Introduction to Unfolding in High Energy Physics

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ÉCOLE POLYTECHNIQUE
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Outline

1. Introduction
2. Basic unfolding methodology
   - Maximum likelihood estimation
   - Regularized frequentist techniques
   - Bayesian unfolding
3. Challenges in unfolding
   - Choice of the regularization strength
   - Uncertainty quantification
   - MC dependence in the smearing matrix
4. Unfolding with RooUnfold
5. Conclusions

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The unfolding problem

- Unfolding refers to the problem of estimating the particle-level distribution of some physical quantity of interest on the basis of observations smeared by an imperfect measurement device
- What would the distribution look like when measured with a device having a perfect experimental resolution?
    - Cf. deconvolution in optics, image reconstruction in medical imaging

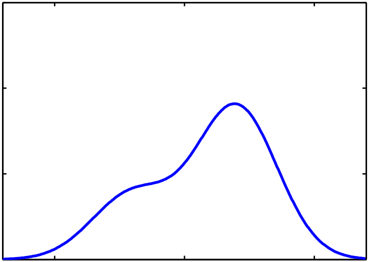
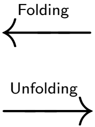


Figure : Smeared density



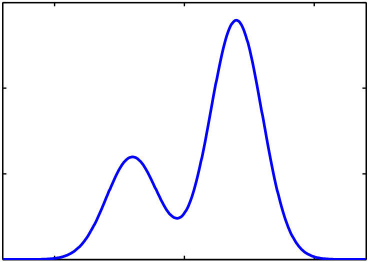


Figure : True density

Why unfold?

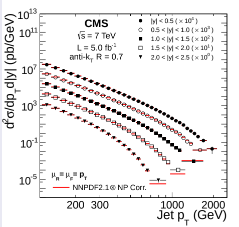
Unfolding is usually done to achieve one or more of the following goals:

1. **Comparison of the measurement with future theories**
2. **Comparison of experiments with different responses**
3. **Input to a subsequent analysis**
4. **Exploratory data analysis**

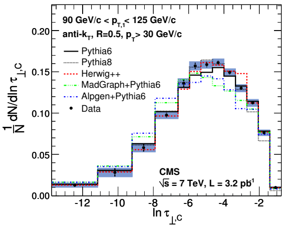
Unfolding is most often used in *measurement* analyses (as opposed to *discovery* analyses): QCD, electroweak, top, forward physics,...

Examples of unfolding in LHC data analysis

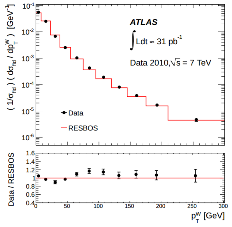
Inclusive jet cross section



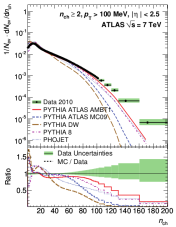
Hadronic event shape



W boson cross section



Charged particle multiplicity



Problem formulation

- Notation:
  - $\boldsymbol{\lambda} \in \mathbb{R}_+^p$ bin means of the true histogram
  - $\mathbf{x} \in \mathbb{N}_0^p$ bin counts of the true histogram
  - $\boldsymbol{\mu} \in \mathbb{R}_+^n$ bin means of the smeared histogram
  - $\mathbf{y} \in \mathbb{N}_0^n$ bin counts of the smeared histogram
- Assume that:
  1. The true counts are independent and Poisson distributed

     $$\mathbf{x}|\boldsymbol{\lambda} \sim \mathrm{Poisson}(\boldsymbol{\lambda}), \quad \perp\!\!\!\perp x_i|\boldsymbol{\lambda}$$

  2. The propagation of events to neighboring bins is multinomial conditional on x_i and independent for each true bin
- It follows that the smeared counts are also independent and Poisson distributed

$$\mathbf{y}|\boldsymbol{\lambda} \sim \mathrm{Poisson}(\mathbf{K}\boldsymbol{\lambda}), \quad \perp\!\!\!\perp y_i|\boldsymbol{\lambda}$$

Problem formulation

- Here the elements of the smearing matrix $\mathbf{K} \in \mathbb{R}^{n \times p}$ are given by

$$K_{ij} = P(\text{smeared event in bin } i \,|\, \text{true event in bin } j)$$

  and assumed to be known
- The unfolding problem:

Problem statement

Given the smeared observations $\mathbf{y}$ and the Poisson regression model

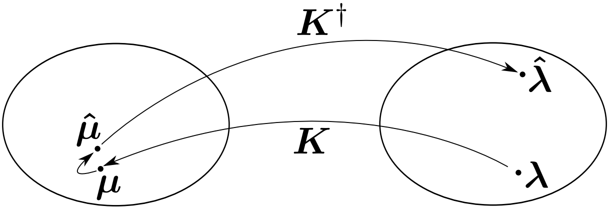
$$\mathbf{y}|\boldsymbol{\lambda} \sim \mathrm{Poisson}(\mathbf{K}\boldsymbol{\lambda}),$$

what can be said about the means $\boldsymbol{\lambda}$ of the true histogram?

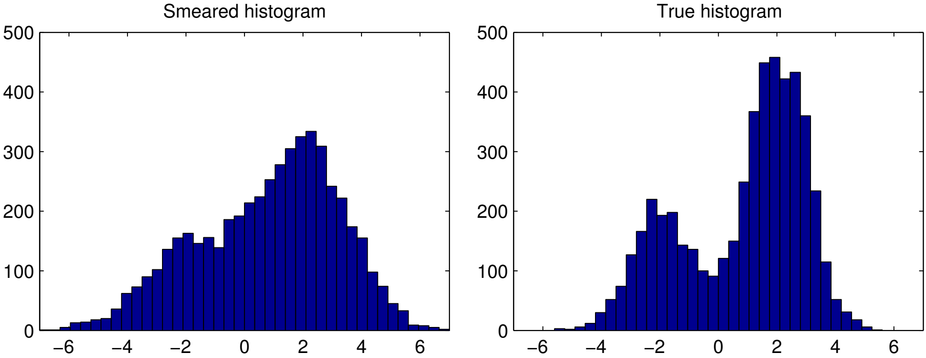
- The problem here is that typically $\mathbf{K}$ is an ill-conditioned matrix

Unfolding is an ill-posed inverse problem

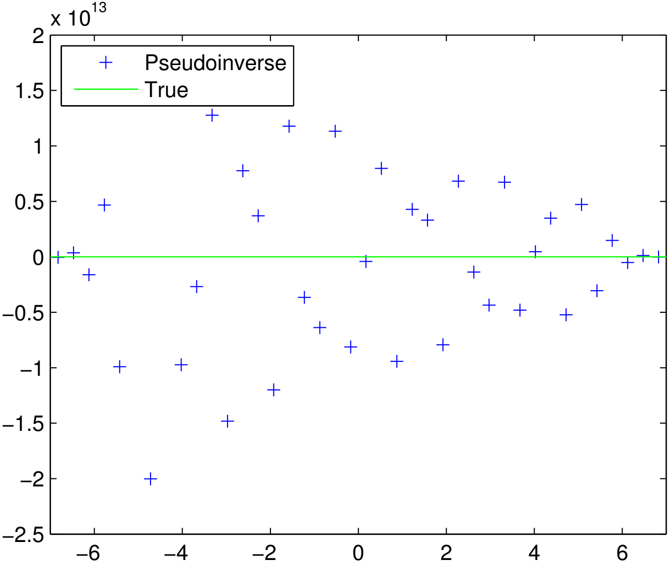
- The unfolding problem is typically ill-posed in the sense that the (pseudo)inverse of $\mathbf{K}$ is very sensitive to small perturbations in the data
- From $\mathbf{y}|\boldsymbol{\lambda} \sim \mathrm{Poisson}(\mathbf{K}\boldsymbol{\lambda})$ we have that $\boldsymbol{\mu} = \mathbf{K}\boldsymbol{\lambda}$
- We could naïvely estimate $\hat{\boldsymbol{\lambda}} = \mathbf{K}^\dagger \hat{\boldsymbol{\mu}} = \mathbf{K}^\dagger \mathbf{y}$
- But this can lead to catastrophic results!



Demonstration of the ill-posedness



Demonstration of the ill-posedness



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The likelihood function

- The *likelihood function* in unfolding is:

$$L(\boldsymbol{\lambda}) = p(\mathbf{y}|\boldsymbol{\lambda}) = \prod_{i=1}^{n} p(y_i|\boldsymbol{\lambda}) = \prod_{i=1}^{n} \frac{\left(\sum_{j=1}^{p} K_{ij}\lambda_j\right)^{y_i}}{y_i!} e^{-\sum_{j=1}^{p} K_{ij}\lambda_j}, \quad \boldsymbol{\lambda} \in \mathbb{R}_+^p$$

- This function uses our Poisson regression model to link the observations $\mathbf{y}$ with the unknown $\boldsymbol{\lambda}$
  - The likelihood function plays a key role in all sensible unfolding methods
- In most statistical problems, the maximum of the likelihood, or equivalently the maximum of the log-likelihood, provides a good estimate of the unknown
  - In ill-posed problems, *this is usually not the case*, but the maximum likelihood solution still provides a good starting point

Maximum likelihood estimation

- Any histogram that maximizes the log-likelihood of the unfolding problem is called a *maximum likelihood estimator* $\hat{\boldsymbol{\lambda}}_{\mathrm{MLE}}$ of $\boldsymbol{\lambda}$
- Hence, we want to solve:

$$\max_{\boldsymbol{\lambda} \in \mathbb{R}_+^p} \log p(\mathbf{y}|\boldsymbol{\lambda}) = \sum_{i=1}^{n} \left[y_i \log \left(\sum_{j=1}^{p} K_{ij} \lambda_j \right) - \sum_{j=1}^{p} K_{ij} \lambda_j \right] + \mathrm{const}$$

Maximum likelihood estimation

Theorem (Vardi et al. (1985))

Assume $K_{ij} > 0$ *and* $\mathbf{y} \neq \mathbf{0}$*. Then the following hold for the log-likelihood* $\log p(\mathbf{y}|\boldsymbol{\lambda})$ *of the unfolding problem:*

1. *The log-likelihood has a maximum.*
2. *The log-likelihood is concave and hence all the maxima are global maxima.*
3. *The maximum is unique if and only if the columns of* $\mathbf{K}$ *are linearly independent*

- So a unique MLE exists when the columns of $\mathbf{K}$ are linearly independent but how do we find it?

Maximum likelihood estimation

Proposition

Let $\mathbf{K}$ *be an invertible square matrix and assume that* $\hat{\boldsymbol{\lambda}} = \mathbf{K}^{-1}\mathbf{y} \geq \mathbf{0}$*. Then* $\hat{\boldsymbol{\lambda}}$ *is the MLE of* $\boldsymbol{\lambda}$*.*

- That is, matrix inversion gives us the MLE if $\mathbf{K}$ is invertible and the resulting estimate is positive
- Note that this result is more restrictive than it may seem
  - $\mathbf{K}$ is often non-square
  - Even if $\mathbf{K}$ was square, it is often not invertible
  - And even if $\mathbf{K}$ was invertible, $\mathbf{K}^{-1}\mathbf{y}$ often contains negative values
- Is there a general recipe for finding the MLE?

Maximum likelihood estimation

- The MLE can always be found computationally by using the *expectation-maximization (EM) algorithm* (Dempster et al. (1977))
  - This is a widely used iterative algorithm for finding maximum likelihood solutions in problems that can be seen as containing incomplete observations
- Starting from some initial value $\boldsymbol{\lambda}^{(0)} > \mathbf{0}$, the EM iteration for unfolding is given by:

$$\lambda_j^{(k+1)} = \frac{\lambda_j^{(k)}}{\sum_{i=1}^{n} K_{ij}} \sum_{i=1}^{n} \frac{K_{ij} y_i}{\sum_{l=1}^{p} K_{il} \lambda_l^{(k)}}, \quad j = 1, \ldots, p$$

- The convergence of this iteration to an MLE (i.e. $\boldsymbol{\lambda}^{(k)} \overset{k\to\infty}{\longrightarrow} \hat{\boldsymbol{\lambda}}_{\mathrm{MLE}}$) was proved by Vardi et al. (1985)

Maximum likelihood estimation

- The EM iteration for finding the MLE in Poisson regression problems has been rediscovered many times in different fields:
  - Optics: Richardson (1972)
  - Astronomy: Lucy (1974)
  - Tomography: Shepp and Vardi (1982); Lange and Carson (1984); Vardi et al. (1985)
  - HEP: Kondor (1983); Mülthei and Schorr (1987); Mülthei et al. (1987, 1989); D'Agostini (1995)
- In modern use, the algorithm is most often called *D'Agostini iteration* in HEP and *Lucy–Richardson deconvolution* in astronomy and optics
- In HEP, also the name "Bayesian unfolding" is used but this is an unfortunate misnomer
  - D'Agostini iteration is a fully frequentist technique for finding the MLE
  - *There is nothing Bayesian about it!*

D'Agostini demo, $k = 0$

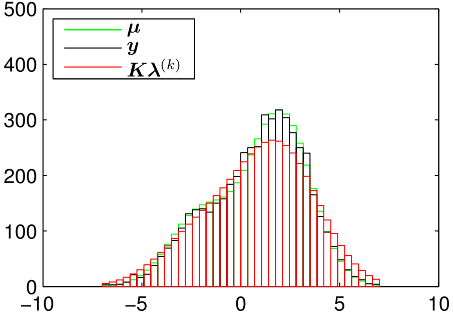

Figure : Smeared histogram

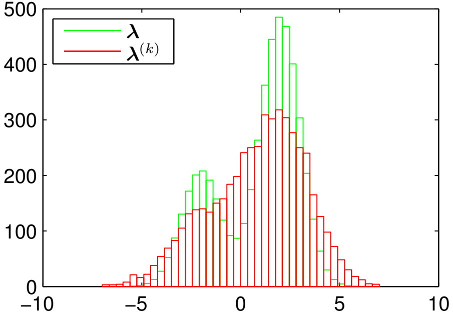

Figure : True histogram

D'Agostini demo, $k = 100$

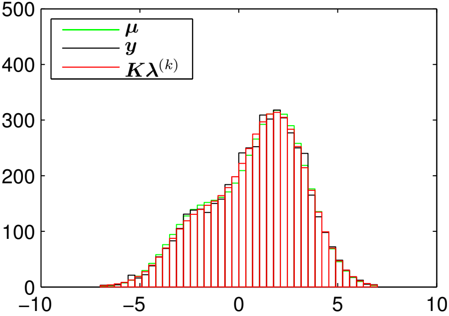

Figure : Smeared histogram

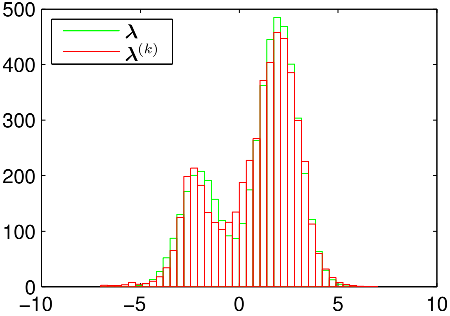

Figure : True histogram

D'Agostini demo, $k = 10000$

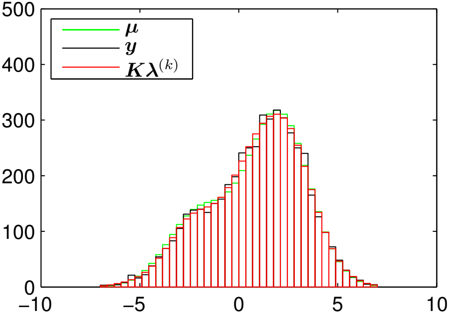

Figure : Smeared histogram

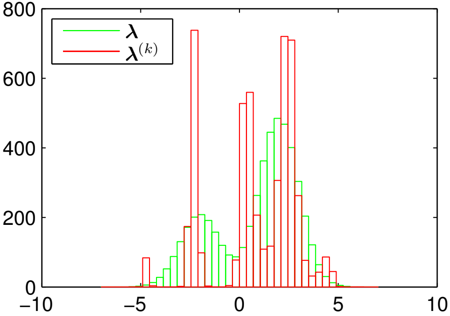

Figure : True histogram

D'Agostini demo, $k = 100000$

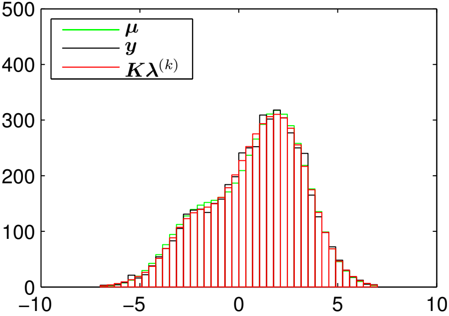

Figure : Smeared histogram

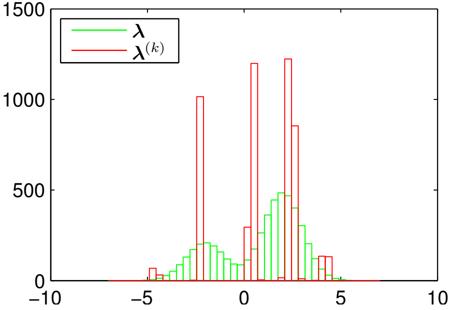

Figure : True histogram

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Regularization by early stopping of the EM iteration

- We have seen that unfortunately the MLE itself is often useless
  - Due to the ill-posedness of the problem, it exhibits large, unphysical fluctuations
  - In other words, the likelihood function alone does not contain enough information to constrain the solution
- As the EM iteration proceeds, the solutions will typically first improve but will start to degrade at some point
  - This is because the algorithm will start overfitting to the Poisson fluctuations in $\mathbf{y}$
- This behavior can be exploited by stopping the iteration before unphysical features start to appear
  - The number of iterations k now becomes a *regularization parameter* that controls the trade-off between fitting the data and taming unphysical features

D’Agostini demo, $k = 100$

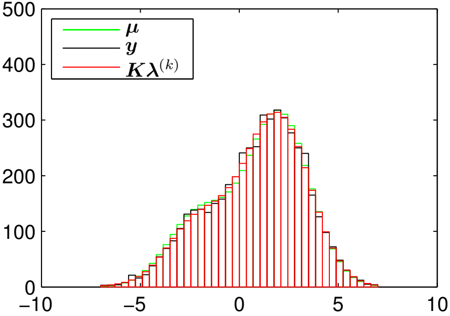


Figure : Smeared histogram

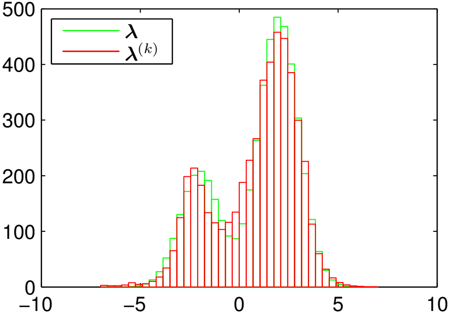


Figure : True histogram

Penalized maximum likelihood estimation

- Early stopping of the EM iteration seems a bit ad-hoc
  - Is there a more principled way of finding good solutions?
- Ideally we would like to find a solution that fits the data but at the same time seems physically plausible
- Let's consider a *penalized maximum likelihood* problem:

$$\max_{\boldsymbol{\lambda} \in \mathbb{R}_+^p} \; F(\boldsymbol{\lambda}) = \log p(\mathbf{y}|\boldsymbol{\lambda}) - \delta P(\boldsymbol{\lambda}),$$

- Here:
  - $P(\boldsymbol{\lambda})$ is a *penalty function* which obtains large values for physically implausible solutions
  - $\delta > 0$ is a *regularization parameter* which controls the balance between maximizing the likelihood and minimizing the penalty
- Typically $P(\boldsymbol{\lambda})$ is a measure of the curvature of the solution
  - I.e., it penalizes for large oscillations

From penalized likelihood to Tikhonov regularization

- To simplify this optimization problem, we use a Gaussian approximation of the Poisson likelihood

$$\mathbf{y}|\boldsymbol{\lambda} \sim \mathrm{Poisson}(\mathbf{K}\boldsymbol{\lambda}) \approx N(\mathbf{K}\boldsymbol{\lambda}, \hat{\mathbf{C}}),$$

  where $\hat{\mathbf{C}} = \mathrm{diag}(\mathbf{y})$

- Hence the objective function becomes:

$$\begin{aligned} F(\boldsymbol{\lambda}) &= \log p(\mathbf{y}|\boldsymbol{\lambda}) - \delta P(\boldsymbol{\lambda}) \\ &= \sum_{i=1}^{n} \left[y_i \log \left(\sum_{j=1}^{p} K_{ij}\lambda_j \right) - \sum_{j=1}^{p} K_{ij}\lambda_j \right] - \delta P(\boldsymbol{\lambda}) + \mathrm{const} \\ &\approx -\frac{1}{2}(\mathbf{y} - \mathbf{K}\boldsymbol{\lambda})^{\mathsf{T}} \hat{\mathbf{C}}^{-1} (\mathbf{y} - \mathbf{K}\boldsymbol{\lambda}) - \delta P(\boldsymbol{\lambda}) + \mathrm{const} \end{aligned}$$

From penalized likelihood to Tikhonov regularization

- We furthermore drop the positivity constraint and absorb the factor $1/2$ into the penalty to obtain

$$\begin{aligned}\hat{\boldsymbol{\lambda}} &= \operatorname*{arg\,max}_{\boldsymbol{\lambda}\in\mathbb{R}^p} -(\mathbf{y}-\mathbf{K}\boldsymbol{\lambda})^{\mathsf{T}}\hat{\mathbf{C}}^{-1}(\mathbf{y}-\mathbf{K}\boldsymbol{\lambda}) - \delta P(\boldsymbol{\lambda}) \\ &= \operatorname*{arg\,min}_{\boldsymbol{\lambda}\in\mathbb{R}^p} (\mathbf{y}-\mathbf{K}\boldsymbol{\lambda})^{\mathsf{T}}\hat{\mathbf{C}}^{-1}(\mathbf{y}-\mathbf{K}\boldsymbol{\lambda}) + \delta P(\boldsymbol{\lambda})\end{aligned}$$

- We see that we have ended up with a penalized χ^2 problem
- This is typically called *(generalized) Tikhonov regularization*

How to choose the penalty?

- The penalty term should reflect the analyst's a priori understanding of the desired solution
- Common choices include:
  - Norm of the solution: $P(\boldsymbol{\lambda}) = \|\boldsymbol{\lambda}\|^2$
  - Curvature of the solution: $P(\boldsymbol{\lambda}) = \|\mathbf{L}\boldsymbol{\lambda}\|^2$, where $\mathbf{L}$ is a discretized 2nd derivative operator
  - SVD unfolding (Höcker and Kartvelishvili, 1996):

$$P(\boldsymbol{\lambda}) = \left\| \mathbf{L} \begin{bmatrix} \lambda_1/\lambda_1^{\mathrm{MC}} \\ \lambda_2/\lambda_2^{\mathrm{MC}} \\ \vdots \\ \lambda_p/\lambda_p^{\mathrm{MC}} \end{bmatrix} \right\|^2 ,$$

    where $\boldsymbol{\lambda}^{\mathrm{MC}}$ is a MC prediction for $\boldsymbol{\lambda}$
  - `TUnfold`[1] (Schmitt, 2012): $P(\boldsymbol{\lambda}) = \|\mathbf{L}(\boldsymbol{\lambda} - \boldsymbol{\lambda}^{\mathrm{MC}})\|^2$

[1] Also more general penalty terms are allowed in `TUnfold`

Least squares estimation with the pseudoinverse

- Consider the least squares problem

$$\min_{\mathbf{x}\in\mathbb{R}^p} \|\mathbf{A}\mathbf{x}-\mathbf{y}\|^2,$$

  where $\mathbf{A} \in \mathbb{R}^{n\times p}$, $\mathbf{x} \in \mathbb{R}^p$ and $\mathbf{y} \in \mathbb{R}^n$

- This problem always has a solution, but it may not be unique
- A solution is always given by the Moore–Penrose pseudoinverse of $\mathbf{A}$:

$$\hat{\mathbf{x}}_{\mathrm{LS}} = \mathbf{A}^{\dagger}\mathbf{y}$$

- When there are multiple solutions, the pseudoinverse gives the one with the smallest norm
- When $\mathbf{A}$ has full column rank, the solution is unique
    - In this special case, the pseudoinverse is given by $\mathbf{A}^{\dagger} = (\mathbf{A}^{\mathsf{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathsf{T}}$
    - Hence, the least squares solution is: $\hat{\mathbf{x}}_{\mathrm{LS}} = (\mathbf{A}^{\mathsf{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathsf{T}}\mathbf{y}$

Finding the Tikhonov regularized solution

- We will now find an explicit form of the Tikhonov regularized estimator

$$\hat{\boldsymbol{\lambda}} = \operatorname*{arg\,min}_{\boldsymbol{\lambda} \in \mathbb{R}^p} \, (\mathbf{y} - \mathbf{K}\boldsymbol{\lambda})^{\mathsf{T}} \hat{\mathbf{C}}^{-1} (\mathbf{y} - \mathbf{K}\boldsymbol{\lambda}) + \delta \|\mathbf{L}\boldsymbol{\lambda}\|^2$$

  by rewriting this as a least squares problem
- This approach also easily generalizes to penalty terms involving $\boldsymbol{\lambda}^{\mathrm{MC}}$
- Let us rewrite:

$$\begin{aligned} \hat{\mathbf{C}}^{-1} &= \mathrm{diag}\left(\frac{1}{y_1}, \ldots, \frac{1}{y_n}\right) \\ &= \underbrace{\mathrm{diag}\left(\frac{1}{\sqrt{y_1}}, \ldots, \frac{1}{\sqrt{y_n}}\right)}_{:=\mathbf{A}} \underbrace{\mathrm{diag}\left(\frac{1}{\sqrt{y_1}}, \ldots, \frac{1}{\sqrt{y_n}}\right)}_{:=\mathbf{A}} \\ &= \mathbf{A}\mathbf{A} = \mathbf{A}^{\mathsf{T}}\mathbf{A} \end{aligned}$$

- Defining $\tilde{\mathbf{y}} := \mathbf{A}\mathbf{y}$ and $\tilde{\mathbf{K}} := \mathbf{A}\mathbf{K}$, our optimization problem becomes

$$\hat{\boldsymbol{\lambda}} = \operatorname*{arg\,min}_{\boldsymbol{\lambda} \in \mathbb{R}^p} \, (\tilde{\mathbf{y}} - \tilde{\mathbf{K}}\boldsymbol{\lambda})^{\mathsf{T}} (\tilde{\mathbf{y}} - \tilde{\mathbf{K}}\boldsymbol{\lambda}) + \delta \|\mathbf{L}\boldsymbol{\lambda}\|^2$$

Finding the Tikhonov regularized solution

- We can rewrite the objective function as follows:

$$\begin{aligned}
&(\tilde{\mathbf{y}} - \tilde{\mathbf{K}}\boldsymbol{\lambda})^{\mathsf{T}}(\tilde{\mathbf{y}} - \tilde{\mathbf{K}}\boldsymbol{\lambda}) + \delta\|\mathbf{L}\boldsymbol{\lambda}\|^2 \\
&= \|\tilde{\mathbf{K}}\boldsymbol{\lambda} - \tilde{\mathbf{y}}\|^2 + \|\sqrt{\delta}\mathbf{L}\boldsymbol{\lambda}\|^2 \\
&= \left\| \begin{bmatrix} \tilde{\mathbf{K}}\boldsymbol{\lambda} - \tilde{\mathbf{y}} \\ \sqrt{\delta}\mathbf{L}\boldsymbol{\lambda} \end{bmatrix} \right\|^2 \\
&= \left\| \begin{bmatrix} \tilde{\mathbf{K}} \\ \sqrt{\delta}\mathbf{L} \end{bmatrix} \boldsymbol{\lambda} - \begin{bmatrix} \tilde{\mathbf{y}} \\ \mathbf{0} \end{bmatrix} \right\|^2
\end{aligned}$$

- Here we recognize a least squares problem, so a minimizer is given by

$$\hat{\boldsymbol{\lambda}} = \begin{bmatrix} \tilde{\mathbf{K}} \\ \sqrt{\delta}\mathbf{L} \end{bmatrix}^{\dagger} \begin{bmatrix} \tilde{\mathbf{y}} \\ \mathbf{0} \end{bmatrix}$$

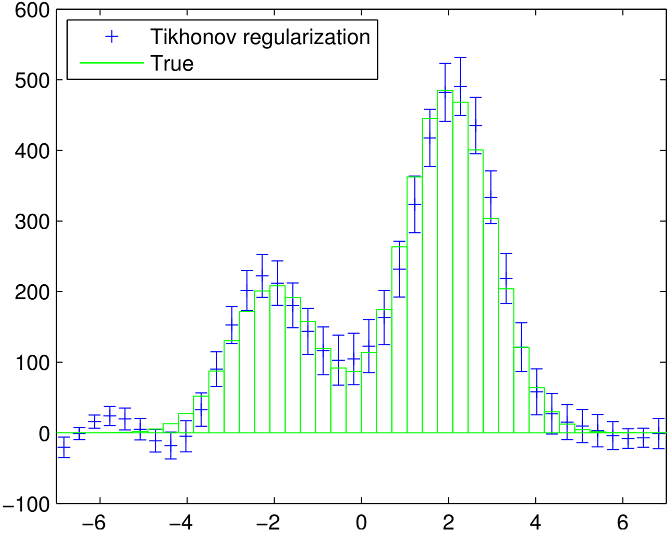
Finding the Tikhonov regularized solution

- Assuming that $\ker(\tilde{\mathbf{K}}) \cap \ker(\mathbf{L}) = \{\mathbf{0}\}$, the minimizer is unique and can be simplified as follows:

$$\begin{aligned}
\hat{\boldsymbol{\lambda}} &= \begin{bmatrix} \tilde{\mathbf{K}} \\ \sqrt{\delta}\mathbf{L} \end{bmatrix}^{\dagger} \begin{bmatrix} \tilde{\mathbf{y}} \\ \mathbf{0} \end{bmatrix} \\
&= \left(\begin{bmatrix} \tilde{\mathbf{K}} \\ \sqrt{\delta}\mathbf{L} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \tilde{\mathbf{K}} \\ \sqrt{\delta}\mathbf{L} \end{bmatrix} \right)^{-1} \begin{bmatrix} \tilde{\mathbf{K}} \\ \sqrt{\delta}\mathbf{L} \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} \tilde{\mathbf{y}} \\ \mathbf{0} \end{bmatrix} \\
&= \left(\begin{bmatrix} \tilde{\mathbf{K}}^{\mathsf{T}} & \sqrt{\delta}\mathbf{L}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{K}} \\ \sqrt{\delta}\mathbf{L} \end{bmatrix} \right)^{-1} \begin{bmatrix} \tilde{\mathbf{K}}^{\mathsf{T}} & \sqrt{\delta}\mathbf{L}^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{y}} \\ \mathbf{0} \end{bmatrix} \\
&= \left(\tilde{\mathbf{K}}^{\mathsf{T}} \tilde{\mathbf{K}} + \delta \mathbf{L}^{\mathsf{T}} \mathbf{L} \right)^{-1} \tilde{\mathbf{K}}^{\mathsf{T}} \tilde{\mathbf{y}} \\
&= \left(\mathbf{K}^{\mathsf{T}} \hat{\mathbf{C}}^{-1} \mathbf{K} + \delta \mathbf{L}^{\mathsf{T}} \mathbf{L} \right)^{-1} \mathbf{K}^{\mathsf{T}} \hat{\mathbf{C}}^{-1} \mathbf{y}
\end{aligned}$$

- Hence we have obtained an explicit, closed-form solution for the Tikhonov regularization problem

Demonstration of Tikhonov regularization, $P(\boldsymbol{\lambda}) = \|\boldsymbol{\lambda}\|^2$



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Bayesian unfolding

- In Bayesian unfolding, the inferences about $\boldsymbol{\lambda}$ are based on the posterior distribution $p(\boldsymbol{\lambda}|\mathbf{y})$
- This is obtained using Bayes' rule:

$$p(\boldsymbol{\lambda}|\mathbf{y}) = \frac{p(\mathbf{y}|\boldsymbol{\lambda})p(\boldsymbol{\lambda})}{p(\mathbf{y})} = \frac{p(\mathbf{y}|\boldsymbol{\lambda})p(\boldsymbol{\lambda})}{\int_{\mathbb{R}_+^p} p(\mathbf{y}|\boldsymbol{\lambda}')p(\boldsymbol{\lambda}')\,\mathrm{d}\boldsymbol{\lambda}'}, \quad \boldsymbol{\lambda} \in \mathbb{R}_+^p$$

  where the likelihood $p(\mathbf{y}|\boldsymbol{\lambda})$ is the same as earlier and $p(\boldsymbol{\lambda})$ is a prior distribution for $\boldsymbol{\lambda}$
- The most common choices as a point estimator of $\boldsymbol{\lambda}$ are:
  - The *posterior mean*: $\hat{\boldsymbol{\lambda}} = \mathrm{E}[\boldsymbol{\lambda}|\mathbf{y}] = \int_{\mathbb{R}_+^p} \boldsymbol{\lambda} p(\boldsymbol{\lambda}|\mathbf{y})\,\mathrm{d}\boldsymbol{\lambda}$
  - The *maximum a posteriori* (MAP) *estimator*: $\hat{\boldsymbol{\lambda}} = \arg\max_{\boldsymbol{\lambda} \in \mathbb{R}_+^p} p(\boldsymbol{\lambda}|\mathbf{y})$
- The width of the posterior distribution $p(\boldsymbol{\lambda}|\mathbf{y})$ can be used to quantify uncertainty regarding $\boldsymbol{\lambda}$
  - But note that the interpretation of the resulting Bayesian *credible intervals* is different from frequentist confidence intervals

Regularization using the prior

- In the Bayesian approach, the prior density $p(\boldsymbol{\lambda})$ regularizes the otherwise ill-posed problem
  - It concentrates the probability mass of the posterior on physically plausible solutions
- The prior is typically of the form

  $$p(\boldsymbol{\lambda}) \propto \exp\left(-\delta P(\boldsymbol{\lambda})\right), \quad \boldsymbol{\lambda} \in \mathbb{R}_+^p,$$

  where $P(\boldsymbol{\lambda})$ is a function characterizing a priori plausible solutions and $\delta > 0$ is a *hyperparameter* controlling the scale of the prior density
- For example, choosing $P(\boldsymbol{\lambda}) = \|\mathbf{L}\boldsymbol{\lambda}\|^2$, where $\mathbf{L}$ a discretized 2nd derivative operator, leads to the positivity-constrained Gaussian smoothness prior

  $$p(\boldsymbol{\lambda}) \propto \exp\left(-\delta\|\mathbf{L}\boldsymbol{\lambda}\|^2\right), \quad \boldsymbol{\lambda} \in \mathbb{R}_+^p$$

Connection between Bayesian unfolding and penalized MLE

- Notice that when $p(\boldsymbol{\lambda}) \propto \exp\left(-\delta P(\boldsymbol{\lambda})\right)$, the Bayesian MAP solution coincides with the penalized maximum likelihood estimator:

$$
\begin{aligned}
\hat{\boldsymbol{\lambda}}_{\mathrm{MAP}} &= \operatorname*{arg\,max}_{\boldsymbol{\lambda} \in \mathbb{R}_+^p} p(\boldsymbol{\lambda}|\mathbf{y}) \\
&= \operatorname*{arg\,max}_{\boldsymbol{\lambda} \in \mathbb{R}_+^p} \log p(\boldsymbol{\lambda}|\mathbf{y}) \\
&= \operatorname*{arg\,max}_{\boldsymbol{\lambda} \in \mathbb{R}_+^p} \log p(\mathbf{y}|\boldsymbol{\lambda}) + \log p(\boldsymbol{\lambda}) \\
&= \operatorname*{arg\,max}_{\boldsymbol{\lambda} \in \mathbb{R}_+^p} \log p(\mathbf{y}|\boldsymbol{\lambda}) - \delta P(\boldsymbol{\lambda}) \\
&= \hat{\boldsymbol{\lambda}}_{\mathrm{PMLE}}
\end{aligned}
$$

- So the penalty term $\delta P(\boldsymbol{\lambda})$ can either be interpreted as a Bayesian prior or as a frequentist regularization term
- The Bayesian interpretation has the advantage that we can visualize the prior $p(\boldsymbol{\lambda})$ by, e.g., drawing samples from it

A note about Bayesian computations

- To be able to compute the posterior mean $\mathrm{E}[\boldsymbol{\lambda}|\mathbf{y}]$ or form the Bayesian credible intervals, we need to be able to evaluate the posterior

$$p(\boldsymbol{\lambda}|\mathbf{y}) = \frac{p(\mathbf{y}|\boldsymbol{\lambda})p(\boldsymbol{\lambda})}{\int_{\mathbb{R}_+^p} p(\mathbf{y}|\boldsymbol{\lambda}')p(\boldsymbol{\lambda}')\,\mathrm{d}\boldsymbol{\lambda}'}$$

- But the denominator is an intractable high-dimensional integral...
- Luckily, it turns out that it is possible to *sample* from the posterior without evaluating the denominator
    - The sample mean and sample quantiles can then be used to compute the posterior mean and the credible intervals
- The class of algorithms that enable this are called Markov chain Monte Carlo (MCMC) samplers and are based on a Markov chain whose equilibrium distribution is the posterior $p(\boldsymbol{\lambda}|\mathbf{y})$
- The single-component Metropolis–Hastings sampler of Saquib et al. (1998) is particularly well-suited for the unfolding problem and seems to also work well in practice

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   - MC dependence in the smearing matrix

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Choice of the regularization strength

- All unfolding methods involve a free parameter controlling the strength of the regularization
  - The parameter δ in Tikhonov regularization and Bayesian unfolding, the number of iterations in D'Agostini
- This parameter is typically difficult to choose using only a priori information
  - But its value usually has a major impact on the unfolded spectrum
- Most LHC analyses choose the regularization parameter using MC studies
  - But this may create an undesired MC bias
- It would be better to choose the regularization parameter based on the observed data $\mathbf{y}$

Data-dependent choice of the regularization strength

- Many methods for using the observed data $\mathbf{y}$ to choose the regularization strength have been proposed in the literature:
  - Goodness-of-fit test in the smeared space (Veklerov and Llacer, 1987)
  - Empirical Bayes estimation (Kuusela and Panaretos, 2014)
  - L-curve (Hansen, 1992)
  - (Generalized) cross validation (Wahba, 1990)
  - ...
- At the moment, we have very limited experience about the relative merits of these methods in HEP unfolding

Goodness-of-fit for choosing the regularization strength

- We present here a simplified version of the procedure proposed by Veklerov and Llacer (1987)
- Let $\hat{\boldsymbol{\mu}} = \mathbf{K}\hat{\boldsymbol{\lambda}}$ be the estimated smeared mean
- Consider the χ^2 statistic

$$T = (\hat{\boldsymbol{\mu}} - \mathbf{y})^{\mathsf{T}} \mathbf{C}^{-1} (\hat{\boldsymbol{\mu}} - \mathbf{y}),$$

  where $\mathbf{C} = \mathrm{diag}(\hat{\boldsymbol{\mu}})$
- If $\mathbf{y} \sim \mathrm{Poisson}(\hat{\boldsymbol{\mu}})$, then asymptotically $T \overset{a}{\sim} \chi^2_n$, where n is the number of bins in $\mathbf{y}$
- Hence, $\mathrm{E}[T] \approx n$
- This suggests that we should choose the regularization strength so that T is as close as possible to n
- Note that this provides a balance between overfitting ($T < n$) and underfitting ($T > n$) the data

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Uncertainty quantification

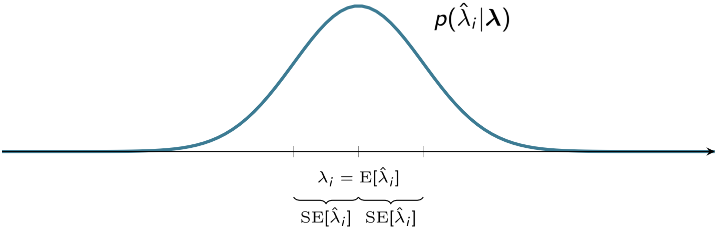
- Proper uncertainty quantification is one of the main challenges in unfolding
- By uncertainty quantification, we mean computing bin-wise frequentist confidence intervals at $1 - \alpha$ confidence level:

$$\inf_{\boldsymbol{\lambda} \in \mathbb{R}_+^p} P_{\boldsymbol{\lambda}}[\hat{\lambda}_{i,L}(\mathbf{y}) \leq \lambda_i \leq \hat{\lambda}_{i,U}(\mathbf{y})] = 1 - \alpha$$

- In practice, we can only hope to satisfy this approximately for finite sample sizes

Uncertainty quantification

- Let $\mathrm{SE}[\hat{\lambda}_i]$ be the standard error of $\hat{\lambda}_i$ (i.e., the standard deviation of the sampling distribution of $\hat{\lambda}_i$)
- In many situations, $\hat{\lambda}_i \pm \widehat{\mathrm{SE}}[\hat{\lambda}_i]$ provides a reasonable 68% confidence interval
  - But this is only true when $\hat{\lambda}_i$ is unbiased and has a symmetric sampling distribution
- But in regularized unfolding the estimators are always biased!
  - Regularization reduces variance by increasing the bias (*bias-variance trade-off*)
  - Hence the SE confidence intervals may have lousy coverage


$p(\hat{\lambda}_i|\boldsymbol{\lambda})$
$\lambda_i = \mathrm{E}[\hat{\lambda}_i]$
$\mathrm{SE}[\hat{\lambda}_i]$
$\mathrm{SE}[\hat{\lambda}_i]$

Uncertainty quantification

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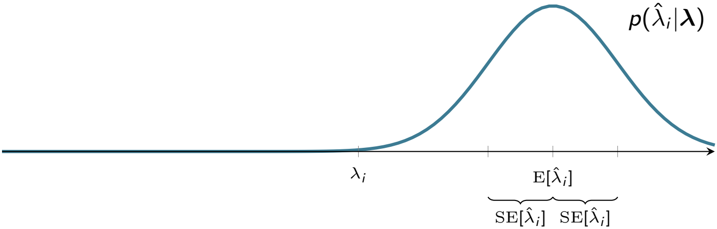
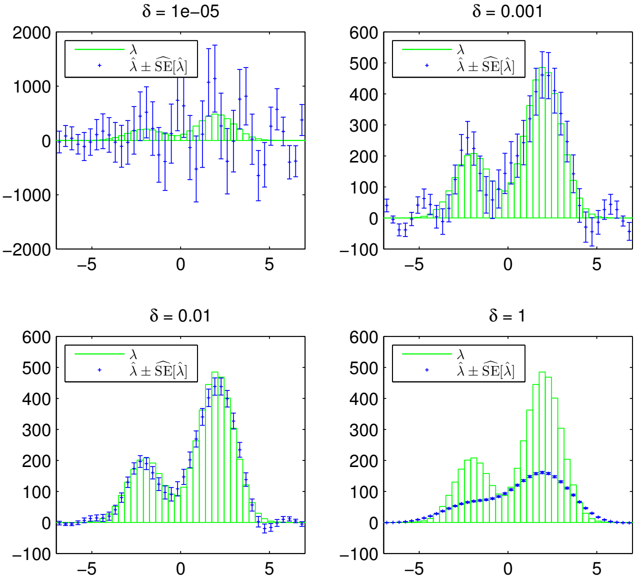

$p(\hat{\lambda}_i|\boldsymbol{\lambda})$
λ_i
$\mathrm{E}[\hat{\lambda}_i]$
$\mathrm{SE}[\hat{\lambda}_i]$
$\mathrm{SE}[\hat{\lambda}_i]$

Demonstration with Tikhonov regularization, $P(\boldsymbol{\lambda}) = \|\boldsymbol{\lambda}\|^2$



Uncertainty quantification

- The uncertainties returned by RooUnfold are estimates of the standard errors computed either using error propagation or resampling
    - Hence these uncertainties should be understood as estimates of the spread of the sampling distribution of $\hat{\boldsymbol{\lambda}}$
    - These should only be understood as approximate confidence intervals if it can be shown that the bias is negligible
- Bootstrap resampling provides an attractive way of forming approximate confidence intervals that take into account the bias and the potential skewness of $p(\hat{\lambda}_i|\boldsymbol{\lambda})$ (Kuusela and Panaretos, 2014)

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MC dependence in the smearing matrix

- The smearing matrix $\mathbf{K}$ is typically estimated using Monte Carlo
- In addition to a statistical error due to the finite sample size, there are two sources of systematics in $\mathbf{K}$:
  1. The matrix depends on the shape of the spectrum within each true bin
  $$K_{ij} = \frac{\int_{F_i} \int_{E_j} k(y,x) f(x) \, \mathrm{d}x \, \mathrm{d}y}{\int_{E_j} f(x) \, \mathrm{d}x}, \quad i = 1, \ldots, n, \quad j = 1, \ldots, p$$
  2. The smearing of the variable of interest may depend on the MC distribution of some auxiliary variables
     - For example, the energy resolution of jets depends on the pseudorapidity distribution of the jets
- The first problem can be alleviated by making the true bins smaller at the cost of increased ill-posedness of the problem

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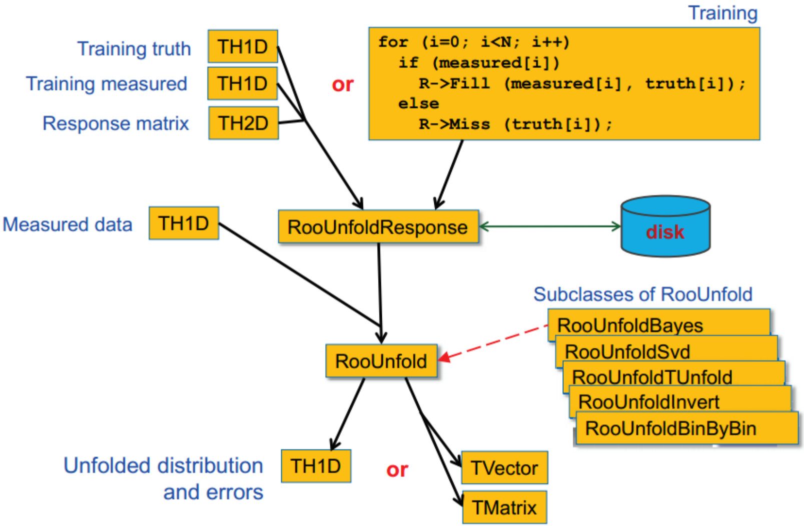
Introduction to RooUnfold

- RooUnfold (Adye, 2011) an unfolding framework for ROOT that provides an interface for many standard unfolding methods
- Written by Tim Adye, Richard Claridge, Kerstin Tackmann and Fergus Wilson
- RooUnfold is currently the most commonly used unfolding framework among the LHC experiments although other implementations are also occasionally used
- RooUnfold includes the following unfolding techniques:
    1. Matrix inversion
    2. D'Agostini iteration
    3. The SVD flavor of Tikhonov regularization
    4. The `TUnfold` flavor of Tikhonov regularization
- There is also an implementation for the so-called bin-by-bin unfolding technique
    - This is an obsolete method that replaces the full response matrix $\mathbf{K}$ by a diagonal approximation and while doing so introduces a huge MC bias
    - This method should not be used!

RooUnfold classes



```
for (i=0; i<N; i++)
  if (measured[i])
    R->Fill (measured[i], truth[i]);
  else
    R->Miss (truth[i]);
```

Figure from Adye (2011)

RooUnfoldInvert

```
RooUnfoldInvert(const RooUnfoldResponse* res, const TH1*
meas, const char* name = 0, const char* title = 0)
```

- This is the most basic method: it estimates $\boldsymbol{\lambda}$ using $\hat{\boldsymbol{\lambda}} = \mathbf{K}^{-1}\mathbf{y}$
- Remember that when $\hat{\boldsymbol{\lambda}}$ is positive, this is the MLE
- `res` contains the response matrix $\mathbf{K}$
- `meas` contains the smeared data $\mathbf{y}$
- The standard error of $\hat{\boldsymbol{\lambda}}$ is estimated using error propagation

RooUnfoldBayes

`RooUnfoldBayes(const RooUnfoldResponse* res, const TH1* meas, Int_t niter = 4, Bool_t smoothit = false, const char* name = 0, const char* title = 0)`

- This implements the D'Agostini/Lucy-Richardson/EM iteration for finding the MLE
- Remember that despite the name this is not a Bayesian technique
- The iteration is started from the MC spectrum, i.e., $\boldsymbol{\lambda}^{(0)} = \boldsymbol{\lambda}^{\mathrm{MC}}$ contained in `res`
- `niter` is the number of iterations
  - For small `niter`, the solution is biased towards $\boldsymbol{\lambda}^{\mathrm{MC}}$; for large `niter`, we get a solution close to the MLE
  - Note that the default `niter = 4` is completely arbitrary and with no optimality guarantees
- `smoothit` can be used to enable a smoothed version of the EM iteration (outside the scope of this course)
- By default, the standard error of $\hat{\boldsymbol{\lambda}}$ is estimated using error propagation at each iteration of the algorithm

RooUnfoldSvd

`RooUnfoldSvd(const RooUnfoldResponse* res, const TH1* meas, Int_t kreg = 0, Int_t ntoyssvd = 1000, const char* name = 0, const char* title = 0)`

- This implements the SVD flavor of Tikhonov regularization, i.e.,

$$\hat{\boldsymbol{\lambda}} = \operatorname*{arg\,min}_{\boldsymbol{\lambda} \in \mathbb{R}^p} (\mathbf{y} - \mathbf{K}\boldsymbol{\lambda})^{\mathsf{T}} \hat{\mathbf{C}}^{-1} (\mathbf{y} - \mathbf{K}\boldsymbol{\lambda}) + \delta \left\| \mathbf{L} \begin{bmatrix} \lambda_1/\lambda_1^{\mathrm{MC}} \\ \lambda_2/\lambda_2^{\mathrm{MC}} \\ \vdots \\ \lambda_p/\lambda_p^{\mathrm{MC}} \end{bmatrix} \right\|^2 ,$$

  where $\boldsymbol{\lambda}^{\mathrm{MC}}$ is again contained in `res`
- This is a wrapper for the `TSVDUnfold` class by K. Tackmann
- `kreg` chooses the number of significant singular values in a certain transformation of the smearing matrix $\mathbf{K}$
  - Small `kreg` corresponds to a large δ and a large `kreg` to a small δ
- The standard error of $\hat{\boldsymbol{\lambda}}$ is estimated by resampling `ntoyssvd` observations
  - Also includes a contribution from the uncertainty of $\mathbf{K}$

RooUnfoldTUnfold

`RooUnfoldTUnfold(const RooUnfoldResponse* res, const TH1* meas, TUnfold::ERegMode reg = TUnfold::kRegModeDerivative, const char* name = 0, const char* title = 0)`

- This implements the `TUnfold` flavor of Tikhonov regularization, i.e.,

  $$\hat{\boldsymbol{\lambda}} = \underset{\boldsymbol{\lambda}\in\mathbb{R}^p}{\arg\min}\ (\mathbf{y}-\mathbf{K}\boldsymbol{\lambda})^{\mathsf{T}}\hat{\mathbf{C}}^{-1}(\mathbf{y}-\mathbf{K}\boldsymbol{\lambda}) + \delta\|\mathbf{L}(\boldsymbol{\lambda}-\boldsymbol{\lambda}^{\mathrm{MC}})\|^2,$$

  where the minimizer is found subject to an additional area constraint[2]
- This is a wrapper for the `TUnfold` class by S. Schmitt
  - `TUnfold` actually provides a lot of extra functionality which cannot be accessed through RooUnfold
- The form of the matrix **L** is chosen using `reg`
  - The supported choices are identity, 1st derivative and 2nd derivative
- The regularization parameter δ is chosen using the `SetRegParm(Double_t parm)` method
  - If δ is not chosen manually, it is found automatically using the L-curve technique, but this only seems to work when $n \gg p$

[2] In the case of the `TUnfold` wrapper, the RooUnfold documentation is not explicit about the choice of $\boldsymbol{\lambda}^{\mathrm{MC}}$ (it does not seem to come from `res` in this case)

RooUnfold practical

- Start by downloading the code template at:

  `www.cern.ch/mkuusela/ETH_workshop_July_2014/RooUnfoldExercise.cxx`
- A set of exercises based on this code can be found at:

  `www.cern.ch/mkuusela/ETH_workshop_July_2014/practical.pdf`
- Useful supplementary material
  - These slides:

    `www.cern.ch/mkuusela/ETH_workshop_July_2014/slides.pdf`
  - RooUnfold website:

    `http://hepunx.rl.ac.uk/~adye/software/unfold/RooUnfold.html`
  - RooUnfold class documentation:

    `http://hepunx.rl.ac.uk/~adye/software/unfold/htmldoc/RooUnfold.html`

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Conclusions

- Unfolding is a complex data analysis task that involves several assumptions and approximations
    - It is crucial to understand the ingredients that go into an unfolding procedure
    - Unfolding algorithms should never be used as black boxes!
- All unfolding methods are based on complementing the likelihood by additional information about physically plausible solutions
- The most popular techniques are the D'Agostini iteration and various flavors of Tikhonov regularization
- Beware when using RooUnfold that:
    - There is a MC dependence in both the smearing matrix and the regularization
    - The uncertainties should be understood as standard errors and do not necessarily provide good coverage properties
    - The regularization parameter has a major impact on the solution and should be chosen in a data-dependent way
- There is plenty room for further improvements in both unfolding methodology and software

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Backup

Uncertainty quantification with the bootstrap

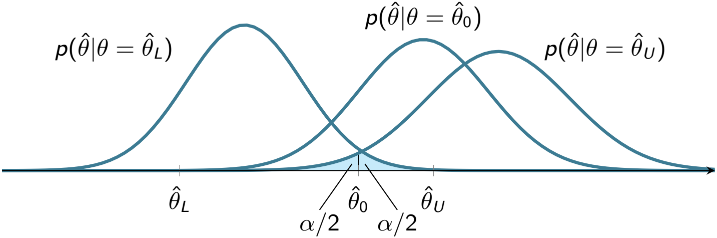
- The bootstrap sample can be obtained as follows:
  1. Unfold $\mathbf{y}$ to obtain $\hat{\boldsymbol{\lambda}}$
  2. Fold $\hat{\boldsymbol{\lambda}}$ to obtain $\hat{\boldsymbol{\mu}} = \mathbf{K}\hat{\boldsymbol{\lambda}}$
  3. Obtain a resampled observation $\mathbf{y}^* \sim \mathrm{Poisson}(\hat{\boldsymbol{\mu}})$
  4. Unfold $\mathbf{y}^*$ to obtain $\hat{\boldsymbol{\lambda}}^*$
  5. Repeat R times from 3
- The bootstrap sample $\{\hat{\boldsymbol{\lambda}}^{*(r)}\}_{r=1}^{R}$ follows the sampling distribution of $\hat{\boldsymbol{\lambda}}$ if the true value of $\boldsymbol{\lambda}$ was the observed value of our estimator
  - I.e., it is our best understanding of the sampling distribution of $\hat{\boldsymbol{\lambda}}$ for the data at hand
- This procedure also enables us to take into account the data-dependent choice of the regularization strength
  - This is very difficult to do using competing methods

Uncertainty quantification with the bootstrap

- The bootstrap sample can be used to compute $1-\alpha$ *basic bootstrap intervals* to serve as approximate $1-\alpha$ confidence intervals for λ_i:

$$[\hat{\lambda}_{i,L}, \hat{\lambda}_{i,U}] = [2\hat{\lambda}_i - \hat{\lambda}^*_{i,1-\alpha/2}, 2\hat{\lambda}_i - \hat{\lambda}^*_{i,\alpha/2}],$$

  where $\hat{\lambda}^*_{i,\alpha}$ denotes the α-quantile of the bootstrap sample $\{\hat{\lambda}_i^{*(r)}\}_{r=1}^R$
- This can be understood as the bootstrap analogue of the Neyman construction of confidence intervals


$p(\hat{\theta}|\theta = \hat{\theta}_0)$
$p(\hat{\theta}|\theta = \hat{\theta}_L)$
$p(\hat{\theta}|\theta = \hat{\theta}_U)$
$\hat{\theta}_L$
$\hat{\theta}_0$
$\hat{\theta}_U$
$\alpha/2$
$\alpha/2$

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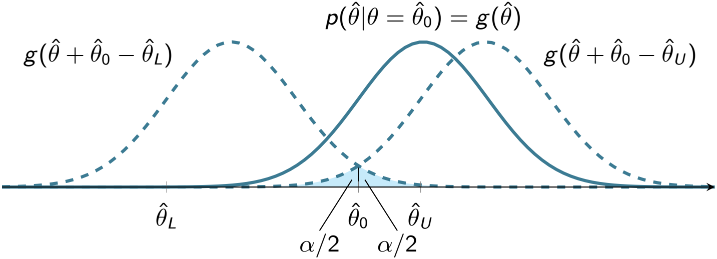
$p(\hat{\theta}|\theta = \hat{\theta}_0) = g(\hat{\theta})$
$g(\hat{\theta} + \hat{\theta}_0 - \hat{\theta}_L)$
$g(\hat{\theta} + \hat{\theta}_0 - \hat{\theta}_U)$
$\hat{\theta}_L$
$\hat{\theta}_0$
$\hat{\theta}_U$
$\alpha/2$
$\alpha/2$

Demonstration

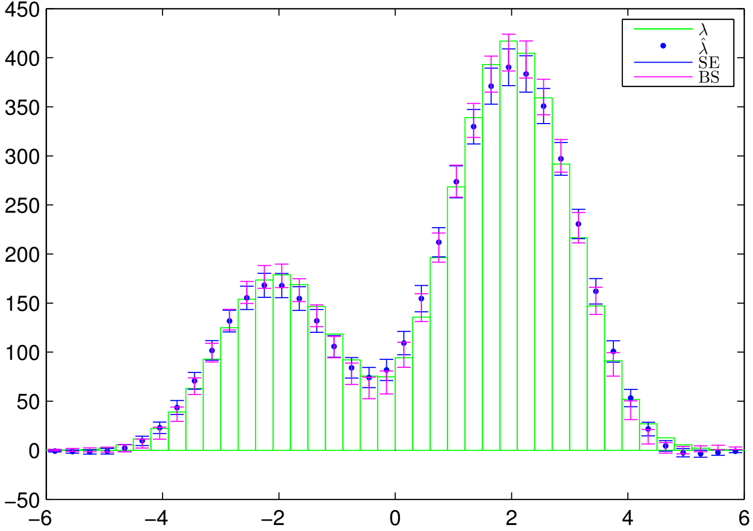

Figure : Tikhonov regularization with 95% bin-wise confidence intervals. The SE intervals cover in 23 bins out of 40, while the bootstrap intervals cover in 32 bins.