# Discretization-invariant Bayesian inversion and Besov space priors


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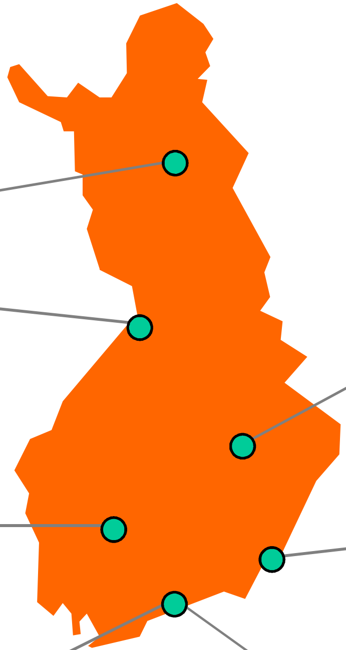
# Finnish Centre of Excellence in Inverse Problems Research



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UNIVERSITY OF HELSINKI
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http://math.tkk.fi/inverse-coe/

# This is a joint work with

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Helsinki University of Technology
Finland

**Eero Saksman**
University of Helsinki
Finland

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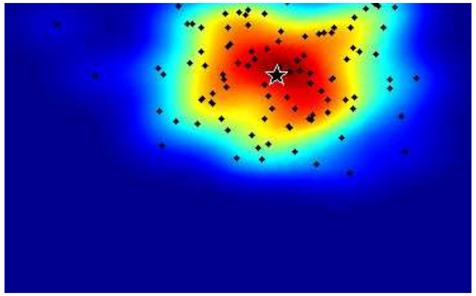
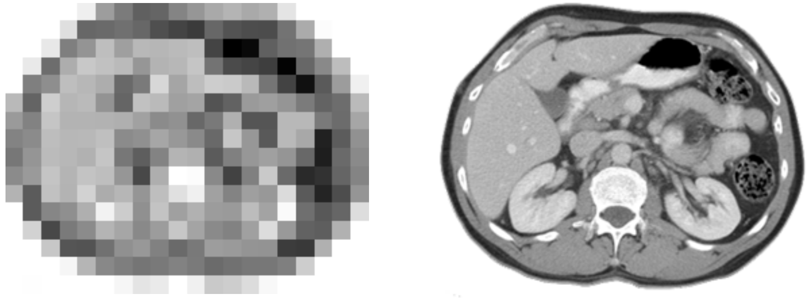
**Finnish Technology Agency, Academy of Finland, Instrumentarium Imaging, GE Healthcare, and Palodex Group**



1. Bayesian inversion



2. Discretization-invariance

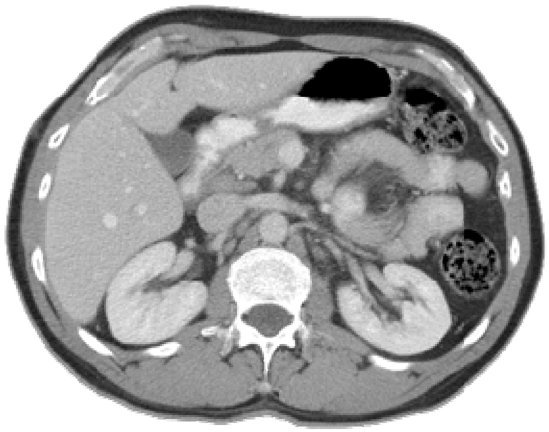
3. Regularization results


4. Besov space priors

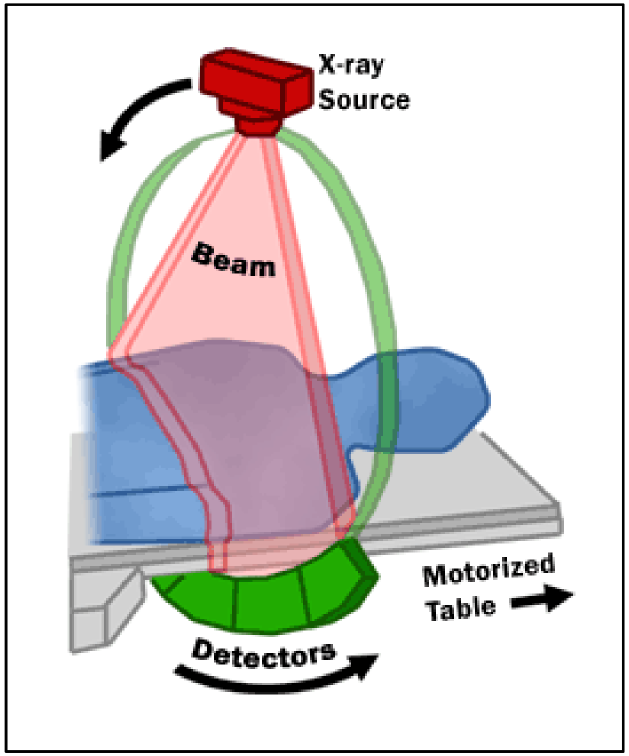
$$e^{-\alpha\|u\|_{B^1_{11}}}$$

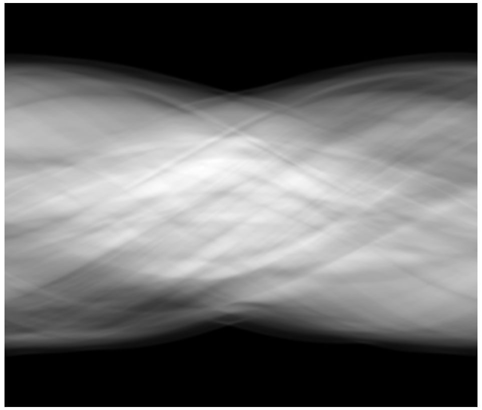
# We discuss indirect measurements of continuum quantities

Example: Radon transform in X-ray tomography



*U*
(attenuation coefficient)



*M*
(noisy sinogram)

$$M = AU + \mathcal{E}$$

# The continuum measurement model must be discretized for practical inversion

We simulate physics by the **continuum model**

$$M = AU + \mathcal{E},$$

where $\mathcal{E}$ is white noise. Here $M(\,\cdot\,,\omega)$ and $U(\,\cdot\,,\omega)$ are random functions defined on $\mathbb{R}^d$.

Data is a realization $M_k(\omega_0) \in \mathbb{R}^k$ described by the **practical measurement model**

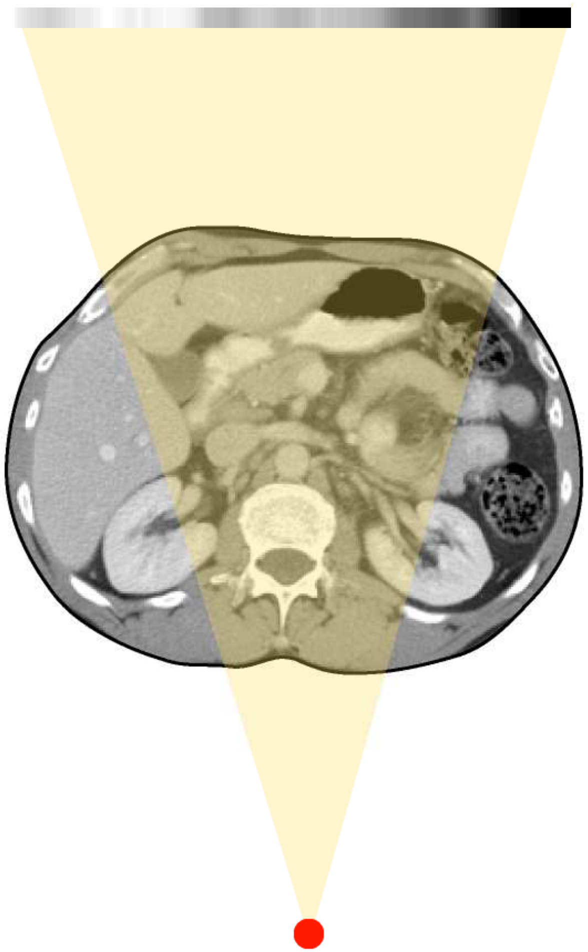
$$M_k = P_k AU + P_k \mathcal{E}.$$

Numerical work needs the **computational model**

$$M_{kn} = P_k AU_n + P_k \mathcal{E},$$

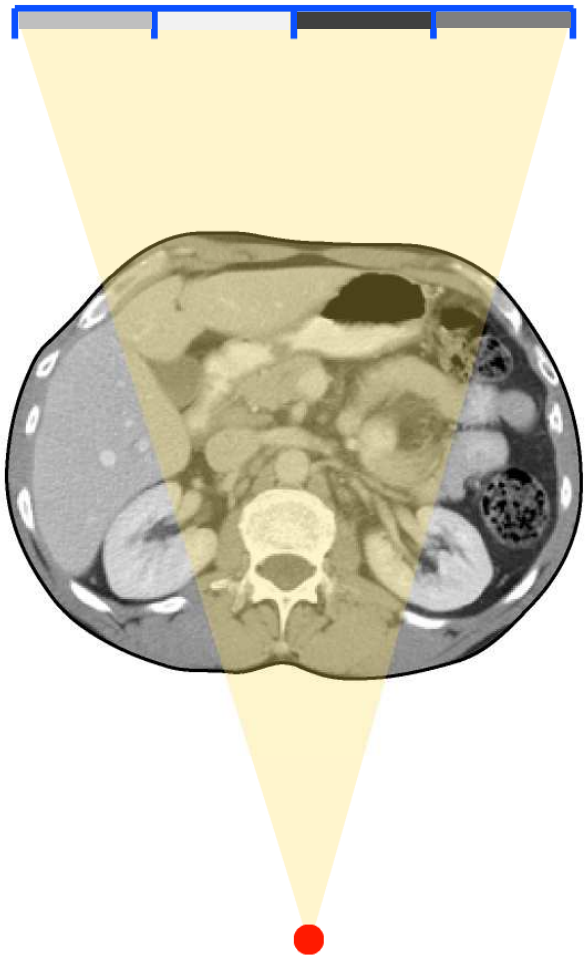
where $U_n = T_n U$ is a discretization of $U$.

# Continuum model for tomography:



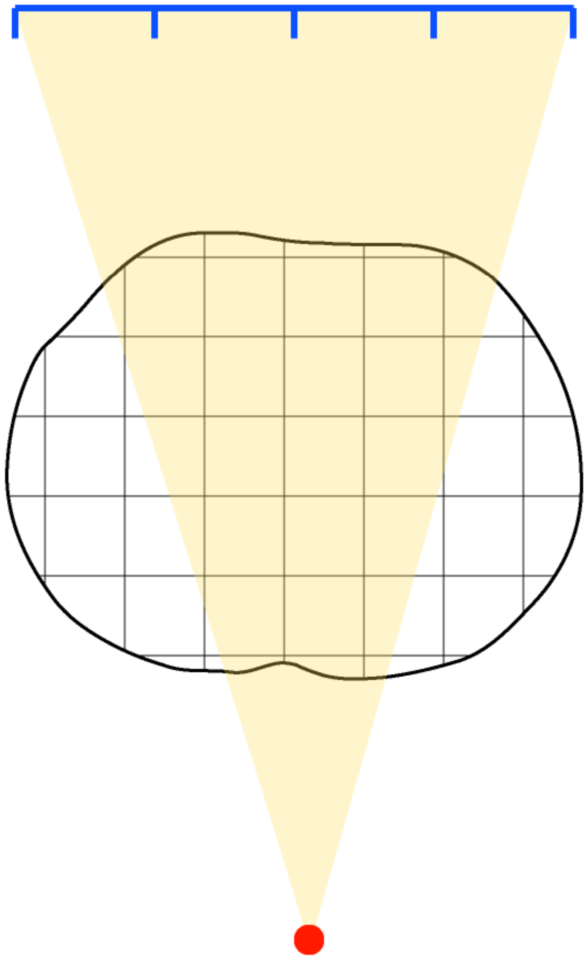
$$M = AU + \mathcal{E}$$

# Practical measurement model:



$$M_k = A_k U + \mathcal{E}_k = P_k A U + P_k \mathcal{E}$$

# Computational model:



$$M_{kn} = P_k A U_n + \mathcal{E}_k$$

# The finite dimensions n and k are independent

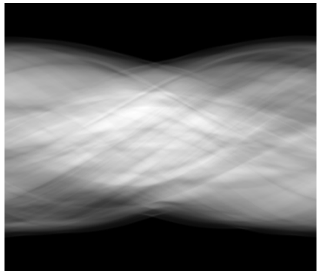
The linear projection operator $P_k$ is related to the measurement device and has $k$-dimensional range.

The linear projection operator $T_n$ is related to the computational discretization of the unknown and has $n$-dimensional range.

# Inverse problem: given a measurement, estimate the quantity U

X-ray tomography: Given measurement

$$M_k(\omega_0) = $$



,

estimate X-ray coefficient U in a two-dimensional slice.

We consider Bayesian estimation of U using a discrete conditional mean estimate (and confidence intervals).

# Bayes formula combines measured and *a priori* information

The posterior distribution corresponding to the finite-dimensional computational model is

$$\pi_{kn}(u_n \,|\, m_{kn}) \sim \Pi_n(u_n)\ \exp(-\frac{1}{2}\|m_{kn} - P_k A u_n\|_2^2),$$

where the prior distribution $\Pi_n$ assigns high probability to functions $u_n$ that are expected in light of *a priori* information, and the likelihood distribution

$$\exp(-\frac{1}{2}\|m_{kn} - P_k A u_n\|_2^2)$$

measures data misfit.

# In this work we estimate U by a discrete conditional mean estimate

Posterior distribution from computational model:

$$\pi_{kn}(u_n \,|\, m_{kn}) = \frac{\Pi_n(u_n)\ \mathrm{exp}(-\frac{1}{2}\|m_{kn} - P_k A u_n\|_2^2)}{\Upsilon_{kn}(m_{kn})}.$$

Conditional mean estimate is defined by

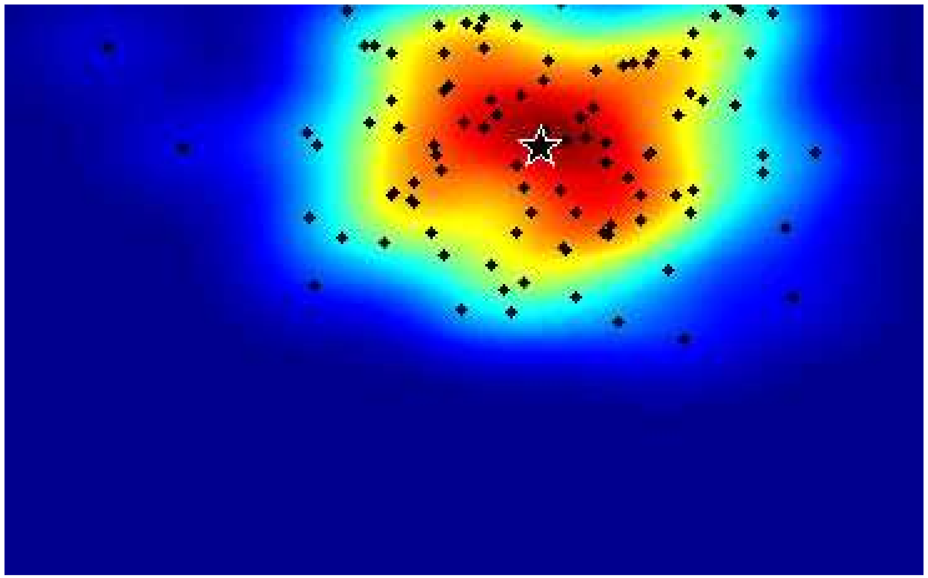
$$\mathbf{u}_{kn}^{\mathrm{CM}} := \int_{\mathbb{R}^n} u_n \pi_{kn}(u_n \,|\, m_k)\, du_n,$$

where the realization $m_k := M_k(\omega_0)$ is data from the practical measurement model.

# The conditional mean estimate is often computed by Markov chain Monte Carlo

$$\mathbf{u}_{kn}^{\mathrm{CM}} = \int_{\mathbb{R}^n} u_n \pi_{kn}(u_n \,|\, m_k)\, du_n \approx \frac{1}{N}\sum_{j=1}^{N} u_n^{(j)}$$

The samples $u_n^{(j)}$ are drawn from the posterior distribution using e.g. Metropolis-Hastings method or Gibbs sampler.



# Conditional mean estimates have been applied to various inverse problems

**Image restoration**

1991 Besag, York & Mollié

**Geological prospecting**

1998 Nicholls

2003 Andersen, Brooks & Hansen

**Atmospheric and ionospheric remote sensing**

1995 Markkanen *et al.*

1997 Nygrén, Markkanen, Lehtinen

1999 D´Ambrogi, Mäenpää & Markkanen

1999 Tamminen

2004 Haario, Laine, Lehtinen, Saksman & Tamminen

**Medical X-ray tomography**

1997 Battle, Cunningham & Hanson

2003 Kolehmainen *et al.*

2003 Siltanen *et al.*

**Electrical impedance imaging**

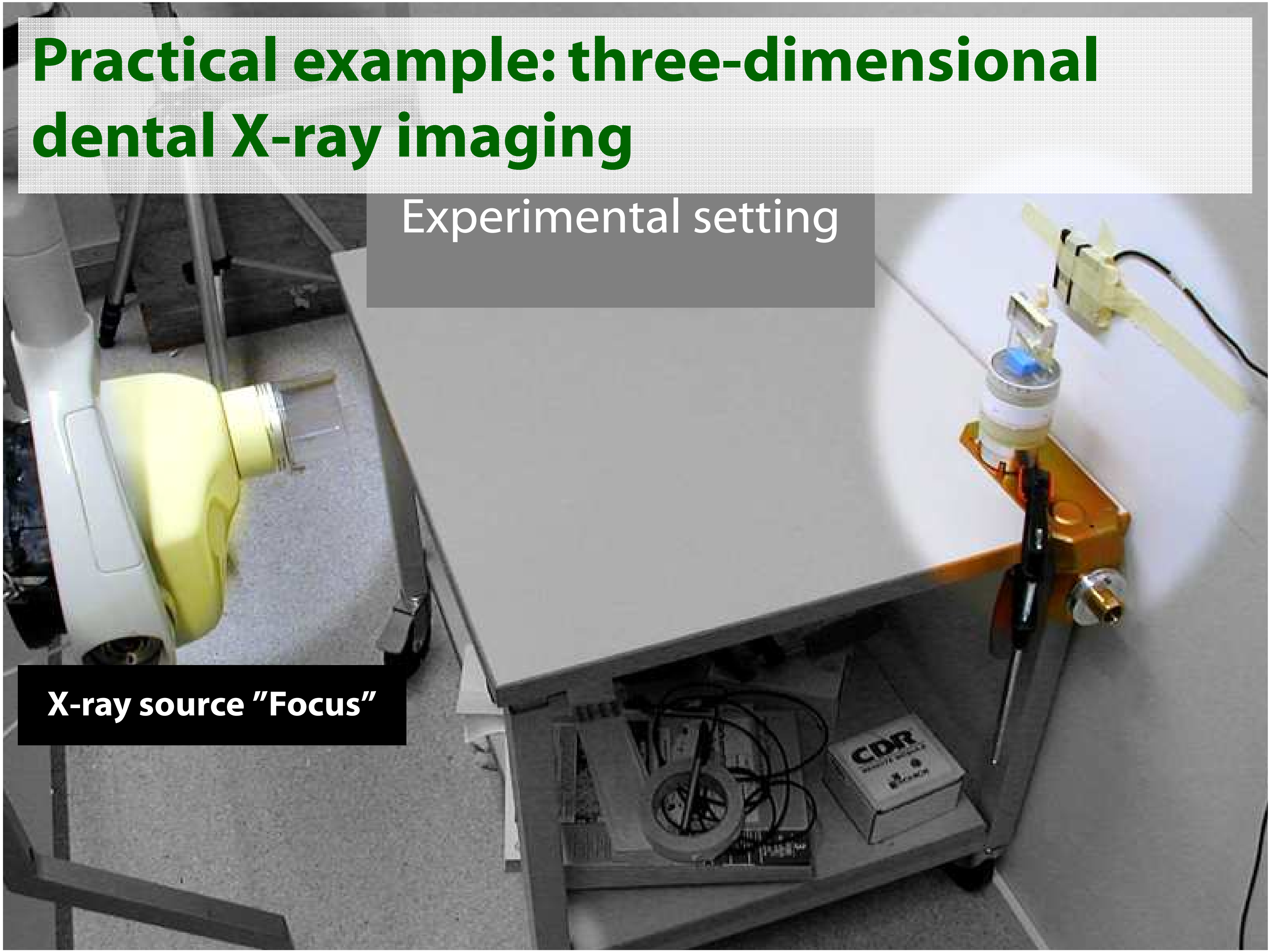
2000 Kaipio, Kolehmainen, Somersalo & Vauhkonen

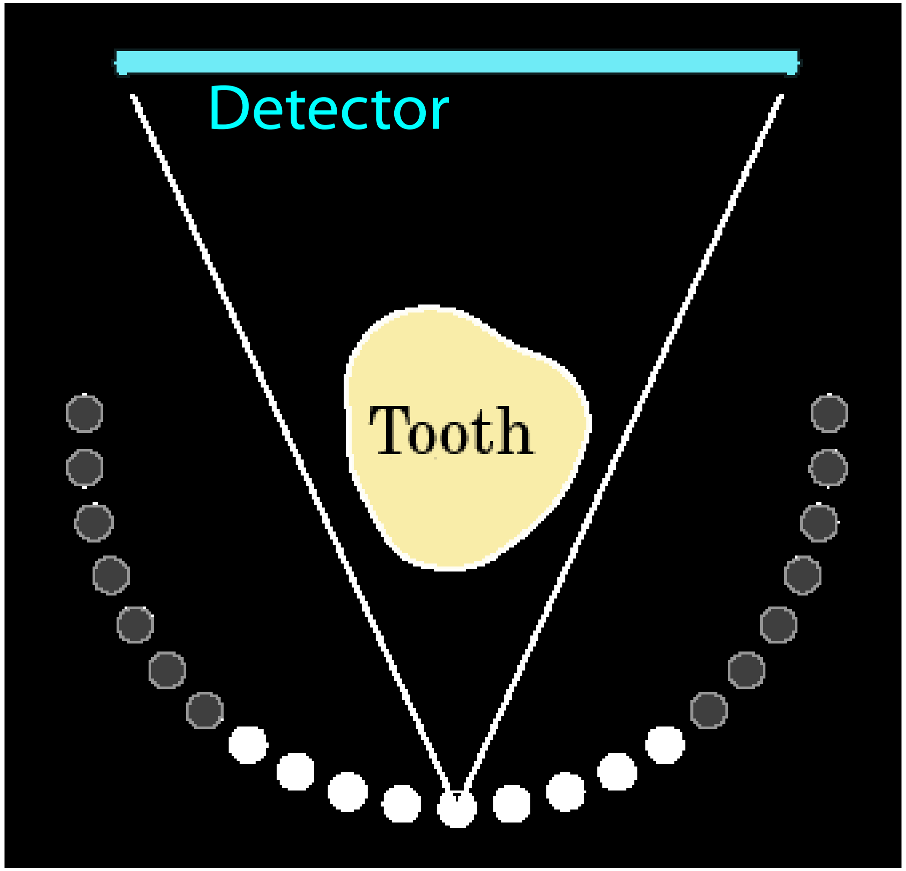
2001 Andersen, Brooks & Hansen

**Personal positioning using cell phone data**

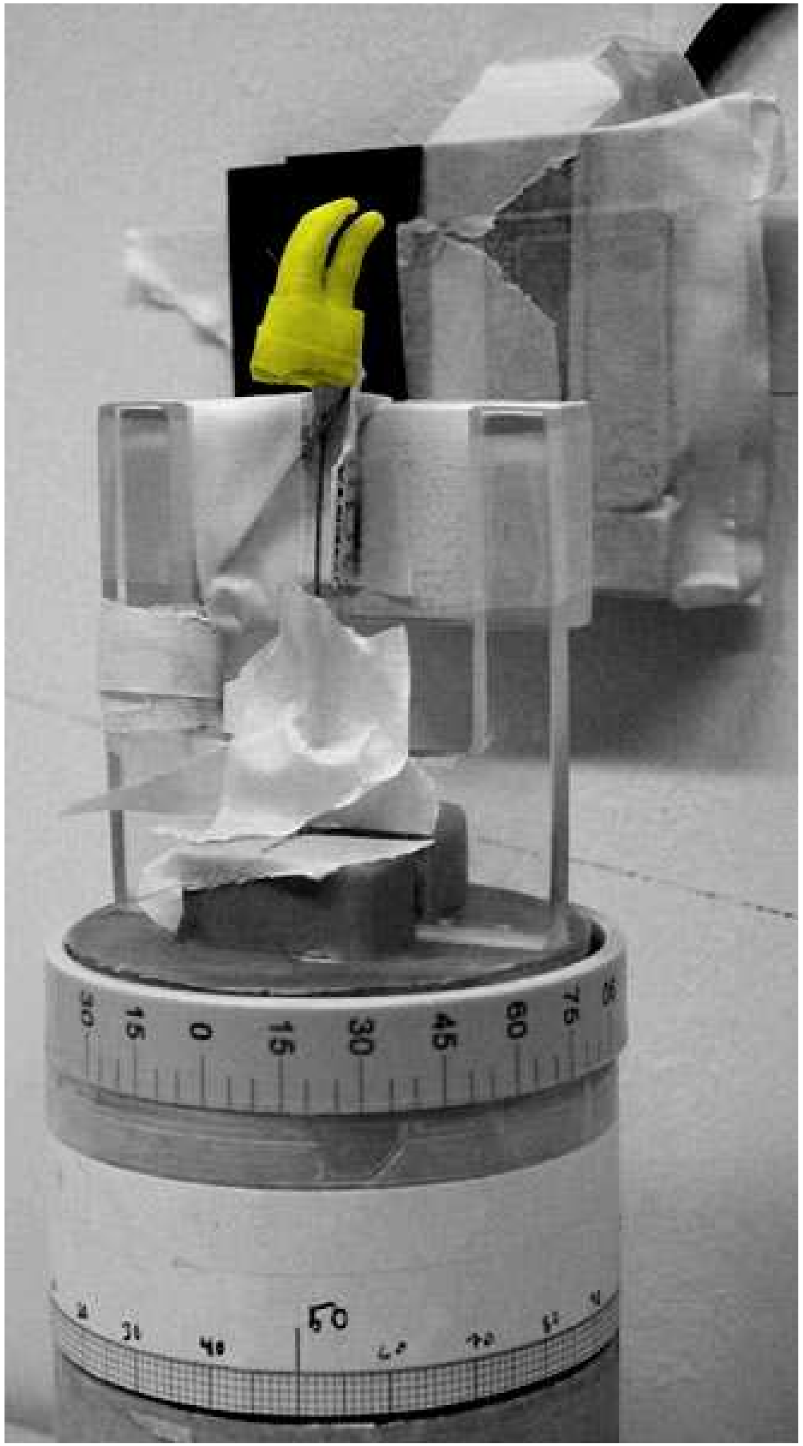
2006 Petrovich and Piché

# Practical example: three-dimensional dental X-ray imaging






X-ray source positions



# We use total variation prior with non-negativity constraint

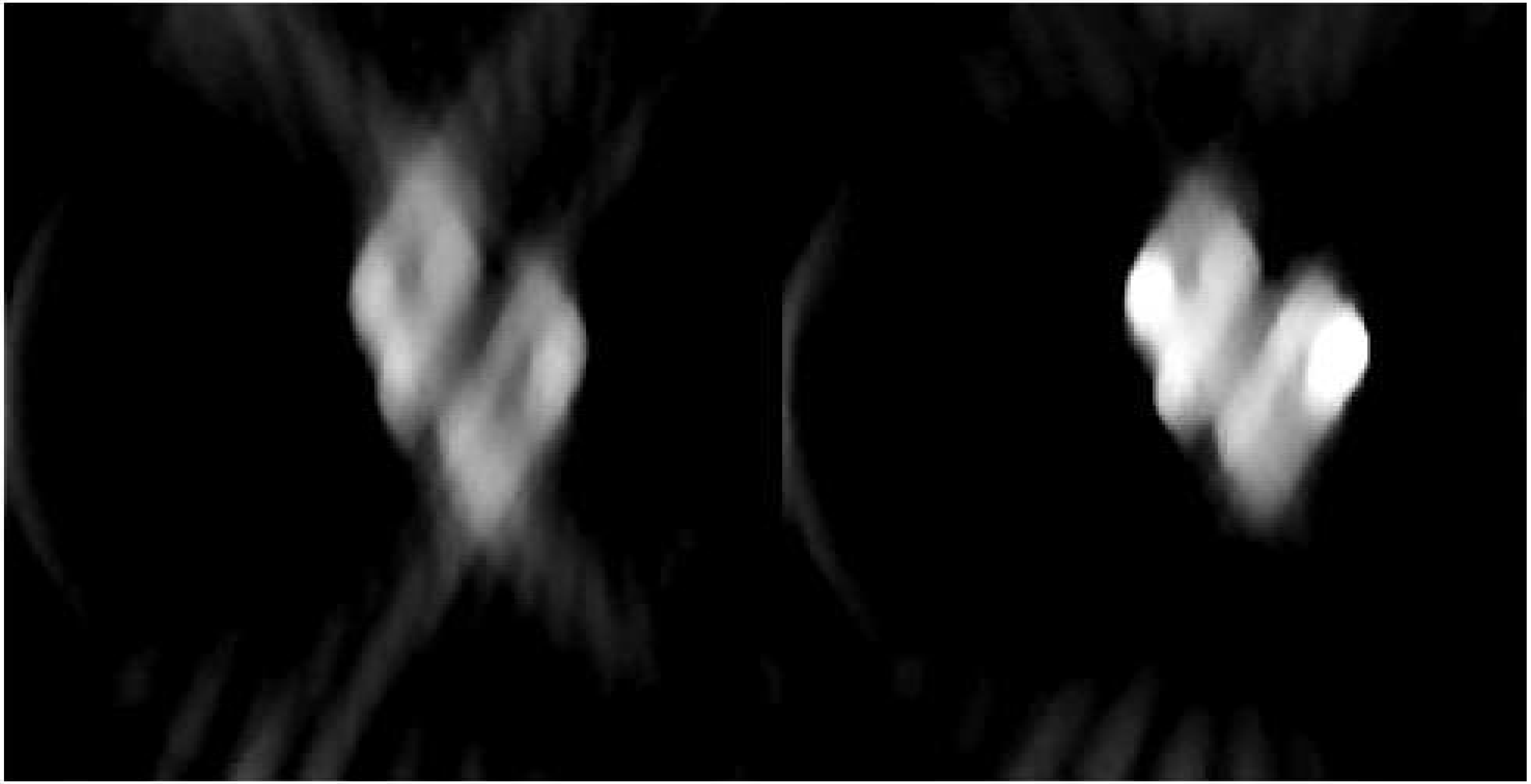
$$\pi_{kn}(u_n \,|\, m_{kn}) = \frac{\Pi_n(u_n)\ \exp(-\frac{1}{2}\|m_{kn} - P_k A u_n\|_2^2)}{\Upsilon_{kn}(m_{kn})},$$

where the prior is given by

$$\Pi_n(u_n) = \chi_{u_n \geq 0} \exp\left( -\alpha_n \sum_{x_\ell, x_\nu \text{ neighbors}} |u_n(x_\ell) - u_n(x_\nu)|_\beta \right).$$

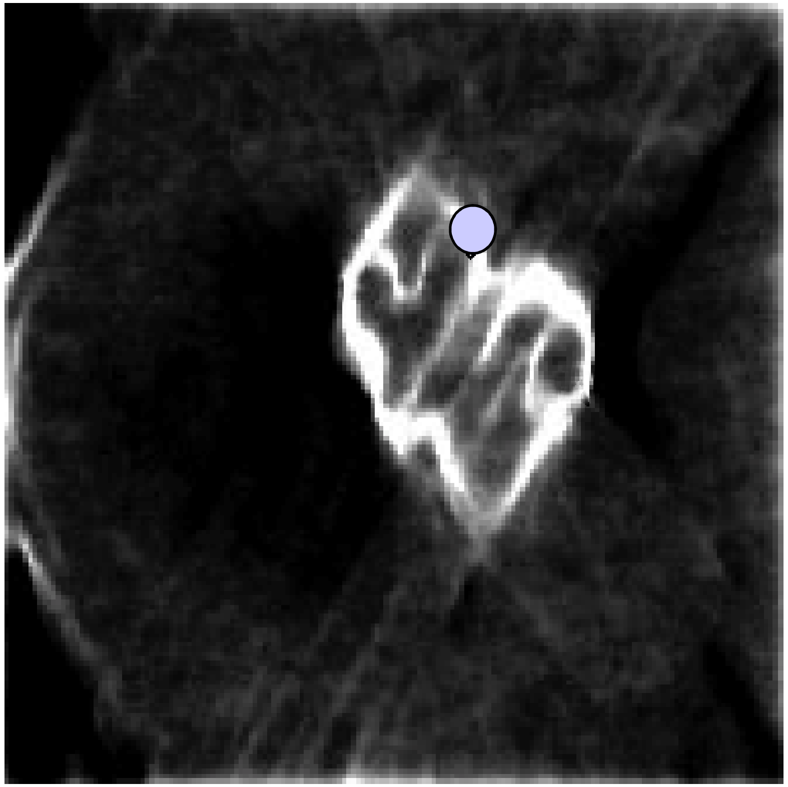
# We can compute several kinds of estimates from the posterior

MAP | Conditional mean

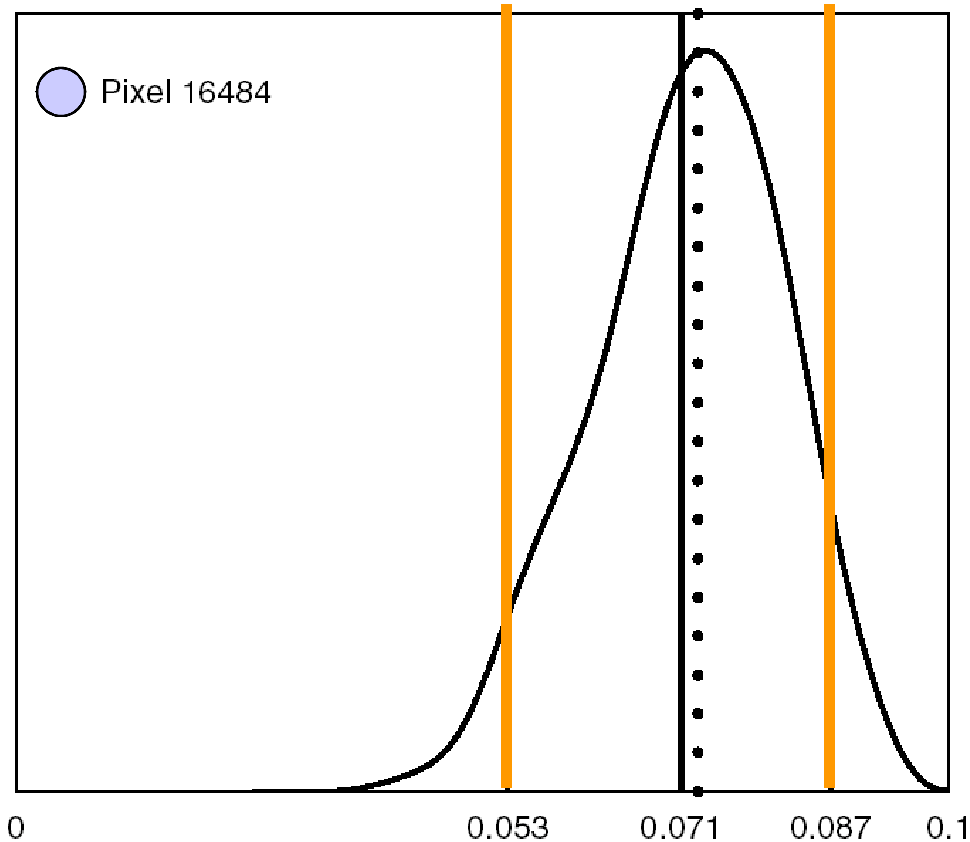


# The Bayesian approach allows further statistical inference

Posterior variance



90% confidence limits




[Kolehmainen *et al.* 2003], thanks to Instrumentarium Imaging

# TV prior seems to work for tomography. However, there is a problem.

Let $Y_n$ be the space of piecewise linear functions on $[0,1]$ with basis $\{\psi_j^n\}$ defined by

$$\psi_j^n(\frac{k}{n}) = \delta_{jk}.$$

We say that $U_n$ is total variation prior in $Y_n$ if

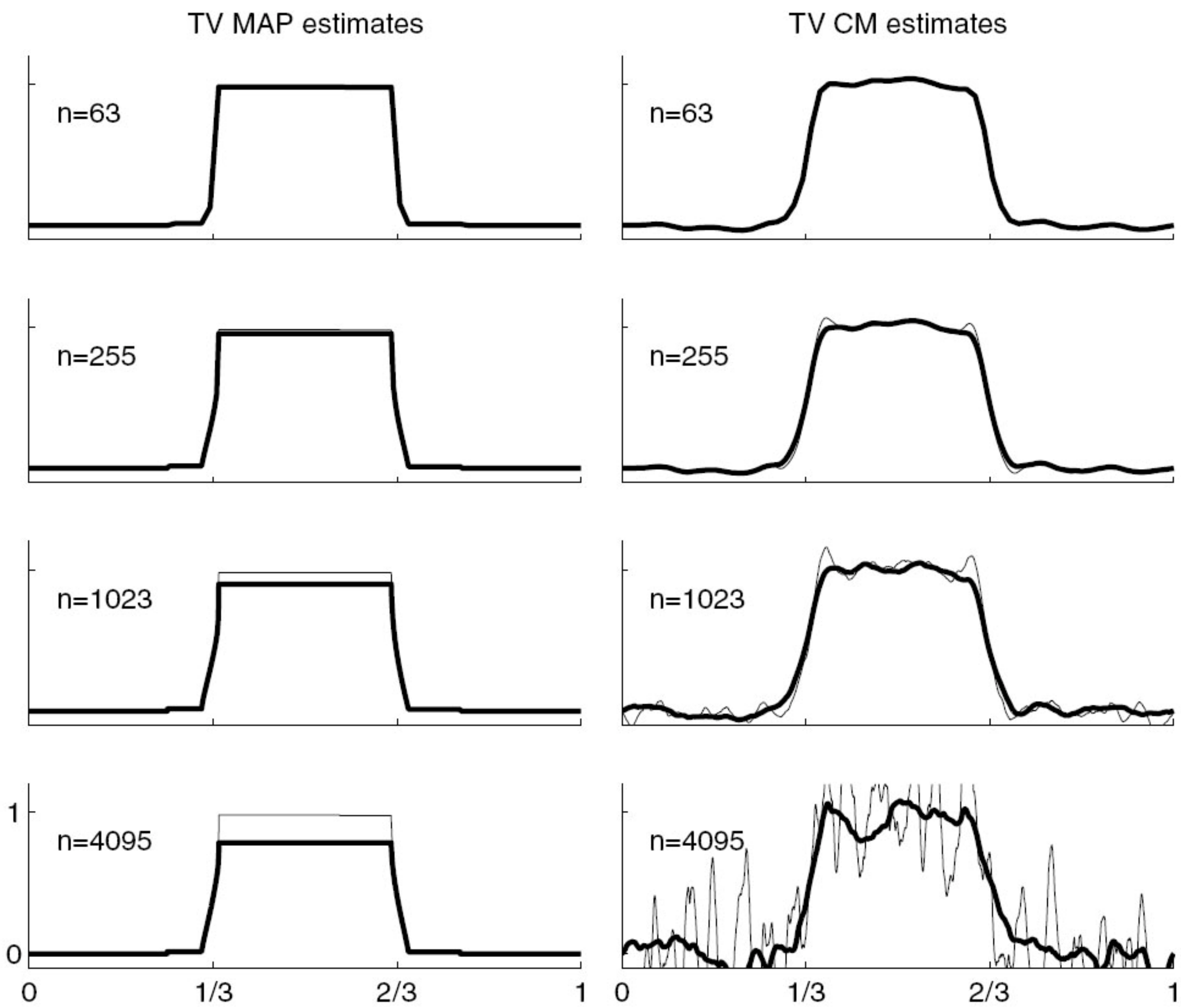
$$U_n(t,\omega) = \sum_{j=1}^{n} u_j^n(\omega)\psi_j^n(t), \quad \omega \in \Omega,$$

where $U_1^n, \dots, U_n^n$ are random numbers with probability density function

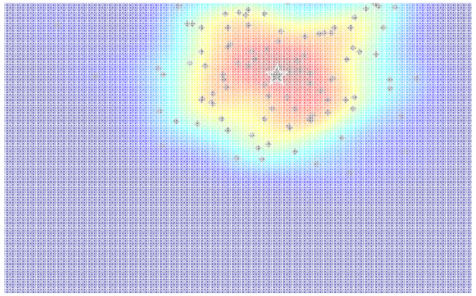
$$\pi(u_1^n, \dots, u_n^n) = c_n \exp(-\alpha_n \|\partial_t u_n\|_{L^1(0,1)}).$$

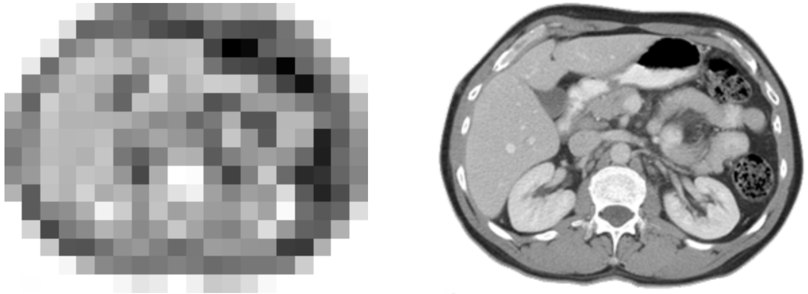
How should $\alpha_n$ be chosen for $n \to \infty$?

# **Total variation prior is not discretization-invariant!** (Lassas & S 2004)




Thin line:
$\alpha_n \sim 1.$
Thick line:
$\alpha_n \sim \sqrt{n}.$





1. Bayesian inversion

2. Discretization-invariance

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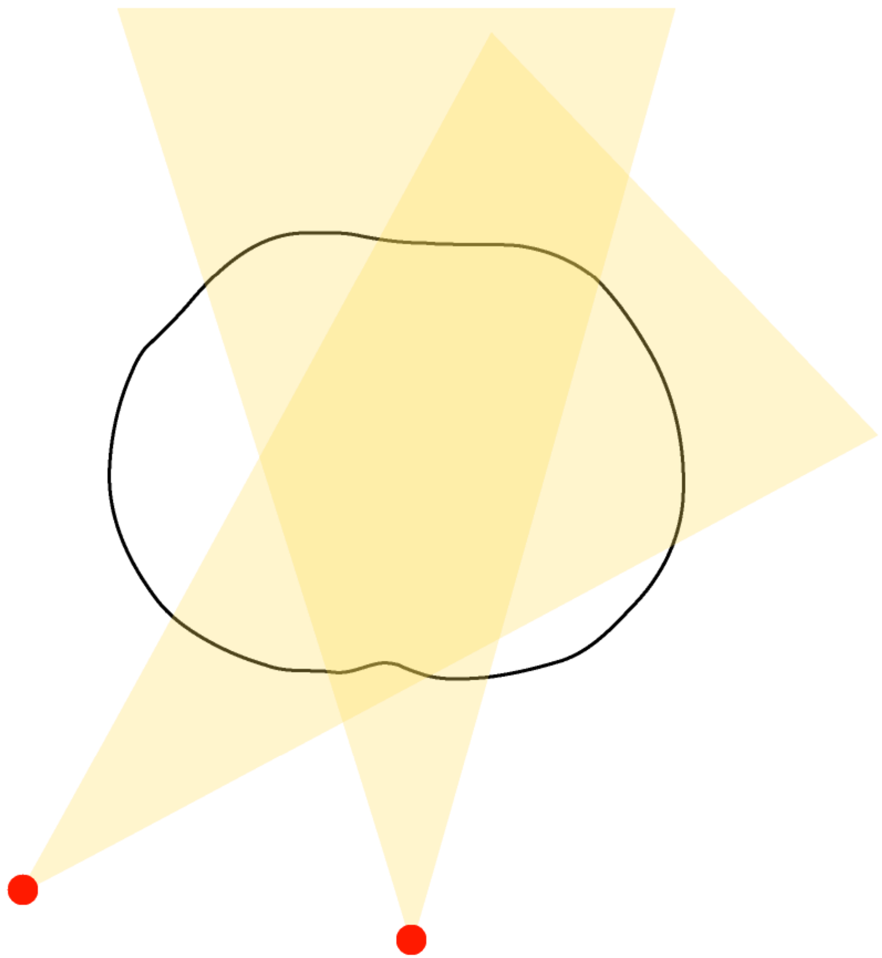
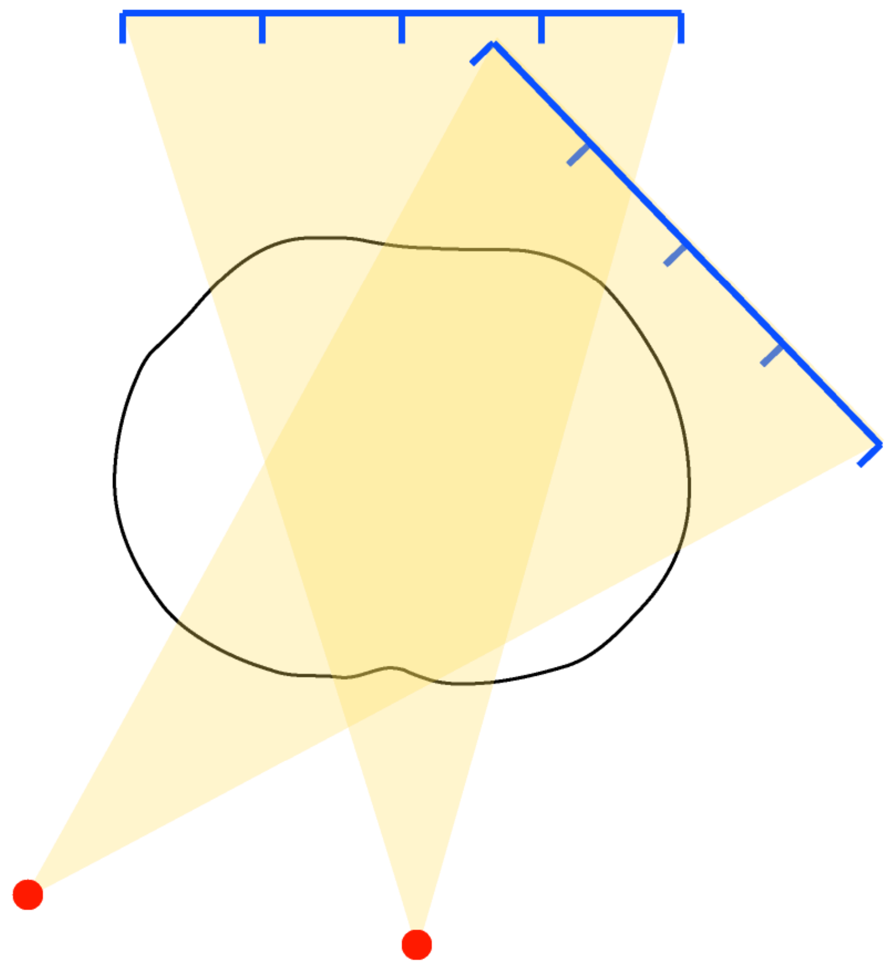
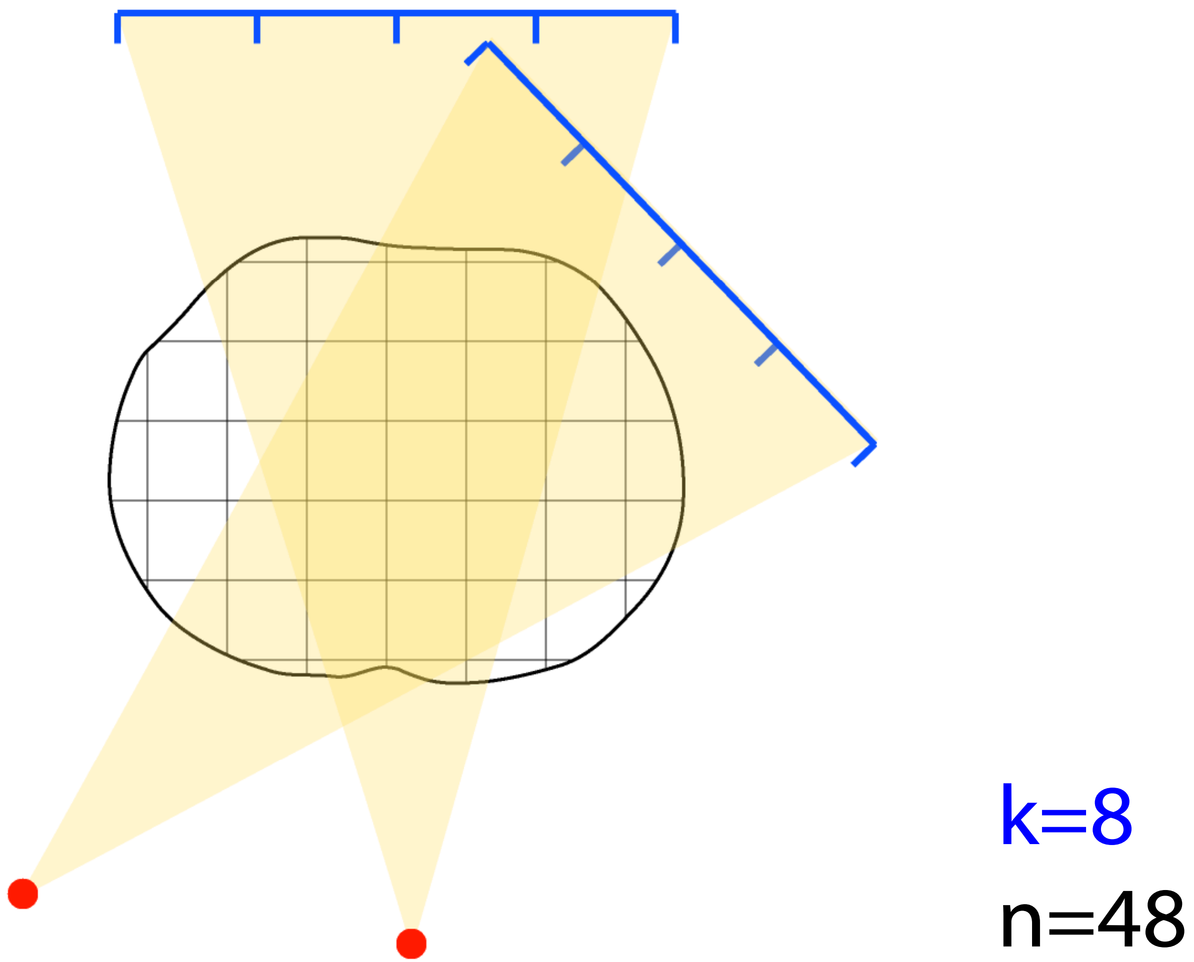
4. Besov space priors

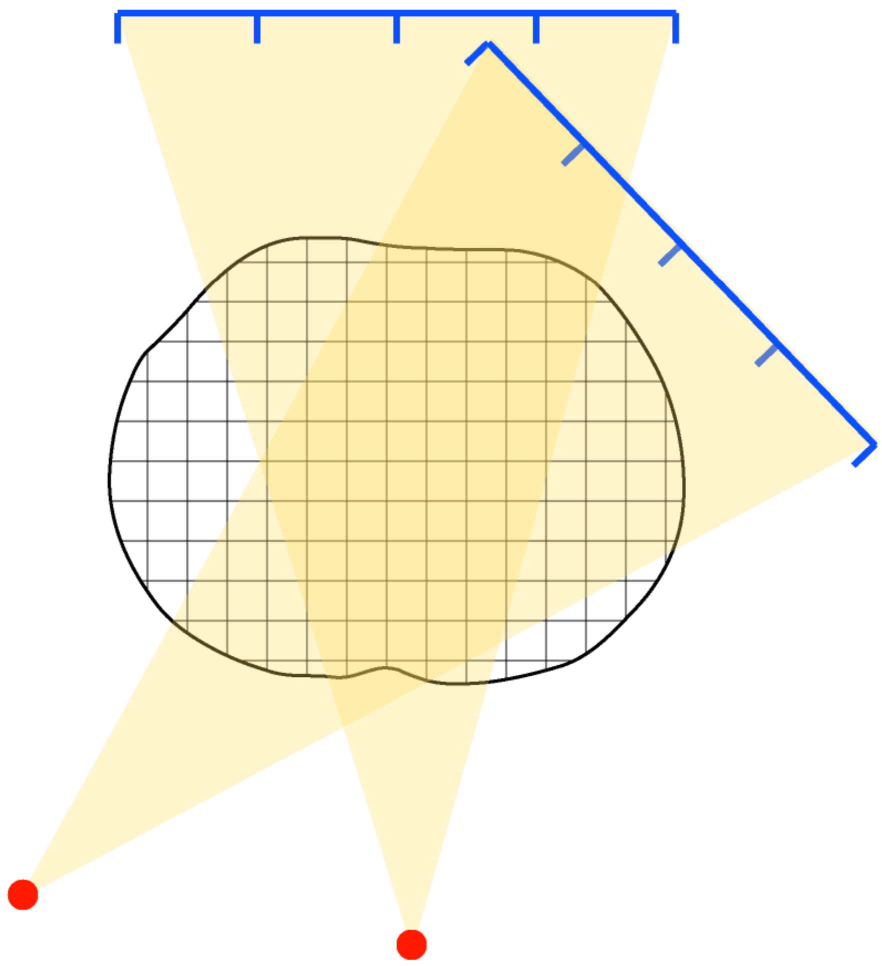

$$e^{-\alpha\|u\|_{B^1_{11}}}$$





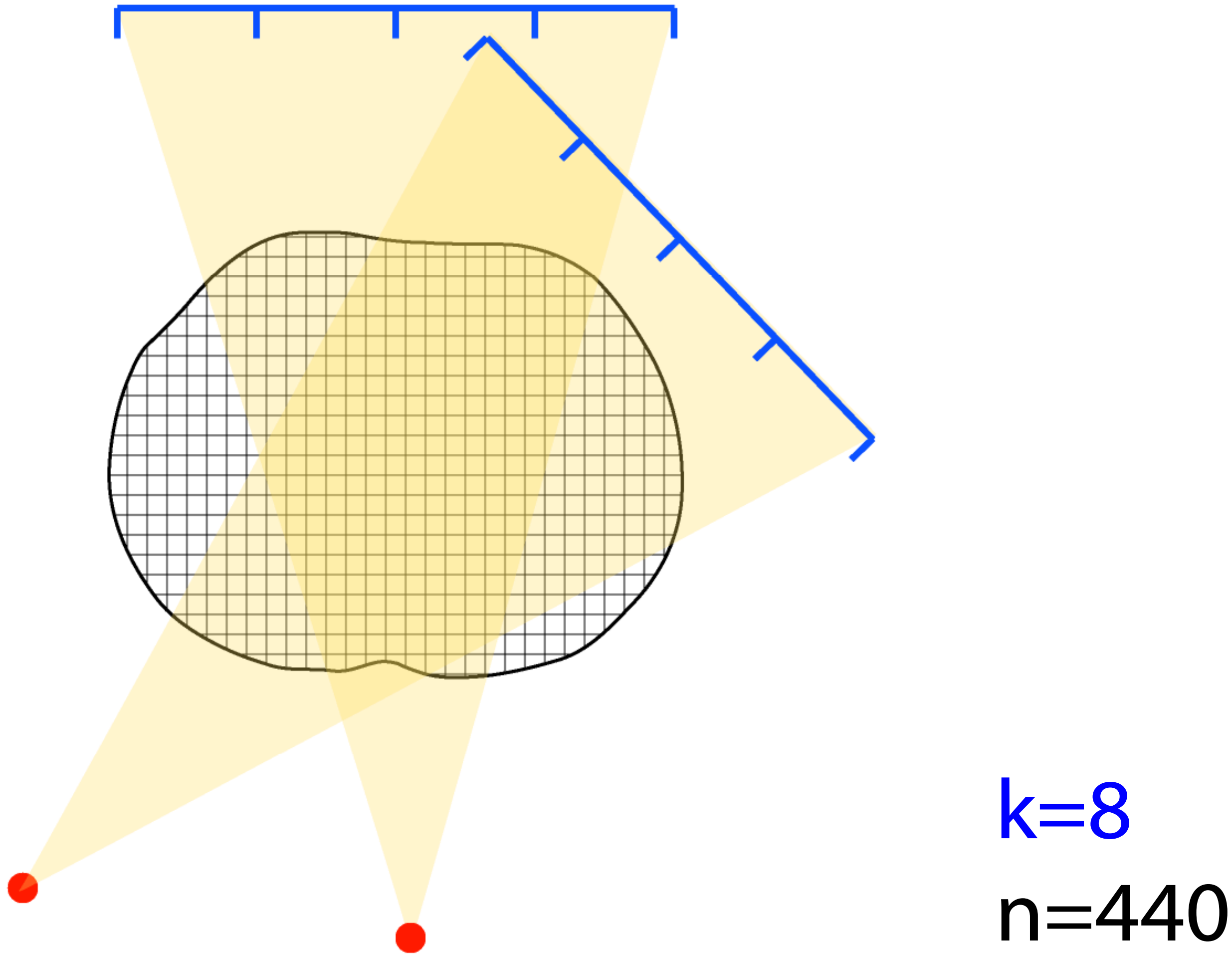
k=8


k=8
n=48

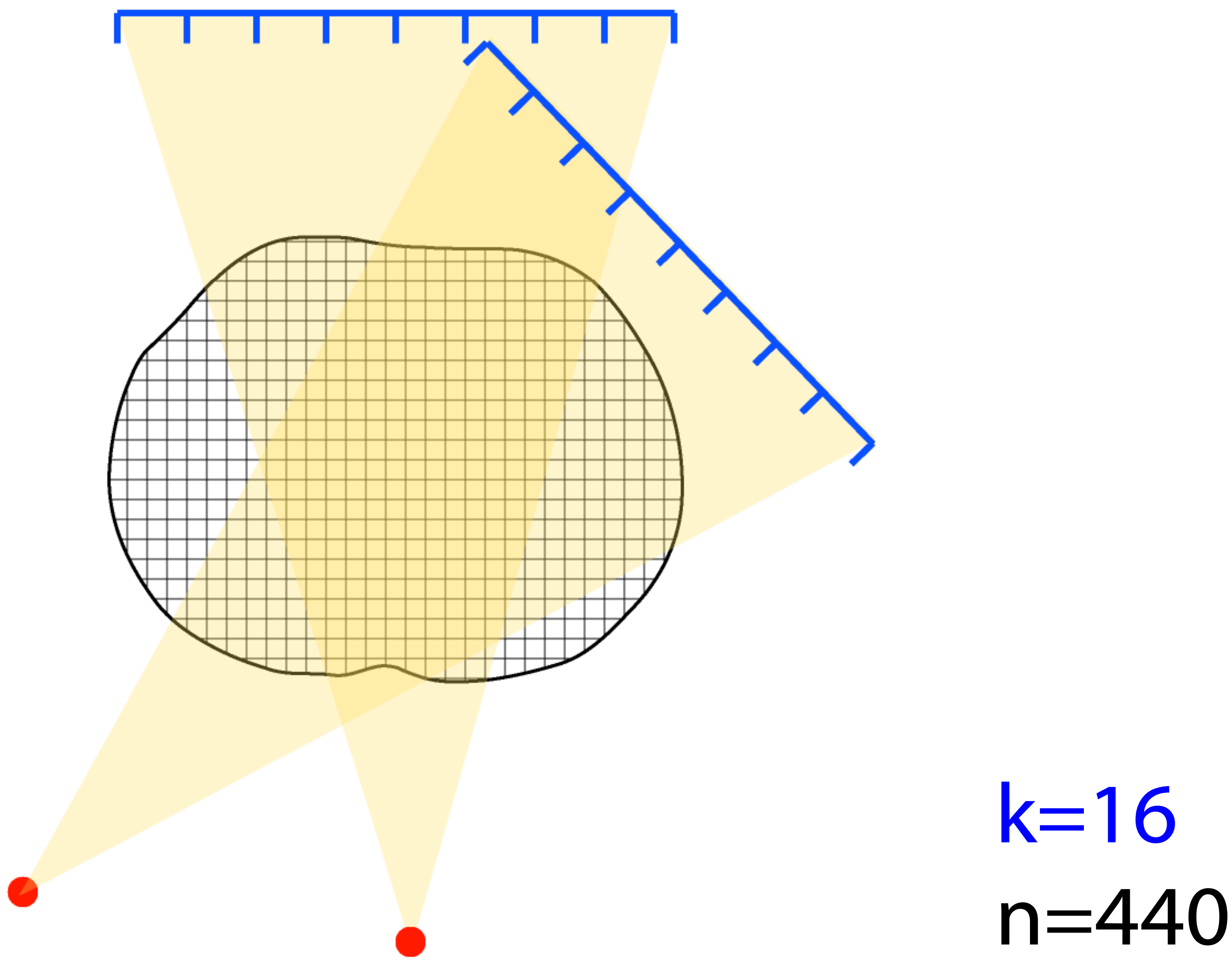


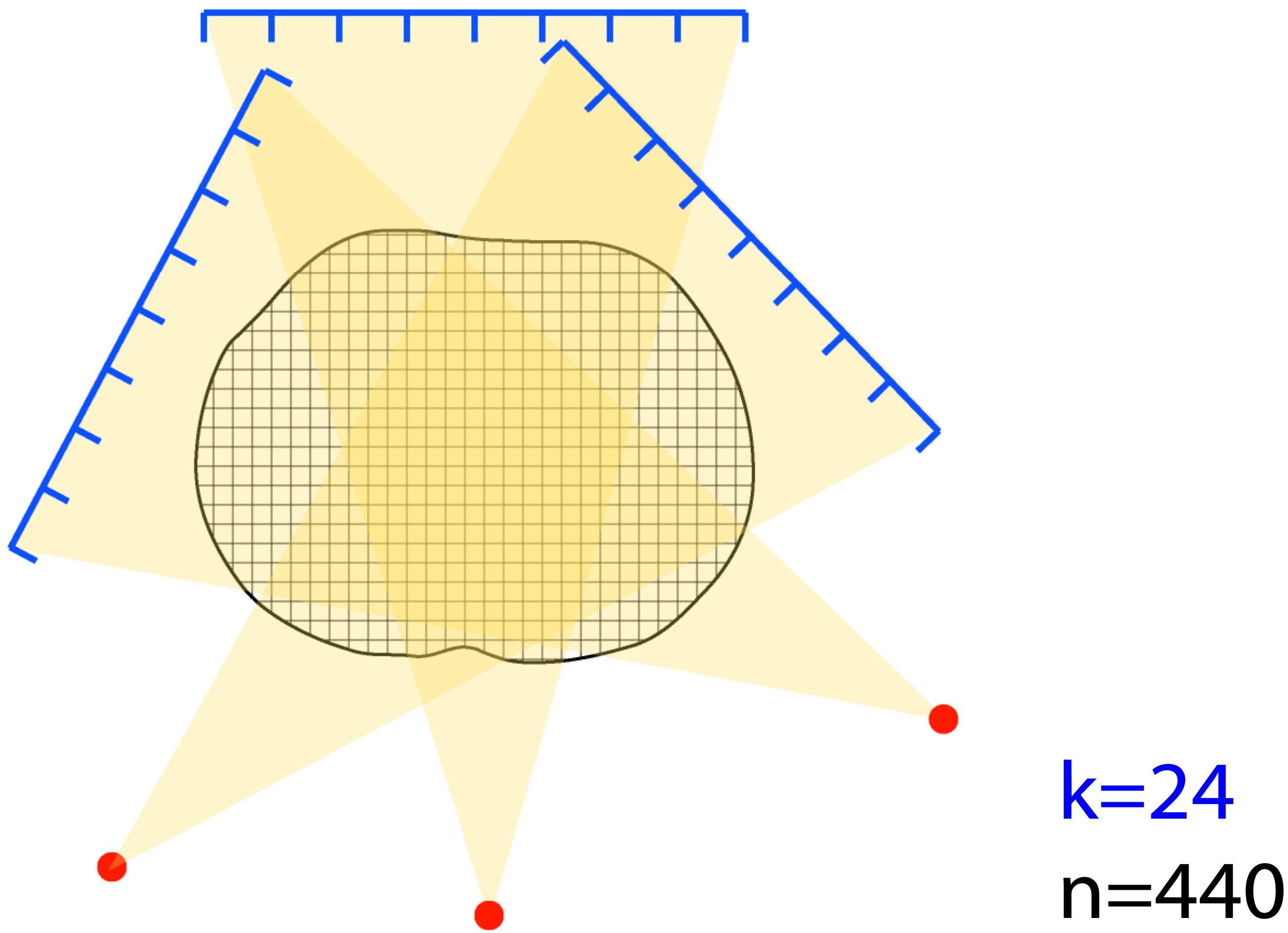
k=8

n=156



k=8
n=440

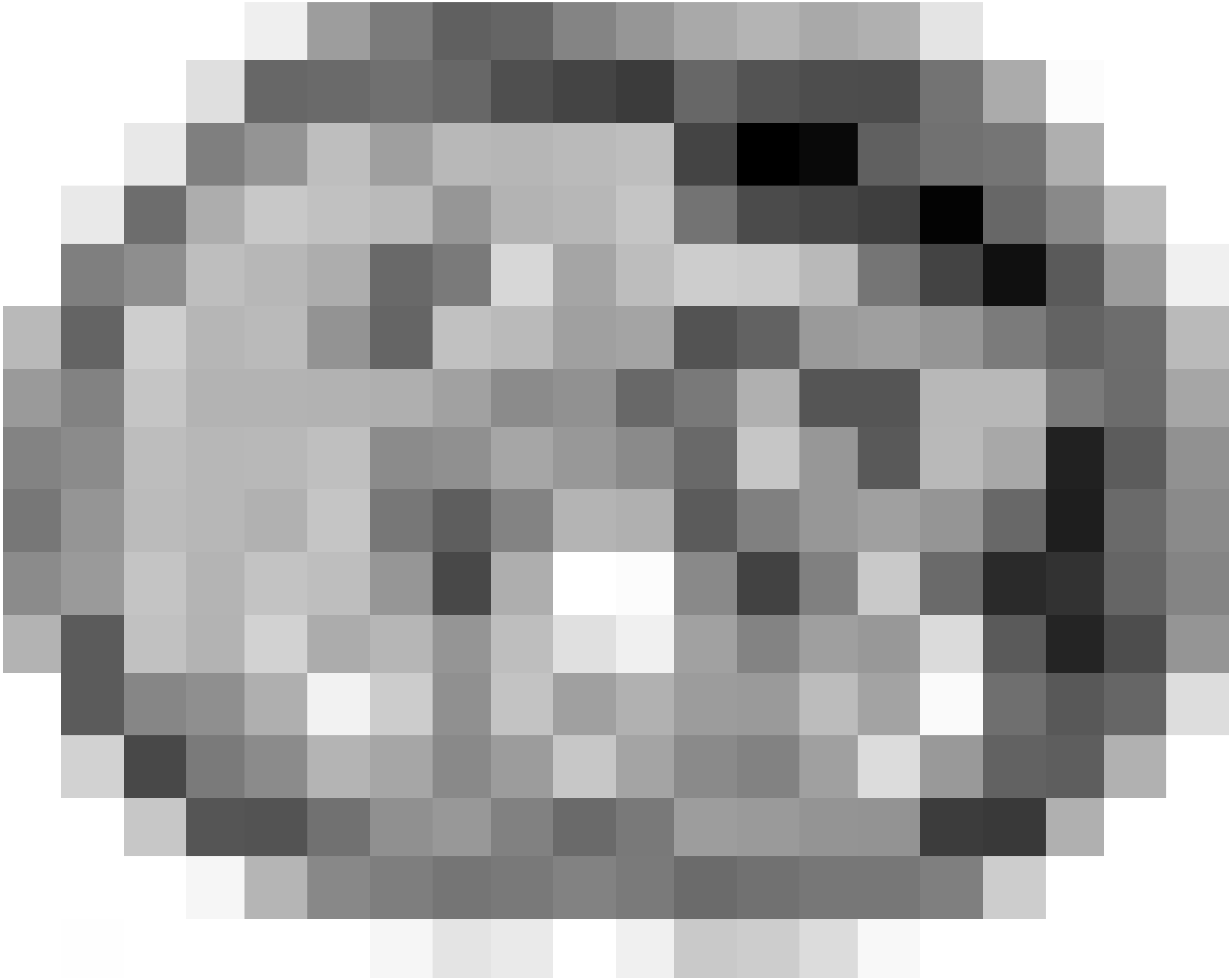

k=16
n=440

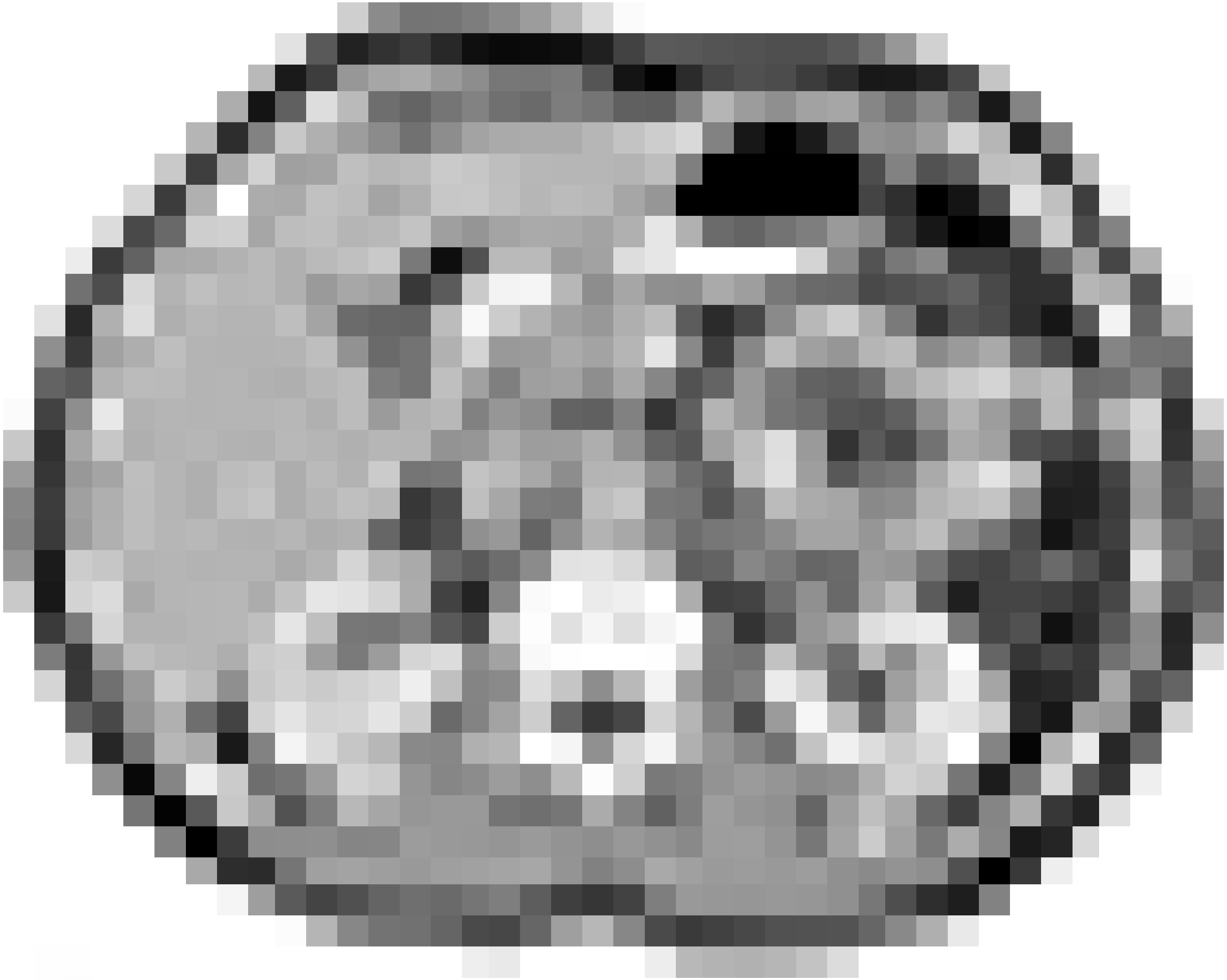

k=24
n=440

**This is the central idea of studying discretization-invariance:**

**The numbers n and k are independent.**

**For the Bayesian inversion strategy to work, the conditional mean estimates must converge as n or k or both tend to infinity.**





# We look for discretization-invariant choices of prior distributions

Recall the conditional mean estimate:

$$\mathbf{u}_{kn}^{\mathsf{CM}} := \int_{\mathbb{R}^n} u_n \pi_{kn}(u_n \,|\, M_k(\omega_0))\, du_n.$$

Possible problems with using $\mathbf{u}_{kn}^{\mathsf{CM}}$:

**Problem 1.** Estimates $\mathbf{u}_{kn}^{\mathsf{CM}}$ diverge as $n \to \infty$.

**Problem 2.** Estimates $\mathbf{u}_{kn}^{\mathsf{CM}}$ diverge as $k \to \infty$.

**Problem 3.** Prior distributions do not express the same prior information for all $n$.

Any choice of $T_n$ and $\Pi_n$ that avoids problems 1–3 is called discretization-invariant.

# Our results continue the tradition of infinite-dimensional statistical inversion

1970 Franklin
1984 Mandelbaum
1989 Lehtinen, Päivärinta and Somersalo
1991 Fitzpatrick
1995 Luschgy
2002 Lasanen
2005 Piiroinen

We achieve discretization invariance for Gaussian and some non-Gaussian prior distributions. Furthermore, we consider realistic measurements.

# Why is discretization invariance useful for finite-dimensional problems?

Sometimes in Bayesian inversion it is necessary to perform computations at two different (finite) resolutions.

For instance,

- Statistical error modeling of Kaipio and Somersalo
- Delayed acceptance Markov chain Monte Carlo

In such case it is important to transform prior information consistently between the two grids.

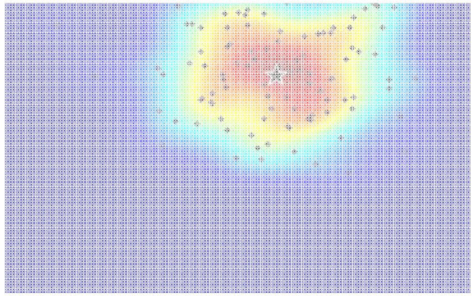
# Our proofs are based on Banach spaces and the concept of reconstructor

We use the following diagram of spaces:

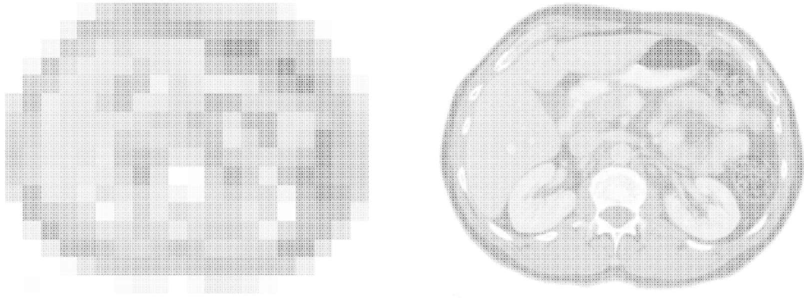
$$\begin{array}{ccccccccc} Y & \xrightarrow{A} & S^1 & \subset & S^{1/2} = Z & \subset & S \\ \Cup & & & & & & \Cup \\ U(\omega_1) & & & & & & \mathcal{E}(\omega_2) \end{array}$$

The reconstructor $\mathcal{R}_{M_{kn}}(U_n | \cdot\ )$ takes the measurement data $m_k = M_k(\omega_0)$ to the mean $\mathbf{u}_{kn}^{\mathsf{CM}}$.

The infinite-dimensional model $M = AU + \mathcal{E}$ has a reconstructor $\mathcal{R}_M(U | \cdot\ )$ as well.



1. Bayesian inversion



2. Discretization-invariance

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4. Besov space priors

$$e^{-\alpha\|u\|_{B^1_{11}}}$$

# The infinite-dimensional limit case can be rigorously defined

Express U as a random Fourier series

$$\sum_{j=-\infty}^{\infty} \sum_{\ell=-\infty}^{\infty} c_{j\ell}(\omega) e^{ij\theta + i\ell\psi},$$

and define projections $T_n$ as simple truncations.

We work with the following diagram:

$$\begin{array}{ccccccc} H^{-1}(\mathbb{T}^2) & \xrightarrow{A} & H^2(\mathbb{T}^2) & \subset & L^2(\mathbb{T}^2) & \subset & H^{-2}(\mathbb{T}^2) \\ \Cup & & & & & & \Cup \\ U(\omega_1) & & & & & & \mathcal{E}(\omega_2) \end{array}$$

Note: applying the classical *smoothness prior* results in realizations of U being continuous with probability zero.

**Theorem** (Lassas, Saksman and S 2008)
Bayesian inversion using Gaussian smoothness prior is discretization-invariant:

$$\lim_{k,n\to\infty} \mathbf{u}_{kn}^{\mathrm{CM}} = \lim_{k,n\to\infty} \mathcal{R}_{M_{kn}}(U_n \,|\, M_k(\omega_0)) = \mathcal{R}_M(U \,|\, M(\omega_0))$$

# Bayesian inversion with smoothness prior is related to Tikhonov regularization

In the Gaussian case, the posterior mean

$$\mathbf{u}_{kn}^{\mathsf{CM}} = \int_{\mathbb{R}^n} u_n \exp(-\alpha \|u_n\|_{H^1}^2) \exp(-\frac{1}{2}\|m_k - P_k A u_n\|_2^2)\, du_n$$

coincides with the MAP estimate

$$\arg\max_{u_n} \left[\exp(-\frac{1}{2}\|m_k - P_k A u_n\|_2^2 - \alpha\|u_n\|_{H^1}^2)\right],$$

where $m_k = M_k(\omega_0)$ is measurement data.

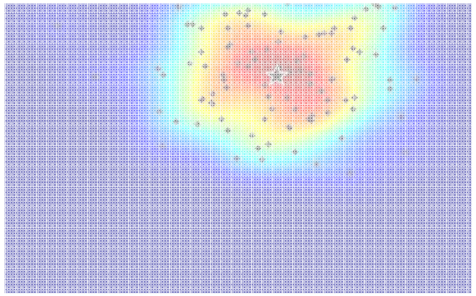
Consider Tikhonov regularization in the form

$$\mathbf{u}_{kn}^{\mathsf{T}} = \arg\min_{u_n} \left[\frac{1}{2}\|m_k - P_k A u_n\|_2^2 + \alpha(\|u_n\|_2^2 + \|\nabla u_n\|_2^2)\right],$$

where $\alpha > 0$ is the regularization parameter. It follows that $\mathbf{u}_{kn}^{\mathsf{T}} = \mathbf{u}_{kn}^{\mathsf{CM}} = \mathcal{R}_{M_{kn}}(U_n \,|\, M_k(\omega_0))$.

Much of the above results about
Gaussian smoothness priors
are due to Sari Lasanen and Petteri Piiroinen.

The essential new contribution here is
using the more realistic measurement model.



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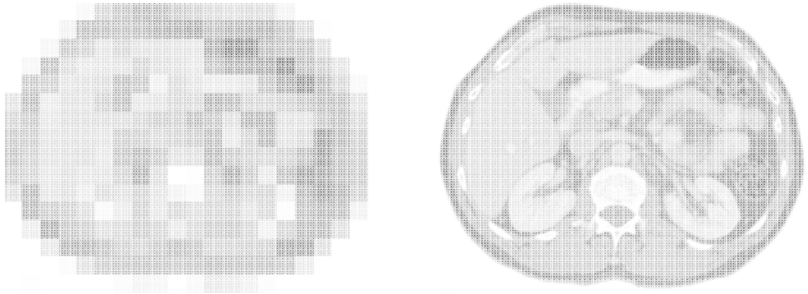

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$$e^{-\alpha\|u\|_{B^1_{11}}}$$

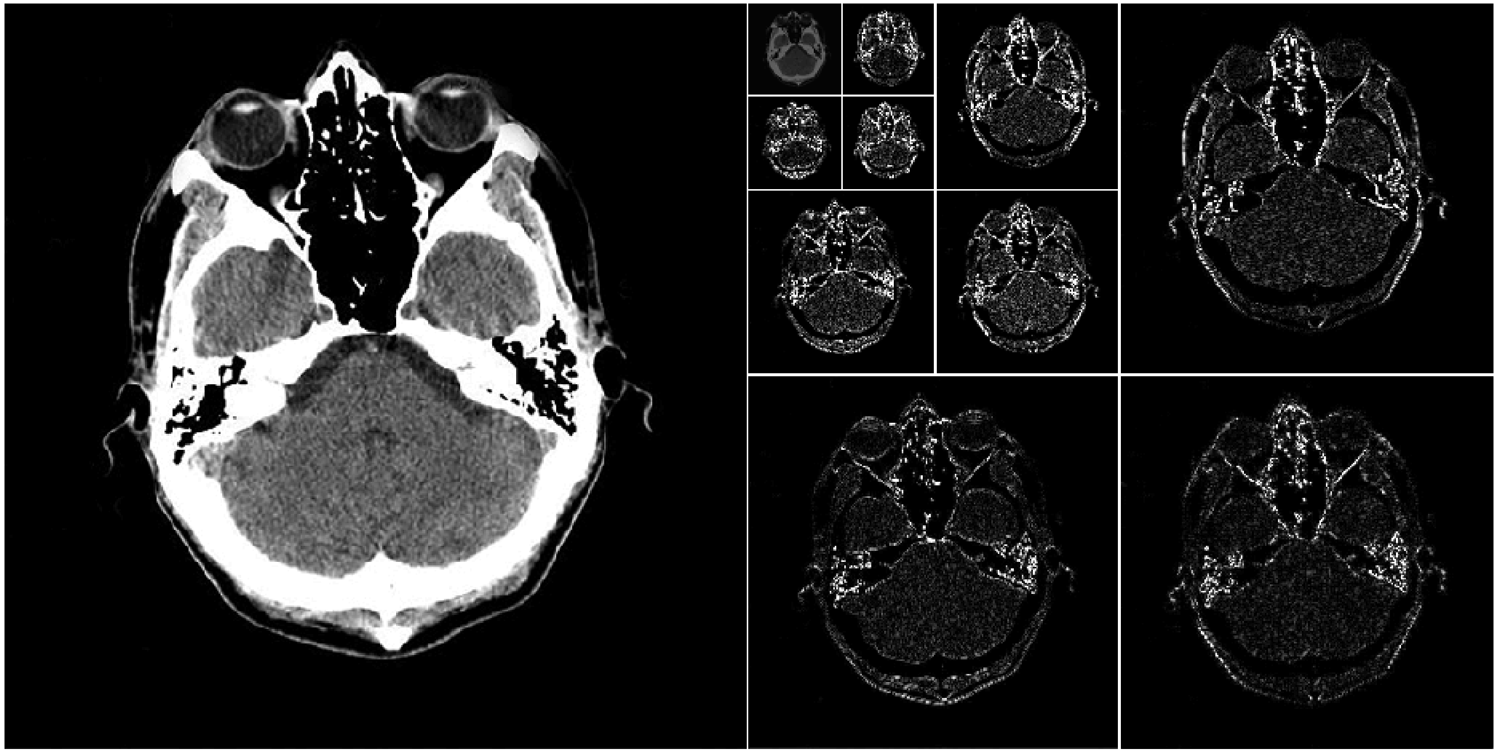
# How to express edge-preserving prior information invariantly?

We suggest replacing the problematic formal total variation density $\exp(-\alpha\|\nabla u\|_1)$ by the formal Besov space density $\exp(-\alpha\|u\|_{B^1_{11}})$.

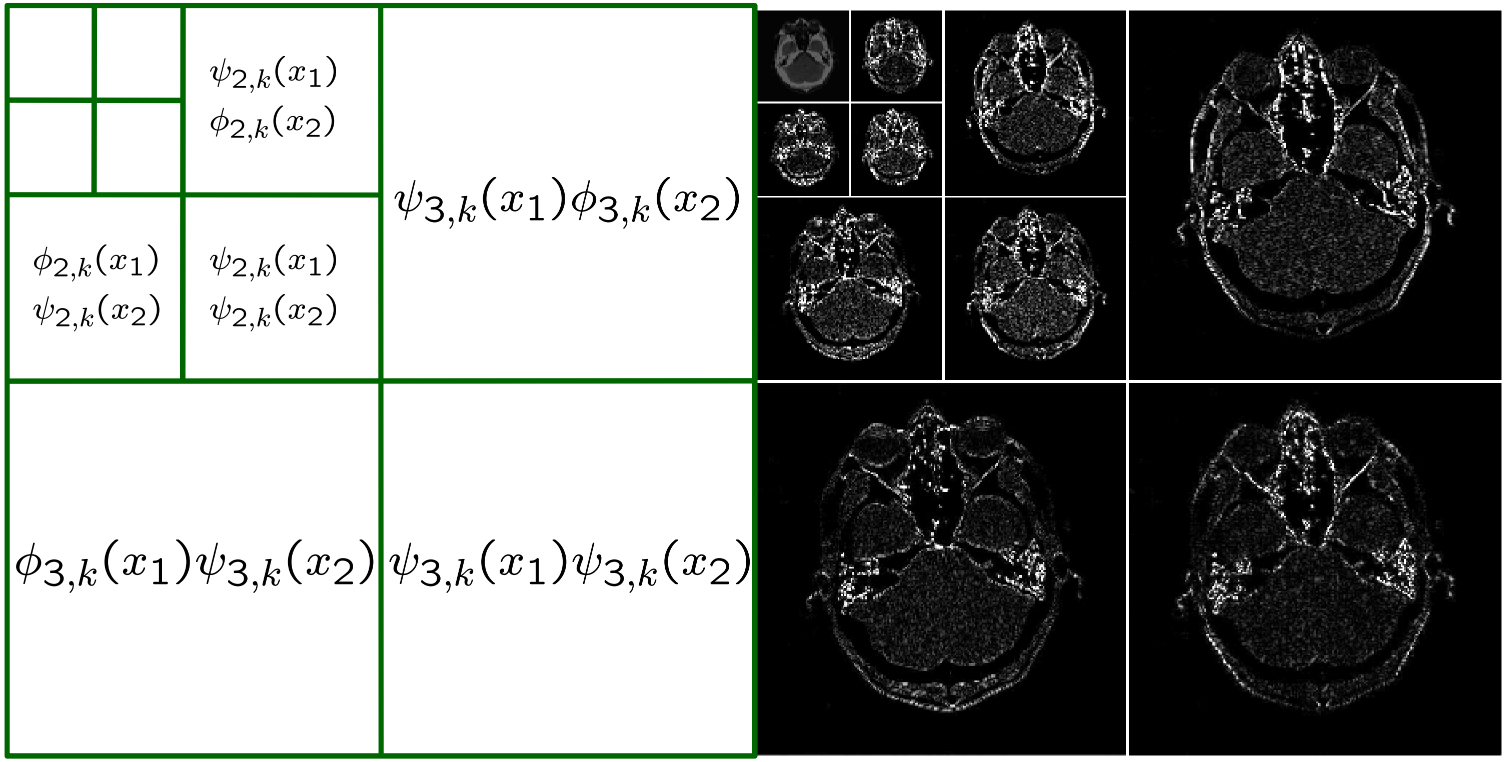
In dimension $d = 2$ the diagram of spaces is

$$\begin{array}{ccccc} B^{-2}_{11}(\mathbb{T}^2) & \xrightarrow{A} & B^{2}_{11}(\mathbb{T}^2) & \subset & B^{-2}_{\infty\infty}(\mathbb{T}^2) \\ \Cup & & & & \Cup \\ U(\omega_1) & & & & \mathcal{E}(\omega_2) \end{array}$$

# Wavelet transform divides a function into details at different scales



# We introduce a convenient renumbering of the basis functions




$$f(x) = \sum_{\ell=1}^{\infty} c_\ell \psi_\ell(x)$$

# Besov space norms can be written in terms of wavelet coefficients

The function

$$f(x) = \sum_{\ell=1}^{\infty} c_\ell \psi_\ell(x)$$

belongs to $B^s_{pq}(\mathbb{T}^d)$ if and only if

$$2^{js} 2^{dj(\frac{1}{2}-\frac{1}{p})} \left( \sum_{\ell=2^{jd}}^{2^{(j+1)d}-1} |c_\ell|^p \right)^{1/p} \in \ell^q(\mathbb{N}).$$

In particular, $f \in B^1_{11}(\mathbb{T}^2)$ if and only if

$$\sum_{\ell=1}^{\infty} |c_\ell| < \infty.$$

# Computation of the CM estimate reduces to sampling from well-known densities

$B^1_{11}(\mathbb{T}^2)$ prior: write $U$ in wavelet basis as

$$U = \sum_{\ell=1}^{\infty} X_\ell \psi_\ell$$

with each $X_\ell$ distributed independently $\sim \exp(-|x|)$.

Posterior distribution of $U_n$ takes the following form in terms of wavelet coefficients $x_1, \ldots, x_n$:

$$C \exp\left( -\frac{1}{2} \| M_k(\omega_0) - A \sum_{\ell=1}^{n} x_\ell \psi_\ell \|^2_{L^2(\mathbb{T}^2)^2} - \alpha \sum_{\ell=1}^{n} |x_\ell| \right)$$

Direct and inverse wavelet transforms are easy and quick to compute.

**Theorem** (Lassas, Saksman and S 2008) Bayesian inversion using $B^1_{11}(\mathbb{T}^2)$ Besov prior is discretization-invariant. More precisely:

Assume that $A : \mathcal{D}'(\mathbb{T}^2) \to C^\infty(\mathbb{T}^2)$ is a bounded linear operator. Let $t < \tilde{t} < -1$, $r > r_1 > 1$ and $\tau > 0$. Assume that $m = M(\omega_0) \in B^{-r_1}_{11}(\mathbb{T}^2)$.

Then

$$\|\mathcal{R}_{M_{kn}}(U_n|m_k) - \mathcal{R}_M(U|m)\|_{B^t_{11}(\mathbb{T}^2)} \leq C[k^{-\tau} + n^{-(\tilde{t}-t)/2}].$$

# We look for discretization-invariant choices of prior distributions

Recall the conditional mean estimate:

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**Problem 2.** Estimates $\mathbf{u}_{kn}^{\mathrm{CM}}$ diverge as $k \to \infty$.

**Problem 3.** Prior distributions do not express the same prior information for all $n$.

Any choice of $T_n$ and $\Pi_n$ that avoids problems 1–3 is called discretization-invariant.

**We show some Besov prior computations to give a flavor of how they work.**

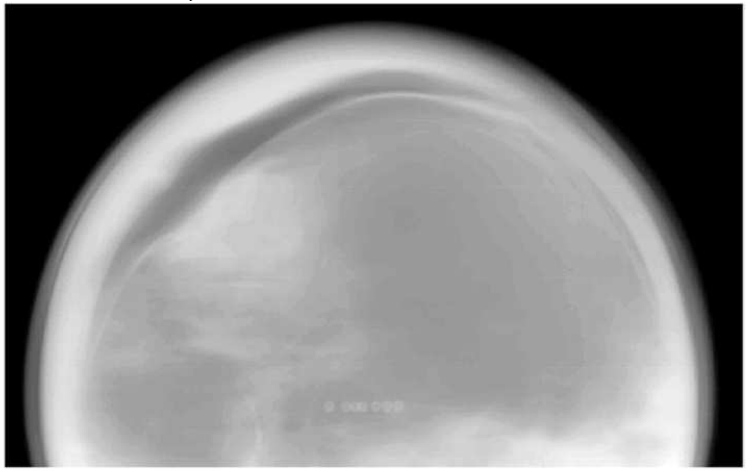
**However, the following examples are maximum a posteriori estimates only.**

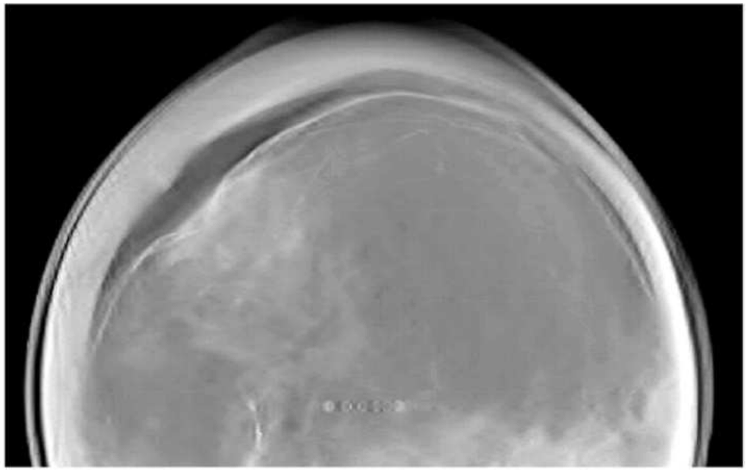
**Computation of conditional mean estimates is a work in progress.**

# Limited angle tomography results for X-ray mammography

[Rantala *et al.* 2006]
Thanks to GE Healthcare

Tomosynthesis



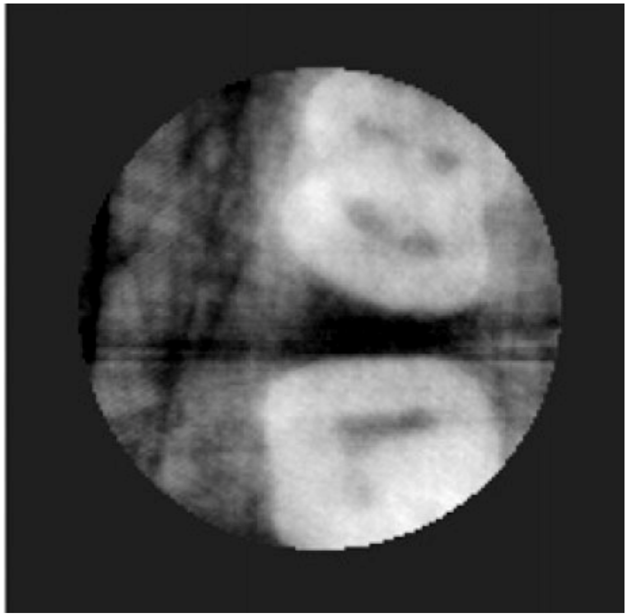


Besov prior

# Local tomography results for dental X-ray imaging

$\Lambda$-tomography

MAP with $B^{1/2}_{3/2,3/2}$ prior



[Niinimäki, S and Kolehmainen 2007]
Thanks to Palodex Group

# Empirical Bayes methodology for specifying Besov prior parameters

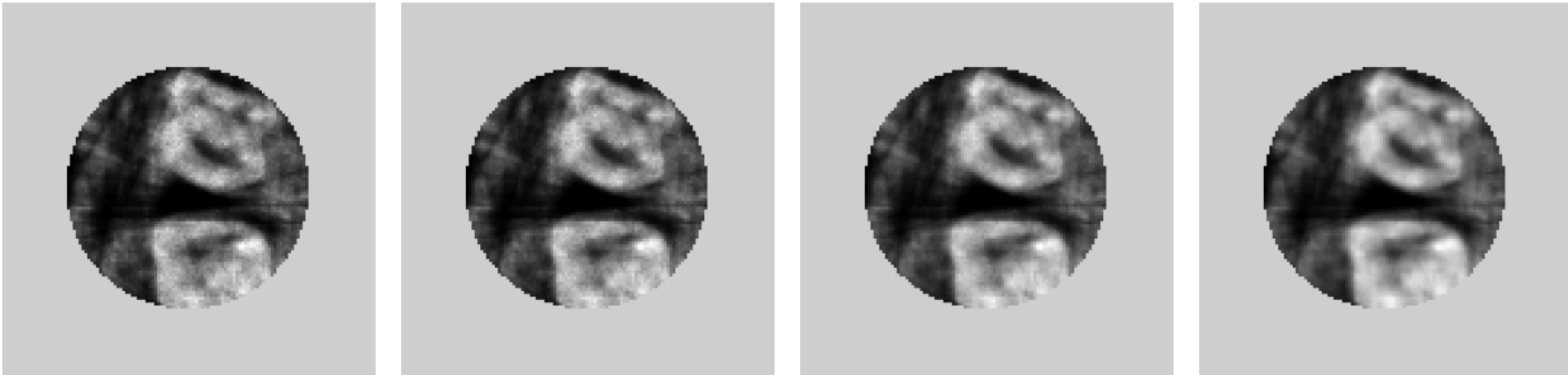


Figure 16: Reconstructions from in vitro dental data. From left: $s = 0$, $s = 0.4$, $s = 0.8$, $s = 1.2$.

[Vänskä, Lassas and S 2008]
Thanks to Palodex Group

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You can download the references at

**www.siltanen-research.net**