Non-Asymptotic Convergence Rate of EM, and Improved Expectation Maximization Algorithms

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Computer Science

Learning with Missing Values

- Missing values are very common in real datasets.
- For example, we could have a dataset like this:

$$X = \begin{bmatrix} N & 33 & 5 \\ L & 10 & 1 \\ F & ? & 2 \\ M & 22 & 0 \end{bmatrix}, y = \begin{bmatrix} -1 \\ +1 \\ -1 \\ ? \end{bmatrix}.$$

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- We'll focus on data that is missing at random (MAR):
  - Assume that the reason ? is missing does not depend on the missing value.

Expectation Maximization: Optimization with MAR Variables

- Expectation maximization (EM) is an optimization algorithm for MAR values:
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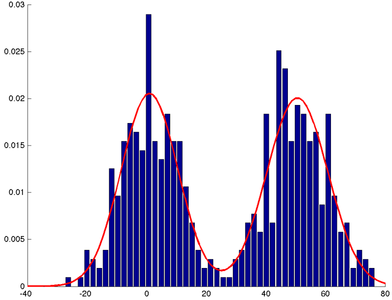
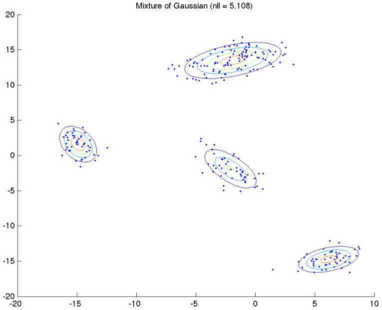
  - Semi-supervised learning.
  - Mixture of Gaussians.
  - Hidden Markov models.
- In the two latter problems, statisticians introduce MAR variables to use EM.

Example: Mixture of Gaussians

- Application: modeling multi-modal data with mixture of Gaussians





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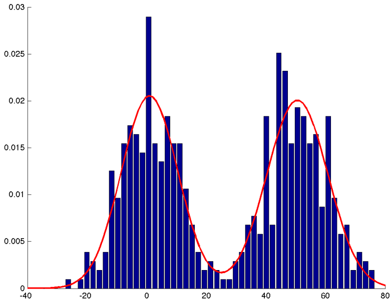

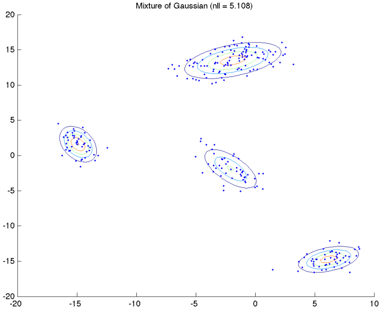

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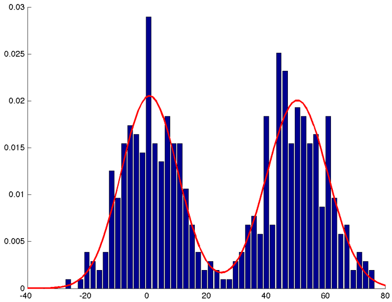

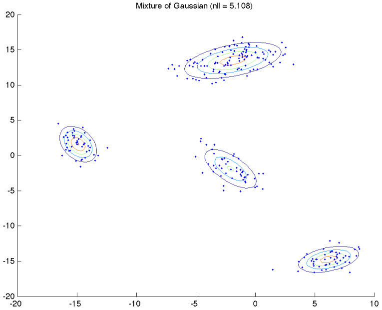

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- As in typical applications of EM, the problem is highly non-convex.

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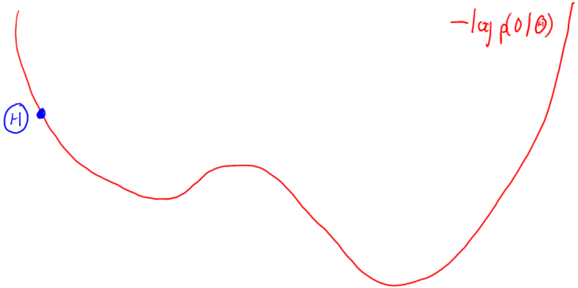
  - At each iteration t we optimize a bound on the function.



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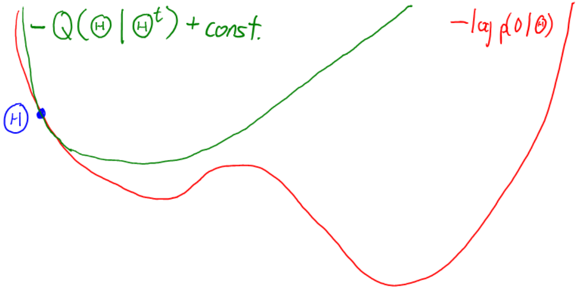

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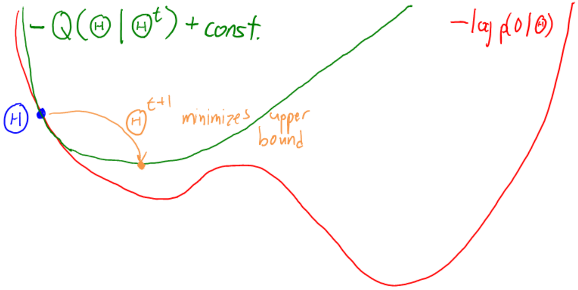

- Unlike gradient descent and Newton, the "surrogate" Q is not quadratic.
- In EM, our bound comes from expectation over hidden variables.

Expectation Maximization (Equation Version)

- We want to maximize likelihood of data X with MAR values z, and parameters λ,

$$\operatorname*{arg\,min}_{\lambda \in \Lambda} p(X \mid \lambda) = \sum_{z \in \mathcal{Z}} p(X, z \mid \lambda),$$

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- Unfortunately, this has a sum inside the log:
  - This will be non-convex even in common settings where $-\log p(X, z \mid \lambda)$ is convex.
  - This won't have closed-form solution even in common settings where minimizer given z does.

Expectation Maximization (Equation Version)

- At each iteration k, the expectation maximization algorithm optimizes a surrogate g_k,

$$\begin{aligned} g_k(\lambda) &= \mathbb{E}_{z \mid X,\, \lambda^k}[p(z \mid X, \lambda)] + \text{const.} \\ &= \sum_{z \in \mathcal{Z}} p(z \mid X, \lambda^k) \log p(X, z \mid \lambda) + \text{const.}, \end{aligned}$$

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- Together, these imply monotonic improvement in the objective (no step size needed).

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    - But we know that EM usually doesn't converge to a global optimum.
- This work: simpler analyses, mild asumptions, true from any starting point.

Surrogate Optimization

We view EM as a surrogate optimization method [Mairal, 2013]:

Algorithm 1 Surrogate Optimization Scheme

1: **Input**: $\lambda^0 \in \Lambda$, number of iterations t.
2: **for** k = 1 to t **do**
3: Compute a surrogate function g_k of f near λ^{k-1}.
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Our results hold in this general framework assuming that (Assumptions 1-3):

- $f(\lambda^{k-1}) = g(\lambda^{k-1})$.
- $f(\lambda) \leq g(\lambda)$ for all λ.
- $f(\lambda) \geq f^*$ for all λ.

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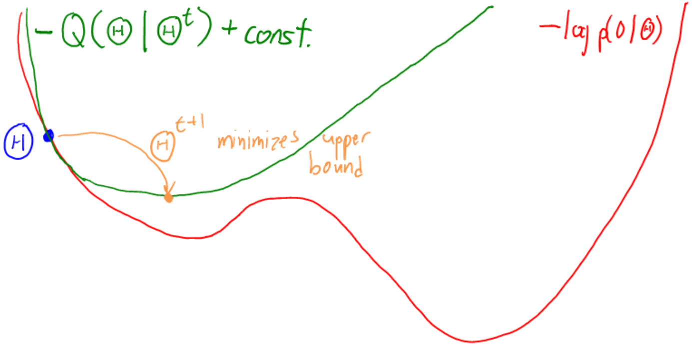
Theorem (Convergence rate of EM for differentiable functions)

Under Assumptions 1-3 and 4a, the EM algorithm starting from any λ^0 is guaranteed to find parameters λ' satisfying $\|\nabla f(\lambda')\|^2 \leq \epsilon$ once we have performed $t \geq \frac{2L[f(\lambda^0)-f^*]}{\epsilon}$ iterations.

- The same rate $O(1/\epsilon)$ rate as gradient descent (with a different constant L).

Non-Asymptotic Convergence Rate

- Proof:



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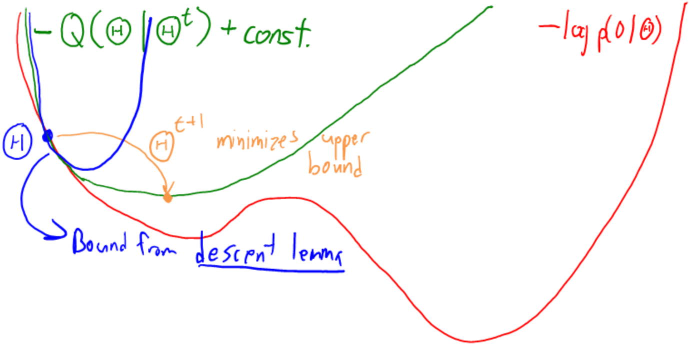

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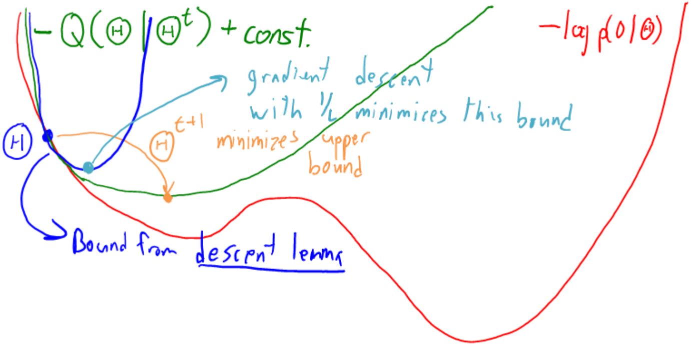

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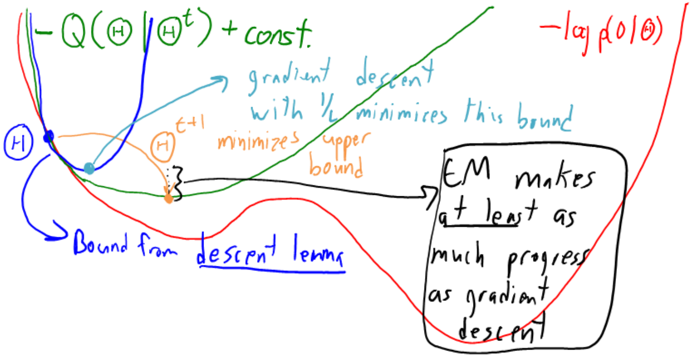
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EM makes at least as much progress as gradient descent

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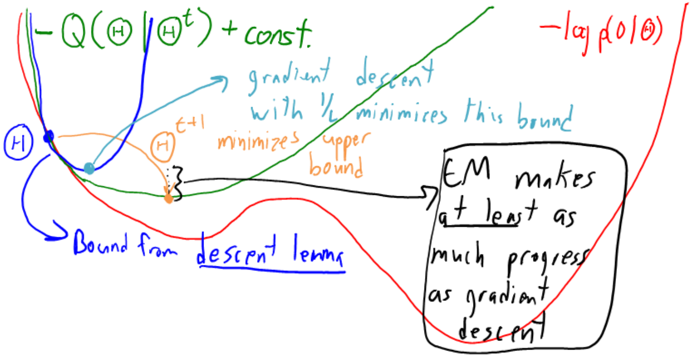

- We obtain faster rates under additional assumptions:
  - Rate in function values for convex f.
  - Linear rate for f satisfying PL.

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Theorem (Convergence rate of EM for non-differentiable functions)

Under Assumptions 1-3 and 4b, the EM algorithm is guaranteed to find parameters λ' satisfying $\|G_k(\lambda')\|^2 \leq \epsilon$ once we have performed $t \geq \frac{2[f(\lambda^0)-f^*]}{\mu\epsilon}$ iterations.

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  - Generalized EM (can't exactly minimize surrogate function).
  - Second-order optimality (variant that escapes saddle points).
  - Accelerated EM (faster rates for locally-convex objectives).
  - Coordinate-wise, stochastic, and stochastic variance-reduced EM (large-scale).
  - Proximal and mirror descent variants.
- See the paper coming soon...

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  2. *Sufficient decrease*: $g_k(\lambda^k) \leq g_k(\lambda^{k-1}) - \alpha\|\nabla g_k(\lambda^{k-1})\|^2$ for some $\alpha > 0$.

The latter condition is easy to check.

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Theorem

SPESO return a (ϵ, γ)-solution after $\frac{3M^2[f(\lambda^0)-f^*]}{\gamma^3}t^*$ total iterations, where t^* is the number of iterations of the first order algorithm for finding a point with gradient smaller than ϵ.

Escaping Saddle Points

Algorithm 3 Saddle Point Escape for Surrogate Optimization (SPESO)

Input: $\lambda^0 \in \Lambda$, $\epsilon > 0$ and $0 < \gamma$
for $s = 1, \ldots.$ **do**
  find $\bar{\lambda}$ such that $\|\nabla f(\bar{\lambda})\| \leq \epsilon$ by executing one of the above algorithm for T^* iteration
  if $\nabla^2 f(\bar{\lambda}) \succ -\gamma I$ **then**
    $\lambda^s = \bar{\lambda}$
    return λ^s
  else
    $\lambda^s = NCJ(\lambda, \gamma)$
  end if
end for

Escaping Saddle Points

Algorithm 4 NJC: Jump along the Negative Curvature

Input: $\lambda \in \Lambda$, $0 < \gamma$
use an algorithm to compute the smallest negative eigenvalue and eigenvector of $\nabla^2 f(\lambda)$ namely μ_{min} and ν s.t. $\|\nu\| = 1$
if $\nabla f(\lambda) \neq 0$ **then**
  return $\lambda^+ = \lambda - \frac{\langle \nu, \nabla f(\lambda) \rangle}{|\langle \nu, \nabla f(\lambda) \rangle|} \frac{\gamma}{M} \nu$
else
  return $\lambda^+ = \lambda + \frac{\gamma}{M} \nu$
end if

- As in recent works, we can avoid Hessian computation by using Hessian-vector products.

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Summary

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- We give non-asymptotic convergence rates for EM under fairly weak assumptions.
  - Differentiable objective and gradient of surrogate is Lipschitz.
  - Non-differentaible objective and surrogate is strongly-convex.
- We've explored a variety of extensions, notably:
  - Generalized EM where we don't exactly optimize the surrogate.
  - Variant that escapes saddle points.
  - Many more...