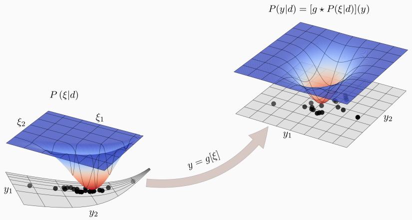


Geometric Variational Inference

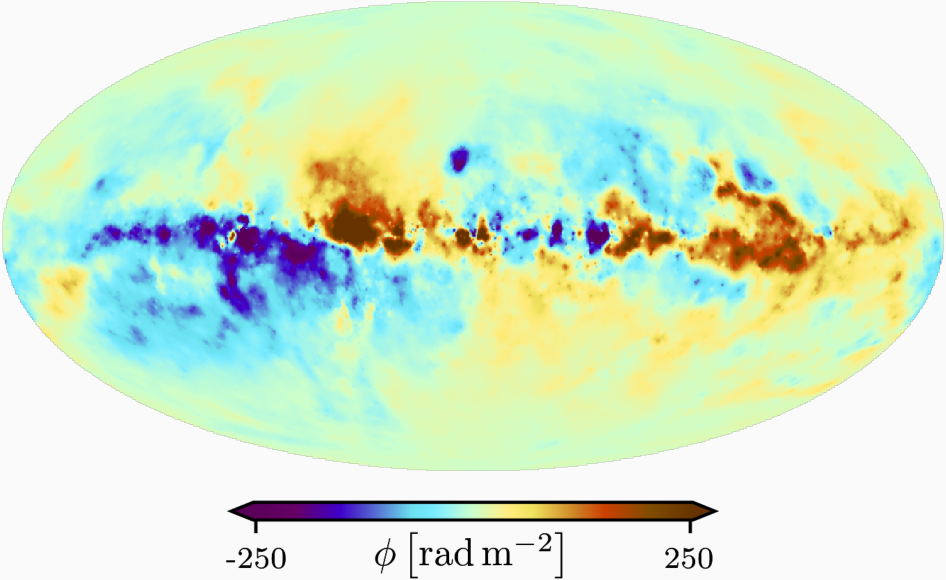
Using Riemannian geometry to enhance variational methods

Philipp Frank

July 16, 2021

Max-Planck Institute for Astrophysics, Garching, Germany

Imaging problems



Imaging problems

Product Rule of Probabilities aka Bayes' theorem

$$\mathcal{P}(s|d,\mathcal{M}) = \frac{\mathcal{P}(d|s,\mathcal{M})\,\mathcal{P}(s|\mathcal{M})}{\mathcal{P}(d|\mathcal{M})}$$

Definitions: $s :=$ parameters, $d :=$ data, $\mathcal{M}$: model assumptions.

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1. Very high dimensional (in both, the parameter space and the data space)

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1. Very high dimensional (in both, the parameter space and the data space)
   1.1 No explicit representation of matrices (e.g. covariance, curvature)
   1.2 Inference algorithm must scale (almost) linear with problem size

Imaging problems

Product Rule of Probabilities aka Bayes' theorem

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Imaging problems:

1. Very high dimensional (in both, the parameter space and the data space)
   - 1.1 No explicit representation of matrices (e.g. covariance, curvature)
   - 1.2 Inference algorithm must scale (almost) linear with problem size
2. Non-linear (non-Gaussian) posterior distributions
   - 2.1 Point estimates (e.g. MAP) not sufficient

Variational Inference

Variational Inference (VI)

Kullback-Leibler divergence

$$\mathrm{KL}\left[\mathcal{Q}_\sigma || \mathcal{P}\right] = -\int \log\left(\frac{\mathcal{P}(\xi|d)}{\mathcal{Q}_\sigma(\xi)}\right)\ \mathcal{Q}_\sigma(\xi)\ \mathrm{d}\xi$$

Posterior: $\mathcal{P}(\xi|d)$; approximation: $\mathcal{Q}_\sigma(\xi)$; variational parameters: σ.

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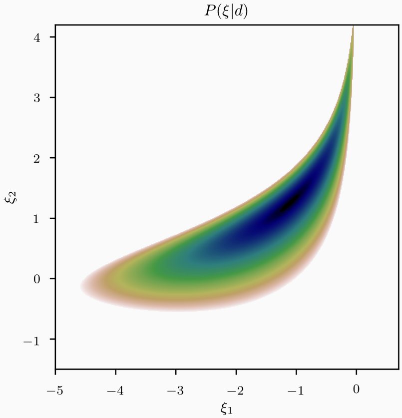
Posterior: $\mathcal{P}(\xi|d)$; approximation: $\mathcal{Q}_\sigma(\xi)$; variational parameters: σ.

Use a transformed standard normal distribution for $\mathcal{Q}$: $\mathcal{Q}(y) = \mathcal{N}(y; 0, \mathbb{1})$
Choose a coordinate system $y = g(\xi)$ such that the *posterior* distribution is close to a Normal distribution.

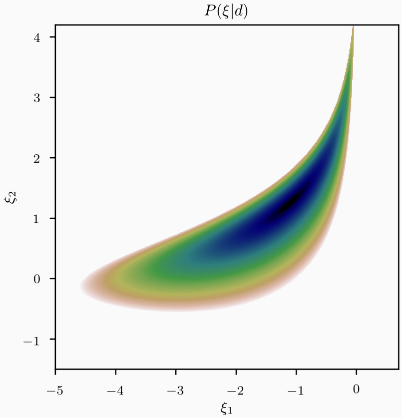
Geometric Variational Inference

Geometric Variational Inference (geoVI)



Information Hamiltonian $\mathcal{H}(\xi|d)$: $\quad -\log\left(\mathcal{P}(\xi|d)\right)$

Geometric Variational Inference (geoVI)

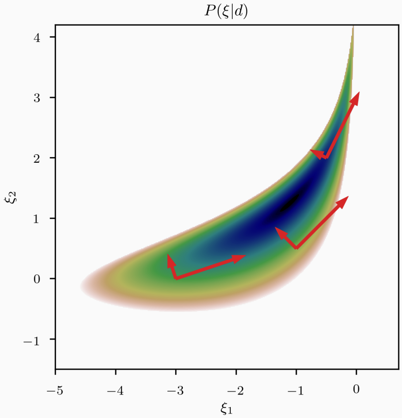


Information Hamiltonian $\mathcal{H}(\xi|d)$: $-\log\left(\mathcal{P}(\xi|d)\right)$

Posterior metric $\mathcal{M}(\xi)$: $\mathcal{M}_{\mathrm{lh}}(\xi) + \mathbb{1}$

Fisher information metric $\mathcal{M}_{\mathrm{lh}}(\xi)$: $\left\langle \frac{\partial^2 \mathcal{H}(d|\xi)}{\partial \xi \partial \xi'} \right\rangle_{\mathcal{P}(d|\xi)}$

Geometric Variational Inference (geoVI)



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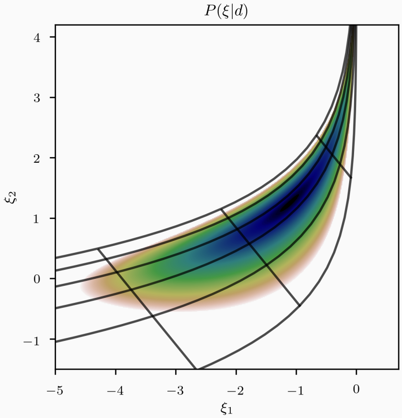

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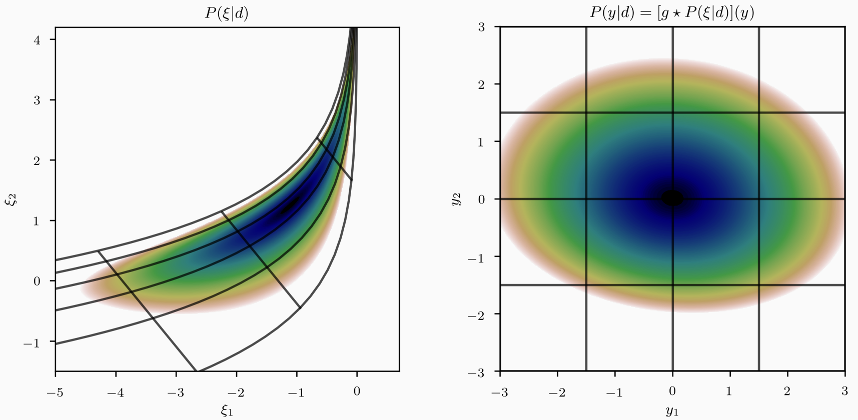
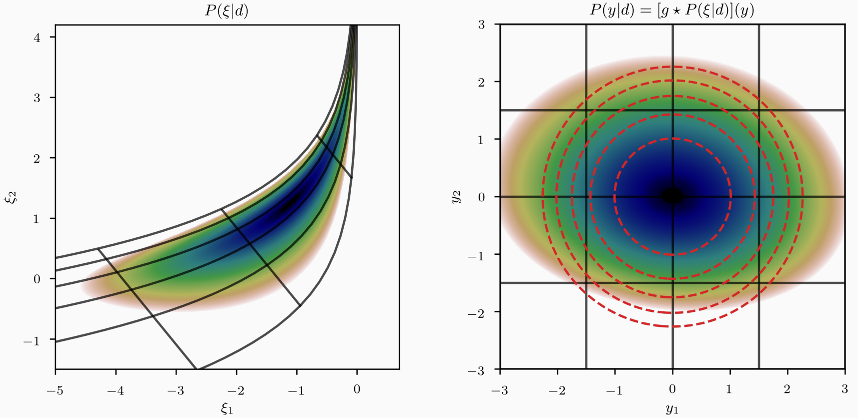
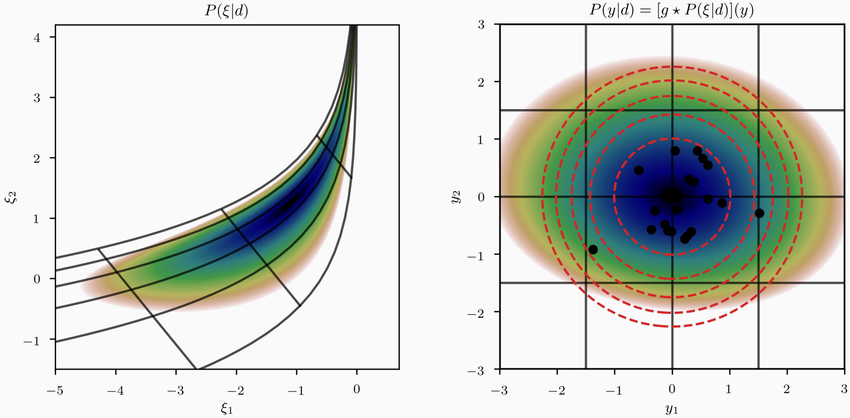


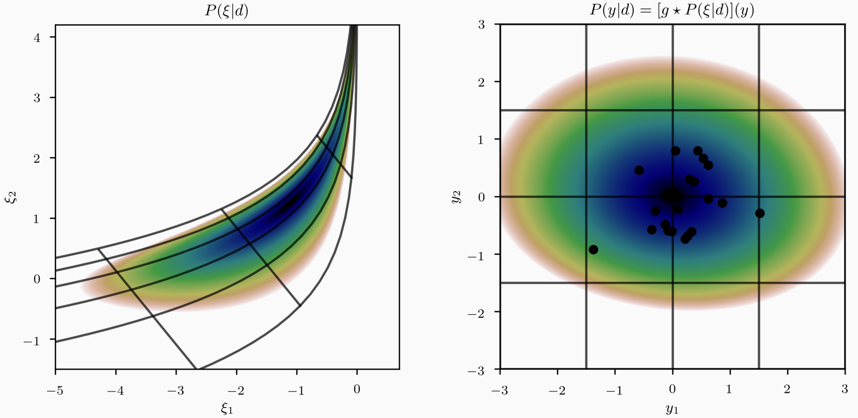
Geometric Variational Inference (geoVI)



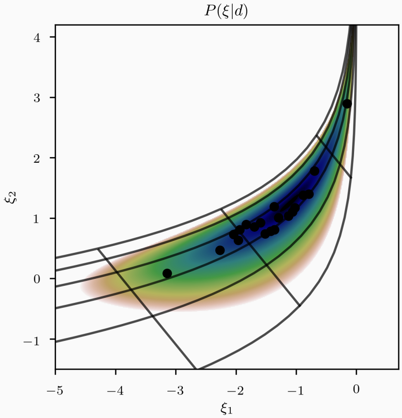
Geometric Variational Inference (geoVI)

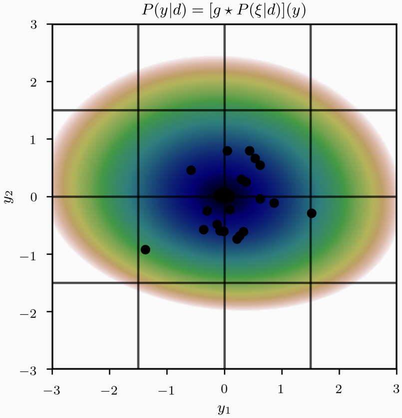


Geometric Variational Inference (geoVI)



Geometric Variational Inference (geoVI)





Geometric Variational Inference (geoVI)

- Write Fisher metric as pullback: $\mathcal{M}(\xi) = \mathcal{M}_{\mathrm{lh}}(\xi) + \mathbb{1} = \left(\frac{\partial x}{\partial \xi}\right)^{T} \frac{\partial x}{\partial \xi} + \mathbb{1}$.
- Find coordinate transformation g such that $\mathcal{M}(\xi) \approx \left(\frac{\partial g}{\partial \xi}\right)^{T} \frac{\partial g}{\partial \xi}$

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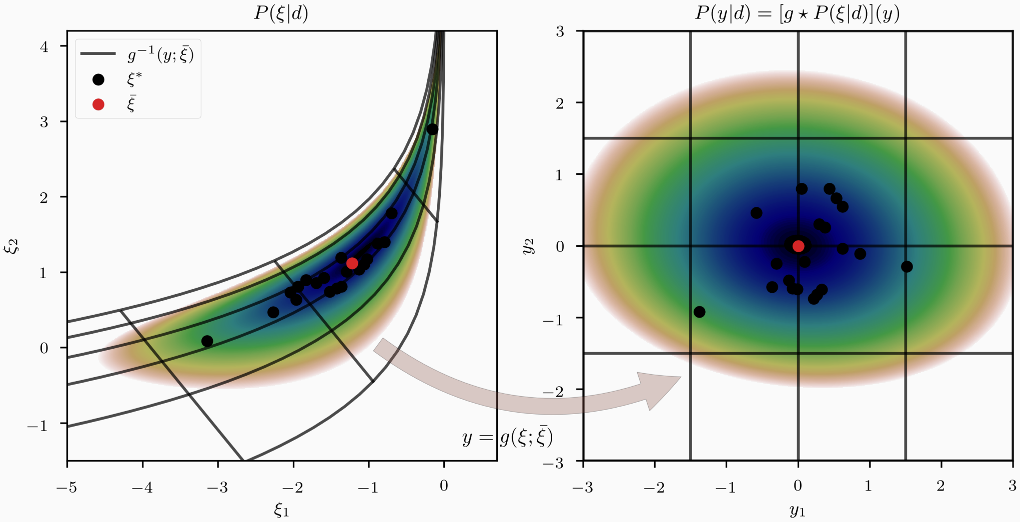
Local Euclidean isometry around $\bar{\xi}$

$$y = g(\xi; \bar{\xi}) = \xi - \bar{\xi} + \left(\frac{\partial x}{\partial \xi}\right)^T \Bigg|_{\xi=\bar{\xi}} (x(\xi) - x(\bar{\xi}))$$

Likelihood transformation: $x(\xi) = x(s(\xi))$, expansion point: $\bar{\xi}$.

Geometric Variational Inference (geoVI)



Geometric Variational Inference (geoVI)

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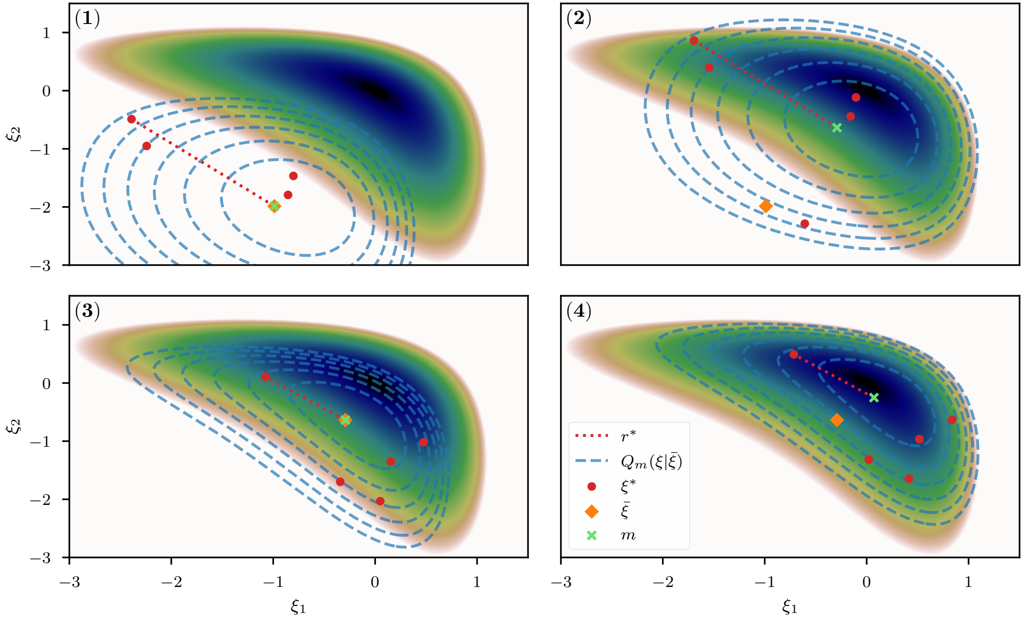
Likelihood transformation: $x(\xi) = x(s(\xi))$, expansion point: $\bar{\xi}$.

Variational approximation with transformed distribution $\mathcal{Q}$

$$\mathcal{Q}_{\bar{\xi}}(\xi) = \mathcal{N}(y|0, \mathbb{1})|_{y=g(\xi;\bar{\xi})} \left|\left|\frac{\partial g(\xi; \bar{\xi})}{\partial \xi}\right|\right|$$


(1)
(2)
(3)
(4)
1
0
−1
−2
−3
ξ_2
−3
−2
−1
0
1
ξ_1
r^*
$Q_m(\xi|\bar{\xi})$
ξ^*
$\bar{\xi}$
m

Application (preliminary)

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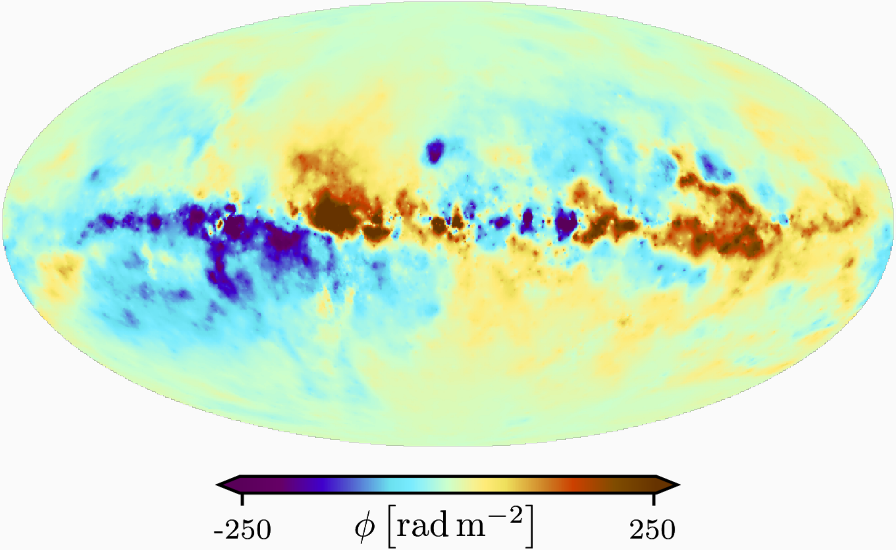
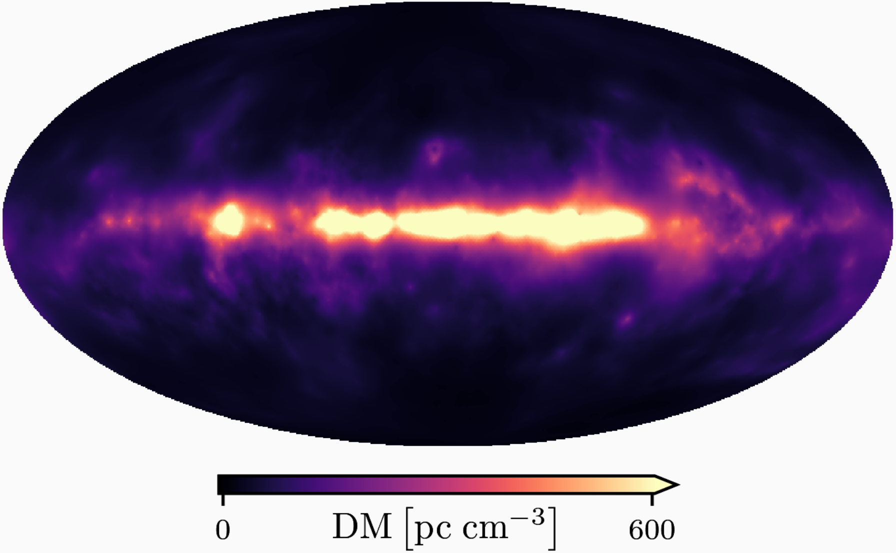
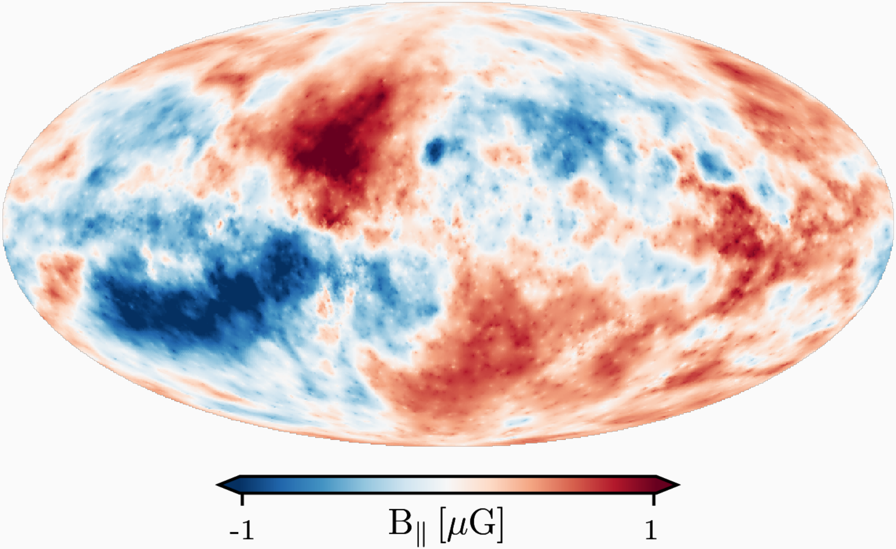


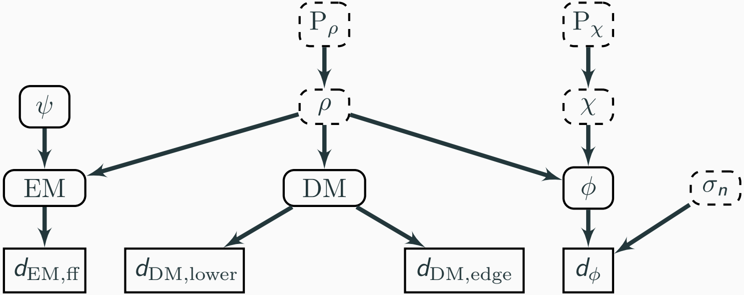
Application (preliminary)



Application (preliminary)



Application (preliminary)

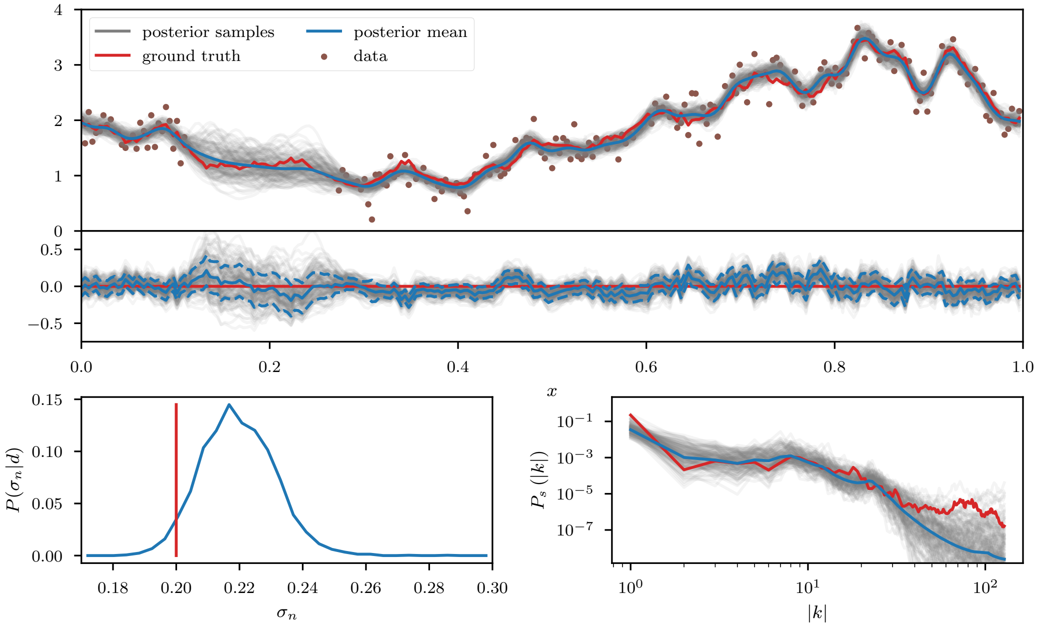


References

- **Geometric variational inference**; Frank, Leike, Enßlin; https://arxiv.org/abs/2105.10470
- **Numerical information field theory (Nifty7)**; https://gitlab.mpcdf.mpg.de/ift/nifty

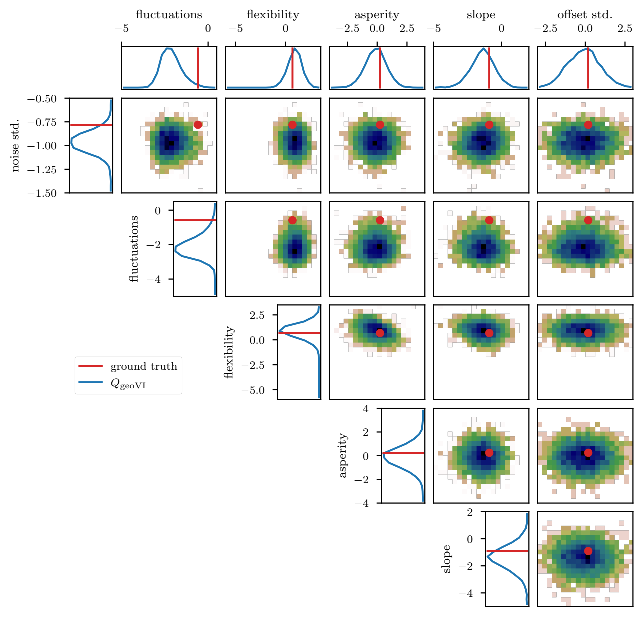
Appendix

Appendix



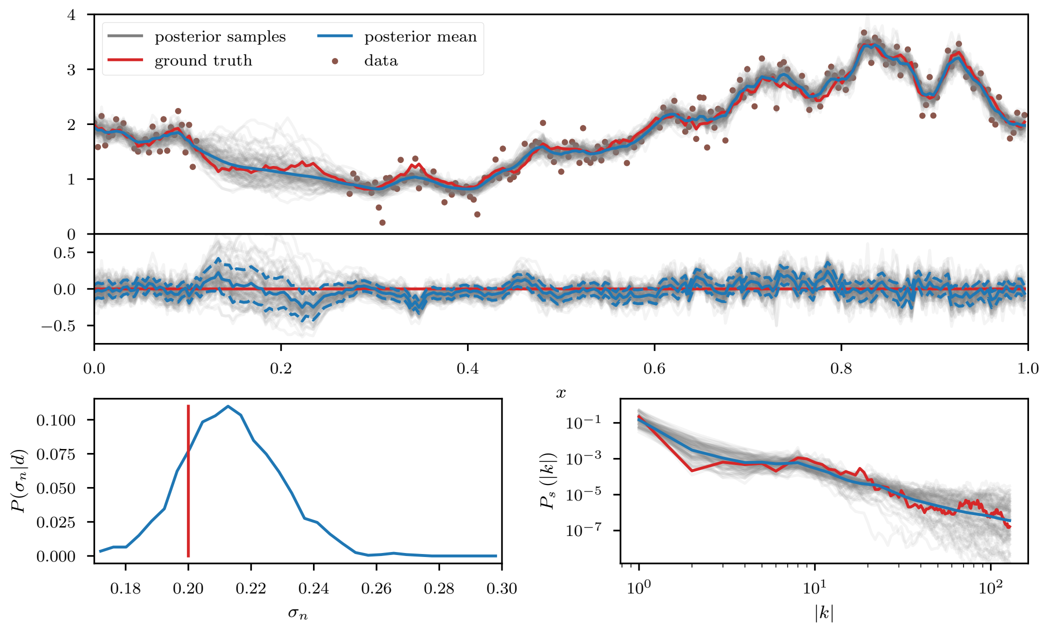
posterior samples
posterior mean
ground truth
data
4
3
2
1
0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
x
0.15
0.10
0.05
0.00
$P(\sigma_n|d)$
0.18
0.20
0.22
0.24
0.26
0.28
0.30
σ_n
10^{-1}
10^{-3}
10^{-5}
10^{-7}
$P_s(|k|)$
10^0
10^1
10^2
$|k|$

Appendix



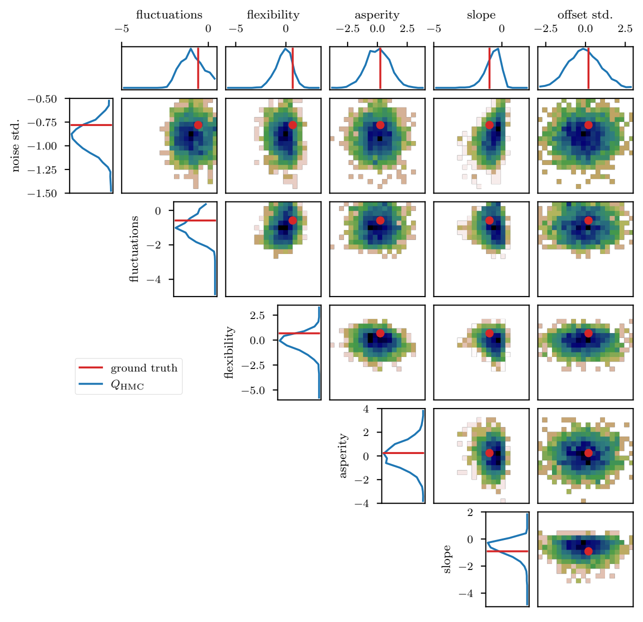
fluctuations
flexibility
asperity
slope
offset std.
noise std.
ground truth
Q_{geoVI}

Appendix



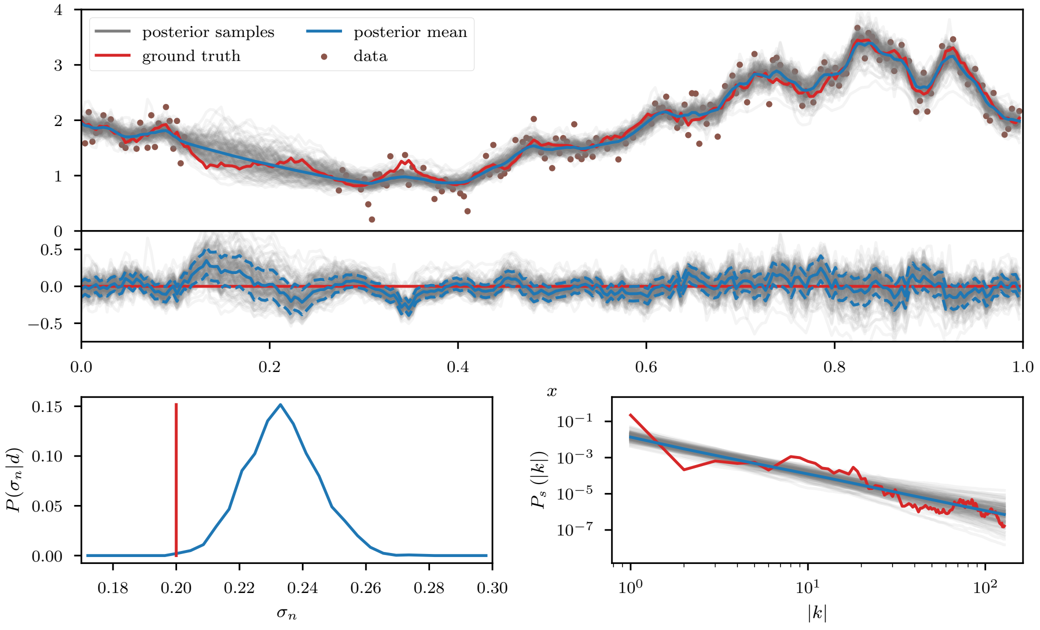
posterior samples
posterior mean
ground truth
data
4
3
2
1
0
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
x
P(σ_n|d)
0.100
0.075
0.050
0.025
0.000
0.18
0.20
0.22
0.24
0.26
0.28
0.30
σ_n
P_s(|k|)
10^{−1}
10^{−3}
10^{−5}
10^{−7}
10^0
10^1
10^2
|k|

Appendix



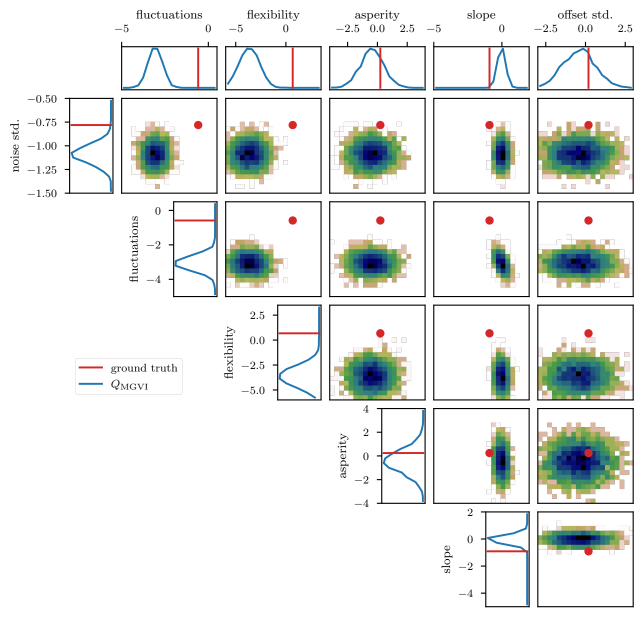
fluctuations
flexibility
asperity
slope
offset std.
noise std.
ground truth
Q_{HMC}

Appendix



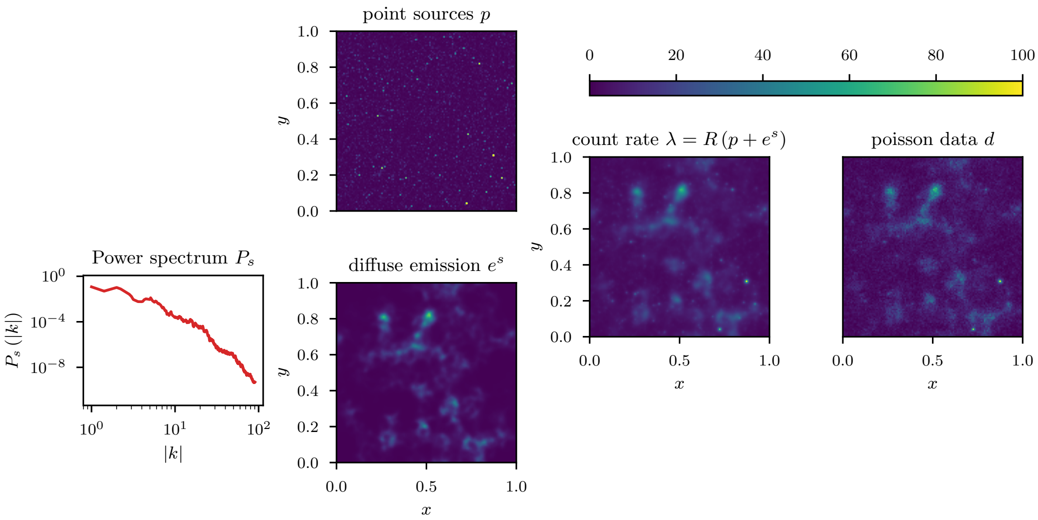
posterior samples
ground truth
posterior mean
data
0
1
2
3
4
0.5
0.0
−0.5
0.0
0.2
0.4
0.6
0.8
1.0
x
$P(\sigma_n|d)$
0.00
0.05
0.10
0.15
0.18
0.20
0.22
0.24
0.26
0.28
0.30
σ_n
$P_s(|k|)$
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^0
10^1
10^2
$|k|$

Appendix



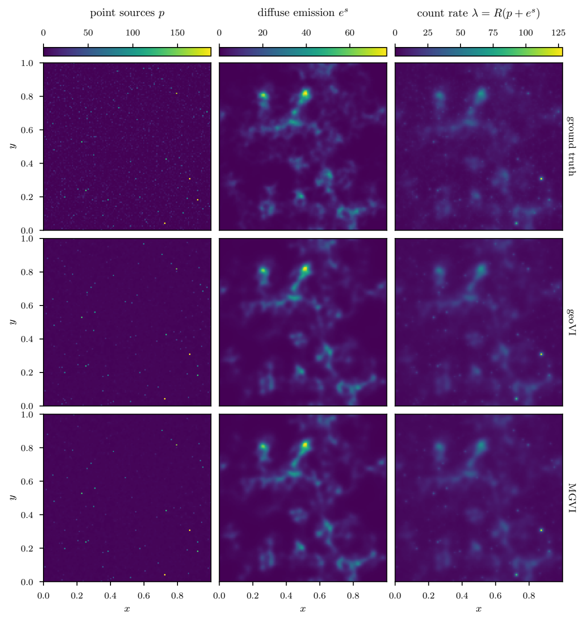
fluctuations
flexibility
asperity
slope
offset std.
noise std.
−0.50
−0.75
−1.00
−1.25
−1.50
fluctuations
flexibility
asperity
slope
ground truth
Q_{MGVI}

Appendix



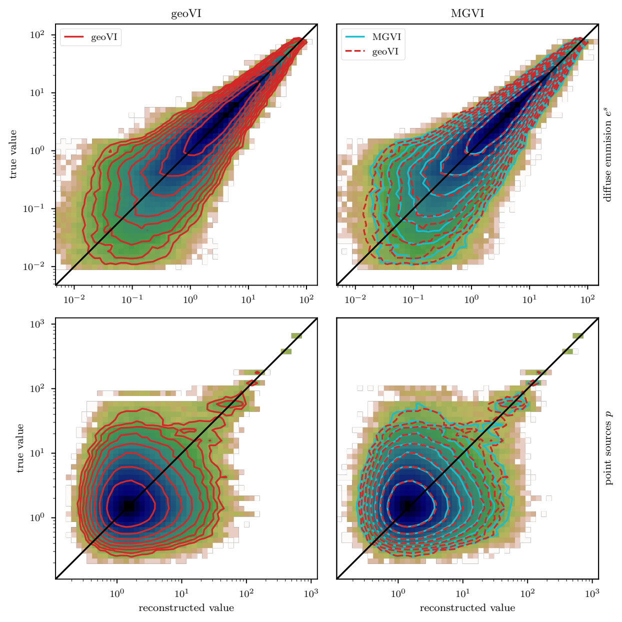
Power spectrum P_s
$P_s(|k|)$
10^0
10^{-4}
10^{-8}
10^0
10^1
10^2
$|k|$
point sources p
diffuse emission e^s
count rate $\lambda = R(p + e^s)$
poisson data d
0
20
40
60
80
100
1.0
0.8
0.6
0.4
0.2
0.0
0.5
x
y

Appendix

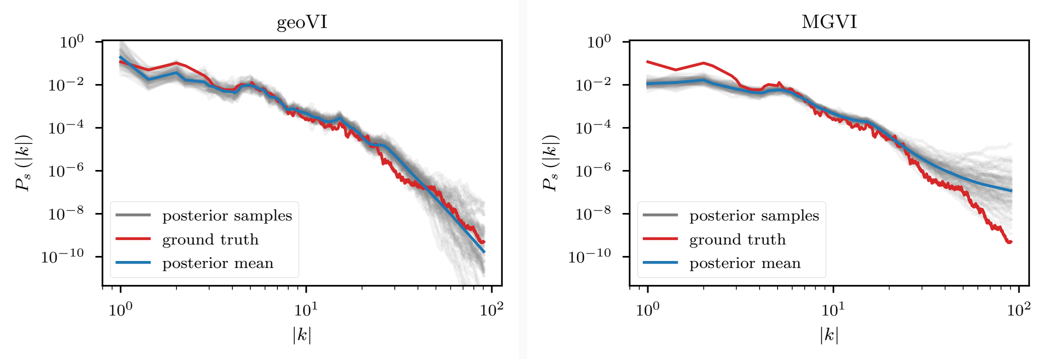


point sources p
diffuse emission e^s
count rate $\lambda = R(p + e^s)$
0 50 100 150
0 20 40 60
0 25 50 75 100 125
ground truth
geoVI
MGVI
y
x
0.0 0.2 0.4 0.6 0.8 1.0

Appendix

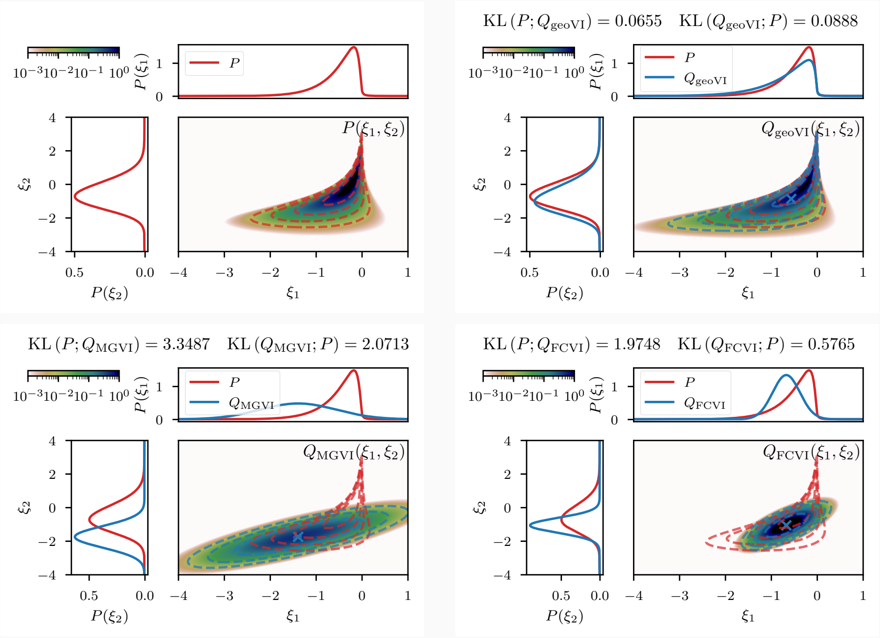

geoVI
MGVI
geoVI
MGVI
geoVI
true value
true value
reconstructed value
reconstructed value
diffuse emmision e^s
point sources p
10^{-2}
10^{-1}
10^0
10^1
10^2
10^3

Appendix



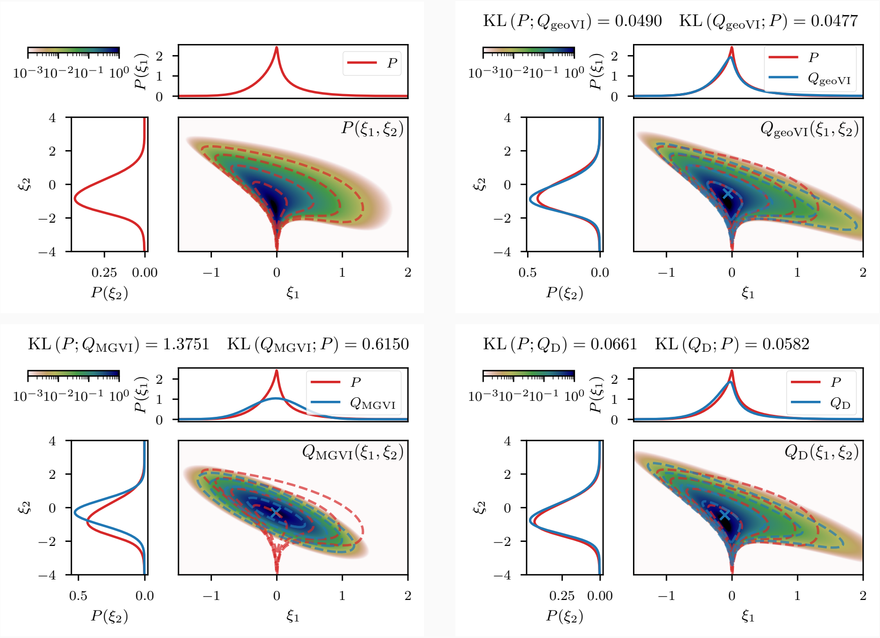
geoVI
MGVI
$P_s(|k|)$
$|k|$
10^0
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^1
10^2
posterior samples
ground truth
posterior mean

Appendix



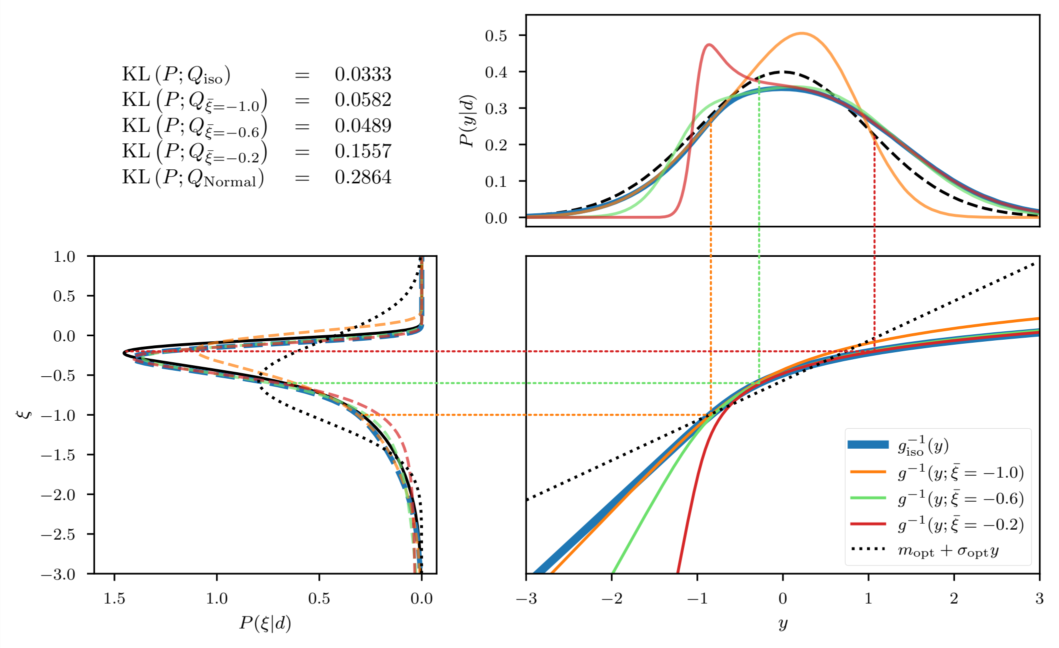
$P(\xi_1, \xi_2)$
KL $(P; Q_{\text{geoVI}}) = 0.0655$ KL $(Q_{\text{geoVI}}; P) = 0.0888$
$Q_{\text{geoVI}}(\xi_1, \xi_2)$
KL $(P; Q_{\text{MGVI}}) = 3.3487$ KL $(Q_{\text{MGVI}}; P) = 2.0713$
$Q_{\text{MGVI}}(\xi_1, \xi_2)$
KL $(P; Q_{\text{FCVI}}) = 1.9748$ KL $(Q_{\text{FCVI}}; P) = 0.5765$
$Q_{\text{FCVI}}(\xi_1, \xi_2)$
P
Q_{geoVI}
Q_{MGVI}
Q_{FCVI}
10^{-3} 10^{-2} 10^{-1} 10^{0}
$P(\xi_1)$
$P(\xi_2)$
ξ_1
ξ_2

Appendix



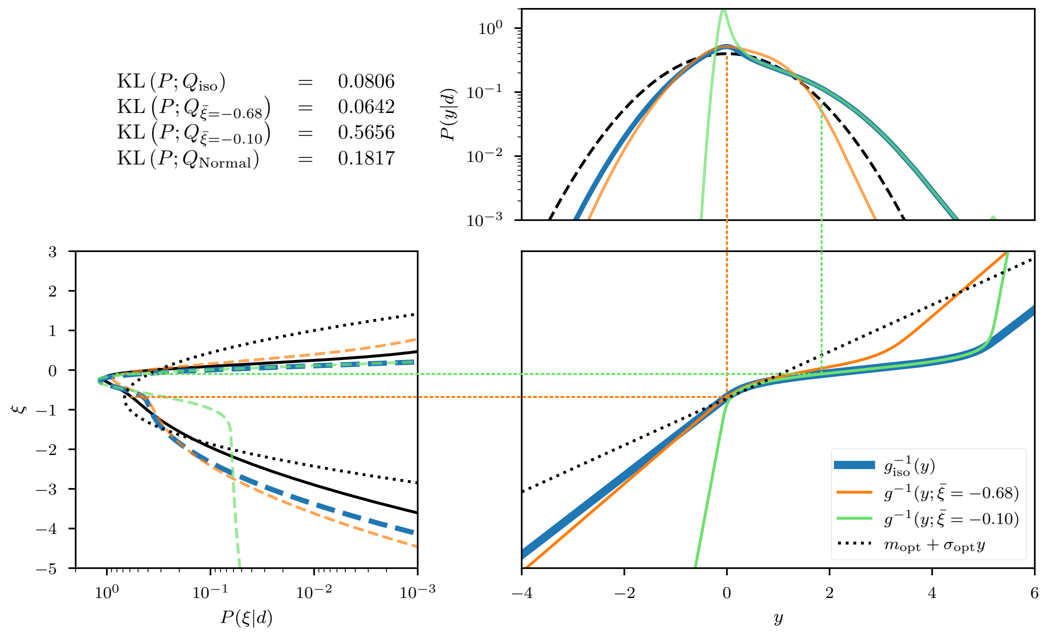
KL $(P; Q_{\mathrm{geoVI}}) = 0.0490$ KL $(Q_{\mathrm{geoVI}}; P) = 0.0477$
KL $(P; Q_{\mathrm{MGVI}}) = 1.3751$ KL $(Q_{\mathrm{MGVI}}; P) = 0.6150$
KL $(P; Q_{\mathrm{D}}) = 0.0661$ KL $(Q_{\mathrm{D}}; P) = 0.0582$
$P(\xi_1, \xi_2)$
$Q_{\mathrm{geoVI}}(\xi_1, \xi_2)$
$Q_{\mathrm{MGVI}}(\xi_1, \xi_2)$
$Q_{\mathrm{D}}(\xi_1, \xi_2)$
$P(\xi_1)$
$P(\xi_2)$
ξ_1
ξ_2
P
Q_{geoVI}
Q_{MGVI}
Q_{D}
10^{-3} 10^{-2} 10^{-1} 10^{0}

Appendix



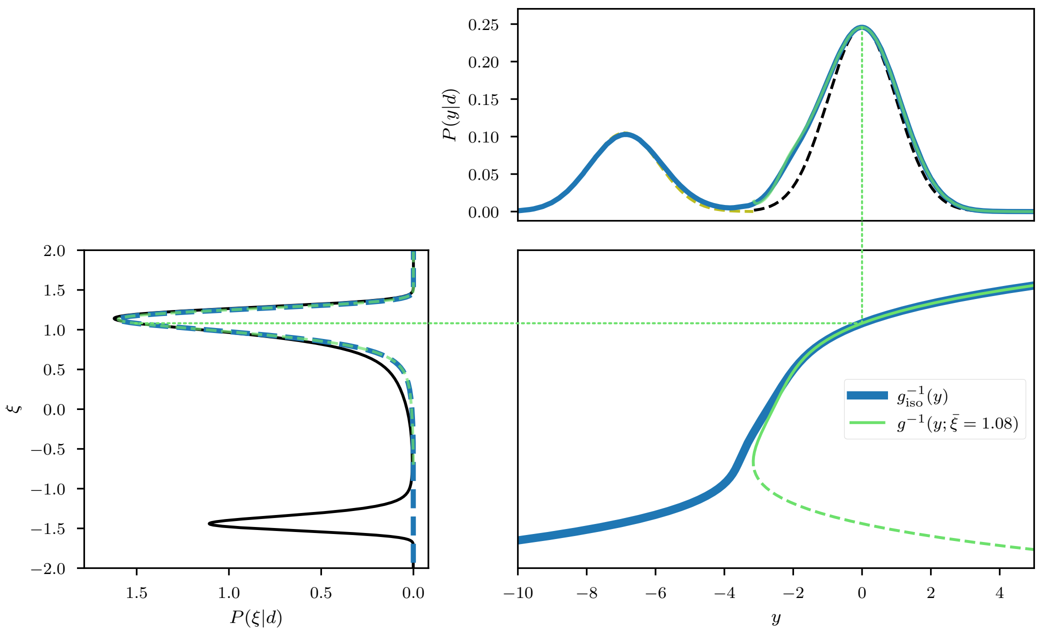
KL (P; Q_iso) = 0.0333
KL (P; Q_ξ̄=−1.0) = 0.0582
KL (P; Q_ξ̄=−0.6) = 0.0489
KL (P; Q_ξ̄=−0.2) = 0.1557
KL (P; Q_Normal) = 0.2864
P(y|d)
ξ
P(ξ|d)
y
g_iso^−1(y)
g^−1(y; ξ̄ = −1.0)
g^−1(y; ξ̄ = −0.6)
g^−1(y; ξ̄ = −0.2)
m_opt + σ_opt y

Appendix



$\mathrm{KL}(P; Q_{\mathrm{iso}}) = 0.0806$
$\mathrm{KL}(P; Q_{\bar{\xi}=-0.68}) = 0.0642$
$\mathrm{KL}(P; Q_{\bar{\xi}=-0.10}) = 0.5656$
$\mathrm{KL}(P; Q_{\mathrm{Normal}}) = 0.1817$
$P(y|d)$
10^{0}
10^{-1}
10^{-2}
10^{-3}
ξ
3
2
1
0
−1
−2
−3
−4
−5
$P(\xi|d)$
y
−4
−2
0
2
4
6
$g_{\mathrm{iso}}^{-1}(y)$
$g^{-1}(y; \bar{\xi} = -0.68)$
$g^{-1}(y; \bar{\xi} = -0.10)$
$m_{\mathrm{opt}} + \sigma_{\mathrm{opt}} y$

Appendix



$P(y|d)$
0.25
0.20
0.15
0.10
0.05
0.00
ξ
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
1.5
1.0
0.5
0.0
$P(\xi|d)$
−10
−8
−6
−4
−2
0
2
4
y
$g_{\text{iso}}^{-1}(y)$
$g^{-1}(y; \bar{\xi} = 1.08)$