Reconstruction of particle's energy spectrum in experiment with Unfolding technique

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1. Main problem and direct method of solving
2. Unfolding methods overview
3. Software implementation: ROOT, RooUnfold
4. Computational experiments results: comparison
Main problem

True value

Measured value

True distribution

Measured distribution
Main problem

True distribution

\( f_{true}(x) \)

Measurement (folding)

\[ f_{meas}(y) = \int_{\Omega} K(x, y) f_{true}(x) dx \]

Measured distribution

\( f_{meas}(y) \)

Spectrum unfolding (deconvolution)

?
Main problem (sampling)

\[ \nu_i = \sum_j R_{ij} \tau_j \]

\[ \tau = (\tau_1, \tau_2, ..., \tau_k) \] — true distribution

\[ \mu = (\mu_1, \mu_2, ..., \mu_n) \] — measured distribution

\[ M\mu = \nu = (\nu_1, \nu_2, ..., \nu_n) \]
Unfolding
“Naive” method

\[ \nu = R \tau \]

\( \tau \) — true distribution
\( \mu \) — measured distribution
\( M \mu = \nu \)

\[ \nu = \mu \]
\[ R \tau = \mu \]

\[ \tau = R^{-1} \mu \]
Unfolding

Maximum likelihood estimation

\[ L(\tau) = \prod_i P(\mu_i, \nu_i(\tau)) = \prod_i e^{-\nu_i} \frac{\nu_i^{\mu_i}}{\mu_i!} \rightarrow \max_{\tau} \]

True distribution (spectrum) estimation: \( \hat{\tau} = R^{-1} \mu \)

(the same as in “naive” method)

**Properties:** consistent and unbiased estimator, minimal error for unbiased estimators class.

**Problems:** unstable for \( \mu \) fluctuations, too large statistical errors.

**Conclusion:** biased estimators (add systematic bias).
Unfolding methods ideas

1. Correction by multiplicative coefficients
   (for measured spectrum)

2. Bayesian methods
   (D Agostini methods + modifications)

3. Methods based on regularization
   1. Tikhonov’s regularization + SVD (Kartvelishvili, Hoecker)
   2. Tikhonov’s regularization, bias limitation + L-curve (Schmitt)
   3. Regularization based on entropy
Bayesian method

(D Agostini)

$(C_1, C_2, \ldots, C_k)$ — causes — particle is in the given energy interval (bin)

$(E_1, E_2, \ldots, E_n)$ — effects — particle is detected in the given energy interval (bin)

$R_{ij} = P(E_i | C_j)$ — migration matrix

Basic idea

$M_{ji} = P(C_j | E_i) = \frac{P(E_i | C_j)P(C_j)}{\sum_{k} P(E_i | C_k)P(C_k)}$

$\hat{\mu} = M \mu$
Iterative bayesian method (D Agostini)

\[ R_{ij} = P(E_i \mid C_j) \] — migration matrix

\[ \varepsilon_i = \sum_k P(E_i \mid C_k) \] — efficiency

1. Initialization: \[ P(C_j) = P_0(C_j) \]

2. Iteration:

\[ M_{ji} = \frac{R_{ij} P(C_j)}{\varepsilon_i \sum_k R_{ik} P(C_k)} \]

\[ \hat{\tau} = M\mu \quad P(C_j) = \hat{\tau}_j / \sum_k \hat{\tau}_k \]

3. Evaluate errors, repeat step 2 if necessary.

Methods based on regularization

\[ R\tau = \mu \quad \overset{\leftrightarrow}{\iff} \quad L(\tau) = (R\tau - \mu)^T (R\tau - \mu) \rightarrow \min_{\tau} \]

\[ \Phi(\tau) = L(\tau) + \alpha \cdot S(\tau) \rightarrow \min_{\tau} \]

\[ S(\tau) \quad \text{— regularization function} \]
\[ \alpha \quad \text{— regularization coefficient} \]

Tasks:

* choose \( S \),

* choose optimal \( \alpha \).
SVD Unfolding

\[ \Phi(\tau) = L(\tau) + \alpha \cdot S(\tau) \rightarrow \min_{\tau} \]

\[ S(\tau) = \sum_{i} (\tau_{i-1} - 2\tau_{i} + \tau_{i+1})^2 = (C\tau)^T (C\tau) \]

Solution \( R\tau = \mu \) system by SVD

\[ R = USV^T \]

\( U, V \) — orthogonal matrices

\( S \) — diagonal matrix

Solution of new system SVD

\[ Z_i = \frac{d_i \cdot S_{ii}^2}{S_{ii}^2 \cdot \alpha} \]

\[ USV^T \tau = \mu \]

\[ z = V^T \tau, \quad d = U^T \mu \]

\[ Sz = d \quad \Rightarrow \quad z_i = \frac{d_i}{S_{ii}} \]

\[ \tau = Vz \]
**SVD Unfolding**

\[ \Phi(\tau) = L(\tau) + \alpha \cdot S(\tau) \rightarrow \min_{\tau} \]

\[ S(\tau) = \sum_{i} (\tau_{i-1} - 2\tau_{i} + \tau_{i+1})^2 = (C\tau)^T (C\tau) \]

**Extras:**

1. Renormalization of the original system

2. Choose regularization coefficient as \( \alpha = s_{kk}^2 \)

   where \( s_{kk} \) — last «large» singular value \( s_{ii} \)

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\[ \Phi(\tau) = L_1(\tau) + \alpha \cdot L_2(\tau) + \lambda \cdot L_3(\tau) \rightarrow \min_{\tau} \]

\[ L_1(\tau) = L(\tau) \]

\[ L_2(\tau) \] — regularization function (smoothness)

\[ L_3(\tau) \] — bias limitation

**Regularization coefficients choosing**

1. L-curve
2. Correlation coefficient minimization
Software implementation

ROOT (5.28, 5.34)
  TUnfold
RooUnfold 1.1.1
  Tunfold
  SVD unfolding
  Bayes unfolding

Data

Exponential spectrums (sp1 and sp2) are generated
  1. Exponential parameters -1 and -2
  2. Generative and measure energy values
  3. Migration matrix constructed by sp2
  4. Migration matrix applied for sp1
Problems

1. Migration matrix construction
   Condition $R_{ii} > 0.5$ (Blobel)
   Possibility of using for another distribution (spectrum)

2. Binning
   The effect of extreme (additional) bin
   Irregular binning
   Different binning for true/measured spectrum
   The effect of binning on the quality of the unfolding

3. Methods particular features
   Bayesian methods: number of iterations
   Regularization methods: coefficient

4. General
   Unfolding quality estimation (comparison)
   Using methods for several measured values
Migration matrix
Different binning

Wide bins, max Rig = 1.6Gv

Short bins, max Rig = 1.6Gv
Results
TUnfold (ROOT)

Wide bins

True
Unfolded
Measured

<table>
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<th>hist_data_LCURVE</th>
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</thead>
<tbody>
<tr>
<td>Entries</td>
</tr>
<tr>
<td>Mean</td>
</tr>
<tr>
<td>RMS</td>
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</table>
Results
TUnfold (ROOT)

Short bins

Method is sensitive to binning
Results

SVD unfolding (RooUnfold)

Wide bins

K_reg = 2

small regularization

Right choose regularization
Wide bins

SVD unfolding (RooUnfold)

**K_reg = 5**

**K_reg = 12**
Results

SVD unfolding (RooUnfold)

Short bins

Same behavior
Results

SVD unfolding (RooUnfold)

Different bins

K_reg = 12

Stable for binning
Results

Bayes unfolding (RooUnfold)

Wide bins

<table>
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<th>Mean</th>
<th>RMS</th>
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<tbody>
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<td>0.9492</td>
<td>0.3368</td>
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iterations = 1
Wide bins

Bayes unfolding (RooUnfold)

Iterations = 10
Results

Bayes unfolding (RooUnfold)

Wide bins

Need to measure the quality

Iterations = 100
Results

Bayes unfolding (RooUnfold)

Short bins

Iterations = 1
Results

Bayes unfolding (RooUnfold)

Iterations convergence depends on binning

Short bins

Bayes unfolding (RooUnfold)

Iterations convergence

iterations = 100

- Entries: 22
- Mean: 0.9578
- RMS: 0.3281
Conclusions

Methods features

* **Bayesian method**
  perceptible dependence on iterations and
  some dependence on binning
  + can be used for several measured parameters (2D)

* **SVD unfolding**
  regularization coefficient choosing

* **TUfold**
  perceptible sensitivity to binning
Thank you for your attention!

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Idea of extending for several parameters

Unpack the matrix in a one-dimensional array

Then possible to use Bayesian method because it’s based on just probabilities (to detect the event in some bin)

Other methods use the information about nearest bins
High energy

Migration matrix

High energy (10-1000 GeV)
Results

TUnfold (RooUnfold)

Applied to cosmic rays spectrum (-2.7)
Results

Bayes unfolding (RooUnfold)

![Graph showing Unfold Response with iteration = 10]

- **Entries:** 9
- **Mean:** 27.92
- **RMS:** 7.8
Results

SVD unfolding (RooUnfold)

\[ k_{\text{reg}} = 7 \]
Results

High energy (10-1000 GeV), cosmic rays

TUnfold
SVD
Bayes

Entries: 9
Mean: 801.9
RMS: 327
Unpacked migration matrix

Migration matrix for Azimuthal and Zenith angle

Use 36 bins for azimuth and 14 bins for zenith angle gives migration matrix $504 \times 504$