TRAINING A GP VIA MAXIMUM LIKELIHOOD

Let us assume

$$y = f(\mathbf{x}) + \epsilon, \; \epsilon \sim \mathcal{N}\left(0, \sigma^2\right),$$

where $f(\mathbf{x}) \sim \mathcal{GP}\left(\mathbf{0}, k\left(\mathbf{x}, \mathbf{x}' | \theta\right)\right)$.

Observing $\boldsymbol{y} \sim \mathcal{N}\left(\mathbf{0}, \boldsymbol{K} + \sigma^2 \boldsymbol{I}\right)$, the marginal log-likelihood (or evidence) is

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

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

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The three terms of the marginal likelihood have interpretable roles, considering that the model becomes less flexible as the length-scale increases:

- the data fit $-\frac{1}{2}\mathbf{y}^T\mathbf{K}_{\mathbf{y}}^{-1}\mathbf{y}$, which tends to decrease if the length scale increases
- the complexity penalty $-\frac{1}{2}\log|\mathbf{K}_{\mathbf{y}}|$, which depends on the covariance function only and which increases with the length-scale, because the model gets less complex with growing length-scale
- a normalization constant $-\frac{n}{2}\log 2\pi$

TRAINING A GP: EXAMPLE

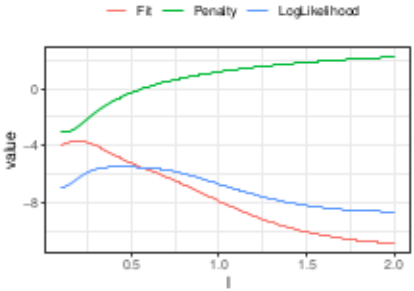
To visualize this, we consider a zero-mean Gaussian process with squared exponential kernel

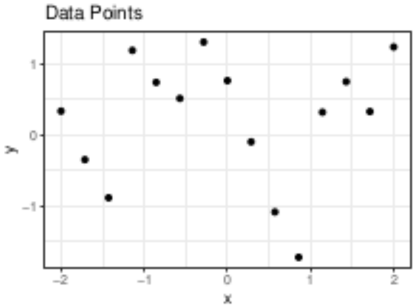
$$k(\mathbf{x}, \mathbf{x}') = \exp\left(-\frac{1}{2\ell^2}\|\mathbf{x} - \mathbf{x}'\|^2\right),$$

- Recall, the model is smoother and less complex for higher length-scale ℓ.
- We show how the
  - data fit $-\frac{1}{2}\boldsymbol{y}^T\boldsymbol{K}_{\boldsymbol{y}}^{-1}\boldsymbol{y}$,
  - the complexity penalty $-\frac{1}{2}\log|\boldsymbol{K}_{\boldsymbol{y}}|$, and
  - the overall value of the marginal likelihood $\log p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{\theta})$

  behave for increasing value of ℓ.

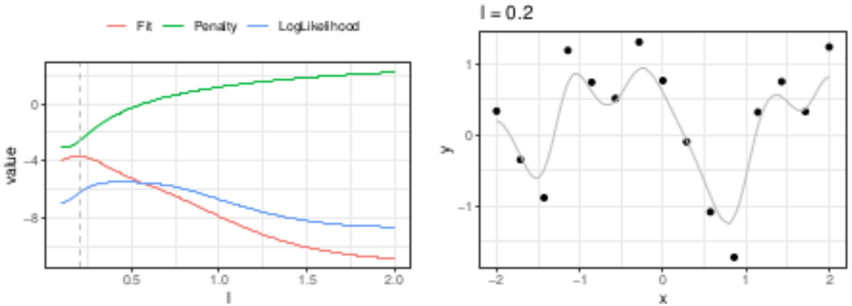
TRAINING A GP: EXAMPLE / 2





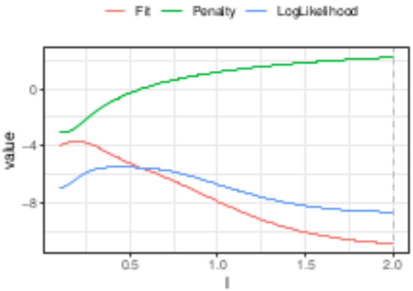
The left plot shows how values of the data fit $-\frac{1}{2}\mathbf{y}^T \mathbf{K}_y^{-1}\mathbf{y}$, the complexity penalty $-\frac{1}{2}\log|\mathbf{K}_y|$ (high value means less penalization) and the overall marginal likelihood $\log p(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\theta})$ behave for increasing values of ℓ.

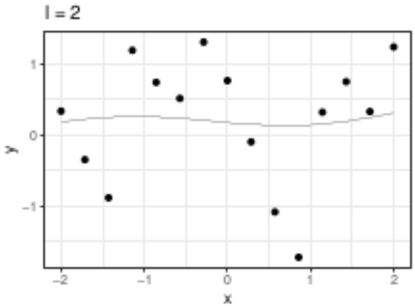
TRAINING A GP: EXAMPLE / 3



- The left plot shows how values of the data fit $-\frac{1}{2}\mathbf{y}^T\mathbf{K}_y^{-1}\mathbf{y}$, the complexity penalty $-\frac{1}{2}\log|\mathbf{K}_y|$ (high value means less penalization) and the overall marginal likelihood $\log p(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\theta})$ behave for increasing values of ℓ.
- A small ℓ results in a good fit, but a high complexity penalty (low $-\frac{1}{2}\log|\mathbf{K}_y|$).

TRAINING A GP: EXAMPLE / 4

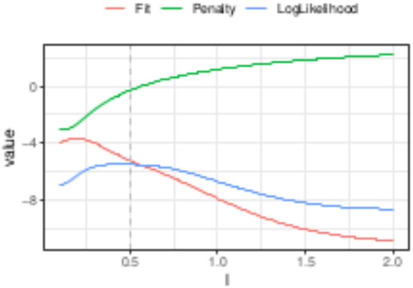


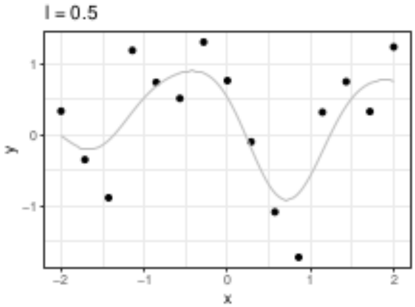


The left plot shows how values of the data fit $-\frac{1}{2}\boldsymbol{y}^T\boldsymbol{K}_y^{-1}\boldsymbol{y}$, the complexity penalty $-\frac{1}{2}\log|\boldsymbol{K}_y|$ (high value means less penalization) and the overall marginal likelihood $\log p(\boldsymbol{y} \mid \boldsymbol{X}, \boldsymbol{\theta})$ behave for increasing values of ℓ.

A large ℓ results in a poor fit.

TRAINING A GP: EXAMPLE / 5





The left plot shows how values of the data fit $-\frac{1}{2}\mathbf{y}^T\mathbf{K}_y^{-1}\mathbf{y}$, the complexity penalty $-\frac{1}{2}\log|\mathbf{K}_y|$ (high value means less penalization) and the overall marginal likelihood $\log p(\mathbf{y} \mid \mathbf{X}, \boldsymbol{\theta})$ behave for increasing values of ℓ.

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

TRAINING A GP VIA MAXIMUM LIKELIHOOD

To set the hyperparameters by maximizing the marginal likelihood, we seek the partial derivatives w.r.t. the hyperparameters

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

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

TRAINING A GP VIA MAXIMUM LIKELIHOOD / 2

- 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, so using a gradient based optimizer is advantageous.

TRAINING A GP VIA MAXIMUM LIKELIHOOD / 3

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 θ: $\mathcal{O}(m^3)$ for subset of size m.
- combining estimates on different subsets of size m:
  Bayesian committee, $\mathcal{O}(nm^2)$.
- using low-rank approximations of $\boldsymbol{K}$ by using only a representative subset ("inducing points") of m training data $\boldsymbol{X}_m$:
  Nyström approximation $\boldsymbol{K} \approx \boldsymbol{K}_{nm}\boldsymbol{K}_{mm}^{-}\boldsymbol{K}_{mn}$,
  $\mathcal{O}(nmk + m^3)$ for a rank-k-approximate inverse of $\boldsymbol{K}_{mm}$.
- exploiting 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.