# AutoML: Gaussian Processes

## Gaussian Process Training

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# Training of a Gaussian Process

- To make predictions for a regression task by a Gaussian process, one simply needs to perform matrix computations.
- But for this to work out, we assume that the covariance functions is fully given, including all of its hyperparameters.
- A very nice property of GPs is that we can learn the numerical hyperparameters of a selected covariance function directly during GP training.

# Training a GP via the Maximum Likelihood I

- Let us assume $y = f(\mathbf{x}) + \epsilon,\ \epsilon \sim \mathcal{N}\left(0, \sigma^2\right)$, where $f(\mathbf{x}) \sim \mathcal{G}\left(\mathbf{0}, k\left(\mathbf{x}, \mathbf{x}' \mid \boldsymbol{\theta}\right)\right)$.

- Noticing that $\boldsymbol{y} \sim \mathcal{N}\left(\mathbf{0}, \boldsymbol{K} + \sigma^2 \boldsymbol{I}\right)$, we can find the marginal log-likelihood (or evidence):

$$
\begin{aligned}
log\, p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{\theta}) &= log\left[(2\pi)^{-n/2} \left|\boldsymbol{K}_y\right|^{-1/2} \exp\left(-\frac{1}{2}\boldsymbol{y}^\top \boldsymbol{K}_y^{-1} \boldsymbol{y}\right)\right] \\
&= -\frac{1}{2}\boldsymbol{y}^\top \boldsymbol{K}_y^{-1} \boldsymbol{y} - \frac{1}{2} log\left|\boldsymbol{K}_y\right| - \frac{n}{2} log\, 2\pi.
\end{aligned}
$$

with $\boldsymbol{K}_y := \boldsymbol{K} + \sigma^2 \boldsymbol{I}$ and $\boldsymbol{\theta}$ denoting the parameters of the covariance function (i.e., the hyperparameters).

# Training a GP via the Maximum Likelihood II

Recalling that the increase of the length-scale reduces the model flexibility, the three terms of the marginal likelihood can be interpreted as follows.

- The data fit $-\frac{1}{2}\boldsymbol{y}^T\boldsymbol{K}_y^{-1}\boldsymbol{y}$. The data fit tends to decrease by increasing the length-scale.
- The complexity penalty $-\frac{1}{2}\,log\,|\boldsymbol{K}_y|$, which depends on the covariance function. This term decreases with the increase of the length-scale (the model gets less complex as the length-scale grows).
- The normalization constant $-\frac{n}{2}\,log\,2\pi$.

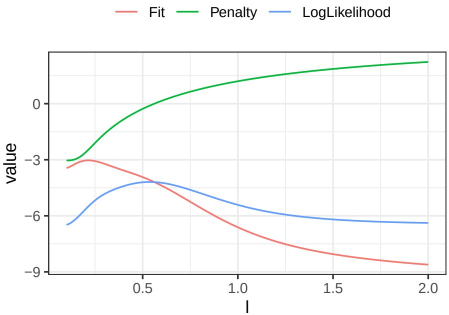
# Training a GP: Example I

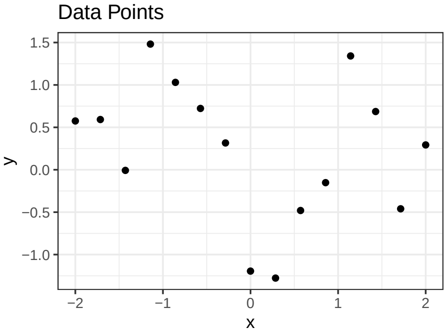
To visualize this, let us consider a zero-mean GP with a squared exponential kernel:

$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2\ell^2}\|\mathbf{x} - \mathbf{x}'\|^2\right).$$

- Recall that the model becomes smoother and less complex as the length-scale $\ell$ increases.
- We will show how each of the following terms behaves if the value of $\ell$ increases:
  - the data fit $-\frac{1}{2}\boldsymbol{y}^\top \boldsymbol{K}_y^{-1}\boldsymbol{y}$,
  - the complexity penalty $-\frac{1}{2}\,log\,|\boldsymbol{K}_y|$,
  - the overall value of the marginal likelihood $log\,p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{\theta})$.

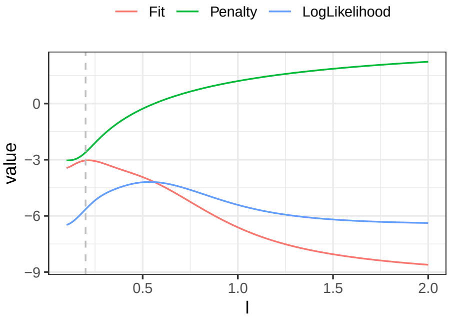
# Training a GP: Example II

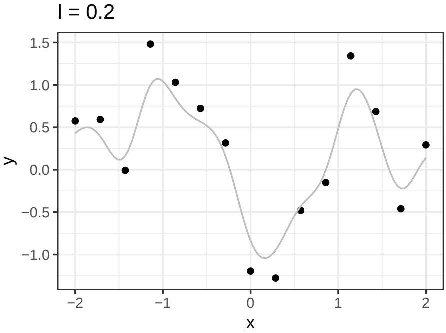



ℹ The left plot depicts how the data fit, the complexity penalty (a higher value means less penalization), and the overall marginal likelihood behave for increasing values of the length-scale.

# Training a GP: Example III

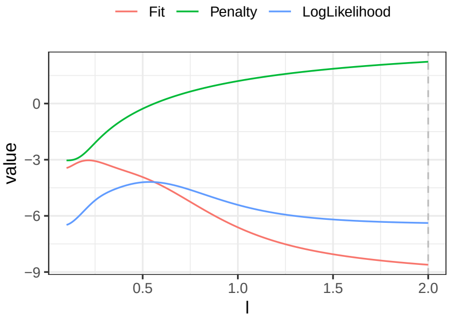


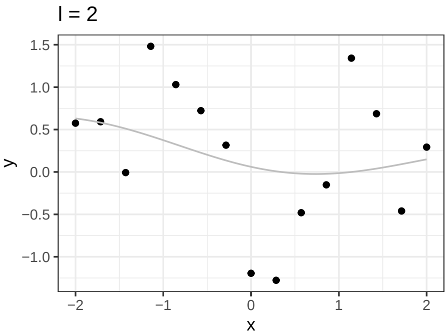




The left plot depicts how the data fit, the complexity penalty (a higher value means less penalization), and the overall marginal likelihood behave for increasing values of the length-scale.

A small $\ell$ leads to a good fit, but, to a high complexity penalty.

# Training a GP: Example IV

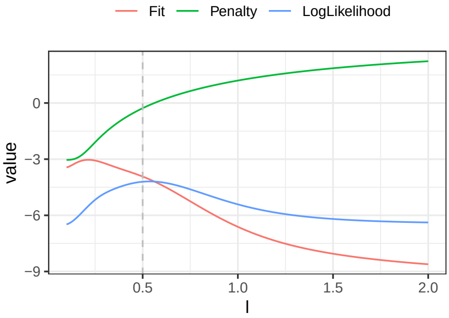


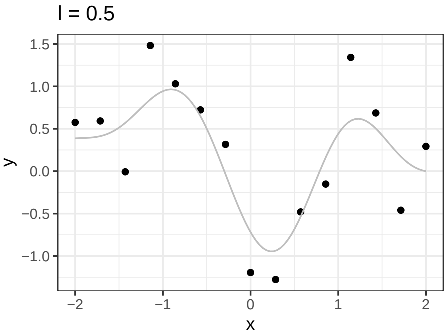




The left plot depicts how the data fit, the complexity penalty (a higher value means less penalization), and the overall marginal likelihood behave for increasing values of the length-scale.

A large $\ell$ results in a poor fit.

# Training a GP: Example V




The left plot depicts how the data fit, the complexity penalty (a higher value means less penalization), and the overall marginal likelihood behave for increasing values of the length-scale.

The maximizer of the log-likelihood ($\ell = 0.5$) balances the complexity and data the fit.

# Training a GP via the Maximum Likelihood I

To choose the hyperparameters by maximizing the marginal likelihood, we need to find the partial derivatives of the likelihood w.r.t. the hyperparameters:

$$
\begin{aligned}
\frac{\partial}{\partial \theta_j} log\, p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{\theta}) &= \frac{\partial}{\partial \theta_j}\left(-\frac{1}{2}\boldsymbol{y}^\top \boldsymbol{K}_y^{-1}\boldsymbol{y} - \frac{1}{2} log\, |\boldsymbol{K}_y| - \frac{n}{2} log\, 2\pi\right) \\
&= \frac{1}{2}\boldsymbol{y}^\top \boldsymbol{K}^{-1}\frac{\partial \boldsymbol{K}}{\partial \theta_j}\boldsymbol{K}^{-1}\boldsymbol{y} - \frac{1}{2}\text{tr}\left(\boldsymbol{K}^{-1}\frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\theta}}\right) \\
&= \frac{1}{2}\text{tr}\left((\boldsymbol{K}^{-1}\boldsymbol{y}\boldsymbol{y}^\top \boldsymbol{K}^{-1} - \boldsymbol{K}^{-1})\frac{\partial \boldsymbol{K}}{\partial \theta_j}\right)
\end{aligned}
$$

Above, we used the following identities:

$$
\frac{\partial}{\partial \theta_j}\boldsymbol{K}^{-1} = -\boldsymbol{K}^{-1}\frac{\partial \boldsymbol{K}}{\partial \theta_j}\boldsymbol{K}^{-1} \text{ and } \frac{\partial}{\partial \boldsymbol{\theta}} log|\boldsymbol{K}| = \text{tr}\left(\boldsymbol{K}^{-1}\frac{\partial \boldsymbol{K}}{\partial \boldsymbol{\theta}}\right)
$$

# Training a GP via the Maximum Likelihood II

- The complexity and the runtime of training a Gaussian process is dominated by the computational task of inverting $\boldsymbol{K}$ - or let's rather say for decomposing it.

- Standard methods require $\mathcal{O}(n^3)$ time (!) for this.

- Once $\boldsymbol{K}^{-1}$ - or rather the decomposition -is known, the computation of the partial derivatives requires only $\mathcal{O}(n^2)$ time per hyperparameter.

- Thus, the computational overhead of computing derivatives is small, and using a gradient based optimizer is advantageous.

# Training a GP via the Maximum Likelihood III

Workarounds to make GP estimation feasible for big data include:

- Using kernels that yield sparse $\boldsymbol{K}$: cheaper to invert.
- Subsampling the data to estimate $\theta$; $\mathcal{O}(m^3)$ for subset of size $m$.
- Combining estimates on different subsets of size $m$: **Bayesian committee**; $\mathcal{O}(nm^2)$.
- Exploiting low-rank approximations of $\boldsymbol{K}$ by using only a representative subset (inducing points) of $m$ training data $\boldsymbol{X}_m$:**Nyström approximation** $\boldsymbol{K} \approx \boldsymbol{K}_{nm}\boldsymbol{K}_{mm}^{-}\boldsymbol{K}_{mn}$, with $\mathcal{O}(nmk + m^3)$ for a rank-k-approximate inverse of $\boldsymbol{K}_{mm}$.
- Utilizing structure in $\boldsymbol{K}$ induced by the kernel: exact solutions but complicated maths, not applicable for all kernels.

... this is still an active area of research.