

Recent Advances in Bayesian Inference for Biomedical Imaging







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Noisy, ill-posed inverse problems:

 $f = N(\mathcal{A}(u), \varepsilon)$

Example: $f = Au + \varepsilon$

 $p_{like}(f|u) \propto$ $\exp\left(-\frac{1}{2}\|f - Au\|_{\Sigma_{\varepsilon}^{-1}}^{2}\right)$

 $p_{prior}(u) \propto$ $\exp(-\lambda \|D^T u\|_2^2)$

 $\begin{aligned} p_{post}(u|f) &\propto \\ &\exp\left(-\frac{1}{2}\|f - Au\|_{\Sigma_{\varepsilon}^{-1}}^{2} - \lambda \|D^{\mathsf{T}}u\|_{2}^{2}\right) \end{aligned}$

Probabilistic representation allows for a rigorous quantification of the solution's uncertainties.







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Inverse problems in the Bayesian framework edited by Daniela Calvetti, Jari P Kaipio and Erkki Somersalo. Special issue of *Inverse Problems*, November 2014.



UQ and a Model Inverse Problem Marco Iglesias and Andrew M. Stuart *SIAM News*, July/August 2014.

Advantageous for high uncertainties:

- Strongly non-linear problems.
- Severely ill-posed problems.
- Little analytical structure
- Additional model uncertainties.



Traditional task: Produce results to be interpreted by trained experts \implies Qualitative usage of the reconstructed information.

Example: Conventional *computer tomography* (CT).



Source: Wikimedia Commons

Traditional task: Produce results to be interpreted by trained experts \implies Qualitative usage of the reconstructed information.

New demand: Produce results for automatized analysis procedures / hypothesis testing; Multimodal imaging.

 \implies *Quantitative* usage of the reconstructed information.





Source: Andre C. Marreiros et al. (2010), Scholarpedia, 5(7):9568.

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New demand: Produce results for automatized analysis procedures / hypothesis testing; Multimodal imaging.

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Example: Statistical analysis of microscopy images.





Source: Wikimedia Commons



- Dynamic Bayesian inversion for prediction or control of dynamical systems
- Infinite dimensional Bayesian inversion.
- Incorporating model uncertainties.
- New ways of encoding a-priori information.
- Large-scale posterior sampling techniques.





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Sparsity / Compressible Representation



(a) 100%



(c) 1%

Sparsity a-priori constraints are used in variational regularization, compressed sensing and variable selection:

$$\hat{u}_{\lambda} = \underset{u}{\operatorname{argmin}} \left\{ \frac{1}{2} \| f - A u \|_{2}^{2} + \lambda \| D^{T} u \|_{1} \right\}$$

(e.g. total variation, wavelet shrinkage, LASSO,...)

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How about sparsity as a-priori information in the Bayesian approach? Felix Lucka, f.lucka@ucl.ac.uk - Recent Advances in Bayesian Inference for Biomedical Imaging





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(2) Sparsity by ℓ_p Priors

3 Hierarchical Bayesian Modeling

4 Discussion, Conclusion and Outlook



 $p_{prior}(u) \propto \exp\left(-\lambda \|D^{\mathsf{T}}u\|_{\rho}^{p}
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Decrease p from 2 to 0 and stop at p = 1 for convenience.

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Decrease p from 2 to 0 and stop at p = 1 for convenience.



$$\exp\left(-\lambda \|D^{\mathsf{T}}u\|_{2}^{2}\right)$$
$$\exp\left(-\frac{1}{2}\|f - Au\|_{\Sigma_{\varepsilon}^{-1}}^{2} - \lambda \|D^{\mathsf{T}}u\|_{2}^{2}\right)$$



$$\exp\left(-\lambda \|\boldsymbol{D}^{\mathsf{T}}\boldsymbol{u}\|_{1}\right) \\ \exp\left(-\frac{1}{2}\|\boldsymbol{f}-\boldsymbol{A}\boldsymbol{u}\|_{\boldsymbol{\Sigma}_{\varepsilon}^{-1}}^{2} - \lambda \|\boldsymbol{D}^{\mathsf{T}}\boldsymbol{u}\|_{1}\right)$$

$$p_{post}(u|f) \propto \exp\left(-\frac{1}{2}\|f - Au\|_{\Sigma_{\varepsilon}^{-1}}^2 - \lambda \|D^T u\|_1\right)$$

Aims: Bayesian inversion in high dimensions $(n \rightarrow \infty)$.

Priors: Simple ℓ_1 , total variation (TV), Besov space priors.

Starting points:

- Lassas & Siltanen, 2004. Can one use total variation prior for edge-preserving Bayesian inversion? Inverse Problems, 20.

Lassas, Saksman & Siltanen, 2009. Discretization invariant Bayesian inversion and Besov space priors. Inverse Problems and Imaging, 3(1).



Kolehmainen, Lassas, Niinimäki & Siltanen, 2012. Sparsity-promoting Bayesian inversion. Inverse Problems, 28(2).



Efficient MCMC Techniques for ℓ_1 Priors

Task: Monte Carlo integration by samples from

$$p_{post}(u|f) \propto \exp\left(-\frac{1}{2}\|f - Au\|_{\Sigma_{\varepsilon}^{-1}}^{2} - \lambda \|D^{T}u\|_{1}\right)$$

Problem: Standard Markov chain Monte Carlo (MCMC) sampler (Metropolis-Hastings) inefficient for large n or λ .

Contributions:

- Development of explicit single component Gibbs sampler.
- Tedious implementation for different scenarios.
- Still efficient in high dimensions $(n > 10^6)$.
- Detailed evaluation and comparison to MH.

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):125012.



Efficient MCMC Techniques for ℓ_1 Priors



(a) Reference

(b) MH-Iso, 1h



(d) MH-Iso, 16h

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(e) Reference

(f) SC Gibbs, 1h

(g) SC Gibbs, 4h

(h) SC Gibbs, 16h

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Deconvolution, simple ℓ_1 prior, $n = 513 \times 513 = 263169$.

Recent Generalization: Slice-Within-Gibbs Sampling

$$p_{prior}(u) \propto \exp\left(-\lambda \|D^{\mathsf{T}}u\|_{1}
ight)$$

Limitations:

- D must be diagonalizable (synthesis priors):
- ℓ_p^q -prior: exp $\left(-\lambda \| D^T u \|_p^q\right)$? TV in 2D/3D?
- Non-negativity or other hard-constraints?

Contributions:

- Replace explicit by generalized slice sampling.
- Implementation & evaluation for most common priors.



Neal, 2003. Slice Sampling. Annals of Statistics 31(3)

L, 2016. Fast Gibbs sampling for high-dimensional Bayesian inversion. submitted, arXiv:1602.08595





$$\hat{u}_{MAP} := \underset{u \in \mathbb{R}^n}{\operatorname{argmax}} \{ p_{post}(u|f) \} \quad \text{OR} \quad \hat{u}_{CM} := \int u p_{post}(u|f) \, \mathrm{d}u$$

Classical Bayes cost formalism discriminates MAP (= variational regularization) and advocates CM.







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Classical Bayes cost formalism discriminates MAP (= variational regularization) and advocates CM.

However...

- Theoretical argument has a logical flaw.
- Discrimination of MAP estimate is not intuitive.
- ► Gaussian priors: MAP = CM. Funny coincidence?
- Non-Gaussian priors: Poor computational validation!







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However...

- Theoretical argument has a logical flaw.
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- ► Gaussian priors: MAP = CM. Funny coincidence?
- Non-Gaussian priors: Poor computational validation!
- \implies Let's compute some examples!







Image Deblurring Example in 2D





(a) Unknown function \tilde{u}

(b) CM estimate by our Gibbs sampler

Deconvolution, simple ℓ_1 prior, $n = 1023 \times 1023 = 1046529$.

Image Deblurring Example in 2D





(a) Unknown function \tilde{u}

(b) MAP estimate by ADMM

Deconvolution, simple ℓ_1 prior, $n = 1023 \times 1023 = 1046529$.

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

- For $\lambda_n = const.$ and $n \longrightarrow \infty$ the TV prior diverges.
- CM diverges.
- MAP converges to edge-preserving limit.



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

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

- For λ_n ∝ √n+1 and n → ∞ the TV prior converges to a smoothness prior.
- CM converges to smooth limit.
- MAP converges to constant.





- **M.** Lassas, E. Saksman, S. Siltanen, 2009. Discretization invariant Bayesian inversion and Besov space priors, Inverse Probl Imaging, 3(1).
- V. Kolehmainen, M. Lassas, K. Niinimäki, S. Siltanen, 2012. Sparsity-promoting Bayesian inversion, Inverse Probl, 28(2).



- ▶ CT using only 45 projection angles and 500 measurement pixel.
- Besov space priors using Haar wavelets.

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



MAP estimate (by ADMM)



CM estimate (by our Gibbs sampler)

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



CM estimate (by our Gibbs sampler)

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



MAP estimate (by ADMM)

CM estimate (by our Gibbs sampler)

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



CM estimate (by our Gibbs sampler)

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



CM estimate (by our Gibbs sampler)

$$\hat{u}_{MAP} := \underset{u \in \mathbb{R}^n}{\operatorname{argmax}} \{ p_{post}(u|f) \} \quad \text{OR} \quad \hat{u}_{CM} := \int u p_{post}(u|f) \, \mathrm{d}u$$

Summary:

- ► Gaussian priors: MAP = CM. Funny coincidence?
- For reasonable priors, CM and MAP look quite similar. Fundamentally different?
- If the CM estimate looks good, it looks like the MAP.
- MAP estimates are sparser, sharper, look and perform better...
- Gribonval, Marchart, Louchet and Moisan, 2011-2013: CM are MAP estimates for different priors.
- \implies Classical theory cannot be complete!







$$\hat{u}_{MAP} := \underset{u \in \mathbb{R}^n}{\operatorname{argmax}} \{ p_{post}(u|f) \} \quad \text{OR} \quad \hat{u}_{CM} := \int u p_{post}(u|f) \, \mathrm{d}u$$

We developed new Bayes cost functions such that

- Both MAP and CM are proper Bayes estimators for proper, convex cost functions.
- Key ingredient: Bregman distances.
- Gaussian case is no strange exception but consistent in this framework.
- M. Burger, F.L., 2014. Maximum a posteriori estimates in linear inverse problems with log-concave priors are proper Bayes estimators, Inverse Problems, 30(11):114004.
- **T. Helin, M. Burger, 2015**. *Maximum a posteriori* probability estimates in infinite-dimensional Bayesian inverse problems, Inverse Problems, 31(8):085009.







Application to Experimental Data: Walnut-CT

- Cooperation with Samuli Siltanen, Esa Niemi et al.
- Implementation of MCMC methods for Fanbeam-CT.
- Besov and TV prior; non-negativity constraints.
- Stochastic noise modeling.
- Bayesian perspective on limited angle CT.



Use the data set for your own work: http://www.fips.fi/dataset.php (documentation: arXiv:1502.04064)



Walnut-CT with TV Prior: Full Angle







(c) CStd







(d) CM

(e) CM, special color scale

(f) CM of $\|\nabla u\|_2$

Walnut-CT with TV Prior: Full vs. Limited Angle



(d) MAP, limited

(e) CM, limited

(f) CStd, limited

Walnut-CT with TV Prior: Non-Negativity Constraints, Limited Angle



(a) CM, uncon







(b) CM, non-neg











(2) Sparsity by ℓ_p Priors

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Gaussian increment prior:

$$p_{prior}(u) \propto \prod_i \exp\left(-rac{(u_{i+1}-u_i)^2}{\gamma}
ight)$$

- Gaussian variables take values on a characteristic scale, determined by γ.
- Similar amplitudes are likely, sparsity (= outliers) is unlikely.



Hierarchical Bayesian Modeling (HBM) of Sparsity

Conditionally Gaussian increment prior:

$$p_{prior}(u|\gamma) \propto \prod_{i} \exp\left(-rac{(u_{i+1}-u_i)^2}{\gamma_i}
ight)$$

Scale-invariant hyperprior to approximate un-informative γ_i^{-1} prior:



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The Implicit Energy Functional behind HBM



Implicit prior is a Student's *t*-prior with $\nu = 2\alpha, \theta = \beta/(2\alpha)$:

$$\begin{split} p_{prior}(u) &\propto \prod_{i} \left(1 + \frac{u_{i}^{2}}{\nu \theta} \right)^{-\frac{\nu - 1}{2}} \\ p_{post}(u|f) &\propto \exp\left(-\frac{1}{2} \|f - A u\|_{\Sigma_{\varepsilon}^{-1}}^{2} - \frac{\nu - 1}{2} \sum_{i} \log\left(1 + \frac{u_{i}^{2}}{\nu \theta} \right) \right) \end{split}$$



feature	ℓ_p prior	HBM
$\mathcal{J}(u)$	$\ u\ _p^p$	$rac{ u+1}{2}\sum\log\left(1+rac{u^2}{ u heta} ight)$
sparsifying parameter	p>0	$\nu > 0$
quadratic limit	p=2	$\nu ightarrow \infty$
sparse limit	ho ightarrow 0	u ightarrow 0
limit functional	$ u _0$	$\sum_{i}^{n}\log\left(\left u_{i}\right ight)$ if all $u_{i} eq0$,
		$-\infty$ else
solutions	sparse	compressible
differentiable	p>1	always
convex	everywhere for $p \geqslant 1$	$\ u\ _{\infty} < \sqrt{\nu\theta}$
homogeneous	yes	no

Other stuff related to HBM: Graphical models, general linear models, latent variable models, Variational Bayes, expectation maximization, scale mixture models, empirical priors, parametric empirical Bayes, automatic relevance determination...

$$p_{post}(u,\gamma|f) \propto \exp\left(-\frac{1}{2}\|f - Au\|_{\Sigma_{\varepsilon}^{-1}}^2 - \sum_i^n \left(\frac{u_i^2 + 2\beta}{2\gamma_i} + (\alpha + 1/2)\log(\gamma_i)\right)\right)$$

All computational approaches (optimization or sampling) exploit the conditional structure:

Fix γ and update u by solving 1 n-dim linear problem.

Fix *u* and update γ by solving *n* 1-dim non-linear problems.

Major difficulty: Multimodality of posterior.

Heuristic Full-MAP computation:

- Use MCMC to explore posterior (avoids very sub-optimal modes).
- Initialize alternating optimization by local MCMC averages to compute local modes.

No guarantee for finding highest mode but usually an acceptable result.

Why HBM? EEG/MEG Source Reconstruction





Notoriously ill-posed problem!



- Inversion with log-concave priors suffers from systematic depth miss-localization, HBM does not.
- HBM shows promising results for focal brain networks with simulated and real data.
- L., Aydin, Vorwerk, Burger, Wolters, 2013. Hierarchical Fully-Bayesian Inference for Combined EEG/MEG Source Analysis of Evoked Responses: From Simulations to Real Data. BaCl 2013, Geneva.
 - L., Pursiainen, Burger, Wolters, 2012. Hierarchical Fully-Bayesian Inference for EEG/MEG combination: Examination of Depth Localization and Source Separation using Realistic FE Head Models. Biomag 2012, Paris
 - L., Pursiainen, Burger, Wolters, 2012. Hierarchical Bayesian inference for the EEG inverse problem using realistic FE head models: Depth localization and source separation for focal primary currents. NeuroImage, 61(4):1364–1382.

Bayesian Modeling:

- Sparsity can be modeled in different ways.
- HBM is an interesting but challenging alternative to ℓ_p priors.

• Combine ℓ_p -type and hierarchical priors: ℓ_p -hypermodels.

Bayesian Computation:

- Elementary MCMC samplers may perform very differently.
- Contrary to common beliefs sample-based Bayesian inversion in high dimensions (n > 10⁶) is feasible if tailored samplers are developed.
- Reason for the efficiency of the Gibbs samplers is unclear.
- Adaptation, parallelization, multimodality, multi-grid.
- Heuristic, fully Bayesian computation for HBM looks promising but needs more careful examination.

Bayesian Estimation / Uncertainty Quantification

- MAP estimates are proper Bayes estimators.
- But: Everything beyond "MAP or CM?" is far more interesting and can really complement variational approaches.

- However: Extracting information from posterior samples (*data mining*) is a non-trivial (future research) topic.
- Application studies had proof-of-concept character up to now.
- Specific UQ task to explore full potential of the Bayesian approach.



L, 2016. Fast Gibbs sampling for high-dimensional Bayesian inversion. submitted, arXiv:1602.08595



L., 2014. Bayesian Inversion in Biomedical Imaging PhD Thesis, University of Münster.

M. Burger, L., 2014. *Maximum a posteriori estimates in linear inverse problems with log-concave priors are proper Bayes estimators Inverse Problems*, 30(11):114004.



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):125012.

L., Pursiainen, Burger, Wolters, 2012. Hierarchical Bayesian inference for the EEG inverse problem using realistic FE head models: Depth localization and source separation for focal primary currents. NeuroImage, 61(4):1364–1382.



Thank you for your attention!



L, 2016. Fast Gibbs sampling for high-dimensional Bayesian inversion. submitted, arXiv:1602.08595



- L., 2014. Bayesian Inversion in Biomedical Imaging PhD Thesis, University of Münster.
- **M. Burger, L., 2014.** *Maximum a posteriori estimates in linear inverse problems with log-concave priors are proper Bayes estimators Inverse Problems*, 30(11):114004.
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Efficient MCMC Techniques for ℓ_1 Priors



Temporal autocorrelation $R^*(t)$ for 1D TV-deblurring, n = 63.

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Efficient MCMC Techniques for ℓ_1 Priors)



Temporal autocorrelation $R^*(t)$ for 1D TV-deblurring.

For images dimensions > 1: No theory yet...but we can compute it.

Test scenario:

▶ CT using only 45 projection angles and 500 measurement pixel.



Need for New Theoretical Predictions



For images dimensions > 1: No theory yet...but we can compute it.



MAP, $n=~64^2$, $\lambda=500$



CM,
$$n = 64^2$$
, $\lambda = 500$

Need for New Theoretical Predictions



For images dimensions > 1: No theory yet...but we can compute it.



CM, $n = 128^2$, $\lambda = 500$

Need for New Theoretical Predictions



For images dimensions > 1: No theory yet...but we can compute it.



MAP, $n = 256^2$, $\lambda = 500$ CM, $n = 256^2$, $\lambda = 500$

cf. Louchet, 2008, Louchet & Moisan, 2013 for the denoising case, A = I.

Examination of Alternative Priors by MCMC: TV-p



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$$p_{post}(u) \propto \exp\left(-\frac{1}{2}\|f - Au\|_{\Sigma_{\varepsilon}^{-1}}^{2} - \lambda \|D^{\mathsf{T}}u\|_{\rho}^{\rho}\right)$$



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 $\Psi(u, v)$.
- Bayes cost is the expected cost:

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

▶ Bayes estimator \hat{u}_{BC} for given Ψ minimizes Bayes cost. Turns out:

$$\hat{u}_{BC}(f) = \underset{\hat{u}}{\operatorname{argmin}} \left\{ \int \Psi(u, \hat{u}(f)) p_{post}(u|f) \, \mathrm{d}u \right\}$$



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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

$$arPsi_\epsilon(u,\hat{u}) = egin{cases} 0, & ext{if} & \|u-\hat{u}\|_\infty \leqslant \epsilon \ 1 & ext{otherwise}, \end{cases}$$

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

- ► MAP and CM seem theoretically and computationally fundamentally different ⇒ 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).

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

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

$$arPsi_\epsilon(u,\hat{u}) = egin{cases} 0, & ext{if} & \|u-\hat{u}\|_\infty < \epsilon \ 1 & ext{otherwise}, \end{cases}$$

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

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

Define

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

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

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

Properties:

Proper, convex cost functions

► For
$$\mathcal{J}(u) = \beta/\lambda \|Lu\|_2^2$$
 (Gaussian case!) we have $\lambda D_{\mathcal{J}}(\hat{u}, u) = \beta \|L(\hat{u} - u)\|_2^2$, and $\Psi_{LS}(u, \hat{u}) = \Psi_{Brg}(u, \hat{u})!$

Theorems:

- (1) The CM estimate is the Bayes estimator for $\Psi_{LS}(u, \hat{u})$
- (II) The MAP estimate is the Bayes estimator for $\Psi_{\scriptscriptstyle \mathsf{Brg}}(u,\hat{u})$

Bregman distances



For a proper, convex functional $\Psi : \mathbb{R}^n \longrightarrow \mathbb{R} \cup \{\infty\}$, the *Bregman* distance $D_{\Psi}^p(f,g)$ between $f,g \in \mathbb{R}^n$ for a subgradient $p \in \partial \Psi(g)$ is defined as



 $D^p_\Psi(f,g) = \Psi(f) - \Psi(g) - \langle p,f-g
angle, \qquad p \in \partial \Psi(g)$

Basically, $D_{\Psi}(f,g)$ measures the difference between Ψ and its linearization in f at another point g