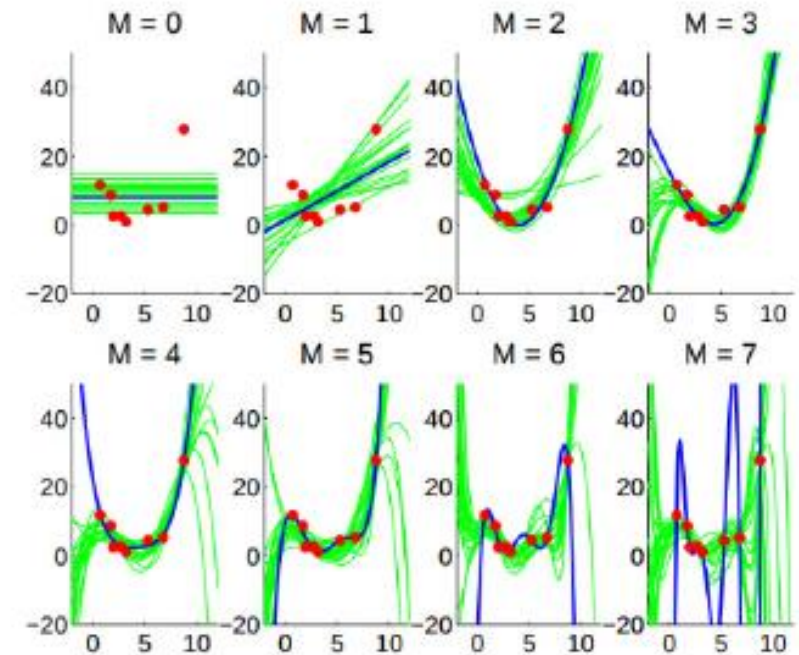
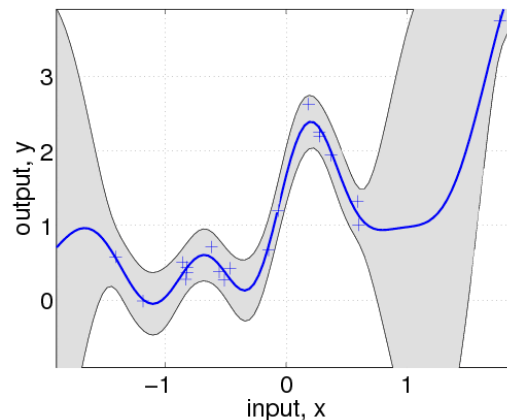


Probabilistic Bayesian Modelling

Probabilistic Model

- x – an observation (random variable/vector)
- $X = \{x_1, x_2, \dots, x_n\}$, set of observations, evidence, data
- Probabilistic model – a mathematical form which provides stochastic information about the random variable x
- θ - parameters of a model
- M – hyperparameters of a model



Modelling Goals

- Estimation (of the underlying model parameters) - $p(\theta, m | X)$
 - Understand
 - Generate new data
- Prediction - $p(x^* | \theta)$ or $p(x^* | X)$, x^* is a new observation
- Model comparison – $p(X | \theta_1) > p(X | \theta_2)$
- Solving the first goal helps solve the second and third goals

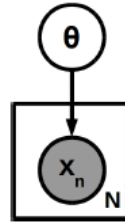
Some probabilities of interest

- **Likelihood function** $p(\mathbf{x}|\theta)$ or the “observation model” specifies how data is generated
 - Measures data fit (or “loss”) w.r.t. the given parameter θ
- **Prior distribution** $p(\theta)$ specifies how likely different parameter values are *a priori*
 - Also corresponds to imposing a “regularizer” over θ
- **Domain knowledge** can help in the specification of the likelihood and the prior

NB: We are talking about probability distributions and not single (point) probabilities

Maximum Likelihood Estimation

- Perhaps the simplest way is to find θ that makes the observed data most likely or most probable



- Formally, find θ that maximizes the probability of the observed data

$$\hat{\theta} = \arg \max_{\theta} \log p(\mathbf{X}|\theta)$$

- However, this gives a single “point” estimate of θ . Doesn't tell us about the uncertainty in θ

Rules of Probability

- Keep in mind these two simple rules of probability: sum rule and product rule

$$P(a) = \sum_b P(a, b) \quad (\text{Sum Rule})$$

$$P(a, b) = P(a)P(b|a) = P(b)P(a|b) \quad (\text{Product Rule})$$

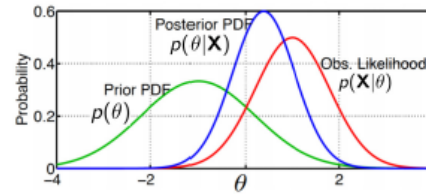
- Note: For continuous random variables, sum is replaced by integral: $P(a) = \int P(a, b)db$
- Another rule is the Bayes rule (can be easily obtained from the above two rules)

$$P(b|a) = \frac{P(b)P(a|b)}{P(a)} = \frac{P(b)P(a|b)}{\int P(a, b)db} = \frac{P(b)P(a|b)}{\int P(b)P(a|b)db}$$

Bayesian Estimation

- Can infer the parameters by computing the **posterior distribution** (Bayesian inference)

$$p(\theta|\mathbf{X}, m) = \frac{p(\mathbf{X}, \theta|m)}{p(\mathbf{X}|m)} = \frac{p(\mathbf{X}|\theta, m)p(\theta|m)}{\int p(\mathbf{X}|\theta, m)p(\theta|m)d\theta} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Marginal likelihood}}$$

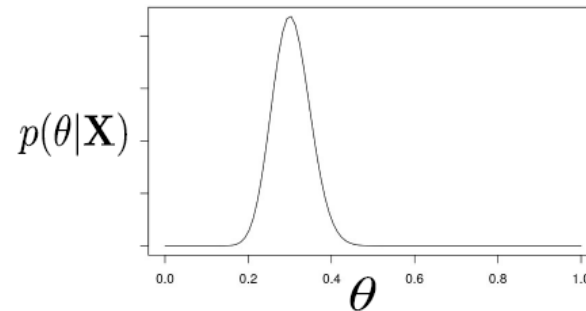


- Cheaper alternative: **Point Estimation** of the parameters. E.g.,
 - **Maximum likelihood estimation (MLE)**: Find θ that makes the observed data most probable
- **Maximum-a-Posteriori (MAP) estimation**: Find θ that has the largest posterior probability

$$\hat{\theta}_{MAP} = \arg \max_{\theta} \log p(\theta|\mathbf{X}) = \arg \max_{\theta} [\log p(\mathbf{X}|\theta) + \log p(\theta)]$$

Posterior Distribution

- Posterior provides us a holistic view about θ given observed data
- A simple unimodal posterior distribution for a scalar parameter θ might look something like



- Various types of estimates regarding θ can be obtained from the posterior, e.g.,
 - Mode of the posterior (same as the MAP estimate)
 - Mean and median of the posterior
 - Variance/spread of the posterior (uncertainty in our estimate of the parameters)

Predictions

- Posterior can be used to compute the **posterior predictive distribution** (PPD) of new observation
- The PPD of a new observation \mathbf{x}_* given previous observations

$$\begin{aligned} p(\mathbf{x}_*|\mathbf{X}, m) &= \int p(\mathbf{x}_*, \theta|\mathbf{X}, m) d\theta = \int p(\mathbf{x}_*|\theta, \mathbf{X}, m) p(\theta|\mathbf{X}, m) d\theta \\ &= \int p(\mathbf{x}_*|\theta, m) p(\theta|\mathbf{X}, m) d\theta \end{aligned}$$

- Note: In the above, we assume that the observations are i.i.d. given θ
- Computing PPD requires doing a posterior-weighted averaging over all values of θ
- If the integral in PPD is intractable, we can approximate the PPD by **plug-in predictive**

$$p(\mathbf{x}_*|\mathbf{X}, m) \approx p(\mathbf{x}_*|\hat{\theta}, m)$$

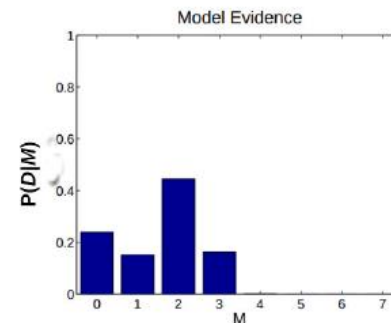
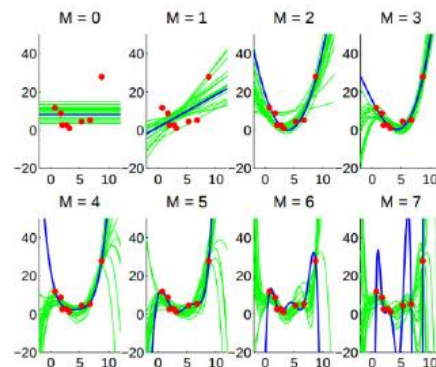
.. where $\hat{\theta}$ is a point estimate of θ (e.g., MLE/MAP)

Marginal Likelihood

- Recall the Bayes rule for computing the posterior

$$p(\theta|\mathbf{X}, m) = \frac{p(\mathbf{X}, \theta|m)}{p(\mathbf{X}|m)} = \frac{p(\mathbf{X}|\theta, m)p(\theta|m)}{\int p(\mathbf{X}|\theta, m)p(\theta|m)d\theta} = \frac{\text{Likelihood} \times \text{Prior}}{\text{Marginal likelihood}}$$

- The denominator in the Bayes rule is the marginal likelihood (a.k.a. “model evidence”)
- Note that $p(\mathbf{X}|m) = \mathbb{E}_{p(\theta|m)}[p(\mathbf{X}|\theta, m)]$ is the **average/expected likelihood** under model m
- For a good model, we would expect this “averaged” quantity to be large (most θ 's will be good)



Model Comparison/Averaging

- Marginal likelihood is hard-to-compute (due to integral) but a very useful quantity
- It can be used for doing [model selection](#)
 - Choose model m that has largest posterior probability

$$\hat{m} = \arg \max_m p(m|\mathbf{X}) = \arg \max_m \frac{p(\mathbf{X}|m)p(m)}{p(\mathbf{X})} = \arg \max_m p(\mathbf{X}|m)p(m)$$

- If all models are equally likely a priori then $\hat{m} = \arg \max_m p(\mathbf{X}|m)$
 - If m is a hyperparam, then $\arg \max_m p(\mathbf{X}|m)$ is MLE-II based hyperparameter estimation
- Marginal likelihood can be used to compute $p(m|\mathbf{X})$ and then perform [Bayesian Model Averaging](#)

$$p(\mathbf{x}_*|\mathbf{X}) = \sum_{m=1}^M p(\mathbf{x}_*|\mathbf{X}, m)p(m|\mathbf{X})$$

Simple Example (MLE)

- Consider a sequence of N coin tosses (call head = 0, tail = 1)
- The n^{th} outcome \mathbf{x}_n is a binary random variable $\in \{0, 1\}$
- Assume θ to be probability of a head (parameter we wish to estimate)
- Each likelihood term $p(\mathbf{x}_n | \theta)$ is Bernoulli: $p(\mathbf{x}_n | \theta) = \theta^{\mathbf{x}_n}(1 - \theta)^{1-\mathbf{x}_n}$
- Log-likelihood: $\sum_{n=1}^N \log p(\mathbf{x}_n | \theta) = \sum_{n=1}^N \mathbf{x}_n \log \theta + (1 - \mathbf{x}_n) \log(1 - \theta)$
- Taking derivative of the log-likelihood w.r.t. θ , and setting it to zero gives

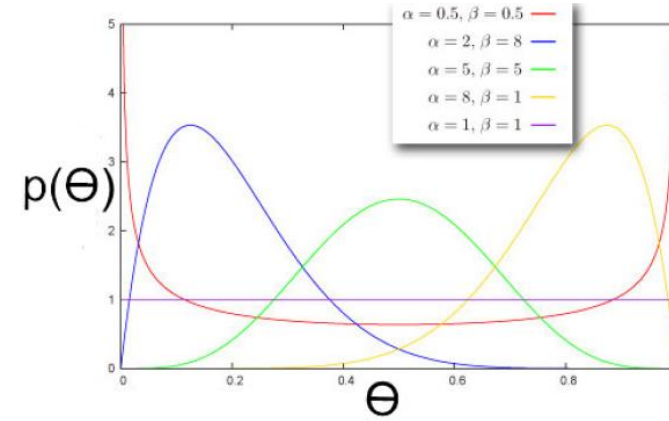
$$\hat{\theta}_{MLE} = \frac{\sum_{n=1}^N \mathbf{x}_n}{N}$$

- $\hat{\theta}_{MLE}$ in this example is simply the fraction of heads!

MAP Estimate

- MAP estimation can incorporate a prior $p(\theta)$ on θ
- Since $\theta \in (0, 1)$, one possibility can be to assume a Beta prior

$$p(\theta) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1} (1 - \theta)^{\beta-1}$$



- α, β are called hyperparameters of the prior (these can have intuitive meaning; we'll see shortly)
- Note that each likelihood term is still a Bernoulli: $p(\mathbf{x}_n|\theta) = \theta^{\mathbf{x}_n}(1 - \theta)^{1-\mathbf{x}_n}$

- The log posterior probability = $\sum_{n=1}^N \log p(\mathbf{x}_n|\theta) + \log p(\theta)$
- Ignoring the constants w.r.t. θ , the log posterior probability:

$$\sum_{n=1}^N \{\mathbf{x}_n \log \theta + (1 - \mathbf{x}_n) \log(1 - \theta)\} + (\alpha - 1) \log \theta + (\beta - 1) \log(1 - \theta)$$

- Taking derivative w.r.t. θ and setting to zero gives

$$\hat{\theta}_{MAP} = \frac{\sum_{n=1}^N \mathbf{x}_n + \alpha - 1}{N + \alpha + \beta - 2}$$

- Note: For $\alpha = 1, \beta = 1$, i.e., $p(\theta) = \text{Beta}(1, 1)$ (equivalent to a uniform prior), $\hat{\theta}_{MAP} = \hat{\theta}_{MLE}$

Bayesian Estimate

- Recall that each likelihood term was Bernoulli: $p(\mathbf{x}_n|\theta) = \theta^{\mathbf{x}_n}(1 - \theta)^{1-\mathbf{x}_n}$
- Let's again choose the prior $p(\theta)$ as Beta: $p(\theta) = \text{Beta}(\alpha, \beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} \theta^{\alpha-1}(1 - \theta)^{\beta-1}$
- The posterior distribution will be proportional to the product of likelihood and prior

$$\begin{aligned} p(\theta|\mathbf{X}) &\propto \prod_{n=1}^N p(\mathbf{x}_n|\theta) p(\theta) \\ &\propto \theta^{\alpha + \sum_{n=1}^N \mathbf{x}_n - 1} (1 - \theta)^{\beta + N - \sum_{n=1}^N \mathbf{x}_n - 1} \end{aligned}$$

- From simple inspection, note that the posterior $p(\theta|\mathbf{X}) = \text{Beta}(\alpha + \sum_{n=1}^N \mathbf{x}_n, \beta + N - \sum_{n=1}^N \mathbf{x}_n)$

Posterior has the same form as prior – conjugate prior

Predictions

- Let's say we want to compute the probability that the next outcome $\mathbf{x}_{N+1} \in \{0, 1\}$ will be a head
- The **plug-in predictive** distribution using a point estimate $\hat{\theta}$ (e.g., using MLE/MAP)

$$p(\mathbf{x}_{N+1} = 1|\mathbf{X}) \approx p(\mathbf{x}_{N+1} = 1|\hat{\theta}) = \hat{\theta} \quad \underline{\text{or equivalently}} \quad p(\mathbf{x}_{N+1}|\mathbf{X}) \approx \text{Bernoulli}(\mathbf{x}_{N+1} \mid \hat{\theta})$$

- The **posterior predictive distribution** (averaging over all θ weighted by their posterior probabilities):

$$\begin{aligned} p(\mathbf{x}_{N+1} = 1|\mathbf{X}) &= \int_0^1 P(\mathbf{x}_{N+1} = 1|\theta)p(\theta|\mathbf{X})d\theta \\ &= \int_0^1 \theta \times \text{Beta}(\theta|\alpha + N_1, \beta + N_0)d\theta \\ &= \mathbb{E}[\theta|\mathbf{X}] \\ &= \frac{\alpha + N_1}{\alpha + \beta + N} \end{aligned}$$

- Therefore the posterior predictive distribution: $p(\mathbf{x}_{N+1}|\mathbf{X}) = \text{Bernoulli}(\mathbf{x}_{N+1} \mid \mathbb{E}[\theta|\mathbf{X}])$

Multinomial Model

- Assume N discrete-valued observations $\{x_1, \dots, x_N\}$ with each $x_n \in \{1, \dots, K\}$, e.g.,
 - x_n represents the outcome of a dice roll with K faces
 - x_n represents the class label of the n -th example (total K classes)
 - x_n represents the identity of the n -th word in a sequence of words
- Assume likelihood to be multinoulli with unknown params $\boldsymbol{\pi} = [\pi_1, \dots, \pi_K]$ s.t. $\sum_{k=1}^K \pi_k = 1$

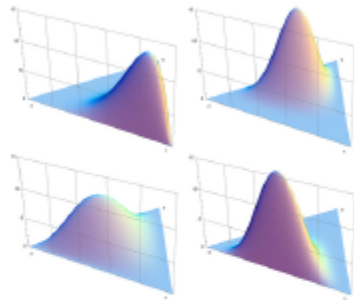
$$p(x_n|\boldsymbol{\pi}) = \text{multinoulli}(x_n|\boldsymbol{\pi}) = \prod_{k=1}^K \pi_k^{\mathbb{I}[x_n=k]}$$

- $\boldsymbol{\pi}$ is a vector of probabilities (“probability vector”), e.g.,
 - Biases of the K sides of the dice
 - Prior class probabilities in multi-class classification
 - Probabilities of observing each words in the vocabulary
- Assume a [conjugate](#) Dirichlet prior on $\boldsymbol{\pi}$ with hyperparams $\boldsymbol{\alpha} = [\alpha_1, \dots, \alpha_K]$ (also, $\alpha_k \geq 0, \forall k$)

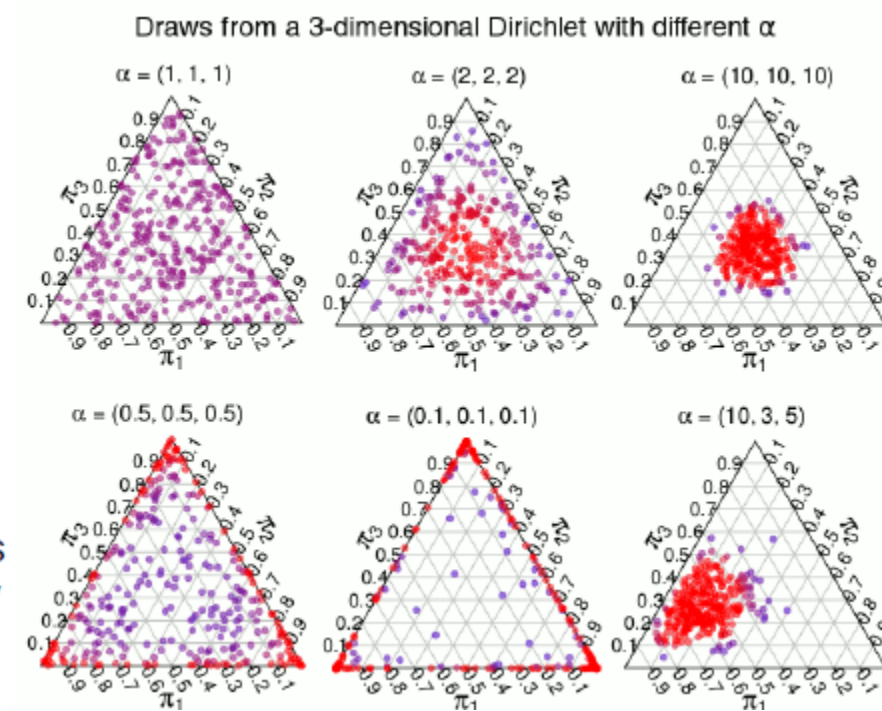
$$p(\boldsymbol{\pi}|\boldsymbol{\alpha}) = \text{Dirichlet}(\boldsymbol{\pi}|\alpha_1, \dots, \alpha_K) = \frac{\Gamma(\sum_{k=1}^K \alpha_k)}{\prod_{k=1}^K \Gamma(\alpha_k)} \prod_{k=1}^K \pi_k^{\alpha_k-1} = \frac{1}{B(\boldsymbol{\alpha})} \prod_{k=1}^K \pi_k^{\alpha_k-1}$$

Dirichlet Distribution

PDF for a 3-dim Dirichlet



Red dots denote regions of high probability density



$$p(\boldsymbol{\pi}|\boldsymbol{\alpha}) = \frac{1}{B(\boldsymbol{\alpha})} \prod_{k=1}^K \pi_k^{\alpha_k-1}$$

$$\text{Mean} = \left[\frac{\alpha_1}{\sum_{k=1}^K \alpha_k}, \dots, \frac{\alpha_K}{\sum_{k=1}^K \alpha_k} \right]$$

$$\text{Mode} = \left[\frac{\alpha_1 - 1}{\sum_{k=1}^K \alpha_k - K}, \dots, \frac{\alpha_K - 1}{\sum_{k=1}^K \alpha_k - K} \right] (\alpha_k > 1)$$

$$\text{var}(\pi_k) = \frac{\alpha_k(\alpha_0 - \alpha_k)}{\alpha_0^2(\alpha_0 + 1)}$$

$$\alpha_0 = \sum_{k=1}^K \alpha_k$$

Estimation

- The posterior over π is easy to compute in this case due to conjugacy b/w multinoulli and Dirichlet

$$p(\pi|\mathbf{X}, \alpha) = \frac{p(\mathbf{X}|\pi, \alpha)p(\pi|\alpha)}{p(\mathbf{X}|\alpha)} = \frac{p(\mathbf{X}|\pi)p(\pi|\alpha)}{p(\mathbf{X}|\alpha)}$$

- Assuming x_n 's are i.i.d. given π , $p(\mathbf{X}|\pi) = \prod_{n=1}^N p(x_n|\pi)$, therefore

$$p(\pi|\mathbf{X}, \alpha) \propto \prod_{n=1}^N \prod_{k=1}^K \pi_k^{\mathbb{I}[x_n=k]} \prod_{k=1}^K \pi_k^{\alpha_k-1} = \prod_{k=1}^K \pi_k^{\alpha_k + \sum_{n=1}^N \mathbb{I}[x_n=k]-1}$$

- Even without computing the normalization constant $p(\mathbf{X}|\alpha)$, we can see that it's a Dirichlet! :-)
- Denoting $N_k = \sum_{n=1}^N \mathbb{I}[x_n = k]$, i.e., number of observations with value k , the posterior will be

$$p(\pi|\mathbf{X}, \alpha) = \text{Dirichlet}(\pi|\alpha_1 + N_1, \dots, \alpha_K + N_K)$$

Gaussian Models

- Univariate with fixed variance
- Univariate with fixed mean
- Univariate with varying mean and variance
- Multivariate

Fixed Variance Gaussian Model

- Consider N i.i.d. observations $\mathbf{X} = \{x_1, \dots, x_N\}$ drawn from a one-dim Gaussian $\mathcal{N}(x|\mu, \sigma^2)$

$$p(x_n|\mu, \sigma^2) = \mathcal{N}(x|\mu, \sigma^2) \propto \exp \left[-\frac{(x_n - \mu)^2}{2\sigma^2} \right]$$

$$p(\mathbf{X}|\mu, \sigma^2) = \prod_{n=1}^N p(x_n|\mu, \sigma^2)$$

- Assume the mean $\mu \in \mathbb{R}$ of the Gaussian is unknown and assume variance σ^2 to be known/fixed
- We wish to estimate the unknown μ given the data \mathbf{X}
 - Let's choose a Gaussian prior on μ , i.e., $p(\mu) = \mathcal{N}(\mu|\mu_0, \sigma_0^2)$ with μ_0, σ_0^2 as fixed

Bayesian Estimate of Mean

- The posterior distribution for the unknown mean parameter μ

$$p(\mu|\mathbf{X}) = \frac{p(\mathbf{X}|\mu)p(\mu)}{p(\mathbf{X})} \propto \prod_{n=1}^N \exp \left[-\frac{(x_n - \mu)^2}{2\sigma^2} \right] \times \exp \left[-\frac{(\mu - \mu_0)^2}{2\sigma_0^2} \right]$$

- Simplifying the above (using completing the squares trick) gives $p(\mu|\mathbf{X}) \propto \exp \left[-\frac{(\mu - \mu_N)^2}{2\sigma_N^2} \right]$ with

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}$$

$$\mu_N = \frac{\sigma^2}{N\sigma_0^2 + \sigma^2} \mu_0 + \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2} \bar{x} \quad \left(\text{where } \bar{x} = \frac{\sum_{n=1}^N x_n}{N} \right)$$

Notion of Sufficient Statistics

Prediction

- What is the **posterior predictive distribution** $p(x_*|\mathbf{X})$ of a new observation x_* ?
- Using the inferred posterior $p(\mu|\mathbf{X})$, we can find the posterior predictive distribution

$$p(x_*|\mathbf{X}) = \int p(x_*|\mu, \sigma^2)p(\mu|\mathbf{X})d\mu = \int \mathcal{N}(x_*|\mu, \sigma^2)\mathcal{N}(\mu|\mu_N, \sigma_N^2)d\mu = \mathcal{N}(x_*|\mu_N, \sigma^2 + \sigma_N^2)$$

- Note; Can also get the above result by thinking of x_* as $x_* = \mu + \epsilon$ where $\mu \sim \mathcal{N}(\mu_N, \sigma_N^2)$, and $\epsilon \sim \mathcal{N}(0, \sigma^2)$ is independently added observation noise
- Note that, as per the above, the uncertainty in distribution of x_* now has two components
 - σ^2 : Due to the noisy observation model, σ_N^2 : Due to the uncertainty in μ
- In contrast, the **plug-in predictive posterior**, given a point estimate $\hat{\mu}$ (e.g., MLE/MAP) would be

$$p(x_*|\mathbf{X}) = \int p(x_*|\mu, \sigma^2)p(\mu|\mathbf{X})d\mu \approx p(x_*|\hat{\mu}, \sigma^2) = \mathcal{N}(x_*|\hat{\mu}, \sigma^2)$$

- Note that as $N \rightarrow \infty$, both approaches would give the same $p(x_*|\mathbf{X})$ since $\sigma_N^2 \rightarrow 0$

Fixed Mean Gaussian Model

- Again consider N i.i.d. observations $\mathbf{X} = \{x_1, \dots, x_N\}$ drawn from a one-dim Gaussian $\mathcal{N}(x|\mu, \sigma^2)$

$$p(x_n|\mu, \sigma^2) = \mathcal{N}(x|\mu, \sigma^2) \quad \text{and} \quad p(\mathbf{X}|\mu, \sigma^2) = \prod_{n=1}^N p(x_n|\mu, \sigma^2)$$

- Assume the variance $\sigma^2 \in \mathbb{R}_+$ of the Gaussian is unknown and assume mean μ to be known/fixed
- Let's estimate σ^2 given the data \mathbf{X} using fully Bayesian inference (not MLE/MAP)
- We first need a prior distribution for σ^2 . What prior $p(\sigma^2)$ to choose in this case?
- If we want a conjugate prior, it should have the same form as the likelihood

$$p(x_n|\mu, \sigma^2) \propto (\sigma^2)^{-1/2} \exp \left[-\frac{(x_n - \mu)^2}{2\sigma^2} \right]$$

- An **inverse-gamma prior** $IG(\alpha, \beta)$ has this form (α, β are shape and scale hyperparams, resp)

$$p(\sigma^2) \propto (\sigma^2)^{-(\alpha+1)} \exp \left[-\frac{\beta}{\sigma^2} \right]$$

$$\text{The posterior } p(\sigma^2|\mathbf{X}) = IG\left(\alpha + \frac{N}{2}, \beta + \frac{\sum_{n=1}^N (x_n - \mu)^2}{2}\right).$$

The posterior $p(\sigma^2|\mathbf{X}) = IG\left(\alpha + \frac{N}{2}, \beta + \frac{\sum_{n=1}^N (x_n - \mu)^2}{2}\right)$. Again IG due to conjugacy.

Gaussian Model: Mean and Variance

- Goal: Infer the mean and precision of a univariate Gaussian $\mathcal{N}(x|\mu, \lambda^{-1})$
- Given N i.i.d. observations $\mathbf{X} = \{x_1, \dots, x_N\}$, the likelihood will be

$$p(\mathbf{X}|\mu, \lambda) = \prod_{n=1}^N \sqrt{\frac{\lambda}{2\pi}} \exp\left[-\frac{\lambda}{2}(x_n - \mu)^2\right] \propto \left[\lambda^{1/2} \exp\left(-\frac{\lambda\mu^2}{2}\right)\right]^N \exp\left[\lambda\mu \sum_{n=1}^N x_n - \frac{\lambda}{2} \sum_{n=1}^N x_n^2\right]$$

- Let's choose the following joint distribution as the prior (compare its form with $p(\mathbf{X}|\mu, \lambda)$)

$$p(\mu, \lambda) \propto \left[\lambda^{1/2} \exp\left(-\frac{\lambda\mu^2}{2}\right)\right]^{\kappa_0} \exp[\lambda\mu c - \lambda d] = \underbrace{\exp\left[-\frac{\kappa_0\lambda}{2}(\mu - c/\kappa_0)^2\right]}_{\text{prop. to a Gaussian}} \underbrace{\lambda^{\kappa_0/2} \exp\left[-\left(d - \frac{c^2}{2\kappa_0}\right)\lambda\right]}_{\text{prop. to a gamma}}$$

- The above is known as the **Normal-gamma** (NG) distribution (product of a Normal and a gamma)

$$p(\mu, \lambda) = \mathcal{N}(\mu|\mu_0, (\kappa_0\lambda)^{-1})\text{Gamma}(\lambda|\alpha_0, \beta_0) = \text{NG}(\mu, \lambda|\mu_0, \kappa_0, \alpha_0, \beta_0) \quad (\text{note: } \mu \text{ and } \lambda \text{ are coupled in the Gaussian part})$$

where $\mu_0 = c/\kappa_0$, $\alpha_0 = 1 + \kappa_0/2$, $\beta_0 = d - c^2/2\kappa_0$ are prior's hyperparameters

- NG is conjugate to Gaussian when both mean & precision are unknown

Gaussian Model: Mean and Variance

- Due to conjugacy, $p(\mu, \lambda|\mathbf{X})$ will also be NG: $p(\mu, \lambda|\mathbf{X}) \propto p(\mathbf{X}|\mu, \lambda)p(\mu, \lambda)$

$$p(\mu, \lambda|\mathbf{X}) = \text{NG}(\mu_N, \kappa_N, \alpha_N, \beta_N) = \mathcal{N}(\mu|\mu_N, (\kappa_N\lambda)^{-1})\text{Gamma}(\lambda|\alpha_N, \beta_N)$$

where the updated posterior hyperparameters are given by¹

$$\begin{aligned}\mu_N &= \frac{\kappa_0\mu_0 + N\bar{x}}{\kappa_0 + N}, \quad \kappa_N = \kappa_0 + N \\ \alpha_N &= \alpha_0 + N/2, \quad \beta_N = \beta_0 + \frac{1}{2} \sum_{n=1}^N (x_n - \bar{x})^2 + \frac{\kappa_0 N (\bar{x} - \mu_0)^2}{2(\kappa_0 + N)}\end{aligned}$$

Posterior Predictive Distribution:

$$p(x_*|\mathbf{X}) = \int \underbrace{p(x_*|\mu, \lambda)}_{\text{Gaussian}} \underbrace{p(\mu, \lambda|\mathbf{X})}_{\text{Normal-Gamma}} d\mu d\lambda = t_{2\alpha_N} \left(x_* | \mu_N, \frac{\beta_N(\kappa_N + 1)}{\alpha_N \kappa_N} \right)$$

Multivariate Gaussian

- The (multivariate) Gaussian with mean $\boldsymbol{\mu}$ and cov. matrix $\boldsymbol{\Sigma}$

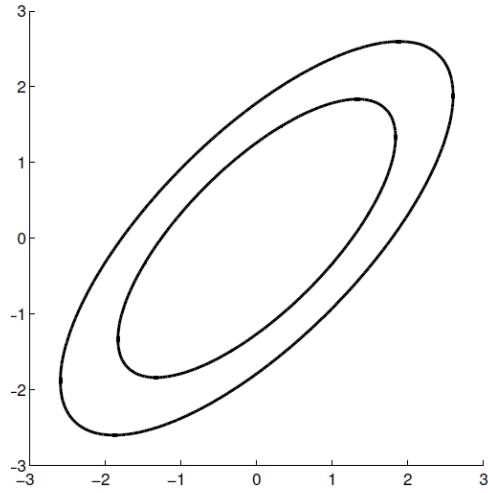
$$\begin{aligned}\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) &= \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right\} \\ &= \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}|}} \exp \left\{ -\frac{1}{2} \text{trace} \left[\boldsymbol{\Sigma}^{-1} \mathbf{S} \right] \right\} \quad \text{where } \mathbf{S} = (\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^\top\end{aligned}$$

- An alternate representation: The “information form”

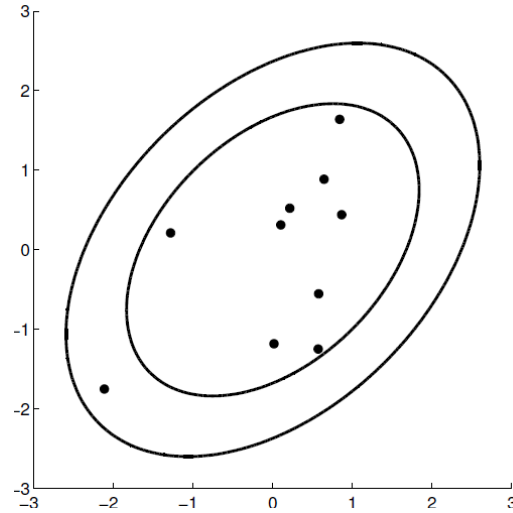
$$\mathcal{N}_c(\mathbf{x}|\boldsymbol{\xi}, \boldsymbol{\Lambda}) = (2\pi)^{-D/2} |\boldsymbol{\Lambda}|^{1/2} \exp \left\{ -\frac{1}{2} \left(\mathbf{x}^\top \boldsymbol{\Lambda} \mathbf{x} + \boldsymbol{\xi}^\top \boldsymbol{\Lambda}^{-1} \boldsymbol{\xi} - 2\mathbf{x}^\top \boldsymbol{\xi} \right) \right\}$$

where $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$ and $\boldsymbol{\xi} = \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu}$ are the “natural parameters” (more when we discuss exp. family).

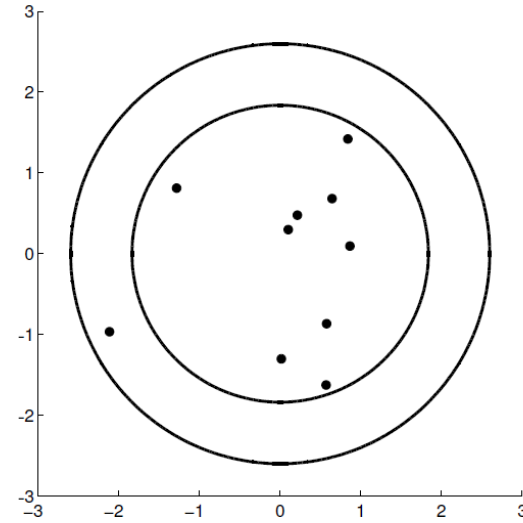
Multivariate Gaussians



$$\Sigma = \begin{bmatrix} 1 & .7 \\ .7 & 1 \end{bmatrix}$$

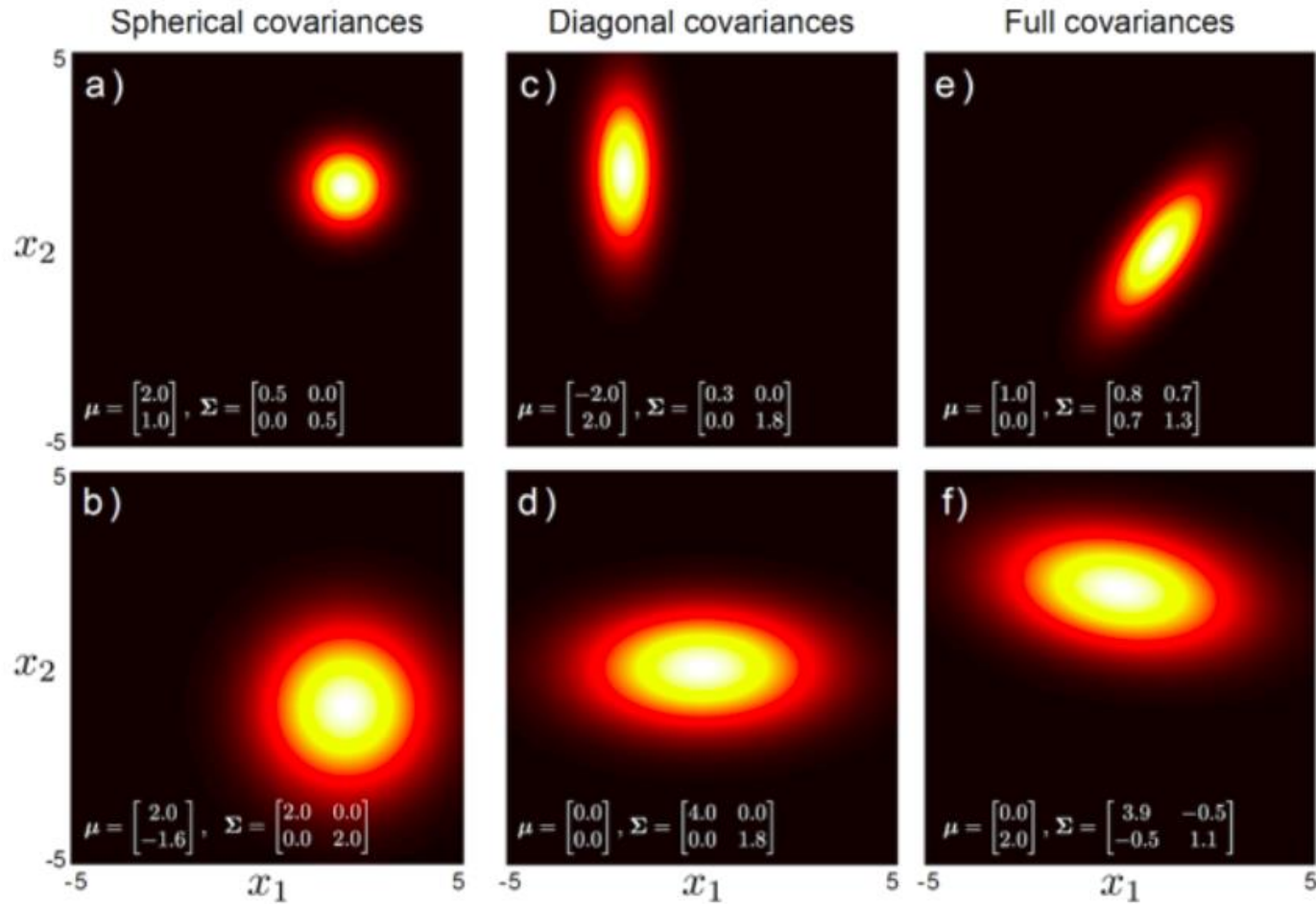


$$\Sigma = \begin{bmatrix} 1 & .4 \\ .4 & 1 \end{bmatrix}$$



$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Covariance Matrix



Multivariate Gaussians: Grouped Variables

- Given \mathbf{x} having multivariate Gaussian distribution $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with $\boldsymbol{\Lambda} = \boldsymbol{\Sigma}^{-1}$. Suppose

$$\begin{aligned}\mathbf{x} &= \begin{bmatrix} \mathbf{x}_a \\ \mathbf{x}_b \end{bmatrix} & \boldsymbol{\mu} &= \begin{bmatrix} \boldsymbol{\mu}_a \\ \boldsymbol{\mu}_b \end{bmatrix} \\ \boldsymbol{\Sigma} &= \begin{bmatrix} \boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab} \\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb} \end{bmatrix} & \boldsymbol{\Lambda} &= \begin{bmatrix} \boldsymbol{\Lambda}_{aa} & \boldsymbol{\Lambda}_{ab} \\ \boldsymbol{\Lambda}_{ba} & \boldsymbol{\Lambda}_{bb} \end{bmatrix}\end{aligned}$$

- The **marginal distribution** of one block, say \mathbf{x}_a , is a Gaussian

$$p(\mathbf{x}_a) = \int p(\mathbf{x}_a, \mathbf{x}_b) d\mathbf{x}_b = \mathcal{N}(\mathbf{x}_a | \boldsymbol{\mu}_a, \boldsymbol{\Sigma}_{aa})$$

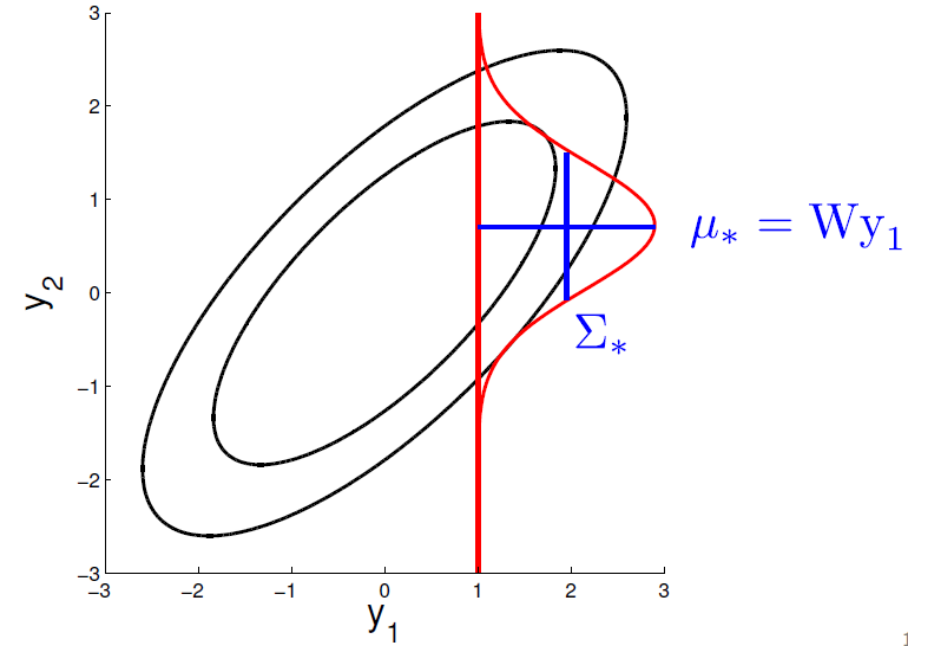
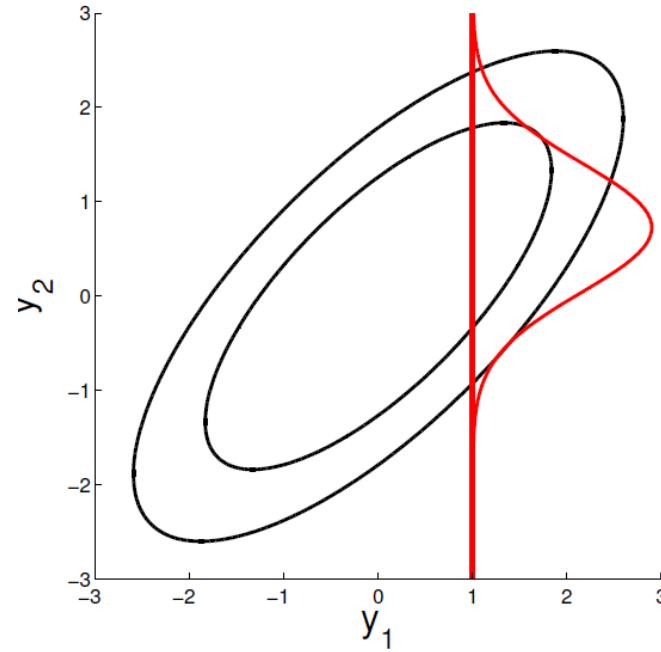
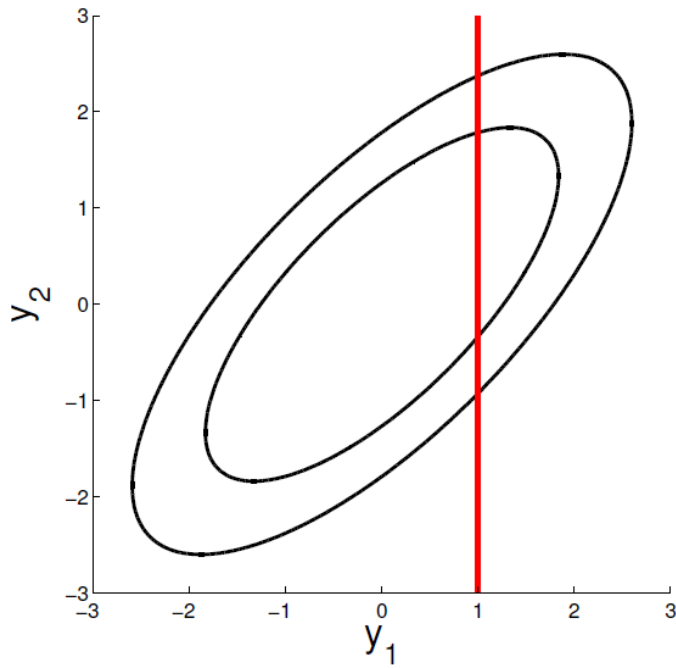
- The **conditional distribution** of \mathbf{x}_a given \mathbf{x}_b , is Gaussian, i.e., $p(\mathbf{x}_a | \mathbf{x}_b) = \mathcal{N}(\mathbf{x}_a | \boldsymbol{\mu}_{a|b}, \boldsymbol{\Sigma}_{a|b})$ where

$$\boldsymbol{\Sigma}_{a|b} = \boldsymbol{\Lambda}_{aa}^{-1} = \boldsymbol{\Sigma}_{aa} - \boldsymbol{\Sigma}_{ab} \boldsymbol{\Sigma}_{bb}^{-1} \boldsymbol{\Sigma}_{ba} \quad (\text{"smaller" than } \boldsymbol{\Sigma}_{aa}; \text{ makes sense intuitively})$$

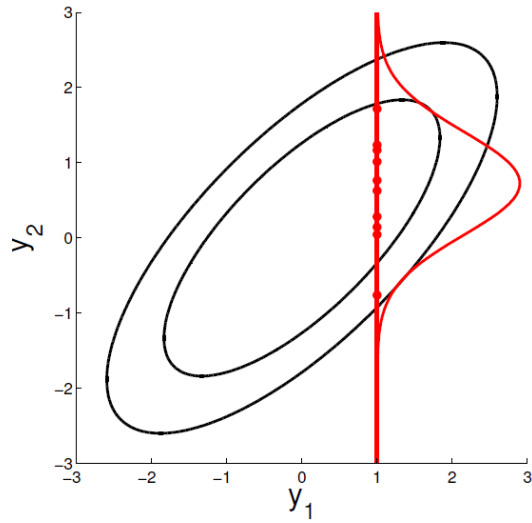
$$\begin{aligned}\boldsymbol{\mu}_{a|b} &= \boldsymbol{\Sigma}_{a|b} \{ \boldsymbol{\Lambda}_{aa} \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b) \} \\ &= \boldsymbol{\mu}_a - \boldsymbol{\Lambda}_{aa}^{-1} \boldsymbol{\Lambda}_{ab} (\mathbf{x}_b - \boldsymbol{\mu}_b) \\ &= \boldsymbol{\mu}_a + \boldsymbol{\Sigma}_{ab} \boldsymbol{\Sigma}_{bb}^{-1} (\mathbf{x}_b - \boldsymbol{\mu}_b)\end{aligned}$$

Conditional Distributions

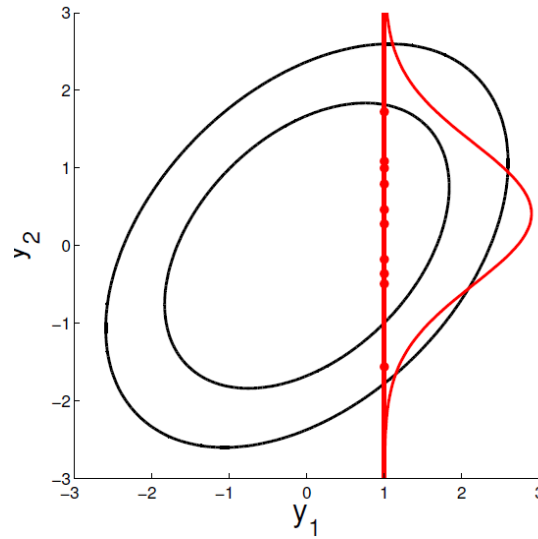
$$p(y_2|y_1, \Sigma) \propto \exp\left(-\frac{1}{2}(y_2 - \mu_*)\Sigma_*^{-1}(y_2 - \mu_*)\right)$$



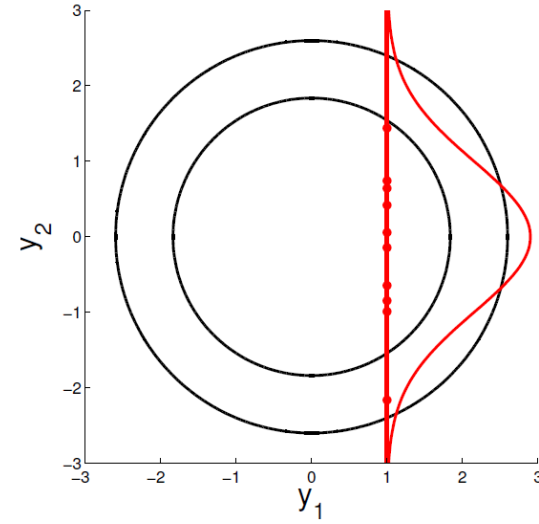
Conditional Distributions



$$\Sigma = \begin{bmatrix} 1 & .7 \\ .7 & 1 \end{bmatrix}$$



$$\Sigma = \begin{bmatrix} 1 & .4 \\ .4 & 1 \end{bmatrix}$$



$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Multivariate Gaussian

- The parameters are now the mean **vector** and the covariance/precision **matrix**
- Posterior updates for these have forms similar to that in the univariate case
- For the mean, commonly a **multivariate Gaussian prior** is used
 - Posterior is also Gaussian due to conjugacy
- For the covariance matrix (with mean fixed), commonly an **inverse-Wishart prior** is used
 - Posterior is also inverse-Wishart due to conjugacy
- For the precision matrix (with mean fixed), commonly a **Wishart prior** is used
 - Posterior is also Wishart due to conjugacy
- When both parameters are unknown, there still exist conjugate joint priors
 - **Normal-Inverse Wishart** for mean + cov matrix, **Normal-Wishart** for mean + precision matrix

Wishart Distribution: Multidimensional extension of Gamma distribution

Linear Transformation of Random Variables

- Suppose $\mathbf{x} = f(\mathbf{z}) = \mathbf{A}\mathbf{z} + \mathbf{b}$ be a linear function of an r.v. \mathbf{z} (not necessarily Gaussian)
- Suppose $\mathbb{E}[\mathbf{z}] = \boldsymbol{\mu}$ and $\text{cov}[\mathbf{z}] = \boldsymbol{\Sigma}$

- Expectation of \mathbf{x}

$$\mathbb{E}[\mathbf{x}] = \mathbb{E}[\mathbf{A}\mathbf{z} + \mathbf{b}] = \mathbf{A}\boldsymbol{\mu} + \mathbf{b}$$

- Covariance of \mathbf{x}

$$\text{cov}[\mathbf{x}] = \text{cov}[\mathbf{A}\mathbf{z} + \mathbf{b}] = \mathbf{A}\boldsymbol{\Sigma}\mathbf{A}^T$$

- Likewise if $x = f(\mathbf{z}) = \mathbf{a}^T \mathbf{z} + b$ is a scalar-valued linear function of an r.v. \mathbf{z} :
 - $\mathbb{E}[x] = \mathbb{E}[\mathbf{a}^T \mathbf{z} + b] = \mathbf{a}^T \boldsymbol{\mu} + b$
 - $\text{var}[x] = \text{var}[\mathbf{a}^T \mathbf{z} + b] = \mathbf{a}^T \boldsymbol{\Sigma} \mathbf{a}$

- These properties are often helpful in obtaining the marginal distribution $p(\mathbf{x})$ from $p(\mathbf{z})$

Linear Gaussian Model

- Consider linear transformation of a Gaussian r.v. \mathbf{z} with $p(\mathbf{z}) = \mathcal{N}(\mathbf{z}|\boldsymbol{\mu}, \boldsymbol{\Lambda}^{-1})$, plus Gaussian noise

$$\boxed{\mathbf{x} = \mathbf{A}\mathbf{z} + \mathbf{b} + \boldsymbol{\epsilon}} \quad \text{where} \quad p(\boldsymbol{\epsilon}) = \mathcal{N}(\boldsymbol{\epsilon}|\mathbf{0}, \mathbf{L}^{-1})$$

- Easy to see that, conditioned on \mathbf{z} , \mathbf{x} too has a Gaussian distribution

$$p(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}|\mathbf{A}\mathbf{z} + \mathbf{b}, \mathbf{L}^{-1})$$

- This is called a Linear Gaussian Model. Very commonly encountered in probabilistic modeling
- The following two distributions are of particular interest. Defining $\boldsymbol{\Sigma} = (\boldsymbol{\Lambda} + \mathbf{A}^\top \mathbf{L} \mathbf{A})^{-1}$, we have

$$p(\mathbf{z}|\mathbf{x}) = \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{p(\mathbf{x})} = \mathcal{N}(\mathbf{z}|\boldsymbol{\Sigma} \{ \mathbf{A}^\top \mathbf{L}(\mathbf{x} - \mathbf{b}) + \boldsymbol{\Lambda}\boldsymbol{\mu} \}, \boldsymbol{\Sigma})$$

$$p(\mathbf{x}) = \int p(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} = \mathcal{N}(\mathbf{x}|\mathbf{A}\boldsymbol{\mu} + \mathbf{b}, \mathbf{A}\boldsymbol{\Lambda}^{-1}\mathbf{A}^\top + \mathbf{L}^{-1})$$

Exponential Family Distributions

- Defines a **class of distributions**. An Exponential Family distribution is of the form

$$p(\mathbf{x}|\theta) = \frac{1}{Z(\theta)} h(\mathbf{x}) \exp[\theta^\top \phi(\mathbf{x})] = h(\mathbf{x}) \exp[\theta^\top \phi(\mathbf{x}) - A(\theta)]$$

- $\mathbf{x} \in \mathcal{X}^m$ is the random variable being modeled (where \mathcal{X} denotes some space, e.g., \mathbb{R} or $\{0, 1\}$)
- $\theta \in \mathbb{R}^d$: **Natural parameters** or **canonical parameters** defining the distribution
- $\phi(\mathbf{x}) \in \mathbb{R}^d$: **Sufficient statistics** (another random variable)
 - **Why "sufficient"**: $p(\mathbf{x}|\theta)$ as a function of θ depends on \mathbf{x} only via $\phi(\mathbf{x})$
- $Z(\theta) = \int h(\mathbf{x}) \exp[\theta^\top \phi(\mathbf{x})] d\mathbf{x}$: **Partition function**
- $A(\theta) = \log Z(\theta)$: **Log-partition function** (also called the cumulant function)
- $h(\mathbf{x})$: A constant (doesn't depend on θ)

Expressing a Distribution in Exp-family form

- Recall the form of exp-fam distribution: $h(\mathbf{x}) \exp[\theta^\top \phi(\mathbf{x}) - A(\theta)]$
- To write any exp-fam dist $p()$ in the above form, write it as $\exp(\log p())$, e.g., for Binomial

$$\begin{aligned}\exp(\log \text{Binomial}(x|N, \mu)) &= \exp\left(\log \binom{N}{x} \mu^x (1 - \mu)^{N-x}\right) \\ &= \exp\left(\log \binom{N}{x} + x \log \mu + (N - x) \log(1 - \mu)\right) \\ &= \binom{N}{x} \exp\left(x \log \frac{\mu}{1 - \mu} - N \log(1 - \mu)\right)\end{aligned}$$

- Now compare the resulting expression with the exponential family form

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp(\theta^\top \phi(\mathbf{x}) - A(\theta))$$

Gaussian as Exponential Form

- Let's try to write a univariate Gaussian in the exponential family form

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp[\theta^\top \phi(\mathbf{x}) - A(\theta)]$$

$$\begin{aligned} \mathcal{N}(x|\mu, \sigma^2) &= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] = \frac{1}{\sqrt{2\pi}} \exp\left[\frac{\mu}{\sigma^2}x - \frac{1}{2\sigma^2}x^2 - \frac{\mu^2}{2\sigma^2} - \log \sigma\right] \\ &= \frac{1}{\sqrt{2\pi}} \exp\left[\begin{bmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{bmatrix}^\top \begin{bmatrix} x \\ x^2 \end{bmatrix} - \left(\frac{\mu^2}{2\sigma^2} + \log \sigma\right)\right] \end{aligned}$$

- $h(x) = \frac{1}{\sqrt{2\pi}}$

- $\theta = \begin{bmatrix} \frac{\mu}{\sigma^2} \\ -\frac{1}{2\sigma^2} \end{bmatrix} = \begin{bmatrix} \theta_1 \\ \theta_2 \end{bmatrix}, \text{ and } \begin{bmatrix} \mu \\ \sigma^2 \end{bmatrix} = \begin{bmatrix} -\frac{\theta_1}{2\theta_2} \\ \frac{1}{-\theta_2} \end{bmatrix}$

- $\phi(x) = \begin{bmatrix} x \\ x^2 \end{bmatrix}$

- $A(\theta) = \frac{\mu^2}{2\sigma^2} + \log \sigma = \frac{-\theta_1^2}{4\theta_2} - \frac{1}{2} \log(-2\theta_2) - \frac{1}{2} \log(2\pi)$

- Many other distribution belong to the exponential family
 - Bernoulli
 - Beta
 - Gamma
 - Multinoulli/Multinomial
 - Dirichlet
 - Multivariate Gaussian
 - .. and many more (https://en.wikipedia.org/wiki/Exponential_family)
- Note: Not all distributions belong to the exponential family, e.g.,
 - Uniform distribution ($x \sim \text{Unif}(a, b)$)

MLE on Exponential Families

- Suppose we have data $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ drawn i.i.d. from an exponential family distribution

$$p(\mathbf{x}|\theta) = h(\mathbf{x}) \exp [\theta^\top \phi(\mathbf{x}) - A(\theta)]$$

- To do MLE, we need the overall likelihood. This is simply a product of the individual likelihoods

$$p(\mathcal{D}|\theta) = \prod_{i=1}^N p(\mathbf{x}_i|\theta) = \left[\prod_{i=1}^N h(\mathbf{x}_i) \right] \exp \left[\theta^\top \sum_{i=1}^N \phi(\mathbf{x}_i) - NA(\theta) \right] = \left[\prod_{i=1}^N h(\mathbf{x}_i) \right] \exp [\theta^\top \phi(\mathcal{D}) - NA(\theta)]$$

- To estimate θ (as we'll see shortly), we only need $\phi(\mathcal{D}) = \sum_{i=1}^N \phi(\mathbf{x}_i)$ and N
- Size of $\phi(\mathcal{D}) = \sum_{i=1}^N \phi(\mathbf{x}_i)$ does not grow with N (same as the size of each $\phi(\mathbf{x}_i)$)
- Only exponential family distributions have finite-sized sufficient statistics
 - No need to store all the data; can simply store and recursively update the sufficient statistics

- The likelihood is of the form $p(\mathcal{D}|\theta) = \left[\prod_{i=1}^N h(\mathbf{x}_i) \right] \exp [\theta^\top \phi(\mathcal{D}) - NA(\theta)]$
- The **log-likelihood** is (ignoring constant w.r.t. θ): $\log p(\mathcal{D}|\theta) = \theta^\top \phi(\mathcal{D}) - NA(\theta)$
- Note: This is concave in θ (since $-A(\theta)$ is concave). Maximization will yield a global maxima of θ
- MLE for exp-fam distributions can also be seen as doing **moment-matching**. To see this, note that

$$\nabla_{\theta} [\theta^\top \phi(\mathcal{D}) - NA(\theta)] = \phi(\mathcal{D}) - N \nabla_{\theta} [A(\theta)] = \phi(\mathcal{D}) - N \mathbb{E}_{p(\mathbf{x}|\theta)}[\phi(\mathbf{x})] = \sum_{i=1}^N \phi(\mathbf{x}_i) - N \mathbb{E}_{p(\mathbf{x}|\theta)}[\phi(\mathbf{x})]$$

- Therefore, at the “optimal” (i.e., MLE) $\hat{\theta}$, where the derivative is 0, the following must hold

$$\mathbb{E}_{p(\mathbf{x}|\theta)}[\phi(\mathbf{x})] = \frac{1}{N} \sum_{i=1}^N \phi(\mathbf{x}_i)$$

matching the **expected** moments of the distribution with **empirical** moments

Bayesian Estimate in Exponential Families

- We saw that the total **likelihood** given N i.i.d. observations $\mathcal{D}\{\mathbf{x}_1, \dots, \mathbf{x}_N\}$

$$p(\mathcal{D}|\theta) \propto \exp \left[\theta^\top \phi(\mathcal{D}) - NA(\theta) \right] \quad \text{where} \quad \phi(\mathcal{D}) = \sum_{i=1}^N \phi(\mathbf{x}_i)$$

- Let's choose the following **prior** (note: it looks similar in terms of θ within the exponent)

$$p(\theta|\nu_0, \boldsymbol{\tau}_0) = h(\theta) \exp \left[\theta^\top \boldsymbol{\tau}_0 - \nu_0 A(\theta) - A_c(\nu_0, \boldsymbol{\tau}_0) \right]$$

- Ignoring the prior's log-partition function $A_c(\nu_0, \boldsymbol{\tau}_0) = \log \int_{\theta} h(\theta) \exp \left[\theta^\top \boldsymbol{\tau}_0 - \nu_0 A(\theta) \right] d\theta$

$$p(\theta|\nu_0, \boldsymbol{\tau}_0) \propto h(\theta) \exp \left[\theta^\top \boldsymbol{\tau}_0 - \nu_0 A(\theta) \right]$$

- Comparing the prior's form with the likelihood, we notice that
 - ν_0 is like the number of “pseudo-observations” coming from the prior
 - $\boldsymbol{\tau}_0$ is the total sufficient statistics of these ν_0 pseudo-observations

Posterior Distribution

- As we saw, the **likelihood** is

$$p(\mathcal{D}|\theta) \propto \exp \left[\theta^\top \phi(\mathcal{D}) - NA(\theta) \right] \quad \text{where} \quad \phi(\mathcal{D}) = \sum_{i=1}^N \phi(\mathbf{x}_i)$$

- And the **prior** we chose is

$$p(\theta|\nu_0, \boldsymbol{\tau}_0) \propto h(\theta) \exp \left[\theta^\top \boldsymbol{\tau}_0 - \nu_0 A(\theta) \right]$$

- For this form of the prior, the **posterior** $p(\theta|\mathcal{D}) \propto p(\theta)p(\mathcal{D}|\theta)$ will be

$$p(\theta|\mathcal{D}) \propto h(\theta) \exp \left[\theta^\top (\boldsymbol{\tau}_0 + \phi(\mathcal{D})) - (\nu_0 + N)A(\theta) \right]$$

- Note that **the posterior has the same form as the prior**; such a prior is called a **conjugate prior** (note: all exponential family distributions have a conjugate prior having a form shown as above)
- Thus posterior hyperparams ν_0', τ_0' are obtained

$$\begin{aligned} \nu_0' &\leftarrow \nu_0 + N \\ \tau_0' &\leftarrow \tau_0 + \phi(\mathcal{D}) \end{aligned}$$

Contd..

- Assuming the prior $p(\theta|\nu_0, \tau_0) \propto h(\theta) \exp [\theta^\top \tau_0 - \nu_0 A(\theta)]$, the posterior was

$$p(\theta|\mathcal{D}) \propto h(\theta) \exp [\theta^\top (\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N)A(\theta)]$$

- Assuming $\tau_0 = \nu_0 \bar{\tau}_0$, we can also write the prior as $p(\theta|\nu_0, \bar{\tau}_0) \propto \exp [\theta^\top \nu_0 \bar{\tau}_0 - \nu_0 A(\theta)]$
- Can think of $\bar{\tau}_0 = \tau_0/\nu_0$ as the average sufficient statistics per pseudo-observation
- The posterior can be written as

$$p(\theta|\mathcal{D}) \propto h(\theta) \exp \left[\theta^\top (\nu_0 + N) \frac{\nu_0 \bar{\tau}_0 + \phi(\mathcal{D})}{\nu_0 + N} - (\nu_0 + N)A(\theta) \right]$$

- Denoting $\bar{\phi} = \frac{\phi(\mathcal{D})}{N}$ as the average suff-stats per real observation, the posterior updates are

$$\begin{aligned} \nu_0' &\leftarrow \nu_0 + N \\ \bar{\tau}_0' &\leftarrow \frac{\nu_0 \bar{\tau}_0 + N \bar{\phi}}{\nu_0 + N} \end{aligned}$$

Posterior Predictive Distribution

- Assume some past (training) data $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$ generated from an exp. family distribution
- Assume some test data $\mathcal{D}' = \{\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_{N'}\}$ from the same distribution ($N' \geq 1$)
- The **posterior predictive distribution** of \mathcal{D}' (probability distribution of new data given old data)

$$p(\mathcal{D}'|\mathcal{D}) = \int p(\mathcal{D}'|\theta)p(\theta|\mathcal{D})d\theta$$

$$\begin{aligned} p(\mathcal{D}'|\mathcal{D}) &= \int p(\mathcal{D}'|\theta)p(\theta|\mathcal{D})d\theta \\ &= \int \underbrace{\left[\prod_{i=1}^{N'} h(\tilde{\mathbf{x}}_i) \right]}_{\text{constant w.r.t. } \theta} \exp \left[\theta^\top \phi(\mathcal{D}') - N' A(\theta) \right] h(\theta) \exp \left[\theta^\top (\tau_0 + \phi(\mathcal{D})) - (\nu_0 + N) A(\theta) - \underbrace{A_c(\nu_0 + N, \tau_0 + \phi(\mathcal{D}))}_{\text{constant w.r.t. } \theta} \right] d\theta \end{aligned}$$

Summary of Single Node Models

- Likelihood, Prior, Posterior, Predictive, Model averaging
 - Hyperparameters (Parametric/Non-parametric models)
 - Conjugate priors and closed form expression
 - Point estimates (MLE, MAP), Distribution Estimates (Bayesian)
 - Generative models
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- Bernoulli (coin)
 - Multinomial (dice)
 - Gaussians (continuous variables)
 - Exponential families

Questions