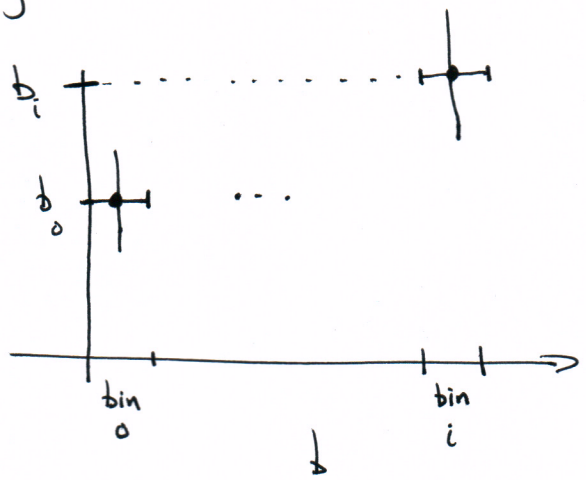
Singular Value Decomposition (SVD)

Let the distribution of a measured observable be stored in vector $\vec{b}$ of dimension n_b

$$\vec{b} = \underbrace{[b_0, \ldots, b_{n_b}]}_{0, \ldots, n_b}$$

Each entry is the count of that bin in a histogram



$\vec{b}$ could be the bins of E_T, $\not{E}_T$, H_T, or whatever.

Note that the true distribution of $\vec{b}$ is approximated by the measured $\vec{b}$, so a particular event in bin i of the true distribution may appear in the same bin i of the measured distribution, any adjacent bin, or nowhere at all in observed $\vec{b}$ due to acceptance.

Assume that the measurement procedure can be simulated with an MC sample.

As such, we generate an MC sample w/ distribution x^{ini} of dimension n_x. This is run through a detector simulation. The observed distribution is b^{ini}. Every event in b^{ini} can be traced back to its original placement in x^{ini}, so $\exists$ a well-defined system of linear relations between the simulated and measured distributions

$$A x^{ini} = b^{ini}$$

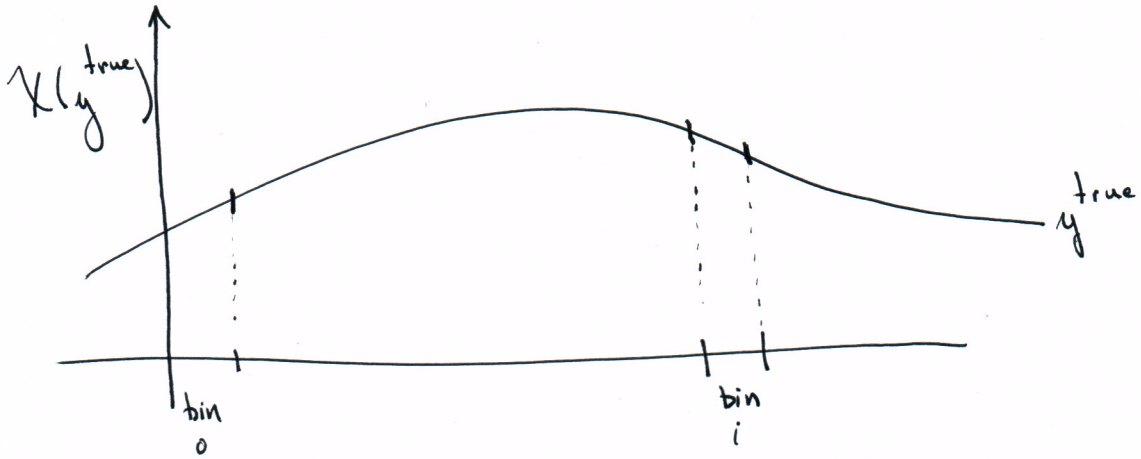
where A is an $n_b \times n_x$ probability matrix. Matrix A acts on the true values, mapping them to the measured value. Hence, matrix A simulates the folding procedure. Later, we will want to use the inverse of A to unfold observed data. Matrix A is also called a response matrix.

> Previous attempts to find the exact inverse of A arrived at solutions that rapidly oscillate in an unworkable manner.

The Singular Value Decomposition (SVD) method offers a more stable solution.

Recall that $\vec{x}$ and $\vec{b}$ are vectors of the bins of some discrete distribution. These bins approximate the continuous probability distribution which underlies it.

Let y^{true} be the continuous variable and separated into the same n_x bins,



such that $x \to y^{true}$ in the limit of infinite events. The j^{th} bin of $\vec{x}$ can be expressed as the integral of the continuous distribution $\chi(y^{true})$ over the width of that bin

$$x_j = \int_{y^{true}_{j-1}}^{y_j} dy^{true}\, \chi(y^{true}), \qquad j = \{1, \dots, n_x\}$$

Letting y be the folder continuous variable underlying b

$$b_i = \int_{y_{i-1}}^{y_i} dy\, B(y), \qquad i = \{1, \dots, n_b\}$$

For these continuous distributions y, y^{true} let $A(y, y^{true})$ be the detector response function that maps the true distribution y^{true} to y.

$$A(y, y^{true})\, X(y^{true}) \longmapsto B(y)$$

$$\Rightarrow \quad B(y) = \int_{y_0^{true}}^{y_{n_x}^{true}} dy^{true}\, A(y, y^{true})\, X(y^{true})$$

And so the detector response matrix relates to the detector response function by:

$$A_{ij}\, x_j = b_i$$

$$\Rightarrow \quad A_{ij} \left[\int_{y_{j-1}^{true}}^{y_j^{true}} dy^{true}\, X(y^{true}) \right] = \left[\int_{y_{i-1}}^{y_i} dy\, B(y) \right]$$

$$\Rightarrow \quad \boxed{A_{ij} = \frac{\int_{y_{i-1}}^{y_i} dy \left[\int_{y_0^{true}}^{y_{n_x}^{true}} dy^{true}\, A(y, y^{true})\, X(y^{true}) \right]}{\int_{y_{j-1}^{true}}^{y_j^{true}} dy^{true}\, X(y^{true})}}$$

A singular value decomposition (SVD) of a real $m \times n$ matrix A is its factorization into the form

$$A = U S V^T$$

where U is an $m \times m$ orthogonal matrix, V is an $n \times n$ orthogonal matrix, and S is an $m \times n$ diagonal matrix w/ non-negative values. Those diagonal values s_i are denoted singular values

Features:

1. If A is orthogonal, then $s_i = 1 \ \forall i$
2. If A is degenerate, then at least one singular value is zero.
3. If some singular values are significantly smaller than others, the system may be difficult to solve.

Simple Example

Consider the following response matrix

$$A = \frac{1}{2}\begin{bmatrix} 1+\varepsilon & 1-\varepsilon \\ 1-\varepsilon & 1+\varepsilon \end{bmatrix} \qquad \varepsilon \in [0, 1]$$

So some value is distributed over two bins and detected over the same two bins.

Ideal Detector ($\varepsilon = 1$): Response matrix A is the identity matrix, so simulation and detection are identical.

Poor Detector ($\varepsilon \ll 1$): $\begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}$ No matter the true bin of an event, it is equally likely to appear in any of the observed bins.

Efficiency: No event escapes detection in this simple example. Each column sums to 1, so there is a 100% probability that an event in column i is in any of the observed bins.

If observed matrix b and the response matrix A is given, one can unfold the true distribution x. (We will return to this example and solve it later.)

Theorem (Kolman, Hill, p.400)

Let A be an $m \times n$ real matrix. There exist orthogonal matrices U of size $m \times m$ and V of size $n \times n$ such that

$$A = U S V^T$$

where S is an $m \times n$ matrix with nondiagonal entries all zero and

$$\lambda_{11} \geq \cdots \geq \lambda_{pp} \geq 0$$

where $p = \min(m, n)$.

Determining U, S, and V in SVD:

1. An $n \times n$ symmetric matrix related to A is $A^T A$

By theorem 6.9, $\exists$ an orthogonal matrix V such that $V^{-1}(A^T A)V = D$, where D is a diagonal matrix w/ entries $\{\lambda_1, \ldots, \lambda_n\}$ as eigenvalues of $A^T A$.

2. Let $\vec{v}_j$ be the j^{th} column of V. Then

$$(A^TA)\vec{v}_j = \lambda_j \vec{v}_j$$

3. Multiply by $\vec{v}_j^T$ from the left

$$\vec{v}_j^T (A^TA)\vec{v}_j = \lambda_j \vec{v}_j^T \vec{v}_j$$

$$(A\vec{v}_j)^T (A\vec{v}_j) = \lambda_j \vec{v}_j^T \vec{v}_j$$

$$\|A\vec{v}_j\|^2 = \lambda_j \|\vec{v}_j\|^2$$

The norm, or length, of a vector is necessarily non-negative. So since $\|A\vec{v}_j\|^2 > 0$ and $\|\vec{v}_j\|^2 > 0$, the eigenvalue λ_j must also be non-negative. $\lambda_j \geq 0$, $\forall j$. This is necessary, because ...

4. Define $\Lambda_{jj} \equiv \sqrt{\lambda_j}$.

$$\Rightarrow \|A\vec{v}_j\|^2 = \Lambda_{jj}^2 \|\vec{v}_j\|^2$$

Because V is defined as orthogonal, each column is a unit vector. It follows that $\|\vec{v}_j\| = |\vec{1}|$.

$$\Rightarrow \boxed{\Lambda_{jj} = \|A\vec{v}_j\|}$$

5. Determine $m \times m$ orthogonal matrix U.

$$AV = US$$

$$A\vec{v}_j = s_{jj}\vec{u}_j \qquad \forall j \in \{1, \dots, p\}$$

$$\vec{u}_j = \frac{1}{s_{jj}} A\vec{v}_j$$

for the first p vectors. For $m > p$, the remaining $m-p$ vectors of U are found by ~~linearly~~ extending the linearly independent vectors in $\{\vec{u}_1, \vec{u}_2, \dots\}$.

Example: Find the ~~sing~~ singular value decomposition of

$$A = \begin{bmatrix} 5 & 5 \\ -1 & 7 \end{bmatrix}.$$

We want to decompose A into

$$A = USV^T$$

where U and V are orthogonal matrices ($U^TU = UU^T = I$)
S is a diagonal matrix with non-negative entries.

We can find this form by using two equations:

1. $A^TA = (USV^T)^T(USV^T)$

$= (SV^T)^TU^TUSV^T$

$= \underline{VS^TSV^T}$ (using $U^TU = I$)

2. $A = USV^T$

$\underline{AV = US}$

Begin with the first

$$A^TA = \begin{bmatrix} 5 & -1 \\ 5 & 7 \end{bmatrix}\begin{bmatrix} 5 & 5 \\ -1 & 7 \end{bmatrix} = \begin{bmatrix} 26 & 18 \\ 18 & 74 \end{bmatrix}$$

Notice that $A^TA = V(S^TS)V^T$ is a diagonalization of A^TA, so S^TS is a diagonal matrix composed of the eigenvalues of A^TA and the columns of V are the associated eigenvectors.

Find the eigenvalues of A^TA via the characteristic equation of A^TA

$$\det(A^TA - \lambda I) = 0 \qquad \text{where } I \text{ is the identity}$$

$$\det\begin{bmatrix} 26-\lambda & 18 \\ 18 & 74-\lambda \end{bmatrix} = 0$$

$$(26-\lambda)(74-\lambda) - 18^2 = 0$$

$$\lambda^2 - 100\lambda + 1600 = 0$$

$$(\lambda - 20)(\lambda - 80) = 0$$

So the eigenvalues of A^TA are 20 and 80. What are the eigenvectors? To find the eigenvector with eigenvalue 20, we need to find a vector in the null space of the matrix

The null space: The set of all vectors $\vec{v}$ for which $A\vec{v} = 0$.

$$A^TA - 20I = \begin{bmatrix} 6 & 18 \\ 18 & 54 \end{bmatrix};$$

$$\Rightarrow \begin{bmatrix} 6 & 18 \\ 18 & 54 \end{bmatrix} \begin{bmatrix} v_{00} \\ v_{10} \end{bmatrix} = 0$$

$$\begin{cases} 6v_{00} + 18v_{10} = 0 \\ 18v_{00} + 54v_{10} = 0 \end{cases}$$

$$\Rightarrow \begin{cases} v_{00} = -3v_{10} \\ v_{10} = r_1, \ \forall r_1 \in \mathbb{R} \end{cases}$$

So we could choose

$$\vec{v}_1 = \begin{bmatrix} v_{00} \\ v_{10} \end{bmatrix} = \begin{bmatrix} -3 \\ 1 \end{bmatrix} \quad (\text{choosing } r=1)$$

but the columns of V should be unit vectors because V is orthogonal, so we can effectively choose a different r by normalizing $\vec{v}_1$

$$\vec{v}_1 = \frac{1}{\sqrt{(-3)^2 + 1^2}} \begin{bmatrix} -3 \\ 1 \end{bmatrix}$$

$$\vec{v}_1 = \frac{1}{\sqrt{10}} \begin{bmatrix} -3 \\ 1 \end{bmatrix}$$

Now find the eigenvector for eigenvalue 80.

$$A^TA - 80I = \begin{bmatrix} 26 & 18 \\ 18 & 74 \end{bmatrix} - \begin{bmatrix} 80 & 0 \\ 0 & 80 \end{bmatrix} = \begin{bmatrix} -54 & 18 \\ 18 & -6 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} -54 & 18 \\ 18 & -6 \end{bmatrix} \begin{bmatrix} v_{01} \\ v_{11} \end{bmatrix} = 0$$

$$\begin{cases} -54v_{01} + 18v_{11} = 0 \\ 18v_{01} - 6v_{11} = 0 \end{cases}$$

$$18v_{11} = 54v_{01}$$

$$\Rightarrow \begin{cases} v_{11} = 3v_{01} \\ v_{01} = r_2, \ \forall r_2 \in \mathbb{R} \end{cases}$$

So the second column vector of V could be $\begin{bmatrix} 1 \\ 3 \end{bmatrix}$ but normalizing it: $\vec{v}_2 = \frac{1}{\sqrt{10}} \begin{bmatrix} 1 \\ 3 \end{bmatrix}$.

$$V = \frac{1}{\sqrt{10}} \begin{bmatrix} -3 & 1 \\ 1 & 3 \end{bmatrix}$$

Since we have eigenvalues 20 and 80 of A^TA,

$$S^TS = \begin{bmatrix} 20 & 0 \\ 0 & 80 \end{bmatrix}$$

$$\Rightarrow S = \begin{bmatrix} \sqrt{20} & 0 \\ 0 & \sqrt{80} \end{bmatrix} = \begin{bmatrix} 2\sqrt{5} & 0 \\ 0 & 4\sqrt{5} \end{bmatrix}$$

What remains is determining U. Use the 2nd equation from the beginning of this example

$$AV = US$$

$$\frac{1}{\sqrt{10}}\begin{bmatrix} 5 & 5 \\ -1 & 7 \end{bmatrix}\begin{bmatrix} -3 & 1 \\ 1 & 3 \end{bmatrix} = US$$

$$\frac{1}{\sqrt{10}}\begin{bmatrix} -10 & 20 \\ 10 & 20 \end{bmatrix} = U\begin{bmatrix} 2\sqrt{5} & 0 \\ 0 & 4\sqrt{5} \end{bmatrix}$$

$$\frac{10}{\sqrt{10}}\begin{bmatrix} -1 & 2 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} \frac{1}{2\sqrt{5}} & 0 \\ 0 & \frac{1}{4\sqrt{5}} \end{bmatrix} = U$$

$$\frac{1}{2\sqrt{5}} \cdot \frac{10}{\sqrt{10}}\begin{bmatrix} -1 & 2 \\ 1 & 2 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{bmatrix} = U$$

$$\frac{10}{2\cdot 5\sqrt{2}}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} = U$$

$$\boxed{\frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} = U}$$

We now have all the pieces of the decomposition. Double check that U is orthogonal:

$$U^TU = \frac{1}{2}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

$$U^TU = I \quad \checkmark$$

Double check the original expression:

$$A = USV^T$$

$$= \frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 2\sqrt{5} & 0 \\ 0 & 4\sqrt{5} \end{bmatrix}\frac{1}{\sqrt{10}}\begin{bmatrix} -3 & 1 \\ 1 & 3 \end{bmatrix}$$

$$= \frac{2\sqrt{5}}{2\sqrt{5}}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}\begin{bmatrix} -3 & 1 \\ 1 & 3 \end{bmatrix}$$

$$= \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} -3 & 1 \\ 2 & 6 \end{bmatrix}$$

$$= \begin{bmatrix} 5 & 5 \\ -1 & 7 \end{bmatrix}$$

Example: Find the SVD of

$$A = \frac{1}{2}\begin{bmatrix} 1+\varepsilon & 1-\varepsilon \\ 1-\varepsilon & 1+\varepsilon \end{bmatrix}$$

We want to decompose A into the form

$$A = USV^T,$$ where U, V are supposed to be orthogonal matrices

Begin by using the form

$$\begin{aligned} A^TA &= (USV^T)^T(USV^T) \\ &= (SV^T)^TU^TUSV^T \\ &= VS^TSV^T \qquad (\text{by orthogonality } U^TU = I) \end{aligned}$$

to find S and V. Notice that this form is a diagonalization of A^TA, so S^TS is a diagonal matrix composed of the eigenvalues of A^TA and the columns of V are the associated eigenvectors.

Find the eigenvalues of A^TA via the characteristic equation of A^TA

$$\det(A^TA - \lambda I) = 0$$

$$A^TA = \frac{1}{4}\begin{bmatrix} 1+\varepsilon & 1-\varepsilon \\ 1-\varepsilon & 1+\varepsilon \end{bmatrix}\begin{bmatrix} 1+\varepsilon & 1-\varepsilon \\ 1-\varepsilon & 1-\varepsilon \end{bmatrix}$$

$$= \frac{1}{4}\begin{bmatrix} (1+\varepsilon)^2+(1-\varepsilon)^2 & 2(1+\varepsilon)(1-\varepsilon) \\ 2(1+\varepsilon)(1-\varepsilon) & (1+\varepsilon)^2+(1-\varepsilon)^2 \end{bmatrix}$$

$$\det\begin{bmatrix} (1+\varepsilon)^2+(1-\varepsilon)^2-\lambda & 2(1+\varepsilon)(1-\varepsilon) \\ 2(1+\varepsilon)(1-\varepsilon) & (1+\varepsilon)^2+(1-\varepsilon)^2-\lambda \end{bmatrix} = 0$$

$$\left((1+\varepsilon)^2+(1-\varepsilon)^2-\lambda\right)^2-4(1+\varepsilon)(1-\varepsilon)=0$$

$$\lambda^2-2\lambda\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)+\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)^2-4(1+\varepsilon)^2(1-\varepsilon)^2=0$$

$$\lambda^2-2\lambda\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)+\left[(1+\varepsilon)^4+(1-\varepsilon)^4+2(1+\varepsilon)^2(1-\varepsilon)^2-4(1+\varepsilon)^2(1-\varepsilon)^2\right]=0$$

$$\lambda^2-2\lambda\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)+\left[(1+\varepsilon)^4+(1-\varepsilon)^4-2(1+\varepsilon)^2(1-\varepsilon)^2\right]=0$$

$$\lambda^2-2\lambda\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)+\left((1+\varepsilon)^2-(1-\varepsilon)^2\right)^2=0$$

For ax^2+bx+c

$$x=\frac{-b\pm\sqrt{b^2-4ac}}{2a}$$

$$\lambda=\frac{1}{2}\left[2\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)\pm\sqrt{4\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)-4\left((1+\varepsilon)^2-(1-\varepsilon)^2\right)^2}\right]$$

$$\lambda=\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)\pm\sqrt{(1+\varepsilon)^4+(1-\varepsilon)^4+2(1+\varepsilon)^2(1-\varepsilon)^2-\left((1+\varepsilon)^4+(1-\varepsilon)^4-2(1+\varepsilon)^2(1-\varepsilon)^2\right)}$$

$$\lambda=\left((1+\varepsilon)^2+(1-\varepsilon)^2\right)\pm\sqrt{4(1+\varepsilon)^2(1-\varepsilon)^2}$$

$$\lambda=(1+\varepsilon)^2+(1-\varepsilon)^2\pm2(1+\varepsilon)(1-\varepsilon)$$ (Hint: Keep in this form)

Define

$$\begin{cases}\lambda_1=(1+\varepsilon)^2+2(1+\varepsilon)(1-\varepsilon)+(1-\varepsilon)^2\\ \lambda_2=(1+\varepsilon)^2-2(1+\varepsilon)(1-\varepsilon)+(1-\varepsilon)^2\end{cases}$$

Find the eigenvector for λ_1:

$$A^TA-\lambda_1 I=\frac{1}{4}\begin{vmatrix}(1+\varepsilon)^2+(1-\varepsilon)^2-(1+\varepsilon)^2-2(1+\varepsilon)(1-\varepsilon)-(1-\varepsilon)^2 & 2(1+\varepsilon)(1-\varepsilon)\\ 2(1+\varepsilon)(1-\varepsilon) & -2(1+\varepsilon)(1-\varepsilon)\end{vmatrix}$$

$$A^TA - \lambda_1 I = \frac{1}{2}(1+\varepsilon)(1-\varepsilon)\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$\Rightarrow \frac{1}{2}(1+\varepsilon)(1-\varepsilon)\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} v_{00} \\ v_{10} \end{bmatrix} = 0$$

$$\Rightarrow \begin{cases} -v_{00} + v_{10} = 0 \\ v_{00} - v_{10} = 0 \end{cases}$$

$$\Rightarrow \begin{cases} v_{00} = v_{10} \\ v_{10} = r_1 \text{ , } \forall\, r_1 \in \mathbb{R} \end{cases}$$

So the normalized eigenvector is

$$\begin{bmatrix} v_{00} \\ v_{10} \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

Similarly, find the eigenvector for λ_2

$$A^TA - \lambda_2 I = \frac{1}{4}\begin{bmatrix} (1+\varepsilon)^2 + (1-\varepsilon)^2 - (1+\varepsilon)^2 + 2(1+\varepsilon)(1-\varepsilon) - (1-\varepsilon)^2 & 2(1+\varepsilon)(1-\varepsilon) \\ 2(1+\varepsilon)(1-\varepsilon) & 2(1+\varepsilon)(1-\varepsilon) \end{bmatrix}$$

$$= \frac{1}{2}(1+\varepsilon)(1-\varepsilon)\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$\Rightarrow \frac{1}{2}(1+\varepsilon)(1-\varepsilon)\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} v_{01} \\ v_{11} \end{bmatrix} = 0$$

$$\Rightarrow \begin{bmatrix} v_{01} \\ v_{11} \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Then $\boxed{V = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}}$

Now recall that the eigenvalues of $A^T A$ are

$$\lambda_{1,2} = (1+\varepsilon)^2 \pm 2(1+\varepsilon)(1-\varepsilon) + (1-\varepsilon)^2$$

$$\lambda_{1,2} = \left[(1+\varepsilon) \pm (1-\varepsilon)\right]^2$$

$$\begin{cases} \lambda_1 = 4 \\ \lambda_2 = 4\varepsilon^2 \end{cases}$$

So the diagonalization is

$$S^T S = 4 \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon^2 \end{bmatrix}$$

$$\Rightarrow \boxed{S = 2 \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix}}$$

Note: This is a factor of 2 larger than in the paper.

Now we can find U:

$$U = AVS^{-1}$$

$$U = \frac{1}{2} \begin{bmatrix} 1+\varepsilon & 1-\varepsilon \\ 1-\varepsilon & 1+\varepsilon \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon^{-1} \end{bmatrix}$$

$$U = \frac{1}{4\sqrt{2}} \begin{bmatrix} 1+\varepsilon & 1-\varepsilon \\ 1-\varepsilon & 1+\varepsilon \end{bmatrix} \begin{bmatrix} 1 & \varepsilon^{-1} \\ 1 & -\varepsilon^{-1} \end{bmatrix}$$

$$U = \frac{1}{4\sqrt{2}} \begin{bmatrix} 2 & 2 \\ 2 & -2 \end{bmatrix}$$

$$\boxed{U = \frac{1}{2\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}}$$

Note: The extra factor of 2 in S results in an extra factor of $\frac{1}{2}$ here

Hence, we have our SVD form

$$A = \frac{1}{2\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} 2 \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

$$\boxed{A = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}}$$

Because the extra factors of 2 and $\frac{1}{2}$ cancel here and also that the form of U is not strictly orthogonal because of only that factor of 2, we can redefine

$$S \equiv \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix} \quad \text{and} \quad U \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

and still have a valid singular value decomposition (I'm guessing).

Solving a Linear System Using SVD

Suppose now that $A = \frac{1}{2}\begin{bmatrix} 1+\varepsilon & 1-\varepsilon \\ 1-\varepsilon & 1+\varepsilon \end{bmatrix}$ is used to measure (via $A\vec{x} = \vec{b}$) the number of observed events in a two-bin histogram $\vec{b} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$. Let's use U, S, and V from the SVD ($A = USV^T$) of A computed earlier.

Begin by substituting the SVD form of A into the problem we are trying to solve:

$$A\vec{x} = \vec{b}$$
$$(USV^T)\vec{x} = \vec{b}$$
$$U^T(USV^T)\vec{x} = U^T\vec{b}$$
$$S(V^T\vec{x}) = (U^T\vec{b})$$

As such, we are using U and V to rotate $\vec{b}$ and $\vec{x}$, respectively.

$$V^T\vec{x} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \underbrace{\frac{1}{\sqrt{2}}\begin{bmatrix} x_1 + x_2 \\ x_1 - x_2 \end{bmatrix}}_{\equiv\, y}$$

$$U^T\vec{b} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \underbrace{\frac{1}{\sqrt{2}}\begin{bmatrix} b_1 + b_2 \\ b_1 - b_2 \end{bmatrix}}_{\equiv\, d}$$

$$\Rightarrow Sy = d$$
$$y = S^{-1}d \quad \text{where } S^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{\varepsilon} \end{bmatrix}, \text{ b/c } \begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{\varepsilon} \end{bmatrix} = I$$

Because S (and therefore S^{-1}) is diagonal, this is a diagonal system of equations.

Recall that we had needed A^{-1} to solve for x exactly, but we can also now find an exact solution with the SVD because $x = Vy$.

$$x = Vy = VS^{-1}d = VS^{-1}U^T b$$

$$= \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & \frac{1}{\varepsilon}\end{bmatrix}\frac{1}{\sqrt{2}}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}b_1\\ b_2\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}1 & \frac{1}{\varepsilon}\\ 1 & -\frac{1}{\varepsilon}\end{bmatrix}\begin{bmatrix}b_1+b_2\\ b_1-b_2\end{bmatrix}$$

$$= \frac{1}{2}\begin{bmatrix}(b_1+b_2)+\frac{1}{\varepsilon}(b_1-b_2)\\ (b_1+b_2)-\frac{1}{\varepsilon}(b_1-b_2)\end{bmatrix}$$

$$= \frac{1}{2}(b_1+b_2)\begin{bmatrix}1\\ 1\end{bmatrix} + \frac{1}{2\varepsilon}(b_1-b_2)\begin{bmatrix}1\\ -1\end{bmatrix}$$

$$= \frac{1}{\sqrt{2}}(b_1+b_2)\begin{bmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{bmatrix} + \frac{1}{\varepsilon\sqrt{2}}(b_1-b_2)\begin{bmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{bmatrix}$$

I expressed the last line as such for a reason. Formally, the SVD of matrix A (i.e. $S(V^T x) = U^T b$) decomposes b into a series of n, orthogonal and normalized functions. The basis is given by the columns of U and the components of $U^T b$ are the coefficients.

We can see this in the example of the previous line of x because:

Orthogonal:

$$\begin{bmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{bmatrix}\cdot\begin{bmatrix}\frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}}\end{bmatrix} = \begin{bmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{bmatrix}\begin{bmatrix}\frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}}\end{bmatrix} = \frac{1}{2} - \frac{1}{2} = 0$$

Normal:

$$\left\|\begin{bmatrix}\frac{1}{\sqrt{2}}\\ \frac{\pm 1}{\sqrt{2}}\end{bmatrix}\right\|^2 = \left(\frac{1}{\sqrt{2}}\right)^2 + \left(\frac{\pm 1}{\sqrt{2}}\right)^2 = \frac{1}{2} + \frac{1}{2} = 1$$

and the coefficients indeed match

$$U^T b = \begin{bmatrix} \frac{1}{\sqrt{2}}(b_1+b_2) \\ \frac{1}{\sqrt{2}}(b_1-b_2) \end{bmatrix}$$

Similarly, x is also decomposed into n_x orthonormal functions whose basis is given by the columns of V. Hence, the original system of equations $Ax=b$ is reduced to the diagonal system

$$Sy = d \iff S(V^T x) = U^T b$$

Since S is diagonal, inverting it is simple.

Problem Areas of This Example

If all the components of $U^T b = \frac{1}{\sqrt{2}} \begin{bmatrix} b_1+b_2 \\ b_1-b_2 \end{bmatrix}$ are statistically significant and the singular values λ_i are not too small, an exact solution by any means is not a problem. However, ε being small introduces problems because the $1/\varepsilon$ term in x blows up. Also, in the same term for this example, statistical uncertainties could cause erratic behavior if the difference between b_1 and b_2 is not statistically significant. Thus, the concurrence of both problems means that erratically behaving terms also over-powers the other in magnitude.

Locating the Difficulty

Suppose b_1 and b_2 are not significantly statistically different from each other by assuming

$$(b_1 - b_2)^2 \leq b_1 + b_2$$

and see what repercussions are in the rotated system $Sy = d$. We can use these assumptions to make some experimental approximations.

Let $B = \begin{bmatrix} b_1 & 0 \\ 0 & b_2 \end{bmatrix}$ be the covariance matrix for the observed bins $b = [b_1, b_2]$. The rotated system of b has a new basis given by the columns of U and was denoted by $d = U^T b$. So the covariance matrix of that is

$$\begin{aligned} D &= U^T B U \\ &= \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} b_1 & 0 \\ 0 & b_2 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} b_1 & b_1 \\ b_2 & -b_2 \end{bmatrix} \\ &= \frac{1}{2}\begin{bmatrix} b_1 + b_2 & b_1 - b_2 \\ b_1 - b_2 & b_1 + b_2 \end{bmatrix} \end{aligned}$$

However, we are now assuming that $(b_1 - b_2)$ is not statistically significant.

$$D \approx \frac{1}{2}\begin{bmatrix} b_1 + b_2 & 0 \\ 0 & b_1 + b_2 \end{bmatrix}$$

So the rotated covariance matrix D is effectively diagonal in this case as well because of statistical uncertainty.

Accounting for this in our rotated problem:

$$S\chi = d$$

$$\begin{bmatrix} 1 & 0 \\ 0 & \varepsilon \end{bmatrix} \begin{bmatrix} \chi_1 \\ \chi_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} (b_1+b_2) \pm \sqrt{b_1+b_2} \\ (b_1-b_2) \pm \sqrt{b_1+b_2} \end{bmatrix}$$

$$\begin{cases} \chi_1 = \frac{1}{\sqrt{2}}(b_1+b_2) \pm \sqrt{\frac{b_1+b_2}{2}} \\ \varepsilon\chi_2 = \frac{1}{\sqrt{2}}(b_1-b_2) \pm \sqrt{\frac{b_1+b_2}{2}} \end{cases}$$

Now we have a sensible expression for χ_1, but the expression for χ_2 is useless for any ε because the right-hand side is a random number. If ε is large, then it is at least a small random; but if ε is small, then this random contribution becomes amplified. The one saving grace of this rotation is that the problem term is isolated to χ_2, leaving χ_1 untouched. Meanwhile, in the original basis for x

$$x = \frac{1}{\sqrt{2}}(b_1+b_2) \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} + \frac{1}{\varepsilon\sqrt{2}}(b_1-b_2) \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{bmatrix}$$

both equations of x are infected with the problem.

In the rotated system above, χ_2 should never be determined by this expression.

Assume a replacement expression for z_2 that replaces the problem terms with zero:

$$0 \cdot z_2 = 0 \pm \sqrt{\frac{b_1+b_2}{2}}$$

This, at least, does not blow up, but also leaves the value of z_2 to be completely arbitrary. The easiest way to proceed is to assign $z_2 \neq 0$, which is fine because orthonormal transformations do not change the norm of the vector:

$$\|x\|^2 = x_1^2 + x_2^2 = z_1^2 + z_2^2$$

Only the chosen transformation itself changes. So, both alternatives lead to the same regularized vector

$$0 = \pm \sqrt{\frac{b_1+b_2}{2}} \gtrless \frac{1}{\sqrt{2}}(b_1 - b_2)$$

$$\Rightarrow \quad x = \frac{1}{\sqrt{2}}(b_1+b_2)\begin{bmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{bmatrix} + \frac{1}{\varepsilon\sqrt{2}}(b_1-b_2)\begin{bmatrix}\frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}}\end{bmatrix}$$

$$\Rightarrow \quad x = \frac{1}{2}(b_1+b_2)\begin{bmatrix}1\\ 1\end{bmatrix}$$

This is the best estimate of the unfolded value x given the statistical accuracy condition and a poor detector $\left(\varepsilon \ll \frac{1}{\sqrt{b_1+b_2}}\right)$.

Rescaling Equations and Normalizing Unknowns

The original problem $A\vec{x} = \vec{b}$ can be thought of as the solution to the least squares problem

$$\sum_{i=1}^{n_b} \left[\sum_{j=1}^{n_x} A_{ij} x_j - b_i \right]^2 = \min$$

but this treats every bin in $\vec{b}$ equally. In experiment, measurement errors can vary from bin to bin, so different equations have different significance.

As such, we should be considering a least squares problem like

$$\sum_{i=1}^{n_b} \left[\frac{\sum_{j=1}^{n_x} A_{ij} - b_j}{\Delta b_i} \right]^2 = \min$$

$$(Ax - b)^T B^{-1} (Ax - b) = \min$$

The exact solution of a well-determined linear system remains unchanged if the equations or unknowns (or both) are rescaled. However, if $n_x \leq n_b$ and some singular values are small (like ε), the system can be over-determined. In this case, rescaling changes the singular values and therefore also the system. This is relevant because if we have a system with trouble terms, then the appropriate rescaling choice could leave statistically significant terms untouched while reducing the trouble-terms.

So far, we have been talking about A as a probability matrix — the probability that an event starting in bin x_j is observed in bin b_i. However, in practice, we don't have an exact analytic knowledge of the underlying nature of events, but rather an MC generation of a signal hypothesis.

In that spirit, let $\vec{x}^{ini}$ be an initial MC input vector and $w_j \equiv x_j / x_j^{ini}$ be the vector that measures the deviation of the j^{th} bin of x from the MC modelling of it. We can then reconceive of A as the matrix that communicates the absolute number of events generated in bin j that are observed in bin i.

$$\sum_{j=1}^{n_x} A_{ij} w_j = b_i$$

This must be unfolded back to w_j, then finish with $x_j = w_j x_j^{ini}$ to obtain the correctly normalized unfolded solution x_j.

There are two reasons for why solving $A\vec{w} = \vec{b}$ is preferrable to $A\vec{x} = \vec{b}$.

1. If the initial MC distribution $\vec{x}^{ini}$ is reasonably close to the one being unfolded, the unknown vector $\vec{w}$ should be smooth and have small bin-to-bin variation. This means that fewer terms are required in the SVD into orthogonal functions. More accurate unfolding should be possible.

2. Even if suitably high MC statistics are generated, some columns or rows of A may have very few events — some elements A_{ij} may contain a single entry. If A is a probability matrix, such elements have the value 1.0, ignoring the fact that it has 100% (i.e. 1 ± 1) uncertainty. Using A as a probability matrix only makes sense when starting with an analytic function without uncertainties. Contrarily, using A as a probability matrix for MC more heavily weights poorly understood (poorly populated bins and less heavily weights the well-understood ones.

> Generated MC statistics should be at least 1 - 2 orders of magnitude higher than the data.

This ensures that the unfolded solution's uncertainties are dominated by measurement uncertainties and not compounded by statistical uncertainties on the MC.

The choice of rescaling is motivated by weighting each equation by its uncertainty Δb_i. After dividing each equation by Δb_i, all equations have equal weight.

Covariance matrices are symmetric and positive definite. So if B is not diagonal, it can be diagonalized:

$$B = QRQ^T$$

$$\Rightarrow B^{-1} = QR^{-1}Q^T \quad \text{for } R_{ii} = r_i^2 \neq 0$$

$$R_{ij} = 0, \ \forall i \neq j$$

Recall that the now-weighted problem we are trying to solve is

$$(Aw-b)^T B^{-1}(Aw-b) = \min$$

where "w" replaces "x" for aforementioned reasons, and now we can use our expression for B^{-1}.

$$(Aw-b)^T Q R^{-1} Q^T (Aw-b) = \min$$

$$\left(Q^T(Aw-b)\right)^T R^{-1}\left((Aw-b)Q\right) = \min$$

$$\left(Q^T Aw - Q^T b\right)^T R^{-1}\left(AwQ - bQ\right) = \min$$

$$\sum_{i=1}^{n_b}\left[\frac{\sum_{j=1}^{n_x}\sum_m Q_{im}A_{mj}w_j - \sum_m Q_{im}b_m}{r_i}\right]^2 = \min$$

Define $\begin{cases} \tilde{A}_{ij} \equiv \frac{1}{r_i}\sum_m Q_{im}A_{mj} \\ \tilde{b}_i \equiv \frac{1}{r_i}\sum_m Q_{im}b_m \end{cases}$

$$\Rightarrow \sum_{i=1}^{n_b}\left[\sum_{j=1}^{n_x}\tilde{A}_{ij}w_j - \tilde{b}_i\right]^2 = \min$$

$$(\tilde{A}w-\tilde{b})^T(\tilde{A}w-\tilde{b}) = \min$$

$$\tilde{A}\vec{w} = \vec{\tilde{b}}$$

This is now the equation we wish to solve.

Regularization and Unfolding

The exact solution of $\tilde{A}\vec{w} = \vec{\tilde{b}}$ still leads to rapidly oscillating solutions because of the problem with small singular values.

Using a priori knowledge of the solution, a "regularization" term is added to the expression to be minimized.

$$(\tilde{A}\vec{w} - \vec{\tilde{b}})^T(\tilde{A}\vec{w} - \vec{\tilde{b}}) + \tau \cdot (C\vec{w})^T(C\vec{w}) = \min$$

The matrix C defines the a priori condition on the solution, while the parameter τ determines the weight of this condition.

The τ parameter will have to be determined for each specific problem at hand, but C is chosen from general considerations. The general consideration is that the solution histogram $\vec{w}$ should be smooth, not wildly oscillating. So we make C the matrix that takes the discrete 2nd derivative of $\vec{w}$. 2nd derivatives measure the curvature at a location. We want the overall curvature of the entire histogram to be a part of the minimization. Thus, $C\vec{w}$ is the vector of 2nd derivatives for each bin, and so $(C\vec{w})^T(C\vec{w})$ is then the sum of the squared curvature over all bins (the squaring ensures we're measuring the magnitude of the curvature, i.e. positive and negative curvatures don't cancel each other out).

Discrete Derivatives:

What do we mean by "derivative" regarding some bin i in a histogram of discrete measures? Just as in the continuous case, a 1^{st} derivative is a measure of slope and a 2^{nd} derivative is a measure of the rate of change of the slope, or curvature. As such, define

$$\frac{dH}{dw_i} \equiv \frac{w_{i+1} - w_i}{\Delta h} \qquad \text{(slope)}$$

$$\frac{d^2H}{dw_i^2} \equiv \frac{w_{i+1} - w_i}{\Delta h} - \frac{w_i - w_{i-1}}{\Delta h} \qquad \text{(difference in slope between the right and left sides of the bin}$$

$$= \frac{1}{\Delta h}\left(w_{i+1} - 2w_i + w_{i-1}\right)$$

where H is the histogram and Δh is the bin width. The bin width is arbitrary and not relevant to the problem, so we drop that (but what if we use a variable bin width histogram?) The 1^{st} derivative can be expressed in matrix form as

$$D_1^{(n)}\vec{w} = \begin{bmatrix} 1 & 0 & 0 & \cdots & \\ -1 & 1 & 0 & & \vdots \\ 0 & -1 & 1 & \ddots & \\ 0 & & & & 0 \\ \vdots & & & 0 & 0 \\ & & \cdots & 0 & -1 \quad 1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} w_1 \\ w_2 - w_1 \\ w_3 - w_2 \\ \vdots \\ w_n - w_{n-1} \end{bmatrix}$$

which we can see gives a kind of slope for each bin except the first one where the concept is ill-defined!

The matrix for the 2nd derivative should then give a difference in this slope for each bin in the form we saw before.

$$(w_{i+1} - w_i) - (w_i - w_{i-1}) = w_{i+1} - 2w_i + w_{i-1}$$

To find it, we can try (let n=4 here for simplicity)

$$D_2^{(4)} \stackrel{?}{\equiv} D_1^{(4)T} D_1^{(4)} = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 1 \end{bmatrix} = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

However,

$$\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ \vdots \\ w_4 \end{bmatrix} = \begin{bmatrix} 2w_1 - w_2 \\ -w_1 + 2w_2 - w_3 \\ -w_2 + 2w_3 - w_4 \\ -w_3 + w_4 \end{bmatrix}$$

This is close to what we want, but the sign is the opposite of what we want and the meaning breaks down at the two boundaries.

$$C^{(n)} \equiv D_2^{(n)} \equiv \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots & & \\ 1 & -2 & 1 & 0 & & & \\ 0 & 1 & -2 & 1 & & & \\ 0 & 0 & 1 & -2 & \ddots & 0 & 1 & 0 \\ \vdots & & & & & 1 & -2 & 1 \\ & & & & & 0 & 1 & -1 \end{bmatrix}$$

Now we have

$$C^{(n)} \vec{w} = \begin{bmatrix} w_2 - w_1 \\ (w_3 - w_2) - (w_2 - w_1) \\ \vdots \\ (w_{i+1} - w_i) - (w_i - w_{i-1}) \\ \vdots \\ -w_n + w_{n-1} \end{bmatrix}$$

which is our vector of the curvatures for each bin i. Then we can measure the magnitude of the curvature for the whole histogram with the norm

$$\left\| C^{(n)} \vec{w} \right\|^2 = \left(C^{(n)} \vec{w} \right)^T \left(C^{(n)} \vec{w} \right)$$

$$= \sum_i \left[(w_{i+1} - w_i) - (w_i - w_{i-1}) \right]^2$$

By choosing a regularization term that measures the total curvature of the histogram and putting it into the problem to be minimized

$$\left(\tilde{A} \vec{w} - \vec{\tilde{b}} \right)^T \left(\tilde{A} \vec{w} - \vec{\tilde{b}} \right) + \tau \left(C \vec{w} \right)^T \left(C \vec{w} \right) = \min$$

the wild oscillations can be controlled. The linear system this corresponds to is now

$$\begin{bmatrix} \tilde{A} \\ \sqrt{\tau} C \end{bmatrix} \vec{w} = \begin{bmatrix} \tilde{b} \\ 0 \end{bmatrix} \qquad (40)$$

where n_x additional equations have been added to the n_b original ones.

Utilize the "Damped Least Squares" method. This will allow us to express the solution of (40) for any value of τ in terms of the original non-regularized problem ($\tau = 0$). Begin by taking one factor of the matrix C out of the vector on the left-hand side so that the regularization term is proportional to the unit matrix

$$\begin{bmatrix} \tilde{A} C^{-1} \\ \sqrt{\tau} \cdot I \end{bmatrix} C \vec{w} = \begin{bmatrix} \tilde{b} \\ 0 \end{bmatrix}$$

Note that every column and row of C sums to zero, indicating it as degenerate and therefore not invertible. Though it seems a bit of a hack job, we fix this problem by adding some ξ to each diagonal element of C. ξ is chosen to be large enough to make the inversion possible, but small enough to not affect the curvature condition being imposed.

Typically, 10^{-3} or 10^{-4} is sufficient.

$$C = \begin{bmatrix} -1+\xi & 1 & 0 & 0 & \cdots \\ 1 & -2+\xi & 1 & 0 & \\ 0 & 1 & -2+\xi & 1 & \\ \vdots & & & \ddots & \\ \vdots & & & & \\ \cdot & & & & \end{bmatrix}$$

Solve this system for $\tau = 0$.

$$\begin{bmatrix} \tilde{A}C^{-1} \\ 0 \end{bmatrix} C\vec{w} = \begin{bmatrix} \tilde{b} \\ 0 \end{bmatrix}$$

$$(\tilde{A}C^{-1})C\vec{w} = \tilde{b}$$

Note that this looks like, and is, $\tilde{A}\vec{w} = \tilde{b}$ — the very kind of problem we solved with SVD earlier. This time, we solve it using SVD for $(\tilde{A}C^{-1})$ instead of just $\tilde{A}$. Later, this will be used in the solution assuming $\tau \neq 0$.

So with SVD, we get a form as before

$$\tilde{A}C^{-1} = USV^T$$

Recall that U and V are orthogonal matrices and S is diagonal with increasing positive definite diagonal elements s_i. Again, as before, define

$$d \equiv U^T \tilde{b} \qquad z \equiv (V^T C)\vec{w}$$

Using d and z:

$$(\tilde{A}C^{-1})C\vec{w} = \tilde{b}$$

$$(USV^T)C\vec{w} = \tilde{b}$$

$$U^T(USV^T)C\vec{w} = U^T\tilde{b}$$

$$\underbrace{(USV^T)C\vec{w}}_{z} = \underbrace{U^T\tilde{b}}_{d}$$

$$\Rightarrow \begin{cases} Sz = d \\ s_i \cdot z_i = d_i \qquad \forall i \in \{1, \ldots, n_x\} \end{cases}$$

Use the superscript (0) to indicate solutions for this non-regularized system

$$z_i^{(0)} = \frac{d_i}{s_i}$$

which is to be used in

$$z^{(0)} = V^T C w^{(0)}$$

$$C^{-1} V z^{(0)} = w^{(0)}$$

From here, recall from p. 26 of these notes that $w_j \equiv x_j / x_j^{ini}$. So the true distribution x can be found by multiplying each of these $w_j^{(0)}$ by the corresponding x_j^{ini}.

This is still the same old useless non-regularized solution, but we can use it to find the regularized ~~system~~ solution.

Let's go back to $d = U^T \tilde{b}$, $z = (V^T C)\vec{w}$, $d_i = z_i s_i$.

The regularization can be introduced in d_i:

$$d_i^{(\tau)} = d_i \frac{s_i^2}{s_i^2 + \tau}$$

I don't understand where this comes from yet, but we can see how it works.

$$\Rightarrow z_i^{(\tau)} = \frac{d_i^{(\tau)}}{s_i} = d_i \frac{s_i}{s_i^2 + \tau}$$

$\frac{s_i}{s_i^2+\tau}$: Regularized inverse of S

$$\Rightarrow w^{(\tau)} = C^{-1} V z^{(\tau)}$$

Note how $d^{(\tau)}$ and $z^{(\tau)}$ reduce to $d^{(0)}$ and $z^{(0)}$, respectively, when $\tau = 0$. Also, if s_i is very small, then we can see how a nonzero τ in the inverse element $\frac{s_i}{s_i^2+\tau}$ prevents it from blowing up too much. The covariance matrices $Z^{(\tau)}$ and $W^{(\tau)}$ for $z^{(\tau)}$ and $w^{(\tau)}$ are

$$Z^{(\tau)}_{ikl} = \frac{s_i^2}{(s_i^2+\tau)^2} \cdot \delta_{ikl}$$

$$W^{(\tau)} = (C^{-1}V) Z^{(\tau)} (C^{-1}V)^T$$

Just as before, we now use these regularized ($\tau \neq 0$) distributions to obtain the [regularized] true unfolded distribution $x^{(\tau)}$ and its covariance matrix $X^{(\tau)}$.

$$\begin{cases} x^{(\tau)}_i = x^{ini}_i \, w^{(\tau)}_i \\ X^{(\tau)}_{ikl} = x^{ini}_i \, W^{(\tau)}_{ikl} \, x^{ini}_{kl} \end{cases}$$

Even though these are regularized and depend on τ, the inverse of the covariance matrix $X^{(\tau)-1}$ should be used for any fits (why?)

$$X^{-1}_{ikl} = \frac{1}{x^{ini}_j \, x^{ini}_{kl}} \sum_i \tilde{A}_{ij} \, \tilde{A}_{ikl}$$

I haven't explicitly done the algebra for this.