Unfolding

1. **Mathematical formulation, response function (matrix)**
2. **Inverting the response matrix**
3. **Correction factors**
4. **Regularized unfolding**
   (a) Tikhonov
   (b) MaxEnt
5. **Variance and bias of the estimators**
6. **Choice of the regularization parameter**
7. **Some examples**

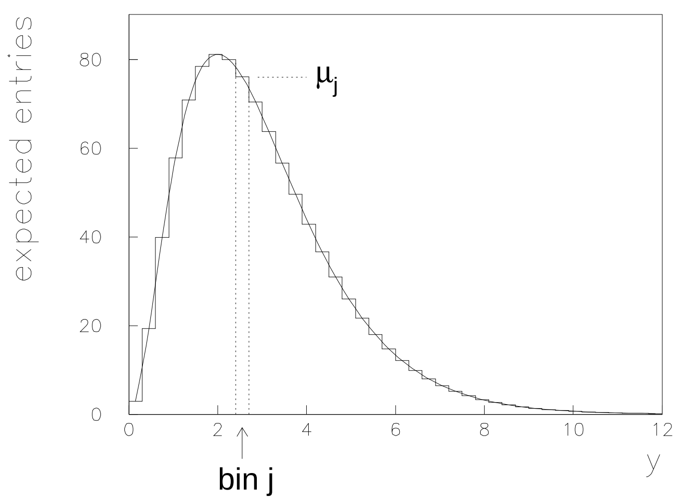
Formulation of the unfolding problem

Consider random variable y. Goal: determine pdf $f(y)$.

If parametrization $f(y;\vec{\theta})$ known,

maximum likelihood $\rightarrow \hat{\vec{\theta}}$

If no parametrization available, construct histogram:



$$p_j = \int_{\text{bin } j} f(y)\,dy \qquad j = 1, \ldots, M$$

$\mu_j = \mu_{\text{tot}}\, p_j \leftarrow$ the 'true histogram'

The goal: construct estimators for the μ_j (or p_j).

$\rightarrow$ number of parameters = number of bins, M

The problem: y cannot be measured without error.

$\rightarrow$ migration of entries between bins

$\rightarrow$ $f(y)$ is 'smeared out', peaks broadened

Response matrix

Effect of measurement errors: y = true value

x = observed value

$$f_{\text{meas}}(x) = \int R(x|y)\, f_{\text{true}}(y)\, dy$$

↓ discretize

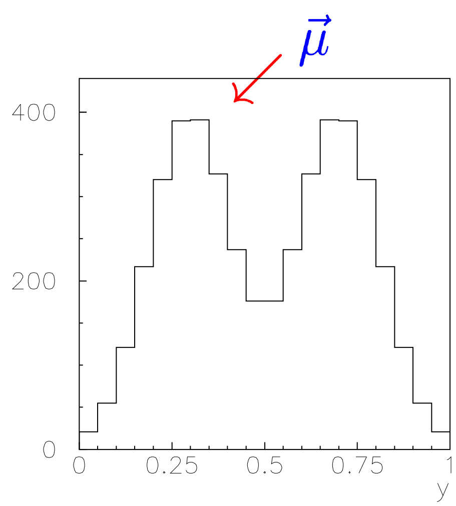
$$\nu_i = \sum_{j=1}^{M} R_{ij}\, \mu_j\,, \quad i = 1, \ldots, N$$

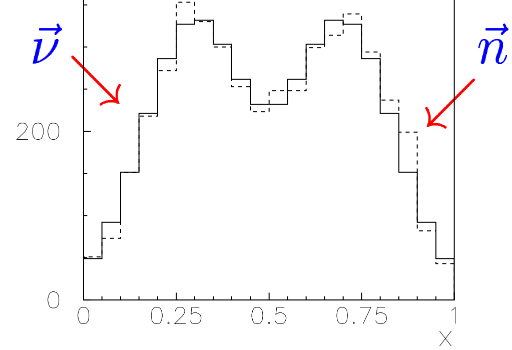
observed histogram (expec. val.) — response matrix — true histogram

$$R_{ij} = P(\text{observed in bin } i \,|\, \text{true value in bin } j)$$

The data: $\vec{n} = (n_1, \ldots, n_N)$, where $\nu_i = E[n_i]$.

N.B. $\vec{\mu}$, $\vec{\nu}$ constants, $\vec{n}$ subject to statistical fluctuations.





Efficiency, background

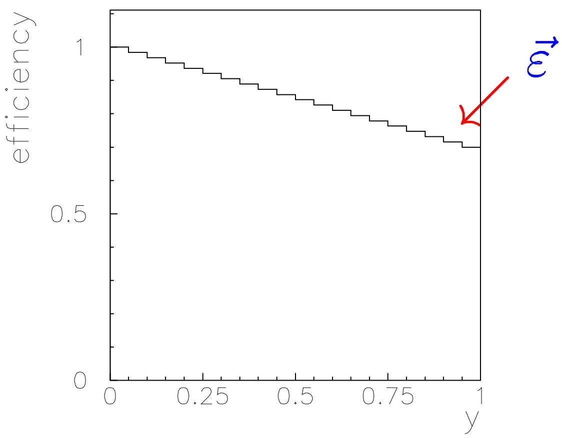
Sometimes an event goes undetected,

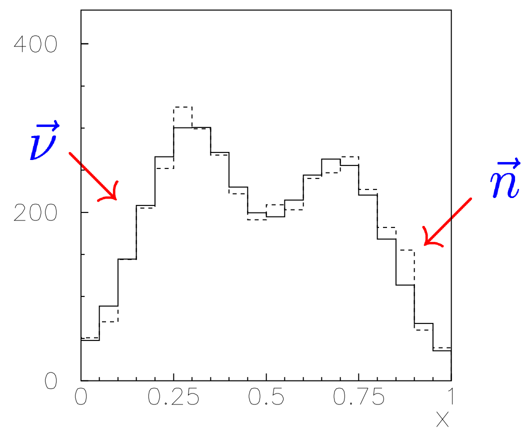
$$\sum_{i=1}^{N} R_{ij} = \sum_{i=1}^{N} P(\text{observed in bin } i \,|\, \text{true value in bin } j)$$

$$= P(\text{observed anywhere} \,|\, \text{true value in bin } j)$$

$$= \varepsilon_j \qquad (\text{efficiency})$$

N.B. ε_j depends on bin j of *true* histogram.





Sometimes we observe something when no true event occurred,

$$\rightarrow \nu_i = \sum_{j=1}^{M} R_{ij}\,\mu_j + \beta_i$$

β_i = expected number of background events in *observed* histogram.

For now, assume $\vec{\beta}$ is known.

Summary of ingredients

'true' histogram: $\vec{\mu} = (\mu_1, \ldots, \mu_M)$, $\quad \mu_{\rm tot} = \sum_{j=1}^{M} \mu_j$

probabilities: $\vec{p} = (p_1, \ldots, p_M) = \vec{\mu}/\mu_{\rm tot}$

expectation values for observed histogram: $\vec{\nu} = (\nu_1, \ldots, \nu_N)$

observed histogram: $\vec{n} = (n_1, \ldots, n_N)$

response matrix: $R_{ij} = P(\text{observed in bin } i \,|\, \text{true value in bin } j)$

efficiencies: $\varepsilon_j = \sum_{i=1}^{N} R_{ij}$

expected background: $\vec{\beta} = (\beta_1, \ldots, \beta_N)$

These are related by:

$$E[\vec{n}] = \vec{\nu} = R\vec{\mu} + \vec{\beta}$$

To find estimators for $\vec{\mu}$, we need probability law, e.g.

$$P(n_i; \nu_i) = \frac{\nu_i^{n_i}}{n_i!} e^{-\nu_i} \quad \text{(Poisson)},$$

or covariance matrix,

$$V_{ij} = \mathrm{cov}[n_i, n_j],$$

in order to construct likelihood function or χ^2.

Why unfold?

Often unfolding not needed, e.g. when

comparing to prediction of existing theory, better to

- 'fold' theory with detector response,
- i.e. include detector effects in its prediction,
- compare this with uncorrected ('raw') data $\vec{n}$.

→ simpler, more robust.

But, 'folding' theory with detector effects requires response matrix,

usually this knowledge not retained after publication of result.

Unfolded distribution can be compared directly to:

- predictions of theories,
- unfolded results from other experiments.

Usually unfolded result is more useful, since new theories

may be invented when response matrix is long gone.

In HEP often unfold:

- structure functions $F_2(x, Q^2)$,
- τ spectral functions (hadronic mass distributions),
- hadronic event-shape distributions,
- particle multiplicity distributions.

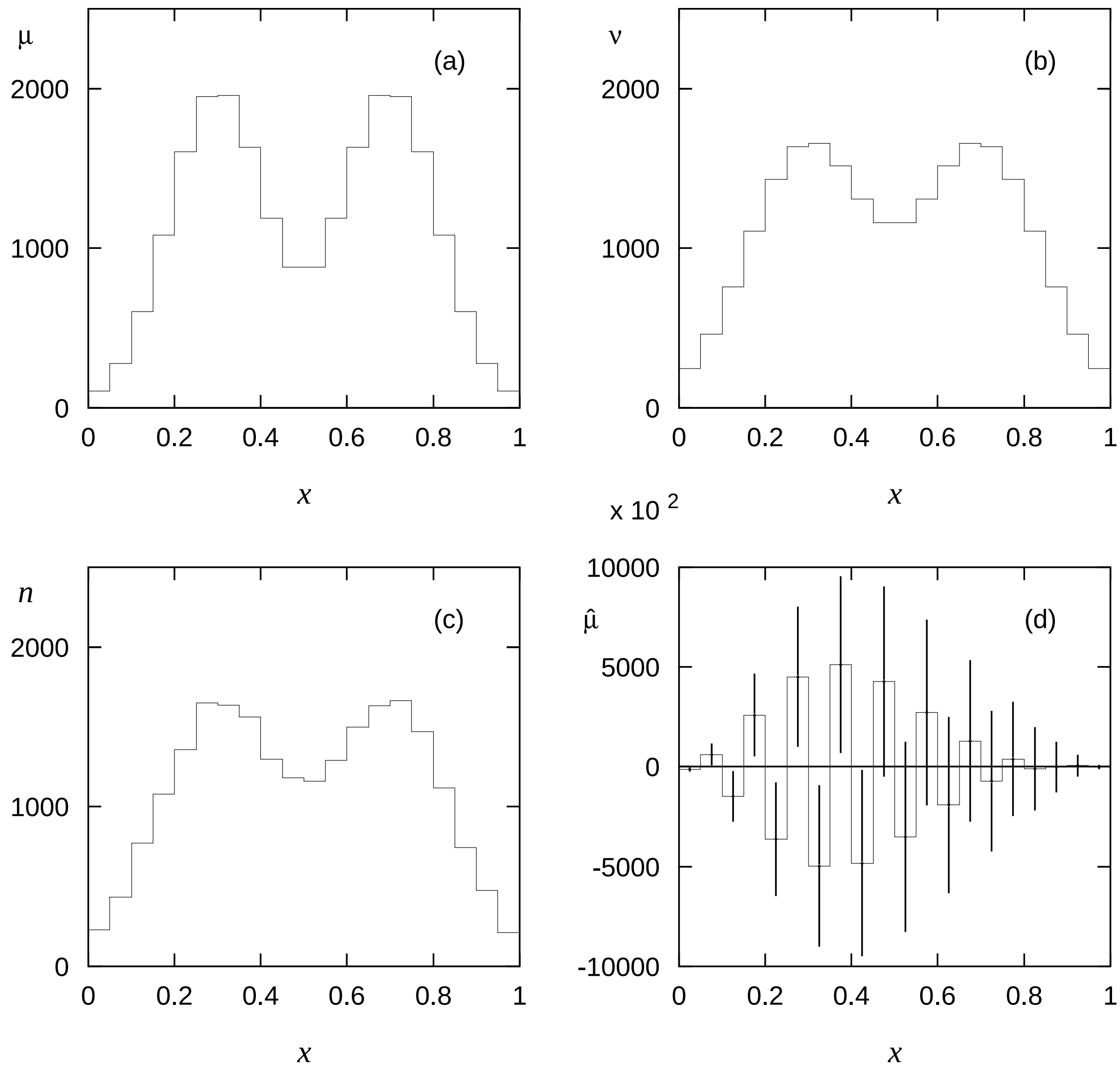
Inverting the response matrix

Assume $\vec{\nu} = R\vec{\mu} + \vec{\beta}$ can be inverted: $\vec{\mu} = R^{-1}(\vec{\nu} - \vec{\beta})$

Suppose data are Poisson: $P(n_i; \nu_i) = \frac{\nu_i^{n_i}}{n_i!} e^{-\nu_i}$

$$\rightarrow \log L(\vec{\mu}) = \sum_{i=1}^{N} (n_i \log \nu_i - \nu_i)$$

ML estimator is $\hat{\vec{\nu}} = \vec{n} \;\rightarrow\; \hat{\vec{\mu}} = R^{-1}(\vec{n} - \vec{\beta})$.

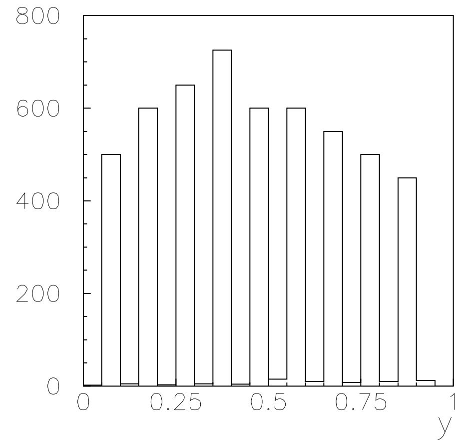


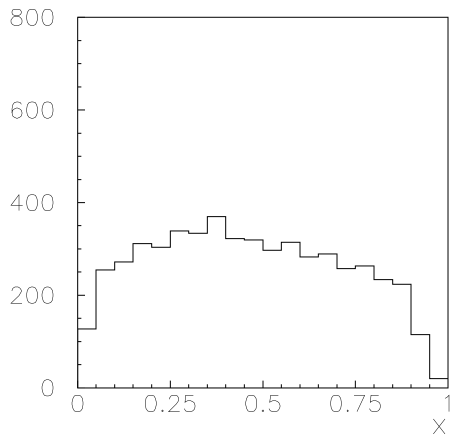
Catastrophic failure (?!)

What went wrong?

Suppose $\vec{\mu}$ really had fine structure:

$\vec{\mu} \rightarrow$





Applying R washes this out, but leaves residual structure.

$\leftarrow \vec{\nu} = R\vec{\mu}$

Applying R^{-1} to $\vec{\nu}$ puts the fine structure back: $\vec{\mu} = R^{-1}\vec{\nu}$.

But we don't have $\vec{\nu}$, only $\vec{n}$.

$\vec{n}$ *has* small bumps due to statistical fluctuations.

$\rightarrow R^{-1}$ 'thinks' this is residual of original fine structure,

$\hat{\vec{\mu}} = R^{-1}\vec{n}$ winds up getting huge 'fine structure'.

ML solution revisited

$$E[\hat{\vec{\mu}}] = R^{-1}(E[\vec{n}] - \vec{\beta}) = \vec{\mu} \;\rightarrow\; \text{unbiased!}$$

Compute variance of estimators,

$$U_{ij} = \text{cov}[\hat{\mu}_i, \hat{\mu}_j] = \sum_{k,l=1}^{N} (R^{-1})_{ik} (R^{-1})_{jl} \, \text{cov}[n_k, n_l]$$

$$= \sum_{k=1}^{N} (R^{-1})_{ik} (R^{-1})_{jk} \, \nu_k$$

Recall RCF bound for unbiased estimators,

$$(U^{-1})_{kl} = -E\left[\frac{\partial^2 \log L}{\partial \mu_k \, \partial \mu_l}\right] = \sum_{i=1}^{N} \frac{R_{ik} R_{il}}{\nu_i}$$

Inverting gives

$$U_{ij} = \sum_{k=1}^{N} (R^{-1})_{ik} (R^{-1})_{jk} \, \nu_k$$

→ ML estimator has minimum variance among unbiased estimators.

But this variance was huge!

→ to reduce variance, we must introduce some bias.

Strategy: accept small bias (systematic error) in exchange for large reduction in variance (statistical error).

Correction factor method

Use equal binning for $\vec{\mu}$, $\vec{\nu}$ and take $\hat{\mu}_i = C_i(n_i - \beta_i)$, where

$$C_i = \frac{\mu_i^{\rm MC}}{\nu_i^{\rm MC}} \quad \text{(correction factor)}$$

$\nu_i^{\rm MC}$ and $\mu_i^{\rm MC}$ from Monte Carlo simulation (no background).

$$U_{ij} = \text{cov}[\hat{\mu}_i, \hat{\mu}_j] = C_i^2 \, \text{cov}[n_i, n_j]$$

Usually $C_i \approx O(1)$, so variances don't blow up.

But the bias $b_i = E[\hat{\mu}_i] - \mu_i$ is

$$b_i = \left(\frac{\mu_i^{\rm MC}}{\nu_i^{\rm MC}} - \frac{\mu_i}{\nu_i^{\rm sig}} \right) \nu_i^{\rm sig} \, , \text{ where } \nu_i^{\rm sig} = \nu_i - \beta_i$$

Need to include systematic error due to MC dependence.

N.B. bias tends to pull $\hat{\vec{\mu}}$ towards $\vec{\mu}^{\rm MC}$

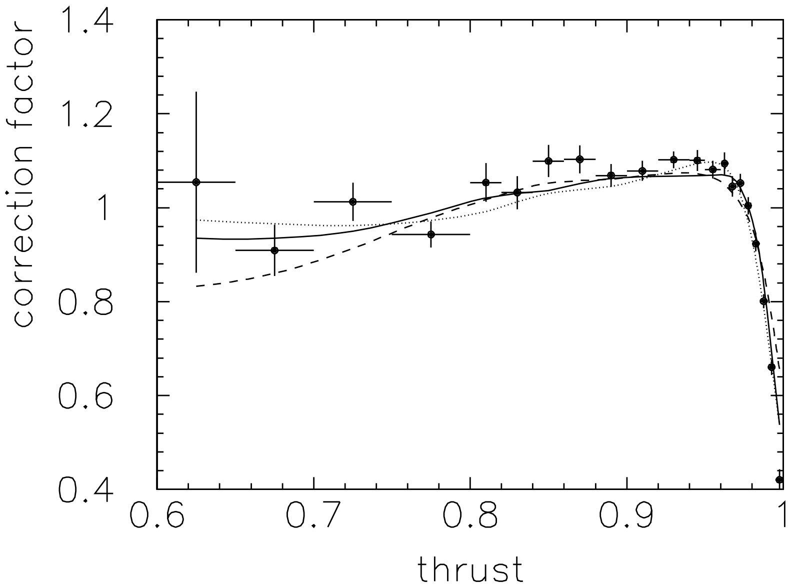
$\rightarrow$ hard to test models.

Not too bad if bin width $\geq$ several times resolution.

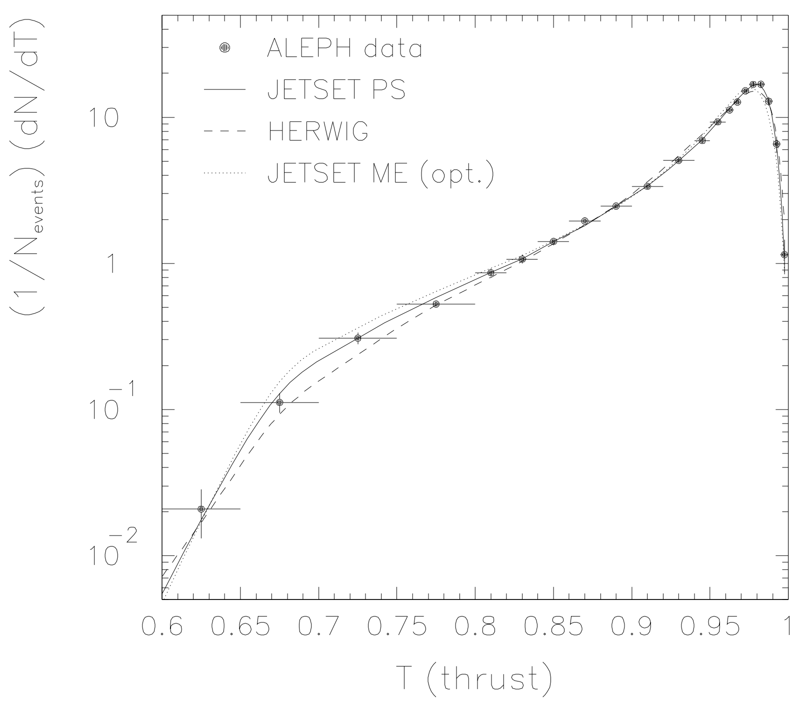
Often used for distributions of event-shape variables.

Example of correction factors in $e^+e^- \to$ hadrons

The correction factors:



The unfolded distribution compared to model predictions:



Regularized unfolding

Consider 'reasonable' estimators such that for some $\Delta \log L$,

$$\log L(\vec{\mu}) \geq \log L_{\max} - \Delta \log L$$

Out of these estimators, choose the 'smoothest', by maximizing

$$\Phi(\vec{\mu}) = \alpha \, \log L(\vec{\mu}) \; + \; S(\vec{\mu}),$$

$S(\vec{\mu})$ = regularization function (measure of smoothness),

α = regularization parameter (choose to give desired $\Delta \log L$)

In addition require $\sum_{i=1}^{N} \nu_i = \sum_{i,j} R_{ij}\mu_j = n_{\mathrm{tot}}$, i.e. maximize

$$\varphi(\vec{\mu}, \lambda) = \alpha \, \log L(\vec{\mu}) \; + \; S(\vec{\mu}) \; + \; \lambda \left[n_{\mathrm{tot}} \; - \; \sum_{i=1}^{N} \nu_i \right]$$

where λ is a Lagrange multiplier,

$$\partial\varphi / \partial\lambda = 0 \rightarrow \sum_{i=1}^{N} \nu_i = n_{\mathrm{tot}}.$$

$\alpha = 0$ gives smoothest solution (ignores data!),

$\alpha \to \infty$ gives ML solution (variance too large).

We need: regularization function $S(\vec{\mu})$,

a prescription for setting α.

Goodness of resulting estimators judged by their bias and variance.

Tikhonov regularization

Take measure of smoothness = mean square of kth derivative,

$$S[f_{\rm true}(y)] = -\int \left(\frac{d^k f_{\rm true}(y)}{dy^k} \right)^2 dy \ , \ \text{where } k = 1, 2, \ldots$$

Often take $k = 2$, → $S \approx$ mean squared curvature.

For histogram this becomes (e.g. for $k = 2$),

$$S(\vec{\mu}) = -\sum_{i=1}^{M-2} (-\mu_i + 2\mu_{i+1} - \mu_{i+2})^2$$

N.B. 2nd derivative not well defined for first and last bins.

If we use Tikhonov ($k = 2$) with $\log L = -\frac{1}{2}\chi^2$,

$$\varphi(\vec{\mu}, \lambda) = -\frac{\alpha}{2}\chi^2(\vec{\mu}) + S(\vec{\mu}) \ \ \text{quadratic in } \mu_i,$$

→ setting derivatives of φ equal to zero gives linear equations.

Several programs available for use in HEP:

RUN, Blobel

SVD, Höcker and Kartvelishvili

Regularization function based on entropy (MaxEnt)

Shannon entropy of a set of probabilities is

$$H = -\sum_{i=1}^{M} p_i \log p_i$$

All p_i equal → maximum entropy (maximum smoothness)

One $p_i = 1$, all others $= 0$ → minimum entropy

Use entropy as regularization function,

$$S(\vec{\mu}) = H(\vec{\mu}) = -\sum_{i=1}^{M} \frac{\mu_i}{\mu_{\rm tot}} \log \frac{\mu_i}{\mu_{\rm tot}}$$

$$\propto \log(\text{number of ways to arrange } \mu_{\rm tot} \text{ entries in } M \text{ bins})$$

Sometimes motivated by Bayesian statistics,

$S(\vec{\mu})$ → prior pdf for $\vec{\mu}$ (?)

Here stay with classical approach:

goodness of estimator judged by bias, variance.

N.B. Entropy does not depend on order of bins.

Variance and bias of $\hat{\vec{\mu}}$

In general, the equations determining $\hat{\vec{\mu}}(\vec{n})$ are nonlinear.

Expand $\hat{\vec{\mu}}(\vec{n})$ about $\vec{n}_{\rm obs}$ (observed data set),

$$\hat{\vec{\mu}}(\vec{n}) \approx \hat{\vec{\mu}}_{\rm obs} - A^{-1}B(\vec{n} - \vec{n}_{\rm obs}) \ ,$$

$$A_{ij} = \begin{cases} \frac{\partial^2 \varphi}{\partial \mu_i \partial \mu_j}, & i,j = 1,\ldots,M, \\ \frac{\partial^2 \varphi}{\partial \mu_i \partial \lambda} = -1, & i = 1,\ldots,M, j = M+1, \\ \frac{\partial^2 \varphi}{\partial \lambda^2} = 0, & i = M+1, j = M+1, \end{cases}$$

$$B_{ij} = \begin{cases} \frac{\partial^2 \varphi}{\partial \mu_i \partial n_j}, & i = 1,\ldots,M, j = 1,\ldots,N, \\ \frac{\partial^2 \varphi}{\partial \lambda \partial n_j} = 1, & i = M+1, j = 1,\ldots,N. \end{cases}$$

Use error propagation to get covariance $U_{ij} = \mathrm{cov}[\hat{\mu}_i, \hat{\mu}_j]$,

$$U = CVC^T \quad \text{where } C = A^{-1}B,$$

and estimators for the bias, $b_i = E[\hat{\mu}_i] - \mu_i$,

$$\hat{b}_i = \sum_{j=1}^{N} C_{ij}(\hat{\nu}_j - n_j) = \sum_{j=1}^{N} \frac{\partial \hat{\mu}_i}{\partial n_j}(\hat{\nu}_j - n_j),$$

where $\hat{\vec{\nu}} = R\hat{\vec{\mu}} + \vec{\beta}$. (N.B. $\hat{\vec{\nu}} \neq \vec{n}$.)

Choosing the regularization parameter α

$\alpha = 0 \rightarrow \hat{\vec{\mu}}$ maximally smooth (ignores data).

$\alpha \rightarrow \infty \rightarrow$ ML solution (no bias, very large variance).

Possible criteria for best trade-off between bias and variance:

Minimize mean squared error,

$$\mathrm{MSE} = \frac{1}{M} \sum_{i=1}^{M} (U_{ii} + \hat{b}_i^2) \,, \quad \text{or}$$

$$\mathrm{MSE}' = \frac{1}{M} \sum_{i=1}^{M} \frac{U_{ii} + \hat{b}_i^2}{\hat{\mu}_i} \,.$$

Or look at changes in χ^2 from unregularized (ML) solution,

$$\Delta\chi^2 = 2\Delta \log L = N \,, \quad \text{or}$$

$$\Delta\chi^2_{\mathrm{eff}} = (\hat{\vec{\nu}} - \vec{n})^T R\, C\, V^{-1} (R\, C)^T (\hat{\vec{\nu}} - \vec{n}) = 1 \,.$$

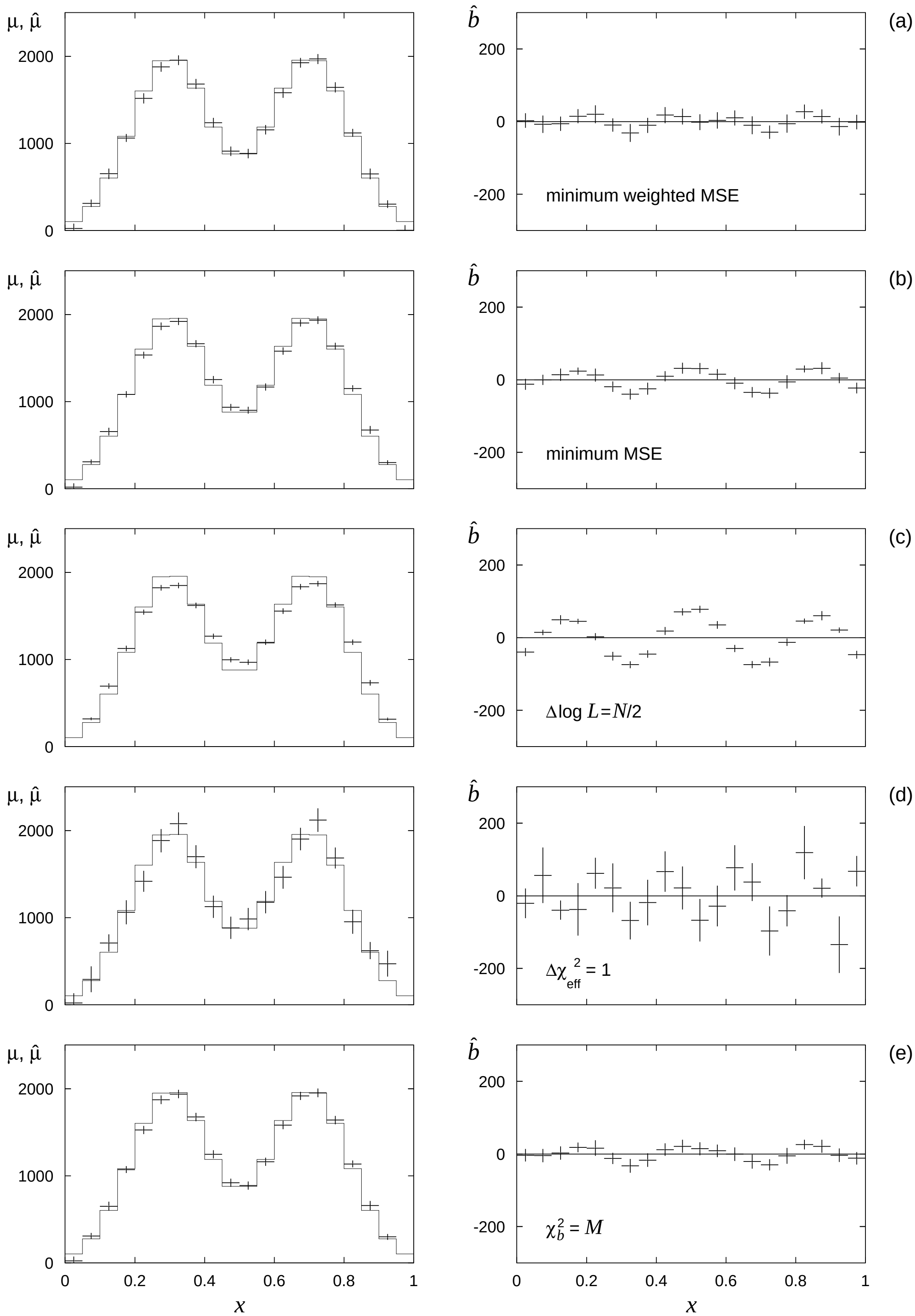
Or require that bias be consistent with zero to within its own error,

$$\chi_b^2 = \sum_{i=1}^{M} \frac{\hat{b}_i^2}{W_{ii}} = M \quad \text{where } W_{ij} = \mathrm{cov}[\hat{b}_i, \hat{b}_j].$$

i.e. if bias significantly different from zero, we would subtract it;

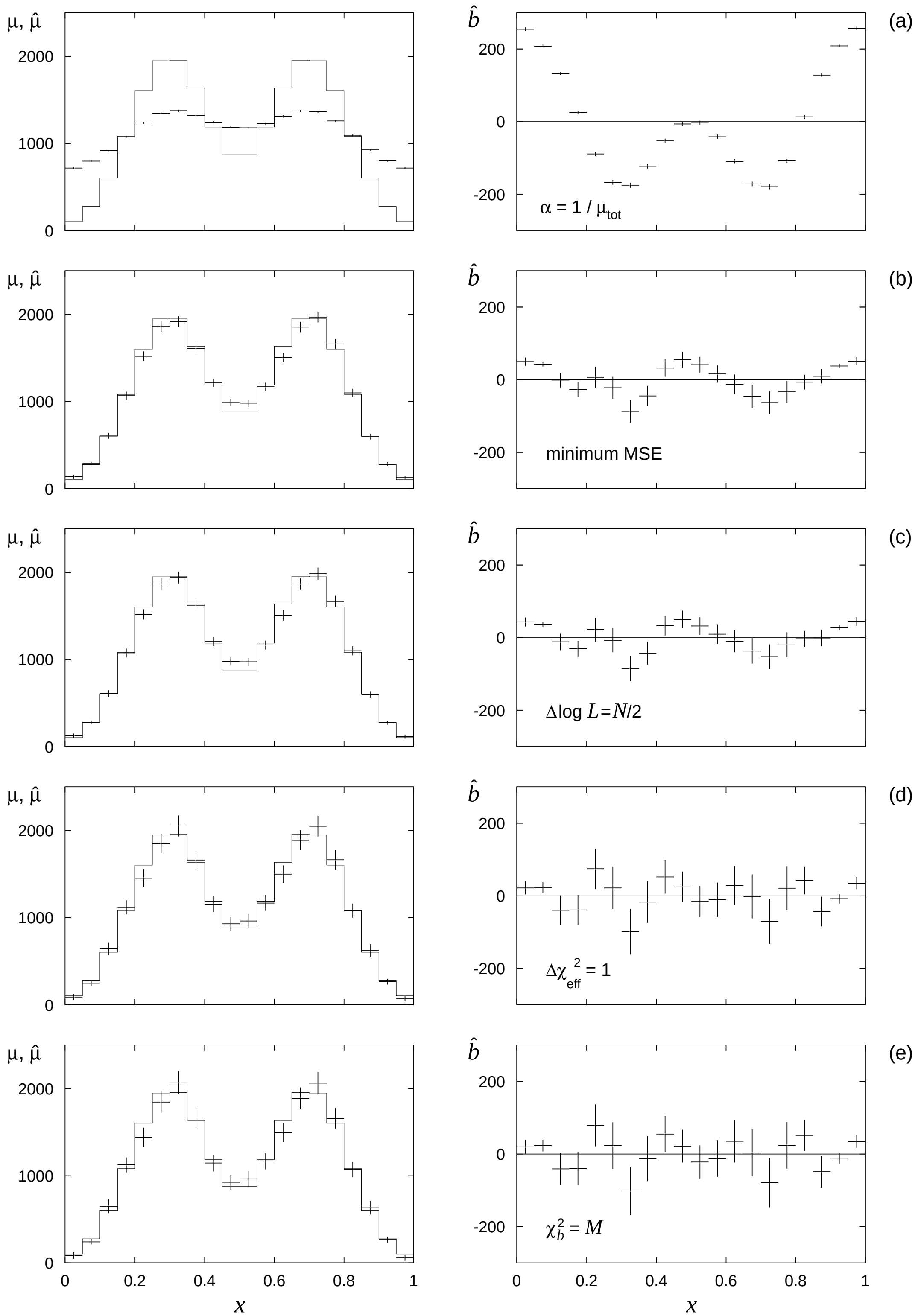
$\rightarrow$ equivalent to going to smaller $\Delta \log L$ or larger α (less bias).

Examples with Tikhonov regularization ($k = 2$)

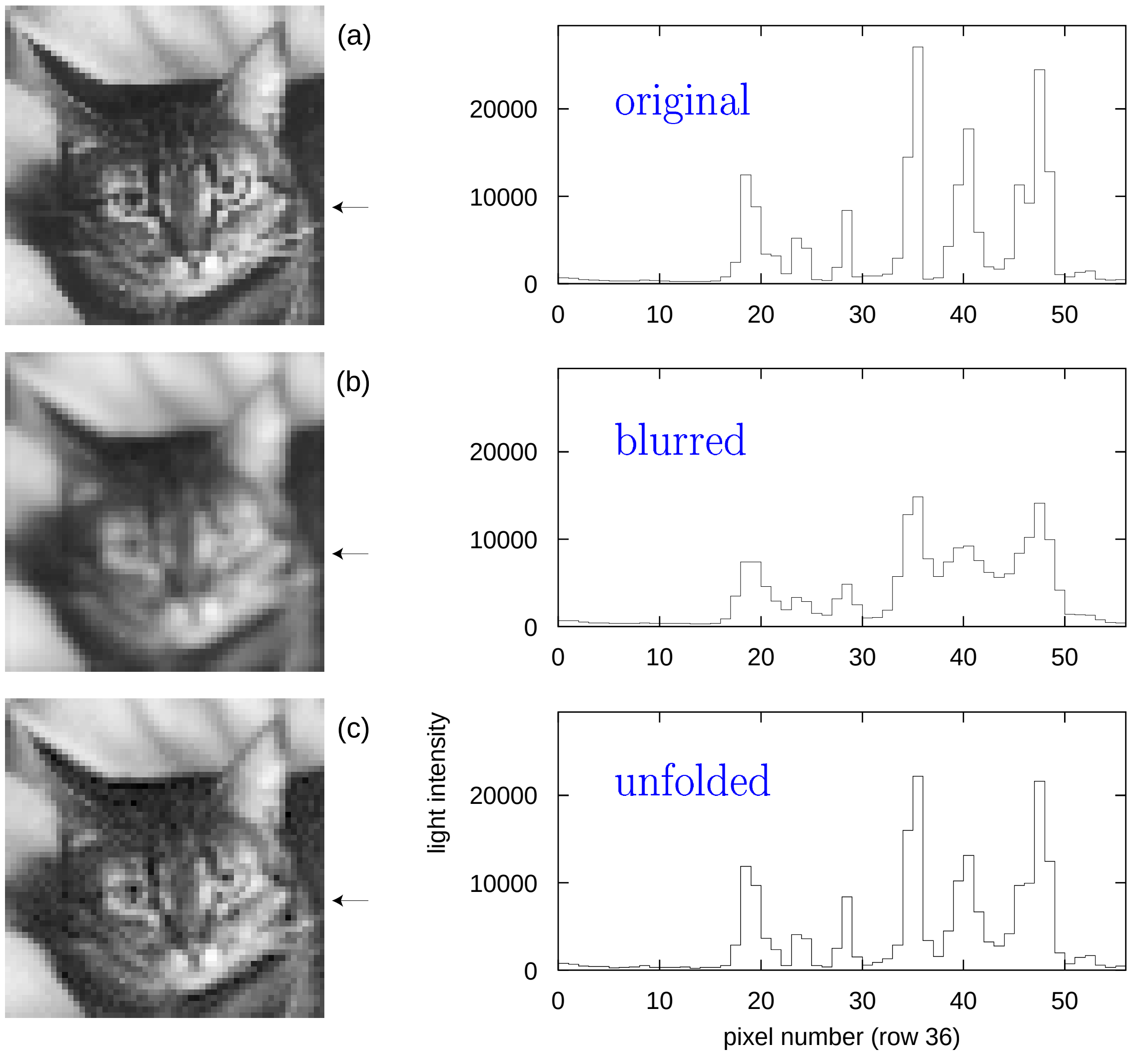


N.B. solution not always positive.

Examples with MaxEnt regularization



A MaxEnt example with image reconstruction (Newton)



MaxEnt often used in astronomical image reconstruction,

only small bias against point sources (peaks),

easy to generalize to two (or more) dimensions.

Unfolding

1. **Mathematical formulation:**

   true histogram: $\vec{\mu} = (\mu_1, \ldots, \mu_M)$

   data: $\vec{n} = (n_1, \ldots, n_N)$

   expectation values of $\vec{n}$: $\vec{\nu} = (\nu_1, \ldots, \nu_N)$

   $\vec{\mu} = R\vec{\nu} + \vec{\beta}$

   Goal: construct estimators for $\vec{\mu}$

2. **Inverting the response matrix:** huge oscillations (large variance) but zero bias and minimum variance among unbiased solutions.

3. **Correction factors:** quick and simple.

4. **Regularized unfolding:**

   Tikhonov: smoothness from mean square kth derivative.

   MaxEnt: smoothness from entropy $H = -\sum_i p_i \log p_i$.

5. **Variance and bias of the estimators:** based on linearized approximation to solution.

6. **Choice of the regularization parameter:** no clear winner (but $\chi_b^2 = M$ my favorite).

7. **Examples:** anything where structure smeared out, detector response is known, no parametrization of true distribution available.