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Optimizing performance in Gaussian Processes

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Symbols and Notation

Matrices are capitalized bold face letters while vectors are lowercase bold face letters.

Syntax	*Meaning*
$\triangleq$	An equality which acts as a statement
$\lvert\boldsymbol{A}\rvert$	The determinate of a matrix.
$\langle\cdot,\cdot\rangle_{\mathcal{H}}$	The inner product with respect to the Hilbert space $\mathcal{H}$, sometimes abbreviated as $\langle\cdot,\cdot\rangle$ if the Hilbert space is clear from context.
$\lVert\cdot\rVert_{\mathcal{V}}$	The norm of a vector with respect to the vector space $\mathcal{V}$, sometimes abbreviated as $\lVert\cdot\rVert$ if the vector space is clear from context.
$\boldsymbol{x}^\intercal, \boldsymbol{X}^\intercal$	The transpose operator.
$\boldsymbol{x}^*, \boldsymbol{X}^*$	The hermitian operator.
$\boldsymbol{a}.*\boldsymbol{b}$ or $\boldsymbol{A}.*\boldsymbol{B}$	Element-wise vector (matrix) multiplication, similar to Matlab.
$\propto$	Proportional to.
∇ or $\nabla_{\boldsymbol{f}}$	The partial derivative (with respect to $\boldsymbol{f}$).
∇	The Hessian.
$\sim$	Distributed according to, example $x \sim \mathcal{N}(0,1)$
$\mathbf{0}$ or $\mathbf{0}_n$ or $\mathbf{0}_{n\times m}$	The zero vector/matrix of appropriate length/size or the zero vector of length n or the zero matrix with dimensions $n \times m$.
$\mathbf{1}$ or $\mathbf{1}_n$ or $\mathbf{1}_{n\times m}$	The one vector/matrix of appropriate length/size or the one vector of length n or the one matrix with dimensions $n \times m$.
$\mathbb{1}_{n\times m}$	The matrix with ones along the diagonal and zeros on off diagonal elements.

$\boldsymbol{A}_{(\cdot,\cdot)}$	Index slicing to extract a submatrix from the elements of $\boldsymbol{A} \in \mathbb{R}^{n \times m}$, similar to indexing slicing from the python and Matlab programming languages. Each parameter can receive a single value or a 'slice' consisting of a start and an end value separated by a semicolon. The first and second parameter describe what row and columns should be selected, respectively. A single value means that only values from the single specified row/column should be selected. A slice tells us that all rows/columns between the provided range should be selected. Additionally if now start and end values are specified in the slice then all rows/columns should be selected. For example, the slice $\boldsymbol{A}_{(1:3,j:j')}$ is the submatrix $\mathbb{R}^{3 \times (j'-j+1)}$ matrix containing the first three rows of $\boldsymbol{A}$ and columns j to j'. As another example, $\boldsymbol{A}_{(:,j)}$ is the j^{th} column of $\boldsymbol{A}$.
$\mathbb{C}$	The complex numbers.
C	The classes in a classification problem.
$\text{cholesky}\left(\boldsymbol{A}\right)$	A function to compute the Cholesky decomposition of the matrix $\boldsymbol{A}$, where $\boldsymbol{L}\boldsymbol{L}^{\intercal} = \boldsymbol{A}$.
$\text{cov}\left(\boldsymbol{f}\right)$	Gaussian process posterior covariance.
d	The number of features in the data set.
D	The dimension of the feature space of the feature mapping constructed in the Random Fourier Feature method.
$\mathcal{D}$	The dataset, $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{n}$.
$\text{diag}\left(\boldsymbol{w}\right)$	Vector argument, a diagonal matrix containing the elements of vector $\boldsymbol{w}$.
$\text{diag}\left(\boldsymbol{W}\right)$	Matrix argument, a vector containing the diagonal elements of the matrix $\boldsymbol{W}$.
$\mathbb{E}$ or $\mathbb{E}_{q(x)}\left[z(x)\right]$	Expectation, or expectation of $z(x)$ where $x \sim q(x)$.
$\mathcal{GP}$	Gaussian process $f \sim \mathcal{GP}\left(m(\boldsymbol{x}), k\left(\boldsymbol{x}, \boldsymbol{x}'\right)\right)$, the function f is distributed as a Guassian process with mean function $m\left(\boldsymbol{x}\right)$ and covariance function $k\left(\boldsymbol{x}, \boldsymbol{x}'\right)$.
$k\left(\cdot,\cdot\right)$	A covariance or kernel matrix.

$\boldsymbol{K}_{\boldsymbol{W}\boldsymbol{W}'}$	For two data sets $\boldsymbol{W} = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_n]^\intercal \in \mathbb{R}^{n \times d}$ and $\boldsymbol{W}' = [\boldsymbol{w}'_1, \boldsymbol{w}'_2, \ldots, \boldsymbol{w}'_m]^\intercal \in \mathbb{R}^{n' \times d}$ the matrix $\boldsymbol{K}_{\boldsymbol{W}\boldsymbol{W}'} \in \mathbb{R}^{n \times n'}$ has elements $(\boldsymbol{K}_{\boldsymbol{W}\boldsymbol{W}'})_{i,j} = k\left(\boldsymbol{w}_i, \boldsymbol{w}'_j\right)$.
$\text{lin-solve}\left(\boldsymbol{A}, \boldsymbol{B}\right)$	A function used to solve $\boldsymbol{X} = \boldsymbol{A}^{-1}\boldsymbol{B}$ in the linear system $\boldsymbol{A}\boldsymbol{X} = \boldsymbol{B}$.
$\mathcal{N}\left(\boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$ or $\mathcal{N}\left(\boldsymbol{x} \mid \boldsymbol{\mu}, \boldsymbol{\Sigma}\right)$	(the variable $\boldsymbol{x}$ has a) Multivariate Gaussian distribution with mean vector $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$.
n and n_*	The number of training (and tests) cases.
N	The dimenion of the feature space.
$\mathbb{N}$	The natural numbers, $\mathbb{N} = \{1, 2, 3, \ldots\}$.
$\mathcal{O}(\cdot)$	Big-O notation. If a function $f \in \mathcal{O}\left(g\right)$ then the absolute value of $f(x)$ is at most a positive multiple of $g(x)$ for all sufficiently large values of x.
$y \mid x$ and $p\left(x \mid y\right)$	A conditonal random variable y given x and its probability density.
$\boldsymbol{Q}, \boldsymbol{V}$	Typically used to denote a matrix with orthonormal structure.
$\mathbb{R}$	The real numbers.
$\text{tr}\left(\boldsymbol{A}\right)$	The trace of a matrix.
$\mathbb{V}$ or $\mathbb{V}_{q(x)}\left[z(x)\right]$	Variance, the variance of $z(x)$ when $x \sim q(x)$.
$\mathcal{X}$	Input space.
$\boldsymbol{X}$	The $n \times d$ matrix of training inputs.
$\boldsymbol{X}_*$	The $n_* \times d$ matrix of test inputs.
$\boldsymbol{x}_i$	The i^{th} training input.
$\mathbb{Z}$	The integers, $\mathbb{Z} = \{\ldots, -2, -1, 0, 1, 2, \ldots\}$.

1. The Nystrom Method

In chapter **??** we saw that GP regression and classification relied on a Gram matrix (see definition **??**) to produce predictions. Unfortunately, from a computational perspective, constructing the Gram matrix for a data set $\mathcal{D} = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^n$ brings about a nasty bottle neck owed by the $\mathcal{O}\left(n^2\right)$ kernel evaluations. Even before the rise of ML, there has been a lot of research devoted to creating numerical methods that quickly construct a low rank approximation of large matrices, $\boldsymbol{A}$, which ordinarily are a computational burdened to build exactly. These methods are centered around the idea of capturing the columns space of the matrix that best describes the the action of $\boldsymbol{A}$ as an operator. For lack of a better explanation, Mahoney gives a fantastic summary of why the column space is of much importance in these approximation techniques

> *"To understand why sampling columns (or rows) from a matrix is of interest,recall that matrices are "about" their columns and rows that is, linear combinations are taken with respect to them; one all but understands a given matrix if one understands its column space, row space, and null spaces; and understanding the subspace structure of a matrix sheds a great deal of light on the linear transformation that the matrix represents."*
> [MWM11, page 13]

Moreover, this class of algorithms lend very nice forms when $\boldsymbol{A}$ possess positive definite structure, which is exactly the case for our Gram matrix.

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