Recent Results on L1-type Priors in Bayesian Inverse Problems

Shanghai International Workshop on Recent Advances
in Inverse Problems and Imaging Science
Shanghai Jiao Tong University

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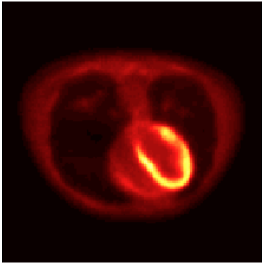
21.09.2013

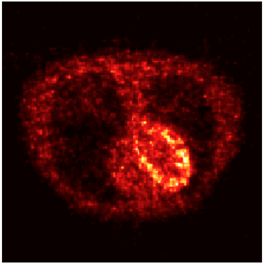
Sparsity Constraints in Inverse Problems

Current trend in high dimensional inverse problems: Sparsity constraints.

- Compressed Sensing: High quality reconstructions from a small amount of data, if a sparse basis/dictionary is a-priori known (e.g., wavelets).
- Total Variation (TV) imaging: Sparsity constraints on the gradient of the unknowns.



(a) 20 min, EM



(b) 5 sec, EM

(c) 5 sec, Bregman EM-TV

Thank's to Jahn Müller for these images!

Sparsity Constraints in Variational Regularization

Commonly applied formulation and analysis by means of variational regularization, mostly by incorporating L1-type norms:

$$\hat{u}_\alpha = \underset{u \in \mathbb{R}^n}{\operatorname{argmin}} \left\{ \|f - K\, u\|_2^2 + \alpha \, |D\, u|_1 \right\}$$

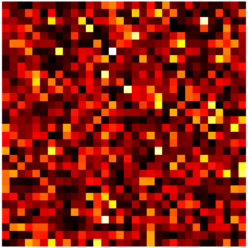
assuming additive Gaussian i.i.d. noise $\sim \mathcal{N}(0, \sigma^2)$

Martin Burger

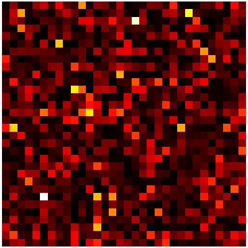
Sparsity Constraints in the Bayesian Approach

Sparsity as a-priori information are encoded into the prior distribution $p_{prior}(u)$:

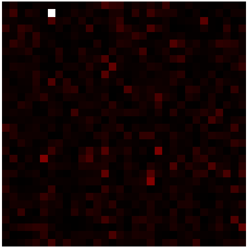
1. Turning the functionals used in variational regularization directly into priors, e.g., L1-type priors:
   - Convenient, as prior is log-concave.
   - MAP estimate is sparse, but the prior itself is not sparse.
2. Hierarchical Bayesian modeling: Sparsity is incorporated at a higher level of the model.
   - Relies on a slightly different concept of sparsity.
   - Resulting implicit priors over unknowns are usually not log-concave.



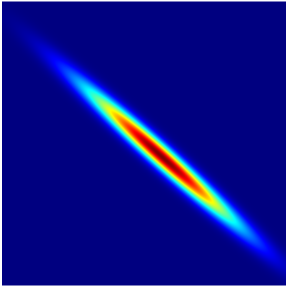
(a) $\exp\left(-\frac{1}{2}\|u\|_2^2\right)$



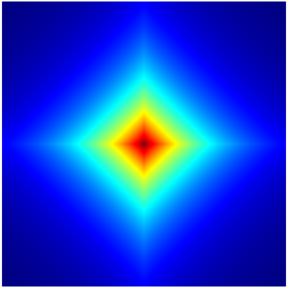
(b) $\exp\left(-|u|_1\right)$



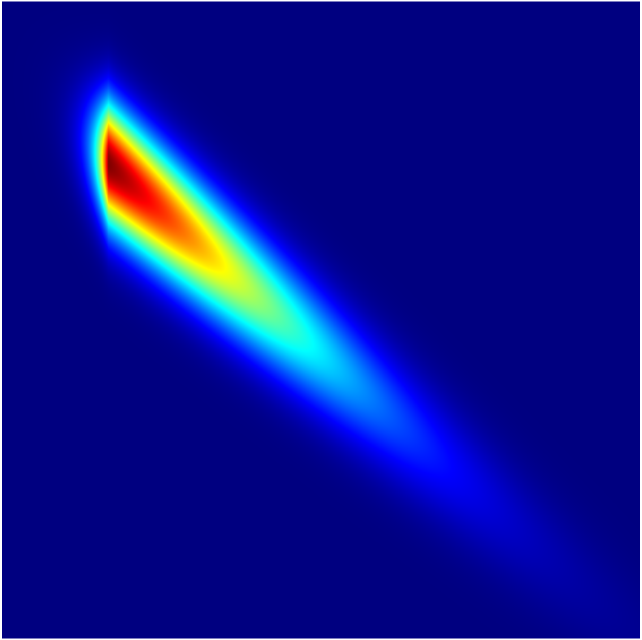
(c) $(1+u^2/3)^{-2}$



Likelihood:
$\exp\left(-\frac{1}{2\,\sigma^2}\|f - K\,u\|_2^2\right)$



Prior: $\exp\left(-\lambda\;|u|_1\right)$
(λ via discrepancy principle)



Posterior: $\exp\left(-\frac{1}{2\,\sigma^2}\|f - K\,u\|_2^2 - \lambda\;|u|_1\right)$

Bayesian Inference and Computational Techniques

Things we might want to do with the posterior:

- Point estimates: MAP and CM.
- Credible regions estimates
- Extreme value probabilities
- Conditional covariance estimates
- Histogram estimates
- Generalized Bayes estimators
- Marginalization of nuisance parameters & Approximation error modeling
- Model selection or averaging
- Experiment design

Computationally, this needs

- high-dimensional optimization[1]
- high-dimensional integration
- a mix of both.

[1] All MAP estimates here computed with Split Bregman method: Goldstein & Osher, *The Split Bregman method for L1-regularized problems*, SIAM J Img Sci, 2009.

MAP vs. CM Estimates: Variational Regularization vs. Bayesian Inference?

Most simple Bayesian inference technique: Point estimates.

1. Maximum a-posteriori-estimate (MAP):

$$\hat{u}_{\mathrm{MAP}} := \operatorname*{argmax}_{u \in \mathbb{R}^n} \; p_{post}(u|f)$$

   Practically: High-dimensional optimization problem.
   Direct correspondence to variational regularization.

2. Conditional mean-estimate (CM):

$$\hat{u}_{\mathrm{CM}} := \mathbb{E}\left[u|f\right] = \int_{\mathbb{R}^n} u \; p_{post}(u|f) \mathrm{d}u$$

   Practically: High-dimensional integration problem.

Difference between MAP and CM estimate?

MAP vs. CM Estimates: Variational Regularization vs. Bayesian Inference?

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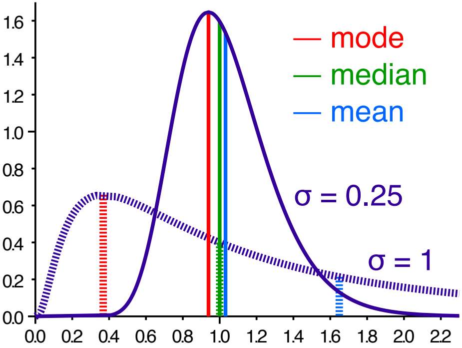
Difference between MAP and CM estimate?

$\rightsquigarrow$ Most interesting question for comparing variational regularization and Bayesian inference?

Outline

MAP vs. CM Estimates: The Classical View

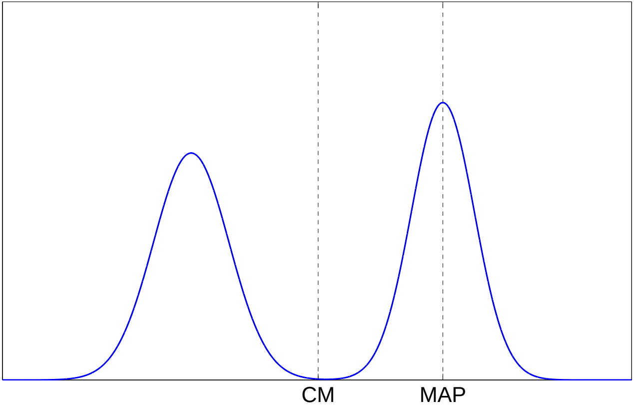


source: Wikimedia Commons

- CM estimate is the mean of the posterior
- MAP estimate the (highest) mode of the posterior.

MAP vs. CM Estimates: The Classical View

Hypothetical distributions to show that none is better in general.



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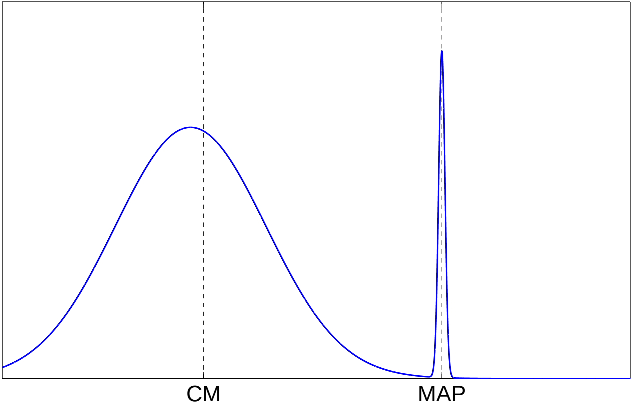

MAP vs. CM Estimates: The Classical View

A theoretical argument “decides” the conflict: The Bayes cost formalism.

- An estimator is a random variable, as it relies on f and u.
- How does it perform on average? Which estimator is “best”?
- $\rightsquigarrow$ Define a cost function $\Psi(u, \hat{u}(f))$.
- Bayes cost is the expected cost:

$$BC(\hat{u}) = \iint \Psi(u, \hat{u}(f)) \, p_{like}(f|u) \, \mathrm{d}f \, p_{prior}(u) \, \mathrm{d}u$$

- Bayes estimator $\hat{u}_{BC}$ for given Ψ minimizes Bayes cost.

MAP vs. CM Estimates: The Classical View

Main classical arguments pro CM and contra MAP estimates:

- CM is Bayes estimator for $\Psi(u, \hat{u}) = \|u - \hat{u}\|_2^2$ (MSE).
- Also the minimum variance estimator.
- The mean value is intuitive, it is the "center of mass", the known "average".
- MAP estimate can be seen as an asymptotic Bayes estimator of

$$\Psi_\epsilon(u, \hat{u}) = \begin{cases} 0, & \text{if} \quad \|u - \hat{u}\|_\infty \leqslant \epsilon \\ 1 & \text{otherwise,} \end{cases}$$

for $\epsilon \to 0$ (uniform cost). $\Longrightarrow$ It is not a proper Bayes estimator.

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- MAP and CM seem theoretically and computationally fundamentally different $\Longrightarrow$ one should decide.
- *"A real Bayesian would not use the MAP estimate"*
- People feel "ashamed" when they have to compute MAP estimates (even when their results are good).

Outline

Some Observations...

The discrimination of the MAP estimate is not intuitive.

Gaussian priors: MAP = CM. Funny coincidence?

Non-Gaussian priors:

- Theoretical considerations could often not be validated numerically
- CM as the mysterious, inaccessible estimate.

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Gaussian priors: MAP $=$ CM. Funny coincidence?

Non-Gaussian priors:

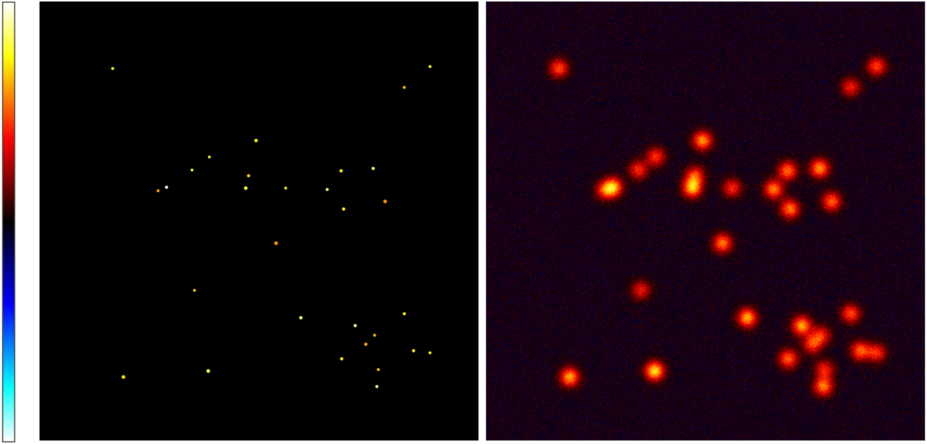
- Theoretical considerations could often not be validated numerically
- CM as the mysterious, inaccessible estimate.

Need for computational tools for CM estimation (and beyond!)

F. L., 2012.
Fast Markov chain Monte Carlo sampling for sparse Bayesian inference in high-dimensional inverse problems using L1-type priors
Inverse Problems, 28(12). arXiv:1206.0262v2.

Outline

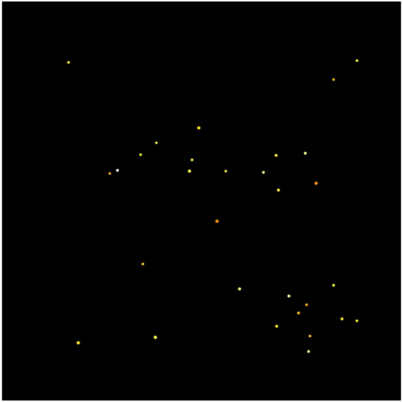
Image Deblurring Example in 2D



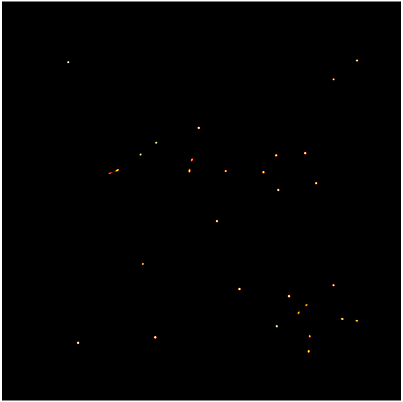
Unknown function $\tilde{u}$ Measurement data f

- Gaussian blurring + relative noise level of 10%
- Reconstruction using simple L1 prior
- $n = 1023 \times 1023 = 1\,046\,529$.

Image Deblurring Example in 2D



(d) Unknown function $\tilde{u}$



(e) MAP estimate by Split Bregman

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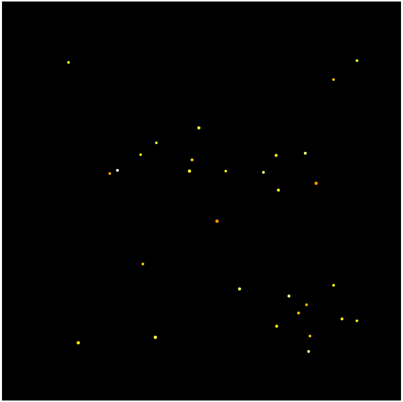
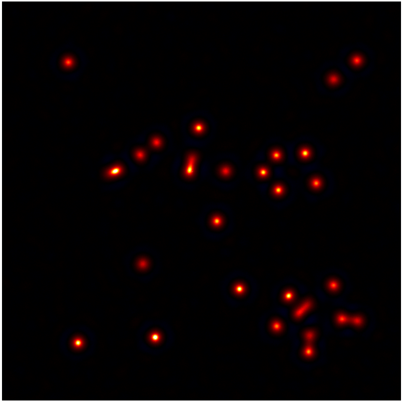


(a) Unknown function $\tilde{u}$



(b) CM estimate by our Gibbs sampler

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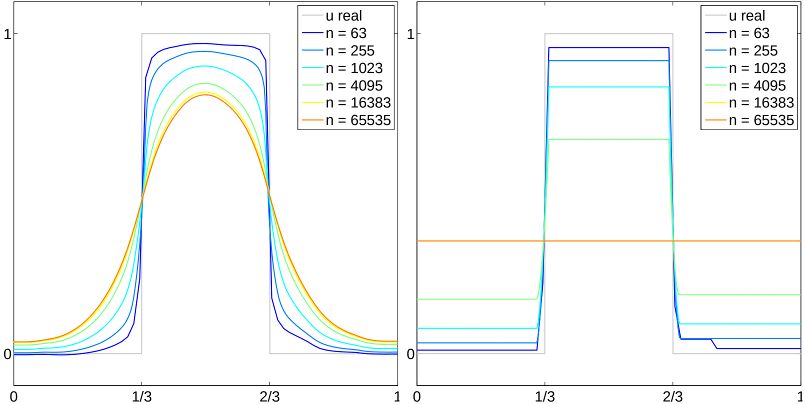
The Discretization Dilemma of the TV prior (Lassas & Siltanen, 2004)

"Can one use total variation prior for edge-preserving Bayesian inversion?"

- For $\lambda_n \propto \sqrt{n+1}$ and $n \longrightarrow \infty$ the TV prior converges to a smoothness prior.
- CM converges to smooth limit.
- MAP converges to constant.



(a) CM by our Gibbs Sampler

(b) MAP by Split Bregman

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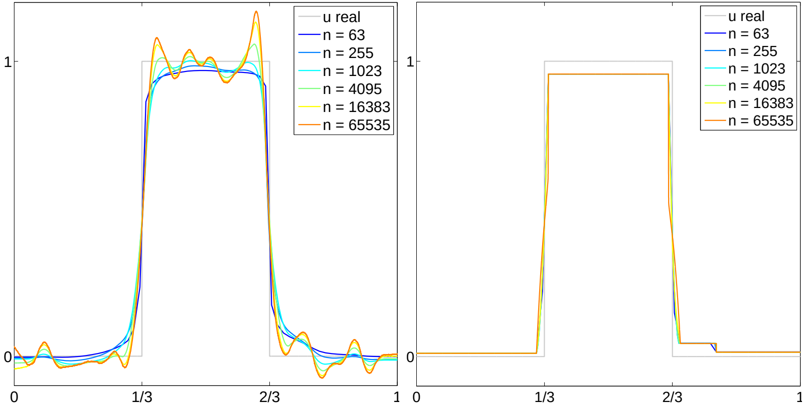

(a) CM by our Gibbs Sampler (b) MAP by Split Bregman

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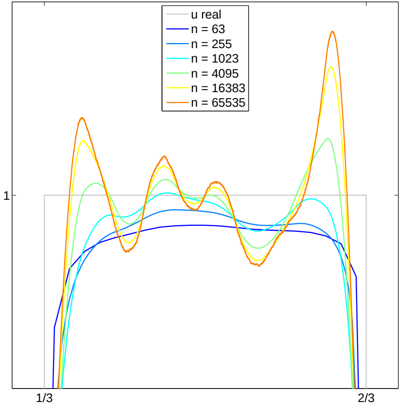
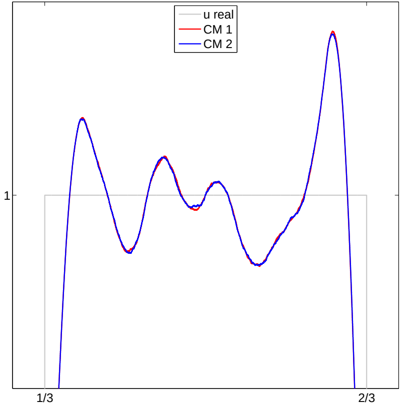


(a) Zoom into CM estimates



(b) MCMC convergence check

Discretization Invariant Besov Priors

Question: Is it possible to construct discretization invariant and edge-preserving priors for Bayesian inversion?

- M. Lassas, E. Saksman, and S. Siltanen, 2009.
  Discretization invariant Bayesian inversion and Besov space priors.
- V. Kolehmainen, M. Lassas, K. Niinimäki, and S. Siltanen, 2012.
  Sparsity-promoting Bayesian inversion.
- K. Hämäläinen, A. Kallonen, V. Kolehmainen, M. Lassas, K. Niinimäki, and S. Siltanen, 2013.
  Sparse tomography.

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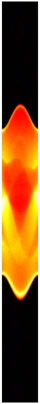
Sparse tomography.

An interesting and important scenario to implement our L1 sampler!

Computational Scenario

real solution u



data f

colormap

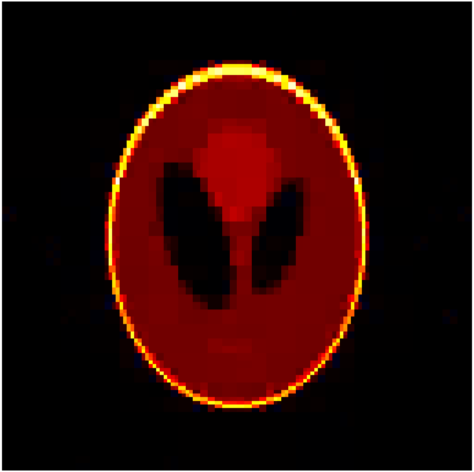
- CT using only 45 projection angles
- 500 measurement pixel
- 1 % relative Gaussian noise added.

Reconstructions for $\lambda = 2e4$, $n = 64\times 64 = 4.096$

MAP estimate (by Split Bregman)

CM estimate (by our Gibbs sampler)

Reconstructions for $\lambda = 2e4$, $n = 128\times128 = 16.384$



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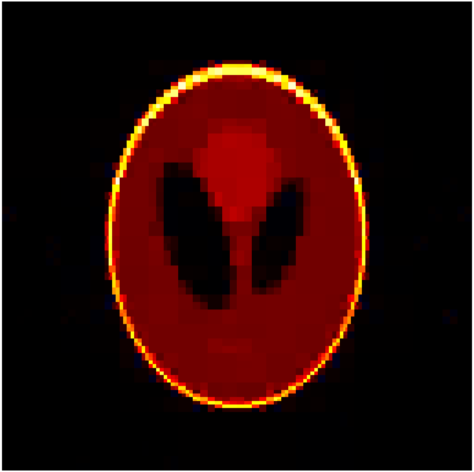
Reconstructions for $\lambda = 2e4$, $n = 256 \times 256 = 65.536$



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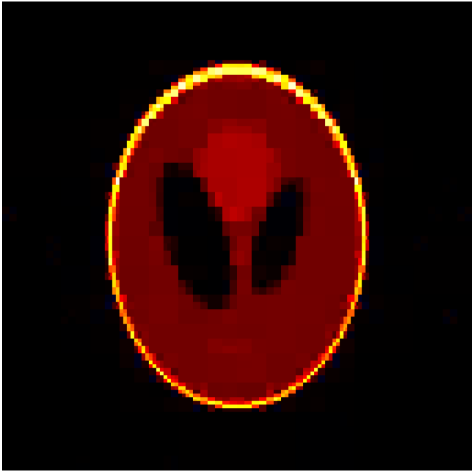
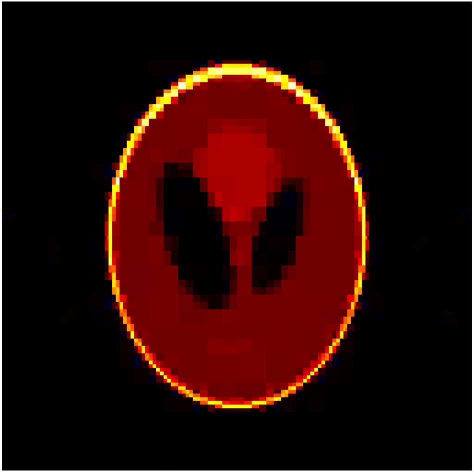
Reconstructions for $\lambda = 2e4$, $n = 512{\times}512 = 262.144$



MAP estimate (by Split Bregman)

CM estimate (by our Gibbs sampler)

Reconstructions for $\lambda = 2e4$, $n = 1024\times1024 = 1.048.576$



MAP estimate (by Split Bregman)

CM estimate (by our Gibbs sampler)

Posterior Samples for $\lambda = 2e4$, $n = 1024{\times}1024 = 1.048.576$

Abbildung : Sample 1

Posterior Samples for $\lambda = 2e4$, $n = 1024{\times}1024 = 1.048.576$

Abbildung : Sample 2

Posterior Samples for $\lambda = 2e4$, $n = 1024 \times 1024 = 1.048.576$

Abbildung : Sample 3

Posterior Samples for $\lambda = 2e4$, $n = 1024{\times}1024 = 1.048.576$

Abbildung : Sample 4

Posterior Samples for $\lambda = 2e4$, $n = 1024{\times}1024 = 1.048.576$

Abbildung : Sample 5

First Results for Sample-Based Tomography with Besov Priors

In line with former results, we have a sampler that works for $n > 10^6$

First reconstructions supports former results of:

V. Kolehmainen, M. Lassas, K. Niinimäki, and S. Siltanen, 2012.
Sparsity-promoting Bayesian inversion.

- discretization invariant.
- MAP and CM coincide for large λ.

A lot of future work to do!

Outline

Summary of Observations and Discussions

- Gaussian priors: MAP = CM. Funny coincidence?
- For reasonable priors, CM and MAP look quite similar. Fundamentally different?
- If a CM estimate looks good, it looks like the MAP estimate.
- MAP estimates are sparser, sharper, look and perform better,...
- Gribonval, 2011: CM are MAP estimates for different priors.

Bayesian Inversion from a Bregman Distance Perspective

Assume

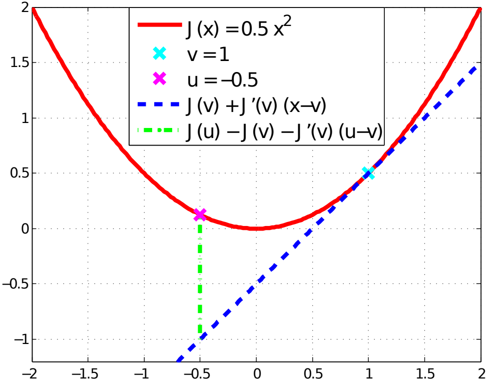
- Linear K
- Additive Gaussian noise: $\mathcal{N}(0, \Sigma_\varepsilon)$
- Log-concave prior, i.e., $p_{prior}(u) \propto \exp\left(-\lambda \mathcal{J}(u)\right)$, where $\mathcal{J}(u)$ is convex.

Martin Burger developed several ideas (joint paper in preparation) to shed new light on the issue.

He uses Bregman distances as a main tool.

I will report some key results here.

Excursus: Bregman Distances



source: Michael Möller

$$D_{\mathcal{J}}^{q}(u,v) = \mathcal{J}(u) - \mathcal{J}(v) - \langle q, u - v \rangle, \qquad q \in \partial\mathcal{J}(v)$$

- Basically: difference between $\mathcal{J}(u)$ and its linearization.
- Proven useful in variational regularization.

A False Conclusion

"A real Bayesian would not use the MAP estimate as it is not a proper Bayes estimator".

"MAP estimate can be seen as an asymptotic Bayes estimator of

$$\Psi_\epsilon(u, \hat{u}) = \begin{cases} 0, & \text{if} \quad \|u - \hat{u}\|_\infty < \epsilon \\ 1 & \text{otherwise,} \end{cases}$$

for $\epsilon \rightarrow 0$.
???$\Longrightarrow$??? It is not a proper Bayes estimator."

"MAP estimator is asymptotic Bayes estimator for some degenerate Ψ"
$\not\Rightarrow$ "MAP can't be Bayes estimator for some proper Ψ" !!!!

Two New Bayes Cost Functions

Define

(a) $\Psi_{\mathrm{LS}}(u,\hat{u}) := \|K(\hat{u}-u)\|^2_{\Sigma_\varepsilon^{-1}} + \beta\|L(\hat{u}-u)\|_2^2$

(b) $\Psi_{\mathrm{Brg}}(u,\hat{u}) := \|K(\hat{u}-u)\|^2_{\Sigma_\varepsilon^{-1}} + \lambda D_{\mathcal{J}}(\hat{u},u)$

for a regular L and $\beta > 0$.

Properties:

- Proper, convex cost functions
- For $\mathcal{J}(u) = \beta/\lambda\|Lu\|_2^2$ we have $\lambda D_{\mathcal{J}}(\hat{u},u) = \beta\|L(\hat{u}-u)\|_2^2$, and $\Psi_{\mathrm{LS}}(u,\hat{u}) = \Psi_{\mathrm{Brg}}(u,\hat{u})$!

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Theorems:

(I) The CM estimate is the Bayes estimator for $\Psi_{\text{LS}}(u,\hat{u})$

(II) The MAP estimate is the Bayes estimator for $\Psi_{\text{Brg}}(u,\hat{u})$

The Posterior is Well Centered around the MAP Estimate

"The posterior is well centered around the CM but not around the MAP estimate"

$$\hat{u}_{\mathrm{MAP}} \in \underset{u}{\operatorname{argmin}} \left\{ \frac{1}{2} \| f - K(u) \|^2_{\Sigma_\varepsilon^{-1}} + \lambda \mathcal{J}(u) \right\}$$

Use optimality condition

$$K^* \Sigma_\varepsilon^{-1} (K \hat{u}_{\mathrm{MAP}} - f) + \lambda \hat{p}_{\mathrm{MAP}} = 0, \qquad \hat{p}_{\mathrm{MAP}} \in \partial \mathcal{J}(\hat{u}_{\mathrm{MAP}}).$$

to rewrite posterior in terms of $\hat{u}_{\mathrm{MAP}}$:

$$p_{post}(u|f) \propto \exp\left(-\frac{1}{2} \| K(u - \hat{u}_{\mathrm{MAP}}) \|^2_{\Sigma_\varepsilon^{-1}} - \lambda D_{\mathcal{J}}^{\hat{p}_{\mathrm{MAP}}}(u, \hat{u}_{\mathrm{MAP}}) \right)$$

Posterior energy is sum of two convex functionals both minimized by $\hat{u}_{\mathrm{MAP}}$.

Average Optimality of the CM Estimate

You can show an "average optimality condition" for the CM estimate:

$$\begin{aligned}\mathbb{E}_{(u|f)}[K^*\Sigma_\varepsilon^{-1}(Ku - f) + \lambda\mathcal{J}'(u)] &= K^*(K\Sigma_\varepsilon^{-1}\,\mathbb{E}_{(u|f)}[u] - f) + \lambda\,\mathbb{E}_{(u|f)}[\mathcal{J}'(u)] \\ &= K^*\Sigma_\varepsilon^{-1}(K\hat{u}_{\mathrm{CM}} - f) + \lambda\hat{p}_{\mathrm{CM}} = 0\end{aligned}$$

where $\hat{p}_{\mathrm{CM}} = \int \mathcal{J}'(u)p_{post}(u|f)\mathrm{d}u$ is the CM estimate for the gradient of $\mathcal{J}$.

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where $\hat{p}_{\mathrm{CM}} = \int \mathcal{J}'(u) p_{post}(u|f)\mathrm{d}u$ is the CM estimate for the gradient of $\mathcal{J}$.

Compare it to optimality condition for MAP estimate:

$$K^*\Sigma_\varepsilon^{-1}(K\hat{u}_{\mathrm{MAP}} - f) + \lambda\hat{p}_{\mathrm{MAP}} = 0$$

Difference: $\mathcal{J}'(\mathbb{E}_{(u|f)}[u]) \neq \mathbb{E}_{(u|f)}[\mathcal{J}'(u)]$ (except for Gaussian case).

Furthermore:

$$\begin{aligned}\mathbb{E}_{(u|f)}\, \|L(\hat{u}_{\mathrm{CM}} - u)\|_2^2 &\leqslant \mathbb{E}_{(u|f)}\, \|L(\hat{u}_{\mathrm{MAP}} - u)\|_2^2 \\ \mathbb{E}_{(u|f)}\, D_{\mathcal{J}}(\hat{u}_{\mathrm{MAP}}, u) &\leqslant \mathbb{E}_{(u|f)}\, D_{\mathcal{J}}(\hat{u}_{\mathrm{CM}}, u)\end{aligned}$$

Take Home Messages

- Sample-based Bayesian inversion with sparsity constraints is feasible in high dimensions.
- Computing CM estimates is NOT the only use of it.
- MAP estimates are proper Bayes estimates for a proper, convex cost function, and the posterior is well-centered around them.
- A "real Bayesian" can use them without feeling ashamed.
- Bregman distances are also an interesting tool to analyze Bayesian inversion.
- "MAP vs. CM" is NOT the most interesting question for comparing variational regularization and Bayesian inference.

Thank you for your attention!

Work was part of the Chinese-Finnish-German project
"Sparsity-constrained inversion with tomographic applications"
(*"Inverse Problems Initiative"* of the DFG).

Coordination by **Samuli Siltanen** (Helsinki); four teams:

- Bremen (Germany), PI: Professor **Peter Maass**
- Helsinki (Finland), PI: Professor **Matti Lassas**
- Münster (Germany), PI: Professor **Martin Burger**
- Shanghai (China), PI: Professor **Jianguo Huang**

Single Component Gibbs Sampling

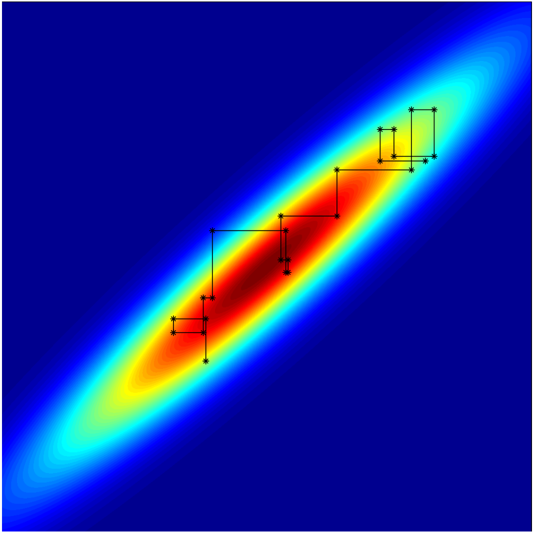
Basic idea:

1. Choose component to update $s \in \{1, \dots, n\}$ (random or systematic).
2. Update u_s by sample from the cond., 1-dim density $p(\,\cdot\,|u_{[-s]})$.

To be fast one needs:

a) fast and explicit comp. of the 1-dim densities.

b) fast, robust and exact sampling from 1-dim densities.



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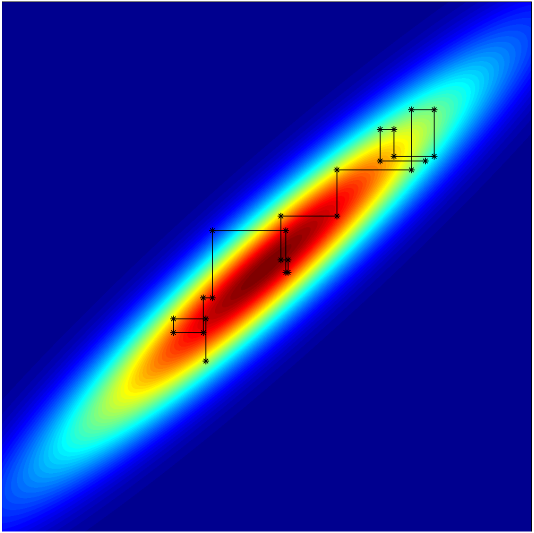
Nasty, involved and time consuming to implement for L1-type priors



Sketch of Gibbs Sampler Implemenation

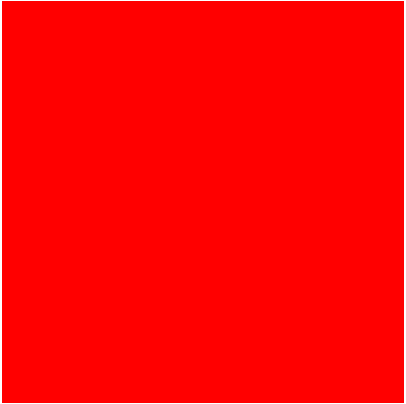
$$p_{post}(u|f) \propto \exp\left(-\frac{1}{2\,\sigma^2}\|f - K\,u\|_2^2 - \lambda\,|Wu|_1\right)$$
$$p_{post}(u|f) \propto \exp\left(-\frac{1}{2\,\sigma^2}\|f - K\,W^{-1}\xi\|_2^2 - \lambda\,|\xi|_1\right)$$

- K: Radon transform of object integrated into measurement sensors.
- W: Haar-Wavelet transform in 2D, $W = [v_1, \ldots, v_n]^T$
- $\xi = Du$: Wavelet coefficients.

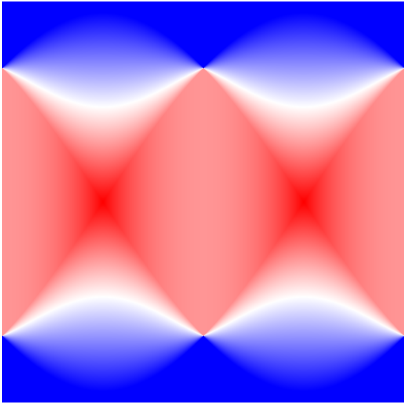
Fast sampling needs fast setup-up of Kv_i, and projection of Kv_i on current residual $(f - K\,W^{-1}\xi)$:

- Haar wavelets consist of 1,2 or 4 rectangles.
- The projection of a rectangle is a symmetric trapezoid.
- Design fast scheme to integrate this into measurement grid.
- Loop over projection angles.

Haar Wavelets & Radon Transforms: $j = 0,\ l = 0,\ k_1 = 0,\ k_2 = 0$

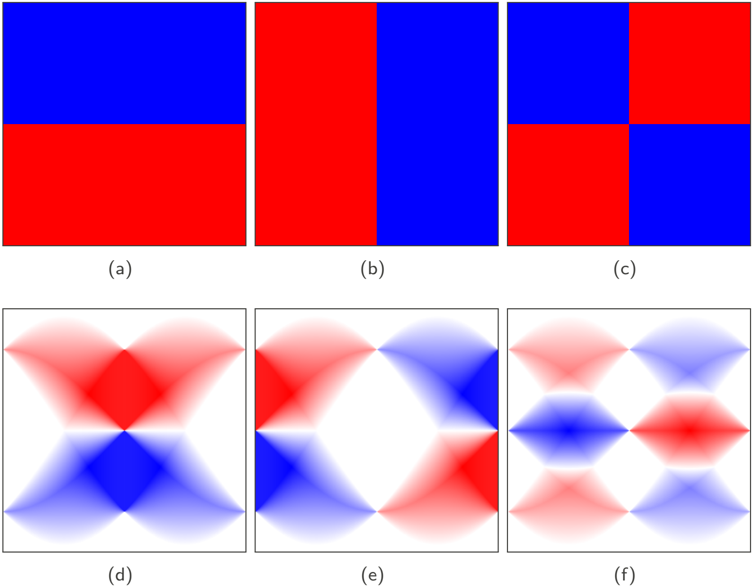


(a)

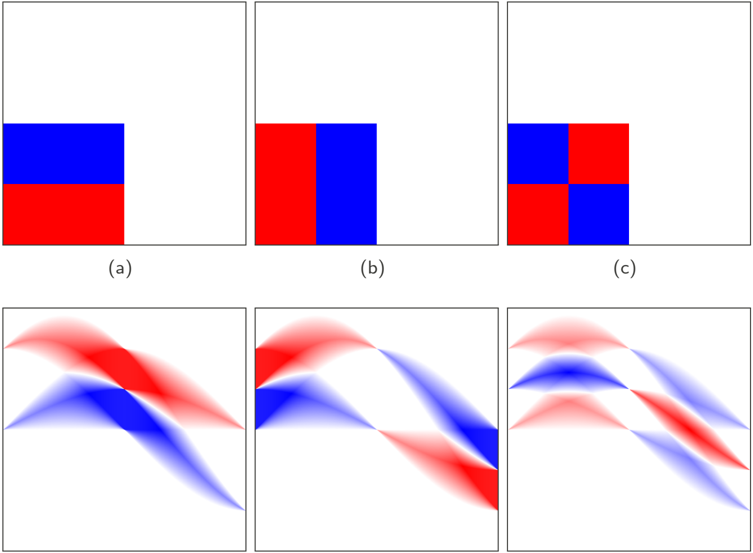


(b)

Haar Wavelets & Radon Transforms: $j = 0,\ l = 1, 2, 3,\ k_1 = 0,\ k_2 = 0$

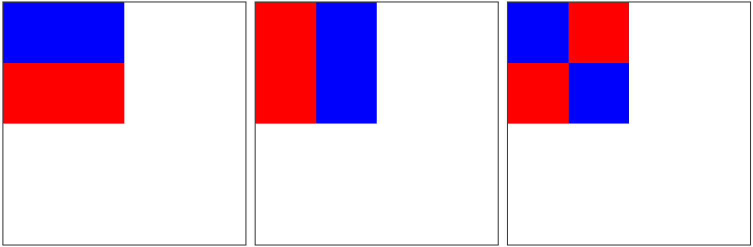


Haar Wavelets & Radon Transforms: $j = 1,\ l = 1, 2, 3,\ k_1 = 0,\ k_2 = 0$



(a) (b) (c) (d) (e) (f)

Haar Wavelets & Radon Transforms: $j = 1,\ l = 1, 2, 3,\ k_1 = 0,\ k_2 = 1$



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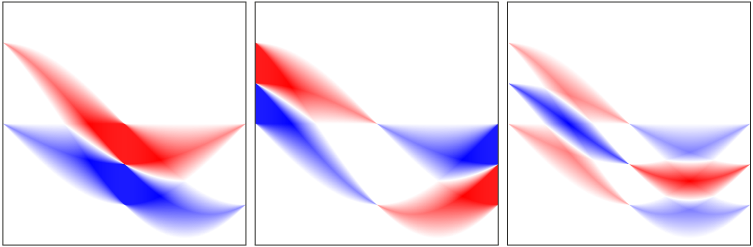
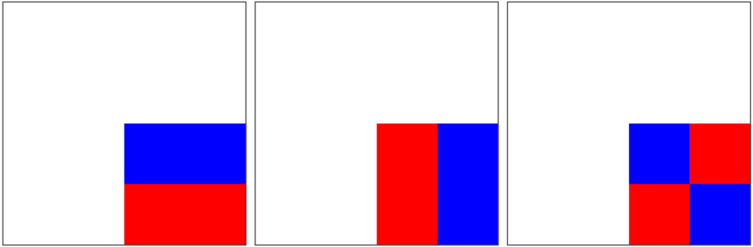


(d) (e) (f)

Haar Wavelets & Radon Transforms: $j = 1,\ l = 1, 2, 3,\ k_1 = 1,\ k_2 = 0$



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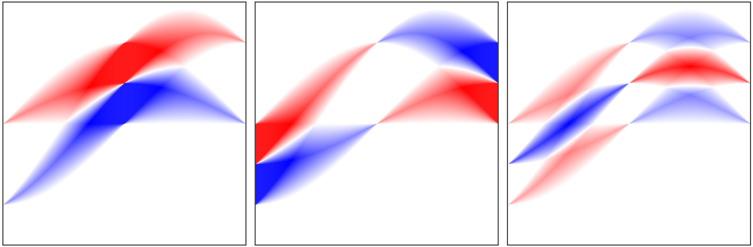

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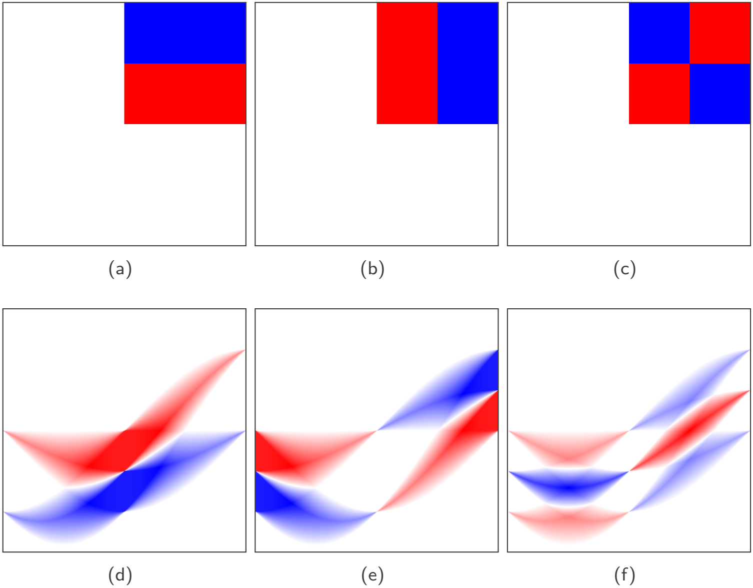
Haar Wavelets & Radon Transforms: $j = 1,\ l = 1, 2, 3,\ k_1 = 1,\ k_2 = 1$



Radon Integration Matrices

For computing MAP estimates we need a fast way to compute $K \cdot u$ and $K^* \cdot v$

Way 1: Matlab's `radon.m`. Turn's out to be problematic:

- ! `iradon.m` is not exact adjoint
- ! Strange offset
- ! Only radon transform, not integrated
- ! Fixed output image size.
- ! Differs from implementation of K used in sampler.

Way 2: Use code to compute integrated radon transform of pixel basis to build K as a sparse matrix.

- ✓ Fast: 3 min vs. 2h with `radon.m`.
- ✓ Size: 400 MB
- ✓ Compatible with sampler implementation
- ✓ Choose offset and output size freely
- ✓ Application of $K \cdot u$ about 2.5 times faster.
- ✓ Code on my website (soon)

Future Work

What happens to the posterior?

- Why do MAP and CM coincide in strongly non-Gaussian situation?
- Role of λ, σ^2: Phase transition?
- Does the covariance concentrate?
- Use Wasserstein distances via embedding?

How can we make more use of the sampler?

- More elaborate inference task.
- Real data.

How to further improve the sampler?

- Single component adaptive Gibbs: Construct Markovian transition kernel from sample history.
- Rao-Blackwellization