GAUSSIAN PROCESS

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OUTLINE

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1. MULTIVARIATE GAUSSIAN (PRE-REQUISITE)

Setting $x = \begin{bmatrix} x_A \\ x_B \end{bmatrix}$ $\mu = \begin{bmatrix} \mu_A \\ \mu_B \end{bmatrix}$ $\Sigma = \begin{bmatrix} \Sigma_{AA} & \Sigma_{AB} \\ \Sigma_{BA} & \Sigma_{BB} \end{bmatrix}.$

$$p(x_A) = \int_{x_B} p(x_A, x_B; \mu, \Sigma) dx_B$$
$$p(x_B) = \int_{x_A} p(x_A, x_B; \mu, \Sigma) dx_A$$

$$p(x_A \mid x_B) = \frac{p(x_A, x_B; \mu, \Sigma)}{\int_{x_A} p(x_A, x_B; \mu, \Sigma) dx_A}$$
$$p(x_B \mid x_A) = \frac{p(x_A, x_B; \mu, \Sigma)}{\int_{x_B} p(x_A, x_B; \mu, \Sigma) dx_B}$$

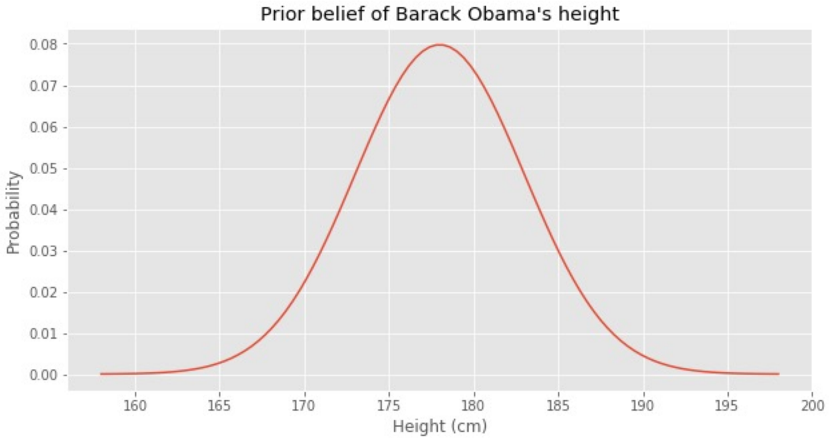
Marginalization $x_A \sim \mathcal{N}(\mu_A, \Sigma_{AA})$
$x_B \sim \mathcal{N}(\mu_B, \Sigma_{BB}).$

Conditional $x_A \mid x_B \sim \mathcal{N}(\mu_A + \Sigma_{AB}\Sigma_{BB}^{-1}(x_B - \mu_B), \Sigma_{AA} - \Sigma_{AB}\Sigma_{BB}^{-1}\Sigma_{BA})$
$x_B \mid x_A \sim \mathcal{N}(\mu_B + \Sigma_{BA}\Sigma_{AA}^{-1}(x_A - \mu_A), \Sigma_{BB} - \Sigma_{BA}\Sigma_{AA}^{-1}\Sigma_{AB}).$

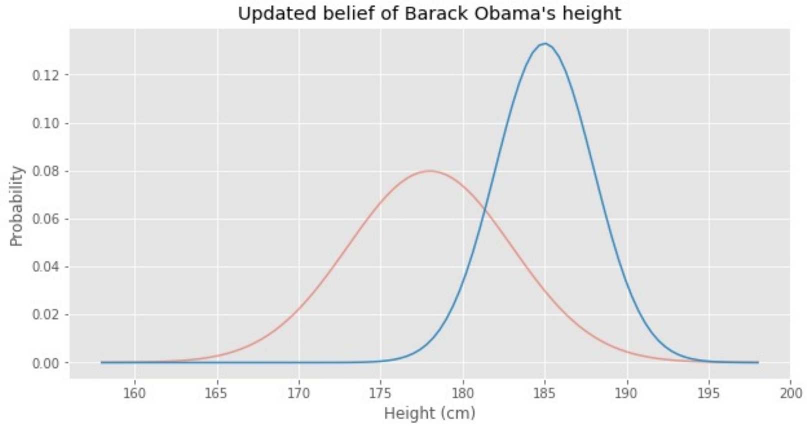
Note: Once Gaussian, always Gaussian

Importance: Central Limit Theorem

WHAT IS OBAMA’S HEIGHT



Prior belief of Barack Obama's height



Updated belief of Barack Obama's height

2. BACKGROUND

- Purpose: Learn underlying distribution from training data

- Parametric vs Nonparametric method
  - Given set of training points, there are potentially infinitely many functions that fit the data

- Bayesian Inference:
  - $p(w|D) = \frac{p(Data|w)p(w)}{p(Data)}$ or $p(w|D) \propto p(Data|w)p(w)$
  - Goal: $p(y^*|x, x^* \ , y)$ – with y*: posterior function, X*: test data, X: training data, y: prior function

3. REQUIREMENTS, ASSUMPTIONS AND SETTINGS

- Regression problem:

- Extension version can be used for classification problem
- $y\ = f(x) + \varepsilon$

$$X = \begin{bmatrix} \text{—} & (x^{(1)})^T & \text{—} \\ \text{—} & (x^{(2)})^T & \text{—} \\ & \vdots & \\ \text{—} & (x^{(n)})^T & \text{—} \end{bmatrix} \in \mathbf{R}^{n \times d} \quad \vec{f} = \begin{bmatrix} f(x^{(1)}) \\ f(x^{(2)}) \\ \vdots \\ f(x^{(n)}) \end{bmatrix}, \quad \vec{\varepsilon} = \begin{bmatrix} \varepsilon^{(1)} \\ \varepsilon^{(2)} \\ \vdots \\ \varepsilon^{(n)} \end{bmatrix}, \quad \vec{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix} \in \mathbf{R}^{n},$$

$$X_* = \begin{bmatrix} \text{—} & (x_*^{(1)})^T & \text{—} \\ \text{—} & (x_*^{(2)})^T & \text{—} \\ & \vdots & \\ \text{—} & (x_*^{(n_*)})^T & \text{—} \end{bmatrix} \in \mathbf{R}^{n_* \times d} \quad \vec{f}_* = \begin{bmatrix} f(x_*^{(1)}) \\ f(x_*^{(2)}) \\ \vdots \\ f(x_*^{(n_*)}) \end{bmatrix}, \quad \vec{\varepsilon}_* = \begin{bmatrix} \varepsilon_*^{(1)} \\ \varepsilon_*^{(2)} \\ \vdots \\ \varepsilon_*^{(n_*)} \end{bmatrix}, \quad \vec{y}_* = \begin{bmatrix} y_*^{(1)} \\ y_*^{(2)} \\ \vdots \\ y_*^{(n_*)} \end{bmatrix} \in \mathbf{R}^{n_*}.$$

$$\begin{bmatrix} \vec{\varepsilon} \\ \vec{\varepsilon}_* \end{bmatrix} \sim \mathcal{N}\left(\vec{0}, \begin{bmatrix} \sigma^2 I & \vec{0} \\ \vec{0}^T & \sigma^2 I \end{bmatrix}\right).$$

4. GAUSSIAN PROCESS

Definition: A GP is a (potentially infinite) collection of random variables such that the joint distribution of every finite subset of random variables is multivariate Gaussian

Prior: Assuming the mean of function is 0 $\mathrm{p(y|x)} \sim \mathcal{N}(\mu = 0, K)$

Posterior: After observing $y^* \ and \ x^*$, we use the Bayesian rules as followed

4. GAUSSIAN PROCESS

Gaussian process: modelling probability distributions over functions $p(y^*|y, x^*, x)$

$$\begin{bmatrix} \vec{y} \\ \vec{y}_* \end{bmatrix} \Bigg| X, X_* = \begin{bmatrix} \vec{f} \\ \vec{f}_* \end{bmatrix} + \begin{bmatrix} \vec{\varepsilon} \\ \vec{\varepsilon}_* \end{bmatrix} \sim \mathcal{N}\left(\vec{0}, \begin{bmatrix} K(X,X) + \sigma^2 I & K(X,X_*) \\ K(X_*,X) & K(X_*,X_*) + \sigma^2 I \end{bmatrix}\right).$$

$$\epsilon \sim \mathcal{N}(\mathbf{0}, \sigma_y^2 \mathbf{I})$$

$$\mu^* = K(X_*,X)\left(K(X,X) + \sigma^2 I\right)^{-1} \vec{y}$$

$$\Sigma^* = K(X_*,X_*) + \sigma^2 I - K(X_*,X)\left(K(X,X) + \sigma^2 I\right)^{-1} K(X,X_*).$$

5. INTUITION, ADVANTAGES AND DISADVANTAGES

- Intuition: Gaussian process versus classical linear regression
  - GP: The posterior distribution over the y* for new input x* reflect the uncertainty in our prediction y* due to the ε and choice of prior θ.
  - Classical linear regression models, estimate θ directly from the training data but provide no estimate of how reliable these learned parameters may be.

- Advantages:
  - Elegant solution
  - Assigning probabilities to each of these functions
  - Incorporate confidence in the prediction

- Disadvantages:
  - Computationally expensive

6. KERNEL

- Definition: Outputs the similarity between 2 given points
- Example: Squared Exponential Kernel

$$k_{SE}(x, x') = \quad \sigma^2 \exp\left(-\frac{||t-t'||^2}{2l^2}\right)$$

- Note: Relation between covariance and kernel
- Parameters:
  - σ^2: average distance away from the function’s mean
  - l : reach of influence on neighbors

7. SUMMARY

-GP: estimation of function, instead of parameters

- Bayesian inference

- Non-parametric method

8. CITATION

https://distill.pub/2019/visual-exploration-gaussian-processes/

http://cs229.stanford.edu/summer2020/gaussian_processes.pdf

https://www.cs.cornell.edu/courses/cs4780/2018fa/lectures/lecturenote15.html