# Using Gaussian Process Regression to invert a Solution of the 1D Heat Equation

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Given an instance of the 1D heat equation with a point source initial condition, the solution is inverted using a Gaussian process. A brief discussion of Gaussian processes (GP) and Gaussian process regression (GPR) is presented. The analytic solution of the heat equation in the presented problem is used to check three GPR interpolated values picked at points with different confidence intervals. The interpolated values are found to have small relative errors in all cases. The problem of inverting a system $Ax = y$ is then discussed in light of GPR.

## INTRODUCTION

The heat equation is relevant in nearly any engineering problem, as temperature can affect both the mechanical and chemical properties of matter. The propagation of heat through a system dictates how the system should be designed, and what materials it should be built with. The particular form of the heat equation also matches other important equations in physics, such as the diffusion equation, which describes Brownian motion. As the equation is so relevant, knowing how to deal with it in different contexts is important.

In this paper, we focus on the simple scenario of a rod with a point heat source. However, we do not solve the standard problem of finding the evolution of the temperature profile over time. Instead, we attempt to find the source of heat given the temperature at a specific time and location. We approach this with Gaussian process regression. The analytic solution is easy to calculate due to the point source initial condition. However, the methodology presented can be applied to much more complex systems, letting us invert any system $Ax = y$ by training a Gaussian process on known solutions.

## PROBLEM STATEMENT

We are given a rod with a source of heat temporarily applied. We then measure the temperature at one location on the bar at one time, with some inaccuracy due to the instrument used for the measurements. Our goal is to find the location where the heat source was applied.

Now, more formally, suppose our bar has length $L$, with one end at the origin, and another end on the positive $z$ axis. Then suppose a source of heat is temporarily applied when $t = 0$ at location $y$ with $0 < y < L$. We know the temperature at location $s_0$ when $t = t_0$ is $x$. Our goal is to find $y$ only given this information.

## RELEVANT BACKGROUND

### Gaussian Processes

A Gaussian process is a distribution over functions, denoted $f(x) \sim \mathcal{GP}(m, k)$. The behavior is completely defined by a mean function, $m = m(x)$, and a covariance function (kernel), $k = k(x, x')$. When taking any finite collection of function values, $\mathbf{f} = \{f(x_0), \ldots, f(x_n)\}$, $\mathbf{f}$ is distributed as a multivariate Gaussian distribution. The covariance function must be finitely positive semi-definite[1]. A common choice is the squared exponential kernel:

$$k(x, x') = \sigma_y^2 e^{-\frac{(x-x')^2}{2\ell^2}} \tag{1}$$

Above, $\ell$ is the characteristic length scale of our data, and $\sigma_y^2$ is the maximum allowed covariance. Smaller distances between $x$ and $x'$ ensure a larger covariance (with $\ell$ dictating how close points need to be in order to influence each other significantly), meaning $f(x)$ will be close to $f(x')$. The mean function is often set to 0, as this avoids assuming a functional form when using Gaussian process regression to extrapolate from a set of data.

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[1] A function $\kappa : X \times X \to \mathbb{R}$ is finitely positive semi-definite iff $\kappa(\mathbf{x}, \mathbf{x}') = \kappa(\mathbf{x}', \mathbf{x})$ for all $\mathbf{x}, \mathbf{x}' \in X$, and the matrix $\kappa(\mathbf{x}, \mathbf{x})$ is positive semi-definite for all $\mathbf{x} \in X$

Similar to how Gaussian distributions define distributions over a finite number of variables, Gaussian processes define distributions over functions. This means that Gaussian processes are infinite-dimensional objects. We understand this by looking at at a multivariate Gaussian distribution, $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \Sigma)$. The random variable $x_i$ is indexed by $i$, its position in $\mathbf{x}$. However, for the Gaussian process $f(x) \sim \mathcal{GP}(m, k)$, the random function $f(x)$ is indexed by the value of x.

### Gaussian Process Regression

Let $\mathbf{f}$ be a vector of function values corresponding to the vector of inputs $\mathbf{x}$, where the function mapping $\mathbf{x}$ to $\mathbf{f}$ is unknown. Our goal is to predict the function values $\mathbf{f}_*$ corresponding to inputs $\mathbf{x}_*$. If we assume that $f(x)$ is drawn from a Gaussian process, the finite set of function values $\mathbf{f}$ must be distributed as a multivariate Gaussian distribution. Thus, the sets $\mathbf{f}$ and $\mathbf{f}_*$ together have a joint Gaussian distribution:

$$\begin{bmatrix} \mathbf{f} \\ \mathbf{f}_* \end{bmatrix} \sim \mathcal{N}\left( \begin{bmatrix} \boldsymbol{\mu} \\ \boldsymbol{\mu}_* \end{bmatrix}, \begin{bmatrix} \Sigma & \Sigma_* \\ \Sigma_*^T & \Sigma_{**} \end{bmatrix} \right) \tag{2}$$

Above, $\boldsymbol{\mu}$ and $\boldsymbol{\mu}_*$ represent the vectors of mean values for $\mathbf{f}$ and $\mathbf{f}_*$, $\Sigma$ and $\Sigma_{**}$ represent the covariance matrices of $\mathbf{x}$ and $\mathbf{x}_*$ with themselves, and $\Sigma_*$ represents the matrix of covariances between $\mathbf{x}$ and $\mathbf{x}_*$. Since we have no knowledge of the function that produced the data, we assume $\boldsymbol{\mu} = \mathbf{0}$ and $\boldsymbol{\mu}_* = \mathbf{0}$. We then have the conditional distribution of $\mathbf{f}_*$ given $\mathbf{f}$:

$$\mathbf{f}_* | \mathbf{f} \sim \mathcal{N}(\Sigma_*^T \Sigma^{-1} \mathbf{f}, \Sigma_{**} - \Sigma_*^T \Sigma^{-1} \Sigma_*) \tag{3}$$

This distribution given the data $(x_i, f_i)$, which we will refer to as $\mathcal{D}$, corresponds to a posterior Gaussian process:

$$f|\mathcal{D} \sim \mathcal{GP}(m_\mathcal{D}, k_\mathcal{D}) \tag{4}$$

$$m_\mathcal{D} = \Sigma(X, x)^T \Sigma^{-1} \mathbf{f} \tag{5}$$

$$k_\mathcal{D} = k(x, x') - \Sigma(X, x)^T \Sigma^{-1} \Sigma(X, x') \tag{6}$$

The notation is taken from Rasmussen [1]. $\Sigma(X, x)$ represents the vector of covariances between the vector of training inputs $X$ and $x$. The best guess for $f(x_u)$ for some $x_u \in \mathbf{x}_*$ would then be $f(x_u) = \Sigma(X, x_u)^T \Sigma^{-1} \mathbf{f}$.

However, our data $\mathcal{D}$ is not always precise. There may be noise associated with each measurement. If we assume the noise is independent for each data point, we can model this by adding a noise term to each $k(x, x)$ for all $x \in \mathbf{x}$. This accounts for training data of the form $y = f(x) + \mathcal{N}(0, \sigma_n^2)$. We capture this by modifying our kernel: $k(x, x') \to k(x, x') + \sigma_n^2 \delta_{xx'}$, where $\delta_{xx'}$ is the Kronecker delta, and $\sigma_n^2$ is the variance of the noise.

### Heat Equation

The heat equation simplifies to the following in one dimension (on the $z$ axis):

$$\nabla^2 u = \frac{1}{\alpha^2} \frac{\partial^2 u}{\partial t^2} \quad \to \quad \frac{\partial^2 u}{\partial z^2} = \frac{1}{\alpha^2} \frac{\partial^2 u}{\partial t^2} \tag{7}$$

Given the scenario described in the problem statement, we have the initial condition $u(z, 0) = T_0 \delta(z - y)$, where $T_0$ is the temperature of the source, and $\delta$ is the Dirac delta function. We then have the solution:

$$u(z, t) = \frac{T_0}{\sqrt{4\pi D t}} e^{-\frac{(z-y)^2}{4Dt}} \tag{8}$$

Given the temperature $x$ at time $t_0$ and location $s_0$ on the rod, we can then calculate the location $y$ of the heat source. We assume the positive branch of the square root. With $\alpha = 2Dt_0$, we have

$$x = \frac{T_0}{\sqrt{2\pi\alpha}} e^{-\frac{(s_0-y)^2}{2\alpha}} \quad \to \quad y = s_0 + \left( 2\alpha \log \frac{T_0}{x\sqrt{2\pi\alpha}} \right)^{\frac{1}{2}} \tag{9}$$

## IMPLEMENTATION

We generate the training data for our GP by uniformly sampling values on the interval $[0, L]$ to compose a vector of heat sources, $\mathbf{y}$. We then use Eq. 9 to generate the corresponding temperatures that would be measured for those heat sources, $\mathbf{x}$. Our training data is then the set of points $\mathcal{D} = (x_i, y_i + \mathcal{N}(0, \sigma_n^2))$. Now, given some measured temperature value $x_*$ at $z = s_0$ when $t = t_0$, we can find our expected value of $y_*$ using Eq. 5.

$$E[y_*] = m_{\mathcal{D}}(x_*) = \Sigma(\mathbf{x}, x_*)^T \Sigma^{-1} \mathbf{y} \tag{10}$$

However, we need to pick appropriate values of $\ell$, $\sigma_y$ and $\sigma_n$ for our covariance function in order to make an appropriate regression. With $s_0 = 10$, $T_0 = 40$, and $\mathbf{y}$ as a uniform sampling of spacing 0.05 on the interval $[10, 13.5]$, we use the values $\ell = 1$, $\sigma_y = 1$, and $\sigma_n = 0.01$.

## RESULTS

The GPR was used to calculate $\mathbf{y}_*$ given $\mathbf{x}_*$ as a vector with values between 0.1 and 40. The GPR is plotted with the training data and three specific values of interest in Fig. 1. The GPR agrees almost exactly with the analytic solution detailed in Eq. 9. The three measured temperature values and the corresponding interpolated initial heat source locations are tabulated below.

| Temp $x_*$ | Analytic $y_*$ | GPR $y_*$ | Rel. Error |
|---|---|---|---|
| 5.0 | 12.03803 | 12.03621 | 1.512e-04 |
| 19.7 | 11.18795 | 11.18934 | 1.1244e-04 |
| 37.0 | 10.38810 | 10.37765 | 1.1007e-03 |

Although the confidence interval is much wider for the interpolated value corresponding to x = 19.7, the relative error in the interpolation is still extremely low. The confidence interval can be made more narrow by gathering more training data where the confidence interval is largest.

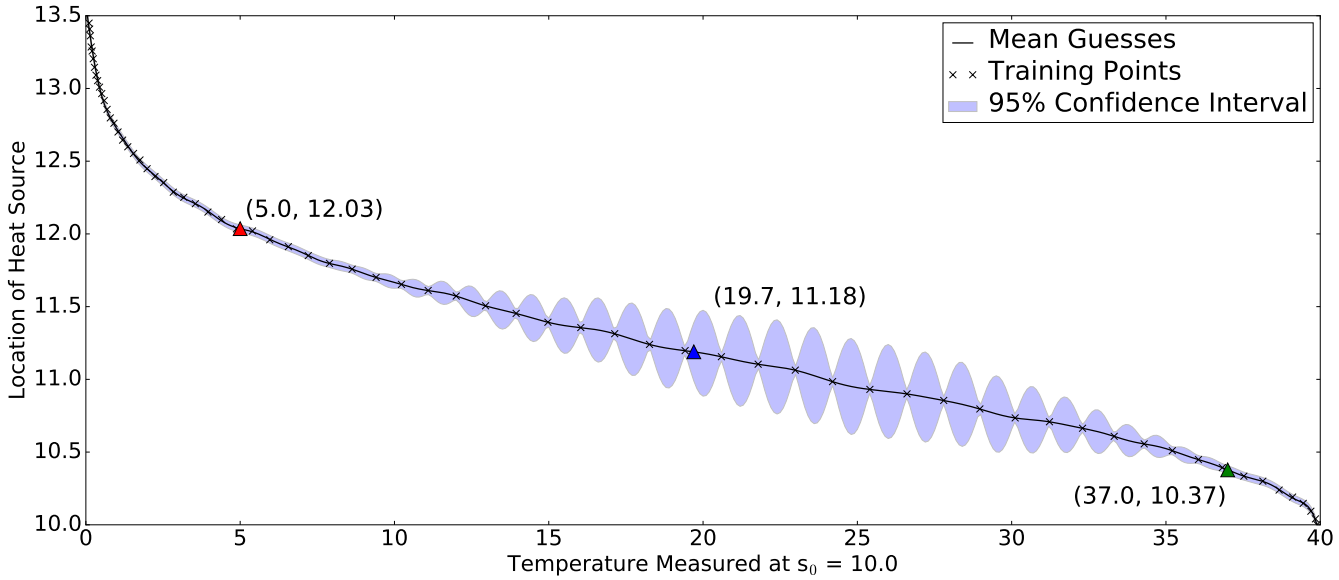


FIG. 1: Temperature measured at location $s_0$ versus location of initial heat source. The training data is plotted alongside a curve representing the interpolation. The confidence interval is more narrow when the training temperature values are closer together. The highest uncertainty occurs when the initial location varies the most with temperature measured.

## CONCLUSION

Our problem was of the form $x = H(y)$, where $H(y)$ represents Eq. 9. We generated data by sampling values of y and generating the corresponding x values. The GPR then allowed us to interpolate values of $y$ given $x_*$: $y_* = H^{-1}(x_*)$. As the problem was easily solved analytically, we checked the accuracy of our guess for $H^{-1}$ against the solution to the heat equation given our initial conditions. We saw that the GPR was accurate throughout the domain of the regression, yielding low relative errors even when the confidence interval was large.

This effectively allowed us to invert $H(y)$. The same methodology can be applied to more complex problems of the form $Ax = y$, where $A$ is not easily invertible. By picking specific $y_i$ that have more readily known solutions $x_i$, a Gaussian process can be trained on the data $(x_i, y_i)$. A GPR could then be used to find $x_* = A^{-1}y_*$ for instances of $y_*$ that make the equation more difficult to solve.

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