^T \), \( \mathbf{d} = (d_1, \ldots, d_M)^T \), \( (\mathbf{K})_{ij} = |\mathbf{r}_i - \mathbf{r}_j|^{2m-3} \), \( (\mathbf{T})_{ij} = \nu_i (\mathbf{r}_j) \), and \( \mathbf{v} = (\nu_1, \ldots, \nu_N)^T \) is the given potential distribution. The superscript \( \mathbf{T} \) indicates transpose operation and \( \mathbf{I} \) is the \( N \times N \) identity matrix. This system has the formal solution (Wahba, 1990)

\[
\mathbf{c} = \mathbf{Q}_N^{-1} \left( \mathbf{K} + \mathbf{N} \mathbf{A} \mathbf{I} \mathbf{Q}_N \right)^{-1} \mathbf{Q}_N \mathbf{v}
\]

\[
\mathbf{Rd} = \mathbf{Q}_N^{-1} \left( \mathbf{v} - \mathbf{K} \mathbf{c} - \mathbf{N} \mathbf{c} \right)
\]

where \( \mathbf{Q}_N \in \mathbb{R}^{N \times N} \), \( \mathbf{Q}_M \in \mathbb{R}^{N \times (N-M)} \), and \( \mathbf{R} \in \mathbb{R}^{N \times M} \) derive from the QR-factorization of \( \mathbf{T} \).

With the above definitions we can express the smoothed potential at the electrode locations as

\[
\nu_h = \mathbf{K} \mathbf{c} + \mathbf{d}
\]

By introducing the matrices \( \mathbf{K}^{-1} \) and \( \mathbf{T} \), we obtain an analogous expression for the Laplacian estimate, which is

\[
\text{Lap}_h (\mathbf{v}) = \mathbf{K} \mathbf{c} + \mathbf{d}
\]

This approach has a major deficiency: it does not work if the data points \( \mathbf{r}_1, \ldots, \mathbf{r}_N \) are located on a spherical or an ellipsoidal surface. To understand this, consider the case \( m = 3 \), for which the matrix \( \mathbf{T} \) can be expressed as Carvalhaes and Suppes (2011)

\[
\mathbf{T} = \left[ \begin{array}{ccc}
1 & x_1 & y_1 \\
1 & x_1 & z_1 \\
1 & y_1 & z_1 \\
1 & z_1 & z_1 \\
1 & x_2 & y_2 \\
1 & x_2 & z_2 \\
1 & y_2 & z_2 \\
1 & z_2 & z_2 \\
1 & x_3 & y_3 \\
1 & x_3 & z_3 \\
1 & y_3 & z_3 \\
1 & z_3 & z_3 \\
\end{array} \right]
\]

Since on spherical and ellipsoidal surfaces the coordinates \( x_i, y_i, z_i \) are subject to

\[
\frac{x^2}{a^2} + \frac{y^2}{b^2} + \frac{z^2}{c^2} = 1, \quad a, b, c > 0
\]

The Matlab command for the QR-factorization of \( \mathbf{T} \) is \( qr(\mathbf{T}) \).

Note that \( a = b = c \) on the sphere.
the 1st, 5th, 8th, and 10th columns of \( \mathbf{T} \) are linearly dependent\(^{14} \). Hence, we can always express one of these columns in terms of the others. This is equivalent to say that \( \mathbf{T} \) has 10 columns but only 9 are linearly independent. This makes the linear system (25) singular, so that the unknowns \( \mathbf{c} \)'s and \( d \)'s cannot be uniquely determined.

The singularity of Eq. (25) on spheres and ellipsoids affects only the transformation parameterized by \( \mathbf{d} \), leaving intact the transformation specified by \( \mathbf{c} \). It is therefore natural to try a minimum norm solution to this problem by determining \( \mathbf{d} \) using the pseudo-inverse of \( \mathbf{R} \), i.e., \( \mathbf{d} = \mathbf{R}^+ \mathbf{Q}_i (\mathbf{v} - \mathbf{Kc} - \mathbf{Nxc}) \). This approach was proposed by Carvalhaes and Suppes (2011) (see also Carvalhaes (2013)) and was evaluated in a problem involving the localization of cortical activity on spherical and ellipsoidal scalp models. Simulations using over 30,000 configurations of radial dipoles resulted in a success rate above 94.5% for the correct localization of cortical activity at the closest electrode. This rate improved to 99.5% for the task of locating the electrical source at one of the two closest electrodes. Prediction error occurred more often for sources generating very small or very large peaks in the amplitude of the potential, but it decreased substantially with increasing the number of electrodes in the simulation. In the same study, but now using empirical data, the SL of Eq. (24) outperformed finite difference and the method of spherical splines discussed below.

Similar to finite difference, splines and other methods discussed below are usually affected by the density of the electrode array. In general, high-density arrays result in more accurate estimates. However, some preparation issues such as electrolyte bridges are mainly a characteristic of high-density estimates and should be a concern, as it is for finite difference (Tenke and Kayser, 2001). Another concern is that by increasing the number of electrodes the system (25) becomes increasingly sensitive to error (noise) in the input vector \( \mathbf{v} \). This problem is that of Fig. 4: the polar angle \( \theta \in [0, \pi] \) is measured down from the vertex, and the azimuthal angle \( \phi \in [0, 2\pi] \) increases counterclockwise from the \( x \) axis, which is directed toward the nasion. With this convention,

\[
\text{Lap}_s(f) = \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial f}{\partial \theta} \right] + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 f}{\partial \phi^2}.
\]

It can be proved that the Legendre polynomials satisfy (Jackson, 1999, p. 110)

\[
\text{Lap}_s(P_i(\hat{\mathbf{r}} \cdot \mathbf{r})) = -\frac{\ell (\ell + 1)}{r^2} P_i(\hat{\mathbf{r}} \cdot \mathbf{r}),
\]

thus leading to

\[
\text{Lap}_s(f)(\mathbf{r}) = -\frac{1}{r^2} \sum_{m=1}^{N} c_m g_{m-1}(\mathbf{r}, \mathbf{r}_m), \quad m > 1,
\]

which is known as the spherical SL of \( f(\mathbf{r}) \).

In comparison to the previous approach, the method of spherical splines has the advantage of providing a simple expression for the SL of \( f(\mathbf{r}) \) restricted to spherical geometry. Additionally, the geodesic distance ensures that the system (25) is non-singular, so that the coefficient \( d \) can be determined without using the pseudo-inverse of \( \mathbf{R} \).

### 3.3. Smoothing spherical splines

For the case of data points on spheres, Wahba (1981b) developed a pseudo-spline method that circumvents the singularity of Eq. (25) by replacing the Euclidean distance with the geodesic distance. This method, called spherical splines, was used by Perrin et al. (1989) to developed one of the most popular SL methods in the literature. In this case, the smoothing/interpolating function is defined as

\[
\hat{f}_{\text{spo}}(\mathbf{r}) = \sum_{i=1}^{N} c_i g_{m}(\mathbf{r}, \mathbf{r}_i) + d.
\]

\(^{14}\) That is, summing these columns with weights \(-1, 1/2, 1/3, 1/4\) yields a zero vector.

\(^{15}\) The condition number of a matrix \( \mathbf{A} \) is a real number that estimates the loss of precision in inverting this matrix numerically. This number, denoted by \( \text{cond}(\mathbf{A}) \), is usually computed as the ratio of the largest to smallest eigenvalue of \( \mathbf{A} \), implying that \( \text{cond}(\mathbf{A}) \approx 1 \).
However, some caution is required. In practice the term $f_{\text{NNLS}}(\mathbf{r}, \mathbf{r}_i)$ in Eq. (35) needs to be truncated for evaluation, and truncation error should not be overlooked. The left-out terms in the truncation are Legendre polynomials of higher-degree (large $\ell$), accounting for high-frequency spatial features. Too much filtering of such features can dilute the potential for improvement in spatial resolution. In view of that, one should keep as many Legendre polynomials as possible. Another point worth considering is the factor $(2\ell + 1)/\ell!(\ell + 1)^m$ that multiplies the Legendre polynomials in Eq. (32b). This factor falls off as $1/\ell^{2m-1}$. As $\ell$ increases, it approaches zero rapidly, resulting in a quick cancelation of higher-degree polynomials. The value assigned to $m$ must take this effect into account; the larger the value of $m$, the more dramatic is the reduction in high-frequency features. Typically, a value of $m$ between 2 and 6 provides satisfactory results for simulation and data analysis (Babiloni et al., 1995; de Barros et al., 2006; Carvalhaes and Suppes, 2011).

3.4. Other approaches

There are many other possible ways to estimate the SL of EEG signals. In this section we briefly review the methods proposed by Yao (2002) and Nunez and collaborators (Law et al., 1993a; Nunez and Srinivasan, 2006). Similar to thin-plate splines, Yao’s approach uses interpolation based on radial functions to estimate the SL of the potential. The interpolating function has the general form

$$f_{\text{RBF}}(\mathbf{r}) = \sum_{i=1}^{N} c_i e^{-\frac{\|\mathbf{r} - \mathbf{r}_i\|^2}{\sigma^2}} + b,$$

(36)

where $S(\mathbf{r}, \mathbf{r}_i)$ measures the arc of circle connecting $\mathbf{r}$ and $\mathbf{r}_i$ and the parameters $c_i$ and $b$ are subject to

$$f_{\text{RBF}}(\mathbf{r}_i) = V_i, \quad i = 1, \ldots, N,$$

(37)

where $\mathbf{r}_i$ is the location of the $i$th electrode and $V_i$ is the value of the potential at that location. Because the system (37) contains $N + 1$ unknowns\(^{16}\) but only $N$ equations, it is solved using pseudo-inversion (see the Appendix in Zhai and Yao (2004)).

In contrast to thin-plate splines, the Gaussian $e^{-\frac{\|\mathbf{r} - \mathbf{r}_i\|^2}{\sigma^2}}$ approaches zero asymptotically as the distance increases from $\mathbf{r}_i$. The parameter $\sigma$, commonly referred to as the spread parameter, controls the rate of decay of $e^{-\frac{\|\mathbf{r} - \mathbf{r}_i\|^2}{\sigma^2}}$. A large $\sigma$ produces a sharp decay, resulting in a short range of influence for each node $\mathbf{r}_i$. Yao recommended to set $\sigma$ according to the number of electrodes in the montage; for instance, $\sigma = 20$ for arrays with 32 sensors, $\sigma = 40$ for 64 sensors, and $\sigma = 50$ for 128 sensors. But he also remarked that a proper choice of $\sigma$ should take into account the source location. In principle, small values of $\sigma$ would be more suitable to fit deep brain sources, whereas shallow sources would be better described by small $\sigma$-values. In other words, interpolation with Gaussian functions is not automatic. The parameter $\sigma$ needs to be tuned properly for good performance, which can be difficult to achieve for non-equidistant electrodes. Nevertheless, Yao showed consistent results favoring the Gaussian method against spherical splines for simulated and empirical data. More recently Bortol and Sovka (2013) questioned the regularization technique used by Yao (2002) and the impossibility of obtaining good estimates without a prior knowledge about the source depth.

The method developed by Nunez and collaborators is called the New Orleans Spline-Laplacian (Law et al., 1993a; Nunez and Srinivasan, 2006). It uses an interpolating function that resembles two-dimensional splines but with knots in $\mathbb{R}^3$ instead of $\mathbb{R}^2$, i.e.,

$$f_{\text{NNLS}}(\mathbf{r}) = \sum_{i=1}^{N} c_i |\mathbf{r} - \mathbf{r}_i| \log \left( |\mathbf{r} - \mathbf{r}_i|^2 + \omega^2 \right) + d_1 + d_2 x + d_3 y + d_4 z + d_5 x^2 + d_6 x y + d_7 x z + d_8 y^2 + d_9 x y z + d_{10} z^2,$$

(38)

where the parameters $c_i$’s and $d_i$’s are determined in the fashion of Eq. (25). This method was implemented for spherical and ellipsoidal scalp models and its performance was studied using simulations and real data (Law et al., 1993a). A remark about the function $f_{\text{NNLS}}(\mathbf{r})$ is that it has no optimality property, except that for $\omega$ and $z$ equal to zero it corresponds to the unique minimizer of Eq. (23) in $\mathbb{R}^2$ (Duchon, 1977; Meinguet, 1979). But $f_{\text{NNLS}}(\mathbf{r})$ does not minimize Eq. (23) in $\mathbb{R}^3$, as the minimizer of Eq. (23) in $\mathbb{R}^3$ is unique and correspond to the spline function (24). In other words, $f_{\text{NNLS}}(\mathbf{r})$ is not actually a spline function.\(^{17}\) Despite that, Nunez and colleagues reported many studies showing a good performance of their method (Law et al., 1993b; Nunez and Westdorp, 1994; Nunez et al., 2001; Nunez and Srinivasan, 2006) and emphasized its agreement with cortical imaging algorithms in terms of correlation (Nunez et al., 1993, 1994).

3.5. The SL matrix

The computational cost of estimating the SL is usually not prohibitive, but in many circumstances it is enough to justify the use of an additional technique to improve performance. The SL matrix $\mathbf{L}$ is an excellent tool for this, and because of the linearity of the SL differentiation, it can be created for any of the SL methods above. For interpretation purposes the SL matrix can be viewed as a discrete representation of the differential operator $\text{Lap}_d$ at the electrode sites. We will illustrate below the method for finite differences and splines. Once the matrix $\mathbf{L}$ is obtained the SL estimate is carried out through the linear transformation

$$\text{Lap}_d(w) = \mathbf{L} w.$$

(39)

An important aspect of $\mathbf{L}$ is that its construction does not involve brain data, as otherwise it could not represent the mathematical operator $\text{Lap}_d$. This way we need to create $\mathbf{L}$ only once for each method and electrode configuration. But notice that $\mathbf{L}$ depends on the parameters $m$ and $\lambda$ for splines.

We will first illustrate the construction of $\mathbf{L}$ for finite difference approximations. In this case, $\mathbf{L}$ is constructed row by row using the scheme in Fig. 3. Electrodes that do not contribute to an approximation are assigned a zero weight in that computation. This way, each row of $\mathbf{L}$ has as many elements as the number of channels in the montage, but only five elements are nonzero in each row. This implies that $\mathbf{L}$ is a sparse matrix, with its sparsity increasing with the number of channels. Because the weights of each approximation sum to zero, the columns of $\mathbf{L}$ also sum to zero, which reflect the fact that the Laplacian transformation is reference-free.

As a simple illustration, consider the electrode arrangement in Fig. 5, with 9 electrodes evenly distributed in a square grid of spacing $h$.

The Laplacian matrix of this arrangement has dimension $9 \times 9$ and is given by

$$\mathbf{L} = \frac{1}{h^2} \begin{pmatrix}
2 & -2 & 1 & -2 & 0 & 0 & 0 & 0 & 0 \\
-1 & 1 & 1 & 0 & -2 & 0 & 0 & 1 & 0 \\
1 & -2 & 0 & 0 & -2 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 1 & 1 & -2 & -1 & 0 & 0 \\
1 & 0 & 0 & -2 & 0 & 0 & 2 & -2 & 1 \\
0 & 1 & 0 & 0 & -2 & 0 & 1 & -1 & 1 \\
0 & 0 & 1 & 0 & 0 & -2 & 1 & -2 & 2 \end{pmatrix}.$$

(40)

A quick inspection on the diagonal elements of $\mathbf{L}$ reveals that none of them is equal to zero, but they sum to zero. This means that $\mathbf{L}$ does not

\(^{16}\) Namely, we have to determine the $N + 1$ parameters $c_0, \ldots, c_N$ and $d$.

\(^{17}\) Due to the constraint (31), the NOSL algorithm is also affected by the singularity of Eq. (25) on spherical and ellipsoidal scalp models (see discussion in Section 3.2). Apparently, in an effort to remedy this problem the Matlab code of Nunez and Srinivasan (2006, p. 585) adds “noise” (error) to zero-valued electrode coordinates, effectively making Eq. (25) nonsingular, but not necessarily leading to a well-conditioned solution.
possess inverse. The inability to invert $L$ is not exclusive of finite differences, but rather a general property that reflects the ambiguity on the choice of reference. Stated in other words, the Laplacian transformation (39) cannot be uniquely undone due to the fact that the potential is not uniquely defined.

Mesh-free methods generate $L$ matrices that are non-sparse, i.e., most of their entries are nonzero. In the context of smoothing splines, Carvalhaes and Suppes (2011) showed that

$$L_\lambda = KC_\lambda + TD_\lambda,$$

(41)

where the subscript $\lambda$ emphasizes dependency on the regularization parameter, and

$$\begin{align*}
\bar{K}_{ij} &= \text{Lap}_\lambda\left(r_i - r_j\right)^{2m-2}, \\
\bar{T}_{ij} &= \text{Lap}_\lambda\left(V_i / (r_i)\right), \\
C_\lambda &= Q_2^{-1} \left( K + N\lambda I \right) Q_2^{-T}, \\
D_\lambda &= \bar{T}^T Q_2^{-1} \left( 1 - KC_\lambda - N\lambda C_\lambda \right).
\end{align*}$$

(42)

(43)

The matrix $L_\lambda$ also has no inverse, thus not allowing unambiguous inverse operation. This is due to the fact that $C_\lambda$ and $T$ are rank-deficient. In other words, since $Q_2$ has only $N - 1$ columns, only $N - 1$ degrees of freedom are available from $C_\lambda$. In turn, because the Laplacian operation $\text{Lap}_\lambda(V_i / r_i)$ vanishes at any polynomial $V_i$ of degree less than 2, the first four columns of $T$ are null.

For spherical splines, $\bar{K}_{ij} = -g_m(r_i, r_j) / r^2$, $T$ is a $N$-vector of ones, and $T$ is null, so that

$$L_\lambda = KC_\lambda,$$

(43)

which has rank $N - 1$ and does not possess inverse. Since $T$ is a vector of ones, its QR-factorization gives $R = -\sqrt{N}$, i.e., $R$ is a scalar instead of a matrix, and $Q_2 = -T / \sqrt{N}$. Consequently, $D_\lambda = T^T (1 - KC_\lambda - N\lambda C_\lambda) / N$, which is also a $N$-vector instead of a matrix.

As anticipated, the construction of $L$ and $L_\lambda$ is carried out without using brain data. Because the matrix $C_\lambda$ depends on the inverse of the matrix $[Q_2^T (K + N\lambda I) Q_2]$ it is subject to the numerical issues discussed in Section 3.2, so that it is recommended to set $\lambda$ nonzero and keep $m$ as small as possible for accurate results. The fact that the matrix $L$ for finite difference is sparse implies that the computational cost of finite difference is generally much smaller than the cost of splines. A quick calculation shows that for a signal containing $\tau$ time frames the cost of computing (39) with finite difference is $5N\tau$ floating-point operations ($\text{flops}$), while for splines this amounts to $N^2\tau$ flops. If we decide not to use the matrix $L_\lambda$ then the system (25) needs to be solved once for each frame, at the total cost of $(2/3)N^3\tau$ flops.

3.6. The regularization of smoothing splines

The use of smoothing splines to estimate the SL requires fixing the regularization parameter $\lambda$, which, as said above, has the beneficial effect of eliminating spatial noise. A key factor to guide toward a good choice of $\lambda$ is the mean square error function

$$R(\lambda) = \frac{1}{N} \sum_{i=1}^N \left(V_i - f_\lambda(r_i)\right)^2.$$  
(44)

Intuitively, this function measures infidelity of $f_\lambda(r)$ to the input data $(V_1, \ldots, V_N)$ due to smoothing. The goal of regularization is to weight this function appropriately to achieve a good balance between fidelity and variance reduction. The popular method of generalized cross-validation (GCV) proposed by Craven and Wahba (1979) addresses this problem in the following way. The GCV estimate of $\lambda$ is the value for which the GCV function

$$\text{GCV}(\lambda) = \frac{1}{N} \sum_{i=1}^N \left(V_i - f_\lambda(r_i)\right)^2 / \left(1 - \text{trace}(S_\lambda) / N\right)^2.$$  
(45)

reaches its minimum value. That is, the GCV criterion is to correct the squared residuals $(V_i - f_\lambda(r_i))^2$ about the estimate by dividing them by the factor $(1 - \text{trace}(S_\lambda) / N)^2$. The matrix $S_\lambda$ is a square matrix satisfying

$$\begin{bmatrix}
  f_\lambda(r_1) \\
  \vdots \\
  f_\lambda(r_N)
\end{bmatrix} = S_\lambda \begin{bmatrix}
  V_1 \\
  \vdots \\
  V_N
\end{bmatrix}.$$  
(46)

The matrix $S_\lambda$ is called the smoother matrix. The value $\lambda = 0$ (no smoothing) is excluded from GCV predictions, as it leads to $\text{trace}(S_\lambda) = N$. It follows from our previous development that

$$S_\lambda = KC_\lambda + TD_\lambda.$$  
(47)

The fact that this expression involves no differentiation means that $S_\lambda$ can be easily computed on any scalp model. We also remark that the columns of $S_\lambda$ sum to 1 (whereas the columns of $L_\lambda$ sum to 0), implying that the transformation (46) preserves the reference potential.

There are two inconveniences to be highlighted about the parameter $\lambda$. First, the parameter $\lambda$ has no upper bound, meaning that the search for the overall optimal value of $\lambda$ should include any real number from 0 to infinity. In practice, this search is performed on a finite interval (Babiloni et al., 1995), but there is no guarantee of convergence to the overall optimal $\lambda$. Second, the optimal value of $\lambda$ has no meaningful interpretation for comparison between different studies. For this reason, instead of thinking in terms of $\lambda$ it is convenient to think in terms of an alternative parameter $DF_\lambda$ that is called the effective degree of freedom of

---

18 This formula is valid only if $L$ is stored in the computer as a sparse matrix.

19 This is valid for an efficient resolution using LU decomposition (Press, 1992).
The parameter \( \text{DF}_x \) is defined by Hastie et al. (2009); James et al. (2013)

\[
\text{DF}_x = \text{trace}(S_x),
\]

where the trace operation sums over the diagonal elements of \( S_x \). The trace operation assigns a finite value to \( \text{DF}_x \), between 1 (\( \lambda = \infty \)) and \( N \) (\( \lambda = 0 \)), the lower bound\(^\text{20}\) representing the linear portion of \( f_x(r) \) and the upper bound reflecting the maximum variance, for which \( S_x \) is the projection matrix from regression over \( (V_1, \ldots, V_N)^T \).

In order to use \( \text{DF}_x \) instead of \( \lambda \) we need to invert the relation \((48)\).

Fig. 6 depicts the result for a montage with 32 sensors. Although \( \text{DF}_x \) is shown as if it were the independent variable, its values were actually determined from Eq. \((48)\) by fixing \( \lambda \). The Matlab code of Appendix B was used to compute \( S_x \). This code implements the spherical splines algorithm of Section 3.3 with a default error tolerance of less than \( 1 \times 10^{-10} \) to evaluate the infinity norm \((32b)\). The electrode locations were normalized to a sphere of radius 10 cm. Fig. 6 shows that \( \text{DF}_x \) decreases monotonically with \( \lambda \). Thanks to monotonicity we can interpolate the pairs \((\text{DF}_x, \lambda)\) to obtain a continuous curve from which we can estimate a given \( \text{DF}_x \). To fix ideas an example using real brain data is discussed in detail in the supplementary material.

4. Concluding remarks

The literature on the SL technique is quite large and this paper could only review or expand a few topics of general importance. It was our goal to give an intuitive view of the technique by providing physical insights that are often missing in the literature. In addition, we discussed some numerical methods to estimate the Laplacian, emphasizing each of its own set of strengths and limitations. Special attention was given to finite difference and spline methods. Finite difference is one of the simplest approaches for SL estimates, and its computational cost is advantageous, particularly for large numbers of electrodes. Its major disadvantage, however, is that estimates are prone to discretization errors and regularized estimates to eliminate spatial noise are not provided. Splines are still the main alternative to finite difference. The need for evenly-spaced electrodes and problems related to discretization are eliminated, the scalp geometry is more realistic, and spatial noise can be reduced through regularization. The cost of such improvement is reflected in an increase in mathematical complexity and a higher computational cost compared to finite difference.

Splines are sensitive to error in electrode locations (e.g., Bortel and Sovka, 2008), a problem affecting finite difference as well. The belief that accurate estimates at peripheral electrodes are made possible by splines is not entirely correct. In fact, note that the construction of \( f_x(r) \) involves \( N + M \) unknowns, which are the coefficients \( c_i \)'s and \( d_i \)'s in Eqs. \((24)\) and \((32a)\), but only \( N \) observations are available for each frame, which are the measured potentials \( V_1, \ldots, V_N \). To avoid underdetermination, the system \((25)\) contains an ad hoc condition \( T^c e = 0 \) that adds \( M \) more constraints to \( f_x(r) \), which has the geometric effect of canceling terms from \( f_x(r) \) that grow faster than a polynomial of degree \( m \) as one moves away from the electrodes. Estimates at central and peripheral electrodes are affected differently by this condition, with estimates at peripheral electrodes being less accurate. It was outside the scope of our work to discuss more realistic scalp-model methods and electrode location error, as they require tools such as MRI that are often not readily available to researchers (e.g., see Le and Gevins (1993); Gevins et al. (1994); Le et al. (1994); Babiloni et al. (1996); Bortel and Sovka (2013)).

Our discussion recommended to set the spline parameter \( m \) as equal to 3 or 4 to avoid numerical issues. Fig. 6 gives further insight into this problem. This example shows a compromise between \( m \), the effective number of degrees of freedom of the spline fit, and the lower bound of \( \lambda \). Although small and large values of \( m \) appear equally suitable to assess low degrees of freedom, say \( \text{DF}_x < 10 \), the fact that \( \lambda \) is bounded from below at \( 10^{-8} \) prevents us from exploiting the region of \( \text{DF}_x > 20 \) properly without setting \( m = 3 \) or 4. One may try to circumvent this limitation by decreasing the lower bound of \( \lambda \) toward zero, but as explained in Section 3.2 this has the problem of impoverishing the numerical conditioning, thus reinforcing our above recommendation.

Despite the broad literature on the subject, some basic problems on Laplacian estimates are still unsolved. One difficult problem that could not be addressed is related to the finite size of electrodes. All computational methods discussed here were built on the idea of a point-like electrode, but an electrode has a finite size, and for this reason EEG potentials should be interpreted as spatial averages instead of point values. A possible approach to this consists of replacing the variational problem \((23)\) with

\[
\text{RSS}(f, \lambda) = \frac{1}{N} \sum_i \left[ V_i - \int f(r_i) dA \right]^2 + \lambda J_m[f],
\]

\(^{20}\) The lower bound \( \text{DF}_x = 1 \) holds for spherical splines. For regular splines \( \text{DF}_x \) is at least equal to 2, depending on the dimension of the space.
where the double integral is over the area of the finite electrode. That is, we replace the interpolation condition \( V_i = f(x) \) by the volume matching condition \( V_i = \int_{\Omega} f(x) dA \). Wahba (1981a) studied this problem in Euclidean space and used the GCV statistics to estimate the optimal value of the parameter \( \lambda \). We seek a solution to the minimization problem on the sphere to deal with finite-sized electrodes on a spherical scalp model. This problem is arguably not trivial and almost certainly will require a numerical solution. Yet this is a simplified model that does not address the much more complicated problem of boundary effects due to the highly conductive electrode over the region \( \Omega \).

Considerable attention was devoted to the method of estimating the Laplacian derivation by means of a linear transformation, for which some figures were given estimating computational costs and encouraging the use of this procedure, mainly in the context of splines. Similar attention was paid to the problem of regularization to eliminate spatial noise. It is worth remarking that spatial regularization is not useful to eliminate noise coming from the reference electrode. In fact, because spline fits preserves the reference signal, the residuals \( \hat{a} = V_i - f_i(x) \) are reference-free, and so is the GCV error function, making evident that any noise due to the reference is fully preserved by regularization. This problem, however, should not cause much concern as it simply does not exist in the context of SI analysis.

Finally, we want to mention our effort in recent papers to develop a vector form of EEG that combines the SI and the tangential components of the electric field projected on the scalp surface (Wang et al., 2012; Carvalhaes et al., 2014). This combination was grounded on the observation that the SI derivation is closely related to the spatial component of the electric field oriented normally to the scalp surface, thus not containing substantial information about features encoded in tangential direction. Not surprisingly, this combination of physically distinct but somewhat supplementary quantities resulted in significant improvement for a variety of classification tasks as described in Carvalhaes et al. (2014).

Appendix A. The mathematics behind finite difference

A systematic way to obtain finite difference approximations for the derivatives of a function is based on the Taylor series expansion. To expand in terms of Taylor series, we formulate the problem in terms of a continuous function \( V \) and then, for compatibility with our notation in Section 3.1, rewrite the final approximation using discrete variables. In its simplest case, the Taylor series of a univariate function \( V(x) \) around a point \( x = a \) is defined by the infinite summation

\[
V(x + h) = V(a) + V'(a)h + \frac{1}{2!} V''(a)h^2 + \frac{1}{3!} V'''(a)h^3 + \ldots \quad (A-1)
\]

where \( h \) is called the increment, \( n! = n(n-1)(n-2) \ldots 1 \) is the factorial of \( n \), and \( V^{(n)}(a) \) denotes the \( n \)-th derivative of \( V(x) \) at \( x = a \). That is, the Taylor series of \( V(x) \) is a power series of \( h \) with coefficients given by the derivatives of \( V(x) \) at \( x = a \). To obtain an approximation for the second derivative (or any other derivative) of \( V(x) \) at \( x = a \) we proceed as follows. Replace \( h \) with \( -h \) in (A-1) and obtain an analogous expression for \( V(x - h) \), i.e.,

\[
V(x - h) = V(a) - V'(a)h - \frac{1}{2!} V''(a)h^2 - \frac{1}{3!} V'''(a)h^3 + \ldots
\]

Adding these two expressions,

\[
V(x + h) + V(x - h) = 2V(a) + V'(a)h^2 + \frac{1}{12} V''(a)h^4 + \ldots
\]

whence

\[
V'(a) = \frac{V(a + h) + V(a - h) - 2V(a)}{h^2} - \frac{1}{12} V''(a)h^2 + \ldots \quad (A-2)
\]

Assuming that \( h \) is sufficiently small we can ignore all terms containing powers of \( h \) and arrive at

\[
V'(a) \approx \frac{V(a + h) + V(a - h) - 2V(a)}{h^2}
\]

Replacing \( a = (i - 1)h \), \( i = 2, \ldots, N - 1 \), and using the notation \( V_i = V(a) \) and \( V_{i \pm 1} = V(a \pm h) \) yields

\[
V'(a) \approx V_{i+1} + V_{i-1} - 2V_i \quad (A-3)
\]

This expression was obtained by truncating the infinite series (A-2) after the first term. This way, starting from \( h^2 \) all powers of \( h \) were eliminated assuming that \( h \) was sufficiently small. The result was a second-order approximation \( ^{21} \), which in the “big-Oh” notation is referred to as \( O(h^2) \).

Approximation (A-3) excludes the case of a peripheral node, for which either \( V_{i+1} \) or \( V_{i-1} \) does not exist. In this case, we have to build the approximation using only nodes to the right or left of \( a \), but not both. For instance, let \( i = 1 \) and use the expansions

\[
V(x + h) = V(a) + V'(a)h + \frac{1}{2} V''(a)h^2 + \frac{1}{6} V'''(a)h^3 + \ldots
\]

\[
V(x + 2h) = V(a) + 2V'(a)h + 2V''(a)h^2 + \frac{4}{3} V'''(a)h^3 + \ldots
\]

from which

\[
V'(a) \approx \frac{V(a + 2h) - 2V(a + h) + V(a)}{h^2}
\]

\[
V'(a) \approx V_{i+2} - 3V_{i+1} + 3V_{i+1} - V_i
\]

In terms of the grid variables,

\[
V'(a) \approx \frac{V_{i+2} - 2V_{i+1} + V_i}{h^2} \quad (A-4)
\]

which is a first order approximation. Note that this expression corresponds to the formula obtained by Freeman and Nicholson (1975) for one-dimensional estimate of intracranial CSD.

A.1. Bivariate functions and approximations for \( \nabla^2 V(a, b) \)

The extension of (A-1) to bivariate functions replaces ordinary derivatives with partial derivatives. Namely,

\[
V(a + h_1, b + h_2) - V(a, b) = \frac{\partial V(a, b)}{\partial x} h_1 + \frac{\partial V(a, b)}{\partial y} h_2 + \frac{1}{2!} \left[ \frac{\partial^2 V(a, b)}{\partial x^2} h_1^2 + \frac{\partial^2 V(a, b)}{\partial x \partial y} h_1 h_2 + \frac{\partial^2 V(a, b)}{\partial y^2} h_2^2 \right] + \ldots
\]

\[
\approx \frac{1}{2!} \left[ \frac{\partial^2 V(a, b)}{\partial x^2} h_1^2 + \frac{\partial^2 V(a, b)}{\partial x \partial y} h_1 h_2 + \frac{\partial^2 V(a, b)}{\partial y^2} h_2^2 \right] + \ldots
\]

\[
\approx \frac{1}{12} \left[ \frac{\partial^3 V(a, b)}{\partial x^3} h_1^3 + \frac{3}{2} \frac{\partial^3 V(a, b)}{\partial x^2 \partial y} h_1^2 h_2 + \frac{3}{2} \frac{\partial^3 V(a, b)}{\partial x \partial y^2} h_1 h_2^2 + \frac{\partial^3 V(a, b)}{\partial y^3} h_2^3 \right] + \ldots
\]

\[
\approx \frac{1}{12} \left[ \frac{\partial^3 V(a, b)}{\partial x^3} h_1^3 + \frac{3}{2} \frac{\partial^3 V(a, b)}{\partial x^2 \partial y} h_1^2 h_2 + \frac{3}{2} \frac{\partial^3 V(a, b)}{\partial x \partial y^2} h_1 h_2^2 + \frac{\partial^3 V(a, b)}{\partial y^3} h_2^3 \right] + \ldots
\]

Similar to the one-dimensional case, with appropriate choices for \( h_1 \) and \( h_2 \) one can use this expansion to approximate the partial derivatives of \( V(x, y) \) at any point in a rectangular grid. An

\[ ^{21} \] The order of a finite difference approximation is given by the smallest power of \( h \) that is left out in the truncation.
approximation for the Laplacian of $V(x, y)$ at a central node of a square grid ($h_1 = h_2 = h$) is obtained as follows. First, use Eq. (A-5) to expand $V(a \pm h, b)$ and $V(a, b \pm h)$:

$$
V(a \pm h, b) = V(a, b) \pm \frac{\partial V(a, b)}{\partial x} h + \frac{1}{2} \frac{\partial^2 V(a, b)}{\partial x^2} h^2 + \frac{1}{6} \frac{\partial^3 V(a, b)}{\partial x^3} h^3 + \cdots
$$

$$
V(a, b \pm h) = V(a, b) \pm \frac{\partial V(a, b)}{\partial y} h + \frac{1}{2} \frac{\partial^2 V(a, b)}{\partial y^2} h^2 + \frac{1}{6} \frac{\partial^3 V(a, b)}{\partial y^3} h^3 + \cdots
$$

Second, add these four expressions to obtain

$$
V(a + h, b) + V(a - h, b) + V(a, b + h) + V(a, b - h) - 4V(a, b) = \frac{\partial^2 V(a, b)}{\partial x^2} h^2 + \frac{\partial^2 V(a, b)}{\partial y^2} h^2 + \cdots
$$

whence

$$
\text{Lap}(V(a, b)) = \frac{\partial^2 V(a, b)}{\partial x^2} h^2 + \frac{\partial^2 V(a, b)}{\partial y^2} h^2 + \cdots
$$

which is a first-order approximation. In terms of the grid variables,

$$
\text{Lap}(V)_{(i,j)} \approx \frac{V(i, j+1) - 2V(i, j) + V(i, j-1)}{h^2} + \frac{V(i+1, j) - 2V(i, j) + V(i-1, j)}{h^2},
$$

(A-8a)

In a similar fashion, for grid points at right, bottom, and upper edges (excluding the corners) we obtain, respectively,

$$
\text{Lap}(V)_{(i,N)} \approx \frac{V(i, N-2) - 2V(i, N-1) + V(i, N)}{h^2},
$$

(A-8b)

$$
\text{Lap}(V)_{(N,j)} \approx \frac{V(N-2, j) - 2V(N-1, j) + V(N, j)}{h^2},
$$

(A-8b)

$$
\text{Lap}(V)_{(1,j)} \approx \frac{V(3, j) - 2V(2, j) + V(1, j)}{h^2},
$$

(A-8c)

Finally, assume that the node of interest is at the left upper corner of the grid, corresponding to $i = j = 1$ ($a = 0, b = (N - 1)h$). To approximate the Laplacian of $V$ at this node we use

$$
\text{Lap}(V)_{(1,1)} \approx \frac{V(3, 1) - 2V(2, 1) + V(1, 1)}{h^2},
$$

(A-10)

Adding these expansions with weights $-2, 1, 1,$ and $-2$ yields

$$
-2V(h, b) + V(2h, b) + V(0, b - 2h) - 2V(0, b - h) - 2V(0, b) = \frac{\partial^2 V(a, b)}{\partial x^2} h^2 + \frac{\partial^2 V(a, b)}{\partial y^2} h^2 + \cdots
$$

Solving for $\text{Lap}(V)$ we obtain the first-order approximation

$$
\text{Lap}(V)_{(0, 0)} \approx \frac{V(2h, b) - V(0, b)}{h^2} + \frac{V(0, b - 2h) - 2V(0, b - h) + V(0, b)}{h^2},
$$

Equivalently,

$$
\text{Lap}(V)_{(1,1)} \approx \frac{V(1, 3) - V(2, 1) + V(3, 1) - 2V(2, 1) + V(1, 1)}{h^2}.
$$

(A-10)

Using symmetry we can obtain similar approximations for the other corners of the grid illustrated in Fig. 3.

Appendix B. A Matlab code to construct $S_\lambda$ and $I_\lambda$

Here we present a Matlab code to build the smoother matrix $S_\lambda$ and the SL matrix $I_\lambda$ using spherical splines. The first function, sphlap0.m, is an auxiliary function to generate the matrices $K, K, T, Q_1, Q_2,$ and $R$ presented above. Since none of these matrices depend on the regularization parameter $\lambda$, they need to be computed only once for each value of $m$ and electrode configuration. The computation of these matrices is not fast because it involves the evaluation of Legendre polynomials. Therefore, for efficiency, this function should never be called inside a regularization loop. The second function, sphlap.m, receives the output of sphlap0.m as argument plus the value of $\lambda$ and return the matrices $S_\lambda$ and $I_\lambda$. This is the function that should be used inside a regularization loop.
Listing 1: Auxiliary function to compute spherical splines

% sphlap0.m - Auxiliary function to compute spherical splines

% Usage: [K, LapK, T, Q1, Q2, R] = sphlap0(x, y, z, m, tol);
% % Required inputs
% x, y, z: electrode coordinates (must be on a sphere)
% m: interpolation order (2<m<6)
% % Optional Input
% tol: error tolerance in the estimate of the Legendre polynomials.
% Default is 1e-10.
% % Output
% K, LapK, T, Q1, Q2, R: matrices required to implement spherical splines
% 
function [K, LapK, T, Q1, Q2, R] = sphlap0(x, y, z, m, tol)

% Handle arguments
if nargin < 4
    help sphlap0.m;
    return;
end

if nargin == 4
    tol = 1e-10;
end

if m < 2 || m > 6
    error('sphlap0:interorder', 'The parameter "m" should be in the range of 2 and 6');
end

r = sqrt(r2); % radial distance
r2 = r2 - (z(1)^2); % squared head radius

G = []; % auxiliary matrices
G0 = 0;
epsilon = tol + 1; % final error tolerance

while (tol < epsilon)
    Pn = legendre(n, cos_gamma(:));
    a = (2*n+1) / (n*(n+1));
    gm = a * Pn(:,1);
    G = horzcat(G, gm);
    LapG = horzcat(LapG, -n * (n+1) * gm);
    epsilon = max(max(abs(G(:,end) - G0)));
    G0 = G(:,end);
    n = n + 1;
end

R = G(:,end); % final residual

K = reshape(sum(G), N, [])./(4*pi);
LapK = reshape(sum(LapG), N, [])./(4*pi*r2);
T = ones(N, 1);

% QR decomposition of T
[Q, R] = qr(T);
R = R(1);
Q1 = Q(:, 1);
Q2 = Q(:, 2:N);

% Alternative
A = -sqrt(W);
Q1 = Q1 / R;
% [V, U] = svd(T);
Q2 = U(:, 2:end);
end
Listing 2: Function to compute the smoother and the Laplacian matrices

```
function [S, L] = sphlap(R, LapK, T, Q1, Q2, R, lambda)

% sphiap.m - Compute the smoother and Laplacian matrices using spherical splines

% Usage: [S, L] = sphlap(R, LapK, T, Q1, Q2, R, lambda);

% Required Inputs
% R, LapK, T, Q1, Q2, and R: matrices generated by sphlap
% lambda: smoothing parameter

% Output:
% S = the smoother matrix
% L = the Laplacian matrix

% Handle arguments
if nargin < 7
    help sphlap.m;
    return;
end

I = eye(size(K,1));
Klamb = K + lambda*I;

C = Q2 / Q2';
Klamb = Q2 * Q2';
D = R(1:Q1').*(I - Klamb*C);

S = K + C + T * D;
L = LapK * C;
% The Laplacian matrix

end
```

Appendix C. Supplementary data

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.ijpsycho.2015.04.023.

References


