Gaussian Processes and MC Dropout

What is a Gaussian Process

- Gaussian processes are stochastic processes - a collection of indexable random variables
- Given any finite collection of random variables from a GP, the joint distribution is Normal

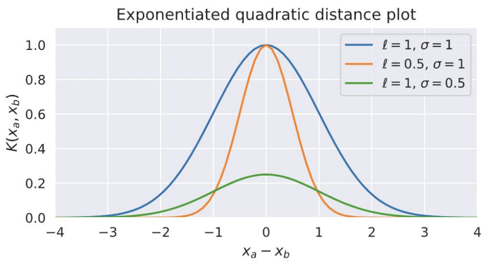
$$\{Y_x | x \in S\} \qquad \{Y_{x_1}, Y_{x_2}, \ldots Y_{x_n}\} \sim \text{MVN}$$

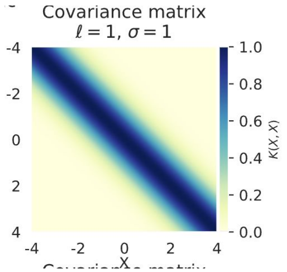
- Another way to view Gaussian Processes is a distribution over functions
- GPs can be used in a variety of applications as they are theoretically able to approximate any smooth function

What is a Gaussian Process

- To specify a GP, make a PSD symmetric matrix describing the covariance between $\mathbf{K} = \begin{bmatrix} k(x_1, x_1) & \dots & k(x_1, x_n) \\ \vdots & \ddots & \vdots \\ k(x_n, x_1) & \dots & k(x_n, x_n) \end{bmatrix}$
    - Use a kernel function ***k*** mapping indices to covariances

- We can define kernel to be the exponential quadratic kernel $K(x_1, x_2) = \sigma^2 \exp\left(\frac{||x_1 - x_2||^2}{\lambda^2}\right)$





https://peterroelants.github.io/posts/gaussian-process-kernels/

GP Regression

- Suppose we want to model the relationship **y = f(x) + ε** where **ε ~ N(0,** σ^2**)** i.e.

  y ~ N(f(x), σ^2**)**

- We can use GP as a prior specification on **f(x)**

  f(x) ~ GP(0, K(x, x))

- After observing the x's, we get the MVN over the f(x)'s by instantiating the covariance matrix

  f(x) ~ N(0, K)

GP Regression

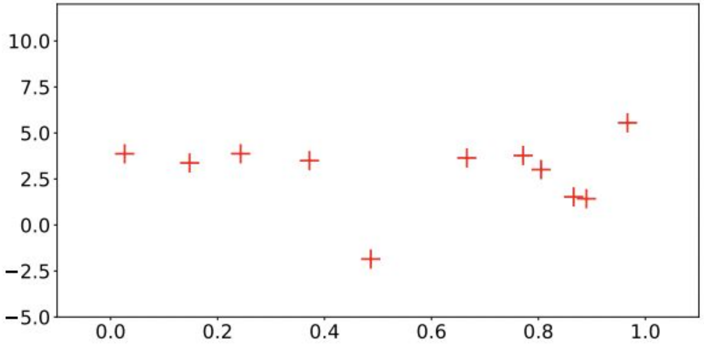
- How to make predictions on new indices $\mathbf{x}_*$? Get the joint distribution over labels and predictions $\mathbf{f}_*$

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{f}_* \end{pmatrix} \sim \mathcal{N}\left(\mathbf{0}, \begin{bmatrix} \mathbf{K} + \sigma_n^2 I & \mathbf{K}_* \\ \mathbf{K}_*^\top & \mathbf{K}_{**} \end{bmatrix}\right) \qquad \mathbf{K}_* = K(\mathbf{X}, \mathbf{X}_*) \text{ and } \mathbf{K}_{**} = K(\mathbf{X}_*, \mathbf{X}_*).$$

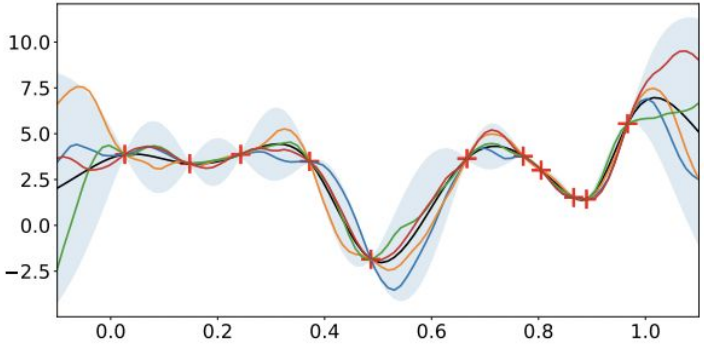
- Marginalize to get the predictive distribution

$$\mathbf{f}_* \mid \mathbf{X}, \mathbf{y}, \mathbf{x}_* \sim \mathcal{N}\left(\bar{\mathbf{f}}_*, \operatorname{cov}(\mathbf{f}_*)\right)$$

$$\begin{aligned} \bar{\mathbf{f}}_* &\triangleq \mathbb{E}[\bar{\mathbf{f}}_* \mid \mathbf{X}, \mathbf{y}, \mathbf{X}_*] \\ &= \mathbf{K}_*^\top [\mathbf{K} + \sigma_n^2 I]^{-1} \mathbf{y} \ , \\ \operatorname{cov}(\mathbf{f}_*) &= \mathbf{K}_{**} - \mathbf{K}_*^\top [\mathbf{K} + \sigma_n^2 I]^{-1} \mathbf{K}_* \end{aligned}$$



(a) Data point observations



(b) Five possible functions by GPR

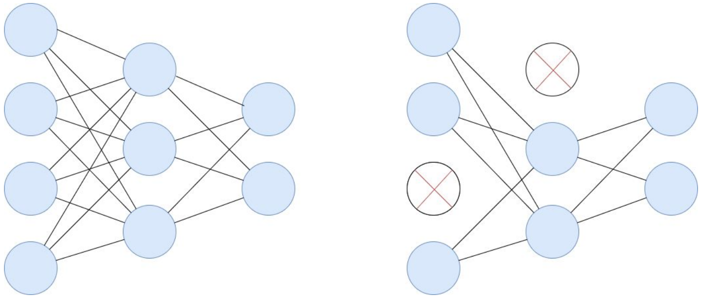
Remarks

- Gaussian Processes can be used in regression to fit any type of non-linearity
- It is a type of non-parametric model - number of parameters scales with the size of dataset
- Kernel hyperparameters can be tuned using MLE

MC Dropout

- In neural networks, dropout is used as regularization
- MC Dropout is just like regular NN dropout, but used also at test time
  - As a result, we can introduce uncertainty in the output
- Dropout in a general sense can be seen as adding random multiplicative noise to the input of each layer

$$\mathbf{B} = (\mathbf{A} \circ \xi)\theta, \quad \text{with } \xi_{i,j} \sim p(\xi_{i,j})$$



https://towardsdatascience.com/monte-carlo-dropout-7fd52f8b6571

Bayesian(?) interpretations of MC Dropout

Kingma, Salimans and Welling (2015) - Variational Dropout and the Local Reparameterization Trick

- Bayesian approximation using Variational Inference on a dropout network
- Uses the dropout rate as part of the variational parameters on the variational distribution
- An improper prior is chosen to prevent shrinkage effect on the weights

$$w_{jk}^{(h)} = \theta_{jk}^{(h)} \times \xi_{jk}^{(h)},\ \underbrace{\xi_{jk}^{(h)} \sim N(1, \alpha)}_{\text{Gaussian "dropout"}} \text{ with (improper log uniform) prior } p(\log |w_{jk}^{(h)}|) \propto c$$

$$q(w_{jk}^{(h)}) \equiv N\left(\theta_{jk}^{(h)}, \alpha(\theta_{jk}^{(h)})^2\right)$$

Bayesian(?) interpretations of MC Dropout

Gal and Ghahramani (2017) - Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning

- Views the entire NN prediction object itself as a variational stochastic process, approximates another variational stochastic known as *Sparse Spectrum GP*
- Equivalency in objective functions between training a NN with dropout layers and SSGP

$$\underset{\text{Monte Carlo point masses}}{\overset{\text{NN prediction based on}}{\text{MC-Dropout NN}}} \xrightarrow[\text{approximates}]{\text{NN optimization}} \text{Sparse Spectrum GP} \xrightarrow[\text{"via VI"}]{\textit{approx.}} \text{GP}$$

$$\underbrace{w_{jk}^{(h)} \sim p^{(h)} N(m_{jk}^{(h)}, \sigma^2) + (1 - p^{(h)}) N(0, \sigma^2)}_{\text{a sparse spectrum GP takes this form and approximates a GP}} \overset{\sigma \to 0}{\approx} \underbrace{z_k^{(h)} m_{jk}^{(h)} + 0 \times (1 - z_{jk}^{(h)}),\ z_{jk}^{(h)} \sim bin(p^{(h)})}_{\text{a dropout NN where } z_{jk}^{(h)} \text{ is always Monte Carlo sampled}}$$

Bayesian(?) interpretations of MC Dropout

- Improper log uniform prior produces improper posteriors (HMG 2017)
- Issues with non-continuity in point mass approximation
- Mode collapse failure of the posterior distribution of dropout parameters (Osband 2016)

References

Schwartz 2021. https://github.com/pointOfive/Summer_2022_STA496H1/blob/main/files/GaussianProcesses.ipynb

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Wang 2020. An Intuitive Tutorial to Gaussian Processes Regression

Osband 2016. Risk vs. Uncertainty in Deep Learning: Bayes, Bootstrap, and the Dangers of Dropout