#### Parallelizable algorithms for image recovery problems

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## **Executive Summary**

• In a wide variety of estimation problems, one estimates an unknown parameter vector  $\mathbf{x}^{true}$  by minimizing a *partially separable* cost function:

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}\geq\mathbf{0}} \Phi(\mathbf{x}), \qquad \Phi(\mathbf{x}) = \sum_{i} \psi_{i}([\mathbf{B}\mathbf{x}-\mathbf{c}]_{i}), \qquad [\mathbf{B}\mathbf{x}-\mathbf{c}]_{i} = \sum_{j} b_{ij}x_{j}-c_{i}.$$

- Fast methods for estimating  $\mathbf{x}^{true}$  by minimizing  $\Phi(\mathbf{x})$  are essential for successful routine use in applications such as medical tomography.
- We have developed fast converging algorithms for minimizing  $\Phi(x)$ .
- One algorithm has the fast convergence of coordinate descent, yet is parallelizable.
- The new algorithms converge faster than general-purpose minimization methods.

# Outline

- Motivating applications and cost functions
- Edge-preserving regularization
- Unified cost function
- Minimization algorithms
  - Optimization transfer
  - Separable paraboloidal surrogates (SPS) algorithm
  - Paraboloidal surrogate coordinate descent (PSCD) algorithm
  - Parallelizable coordinate descent algorithm
- Representative results
- Summary and future work

# **Application: X-ray Computed Tomography**



Statistical model:  $Y_i \sim \text{Poisson}\{b_i \exp(-[\mathbf{A}\mathbf{x}]_i) + r_i\}$ 

- $Y_i$ : measurement along *i*th ray (statistically independent),  $i = 1, ..., n_d$
- x<sub>j</sub>: unknown attenuation coefficient in the *j*th voxel
- $b_i$ : mean number of transmitted photons along *i*th ray
- *a<sub>ij</sub>*: Radon projection matrix
- *r<sub>i</sub>*: random coincidences and scatter
- Beer's Law for photon survival probability:  $e^{-\int \mu(\cdot) dl'}$
- [Ax]<sub>i</sub>: discrete approximation to line integral along *i*th ray

## X-ray CT Statistical Image Reconstruction

It is natural to estimate the attenuation image  $\mathbf{x}$  by finding the "best fit" to the sinogram data, as measured by the log-likelihood:

$$\mathbf{\hat{x}}_{\mathrm{ML}} \stackrel{ riangle}{=} rg\min_{\mathbf{x} \ge \mathbf{0}} \Phi^{\mathrm{data}}(\mathbf{x}) \quad \mathrm{where} \quad \Phi^{\mathrm{data}}(\mathbf{x}) = \sum_{i=1}^{n_d} \psi_i([\mathbf{A}\mathbf{x}]_i)$$

$$\Psi_i(l) \stackrel{\triangle}{=} (b_i e^{-l} + r_i) - Y_i \log (b_i e^{-l} + r_i).$$



- Summation form due to independence of recorded photon counts.
- Inner products  $[Ax]_i$  due to Beer's law and line integrals
- $\psi_i$ 's determined by Poisson negative log-likelihood

# **Application: PET Image Reconstruction**



 $n_d \approx (n_{\rm crystals})^2$ 

# **PET Image Reconstruction**

Most statistical methods for PET image reconstruction are based on the following Poisson statistical model.

$$Y_i \sim \text{Poisson}\left\{\varepsilon_i s_i \sum_j g_{ij} x_j + r_i\right\}, \ i = 1, \dots, n_d.$$

- *Y<sub>i</sub>*: measured counts in sinogram bins (statistically independent)
- $x_j$ : unknown radiotracer concentration in the *j*th voxel
- ε<sub>i</sub>: *i*th detector efficiency
- *s<sub>i</sub>*: photon survival probability along *i*th ray (attenuation)
- *g<sub>ij</sub>*: projection matrix
- *r<sub>i</sub>*: random coincidences and scatter
- *n<sub>d</sub>*: number of detector pairs

## **Maximum-Likelihood PET Image Reconstruction**

If the Poisson model is valid, it is natural to estimate the emission image  $\mathbf{x}$  by finding the "best fit" to the sinogram data, as measured by the log-likelihood:

$$\hat{\mathbf{x}}_{\mathrm{ML}} \stackrel{\triangle}{=} \arg\min_{\mathbf{x} \ge \mathbf{0}} \Phi^{\mathrm{data}}(\mathbf{x}) \quad \text{where} \quad \Phi^{\mathrm{data}}(\mathbf{x}) = \sum_{i=1}^{n_d} \psi_i([\mathbf{A}\mathbf{x}]_i)$$
$$\psi_i(l) \stackrel{\triangle}{=} (l+r_i) - Y_i \log(l+r_i), \quad a_{ij} \stackrel{\triangle}{=} \varepsilon_i s_i g_{ij}.$$



- Summation form due to independence of recorded photon counts.
- Inner products [Ax]<sub>i</sub> due to Radon tomographic projection
- $\psi_i$ 's determined by Poisson negative log-likelihood

# **Application: Confocal Microscopy 3D Image Restoration**



Cost function is comparable to that of PET / SPECT.

## **Application: Robust Multiuser Detection**

Wang and Poor, Feb. 1999 IEEE Tr. Sig. Proc. "Robust multi-user detection in non-Gaussian channels"

Model for direct-sequence code-division multiple access (CDMA):

$$Y_i = \sum_{j=1}^{K} a_{ij} x_j + N_i, \ i = 1, \dots, n_d$$

- *Y<sub>i</sub>*: sampled output of chip-matched filter
- x<sub>j</sub>: jth information bit scaled by received amplitude
- *N<sub>i</sub>*: possibly non-Gaussian noise
- *a<sub>ij</sub>*: signature sequence of *j*th user

Robust bit estimator (using, *e.g.*, the Huber function):

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}} \Phi(\mathbf{x}), \quad \Phi(\mathbf{x}) = \sum_{i=1}^{n_d} \Psi(Y_i - [\mathbf{A}\mathbf{x}]_i)$$

### **Application: Physics-based MR image reconstruction**

y = Ax + noise

- y: samples in spatial frequency space
- x: object transverse magnetization
- A: Fourier transform modified by magnetic field inhomogeneity

$$Y_i = \sum_{j=1}^{n_p} x_j \exp\left(\sqrt{-1}2\pi \left[\underline{k}_i \cdot \underline{r}_j + \Delta_j t_i\right]\right)$$

- $\underline{k}_i$ : frequency space location of *i*th sample
- $\underline{r}_i$ : coordinates of *j*th voxel
- $\Delta_i$ : field inhomogeneity induced off-resonance frequency for *j*th voxel
- *t<sub>i</sub>*: time of *i*th sample

Gaussian noise, so  $\psi_i(t) = t^2/2$  (least squares estimation)

# **Edge-preserving Regularization**

Minimizing  $\Phi^{data}$  alone is inadequate for ill-conditioned inverse problems.

Generic prior "knowledge" of piece-wise smoothness:

•  $x_j - x_{j-1} \approx 0$ 

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- $x_{j-1} 2x_j + x_{j+1} \approx 0$
- $x_j \approx 0, \ j \in J \subset \{1, \dots, n_p\}$

(piece-wise constant) (piece-wise linear) (support constraints)

Combining:  $Cx \approx z$  (where typically z = 0).

Expressed as penalty function:

$$\Phi^{\text{penalty}}(\mathbf{x}) = \sum_{k} \Psi_{k}^{\text{penalty}}?([\mathbf{C}\mathbf{x} - \mathbf{z}]_{k}).$$

To "preserve" edges,  $\psi_k^{\text{penalty}}$  should be nonquadratic.

# **Example of edge-preserving potential function**



# Penalty Function: General Form $\Phi^{\text{penalty}}(\mathbf{x}) = \sum_{k} \psi_k([\mathbf{C}\mathbf{x}]_k), \text{ where } [\mathbf{C}\mathbf{x}]_k = \sum_{j} c_{kj} x_j$

Example:



# **Unified Cost Function**

$$\Phi(\mathbf{x}) = \sum_{i=1}^{N} \psi_i([\mathbf{B}\mathbf{x} - \mathbf{c}]_i)$$
 "partially separable"

Regularized edge-preserving cost function is a special case:

$$\Phi(\mathbf{x}) = \Phi^{\text{data}}(\mathbf{x}) + \Phi^{\text{penalty}}(\mathbf{x}), \quad \mathbf{B} = \begin{bmatrix} \mathbf{A} \\ \mathbf{C} \end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} \mathbf{y} \\ \mathbf{z} \end{bmatrix}$$

Optimization problem:

$$\hat{\mathbf{x}} = \arg\min_{\mathbf{x}} \Phi(\mathbf{x})$$
 or  $\hat{\mathbf{x}} = \arg\min_{\mathbf{x} \ge \mathbf{0}} \Phi(\mathbf{x}).$ 

This formulation encompasses a wide variety of inverse problems.

Challenges: nonnegativity constraint, nonquadratic  $\psi_i$ 's, size of **B**.

# **Ideal Algorithm**

 $\hat{\mathbf{x}} \stackrel{\triangle}{=} \arg\min_{\mathbf{x} \ge \mathbf{0}} \Phi(\mathbf{x})$  (global minimizer)

stable and convergent converges quickly globally convergent fast robust user friendly monotonic parallelizable simple flexible  $\{\mathbf{x}^{(n)}\}\$  converges to  $\hat{\mathbf{x}}$  if run indefinitely  $\{\mathbf{x}^{(n)}\}\$  gets "close" to  $\hat{\mathbf{x}}$  in just a few iterations  $\lim_{n} \mathbf{x}^{(n)}$  independent of starting image requires minimal computation per iteration insensitive to finite numerical precision nothing to adjust (*e.g.* acceleration factors)  $\Phi(\mathbf{x}^{(n)})$  increases every iteration (when necessary)

easy to program and debug accommodates any type of system model (matrix stored by row or column or projector/backprojector)

Choices: forgo one or more of the above

# **Optimization Transfer (1D illustration)**



## **Optimization Transfer**

(cf EM Algorithm)

- E-step: choose surrogate function  $\phi(\mathbf{x}; \mathbf{x}^{(n)})$
- M-step: minimize surrogate function

$$\mathbf{x}^{(n+1)} = \arg\min_{\mathbf{x} \ge \mathbf{0}} \phi(\mathbf{x}; \mathbf{x}^{(n)})$$

Surrogate design goals:

- Easy to "compute"
- Easy to minimize
- Fast convergence rate
- Monotone convergence

$$\Phi(\mathbf{x}^{(n)}) - \Phi(\mathbf{x}) \ge \phi(\mathbf{x}^{(n)}; \mathbf{x}^{(n)}) - \phi(\mathbf{x}; \mathbf{x}^{(n)})$$

Often mutually incompatible goals .. compromises

# **Optimization Transfer in 2D**



# **Exploiting Partial Separability (E-step)**

Cost FunctionParaboloidal Surrogate Function $\Phi(\mathbf{x}) = \sum_{i=1}^{N} \psi_i([\mathbf{B}\mathbf{x} - \mathbf{c}]_i) \leq \phi(\mathbf{x}; \mathbf{x}^{(n)}) \stackrel{\triangle}{=} \sum_{i=1}^{N} q_i([\mathbf{B}\mathbf{x} - \mathbf{c}]_i; t_i^{(n)}),$ where  $t_i^{(n)} \stackrel{\triangle}{=} [\mathbf{B}\mathbf{x}^{(n)} - \mathbf{c}]_i).$ 

1-D tangent parabola surrogate:

$$\psi_i(t) \leq q_i(t;t_i^{(n)}), \quad q_i(t;s) \stackrel{ riangle}{=} \psi_i(s) + \dot{\psi}_i(s)(t-s) + \kappa_i(s) \frac{(t-s)^2}{2}.$$

Optimal parabola curvature (for fastest convergence rate):

$$\kappa_i(s) \stackrel{ riangle}{=} \min\{\kappa \ge 0 : q_i(t;s) \ge \psi_i(t) \ \forall t\}.$$

For Huber-like functions:  $\kappa_i(s) = \dot{\psi}_i(s)/s \stackrel{\triangle}{=} \omega_i(s)$ .

For emission and transmission tomography, optimal  $\kappa_i$  derived by Erdoğan (Tr. Med. Im., 1999)

# **Tangent Parabolas**



 $\omega_{\psi}(t_0)$  is the curvature of the parabola that is tangent at  $t_0$ 

# **Nonmonotonicity of Newton-Raphson**



# Minimizing the Paraboloidal Surrogate (M-step) $\phi(\mathbf{x};\mathbf{x}^{(n)}) = c_0 + \nabla \Phi(\mathbf{x}^{(n)})(\mathbf{x} - \mathbf{x}^{(n)}) - \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(n)})'\mathbf{B}' \operatorname{diag}\left\{\kappa_i^{(n)}\right\} \mathbf{B}(\mathbf{x} - \mathbf{x}^{(n)}),$

where the tangent parabola curvatures are:

$$\mathbf{\kappa}_i^{(n)} = \mathbf{\kappa}_i(t_i^{(n)}) = \mathbf{\kappa}_i([\mathbf{B}\mathbf{x}^{(n)} - \mathbf{c}]_i).$$

M-step: Minimize  $\phi(\mathbf{x}; \mathbf{x}^{(n)})$  using any iterative "least squares" algorithm that accommodates nonnegativity constraints.

#### Reasonable choices of algorithms

- PSCD Paraboloidal surrogates coordinate descent:
  - fast converging, but non-parallelizable
- SPS (separable paraboloidal surrogates):

slow converging, but fully parallelizable

 PPCD (partitioned-separable paraboloidal surrogate coordinate descent) best of both worlds?

# Paraboloidal surrogates coordinate descent (PSCD)

- Update one pixel at a time, w.r.t. the surrogate, holding other pixels fixed:  $x_{j}^{(n+1)} = \arg\min_{x_{i}>0} \phi(x_{1}^{(n+1)}, \dots, x_{j-1}^{(n+1)}, x_{j}, x_{j+1}^{(n)}, \dots, x_{n_{p}}^{(n)}; \mathbf{x}^{(n)}).$
- Cycle through all pixels, then update the paraboloidal surrogate ( $\kappa_i^{(n)}$ 's).

Advantages:

- Intrinsically monotonic, global convergence (for a broad family of  $\psi_i$ 's)
- Fast converging (from good initial image)
- Nonnegativity constraint trivial

Disadvantages:

- Requires column access of system matrix
- Poorly parallelizable

#### Separable paraboloid surrogate

One can use the convexity of the paraboloidal surrogate  $\phi$  to define a second surrogate function that is **separable**:

$$\phi(\mathbf{x};\mathbf{x}^{(n)}) \le \phi^{SP}(\mathbf{x};\mathbf{x}^{(n)}) \stackrel{\triangle}{=} \sum_{j=1}^{n_p} \phi_j(x_j - x_j^{(n)};\mathbf{x}^{(n)})$$

where

$$\phi_j(t; \mathbf{x}^{(n)}) \stackrel{\triangle}{=} \sum_{i=1}^N \pi_{ij} \kappa_i^{(n)} \frac{1}{2} \left( \frac{b_{ij}}{\pi_{ij}} t + [\mathbf{B}\mathbf{x}^{(n)} - \mathbf{c}]_i \right)^2,$$
$$\pi_{ij} = \frac{|b_{ij}|}{\sum_{j=1}^{n_p} |b_{ik}|}.$$

Minimizing the separable paraboloid  $\phi^{SP}$  is trivial, especially compared to minimizing a paraboloid.

$$\mathbf{x}^{(n+1)} = \arg\min_{\mathbf{x}\geq\mathbf{0}} \phi(\mathbf{x};\mathbf{x}^{(n)}) \implies x_j^{(n+1)} = \arg\min_{x_j\geq\mathbf{0}} \phi_j(x_j - x_j^{(n)};\mathbf{x}^{(n)}), \ j = 1, \dots, n_p.$$

# Separable paraboloid surrogate (SPS) algorithm

$$x_{j}^{(n+1)} = \left[ x_{j}^{(n)} - \frac{\dot{q}_{j}(0; \mathbf{x}^{(n)})}{\ddot{q}_{j}(0; \mathbf{x}^{(n)})} \right]_{+} \Rightarrow \mathbf{x}^{(n+1)} = \left[ \mathbf{x}^{(n)} - \operatorname{diag} \left\{ \frac{1}{\ddot{q}_{j}(0; \mathbf{x}^{(n)})} \right\} \nabla \Phi(\mathbf{x}^{(n)}) \right]_{+}$$

Advantages:

- Monotonically decreases  $\Phi$
- Converges globally to unique minimizer (for broad family of convex  $\psi_i$ 's)
- No matrix inversion required
- Easily enforces nonnegativity constraint
- Completely parallelizable (all pixels updated simultaneously)

Disadvantages:

• Very slow convergence (ala EM algorithm)

# **Convergence Rate / Surrogate Curvature**



# Separable vs Nonseparable Surrogates



Separable surrogates (*e.g.* EM) have high curvature : slow convergence. Nonseparable surrogates can have lower curvature : faster convergence. Harder to minimize? Use paraboloids (quadratic surrogates).

# **PSCD vs SPS Algorithm**



# **Naive Parallelizable Coordinate Descent**

- Goal: fast convergence of coordinate descent, yet parallelizable
- Suitable for coarse-grain parallelization



- Each processor applies coordinate descent independently to its block
- Not guaranteed to be monotonic!

#### Partitioned-separable paraboloidal surrogate

Partion pixels into *K* subsets indexed by  $J_k$ , where  $\bigcup_{k=1}^{K} J_k = \{1, 2, ..., n_p\}$ .

E-step: Form a surrogate function that is separable *between blocks*:

$$\Phi(\mathbf{x}) \leq \phi(\mathbf{x}; \mathbf{x}^{(n)}) \leq Q(\mathbf{x}; \mathbf{x}^{(n)}) = \sum_{k=1}^{K} Q_k(\mathbf{x}_{J_k}; \mathbf{x}^{(n)}).$$

By construction, decreasing this new surrogate  $Q(\mathbf{x}; \mathbf{x}^{(n)})$  will monotonically decrease the cost function  $\Phi$ :

$$\Phi(\mathbf{x}^{(n)}) - \Phi(\mathbf{x}) \ge Q(\mathbf{x}^{(n)}; \mathbf{x}^{(n)}) - Q(\mathbf{x}; \mathbf{x}^{(n)}).$$

M-step: Partitioned-separable form allows processor parallelization:

$$\mathbf{x}^{(n+1)} = \arg\min_{\mathbf{x}\geq\mathbf{0}} Q(\mathbf{x};\mathbf{x}^{(n)}) \implies \mathbf{x}_{J_k}^{(n+1)} = \arg\min_{\mathbf{x}_{J_k}\geq\mathbf{0}} Q_k(\mathbf{x}_{J_k};\mathbf{x}^{(n)}), \ k = 1,\ldots,K.$$

## **PPCD Derivation**

Adaptation of De Pierro's convexity trick for modified EM algorithm:

$$[\mathbf{B}\mathbf{x} - \mathbf{c}]_{i} = \sum_{j=1}^{n_{p}} b_{ij}x_{j} - c_{i} = \sum_{k=1}^{K} \pi_{ik} \left( \frac{s_{ik}^{(n)}(\mathbf{x}_{J_{k}})}{\pi_{ik}} + t_{i}^{(n)} \right)$$
  
where  $\pi_{ik} = \frac{\sum_{j \in J_{k}} |b_{ij}|}{\sum_{j=1}^{n_{p}} |b_{ij}|} \ge 0$  and  $\sum_{k=1}^{K} \pi_{ik} = 1$ ,  
 $s_{ik}^{(n)} = [\mathbf{B}_{J_{k}}(\mathbf{x}_{J_{k}} - \mathbf{x}_{J_{k}}^{(n)}) - \mathbf{c}]_{i} = \sum_{j \in J_{k}} b_{ij}(x_{j} - x_{j}^{(n)}) - c_{i}.$ 

When q is a quadratic (and hence convex function):

$$q([\mathbf{B}\mathbf{x} - \mathbf{c}]_i) = q\left(\sum_{k=1}^K \pi_{ik}\left(\frac{s_{ik}^{(n)}(\mathbf{x}_{J_k})}{\pi_{ik}} + t_i^{(n)}\right)\right) \le \sum_{k=1}^K \pi_{ik} q\left(\frac{s_{ik}^{(n)}(\mathbf{x}_{J_k})}{\pi_{ik}} + t_i^{(n)}\right).$$

The latter term is the foundation for  $Q_k$ , being partitioned separable.

# Partitioned separable Paraboloidal-surrogate Coordinate Descent (PPCD) Algorithm

#### E-step

- Form paraboloidal surrogate  $\phi(\mathbf{x}; \mathbf{x}^{(n)})$  from cost function  $\Phi(\mathbf{x})$
- Form partitioned separable surrogate  $Q(\mathbf{x}; \mathbf{x}^{(n)}) = \sum_{k=1}^{K} Q_k(\mathbf{x}_{J_k}; \mathbf{x}^{(n)})$

#### M-step

• *K* processors independently "minimize" (or decrease)  $\{Q_k(\mathbf{x}_{J_k}; \mathbf{x}^{(n)})\}$ , using any nonnegative least-squares method such as coordinate descent

$$\mathbf{x}_{J_k}^{(n+1)} = \arg\min_{\mathbf{x}_{J_k} \ge \mathbf{0}} Q_k(\mathbf{x}_{J_k}; \mathbf{x}^{(n)}), \ k = 1, \dots, K.$$

• Broadcast  $\mathbf{x}_{J_k}^{(n+1)}$  to other processors

For a broad class of convex  $\psi_i$ 's, global convergence follows from SAGE convergence proof, Fessler and Hero, 1995 (IEEE T-SP).

## **Representative 2D Simulation Results**

Object



#### Restoration







Poisson measurement noise with PSNR = 25 dB

Restored by maximum penalized likelihood using nonquadratic edge-preserving penalty function:

$$\Psi(t) = \delta^2 \left[ \left| \frac{t}{\delta} \right| - \log \left( 1 + \left| \frac{t}{\delta} \right| \right) \right], \text{ with } \delta = 1.5.$$

# **Convergence rate vs number of processors (2D)**



# **Confocal microscopy simulation (3D)**



xy:

XZ:

# **Cost function decrease vs Elapsed time**



# **Elapsed time per iteration vs # of Processors**



# Summary

#### **Optimization transfer**

- Natural framework for algorithm development
- Exploits structure of "partially separable" cost functions

Partitioned separable paraboloidal surrogate coordinate descent algorithm

- Accommodates non-quadratic cost functions
- Monotonically decreases  $\Phi$
- Converges globally to unique minimizer (for broad class of  $\psi_i$ 's)
- Easily accommodates nonnegativity constraint
- Parallelizable
- Converges faster than a general-purpose optimization method

# **Future Work**

Convergence proof for multiple minima:



Slides and paper available from: http://www.eecs.umich.edu/~fessler

# **Monotone Convergence**

From R. Meyer "Sufficient conditions for the convergence of monotonic mathematical programming algorithms," J. Comput. System. Sci., 1976.

Let M be a point to set mapping such that, on G,

- M is uniformly compact,
- *M* is upper semi-continuous,
- M is strictly monotonic with respect to the function  $\Phi$ .

If  $\{\mathbf{x}^{(n)}\}\$  is any sequence generated by the algorithm  $\mathbf{x}^{(n+1)} \in M(\mathbf{x}^{(n)})$ :

- all accumulation points of  $\{\mathbf{x}^{(n)}\}$  will be fixed points,
- $\Phi(\mathbf{x}^{(n)}) \rightarrow \Phi(\mathbf{x}^{\star})$  where  $\mathbf{x}^{\star}$  is a fixed point,  $\|\mathbf{x}^{(n+1)} \mathbf{x}^{(n)}\| \rightarrow 0$ , and
- either  $\{\mathbf{x}^{(n)}\}\$  converges or the accumulation points of  $\{\mathbf{x}^{(n)}\}\$  form a continuum.