

Speedy Gibbs Sampling for $A^T CA$ Equilibrium Systems

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Outline

- Short introduction to inverse Problems
- Introduction to $\mathbf{A}^T \mathbf{C} \mathbf{A}$ systems
- Computational issues
- Fast conditional sampling
- Example on Electrical Capacitance Tomography (ECT)

Inverse Problems

Determine $\mathbf{x} \in \mathbb{R}^N$ from

$$\tilde{\mathbf{d}} = P(\mathbf{x}) + \mathbf{v}, \tilde{\mathbf{d}}, \mathbf{v} \in \mathbb{R}^M \quad (1)$$

Forward map (model) $F : \mathbf{x} \mapsto \mathbf{y}$.

$$\mathbf{y} = F(\mathbf{x}) \quad (2)$$

$$F(\mathbf{x}) = P(\mathbf{x}) \quad \forall \mathbf{x}, \quad (3)$$

Where does the name come from:

$$\mathbf{x} = F^{-1}(\tilde{\mathbf{d}}), \quad (4)$$

Does not work as inverse problems are ill posed.

- Regularization
- Prior knowledge

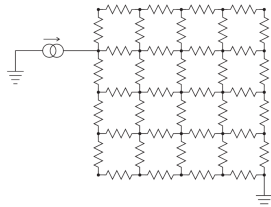
$$\rightarrow \mathcal{F}^{-1}(\tilde{\mathbf{d}})$$

$A^T CA$ what are they? Why are they important?

- What are they: Systems where the underlying stiffness matrix K can be expressed by the form $A^T CA$. C is diagonal and contains the parameter (material values, etc.). A is a mapping.
 - The stiffness matrix depends linear to C
 - The system itself is nonlinear.
- Why are they so important?: They appear in many inverse problems with an underlying electrical, mechanical, heat transfer, hydraulic, etc. problem (Gilbert Strang).
- More general: everything with an underlying resistor network structure
→ so even in finite element discretizations of pde's.

Resistor Network

$$\mathbf{K}_{(l,m)} = \begin{cases} -\frac{1}{R_{(l,m)}} & l \neq m \\ \sum_{k=1}^N \frac{1}{R_{(l,k)}} & l = m \end{cases} \quad (5)$$



$\mathbf{A}^T \mathbf{C} \mathbf{A}$ decomposition:

$$C_{(l,m)} = \begin{cases} \frac{1}{R_{(l,m)}} & (l,m) \in \mathcal{D} \\ 0 & \text{otherwise} \end{cases} \quad (6)$$

$$A_{(l,m)} = \begin{cases} +1 & \text{'+' end of resistor } l \text{ is connected to node } m \\ -1 & \text{'-' end of resistor } l \text{ is connected to node } m \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

How to obtain a full rank system?

- Reduction of the reference node (nodal analysis)

$$\mathbf{Y}\mathbf{u} = \mathbf{i} \quad (8)$$

Most common method in circuit analysis. Easy to implement - just skip the reference column from \mathbf{A} .

- Penalty method: Add some large number to the reference node. Simple, but not exact, Problem with the condition number.
- Variational formulation

$$\mathbf{u} = \operatorname{argmin} \mathbf{u}^T \mathbf{K} \mathbf{u} - \mathbf{i}^T \mathbf{u} \quad (9)$$

$$\text{s.t. } \mathbf{u}^T \boldsymbol{\chi} = 0 \quad (10)$$

→ Constraint optimization problem

- Non-standard penalty method*

*We have not found a better name yet

Non-standard penalty method*

- Approach

$$\mathbf{u} = \operatorname{argmin} \mathbf{u}^T \mathbf{K} \mathbf{u} - \mathbf{i}^T \mathbf{u} \quad (11)$$

$$\text{s.t. } \mathbf{u}^T \mathbf{c} = 0 \quad (12)$$

with $\mathbf{i}^T \mathbf{c} \neq 0$

- Unconstrained optimization problem

$$\mathbf{u} = \operatorname{argmin} (\mathbf{u}^T \mathbf{K} \mathbf{u} - \mathbf{i}^T \mathbf{u}) + \lambda \mathbf{u}^T \mathbf{c}^T \mathbf{c} \mathbf{u} \quad (13)$$

- Exact method for any value of λ (conditioning), the equation system preserves all nice properties (symmetry, poss. def.).
- \mathbf{i} has to contain the input currents and the output current at the reference node!

*We have not found a better name yet

Solution with Green's Functions

- For all further derivations we assume that $\mathbf{K} = \mathbf{A}^T \mathbf{C} \mathbf{A}$ has full rank.
- Our problem

$$\mathbf{K} \mathbf{u} = \mathbf{b} \quad (14)$$

is often a self adjoint (\mathbf{K} is symmetric) problem

- Solve for Green's functions \mathbf{g}
- Solve

$$\mathbf{K} \mathbf{g}_j = \mathbf{e}_j, \quad (15)$$

where \mathbf{e}_j is the j^{th} unit vector

- Solution

$$u_j = \mathbf{g}^T \mathbf{b} \quad (16)$$

Jacobian operation for $Ku = b$

Lets start with $J : \mathbf{c} \mapsto \mathbf{u}$

$$(\mathbf{K} + d\mathbf{K})(\mathbf{u} + d\mathbf{u}) = \mathbf{b}, \quad (17)$$

can be rearranged to

$$\mathbf{K}d\mathbf{u} = -d\mathbf{K}(\mathbf{u} + d\mathbf{u}). \quad (18)$$

$$\frac{d\mathbf{u}}{dc_j} = -\mathbf{K}^{-1} \frac{d\mathbf{K}}{dc_j} \mathbf{u}. \quad (19)$$

Chain rule

$$d\mathbf{u} = \mathbf{J}d\mathbf{c} = -\sum_j \mathbf{K}^{-1} \frac{d\mathbf{K}}{dc_j} \mathbf{u} dc_j = -\mathbf{K}^{-1} \left[\sum_j \frac{d\hat{\mathbf{K}}}{du_j} du_j \right] \mathbf{u} \quad (20)$$

$$= -\mathbf{K}^{-1} \mathbf{K}_{d\mathbf{c}} \mathbf{u}. \quad (21)$$

Jacobian operation 2

The last equation still requires $\hat{\mathbf{K}}^{-1} \rightarrow$ replace by \mathbf{G}

$$d\mathbf{u} = -\mathbf{G}^T \mathbf{K}_{dc} \mathbf{G}. \quad (22)$$

Similar $\mathbf{J}^T : \mathbf{r} \mapsto \mathbf{C}$

$$\mathbf{J}^T \mathbf{r} = -\text{diag}((\mathbf{G}^T \mathbf{A}^T)^T (\mathbf{R} \mathbf{G}^T \mathbf{A})), \quad (23)$$

with $\mathbf{R} = \text{diag}(\mathbf{r})$

We have

- a **linear approximation** and can do
- **gradient based optimization**

for free by maintaining Green's functions.

Exact low rank updates for $\mathbf{K}\mathbf{u} = \mathbf{b}$

How does \mathbf{u} change when a low number of elements of \mathbf{C} are updated?

Purpose: line search, conditional sampling

Woodbury Formula:

$$(\mathbf{K} + \mathbf{U}\mathbf{W}^T)^{-1} = \mathbf{K}^{-1} - \underbrace{\mathbf{K}^{-1}\mathbf{U}(\mathbf{I} + \mathbf{W}^T\mathbf{K}^{-1}\mathbf{U})^{-1}\mathbf{W}^T\mathbf{K}^{-1}}_{\text{update term}}, \quad (24)$$

How can we use this:

$$\mathbf{K}_{\text{new}} = \mathbf{K}_{\text{old}} + \gamma\mathbf{A}^T\mathbf{C}_\Delta\mathbf{A}^T = \hat{\mathbf{K}}_{\text{old}} + \gamma\mathbf{U}\mathbf{W}^T \quad (25)$$

With \mathbf{G} to replace $\mathbf{K}_{\text{old}}^{-1}$

$$\Delta\mathbf{u} = -\gamma\mathbf{G}^T\mathbf{U}(\mathbf{I} + \gamma\mathbf{W}_{:,C}^T\mathbf{G}_{C,C}\mathbf{U}_{C,:})^{-1}\mathbf{W}^T\mathbf{G}, \quad (26)$$

Drawback: $\mathbf{G}_{C,C}$ (Green's functions for the effected nodes C) is needed

Woodbury for $\mathbf{A}^T \mathbf{S} \mathbf{A}$ systems 1

Can we do better for our system structure?

Assume

$$\mathbf{K}_{\text{old}} = \mathbf{A}^T \mathbf{C} \mathbf{A}^T, \quad (27)$$

with \mathbf{S} being a $m \times m$ diagonal matrix and \mathbf{A} being a $m \times n$ matrix.

$$\mathbf{K}_{\text{new}} = \mathbf{A}^T \mathbf{C} \mathbf{A} + \mathbf{A}^T \mathbf{C}_{\Delta} \mathbf{A}, \quad (28)$$

With the decomposition: $\mathbf{U} = \mathbf{A}^T$ and $\mathbf{W}^T = \mathbf{C}_{\Delta} \mathbf{A}$, the Woodbury is given as

$$\mathbf{K}_{\text{new}}^{-1} = \mathbf{K}_{\text{old}}^{-1} - \mathbf{K}_{\text{old}}^{-1} \mathbf{A}^T (\mathbf{I} + \mathbf{C}_{\Delta} \mathbf{A} \mathbf{K}_{\text{old}}^{-1} \mathbf{A}^T)^{-1} \mathbf{C}_{\Delta} \mathbf{A} \mathbf{K}_{\text{old}}^{-1}, \quad (29)$$

Is there a way to replace $\mathbf{K}_{\text{old}}^{-1}$?

Woodbury for $A^T CA$ systems 2

Assume

$$K_{\text{old}}^{-1} = J_1^{-1} C^{-1} J_2^{-T}, \quad (30)$$

Thus

$$A^T CA J_1^{-1} C^{-1} J_2^{-T} = I. \quad (31)$$

- $CC^{-1} = I \dots \checkmark$
- $A^T J_2^{-T} = I \dots J_2^{-T}$? Pseudo inverse

$$J_2^{-1} = \underbrace{(AA^T)^{-1}}_{\text{Laplacian}} A \quad (32)$$

- $AJ_1^{-1} = I \dots$ not possible

Woodbury for $A^T C A$ systems 3

J_1^{-1} is a problem. However, lets insert it into the inverse of the Woodbury matrix

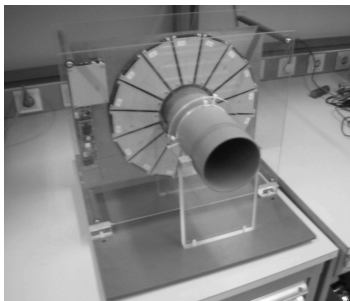
$$(I + C_{\Delta} A K_{\text{old}}^{-1} A^T)^{-1} = (I + C_{\Delta} A J_1^{-1} C^{-1} J_2^{-T} A^T)^{-1}, \quad (33)$$

$$= (I + C_{\Delta} C^{-1} J_2^{-T} A^T)^{-1}, \quad (34)$$

- Instead of $G_{C,C}$ now only the diagonal matrix S has to be inverted. J_2^{-T} can be computed in advance.
- Again, this form can be reduced and Green's functions can be used on the left and right hand side!

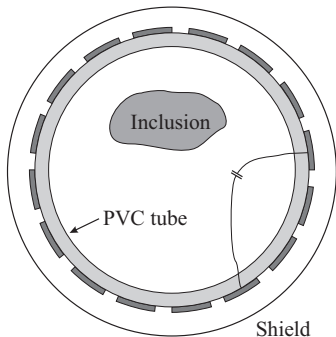
Electrical Capacitance Tomography

- Inverse problem using capacitance measurements.
- Ill-posed \rightarrow regularization or prior knowledge required.
- Suitable for process tomography due to good contrast of the permittivity (i.e. oil/water).
- Noninvasive.
- Cheap instrumentation but low spatial resolution due to soft field.
- Non ionizing \rightarrow safe.



Neumayer et. al.: Current Reconstruction Algorithms in Electrical Capacitance Tomography, Springer 2010

Electrical Capacitance tomography



- Ω : whole domain
- Ω_{ROI} : interior of the pipe.
- $\partial\Omega_{ROI}$: interior of the pipe.

PDE:

$$\nabla \cdot (\epsilon_0 \epsilon_r \nabla V) = 0, \quad (35)$$

BC:

$$V_{\partial\Omega} = 0, \quad (36)$$

$$V_{\Gamma_i} = V_{\Gamma_i}, \quad (37)$$

$$V_{\Gamma_j} = 0 \quad \forall j \neq i, \quad (38)$$

Gauss law:

$$C_{i,j} = -\frac{1}{V_{\Gamma_i}} \oint_{\Gamma_j} \epsilon_0 \epsilon_r \nabla V \cdot \vec{n} d\Gamma. \quad (39)$$

Gives a $N_{elec} \times N_{elec}$ matrix.

Standard computations: $F : \varepsilon \mapsto \mathbf{C}$

Finite element system:

$$\mathbf{K} = \sum_{i=1}^{N_e} \varepsilon_i \mathbf{K}_{e,i}, \quad (40)$$

With BC:

$$\hat{\mathbf{K}} \mathbf{v} = \mathbf{r}. \quad (41)$$

Charge method:

$$Q_{elec} = \sum_{n_{elec}} (\mathbf{K} \mathbf{v})_{n_{elec}}, \quad (42)$$

Derivatives:

$$dC_{i,j} = \gamma_j^T \left[\left[\frac{\partial \mathbf{r}}{\partial \varepsilon_k} \right] - \left[\frac{\partial \hat{\mathbf{K}}}{\partial \varepsilon_k} \right] \mathbf{v}_i \right] d\varepsilon_k, \quad (43)$$

Fast material update

Eigenvector decomposition:

$$\mathbf{K}_e = \mathbf{V}_e \mathbf{D}_e \mathbf{V}_e^{-1}, \quad (44)$$

If $\mathbf{K}_e = \mathbf{K}_e^T$:

$$\mathbf{K}_e = \mathbf{A}_e^T \mathbf{S}_e \mathbf{A}_e, \quad (45)$$

For FE system

$$\mathbf{K} = \mathbf{K}_{ini} + \sum_{l=1}^p \mathbf{A}_l^T \mathcal{E} \mathbf{A}_l, \quad (46)$$

with \mathbf{K}_{ini} such that \mathbf{K} has full rank (includes the BC).

Charge map: $Q_C : V_{\partial\Omega_{ROI}} \mapsto \Delta Q$

How does the potential on the tube influences the charge on the electrodes?

Solve

$$\nabla \cdot (\epsilon_0 \epsilon_r \nabla V) = 0 \quad (47)$$

in $\Omega \setminus \Omega_{ROI}$ with BC:

$$V_{\partial\Omega} = 0, \quad (48)$$

$$V_{\partial\Omega_{ROI}} = \delta(\mathbf{x} - \mathbf{x}_i) \quad \forall \mathbf{x}_i \in \partial\Omega_{ROI} \quad (49)$$

$$V_{\Gamma_j} = 0 \quad \forall j, \quad (50)$$

Discrete version $Q_C : \mathbf{v}_{\partial\Omega_{ROI}} \mapsto \Delta Q$

$$\mathbf{Q} = \mathbf{Q}_a + \mathbf{Q}_C \mathbf{V}_{\partial\Omega_{ROI}}, \quad (51)$$

$\mathbf{V}_{\partial\Omega_{ROI}}$ contains the nodal potentials on $\partial\Omega_{ROI}$

Solution with Green's functions

$$\hat{\mathbf{K}}\mathbf{G} = \mathbf{E}_{\partial\Omega_{ROI}}, \quad (52)$$

$$\mathbf{V}_{\partial\Omega_{ROI}} = \mathbf{G}^T \mathbf{R}, \quad (53)$$

\mathbf{R} contains the right hand side terms for each electrode.

$$\mathbf{Q} = \mathbf{Q}_a + \mathbf{Q}_c \underbrace{\mathbf{G}^T \mathbf{R}}_{\mathbf{V}_{\partial\Omega_{ROI}}}, \quad (54)$$

... is bad, because $\mathbf{E}_{\partial\Omega_{ROI}}$ in equation (52) means the solution for all nodes on $\partial\Omega_{ROI}$.

Trick:

$$\hat{\mathbf{K}}\mathbf{G}\mathbf{Q}_c^T = \mathbf{E}_k \mathbf{Q}_c^T, \quad (55)$$

$$\hat{\mathbf{K}}\mathbf{G}_Q = \mathbf{E}_k \mathbf{Q}_c^T = \mathbf{R}_Q, \quad (56)$$

Hence:

$$\mathbf{Q} = \mathbf{Q}_a + \mathbf{G}_Q^T \mathbf{R}. \quad (57)$$

Jacobian operations for ECT

- Linearization: $J : \varepsilon \mapsto \mathbf{Q}$

$$d\mathbf{Q} = -\mathbf{G}_Q^T \hat{\mathbf{K}}_{d\varepsilon} \mathbf{G}_Q \quad (58)$$

$$d\mathbf{Q} = -\mathbf{G}_Q^T \left[\sum_I^p \mathbf{A}_I^T d^{\mathcal{E}} \mathbf{A}_I \right] \mathbf{G}_Q. \quad (59)$$

- Gradient: $J^T : \mathbf{Q} \mapsto \varepsilon$

$$\mathbf{J}^T \mathbf{q} = -\text{diag} \left(\left(\sum_{I=1}^p (\mathbf{G}_Q^T \mathbf{A}_I^T)^T (\mathbf{Q} \mathbf{G}_Q^T \mathbf{A}_I) \right) \right), \quad (60)$$

Low Rank updates for ECT

- With computation of the additional Green's Funcions

$$\Delta \mathbf{Q} = -\gamma \mathbf{G}_Q^T \mathbf{L} (\mathbf{I} + \gamma \mathbf{U}_{:,C} \mathbf{G}_{C,C} \mathbf{L}_{C,:})^{-1} \mathbf{U} \mathbf{G}_Q, \quad (61)$$

- $\mathbf{A}^T \mathbf{C} \mathbf{A}$ form

$$\Delta \mathbf{Q} = -\mathbf{G}_{Q,C_2,:}^T \mathbf{A}_{1,:C}^T \left(\mathbf{I} + \mathbf{S}_C \mathbf{S}_{0,C}^{-1} \mathbf{W}_{3,:C}^T \mathbf{W}_{1,:C} \right)^{-1} \mathbf{S} \mathbf{W}_{1,:C}^T \mathbf{G}_{Q,C_2,:}, \quad (62)$$

A speed comparison

| Operation/Method | t_{mesh1} | t_{mesh2} |
|---|-------------|-------------|
| | ms | ms |
| Forward problem standard | 96 | 640 |
| Forward problem new | 4.8 | 26 |
| Standard material update | 35.5 | 230 |
| Fast material update | 0.039 | 2 |
| Matrix inversion | 3.3 | 19 |
| Jacobian by AVM | 360 | > 2000 |
| Jacobian op. $J : \varepsilon \mapsto \mathbf{Q}$ | 0.48 | 3.9 |
| Jacobian transp. op. $J^T : \mathbf{Q} \mapsto \varepsilon$ | 3.3 | 15.5 |
| Exact low rank update (1 elem.) | 3.5 | 16.3 |
| WSW^T Woodbury (1 elem.) | 0.66 | 4.2 |
| Exact low rank update (20 elem.) | 11.6 | 55.4 |
| WSW^T Woodbury (20 elem.) | 2.7 | 14.1 |
| Exact update 1 elem \times 20 | 5.6 | 18 |
| WSW^T Woodbury 1 elem \times 20 | 1.1 | 3 |
| Domain d. by Schur c. | 23.8 | 66 |
| Schur c. with Cho. | 2.9 | 8 |
| Woodb. for Schur c. with Chol. | 0.895 | 17.1 |

Fast Deterministic Method

$$\mathbf{x}^* = \operatorname{argmin}_{\mathbf{x}} \left\| F(\mathbf{x}) - \tilde{\mathbf{d}} \right\|_2^2 + \alpha \mathbf{x}^T \mathbf{L}^T \mathbf{L} \mathbf{x}, \quad (63)$$

Gauss Newton method:

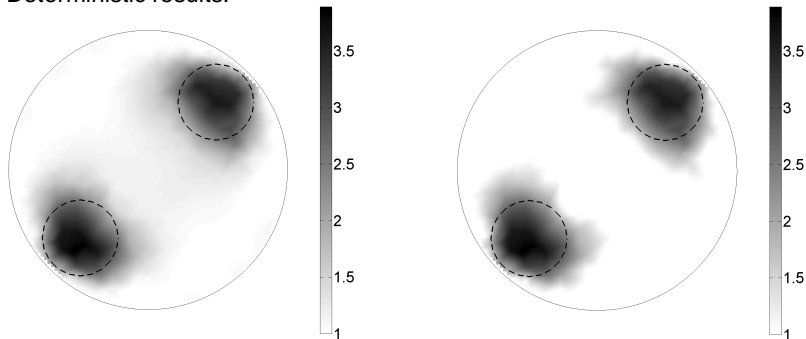
$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{s} \left(\mathbf{J}^T \mathbf{J} + \alpha \mathbf{L}^T \mathbf{L} \right)^{-1} \left(\mathbf{J}^T \mathbf{r}_k + \mathbf{L}^T \mathbf{L} \mathbf{x}_k \right), \quad (64)$$

BFGS scheme:

- 1 Evaluate the Newton direction $\mathbf{p}_k = -\mathbf{H}_k^{-1} \mathbf{g}_k$
- 2 Find s to set $\mathbf{x}_{k+1} = \mathbf{x}_k + s \mathbf{p}_k$ and set $\mathbf{s}_k = s \mathbf{p}_k$
- 3 Compute $\mathbf{y}_k = \mathbf{g}(\mathbf{x}_{k+1}) - \mathbf{g}(\mathbf{x}_k)$.
- 4 Evaluate $\mathbf{H}_{k+1}^{-1} = \mathbf{H}_k^{-1} + \frac{\mathbf{s}_k^T \mathbf{y}_k + \mathbf{y}_k^T \mathbf{H}_k^{-1} \mathbf{y}_k}{(\mathbf{s}_k^T \mathbf{y}_k)^2} \mathbf{s}_k \mathbf{s}_k^T - \frac{\mathbf{H}_k^{-1} \mathbf{y}_k \mathbf{s}_k^T + \mathbf{s}_k \mathbf{y}_k^T \mathbf{H}_k^{-1}}{(\mathbf{s}_k^T \mathbf{y}_k)^2}$.

Bayesian Inversion

Deterministic results:



About 50 iterations per second are possible on a standard PC.

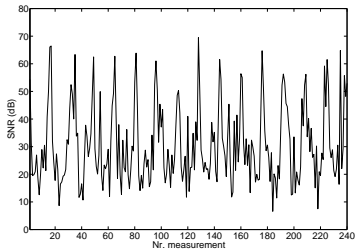
Bayesian Inversion

- Posterior to sample from

$$\pi(\mathbf{x}|\tilde{\mathbf{d}}) \propto \exp\left(-\frac{1}{2}\mathbf{e}^T\boldsymbol{\Sigma}_v^{-1}\mathbf{e}\right) \exp\left(-\frac{1}{2}\alpha\mathbf{x}^T\mathbf{L}^T\mathbf{L}\mathbf{x}\right) l(\mathbf{x}). \quad (65)$$

- \mathbf{L} : smoothing prior

Signal disturbed by additive Gaussian noise.



How to implement a Gibbs sampler

- General Steps

- 1 Draw a conditional sample.
- 2 If the new sample is accepted, compute the new forward map to obtain the new Green's functions \mathbf{G}_Q for the cheap evaluation of the next conditional sample.

Versions:

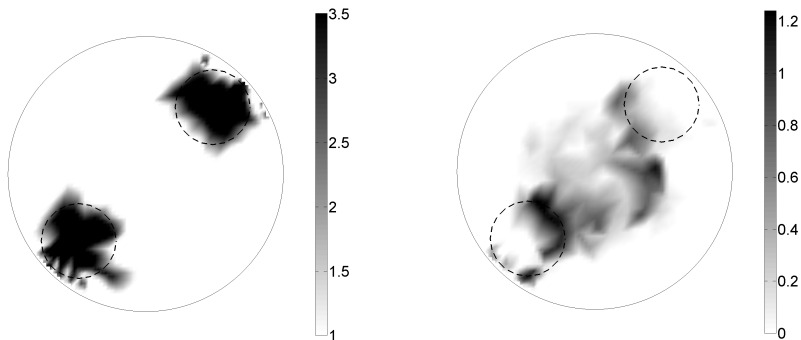
- Bimodal (two valued) material distributions
- General material values

Bimodal Material Distributions

■ Computation steps:

- 1 Flip one element of \mathbf{x} to generate the proposal \mathbf{x}' .
- 2 Compute the likelihood ratio $\alpha = \min \left[1, \frac{\pi(\mathbf{x}'|\tilde{\mathbf{d}})}{\pi(\mathbf{x}|\tilde{\mathbf{d}})} \right]$.
- 3 Accept \mathbf{x}' with probability α .

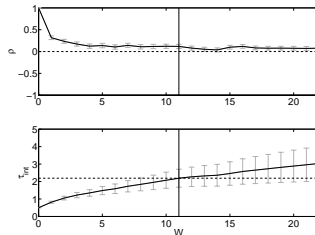
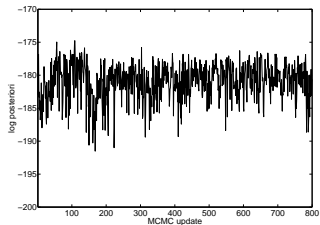
Bimodal Material Distributions



- Mean estimate and standard deviation
- About 3 frames per second are possible using the Jacobian operations

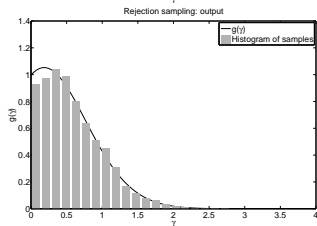
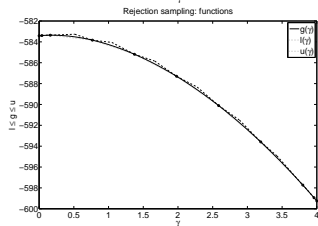
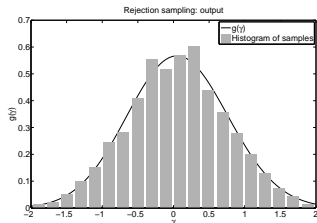
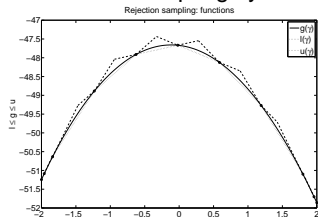
Bimodal Material Distributions

Behavior of the chain

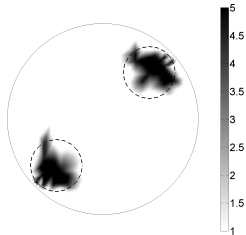
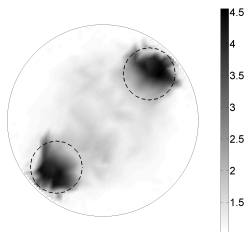


General Gibbs Sampler

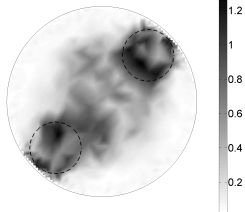
Conditional sampling by ARS



Gibbs Sampler

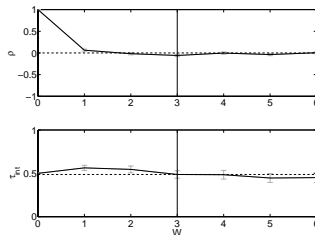
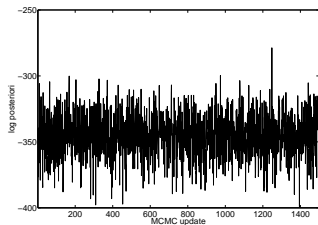


We use a reduced version of ARS
- not the correct statistic (can be worked out), but fast. A sample in the time of an optimization result!



Gibbs Sampler

Behavior of the chain



- And this is just the most trivial version of a Gibbs sampler!

Summary

- Inverse problems
- General introduction to $\mathbf{A}^T \mathbf{C} \mathbf{A}$ systems
- Computational aspects
- Fast low rank updates
- Example on ECT

→ with some tricks we can generate samples in the time of an optimization run.

Neumayer and Fox, JUQ 2013