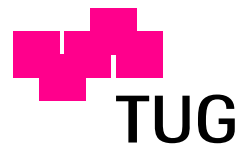


Evidence maximisation, α marginalisation, priors

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Talk overview

- Introduction, maximum likelihood estimation (MLE)
- MLE → Bayesian-, MAP-estimate
- Bayesian estimation, regularisation
- Hierarchical Bayesian models
- Approximative scheme: α -marginalisation
- Approximative scheme: Evidence procedure
- Illustrative example (Mathematica)
- Automatic relevance determination
- Priors
- Conclusion

MLE review through example [1|5]

Suppose one measures a noisy output z of a functional relation $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $y = f(\mathbf{x})$. We assume:

$$z = y + \epsilon$$

Goal: reconstruct the functional relation from $\{\mathbf{x}, z\}$

Synonyms: interpolation, nonlinear regression, supervised learning

Ansatz for $f(\mathbf{x})$ (no model mismatch):

$$y = \hat{f}(\mathbf{x}, \mathbf{w}) = \sum_{i=1}^{M-1} w_i K(\mathbf{c}_i, \mathbf{x}) + w_0$$

MLE review through example [2|5]

Why this model class?

AREAS OF APPLICATION:

- Straight line fitting, curve fitting
- Multivariate linear regression
- Discrete-time integral models (e.g. FIR)
- Kernel regression methods (e.g. RBF networks)
- Regression using orthogonal functions

MLE review through example [3|5]

Assume Gaussian noise

$\epsilon \sim \mathcal{N}(0, \sigma^2)$ with σ^2 known

$$p(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(z - y)^2}{2\sigma^2}\right]$$

Likelihood function

$$l(\mathbf{w}|z) \equiv p(z|\mathbf{w}) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(z - \hat{f}(\mathbf{x}, \mathbf{w}))^2}{2\sigma^2}\right]$$

MLE review through example [4|5]

More measurements $\{\mathbf{x}_i, z_i\}_{k=1}^N$,

White noise:

$$p(z_1, \dots, z_N | \mathbf{w}) = \prod_{i=1}^N p(z_i | \mathbf{w})$$

Thus

$$p(\mathbf{z} | \mathbf{w}) = (2\pi\sigma^2)^{-\frac{N}{2}} \exp \left[-\frac{\sum_{i=1}^N (z_i - \hat{f}(\mathbf{x}_i, \mathbf{w}))^2}{2\sigma^2} \right]$$

MLE:

$$\hat{\mathbf{w}} = \underset{\mathbf{w}}{\operatorname{argmax}} p(\mathbf{z} | \mathbf{w}) = \underset{\mathbf{w}}{\operatorname{argmin}} (-\ln p(\mathbf{z} | \mathbf{w}))$$

MLE review through example [5|5]

Linear problem:

$$\hat{w} = \underset{w}{\operatorname{argmin}} \|z - \Phi w\|^2 \text{ with } \Phi \in \mathbb{R}^{N \times M}$$

Maximum likelihood estimate:

$$\hat{w}_{MLE} = (\Phi^T \Phi)^{-1} \Phi^T z$$

MLE → Bayes, MAP [1|3]

$$p(\mathbf{z}|\mathbf{w}) = \frac{p(\mathbf{z}, \mathbf{w})}{p(\mathbf{w})} = \frac{p(\mathbf{w}|\mathbf{z})p(\mathbf{z})}{p(\mathbf{w})}$$

Thus

$$p(\mathbf{w}|\mathbf{z}) = \frac{p(\mathbf{z}|\mathbf{w})p(\mathbf{w})}{p(\mathbf{z})}$$

Posterior \propto Likelihood \times Prior

Bayesian estimate:

$$\hat{\mathbf{w}} = \mathbb{E}_{\mathbf{w}|\mathbf{z}}[\mathbf{w}] = \int_{\mathbf{w}} \mathbf{w}p(\mathbf{w}|\mathbf{z})d\mathbf{w}$$

MLE → Bayes, MAP [2|3]

When does a posteriori and likelihood coincide?

$$p(\mathbf{w}|\mathbf{z}) = p(\mathbf{z}|\mathbf{w}) \text{ if } p(\mathbf{w})/p(\mathbf{z}) = 1$$

- $p(\mathbf{z})$ is not a function of w thus $p(\mathbf{w}) = \text{const.}$
- flat prior distribution → no preferences

What is MAP ?

Maximum a posteriori estimate:

$$\hat{\mathbf{w}}_{MAP} = \underset{\mathbf{w}}{\operatorname{argmax}} p(\mathbf{w}|\mathbf{z})$$

MLE → Bayes, MAP [3|3]

When does a posteriori estimate and MAP coincide?

$p(\mathbf{w}|\mathbf{z})$ is unimodal and symmetric

When does a posteriori estimate and MLE coincide?

flat prior + $p(\mathbf{w}|\mathbf{z})$ is unimodal and symmetric

Our first Bayesian model [1|5]

$$p(\mathbf{w}|\mathbf{z}) = \frac{p(\mathbf{z}|\mathbf{w})p(\mathbf{w})}{\int_{\mathcal{W}} p(\mathbf{z}|\mathbf{w})p(\mathbf{w})d\mathbf{w}}$$

All we need is to specify a prior $p(\mathbf{w})$

One choice:

$$p(\mathbf{w}) = (2\pi/\alpha)^{-\frac{M}{2}} \exp\left(-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right)$$

α is a known and fixed parameter

Our first Bayesian model [2|5]

How to compute the posterior $p(\mathbf{w}|\mathbf{z})$?

Can we do the normalisation integral? (Yes, but ...)

$$\int_{\mathbf{w}} p(\mathbf{z}|\mathbf{w})p(\mathbf{w})d\mathbf{w} = C \int_{\mathbb{R}^M} \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{z} - \Phi\mathbf{w}\|^2 - \frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right) d\mathbf{w}$$

First check the integrand. **What is the minimiser of**

$$\frac{1}{2\sigma^2}(\mathbf{z} - \Phi\mathbf{w})^T(\mathbf{z} - \Phi\mathbf{w}) + \frac{\alpha}{2}\mathbf{w}^T\mathbf{w}$$

$$\frac{\partial}{\partial \mathbf{w}} : \quad -\frac{1}{\sigma^2}\Phi^T(\mathbf{z} - \Phi\mathbf{w}) + \alpha\mathbf{w}$$

Our first Bayesian model [3|5]

STILL: How to compute the posterior $p(\mathbf{w}|\mathbf{z})$?

$$\underbrace{(\Phi^T \Phi + \alpha \sigma^2 \mathbf{I})}_{\equiv \Sigma} \mathbf{w}_m = \Phi^T \mathbf{z}$$

$$\mathbf{w}_m = (\Phi^T \Phi + \alpha \sigma^2 \mathbf{I})^{-1} \Phi^T \mathbf{z}$$

We now try to rewrite the exponent of the integrand

$$\frac{1}{2\sigma^2} (\mathbf{z} - \Phi \mathbf{w})^T (\mathbf{z} - \Phi \mathbf{w}) + \frac{\alpha}{2} \mathbf{w}^T \mathbf{w}$$

$$\frac{1}{2\sigma^2} (\mathbf{z}^T \mathbf{z} - 2\mathbf{w}^T \Phi^T \mathbf{z} + \mathbf{w}^T \Phi^T \Phi \mathbf{w}) + \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} + \frac{1}{2\sigma^2} \mathbf{w}_m^T \Sigma \mathbf{w}_m - \frac{1}{2\sigma^2} \mathbf{w}_m^T \Sigma \mathbf{w}$$

Our first Bayesian model [4|5]

STILL: How to compute the posterior $p(\mathbf{w}|\mathbf{z})$?

$$\frac{1}{2\sigma^2}(\mathbf{z} - \Phi\mathbf{w})^T(\mathbf{z} - \Phi\mathbf{w}) + \frac{\alpha}{2}\mathbf{w}^T\mathbf{w}$$

can be written as

$$\frac{1}{2\sigma^2}(\mathbf{z}^T\mathbf{z} - \mathbf{w}_m^T\Sigma\mathbf{w}_m) + \frac{1}{2\sigma^2}(\mathbf{w} - \mathbf{w}_m)^T\Sigma(\mathbf{w} - \mathbf{w}_m)$$

Thus

$$p(\mathbf{w}|\mathbf{z}) \propto p(\mathbf{z}|\mathbf{w})p(\mathbf{w}) \propto \exp\left(-\frac{1}{2\sigma^2}(\mathbf{w} - \mathbf{w}_m)^T\Sigma(\mathbf{w} - \mathbf{w}_m)\right)$$

Our first Bayesian model [5|5]

STILL: How to compute the posterior $p(\mathbf{w}|\mathbf{z})$?

$$p(\mathbf{w}|\mathbf{z}) \propto \exp\left(-\frac{1}{2\sigma^2}(\mathbf{w} - \mathbf{w}_m)^T \Sigma (\mathbf{w} - \mathbf{w}_m)\right)$$

- Multivariate Gaussian with covariance Σ^{-1}
- Centered at \mathbf{w}_m thus $\mathbf{w}_m \equiv \mathbf{w}_{MAP}$
- and $E_{\mathbf{w}|\mathbf{z}}[\mathbf{w}] = \int_{\mathcal{W}} \mathbf{w} p(\mathbf{w}|\mathbf{z}) d\mathbf{w} \equiv \mathbf{w}_{MAP}$

What to take home?

The regularised linear least squares problem (Tikhonov)

$$\min_{\mathbf{w}} \{ \|\mathbf{z} - \Phi\mathbf{w}\|^2 + \lambda\|\mathbf{w}\|^2 \}$$

with the solution

$$\hat{\mathbf{w}} = (\Phi^T\Phi + \lambda\mathbf{I})^{-1}\Phi^T\mathbf{z}$$

can be seen as the Bayesian problem with Gaussian likelihood and Gaussian prior, where $\lambda = \alpha\sigma^2$.

Extending our model [1|4]

What if we do not know σ^2 and α ?

Bayesian answer: define prior distributions $p(\sigma^2)$, $p(\alpha)$

Our old w -prior

$$p(\mathbf{w}) = (2\pi/\alpha)^{-\frac{M}{2}} \exp\left(-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right)$$

gets

$$p(\mathbf{w}|\alpha) = (2\pi/\alpha)^{-\frac{M}{2}} \exp\left(-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right)$$

and

$$p(\mathbf{w}, \alpha) = p(\mathbf{w}|\alpha)p(\alpha)$$

Extending our model [2|4]

Marginalisation of $p(\mathbf{w}, \alpha)$ with respect to α is our new \mathbf{w} -prior

$$p(\mathbf{w}) = \int p(\mathbf{w}|\alpha)p(\alpha)d\alpha$$

What about the noise variance σ^2 ?

The old likelihood function $p(\mathbf{z}|\mathbf{w})$ gets

$$p(\mathbf{z}|\mathbf{w}, \sigma^2)$$

and

$$p(\mathbf{z}, \sigma^2|\mathbf{w}) = p(\mathbf{z}|\mathbf{w}, \sigma^2)p(\sigma^2)$$

Extending our model [3|4]

Marginalisation of $p(\mathbf{z}, \sigma^2 | \mathbf{w})$ with respect to σ^2 is our new likelihood

$$p(\mathbf{z} | \mathbf{w}) = \int p(\mathbf{z} | \mathbf{w}, \sigma^2) p(\sigma^2) d\sigma^2$$

The posterior computes again to

$$p(\mathbf{w} | \mathbf{z}) = \frac{p(\mathbf{z} | \mathbf{w}) p(\mathbf{w})}{\int_{\mathcal{W}} p(\mathbf{z} | \mathbf{w}) p(\mathbf{w}) d\mathbf{w}}$$

where likelihood and w -prior are in general non-Gaussian.

THE POSTERIOR IS IN GENERAL NOT GAUSSIAN

Even if can find the posterior analytically we have to compute

$$E_{\mathbf{w} | \mathbf{z}}[\mathbf{w}]$$

Extending our model [4|4]

INTERMEDIATE SUMMARY: Perfect Bayesian estimation

- Define a likelihood function from the model with a parameter σ^2 ("hyperparameter", "nuisance-parameter")
- Define a prior over weights with the hyperparameter α
- Integrate over σ^2 to get the actual likelihood
- Integrate over α to get the actual prior
- Compute the normalisation integral of likelihood \times prior
- Get the posterior
- Compute the expectation for weights $\hat{w} = E_{w|z}[w]$

MODELS WITH HYPERPRIORS: HIERARCHICAL BAYES

Approximate Solutions [1|2]

Suppose we choose this new $p(\alpha)$ and $p(\sigma^2)$ such that

- we can do the integrals for true likelihood and w -prior
- we can find the posteriori analytically
- we can not integrate the posterior for $E_{w|z}[w]$

One Solution:

- Find w_{MAP} s for posterior $p(w|z)$ (in general multimodal)
- approximate at each w_{MAP} a Gaussian
- decide heuristically which one is right

[Buntine, Weigend 1994] ("MAP method" for further reference)

" α -marginalisation approximation"

Approximate Solutions [2|2]

Disadvantages of MAP method:

- Always goes for the peak
- Does not care about the probability mass
- This discrepancy gets amplified for high dimensions of w -space. (usual)

DIFFERENT APPROACH:

"Evidence procedure", "type II maximum likelihood"

- Find good values for σ^2 and α
- Freeze values of the hyperparameters
- Posterior is given by our first simple model: **GAUSSIAN**
- How: Maximise the evidence of the hyperparameters given the data: $\max_{\alpha, \sigma^2} p(\alpha, \sigma^2 | \mathbf{z})$

The Evidence procedure [1|8]

Expand the posterior

$$\begin{aligned} p(\mathbf{w}|\mathbf{z}, \alpha, \sigma^2) &= \frac{p(\mathbf{w}, \mathbf{z}, \alpha, \sigma^2)}{p(\mathbf{z}, \alpha, \sigma^2)} = \frac{p(\mathbf{z}|\mathbf{w}, \alpha, \sigma^2)p(\mathbf{w}, \alpha, \sigma^2)}{p(\mathbf{z}|\alpha, \sigma^2)p(\alpha, \sigma^2)} \\ &= \frac{p(\mathbf{z}|\mathbf{w}, \alpha, \sigma^2)p(\mathbf{w}|\alpha, \sigma^2)p(\alpha, \sigma^2)}{p(\mathbf{z}|\alpha, \sigma^2)p(\alpha, \sigma^2)} = \frac{p(\mathbf{z}|\mathbf{w}, \sigma^2)p(\mathbf{w}|\alpha)}{p(\mathbf{z}|\alpha, \sigma^2)} \end{aligned}$$

Suppose the evidence procedure gives us values α_{ev} and σ_{ev}^2 :
The posterior is then given

$$p(\mathbf{w}|\mathbf{z}, \alpha_{ev}, \sigma_{ev}^2) = \frac{p(\mathbf{z}|\mathbf{w}, \sigma_{ev}^2)p(\mathbf{w}|\alpha_{ev})}{p(\mathbf{z}|\alpha_{ev}, \sigma_{ev}^2)}$$

How does it relate to the correct posterior, with marginalised hyperparameters?

The Evidence procedure [2|8]

How does it relate to the correct posterior, with marginalised hyperparameters?

Consider the marginalisation:

$$p(\mathbf{w}, \mathbf{z}) = \int p(\mathbf{w}, \mathbf{z}, \alpha, \sigma^2) d\alpha d\sigma^2$$

then

$$\begin{aligned} p(\mathbf{w}|\mathbf{z}) &= \frac{1}{p(\mathbf{z})} \int p(\mathbf{w}|\mathbf{z}, \alpha, \sigma^2) p(\mathbf{z}, \alpha, \sigma^2) d\alpha d\sigma^2 \\ &= \frac{1}{p(\mathbf{z})} \int p(\mathbf{w}|\mathbf{z}, \alpha, \sigma^2) p(\alpha, \sigma^2|\mathbf{z}) p(\mathbf{z}) d\alpha d\sigma^2 \\ &= \int p(\mathbf{w}|\mathbf{z}, \alpha, \sigma^2) p(\alpha, \sigma^2|\mathbf{z}) d\alpha d\sigma^2 \end{aligned}$$

The Evidence procedure [3|8]

$p(\alpha, \sigma^2 | \mathbf{z})$ is "the evidence for α, σ^2 in the data"

If $p(\alpha, \sigma^2 | \mathbf{z})$ is peaked at $\alpha_{ev}, \sigma_{ev}^2$ (ideally $\delta(\alpha_{ev}, \sigma_{ev}^2)$)

$$p(\mathbf{w} | \mathbf{z}) \approx p(\mathbf{w} | \mathbf{z}, \alpha_{ev}, \sigma_{ev}^2)$$

How to find the peak of $p(\alpha, \sigma^2 | \mathbf{z})$ for our model?

$$p(\alpha, \sigma^2 | \mathbf{z}) \propto p(\mathbf{z} | \alpha, \sigma^2) p(\alpha) p(\sigma^2)$$

If we assume flat hyperpriors we only have to find the maximum of

$$p(\mathbf{z} | \alpha, \sigma^2) = \int_{\mathbf{w}} p(\mathbf{z} | \mathbf{w}, \sigma^2) p(\mathbf{w} | \alpha) d\mathbf{w}$$

The Evidence procedure [4|8]

I have seen you around...

$$p(\mathbf{z}|\mathbf{w}, \sigma^2) = (2\pi\sigma^2)^{-\frac{N}{2}} \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{z} - \Phi\mathbf{w}\|^2\right)$$

and

$$p(\mathbf{w}|\alpha) = (2\pi/\alpha)^{-\frac{M}{2}} \exp\left(-\frac{\alpha}{2}\mathbf{w}^T\mathbf{w}\right)$$

That is just the normalisation integral of the simple model!
(fixed α, σ^2)

$$p(\mathbf{z}|\mathbf{w}, \sigma^2)p(\mathbf{w}|\alpha) = \frac{1}{C} e^{-\frac{1}{2\sigma^2}(\mathbf{z}^T\mathbf{z} - \mathbf{w}_m^T\mathbf{\Sigma}\mathbf{w}_m + (\mathbf{w} - \mathbf{w}_m)^T\mathbf{\Sigma}(\mathbf{w} - \mathbf{w}_m))}$$

The Evidence procedure [5|8]

With the integral for multivariate Gaussian

$$\int_{\mathbb{R}^k} \exp\left(-\frac{1}{2}\mathbf{w}^T \mathbf{B}\mathbf{w}\right) d\mathbf{w} = (2\pi)^{k/2} \frac{1}{\sqrt{|\mathbf{B}|}}$$

The "evidence integral", or "marginal likelihood" $p(\mathbf{z}|\alpha, \sigma^2)$ reads,

$$\int_{\mathbf{w}} p(\mathbf{z}|\mathbf{w}, \sigma^2) p(\mathbf{w}|\alpha) d\mathbf{w} = \frac{1}{C' \sqrt{|\Sigma|}} \exp\left[-\frac{1}{2\sigma^2}(\mathbf{z}^T \mathbf{z} - \mathbf{w}_m \Sigma \mathbf{w}_m)\right]$$

$$\{\alpha_{ev}, \sigma_{ev}^2\} = \underset{\alpha, \sigma^2}{\operatorname{argmax}} p(\mathbf{z}|\alpha, \sigma^2) = \underset{\alpha, \sigma^2}{\operatorname{argmax}} (\ln(p(\mathbf{z}|\alpha, \sigma^2)))$$

The Evidence procedure [6|8]

No explicit solution for

$$\{\alpha_{ev}, \sigma_{ev}^2\} = \operatorname{argmax}_{\alpha, \sigma^2} p(\mathbf{z} | \alpha, \sigma^2)$$

found but implicit expression can be used for re-estimation of the form

$$\alpha_{new} = g(\mathbf{w}_m, \alpha_{old}) \quad \text{and} \quad \sigma_{new}^2 = h(\mathbf{w}_m, \sigma_{old}^2)$$

As $\mathbf{w}_m = \Sigma^{-1}(\alpha, \sigma^2) \Phi^T \mathbf{z}$:

Concurrently update of $\{\alpha, \sigma^2\}$ and $\{\Sigma, \mathbf{w}_m\}$

The Evidence procedure [7|8]

SUMMARY OF EVIDENCE PROCEDURE

- It is an approximation to the true posterior. Works good if $p(\alpha, \sigma^2 | z)$ has a clear peak
- The hyperparameter are fixed to the most probable values given the data
- For Gaussian likelihood + w -prior and flat hyperpriors
 - ◇ efficient iterative scheme for $\{\alpha_{ev}, \sigma_{ev}^2\}$ (convergence to a local maximum of $p(z | \alpha, \sigma^2)$)
 - ◇ posterior is approximated with one Gaussian

[Mackay 1992]

The Evidence procedure [8|8]

Illustration, simple example

Extending evidence procedure [1|2]

AUTOMATIC RELEVANCE DETERMINATION

Introduce weight prior

$$p(\mathbf{w}|\boldsymbol{\alpha}) = \left[(2\pi)^{-\frac{M}{2}} \prod_{i=0}^M \alpha_i \right] \exp\left(-\frac{1}{2} \sum_{i=0}^M \alpha_i w_i^2\right)$$

Each weight gets a hyperparameter controlling its variance

What if one $\alpha_k \rightarrow \infty$ through applying evidence update rule?:

The weight w_k is centered at zero with variance $\rightarrow 0$

$\rightarrow w_k$ can be removed from the model!

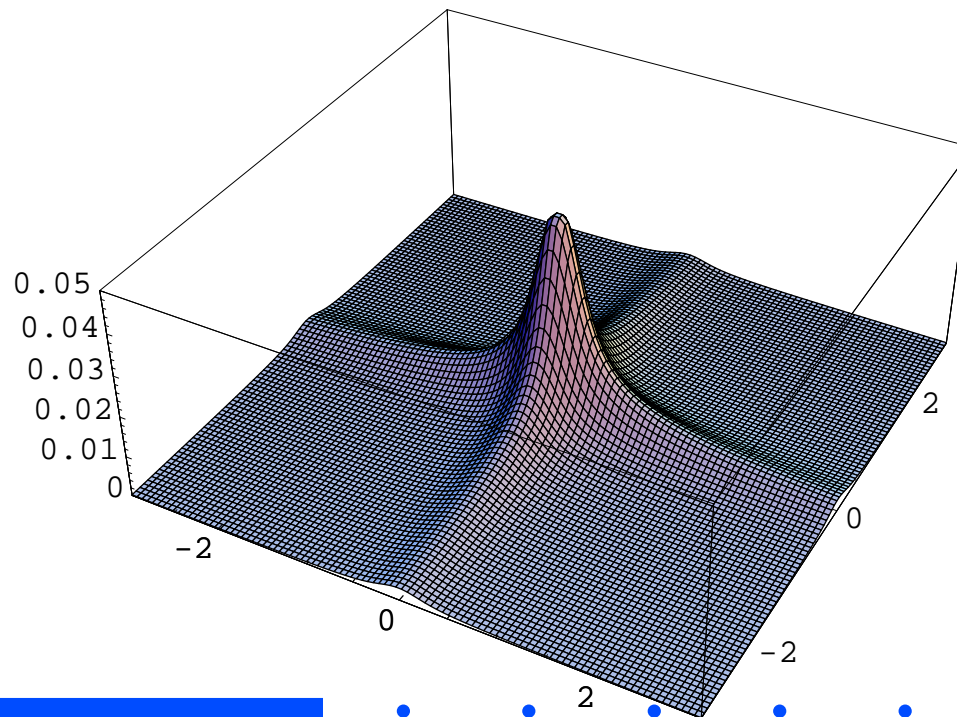
GENERATION OF HIGHLY SPARSE MODELS

[Mackay 1994, Neal 1996, Tipping 2001]

Extending evidence procedure [2|2]

What's the real w -prior (noninformative $p(\alpha)$ + Gaussian $p(w|\alpha)$)?

$$p(w) = \int_{D(\alpha)} p(w|\alpha)p(\alpha)d\alpha$$



Priors

- Noninformative Priors
- Improper Priors
- Invariance under group action
- Conjugate priors
- Maximum entropy priors

Conclusion

- Overview of MLE, Bayes, MAP for linear models
- Simple Bayesian models
- Hierarchical Bayesian models
- Approximative schemes
 - ◇ " α -marginalisation approximation"
 - ◇ Evidence procedure
- Automatic relevance determination