Summary of: Direct Methods for Gaussian Processes by O'Neil et. al.

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Overview

Gaussian Process motivation and definition

- Given data $(\mathbf{X}_n, \mathbf{Y}_n) = (X_1, Y_1), \ldots, (X_n, Y_n)$, how do you infer what type of process generated the data and responses? – enable predictions for future data.
- Frequentists just use regression; alternative approach is probabilistic...
- The posterior probability distribution for the process $f : \mathcal{X}^n \to \mathcal{Y}^n$ is

$$P(f|\mathbf{X}_n, \mathbf{Y}_n) = \frac{P(\mathbf{Y}_n|f, \mathbf{X}_n)P(f)}{P(\mathbf{Y}_n|\mathbf{X}_n)}$$

- What is the function space to which f belongs? Need to restrict the space if we want to be able to measure the numerator terms.
- Simplifying assumption: f is a Gaussian Process.
- A mapping f is called a **Gaussian Process** if for any $m \in \mathbb{N}$, for any m-length input set $(X_1, \ldots, X_m)$, the distribution of $(f(X_1), \ldots, f(X_m))$ is multivariate normal.

Gaussian Process Intuition

- Gaussian Process generalizes the notion of a finite dimensional Gaussian distribution to an infinite dimensional analog

$$X \sim \mathcal{N}(\mu, \Sigma) \iff f(\mathbf{X}_n) \sim \mathcal{N}(\mu(\mathbf{X}_n), \Sigma(\mathbf{X}_n))$$

  The mean and covariance functions are defined by the data.
- $\Sigma(\mathbf{X}_n)_{ij} = K(\mathbf{X}_n)_{ij} = k(x_i, x_j)$ for some kernel k where k is a positive semidefinite kernel, meaning that K is a PSD kernel matrix.
- We will see that, for prediction, the covariance function $\Sigma_p(\mathbf{X}_n)$ is often of the form $\Sigma(\mathbf{X}_n) = \sigma^2 I + K$.

- We can now define the prior on f, $P(f)$, using this formalism. Assuming for simplicity that $\mu(x) = 0$, the prior for f is the density for an n-dimensional multivariate normal:

$$P(f(\mathbf{X}_n)) = (2\pi)^{-\frac{n}{2}} \det(\Sigma(\mathbf{X}_n))^{-\frac{1}{2}} \exp\left(-\frac{1}{2} f(\mathbf{X}_n)\Sigma(\mathbf{X}_n)^{-1} f(\mathbf{X}_n)\right)$$

- To make predictions, we consider the distribution for $\mathbf{Y}_n|\mathbf{X}_n$

$$Y_{n+1}|\mathbf{X}_n, \mathbf{Y}_n, X_{n+1} \sim N(\tilde{\mu}(x), \tilde{\Sigma}(x))$$

where $\tilde{\mu}, \tilde{\Sigma}$ are functions of the data. The resulting likelihood function involves inverting a matrix of the form $(\sigma^2 I + \Sigma(\mathbf{X}_n))^{-1}$.

Computational Bottleneck

Common computational complexities

- Using Gauss-Jordan elimination, matrix inversion has complexity $O(n^3)$.
- Finding determinant of a matrix by LU decomposition has complexity $O(n^3)$.

- For large n, this makes computation of posterior distributions for Gaussian Processes intractable – recall the inverse and determinant in the likelihood function.
- What can be done?

Accelerated Methods for inversion/determinant of matrix of form $C = I + K$

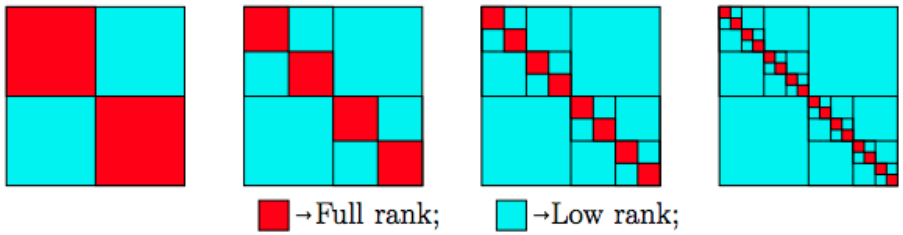
Types

1. Direct Methods
   - $rank(K) = p << n \Rightarrow$ use Sherman-Morrison-Woodbury formula and Sylvester det. theorem in $O(p^2 n)$ each. It is typically not easy to identify if K is low rank, or if it is approximately low rank.
2. Iterative Methods
   - Fast Gauss Transform and Fast Fourier Transform: can speed up matrix multiplication to help with determinant but inverse will still be hard?

Broad distinction between two main approaches: low rank approximations that assume K is a finite rank operator (will be a dense entry-wise but "data-sparse") vs. thresholding actual entries of the matrix (matrix will be sparse, but has high numerical rank).
The paper's method makes an approximation at the "level of the covariance matrix."

HODLR Matrix definition

Hierarchical Off-Diagonal Low-Rank Matrices (**HODLR**) are a class of matrices that have off-diagonal blocks that are easily represented recursively, each of which have low rank (we focus on symmetric matrices).



HODLR examples

Example: For $K_0 \in \mathbb{S}^n$, K_0 is a two level HODLR matrix if

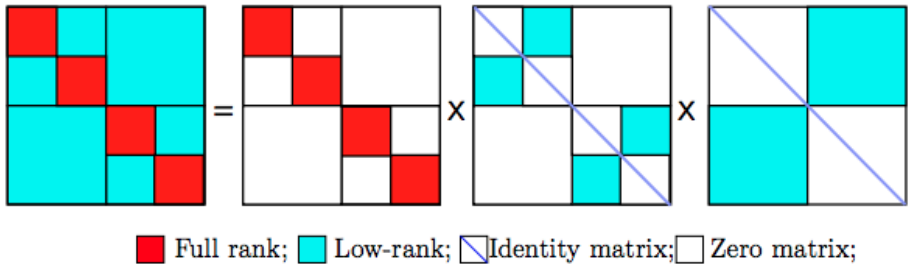
$$K_0 = \begin{pmatrix} K_1^{(1)} & U_1^{(1)} V_1^{(1)^T} \\ V_1^{(1)} U_1^{(1)^T} & K_2^{(1)} \end{pmatrix}, \; U_1^{(1)}, V_1^{(1)} \in \mathbb{R}^{\frac{n}{2} \times r}, \; r << n$$

$$K_1^{(1)} = \begin{pmatrix} K_{1,1}^{(2)} & U_1^{(2)} V_1^{(2)^T} \\ V_1^{(2)} U_1^{(2)^T} & K_{1,2}^{(2)} \end{pmatrix}, K_2^{(1)} = \begin{pmatrix} K_{2,1}^{(2)} & U_2^{(2)} V_2^{(2)^T} \\ V_2^{(2)} U_2^{(2)^T} & K_{2,2}^{(2)} \end{pmatrix}$$

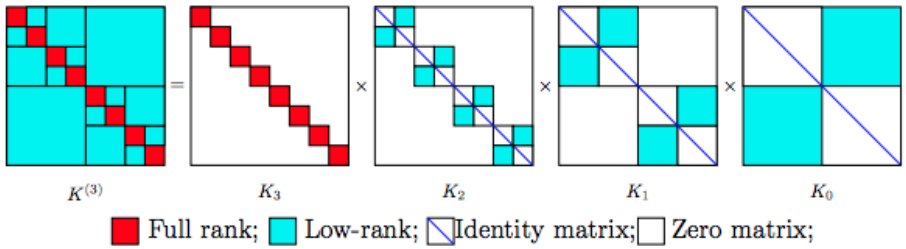
$$U_i^{(2)}, V_i^{(2)} \in \mathbb{R}^{\frac{n}{4} \times r}, \; \forall (i,j) \in \{1,2\}^2, \; K_{i,j}^{(2)} \in \mathbb{R}^{\frac{n}{4} \times \frac{n}{4}}$$

A suggested factorization for HODLR matrices

Without explaining how it will be obtained, suppose that we are given a factorization of $K = \prod_{i=0}^{\kappa} K_i$.
For $\kappa = 2$, $K = K_2 K_1 K_0 \Leftrightarrow$:



For $\kappa = 3$, $K = K_3 K_2 K_1 K_0 \Leftrightarrow$:



Why is this helpful? Matrix Inversion!

- Consider $K = \begin{pmatrix} A & UV^T \\ VU^T & B \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} + \begin{pmatrix} 0 & UV^T \\ VU^T & 0 \end{pmatrix} = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} + \begin{pmatrix} U & 0 \\ 0 & V \end{pmatrix} \begin{pmatrix} 0 & V^T \\ U^T & 0 \end{pmatrix}$
- Since U, V are low rank, the matrix can be more easily inverted using the Sherman-Morrison-Woodbury Formula:

$$(A + BC)^{-1} = A^{-1} - A^{-1}B(I + CA^{-1}B)^{-1}CA^{-1}$$

$$\Leftrightarrow (I + BC)^{-1} = I - B(I + CB)^{-1}C$$

  Because of B, C having very few columns, the middle term can be inverted very quickly.
- To invert entire matrix, we can perform this procedure on each of the block of each component in $K = K_\kappa K_{\kappa-1} \cdots K_2 K_1 K_0$. We will usually have $\kappa \approx \log n$ so inversion can be computed in $\mathcal{O}(n \log n)$ because S-M-W formula inverse in $\mathcal{O}(n)$.

Why is this helpful? Computing Determinant!

Sylvester's Determinant Theorem

For $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times m}$, $\det(I_m + AB) = \det(I_n + BA)$.

- $K = \prod_{i=0}^{\kappa} K_i \Rightarrow \det K = \prod_{i=0}^{\kappa} \det K_i$. $\det K_\kappa = \prod_{i=1}^{2^\kappa} \det K_{\kappa,i}$. For $k \neq \kappa$, $\det K_k$ is a low rank perturbation to the identity matrix, and we can use Sylvester's theorem on each diagonal block $j \in [1, 2^{k+1}]$:

$$\det\left(I_{\frac{n}{2^k}} + \begin{pmatrix} U_j^{(k)} & 0 \\ 0 & V_j^{(k)} \end{pmatrix} \begin{pmatrix} 0 & V_j^{(k)^T} \\ U_j^{(k)^T} & 0 \end{pmatrix}\right)$$

$$= \det\left(I_{2r} + \begin{pmatrix} 0 & V_j^{(k)^T} V_j^{(k)} \\ U_j^{(k)^T} U_j^{(k)} & 0 \end{pmatrix}\right)$$

- Each matrix's computational cost using the theorem is $\mathcal{O}(n)$, so doing so for all κ matrices costs $\mathcal{O}(n \log n)$.

Algorithm for computing the factorization

- Given a HODLR matrix $K \in \mathbb{R}^{n \times n}$, $K = \begin{pmatrix} A_{11} & A_{12} \\ A_{12}^T & A_{22} \end{pmatrix}$ where A_{11}, A_{22} are full rank and $A_{12} = UV^T$ is low rank. The key is to note that:

$$K = \begin{pmatrix} A_{11} & UV^T \\ VU^T & A_22 \end{pmatrix} = \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix} \begin{pmatrix} I_{\frac{n}{2}} & A_{11}^{-1}UV^T \\ A_{22}^{-1}VU^T & I_{\frac{n}{2}} \end{pmatrix}$$

This might seem like an expensive algorithm, because A_{11} might be large, but we do it recursively, and so only invert matrices that are $\kappa \times \kappa$.

Numerical Results in Computation

- Experimented with matrix inversion and determinant computation for different covariance matrices $C = \sigma^2 I + K$ where K is a PSD kernel matrix. Tested with kernel functions: (1) Gaussian covariance, (2) multiquadric covariance, (3) exponential covariance, (4) Inverse multiquadric and biharmonic kernels.
- Results are extremely impressive. They are tables II-V in O'Neil's paper.
- When the dimension of the points was increased, the computation time explodes, and the meaningfulness of the spatial structure is compromised due to curse of dimensionality. Not an interesting application of this method at this time...
- In a regression experiment, the RMSE of the regression line is inversely related to the factorization precision.

Conclusions

- Many covariance matrices used in GPs have the HODLR property, justifying the use of this method in many applications.
- Future research needed to identify how to deal with cases when dimensionality of data is large.
- No comparison is given to other methods' computation time and accuracy.
- How does this compare to a more general multiscale method like MMF – we may want to deal with structures other than HODLR.
- Next step: compare computational results of MMF factorized matrices with this method on HODLR matrices.