(1) Parameter Estimation for Gaussians (2) Probabilistic Linear Regression

CS772A: Probabilistic Machine Learning

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Plan Today

- Estimating parameters of a Gaussian distribution
 - Will only focus on fully Bayesian inference, not MLE/MAP (left as an exercise)
- Probabilistic Linear Regression
 - Using Gaussian likelihood and Gaussian prior



Bayesian Inference for Mean of a Univariate Gaussian

• Consider N i.i.d. scalar obs $\mathbf{X} = \{x_1, x_2, \dots, x_N\}$ drawn from $p(x|\mu, \sigma^2) = \mathcal{N}(x|\mu, \sigma^2)$

$$p(x|\mu,\sigma^2) \qquad p(x_n|\mu,\sigma^2) = \mathcal{N}(x|\mu,\sigma^2) \propto \exp\left[-\frac{(x_n-\mu)^2}{2\sigma^2}\right] \qquad p(\mu|\mu_0,\sigma_0^2) \qquad p$$

• Each x_n is a noisy measurement of $\mu \in \mathbb{R}$, i.e., $x_n = \mu + \epsilon_n$ where $\epsilon_n \sim \mathcal{N}(0, \sigma^2)$

- Would like to estimate μ given **X** using fully Bayesian inference (not point estimation)
- Need a prior over μ . Let's choose a Gaussian $p(\mu | \mu_0, \sigma_0^2) = \mathcal{N}(\mu | \mu_0, \sigma_0^2)$
 - The prior basically says that *a priori* μ is close to μ_0
 - The prior's variance σ_0^2 tells us how certain we are about the above assumption
 - Since σ^2 in the likelihood model $\mathcal{N}(x|\mu, \sigma^2)$ is known, the Gaussian prior $\mathcal{N}(x|\mu_0, \sigma_0^2)$ on μ is also conjugate to the likelihood (thus posterior of μ will also be Gaussian)

Assumed fixed

Assume μ_0

and σ_0^2 to be

Bayesian Inference for Mean of a Univariate Gaussian

- The posterior distribution for the unknown mean parameter μ

On conditioning side,
skipping all fixed params
and hyperparams from
the notation
$$p(\mu|\mathbf{X}) = \frac{p(\mathbf{X}|\mu)p(\mu)}{p(\mathbf{X})} \propto \prod_{n=1}^{N} \exp\left[-\frac{(x_n - \mu)^2}{2\sigma^2}\right] \times \exp\left[-\frac{(\mu - \mu_0)^2}{2\sigma_0^2}\right]$$

Simplifying the above (using completing the squares trick – see note) gives



Meaning, we become very-very

certain about the estimate of μ

- What happens to the posterior as N (number of observations) grows very large?
 - Data (likelihood part) overwhelms the prior
 - Posterior's variance σ_N^2 will approximately be σ^2/N (and goes to 0 as $N \to \infty$)
 - The posterior's mean μ_N approaches $ar{x}$ (which is also the MLE solution)

Bayesian Inference for Mean of a Univariate Gaussian

• Using the inferred posterior $p(\mu|\mathbf{X})$, we can find the posterior predictive distribution

■ In

Assumed fixed, only
$$\mu$$
 is
the unknown here

$$p(x_*|\mathbf{X}) = \int p(x_*|\mu, \sigma^2) p(\mu|\mathbf{X}) d\mu$$
On conditioning side,
skipping all fixed params
and hyperparams from
the notation

$$= \int \mathcal{N}(x_*|\mu, \sigma^2) \mathcal{N}(\mu|\mu_N, \sigma_N^2) d\mu$$
This "extra" variance is due to the
averaging over the posterior's uncertainty

$$= \mathcal{N}(x_*|\mu_N, \sigma^2 + \sigma_N^2)$$
This "extra" variance is due to the
averaging over the posterior's uncertainty

$$= \mathcal{N}(x_*|\mathbf{X}) = \mathcal{N}(x_*|\mu_N, \sigma^2 + \sigma_N^2)$$
For an alternative way to get the above result, note that

$$x_* = \mu + \epsilon \qquad \mu \sim \mathcal{N}(\mu_N, \sigma_N^2) \qquad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

$$\Rightarrow \qquad p(x_*|\mathbf{X}) = \mathcal{N}(x_*|\mu_N, \sigma^2 + \sigma_N^2)$$
Since both μ and ϵ are Gaussian tw, and are independent.
 x_* also has a Gaussian predictive, and the respective
means and variances of μ and ϵ get added up
In contrast, the plug-in predictive given a point estimate $\hat{\mu}$ will be

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

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Bayesian Inference for Variance of a Univariate Gaussian⁶

• Consider N i.i.d. scalar obs $\mathbf{X} = \{x_1, x_2, \dots, x_N\}$ drawn from $\mathcal{N}(x|\mu, \sigma^2)$

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

- Assume the variance $\sigma^2 \in \mathbb{R}_+$ to be unknown and mean μ to be fixed/known

- Would like to estimate σ^2 given **X** using fully Bayesian inference (not point estimation)
- Need a prior over 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

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

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

$$p(\sigma^2) \propto (\sigma^2)^{-(\alpha+1)} \exp\left[-\frac{\beta}{\sigma^2}\right] \qquad (\text{note: mean of } IG(\alpha,\beta) = \frac{\beta}{\alpha-1})$$

• Due to conjugacy, posterior will also be IG: $p(\sigma^2|\mathbf{X}) = IG(\alpha + \frac{N}{2}, \beta + \frac{\sum_{n=1}^{N}(x_n - \mu)^2}{2})$



Working with Gaussians: Variance vs Precision

• Often, it is easier to work with the precision (=1/variance) rather than variance

$$p(x_n|\mu,\lambda^{-1}) = \mathcal{N}(x|\mu,\lambda^{-1}) = \sqrt{\frac{\lambda}{2\pi}} \exp\left[-\frac{\lambda}{2}(x_n-\mu)^2\right]$$

• If mean is known, for precision, $Gamma(\alpha, \beta)$ is a conjugate prior to Gaussian lik.

PDF of gamma distribution $p(\lambda) \propto (\lambda)^{(\alpha-1)} \exp[-\beta\lambda]$ (Note: mean of $\operatorname{Gamma}(\alpha,\beta) = \frac{\alpha}{\beta}$) $\overset{\alpha \text{ and } \beta}{\longrightarrow}$ and rate params, resp., of the Gamma distribution

- (Verify) The posterior $p(\lambda | X)$ will be $Gamma(\alpha + \frac{N}{2}, \beta + \frac{\sum_{n=1}^{N} (x_n \mu)^2}{2})$
- Note: Unlike the case of unknown mean and fixed variance, the PPD for this case (and also the unknown variance case) will not be a Gaussian
- Note: Gamma distribution can be defined in terms of shape and scale or shape and rate parametrization (scale = 1/rate). Likewise, inverse Gamma can also be defined both shape and scale (which we saw) as well as shape and rate parametrizations.

Bayesian Inference for Both Parameters of a Gaussian

- Gaussian with unknown scalar mean and unknown scalar precision (two parameters)
- Consider N i.i.d. scalar obs $\mathbf{X} = \{x_1, x_2, \dots, x_N\}$ drawn from $\mathcal{N}(x|\mu, \lambda^{-1})$
- Assume both mean μ and precision λ to be unknown. The likelihood can be written as

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

- Would like a joint conjugate prior distribution $p(\mu, \lambda)$
 - It must have the same form as the likelihood as written above. Basically, something that looks like

Thankfully, this is a known distribution: normal-gamma (NG)
$$p(\mu, \lambda) \propto \left[\lambda^{1/2} \exp\left(-\frac{\lambda\mu^2}{2}\right)\right]^{\kappa_0} \exp\left[\lambda\mu c - \lambda d\right]$$

Called so since it can be written



Called so since it can be writter as a product of a normal and a gamma (next slide)

The NG also has a multivariate version called normal-Wishart distribution to jointly model a real-valued vector and a PSD matrix

Detour: Normal-gamma (Gaussian-gamma) Distribution⁹

We saw that the conjugate prior needed to have the form

$$p(\mu, \lambda) \propto \left[\lambda^{1/2} \exp\left(-\frac{\lambda\mu^2}{2}\right)\right]^{\kappa_0} \exp\left[\lambda\mu c - \lambda d\right]$$

$$= \underbrace{\exp\left[-\frac{\kappa_0\lambda}{2}(\mu - c/\kappa_0)^2\right]}_{\text{prop. to a Gaussian}} \underbrace{\lambda^{\kappa_0/2} \exp\left[-\left(d - \frac{c^2}{2\kappa_0}\right)\lambda\right]}_{\text{prop. to a gamma}} \text{ (re-arranging terms)}$$
Assuming shape-rate commutivation of the commut

The above is product of a normal and a gamma distribution
parametrization of the gamma

$$p(\mu,\lambda) = \mathcal{N}(\mu|\mu_0, (\kappa_0\lambda)^{-1})\mathsf{Gamma}(\lambda|\alpha_0, \beta_0) = \mathsf{NG}(\mu_0, \kappa_0, \alpha_0, \beta_0)$$

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

- The NG $p(\mu, \lambda) = NG(\mu_0, \kappa_0, \alpha_0, \beta_0)$ is conjugate to a Gaussian distribution if both its mean and precision parameters are unknown and are to be estimated
 - Thus a useful prior in many problems involving Gaussians with unknown mean and precision

Bayesian Inference for Both Parameters of a Gaussian ¹⁰

• Due to conjugacy, the joint posterior $p(\mu, \lambda | \mathbf{X})$ will also be normal-gamma

Skipping all hyperparameters on the conditioning side $p(\mu, \lambda | \mathbf{X}) \propto p(\mathbf{X} | \mu, \lambda) p(\mu, \lambda)$

• Plugging in the expressions for $p(\mathbf{X}|\mu, \lambda)$ and $p(\mu, \lambda)$, we get

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

The above's posterior's parameters will be

$$\mu_{N} = \frac{\kappa_{0}\mu_{0} + N\bar{x}}{\kappa_{0} + N}$$

$$\kappa_{N} = \kappa_{0} + N$$

$$\alpha_{N} = \alpha_{0} + N/2$$

$$\beta_{N} = \beta_{0} + \frac{1}{2} \sum_{n=1}^{N} (x_{n} - \bar{x})^{2} + \frac{\kappa_{0}N(\bar{x} - \mu_{0})^{2}}{2(\kappa_{0} + N)}$$



(For full derivation of posterior, refer to "Conjugate Bayesian analysis of the Gaussian distribution" - Murphy (2007))

Other Quantities of Interest

We saw that the joint posterior for mean and precision is NG

$$\mathcal{P}(\mu,\lambda|\mathbf{X}) = \mathsf{NG}(\mu_{N},\kappa_{N},\alpha_{N},\beta_{N}) = \mathcal{N}(\mu|\mu_{N},(\kappa_{N}\lambda)^{-1})\mathsf{Gamma}(\lambda|lpha_{N},eta_{N})$$

 ${\ }$ From the above, we can also obtain the marginal posteriors for μ and λ

$$p(\lambda|\mathbf{X}) = \int p(\mu, \lambda|\mathbf{X}) d\mu = \operatorname{Gamma}(\lambda|\alpha_N, \beta_N)$$

$$p(\mu|\mathbf{X}) = \int p(\mu, \lambda|\mathbf{X}) d\lambda = \int p(\mu|\lambda, \mathbf{X}) p(\lambda|\mathbf{X}) d\lambda = \underbrace{t_{2\alpha_N}(\mu|\mu_N, \beta_N/(\alpha_N\kappa_N))}_{\text{t distribution}}$$

- Marginal likelihood of the model $p(\mathbf{X}) = \frac{\Gamma(\alpha_N)}{\Gamma(\alpha_0)} \frac{\beta_0^{\alpha_0}}{\beta_N^{\alpha_N}} \left(\frac{\kappa_0}{\kappa_N}\right)^{\frac{1}{2}} (2\pi)^{-N/2} \qquad \text{Marginal lik has closed form}$ $p(\mathbf{X}) = \frac{\Gamma(\alpha_N)}{\Gamma(\alpha_0)} \frac{\beta_0^{\alpha_0}}{\beta_N^{\alpha_N}} \left(\frac{\kappa_0}{\kappa_N}\right)^{\frac{1}{2}} (2\pi)^{-N/2} \qquad \text{Marginal lik has closed form}$ $p(\mathbf{X}) = \frac{\Gamma(\alpha_N)}{\Gamma(\alpha_0)} \frac{\beta_0^{\alpha_0}}{\beta_N^{\alpha_N}} \left(\frac{\kappa_0}{\kappa_N}\right)^{\frac{1}{2}} (2\pi)^{-N/2} \qquad \text{Marginal lik has closed form}$
- PPD of a new observation x_*

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



An Aside: Student-t distribution

An infinite sum of Gaussian distributions, with same means but different precisions

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Same as saying that we are integrating out the precision parameter of a Gaussian with the mean held as fixed

• $\nu > 0$ is called the degree of freedom, μ is the mean, and σ^2 is the scale



Inferring Params of Gaussian: Some Other Cases

- We only considered parameter estimation for univariate Gaussian distribution
 - The approach also extends to inferring parameters of a multivariate Gaussian
 - For the unknown mean and precision matrix, normal-Wishart can be used as prior
- Posterior updates have forms similar to that in the univariate case
- When working with mean-variance, can use normal-inverse gamma as conjugate prior
 For multivariate Gaussian, can use normal-inverse Wishart for mean-covariance pair
- Other priors can also be used as well when inferring parameters of Gaussians, e.g.,
 normal-Inverse χ^2 commonly used in Statistics community for scalar mean-variance estimation
- May also refer to "Conjugate Bayesian analysis of the Gaussian distribution" Murphy (2007) for various examples and more detailed derivations



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Linear Gaussian Model

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

Independently added

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and drawn from

 $\mathcal{N}(\boldsymbol{\epsilon}|\boldsymbol{0},\boldsymbol{L}^{-1})$

 $x = Az + b + \epsilon$

Easy to see that, conditioned on z, x too has a Gaussian distribution

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

- A Linear Gaussian Model. Very commonly encountered in probabilistic modeling
- The following two distributions are of interest. Assuming $\Sigma = (\Lambda + A^{T}LA)^{-1}$

$$p(z|x) = \frac{p(x|z)p(z)}{p(z)} = \mathcal{N}(z|\Sigma\{A^{\top}L(x-b)+\Lambda\mu\},\Sigma)$$
If $p(z)$ is a prior and $p(x|z)$ is likelihood then this is the posterior
$$p(x) = \int p(x|z)p(z)dz = \mathcal{N}(x|A\mu+b,A\Lambda^{-1}A^{\top}+L^{-1})$$
If $p(z)$ is a prior and $p(x|z)$ is likelihood then this is the marginal likelihood then this is the marginal likelihood then the posterior

Exercise: Prove the above results (PRML Chap. 2 contains a proof)

Applications of Gaussian-based Models

- Gaussians and Linear Gaussian Models widely used in probabilistic models, e.g.,
 - Probability density estimation: Given $x_1, x_2, ..., x_N$, estimate p(x) assuming Gaussian lik./noise
 - Given N sensor obs. $\{x_n\}_{n=1}^N$ with $x_n = \mu + \epsilon_n$ (zero-mean Gaussian noise ϵ_n) estimate the underlying true value μ (possibly along with the variance of the estimate of μ)
 - Estimating missing data: $p(x_n^{\text{miss}}|x_n^{\text{obs}})$ or $\mathbb{E}[x_n^{\text{miss}}|x_n^{\text{obs}}]$
 - Linear Regression with Gaussian Likelihood
 Training feat. mat
 Training responses
 Training $y = Xw + \epsilon$ The prior p(w) i.i.d. Gaussian noise
 - Linear latent variable models (probabilistic PCA, factor analysis, Kalman filters) and their mixtures
 - Gaussian Processes (GP) extensively use Gaussian conditioning and marginalization rules

y = f + noise (GP assumes $f = [f(x_1), \dots, f(x_N)]$ is jointly Gaussian)

More complex models where parts of the model use Gaussian likelihoods/priors



Probabilistic Linear Regression



Note: Only y_n being modeled, not 16 $\boldsymbol{x_n}$ (discriminative model). A conditional model where y_n is being modeled, conditioned on \boldsymbol{x}_n

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- Assume training data $\{x_n, y_n\}_{n=1}^N$, with features $x_n \in \mathbb{R}^D$ and responses $y_n \in \mathbb{R}$
- Assume each y_n generated by a noisy linear model with wts $\mathbf{w} = [w_1, \dots, w_n]$

mean $\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}_{n}$

$$y_n = oldsymbol{w}^{ op} oldsymbol{x}_n + \epsilon_n$$
where $\epsilon_n \sim \mathcal{N}(\mathbf{0}, eta^{-1})$

- Precision (β) variance of the Gaussian noise tells is how noisy the outputs are (i.e., how far from the mean they are)
- Other noise models also possible (e.g., Laplace distribution for noise)



Probabilistic Linear Regression



 $N \times 1$ response vector

regularizer with λ being the reg. constant

Neq. log-prior corresponds to ℓ_2

Plate diagram. Hyperparams (λ, β) are fixed and not shown for brevity

 $N \times D$ feature matrix

0.35

0.15

The linear model with Gaussian noise corresponds to a Gaussian likelihood

$$p(y_n | \mathbf{x}_n, \mathbf{w}, \beta) = \mathcal{N}(y_n | \mathbf{w}^\top \mathbf{x}_n, \beta^{-1})$$
 NLL corresponds to squared loss prop. to $(y_n - \mathbf{w}^\top \mathbf{x}_n)^2$

Assuming responses to be i.i.d. given features and weights

$$p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(y_n | \mathbf{w}^{\top} \mathbf{x}_n, \beta^{-1}) = \mathcal{N}(\mathbf{y} | \mathbf{X} \mathbf{w}, \beta^{-1} \mathbf{I}_N)$$

The above is equivalent to the following

$$y = Xw + \epsilon$$
 where $\epsilon \sim \mathcal{N}(0, \beta^{-1}\mathbf{I}_{N})$

Assume the following Gaussian prior on w,

$$p(\boldsymbol{w}) = \prod_{d=1}^{D} p(w_d) = \prod_{d=1}^{D} \mathcal{N}(w_d | 0, \lambda^{-1}) = \mathcal{N}(\boldsymbol{w} | 0, \lambda^{-1} \mathbf{I}_D) = \left(\frac{\lambda}{2\pi}\right)^{\frac{D}{2}} \exp\left[-\frac{\lambda}{2} \boldsymbol{w}^\top \boldsymbol{w}\right]$$

Can even use different λ 's for different
 w_d 's. Useful in sparse modeling (later)

• Then $y = Xw + \epsilon$ is simply a linear Gaussian model

Can use all the rules of linear Gaussian models to perform inference/predictions ③

The precision λ of the Gaussian prior controls how aggressively the prior pushes the elements towards mean (0)

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 $p(w_d) = \mathcal{N}(w_d | 0, \lambda^{-1})$