SVD-Based Unfolding: Implementation and Experience

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CERN

Phystat 2011 – January 20, 2011 – Geneva, Switzerland

TSVDUnfold – A root-based Implementation

- SVD-based unfolding method in detail described by Vato Kartvelishvili
- TSVDUnfold provides one implementation, available in root 5.28
- Rather minimal implementation, provided in addition to unfolding result
  - ⋆ Propagation of covariance matrices on measured spectrum to unfolded spectrum using pseudo experiments
  - ⋆ Evaluation of impact of statistical uncertainty on detector response matrix on unfolded spectrum using pseudo experiments
  - ⋆ Access to $|d_i|$ for determination of regularization
  - ⋆ Access to singular values of detector response matrix
  - ⋆ Allow normalization of unfolded spectrum
- Tutorial for usage of TSVDUnfold available (with math tutorials)
- TSVDUnfold is interfaced from RooUnfold (→ talk by Tim Adye)

TSVDUnfold: Future Improvements

Currently under development (and used here)

- Covariance matrix and inverse as discussed by Vato Kartvelishvili
  - ⋆ Propagation with toys still has its place for propagation of individual uncertainties
- Improved normalization of unfolded spectrum

To be added

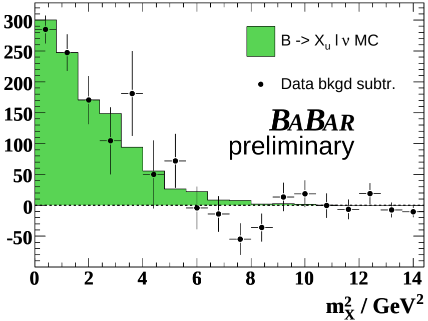
- Different number of bins in measured and unfolded spectrum
- Rescaling of equations (see Vato's talk) using correlations in measured spectrum

Unfolding $B \to X_u \ell \nu$ Spectra in BaBar

- SVD-based unfolding was used at BaBar:
  - ⋆ Hadronic mass (m_X^2) spectrum in inclusive $B \to X_u \ell \nu$ decays
  - ⋆ q^2 spectra in $B \to \pi \ell \nu$ and $B \to \rho \ell \nu$ decays
  - ⋆ Of course also other unfolding methods used in different analyses
- Use hadronic mass spectrum here as an example

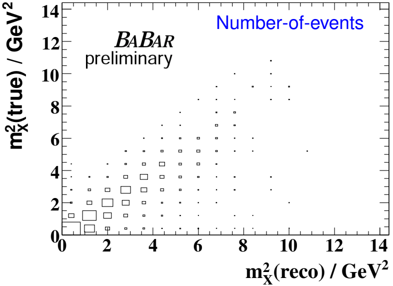
- Rather small statistics
  - ⋆ $\mathbf{1027 \pm 176(stat)}$ signal events
- Rather large statistical and systematic uncertainties from $B \to X_c \ell \nu$ background subtraction
  - ⋆ Also negative bins from oversubtraction
- Resolution $\sim$ bin size

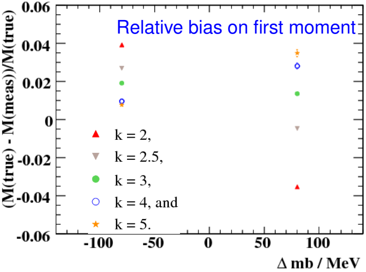
Measured m_X^2 spectrum



Determination of Regularization

- Determination of regularization with pseudo-experiments
- Input: “data” and “MC” with different b-quark mass
  - ⋆ Significant change in shape of spectrum
- Test bias on spectral moments for different values of regularization
  - ⋆ Choose operating point where bias small compared to statistical uncertainties





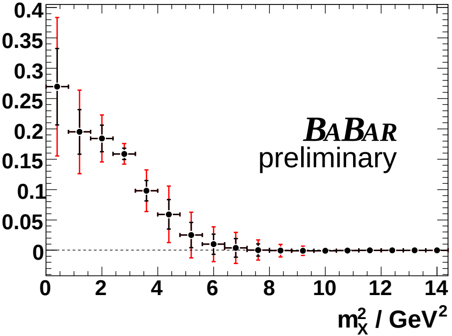
For $\tau = s_2 s_3$

	$\sigma(M_1)/M_1$	$\sigma(U_2)/U_2$	$\sigma(U_3)/U_3$
stat	$\mathbf{0.17}$	$\mathbf{0.30}$	$\mathbf{0.34}$
bias	$\mathbf{0.01}$	$\mathbf{0.02}$	$\mathbf{0.05}$

A Few Observations

- Both statistical and systematic uncertainties should be used for rescaling of equations
  - ⋆ Significantly more stable result
- Propagate covariance matrices from different sources of uncertainties to avoid effect of instabilities (overestimated uncertainties)

Unfolded m_X^2 spectrum



- Large correlations between bins and hence between moments: $\rho_{12} = 0.99$, $\rho_{23} = 0.94$ and $\rho_{13} = 0.88$
- Unfolded spectrum normalized to unit area since overall efficiency poorly known (and irrelevant)

Covariance Matrices for Unfolded Spectrum

- Current implementation propagates covariance matrices on measured spectrum to unfolded spectrum using pseudo experiments
- SVD method provides regularized covariance matrix $X^{(\tau)}$ and the inverse of the covariance matrix X^{-1} (independent of regularization) $\rightarrow$ Vato's talk:

$$X_{ik}^{(\tau)} = x_i^{\text{ini}} W_{ik}^{(\tau)} x_k^{\text{ini}}$$

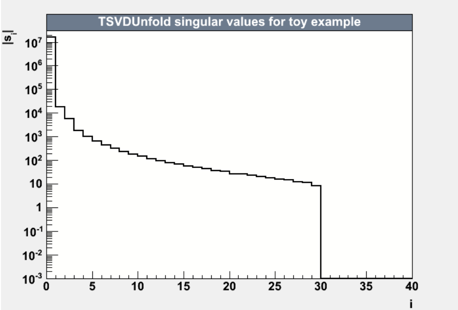
and

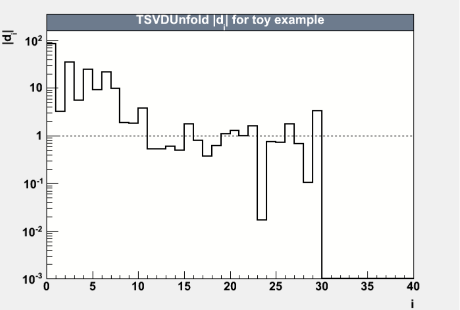
$$X_{jk}^{-1} = \frac{1}{x_j^{\text{ini}} x_k^{\text{ini}}} \sum_i \tilde{A}_{ij} \tilde{A}_{ik}$$

- X^{-1} to be used for computation of χ^2 (used in the following), $X^{(\tau)}$ (also from pseudo experiments) often observed not to be invertable
- Compare covariance matrices from the two methods for different regularizations (1000 pseudo experiments)

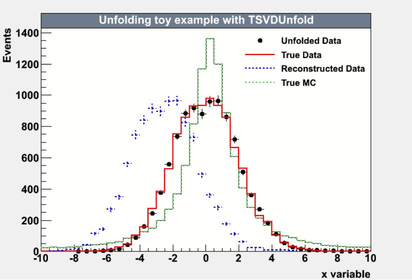
Toy Example for SVD Unfolding

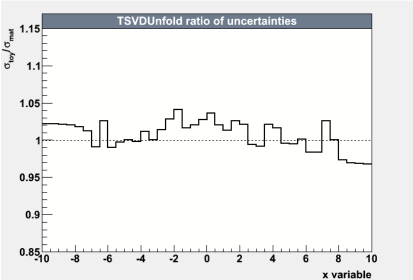
- Regularization for SVD determined by distribution of $|d_i|$ and good χ^2 between unfolded result and truth input ($k = 16$, $\chi^2 = 21.4$)

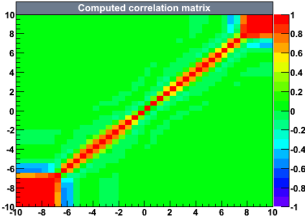


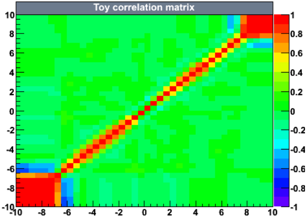


Well-Regularized Unfolding ($k = 16$)





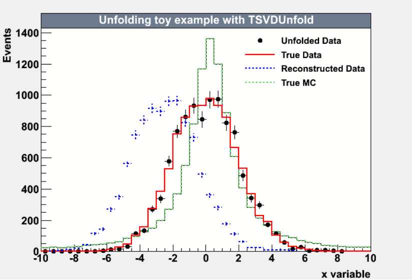


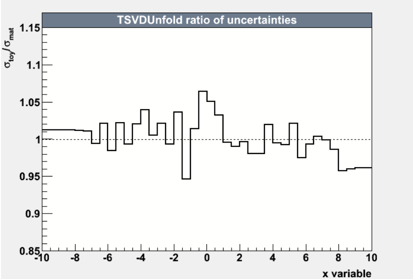


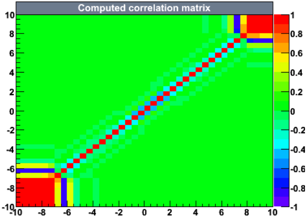
$\chi^2/\mathrm{ndof} = 0.53$

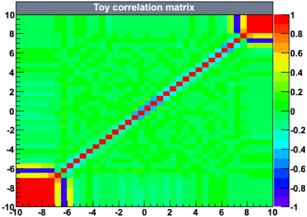
Prob$= 0.993$

Underregularized Unfolding ($k = 30$)





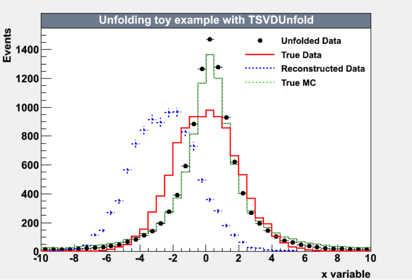


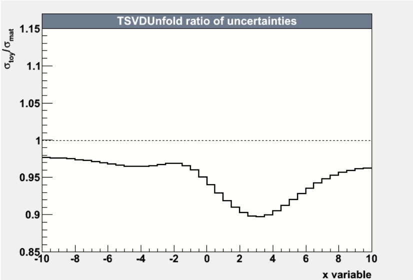


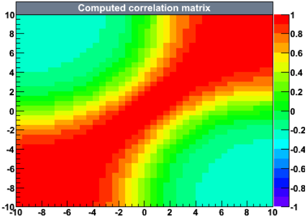
$\chi^2/\mathrm{ndof} = 0.93$

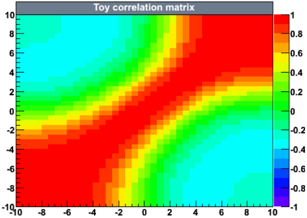
Prob$= 0.60$

Overregularized Unfolding ($k = 3$)









$\chi^2/\mathrm{ndof} = 28.5$

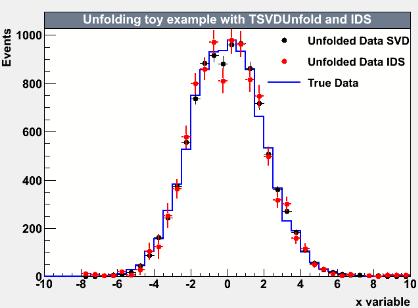
Prob$\sim$ 0

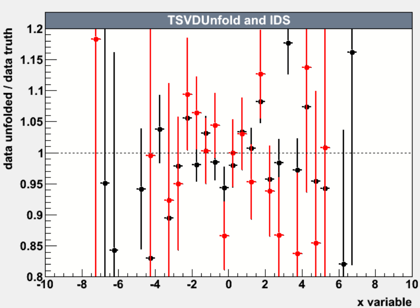
Comparison Between SVD and IDS Methods

- Iterative dynamically stabilized unfolding presented by Bogdan Malaescu
- Compare SVD and IDS methods for a common example (see before)
- Regularization for IDS determined using data and reconstructed "inproved" MC input as described by Bogdan, performance can probably be improved over what is shown here

Comparison Between SVD and IDS Methods

- Neither IDS nor SVD method shows obvious bias with chosen regularization and similar fluctuations around “data truth”
- SVD method yields substantially smaller uncertainties
  - ⋆ Uncertainties from finite MC statistics included in both cases
  - ⋆ Depends on chosen regularization

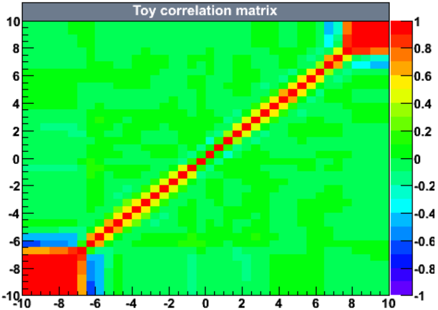




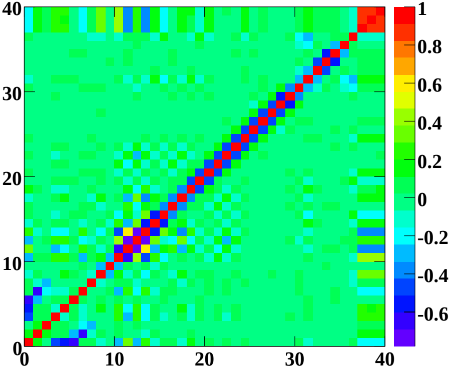
Thanks a lot to Bogdan for unfolding our example spectrum with IDS!

Comparison Between SVD and IDS Methods

SVD



IDS



- Very different correlation patterns
- SVD: correlations along diagonal, anti-correlations in medium range, small correlations in longe range
- IDS: correlations smaller in general, with shorter range than in SVD, often anti-correlations with direct neighbors

Summary

- `TSVDUnfold` available since `root` 5.28
  - ⋆ Also usable through `RooUnfold` interface
- Good agreement between computed uncertainties (within 10%) and correlations from pseudo experiments, even for non-optimal regularization
  - ⋆ Computed covariance matrix and its effective pseudo-inverse will be available in next version
- IDS and SVD unfolding show similar results on toy example in terms of fluctuation and bias, but differences in uncertainties and correlations
  - ⋆ In both cases, uncertainties and correlations depend on chosen regularization