Lecture 2 : Probabilistic computations.

The 2D pdf studied in slice, Gibbs & Hamiltonian sampling.

$$\boxed{p(x,y) \propto x^2 \exp(-xy^2 - y^2 + 2y - 4x)}.$$

$0 < x < +\infty$
$-\infty < y < +\infty$.

marginals:

$$p(x) \propto x^2 e^{-4x} \int_{-\infty}^{+\infty} e^{-y^2(x+1) + 2y}\, dy.$$

$$\boxed{p(x) \propto x^2 e^{-4x} \frac{1}{\sqrt{x+1}} e^{\frac{1}{x+1}}}$$

using $\int_{-\infty}^{+\infty} e^{-ax^2+bx+c} = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a}+c}$

$$p(y) \propto e^{-y^2+2y} \int_0^{+\infty} x^2 e^{-xy^2-4x}\, dx.$$

2 integration by parts:

$$\int_0^{+\infty} x^2 e^{-xy^2-4x} dx = \underbrace{\left[\frac{-x^2 e^{-xy^2-4x}}{y^2+4}\right]_0^{+\infty}}_{=0} + \int_0^{+\infty} 2x \frac{e^{-xy^2-4x}}{y^2+4} dx$$

$$= \left[-\frac{2x\, e^{-xy^2-4x}}{(y^2+4)^2}\right]_0^{+\infty} + 2\int_0^{+\infty} \frac{e^{-xy^2-4x}}{(y^2+4)^2} dx$$

$$= \left[-2\frac{e^{-xy^2-4x}}{(y^2+4)^3}\right]_0^{+\infty}$$

$$= \frac{2}{(y^2+4)^3}$$

(alternatively, one could have used "integration by differentiation")

$$\boxed{p(y) \propto \frac{e^{-y^2+2y}}{(y^2+4)^3}}$$

conditionals. (Gibbs sampling).

$$p(y|x) = \frac{p(x,y)}{p(x)} \propto \frac{1}{\sqrt{x+1}} \exp\left(-xy^2 - y^2 + 2y - 4x + 4x - \frac{1}{x+1}\right)$$

$$\propto \frac{1}{\sqrt{x+1}} \exp\left(-y^2(x+1) + 2y - \frac{1}{x+1}\right).$$

$$y^2(x+1) + 2y - \frac{1}{x+1} = \Big(y - \underbrace{\frac{1}{x+1}}_{\mu}\Big)^2 \underbrace{(x+1)}_{(2\sigma^2)^{-1}}$$

$$\Rightarrow \quad \boxed{f(y|x) = G\left(\mu = \frac{1}{1+x}, \ \sigma^2 = \frac{1}{2(1+x)}\right)}$$

Gaussian distribution G: $\quad f(t) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\frac{(t-\mu)^2}{\sigma^2}\right)$. $\quad \mu$: mean, σ: standard deviation

$$f(x|y) = \frac{f(x,y)}{f(y)} \propto \frac{x^2}{(y^2+4)^3} \exp\left(-xy^2 - y^2 + 2y - 4x + y^2 - 2y\right).$$

$$\propto x^2 (y^2+4)^3 \exp\left(-x(y^2+4)\right).$$

$$\Rightarrow \quad \boxed{f(x|y) = \Gamma\left(k = 3, \ \theta = y^2+4\right)}$$

Gamma distribution Γ: $\quad f(t) = \frac{1}{\Gamma(k)\theta^k} t^{k-1} e^{-\frac{t}{\theta}}$ $\quad t \geq 0$, $k > 0$: ~~shape~~, $\theta > 0$: scale.

<u>gradients</u> (for Hamiltonian sampling).

$\psi(x,y) \equiv -\ln f(x,y)$ "potential energy"

$$\boxed{\psi(x,y) = -2\ln x + xy^2 + y^2 - 2y + 4x}$$

$$\boxed{\frac{\partial \psi}{\partial x}(x,y) = -\frac{2}{x} + y^2 + 4}$$

$$\boxed{\frac{\partial \psi}{\partial y}(x,y) = 2xy + 2y - 2}$$