

Introduction to Unfolding: A Statistician's Perspective

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The unfolding problem

- Any differential cross section measurement is affected by the finite resolution of the particle detectors
 - This causes the observed spectrum of events to be “smeared” or “blurred” with respect to the true one
- The *unfolding problem* is to estimate the true spectrum using the smeared observations
- Ill-posed inverse problem with major methodological challenges

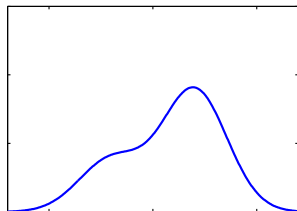


Figure: Smeared spectrum

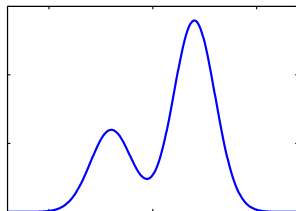
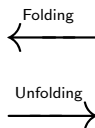


Figure: True spectrum

Problem formulation

- Let f be the true, particle-level spectrum and g the smeared, detector-level spectrum
 - Denote the true space by T and the smeared space by S (both taken to be intervals on the real line)
 - Mathematically f and g are the intensity functions of the underlying Poisson point process
- The two spectra are related by

$$g(s) = \int_T k(s, t) f(t) dt,$$

where the smearing kernel k represents the response of the detector and is given by

$$k(s, t) = p(Y = s | X = t, X \text{ observed}) P(X \text{ observed} | X = t),$$

where X is a true event and Y the corresponding smeared event

Task: Infer the true spectrum f given smeared observations from g

Discretization

- Problem usually discretized using histograms (splines are also sometimes used)
- Let $\{T_i\}_{i=1}^p$ and $\{S_i\}_{i=1}^n$ be binnings of the true space T and the smeared space S
- Smeared histogram $\mathbf{y} = [y_1, \dots, y_n]^T$ with mean

$$\boldsymbol{\mu} = \left[\int_{S_1} g(s) ds, \dots, \int_{S_n} g(s) ds \right]^T$$

- Quantity of interest:

$$\boldsymbol{\lambda} = \left[\int_{T_1} f(t) dt, \dots, \int_{T_p} f(t) dt \right]^T$$

- The mean histograms are related by $\boldsymbol{\mu} = \mathbf{K}\boldsymbol{\lambda}$, where the elements of the *response matrix* \mathbf{K} are given by

$$K_{i,j} = \frac{\int_{S_i} \int_{T_j} k(s, t) f(t) dt ds}{\int_{T_j} f(t) dt} = P(\text{smeared event in bin } i \mid \text{true event in bin } j)$$

- The discretized statistical model becomes

$$\mathbf{y} \sim \text{Poisson}(\mathbf{K}\boldsymbol{\lambda})$$

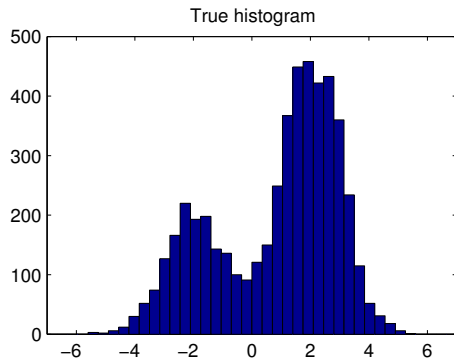
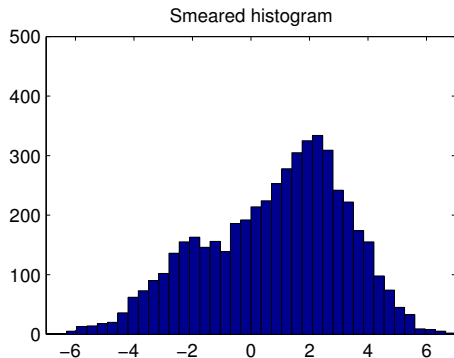
and we wish to make inferences about $\boldsymbol{\lambda}$ under this model

Why is unfolding difficult?

Two key challenges:

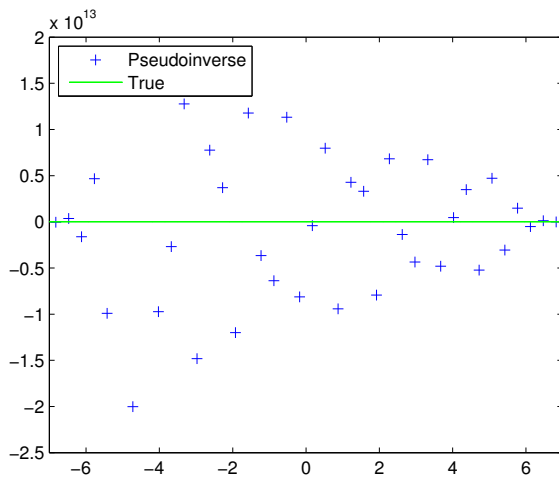
- **Problem 1:** \mathbf{K} is an ill-conditioned matrix $\Rightarrow \hat{\boldsymbol{\lambda}} = \mathbf{K}^{-1}\mathbf{y}$ tends to have unphysical high-frequency oscillations \Rightarrow Regularization
- **Problem 2:** \mathbf{K} depends on the shape of the spectrum inside the true bins $\Rightarrow \mathbf{K}$ estimated using a MC ansatz \Rightarrow Systematic uncertainty

Demonstration of ill-posedness

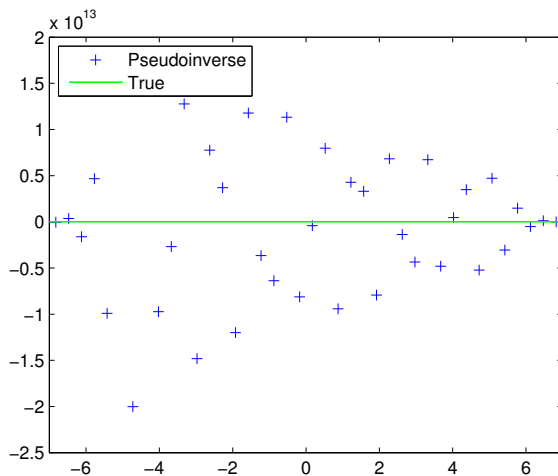


$$\mu = K\lambda, \quad y \sim \text{Poisson}(\mu) \quad \xRightarrow{??} \quad \hat{\lambda} = K^{-1}y$$

Demonstration of ill-posedness



Demonstration of ill-posedness



$$\text{MSE}(\hat{\theta}) = \mathbb{E}((\hat{\theta} - \theta)^2) = [\text{bias}(\hat{\theta})]^2 + \text{var}(\hat{\theta})$$

Regularization: bias \uparrow , variance $\downarrow \Rightarrow$ MSE \downarrow

Current unfolding methods

- Two main approaches (more information in the [backup](#)):

- 1 Tikhonov regularization (i.e., SVD by Höcker and Kartvelishvili (1996) and TUnfold by Schmitt (2012)):

$$\min_{\lambda \in \mathbb{R}^p} (\mathbf{y} - \mathbf{K}\lambda)^T \hat{\mathbf{C}}^{-1} (\mathbf{y} - \mathbf{K}\lambda) + \delta P(\lambda)$$

with

$$P_{\text{SVD}}(\lambda) = \left\| \mathbf{L} \begin{bmatrix} \lambda_1 / \lambda_1^{\text{MC}} \\ \lambda_2 / \lambda_2^{\text{MC}} \\ \vdots \\ \lambda_p / \lambda_p^{\text{MC}} \end{bmatrix} \right\|^2 \quad \text{or} \quad P_{\text{TUnfold}}(\lambda) = \|\mathbf{L}(\lambda - \lambda^{\text{MC}})\|^2,$$

where \mathbf{L} is usually the discretized second derivative (also other choices possible)

- 2 Expectation-maximization iteration with early stopping (D'Agostini, 1995):

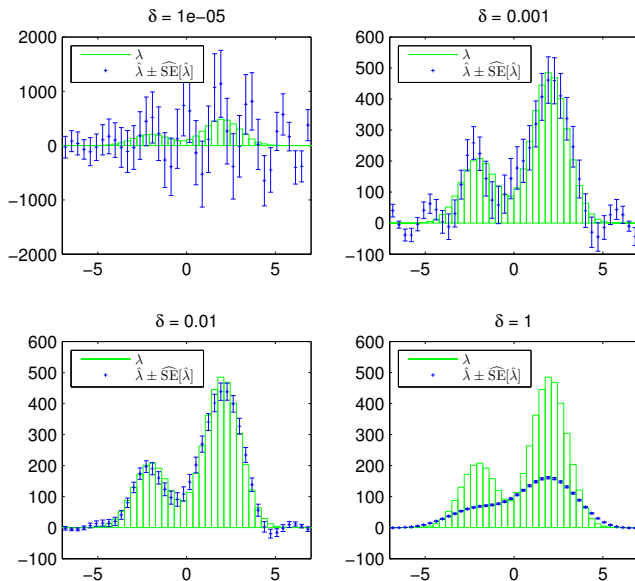
$$\lambda_j^{(t+1)} = \frac{\lambda_j^{(t)}}{\sum_{i=1}^n K_{i,j}} \sum_{i=1}^n \frac{K_{i,j} y_i}{\sum_{k=1}^p K_{i,k} \lambda_k^{(t)}}, \quad \text{with } \lambda^{(0)} = \lambda^{\text{MC}}$$

- All these methods typically regularize by biasing towards a MC ansatz λ^{MC}
- Regularization strength controlled by the choice of δ in Tikhonov or by the number of iterations in D'Agostini
- Uncertainty quantification: $[\underline{\lambda}_i, \bar{\lambda}_i] = \left[\hat{\lambda}_i - z_{1-\alpha/2} \sqrt{\widehat{\text{var}}(\hat{\lambda}_i)}, \hat{\lambda}_i + z_{1-\alpha/2} \sqrt{\widehat{\text{var}}(\hat{\lambda}_i)} \right]$, with $\widehat{\text{var}}(\hat{\lambda}_i)$ estimated using error propagation or resampling

Choice of the regularization strength

- A key issue in unfolding is the choice of the regularization strength (δ in Tikhonov, # of iterations in D'Agostini)
 - The solution and especially the uncertainties depend heavily on this choice
- This choice should be done using an objective data-driven criterion
 - In particular, one must not rely on the software defaults for the regularization strength (such as 4 iterations of D'Agostini in RooUnfold)
- Many data-driven methods have been proposed:
 - 1 (Weighted/generalized) cross-validation (e.g., Green and Silverman, 1994)
 - 2 L-curve (Hansen, 1992)
 - 3 Empirical Bayes estimation (Kuusela and Panaretos, 2015)
 - 4 Goodness-of-fit test in the smeared space (Veklerov and Llacer, 1987)
 - 5 Akaike information criterion (Volobouev, 2015)
 - 6 Minimization of a global correlation coefficient (Schmitt, 2012)
 - 7 ...
- Limited experience about the relative merits of these in typical unfolding problems
- **Note:** *All of these are designed for point estimation!*
 - Not necessarily optimal for uncertainty quantification

Tikhonov regularization, $P(\lambda) = \|\lambda\|^2$, varying δ

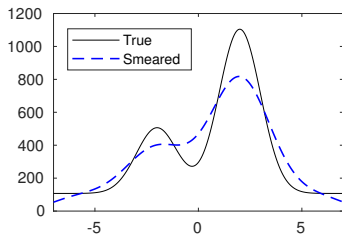


For the rest of this talk, I will focus on the following question: *Do the unfolded confidence intervals have the advertised coverage probability*

$$P(\lambda_i \in [\underline{\lambda}_i(\mathbf{y}), \bar{\lambda}_i(\mathbf{y})]) \approx 1 - \alpha$$

?

Simulation setup



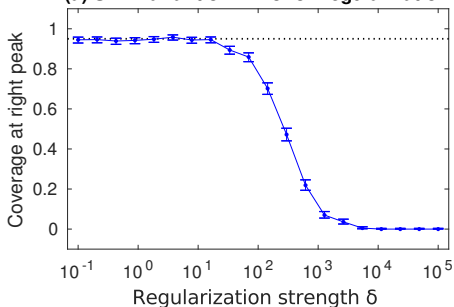
$$f(t) = \lambda_{\text{tot}} \left\{ \pi_1 \mathcal{N}(t|-2, 1) + \pi_2 \mathcal{N}(t|2, 1) + \pi_3 \frac{1}{|T|} \right\}$$

$$g(s) = \int_T \mathcal{N}(s-t|0, 1) f(t) dt$$

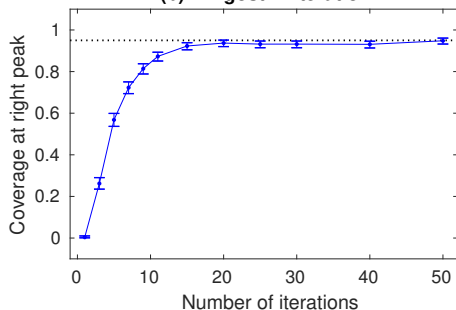
$$f^{\text{MC}}(t) = \lambda_{\text{tot}} \left\{ \pi_1 \mathcal{N}(t|-2, 1.1^2) + \pi_2 \mathcal{N}(t|2, 0.9^2) + \pi_3 \frac{1}{|T|} \right\}$$

Coverage as a function of regularization strength

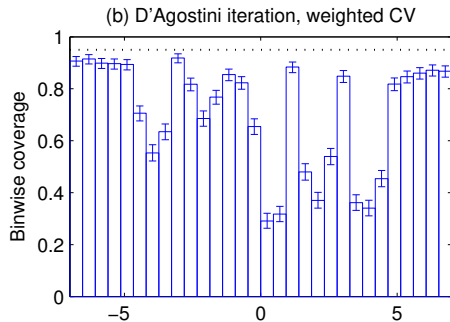
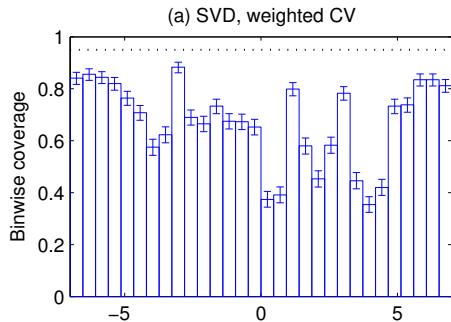
(a) SVD variant of Tikhonov regularization



(b) D'Agostini iteration



Undercoverage of existing methods



There is major undercoverage if regularization strength chosen using (weighted) cross-validation; same is true for L-curve and MMLE

I have previously proposed two complementary ways of obtaining improved uncertainties in unfolding (Kuusela and Panaretos, 2015; Kuusela, 2016; Kuusela and Stark, 2017):

- 1 **Debiased confidence intervals** for smooth spectra
 - Gives improved coverage in Tikhonov-type methods by adjusting the bias-variance trade-off to the direction of less bias and more variance
- 2 **Shape-constrained confidence intervals** for steeply falling spectra
 - Gives guaranteed conservative coverage if something is known about the shape of the true spectrum (monotonicity, convexity,...)

Undersmoothed unfolding

- The simplest form of debiasing is to reduce δ from the cross-validation/L-curve/MMLE value until the intervals have close-to-nominal coverage
- The challenge is to come up with a data-driven rule for deciding *how much to undersmooth*
- I have been working with a student Lyle Kim to implement the data-driven methods from Kuusela (2016) as an extension of TUnfold
- The code is available at:

<https://github.com/lylejkim/UndersmoothedUnfolding>

- If you're already working with TUnfold, then trying this approach requires adding only one extra line of code to your analysis
 - See the Github repository for example usage

Unfolded histograms, $\lambda^{\text{MC}} = 0$

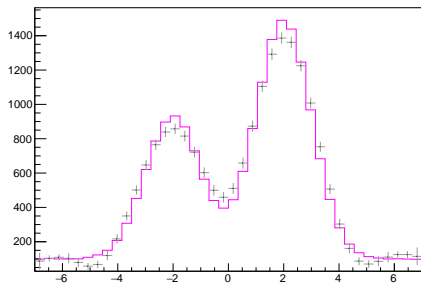


Figure: L-curve, $\tau = \sqrt{\delta} = 0.01186$

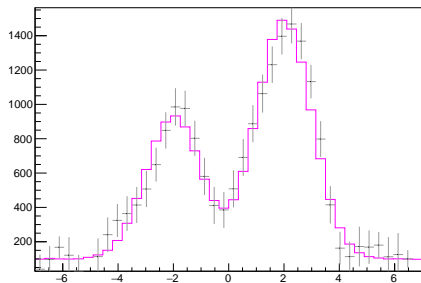


Figure: Undersmoothing, $\tau = \sqrt{\delta} = 0.00177$

Binwise coverage, $\lambda^{MC} = 0$

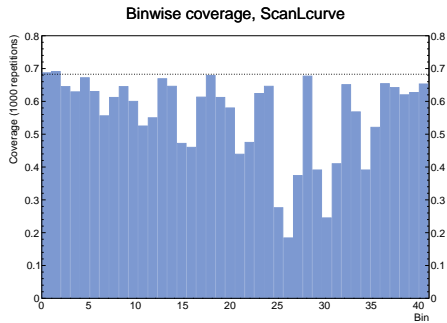


Figure: L-curve

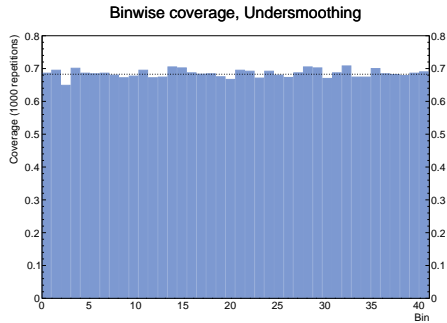


Figure: Undersmoothing

Unregularized unfolding?

- At the end of the day, *any regularization technique makes unverifiable assumptions about the true spectrum*
 - If these assumptions are not satisfied, the uncertainties will be wrong
- It seems to me that the fundamental problem is that we are asking too hard questions about the true spectrum
 - One simply cannot recover extremely detailed information about f without further outside knowledge
- So the question becomes: What features of f can be recovered based on the smeared data \mathbf{y} and how to do this with *honest unregularized* uncertainties?

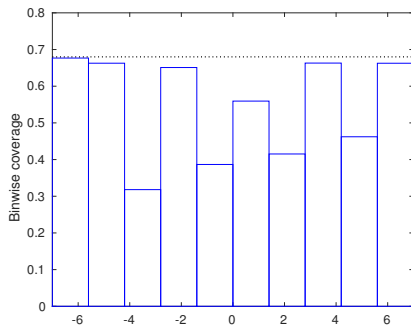
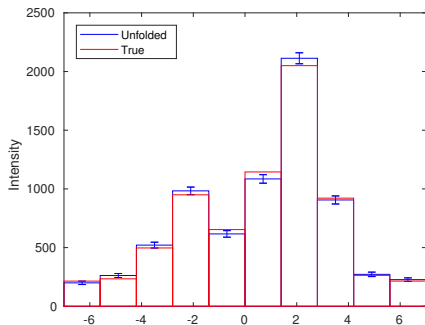
Wide bin unfolding

- One functional we should be able to recover without explicit regularization is the integral of f over a *wide* unfolded bin:

$$H_j[f] = \int_{T_j} f(t) dt, \quad \text{width of } T_j \text{ large}$$

- But one cannot simply arbitrarily increase the particle-level bin size in the conventional approaches, since this increases the MC dependence of \mathbf{K}
- To circumvent this, *it is possible to first unfold with fine bins and then aggregate into wide bins*
- Let's see how this works!
 - Simulation setup: $\hat{\lambda} = \mathbf{K}^\dagger \mathbf{y}$, convolution kernel $\mathcal{N}(0, 0.35^2)$, slightly different f^{MC} , otherwise as before

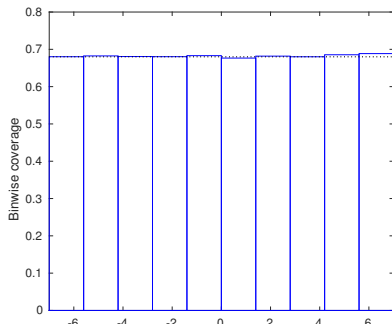
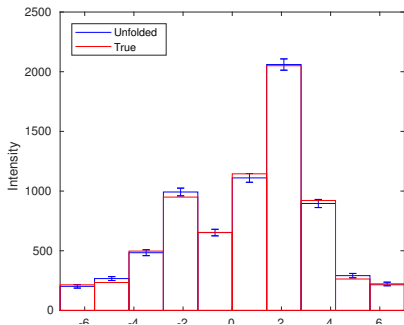
Wide bins, standard approach, perturbed MC



The response matrix $K_{i,j} = \frac{\int_{S_i} \int_{T_j} k(s,t) f^{\text{MC}}(t) dt ds}{\int_{T_j} f^{\text{MC}}(t) dt}$ depends on f^{MC}

\Rightarrow Undercoverage if $f^{\text{MC}} \neq f$

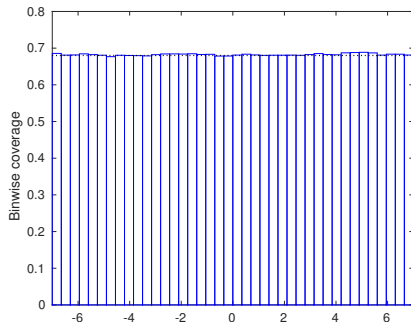
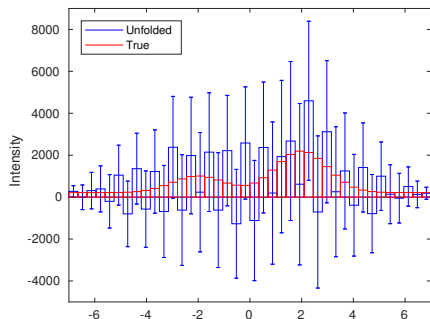
Wide bins, standard approach, correct MC



If $f^{\text{MC}} = f$, coverage is correct

⇒ But this situation is unrealistic because f of course is unknown

Fine bins, standard approach, perturbed MC

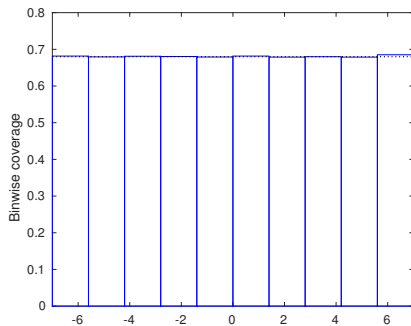
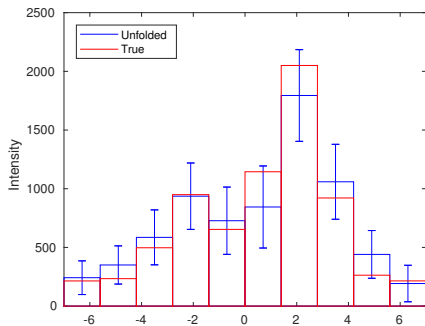


With narrow bins, less dependence on f^{MC} so coverage is correct, but the intervals are very wide¹

⇒ Let's aggregate these into wide bins, keeping track of the correlations

¹More unfolded realizations given in the [backup](#).

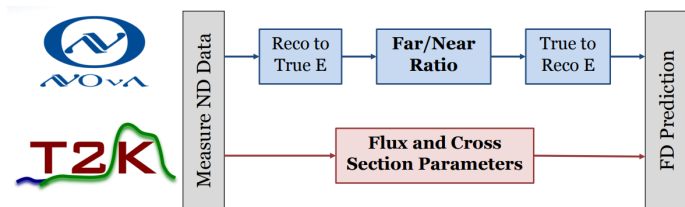
Wide bins via fine bins, perturbed MC



Wide bins via fine bins gives both correct coverage and intervals with reasonable length²

²More unfolded realizations given in the [backup](#).

Application to long-baseline neutrino experiments?



From A. Himmel's talk yesterday

- Notice the steps in NOvA: ND unfolding \rightarrow ND/FD mapping \rightarrow FD smearing
- This means that we are really interested in functionals of the form

$$H_i[f] = \int_{S_i} \int_T k_{FD}(s, t) r_{ND \rightarrow FD}(t) f_{ND}(t) dt ds$$

- This should be a well-behaved functional since it is *resmearing* the unfolded spectrum
- Hence the previous discussion should apply: first unfold in ND using fine bins and no regularization, map to FD, resmear

Conclusions

- Unfolding is a complex data analysis task with many potential pitfalls
 - It is crucial to understand all the ingredients that go into an unfolding procedure
- Coverage is a useful criterion for validating, optimizing and comparing unfolding methods
- Standard methods can have drastically lower coverage than expected
- Undersmoothing (which is now available for ROOT) provides one way of obtaining intervals with both reasonable coverage and reasonable length
- But it seems to me that ultimately there is a need for a major rethinking of the role of regularization
 - Any regularization really means some amount of “cheating” on the uncertainties
 - We should probably think of ways to provide unregularized uncertainties on relevant, well-chosen functionals of f , such as integral over wide bins
 - A simple step in this direction is to first unfold with narrow bins and then compute the functionals
 - This line of thinking seems relevant to predicting FD spectra using ND data

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Backup

Two main approaches to unfolding:

- 1 Tikhonov regularization (Höcker and Kartvelishvili, 1996; Schmitt, 2012)
- 2 Expectation-maximization iteration with early stopping (D'Agostini, 1995; Richardson, 1972; Lucy, 1974; Shepp and Vardi, 1982; Lange and Carson, 1984; Vardi et al., 1985)

Tikhonov regularization

- Tikhonov regularization estimates λ by solving:

$$\min_{\lambda \in \mathbb{R}^p} (\mathbf{y} - \mathbf{K}\lambda)^T \hat{\mathbf{C}}^{-1} (\mathbf{y} - \mathbf{K}\lambda) + \delta P(\lambda)$$

- The first term as a Gaussian approximation to the Poisson log-likelihood
- The second term penalizes physically implausible solutions
- Common penalty terms:
 - **Norm**: $P(\lambda) = \|\lambda\|^2$
 - **Curvature**: $P(\lambda) = \|\mathbf{L}\lambda\|^2$, where \mathbf{L} is a discretized 2nd derivative operator
 - **SVD unfolding** (Höcker and Kartvelishvili, 1996):

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

where λ^{MC} is a MC prediction for λ

- **TUnfold**³ (Schmitt, 2012): $P(\lambda) = \|\mathbf{L}(\lambda - \lambda^{\text{MC}})\|^2$

³TUnfold implements also more general penalty terms

- Starting from some initial guess $\lambda^{(0)} > \mathbf{0}$, iterate

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

- Regularization by stopping the iteration before convergence:
 - $\hat{\lambda} = \lambda^{(K)}$ for some small number of iterations K
 - I.e., bias the solution towards $\lambda^{(0)}$
 - Regularization strength controlled by the choice of K
- In RooUnfold (Adye, 2011), $\lambda^{(0)} = \lambda^{\text{MC}}$

D'Agostini iteration

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

- This iteration has been discovered in various fields, including optics (Richardson, 1972), astronomy (Lucy, 1974) and tomography (Shepp and Vardi, 1982; Lange and Carson, 1984; Vardi et al., 1985)
- In particle physics, it was popularized by D'Agostini (1995) who called it “Bayesian” unfolding
- **But:** This is in fact an expectation-maximization (EM) iteration (Dempster et al., 1977) for finding the *maximum likelihood estimator* of $\boldsymbol{\lambda}$ in the Poisson regression problem $\mathbf{y} \sim \text{Poisson}(\mathbf{K}\boldsymbol{\lambda})$
- As $k \rightarrow \infty$, $\boldsymbol{\lambda}^{(k)} \rightarrow \hat{\boldsymbol{\lambda}}_{\text{MLE}}$ (Vardi et al., 1985)
- *This is a fully frequentist technique for finding the (regularized) MLE*
 - The name “Bayesian” is an unfortunate misnomer

D'Agostini demo, $k = 0$

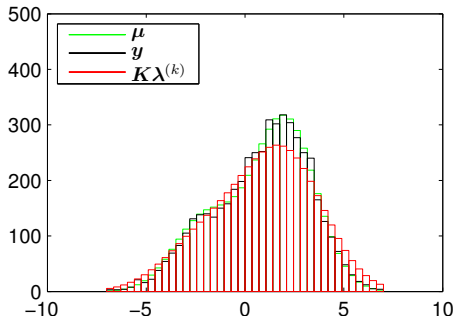


Figure: Smearing histogram

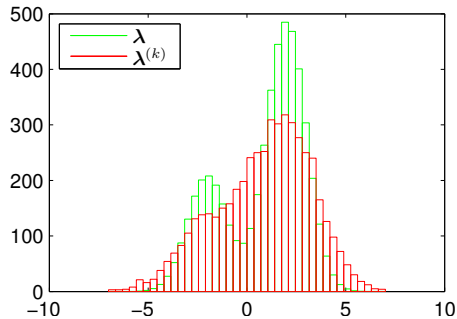


Figure: True histogram

D'Agostini demo, $k = 100$

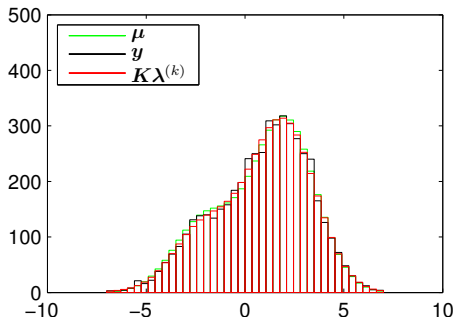


Figure: Smearing histogram

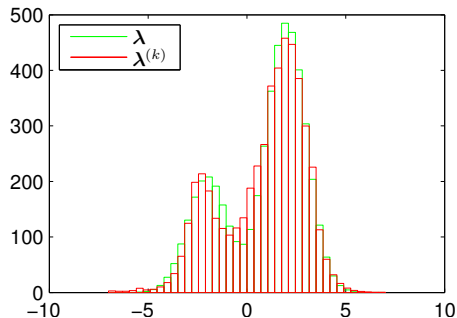


Figure: True histogram

D'Agostini demo, $k = 10000$

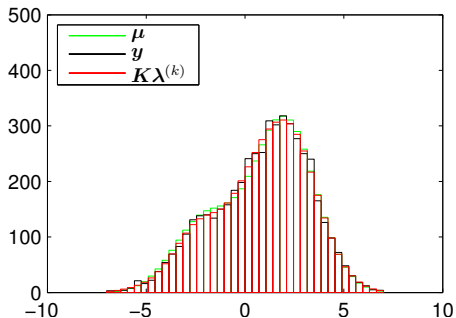


Figure: Smeared histogram

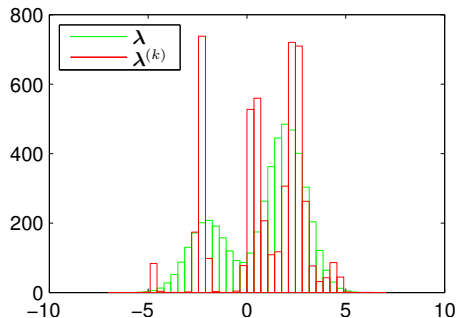


Figure: True histogram

D'Agostini demo, $k = 100000$

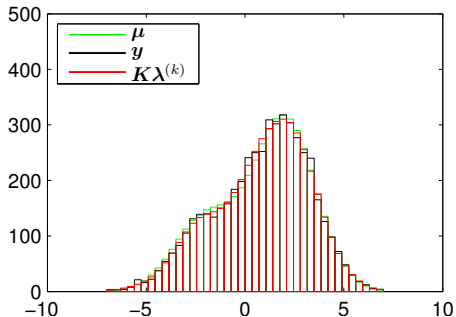


Figure: Smeared histogram

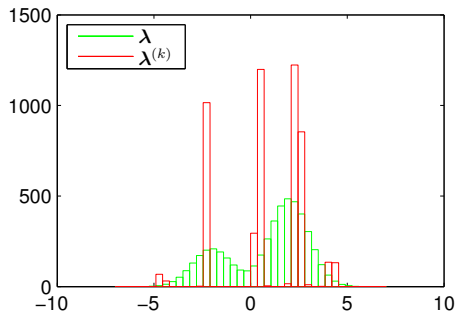


Figure: True histogram

Other methods

- Bin-by-bin correction factors
 - Attempts to unfold resolution effects by performing multiplicative efficiency corrections
 - This method is simply wrong and must not be used (it is no longer allowed in CMS)
- Fully Bayesian unfolding (Choudalakis, 2012)
 - Unfolding using Bayesian statistics where the prior regularizes the ill-posed problem
 - Certain priors lead to solutions similar to Tikhonov, but with Bayesian credible intervals as the uncertainties
 - Note: D'Agostini has nothing to do with proper Bayesian inference
- RUN/TRUEE (Blobel, 1985, 1996; Milke et al., 2013)
 - Penalized maximum likelihood with B-spline discretization
- Shape-constrained unfolding (Kuusela and Stark, 2017)
 - Correct-coverage uncertainties by imposing constraints on positivity, monotonicity and convexity
- Expectation-maximization with smoothing (Volobouev, 2015)
 - Adds a smoothing step to each iteration of D'Agostini
- Iterative dynamically stabilized unfolding (Malaescu, 2011)
 - Seems quite ad-hoc, with many free tuning parameters and unknown (at least to me) statistical properties
 - I have not seen this used in CMS, but it seems to be quite common in ATLAS
- ...

Coverage as a function of $\tau = \sqrt{\delta}$

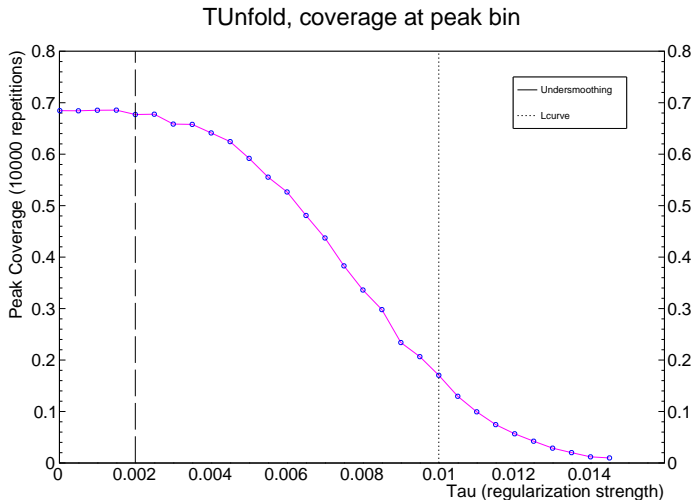
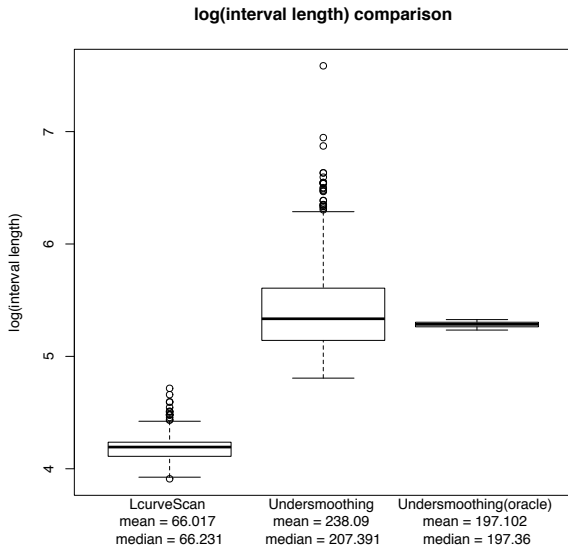
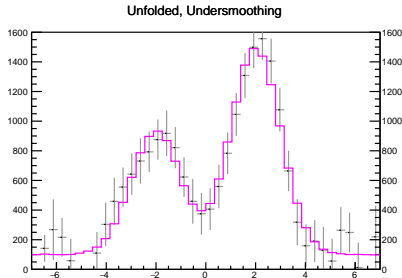
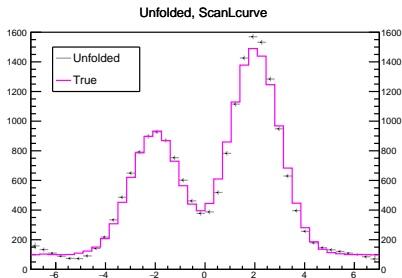
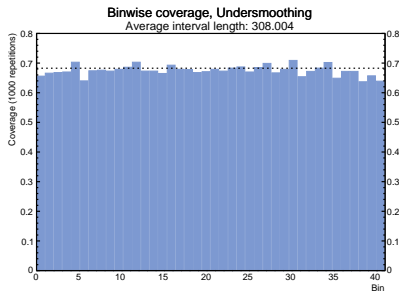
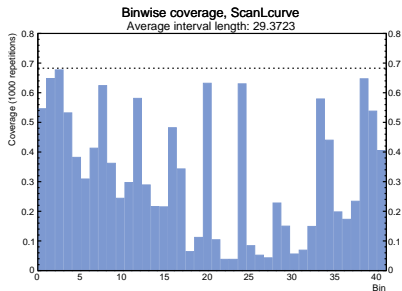


Figure: Coverage at the right peak of a bimodal density

Interval lengths, $\lambda^{\text{MC}} = 0$



Histograms, coverage and interval lengths when $\lambda^{MC} \neq 0$



Coverage study from Kuusela (2016)

Method	Coverage at $t = 0$	Mean length
BC (data)	0.932 (0.915, 0.947)	0.079 (0.077, 0.081)
BC (oracle)	0.937 (0.920, 0.951)	0.064 (0.064, 0.064)
US (data)	0.933 (0.916, 0.948)	0.091 (0.087, 0.095)
US (oracle)	0.949 (0.933, 0.962)	0.070 (0.070, 0.070)
MMLE	0.478 (0.447, 0.509)	0.030 (0.030, 0.030)
MISE	0.359 (0.329, 0.390)	0.028
Unregularized	0.952 (0.937, 0.964)	40316

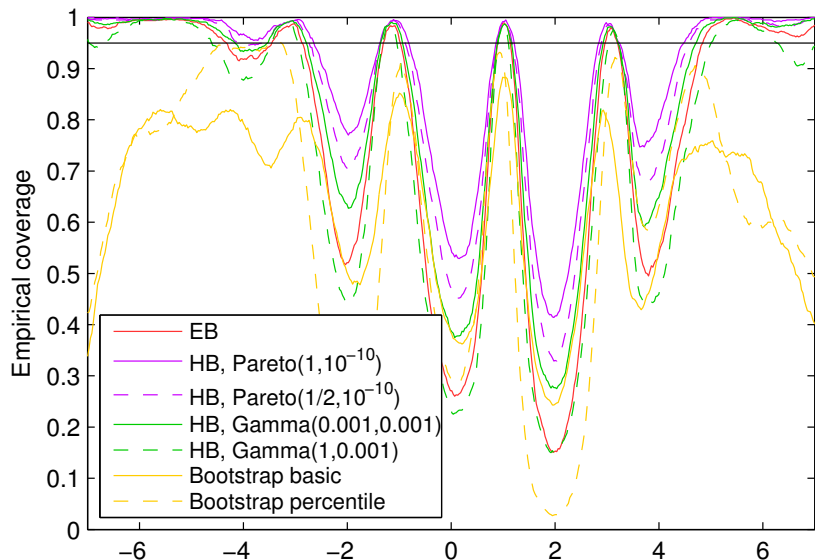
BC = iterative bias-correction

US = undersmoothing

MMLE = choose δ to maximize the marginal likelihood

MISE = choose δ to minimize the mean integrated squared error

UQ in inverse problems is challenging



[Kuusela and Panaretos (2015)]

Some remarks based on experience from the LHC

- One should think carefully if unfolding is *really* needed
 - E.g., if the goal of the experiment is to measure just a few 1-dimensional parameters, then one should perform the fit in the smeared space (as opposed to inferring the quantities from the regularized unfolded spectrum)
 - What about smearing the theory instead of unfolding the data? (Complicated by systematics in the response matrix)
 - Unfolding can be useful for comparison of experiments, propagation to further analyses, cross section ratios, tuning of MC generators, exploratory data analysis,...
- One should analyze carefully if regularization is necessary
 - If there is little smearing (response matrix almost diagonal), then the MLE obtained by running D'Agostini until convergence will do the job⁴
 - Some insight can be obtained by studying the condition number of \mathbf{K}

⁴The matrix inverse $\hat{\lambda} = \mathbf{K}^{-1}\mathbf{y}$ also gives the MLE provided that \mathbf{K} is invertible and $\hat{\lambda} \geq \mathbf{0}$

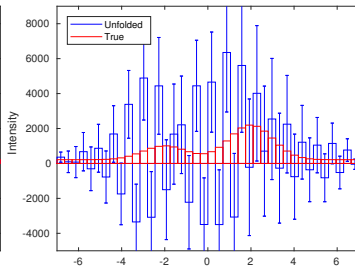
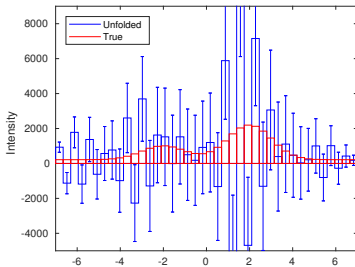
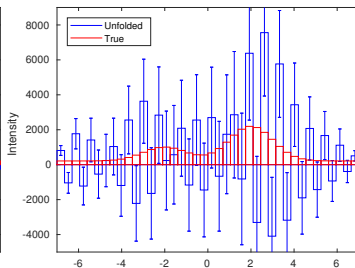
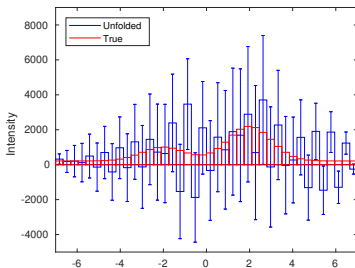
Some remarks based on experience from the LHC

- One must not rely on software defaults for the regularization strength
 - The unfolded solution is very sensitive to this choice and the optimal choice is very problem dependent
 - In particular, the default 4 iterations for D'Agostini in RooUnfold is just an arbitrary choice and does not guarantee a good solution
- The standard methods (at least as implemented in RooUnfold) regularize by biasing the solution towards the MC prediction λ^{MC}
 - Danger of producing over-optimistic results, as too strong regularization will always make the unfolded histogram match the MC, whether the MC is correct or not
 - Safer to use MC-independent regularization

Some remarks based on experience from the LHC

- Choice of unfolding software important
 - TUnfold is more versatile and better documented than RooUnfold
 - In particular, TUnfold allows one to change the bias vector λ^{MC} , while in RooUnfold it is fixed to the same MC that is used to construct the response matrix
 - PyUnfold implements D'Agostini with free choice of $\lambda^{(0)}$
- One cannot simply do away with ill-posedness by using wider bins
 - The wider the bins, the more dependent the response matrix \mathbf{K} becomes on the assumed shape of the spectrum inside the bins
 - But: see later in this talk
- Uncertainty quantification (i.e., providing confidence intervals) in the unfolded space is a very delicate matter
 - When regularization is used, the variance alone may not be a good measure of uncertainty because it ignores the bias
 - But the bias is needed to regularize the problem...

Fine bins, standard approach, perturbed MC, 4 realizations



Wide bins via fine bins, perturbed MC, 4 realizations

