Methods for inverse problems: V. Kaczmarz and Expectation Maximization methods

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overview

1. Problem setting: System of nonlinear operator equations
2. Gradient type Kaczmarz methods
3. Newton type Kaczmarz methods
   - Levenberg-Marquardt type Kaczmarz methods
   - IRGNM type Kaczmarz methods
4. EM algorithms

System of nonlinear operator equations

Instead of $\mathbf{F}(x) = \mathbf{y}$ consider systems of operator equations

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\begin{aligned}
F_0(x) &= y_0 \\
F_1(x) &= y_1 \\
F_2(x) &= y_2 \\
&\vdots \\
F_{N-1}(x) &= y_{N-1}
\end{aligned}
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Example: EIT

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\begin{cases}
\nabla \cdot (\sigma \nabla u_i) = 0 & \text{in } \Omega \\
\nu \cdot (\sigma \nabla u_i) = j_i\,, \quad u_i = v_i & \text{on } \partial\Omega
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Problem setting: System of nonlinear operator equations

$$F_i(x) = y_i\,, \quad i = 0, \ldots, N-1\,,$$

noisy data

$$\|y_i^\delta - y_i\| \leq \delta\,, \quad i = 0, \ldots, N-1\,,$$

e.g. $x \ldots$ coefficient in a PDE,
$\mathbf{F}(x) = (F_0(x), \ldots, F_{N-1}(x)) \ldots$ discr. Dirichlet-to Neumann map
Kaczmarz methods (algebraic reconstruction technique):
cyclic iteration over subproblems [Kaczmarz'93], [Natterer '97]

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Gradient type Kaczmarz methods

Landweber iteration for a single operator equation

$$x_{k+1}^{\delta} = x_k^{\delta} - \mathbf{F}'(x_k^{\delta})^*(\mathbf{F}(x_k^{\delta}) - \mathbf{y}^{\delta})$$

Discrepancy principle:

stop the iteration as soon as $\|\mathbf{F}(x_k^{\delta}) - \mathbf{y}^{\delta}\| \leq \tau\delta \rightsquigarrow k_* \sim \delta^{-1}$

Nonlinearity condition:

$\|\mathbf{F}(\tilde{x}) - \mathbf{F}(x) - \mathbf{F}'(x)(\tilde{x} - x)\| \leq \eta\|\mathbf{F}(\tilde{x}) - \mathbf{F}(x)\|$

Convergence Results:

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$$x_{k+1}^\delta = x_k^\delta - \omega_k F_{[k]}'(x_k^\delta)^*(F_{[k]}(x_k^\delta) - y_{[k]}^\delta)$$

$$\omega_k \;:=\; \begin{cases} 1 & \text{if } \|F_{[k]}(x_k^\delta) - y_{[k]}^\delta\| \geq \tau\delta \\ 0 & \text{otherwise} \end{cases} .$$

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[Haltmeier Leitao Scherzer'07], [De Cesaro Haltmeier Leitao Scherzer'08], [Haltmeier'09]

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Choice of α_k: (inexact Newton) $\rho \in (0,1)$
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[Burger BK'04], [Baumeister BK Leitão'09]

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Example 1

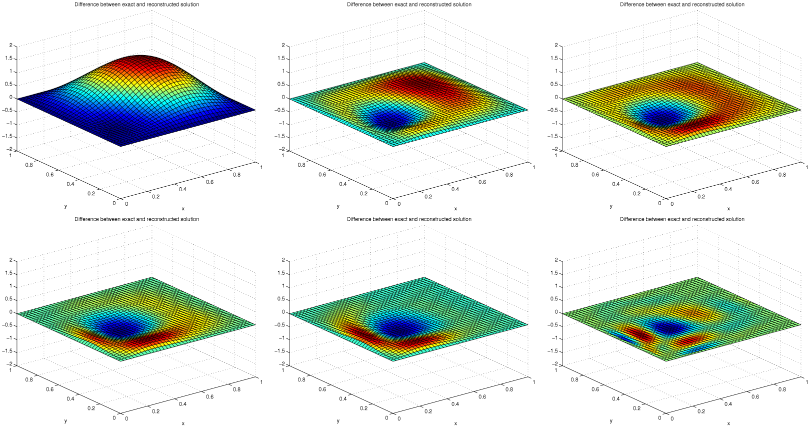
Reconstruction from Dirichlet-Neumann Map:
Estimate space-dependent coefficient $q \geq 0$

$$\begin{aligned} -\Delta u + qu &= 0, \qquad \text{in } \Omega, \\ u &= f \qquad \text{on } \partial\Omega, \end{aligned}$$

from N Dirirchlet-Neumann pairs $(f_i, \frac{\partial u_i}{\partial \nu}|_{\partial\Omega})$.

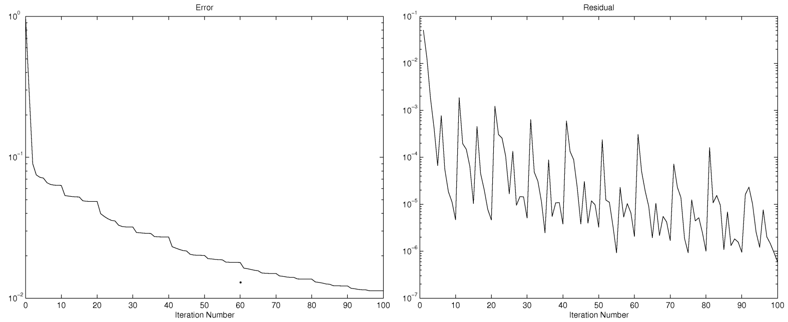
$\Omega = (0,1)^2$
$f_i \approx \delta(\cdot - x^i)\,, \quad x^i$ uniformly spaced on $\partial\Omega$
$N = 20$
$q^* = 3 + 5\sin(\pi x)\sin(\pi y)$
$q_0 \equiv 3$

Results with Levenberg-Marquardt-Kaczmarz



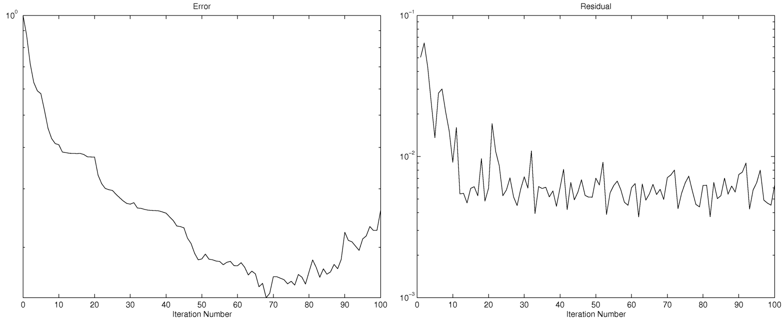
Difference $q^* - q_k$ at iterates 1, 2, 3, 5, 10, and 100.

Convergence with exact data



Semi-logarithmic plot of error (left) and residual (right) vs. iteration number

Semiconvergence with noisy data



Semi-logarithmic plot of error (left) and residual (right) vs. iteration number, $\delta = 1\%$

Loping Levenberg-Marquardt Kaczmarz iteration

$$x_{k+1}^\delta = x_k^\delta + \omega_k (F_{[k]}'(x_k^\delta)^* F_{[k]}'(x_k^\delta) + \alpha I)^{-1} F_{[k]}'(x_k^\delta)^* (y_{[k]}^\delta - F_{[k]}(x_k^\delta))$$

$$\omega_k := \begin{cases} 1 & \text{if } \|F_{[k]}(x_k^\delta) - y_{[k]}^\delta\| \geq \tau\delta \\ 0 & \text{otherwise} \end{cases} .$$

Discrepancy principle:

stop the iteration as soon as $\|F_i(x_k^\delta) - y_i^\delta\| \leq \tau\delta \quad \forall i$

i.e., $k_*^\delta := \min\{jN \in \mathbb{N} : x_{jN}^\delta = x_{jN+1}^\delta = \cdots = x_{jN+N}^\delta\}$

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Convergence Results:

- monotonicity of the error and ^{2} summability of the residuals
- convergence with exact/noisy data

[Baumeister BK Leitão'09]

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Inverse doping problem for semiconductor devices

(drift-diffusion equations, equilibrium at vanishing applied potential U)
Reconstruct $\gamma = e^{V_0}$ ($V_0 \ldots$ potential) in

$$\begin{aligned} \operatorname{div}(\mu_n \gamma \nabla \hat{u}) &= 0 && \text{in } \Omega \\ \hat{u} &= -U(x) && \text{on } \partial\Omega_D \\ \nabla \hat{u} \cdot \nu &= 0 && \text{on } \partial\Omega_N \end{aligned} \qquad \begin{aligned} \operatorname{div}(\mu_p \gamma^{-1} \nabla \hat{v}) &= 0 && \text{in } \Omega \\ \hat{v} &= U(x) && \text{on } \partial\Omega_D \\ \nabla \hat{v} \cdot \nu &= 0 && \text{on } \partial\Omega_N \end{aligned}$$

from N Dirirchlet-Neumann pairs $(U_i, \Lambda(U_i))$
where

$$\Lambda(U) = \int_{\Gamma_1} (\mu_n \gamma \hat{u}_\nu - \mu_p \gamma^{-1} \hat{v}_\nu)\, ds$$

$\hat{u}$, $\hat{v}$ ... concentrations of electrons and holes,
U ... applied potential,
μ_n, μ_p ... (known) electron and hole mobilities.

The doping profile C can then be determined from
$C(x) = \gamma(x) - \gamma^{-1}(x) - \lambda^2 \Delta(\ln \gamma(x))$, $x \in \Omega$.

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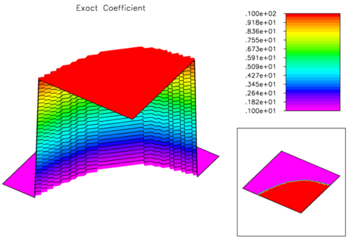
Exact coefficient and PDE solution for one voltage source

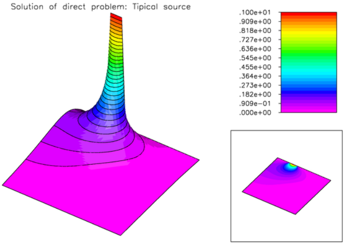
$$\Omega = (0,1)^2, \qquad N = 9$$

$$\Gamma_1 := \{(x,1)\,;\; x \in (0,1)\}, \;\; \Gamma_0 := \{(x,0)\,;\; x \in (0,1)\},$$

$$\partial\Omega_N := \{(0,y)\,;\; y \in (0,1)\} \cup \{(1,y)\,;\; y \in (0,1)\},$$

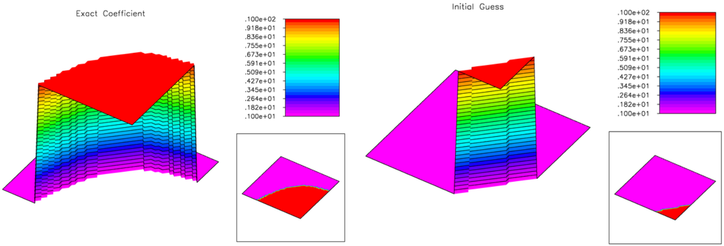
$$U_i(x) := \begin{cases} 1, & |x - x_i| \le 2^{-4} \\ 0, & \text{else} \end{cases}, \quad x_i = \tfrac{2i+1}{2M} \; i = 0, \dots, M-1.$$





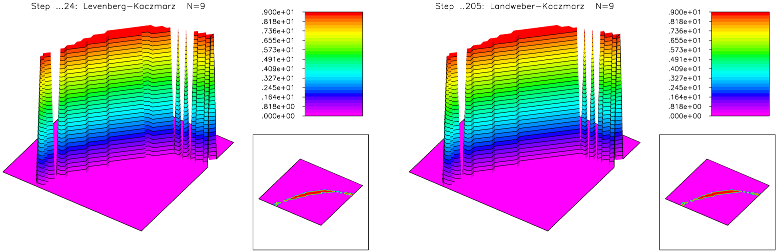
exact coefficient γ to be identified (left);
typical voltage source U_i and corresponding solution $\hat{u}$ (right)

Exact coefficient and initial guess



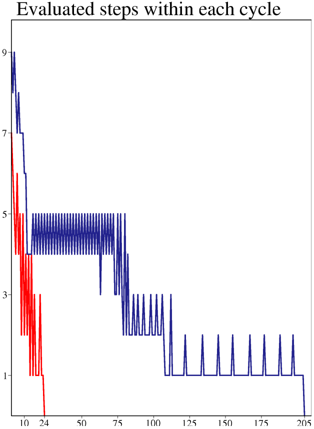
exact coefficient γ to be identified (left);
initial guess (right)

Comparison of loping Levenberg-Marquardt-Kaczmarz with Landweber-Kaczmarz



Numerical experiment with noisy data (5%):
error obtained with L-LMK after 24 cycles (left);
error obtained with L-LWK after 205 cycles (right)

Comparison of loping Levenberg-Marquardt-Kaczmarz with Landweber-Kaczmarz



Numerical experiment with noisy data (5 per cent):
number of non-loped inner steps in each cycle for L-LMK (solid red) and L-LWK (dashed blue), respectively.

The IRGNM for single operator equations

$$x_{k+1}^{\delta} = x_0 - G_{\alpha_k}(\mathbf{F}'(x_k^{\delta}))(\mathbf{F}(x_k^{\delta}) - \mathbf{y}^{\delta} - \mathbf{F}'(x_k^{\delta})(x_k^{\delta} - x_0))$$

e.g., $G_{\alpha}(K) = (K^*K + \alpha I)^{-1}$

Choice of α_k: $\alpha_k = \alpha_0 q^k$

Discrepancy principle:

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- convergence with exact/noisy data
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[Bakushinski'92], [BK Neubauer Scherzer'94], [Hohage'99]

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[BK '97]

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Condition on a priori guess

$x_{0,i} - x^* \in \mathcal{N}(F'_i(x^*))^\perp \;\; \forall i$

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- convergence with exact/noisy data [Burger BK '06]

Nonlinearity conditions

$$\mathbf{F}'(\tilde{x}) = \mathbf{F}'(x)\mathbf{R}^x_{\tilde{x}}\,, \quad \|\mathbf{R}^x_{\tilde{x}} - I\| \leq C_R\|\tilde{x} - x\|\,, \quad \tilde{x}, x \in \mathcal{B}_\rho(x^*)$$

$\Longrightarrow$ (with $R_i{}^x_{\tilde{x}} := \mathbf{R}^x_{\tilde{x}}$)

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i.e., range invariance of all individual F_i is a weaker condition than range invariance of collection $\mathbf{F}$

Lemma

Let X, Y, Z be Hilbert spaces, and let $L_i \in \mathcal{L}(Z_i, Y_i)$. Moreover, let $H_i : X_i \to Z_i$, $i = 0, \ldots, p-1$ be continuously Fréchet differentiable. Then,

$$\forall i \; : \; H_i \text{ satisfies } (*) \quad \Rightarrow \quad \forall i \; : \; F_i = L_i \circ H_i \text{ satisfies } (*)$$

Moreover,

$$\exists C_i\,, (\forall x \in \mathcal{B}_\rho(x^*)\,,: \; \|H_i'(x)^{-1}\| \leq C_i) \; \text{ and } H_i' \text{ Lipschitz}$$
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Example 1

Reconstruction from Dirichlet-Neumann Map:
Estimate space-dependent coefficient $q \geq 0$

$$\begin{aligned} -\Delta u + qu &= 0, \qquad \text{in } \Omega, \\ u &= f \qquad \text{on } \partial\Omega, \end{aligned}$$

from N Dirichlet-Neumann pairs $(f_i, \frac{\partial u_i}{\partial \nu}|_{\partial\Omega})$.
$L : u \mapsto \frac{\partial u}{\partial \nu}|_{\partial\Omega}$ ... trace operator
$H_i : q \mapsto u_i$ ... parameter-to-solution map for PDE with Dirichlet data f_i

Example 2

Reconstruction from multiple sources:
Estimate space-dependent coefficient $q \geq 0$

$$\begin{aligned} -\Delta u + qu &= h, \qquad \text{in } \Omega, \\ \frac{\partial u}{\partial \nu} &= 0 \qquad \text{on } \partial\Omega, \end{aligned}$$

from N source-Dirichlet pairs (h_i, u_i).
$L : u \mapsto u|_{\partial\Omega}$ ... trace operator
$H_i : q \mapsto u_i$ ... parameter-to-solution map for PDE with source h_i,

Further Examples

SPECT: Reconstruct source f and coefficient $a \geq 0$ in

$$\theta_i \cdot \nabla u_i + a u_i = f \qquad \text{in } \Omega \subset \mathbb{R}^d,$$

from N pairs $(\theta_i, u_i|_{\Gamma_i^+})$
where $\theta_i \in S(0,1)$, $\Gamma_i^+ := \{x \in \partial\Omega \,:\, \nu(x) \cdot \theta_i \geq 0\}$, and $u_i|_{\partial\Omega \setminus \Gamma_i^+} = 0$.

Ultrasound tomography: Reconstruct f in

$$\begin{aligned} \Delta v_i + k^2(1-f)v_i &= k^2 f e^{\mathbf{i}kx\cdot\theta_i} && \text{in } \Omega, \\ \frac{\partial v_i}{\partial \nu} &= B v_i && \text{on } \partial\Omega, \end{aligned}$$

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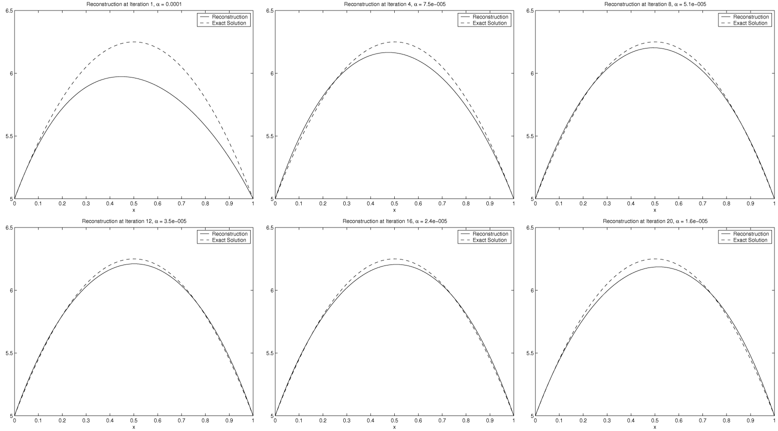
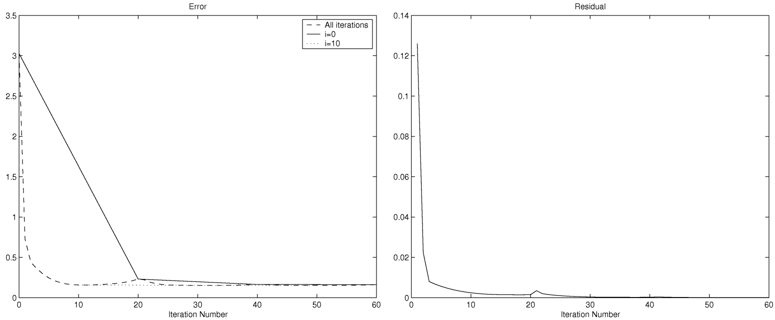
$\Omega = (0, 1)$
$h_i \approx \delta(\cdot - x^i)\,, \quad x^i$ uniformly spaced in Ω
$N = 20$
$q^* = 5 + 5x(1 - x)$
$q_0 \equiv 5$

Results with IRGNM-Kaczmarz (exact data)



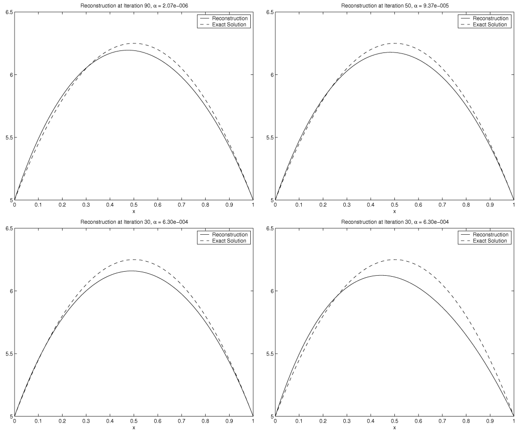
Reconstructions q_k at iterates 1, 4, 8, 12, 16, and 20.

Convergence of IRGNM-Kaczmarz (exact data)



Plot of error (left) and residual (right) vs. iteration number

Results with IRGNM-Kaczmarz (noisy data)



Reconstructions q_k for noise levels $\delta = 0.5\%$ (top left), $\delta = 1\%$ (top right), $\delta = 3\%$ (bottom left), $\delta = 5\%$ (bottom right).

Expectation Maximization (EM) algorithms

EM (Richardson-Lucy) algorithm for linear problems

for image reconstruction with nonnegativity constraints:
[Bertero 1998], [Natterer&Wuebbeling 2001], [Dempster&Laird&Rubin 1977]

$F : L^1(\Omega) \to L^1(\Sigma)$ linear operator

$$x_{k+1}^\delta = x_k^\delta F^* \left(\frac{y^\delta}{F x_k^\delta} \right). \tag{1}$$

$\rightsquigarrow$ multiplicative fixed-point scheme.
$\rightsquigarrow$ well-suited for multiplicative noise models (e.g. Poisson models)

$F,\ F^*$ positivity preserving, $x_0^\delta \geq 0,\ y^\delta \geq 0 \ \Rightarrow\ \forall k \in \mathbb{N} :\ x_k^\delta \geq 0$

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$F,\ F^*$ positivity preserving, $x_0^\delta \geq 0,\ y^\delta \geq 0 \ \Rightarrow\ \forall k \in \mathbb{N} :\ x_k^\delta \geq 0$

Derivation

$$x_{k+1}^\delta = x_k^\delta F^* \left(\frac{y^\delta}{F x_k^\delta} \right) . \tag{2}$$

is descent method for the functional

$$J(x) := \int_\Sigma \left[y^\delta \log \left(\frac{y^\delta}{Fx} \right) - y^\delta + Fx \right] d\sigma \, ,$$

Kullback-Leibler divergence (relative entropy) between Fx and y^δ.
optimality condition

$$x \left(-F^* \left(\frac{y^\delta}{Fx} \right) + F^* 1 \right) = 0 \, .$$

with operator scaling $F^* 1 = 1 \;\rightsquigarrow\; (2)$

Idea of convergence proof

[Mülthei&Schorr89], [Natterer&Wuebbeling 2001], [Resmerita&Engl&Iusem 2007], [Bissantz&Mair&Munk]
similar to Landweber with $\|\cdot\|^2 \leftrightarrow$ Kullback-Leibler divergence

$$KL(x,\tilde{x}) = \int_\Omega \left[x \log \frac{x}{\tilde{x}} - x + \tilde{x}\right],$$

For $x^\dagger$ with $Fx^\dagger = y$ by convexity

$$KL(x^\dagger, x_{k+1}) + J(x_k) \leq KL(x^\dagger, x_k).$$

$\Rightarrow$

$$KL(x^\dagger, x_k) + \sum_{j=0}^{k-1} J(x_j) \leq KL(x^\dagger, x_0),$$

$\Rightarrow$ boundedness of $KL(x^\dagger, x_k)$ and summability of $J(x_j)$.

EM algorithm for nonlinear problems

nonlinear operator $F : L^1(\Omega) \to L^1(\Sigma)$, no scaling $\rightsquigarrow$ fixed-point equation

$$xF'(x)^* 1 = xF'(x)^* \left(\frac{y^\delta}{Fx} \right) .$$

nonlinear EM algorithm

$$x_{k+1}^\delta = \frac{x_k^\delta}{F'(x_k^\delta)^* 1} F'(x_k^\delta)^* \left(\frac{y^\delta}{F(x_k^\delta)} \right) .$$

[Haltmeier&Leitao&Resmerita 2009]