Condition estimation of linear algebraic equations and its application to feature selection

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Introduction

Several problems require the prediction of the output of a physical system for which the sample size n is much smaller than the dimension of the data p:

- Chemometrics
- Brain imaging
- Genomics
- Gene selection from microarray data
- Text analysis

The condition n < p implies that there are many models that satisfy the given data and important issues therefore arise:

- Which model from this infinite set of models should be chosen?
- What is the criterion that should be used for this selection?
- Can the selection be generic, that is, not problem dependent, such that prior information is not required?

Mathematical background

These problems yield an equation of the form

$$Ax = b + \varepsilon, \qquad A \in \mathbb{R}^{m \times n}, \qquad b \in \mathbb{R}^m, \qquad x \in \mathbb{R}^n$$

where m < n, $\operatorname{rank} A = m$ and ε is the noise. The least squares minimisation of $\|\varepsilon\|$ leads to the normal equation

$$A^T A x = A^T b$$

whose solution is

$$x_{\text{soln}} = A^{\dagger} b = V S^{\dagger} U^{T} b$$

where the superscript † denotes the pseudo-inverse. The solution is

$$x_{\text{soln}} = x_{\text{ln}} + x_0, \quad x_{\text{ln}} = V \begin{bmatrix} S_1^{-1} U^T b \\ 0_{n-m} \end{bmatrix}, \quad x_0 = V \begin{bmatrix} 0_m \\ r \end{bmatrix}$$

where x_{ln} is the minimum norm solution, x_0 lies in the null space of A, r is arbitrary, and

$$S = \begin{bmatrix} S_1 & 0_{m,n-m} \end{bmatrix}$$



The solution x_{ln} is unsatisfactory for two reasons:

- Prediction accuracy: This solution may have low bias and high variance. Prediction accuracy can sometimes be improved by reducing or setting to zero some coefficients of x_{ln} .
- Interpretation: It is usually desirable to choose the most important components of x_{ln} that characterise the physical system being considered.

Methods that are used to overcome these problems:

- Ridge regression: The magnitude of the components of x_{ln} is reduced continuously:
 - It is more stable than subset selection.
 - It does not set any components to zero and thus it does not yield a sparse model that can be easily interpreted.
- Subset selection: Components of x_{ln} are deleted in discrete steps:
 - The models are strongly dependent on the components that are deleted because the elimination procedure is discrete.
 - A small change in the data can cause a large change in the selected model, which reduces the prediction accuracy.

Ridge regression (Tikhonov regularisation)

The sensitivity of the solution $x_{\rm ln}$ to perturbations in b can be reduced by a constraint on the magnitude of the solution $x_{\rm reg}$:

$$x_{\text{reg}} = \arg\min_{x} \ \left\{ \left(Ax - b\right)^{T} \left(Ax - b\right) + \lambda \left\|x\right\|^{2} \right\}, \qquad \lambda > 0$$

and thus

$$(A^T A + \lambda I) x_{reg} = A^T b, \qquad \lambda > 0$$

The lasso ('least absolute shrinkage and selection operator')

The retension of the advantages of ridge regression (stability) and subset selection (sparsity) are combined in the lasso:

$$x_{\text{lasso}} = \arg\min_{x} \ \left\{ \left(Ax - b \right)^T \left(Ax - b \right) \right\} \quad \text{subject to} \quad \|x\|_1 \le t$$

which can also be written as

$$x_{\mathrm{lasso}} = \arg \min_{x} \ \left\{ \left(Ax - b\right)^{T} \left(Ax - b\right) + \lambda \left\|x\right\|_{1} \right\}, \qquad \lambda > 0$$

The elastic net

This method is an improvement on the lasso and it combines L_1 and L_2 regularisation:

$$x_{\text{elastic}} = \arg\min_{x} \left\{ (Ax - b)^{T} (Ax - b) + \lambda_{1} \|x\|_{1} + \lambda_{2} \|x\|^{2} \right\}$$

where

$$\lambda_1, \lambda_2 > 0$$

The solutions from Tikhonov regularisation, the lasso and the elastic net reduce the sensitivity of the least norm solution $x_{\rm ln}$ to perturbations in b, but there are differences between these forms of regularisation.

Compare Tikhonov regularisation

- Tikhonov regularisation imposes a Gaussian prior on the parameters of the model.
- Tikhonov regularisation does not impose sparsity on x_{reg} .
- The solution x_{reg} has a closed form expression.

with the lasso

- The lasso imposes a Laplacian prior on the parameters of the model.
- The lasso favours sparse solutions because some coefficients of $x_{\rm lasso}$ are set to zero. The sparsity of $x_{\rm lasso}$ increases as λ increases.
- The solution x_{lasso} does not have a closed form expression and quadratic programming is required for its computation.

and the elastic net

- The sparsity of x_{elastic} is similar to the sparsity of x_{lasso} .
- The solution $x_{\rm elastic}$ favours a model in which strongly correlated predictors are usually either all included, or all excluded.
- The solution x_{elastic} is much better than x_{lasso} for some problems.

A regularised solution (Tikhonov, the lasso and the elastic net) is stable with respect to perturbations in b, but several points arise:

- Is regularisation always required when the data b are corrupted by noise?
- Must specific conditions on A and b be satisfied in order that regularisation is imposed only when it is required?
- What are consequences of applying regularisation when it is not required?
- If regularisation is required, then

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r_{\text{method}} = x_{\text{ln}} - x_{\text{method}} \neq 0, method = {reg, lasso, elastic}
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Can bounds be imposed on $||r_{reg}||$, $||r_{lasso}||$ and $||r_{elastic}||$, such that these errors induced by regularisation are quantified?

The answers to these questions are most easily obtained if Tikhonov regularisation is considered because the constraint in the 2-norm lends itself naturally to the ${\rm SVD}.$

Regression

The use of regularisation is usually justified for three reasons:

- It reduces or eliminates over-fitting in regression.
- It reduces the sensitivity of the regression curve to noise in the data.
- It imposes a unique solution in feature selection

$$Ax = b$$

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $x \in \mathbb{R}^n$, m < n and rank A = m.

But

 There are well-defined problems for which regularisation must not be used because it causes a large degradation in the solution.

and thus

• Can a quantitative test be established such that regularisation is used only when it is required?

Regression provides a good example of the correct use, and the incorrect use, of regularisation.

Example 1 Consider the points (x_i, y_i) , i = 1, ..., 100, where the independent variables x_i are not uniformly distributed in the interval I = [1, ..., 20], the dependent variables y_i are given by

$$y_i = \sum_{k=1}^{33} a_k \exp\left(-\frac{(x_i - d_k)^2}{2\sigma_d^2}\right), \quad i = 1, \dots, 100$$

the centres d_k of the 33 basis functions are uniformly distributed in I and $\sigma_d = 1.35$.

Consider two sets of data points, $y=y_1$ and $y=y_2$, and the perturbations δy_1 and δy_2 ,

$$\delta y_1, \delta y_2 \sim \mathcal{N}\left(\mu = 0, \sigma^2 = 25 \times 10^{-8}\right)$$

and

$$\frac{\|\delta y_1\|}{\|y_1\|} = 3.41 \times 10^{-6} \qquad \text{and} \qquad \frac{\|\delta y_2\|}{\|y_2\|} = 8.27 \times 10^{-4}$$

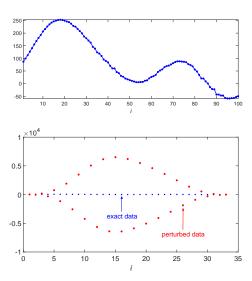


Figure: The exact curve (top), and the coefficients a_i (bottom) for the exact data $y=y_1$ and the perturbed data $y=y_1+\delta y_1$.

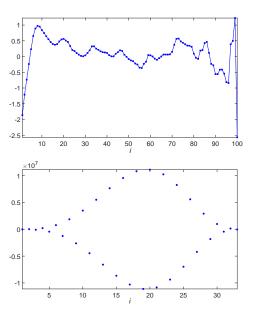


Figure: The exact curve (top), and the coefficients $\log_{10}|a_i|$ (bottom) for the exact data $y=y_2$ and the perturbed data $y=y_2+\delta y_2$.

- The interpolated curve is unstable for the data set $y = y_1$.
- The interpolated curve is stable for the data set $y = y_2$.

The coefficient matrix $A \in \mathbb{R}^{100 \times 33}$ is the same for $y = y_1$ and $y = y_2$, and its condition number is

$$\kappa(A) = 5.11 \times 10^8$$

Thus

- The presence of noise in the vector b, where Ax = b, does not imply that x is sensitive to changes in b.
- The condition $\kappa(A) \gg 1$ does not imply that the equation Ax = b is ill-conditioned.
- Tikhonov regularisation yields a very good result (numerically stable and a small error between the theoretically exact solution and the regularised solution) for $y = y_1$, but an unsatisfactory result for $y = y_2$ (a very large error between the theoretically exact solution and the regularised solution).

Condition numbers and regularisation

The 2-norm condition number of $A \in \mathbb{R}^{m \times n}$ is

$$\kappa(A) = \frac{s_1}{s_n}, \qquad p = \min(m, n)$$

where s_i , i = 1, ..., p, are the singular values of A and rank A = p.

- The condition number $\kappa(A)$ cannot be a measure of the stability of Ax = b because it is independent of b.
- It is necessary to develop a measure of stability that is a function of A and b.
- This leads to:
 - A refined normwise condition number the effective condition number - which is a function of A and b.
 - Componentwise condition numbers one condition number for each component of x.

The effective condition number

The effective condition number $\eta(A, b)$ of

$$A^T A x = A^T b, \qquad A \in \mathbb{R}^{m \times n}, \qquad m \ge n$$

is a refined normwise condition number.

Theorem 1 Let the relative errors Δx and Δb be

$$\Delta x = \frac{\|\delta x\|}{\|x\|}$$
 and $\Delta b = \frac{\|\delta b\|}{\|b\|}$

The effective condition number $\eta(A,b)$ of $A^TAx = A^Tb$ is equal to the maximum value of the ratio of Δx to Δb with respect to all perturbations $\delta b \in \mathbb{R}^m$

$$\eta(A, b) = \max_{\delta b \in \mathbb{R}^m} \frac{\Delta x}{\Delta b} = \frac{1}{s_n} \frac{\|c\|}{\|S^{\dagger}c\|}$$

where $A = USV^T$ is the SVD of A and $c = U^T b$.



Proof It follows from

$$A^T A x = A^T b$$

that $x = VS^{\dagger}U^{T}b = VS^{\dagger}c$ and thus

$$\|\delta x\| = \|VS^{\dagger}U^{T}\delta b\| = \|S^{\dagger}\delta c\| \le \frac{\|\delta c\|}{s_{n}}$$

and the division of both sides of this inequality by ||x|| yields

$$\frac{\|\delta x\|}{\|x\|} \le \frac{1}{s_n} \frac{\|\delta c\|}{\|c\|} \frac{\|c\|}{\|x\|} = \frac{1}{s_n} \frac{\|\delta b\|}{\|b\|} \frac{\|c\|}{\|x\|}$$

and thus

$$\eta(A,b) = \max_{\delta b \in \mathbb{R}^m} \frac{\Delta x}{\Delta b} = \frac{1}{s_n} \frac{\|c\|}{\|S^{\dagger}c\|} = \max_{\delta b \in \mathbb{R}^m} \frac{\Delta x}{\Delta b} = \frac{1}{s_n} \frac{\|b\|}{\|S^{\dagger}U^Tb\|}$$

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- The minimum value of $\eta(A, b)$ occurs when $c = e_n$ (e_i is the ith unit basis vector).
- If some conditions on b are satisfied, the maximum value of $\eta(A, b)$ occurs when $c = e_1$, and thus

$$1 \leq \eta(A, b) \leq \frac{s_1}{s_n} = \kappa(A)$$

More generally, since b = Uc:

- $\eta(A, b) \approx 1$ if the dominant components of b lie along the columns u_i of U that are defined by large values of i.
- $\eta(A, b) \approx \kappa(A)$ if the dominant components of b lie along the columns u_i of U that are defined by small values of i.

The discrete Picard condition

$$\eta(A, b) = \max_{\delta b \in \mathbb{R}^m} \frac{\Delta x}{\Delta b} = \frac{1}{s_n} \frac{\|c\|}{\|S^{\dagger}c\|}, \qquad c = U^{\mathsf{T}}b$$

Consider the ratio $|c_i|/s_i$, i = 1, ..., n.

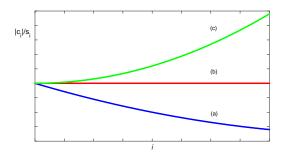


Figure: Three forms for the ratio $|c_i|/s_i$: (a) monotonically decreasing, (b) constant and (c) monotonically increasing.



• If $|c_i|/s_i \to 0$ as $i \to n$, then the constants $|c_i|$ decay to zero faster than the singular values s_i . The condition

$$\frac{|c_i|}{s_i} \to 0$$
 as $i \to n$

is called the discrete Picard condition. If this condition is satisfied, then $\eta(A,b) \approx \kappa(A)$ and thus Ax = b is ill-conditioned. Tikhonov regularisation can be used to yield a well-conditioned solution x.

- If $|c_i|/s_i \approx 1$, i = 1, ..., n, then $\eta(A, b) \approx \kappa(A)/\sqrt{n}$. Tikhonov regularisation cannot be used to yield a well-conditioned solution x.
- If

$$|c_{i+1}| \gg |c_i|, \qquad i = 1, \ldots, n-1$$

then $\eta(A, b) \approx 1$ and regularisation must not be applied.

Computation of the discrete Picard condition

The important term for the evaluation of the discrete Picard condition is

$$||x|| = ||A^{\dagger}b|| = ||S^{\dagger}c||$$

If noise is present, then the square of the magnitude of the perturbed solution is

$$\|x + \delta x\|^2 = \|A^{\dagger}(b + \delta b)\|^2 = \|S^{\dagger}(c + \delta c)\|^2 = \sum_{i=1}^{n} \left(\frac{c_i + \delta c_i}{s_i}\right)^2$$

Assume the magnitude of the perturbation $|\delta c_i|$ is approximately constant, such that

$$\begin{array}{lll} |\delta c_i| & \ll & |c_i| \,, & i=1,\ldots,p-1 \\ |\delta c_i| & \approx & |c_p| \,, & i=p \\ |\delta c_i| & \gg & |c_i| \,, & i=p+1,\ldots,n \end{array}$$

It follows that if the discrete Picard condition is satisfied

$$\frac{|c_i + \delta c_i|}{s_i} \approx \begin{cases} \frac{|c_i|}{s_i}, & i = 1, \dots, p - 1\\ \frac{|c_p + s_p|}{s_p}, & i = p\\ \frac{|\delta c_i|}{s_i}, & i = p + 1, \dots, n \end{cases}$$

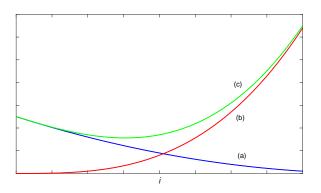


Figure: The ratios (a) $|c_i|/s_i$, (b) $|\delta c_i|/s_i$ and (c) $|c_i+\delta c_i|/s_i$ if the discrete Picard condition is satisfied.

If the discrete Picard condition

$$\frac{|c_i|}{s_i} \to 0$$
 as $i \to n$

is satisfied, the function $|c_i+\delta c_i|/s_i$ cannot be computed because it is sensitive to noise.

A similar result occurs if

$$|c_i| \approx s_i, \qquad i = 1, \ldots, n$$

because

$$\frac{|c_i + \delta c_i|}{s_i} \approx \frac{|\delta c_i|}{s_i}, \quad i = p + 1, \dots, n$$

If

$$|c_{i+1}| \gg |c_i|, \qquad i = 1, \ldots, n-1$$

computational problems do not occur because

$$\frac{|c_i + \delta c_i|}{s} \approx \frac{|c_i|}{s}, \quad i = 1, \dots, n$$

Summary (discrete Picard condition)

- The form of the term $|c_i|/s_i$ defines the stability of Ax = b.
- If

$$\frac{|c_i|}{s_i} \to 0$$
 as $i \to n$

then Ax = b is ill-conditioned. The dominant components of b lie along the columns u_i of U that are defined by small values of i (large singular values). Tikhonov regularisation enables a well-conditioned solution to be computed.

If

$$|c_{i+1}| \gg |c_i|, \quad i = 1, \ldots, n-1$$

then Ax = b is well-conditioned and $|c_i|/s_i$ is numerically stable. The dominant components of b lie along the columns u_i of U that are defined by large values of i (small singular values).

Example 2 Consider the regression problem in Example 1.

- The data points $y=y_1$ yield an ill-conditioned equation $A^TAx=A^Tb$. The effective condition number is $\eta(A,b)=4.61\times 10^8$.
- The data points $y = y_2$ yield a well-conditioned equation $A^T A x = A^T b$. The effective condition number is $\eta(A, b) = 7.94$.

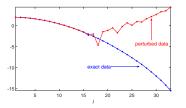


Figure: The ratio $\log_{10} |c_i|/s_i$ for the exact data $y=y_1$ and the ratio $\log_{10} |c_i+\delta c_i|/s_i$ for the perturbed data $y=y_1+\delta y_1$.

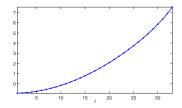


Figure: The ratio $\log_{10} |c_i|/s_i$ for the exact data $y=y_2$ and the ratio $\log_{10} |c_i+\delta c_i|/s_i$ for the perturbed data $y=y_2+\delta y_2$.

Tikhonov regularisation

If the discrete Picard condition is satisfied, the equation $A^TAx = A^Tb$ is ill-conditioned and Tikhonov regularisation requires the solution $x(\lambda)$ of

$$(A^T A + \lambda I)x(\lambda) = A^T b$$

and thus

$$x(\lambda) = V((S^TS + \lambda I)^{-1}S^T)U^Tb, \qquad \lambda \ge 0$$

- What is the error between the regularised solution $(\lambda > 0)$ and the exact solution $(\lambda = 0)$ if:
 - the discrete Picard condition is satisfied
 - the discrete Picard condition is not satisfied

Assume that λ^* is the optimal value of the regularisation parameter λ .

• If the discrete Picard condition, $\frac{|c_i|}{s_i} \to 0$ as $i \to n$, is satisfied, the solution x(0) is dominated by the large singular values and it is independent of the small singular values. The error is small

$$\frac{\|x(\lambda^*) - x(0)\|}{\|x(0)\|} \approx \frac{\lambda^*}{\lambda^* + s_1^2} \ll 1$$

because Tikhonov regularisation filters out the small singular values.

• If $|c_i| \approx s_i, i = 1, ..., n$, the error is smaller because all the singular values contribute to x(0)

$$\frac{\|x(\lambda^*) - x(0)\|}{\|x(0)\|} \approx \left(\frac{n-p}{n}\right)^{\frac{1}{2}}$$

Tikhonov regularisation filters out the components of x(0) associated with the small singular values, but the components associated with the large singular values are not affected.

• If $|c_{i+1}|/s_{i+1} \gg |c_i|/s_i$, i = 1, ..., n-1, the error is large

$$\frac{\|x(\lambda^*) - x(0)\|}{\|x(0)\|} \approx 1, \qquad \|x(\lambda^*)\| \approx 0$$

because x(0) is dominated by the small singular values, all of which are filtered out by Tikhonov regularisation.

Componentwise condition numbers

The condition number $\kappa(A)$ and effective condition number $\eta(A,b)$ are defined in the normwise sense. Condition numbers defined in the componentwise sense are more refined.

• A condition number is assigned to each component of x, where $A^TAx = A^Th$

The condition number $\rho(A, b, x_i)$ of the component x_i of x is defined as

$$\rho(A, b, x_j) = \max_{\delta b \in \mathbb{R}^m} \frac{\Delta x_j}{\Delta b}, \qquad j = 1, \dots, n$$

where

$$\Delta x_j = \frac{|\delta x_j|}{|x_i|}$$
 and $\Delta b = \frac{\|\delta b\|}{\|b\|}$

Theorem 2 The condition number $\rho(A, b, x_j)$ of the component x_j , j = 1, ..., n, of $A^T A x = A^T b$ is

$$\rho(A, b, x_j) = \frac{\left\|e_j^T A^{\dagger}\right\| \|b\|}{|x_j|} = \frac{\left\|e_j^T A^{\dagger}\right\| \|b\|}{\left|e_j^T A^{\dagger} b\right|} = \frac{1}{\cos \gamma_j} > 1$$

where γ_i is the angle between b and the jth row of A^{\dagger} .

Proof If e_j is the jth unit basis vector, then a change δb in b causes a change δx_j in x_j

$$\delta x_j = e_i^T \delta x = e_i^T A^{\dagger} \delta b, \qquad j = 1, \dots, n$$

and thus

$$\Delta x_j = \frac{|\delta x_j|}{|x_j|} \le \frac{\left\| e_j^T A^{\dagger} \right\| \|\delta b\|}{|x_j|}, \qquad j = 1, \dots, n$$

and the result follows.



Example 3 Consider the regression problem in Example 1.

- The data points $y = y_1$ yield an ill-conditioned equation $A^T A x = A^T b$.
- The data points $y = y_2$ yield a well-conditioned equation $A^T A x = A^T b$.

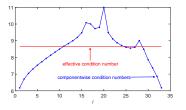


Figure: The effective condition number and the componentwise condition numbers, on a logarithmic scale, for $y = y_1$.

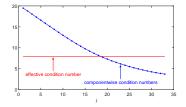


Figure: The effective condition number and the componentwise condition numbers for $y = y_2$.

Feature selection

Many problems in feature selection yield the equation

$$Ax = b + \varepsilon$$

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $x \in \mathbb{R}^n$, m < n, $\operatorname{rank} A = m$ and ε is the noise in the data b. The normal equations are

$$(A^T A) x = A^T b$$

This equation has an infinite number of solutions x_{soln}

$$x_{\text{soln}} = V \begin{bmatrix} S_1^{-1} U^T b \\ 0_{n-m} \end{bmatrix} + V \begin{bmatrix} 0_m \\ r \end{bmatrix} = x_{\text{ln}} + x_0$$

where x_{ln} is the solution of minimum norm, x_0 lies in the null space of A and is orthogonal to x_{ln} , $r \in \mathbb{R}^{n-m}$ is arbitrary and

$$A = USV^T = U \begin{bmatrix} S_1 & 0_{m,n-m} \end{bmatrix} V^T, \qquad S_1 = \operatorname{diag} \{s_i\}_{i=1}^m$$

- The most important features (components of x_{soln}) of the system are usually sought and a sparse solution is therefore desired.
- Use the n-m degrees of freedom in r in the null space vector x_0 to obtain a sparse and regularised solution x_{soln}

$$x_{\mathrm{soln}} = V \left[\begin{array}{c} S_1^{-1} U^T b \\ 0_{n-m} \end{array} \right] + V \left[\begin{array}{c} 0_m \\ r \end{array} \right] = x_{\mathrm{ln}} + x_0$$

The solutions x_{lasso} and x_{elastic} ignore the vector x_0 .

- The vector r is chosen such that if the d components k_1, k_2, \ldots, k_d , of x_{ln} have large condition numbers, then these d components of the solution x_{soln} are equal to zero.
- The lasso and the elastic net yield sparse solutions from constrained minimisation problems but they are approximate solutions of the normal equations

$$(A^T A) x = A^T b$$

The need, or otherwise, for regularisation, and the errors between (a) the solutions $x_{\rm soln}$ and $x_{\rm lasso}$, and (b) the solutions $x_{\rm soln}$ and $x_{\rm elastic}$, are not considered.

Feature selection and condition estimation

Since

$$x_{\text{soln}} = x_{\text{ln}} + x_0 = x_{\text{ln}} + V \begin{bmatrix} 0_m \\ r \end{bmatrix} = x_{\text{ln}} + \begin{bmatrix} V_1 & V_2 \end{bmatrix} \begin{bmatrix} 0_m \\ r \end{bmatrix}$$

it follows that

$$x_{\text{soln}} = x_{\text{ln}} + V_2 r, \qquad V_2 \in \mathbb{R}^{n \times (n-m)}$$

By definition, the components of x_{ln} that have the d largest condition numbers, $1 \le d \le n - m$, satisfy

$$x_{\ln,k} + x_{0,k} = 0,$$
 $k = k_1, k_2, \dots, k_d$

that is, these components of x_{soln} are set to zero, thereby inducing sparsity in x_{soln} .

• The vector r is chosen to satisfy these d equations.

Summary

- A large condition number of A, $\kappa(A) \gg 1$, does not imply that the equation Ax = b is ill-conditioned.
- The effective condition number $\eta(A, b)$ is a better measure of the stability of Ax = b because it is a function of A and b, which must be compared with $\kappa(A)$, which is a function of A only.
- If the discrete Picard condition is satisfied, then $\eta(A,b) \approx \kappa(A)$ and Tikhonov regularisation yields a stable solution whose error is small.
- More refined measures of the stability of Ax = b are the componentwise condition numbers, which measure the stability of each component of x due to a perturbation in b.
- The equation Ax = b for feature selection has an infinite number of solutions. The lasso and elastic net apply regularisation to the least norm solution $x_{\rm ln}$, and they do not consider the vectors $x_{\rm null}$ that lie in the null space of A.
- Consideration of the componentwise condition numbers of $x_{\rm soln} = x_{\rm ln} + x_{\rm null}$ yields a sparse solution that satisfies the normal equations, and regularisation is satisfied in the componentwise sense.