Supplement

The purpose of this supplement is to put our method on a sound theoretical footing by studying the mathematical problem of constructing the gcGCFMs (and a fortiori the transformation matrix $L$) from diffusion measurements of an isotropic phantom. We will show that, in general, seven images (one $b=0$ image and six images with specific diffusion sensitization directions) are sufficient to uniquely determine all the elements of $L$ to within an additive constant that is known to be zero for a properly constructed coil, and that only four images (one $b=0$ image and three diffusion weighted images) are required if it is known a priori that the fields possess certain symmetries under reflection.

Uniqueness proof

The purpose of the following analysis is to show that a particular set of diffusion measurements contains enough information to compute $L$; it is not a practical algorithm. In the next section we apply the results to the method described in the main body of the paper.

We start by describing the gradient of the $z$-component of the magnetic field produced by a real gradient coil as the sum of the fields generated by an "ideal" gradient coil and "nonlinear" terms describing the deviation from the "ideal" field:

$$L_{jk} \equiv \frac{\partial B_k}{\partial r_j} = g_k (\delta_{jk} + \epsilon_{jk}(r))$$  \hspace{1cm} (S1)

where the "gain factors" $g_k$ are the values of $L_{kk}$ at the center of the gradient set, which we use as the origin of our coordinate system.

We restrict our analysis to a region where the contribution of the "nonlinear" terms is small compared to the "ideal" field:

$$\epsilon_{jk}(r) << 1$$  \hspace{1cm} (S2)

Plugging Eq (S1) into Eq (6) and omitting terms that are quadratic in $\epsilon$, we find that

$$tr(b) = B_x^2 (1 + 2\epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}) + B_y^2 (1 + 2\epsilon_{yy} + \epsilon_{zz}) + B_z^2 (1 + 2\epsilon_{zz} + \epsilon_{xx}) + B_x B_y (\epsilon_{xy} + \epsilon_{yx}) + B_x B_z (\epsilon_{xz} + \epsilon_{zx}) + B_y B_z (\epsilon_{yz} + \epsilon_{zy}) + O(\epsilon^2)$$  \hspace{1cm} (S3)

Examining Eq (S3), we see that $tr(b(r))$ (and therefore $E(r)$) depends only on the symmetric part of the matrix $\epsilon$. Since $\epsilon$ in general is not symmetric, the off-diagonal elements $\epsilon_{jk}(r)$, $k \neq j$, cannot be determined from measurements of the diffusion attenuation at $r$; we need more information. We will use the fact that each of the gcGCFMs ($B_x^*, B_y^*$, and $B_z^*$) is the $z$-component of a magnetic field in a source-free region and therefore obeys Laplace’s equation.

We assume that we have diffusion measurements that permit us to compute the attenuation function $E(r)$ defined by Eq (1) for different diffusion weightings in a convex region. Consider first the signal attenuation for an image with prescribed $b$-vector pointing in the $x$-direction. The diffusion weighting $G$ for such an image is

$$G = G^x = \sqrt{b}(1, 0, 0).$$  \hspace{1cm} (S4)
and the corresponding prescribed b-matrix (see Eq (5)) is

\[ b^* = \begin{pmatrix} b & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

We denote the resulting attenuation function \( E^{xx}(r) \). Using Eqs (1), (S1), and (S3) we find

\[ L_{xx} \equiv \frac{\partial^2 B^x}{\partial x^2} = \frac{g_x}{2} \left( 1 - \frac{\log(E^{xx}(r))}{Dg_x^2 b} \right) \equiv h_x(r). \]

Since \( E^{xx}(r) \) and \( g_x \) can be computed from the data, \( h_x(r) \) is a known function of \( r \). Integrating Eq (S6) with respect to \( x \) we find

\[ B^x(x, y, z) = H_x(x, y, z) + F_x(y, z) \]

where

\[ H_x(x, y, z) = \int h_x(x, y, z) \, dx, \]

and \( F_x(y, z) \) is a function that (1) does not depend on \( x \) and (2) obeys Laplace’s equation in 2-dimensions:

\[ \left( \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) F_x = 0 \]

Analogous arguments are valid for measuring \( B^y \) and \( B^z \) from images with b-vectors \( e_y = (0, 1, 0) \) and \( e_z = (0, 0, 1) \), respectively. The analogs to Eqs (S6) and (S7) are

\[ L_{yy} = \frac{\partial B^y}{\partial y} = \frac{g_y}{2} \left( 1 + \frac{\log(E^{yy}(r))}{Dg_y^2 b} \right) \equiv h_y(r) \]

\[ L_{zz} = \frac{\partial B^z}{\partial z} = \frac{g_z}{2} \left( 1 + \frac{\log(E^{zz}(r))}{Dg_z^2 b} \right) \equiv h_z(r) \]

where

\[ B^y(x, y, z) = H_y(x, y, z) + F_y(x, z) \]

\[ B^z(x, y, z) = H_z(x, y, z) + F_z(x, y) \]

and

\[ H_y(x, y, z) = \int h_y(x, y, z) \, dy, \]

\[ H_z(x, y, z) = \int h_z(x, y, z) \, dz, \]
and $F_y(x, z)$ and $F_z(x, y)$ are functions that obey Laplace’s equation in 2-dimensions:

\[
\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) F_y = 0 \quad \text{(S16)}
\]

\[
\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) F_z = 0. \quad \text{(S17)}
\]

The off-diagonal elements of $L$ are computed by taking derivatives of Eqs (S7), (S12), and (S13):

\[
L_{jk} = \frac{\partial B^k}{\partial r^j} = \frac{\partial H^k}{\partial r^j} + \frac{\partial F^k}{\partial r^j}, \quad k \neq j \quad \text{(S18)}
\]

Since Eq (S18) contains the derivatives of the unknown functions $F_k$, more information is needed to uniquely determine the off-diagonal elements of $L$.

We now consider what we can learn from images with diffusion weighting in two directions. Consider images acquired with prescribed diffusion sensitization $G_{xy}$ defined by

\[
G_{xy} = \sqrt{b} \left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right) \quad \text{(S19)}
\]

which results in the the b-matrix

\[
b^{xy} = \begin{pmatrix}
\frac{b}{2} & \frac{b}{2} & 0 \\
\frac{b}{2} & \frac{b}{2} & 0 \\
0 & 0 & 0
\end{pmatrix} \quad \text{(S20)}
\]

Using Eqs (1),(S1),(S3),(S7), and (S12), we find

\[
K_{xy}(r) = g_x \frac{\partial F_y}{\partial x} + g_y \frac{\partial F_x}{\partial y} \quad \text{(S21)}
\]

where $K_{xy}$ is a known function of $r$:

\[
K_{xy}(r) \equiv -\left( \frac{2 \log(E^{xy})}{D} + g_x \left( 2h_x + \frac{\partial H_y}{\partial x} - g_y \right) + g_y \left( 2h_y + \frac{\partial H_x}{\partial y} - g_x \right) \right) \quad \text{(S22)}
\]

The right side of Eq (S21) is the sum of two terms, one of which, $K_{xy}^y(x, z) = g_x \frac{\partial F_y}{\partial x}$, doesn’t depend on $y$ and the other, $K_{xy}^x(y, z) = g_y \frac{\partial F_x}{\partial y}$, doesn’t depend on $x$.

We now investigate the uniqueness of the decomposition. Assume that there is another pair of functions, $\tilde{K}_{xy}^y(x, z)$ and $\tilde{K}_{xy}^x(y, z)$ that share that property:

\[
K_{xy}(x, y, z) = K_{xy}^x(y, z) + K_{xy}^y(x, z) \quad \text{(S23)}
\]

\[
K_{xy}(x, y, z) = \tilde{K}_{xy}^x(y, z) + \tilde{K}_{xy}^y(x, z) \quad \text{(S24)}
\]

Subtracting Eq (S24) from Eq (S23) we find

\[
0 = X_{diff}(y, z) + Y_{diff}(x, z) \quad \text{(S25)}
\]
where

\[ X_{diff}(y, z) = K'_{xy}(y, z) - \tilde{K}'_{xy}(y, z) \] (S26)

\[ Y_{diff}(y, z) = K'_{xy}(x, z) - \tilde{K}'_{xy}(x, z) \] (S27)

The solution to Eq (S25) is

\[ X_{diff}(y, z) = -Y_{diff}(x, z) = f_z(z) \] (S28)

where \( f_z(z) \) is any function that does not depend on \( x \) or \( y \). We can therefore separate Eq (S21) into two equations

\[ \frac{\partial F_x}{\partial y} = \left( \frac{1}{g_y} \right) K_{xy}^x(y, z) + f_z(z) \] (S29)

\[ \frac{\partial F_y}{\partial x} = \left( \frac{1}{g_x} \right) K_{xy}^y(x, z) - f_z(z) \] (S30)

where \( K_{xy}^x(y, z) \) and \( K_{xy}^y(x, z) \) are any solution to Eq (S23). Integrating Eqs (S29) with respect to \( y \) and (S30) with respect to \( x \) we find

\[ F_x(y, z) = X_y(y, z) + f_z(z) y + f_{z2}(z) \] (S31)

\[ F_y(x, z) = Y_x(x, z) - f_z(z) x + f_{z3}(z) \] (S32)

where

\[ X_y(y, z) \equiv \left( \frac{1}{g_y} \right) \int K_{xy}^x(y, z) \, dy \] (S33)

and

\[ Y_x(x, z) \equiv \left( \frac{1}{g_x} \right) \int K_{xy}^y(x, z) \, dx \] (S34)

are known functions and \( f_{z2}(z) \) and \( f_{z3}(z) \) are functions that do not depend on either \( x \) or \( y \). Plugging Eq (S31) into (S9) and Eq (S32) into (S16) we find

\[ f_{z1} = A_{z1} z + B_{z1} \] (S35)

\[ f_{z2} = A_{z2} z + B_{z2} \] (S36)

\[ f_{z3} = A_{z3} z + B_{z3} \] (S37)

where \( A_{z1}, B_{z1}, A_{z2}, B_{z2}, A_{z3}, \) and \( B_{z3} \) are real numbers that cannot be determined from the three diffusion measurements with b-vectors \( e_x, e_y \) and \( e_{xy} \). Plugging Eqs (S35) and (S36) into Eq (S31) and Eqs (S35) and (S37) into Eq (S32) yields
\[ F_x(y, z) = X_y(y, z) + A_{21}yz + B_{21}y + A_{22}z + B_{22} \]  
(S38)

\[ F_y(x, z) = Y_x(x, z) - A_{21}xz - B_{21}x + A_{23}z + B_{23} \]  
(S39)

If we also acquire two additional images with prescribed diffusion weightings \( G^xz \) and \( G^yz \) defined by

\[ G^xz = \sqrt{b} \left( \frac{1}{\sqrt{2}}, 0, \frac{1}{\sqrt{2}} \right) \]  
(S40)

and

\[ G^yz = \sqrt{b} \left( 0, \frac{1}{\sqrt{2}}, 1 \right) \]  
(S41)

with corresponding \( b \)-matrices

\[ b^xz = \begin{pmatrix} \frac{b}{2} & 0 & \frac{b}{2} \\ 0 & 0 & 0 \\ \frac{b}{2} & 0 & \frac{b}{2} \end{pmatrix} \]  
(S42)

and

\[ b^yz = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{b}{2} & \frac{b}{2} \\ 0 & \frac{b}{2} & \frac{b}{2} \end{pmatrix} \]  
(S43)

Subtracting Eq (S44) from (S38), (S45) from (S39), and (S46) from (S47) we get the equations

\[ F_x(y, z) = X_z(y, z) - X_y(y, z) = (A_{21} + A_{y1})yz + \]  
\[ + (B_{21} - A_{y1})y + (A_{22} + B_{y1})z + (B_{22} - B_{y1}) \]  
(S48)

\[ F_y(x, z) = Y_z(x, z) - Y_x(x, z) = (A_{21} + A_{x1})xz + \]  
\[ + (A_{22} + B_{x1})x + (B_{22} - B_{x1})z + (B_{22} - B_{x1}) \]  
(S49)

\[ F_z(x, y) = Z_x(x, y) - Z_y(x, y) = (A_{21} + A_{y1})yz + \]  
\[ + (B_{21} - A_{y1})y + (A_{22} + B_{y1})z + (B_{22} - B_{y1}) \]  
(S50)

Since left hand sides of Eqs (S48), (S49), and (S50) are known functions, the coefficients in each term on the right hand side is also known. In particular, the equations for the first terms on the right hand side of Eqs (S48), (S49), and
Without loss of generality, we can require that to first order in $(S_{12})$, and $(S_{13})$ can be written as

$$
\frac{\partial H_1}{\partial x} = A_{x1}, \quad \frac{\partial H_1}{\partial y} = A_{y1}, \quad \frac{\partial H_1}{\partial z} = A_{z1},
$$

Since the determinant of the matrix of the coefficients in Eq (S51) is not zero, the equation has a unique solution; the constants $A_{x1}$, $A_{y1}$, and $A_{z1}$ are determined by the measurements. Equations corresponding to the other terms in Eqs (S48), (S49), and (S50) constitute constraints on the other coefficients, but do not uniquely determine any of them. Using Eqs (S38), (S39), (S44) - (S47), and the fact that $A_{x1}$, $A_{y1}$, and $A_{z1}$ are known from the measurements, Eqs (S7), (S12), and (S13) can be written as

$$
B^x(x, y, z) = \tilde{H}_x(x, y, z) + a_{yx}y + a_{zx}z + a_x
$$

$$
B^y(x, y, z) = \tilde{H}_y(x, y, z) + a_{xy}x + a_{zy}y + a_y
$$

$$
B^z(x, y, z) = \tilde{H}_z(x, y, z) + a_{xz}x + a_{yz}y + a_z
$$

where the functions $\tilde{H}_i(x, y, z)$ are known from the measurements while all the $a_{ij}$s and $a_k$s are unknown constants. Without loss of generality, we can require that $\tilde{H}_x(x, y, z)$ contains no linear functions of $y$ and $z$, $\tilde{H}_y(x, y, z)$ contains no linear functions of $x$ and $z$, and $\tilde{H}_z(x, y, z)$ contains no linear functions of $x$ and $y$. Furthermore, the uniform fields described by the constants $a_i$ do not contribute to $\mathbf{L}$, which depends only on the derivatives of the $B^k$.

Eqs (S52) - (S54) imply that diffusion measurements of an isotropic phantom determine the GCFMs to within an additive linear function, and hence the off-diagonal elements of the gradients of the GCFMs to within a constant; they cannot measure the direction of the gradients at the origin. If the gradient coils are properly constructed, the direction of the gradient at the origin is known, and the unknown constants in Eqs (S52) - (S54) can be set to zero.

Although the direction of the gradient at the origin cannot be measured, it can be determined whether the gradients of the fields produced at the origin by the three gradient coils are orthogonal. Using Eqs (S1),(S7), (S12), and (S13), the gradients at origin are

$$
\nabla B^x = (1, \epsilon_{yx}(r = 0), \epsilon_{zx}(r = 0) )
$$

$$
\nabla B^y = (\epsilon_{xy}(r = 0), 1, \epsilon_{zy}(r = 0) )
$$

$$
\nabla B^z = (\epsilon_{xz}(r = 0), \epsilon_{yz}(r = 0), 1 )
$$

To first order in $\epsilon_{ij}$, the dot products of the gradient fields at the origin are

$$
\nabla B^x(r = 0) \cdot \nabla B^y(r = 0) = \epsilon_{yx}(r = 0) + \epsilon_{xy}(r = 0)
$$

$$
\nabla B^x(r = 0) \cdot \nabla B^z(r = 0) = \epsilon_{xz}(r = 0) + \epsilon_{zx}(r = 0)
$$

$$
\nabla B^y(r = 0) \cdot \nabla B^z(r = 0) = \epsilon_{yz}(r = 0) + \epsilon_{zy}(r = 0)
$$

But from Eq (S3), we see that the right hand sides of Eqs (S58) - (S60) can be directly measured; if the measured value is nonzero to within experimental error, the gradients are not orthogonal.

We have shown that six diffusion weighted images plus one $b = 0$ image contain enough information to measure the GCFMs to within a linear function. If the gradients are orthogonal at the origin, which can also be determined
from the measurements, the unknown function can probably be safely set to zero.

We now discuss an assumption, reasonable for many coil designs, that permit the GCFMs to be determined from only four images. The fields produced by most gradient coils (some high performance insert gradient coils are the exception) have the following symmetries:

\[ B^x(-x,y,z) = -B^x(x,y,z) \]  
\[ B^x(x,-y,z) = B^x(x,y,z) \]  
\[ B^x(x,y,-z) = B^x(x,y,z) \]  
\[ B^y(-x,y,z) = B^y(x,y,z) \]  
\[ B^y(x,-y,z) = -B^y(x,y,z) \]  
\[ B^y(x,y,-z) = B^y(x,y,z) \]  
\[ B^z(-x,y,z) = B^z(x,y,z) \]  
\[ B^z(x,-y,z) = B^z(x,y,z) \]  
\[ B^z(x,y,-z) = -B^z(x,y,z) \]

Since the unknown function \( F_x(y,z) \) in Eq (S7) lacks symmetry Eq (S61), the unknown function \( F_y(x,z) \) in Eq (S12) lacks symmetry Eq (S65), and the unknown function \( F_z(x,y) \) in Eq (S13) lacks symmetry Eq (S69), these functions are all zero for symmetrical coils, and in this case three diffusion weighted images are sufficient to uniquely determine the GCFMs.

**Application to Least-squares fitting**

In practice, the gcGCFMs are computed not by integration, but by minimizing the cost function \( \Phi \) defined by Eq (7) to find the coefficients in an expansion of \( B^k \) in solid harmonics (See Appendix A). If too few images are acquired to uniquely determine the coefficients of all the basis functions included in the expansion, the equations that have to be solved to minimize \( \Phi \) will be singular. The equations can be regularized either by solving the linear system using singular value decomposition or by explicitly omitting from the expansion terms whose coefficients cannot be determined, which we now identify.

We analyze first the 7-image method. The basis functions in Eq (A6) whose contributions cannot be evaluated are

for \( B^x \): \( u^{\cos}_0, u^{\cos}_{10}, \) and \( u^{\sin}_{11} \),

for \( B^y \): \( u^{\cos}_0, u^{\cos}_{10}, \) and \( u^{\cos}_{11} \), and

for \( B^z \): \( u^{\cos}_0, u^{\cos}_{11}, \) and \( u^{\sin}_{11} \).

As discussed above, the coefficients for these terms can all safely be set to 0.

Before we analyze the 4-image method, we observe that the derivative \( \frac{\partial u_{lm}}{\partial r} \) is a linear combination of the basis functions \( u_{l-1,m} \). To prove this, notice that \( u_{lm} \) is a homogeneous polynomial of degree \( l \), so its derivative is a homogeneous polynomial of degree \( l-1 \). The result follows from the observation that the derivatives of \( u_{lm}(r) \) also obey Laplace’s equation.

In the 4-image method, we try to reconstruct \( B^k(r) \) from measurements of \( \epsilon_{zz} \), which depends only on \( \frac{\partial B^z}{\partial z} \). But for a given value of \( l \), the contribution to \( B^z(r) \) is a linear combination of the \( 2l+1 \) functions \( u_{lm} \), while \( \frac{\partial B^z}{\partial z} \) is a linear combination of the \( 2l-1 \) functions \( u_{l-1,m} \); vectors in a two dimensional subspace of the \( 2l+1 \) dimensional
vector space spanned by $u_{lm}$ do not contribute to the cost function, and their coefficients cannot be determined. The unknown function $F_z(r)$ in Eq (S13) lies in this subspace. The coefficients that cannot be determined are $c_{ll}$ and $s_{ll}$; the corresponding basis functions $u_{ll}^{\cos}$ and $u_{ll}^{\sin}$ do not depend on $z$. This can be proved using the explicit formula for the associated Legendre function [1]:

$$P_l^m(x) = (-1)^m \left(1 - x^2\right)^{\frac{m}{2}} \frac{d^m}{dx^m} P_l(x)$$

(S70)

where $P_l(x)$ is the Legendre polynomial of degree $l$. Since $P_l(x)$ is a polynomial of degree $l$, its $l$-th derivative is a constant, and Eq (S70) becomes

$$P_l^l(\cos(\theta)) = a \sin^m(\theta),$$

(S71)

and

$$u_{ll}^{\cos} = a(r \sin(\theta))^m \cos(m\phi)$$

(S72)

$$u_{ll}^{\sin} = a(r \sin(\theta))^m \sin(m\phi)$$

(S73)

$r \sin(\theta) = \sqrt{x^2 + y^2}$ and $\phi = \arctan(y/x)$, so the $u_{ll}$ are not functions of $z$. Since the fields generated by most $z$-gradient coils obey Eq (S69), $c_{ll}$ and $s_{ll}$ are in fact zero, and the 4-image method, like the 7-image method, determines $B^z(r)$ to within a linear function of $x$ and $y$.

If we apply the above argument to the $x$- and $y$- gradient coils, we see that the functions $F_x(r)$ and $F_y(r)$ that cannot be determined using the 4-image method can be expressed simply in solid harmonics if we use $x$- or $y$- as the direction of the polar axis. Unfortunately, there is no simple formula for expressing these functions in terms of the solid harmonic basis we use in which the polar axis is the $z$-axis.

Many terms can be excluded from the expansion of the ggGCFMs of coils that have the symmetries described by Eqs (S61)-(S69) by studying the reflection symmetries of the solid harmonics. All of the solid harmonics have either even or odd symmetry under reflections in the $x$-, $y$-, or $z$- directions:

$$u_{lm}^{\cos}(-x, y, z) = (-1)^m u_{lm}^{\cos}(x, y, z)$$

(S74)

$$u_{lm}^{\cos}(x, -y, z) = u_{lm}^{\cos}(x, y, z)$$

(S75)

$$u_{lm}^{\cos}(x, y, -z) = (-1)^{(l+m)} u_{lm}^{\cos}(x, y, z)$$

(S76)

$$u_{lm}^{\sin}(-x, y, z) = (-1)^{(l+1)} u_{lm}^{\sin}(x, y, z)$$

(S77)

$$u_{lm}^{\sin}(x, -y, z) = (-1) u_{lm}^{\sin}(x, y, z)$$

(S78)

$$u_{lm}^{\sin}(x, y, -z) = (-1)^{(l+m)} u_{lm}^{\sin}(x, y, z)$$

(S79)

Using Eqs (S67), (S68), (S69), (S76), and (S79), we see that the only basis functions that contribute to $B^z(r)$ are $u_{lm}^{\cos}$ with $l$ odd and $m$ even.

Using Eqs (S61), (S62), (S63), (S74), and (S77), we see that the only basis functions that contribute to $B^x(r)$ are $u_{lm}^{\cos}$ with $l$ odd and $m$ odd.

Using Eqs (S64), (S65), (S66), (S75), and (S78), we see that the only basis functions that contribute to $B^y(r)$ are $u_{lm}^{\sin}$ with $l$ odd and $m$ odd.
Since the radial dependence of the solid harmonics is $r^l$, larger values of $l$ are required to adequately describe larger regions of interest. In addition, since the primary design constraint that leads to gradient inhomogeneity is the finite length of the coil in the $z$-direction, and, for any value of $l$, smaller values of $m$ vary more rapidly in $z$- than do larger values of $m$, we expect less contribution from large $m$. In the current study, the only basis functions that make a significant contribution to the gradient nonlinearity were the $l = 3$ terms. For larger ROIs or shorter gradient coils, larger values of $l$ will contribute, but we expect the dominant contributions to come from $m = 1$ for the $x$- and $y$-gradients and $m = 0$ for the $z$-gradient.

References

[1] Abramowitz M, Stegun IA, editors. Handbook of mathematical functions: with formulas, graphs, and mathematical tables. New York, NY: Dover Publ; 2013.