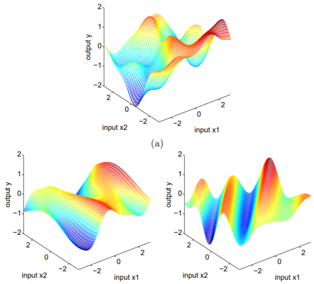
Introduction to Machine Learning

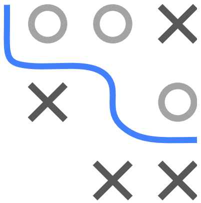
Gaussian Processes
Covariance functions for GPs



Learning goals

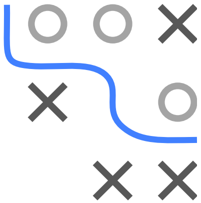
- Covariance functions encode key assumptions about the GP
- Common covariance functions like squared exponential and Matérn

VALID COVARIANCE FUNCTIONS



- Recall marginalization property of GPs: for any $\mathbf{X} = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(n)}\} \subset \mathcal{X}$,
$$\mathbf{f} = f(\mathbf{X}) \sim \mathcal{N}(\mathbf{m}, \mathbf{K})$$
with $\mathbf{m} = m(\mathbf{X})$, $\mathbf{K} = k(\mathbf{X}, \mathbf{X})$
- Cov. function (or kernel) determines cov / kernel / Gram matrix: $\mathbf{K} = k(\mathbf{X}, \mathbf{X})$
- For $\mathbf{K}$ to be a valid cov matrix it needs to be positive semi-definite (PSD) for any choice of inputs $\mathbf{X}$
- Implication: only **PSD functions** (i.e., those that induce PSD $\mathbf{K}$) are valid cov functions
- Also look at SVM chapter for background info on kernels, many further details in e.g. ▸ Duvenaud 2014

STATIONARY COVARIANCE FUNCTIONS



- Recall concept of spatial correlation

$$\mathbf{x}, \tilde{\mathbf{x}} \text{ close in } \mathcal{X} \Rightarrow f(\mathbf{x}), f(\tilde{\mathbf{x}}) \text{ close / more correlated in } \mathcal{Y}$$

- Measure "closeness" via $\boldsymbol{d} = \mathbf{x} - \tilde{\mathbf{x}}$

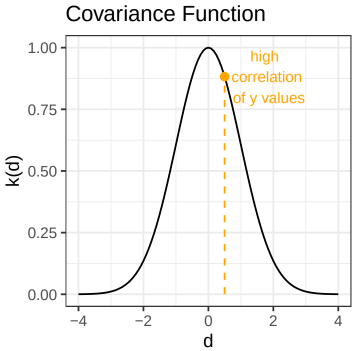
- $k(\cdot, \cdot)$ called **stationary** $\Leftrightarrow$ function of $\boldsymbol{d}$

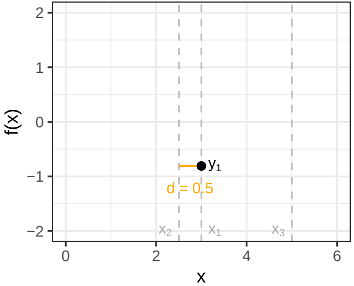
$$k(\mathbf{x}, \tilde{\mathbf{x}}) = k(\boldsymbol{d})$$

- Intuition: stationary $k(\cdot, \cdot)$ implies functions that do not depend on where the points lie in input space but only their difference

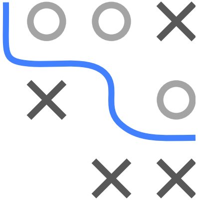
EXAMPLE: STATIONARY COVARIANCE

- Let $f \sim \mathcal{GP}(m(\cdot), k(\cdot, \cdot))$ with $k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp(-\frac{1}{2}\|\boldsymbol{d}\|^2)$
- Consider two points $\mathbf{x}^{(1)} = 3$ and $\mathbf{x}^{(2)} = 2.5$
- To get corr. between $f(\mathbf{x}^{(1)})$ and $f(\mathbf{x}^{(2)})$ look at $\boldsymbol{d}(\mathbf{x}^{(1)}, \mathbf{x}^{(2)})$

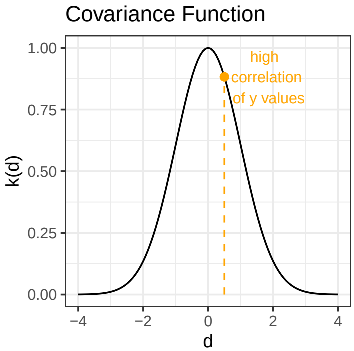


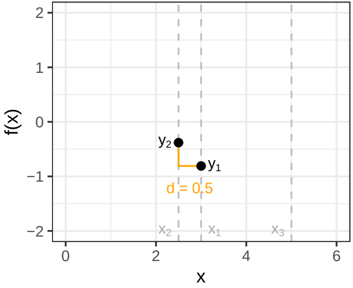


EXAMPLE: STATIONARY COVARIANCE



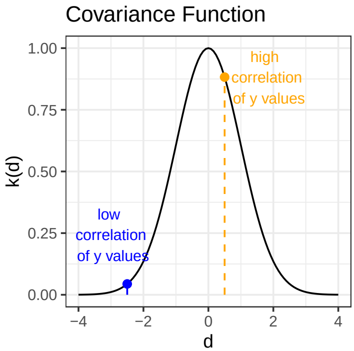
- Suppose we observe $y^{(1)} = -0.8$
- $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}$ are close in $\mathcal{X}$ space
- Under the above GP assumption, $y^{(2)}$ should be close to $y^{(1)}$

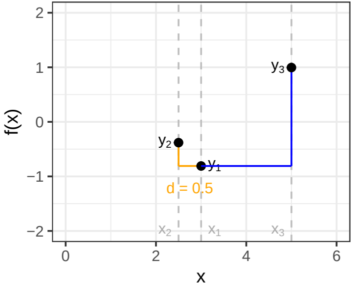




EXAMPLE: STATIONARY COVARIANCE

- Consider now $\mathbf{x}^{(3)} = 5$
- This is now further from $\mathbf{x}^{(1)}$
- $\Rightarrow$ expect lower correlation between $y^{(3)}$, $y^{(1)}$

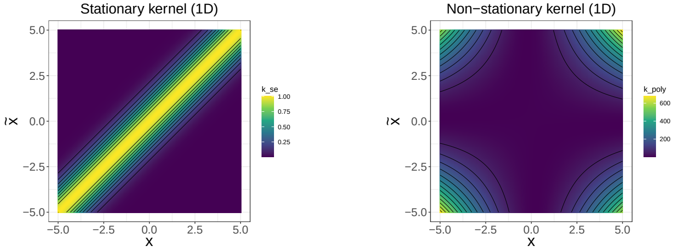




PROPERTIES OF COVARIANCE FUNCTIONS I

- **Stationary**: $k = k(\boldsymbol{d})$ with $\boldsymbol{d} = \mathbf{x} - \tilde{\mathbf{x}}$
  $\Rightarrow$ invariant to translations in $\mathcal{X}$: $k(\mathbf{x}, \mathbf{x} + \boldsymbol{d}) = k(\mathbf{0}, \boldsymbol{d})$
  (so we sometimes abuse notation and write $k(\boldsymbol{d})$)

- Consider $\mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}$ and plot contours of $k(\mathbf{x}, \tilde{\mathbf{x}})$:

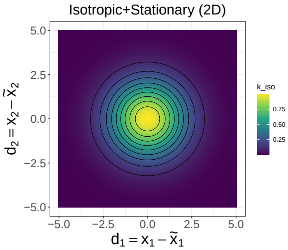


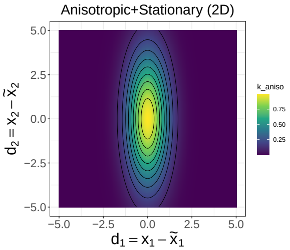
- Contour set of $\mathbf{x} \to k(\mathbf{x}, \tilde{\mathbf{x}}_1)$ must be same as for $\mathbf{x} \to k(\mathbf{x}, \tilde{\mathbf{x}}_2)$ translated by $\tilde{\mathbf{x}}_1 - \tilde{\mathbf{x}}_2$

PROPERTIES OF COVARIANCE FUNCTIONS II

- **Isotropic**: $k = k(\boldsymbol{r})$ with $r = \|\mathbf{x} - \tilde{\mathbf{x}}\|$
  $\Rightarrow$ invariant to rotations, implies stationarity
  (again slight notational abuse)

- Consider $\mathbf{x}, \tilde{\mathbf{x}} \in \mathbb{R}^2$



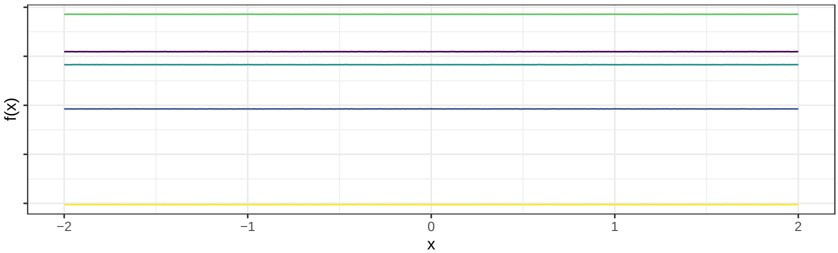


- Isotropic = circular/concentric contours, anisotropic = elliptic

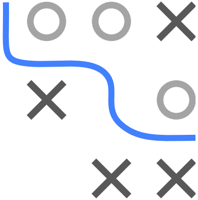
- **Dot product**: $k = k(\mathbf{x}^T \tilde{\mathbf{x}})$

CONSTANT KERNEL

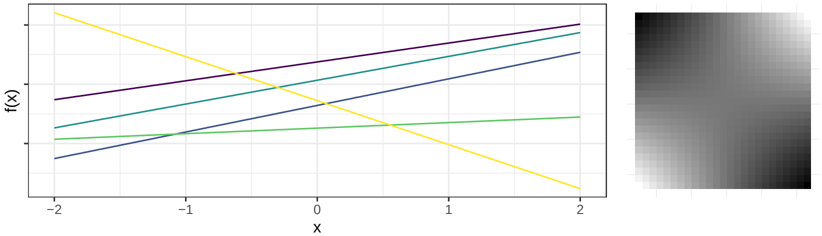
- $k(\mathbf{x}, \tilde{\mathbf{x}}) = \theta_0 \quad > 0$
- Constant function priors
- Global correlation irresp. of concrete inputs $\mathbf{x}, \tilde{\mathbf{x}}$
- Practically pretty useless



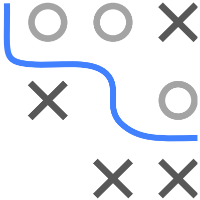
LINEAR KERNEL



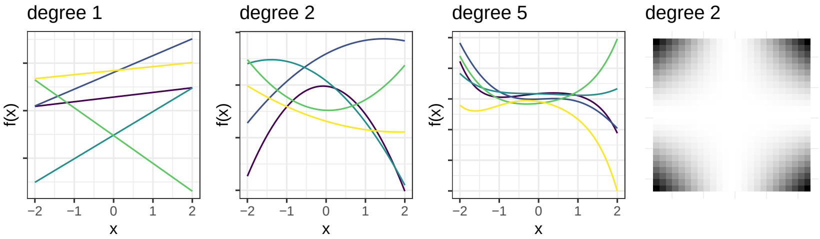
- $k(\mathbf{x}, \tilde{\mathbf{x}}) = \theta_0 + \mathbf{x}^T \tilde{\mathbf{x}}$
- Linear function priors
- Measures directional similarity: higher if vectors point in similar dirs
- In general, non-stationary $\Rightarrow$ depends on locations of $\mathbf{x}, \tilde{\mathbf{x}}$
- See Bayesian linear model part



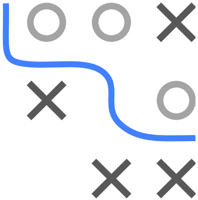
POLYNOMIAL KERNEL



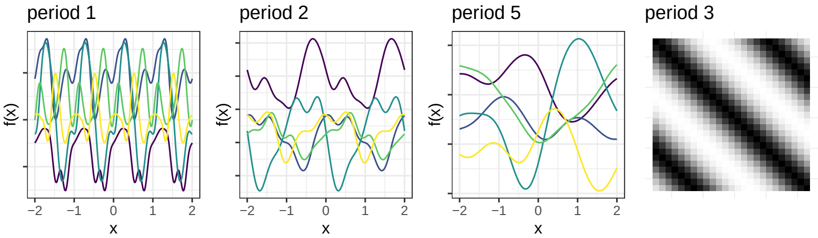
- $k(\mathbf{x}, \tilde{\mathbf{x}}) = (\theta_0 + \mathbf{x}^T \tilde{\mathbf{x}})^p, \quad p \in \mathbb{N}$
- Polynomial function priors
- Allows for non-linearity through higher-order monomials & interaction terms



PERIODIC KERNEL

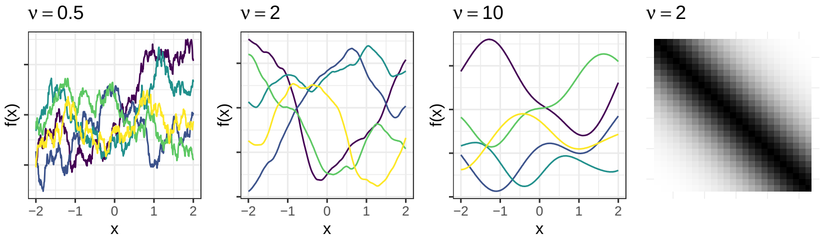


- E.g., radial periodic kernel: $k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(\frac{-2\sin^2(\pi\|\mathbf{x}-\tilde{\mathbf{x}}\|/m)}{\ell^2}\right)$
- m: period, ℓ: length-scale
- $f(\mathbf{x})$ should be periodically similar to points with a distance which is a multiple of m;
  for distances in between, this is modulated by ℓ
- Alternative: Product of 1D periodic kernels, with m_j period in dimension j: $k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(\sum_j \frac{-2\sin^2(\pi|x_j-\tilde{x}_j|/m_j)}{\ell^2}\right)$



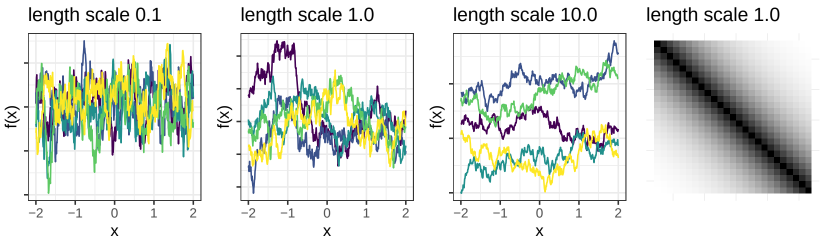
MATÉRN KERNEL

- $k(\mathbf{x}, \tilde{\mathbf{x}}) = \frac{1}{2^\nu \Gamma(\nu)} \left(\sqrt{2\nu} \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\ell} \right)^\nu K_\nu \left(\sqrt{2\nu} \frac{\|\mathbf{x} - \tilde{\mathbf{x}}\|}{\ell} \right)$
- ν: smoothness param, Γ: gamma function, ℓ: length scale, K_ν: modified Bessel function
- Stationary & isotropic
- Allows for controlled degree of smoothness via choice of ν
- ν also determines differentiability
- Use for: non-linear functions with desired degree of smoothness



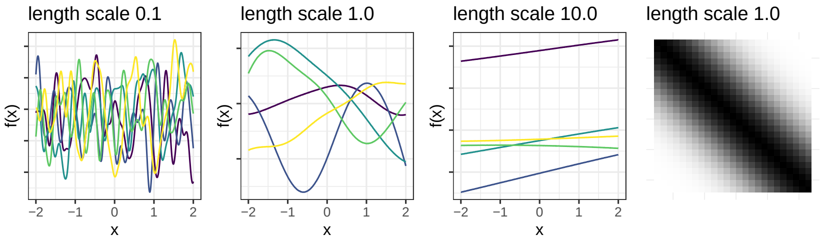
EXPONENTIAL KERNEL

- Aka Ornstein-Uhlenbeck kernel
- $k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\frac{\|\mathbf{x}-\tilde{\mathbf{x}}\|}{\ell}\right)$
- Special case of Matérn kernel with $\nu = 0.5$
- Non-smooth: continuous but not differentiable, can model functions with abrupt variations
- Cov decays exponentially with distance (modulated by ℓ)



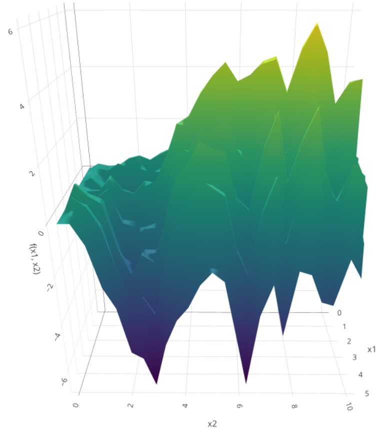
SQUARED EXPONENTIAL KERNEL

- Aka Gaussian kernel, RBF kernel
- $k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\frac{\|\mathbf{x}-\tilde{\mathbf{x}}\|^2}{2\ell^2}\right)$
- Special case of Matérn kernel with $\nu = \infty$
- Very smooth: continuous, ∞ differentiable (not always realistic)
- Cov decays quickly $\Rightarrow$ quadratic in distance



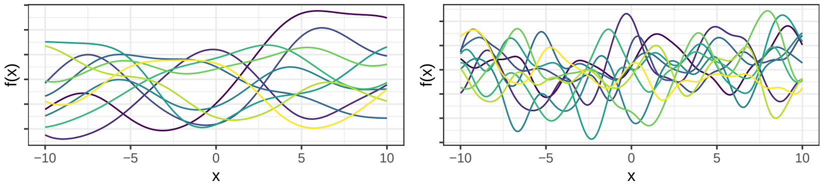
EXAMPLE: BROWNIAN MOTION

- $k(\mathbf{x}, \tilde{\mathbf{x}}) = \prod_j \min(x_j, \tilde{x}_j)$
- Physics application: random fluctuations of particles
- With non-1D inputs aka Brownian sheet
- Correlation in each dimension is 1D-like Brownian motion



CHARACTERISTIC LS : ISOTROPIC CASE

- Every (isotropic) kernel can be written as $k(r)$ where
- $r = ||\mathbf{x} - \tilde{\mathbf{x}}||$
- E.g. $k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\frac{||\mathbf{x}-\tilde{\mathbf{x}}||^2}{2\ell^2}\right)$ or $k(r) = \exp\left(-\frac{1}{2}(\frac{r}{\ell})^2\right)$
- Controls how quickly function values become uncorrelated
- High (low) ℓ: smooth (wiggly) functions



- In SVM kernels we sometimes called this bandwith

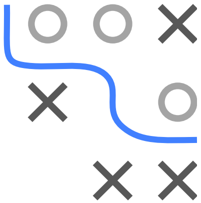
CHARACTERISTIC LS : STATIONARY CASE

- For stationary kernels $k(\boldsymbol{d})$
- We modulate every distance component d_j by an individual ℓ_j
- We can turn the isotropic examples from above into stationary ones – with individual length scales
- Write $||\boldsymbol{d}||^2 = \sum d_j^2$ and put an $1/\ell_j$ before each d_j
- E.g. for squared exp:

$$k(\boldsymbol{d}) = \exp\left(-\frac{1}{2}\sum_{j=1}^{p}\frac{d_j^2}{\ell_j^2}\right)$$

- Also note: this is a product of 1D kernels, one for each input dim. The correlation in each dim is described by the 1D kernel and its distance component is modulated by ℓ_j

BENEFITS OF DIM-WISE LENGTH-SCALES



- $\ell_1, \ldots, \ell_p$: characteristic length-scales

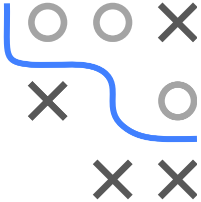
- Intuition for ℓ_i: how far to move along *i*-th axis for fun. values to become uncorrelated?

- Implements **automatic relevance determination** (ARD): inverse of ℓ_i determines importance of *i*-th feature

- Very large $\ell_i \Rightarrow$ cov effectively independent of *i*-th feature

- For features on different scales: rescale automatically by estimating $\ell_1, \ldots, \ell_p$

CHARACTERISTIC LS : WEIGHTED EUCLID DIST



- Can even generalize the above principle
- Move to weighted (squared) Euclidean distance
- E.g. for squared exp again:

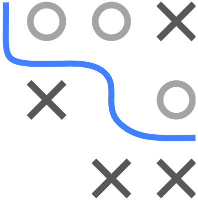
$$k(\mathbf{x}, \tilde{\mathbf{x}}) = \exp\left(-\tfrac{1}{2}(\mathbf{x} - \tilde{\mathbf{x}})^T \boldsymbol{M}(\mathbf{x} - \tilde{\mathbf{x}})\right)$$

- This covers the case before
- Possible choices for $\boldsymbol{M}$:

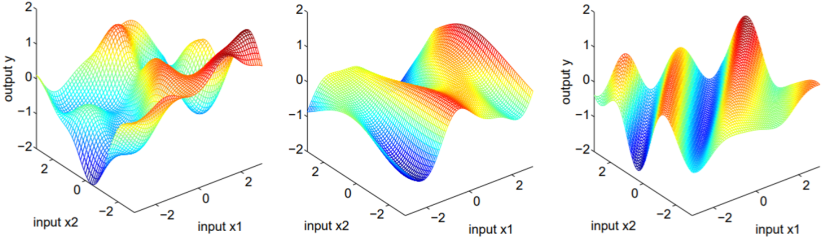
$$\boldsymbol{M}_1 = \ell^{-2}\boldsymbol{I}_p \qquad \boldsymbol{M}_2 = \mathrm{diag}(\boldsymbol{\ell})^{-2} \qquad \boldsymbol{M}_3 = \Gamma\Gamma^T + \mathrm{diag}(\boldsymbol{\ell})^{-2}$$

where $\boldsymbol{\ell} \in \mathbb{R}_+^p$, $\Gamma \in \mathbb{R}^{p \times k}$

EXAMPLES: CHARACTERISTIC LS



- Left: $\boldsymbol{M} = \boldsymbol{I} \Rightarrow$ same variation in all directions
- Middle: $\boldsymbol{M} = \mathrm{diag}(\boldsymbol{\ell})^{-2} \Rightarrow$ less variation in x_2 direction ($\ell_2 > \ell_1$)
- Right: $\boldsymbol{M} = \Gamma\Gamma^T + \mathrm{diag}(\boldsymbol{\ell})^{-2}$ with $\Gamma = (1, -1)^T$ and $\boldsymbol{\ell} = (6, 6)^T$
  $\Rightarrow \Gamma$ determines dir. of most rapid variation



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