IMPERIAL

Bayesian Model Selection:

Selecting the “best” model in a systematic way

SA AIMS

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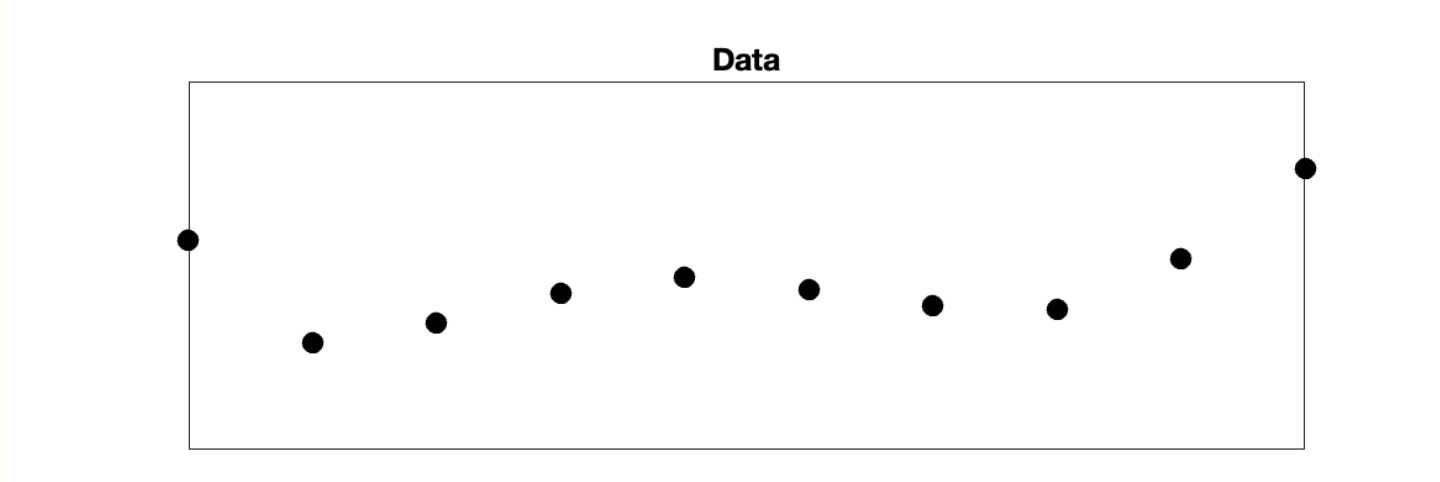
Learning Outcome

- Understand the principle of Occam razor and its Bayesian interpretation
- Gain an intuition to the scaling of prior and likelihood with data and noise
- Able to interpret Information Criterions from the Bayesian evidence perspective
- (Understand the mechanism of sparsification from Bayes' point of view)
- (Applying sparsifying prior to promote sparsity in model creation)

What line would you put through these datapoints?



Taken from Prof. Matthew Juniper's lecture on Bayesian Data Assimilation

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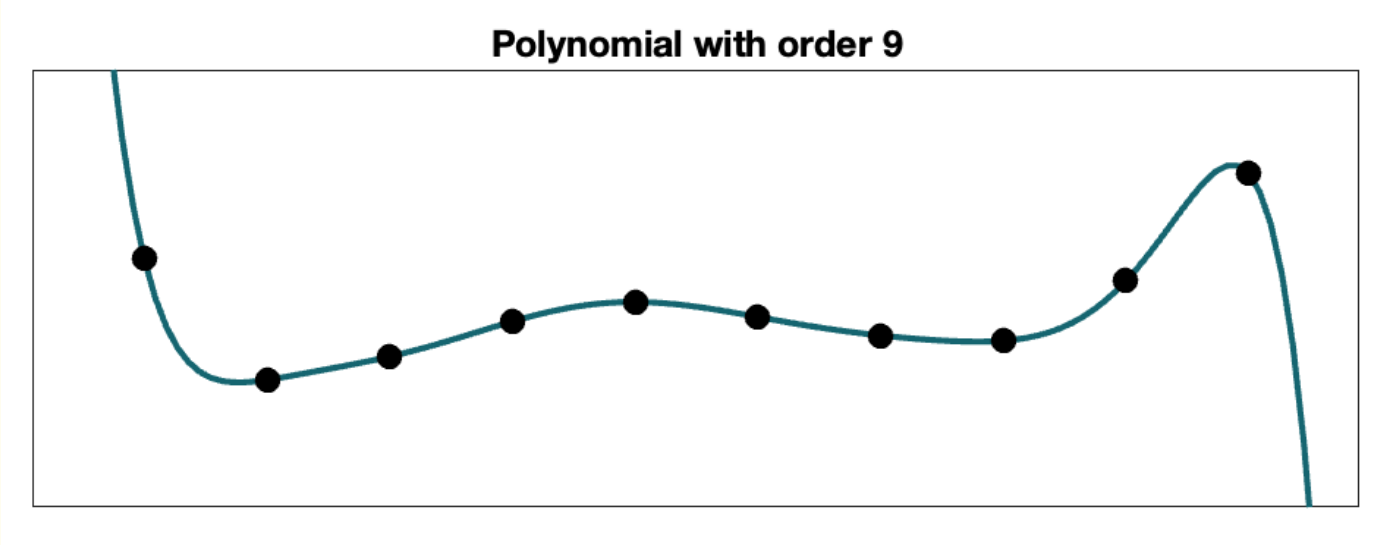

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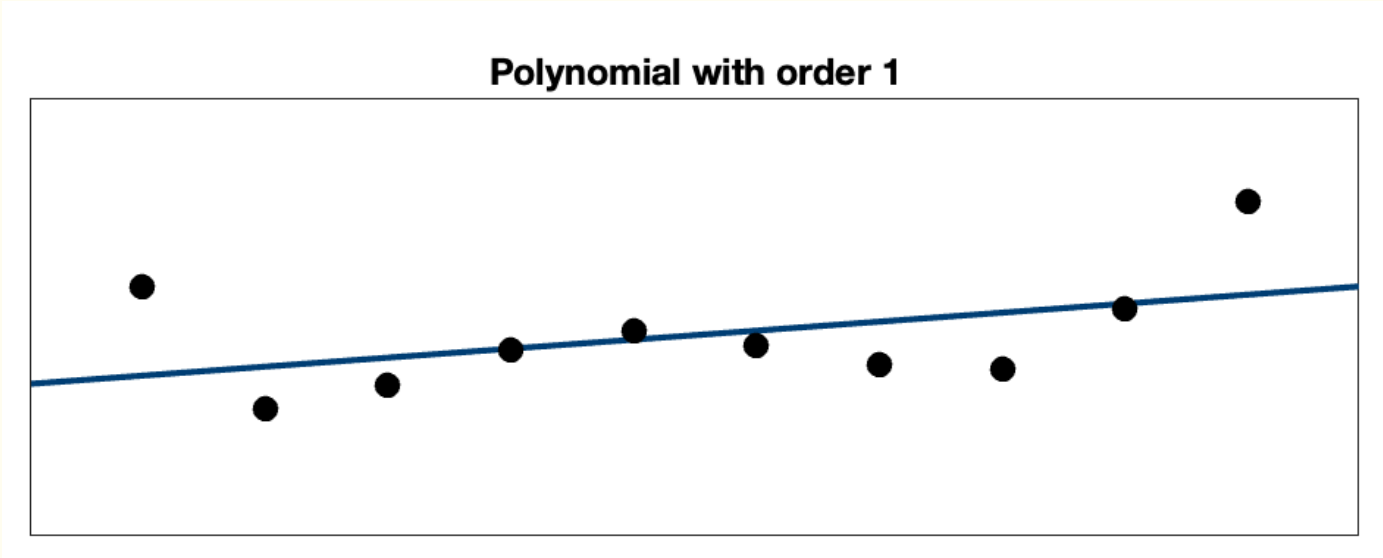

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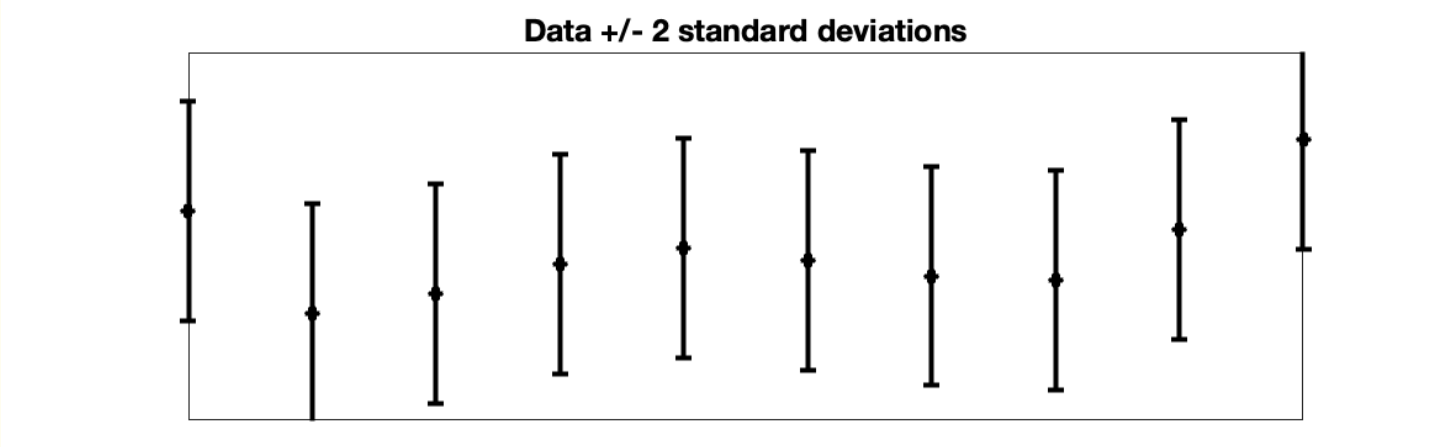

Juniper (2022)

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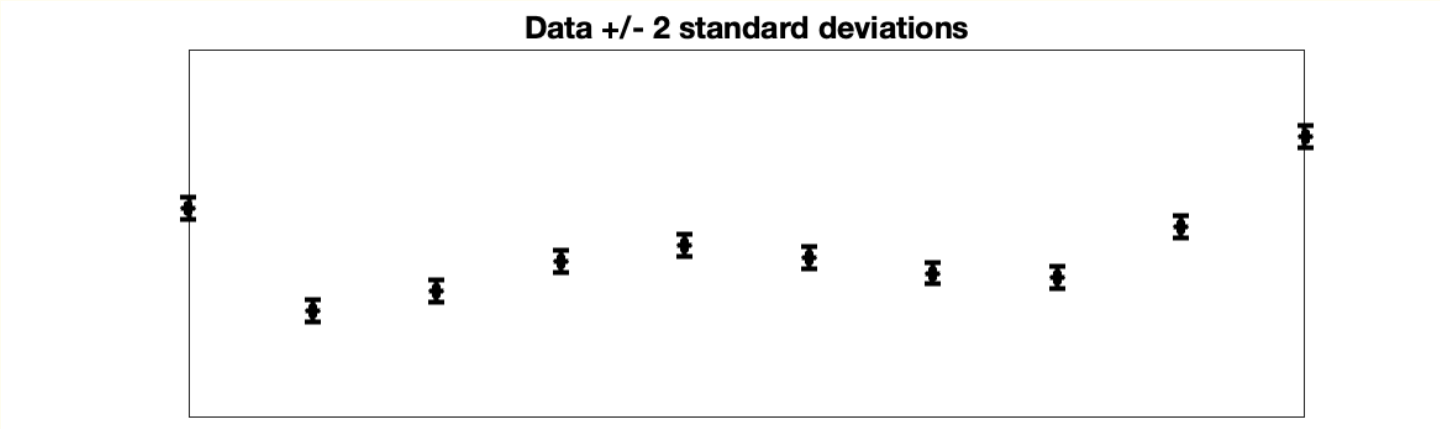

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Occam Razor

“When faced with two (or more) possible explanations, the simpler one is the one most likely to be true.”

(Paraphrasing) **William of Ockham**

We want as simple a model as possible (that still fits the data).

Principle of parsimony in modelling

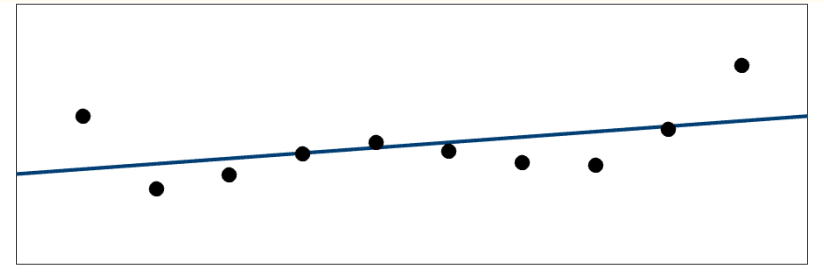
“Truth is much too complicated to allow anything but approximations.”

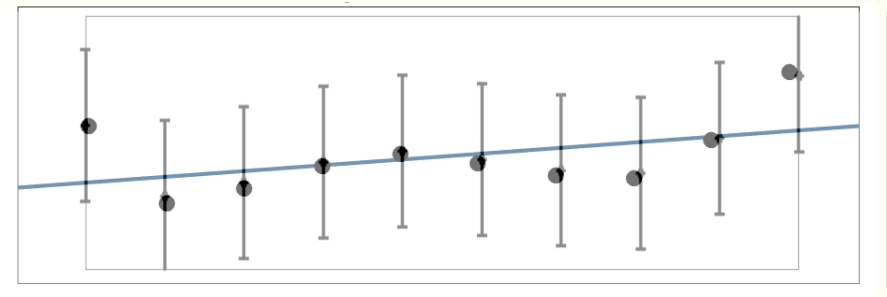
John von Neumann

We want to balance **model complexity** against **accuracy.**

What we want is… parsimonious model !

- **Ockham:** We want as **simple** a model as possible
- **von Neumann**: We want to balance **model complexity** against **accuracy**





How does Bayes help us?

Bayesian perspective
in the pursue of parsimonious models

Bayes' Theorem

$$P(\boldsymbol{\xi}|D) = \frac{P(D|\boldsymbol{\xi})P(\boldsymbol{\xi})}{P(D)}$$

posterior

likelihood prior

evidence

Just a normalising constant?

$D = \{\boldsymbol{x}, \boldsymbol{y}\}$ Data

$\boldsymbol{\xi}$ Fitting parameters

Bayes' Theorem

$$P\left(\boldsymbol{\xi}_{\mathcal{M}_i}|D,\mathcal{M}_i\right) = \frac{P\left(D|\boldsymbol{\xi}_{\mathcal{M}_i},\mathcal{M}_i\right)P(\boldsymbol{\xi}_{\mathcal{M}_i}|\mathcal{M}_i)}{P(D|\mathcal{M}_i)}$$

likelihood — prior

posterior

evidence

Key 'score' to compare btw models !

Model selection under Bayes

$$\underset{\mathcal{M}_i}{\operatorname{argmax}}\, P(\mathcal{M}_i|D)$$

where

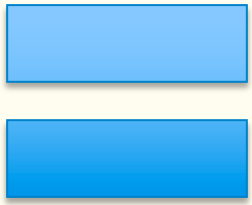
$$P(\mathcal{M}_i|D) \propto P(D|\mathcal{M}_i)P(\mathcal{M}_i)$$

$D = \{\boldsymbol{x}, \boldsymbol{y}\}$ Data

$\mathcal{M}_i$ Hypothesis (model basis)

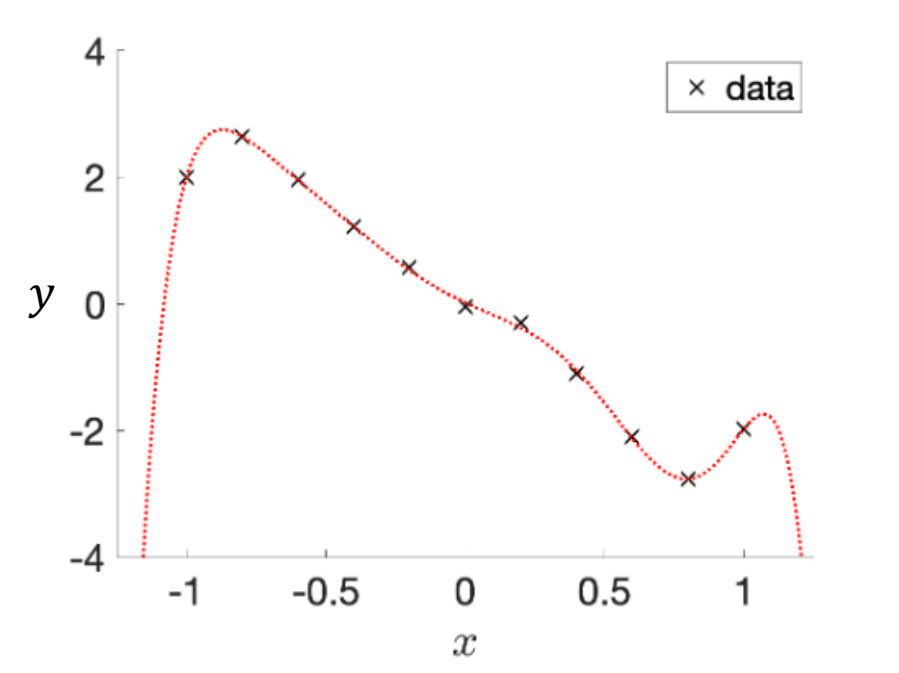
$\boldsymbol{\xi}_{\mathcal{M}_i}$ Fitting parameters

Model with max. $P(D|\mathcal{M}_i)$



Most parsimonious model

An example with linear regression – Model 1 (Complex)

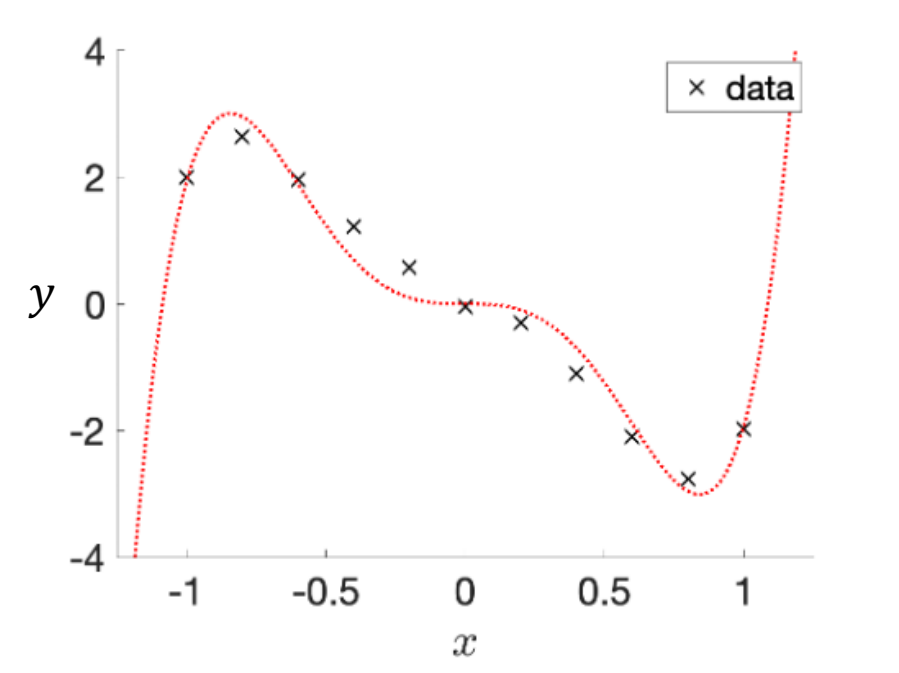


target = Polynomial Functions · Learnt Coefficients

$\mathbf{y} = \boldsymbol{\Theta}(\boldsymbol{x}) \cdot \boldsymbol{\xi}$

$\begin{bmatrix} \mathbf{y} \end{bmatrix} = \begin{bmatrix} 1 & x & x^2 & x^3 & x^4 & x^5 & x^6 & x^7 & x^8 & \cdots \end{bmatrix} \begin{bmatrix} \xi \end{bmatrix}$

An example with linear regression – Model 2 (parsimonious)



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Why is max. evidence = Occam Razor?
An example with linear regression

$D = \{\boldsymbol{x}, \boldsymbol{y}\}$ Data

$\mathcal{M}_i$ Model

$\boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x})$ Model Basis

$\boldsymbol{\xi}$ Fitting parameters

Bayes' rule

$$P(\boldsymbol{\xi}|D,\mathcal{M}_i) = \frac{P(D|\boldsymbol{\xi},\mathcal{M}_i)P(\boldsymbol{\xi}|\mathcal{M}_i)}{P(D|\mathcal{M}_i)}$$

posterior; likelihood; prior; evidence

Gaussian Linear model:
$\boldsymbol{y} \sim \boldsymbol{\mathcal{N}}(\boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x}) \cdot \boldsymbol{\xi}, \sigma^2\mathbf{I})$

$$-\ln P(\boldsymbol{\xi}|D,\mathcal{M}_i) = \frac{1}{2\sigma^2}\|\boldsymbol{y} - \boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x}) \cdot \boldsymbol{\xi}\|_F^2 + \frac{1}{2\sigma_p^2}\|\boldsymbol{\xi}\|_2^2 + normalise$$

error

posterior; likelihood; Prior (L_2 regularisation)

Maximum a posteriori (MAP):

$$\boldsymbol{\xi}_{MAP} = \underset{\boldsymbol{\xi}}{\operatorname{argmax}}\, P(\boldsymbol{\xi}|D,\mathcal{M}_i)$$

=

Regularised Regression
(Regularisation ↔ prior)

Why is max. evidence = Occam Razor?
An example with linear regression

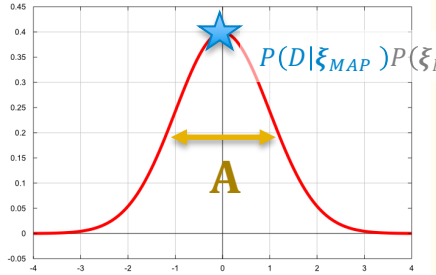
$$\mathbf{A} = \sigma_p^{-2}\mathbf{I} + \sigma^{-2}\boldsymbol{\Theta}_{\mathcal{M}}{}^{\mathrm{T}}\boldsymbol{\Theta}_{\mathcal{M}}$$

Assuming the prior to all models $P(\mathcal{M}_i)$ is uniform:

$$P(\mathcal{M}_i|D) \propto P(D|\mathcal{M}_i) = \int_{\xi} P(D|\boldsymbol{\xi}, \mathcal{M}_i) P(\boldsymbol{\xi}|\mathcal{M}_i) d\boldsymbol{\xi}$$

← Difficult to eval.

Posterior:



$D = \{\boldsymbol{x}, \boldsymbol{y}\}$ Data

$\mathcal{M}_i$ Model

$\boldsymbol{\xi}$ Fitting parameters

$\mathbf{A}$ Parameter Covariance

Why is max. evidence = Occam Razor?
An example with linear regression

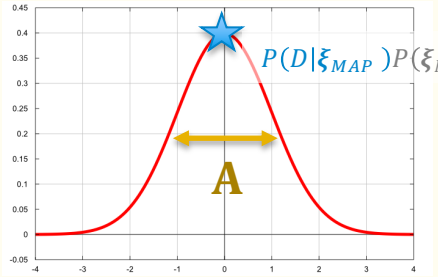
$$\mathbf{A} = \sigma_p^{-2}\mathbf{I} + \sigma^{-2}\boldsymbol{\Theta}_{\mathcal{M}}{}^{\mathrm{T}}\boldsymbol{\Theta}_{\mathcal{M}}$$

Assuming the prior to all models $P(\mathcal{M}_i)$ is uniform:

$$P(\mathcal{M}_i|D) \propto P(D|\mathcal{M}_i) = \int_{\xi} P(D|\xi, \mathcal{M}_i) P(\xi|\mathcal{M}_i) d\xi$$

Occam Razor!

Posterior:



$$= P(D|\xi_{MAP}, \mathcal{M}_i) \quad P(\xi_{MAP}|\mathcal{M}_i) \quad \left[\det\left(\frac{\mathbf{A}}{2\pi}\right)\right]^{-1/2}$$

Likelihood @ MAP — Prior on ξ @ MAP — Uncertainty in ξ around MAP

$\uparrow \#\xi \Rightarrow$
$\uparrow likelihood$

$\uparrow \#\xi \Rightarrow$
$\downarrow prior$

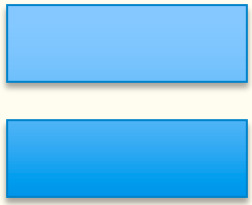
$\uparrow \#\xi \Rightarrow$
$\uparrow rank(\mathbf{A}) \Rightarrow$
$\downarrow |\mathbf{A}|^{-1/2}$

How well $\mathcal{M}_i$ fit

Penalise models with too many param.

$D = \{\boldsymbol{x}, \boldsymbol{y}\}$ Data
$\mathcal{M}_i$ Model
$\boldsymbol{\xi}$ Fitting parameters
$\mathbf{A}$ Parameter Covariance

Model with max. $P(D|\mathcal{M}_i)$



Indeed!

Most parsimonious model

Computing Evidence – Gaussian case

Aim: $\underset{\mathcal{M}_i}{\operatorname{argmax}} P(\mathcal{M}_i|D)$

$$P(\mathcal{M}_i|D) \propto P(D|\mathcal{M}_i) = \int_{\xi} P(D|\boldsymbol{\xi}, \mathcal{M}_i) P(\boldsymbol{\xi}|\mathcal{M}_i) d\boldsymbol{\xi}$$

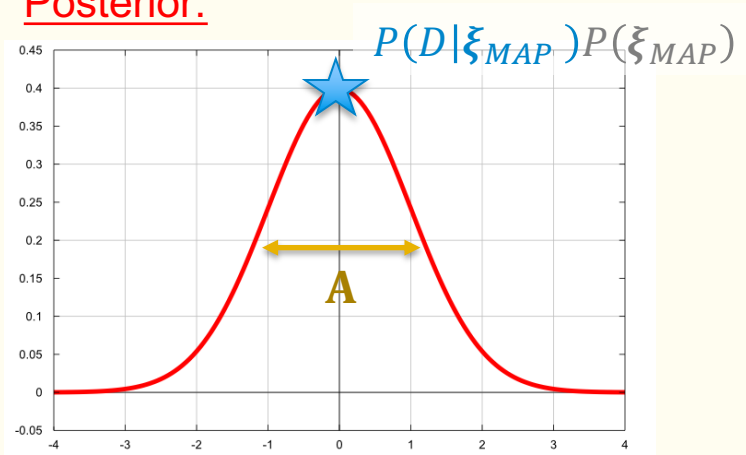
$$= P(D|\boldsymbol{\xi}_{MAP}, \mathcal{M}_i) \quad P(\boldsymbol{\xi}_{MAP}|\mathcal{M}_i) \quad \left[\det\left(\frac{\mathbf{A}}{2\pi}\right)\right]^{-1/2}$$

Likelihood @ MAP — Prior on $\boldsymbol{\xi}$ @ MAP — Uncertainty in $\boldsymbol{\xi}$ around MAP

Occam Factor

Obtained from linear regression

Posterior:



Penalizes models with too many param.

$D = \{\boldsymbol{x}, \boldsymbol{y}\}$ Data

$\mathcal{M}_i$ Model

$\boldsymbol{\xi}$ Fitting parameters

$\mathbf{A}$ Parameter Covariance

$$\mathbf{A} = \sigma_p^{-2}\mathbf{I} + \sigma^{-2}\boldsymbol{\Theta}_{\mathcal{M}}{}^{\mathrm{T}}\boldsymbol{\Theta}_{\mathcal{M}}$$

Approximating Evidence – Laplace Method

Aim: $\underset{\mathcal{M}_i}{\operatorname{argmax}} P(\mathcal{M}_i|D)$

$$P(\mathcal{M}_i|D) \propto P(D|\mathcal{M}_i) = \int_{\xi} \underbrace{P(D|\boldsymbol{\xi},\mathcal{M}_i)P(\boldsymbol{\xi}|\mathcal{M}_i)}_{\propto P(\boldsymbol{\xi}|D)} d\boldsymbol{\xi}$$

Difficult to eval.

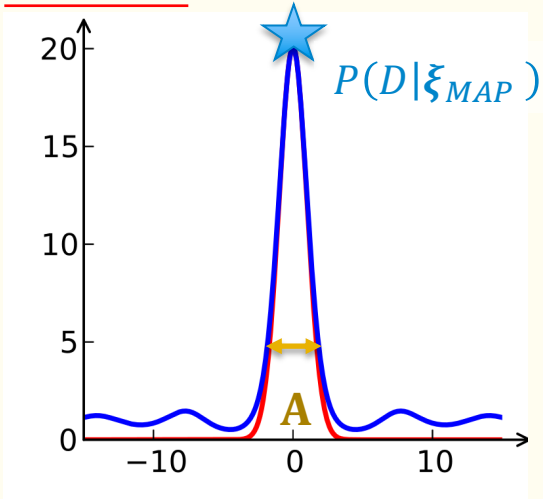
$$\approx P(D|\boldsymbol{\xi}_{MAP},\mathcal{M}_i) \quad P(\boldsymbol{\xi}_{MAP}|\mathcal{M}_i) \quad \left[\det\left(\frac{\mathbf{A}}{2\pi}\right)\right]^{-1/2}$$

Likelihood @ MAP — Prior on $\boldsymbol{\xi}$ @ MAP — Uncertainty in $\boldsymbol{\xi}$ around MAP

Occam Factor

Obtained from variational inference

Posterior:



Penalizes models with too many param.

$$\mathbf{A} = -\left.\frac{d^2 \ln P(D|\boldsymbol{\xi},\mathcal{M}_i)P(\boldsymbol{\xi}|\mathcal{M}_i)}{d\xi^2}\right|_{\xi_{MAP}}$$

$D = \{\boldsymbol{x}, \boldsymbol{y}\}$ Data

$\mathcal{M}_i$ Model

$\boldsymbol{\xi}$ Fitting parameters

$\mathbf{A}$ Parameter Uncertainty

Scaling of Likelihood and Occam Factor and BIC

$\mathbf{A}$ is a $k \times k$ matrix scales with n

$$\ln P(D|\mathcal{M}_i) \approx \underbrace{\ln P(D|\boldsymbol{\xi}_{MAP}, \mathcal{M}_i)}_{\sim O(n)} + \underbrace{\ln P(\boldsymbol{\xi}_{MAP}|\mathcal{M}_i)}_{\sim O(k)} + \underbrace{\ln \left[\det\left(\frac{\mathbf{A}}{2\pi}\right)\right]^{-1/2}}_{\sim O(-\frac{k}{2}\ln\frac{n}{2\pi})}$$

Likelihood @ MAP

Occam Factor

When $n \to \infty \gg k$,

$$-2 \ln P(D|\mathcal{M}_i) \approx -2 \ln \hat{L} + k \ln n + O(1)$$

$$BIC = k \ln n - 2 \ln \hat{L}$$

$\therefore$ Minimise BIC $\approx$ Maximise Evidence

n	Number of data
k	Number of parameters
D	Data
$\mathcal{M}_i$	Model
$\boldsymbol{\xi}$	Fitting parameters
$\mathbf{A}$	Parameter Covariance

Model Sparsification through priors

Selecting a model in a set of models defined by combinations of terms

The Role of Prior in Regression

$D = \{\boldsymbol{x}, \boldsymbol{y}\}$ Data

$\mathcal{M}_i$ Model

$\boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x})$ Model Basis

$\boldsymbol{\xi}$ Fitting parameters

Bayes' rule

likelihood prior

$$P(\boldsymbol{\xi}|D,\mathcal{M}_i) = \frac{P(D|\boldsymbol{\xi},\mathcal{M}_i)P(\boldsymbol{\xi}|\mathcal{M}_i)}{P(D|\mathcal{M}_i)}$$

posterior

evidence

Gaussian Linear model:
$\boldsymbol{y} \sim \boldsymbol{\mathcal{N}}(\boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x}) \cdot \boldsymbol{\xi}, \sigma^2\mathbf{I})$

error

$$-\ln P(\boldsymbol{\xi}|D,\mathcal{M}_i) = \frac{1}{2\sigma^2}\|\boldsymbol{y} - \boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x}) \cdot \boldsymbol{\xi}\|_F^2 + \gamma\|\boldsymbol{\xi}\| + normalise$$

posterior likelihood Prior (Regularisation)

Maximum a posteriori (MAP):

$$\boldsymbol{\xi}_{MAP} = \underset{\boldsymbol{\xi}}{\operatorname{argmax}}\, P(\boldsymbol{\xi}|D,\mathcal{M}_i)$$

=

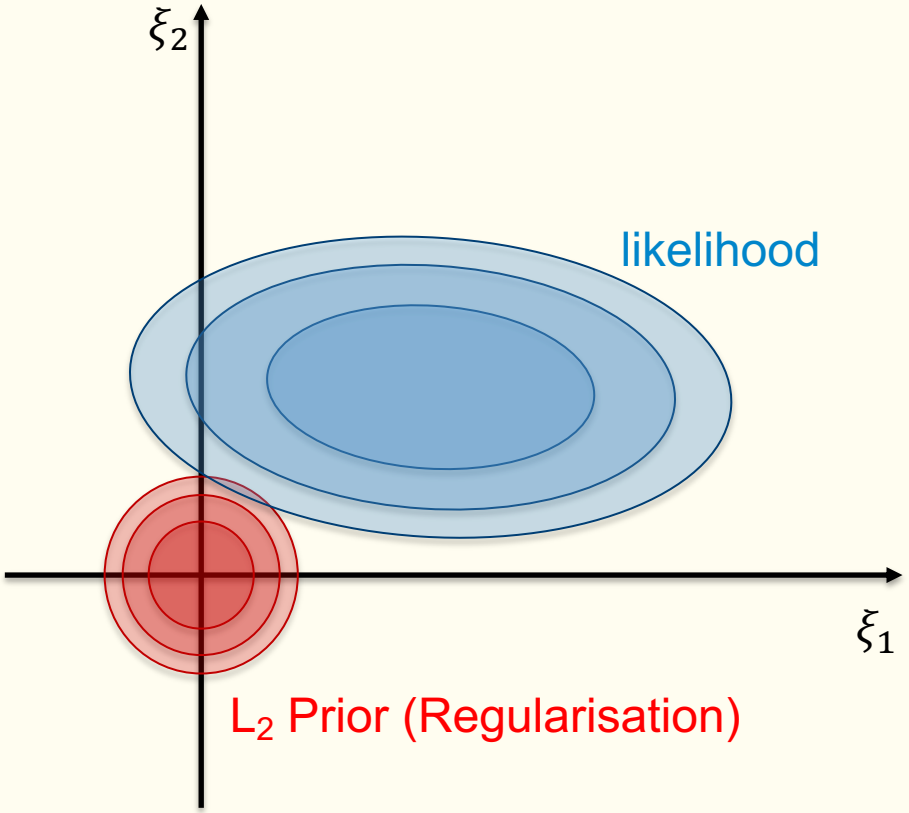
Regularised Regression
(Regularisation ↔ prior)

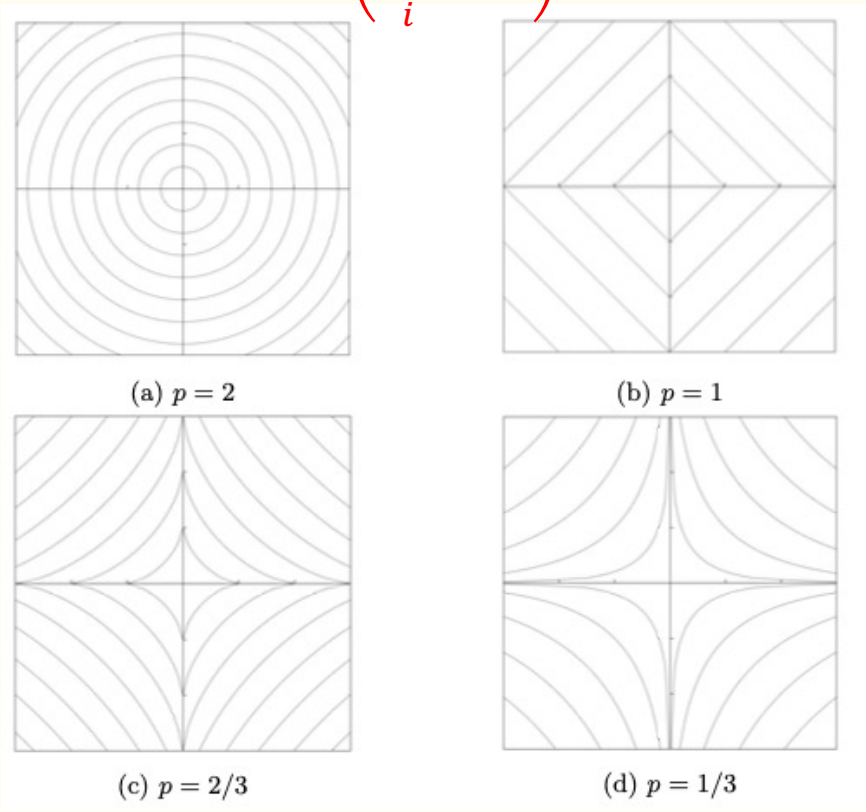
Types of prior

Regression	Loss	Regulariser	Prior
Ridge	$\frac{1}{2\sigma^2}\|\boldsymbol{y}-\boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x})\cdot\boldsymbol{\xi}\|_F^2+\frac{\gamma}{2}\|\boldsymbol{\xi}\|_2^2$	$\frac{1}{2}\|\boldsymbol{\xi}\|_2^2=\frac{1}{2}\sum_i \xi_i^2$	Gaussian (L2) $\xi\sim\mathcal{N}(0,1)$
LASSO	$\frac{1}{2\sigma^2}\|\boldsymbol{y}-\boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x})\cdot\boldsymbol{\xi}\|_F^2+\gamma\|\boldsymbol{\xi}\|_1$	$\|\boldsymbol{\xi}\|_1=\sum_i \|\xi_i\|$	Laplace (L1) $\xi\sim Laplace(0,1)$
Sequential Threshold	$\frac{1}{2\sigma^2}\|\boldsymbol{y}-\boldsymbol{\Theta}_{\mathcal{M}}(\boldsymbol{x})\cdot\boldsymbol{\xi}\|_F^2+\gamma\|\boldsymbol{\xi}\|_0$	$\|\boldsymbol{\xi}\|_0$ $=\#\ of\ nonzero$	(No formal prior, L0)
Spike and Slab	(Ridge with $\|\boldsymbol{\xi}\|_2^2$ + loss for λ)	$\xi\|\lambda\sim\mathcal{N}(0,1)\lambda+\mathcal{N}(0,\epsilon^2)(1-\lambda)$ $\lambda\sim Ber(\pi)$	
Normal-Gamma	(Ridge with $\|\boldsymbol{\xi}\|_2^2$ + loss for α)	$\xi\|\alpha\sim\mathcal{N}(0,diag(\alpha^{-1}))$ $\alpha\sim Gamma(k,\theta)$	

Prior as sparsifier

$$\|\boldsymbol{\xi}\|_{\boldsymbol{p}} = \left(\sum_i |\xi_i|^p\right)^{1/p}$$





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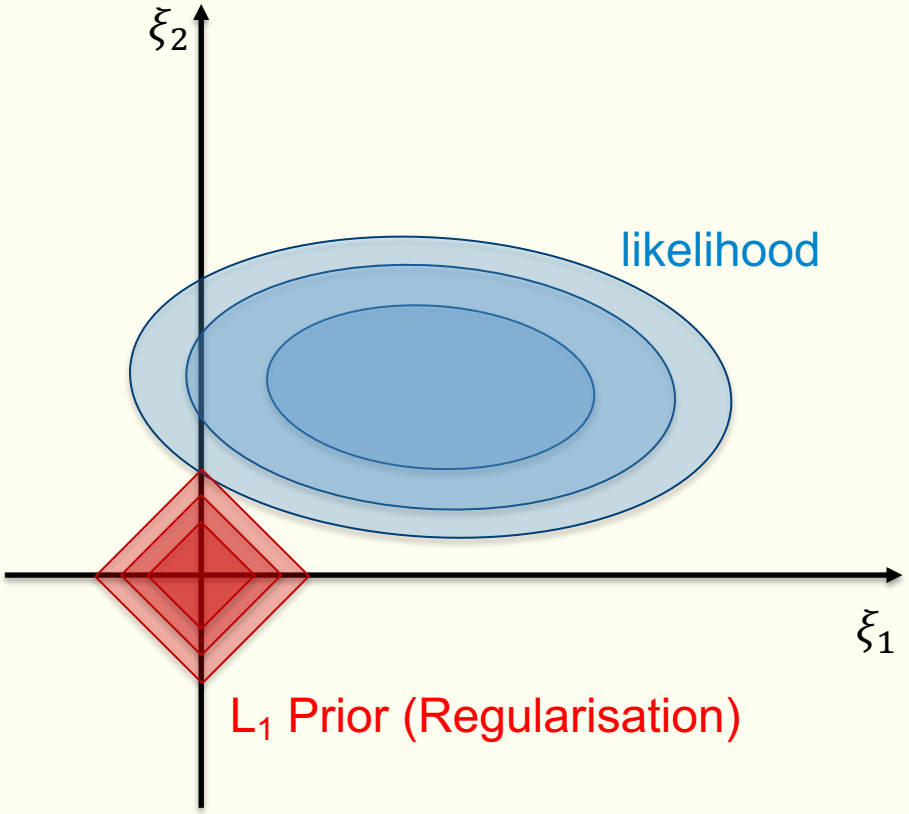
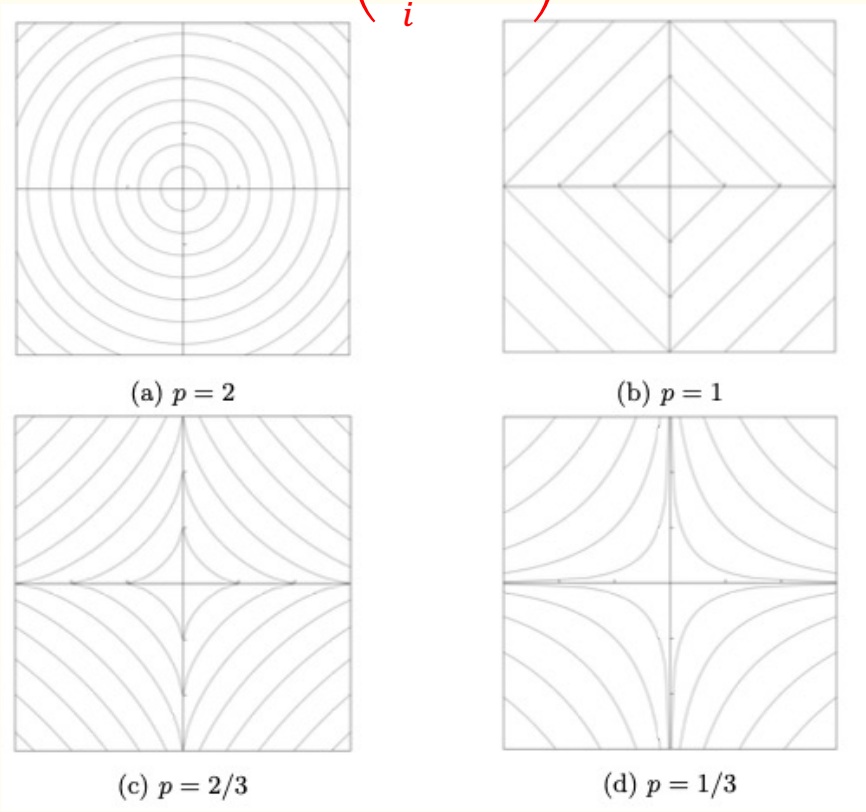
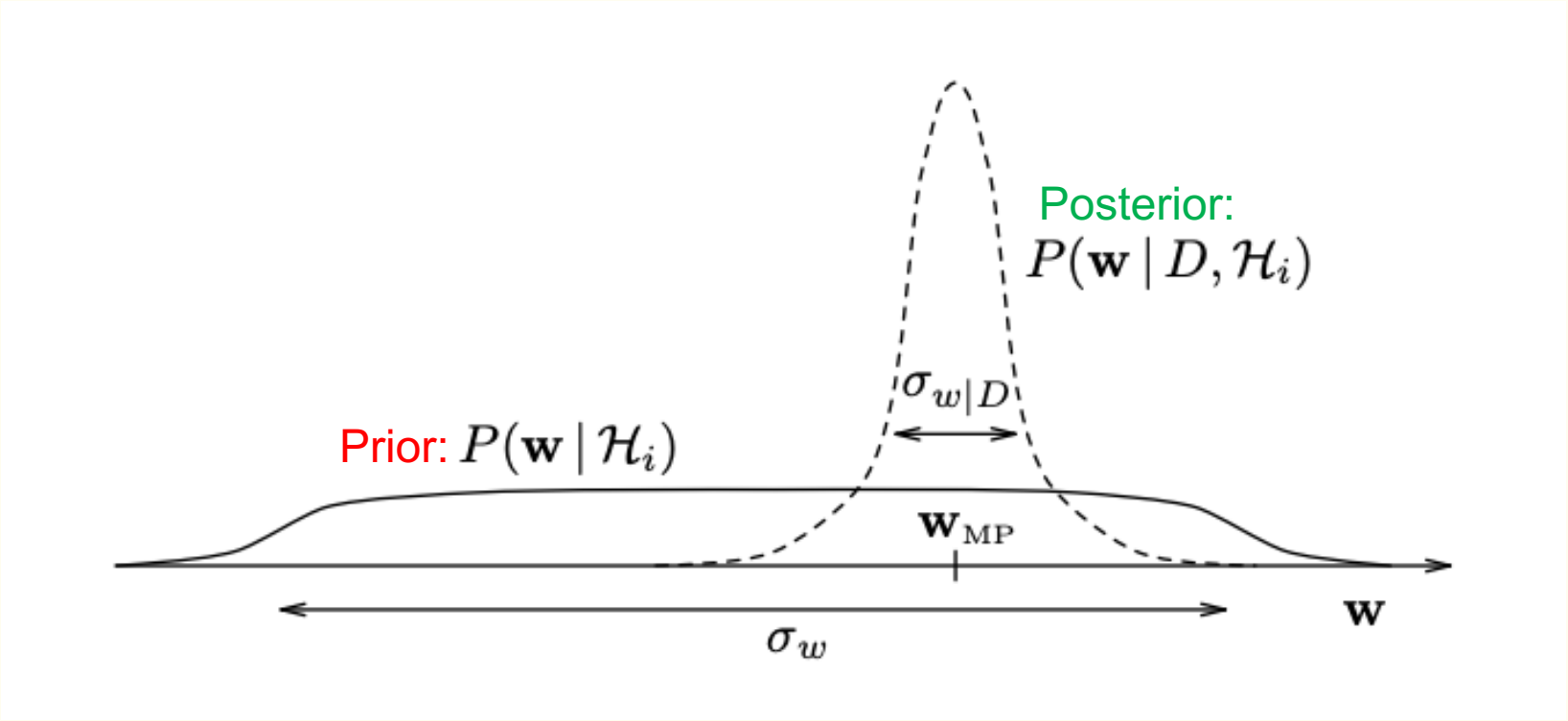




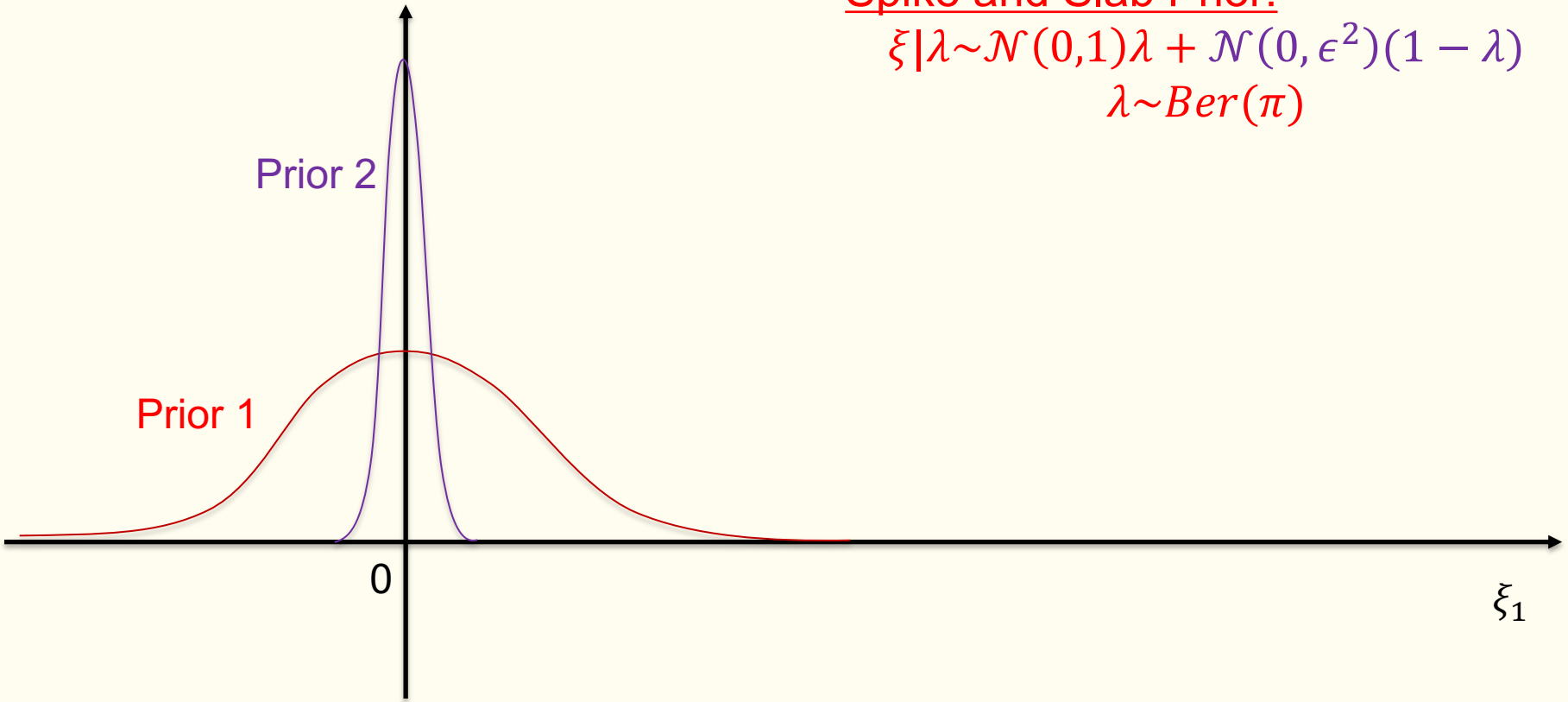
Prior as sparsifier – Hierarchical Prior



Prior as sparsifier – Hierarchical Prior

Spike and Slab Prior:

$$\xi|\lambda \sim \mathcal{N}(0,1)\lambda + \mathcal{N}(0,\epsilon^2)(1-\lambda)$$
$$\lambda \sim Ber(\pi)$$



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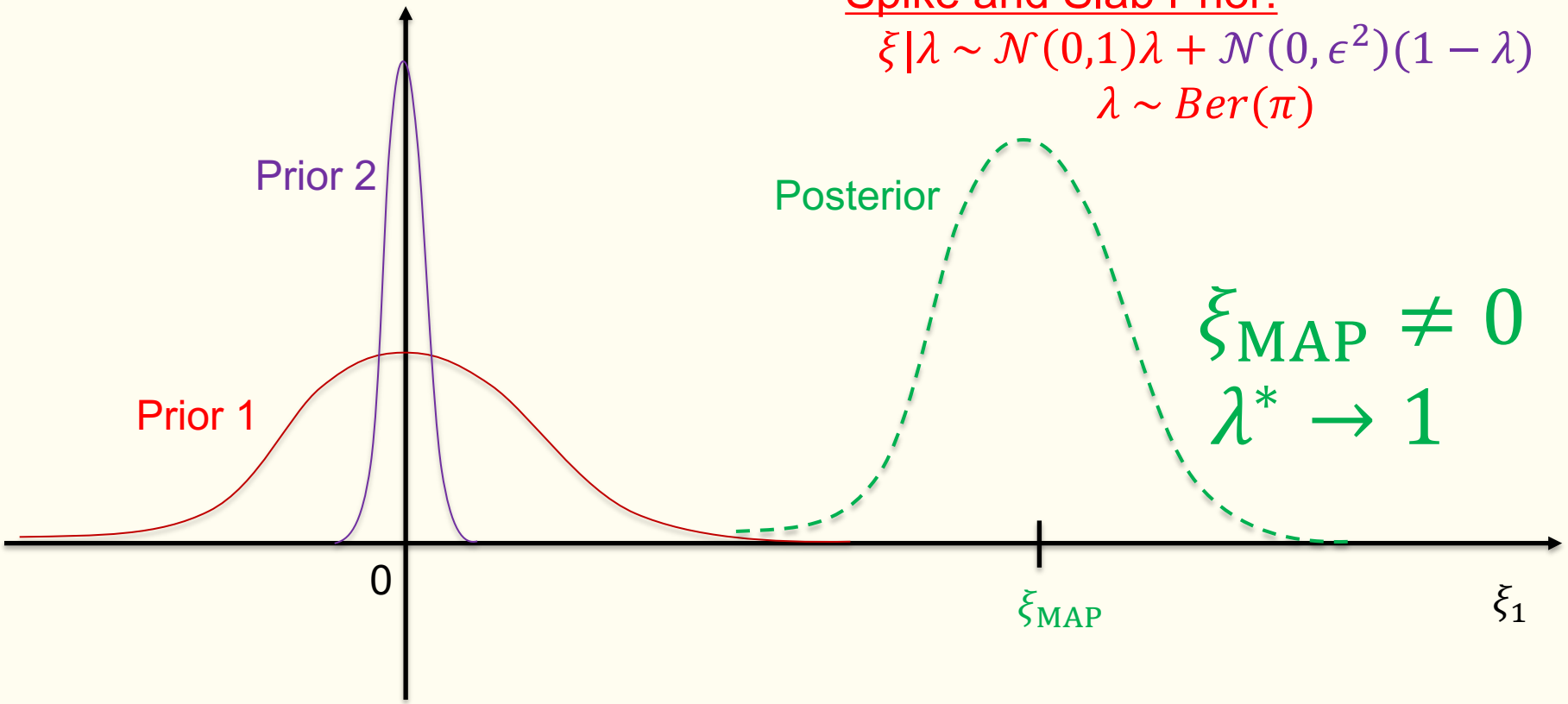

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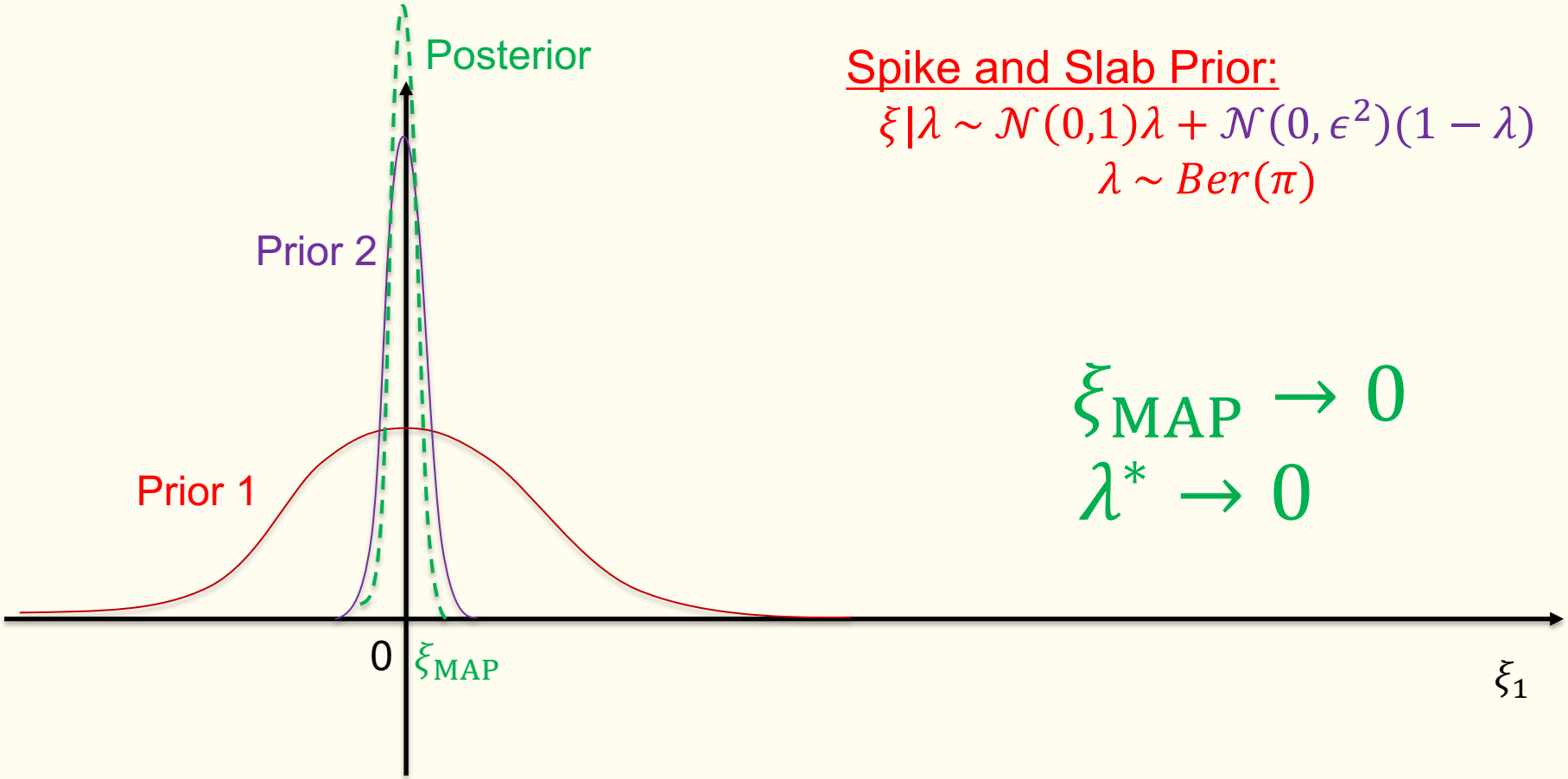
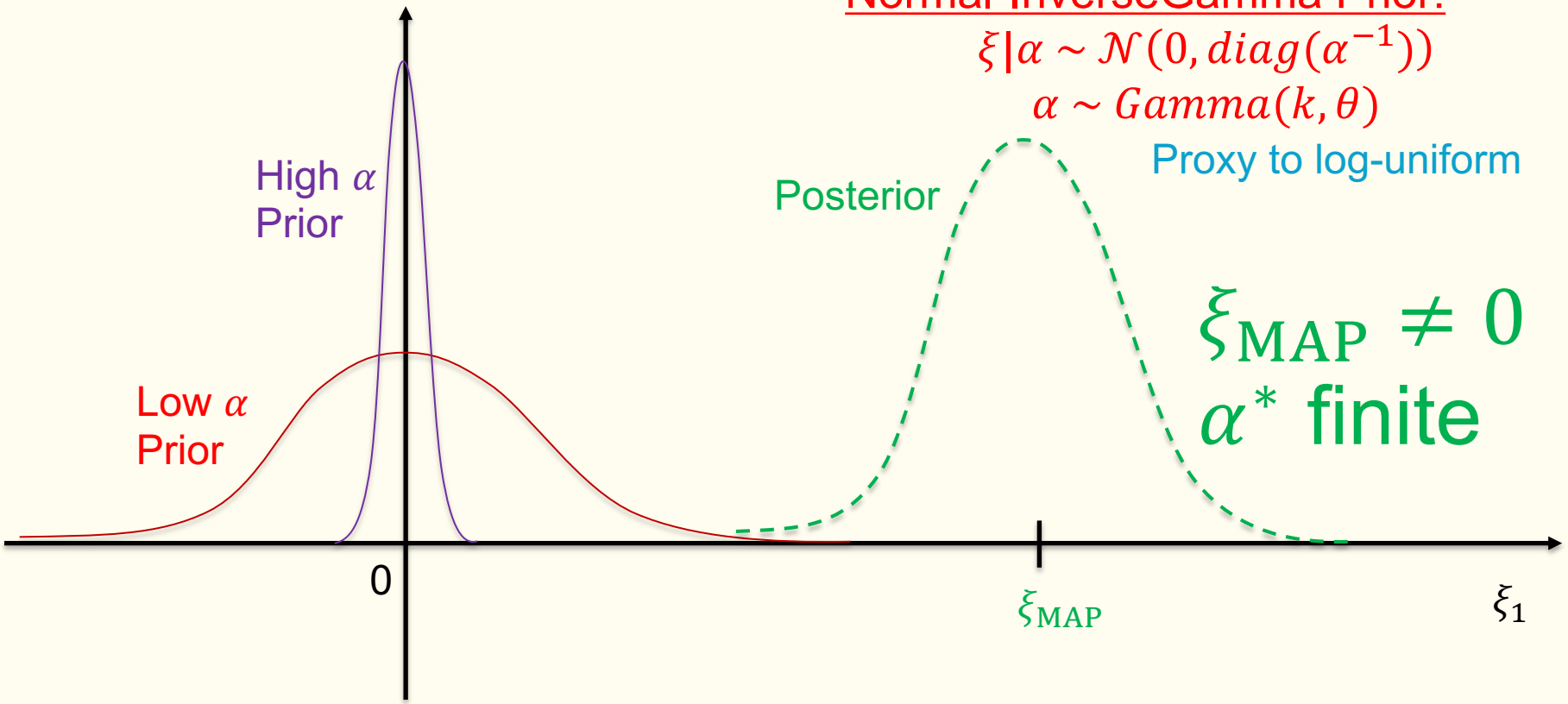


Spike and Slab Prior:

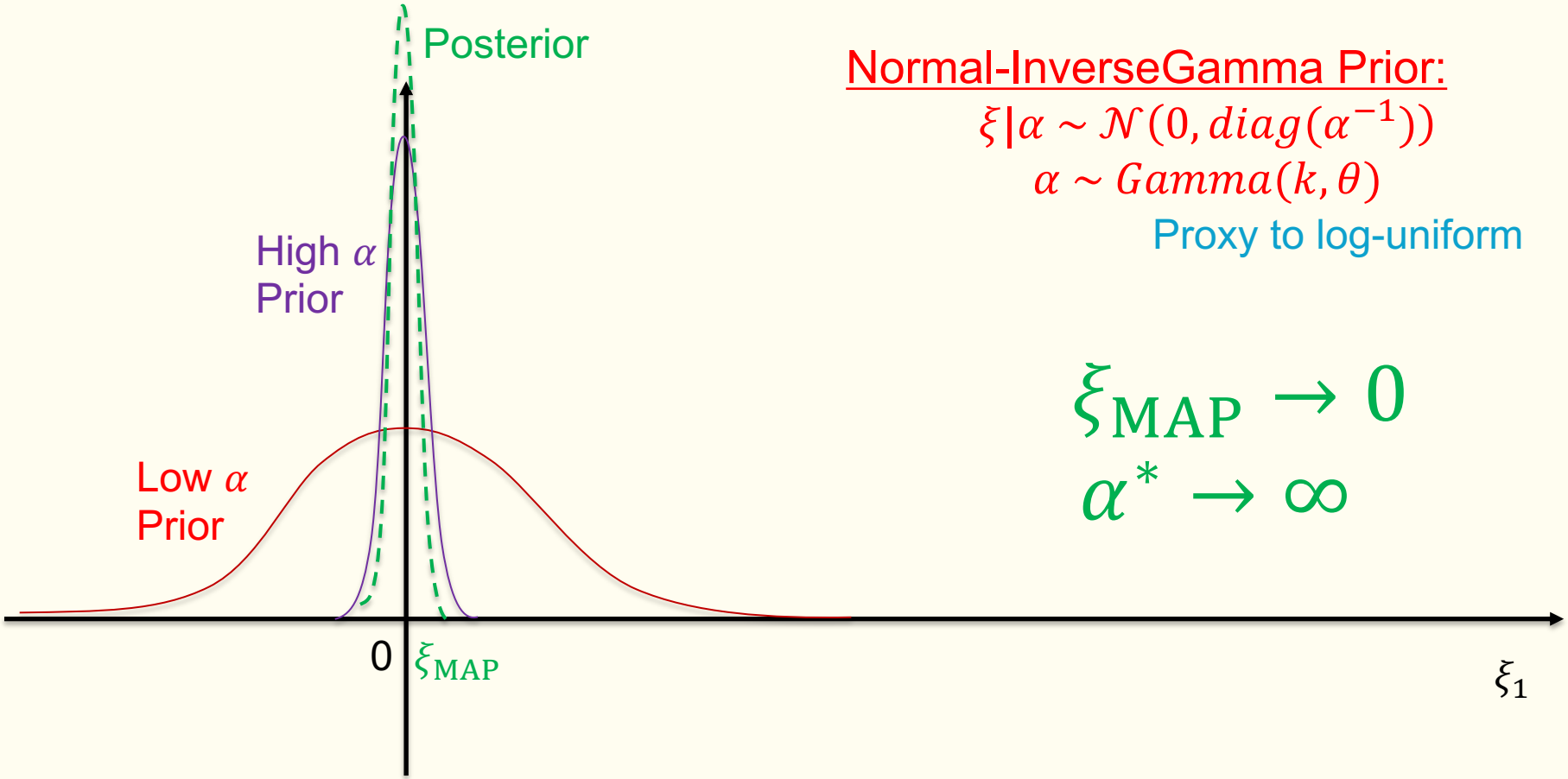
$$\xi|\lambda \sim \mathcal{N}(0,1)\lambda + \mathcal{N}(0,\epsilon^2)(1-\lambda)$$
$$\lambda \sim Ber(\pi)$$

$$\xi_{\mathrm{MAP}} \to 0$$
$$\lambda^* \to 0$$

Prior as sparsifier – Hierarchical Prior



Prior as sparsifier – Hierarchical Prior



Normal-InverseGamma Prior:

$$\xi|\alpha \sim \mathcal{N}(0, diag(\alpha^{-1}))$$

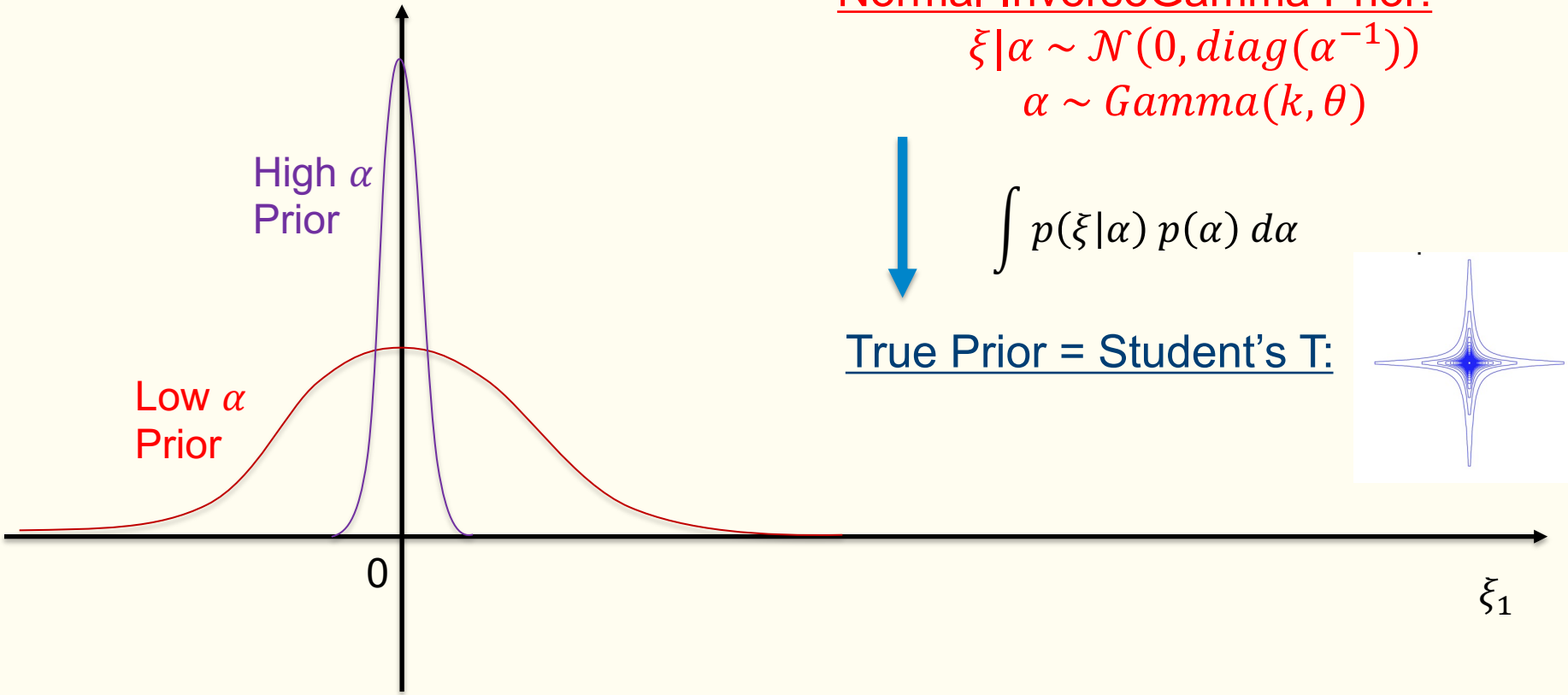
$$\alpha \sim Gamma(k, \theta)$$

Proxy to log-uniform

$$\xi_{\mathrm{MAP}} \to 0$$

$$\alpha^* \to \infty$$

Prior as sparsifier – Hierarchical Prior



Normal-InverseGamma Prior:

$$\xi|\alpha \sim \mathcal{N}(0, diag(\alpha^{-1}))$$
$$\alpha \sim Gamma(k, \theta)$$

$$\int p(\xi|\alpha)\, p(\alpha)\, d\alpha$$

True Prior = Student's T:

Final remark on sparsifying priors VS Bayesian evidence

- Selecting model by Bayesian evidence is to formally think about

$$P(\mathcal{M}_i|D) = P(D|\mathcal{M}_i)P(\mathcal{M}_i)$$

  - FORMAL!
  - Fundamentally Bayesian, Fundamentally probabilistic
  - Can deal with heterogeneous datasets (parameters are marginalised out)

- Sparsifying (selecting) model by sparsifying prior
  - Rooted in “regression” typed problem
  - (not as) formal
  - More popular (because they’re “faster”?)

Tutorial: 1D Polynomial Regression

Data Generation

- Generate {x,y} data pair from some randomly selected sum of polynomial terms
- Add Gaussian noise to y with known variance σ^2

Regression

- Perform linear regression (Frequentist: OLS; Bayesian: Ridge) on a polynomial library
- Find Evidence
- Remove terms in the library and redo regression; Find the combination of terms (model) that give max evidence

Experimentation

- How does changing σ^2 in the input of the regression changes the model selection?
  - How does that correspond to the intuition of Occam Razor?
- How can one further optimise the prior variance (a hyperparameter)?