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 ith row of y and X correspond to the ith observation (y_i, x_i).

In a Bayesian setting, we model this data as:

$$\textbf{Likelihood}: \quad y \sim N(Xw, \sigma^2 I)$$
$$\textbf{Prior}: \quad w \sim N(0, \lambda^{-1} I)$$

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.

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 vs Bayesian inference

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: $p(y|w, X)$.
- **MAP**: Takes into account model prior: $p(y, w|X) = p(y|w, X)p(w)$.

Bayesian inference

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

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

$$\text{prior} \quad \rightarrow \quad \text{likelihood} \quad \rightarrow \quad \text{posterior}$$

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

Bayesian linear regression

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

We work with the proportionality first:

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

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.

We need to normalize:

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

There are two key terms in the exponent:

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

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.

Compare: In other words, a Gaussian looks like this:

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

and we've shown that, for some setting of Z,

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

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

$$\Sigma^{-1} = (\lambda I + \sigma^{-2}X^TX), \qquad \mu = (\lambda\sigma^2 I + X^TX)^{-1}X^Ty\,?$$

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

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

The posterior distribution

Therefore, the posterior distribution of w is:

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

Things to notice:

- $\mu = w_{\text{MAP}}$
- 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.

USES OF THE POSTERIOR DISTRIBUTION

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:

$$\left[\begin{array}{c} w_i \\ w_j \end{array}\right] \sim N\left(\left[\begin{array}{c} \mu_i \\ \mu_j \end{array}\right], \left[\begin{array}{cc} \Sigma_{ii} & \Sigma_{ij} \\ \Sigma_{ji} & \Sigma_{jj} \end{array}\right]\right)$$

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

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

Predictive distribution (intuition)

This is called the *predictive distribution*:

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

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

$$\begin{aligned}\text{Model:} \quad p(y_0|x_0, w) &= N(y_0|x_0^T w, \sigma^2),\\ \text{Bayes rule:} \quad p(w|y, X) &= N(w|\mu, \Sigma).\end{aligned}$$

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:

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

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

PRIOR $\rightarrow$ POSTERIOR $\rightarrow$ PRIOR

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

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

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

Simple modifications can be made sequentially in this case:

$$\begin{aligned} p(w|y_0, x_0, y, X) &= N(w|\mu, \Sigma), \\ \Sigma &= (\lambda I + \sigma^{-2}(x_0 x_0^T + \textstyle\sum_{i=1}^n x_i x_i^T))^{-1}, \\ \mu &= (\lambda\sigma^2 I + (x_0 x_0^T + \textstyle\sum_{i=1}^n x_i x_i^T))^{-1}(x_0 y_0 + \textstyle\sum_{i=1}^n x_i y_i). \end{aligned}$$

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 $\mathcal{D} = \{x_1, \ldots, x_n\}$, can we come up with a good strategy?

An "active learning" strategy

Imagine we already have data (y, X) for $X \subset \mathcal{D}$, and the 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

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

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

$$\begin{aligned}
\text{Prior}: &\quad (\lambda I + \sigma^{-2}X^TX)^{-1} && \equiv \; \Sigma \\
&\qquad\qquad \Downarrow \\
\text{Posterior}: &\quad (\lambda I + \sigma^{-2}(x_0x_0^T + X^TX))^{-1} && \equiv \; (\Sigma^{-1} + \sigma^{-2}x_0x_0^T)^{-1}
\end{aligned}$$

Using the “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*:

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

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.

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