Data-Driven Design & Analyses of Structures & Materials (3dasm)

Lecture 11

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Outline for today

- Derivation of different Linear Regression models
    - Picking up where we left off in Lectures 8 and 9.

Reading material: This notebook + Chapter 11 of the book.

Recap of Lectures 8 and 9

Recall our view of Linear regression models from a Bayesian perspective: it's all about the choice of **likelihood** and **prior**!

Likelihood	Prior (on the weights)	Posterior	Name of the model	Book section
Gaussian	Uniform	Point estimate	Least Squares regression	11.2.2
Gaussian	Gaussian	Point estimate	Ridge regression	11.3
Gaussian	Laplace	Point estimate	Lasso regression	11.4
Student-t	Uniform	Point estimate	Robust regression	11.6.1
Laplace	Uniform	Point estimate	Robust regression	11.6.2
Gaussian	Gaussian	Gaussian	Bayesian linear regression	11.7

Let's continue along the lines of Lectures 8 and 9, and derive a few of these models for the multidimensional case.

We are now totally prepared to derive any ML model in any dimension!
In Lecture 8 and its Homework we derived linear regression models using 1D input x, 1D output y, and a polynomial basis function $\boldsymbol{\phi}(x)$.
We will quickly recap what we did then, and then show how this generalizes to multidimensional inputs $\mathbf{x}$ and for any kind of basis function $\boldsymbol{\phi}(\mathbf{x})$.

- Note: without loss of generality, we will keep considering a single output y.

Linear Least Squares: Linear regression with Gaussian likelihood, Uniform prior and posterior via Point estimate

Likelihood	Prior (on the weights)	Posterior	Name of the model	Book section
Gaussian	Uniform	Point estimate	Least Squares regression	11.2.2

This model assumes a Gaussian observation distribution with constant variance and "linear" mean (recall: linear in the unknowns $\mathbf{z}$). If considering 1D input x and 1D output y the model is written as:

1. Gaussian observation distribution: $p(y|x,\mathbf{z}) = \mathcal{N}(y|\mu_{y|z} = \mathbf{w}^T\boldsymbol{\phi}(x), \sigma^2_{y|z} = \sigma^2)$

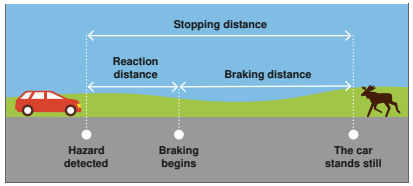
where $\mathbf{z} = (\mathbf{w}, \sigma)$ are all the unknown model parameters (hidden rv's).

1. Uniform prior distribution for each hidden rv in $\mathbf{z}$: $p(\mathbf{z}) \propto 1$
2. MLE point estimate for posterior: $\hat{\mathbf{z}}_{\text{mle}} = \underset{z}{\text{argmin}} \left[-\sum_{i=1}^{N} \log p(y = y_i | x = x_i, \mathbf{z}) \right]$

Final prediction is given by the PPD: $p(y^*|x^*, \mathcal{D}) = \int p(y^*|x^*, \mathbf{z}) \delta(\mathbf{z} - \hat{\mathbf{z}}) dz = p(y^*|x^*, \mathbf{z} = \hat{\mathbf{z}})$

Recall the car stopping distance problem

Let's focus (again) on our favorite problem, but now we will not keep the velocity of the car x fixed.
If we knew the "ground truth" of this problem, then it would be given by:
$y = z_1 \cdot x + z_2 \cdot x^2$



- y is the **output**: the car stopping distance (in meters)
- z_1 is a hidden variable: an rv representing the driver's reaction time (in seconds)
- z_2 is another hidden variable: an rv that depends on the coefficient of friction, the inclination of the road, the weather, etc. (in $\text{m}^{-1}\text{s}^{-2}$).
- x is the **input**: constant car velocity (in m/s).

Remember: We don't know the "true" nature of the unknowns (the $\mathbf{z}$ rv's). For example, they could be $z_1 \sim \mathcal{N}(\mu_{z_1} = 1.5, \sigma^2_{z_1} = 0.5^2)$, and $z_2 \sim \delta(z_2 - 0.1)$, i.e. z_2 could just be $z_2 = 0.1$. Either way, when we don't know them we assume that they are rv's with some prior distribution and we use Bayesian inference (or point estimates) to determine a posterior estimate.

Unsurprisingly, in Lecture 9 we saw that a linear model with a **quadratic polynomial basis function** predicts the stopping distance for this problem very well. For example, we considered the following model:

1. Gaussian observation distribution: $p(y|x, \mathbf{z}) = \mathcal{N}(y|\mu_{y|z} = \mathbf{w}^T\boldsymbol{\phi}(x), \sigma^2_{y|z} = \sigma^2)$

where $\mathbf{z} = (\mathbf{w}, \sigma)$ are all the hidden rv's of the model, i.e. the model parameters.

- the vector $\mathbf{w} = [w_0, w_1, w_2 \ldots, w_{M-1}]^T$ includes the **bias** term w_0 and the remaining **weights** w_m with $m = 1, \ldots, M-1$.
- the vector $\boldsymbol{\phi}(x) = [1, x, x^2, \ldots, x^{M-1}]^T$ includes the **basis functions**, which for a 1D input x correspond to a polynomial of degree $M-1$. So, when $M = 3$ we have a quadratic polynomial basis for 1D input x, i.e. $\mu_{y|z} = w_0 + w_1 x + w_2 x^2$.

1. Uniform prior distribution for each hidden rv in $\mathbf{z}$: $p(\mathbf{z}) \propto 1$

1. MLE point estimate for posterior: $\hat{\mathbf{z}}_{\text{mle}} = \underset{z}{\text{argmin}} \left[-\sum_{n=1}^{N} \log p(y = y_n|x_n, \mathbf{z}) \right]$

For other problems, the polynomial degree of the basis functions may need to be different.

- For example, in Lecture 10 we saw that when the ground truth was $x \sin x$ then the polynomial basis functions need to have a higher degree. However, even then the approximation is not brilliant because the ground truth is not really a polynomial!

There are other basis functions that can be adopted. For example, spline basis functions (Section 11.5 in the book), among many other possibilities (kernels!).

As we also mentioned, as long as the basis functions $\boldsymbol{\phi}(x)$ do not depend on any rv $\mathbf{z}$ and the mean of observation distribution is defined linearly as a function of the rv's, then we still have a linear regression model.

But now let's consider problems that still have only one output y but that can have multiple inputs $\mathbf{x} = [x_1, x_2, \ldots, x_D]^T$ where x_d is feature d and where $d = 1, \ldots, D$.

In this case, we can write the linear regression model for multi-dimensional input as:

1. Gaussian observation distribution: $p(y|\mathbf{x}, \mathbf{z}) = \mathcal{N}(y|\mu_{y|z} = \mathbf{w}^T\boldsymbol{\phi}(\mathbf{x}), \sigma^2_{y|z} = \sigma^2)$

where $\mathbf{z} = (\mathbf{w}, \sigma)$ are all the hidden rv's of the model, i.e. the model parameters.

- the vector $\mathbf{w} = [w_0, w_1, w_2 \ldots, w_{M-1}]^T$ includes the **bias** term w_0 and the remaining **weights** w_m with $m = 0, \ldots, M-1$.
- and the basis functions remain a vector but where each element also acts on a vector $\mathbf{x}$, where x_d has D features: $\boldsymbol{\phi}(\mathbf{x}) = [\phi_0(\mathbf{x}), \phi_1(\mathbf{x}), \phi_2(\mathbf{x}) \ldots, \phi_{M-1}(\mathbf{x})]^T$

For example, for a 2D input $\mathbf{x} = [x_1, x_2]^T$ the quadratic polynomial basis has $M = 6$ leading to:

$$\mu_{y|z} = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_1 x_2 + w_4 x_1^2 + w_5 x_2^2$$

and where the remaining choices for the linear regression model remain the same:

1. Uniform prior distribution for each hidden rv in $\mathbf{z}$: $p(\mathbf{z}) \propto 1$
2. MLE point estimate for posterior: $\hat{\mathbf{z}}_{\text{mle}} = \underset{z}{\text{argmin}} \left[-\sum_{n=1}^{N} \log p(y = y_n | \mathbf{x} = \mathbf{x}_n, \mathbf{z}) \right]$

Final prediction is given by the PPD:

$$p(y^* | \mathbf{x}^*, \mathcal{D}) = \int p(y^* | \mathbf{x}^*, \mathbf{z}) \delta(\mathbf{z} - \hat{\mathbf{z}}) dz = p(y^* | \mathbf{x}^*, \mathbf{z} = \hat{\mathbf{z}})$$

Therefore, we are capable of predicting the PPD by discovering the unknowns $\mathbf{z}$ via the point estimate of the posterior, which requires solving the argmin of the negative log likelihood.

Now, let's focus on estimating the unknowns $\mathbf{z}$ via the MLE point estimate of the posterior (maximum likelihood estimation).
As we saw in Lecture 8, finding the MLE is the same as finding the location of the minimum of the negative log likelihood.
Since our observation distribution is a multivariate Gaussian,
$p(y|\mathbf{x}, \mathbf{z}) = \mathcal{N}(y|\mu_{y|z} = \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}), \sigma^2_{y|z} = \sigma^2)$
then the likelihood is given by (Lecture 5 but now with vectors):

$$p(y = \mathcal{D}_y|\mathbf{x} = \mathcal{D}_x, \mathbf{z}) = \prod_{n=1}^{N} p(y = y_n|\mathbf{x} = \mathbf{x}_n, \mathbf{z}) \tag{1}$$

$$= p(y = y_1|\mathbf{x} = \mathbf{x}_1, \mathbf{z}) p(y = y_2|\mathbf{x} = \mathbf{x}_2, \mathbf{z}) \cdots p(y = y_N|\mathbf{x} = \mathbf{x}_N, \mathbf{z}) \tag{2}$$

which we already know that is also a multivariate Gaussian (unnormalized).

But, since we are not going fully Bayesian, the only thing we need to estimate is the location of the maximum of the likelihood (point estimate!):

$$\hat{\mathbf{z}}_{\text{mle}} = \underset{z}{\text{argmin}} \left[\text{NLL}(\mathbf{z})\right] \tag{3}$$

$$= \underset{z}{\text{argmin}} \left[-\sum_{n=1}^{N} \log p(y = y_n | \mathbf{x} = \mathbf{x}_n, \mathbf{z})\right] \tag{4}$$

In Lecture 9 we allowed scikit-learn to find the minimum for us! But today we will actually determine this minimum...
You already did this in the Homework of Lecture 8 for the 1D case with a linear polynomial basis and fixing x. The multivariate case for a general basis function and for different $\mathbf{x}$ is just as easy! Especially when considering the variance of the observation distribution to be the same everywhere!

$$\hat{\mathbf{z}}_{\text{mle}} = \underset{z}{\text{argmin}} \left[-\sum_{n=1}^{N} \log p(y = y_n | \mathbf{x} = \mathbf{x}_n, \mathbf{z}) \right] \tag{5}$$

$$= \underset{z}{\text{argmin}} \left[-\sum_{n=1}^{N} \log \left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{ -\frac{1}{2\sigma^2} \left[y_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) \right]^2 \right\} \right) \right] \tag{6}$$

$$= \underset{z}{\text{argmin}} \left[\frac{N}{2} \log \left(2\pi\sigma^2 \right) + \frac{1}{2\sigma^2} \sum_{n=1}^{N} \left[y_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) \right]^2 \right] \tag{7}$$

where we recall that the unknowns are $\mathbf{z} = (\mathbf{w}, \sigma)$.

To find the minimum location we need to take the gradient of the $\mathrm{NLL}(\mathbf{z})$ wrt $\mathbf{z}$ and equal it to zero:

$$\nabla_{\mathbf{z}} \mathrm{NLL}(\mathbf{z}) = \mathbf{0}$$

which can be written as,

$$\begin{bmatrix} \frac{\partial \mathrm{NLL}(\mathbf{z})}{\partial w_0} \\ \frac{\partial \mathrm{NLL}(\mathbf{z})}{\partial w_1} \\ \vdots \\ \frac{\partial \mathrm{NLL}(\mathbf{z})}{\partial w_{M-1}} \\ \frac{\partial \mathrm{NLL}(\mathbf{z})}{\partial \sigma^2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}$$

We can first solve this system of equations wrt $\mathbf{w}$, and then solve wrt σ

Then, solving first for the weights $\mathbf{w}$:

$$\nabla_{\mathbf{w}} \text{NLL}(\mathbf{w}, \sigma^2) = \mathbf{0}$$

we note that,

$$\nabla_{\mathbf{w}} \text{NLL}(\mathbf{w}, \sigma^2) = \mathbf{0} \tag{8}$$

$$\nabla_{\mathbf{w}} \left[\frac{N}{2} \log\left(2\pi\sigma^2\right) + \frac{1}{2\sigma^2} \sum_{n=1}^{N} \left[y_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) \right]^2 \right] = \mathbf{0} \tag{9}$$

$$\nabla_{\mathbf{w}} \left[\underbrace{\frac{1}{2} \sum_{n=1}^{N} \left[y_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) \right]^2}_{\text{RSS}(\mathbf{w})} \right] = \mathbf{0} \tag{10}$$

Note: in Statistics the term in the argument is called **residual sum of squares**.

We can rewrite the above expression in simpler form:

$$\nabla_{\mathbf{w}} \left[\frac{1}{2} \sum_{n=1}^{N} \left[y_n - \mathbf{w}^T \boldsymbol{\phi}(\mathbf{x}_n) \right]^2 \right] = 0 \tag{11}$$

$$\nabla_{\mathbf{w}} \left[\frac{1}{2} (\boldsymbol{\Phi}\mathbf{w} - \mathbf{y})^T (\boldsymbol{\Phi}\mathbf{w} - \mathbf{y}) \right] = 0 \tag{12}$$

where we group all output measurements y_n into a $N \times 1$ vector $\mathbf{y}$ and where we group all N evaluations of the basis functions into the $N \times M$ matrix:

$$\boldsymbol{\Phi} = \begin{bmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{bmatrix}$$

Setting the gradient wrt all $\mathbf{w}$ to zero gives,

$$\nabla_{\mathbf{w}} \left[\frac{1}{2} (\mathbf{\Phi w} - \mathbf{y})^T (\mathbf{\Phi w} - \mathbf{y}) \right] = \mathbf{0} \tag{13}$$

$$\frac{1}{2} \left[\left(\mathbf{\Phi}^T \mathbf{\Phi} + \mathbf{\Phi}^T \mathbf{\Phi} \right) \mathbf{w} - \mathbf{\Phi}^T \mathbf{y} - \mathbf{\Phi}^T \mathbf{y} \right] = \mathbf{0} \tag{14}$$

where we used the identity $\frac{\partial \mathbf{u}^T \mathbf{A} \mathbf{u}}{\partial \mathbf{u}} = \left(\mathbf{A} + \mathbf{A}^T \right) \mathbf{u}$ where $\mathbf{A}$ is an arbirary matrix and $\mathbf{u}$ an arbitrary vector. (See Section 7.8 of Murphy's book if you need to revise matrix calculus).
From which we reach the MLE prediction for the weights:

$$\hat{\mathbf{w}}_{\text{mle}} = \left(\mathbf{\Phi}^T \mathbf{\Phi} \right)^{-1} \mathbf{\Phi}^T \mathbf{y}$$

We conclude that our point estimate for the posterior (MLE) is: $\hat{\mathbf{w}}_{\mathrm{MLE}} = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{y}$
where the quantity

$$\mathbf{\Phi}^\dagger = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T$$

is known as the Moore-Penrose pseudo-inverse of the matrix $\mathbf{\Phi}$. It can be regarded as a generalization of the notion of matrix inverse to **nonsquare matrices**. In the special case of $\mathbf{\Phi}$ being square and invertible, then using the property $(\mathbf{AB})^{-1} = \mathbf{B}^{-1}\mathbf{A}^{-1}$ we see that $\mathbf{\Phi}^\dagger = \mathbf{\Phi}^{-1}$.

Also note that we could have calculated separetely the bias term w_0 (which is convenient because for other models the bias usually has a uniform prior, unlike the remaining weights). If we do that we obtain:

$$\hat{w}_0 = \bar{y} - \sum_{m=1}^{M-1} w_m \bar{\phi}_m$$

where we defined $\bar{y} = \frac{1}{N} \sum_{n=1}^{N} y_n$ and $\bar{\phi}_m = \frac{1}{N} \sum_{n=1}^{N} \phi_m(\mathbf{x}_n)$.

Having found the solution for all $\mathbf{w}$, we just need to find one last unknown from the point estimate of the posterior:

$$\nabla_{\sigma^2} \mathrm{NLL}(\mathbf{w}, \sigma^2) = 0$$

which is particularly simple:

$$\hat{\sigma}^2_{\mathrm{mle}} = \frac{1}{N} \sum_{n=1}^{N} \left[y_n - \hat{\mathbf{w}}^T_{\mathrm{mle}} \boldsymbol{\phi}(\mathbf{x}_n) \right]^2$$

In summary, the MLE point estimate of the posterior leads to the following estimation of parameters:

$$\hat{\mathbf{w}}_{\text{mle}} = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{y}$$

$$\hat{\sigma}^2_{\text{mle}} = \frac{1}{N}\sum_{n=1}^{N}\left[y_n - \hat{\mathbf{w}}^T_{\text{mle}}\boldsymbol{\phi}(\mathbf{x}_n)\right]^2$$

where the Moore-Penrose pseudo inverse needs to be calculated $\mathbf{\Phi}^\dagger = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T$.
This calculation can be done efficiently by many libraries, including Numpy.

- For example, scikit-learn uses a solver based on SVD (Single Value Decomposition: the most common dimensionality reduction method) which is efficient when $N > M$ (overdetermined system). Book section 7.5 has an excellent summary of SVD, if you are curious.
- Of course, if $N = M$ then there is a unique solution (you'll verify this in Homework 4) and the error on the training set becomes zero (linear regression becomes fully interpolatory).

See you next class

Have fun!