Expectation Maximization (EM) Algorithm

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Known Coin Tossing

Figure 1: Ancient coins

Example 1: Tossing coin type known, estimate probabilities

Known Coin Tossing

Example 1: Two coins - two different distributions

- Probability p_1 or p_2 for "head"
- The regime (coin type) is known for every toss
- Maximum Likelihood (ML) for $\theta = (p_1, p_2)^\top$

Unknown Coin Tossing

Example 2: Current regime (coin) is unknown

- Probability to select the second coin δ
- Challenge: unobserved indicator variable (latent)
- Expectation Maximization (EM) for $\theta = (p_1, p_2, \delta)^\top$

Unknown Coin Tossing

Figure 2: Ancient coins

Example 2: Tossing coin type unknown, estimate probabilities

Known Coin Tossing

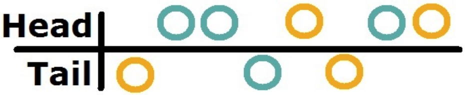

Figure 3: Parameter estimation - Maximum Likelihood (ML)

Unknown Coin Tossing

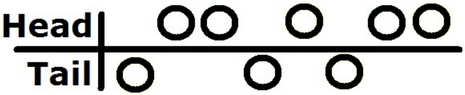

Figure 4: Parameter estimation - Expectation Maximization (EM)

EM Algorithm

- Maximum likelihood estimates under incomplete data
  - Hartley and Rao (1967)
  - Dempster et al. (1977)

- Applications
  - Missing data, grouping, censoring and truncation
  - Finite mixtures

Hermann Otto Hirschfeld on BBI: 

Outline

1. Motivation ✓
2. EM for a Mixture
3. EM Algorithm
4. Conclusions

Mixtures

- Two sequences of (dependent) observations
  - Latent $X_i, i = 1, \dots, n$
  - Observable $Y_i, i = 1, \dots, n$

- Linear mixture: Combination of distributions (components)

$$Y = (1 - X)Z_0 + XZ_1, \quad X \in \{0, 1\}, \mathrm{P}\,(X = 1) = \delta$$

with pdfs $f_{Z_j}(\bullet|\theta_j)$ and parameter θ_j, $j \in \{0, 1\}$

Mixtures

Coin example

- X_i selects one coin:

$$X_i = \begin{cases} 1, & \text{first coin with probability } \delta \\ 0, & \text{second coin} \end{cases}$$

- $Y_i \mid X_i$ is the observed result

$$Y_i \mid X_i = \begin{cases} 1, & \text{heads with probability } p_1 \text{ or } p_2 \\ 0, & \text{tails} \end{cases}$$

Mixtures

- Parameter of interest $\theta = (\theta_1, \theta_2, \delta)^\top$
  - Component parameter, e.g. $\theta_1 = p_1, \theta_2 = p_2$
  - Probability $\delta = \mathrm{P}(X = 1)$

- State X selects a component of Y

$$f_{Y|X}(y|X = x, \theta) = \begin{cases} f_{Z_0}(y|\theta_1), & \text{if } x = 0 \\ f_{Z_1}(y|\theta_2), & \text{if } x = 1 \end{cases}$$

Maximum Likelihood for a Mixture

- Marginal density of Y

$$f_Y(y|\theta) = (1-\delta)\, f_{Z_0}(y|\theta_1) + \delta f_{Z_1}(y|\theta_2)$$

- Maximum likelihood (ML) using marginal $f_Y(y|\theta)$
  - Requires observed data
  - Challenge: the likelihood function has an additive structure

Proof

Maximum Likelihood for a mixture

- Joint density of X, Y

$$f_{XY}(y, x|\theta) = \{(1-\delta)f_{Z_0}(y|\theta_1)\}^{1-x}\{\delta f_{Z_1}(y|\theta_2)\}^{x}$$

- Maximum likelihood using joint $f_{XY}(x, y|\theta)$
  - The likelihood function has a multiplicative structure
  - State x is unobserved

Proof

EM for a Mixture

- E-Step: Compute the conditional expectation $\mathrm{E}\left[X|Y,\theta\right]$
  - Expectation step
  - Requires parameter θ
- M-Step: Estimate parameter θ
  - Use $\mathrm{E}\left[X|Y,\theta\right]$ instead of X in the likelihood
  - ML for the joint density $f_{XY}(x,y|\theta)$

E-Step

- Conditional expectation $\gamma(\theta, Y) \overset{\text{def}}{=} \mathsf{E}\left[X | Y, \theta\right]$
  - Parameter $\theta = (\theta_1, \theta_2, \delta)^\top$ is required

$$\gamma(\theta, Y = y) = \frac{\delta f_{Z_1}(y|\theta_2)}{(1-\delta) f_{Z_0}(y|\theta_1) + \delta f_{Z_1}(y|\theta_2)}$$

▸ Proof

E-Step

- Employ (arbitrary) initial parameter $\theta^{(0)}$

  1) Component parameter $\theta_1^{(0)}, \theta_2^{(0)}$
  2) Mixture weight $\delta^{(0)}$

$$\gamma(\theta^{(0)}, Y = y) = \frac{\delta^{(0)} f_{Z_1}(y|\theta_2^{(0)})}{(1 - \delta^{(0)}) f_{Z_0}(y|\theta_1^{(0)}) + \delta^{(0)} f_{Z_1}(y|\theta_2^{(0)})}$$

M-Step

- Maximize log-likelihood $\ell(\theta) = \sum_{i=1}^{n} \log f_{XY}(x_i, y_i|\theta)$

$$\theta^{(1)} = \arg\max_{\theta} \ell\left\{\theta | x = \gamma(\theta^{(0)}, y_i), y\right\}$$

- Mixture weight δ estimate

$$\delta^{(1)} = n^{-1} \sum_{i=1}^{n} \gamma(\theta^{(0)}, y_i)$$

▸ Proof

Iteration

- Iteration of the E- and M-steps
  - Step 1: $\theta^{(1)}$
  - Step 2: $\theta^{(2)}$

    ...
  - Step k: $\theta^{(k)}$

- Repetition of the steps until convergence

EM algorithm - Example

Mixture of normals, e.g. Gentle et al. (2004)

- Mixture with two $\mathrm{N}(\mu_j, 1)$ components
- Parameter $\theta = (\mu_1, \mu_2, \delta)^\top$, $\theta_1 = \mu_1$, $\theta_2 = \mu_2$

$$f_{Z_j}(y|\theta_j) = \frac{1}{\sqrt{2\pi}} \exp\left\{ \frac{(y-\mu_j)^2}{2} \right\}, \quad j \in \{1, 2\}$$

EM algorithm - Example

Mixture of normals

- Maximum likelihood using the joint density

$$f_{XY}(x, y|\theta) = \sum_{j=0}^{1} \mathbf{I}\{x = j\} f_{Z_j}(y|\mu_{j+1})$$

- Component mean

$$\mu_1^{(1)} = \frac{\sum_{i=1}^{n} \left\{y_i - y_i\gamma(\theta^{(0)}, y_i)\right\}}{\sum_{i=1}^{n} \left\{1 - \gamma(\theta^{(0)}, y_i)\right\}}, \quad \mu_2^{(1)} = \frac{\sum_{i=1}^{n} y_i\gamma(\theta^{(0)}, y_i)}{\sum_{i=1}^{n} \gamma(\theta^{(0)}, y_i)}$$

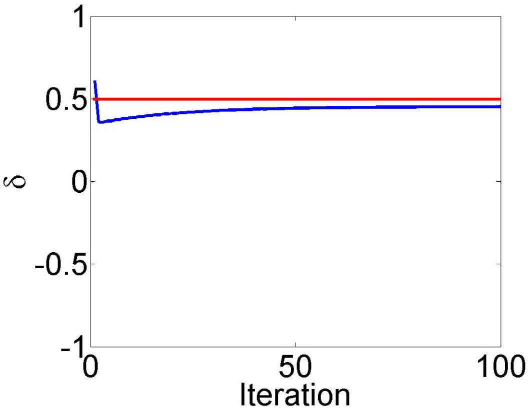

Figure 5: Parameter convergence example, true value in red, $n = 250$

EM_Normal

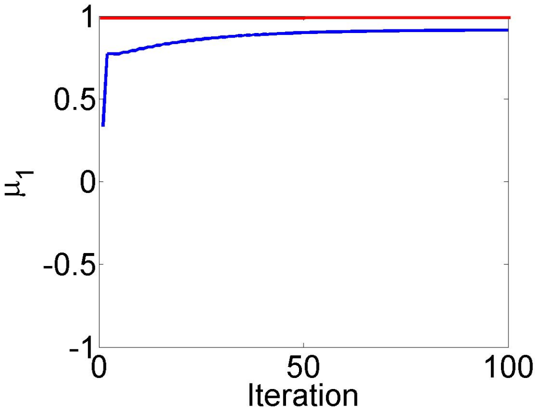

Figure 6: Parameter convergence example, true value in red, $n = 250$

EM_Normal

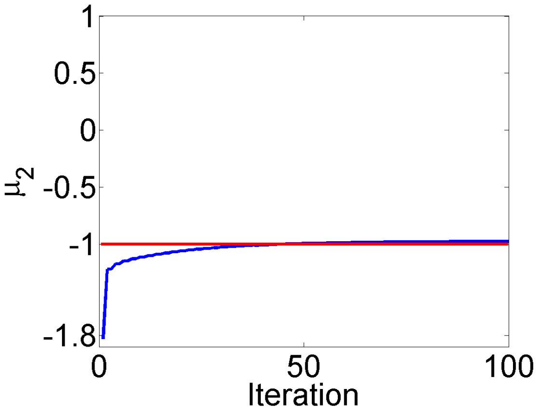

Figure 7: Parameter convergence, true value in red, $n = 250$

▸ Example 2 ▸ Example 3 ▸ Example 4

EM_Normal

The general Algorithm

- Blimes (1998): Maximum likelihood estimation
  - Infeasible likelihood, simplifies with hidden parameter
  - Hidden or missing values
- Complete data log-likelihood

$$\ell(\theta) = \sum_{i=1}^{n} \log \{ f_{XY}(x_i, y_i|\theta) \}$$

EM algorithm - E-Step

- Expectation step, general algorithm
  - Expectation of the log-likelihood ℓ
  - Gentle et al. (2012)

$$\begin{aligned} \mathcal{Q}(\theta \mid \theta^{(k)}) =& \mathsf{E}_X \left[\ell\left(\theta|X, Y\right) | Y, \theta^{(k)} \right] \\ =& \int_{z \in \mathfrak{X}} \ell\left(\theta|z, y\right) f_{X|Y}(z|Y = y, \theta^{(k)}) dz, \end{aligned}$$

with $\mathfrak{X}$ the support of X

EM algorithm - E-Step

Example: Linear mixtures

$$\ell(\theta) = \sum_{i=1}^{n} \log \{ \mathbf{I}\{x_i = 0\}(1-\delta) f_{Z_0}(y_i|\theta_1) + \mathbf{I}\{x_i = 1\}\, \delta f_{Z_1}(y_i|\theta_2) \}$$

- The joint likelihood is a linear function of x

EM algorithm - M-Step

- Maximization: Estimate the parameter of interest θ
  - Maximization of $\mathcal{Q}(\theta|\theta^{(0)})$ w.r.t. θ
  - Updated (optimal) estimate $\theta^{(1)}$

$$\theta^{(1)} = \arg\max_{\theta} \mathcal{Q}(\theta \mid \theta^{(0)})$$

Properties

S. Kullback and R. Leibler on BBI: 

Conclusions

- EM Algorithm
  - Finding parameter estimates
  - Latent variables, missing data
- Application
  - Coin example
  - Normal mixtures

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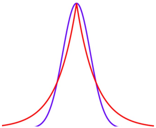

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Distributions

- Marginal density of X and $Y|X$ with $\theta = (\theta_1, \theta_2, \delta)^\top$ are given

$$f_X(x|\theta) = \mathbb{I}\{x = 1\}\delta + \mathbb{I}\{x = 0\}(1 - \delta) = \delta^x(1 - \delta)^{1-x}$$

$$f_{Y|X}(y|X = x, \theta) = f_{Z_0}(y|\theta_1)^{1-x} f_{Z_1}(y|\theta_2)^x$$

- Marginal of Y applying the law of total probability

$$f_Y(y|\theta) = \sum_{j=0}^{1} \mathrm{P}(X = j) f_{Y|X}(y|X = j, \theta)$$

$$f_Y(y|\theta) = (1 - \delta) f_{Z_0}(y|\theta_1) + \delta f_{Z_1}(y|\theta_2)$$

Back

Distributions

- Marginal density of X and $Y|X$ with $\theta = (\theta_1, \theta_2, \delta)^\top$ are given

$$f_X(x|\delta) = \mathbf{I}\{x = 1\}\delta + \mathbf{I}\{x = 0\}(1-\delta) = \delta^x(1-\delta)^{1-x}$$
$$f_{Y|X}(y|X = x, \theta) = f_{Z_0}(y|\theta_1)^{1-x} f_{Z_1}(y|\theta_2)^x$$

- Joint distribution of X and Y

$$f_{XY}(x, y|\theta) = f_{Y|X}(y|X = x, \theta) f_X(x|\theta)$$
$$f_{XY}(x, y|\theta) = \{(1-\delta) f_{Z_0}(y|\theta_1)\}^{1-x} \{\delta f_{Z_1}(y|\theta_2)\}^x$$

Back

Conditional Expectation

- Conditional distribution of $X|Y$ via Bayes rule

$$f_{X|Y}(x|Y=y,\theta)=\frac{f_{XY}(x,y|\theta)}{f_Y(y|\theta)}$$

- Resulting distribution of $X|Y$

$$f_{X|Y}(x|Y=y,\theta)=\frac{\{(1-\delta)f_{Z_0}(y|\theta_1)\}^{1-x}\{\delta f_{Z_1}(y|\theta_2)\}^{x}}{(1-\delta)f_{Z_0}(y|\theta_1)+\delta f_{Z_1}(y|\theta_2)}$$

E-Step

Conditional Expectation

- Since X is binomial

$$\gamma(Y,\theta) = \mathrm{E}\left[X|Y,\theta\right] = \mathrm{P}\left(X = 1|Y,\theta\right)$$

- Expectation of the unobserved variable

$$\mathrm{E}[X|Y,\theta] = \frac{\delta f_{Z_1}(y|\theta_2)}{(1-\delta) f_{Z_0}(y|\theta_1) + \delta f_{Z_1}(y|\theta_2)}$$

E-Step

M-Step for mixture probabilities

- Maximize the expectation of the likelihood $\mathcal{Q}$
- M components, following Blimes (1998)
  - The sum of component probabilities must be equal to 1

$$\arg\max_{\theta} \mathcal{Q}(\theta \mid \theta^{(k)}) \qquad \text{s.t.} \sum_{j=1}^{M} \delta_j = 1$$

▸ M-Step

M-Step for mixture probabilities

- Optimization w.r.t. δ_j, Lagrange parameter λ

$$\frac{1}{\delta_j}\sum_{i=1}^{n} f_X(j|y_i,\theta^{(k)}) = \lambda$$

$\lambda = n$ completes the proof

$$\sum_{i=1}^{n}\sum_{j=1}^{M}\frac{1}{\delta_j} f_X(j|y_i,\theta^{(k)}) = M\lambda$$

▸ M-Step

Properties

- The likelihood of Y has a lower bound, e.g. Hastie (2008)
  - EM maximizes the bound

$$E_{f_X(x\,|\theta)}\left[\log f_{XY}\left(x, y \mid \theta\right) - \log f_X\left(x|\theta\right)\right] \leq \log\{f_Y(y|\theta)\}$$

▸ M-Step

Lower bound of the marginal likelihood

Kullback-Leibler divergence of a variational distribution $\tilde{f}_x(x_i|\theta)$ and the parametric model $f_X(x|y,\theta)$, e.g., Barber (2012):

$$KL\left\{\tilde{f}_X(x|\theta)||f_X(x|y,\theta)\right\} \geq 0$$

$$\underset{\tilde{f}_X(x|\theta)}{\mathsf{E}}\left[\log\{\tilde{f}_X(x|\theta)\} - \log\left\{\frac{f_{XY}(x,y|\theta)}{f_Y(y|\theta)}\right\}\right] \geq 0$$

M-Step

Kullback-Leibler Divergence

- Also known as relative entropy
  - Difference measure of distributions P and Q
  - Not symmetric, not a metric

$$KL(P||Q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx \geq 0$$

M-Step

Kullback-Leibler Divergence

The Kullback-Leibler divergence is positive

$$\log(z) \leq z - 1$$
$$q(x) \log \frac{p(x)}{q(x)} \leq p(x) - q(x)$$

$p(x)$ and $q(x)$ are densities, thus

$$\int_{-\infty}^{\infty} \{p(x) - q(x)\}\, dx = 1 - 1 = 0$$

M-Step

Convergence Example 2: $\delta = 0.5, \mu_1 = 0.5, \mu_2 = -0.5, n = 250$

- True μ_1 and μ_2 closer together
- Components harder to "disentangle"

Back

EM_Normal

Convergence Example 2: $\delta = 0.5, \mu_1 = 0.5, \mu_2 = -0.5, n = 250$

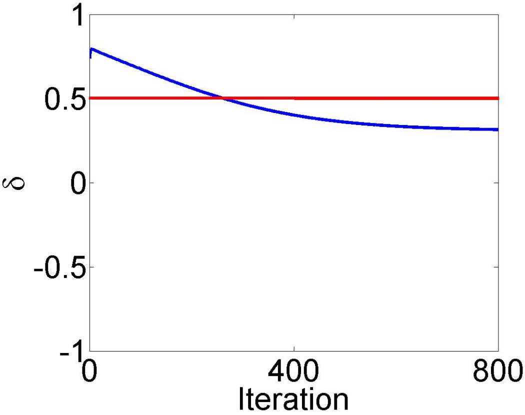

Figure 8: Parameter convergence example, $n = 250$, true value in red

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Convergence Example 2: $\delta = 0.5, \mu_1 = 0.5, \mu_2 = -0.5, n = 250$

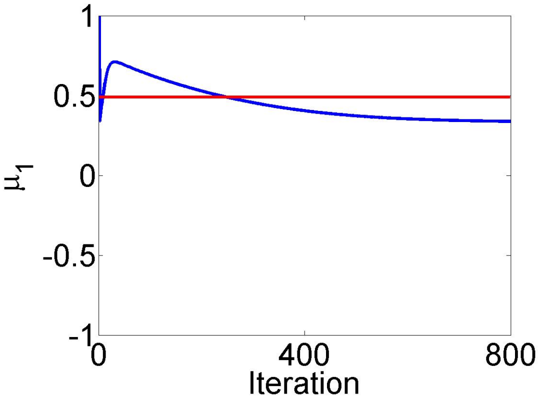

Figure 9: Parameter convergence example, $n = 250$, true value in red

Back

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Convergence Example 2: $\delta = 0.5, \mu_1 = 0.5, \mu_2 = -0.5, n = 250$

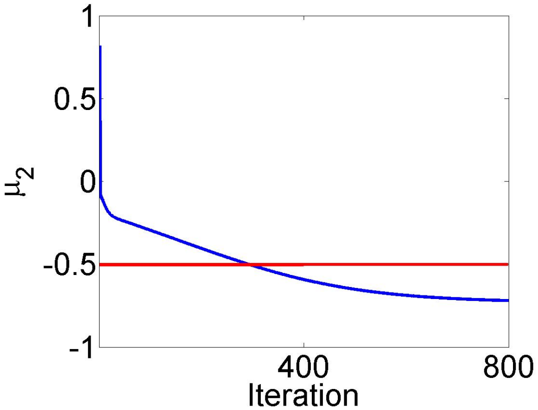

Figure 10: Parameter convergence example, $n = 250$, true value in red

Back

EM_Normal

Convergence Example 3:

$\delta = 0.5, \mu_1 = 0.25, \mu_2 = -0.25, n = 250$

- True μ_1 and μ_2 even closer together
- Components harder to "disentangle"

Back

EM_Normal

Convergence Ex. 3: $\delta = 0.5, \mu_1 = 0.25, \mu_2 = -0.25, n = 250$

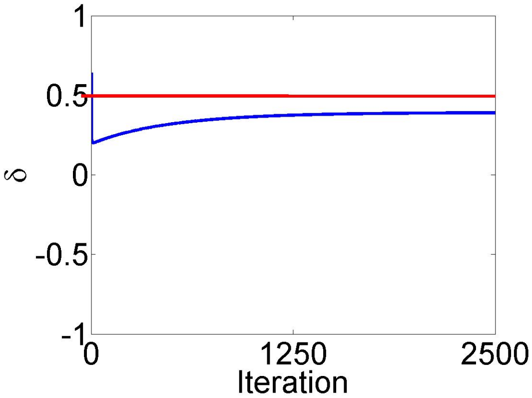

Figure 11: Parameter convergence example, $n = 250$, true value in red

Back

EM_Normal

Convergence Ex. 3: $\delta = 0.5, \mu_1 = 0.25, \mu_2 = -0.25, n = 250$

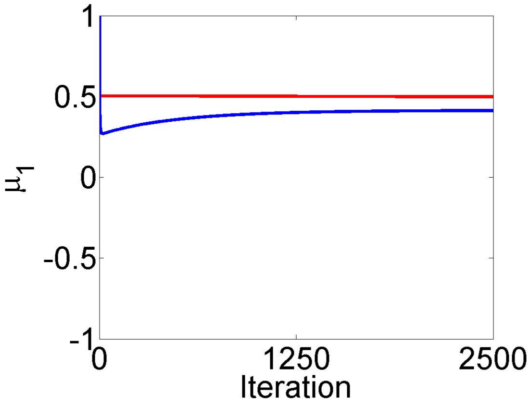

Figure 12: Parameter convergence example, $n = 250$, true value in red

Back

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Convergence Ex. 3: $\delta = 0.5, \mu_1 = 0.25, \mu_2 = -0.25, n = 250$

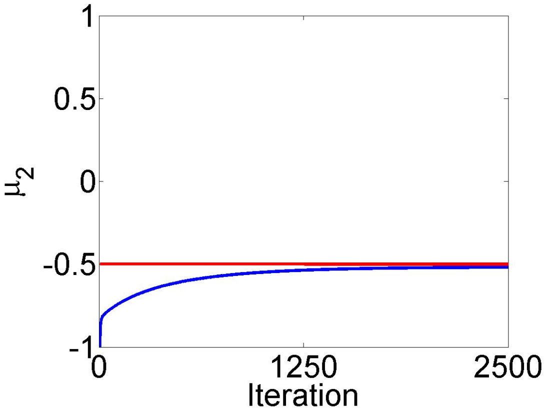

Figure 13: Parameter convergence example, true value in red

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Convergence Example 2: $\delta = 0.9, \mu_1 = 0.5, \mu_2 = -0.5, n = 250$

- $\delta = 0.9$, low probability of first component
- Few observations from first component

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Convergence Example 4: $\delta = 0.9, \mu_1 = 1, \mu_2 = -1, n = 250$

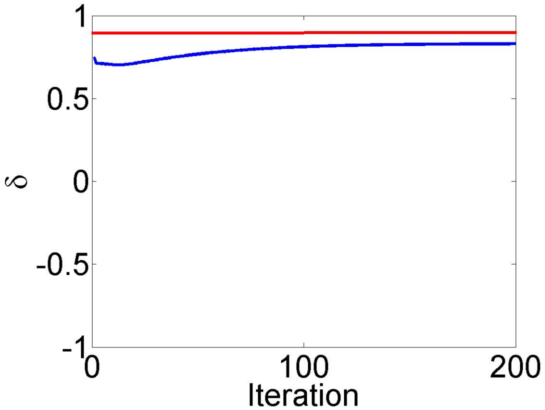

Figure 14: Parameter convergence example, true value in red

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Convergence Example 4: $\delta = 0.9, \mu_1 = 1, \mu_2 = -1, n = 250$

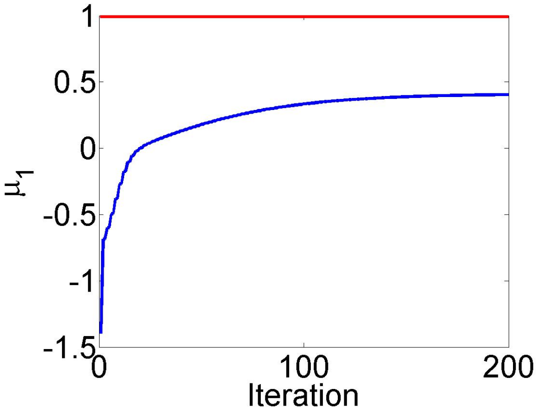

Figure 15: Parameter convergence example, true value in red

Back

EM_Normal

Convergence Example 4: $\delta = 0.9, \mu_1 = 1, \mu_2 = -1, n = 250$

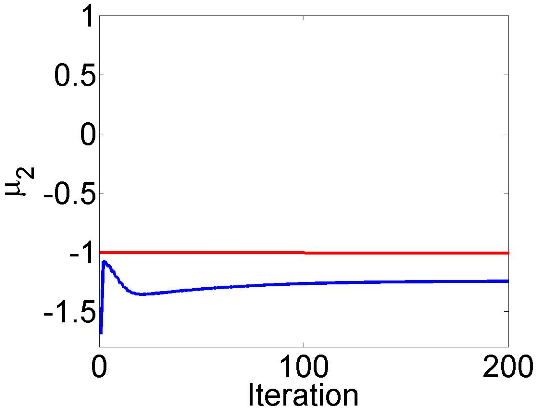

Figure 16: Parameter convergence example, true value in red

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