

Lecture 7

PSEUDOINVERSES II

Computational methods and applications

Harrison H. Barrett
University of Arizona

OUTLINE

- Review of definitions
- Properties of the Moore-Penrose pseudoinverse
- Pseudoinverses and linear equations
- Iterative computation of the pseudoinverse
- Effects of noise
- Regularization

Decomposition of object and image space

An arbitrary object can be written as

$$\mathbf{f} = \sum_{n=1}^N \alpha_n \mathbf{u}_n = \sum_{n=1}^R \alpha_n \mathbf{u}_n + \sum_{n=R+1}^N \alpha_n \mathbf{u}_n$$

$$\mathbf{f} = \mathbf{f}_{meas} + \mathbf{f}_{null}, \quad \mathcal{H}\mathbf{f}_{null} = 0, \quad \mathbf{f}_{meas} \perp \mathbf{f}_{null}.$$

An arbitrary vector in image space can be represented as:

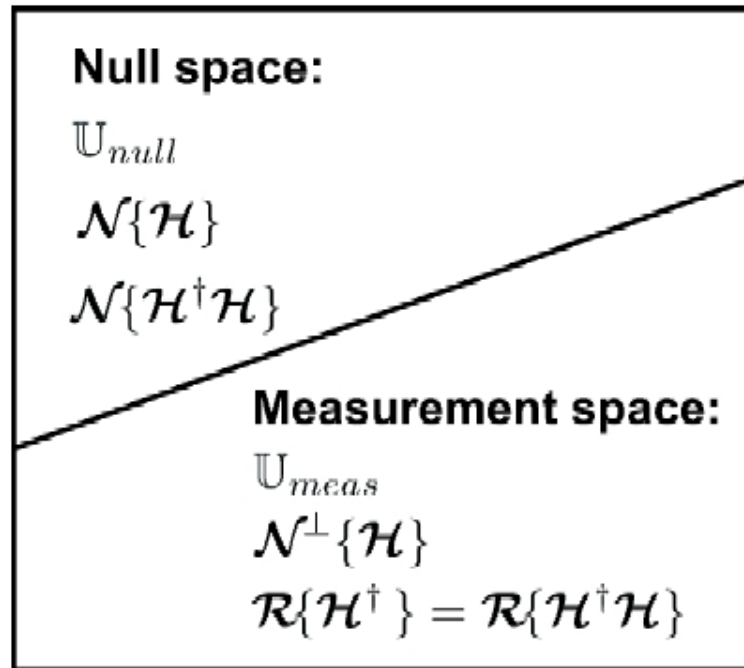
$$\mathbf{g} = \sum_{m=1}^M \beta_m \mathbf{v}_m = \sum_{m=1}^R \beta_m \mathbf{v}_m + \sum_{m=R+1}^M \beta_m \mathbf{v}_m$$

$$\mathbf{g} = \mathbf{g}_{con} + \mathbf{g}_{incon}, \quad \mathcal{H}^\dagger \mathbf{g}_{incon} = 0, \quad \mathbf{g}_{con} \perp \mathbf{g}_{incon}$$

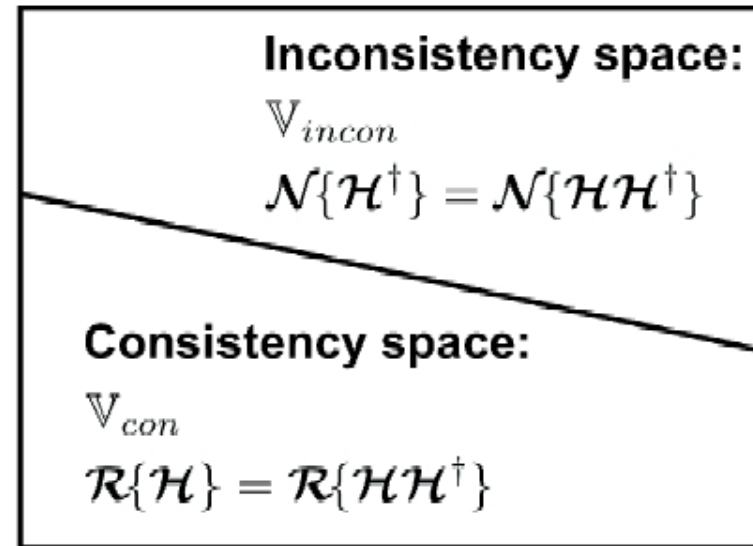
Thus we can decompose object and image space into orthogonal subspaces:

$$\mathbb{U} = \mathbb{U}_{meas} \oplus \mathbb{U}_{null}, \quad \mathbb{V} = \mathbb{V}_{con} \oplus \mathbb{V}_{incon}$$

Four subspaces



\mathbb{U} : Domain of the operator \mathcal{H}

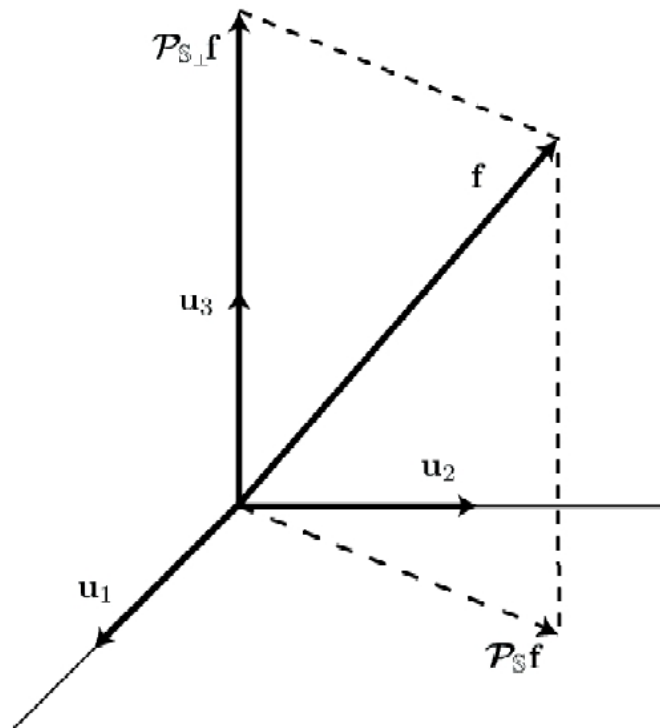


\mathbb{V} : Domain of the adjoint operator \mathcal{H}^\dagger

Recall $R \leq \min(M, N)$. If $R = N$, there is no nontrivial null space. If $R = M$, there is no nontrivial inconsistency space.

Projection operators

A general projection operator \mathcal{P} is Hermitian ($\mathcal{P}^\dagger = \mathcal{P}$) and *idempotent* ($\mathcal{P}^2 = \mathcal{P}$). We are interested here in projections onto subspaces:



Projections onto subspaces

$$\mathbf{f}_{meas} = \sum_{n=1}^R \alpha_n \mathbf{u}_n = \mathcal{P}_{meas} \mathbf{f} , \quad \mathbf{f}_{null} = \sum_{n=R+1}^N \alpha_n \mathbf{u}_n = \mathcal{P}_{null} \mathbf{f} ,$$

where \mathcal{P}_{meas} and \mathcal{P}_{null} are the projectors onto measurement and null space, respectively. Can show that

$$\mathcal{P}_{meas} = \sum_{n=1}^R \mathbf{u}_n \mathbf{u}_n^\dagger , \quad \mathcal{P}_{null} = \sum_{n=R+1}^N \mathbf{u}_n \mathbf{u}_n^\dagger = \mathbf{I}_U - \mathcal{P}_{meas}$$

Similarly,

$$\mathbf{g}_{con} = \sum_{m=1}^R \beta_m \mathbf{v}_m = \mathcal{P}_{con} \mathbf{g} , \quad \mathbf{g}_{incon} = \sum_{m=R+1}^M \beta_m \mathbf{v}_m = \mathcal{P}_{incon} \mathbf{g} .$$

$$\mathcal{P}_{con} = \sum_{m=1}^R \mathbf{v}_m \mathbf{v}_m^\dagger , \quad \mathcal{P}_{incon} = \sum_{m=R+1}^M \mathbf{v}_m \mathbf{v}_m^\dagger = \mathbf{I}_V - \mathcal{P}_{con}$$

Moore's definition of pseudoinverse

Moore (1920) defined an operator \mathcal{H}^+ (a matrix in his case) such that:

$$\mathcal{P}_{meas} = \mathcal{H}^+ \mathcal{H}, \quad \mathcal{P}_{null} = \mathbf{I}_{\mathbb{U}} - \mathcal{H}^+ \mathcal{H},$$

$$\mathcal{P}_{con} = \mathcal{H} \mathcal{H}^+, \quad \mathcal{P}_{incon} = \mathbf{I}_{\mathbb{V}} - \mathcal{H} \mathcal{H}^+.$$

These four definitions turn out to completely determine \mathcal{H}^+ .

The Penrose equations and the Moore-Penrose pseudoinverse

A *generalized inverse* is defined as any operator $\mathcal{H}^\#$ that satisfies one or more of the following equations:

$$\text{Penrose Eq. 1: } \mathcal{H}\mathcal{H}^\#\mathcal{H} = \mathcal{H}. \quad (1.130a)$$

$$\text{Penrose Eq. 2: } \mathcal{H}^\#\mathcal{H}\mathcal{H}^\# = \mathcal{H}^\#. \quad (1.130b)$$

$$\text{Penrose Eq. 3: } (\mathcal{H}\mathcal{H}^\#)^\dagger = \mathcal{H}\mathcal{H}^\#. \quad (1.130c)$$

$$\text{Penrose Eq. 4: } (\mathcal{H}^\#\mathcal{H})^\dagger = \mathcal{H}^\#\mathcal{H}. \quad (1.130d)$$

The Moore-Penrose pseudoinverse, denoted \mathcal{H}^+ , is the generalized inverse that satisfies all four Penrose equations. It is equal to the true inverse if one exists.

The Moore-Penrose pseudoinverse exists for all operators with finite-dimensional range ($M < \infty$), including CD operators and matrices. It may not exist for some CC operators.

SVD expressions

Recall:

$$\mathcal{H} = \sum_{n=1}^R \sqrt{\mu_n} \mathbf{v}_n \mathbf{u}_n^\dagger, \quad \mathcal{H}^\dagger = \sum_{n=1}^R \sqrt{\mu_n} \mathbf{u}_n \mathbf{v}_n^\dagger$$

Can define a pseudoinverse as

$$\mathcal{H}^+ = \sum_{n=1}^R \frac{1}{\sqrt{\mu_n}} \mathbf{u}_n \mathbf{v}_n^\dagger$$

This operator satisfies both Moore and Penrose definitions.

Limiting representations

The Moore-Penroose pseudoinverse can be written in terms of true inverses in two different ways:

$$\mathcal{H}^+ = \lim_{\eta \rightarrow 0^+} \left[\mathcal{H}^\dagger \mathcal{H} + \eta \mathcal{I}_{\mathbb{U}} \right]^{-1} \mathcal{H}^\dagger. \quad (1.135)$$

$$\mathcal{H}^+ = \lim_{\eta \rightarrow 0^+} \mathcal{H}^\dagger \left[\mathcal{H} \mathcal{H}^\dagger + \eta \mathcal{I}_{\mathbb{V}} \right]^{-1}. \quad (1.141)$$

Term $\eta \mathcal{I}$ guarantees that the indicated inverses exist.

See B&M for proof that the limits reproduce the SVD expressions.

These representations are useful for constructing practical iterative algorithms.

Pseudoinverse identities

$$[\mathcal{H}^+]^+ = \mathcal{H}; \quad (1.147)$$

$$\mathcal{H}^+ = (\mathcal{H}^\dagger \mathcal{H})^+ \mathcal{H}^\dagger; \quad (1.148)$$

$$\mathcal{H}^+ = \mathcal{H}^\dagger [\mathcal{H} \mathcal{H}^\dagger]^+; \quad (1.149)$$

$$[\mathcal{H}^\dagger]^+ = [\mathcal{H}^+]^\dagger; \quad (1.150)$$

$$[\mathcal{H}^\dagger]^+ = [\mathcal{H} \mathcal{H}^\dagger]^+ \mathcal{H}; \quad (1.151)$$

$$[\mathcal{H}^+ \mathcal{H}]^+ = \mathcal{H}^+ \mathcal{H}; \quad (1.152)$$

$$\mathcal{H}^+ \mathcal{H} \mathcal{H}^\dagger = \mathcal{H}^\dagger; \quad (1.153)$$

$$\mathcal{H}^\dagger \mathcal{H} \mathcal{H}^+ = \mathcal{H}^\dagger; \quad (1.154)$$

$$\mathcal{H}^+ \mathcal{H} = (\mathcal{H}^\dagger \mathcal{H})^+ (\mathcal{H}^\dagger \mathcal{H}) = (\mathcal{H}^\dagger \mathcal{H}) (\mathcal{H}^\dagger \mathcal{H})^+; \quad (1.155)$$

$$\mathcal{H} \mathcal{H}^+ = (\mathcal{H} \mathcal{H}^\dagger)^+ \mathcal{H} \mathcal{H}^\dagger = \mathcal{H} \mathcal{H}^\dagger (\mathcal{H} \mathcal{H}^\dagger)^+; \quad (1.156)$$

$$[\mathcal{H}^\dagger \mathcal{H}]^+ = \mathcal{H}^+ [\mathcal{H}^\dagger]^+; \quad (1.157)$$

$$[\mathcal{H}^\dagger \mathcal{H}]^+ = \mathcal{H}^+ [\mathcal{H} \mathcal{H}^\dagger]^+ \mathcal{H} = \mathcal{H}^\dagger [\mathcal{H} \mathcal{H}^\dagger]^+ [\mathcal{H}^\dagger]^+; \quad (1.158)$$

$$[\mathcal{H} \mathcal{H}^\dagger]^+ = [\mathcal{H}^\dagger]^+ \mathcal{H}^+. \quad (1.159)$$

All of these identities can be proved either directly from the Penrose equations or from the SVD representations of \mathcal{H} and \mathcal{H}^+ .

Pseudoinverse of a product

It is not true in general that $(AB)^+ = B^+A^+$. Instead:

$$(AB)^+ = (A^+AB)^+(ABB^+)^+$$

Solutions of linear equations

Consider a matrix representation of an imaging system with noise:

$$g_m = \sum_{n=1}^N H_{mn} f_n + \epsilon_m, \quad m = 1, \dots, M, \quad (1.179)$$

where ϵ_m represents noise and modeling error. In matrix-vector form:

$$\mathbf{g} = \mathbf{H}\mathbf{f} + \boldsymbol{\epsilon}. \quad (1.180)$$

What is meant by a “solution” of this equation?

Mathematicians would define an “exact” solution as one that satisfies

$$\mathbf{g} = \mathbf{H}\hat{\mathbf{f}}. \quad (1.181)$$

- Does an exact solution exist?
- Is it unique?
- Is it stable?

Existence

$$\mathbf{g} = \mathbf{H}\hat{\mathbf{f}}. \quad (1.181)$$

Equation (1.181) has *at least* one exact solution for *a particular* \mathbf{g} if and only if:

- The data are consistent;
- \mathbf{g} lies in \mathbb{V}_{con} ;
- $\mathbf{H}\mathbf{H}^+\mathbf{g} = \mathbf{g}$.

Equation (1.181) has *at least* one exact solution for *every* \mathbf{g} if and only if:

- Rank = number of measurements ($R = M$);
- \mathbb{V}_{incon} is trivial;
- $\mathbf{H}\mathbf{H}^\dagger$ is nonsingular.

These conditions can be satisfied only if $M \leq N$, i.e., the problem is *underdetermined*, more unknowns than measurements.

Uniqueness

$$\mathbf{g} = \mathbf{H}\hat{\mathbf{f}} . \quad (1.181)$$

Equation (1.181) has *at most* one solution for every \mathbf{g} if and only if:

- Rank = number of unknowns ($R = N$);
- \mathbb{U}_{null} is trivial;
- $\mathbf{H}^\dagger \mathbf{H}$ is nonsingular.

These conditions can be satisfied only if $M \geq N$ (i.e., the problem is overdetermined).

Putting the existence and uniqueness conditions together, we see that a unique, exact solution exists only if \mathbf{H} is square and full rank, $M = N = R$.

An explicit solution for consistent data

A particular data vector is consistent if:

$$\mathbf{H}\mathbf{H}^+\mathbf{g} = \mathbf{g}, \quad (1.185)$$

which can happen in two ways:

- There is no nontrivial inconsistency space
- We cheated and generated noise-free data

If the data are consistent, one solution to (1.181) is

$$\hat{\mathbf{f}} = \mathbf{H}^+\mathbf{g}. \quad (1.186)$$

To show that this is a solution, operate on it with \mathbf{H} . The result is

$$\mathbf{H}\hat{\mathbf{f}} = \mathbf{H}\mathbf{H}^+\mathbf{g} = \mathbf{g}, \quad (1.187)$$

where the last step follows from the consistency condition (1.185).

General solution for consistent data

$\mathbf{H}\hat{\mathbf{f}}$ is one solution to $\mathbf{g} = \mathbf{H}\hat{\mathbf{f}}$, but it is not unique if \mathbf{H} has null vectors.

The most general solution is

$$\hat{\mathbf{f}} = \mathbf{H}^+ \mathbf{g} + [\mathbf{I}_N - \mathbf{H}^+ \mathbf{H}] \mathbf{y}, \quad (1.188)$$

where \mathbf{y} is an arbitrary vector in \mathbb{U} . Since $\mathbf{I}_N - \mathbf{H}^+ \mathbf{H}$ is just \mathbf{P}_{null} , the second term in (1.188) is a null vector of \mathbf{H} .

To demonstrate that (1.188) is a solution to (1.181) for consistent data, we again operate on it with \mathbf{H} , yielding

$$\mathbf{H}\hat{\mathbf{f}} = \mathbf{H}\mathbf{H}^+ \mathbf{g} + [\mathbf{H} - \mathbf{H}\mathbf{H}^+ \mathbf{H}] \mathbf{y}. \quad (1.189)$$

The first term is \mathbf{g} by the consistency condition (1.185), while the second term is zero by the first Penrose equation, so (1.188) is indeed a solution to (1.181) if the data are consistent.

Least-squares solutions

For inconsistent data, no “exact” solution exists – there is no $\hat{\mathbf{f}}$ such that $\mathbf{H}\hat{\mathbf{f}} \equiv \mathbf{g}$.

One approach in that case is to look for a *least-squares solution* such that the norm of $\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}$ is minimized:

$$\hat{\mathbf{f}}_{LS} = \underset{\hat{\mathbf{f}}}{\operatorname{argmin}} \|\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}\|^2. \quad (1.191)$$

In words, look for a solution that matches the data as closely as possible.

A statistical justification for this approach will be given next week.

Terminology: $\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}$ is called the *residual*

The normal equation

If there are no constraints (such as positivity) on the solution, a least-squares solution must satisfy:

$$\frac{\partial}{\partial \hat{f}_n} \|\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}\|^2 = 0 \quad \forall n.$$

Carrying out the derivative yields

$$\mathbf{H}^\dagger \mathbf{H} \hat{\mathbf{f}} = \mathbf{H}^\dagger \mathbf{g}. \quad (1.194)$$

This important result is called the *normal equation*. Solving the normal equation is equivalent to finding a least-squares solution to the original equation, $\mathbf{g} = \mathbf{H}\hat{\mathbf{f}}$.

Existence and uniqueness revisited

A solution to the normal equation always exists, but it is not unique if \mathbf{H} has null vectors.

if $\mathbf{H}^\dagger \mathbf{H}$ is nonsingular or $R = N$, the least-squares solution is given uniquely by

$$\hat{\mathbf{f}}_{LS} = \left(\mathbf{H}^\dagger \mathbf{H} \right)^{-1} \mathbf{H}^\dagger \mathbf{g}, \quad (R = N). \quad (1.195)$$

With a null space ($R < N$), the general least-squares solution has exactly the same form as (1.188):

$$\hat{\mathbf{f}}_{LS} = \mathbf{H}^+ \mathbf{g} + \left[\mathbf{I}_N - \mathbf{H}^+ \mathbf{H} \right] \mathbf{y}, \quad (1.196)$$

where again \mathbf{y} is an arbitrary vector in \mathbb{U} .

Minimum-norm solutions

General solution repeated:

$$\hat{\mathbf{f}}_{LS} = \mathbf{H}^+ \mathbf{g} + [\mathbf{I}_N - \mathbf{H}^+ \mathbf{H}] \mathbf{y}, \quad (1.196)$$

One way to get a unique LS solution is simply to demand that there be no null component and set $\mathbf{y} = 0$.

Note that this choice minimizes the norm *of the solution* (as well as the norm of the residual):

$$||\hat{\mathbf{f}}||^2 = ||\hat{\mathbf{f}}_{meas}||^2 + ||\hat{\mathbf{f}}_{null}||^2.$$

Thus the *minimum-norm, least-squares* (MNLS) solution is

$$\hat{\mathbf{f}}_{MNLS} = \mathbf{H}^+ \mathbf{g}.$$

Another view of MNLS

A least-squares solution is given by

$$\hat{\mathbf{f}}_{LS} = \underset{\hat{\mathbf{f}}}{\operatorname{argmin}} \|\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}\|^2. \quad (1.191)$$

To get the unique MNLS solution, we can require

$$\hat{\mathbf{f}}_{MNLS} = \lim_{\eta \rightarrow 0} \underset{\hat{\mathbf{f}}}{\operatorname{argmin}} \left\{ \|\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}\|^2 + \eta \|\hat{\mathbf{f}}\|^2 \right\}.$$

Since $\eta \rightarrow 0$, the extra term does not disrupt the LS requirement, but for any $\eta > 0$ it penalizes null functions.

Computation of the MP pseudoinverse

We now know that the MNLS solution to $\mathbf{g} = \mathbf{H}\hat{\mathbf{f}}$ always exists and is always unique. It is given formally by $\hat{\mathbf{f}}_{MNLS} = \mathbf{H}^+ \mathbf{g}$, but how do we compute it?

Two possible answers:

- Do an SVD and use $\mathcal{H}^+ = \sum_{n=1}^R \frac{1}{\sqrt{\mu_n}} \mathbf{u}_n \mathbf{v}_n^\dagger$
- Find an iterative algorithm that converges to $\mathbf{H}^+ \mathbf{g}$

The Landweber algorithm

Consider the following iteration:

$$\hat{\mathbf{f}}^{(k+1)} = \hat{\mathbf{f}}^{(k)} + \mathbf{H}^\dagger \left[\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}^{(k)} \right] . \quad (1.231)$$

If this algorithm converges, we must have

$$\hat{\mathbf{f}}^{(k+1)} = \hat{\mathbf{f}}^{(k)}$$

and hence

$$\mathbf{H}^\dagger \mathbf{g} = \mathbf{H}^\dagger \mathbf{H} \hat{\mathbf{f}}^{(k)} ,$$

which is just the normal equation. Moreover, the solution cannot contain any null functions, provided the initial estimate contains none, since the operator \mathbf{H}^\dagger “erases” the null functions in the correction term. A suitable initial estimate is $\hat{\mathbf{f}}^{(0)} = \mathbf{H}^\dagger \mathbf{g}$. With this choice,

$$\hat{\mathbf{f}}^{(\infty)} = \hat{\mathbf{f}}_{MMLS}$$

For derivation of the Landweber algorithm and discussion of convergence, see B&M Sec. 1.7.6.

Noise amplification

If we represent the actual vector \mathbf{f} (not its estimate) by

$$\mathbf{f} = \sum_{k=1}^N \alpha_k \mathbf{u}_k, \quad \alpha_k = \mathbf{u}_k^\dagger \mathbf{f}, \quad (1.207)$$

and the noise by

$$\boldsymbol{\epsilon} = \sum_{k=1}^M \gamma_k \mathbf{v}_k, \quad \gamma_k = \mathbf{v}_k^\dagger \boldsymbol{\epsilon}, \quad (1.208)$$

then the expansion coefficients for \mathbf{g} are given by

$$\beta_k = \sqrt{\mu_k} \alpha_k + \gamma_k. \quad (1.209)$$

With the SVD form of \mathbf{H}^+ , we find

$$\hat{\mathbf{f}}_{MNLS} = \sum_{k=1}^R \left[\alpha_k + \frac{\gamma_k}{\sqrt{\mu_k}} \right] \mathbf{u}_k = \mathbf{f}_{meas} + \sum_{k=1}^R \frac{\gamma_k}{\sqrt{\mu_k}} \mathbf{u}_k, \quad (1.210)$$

Noise in the pseudoinverse solution is very large if μ_k is near zero.

Tikhonov regularization

Recall

$$\hat{\mathbf{f}}_{MNLS} = \lim_{\eta \rightarrow 0} \operatorname{argmin}_{\hat{\mathbf{f}}} \left\{ \|\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}\|^2 + \eta \|\hat{\mathbf{f}}\|^2 \right\} .$$

One way to control the noise is just to omit the limit:

$$\hat{\mathbf{f}}_{RLS} = \operatorname{argmin}_{\hat{\mathbf{f}}} \left\{ \|\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}\|^2 + \eta \|\hat{\mathbf{f}}\|^2 \right\} ,$$

where *RLS* stands for *regularized least squares*.

The RLS solution can be found by a modified Landweber algorithm:

$$\hat{\mathbf{f}}^{(k+1)} = (1 - \eta) \hat{\mathbf{f}}^{(k)} + \mathbf{H}^\dagger \left[\mathbf{g} - \mathbf{H}\hat{\mathbf{f}}^{(k)} \right] .$$

Tikhonov regularization – cont.

The Tikhonov RLS solution in SVD form is

$$\hat{\mathbf{f}}_{RLS} = \sum_{k=1}^R \frac{\mu_k \alpha_k}{\mu_k + \eta} \mathbf{u}_k + \sum_{k=1}^R \frac{\sqrt{\mu_k} \gamma_k}{\mu_k + \eta} \mathbf{u}_k .$$

Good news: Noise is attenuated

Bad news: Some components in measurement space are attenuated

Summary

- The Moore-Penrose pseudoinverse is an elegant theoretical construct
- It can be realized by SVD methods or iterative algorithms
- When applied to noisy data, it yields the MNLS solution
- MNLS solutions have no null functions but large noise
- Tikhonov and other regularizing methods can control noise, but at the expense of resolution