

COMS 4721: Machine Learning for Data Science

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Model

Have vector $y \in \mathbb{R}^n$ and covariates matrix $X \in \mathbb{R}^{n \times d}$. The i th row of y and X correspond to the i th observation (y_i, x_i) .

In a Bayesian setting, we model this data as:

$$\textbf{Likelihood} : y \sim N(Xw, \sigma^2 I)$$

$$\textbf{Prior} : w \sim N(0, \lambda^{-1} I)$$

The unknown model variable is $w \in \mathbb{R}^d$.

- ▶ The “likelihood model” says how well the observed data agrees with w .
- ▶ The “model prior” is our prior belief (or constraints) on w .

This is called Bayesian linear regression because we have defined a prior on the unknown parameter and will try to learn its posterior.

Earlier we estimated w using MAP (or under posterior)

MAP solution

MAP inference returns the maximum of the log joint likelihood.

$$\textbf{Joint Likelihood} : \quad p(y, w|X) = p(y|w, X)p(w)$$

Using Bayes rule, we see that this point also maximizes the **posterior** of w .

$$\begin{aligned} w_{\text{MAP}} &= \arg \max_w \ln p(w|y, X) \\ &= \arg \max_w \ln p(y|w, X) + \ln p(w) - \ln p(y|X) \\ &= \arg \max_w -\frac{1}{2\sigma^2}(y - Xw)^T(y - Xw) - \frac{\lambda}{2}w^T w + \text{const.} \end{aligned}$$

We saw that this solution for w_{MAP} is the same as for ridge regression:

$$w_{\text{MAP}} = (\lambda\sigma^2 I + X^T X)^{-1} X^T y \quad \Leftrightarrow \quad w_{\text{RR}}$$

Point estimates

w_{MAP} and w_{ML} are referred to as point estimates of the model parameters.

They find a specific value (point) of the vector w that maximizes an objective function — the posterior (MAP) or likelihood (ML).

- ▶ **ML:** Only considers the data model: $p(\underline{y}|w, X)$.
- ▶ **MAP:** Takes into account model prior: $p(y, w|X) = p(\underline{y}|w, X)p(w)$.

Bayesian inference

Bayesian inference goes one step further by characterizing uncertainty about the values in w using Bayes rule.

BAYES RULE AND LINEAR REGRESSION

Posterior calculation

Since w is a continuous-valued random variable in \mathbb{R}^d , Bayes rule says that the *posterior* distribution of w given y and X is

$$p(w|y, X) = \frac{p(y|w, X)p(w)}{\int_{\mathbb{R}^d} p(y|w, X)p(w) dw}$$

That is, we get an updated distribution on w through the transition

prior \rightarrow likelihood \rightarrow posterior

Quote: “The posterior of ___ is proportional to the likelihood times the prior.”

FULLY BAYESIAN INFERENCE

Bayesian linear regression

In this case, we can update the posterior distribution $p(w|y, X)$ analytically.

We work with the proportionality first:

$$\begin{aligned} p(w|y, X) &\propto p(y|w, X)p(w) \\ &\propto \left[e^{-\frac{1}{2\sigma^2} (y-Xw)^T (y-Xw)} \right] \left[e^{-\frac{\lambda}{2} w^T w} \right] \\ &\propto e^{-\frac{1}{2} \{ w^T (\lambda I + \sigma^{-2} X^T X) w - 2\sigma^{-2} w^T X^T y \}} \end{aligned}$$

The \propto sign lets us multiply and divide this by anything *as long as it doesn't contain w* . We've done this twice above. Therefore the 2nd line \neq 3rd line.

BAYESIAN INFERENCE FOR LINEAR REGRESSION

We need to normalize:

$$p(w|y, X) \propto e^{-\frac{1}{2}\{w^T(\lambda I + \sigma^{-2}X^T X)w - 2\sigma^{-2}w^T X^T y\}}$$

There are two key terms in the exponent:

$$\underbrace{w^T(\lambda I + \sigma^{-2}X^T X)w}_{\text{quadratic in } w} - \underbrace{2w^T X^T y/\sigma^2}_{\text{linear in } w}$$

We can conclude that $p(w|y, X)$ is Gaussian. Why?

1. We can multiply and divide by anything not involving w .
2. A Gaussian has $(w - \mu)^T \Sigma^{-1} (w - \mu)$ in the exponent.
3. We can “complete the square” by adding terms not involving w .

BAYESIAN INFERENCE FOR LINEAR REGRESSION

Compare: In other words, a Gaussian looks like:

$$p(w|\mu, \Sigma) = \frac{1}{(2\pi)^{\frac{d}{2}} |\Sigma|^{\frac{1}{2}}} e^{-\frac{1}{2}(w^T \Sigma^{-1} w - 2w^T \Sigma^{-1} \mu + \mu^T \Sigma^{-1} \mu)}$$

and we've shown for some setting of Z that

$$p(w|y, X) = \frac{1}{Z} e^{-\frac{1}{2}(w^T (\lambda I + \sigma^{-2} X^T X) w - 2w^T X^T y / \sigma^2)}$$

Conclude: What happens if in the above Gaussian we define:

$$\Sigma^{-1} = (\lambda I + \sigma^{-2} X^T X), \quad \Sigma^{-1} \mu = X^T y / \sigma^2 ?$$

Using these specific values of μ and Σ we only need to set

$$Z = (2\pi)^{\frac{d}{2}} |\Sigma|^{\frac{1}{2}} e^{\frac{1}{2} \mu^T \Sigma^{-1} \mu}$$

The posterior distribution

Therefore, the posterior distribution of w is:

$$\begin{aligned} p(w|y, X) &= N(w|\mu, \Sigma), \\ \Sigma &= (\lambda I + \sigma^{-2} X^T X)^{-1}, \\ \mu &= (\lambda \sigma^2 I + X^T X)^{-1} X^T y \quad \Leftarrow \quad w_{\text{MAP}} \end{aligned}$$

Things to notice:

- ▶ $\mu = w_{\text{MAP}}$ after a redefinition of the regularization parameter λ .
- ▶ Σ captures uncertainty about w , like $\text{Var}[w_{\text{LS}}]$ and $\text{Var}[w_{\text{RR}}]$ did before.
- ▶ However, now we have a full probability distribution on w .

Least Squares & RR also captured some uncertainty of w ,
but now we have actually a functional distribution that
we can work with to calculate prob, have a density function for w etc.



Understanding w

We saw how we could calculate the variance of w_{LS} and w_{RR} . Now we have an entire distribution. Some questions we can ask are:

Q: Is $w_i > 0$ or $w_i < 0$? Can we confidently say $w_i \neq 0$?

A: Use the *marginal posterior distribution*: $w_i \sim N(\mu_i, \Sigma_{ii})$.

Q: How do w_i and w_j relate?

A: Use their joint marginal posterior distribution:

$$\begin{bmatrix} w_i \\ w_j \end{bmatrix} \sim N \left(\begin{bmatrix} \mu_i \\ \mu_j \end{bmatrix}, \begin{bmatrix} \Sigma_{ii} & \Sigma_{ij} \\ \Sigma_{ji} & \Sigma_{jj} \end{bmatrix} \right)$$

Having the distribution we can comment about >0 or <0 of ranges, confidence intervals.

Predicting new data

The posterior $p(w|y, X)$ is perhaps most useful for predicting new data.

PREDICTING NEW DATA

PREDICTING NEW DATA

Recall: For a new pair (x_0, y_0) with x_0 measured and y_0 unknown, we can predict y_0 using x_0 and the LS or RR (i.e., ML or MAP) solutions:

$$y_0 \approx x_0^T w_{\text{LS}} \quad \text{or} \quad y_0 \approx x_0^T w_{\text{RR}}$$

With Bayes rule, we can make a *probabilistic* statement about y_0 :

$$\begin{aligned} p(y_0|x_0, y, X) &= \int_{\mathbb{R}^d} p(y_0, w|x_0, y, X) dw \\ &= \int_{\mathbb{R}^d} p(y_0|w, x_0, y, X) p(w|x_0, y, X) dw \end{aligned}$$

Notice that *conditional independence* lets us write

$$p(y_0|w, x_0, y, X) = \underbrace{p(y_0|w, x_0)}_{\text{likelihood}} \quad \text{and} \quad p(w|x_0, y, X) = \underbrace{p(w|y, X)}_{\text{posterior}}$$

PREDICTING NEW DATA

Predictive distribution (intuition)

This is called the *predictive distribution*:

$$p(y_0|x_0, y, X) = \int_{\mathbb{R}^d} \underbrace{p(y_0|x_0, w)}_{\text{likelihood}} \underbrace{p(w|y, X)}_{\text{posterior}} dw$$

Intuitively:

1. Evaluate the likelihood of a value y_0 given x_0 for a particular w .
2. Weight that likelihood by our current belief about w given data (y, X) .
3. Then sum (integrate) over all possible values of w .

PREDICTING NEW DATA

We know from the model and Bayes rule that

$$\text{Model: } p(y_0|x_0, w) = N(y_0|x_0^T w, \sigma^2),$$

$$\text{Bayes rule: } p(w|y, X) = N(w|\mu, \Sigma).$$

With μ and Σ calculated on a previous slide.

The predictive distribution can be calculated exactly with these distributions.
Again we get a Gaussian distribution:

$$p(y_0|x_0, y, X) = N(y_0|\mu_0, \sigma_0^2),$$

$$\mu_0 = x_0^T \mu,$$

$$\sigma_0^2 = \sigma^2 + x_0^T \Sigma x_0.$$

Notice that the expected value is the MAP prediction since $\mu_0 = x_0^T w_{\text{MAP}}$, but we now quantify our confidence in this prediction with the variance σ_0^2 .

ACTIVE LEARNING

Bayesian learning is naturally thought of as a sequential process. That is, the posterior after seeing some data becomes the prior for the next data.

Let y and X be “old data” and y_0 and x_0 be some “new data”. By Bayes rule

$$p(w|y_0, x_0, y, X) \propto p(y_0|w, x_0) \underline{p(w|y, X)}.$$

The posterior after (y, X) has become the prior for (y_0, x_0) .

Simple modifications can be made sequentially in this case:

$$p(w|y_0, x_0, y, X) = N(w|\mu, \Sigma),$$

$$\Sigma = (\lambda I + \sigma^{-2}(x_0 x_0^T + \sum_{i=1}^n x_i x_i^T))^{-1},$$

$$\mu = (\lambda \sigma^2 I + (x_0 x_0^T + \sum_{i=1}^n x_i x_i^T))^{-1} (x_0 y_0 + \sum_{i=1}^n x_i y_i).$$

INTELLIGENT LEARNING

Notice we could also have written

$$p(w|y_0, x_0, y, X) \propto p(y_0, y|w, X, x_0)p(w)$$

but often we want to use the sequential aspect of inference to help us learn.

Learning w and making predictions for new y_0 is a two-step procedure:

- ▶ Form the predictive distribution $p(y_0|x_0, y, X)$.
- ▶ Update the posterior distribution $p(w|y, X, y_0, x_0)$.

Question: Can we learn $p(w|y, X)$ intelligently?

That is, if we're in the situation where we can pick which y_i to measure with knowledge of $\mathcal{D} = \{x_1, \dots, x_n\}$, can we come up with a good strategy?

An “active learning” strategy

Imagine we already have a measured dataset (y, X) and posterior $p(w|y, X)$. We can construct the predictive distribution for every remaining $x_0 \in \mathcal{D}$.

$$\begin{aligned}p(y_0|x_0, y, X) &= N(y_0|\mu_0, \sigma_0^2), \\ \mu_0 &= x_0^T \mu, \\ \sigma_0^2 &= \sigma^2 + x_0^T \Sigma x_0.\end{aligned}$$

For each x_0 , σ_0^2 tells how confident we are. This suggests the following:

1. Form predictive distribution $p(y_0|x_0, y, X)$ for all unmeasured $x_0 \in \mathcal{D}$
2. Pick the x_0 for which σ_0^2 is largest and measure y_0
3. Update the posterior $p(w|y, X)$ where $y \leftarrow (y, y_0)$ and $X \leftarrow (X, x_0)$
4. Return to #1 using the updated posterior

Entropy (i.e., uncertainty) minimization

When devising a procedure such as this one, it's useful to know what *objective function* is being optimized in the process.

We introduce the concept of the *entropy* of a distribution. Let $p(z)$ be a continuous distribution, then its (differential) entropy is:

$$\mathcal{H}(p) = - \int p(z) \ln p(z) dz.$$

This is a measure of the spread of the distribution. More positive values correspond to a more “uncertain” distribution (larger variance).

The entropy of a multivariate Gaussian is

$$\mathcal{H}(N(w|\mu, \Sigma)) = \frac{1}{2} \ln \left((2\pi e)^d |\Sigma| \right).$$

ACTIVE LEARNING

The entropy of a Gaussian changes with its covariance matrix. With sequential Bayesian learning, the covariance transitions from

$$\text{Prior : } (\lambda I + \sigma^{-2} X^T X)^{-1} \equiv \Sigma$$

\Downarrow

$$\text{Posterior : } (\lambda I + \sigma^{-2}(x_0 x_0^T + X^T X))^{-1} \equiv (\Sigma^{-1} + \sigma^{-2} x_0 x_0^T)^{-1}$$

Using a “rank-one update” property of the determinant, we can show that the entropy of the prior $\mathcal{H}_{\text{prior}}$ relates to the entropy of the posterior $\mathcal{H}_{\text{post}}$ as:

$$\mathcal{H}_{\text{post}} = \mathcal{H}_{\text{prior}} - \frac{d}{2} \ln(1 + \sigma^{-2} x_0^T \Sigma x_0)$$

Therefore, the x_0 that minimizes $\mathcal{H}_{\text{post}}$ also maximizes $\sigma^2 + x_0^T \Sigma x_0$. We are minimizing \mathcal{H} myopically, so this is called a “greedy algorithm”.

MODEL SELECTION

SELECTING λ

We've discussed λ as a “nuisance” parameter that can impact performance.

Bayes rule gives a principled way to do this via *evidence maximization*:

$$p(w|y, X, \lambda) = \underbrace{p(y|w, X)}_{\text{likelihood}} \underbrace{p(w|\lambda)}_{\text{prior}} / \underbrace{p(y|X, \lambda)}_{\text{evidence}}.$$

The “evidence” gives the likelihood of the data with w integrated out. It's a measure of how good our model and parameter assumptions are.

SELECTING λ

If we want to set λ , we can also do it by maximizing the evidence.¹

$$\hat{\lambda} = \arg \max_{\lambda} \ln p(y|X, \lambda).$$

We notice that this looks exactly like maximum likelihood, and it is:

Type-I ML: Maximize the likelihood over the “main parameter” (w).

Type-II ML: Integrate out “main parameter” (w) and maximize over the “hyperparameter” (λ). Also called *empirical Bayes*.

The difference is only in their perspective.

This approach requires us to solve this integral, but we often can't for more complex models. Cross-validation is an alternative that's always available.

¹We can show that the distribution of y is $p(y|X, \lambda) = N(y|0, \sigma^2 I + \lambda^{-1} X X^T)$. This would require an algorithm to maximize over λ . The key point here is the general technique.