VE414 Lecture 7

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- You should have noticed that the following is indispensable

$$\text{Posterior} \propto \text{Likelihood} \times \text{Prior}$$

- However, to obtain any posterior, in addition to identifying a likelihood to model the data generating process, and choosing a prior for the unknown, we need to "normalise" the product of the two to have the posterior.
- So far, the only way we can obtain the posterior is to use a conjugate prior, any other prior in general will very likely lead us to an expression

$$\text{Likelihood} \times \text{Prior}$$

that cannot be integrated analytically, e.g

$$f_{Y|X} \propto \exp\left(-\frac{(x-y)^2}{2}\right) \times \frac{1}{1+y^2}$$

- Often only the posterior up to an multiplicative constant is readily available.

- In terms of point estimates, having only the posterior

$$\text{Posterior} \propto \text{Likelihood} \times \text{Prior}$$

up to an multiplicative constant means we will not have the mean in general.

Q: What should we do if a point estimate is required?

- If a point estimate is required, we could use the mode instead of the mean.

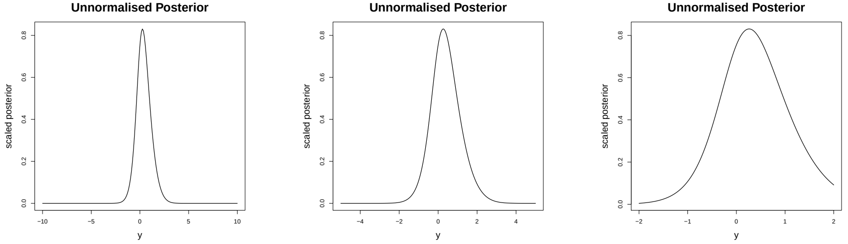
$$\arg\max_y f_{Y|X}(y \mid x)$$

Q: Why will we be able to avoid the integral in this case?

$$\hat{y}_{MAP} = \arg\max_y f_{Y|X}(y \mid x) = \arg\max_y f_{X|Y}(x \mid y) f_Y(y)$$

- The optimisation is easier than the integration, especially in high dimension.

- For univariate optimisation, it is always a good idea to plot the function.
- The posterior is not available, but the unnormalised posterior can provide



information on where the posterior peaks and how quickly it drops towards 0.

- In this case, we could simply start with a small interval, say

$$[-1, 1]$$

and use a reliable optimisation method to find where the peak is.

- Julia has a large number of optimisation algorithms, the following package

```
julia> using Pkg
julia> Pkg.add("Optim")
```

is sufficient for us.

- Load the package **Optim** into the current session,

```
julia> using Optim
```

- Let us solve for $x = 0.75$, and set the lower and upper bound,

```
julia> x = 0.75; lower = -1; upper = 1;
```

- Define the objective function, which is simply the negative of our integrand,

```
julia> un_posterior(y) = -exp(-(x-y)^2/2)/(1+y^2)
```

```
un_posterior (generic function with 1 method)
```

```
julia> ymap = optimize(un_posterior,
           lower, upper, GoldenSection())
```

```
Results of Optimization Algorithm
 * Algorithm: Golden Section Search
 * Search Interval: [-1.000000, 1.000000]
 * Minimizer: 2.611106e-01
 * Minimum: -8.307208e-01
 * Iterations: 40
 * Convergence:
 max(|x-x_upper|,|x-x_lower|) <=
 2*(1.5e-08*|x|+2.2e-16) :true
```

- Numerical optimisation will not be covered in this course, but you should know it is easier than numerical integration, especially so in high dimension.

Q: Does that mean we can always avoid the integral?

Q: How should we deal with the integral when the MAP estimate is not ideal?

- The easiest way to obtain a rough idea $f_{Y|X}$ without analytically computing

$$\int_{-\infty}^{\infty} f_{X|Y}(x \mid y) f_Y(y)\, dy$$

is to use a grid approximation, in which the integral is approximated by

$$\int_{-\infty}^{\infty} f_{X|Y}(x \mid y) f_Y(y)\, dy \approx \frac{b-a}{n} \sum_{i=1}^{n} f_{X|Y}(x \mid y_i) f_Y(y_i)$$

where y_is are equally spaced values over the support $[a, b]$

- Consider the following model with $X_3 = 2$ again,

$$\begin{aligned} P &\sim \text{Uniform}\,(0,1) \\ X_k \mid P &\sim \text{Binomial}\,(k,p) \\ \Longrightarrow\ P \mid X_3 = 2 &\sim \text{Beta}\,(3,2) \end{aligned}$$

- If you are Bayes, the integral that you have to deal with is

$$\int_0^1 \binom{3}{2} p^2 (1-p)^1 \cdot 1 \, dp$$

- In this case, we actually can work out the exact normalising constant easily

$$A = \binom{3}{2} \int_0^1 p^2 (1-p)^1 \cdot 1 \, dp = \binom{3}{2} \frac{1}{12}$$

- So the exact posterior is given by

$$f_{P|X_3=2}(p \mid 2) = 12p^2(1-P) \qquad \text{for} \quad p \in [0,1]$$

- Let us see how well a grid approximation performs

```
julia> range(0, length=6, stop=1)
```

```
0.0:0.2:1.0
```

- Put the last answer, which is a range object of the grid values, into an array

```
julia> p_grid = collect(ans[2:6])
```

```
5-element Array{Float64,1}:
 0.2
 0.4
 0.6
 0.8
 1.0
```

- Assume uniform prior

```
julia> prior = fill(1, 5)
```

```
5-element Array{Int64,1}:
 1
 1
 1
 1
 1
```

- Initialise an array for likelihood

```
julia> likelihood = Array{Float64, 1}(undef, 5);
```

- You need the next two lines only if you haven't installed **Distributions**

```
julia> using Pkg
julia> Pkg.add("Distributions")
```

- Load the package **Distributions**

```
julia> using Distributions
```

- Compute the likelihood at each point in the grid

```
julia> k = 3; x = 2;
julia> for i in 1:1:5
           p = p_grid[i];
           d = Binomial(k, p);
           likelihood[i] = pdf(d, x);
       end
```

- Compute the product of likelihood and prior

```
julia> unnormalised_posterior = likelihood .* prior
```

```
5-element Array{Float64,1}:
 0.09600000000000002
 0.2880000000000014
 0.43199999999999994
 0.384
 0.0
```

- Normalising constant

```
julia> A = (1-0) * sum(unnormalised_posterior) / 5
```

```
0.24000000000000005
```

- Posterior Values

```
julia> posterior = unnormalised_posterior / A;
```

- We expect our approximation on the normalising constant to improve

```
julia> A
0.24000000000000005
```

when the number of points in the grid increases, we have 5 points currently.

- With 10 points, we have

```
julia> A
0.2475
```

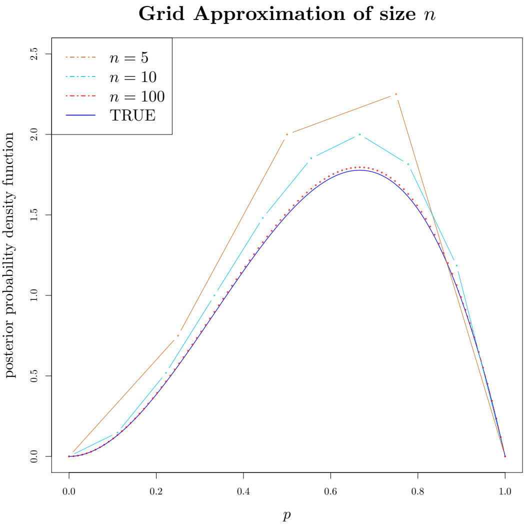
- With 100 points, we have

```
julia> A
0.24997500000000003
```

- With 10000 points, we have

```
julia> A
0.24999999997500003
```

- The approximation seems to be reasonably good when n reaches 100.



- Now consider the following case again,

$$f_{Y|X} \propto \exp\left(-\frac{(x-y)^2}{2}\right) \times \frac{1}{1+y^2}$$

which requires to compute the following integral to obtain the posterior

$$A = \int_{-\infty}^{\infty} \exp\left(-\frac{(x-y)^2}{2}\right) \times \frac{1}{1+y^2}\, dy$$

Q: Do you see an issue of using a grid approximation in this case?

- We could resolve it by splitting the integral and transforming y

$$\begin{aligned} A = &\int_{-\infty}^{c} \exp\left(-\frac{(x-y)^2}{2}\right) \times \frac{1}{1+y^2}\, dy \qquad \text{for some } c \in \mathbb{R}. \\ &+ \int_{c}^{\infty} \exp\left(-\frac{(x-y)^2}{2}\right) \times \frac{1}{1+y^2}\, dy \end{aligned}$$

so that we only have to deal with integrals over a finite interval.

- That is, we have to choose some c value and find two transformations,

$$u = g(y) \implies y = g^{-1}(u) \qquad \text{and} \qquad v = h(y) \implies y = h^{-1}(v)$$

one for each of the followings

$$A_1 = \int_{-\infty}^{c} f(y)\,dy \qquad \text{and} \qquad A_2 = \int_{c}^{\infty} f(y)\,dy$$

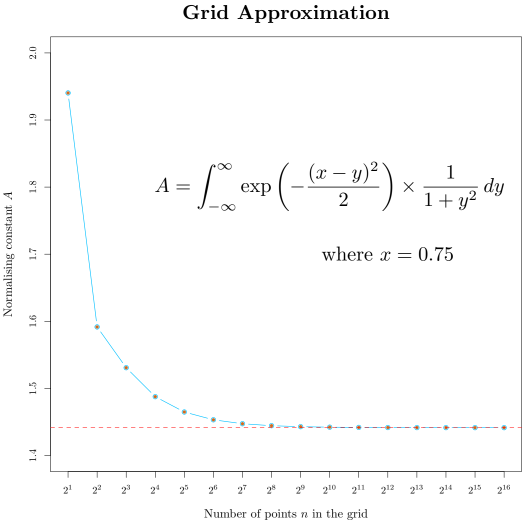
so that the two integrals are replaced by

$$A_1 = \int_a^b \left(\frac{f}{g'}\right) \circ g^{-1}(u)\,du \qquad \text{and} \qquad A_2 = \int_d^e \left(\frac{f}{h'}\right) \circ h^{-1}(v)\,dv$$

where a, b, c and d are finite

$$\begin{aligned} b &= g(c) \\ a &= \lim_{y\to-\infty} g(y) \end{aligned} \qquad \text{and} \qquad \begin{aligned} e &= \lim_{y\to\infty} h(y) \\ d &= h(c) \end{aligned}$$

- The approximation seems to be reasonably good when n reaches $2^{10} = 1024$.



Q: Can we do better than a simple grid approximation?

- A simple grid approximation can be understood as a weighted sum

$$\int_a^b f(x)\,dx \approx \frac{b-a}{n}\sum_{i=1}^{n} f(x_i) = \sum_{i=1}^{n} w_i f(x_i)$$

  where the weight is chosen to be the same

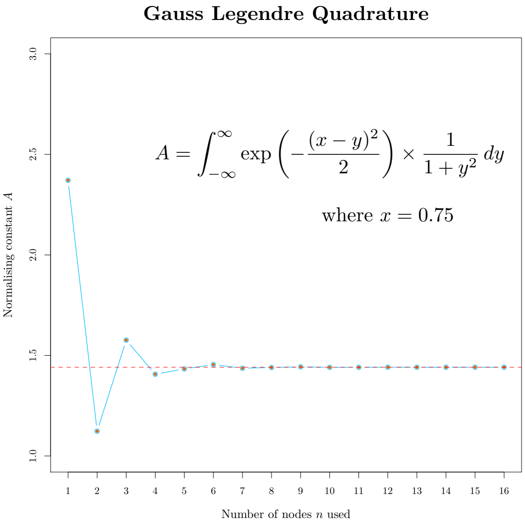
$$w_i = \frac{b-a}{n}$$

  and the points x_is are chosen to be equally spaced.

- Gaussian quadrature chooses the points for evaluation in an optimal, rather than equally spaced, way. The points, x_i, which are known as nodes, are chosen along with the weights w_i to minimise the error in general obtained in

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} w_i f(x_i)$$

- Pay attention to the scale in x-axis, Gauss has a lot to offer as usual!

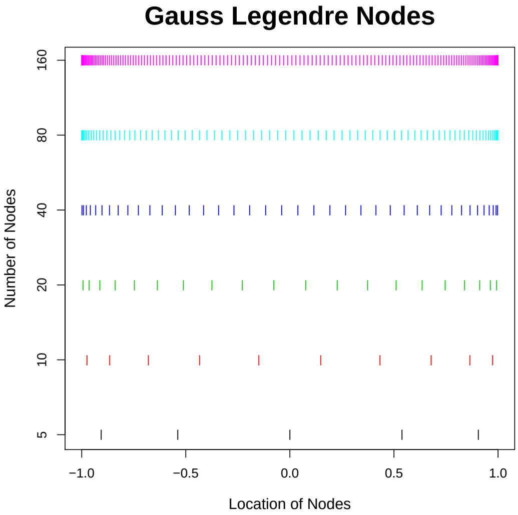


- Just like optimisation, quadrature in detail will not be covered in this course, but you need know Julia can find the nodes and weights for you easily.

```
julia> using FastGaussQuadrature
julia> # You need to install it if you have not

julia> x = 0.75; n = 5; # Number of nodes

julia> nodes, weights = gausslegendre(n);

julia> nodes
```

```
5-element Array{Float64,1}:
 -0.906179845938664
 -0.538469310105683
  0.0
  0.538469310105683
  0.906179845938664
```

- Note Gauss put more nodes near the ends, there is more than luck in play.



- Neither nodes nor weights depend on the integrand.

```
julia> weights
```

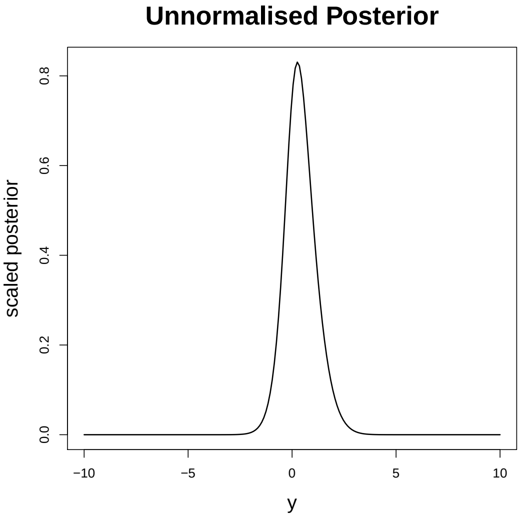
```
5-element Array{Float64,1}:
 0.2369268850561890B
 0.47862867049936647
 0.5688888888888889
 0.47862867049936647
 0.23692688505618908
```

```
julia> u_integrand = Array{Float64, 1}(undef, n);

julia> for i in 1:1:n
           u = nodes[i];
           ginv = (u-1)/(u+1);
           logscale = log(1/2) + 2*log(1-ginv) -
               (x-ginv)^2/2 - log(1+ginv^2);
           u_integrand[i] = exp(logscale);
       end
```

```
julia> v_integrand = Array{Float64, 1}(undef, n);

julia> for i in 1:1:n
           v = nodes[i];
           hinv = (1-v)/(1+v);
           logscale = log(1/2) + 2*log(1+hinv) -
               (x-hinv)^2/2 - log(1+hinv^2);
           v_integrand[i] = exp(logscale);
       end

julia> A1 = sum(weights.*u_integrand);

julia> A2 = sum(weights.*v_integrand);

julia> A = A1 + A2
```

```
1.4331167574845127
```

Q: What can we do without Julia? What would you do if you were Laplace?



- Laplace noticed three things that are common in a lot of the problems:
  1. Posterior is smooth and unimodal, or at least well separated modes.
  2. Has a strictly positive second derivative at its modal value $\hat{y}_{MAP}$.
  3. The integrand peaks sharply around $\hat{y}_{MAP}$ when there is enough data.
- In general, suppose the integral we have to compute is in the following form

$$I(s) = \int_{-\infty}^{\infty} \exp\left(-sh(y)\right)\, dy$$

and $s \to \infty$ as the number of data $\to \infty$, for example,

$$\mathcal{L}\left(\mu; \bar{x}, \sigma^2\right) \propto \exp\left(-\frac{\left(\bar{x}-\mu\right)^2}{2\left(\sigma/\sqrt{n}\right)^2}\right) = \exp\left(-\frac{1}{2\left(\sigma/\sqrt{n}\right)^2}\left(\bar{x}-\mu\right)^2\right)$$

- That is, it is going to be a method when we have sufficiently large dataset.

- Suppose $h(y)$ is sufficiently smooth so that Taylor's theorem is applicable,

$$h(y) \approx h(\hat{y}) + \frac{1}{2}h''(\hat{y})(y-\hat{y})^2 + \frac{1}{6}h^{(3)}(\hat{y})(y-\hat{y})^3 + \frac{1}{24}h^{(4)}(\hat{y})(y-\hat{y})^4$$

  where $\hat{y}$ denotes the MAP estimate, so the 1st order derivative vanished.

- In terms of the integral, we have

$$\begin{aligned}
I(s) &= \int_{-\infty}^{\infty} \exp\left(-sh(y)\right) dy \\
&\approx \int_{-\infty}^{\infty} \exp\left[-s\left(h(\hat{y}) + \frac{1}{2}h''(\hat{y})(y-\hat{y})^2\right.\right. \\
&\qquad \left.\left. + \frac{1}{6}h^{(3)}(\hat{y})(y-\hat{y})^3 + \frac{1}{24}h^{(4)}(\hat{y})(y-\hat{y})^4\right)\right] dy \\
&= e^{-s\hat{h}} \int_{-\infty}^{\infty} e^{-s\hat{h}^{(2)}u^2/2} \exp\left(-\frac{s}{6}\hat{h}^{(3)}u^3 - \frac{s}{24}\hat{h}^{(4)}u^4\right) du
\end{aligned}$$

  where the hat denotes the function evaluated at $\hat{y}$, and $u = y - \hat{y}$.

- Invoking Taylor's again, this time on the exponential function around zero,

$$
\begin{aligned}
J(u) &= \exp\left(-\frac{s}{6}\hat{h}^{(3)}u^3 - \frac{s}{24}\hat{h}^{(4)}u^4\right) \\
&\approx 1 - \frac{s}{6}\hat{h}^{(3)}u^3 - \frac{s}{24}\hat{h}^{(4)}u^4 + \frac{1}{2}\left(\frac{s}{6}\hat{h}^{(3)}u^3 + \frac{s}{24}\right)^2 \\
&= 1 - \frac{s}{24}\hat{h}^{(4)}u^4 + \frac{s^2}{72}\left(\hat{h}^{(3)}\right)^2 u^6 + \frac{s^2}{1052}\left(\hat{h}^{(4)}\right)^2 u^8 + \text{odd powers}
\end{aligned}
$$

- Since the Gaussian function is an even function, the odd powers will vanish

$$
I(s) \approx e^{-s\hat{h}} \int_{-\infty}^{\infty} J(u) \cdot e^{-s\hat{h}^{(2)}u^2/2}\, du
$$

- The reason for using Taylor's again is to be able to use the moment formula

$$
\int_{-\infty}^{\infty} x^{2m} e^{-\alpha x^2}\, dx = \frac{2m!}{m!2^{2m}}\sqrt{\pi}\alpha^{-(m+1)/2}
$$

- Using this moment formula and setting $\sigma^2 = \frac{1}{\hat{h}^{(2)}}$, we have

$$I(s) \approx e^{-s\hat{h}}\sqrt{2\pi}\sigma s^{-1/2}\left(1 + \frac{5\sigma^6}{24s}\left(\hat{h}^{(3)}\right)^2 - \frac{\sigma^4}{8s}\hat{h}^{(4)}\right)$$

- If only the first order term in the above approximation is used

$$I(s) = \int_{-\infty}^{\infty} \exp\left(-sh(y)\right)\, dy \approx e^{-s\hat{h}}\sqrt{2\pi}\sigma s^{-1/2} \qquad \text{for a large } s$$

  then the approximation is known as Laplace approximation.

- Essentially, many posteriors can be approximated locally near the mode by a normal distribution, when we have enough data, the posterior is dominated near the mode, thus the approximation becomes better and better $s \to \infty$.

- It can be extended to high dimensional cases as well as the following case

$$I(s) = \int_{-\infty}^{\infty} g(y) \exp\left(-sh(y)\right)\, dy$$