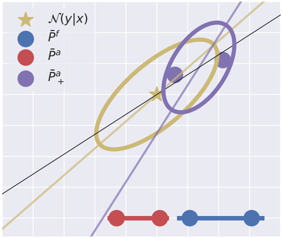
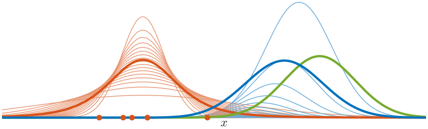
EnKF – FAQ

(Ensemble Kalman filter – Frequently asked questions)





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Leeds, May 16, 2019

Revising the stochastic iterative ensemble smoother

Patrick N. Raanes*[1,2], Geir Evensen[1,2], and Andreas S. Stordal[1]

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February 4, 2019

Abstract

Ensemble randomized maximum likelihood (EnRML) is an iterative (stochastic) ensemble smoother, used for large and nonlinear inverse problems, such as history matching and data assimilation. Its current formulation is overly complicated and has issues with computational costs, noise, and covariance localization, even causing some practitioners to omit crucial prior information. This paper resolves these difficulties and streamlines the algorithm, without changing its output. These simplifications are achieved through the careful treatment of the linearizations and subspaces. For example, it is shown (a) how ensemble linearizations relate to average sensitivity, and (b) that the ensemble does not loose rank during updates. The paper also draws significantly on the theory of the (deterministic) iterative ensemble Kalman smoother (IEnKS). Comparative benchmarks are obtained with the Lorenz-96 model with these two smoothers and the ensemble smoother using multiple data assimilation (ES-MDA).

1 Introduction

Ensemble (Kalman) smoothers are approximate methods used for data assimilation (state estimation in geoscience), history matching (parameter estimation for reservoirs), and other inverse problems constrained by partial differential equations. Iterative versions of the ensemble smoother, derived from optimization perspectives, have proven useful in improving the estimation accuracy when the forward operator is nonlinear. Ensemble randomized maximum likelihood (EnRML), also known as the iterative ensemble smoother (IES), is one such method. This paper fixes several issues with EnRML, described in the following. *Readers unfamiliar with EnRML may jump to the beginning of the derivation:*

linearization $\overline{\mathbf{M}}_i$ only appears in the product $\overline{\mathbf{M}}_i \overline{\mathbf{C}}_{x,i} \overline{\mathbf{M}}_i^\top$, which does not require $\mathbf{X}_i^+$. For the *prior increment*, on the other hand, the modification breaks its Kalman gain form. Meanwhile, the precision matrix form, i.e. their equation 10, is already invalid because it requires the inverse of $\overline{\mathbf{C}}_{x,i}$. Still, in their equation 15, the prior increment is formulated with an inversion in ensemble space, and also unburdened of the explicit computation of $\overline{\mathbf{M}}_i$. Intermediate explanations are lacking, but could be construed to involve approximate inversions. Another issue is that the pseudo-inverse of $\overline{\mathbf{C}}_x$ is now required (via $\mathbf{X}$), and covariance localization is further complicated.

An approximate version was therefore also proposed, where the prior mismatch term is omitted from the update formula altogether. This is not principled, and severely

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RESEARCH ARTICLE

Quarterly Journal of the Royal Meteorological Society RMetS

Adaptive covariance inflation in the ensemble Kalman filter by Gaussian scale mixtures

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Funding information

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- Why do we use $(N-1)$ in $\frac{1}{N-1}\sum_n (x_n - \bar{x})^2$?
- About nonlinearity:
  - Why does it create sampling error?
  - Why does it cause divergence?

$\mathcal{N}$ despite nonlinearity

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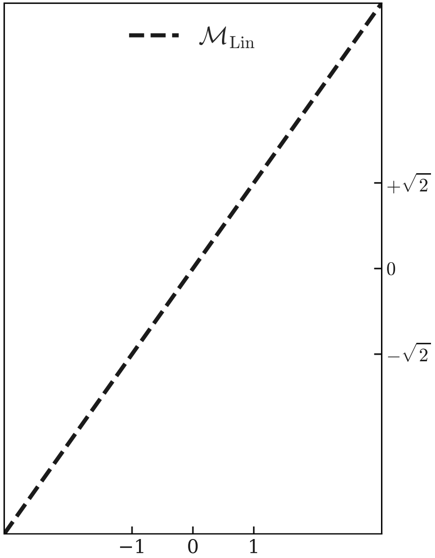

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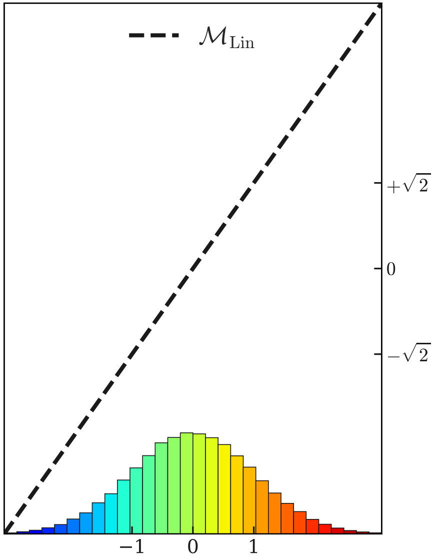

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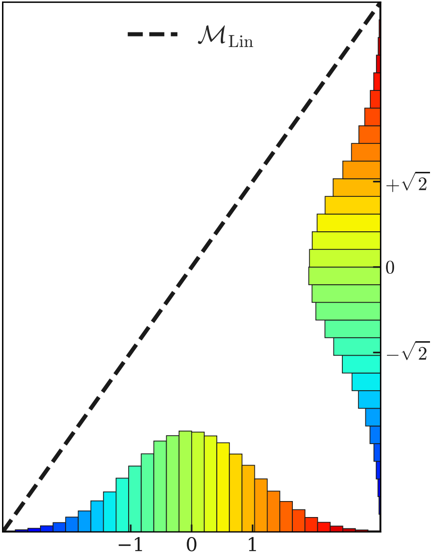

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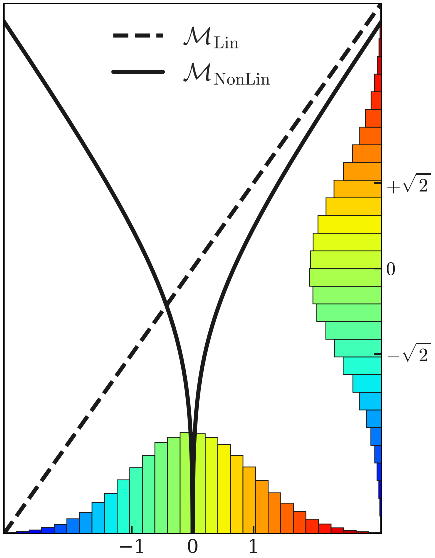

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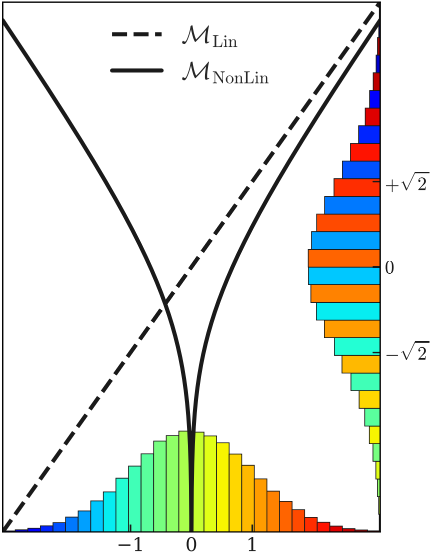

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Consider the problem with:

$$\begin{aligned} \text{prior} &= \mathcal{N}(x|0, \underline{\;2\;}), \\ \text{likelihood} &= \mathcal{N}(0|x, 2), \\ \implies \text{posterior} &= \mathcal{N}(x|\underline{\;0\;}, \underline{\;1\;}). \end{aligned}$$

Now apply a (square-root) EnKF to it.

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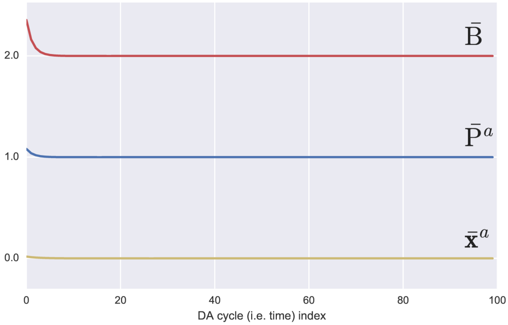

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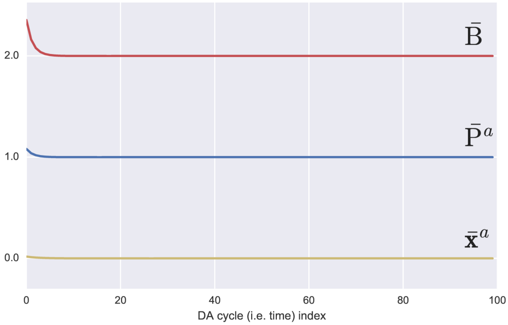

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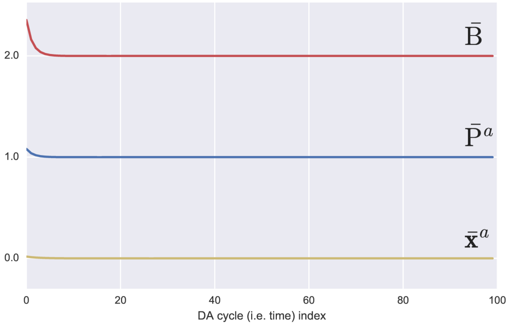

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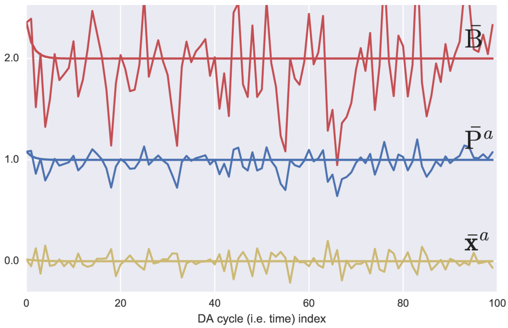

Riccati eqn.

Assume linear $(\mathbf{M})$ dynamics, $\mathbf{Q} = 0$, $\mathbf{H} = \mathbf{I}$, and a deterministic EnKF.

The ensemble covariance obeys:

- the forecast step: $$\bar{\mathbf{B}}_k = \mathbf{M}^2 \bar{\mathbf{P}}_{k-1} \, ; \tag{1}$$
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$$\iff \quad \bar{\mathbf{P}}_k^{-1} = \bar{\mathbf{B}}_k^{-1} + \mathbf{R}^{-1} \, . \tag{3}$$

$\Longrightarrow$ the "Riccati recursion":

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Deductions from Riccati: Attenuation

Stationary solution:

$$\bar{\mathbf{P}}_\infty^{-1} = (\mathbf{M}^2 \bar{\mathbf{P}}_\infty)^{-1} + \mathbf{R}^{-1} \tag{5}$$

$$\iff \quad \bar{\mathbf{P}}_\infty = \bar{\mathbf{K}}_\infty \mathbf{R} \,, \quad \bar{\mathbf{K}}_\infty = \begin{cases} \mathbf{I} - \mathbf{M}^{-2} & \text{if } \mathbf{M} \geq 1 \,, \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

Initial conditions (ICs) don't appear
$\implies$ ICs are "forgotten".
$\implies$ Sampling error is attenuated.

Deductions from Riccati: Attenuation

Stationary solution:

$$\bar{\mathbf{P}}_\infty^{-1} = (\mathbf{M}^2 \bar{\mathbf{P}}_\infty)^{-1} + \mathbf{R}^{-1} \tag{5}$$

$$\iff \quad \bar{\mathbf{P}}_\infty = \bar{\mathbf{K}}_\infty \mathbf{R}\,, \quad \bar{\mathbf{K}}_\infty = \begin{cases} \mathbf{I} - \mathbf{M}^{-2} & \text{if } \mathbf{M} \geq 1\,, \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

Initial conditions (ICs) don't appear

$\implies$ ICs are "forgotten".

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Perturbation analysis:

$$\text{Recall:} \qquad \bar{\mathbf{P}}_k = \underbrace{(\mathbf{I} - \bar{\mathbf{K}}_k)}\, \mathbf{M}^2 \bar{\mathbf{P}}_{k-1} \, . \tag{7}$$

$$\text{By contrast,} \qquad \delta\bar{\mathbf{P}}_k \approx (\mathbf{I} - \bar{\mathbf{K}}_k)^2 \left[\mathbf{M}^2 + \mathcal{M}\mathcal{M}''\right] \delta\bar{\mathbf{P}}_{k-1} \, , \tag{8}$$

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Deductions from Riccati: Why $(N-1)$?

Riccati invariant to change $\tilde{\mathbf{P}} = \alpha\bar{\mathbf{P}}$, hence:

$$1/\tilde{\mathbf{P}}_\infty = 1/(\mathbf{M}^2\tilde{\mathbf{P}}_\infty) + 1/\mathbf{R} \tag{9}$$

Sampling error from nonlinearity – why?

- Consider the m-th "true" and "sample" moments:

$$\mu_m = \mathbb{E}[x^m], \tag{10}$$

$$\hat{\mu}_m = N^{-1} \sum_{n=1}^{N} x_n^m. \tag{11}$$

- Define: $\text{Error}_m = \hat{\mu}_m - \mu_m$.
- Define: $\mu_m^{\mathsf{f}} = \mathbb{E}[(\mathcal{M}(x))^m]$.
- Assume degree-d Taylor-exp. of $\mathcal{M}$ is accurate. Then

$$\mu_m^{\mathsf{f}} = \sum_{i=1}^{md} C_{m,i}\mu_i. \tag{12}$$

- Due to coupling of moments,

$$\text{Error}_m^{\mathsf{f}} = \sum_{i=1}^{md} C_{m,i}\text{Error}_i^{a}, \tag{13}$$

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Why do we prefer the Kalman gain "form"?

Not equivalent when $(N-1) < M$:

$$\bar{\mathbf{P}} = [\mathbf{I} - \bar{\mathbf{K}}\mathbf{H}]\bar{\mathbf{B}} \tag{14}$$

$$\bar{\mathbf{P}} = (\bar{\mathbf{B}}^{+} + \mathbf{H}^{\mathsf{T}}\mathbf{R}^{-1}\mathbf{H})^{-1} \tag{15}$$

Which is better?

Note that eqn. (15) follows from

$$\text{prior} \propto \exp[-\tfrac{1}{2}(x - \bar{x})^{\mathsf{T}}\,\bar{\mathbf{B}}^{+}\,(x - \bar{x})]\,, \tag{16}$$

which is "flat" in the directions outside of $\text{col}(\bar{\mathbf{B}})$.
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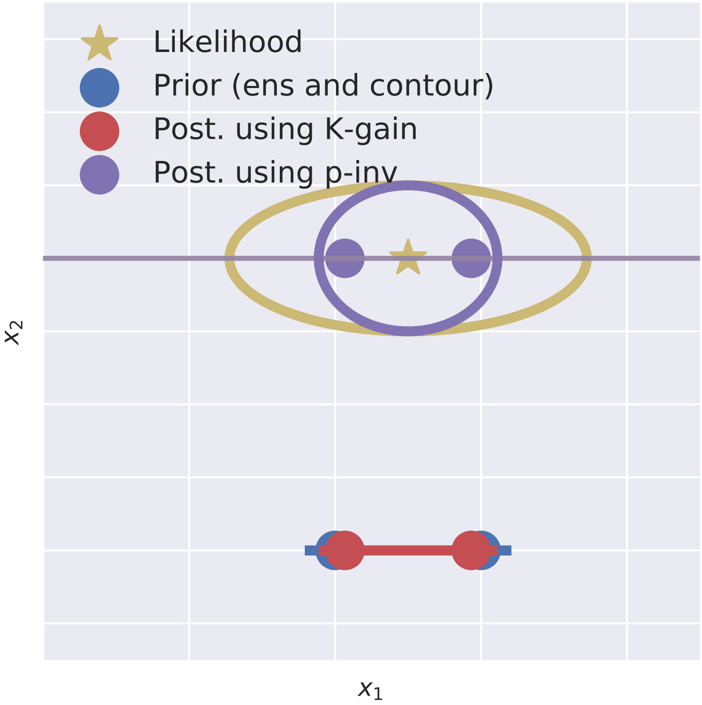
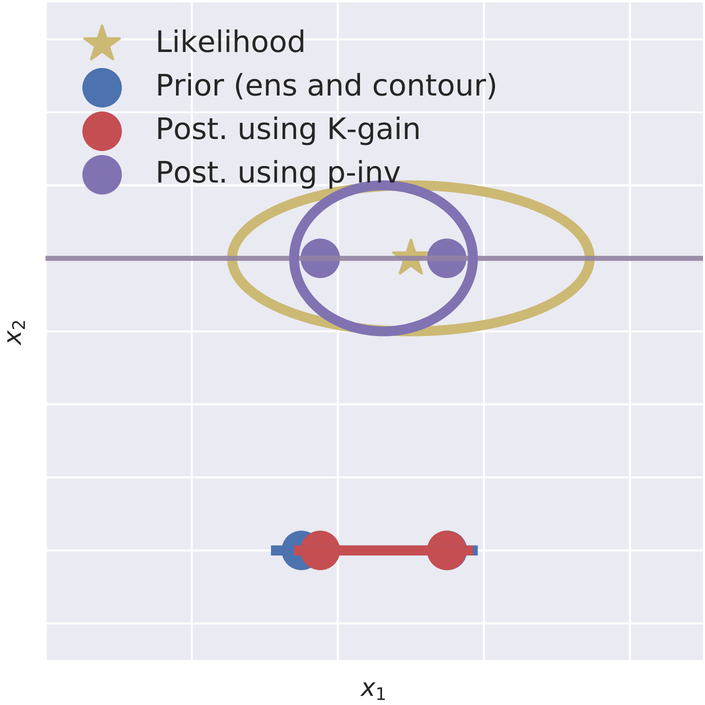

Likelihood
Prior (ens and contour)
Post. using K-gain
Post. using p-inv
x_2
x_1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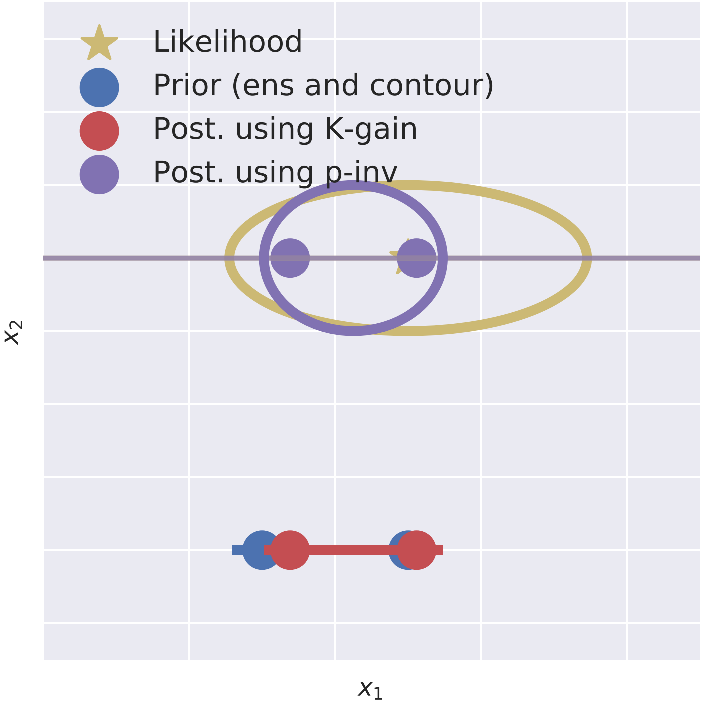

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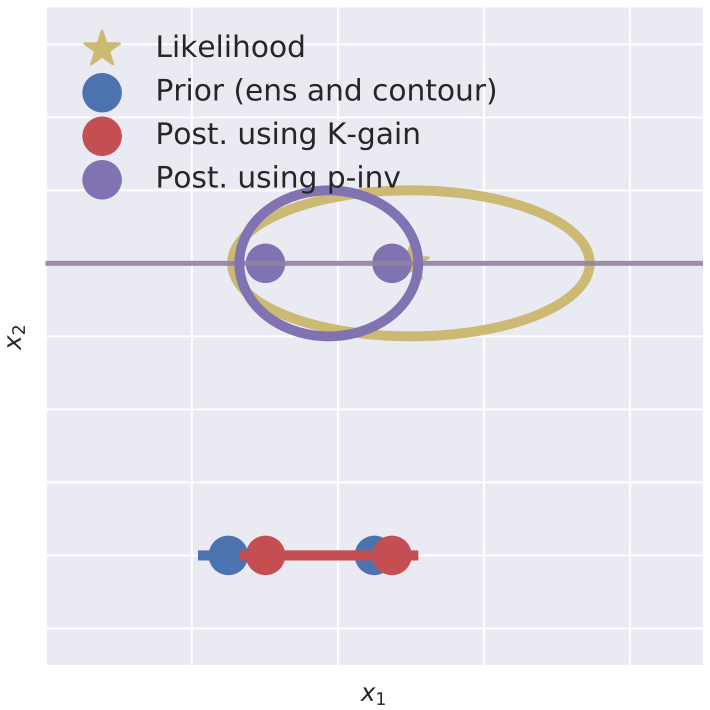

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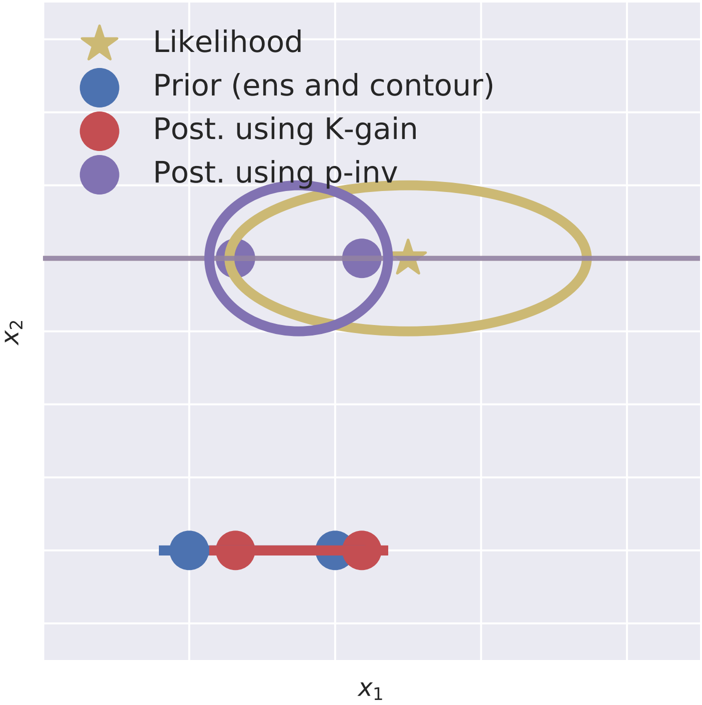

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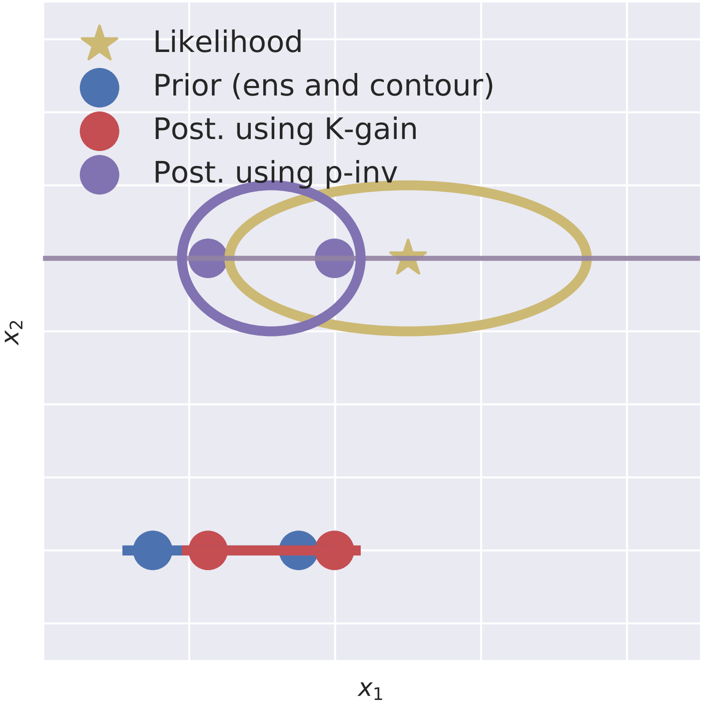

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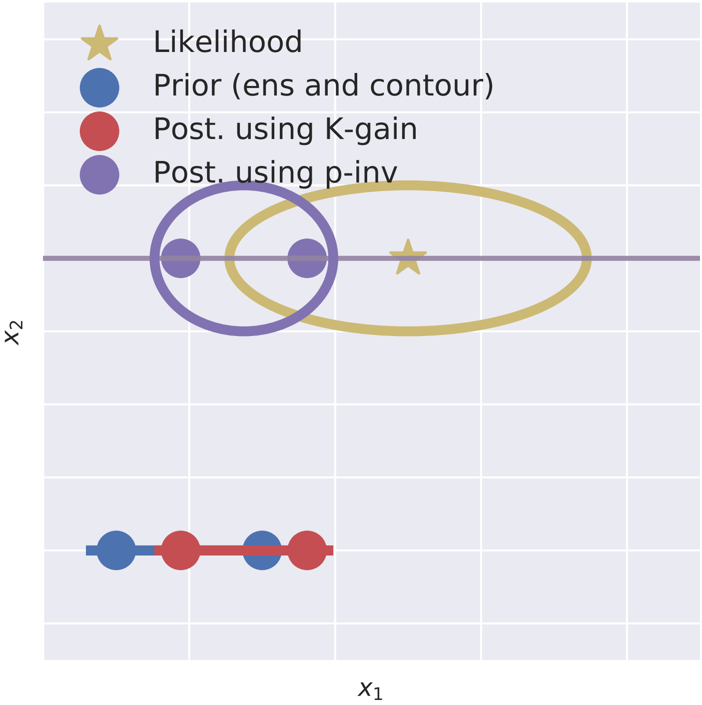
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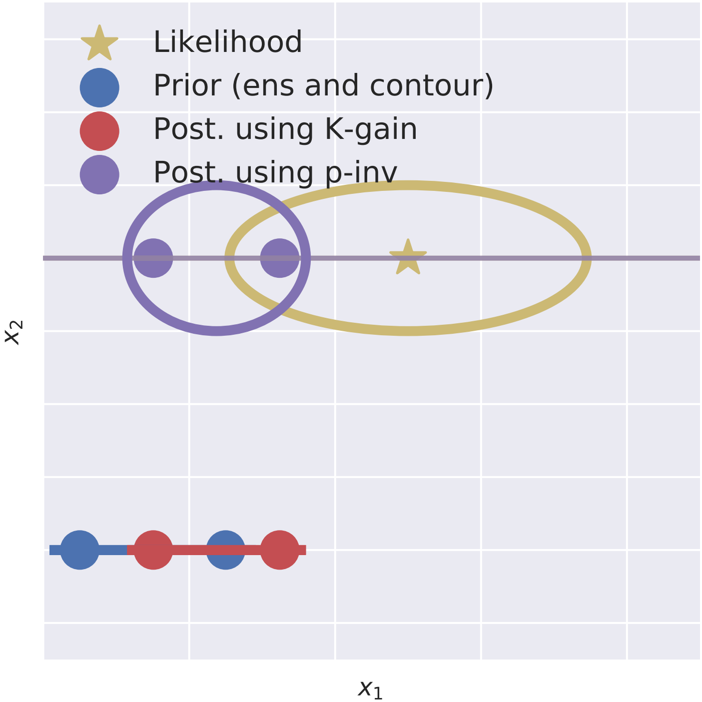
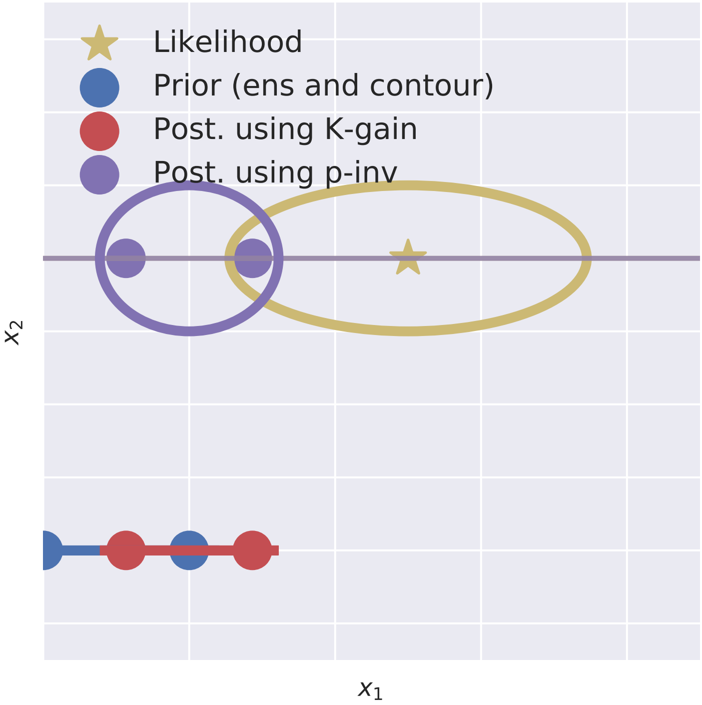


Likelihood
Prior (ens and contour)
Post. using K-gain
Post. using p-inv
x_2
x_1


Likelihood
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Post. using K-gain
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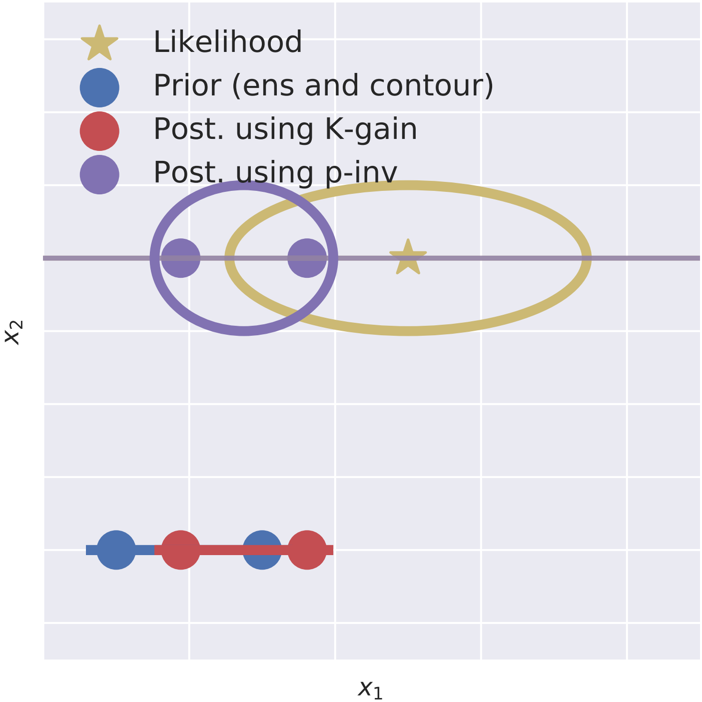
x_2
x_1



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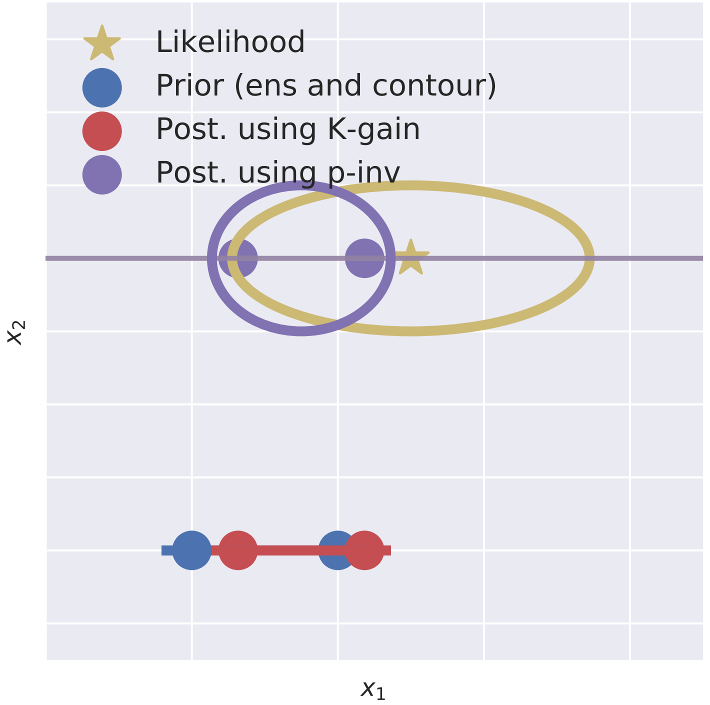
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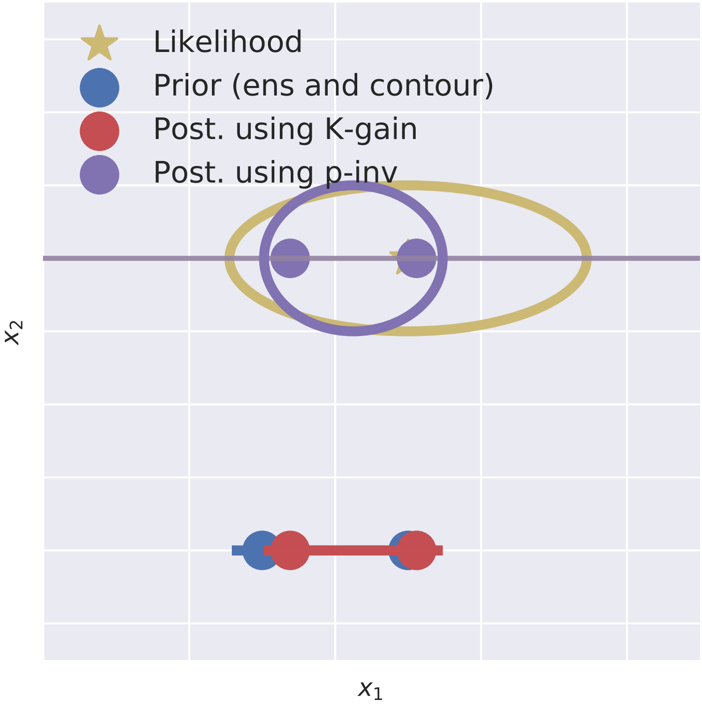

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x_2
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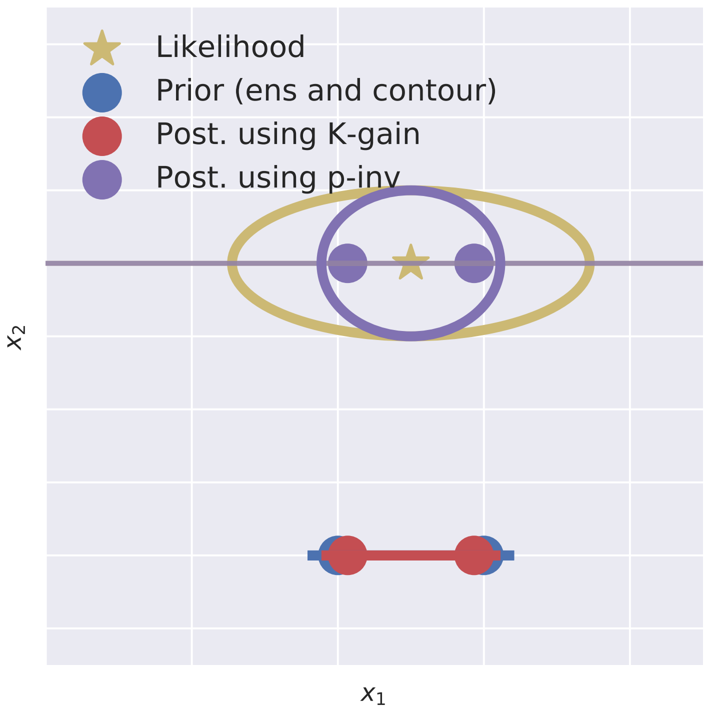

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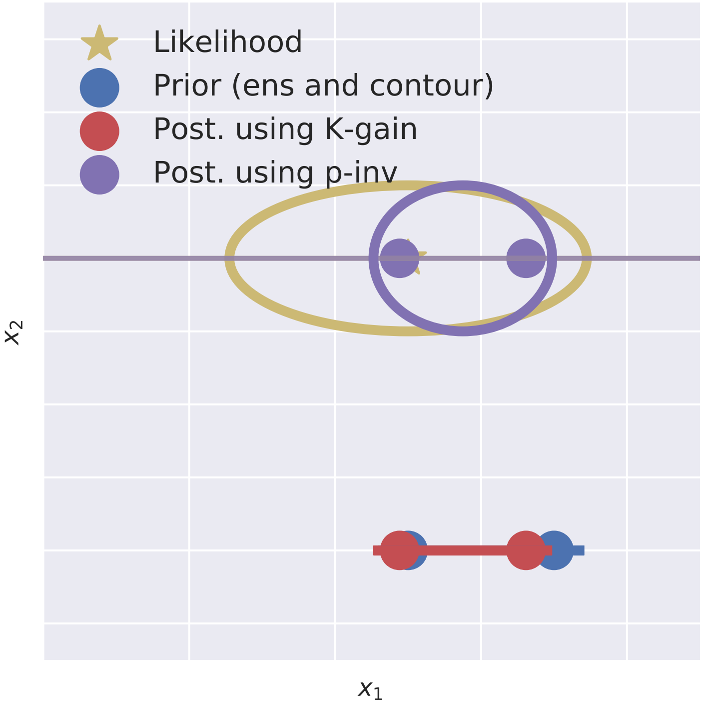
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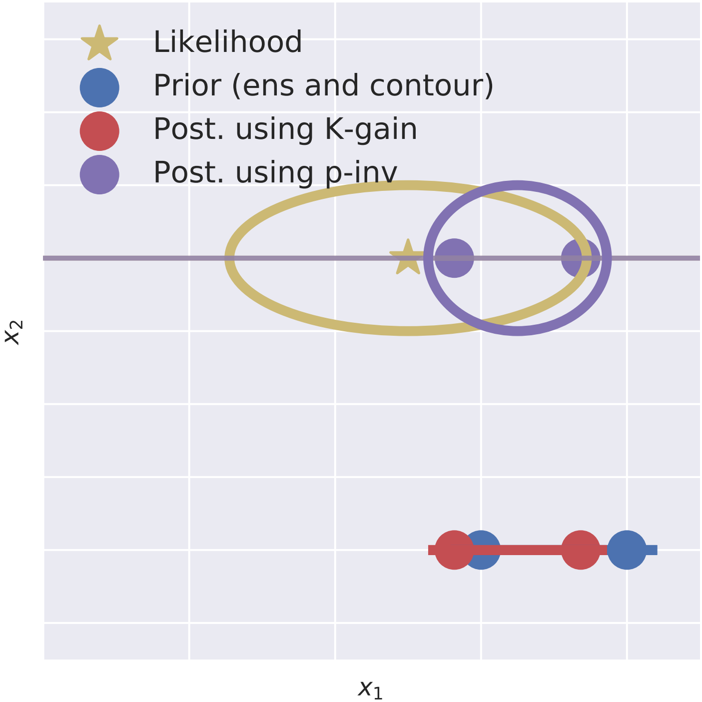
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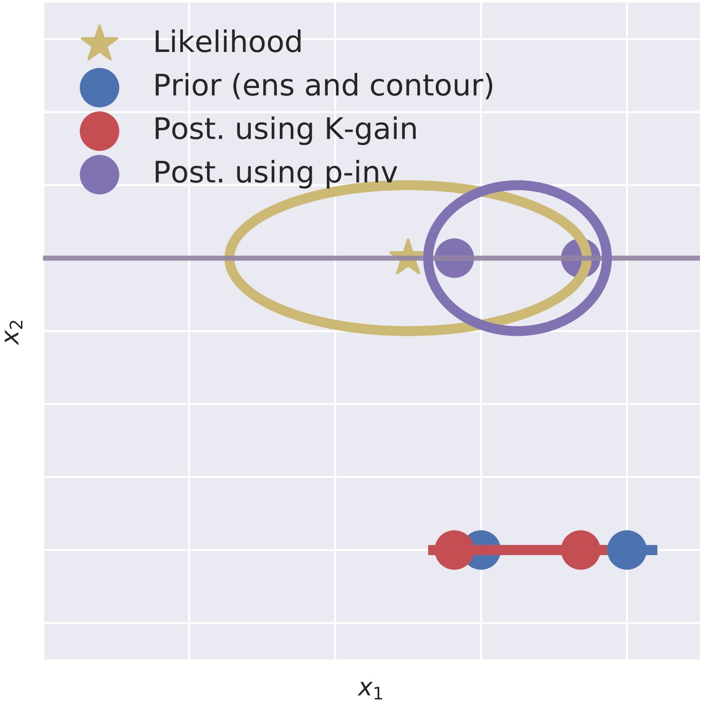
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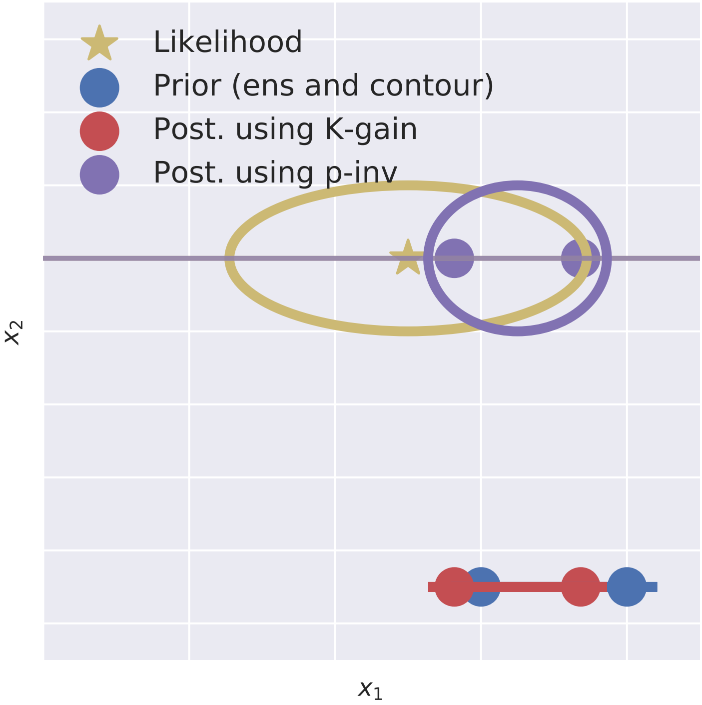

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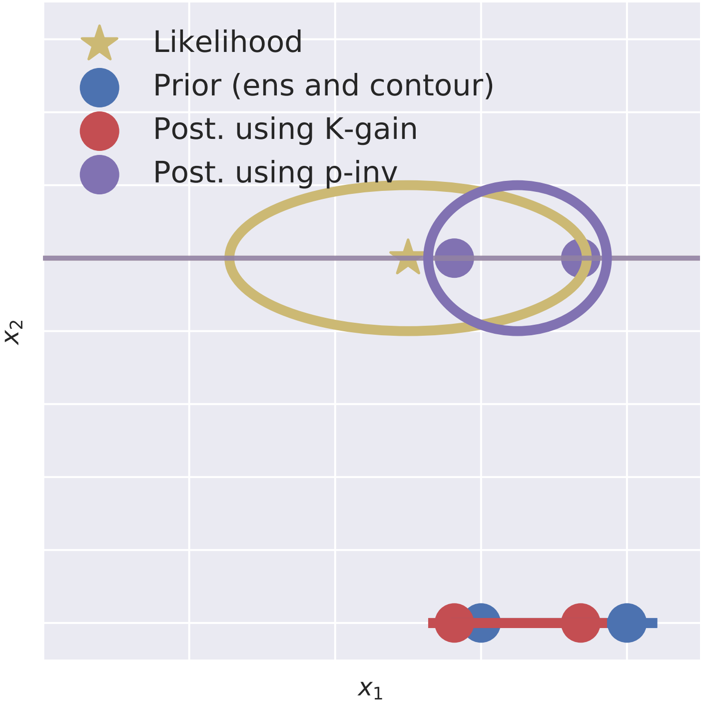

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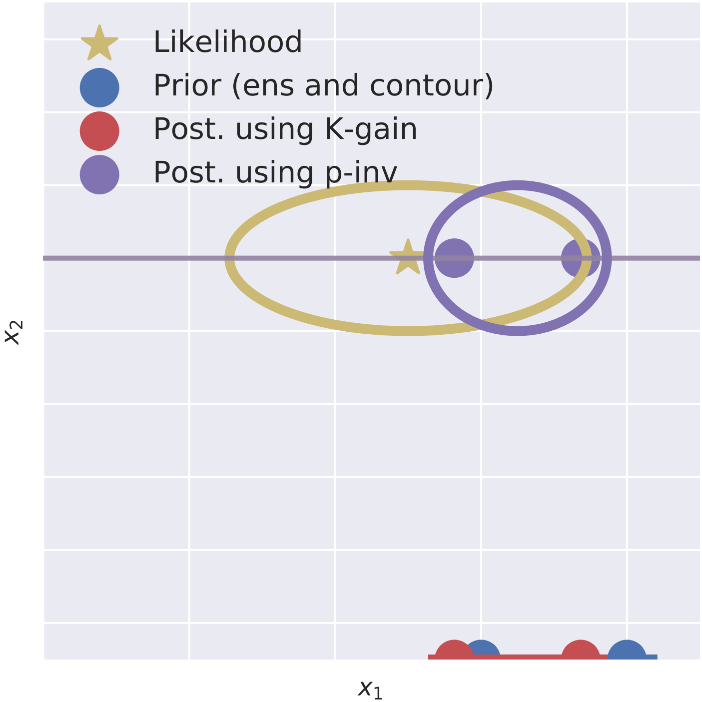
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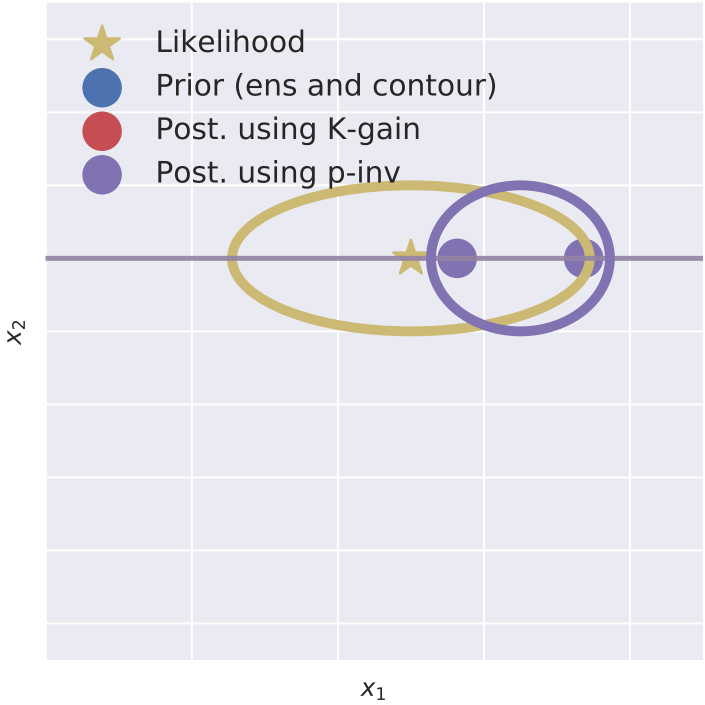

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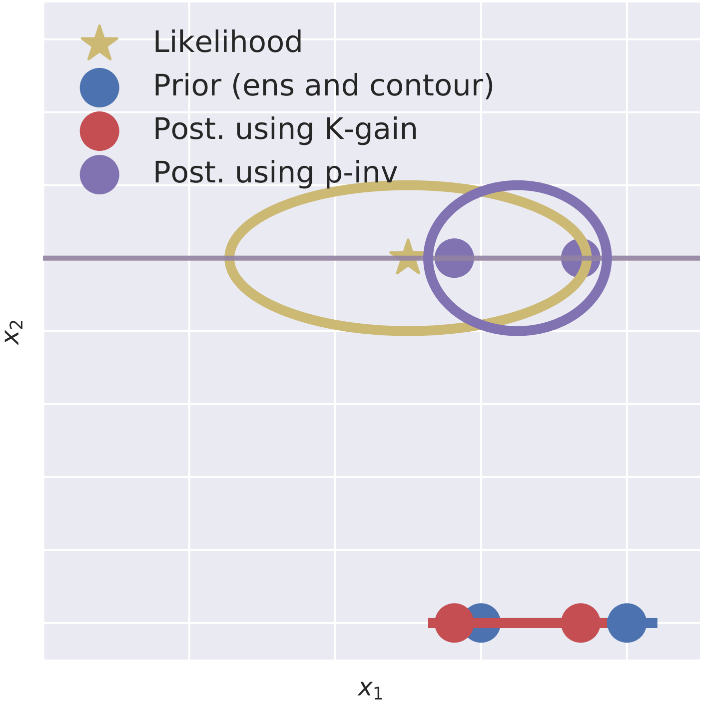
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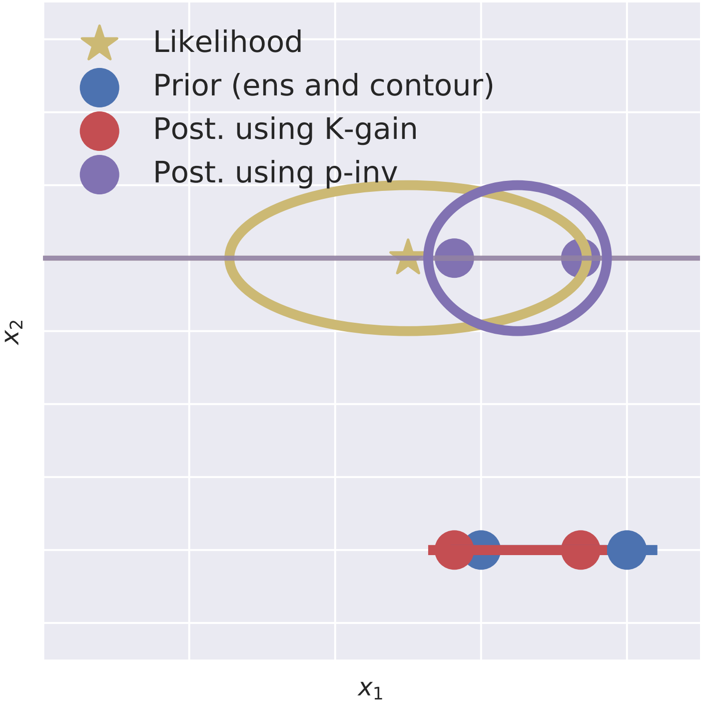
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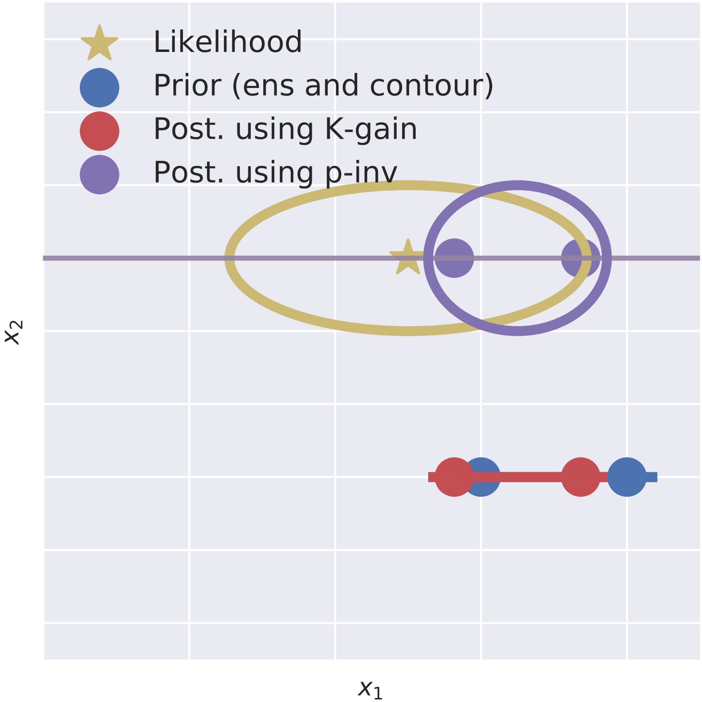
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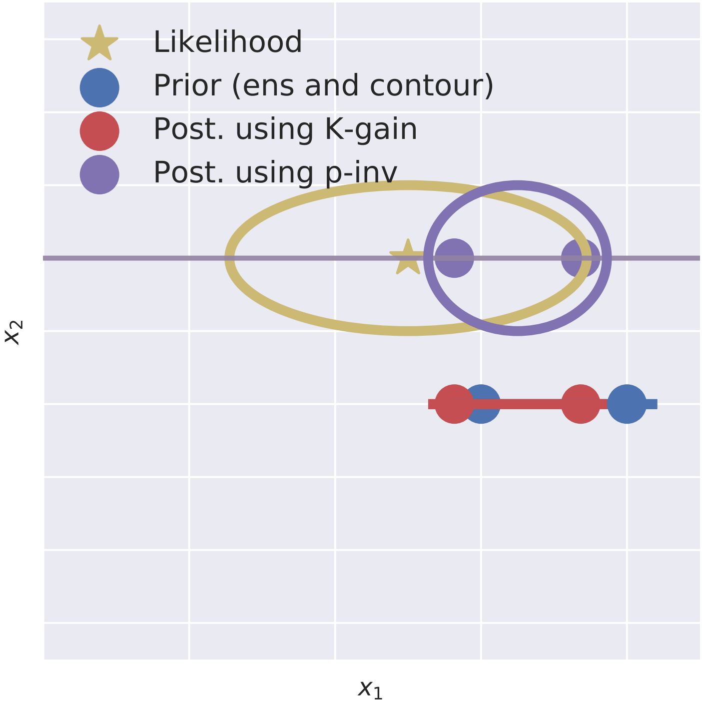

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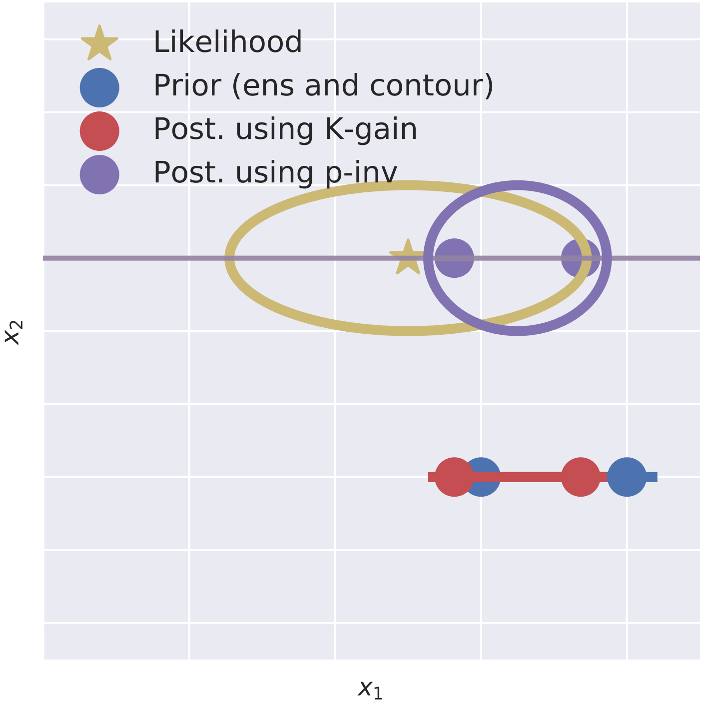

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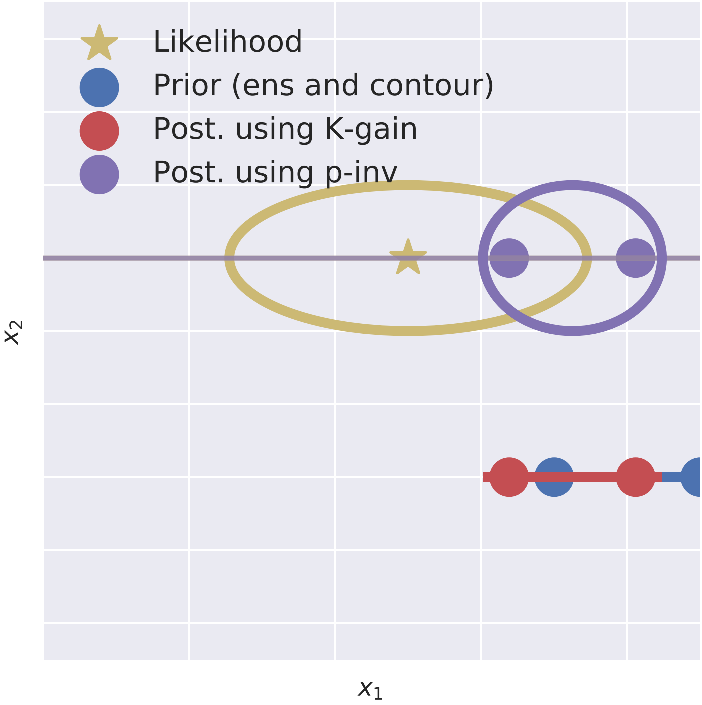

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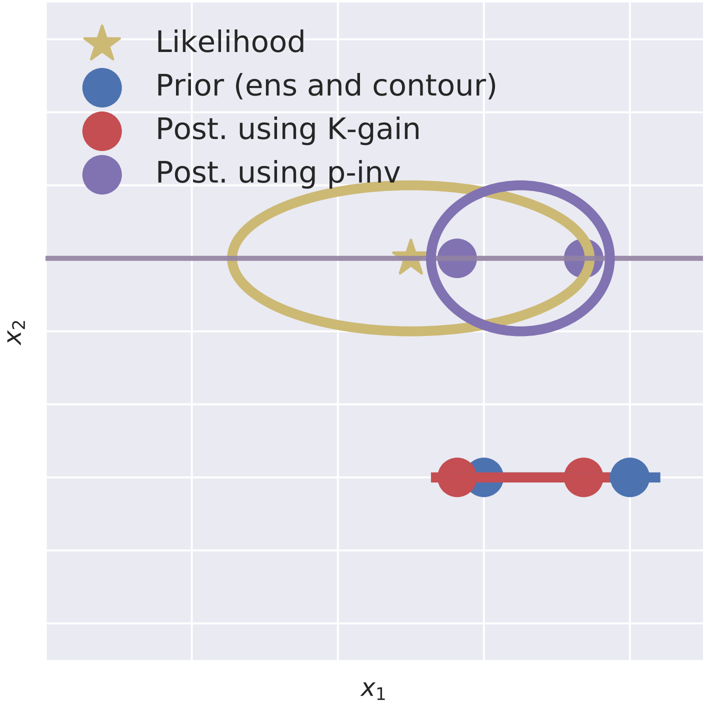
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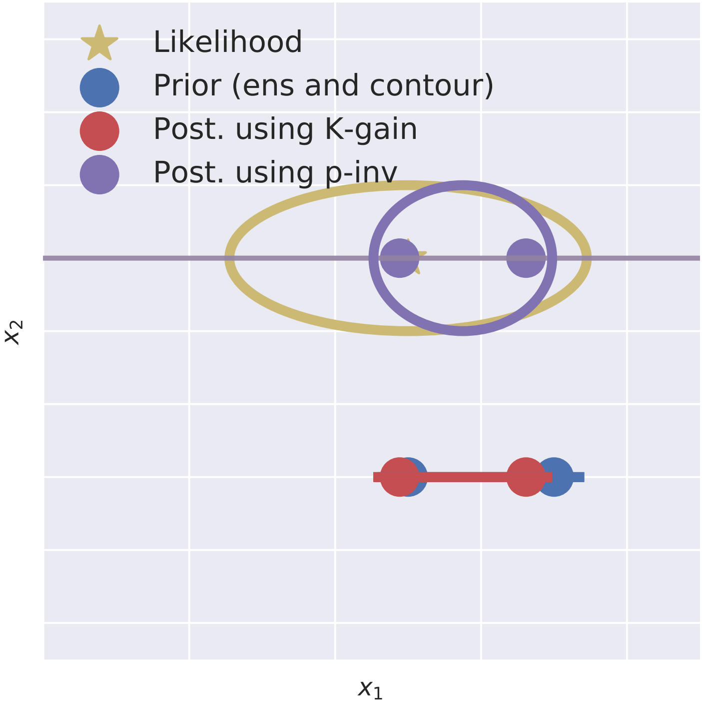

Likelihood
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Post. using K-gain
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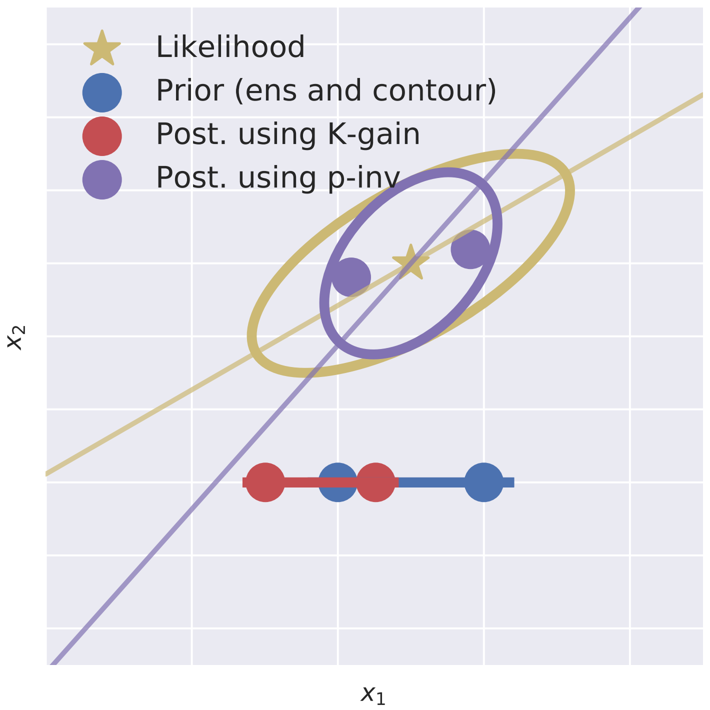
x_2
x_1



Likelihood
Prior (ens and contour)
Post. using K-gain
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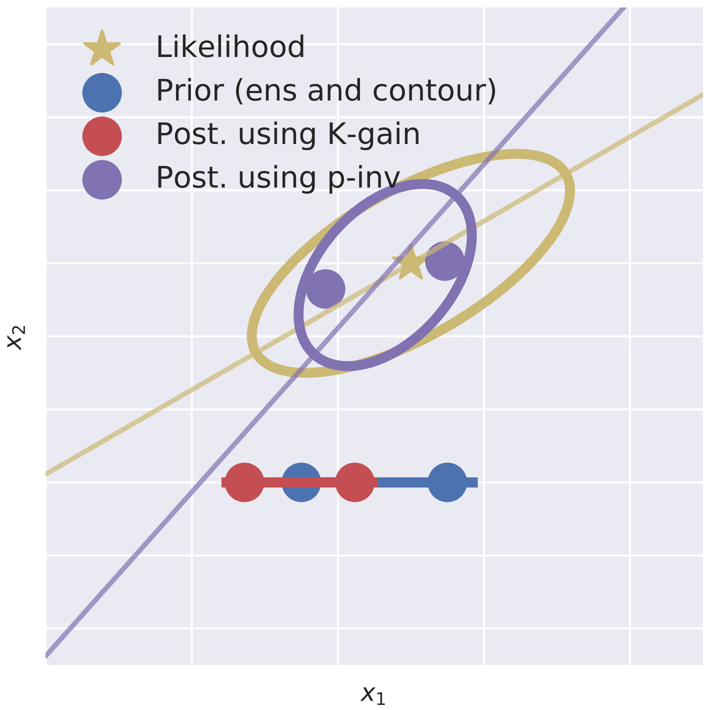
x_2
x_1



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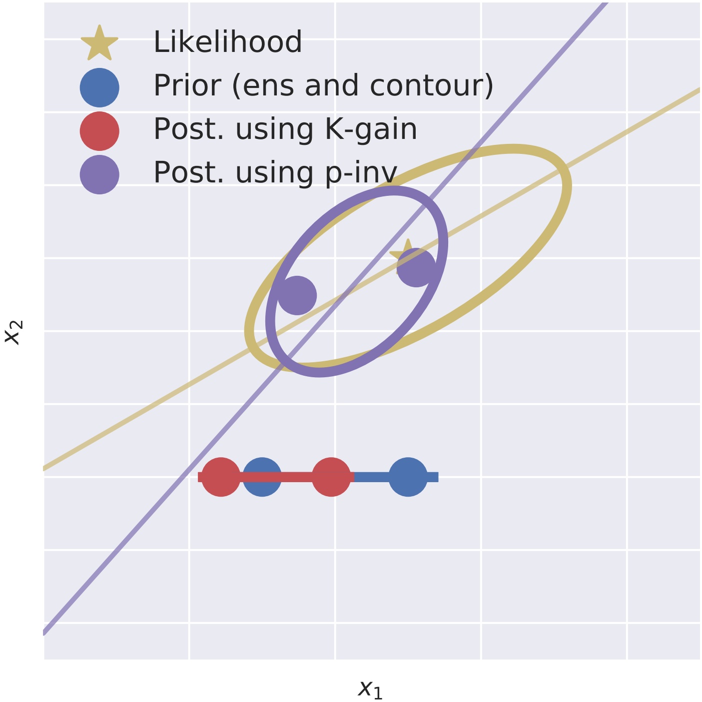
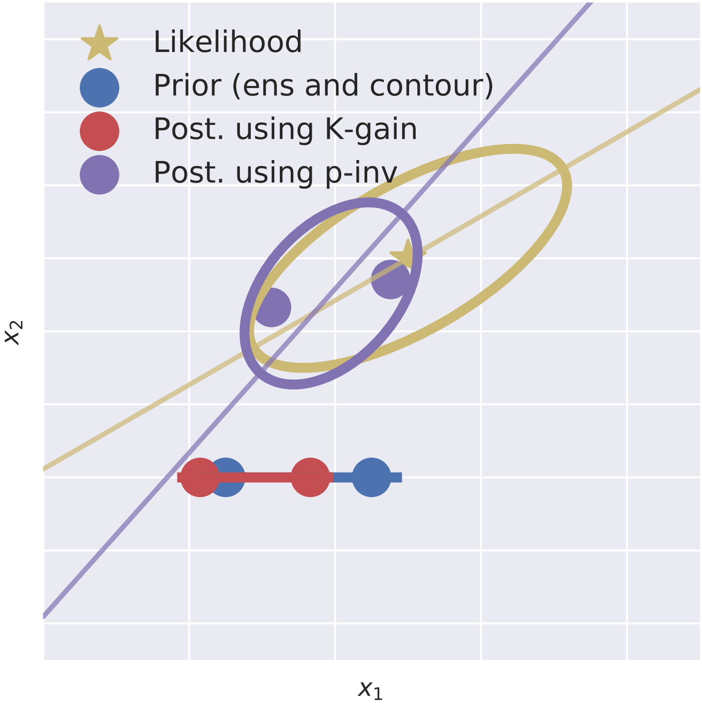
x_2
x_1



Likelihood
Prior (ens and contour)
Post. using K-gain
Post. using p-inv
x_2
x_1



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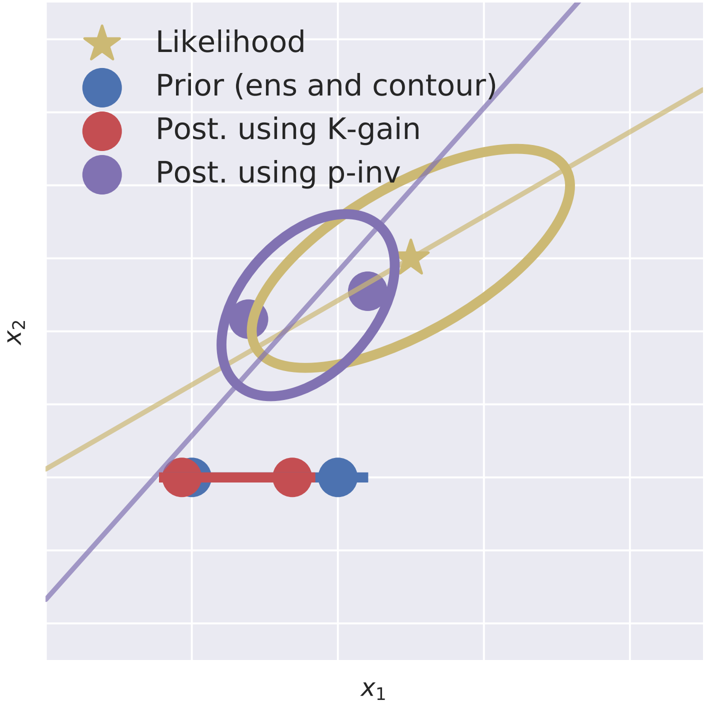
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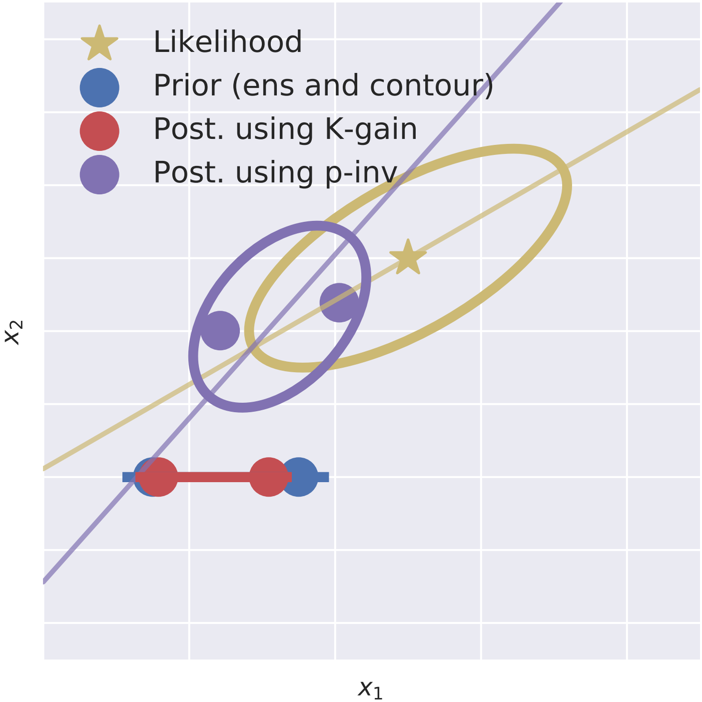

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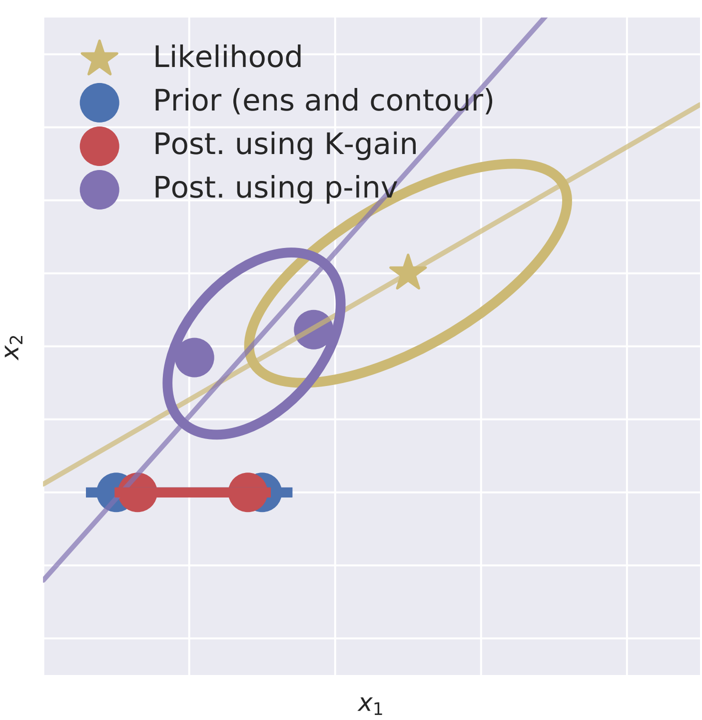
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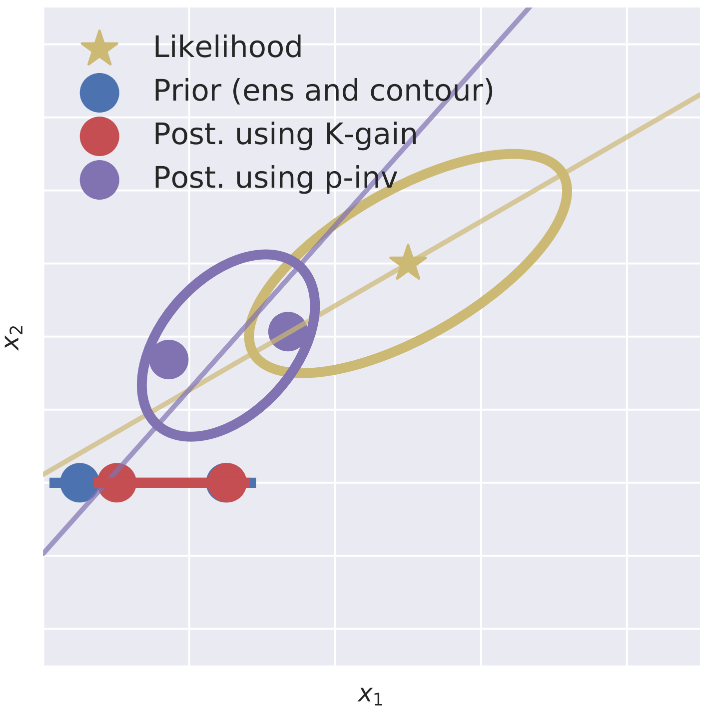
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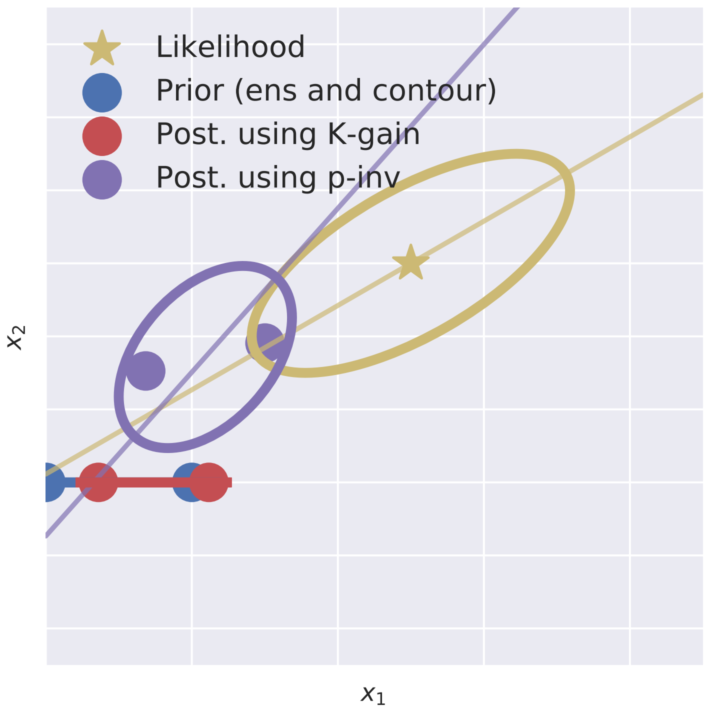

Likelihood
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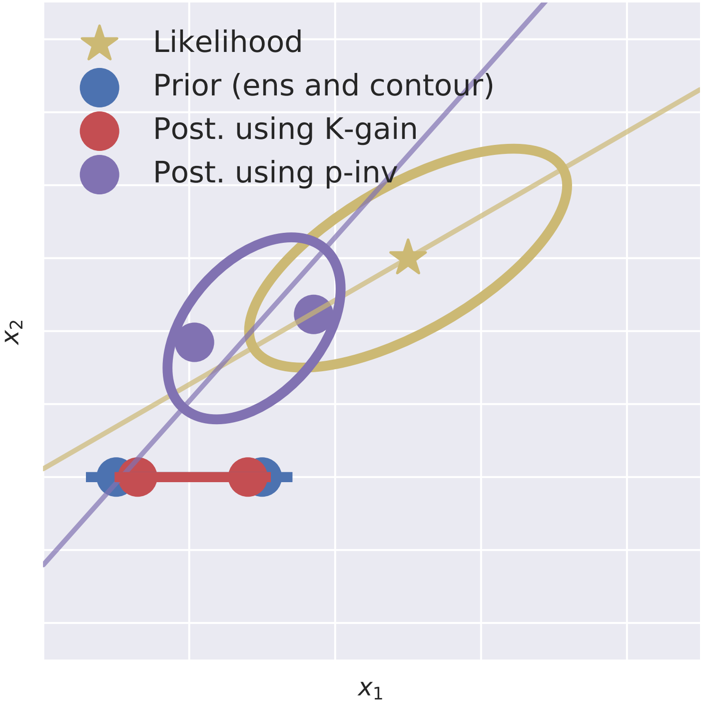
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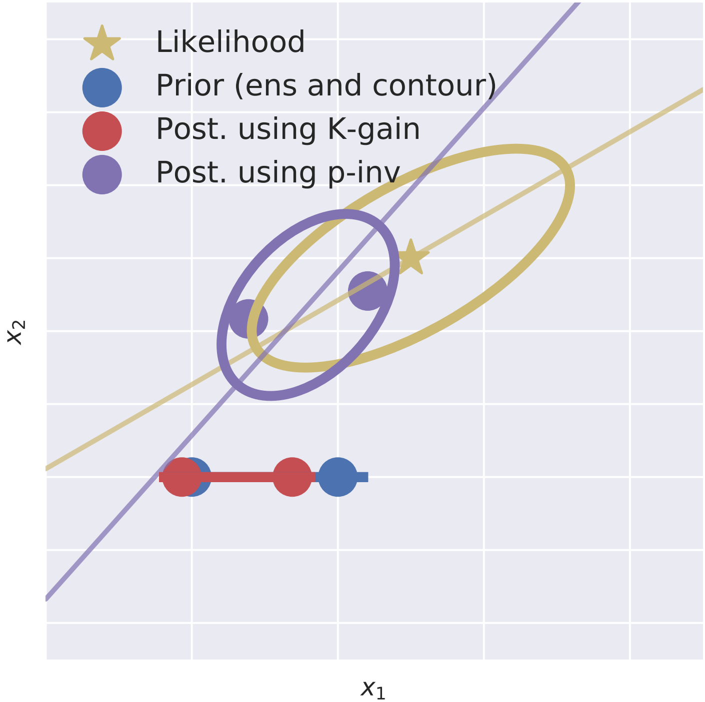

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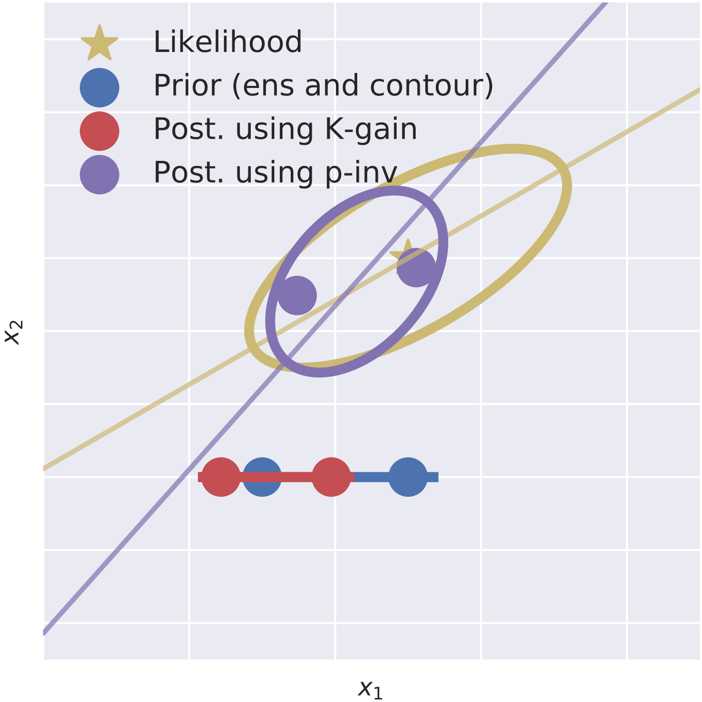

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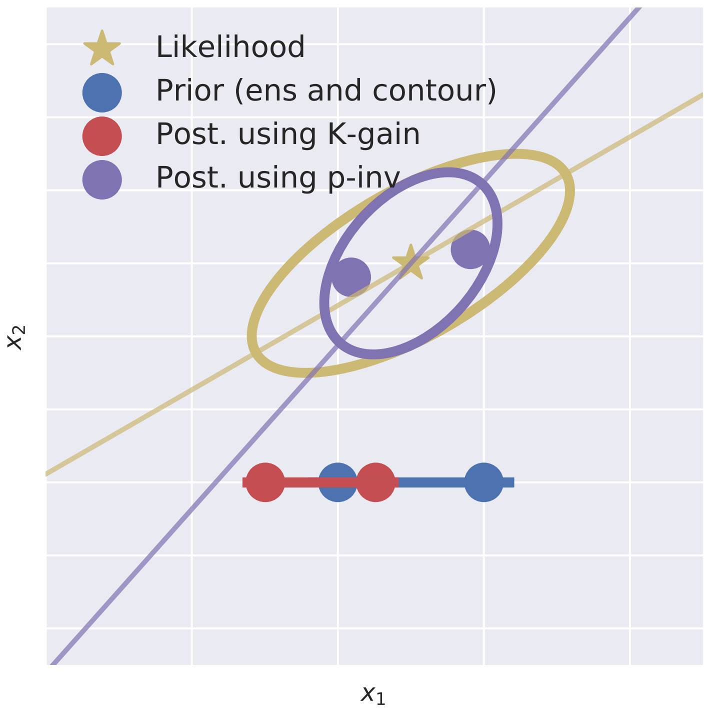

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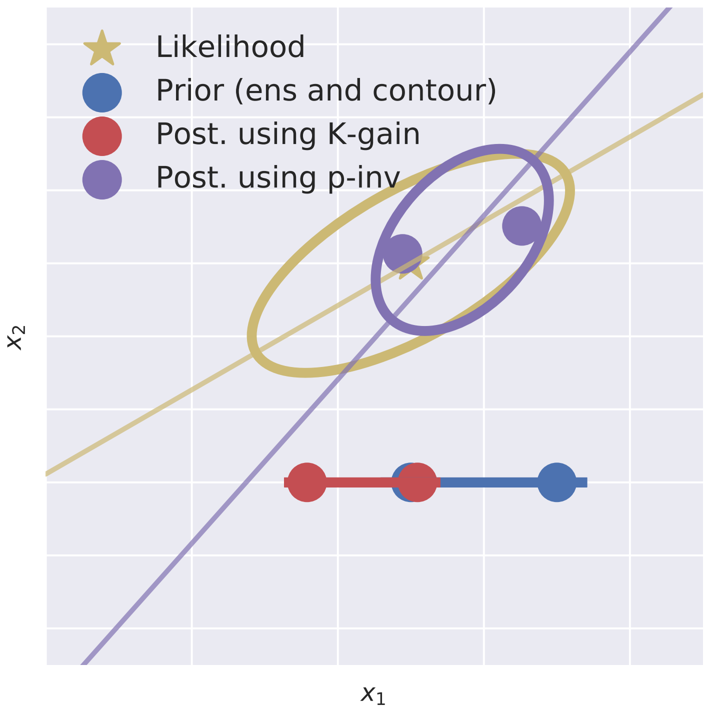
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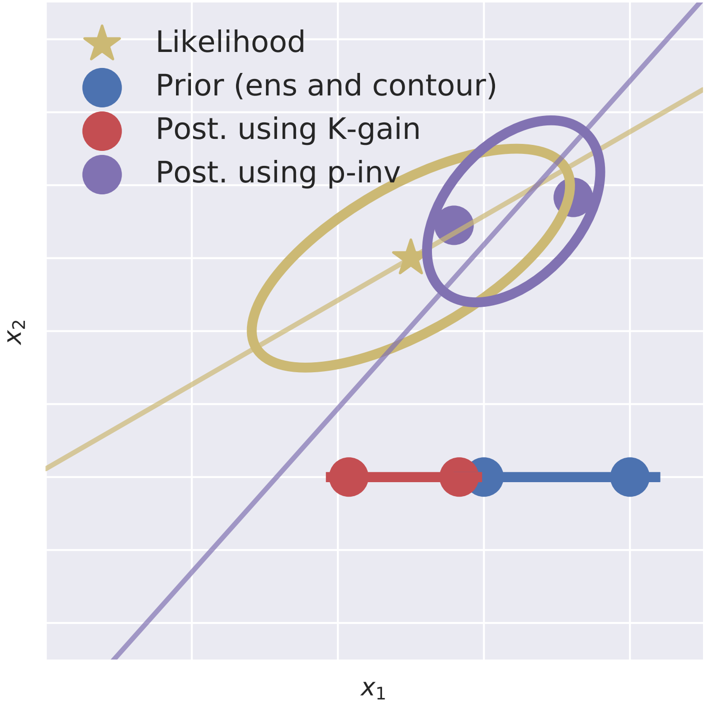
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Ensemble linearizations

Recall the EnKF gain:

$$\bar{\mathbf{K}} = \underbrace{\bar{\mathbf{C}}_{\boldsymbol{xy}}}_{\frac{1}{N-1}\mathbf{X}\mathbf{Y}^\mathsf{T}} \Big(\underbrace{\bar{\mathbf{C}}_{\boldsymbol{y}}}_{\frac{1}{N-1}\mathbf{Y}\mathbf{Y}^\mathsf{T}} + \mathbf{R} \Big)^{-1} . \tag{17}$$

Question: Is there a matrix $\bar{\mathbf{H}}$ such that

$$\bar{\mathbf{K}} = \bar{\mathbf{C}}_{\boldsymbol{x}} \bar{\mathbf{H}}^\mathsf{T} \Big(\bar{\mathbf{H}} \bar{\mathbf{C}}_{\boldsymbol{x}} \bar{\mathbf{H}}^\mathsf{T} + \mathbf{R} \Big)^{-1} ? \tag{18}$$

Answer: yes (mostly):

$$\bar{\mathbf{H}} = \mathbf{Y}\mathbf{X}^{+} , \tag{19}$$

Follow up questions:

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Follow up questions:

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- Why is this rarely discussed?
- Does it relate to the analytic derivative ($\mathcal{H}'$) ?

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$\bar{\mathbf{H}}$ is:

- Linear least-squares (LLS) estimate of $\mathcal{H}$ given $\mathbf{Y}$ and $\mathbf{X}$.
- BLUE ?
- MVUE ?

EnKF also doing LLS of x given (x^f, y) and $\bar{\mathbf{H}}$.

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Why is $\bar{\mathbf{H}}$ estimate rarely explicit?

Insert $\bar{\mathbf{H}} = \mathbf{Y}\mathbf{X}^{+}$ in $\bar{\mathbf{K}}$:

$$\bar{\mathbf{K}} = \bar{\mathbf{C}}_{\boldsymbol{x}} \bar{\mathbf{H}}^{\mathsf{T}} \big(\bar{\mathbf{H}} \bar{\mathbf{C}}_{\boldsymbol{x}} \bar{\mathbf{H}}^{\mathsf{T}} + \mathbf{R}\big)^{-1} \tag{20}$$

$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}} \big(\mathbf{Y} \boldsymbol{\Pi}_{\mathbf{X}^{\mathsf{T}}} \mathbf{Y}^{\mathsf{T}} + (N{-}1)\mathbf{R}\big)^{-1}, \tag{21}$$

where $\boldsymbol{\Pi}_{\mathbf{X}^{\mathsf{T}}} = \mathbf{X}^{+}\mathbf{X}$.

Note:

- Appearance of $\boldsymbol{\Pi}_{\mathbf{X}^{\mathsf{T}}}$ can be understood from chain rule.
- Vanishing of $\boldsymbol{\Pi}_{\mathbf{X}^{\mathsf{T}}}$ if $\mathcal{H}$ is linear, or $(N{-}1) \leq M$.
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$$\bar{\mathbf{K}} = \bar{\mathbf{C}}_{\boldsymbol{x}}\bar{\mathbf{H}}^{\mathsf{T}}\big(\bar{\mathbf{H}}\bar{\mathbf{C}}_{\boldsymbol{x}}\bar{\mathbf{H}}^{\mathsf{T}} + \mathbf{R}\big)^{-1} \tag{20}$$

$$= \mathbf{X}\mathbf{Y}^{\mathsf{T}}\big(\mathbf{Y}\boldsymbol{\Pi}_{\mathbf{X}^{\mathsf{T}}}\mathbf{Y}^{\mathsf{T}} + (N-1)\mathbf{R}\big)^{-1}\,, \tag{21}$$

where $\boldsymbol{\Pi}_{\mathbf{X}^{\mathsf{T}}} = \mathbf{X}^{+}\mathbf{X}$.

Note:

- Appearance of $\boldsymbol{\Pi}_{\mathbf{X}^{\mathsf{T}}}$ can be understood from chain rule.
- Vanishing of $\boldsymbol{\Pi}_{\mathbf{X}^{\mathsf{T}}}$ if $\mathcal{H}$ is linear, or $(N-1) \leq M$.
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Does $\bar{\mathbf{H}}$ relate to $\mathcal{H}'$?

Theorem:

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\begin{array}{ccc}
\lim_{N\to\infty} \bar{\mathbf{H}} & = & \mathbb{E}[\mathcal{H}'(x)] \\
\| & & \| \\
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\| & & \\
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I.e. $\bar{\mathbf{H}}$ is (indeed) the average derivative.

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