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## The Bayesian Approach to Inverse Problems and Imaging: Computational Aspects

Level Set Collective Seminar, UCLA



# Outline

Exemplary Application: Inverse Problems with Sparsity Constraints

Basic Algorithms for Integration-based Posterior Inference

Iterative Optimization and Sampling

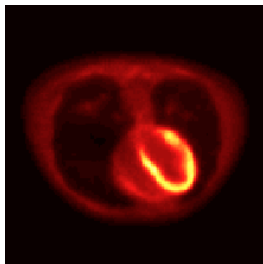
Selected Advanced Topics and Trends (optional)

Take Home Messages, Conclusions & Ongoing Work

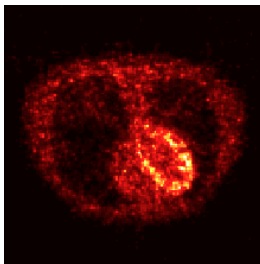
## Sparsity Constraints in Inverse Problems

Current trend in high dimensional inverse problems: **Sparsity constraints**.

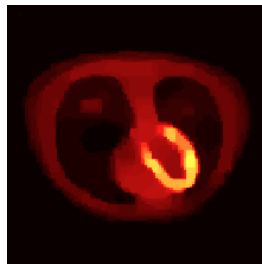
- ▶ **Compressed Sensing**: High quality reconstructions from a small amount of data, if a sparse basis/dictionary is a-priori known (e.g., wavelets).
- ▶ **Total Variation (TV)** imaging: Sparsity constraints on the gradient of the unknowns.



(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:

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

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

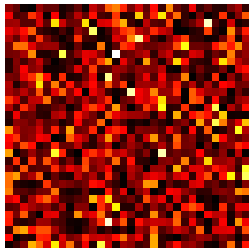
Notation:

- ▶  $f \in \mathbb{R}^k$ : The noisy measurement data given
- ▶  $u \in \mathbb{R}^n$ : The unknowns to recover w.r.t. the chosen discretization
- ▶  $K \in \mathbb{R}^{k \times n}$ : Discretization of the forward operator w.r.t. the domains of  $u$  and  $f$ .
- ▶  $D \in \mathbb{R}^{l \times n}$ : Discrete formulation of the mapping onto the (potentially) sparse quantity.

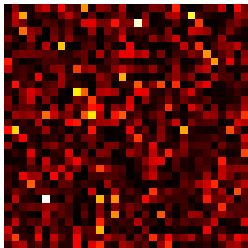
## Sparsity Constraints in the Bayesian Approach

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

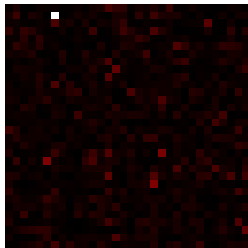
1. Turning the functionals used in variational regularization directly into priors, e.g., **L1-type priors**:
  - ▶ Convenient, as prior is **log-concave**.
  - ▶ MAP estimate is sparse, but the **prior itself is not sparse**.
2. Hierarchical Bayesian modeling: Sparsity is incorporated at a higher level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



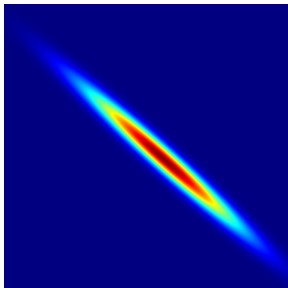
(a)  $\exp\left(-\frac{1}{2}\|u\|_2^2\right)$



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

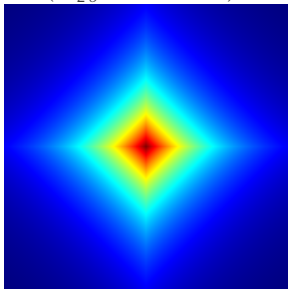


(c)  $(1 + u^2/3)^{-2}$



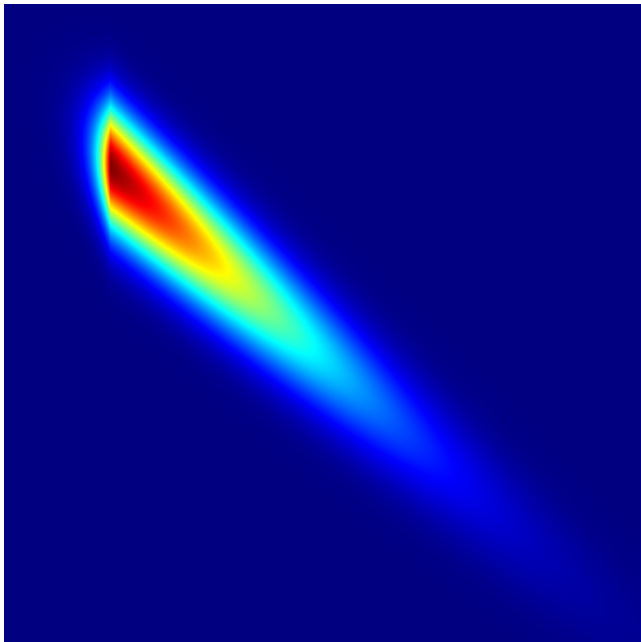
Likelihood:

$$\exp\left(-\frac{1}{2\sigma^2}\|f - Ku\|_2^2\right)$$



Prior:  $\exp(-\lambda |u|_1)$

( $\lambda$  via discrepancy principle)



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

## Reminder: Bayesian Inference and Advanced 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**
- ▶ high-dimensional **integration**
- ▶ a mix of both.

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## Integration-based Inference for Sparse Bayesian Inversion: How I got into this...

I assisted for the computational parts in (S. Comelli, 2011; *A Novel Class of Priors for Edge-Preserving Methods in Bayesian Inversion*) and faced many problems:

- ▶ Standard techniques for high-dimensional integration break down for ill-posed inverse problems.
- ▶ Especially for those with sparsity constraints.

## Integration-based Inference for Sparse Bayesian Inversion: How I got into this...

I assisted for the computational parts in (S. Comelli, 2011; *A Novel Class of Priors for Edge-Preserving Methods in Bayesian Inversion*) and faced many problems:

- ▶ Standard techniques for high-dimensional integration break down for ill-posed inverse problems.
- ▶ Especially for those with sparsity constraints.

⇒ Good example to explain and illustrate the computational aspects of integration-based Bayesian inference. To do so, this talk uses partial results from:



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), 2012; [arXiv:1206.0262v2](https://arxiv.org/abs/1206.0262v2)



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## Monte Carlo Integration in a Nutshell

$$\mathbb{E}[f(x)] = \int_{\mathbb{R}^n} f(x) p(x) dx$$

- ▶ *Traditional Gauss-type quadrature:*

Construct suitable grid  $\{x_i\}_i$ , w.r.t  $\omega(x) := p(x)$  and approximate by  $\sum_{i=1}^K \omega_i f(x_i)$ .  
 $\implies$  Grid construction and evaluation **infeasible** in high dimensions.

- ▶ *Monte Carlo integration idea:*

Generate suitable grid  $\{x_i\}_i$ , w.r.t  $p(x)$  by drawing  $x_i \sim p(x)$  and approximate by  $\frac{1}{K} \sum_{i=1}^K f(x_i)$ . By the *Law of large numbers*:

$$\frac{1}{K} \sum_{i=1}^K f(x_i) \xrightarrow{K \rightarrow \infty} \mathbb{E}_{p(x)}[f(x)] = \int_{\mathbb{R}^n} f(x) p(x) dx$$

in L1 with rate  $O(K^{-1/2})$  (**independent of  $n$** ).

## Markov Chain Monte Carlo

Not able to draw **independent** samples?

↪ With  $\{x_j\}_j$  being an **ergodic Markov chain**, it still works!

**Markov chain Monte Carlo** (MCMC) methods are algorithms to construct such a chain:

- ▶ Huge number of MCMC methods exists.
- ▶ No “universal” method.
- ▶ Most methods rely on one two basic schemes:
  - ▶ Metropolis-Hastings (MH) Sampling [Metropolis et al., 1953; Hastings, 1970]
  - ▶ Gibbs Sampling [Geman & Geman, 1984]
- ▶ Posteriors from inverse problems seem to be “special”.

In this section: Comparison between the **most basic variants** of MH and Gibbs sampling for our specific scenario.

# Symmetric, Random-Walk Metropolis-Hastings Sampling

Basic idea:

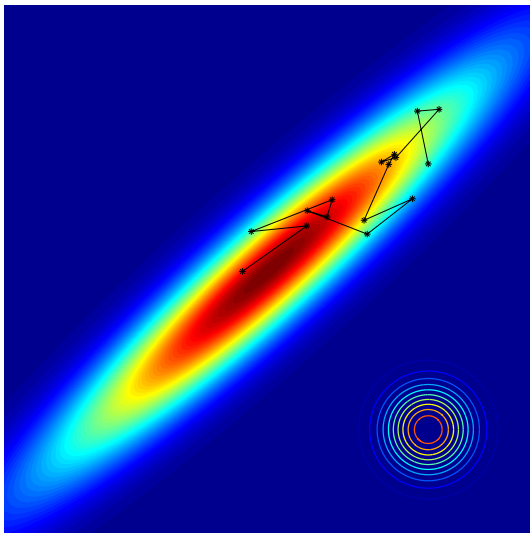
1  $y = u_{i-1} + z; z \sim p_{pro}(z)$

2 Acceptance ratio  $r = \frac{p(y)}{p(u_{i-1})}$

3  $\theta \sim U([0, 1])$

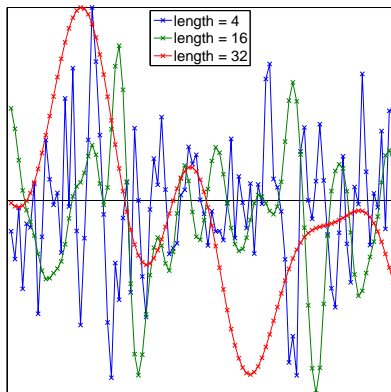
4 If  $r \geq \theta$ , set  $u_i = y$   
else, set  $u_i = u_{i-1}$ .

- ▶ “Black box” sampling:  
Only evaluation of  $p$ .
- ▶ Most widely used.
- ▶ Tuning of  $p_{pro}$ .
- ▶ Basis for very sophisticated sampling algorithms.

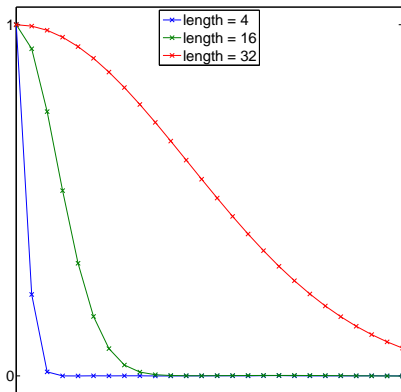


Evaluate performance of a sampler via **autocorrelation functions (acf)**:

- ▶ Desired: Independent samples of  $p(x)$ .
- ▶  $R(\tau) \in [0, 1]$  measures the average correlation between samples  $x_i, x_{i+\tau}$  w.r.t. to a test function.
- ▶ A rapid decay of  $R(\tau) \implies$  Samples get uncorrelated fast!



(a) Stochastic processes...

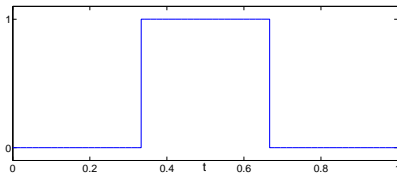


(b) ...and their autocorrelation functions

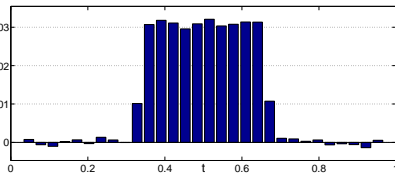
## Total Variation Deblurring Example in 1D (from Lassas & Siltanen, 2004)

- ▶ Model of a **charge coupled device** (CCD) in 1D.
- ▶ Unknown light intensity  $\tilde{u} : [0, 1] \rightarrow \mathbb{R}^+$ , indicator on  $[\frac{1}{3}, \frac{2}{3}]$ .
- ▶ Integrated into  $k = 30$  CCD pixels  $[\frac{1}{k+2}, \frac{k+1}{k+2}] \subset [0, 1]$ .
- ▶ Noise is added.
- ▶  $\tilde{u}$  is reconstructed on a regular,  $n$ -dim. grid.
- ▶  $D$  is the forward finite difference operator with NB cond.

$$p_{post}(u|f) \propto \exp\left(-\frac{1}{2\sigma^2}\|f - Ku\|_2^2 - \lambda |Du|_1\right)$$



(c) The unknown function  $\tilde{u}(t)$



(d) The measurement data  $f$



## Performance of the MH Sampler

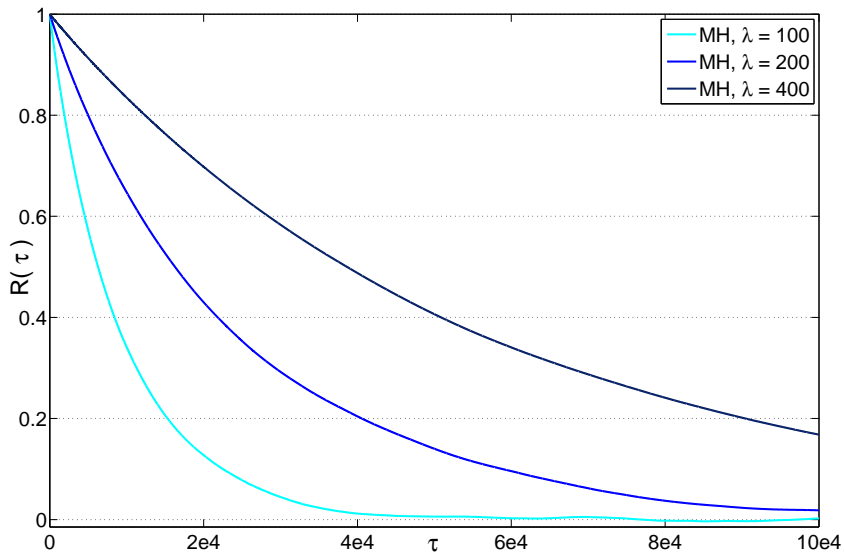


Figure: Autocorrelation plots  $R(\tau)$  for MH Sampler and  $n = 63$ .

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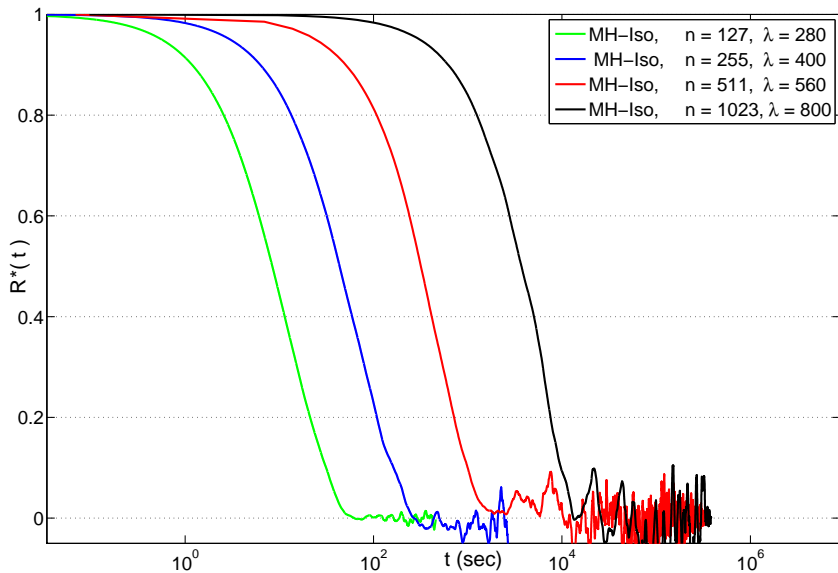


Figure: Temporal autocorrelation plots  $R^*(t)$  for MH Sampler.

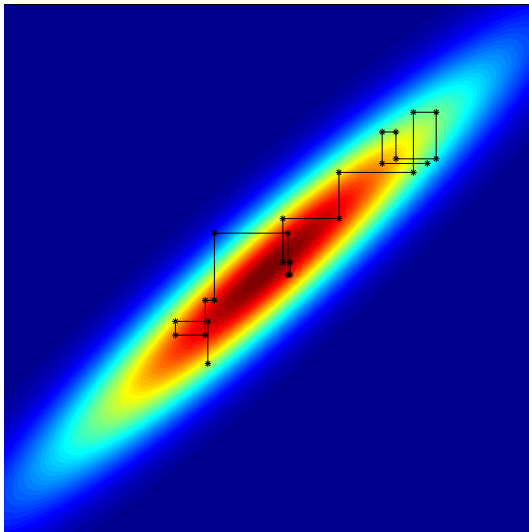
# Single Component Gibbs Sampling

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.



# Single Component Gibbs Sampling

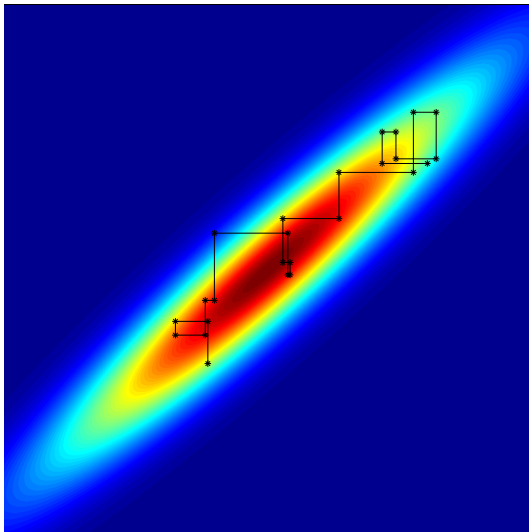
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**Nasty, involved and time consuming to implement** for L1-type priors



## Total Variation Deblurring Example in 1D (from Lasso & Siltanen, 2004)

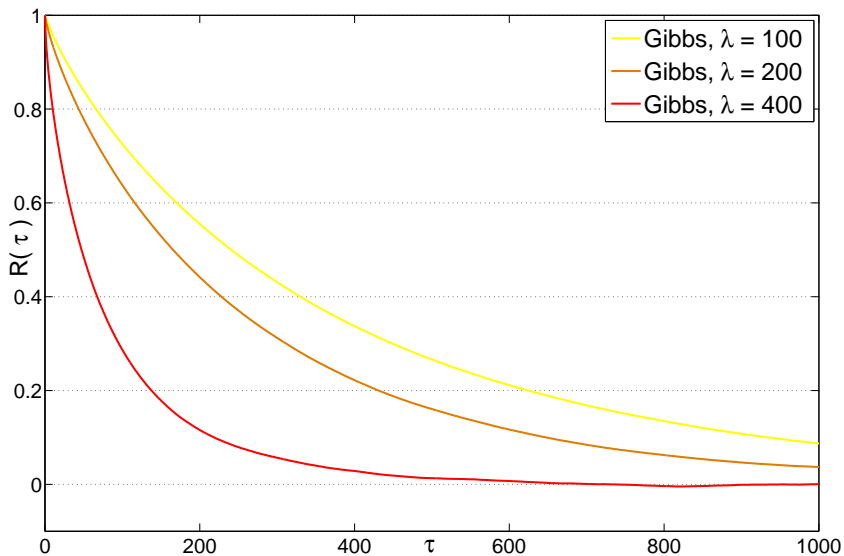


Figure: Autocorrelation plots  $R(\tau)$  for Gibbs Sampler and  $n = 63$ .

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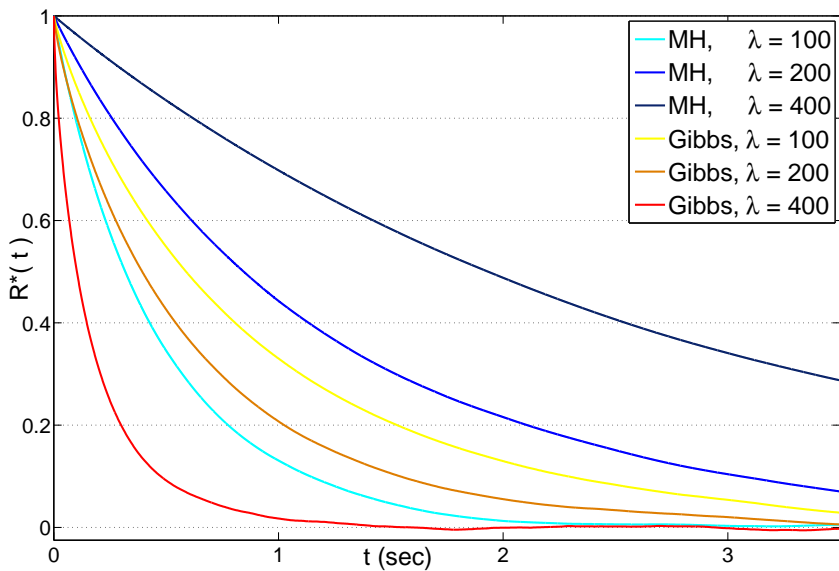


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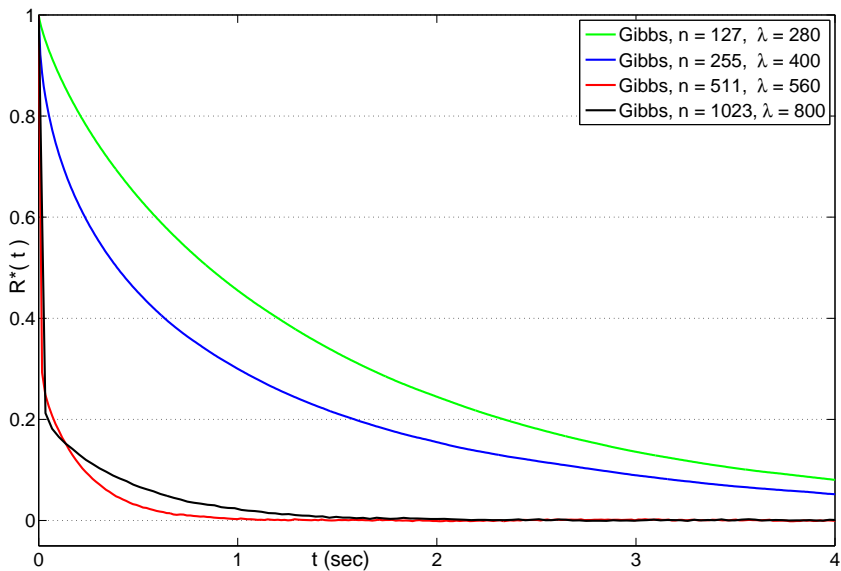


Figure: Temporal autocorrelation plots  $R^*(t)$  for Gibbs Sampler

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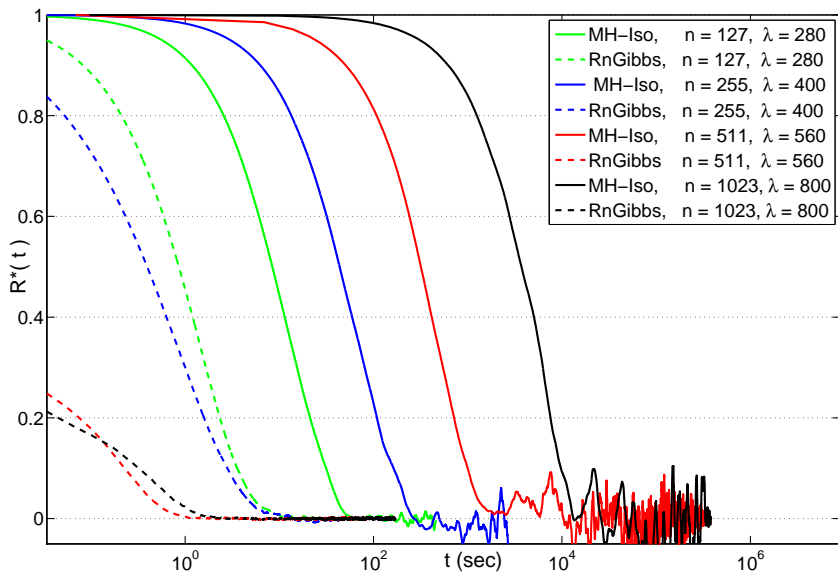


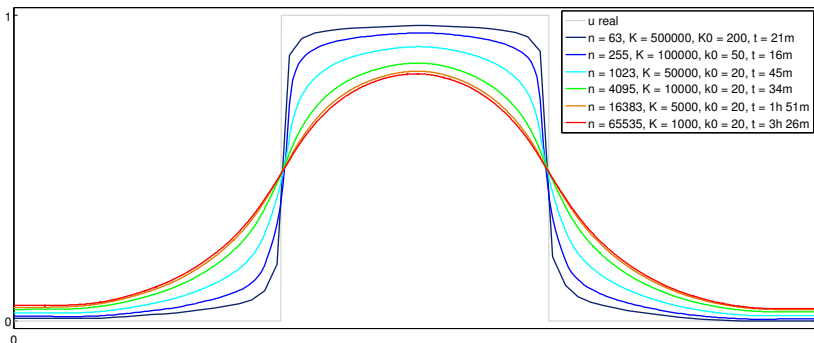
Figure: Temporal autocorrelation plots  $R^*(t)$ .



## Total Variation Deblurring Example in 1D (from Lasso & Siltanen, 2004)

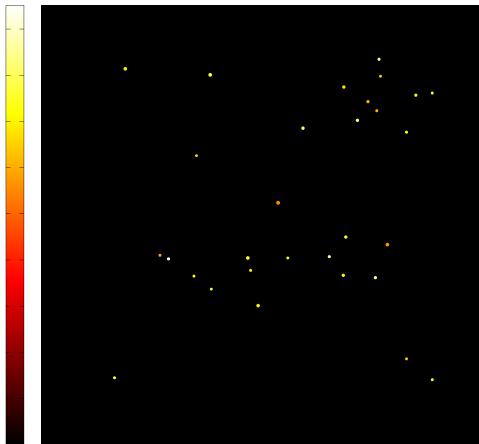
New sampler can be used to address theoretical questions:

- ▶ Lasso & Siltanen, 2004: For  $\lambda_n \propto \sqrt{n+1}$ , the TV prior converges to a smoothness prior in the limit  $n \rightarrow \infty$ .
- ▶ MH sampling to compute CM estimate for  $n = 63, 255, 1023, 4095$ .
- ▶ Even after a month of computation time only partly satisfying results.

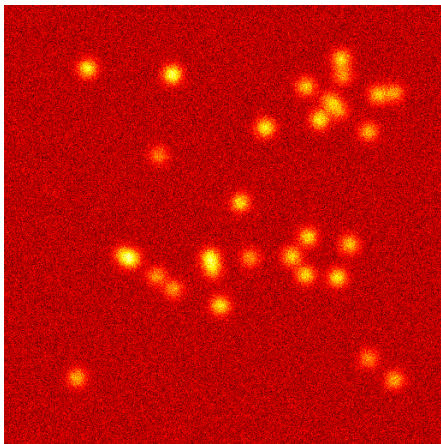


**Figure:** CM estimate computed for  $n = 63, 255, 1023, 4095, 16383, 65535$  using Gibbs sampler on a comparable CPU.

## Image Deblurring Example in 2D



Unknown function  $\tilde{u}$



Measurement data  $m$

- ▶ Gaussian blurring kernel
- ▶ Relative noise level of 10%
- ▶ Reconstruction using  $n = 511 \times 511 = 261\,121$ .

## Image Deblurring Example in 2D

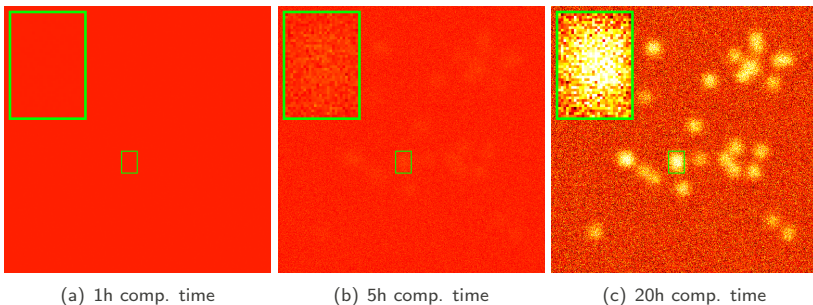


Figure: CM estimates by MH sampler

## Image Deblurring Example in 2D

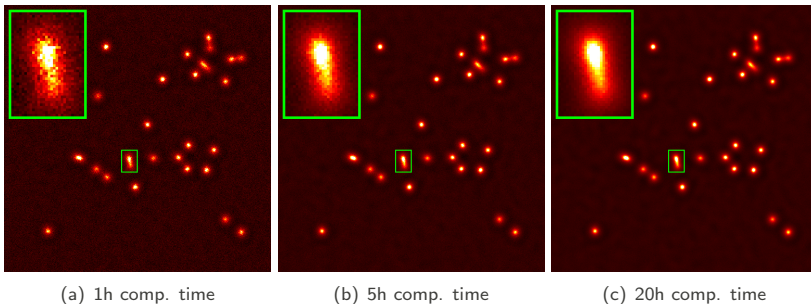


Figure: CM estimates by Gibbs sampler



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## Iterative Optimization and MCMC Sampling...

...often look very different at first glance:

- ▶ Iterative optimization follows a clear and determined path in search space.
- ▶ MCMC samplers randomly “stray around like pub crawlers”.



Source: Wikimedia Commons

## Iterative Optimization and MCMC Sampling...

However, both try to find points that are optimally representative for  $p(x)$  in a computationally efficient way:

- ▶ Optimization:  $\{x_i\}_i$  such that  $x_i \rightarrow \hat{x} = \operatorname{argmax} p(x)$  as fast as possible.
- ▶ Samplers:  $\{x_i\}_i$  such that  $\frac{1}{K} \sum_i^K f(x_i) \rightarrow \int f(x)p(x)dx$  as fast as possible.

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- ▶ Samplers:  $\{x_i\}_i$  such that  $\frac{1}{K} \sum_i^K f(x_i) \rightarrow \int f(x)p(x)dx$  as fast as possible.

“Straying around” is not the main aim of MCMC samplers: There are two types of randomness in **MCMC**:

- ▶ **Markov chain**: The **unwanted**, random-walk-like randomness that we have to tolerate (but want to get rid off) because we’re not able to draw independent samples.
- ▶ **Monte Carlo**: The **wanted** independent-samples-like randomness that leads to the convergence of the integral.



## Iterative Optimization and MCMC Sampling: Practical Observations

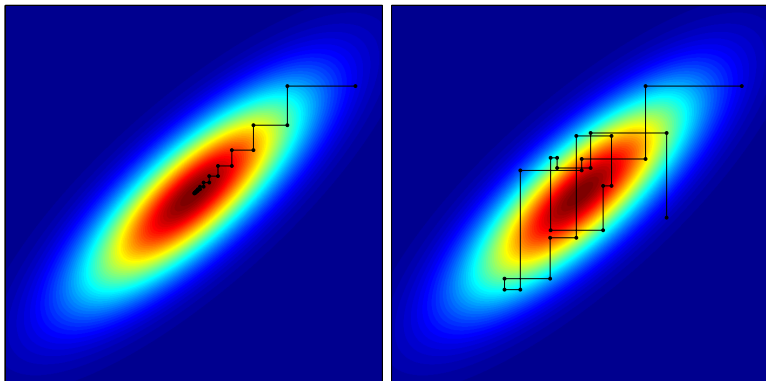
People that work with both of them realize:

- ▶ Both suffers from similar problems, e.g., strong dependencies between single components.
- ▶ Both are only fast if they take the analytical structure of  $p(x)$  into account.
- ▶ Some algorithms for sampling and optimization are surprisingly similar. (↪ in the next talk, the only difference is a slight modification of the right hand side).
- ▶ For both of them holds: Algorithms that work well in other areas may fail for inverse problems.

## Example: Deterministic and Stochastic Overrelaxation

As an example, consider a Gaussian density  $p(x)$  and iterative

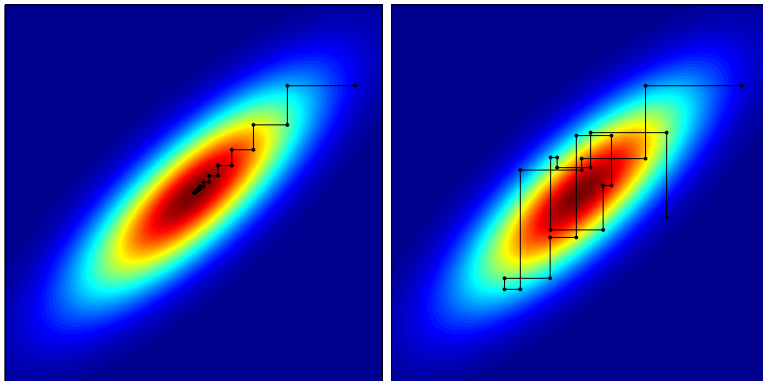
1. optimization over conditional single component densities (left image).
2. sampling over conditional single component densities (right image).



Both suffer from **strong correlations between single components**.

⇒ This is a natural feature of inverse problems, the compact forward operator “wraps up and compresses” many dimensions.

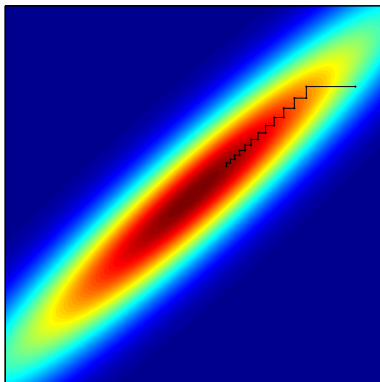
## Example: Deterministic and Stochastic Overrelaxation



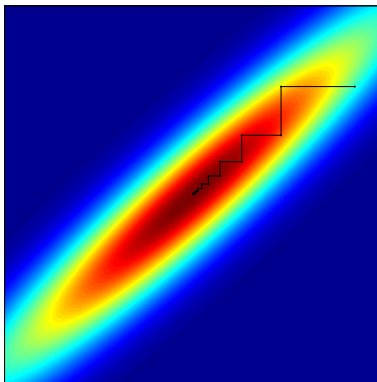
The optimization is the well known Gauss-Seidel solver for linear systems  
↪ Geometric convergence of optimization and Gibbs sampling.

## Example: Deterministic and Stochastic Overrelaxation

**Successive over-relaxation (SOR)** is a technique to counteract the coupling between components and to increase the convergence rate.



(g) SOR,  $w = 1$  (normal Gauss Seidel)



(h) SOR,  $w = 1.5$

## Example: Deterministic and Stochastic Overrelaxation

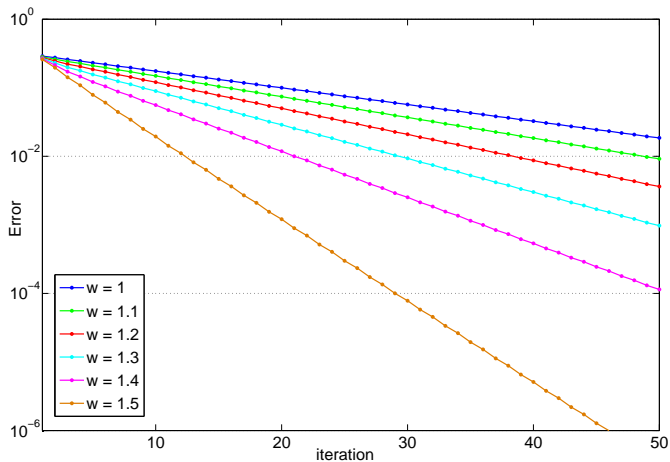


Figure: SOR error for different values of  $w$ .

## Example: Deterministic and Stochastic Overrelaxation

You can use the same idea to accelerate the convergence of Gibbs sampling:

- ▶ **Adler, 1981.** *Over-relaxation method for the Monte Carlo evaluation of the partition function for multiquadratic actions*  
⇒ Formulation for Gaussian distributions.
- ▶ **Neal, 1995.** *Suppressing Random Walks in Markov Chain Monte Carlo Using Ordered Overrelaxation*  
⇒ Generalization to arbitrary distributions.

In my paper on Gibbs sampling for L1-type priors, ordered over-relaxation is derived and used.

## Example: Deterministic and Stochastic Overrelaxation

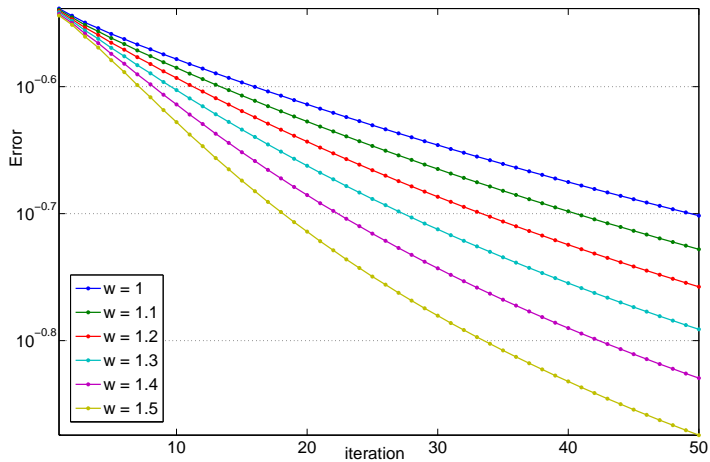


Figure: CM estimate error for different values of  $w$ .

## Example: Deterministic and Stochastic Overrelaxation

Using SOR (or other stationary solvers) for large sparse linear systems:

Outdated due to the **conjugate gradient** (CG) method...

...and so is sampling high dimensional Gaussians with sparse correlation matrix by Gibbs samplers due **CG sampling**, see Schneider and Willsky, 2002 and Parker and Fox, 2012.

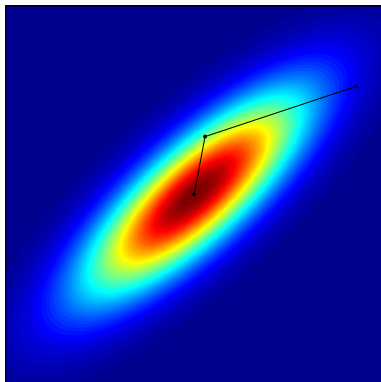


Figure: Conjugate gradient method



## Iterative Optimization and MCMC Sampling: My Conclusion

- ▶ Iterative optimization and sampling are not that different.
- ▶ MCMC sampling for inverse problems is just far less elaborate up to now.
- ▶ There is a lot to learn from optimization to improve sampling.
- ▶ Especially to suppress superfluous randomness  
→ Getting rid of the first “MC” in “MCMC”.
- ▶ The blindfolded use of “black-box” MCMC sampling may have ruined its reputation in certain areas.



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## Adaptive Metropolis Hastings Sampling

- ▶ Crucial issue for MH performance: Proposal distribution.
- ▶ **Global adaptation** strategies (**adaptive Metropolis** tune the proposal distribution to optimize the global acceptance rate.
- ▶ Basis: Sampling history.
- ▶ Chains are **not Markovian** anymore, but still **ergodic**.
- ▶ Especially developed for inverse problems.



H. Haario, E. Saksman and J. Tamminen, 2001.  
An Adaptive Metropolis Algorithm.



H. Haario, E. Saksman and J. Tamminen, 2005.  
Componentwise adaptation for high dimensional MCMC.

## Delayed Rejection Metropolis Hastings Sampling

- ▶ Crucial issue for MH performance: Proposal distribution.
- ▶ **Local adaptation** strategies design proposal distributions that locally adapt to the target distribution.
- ▶ Most often used: **delayed rejection**.
- ▶ Can be combined with global adaptation strategies.



A. Mira, 2001.

On Metropolis-Hastings algorithms with delayed rejection.



H. Haario, M. Laine, A. Mira and E. Saksman, 2006.

DRAM: Efficient adaptive MCMC.

## Delayed Acceptance Metropolis Hastings Sampling

- ▶ Large scale non-linear problems come with a high computational cost for evaluating the forward model.
- ▶ **Delayed acceptance** schemes first “test“ possible new states with a reduced forward model.
- ▶ Only accepted proposals are evaluated with the full model.
- ▶ Can be combined with other adaptation strategies.



A.J. Christen and C. Fox, 2005.  
MCMC using an Approximation,



T. Cui, C. Fox, M.J. O'Sullivan, 2011.  
Bayesian calibration of a large-scale geothermal reservoir model by a new adaptive delayed acceptance Metropolis Hastings algorithm.

## Parallelization: Naive, Tempering & Interacting

In principle, MCMC algorithms are great for parallelization.

- ▶ **Naive parallelization:** Run independent chains and merge results.
  - ▶ For "nice" samplers and distributions perfect speed up.
  - ▶ Might show problems for multimodal distributions or strongly correlated samplers.
- ▶ **Parallel tempering:** Run independent chains at different "temperatures" and swap states.
- ▶ **Interacting tempering:** More complex interactions between chains.



Jun S. Liu. 2008.

Monte Carlo Strategies in Scientific Computing.  
Springer Series in Statistics. Springer New York.



# Outline

Exemplary Application: Inverse Problems with Sparsity Constraints

Basic Algorithms for Integration-based Posterior Inference

Iterative Optimization and Sampling

Selected Advanced Topics and Trends (optional)

Take Home Messages, Conclusions & Ongoing Work

## Take Home Messages I

- ▶ Monte Carlo (MC) integration approximates high dimensional integrals by constructing an integration grid using statistical reasoning.
- ▶ Markov Chain Monte Carlo (MCMC) schemes realize MC integration by constructing suitable Markov chains.
- ▶ MCMC techniques rely on two elementary schemes: Metropolis Hastings (MH) and Gibbs sampling.
- ▶ MCMC can be used to compute many quantities in Bayesian inverse problems.



## Take Home Messages II

- ▶ High dimensional inverse problems using sparsity constraints pose specific challenges for MCMC schemes.
- ▶ However, MCMC schemes are not in general slow and scale bad with increasing dimension.
- ▶ The elementary MCMC schemes may show very different performance.
- ▶ The dependence on dimension and prior impact is not trivial.
- ▶ Inference in every high dimensions is feasible ( $n > 1\,000\,000$  still works...).

### CAUTION!

- ▶ These results do not generalize.
- ▶ MH and Gibbs sampling have both pro's and con's.
- ▶ For MH samplers, the right choice of the proposal kernel is essential.
- ▶ Especially for MH sampling, there are powerful techniques to increase performance while preserving the “black-box” property.

## Take Home Messages III

- ▶ Iterative optimization and MCMC sampling are not that different.
- ▶ Concepts from optimization can be used to speed up sampling.
- ▶ Example: Overrelaxation.

For inverse problems, I think that for both optimization and sampling,

- ▶ the degenerate nature of the posterior is the main problem.
- ▶ tailoring the algorithms to the structure of the posterior is key for good performance.

## Ongoing Own Work

Use the current L1 Sampler to tackle...

- ▶ Real applications: Sparse tomography using Besov space priors like in [Kolehmainen, Lassas, Niinimäki, Siltanen, 2012]
- ▶ Theoretical questions, e.g., of how stair-casing in TV can be seen from a Bayesian perspective or on the relation between MAP and CM estimates (see last talk).

Further develop the L1 sampler

- ▶ Add adaptive elements
- ▶ Comparison to more sophisticated variants of MH schemes.
- ▶ Formulation for block-sparse priors, e.g., to apply it to EEG/MEG.
- ▶ Generalization to arbitrary  $D$  in  $|Du|_1$ .
- ▶ Learn more from optimization methods!

# Thank you for your attention!

-  Jari Kaipio and Erkki Somersalo. 2005  
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-  Daniela Calvetti and Erkki Somersalo. 2007.  
Introduction to Bayesian Scientific Computing.
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Fast Markov chain Monte Carlo sampling for sparse Bayesian inference in high-dimensional inverse problems using L1-type priors