Large Matrix Manipulation for Unfolding Optimization

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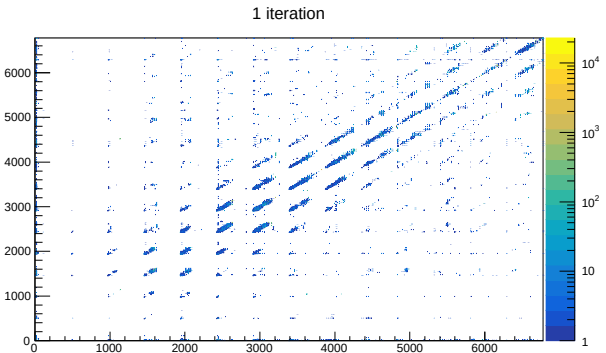
Overview

- I have been dealing with covariance matrices of size 6776×6776 for optimizing the number of iterations in iterative unfolding.
- In this study, RooUnfold is used to calculate the covariance matrix.
- Matrix manipulation is done with `PyROOT`, `root_numpy`, and `numpy.linalg`.
- It turns out large matrices are hard to manipulate numerically.

Welcome to numerical linear algebra!

Visualizing a Covariance Matrix



- Log scale is used to make the structure more visible.
- Obviously this matrix is singular due to rows and columns with elements all zero. Those are unoccupied bins and unavoidable.

Metric for Iteration Optimization and Inverting (Nearly) Singular Matrices

- For the metric, we use average global correlation coefficient[1].

$$\rho_{avg} = \frac{1}{N}\sum_{j=1}^{N}\rho_j$$

$$\rho_j = \sqrt{1 - \frac{1}{[\mathbf{V}]_{jj}[\mathbf{V}^{-1}]_{jj}}}$$

, where j runs through all bins and $\mathbf{V}$ the covariance matrix.

- Since $\mathbf{V}$ is singular, I have tried several ways to deal with this.
- I tried removing the zero rows and columns. I will talk about this later.
- I also tried pseudoinverse (Moore-Penrose inverse). I will not define it, but cite important properties here.
  1. For any matrix $\mathbf{A}$, there exists a unique pseudoinverse of it, denoted $\mathbf{A}^{+}$.
  2. If $\mathbf{A}$ is invertible, $\mathbf{A}^{-1} = \mathbf{A}^{+}$.

[1] Data Unfolding Methods in High Energy Physics

Playing with Pseudoinverse

```
a
 [[ 33.    0.   25.5  -7.   17.5]
 [  0.    0.    0.    0.    0. ]
 [ 25.5   0.   42.  -18.5   7.5]
 [ -7.    0.  -18.5  35.  -10. ]
 [ 17.5   0.    7.5 -10.   45. ]]

pseudoinverse of a
 [[ 0.082  0.    -0.054 -0.02  -0.027]
 [-0.     -0.    -0.    -0.    -0.   ]
 [-0.054 -0.     0.066  0.029  0.016]
 [-0.02  -0.     0.029  0.043  0.013]
 [-0.027 -0.     0.016  0.013  0.033]]

rho vector
 [0.7942625476679229, 0.8002848352198804, 0.5855932326975848, 0.5704565563999852]

average global correlation coefficient of a
 0.687649292996343 4

b
 [[ 33.     0.    25.5   -7.    17.5 ]
 [  0.     0.05   0.     0.     0.   ]
 [ 25.5    0.    42.   -18.5    7.5  ]
 [ -7.     0.   -18.5   35.   -10.   ]
 [ 17.5    0.     7.5  -10.    45.  ]]

inverse of b
 [[ 0.082  0.    -0.054 -0.02  -0.027]
 [ 0.     20.    0.     0.     0.   ]
 [-0.054  0.     0.066  0.029  0.016]
 [-0.02   0.     0.029  0.043  0.013]
 [-0.027  0.     0.016  0.013  0.033]]

rho vector
 [0.7942625476679226, 0.0, 0.8002848352198803, 0.5855932326975843, 0.5704565563999848]

average global correlation coefficient of b
 0.5501194343970744
```

1. I generated a random symmetric matrix $\mathbf{A}$, and manually set the second row and column to zero.
2. The pseudoinverse of $\mathbf{A}$ is calculated.
3. The $\boldsymbol{\rho}$ vector of $\mathbf{A}$ is calculated.
4. A second matrix $\mathbf{B}$ is generated by copying $\mathbf{A}$ and setting the 0 on the diagonal to 0.05. (Following Matt Judah)
5. The inverse of $\mathbf{B}$ is calculated.
6. The $\boldsymbol{\rho}$ vector of $\mathbf{B}$ is calculated.

- The two results are identical except where they are different to start with.
- I did the bench testing because even I made the zero diagonal elements 0.05 in the real covariance matrices, they were still singular.

Nonphysical Values of ρ_j's

- As the paper and the name (correlation coefficient) suggest, a valid ρ_j should be in the range

$$0 \leq \rho_j = \sqrt{1 - \left(\mathbf{V}_{jj}\mathbf{V}_{jj}^{-1}\right)^{-1}} \leq 1 \tag{1}$$

- Eq. (1) is satisfied if and only if

$$\mathbf{V}_{jj}\mathbf{V}_{jj}^{-1} \geq 1 \tag{2}$$

- I went on to use pseudoinverse to calculate ρ_{avg}, and found that only a fraction of all ρ_j's satisfy Eq. (2).
- I started to suspect that the inverse process involved is numerically unstable.

Condition Number and $\mathbf{V}_{jj}\mathbf{V}_{jj}^{-1}$

- Consider the linear equation $\mathbf{Ax} = \mathbf{b}$. If small changes in $\mathbf{b}$ imply small changes in the solution $\mathbf{x}$, then $\mathbf{A}$ has a small condition number. Otherwise $\mathbf{A}$ has a big condition number.
- Not surprisingly, nearly singular matrices have large condition numbers.
- Since I don't know how to prove Eq. (2) mathematically, I did what an experimentalist does: do some experiments.
- I generated random positive semidefinite matrices to simulate covariance matrices, and look at their condition numbers and $\mathbf{V}_{jj}\mathbf{V}_{jj}^{+}$'s.

Condition Number and $\mathbf{V}_{jj}\mathbf{V}_{jj}^{-1}$ (Cont.)

well−conditioned example

```
positive semidefinite matrix V
[[ 80.844 101.687  −7.097   3.693 −37.207]
 [101.687 227.373 −87.639  15.71  −42.425]
 [ −7.097 −87.639 223.402  64.78   61.958]
 [  3.693  15.71   64.78  118.352  24.211]
 [−37.207 −42.425  61.958  24.211  78.489]]

condition number of V
34.26

V_ii*(V^+)_ii
[4.675 4.628 2.953 1.431 2.122]
```

ill−conditioned example

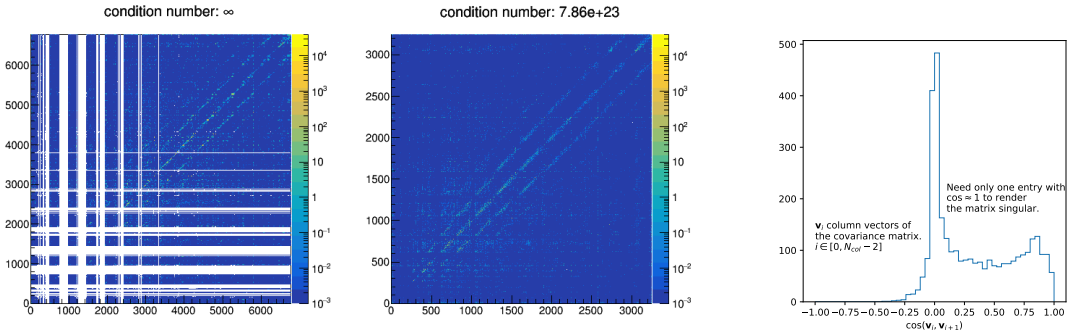
```
positive semidefinite matrix V
[[ 53.276 −19.187 −71.864 −33.168 −44.791]
 [−19.187  10.654  23.82    3.057  17.234]
 [−71.864  23.82   98.07   49.632  59.81 ]
 [−33.168   3.057  49.632  41.747  25.265]
 [−44.791  17.234  59.81   25.265  37.982]]

condition number of V
1.582e+17

V_ii*(V^+)_ii
[0.13 0.097 0.204 1.237 0.142]
```

Out of those tens of random positive semidefinite matrices, they showed invariably that,

- If the condition number is small (say, < 1000), $\mathbf{V}_{jj}\mathbf{V}_{jj}^{+} \geq 1$ is always true for all j.
- If the condition number is large (i.e., in scientific notation), $\mathbf{V}_{jj}\mathbf{V}_{jj}^{+} \geq 1$ is not satisfied for some or all j.

Bottom line: $\mathbf{V}_{jj}\mathbf{V}_{jj}^{+} \geq 1$ is true for all j only if $\mathbf{V}$ is well-conditioned.

Removing Zero Rows and Columns Does Not Help!

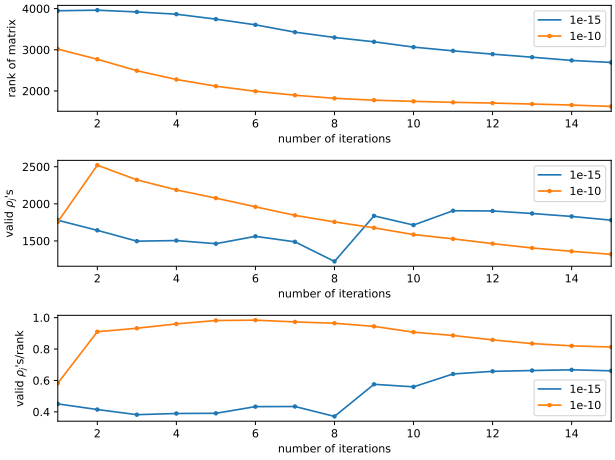


- Plots are with 2 iterations. Similar situation applies to all iterations.
- The reason is a large matrix becomes nearly singular if it contains highly correlated rows or columns.
- The adjacent columns of a covariance matrix are very often highly correlated.
- Of course, smaller matrices are always better. Will move to using the zero suppressed matrices.

The Rank and Inverse of a Large Matrix Actually Depend on a Small Tolerance!

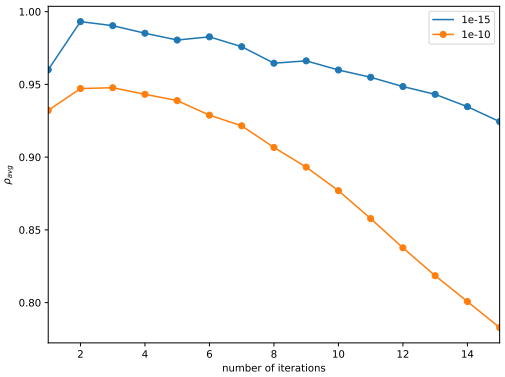
- Intuitively, the number of valid ρ_j's should not exceed the rank of the matrix. Therefore, knowing the rank of the matrix helps understand the problem.
- Turns out the rank of a large matrix depends on a small tolerance ϵ. Singular values obtained by SVD (singular value decomposition) that are smaller than ϵ are set to exact zero to avoid numerical instability. This is called low-rank approximation (or truncated SVD), and regarded as a way of regularizing the linear system.
- The same tolerance applies to obtaining the pseudoinverse of the matrix since the most common algorithm used to calculated the pseudoinverse is using SVD.
- I am going to show you the ranks, the ρ_{avg}'s among valid ρ_j's of the covariance matrices as a function of number of iterations and compare results obtained with two different tolerance values.

Different Tolerance Values Result in Different Number of Valid ρ_j



- Different iterations give different covariance matrices.
- With $\epsilon = 10^{-15}$, some matrices have ranks larger than the size of the zero-suppressed counterparts! This is evidence of numerical instability.
- A criterion for how well a matrix is regularized in this study can be *the ratio of the number of valid ρ_j's to the rank*. In this sense, $\epsilon = 10^{-10}$ should give a more reliable measure.

ρ_{avg} Results, Work to Do



- Although the results depend on tolerance, the *trends* with iterations are the same.
- Obviously I need to extend the plots to at least 100. I will sample iterations in $[1, 1000]$ and see if a minimum exists.
- I have to run the analysis on grid, or implement a much faster covariance matrix calculation algorithm.
- If there are any other iteration optimization metrics that are much easier to wield, I am happy to switch over...