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Tradeoffs Between Measurement Residual and Reconstruction Error in Inverse Problems with Prior Information

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ABSTRACT

In many inverse problems with prior information, the measurement residual and the reconstruction error are two natural metrics for reconstruction quality, where the measurement residual is defined as the weighted sum of the squared differences between the data actually measured and the data predicted by the reconstructed model, and the reconstruction error is defined as the sum of the squared differences between the reconstruction and the truth, averaged over some *a priori* probability space of possible solutions. A reconstruction method that minimizes only one of these cost functions may produce unacceptable results on the other. This paper develops reconstruction methods that control both residual and error, achieving the minimum residual for any fixed error or vice versa. These jointly optimal estimators can be obtained by minimizing a weighted sum of the residual and the error; the weights are determined by the slope of the tradeoff curve at the desired point and may be determined iteratively. These results generalize to other cost functions, provided that the cost functions are quadratic and have unique minimizers; some results are obtained under the weaker assumption that the cost functions are convex.

1. INTRODUCTION

In many inverse problems there are two or more natural cost functions for the reconstruction quality. Two very common ones are the measurement residual, defined as the weighted sum of the squared differences between the data actually measured and the data predicted by the reconstructed model, and the reconstruction error, defined as the sum of the squared differences between the reconstruction and the truth, averaged over some *a priori* probability space of possible solutions. The minimum-norm least squares method [2] minimizes the residual without respect to the error and can produce very large reconstruction errors in ill-posed problems [1]. Minimum mean-square error methods such as OCLIM [1], on the other hand, minimize the reconstruction error without regard to the residual and can possibly produce reconstructions in which the measured and predicted data match only poorly.

The purpose of this paper is to develop reconstruction methods that control both the residual and the error and that yield the minimum error for a fixed residual or vice versa. The paper also develops some useful properties of the tradeoff curve which defines the minimum possible residual for every value of error, and vice versa.

The first part of the paper demonstrates that the tradeoff curve is convex and monotone decreasing, given only the assumption that the cost functions are convex. Furthermore, every estimator that minimizes a weighted sum of the cost functions achieves some point on the tradeoff curve. The second part of the paper considers the additional assumptions that the cost functions are quadratic and have unique minimizers; then every interior point on the tradeoff curve can be achieved by an estimator which minimizes the weighted sum of the cost functions. The third part of the paper considers the measurement residual and the reconstruction error as the cost functions and derives the optimal estimator for any point on their tradeoff curve. The final part of the paper applies these results to a model problem from biomagnetic source imaging and exhibits the tradeoff curve for this problem.

2. FOUNDATIONS

We begin by developing some fundamental properties of the tradeoff curve between two cost functions for reconstruction quality. Suppose that $\mathcal{D}$ is a space of possible data sets and $\mathcal{M}$ is a Banach space of possible models to explain a data set. Let $\mathcal{H}$ be a set of reconstruction operators from $\mathcal{D}$ to $\mathcal{M}$, either linear or nonlinear. Since $\mathcal{M}$ is a linear space, it is always possible to define the addition of two operators or the multiplication of an operator by a constant as the corresponding addition or multiplication of the solutions. That is, for any scalars α and β and any estimators H_1 and H_2,

$$(\alpha H_1 + \beta H_2) : d \mapsto \alpha H_1(d) + \beta H_2(d) \quad , \tag{1}$$

where $d \in \mathcal{D}$ is a data set. Further let span($\mathcal{H}$) be the set of all linear combinations of operators in $\mathcal{H}$ and observe that span($\mathcal{H}$) is a linear space, whether or not the operators H in $\mathcal{H}$ are themselves linear or nonlinear.

Let the cost functions $\mu(H)$ and $\nu(H)$ be any real-valued convex functions of the reconstruction filter H and suppose that smaller values of μ and ν indicate better quality. Recall that a function μ is convex if

$$\mu(\alpha H_1 + (1-\alpha)H_2) \leq \alpha\mu(H_1) + (1-\alpha)\mu(H_2) \tag{2}$$

for all $1 \leq \alpha \leq 1$ and all H_1 and H_2 in span($\mathcal{H}$).

Definition 1: A point (μ_1, ν_1) is feasible if there exists an operator $H \in$ span($\mathcal{H}$) such that $\mu(H) = \mu_1$ and $\nu(H) = \nu_1$.

Definition 2: A point (μ_1, ν_1) is (μ, ν)-optimal (or just optimal) if it is feasible and there is no other feasible point (μ_2, ν_2) such that $\mu_2 \leq \mu_1$ and $\nu_2 \leq \nu_1$. Equivalently, if there is no other feasible point in the closed quadrant below and to the left of (μ_1, ν_1). An operator H is (μ, ν)-optimal if $(\mu(H), \nu(H))$ is an optimal point.

Definition 3: The (μ, ν) tradeoff curve is the set of optimal points.

It is now easy to show that the tradeoff curve is single-valued and monotone decreasing.

Lemma 4: Let (μ_1, ν_1) and (μ_2, ν_2) be two points on the tradeoff curve. Then exactly one of the following three statements is true: (1) $\mu_1 = \mu_2$ and $\nu_1 = \nu_2$; (2) $\mu_1 < \mu_2$ and $\nu_1 > \nu_2$; or (3) $\mu_1 > \mu_2$ and $\nu_1 < \nu_2$.

Proof: Let H_1 and H_2 be the estimators that realize the two given points. Since the points are optimal, so are the estimators. (1) Consider the case that $\mu_1 = \mu_2$. If $\nu_1 < \nu_2$ then H_2 cannot be optimal, and if $\nu_1 > \nu_2$ then H_1 cannot be optimal. (2) Consider the case that $\mu_1 < \mu_2$. If $\nu_1 \leq \nu_2$ then H_2 cannot be optimal. (3) Consider the case that $\mu_1 > \mu_2$. If $\nu_1 \geq \nu_2$ then H_1 cannot be optimal. ■

The tradeoff curve is also convex, in the sense defined by the following proposition.

Lemma 5: Let H_1 and H_2 be optimal estimators such that $\mu(H_1) < \mu(H_2)$ and (necessarily) $\nu(H_1) > \nu(H_2)$. Then for every $0 < \alpha < 1$ there exist a feasible estimator H_3 and an optimal estimator H_4 such that

$$\mu(H_1) < \mu(H_4) \leq \mu(H_3) \leq \alpha\mu(H_1) + (1-\alpha)\mu(H_2) \tag{3}$$

and

$$\nu(H_2) < \nu(H_4) \leq \nu(H_3) \leq \alpha\nu(H_1) + (1-\alpha)\nu(H_2) \quad . \tag{4}$$

Proof: Define $H_3 = \alpha H_1 + (1-\alpha)H_2$. Then by the convexity of μ and ν,

$$\mu(H_3) \leq \alpha\mu(H_1) + (1-\alpha)\mu(H_2) \tag{5}$$

and

$$\nu(H_3) \leq \alpha\nu(H_1) + (1-\alpha)\nu(H_2) \quad . \tag{6}$$

If it happens that H_3 is optimal, take $H_4 = H_3$. Otherwise H_3 is not optimal and there must exist some optimal estimator H_4 such that $\mu(H_4) \leq \mu(H_3)$ and $\nu(H_4) \leq \nu(H_3)$. In either case we have $\mu(H_4) \leq \mu(H_3)$ and $\nu(H_4) \leq \nu(H_3)$. Finally observe that we must have $\mu(H_1) < \mu(H_4)$; since $\nu(H_4) < \nu(H_1)$, H_1 cannot be optimal otherwise. Similarly, we must have $\nu(H_2) < \nu(H_4)$ since H_2 is optimal. ■

3. TRADEOFF FUNCTION

Since the tradeoff curve is single-valued, we can define a continuous tradeoff function that gives the minimum possible value of the second cost function ν for any given value of the first cost function μ. Then there is an estimator that comes arbitrarily close to any point on the curve traced out by this function.

Definition 6: The tradeoff function $\hat{\nu}$ from μ to ν is the real-valued function given by

$$\hat{\nu}(\mu_0) = \inf_{\mu(H) \leq \mu_0} \nu(H) \quad . \tag{7}$$

It is undefined whenever no such H exists.

Lemma 7: Let A be an optimal estimator. Then for every $\mu_0 \geq \mu(A)$ and every $\epsilon > 0$, there exists an $H \in \mathrm{span}(\mathcal{H})$ such that $\mu(H) \leq \mu_0$ and $\nu(H) \leq \hat{\nu}(\mu_0) + \epsilon$.

Proof: The existence of $\hat{\nu}(\mu_0)$ follows from the fact that $\mu(A) \leq \mu_0$. Then the inequalities $\mu(H) \leq \mu_0$ and $\nu(H) \leq \hat{\nu}(\mu_0) + \epsilon$ follow from the definition of infimum. ■

Proposition 8: Let A and B be optimal estimators such that $\mu(A) < \mu(B)$. Then (1) $\hat{\nu}$ is defined, convex, and monotone non-increasing on the closed interval $[\mu(A), \mu(B)]$; (2) $\nu(B) \leq \hat{\nu}(\mu_0) \leq \nu(A)$ for all $\mu_0 \in [\mu(A), \mu(B)]$; (3) the left derivative

$$\hat{\nu}'_- = \lim_{\mu_1 \uparrow \mu_0} \frac{\hat{\nu}(\mu_1) - \hat{\nu}(\mu_0)}{\mu_1 - \mu_0} \tag{8}$$

exists for all $\mu_0 \in (\mu(A), \mu(B)]$; and (4) the right derivative

$$\hat{\nu}'_+ = \lim_{\mu_1 \downarrow \mu_0} \frac{\hat{\nu}(\mu_1) - \hat{\nu}(\mu_0)}{\mu_1 - \mu_0} \tag{9}$$

exists for all $\mu_0 \in [\mu(A), \mu(B))$.

Proof: (1) To see that $\hat{\nu}(\mu_0)$ is defined for $\mu_0 \geq \mu(A)$, observe that A satisfies the condition that $\mu(A) \leq \mu_0$ and so the infimum always exists. Furthermore $\hat{\nu}(\mu_0) \leq \nu(A)$.

(2) To see that $\hat{\nu}$ is monotone non-increasing, consider two points μ_1 and μ_2 such that $\mu(A) \leq \mu_1 \leq \mu_2 \leq \mu(B)$. Then

$$\hat{\nu}(\mu_1) = \inf_{\mu(H) \leq \mu_1} \nu(H) \geq \inf_{\mu(H) \leq \mu_2} \nu(H) = \hat{\nu}(\mu_2) \quad . \tag{10}$$

The inequality $\nu(B) \leq \hat{\nu}(\mu_0)$ follows immediately from monotonicity.

(3) To see that $\hat{\nu}$ is convex, consider any μ_1 and μ_2 such that $\mu(A) \leq \mu_1 < \mu_2 \leq \mu(B)$ and any $\epsilon > 0$. Then there exist H_1 and H_2 such that

$$\mu(H_1) \leq \mu_1 \qquad \text{and} \qquad \nu(H_1) < \hat{\nu}(\mu_1) + \epsilon \tag{11}$$

$$\mu(H_2) \leq \mu_2 \qquad \text{and} \qquad \nu(H_2) < \hat{\nu}(\mu_2) + \epsilon \quad . \tag{12}$$

Furthermore, by Lemma 5, there exists for any $0 \leq \alpha \leq 1$ an estimator H_α such that

$$\begin{aligned} \mu(H_\alpha) &\leq (1-\alpha)\mu(H_1) + \alpha\mu(H_2) \\ &\leq (1-\alpha)\mu_1 + \alpha\mu_2 \end{aligned} \tag{13}$$

and

$$\nu(H_\alpha) \leq (1-\alpha)\nu(H_1) + \alpha\nu(H_2) \quad . \tag{14}$$

Then consider

$$\begin{aligned} \hat{\nu}((1-\alpha)\mu_1 + \alpha\mu_2) &= \inf_{\mu(H) \leq (1-\alpha)\mu_1 + \alpha\mu_2} \nu(H) \\ &\leq \nu(H_\alpha) \\ &\leq (1-\alpha)\nu(H_1) + \alpha\nu(H_2) \\ &\leq (1-\alpha)(\hat{\nu}(\mu_1) + \epsilon) + \alpha(\hat{\nu}(\mu_2) + \epsilon) \\ &= (1-\alpha)\hat{\nu}(\mu_1) + \alpha\hat{\nu}(\mu_2) + \epsilon \quad , \end{aligned} \tag{15}$$

and, since ϵ was arbitrary,

$$\hat{\nu}((1-\alpha)\mu_1 + \alpha\mu_2) \leq (1-\alpha)\hat{\nu}(\mu_1) + \alpha\hat{\nu}(\mu_2) \quad , \tag{16}$$

which is the required condition for convexity. Continuity and the existence of the left and right derivatives follow from convexity. ■

Lemma 9: Suppose that the estimator H is (μ, ν)-optimal. Then $\nu(H) = \hat{\nu}(\mu(H))$.

Proof: First observe that

$$\begin{aligned}\hat{\nu}(\mu(H)) &= \inf_{G:\mu(G)\leq\mu(H)} \nu(G) \\ &\leq \nu(H)\end{aligned} \tag{17}$$

since $\mu(H) \leq \mu(H)$. Now suppose that $\hat{\nu}(\mu(H)) < \nu(H)$. Then there must exist a G such that $\mu(G) \leq \mu(H)$ and $\nu(G) < \nu(H)$. But then H cannot be optimal. Therefore we must have $\hat{\nu}(\mu(H)) = \nu(H)$. ■

4. A CLASS OF OPTIMAL ESTIMATORS

Given a point (μ, ν) on the tradeoff curve, we often wish to construct an estimator that achieves that performance. In fact, it is possible to define a class of estimators which are always (μ, ν)-optimal. Unfortunately, it is not known in the general case whether every optimal point can be achieved by an estimator in this class.

Definition 10: The class $\Theta \subset \text{span}(\mathcal{H})$ is the set of estimators $H \in \text{span}(\mathcal{H})$ that minimize the weighted sum $\mu(H) + \theta\nu(H)$ for some fixed positive real θ.

Theorem 11: Suppose that the estimator $H_\theta \in \Theta$ minimizes $\mu(H) + \theta\nu(H)$ for some fixed $\theta > 0$. Then H_θ is (μ, ν)-optimal. Furthermore,

$$\hat{\nu}'_-(\mu(H_\theta)) \leq -\frac{1}{\theta} \leq \hat{\nu}'_+(\mu(H_\theta)) \quad . \tag{18}$$

Proof: (1) Suppose that H_θ is not (μ, ν)-optimal. Then there exists a $G \in \text{span}(\mathcal{H})$ such that either $\mu(G) < \mu(H_\theta)$ and $\nu(G) \leq \nu(H_\theta)$ or $\mu(G) \leq \mu(H_\theta)$ and $\nu(G) < \nu(H_\theta)$. In either case

$$\mu(G) + \theta\nu(G) < \mu(H_\theta) + \theta\nu(H_\theta) \tag{19}$$

and therefore H_θ does not minimize $\mu(H) + \theta\nu(H)$.

(2) For the inequality on the derivatives, define $\mu_\theta = \mu(H_\theta)$ and consider some $\mu_1 \neq \mu_\theta$. Fix $\epsilon > 0$. Then there exists an optimal estimator H_1 such that $\mu(H_1) \leq \mu_1$ and $\nu(H_1) \leq \hat{\nu}(\mu_1) + \epsilon$. Then

$$\mu(H_1) + \theta\nu(H_1) \leq \mu_1 + \theta(\hat{\nu}(\mu_1) + \epsilon) \quad . \tag{20}$$

Now since H_θ minimizes $\mu(H) + \theta\nu(H)$ we have

$$\mu(H_\theta) + \theta\nu(H_\theta) \leq \mu(H_1) + \theta\nu(H_1) \tag{21}$$

and so

$$\mu(H_\theta) + \theta\nu(H_\theta) \leq \mu_1 + \theta\left[\hat{\nu}(\mu_1) + \epsilon\right] \quad . \tag{22}$$

Since $\hat{\nu}(\mu_\theta) = \hat{\nu}(\mu(H_\theta)) \leq \nu(H_\theta)$,

$$\mu_\theta + \theta\hat{\nu}(\mu_\theta) \leq \mu_1 + \theta\left[\hat{\nu}(\mu_1) + \epsilon\right] \quad . \tag{23}$$

Since ϵ is arbitrary,

$$\mu_\theta + \theta\hat{\nu}(\mu_\theta) \leq \mu_1 + \theta\hat{\nu}(\mu_1) \tag{24}$$

and

$$-\theta\left[\hat{\nu}(\mu_1) - \hat{\nu}(\mu_\theta)\right] \leq \mu_1 - \mu_\theta \quad . \tag{25}$$

(3) If $\mu_1 > \mu_\theta$, the last inequality can be rearranged to yield

$$\frac{\hat{\nu}(\mu_1) - \hat{\nu}(\mu_\theta)}{\mu_1 - \mu_\theta} \geq -\frac{1}{\theta} \quad . \tag{26}$$

Taking the limit as $\mu_1 \downarrow \mu_\theta$ yields

$$-\frac{1}{\theta} \leq \hat{\nu}'_+(\mu(H_\theta)) \quad . \tag{27}$$

(4) If $\mu_1 < \mu_\theta$, the inequality can be rearranged to yield

$$\frac{\hat{\nu}(\mu_1) - \hat{\nu}(\mu_\theta)}{\mu_1 - \mu_\theta} \leq -\frac{1}{\theta} \tag{28}$$

and taking the limit as $\mu_1 \uparrow \mu_\theta$ yields

$$\hat{\nu}'_-(\mu(H_\theta)) \leq -\frac{1}{\theta} \quad . \tag{29}$$

■

5. QUADRATIC COST FUNCTIONS

Many interesting inverse problems involve finite-dimensional linear estimators and quadratic cost functions and it is true for this case that every interior point on the tradeoff curve can be achieved by an estimator $H_\theta \in \Theta$ for some θ. To be definite, suppose that the model space $\mathcal{M}$ and the data space $\mathcal{D}$ are both finite-dimensional vector spaces, and that the model $\mathbf{m}$ and the data $\mathbf{d}$ are related by the linear equation $\mathbf{d} = \mathbf{F}\mathbf{m} + \mathbf{w}$, where $\mathbf{w}$ is the measurement error. Furthermore, the estimate of the model is always in the form $\hat{\mathbf{m}} = \mathbf{H}\mathbf{d}$ where $\mathbf{H}$ is a matrix. Stacking the columns of the matrix $\mathbf{H}$ yields a vector $\mathbf{h}$.

Definition 12: Suppose that span($\mathcal{H}$) is a finite-dimensional vector space and that every element $H \in$ span($\mathcal{H}$) can be uniquely represented as a stacked vector $\mathbf{h}$. Then a cost function $\mu(H)$ is quadratic if it can be written in the form

$$\mu(H) = \mathbf{h}^T\mathbf{A}\mathbf{h} + \mathbf{b}^T\mathbf{h} + c \tag{30}$$

for some symmetric positive semidefinite matrix $\mathbf{A}$, some real vector $\mathbf{b}$, and some real constant c. The cost function $\mu(H)$ is quadratic positive definite if the matrix $\mathbf{A}$ is positive definite.

Proposition 13: Let $\mu(H)$ be a quadratic cost function. Then $\mu(H)$ is a convex function of H.

Proof: Let H_1 and H_2 be any two estimators and let $\mathbf{h}_1$ and $\mathbf{h}_2$ be the vectors that represent them. Assume that $0 \leq \alpha \leq 1$. Then

$$\begin{aligned}\mu(\alpha H_1 + (1-\alpha)H_2) &= [\alpha\mathbf{h}_1 + (1-\alpha)\mathbf{h}_2]^T\mathbf{A}[\alpha\mathbf{h}_1 + (1-\alpha)\mathbf{h}_2] \\ &\quad + \mathbf{b}^T[\alpha\mathbf{h}_1 + (1-\alpha)\mathbf{h}_2] + c \\ &= \alpha[\mathbf{h}_1^T\mathbf{A}\mathbf{h}_1 + \mathbf{b}^T\mathbf{h}_1 + c] + (1-\alpha)[\mathbf{h}_2^T\mathbf{A}\mathbf{h}_2 + \mathbf{b}^T\mathbf{h}_2 + c] \\ &\quad - \alpha(1-\alpha)[\mathbf{h}_1^T\mathbf{A}\mathbf{h}_1 - 2\mathbf{h}_1^T\mathbf{A}\mathbf{h}_2 + \mathbf{h}_2^T\mathbf{A}\mathbf{h}_2] \\ &= \alpha\mu(H_1) + (1-\alpha)\mu(H_2) - \alpha(1-\alpha)[\mathbf{h}_1 - \mathbf{h}_2]^T\mathbf{A}[\mathbf{h}_1 - \mathbf{h}_2] \\ &\leq \alpha\mu(H_1) + (1-\alpha)\mu(H_2) \end{aligned} \tag{31}$$

since $\mathbf{A}$ is positive semidefinite. ∎

Proposition 14: Consider a quadratic cost function

$$\mu(H) = \mathbf{h}^T\mathbf{A}\mathbf{h} + \mathbf{b}^T\mathbf{h} + c \quad . \tag{32}$$

Then the estimator H represented by

$$\mathbf{h} = \tfrac{1}{2}\mathbf{A}^\dagger\mathbf{b} \tag{33}$$

minimizes $\mu(H)$, where $\mathbf{A}^\dagger$ is the Moore-Penrose pseudoinverse of $\mathbf{A}$. If μ is positive definite, then the estimator H is unique and can be written as

$$\mathbf{h} = \tfrac{1}{2}\mathbf{A}^{-1}\mathbf{b} \quad . \tag{34}$$

Proof: To find the minimum, consider a variation $\mathbf{h} + \delta\mathbf{h}$ to obtain

$$\begin{aligned}\mu(H + \delta H) &= (\mathbf{h} + \delta\mathbf{h})^T\mathbf{A}(\mathbf{h} + \delta\mathbf{h}) + \mathbf{b}^T(\mathbf{h} + \delta\mathbf{h}) + c \\ &= \mathbf{h}^T\mathbf{A}\mathbf{h} + \mathbf{b}^T\mathbf{h} + c + 2\delta\mathbf{h}^T\mathbf{A}^T\mathbf{h} + \delta\mathbf{h}^T\mathbf{b} + \delta\mathbf{h}^T\mathbf{A}\delta\mathbf{h} \quad . \end{aligned} \tag{35}$$

The estimator corresponding to $\mathbf{h}$ is a stationary point of μ if the linear term in $\delta\mathbf{h}$ is zero independent of the value of $\delta\mathbf{h}$. This requires $2\mathbf{A}^T\mathbf{h} = \mathbf{b}$, or, since $\mathbf{A}$ is symmetric, $2\mathbf{A}\mathbf{h} = \mathbf{b}$.

Now suppose that μ is positive definite. Then $\mathbf{A}$ is positive definite and the quadratic term in $\delta\mathbf{h}$ is positive whenever $\delta\mathbf{h}$ is not zero. Thus any stationary point must be a minimum and the solution $\mathbf{h} = \frac{1}{2}\mathbf{A}^{-1}\mathbf{b}$ must be unique. Suppose instead that μ is not positive definite. Then $\mathbf{A}$ is only positive semidefinite and the solution $\mathbf{h} = \frac{1}{2}\mathbf{A}^\dagger\mathbf{b}$ is not unique. ∎

Corollary 15: A quadratic cost function μ is positive definite if and only if there is a unique estimator H that minimizes it.

Proposition 16: Consider a quadratic positive definite cost function

$$\mu(H) = \mathbf{h}^T\mathbf{A}_\mu\mathbf{h} + \mathbf{b}_\mu^T\mathbf{h} + c_\mu \quad , \tag{36}$$

a quadratic cost function

$$\nu(H) = \mathbf{h}^T \mathbf{A}_\nu \mathbf{h} + \mathbf{b}_\nu^T \mathbf{h} + c_\nu \quad , \tag{37}$$

and a non-negative real constant θ. Then there is a unique estimator H_θ that minimizes $\mu(H) + \theta\nu(H)$ and that estimator H_θ is represented by

$$\mathbf{h} = \tfrac{1}{2}(\mathbf{A}_\mu + \theta \mathbf{A}_\nu)^{-1}(\mathbf{b}_\mu + \theta \mathbf{b}_\nu) \quad . \tag{38}$$

Proof: The weighted cost function

$$\mu(H) + \theta\nu(H) = \mathbf{h}^T(\mathbf{A}_\mu + \theta\mathbf{A}_\nu)\mathbf{h} + (\mathbf{b}_\mu + \theta\mathbf{b}_\nu)^T\mathbf{h} + (c_\mu + \theta c_\nu) \tag{39}$$

is quadratic and positive definite. ■

Theorem 17: Let μ be a quadratic positive definite cost function and ν be a quadratic cost function. Let A and B be optimal linear estimators and (μ_0, ν_0) a point on the tradeoff curve such that $\mu(A) \leq \mu_0 < \mu(B)$. Then there is a linear estimator $H_\theta \in \Theta$ such that $\mu(H_\theta) = \mu_0$ and $\nu(H_\theta) = \nu_0$.

Proof: The optimal estimator H_θ is a continuous function of the parameter θ. Similarly, μ and ν are continuous functions of H_θ. Thus $\mu(H_\theta)$ is a continuous function of θ and there must exist a θ such that $\mu(H_\theta) = \mu_0$. Since H_θ is optimal, $\nu(H_\theta) = \nu_0$. ■

The problem of finding the particular value of θ to realize a desired optimal point may be solved numerically by iterative methods.

6. ERROR VERSUS RESIDUAL

The results of the previous section may be applied to the specific problem of trading off the measurement residual versus the reconstruction error in the inverse problem with prior information. To make the problem definite, assume that $\mathbf{d} = \mathbf{F}\mathbf{m} + \mathbf{w}$ as before and that $\mathbf{m}$ and $\mathbf{w}$ are independent zero-mean Gaussian random vectors with covariances $\mathbf{C_m} = \mathsf{E}\,\mathbf{m}\mathbf{m}^T$ and $\mathbf{C_w} = \mathsf{E}\,\mathbf{w}\mathbf{w}^T$.

The measurement residual (or data misfit) may then defined as

$$\chi^2 = (\mathbf{d} - \mathbf{F}\hat{\mathbf{m}})^T \mathbf{C_w}^{-1} (\mathbf{d} - \mathbf{F}\hat{\mathbf{m}}) \tag{40}$$

and is a measure of the discrepancy between the data actually measured and the data predicted by the model. The Moore-Penrose pseudoinverse minimizes χ^2 but is not unique; therefore χ^2 is not a positive definite cost function.

The mean square reconstruction error for a given data set $\mathbf{d}$ may be defined as

$$\hat{\eta}^2 = \mathsf{E}\left[\|\mathbf{m} - \hat{\mathbf{m}}\|^2 \,\middle|\, \mathbf{d} \right] \tag{41}$$

and is a measure of the uncertainty in the solution $\hat{\mathbf{m}}$. We will see shortly that $\hat{\eta}^2$ is positive definite.

To find an estimator that jointly minimizes χ^2 and $\hat{\eta}^2$ it is sufficient to consider the weighted sum

$$S(\hat{\mathbf{m}}) = \mathsf{E}\left[\|\mathbf{m}-\hat{\mathbf{m}}\|^2 \,\Big|\, \mathbf{d}\right] + \theta\,(\mathbf{d}-\mathbf{F}\hat{\mathbf{m}})^T\mathbf{C}_{\mathbf{w}}^{-1}(\mathbf{d}-\mathbf{F}\hat{\mathbf{m}}) \quad . \tag{42}$$

Taking the variation $\hat{\mathbf{m}} + \delta\hat{\mathbf{m}}$ yields

$$\begin{aligned} S(\hat{\mathbf{m}}+\delta\hat{\mathbf{m}}) = {} & \mathsf{E}\left[\|\mathbf{m}-\hat{\mathbf{m}}\|^2 \,\Big|\, \mathbf{d}\right] + \theta\,(\mathbf{d}-\mathbf{F}\hat{\mathbf{m}})^T\mathbf{C}_{\mathbf{w}}^{-1}(\mathbf{d}-\mathbf{F}\hat{\mathbf{m}}) \\ & - 2\delta\hat{\mathbf{m}}^T\,\mathsf{E}\,[\mathbf{m}-\hat{\mathbf{m}} \mid \mathbf{d}] - 2\theta\,\delta\hat{\mathbf{m}}^T\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}(\mathbf{d}-\mathbf{F}\hat{\mathbf{m}}) \\ & + \delta\hat{\mathbf{m}}^T\delta\hat{\mathbf{m}} + \theta\,\delta\hat{\mathbf{m}}^T\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}\mathbf{F}\delta\hat{\mathbf{m}} \quad . \end{aligned} \tag{43}$$

Observe that the sum of the quadratic terms in $\delta\hat{\mathbf{m}}$ is positive whenever $\delta\hat{\mathbf{m}} \neq 0$ and so any stationary point must be unique and must be a minimum. To find this minimum, set the coefficient of the linear term to zero, or

$$\begin{aligned} & \mathsf{E}\,[\mathbf{m}-\hat{\mathbf{m}} \mid \mathbf{d}] + \theta\,\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}(\mathbf{d}-\mathbf{F}\hat{\mathbf{m}}) = 0 \\ \Rightarrow\quad & \mathsf{E}(\mathbf{m} \mid \mathbf{d}) - \hat{\mathbf{m}} + \theta\,\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}\mathbf{d} - \theta\,\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}\mathbf{F}\hat{\mathbf{m}} = 0 \\ \Rightarrow\quad & \mathbf{C}_{\mathbf{m}}\mathbf{F}^T(\mathbf{F}\mathbf{C}_{\mathbf{m}}\mathbf{F}^T+\mathbf{C}_{\mathbf{w}})^{-1}\mathbf{d} + \theta\,\mathbf{F}\mathbf{C}_{\mathbf{w}}^{-1}\mathbf{d} = \hat{\mathbf{m}} + \theta\,\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}\mathbf{F}\hat{\mathbf{m}} \\ \Rightarrow\quad & \hat{\mathbf{m}} = \left[\mathbf{I} + \theta\,\mathbf{F}\mathbf{C}_{\mathbf{w}}^{-1}\mathbf{F}\right]^{-1}\left[\mathbf{C}_{\mathbf{m}}\mathbf{F}^T(\mathbf{F}\mathbf{C}_{\mathbf{m}}\mathbf{F}^T+\mathbf{C}_{\mathbf{w}})^{-1} + \theta\,\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}\right]\mathbf{d} \quad . \end{aligned} \tag{44}$$

The optimal estimator is

$$\mathbf{H}_\theta = \left[\mathbf{I} + \theta\,\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}\mathbf{F}\right]^{-1}\left[\mathbf{C}_{\mathbf{m}}\mathbf{F}^T(\mathbf{F}\mathbf{C}_{\mathbf{m}}\mathbf{F}^T+\mathbf{C}_{\mathbf{w}})^{-1} + \theta\,\mathbf{F}^T\mathbf{C}_{\mathbf{w}}^{-1}\right] \quad . \tag{45}$$

Setting $\theta = 0$ in the preceding derivation yields the unique estimator that minimizes $\hat{\eta}^2$, which is

$$\mathbf{H}_\eta = \mathbf{C}_{\mathbf{m}}\mathbf{F}^T(\mathbf{F}\mathbf{C}_{\mathbf{m}}\mathbf{F}^T+\mathbf{C}_{\mathbf{w}})^{-1} \quad . \tag{46}$$

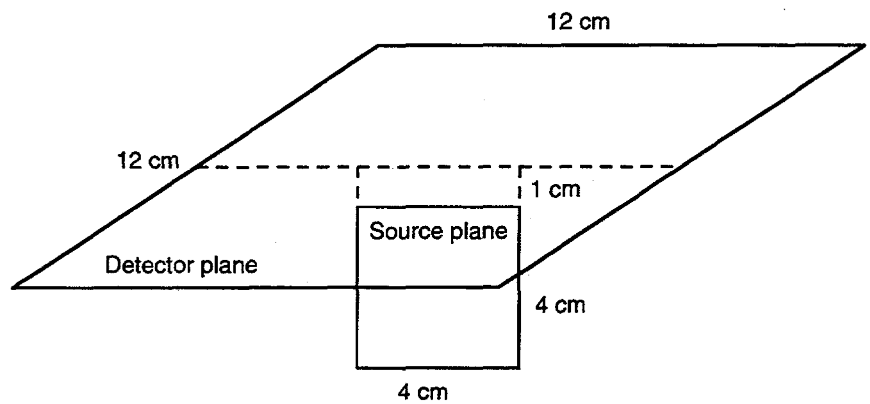
Since this estimator is unique, the cost function $\hat{\eta}^2$ must be positive definite. Note that this is identical to the OCLIM estimator [1].

Given the data $\mathbf{d}$ and the optimal estimate $\hat{\mathbf{m}}$ it is easy to compute χ^2 directly from its definition. To compute $\hat{\eta}^2$, let $\bar{\mathbf{m}} = \mathsf{E}(\mathbf{m} \mid \mathbf{d})$ and consider

$$\begin{aligned} \hat{\eta}^2 &= \mathsf{E}\left[\|\mathbf{m}-\hat{\mathbf{m}}\|^2 \,\Big|\, \mathbf{d}\right] \\ &= \mathsf{E}\left[(\mathbf{m}-\bar{\mathbf{m}}+\bar{\mathbf{m}}-\hat{\mathbf{m}})^T(\mathbf{m}-\bar{\mathbf{m}}+\bar{\mathbf{m}}-\hat{\mathbf{m}}) \,\Big|\, \mathbf{d}\right] \\ &= \mathsf{E}\left[(\mathbf{m}-\bar{\mathbf{m}})^T(\mathbf{m}-\bar{\mathbf{m}}) \,\Big|\, \mathbf{d}\right] + \mathsf{E}\left[(\hat{\mathbf{m}}-\bar{\mathbf{m}})^T(\hat{\mathbf{m}}-\bar{\mathbf{m}}) \,\Big|\, \mathbf{d}\right] \\ &\qquad + 2\,\mathsf{E}\left[(\mathbf{m}-\bar{\mathbf{m}})^T(\hat{\mathbf{m}}-\bar{\mathbf{m}}) \,\Big|\, \mathbf{d}\right] \\ &= \mathrm{Tr}(\mathrm{Var}(\mathbf{m} \mid \mathbf{d})) + \|\hat{\mathbf{m}}-\bar{\mathbf{m}}\|^2 \quad , \end{aligned} \tag{47}$$

which can be expanded into a convenient form for computation

$$\begin{aligned} \hat{\eta}^2 = {} & \mathrm{Tr}\left(\mathbf{C}_{\mathbf{m}} - \mathbf{C}_{\mathbf{m}}\mathbf{F}^T(\mathbf{F}\mathbf{C}_{\mathbf{m}}\mathbf{F}^T+\mathbf{C}_{\mathbf{w}})^{-1}\mathbf{F}\mathbf{C}_{\mathbf{m}}\right) \\ & + \left\|\hat{\mathbf{m}} - \mathbf{C}_{\mathbf{m}}\mathbf{F}^T(\mathbf{F}\mathbf{C}_{\mathbf{m}}\mathbf{F}^T+\mathbf{C}_{\mathbf{w}})^{-1}\mathbf{d}\right\|^2 \quad . \end{aligned} \tag{48}$$



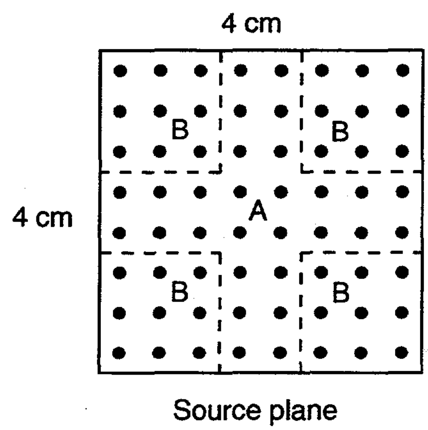


Figure 1 A simple biomagnetic imaging problem. The source plane is perpendicular to the detector plane and contains 64 dipoles perpendicular to the source plane.

7. SOME SIMULATION RESULTS

The theoretical results obtained in this paper will be illustrated by a problem in magnetoencephalographic source imaging, using the simplified geometry shown in Figure 1. The sources are arranged in a 4 $\times$ 4 cm^2 planar array perpendicular to the detector plane, and centered below that plane with its nearest edge 1 cm away. The source plane contains an 8 $\times$ 8 array of current dipoles directed perpendicular to the plane. The 28 sources in the central cruciform region labelled A are assigned an *a priori* RMS source amplitude $\alpha_A = 20 \times 10^{-9}$ A-m; the 36 remaining sources are assigned a different *a priori* amplitude $\alpha_B = 2 \times 10^{-9}$ A-m.

Figure 2 shows the detector array, which has a 12 $\times$ 12 cm^2 planar array of 144 detectors arranged in a 12 $\times$ 12 grid. Each detector measures the magnetic field perpendicular to the plane of the array. The RMS measurement noise at each detector is $\sigma = 100 \times 10^{-15}$ T; the noise is assumed to be independent, zero-mean, and Gaussian.

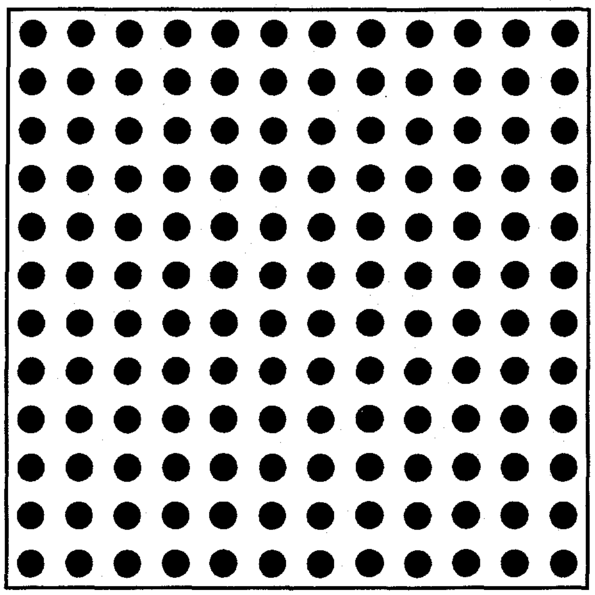


Figure 2 Detector grid. The detector grid contains a 12 by 12 array of sensors that sample the field perpendicular to the array.

The true source distribution was modelled as a single active dipole at row 4 (counting from the top) and column 4, with an amplitude of 100×10^{-9} A-m. A measurement data set, including noise, was computed using the Biot-Savart Law. Figure 3 shows the tradeoff curve between residual χ^2 and error $\hat{\nu}^2$ in (A-m)^2 for this model problem and this data set, plotted in semilog coordinates to accomodate the wide range of values of $\hat{\nu}^2$. The curve is convex, although the use of semilog coordinates conceals this fact. The values of θ used to draw the curve were, going from left to right, $0, 10^{-20}, 10^{-19}, 10^{-18}, \ldots, 10^{-6}$. Optimal points for larger values of θ could not be obtained since the matrix $\mathbf{I} + \theta \mathbf{F}^T \mathbf{C}_{\mathbf{w}}^{-1} \mathbf{F}$ becomes too ill-conditioned to allow accurate computation. The upper left end of the tradeoff curve corresponds to the OCLIM estimator and achieves the minimum possible $\hat{\nu}^2$.

8. DISCUSSION

The best possible mean square error $\hat{\nu}^2$ is 8×10^{-15} (A-m)^2 and is achieved at a residual of $\chi^2 = 134$. Increasing θ increases the square error by 5 orders of magnitude before the residual changes significantly. Further to the right, the curve descends roughly linearly, indicating that the mean square error increases exponentially as the residual decreases.

It is useful to compare the mean square error to the expected squared source amplitude, which is $\mathsf{E}\,\|\hat{\mathbf{m}}\|^2 = (28)(20 \times 10^{-9})^2 + (36)(2 \times 10^{-9})^2 = 11.3 \times 10^{-15}$ (A-m)^2. Since this is only slightly greater than the best possible squared error, it is not possible in this problem to reduce the residual below 134 without increasing the error to the point that it swamps the amplitudes being sought. That being the case, there is no reason not to use the OCLIM estimator to obtain the minimum square error.

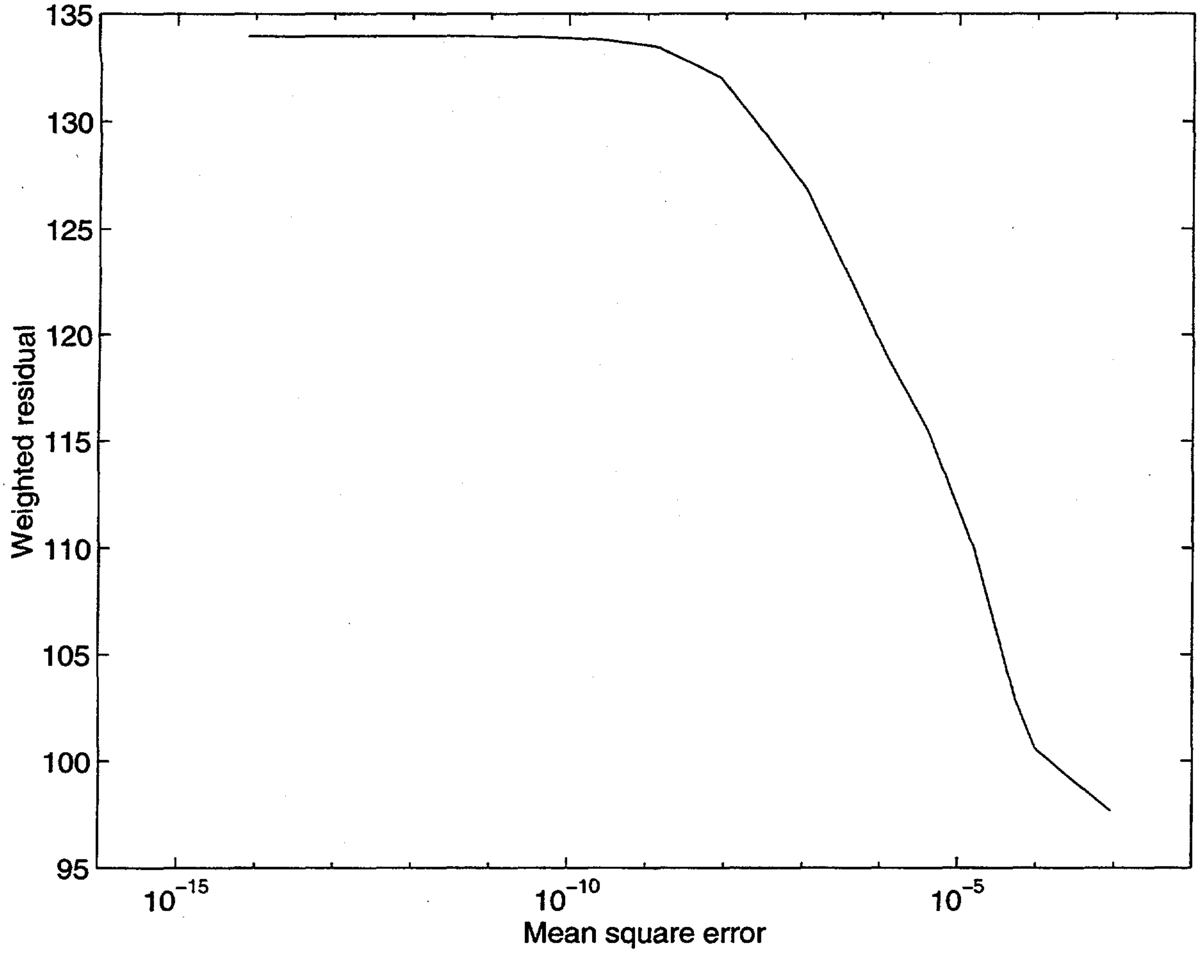


Figure 3 Tradeoff curve for the model problem. This curve plots the best possible residual χ^2 for each value of mean square error $\hat{\nu}^2$. The curve is convex but does not appear so because it is a semilog rather than linear plot.

9. ACKNOWLEDGEMENTS

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10. REFERENCES

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