KOÇ ÜNİVERSİTESİ

Uzam-zamansal modelleme için yapay öğrenme modelleri

Mehmet Gönen
mehmetgonen@ku.edu.tr

Endüstri Mühendisliği Bölümü, Mühendislik Fakültesi
Hesaplamalı Biyoloji Bölümü, Tıp Fakültesi

27 Şubat 2021

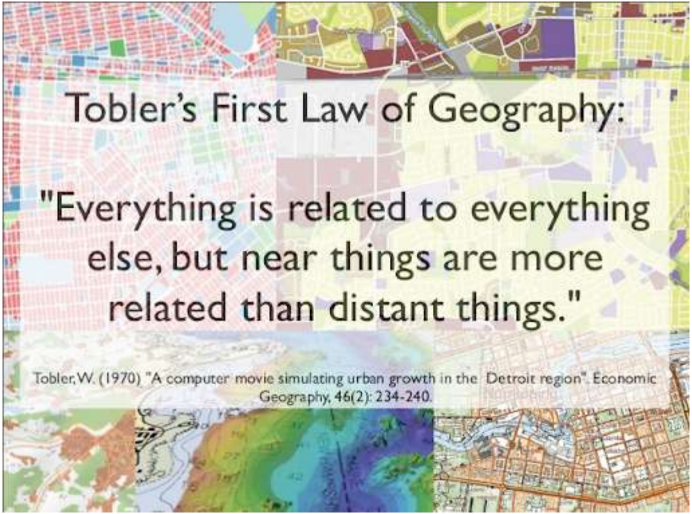
Uzam-zamansal modelleme

- Guatemala yerlileri tarafından çizilen 1527 ve 1530 yılları arasındaki İspanyol işgalinin haritası

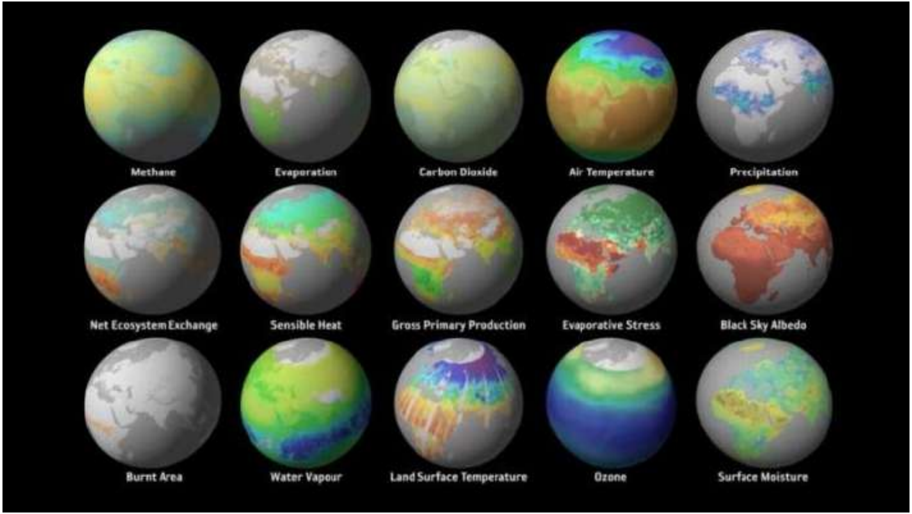
Uzam-zamansal modelleme

- “After choosing the area we usually have no guidance beyond the verifiable fact that patches in close proximity are commonly more alike, as judged by the yield of the crops, than those which are far apart.” (R. A. Fisher, 1935)

Uzam-zamansal modelleme

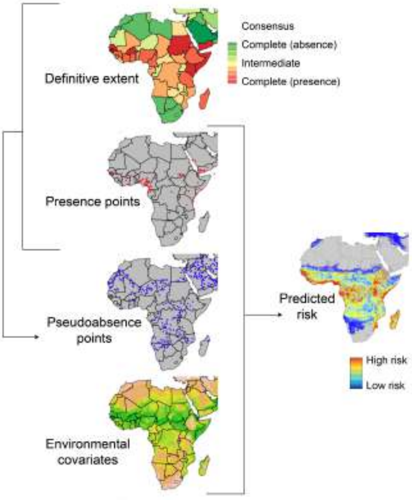


Uzam-zamansal modelleme

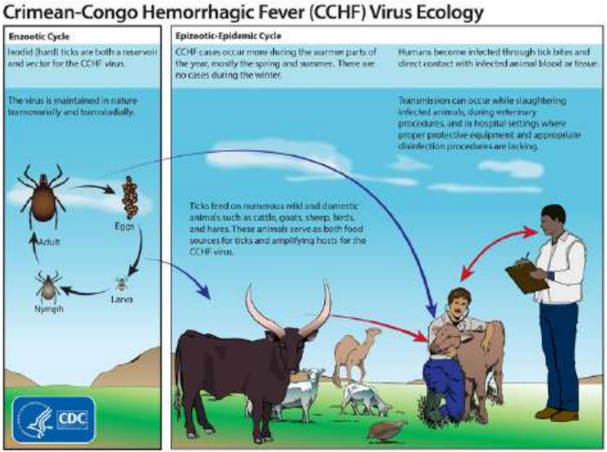


Uzam-zamansal modelleme

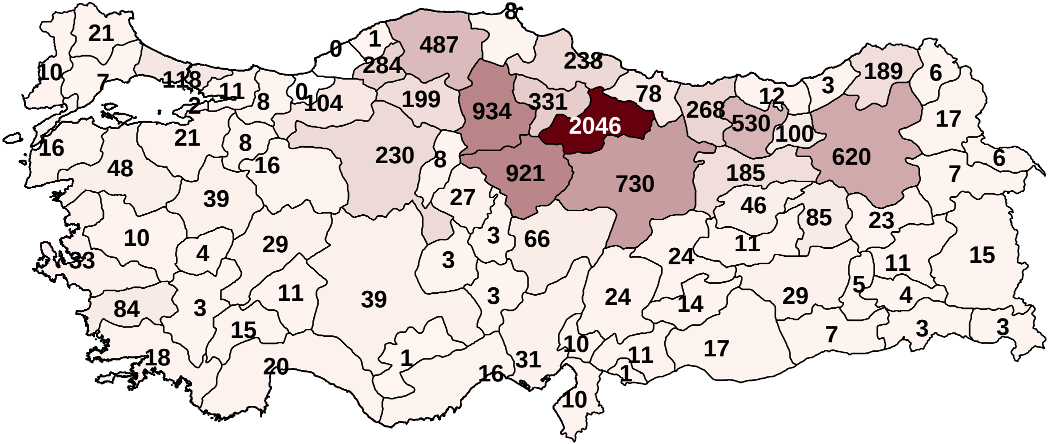
Enfeksiyon hastalıklarının modellenmesi



Kırım–Kongo Kanamalı Ateşi (KKKA) hastalığı



Türkiye’de KKKA



Türkiye'de KKKA

Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec	Total	Season
0	0	2	9	24	62	101	44	6	1	0	0	249	2004
0	0	0	8	27	77	95	51	3	4	0	0	265	2005
0	0	1	19	65	160	114	72	8	0	0	0	439	2006
0	0	2	25	119	216	224	90	40	1	0	0	717	2007
0	0	1	37	241	432	411	151	40	2	0	0	1315	2008
0	0	0	37	205	496	366	177	33	3	1	0	1318	2009
0	0	0	61	240	272	222	59	11	2	0	0	867	2010
0	0	1	29	149	341	349	180	19	5	2	0	1075	2011
0	0	1	31	223	233	201	90	13	3	1	0	796	2012
0	0	1	74	225	260	254	81	11	2	2	0	910	2013
0	4	6	95	218	238	280	108	13	5	0	0	967	2014
0	0	2	16	97	231	218	119	20	12	2	1	718	2015
0	4	17	441	1833	3018	2835	1222	217	40	8	1	9636	Total

Regresyon problemi

- Eğitim kümesi: $\mathcal{X} = \{(\boldsymbol{x}_i, y_i) \in \mathbb{R}^D \times \mathbb{R}\}_{i=1}^N$

$$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1D} \\ x_{21} & x_{22} & \cdots & x_{2D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N1} & x_{N2} & \cdots & x_{ND} \end{bmatrix} \qquad \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$$

- Önceden görmediğimiz bir veri noktası $\boldsymbol{x}_* \in \mathbb{R}^D$ için çıktı değerini kestirmek

$$\boldsymbol{x}_* = \begin{bmatrix} x_{*1} & x_{*2} & \cdots & x_{*D} \end{bmatrix} \qquad y_* = \begin{bmatrix} ? \end{bmatrix}$$

Gauss süreci

- Normal dağılım: $\mathcal{N}(x;\mu,\sigma^2)$

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

- Çok değişkenli normal dağılım: $\mathcal{N}(\boldsymbol{x};\boldsymbol{\mu},\boldsymbol{\Sigma})$

$$p(\boldsymbol{x}) = \frac{1}{\sqrt{(2\pi)^D|\boldsymbol{\Sigma}|}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\top\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right)$$

Gauss süreci

$$y_i = f(\boldsymbol{x}_i) + \xi_i \qquad \forall i$$
$$f \sim \mathcal{GP}(f; m(\cdot), k(\cdot, \cdot))$$
$$\xi_i \sim \mathcal{N}(\xi_i; 0, \sigma^2) \qquad \forall i$$

y_i: $\boldsymbol{x}_i$ için ölçülen çıktı değeri

$f(\boldsymbol{x}_i)$: $\boldsymbol{x}_i$ için gerçek çıktı değeri

$m(\cdot)$: ortalama fonksiyonu

$k(\cdot, \cdot)$: kovaryans fonksiyonu

ξ_i: gürültü (ölçüm hatası, kayıt hatası, sistemdeki gürültü)

Gauss süreci

- Gauss süreci fonksiyonlar üzerinde tanımlanmış bir dağılımdır.

- Gözlemlenen değişkenler beraberce normal dağılım izlemektedir.

$$\begin{bmatrix} f(\boldsymbol{x}_1) \\ f(\boldsymbol{x}_2) \\ \vdots \\ f(\boldsymbol{x}_N) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} f(\boldsymbol{x}_1) \\ f(\boldsymbol{x}_2) \\ \vdots \\ f(\boldsymbol{x}_N) \end{bmatrix}; \begin{bmatrix} m(\boldsymbol{x}_1) \\ m(\boldsymbol{x}_2) \\ \vdots \\ m(\boldsymbol{x}_N) \end{bmatrix}, \begin{bmatrix} k(\boldsymbol{x}_1, \boldsymbol{x}_1) & k(\boldsymbol{x}_1, \boldsymbol{x}_2) & \dots & k(\boldsymbol{x}_1, \boldsymbol{x}_N) \\ k(\boldsymbol{x}_2, \boldsymbol{x}_1) & k(\boldsymbol{x}_2, \boldsymbol{x}_2) & \dots & k(\boldsymbol{x}_2, \boldsymbol{x}_N) \\ \vdots & \vdots & \ddots & \vdots \\ k(\boldsymbol{x}_N, \boldsymbol{x}_1) & k(\boldsymbol{x}_N, \boldsymbol{x}_2) & \dots & k(\boldsymbol{x}_N, \boldsymbol{x}_N)) \end{bmatrix} \right)$$

Gauss süreci

- Ortalama fonksiyonu olarak genelde 0 fonksiyonu kullanılmaktadır.

  $m(\boldsymbol{x}_i) = 0$

- Kovaryans fonksiyonu olarak Gauss çekirdeği sıklıkla kullanılmaktadır.

  $k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \exp(-\|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2^2 / s^2)$

$$\boldsymbol{y} = \boldsymbol{f} + \boldsymbol{\xi}$$
$$\boldsymbol{f} \sim \mathcal{N}(\boldsymbol{f}; \mathbf{0}, \mathbf{K})$$
$$\boldsymbol{\xi} \sim \mathcal{N}(\boldsymbol{\xi}; \mathbf{0}, \sigma^2 \mathbf{I})$$

Gauss süreci

- Bayes teoremini kullandığımızda:

$$p(\boldsymbol{f}|\boldsymbol{y}) = \frac{p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f})}{p(\boldsymbol{y})}$$

$$\begin{aligned} p(\boldsymbol{f}|\boldsymbol{y}) &\propto p(\boldsymbol{y}|\boldsymbol{f})p(\boldsymbol{f}) \\ &\propto p(\boldsymbol{y}-\boldsymbol{f})p(\boldsymbol{f}) \\ &\propto \mathcal{N}(\boldsymbol{y}-\boldsymbol{f};\mathbf{0},\sigma^2\mathbf{I})\mathcal{N}(\boldsymbol{f};\mathbf{0},\mathbf{K}) \end{aligned}$$

Gauss süreci

- En büyük ardıl olasılık kestirimini kullanarak:

$$\boldsymbol{f}^\star = \arg\max_{\boldsymbol{f}} p(\boldsymbol{f}|\boldsymbol{y}) = \arg\max_{\boldsymbol{f}} \log p(\boldsymbol{f}|\boldsymbol{y})$$

$$\log p(\boldsymbol{f}|\boldsymbol{y}) = -\frac{1}{2\sigma^2}\|\boldsymbol{y} - \boldsymbol{f}\|_2^2 - \frac{1}{2}\boldsymbol{f}^\top \mathbf{K}^{-1}\boldsymbol{f} + \text{constant}$$

- $\boldsymbol{f}$ değişkenini $\mathbf{K}\boldsymbol{\alpha}$ ile yer değiştirdiğimizde:

$$\log p(\boldsymbol{\alpha}|\boldsymbol{y}) = -\frac{1}{2\sigma^2}\|\boldsymbol{y} - \mathbf{K}\boldsymbol{\alpha}\|_2^2 - \frac{1}{2}\boldsymbol{\alpha}^\top \mathbf{K}\boldsymbol{\alpha} + \text{constant}$$

Gauss süreci

- Kısıtsız en iyileme problemi

$$
\begin{aligned}
\boldsymbol{\alpha}^{\star} &= \arg\max_{\boldsymbol{\alpha}} \log p(\boldsymbol{\alpha}|\boldsymbol{y}) \\
&= \arg\max_{\boldsymbol{\alpha}} -\frac{1}{2\sigma^2}\left(\boldsymbol{y}^\top\boldsymbol{y} - 2\boldsymbol{y}^\top\mathbf{K}\boldsymbol{\alpha} + \boldsymbol{\alpha}^\top\mathbf{K}\mathbf{K}\boldsymbol{\alpha}\right) - \frac{1}{2}\boldsymbol{\alpha}^\top\mathbf{K}\boldsymbol{\alpha}
\end{aligned}
$$

- $\boldsymbol{\alpha}$ değişkenine göre türev alıp en iyi değeri bulabiliriz.

$$
\boldsymbol{\alpha}^{\star} = (\mathbf{K} + \sigma^2\mathbf{I})^{-1}\boldsymbol{y}
$$

Gauss süreci

$$\boldsymbol{a} \sim \mathcal{N}(\boldsymbol{a}; \boldsymbol{\mu}_a, \boldsymbol{\Sigma}_a)$$
$$\boldsymbol{b} \sim \mathcal{N}(\boldsymbol{b}; \boldsymbol{\mu}_b, \boldsymbol{\Sigma}_b)$$
$$\boldsymbol{a} + \boldsymbol{b} \sim \mathcal{N}(\boldsymbol{a} + \boldsymbol{b}; \boldsymbol{\mu}_a + \boldsymbol{\mu}_b, \boldsymbol{\Sigma}_a + \boldsymbol{\Sigma}_b)$$

- $\boldsymbol{y}$ and y_* için bileşik olasılık dağılımı

$$\begin{bmatrix} \boldsymbol{y} \\ y_* \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \boldsymbol{y} \\ y_* \end{bmatrix}; \begin{bmatrix} \mathbf{0} \\ 0 \end{bmatrix}, \begin{bmatrix} \mathbf{K} + \sigma^2 \mathbf{I} & \boldsymbol{k}_* \\ \boldsymbol{k}_*^\top & k(\boldsymbol{x}_*, \boldsymbol{x}_*) \end{bmatrix} \right)$$

$$\boldsymbol{k}_* = \begin{bmatrix} k(\boldsymbol{x}_1, \boldsymbol{x}_*) \\ k(\boldsymbol{x}_2, \boldsymbol{x}_*) \\ \vdots \\ k(\boldsymbol{x}_N, \boldsymbol{x}_*) \end{bmatrix}$$

Gauss süreci

$$\begin{bmatrix}\boldsymbol{a}\\ \boldsymbol{b}\end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix}\boldsymbol{a}\\ \boldsymbol{b}\end{bmatrix}; \begin{bmatrix}\boldsymbol{\mu}_a\\ \boldsymbol{\mu}_b\end{bmatrix}, \begin{bmatrix}\boldsymbol{\Sigma}_{aa} & \boldsymbol{\Sigma}_{ab}\\ \boldsymbol{\Sigma}_{ba} & \boldsymbol{\Sigma}_{bb}\end{bmatrix}\right)$$

$$\boldsymbol{b}|\boldsymbol{a} \sim \mathcal{N}\big(\boldsymbol{b}; \boldsymbol{\mu}_b + \boldsymbol{\Sigma}_{ba}\boldsymbol{\Sigma}_{aa}^{-1}(\boldsymbol{a} - \boldsymbol{\mu}_a), \boldsymbol{\Sigma}_{bb} - \boldsymbol{\Sigma}_{ba}\boldsymbol{\Sigma}_{aa}^{-1}\boldsymbol{\Sigma}_{ab}\big)$$

- y_* değerini kestirmek için aşağıdaki dağılımı kullanabiliriz.

$$y_*|\boldsymbol{y} \sim \mathcal{N}\Big(y_*; \boldsymbol{k}_*^\top \underbrace{(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\boldsymbol{y}}_{\boldsymbol{\alpha}}, k(\boldsymbol{x}_*, \boldsymbol{x}_*) - \boldsymbol{k}_*^\top(\mathbf{K} + \sigma^2\mathbf{I})^{-1}\boldsymbol{k}_*\Big)$$

PLOS NEGLECTED TROPICAL DISEASES

RESEARCH ARTICLE

Spatiotemporal prediction of infectious diseases using structured Gaussian processes with application to Crimean–Congo hemorrhagic fever

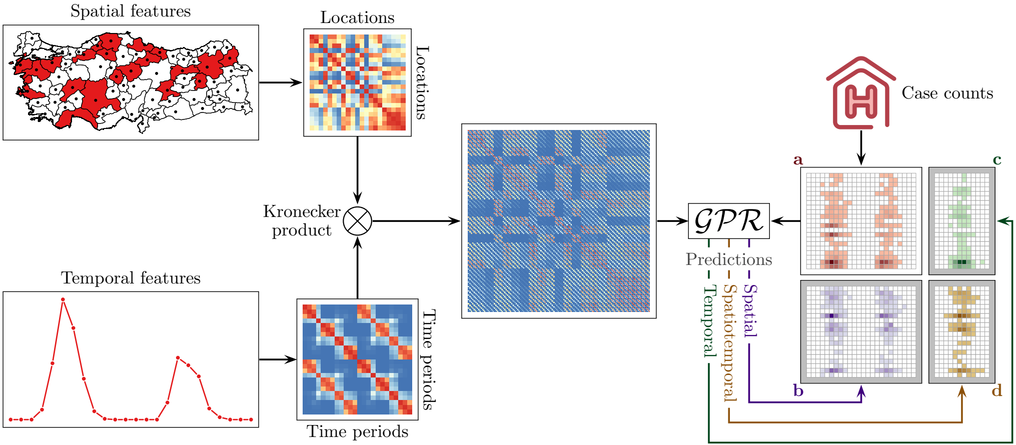
Çiğdem Ak[1], Önder Ergönül[2], İrfan Şencan[3], Mehmet Ali Torunoğlu[3], Mehmet Gönen[4,5]*

1 Graduate School of Sciences and Engineering, Koç University, İstanbul, Turkey, **2** Department of Infectious Diseases and Clinical Microbiology, School of Medicine, Koç University, İstanbul, Turkey, **3** Public Health Directorate, Ministry of Health, Ankara, Turkey, **4** Department of Industrial Engineering, College of Engineering, Koç University, İstanbul, Turkey, **5** School of Medicine, Koç University, İstanbul, Turkey

* mehmetgonen@ku.edu.tr

Check for updates

Yapısal Gauss süreci modelimiz



Yapısal Gauss süreci

- Her bir veri noktası $\boldsymbol{x}_i$, bir lokasyon ve bir zaman vektöründen oluşmaktadır.

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = k((\boldsymbol{s}_l, \boldsymbol{t}_p), (\boldsymbol{s}_m, \boldsymbol{t}_q)) = k_s(\boldsymbol{s}_l, \boldsymbol{s}_m) k_t(\boldsymbol{t}_p, \boldsymbol{t}_q)$$

Yapısal Gauss süreci

- Her bir veri noktası $\boldsymbol{x}_i$, bir lokasyon ve bir zaman vektöründen oluşmaktadır.

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = k((\boldsymbol{s}_l, \boldsymbol{t}_p), (\boldsymbol{s}_m, \boldsymbol{t}_q)) = k_s(\boldsymbol{s}_l, \boldsymbol{s}_m) k_t(\boldsymbol{t}_p, \boldsymbol{t}_q)$$

- Çekirdek matrisini iki küçük matrisin Kronecker çarpımı şeklinde yazabiliriz.

$$\mathbf{K} = \mathbf{K}_s \otimes \mathbf{K}_t$$

Yapısal Gauss süreci

- Her bir veri noktası $\boldsymbol{x}_i$, bir lokasyon ve bir zaman vektöründen oluşmaktadır.

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = k((\boldsymbol{s}_l, \boldsymbol{t}_p), (\boldsymbol{s}_m, \boldsymbol{t}_q)) = k_s(\boldsymbol{s}_l, \boldsymbol{s}_m) k_t(\boldsymbol{t}_p, \boldsymbol{t}_q)$$

- Çekirdek matrisini iki küçük matrisin Kronecker çarpımı şeklinde yazabiliriz.

$$\mathbf{K} = \mathbf{K}_s \otimes \mathbf{K}_t$$

- y_* değerini kestirmek için aşağıdaki dağılımı kullanabiliriz.

$$\mathrm{E}[y_\star | \boldsymbol{x}_\star, \mathbf{X}, \mathbf{Y}, \sigma^2] = (\boldsymbol{k}_{s,\star} \otimes \boldsymbol{k}_{t,\star})^\top (\mathbf{K}_s \otimes \mathbf{K}_t + \sigma^2 \mathbf{I})^{-1} \operatorname{vec}(\mathbf{Y})$$

$$\mathrm{Var}[y_\star | \boldsymbol{x}_\star, \mathbf{X}, \mathbf{Y}, \sigma^2] = k_s(s_\star, s_\star) k_t(t_\star, t_\star) - (\boldsymbol{k}_{s,\star} \otimes \boldsymbol{k}_{t,\star})^\top (\mathbf{K}_s \otimes \mathbf{K}_t + \sigma^2 \mathbf{I})^{-1} (\boldsymbol{k}_{s,\star} \otimes \boldsymbol{k}_{t,\star})$$

Kronecker çarpımı

- $\mathbf{A}$: $m \times n$ büyüklüğünde bir matris
- $\mathbf{B}$: $p \times q$ büyüklüğünde bir matris
- $\mathbf{A} \otimes \mathbf{B}$: $mp \times nq$ büyüklüğünde bir blok matris

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{bmatrix}$$

- Örnek

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \otimes \begin{bmatrix} 0 & 5 \\ 6 & 7 \end{bmatrix} = \begin{bmatrix} 1 \times 0 & 1 \times 5 & 2 \times 0 & 2 \times 5 \\ 1 \times 6 & 1 \times 7 & 2 \times 6 & 2 \times 7 \\ 3 \times 0 & 3 \times 5 & 4 \times 0 & 4 \times 5 \\ 3 \times 6 & 3 \times 7 & 4 \times 6 & 4 \times 7 \end{bmatrix} = \begin{bmatrix} 0 & 5 & 0 & 10 \\ 6 & 7 & 12 & 14 \\ 0 & 15 & 0 & 20 \\ 18 & 21 & 24 & 28 \end{bmatrix}$$

Yapısal Gauss süreci

$$\mathbf{K}_s = \mathbf{U}_s \mathbf{D}_s \mathbf{U}_s^\top$$
$$\mathbf{K}_t = \mathbf{U}_t \mathbf{D}_t \mathbf{U}_t^\top$$

Yapısal Gauss süreci

$$\mathbf{K}_s = \mathbf{U}_s \mathbf{D}_s \mathbf{U}_s^\top$$
$$\mathbf{K}_t = \mathbf{U}_t \mathbf{D}_t \mathbf{U}_t^\top$$

$$\mathbf{K}_s \otimes \mathbf{K}_t = (\mathbf{U}_s \otimes \mathbf{U}_t)(\mathbf{D}_s \otimes \mathbf{D}_t)(\mathbf{U}_s \otimes \mathbf{U}_t)^\top$$

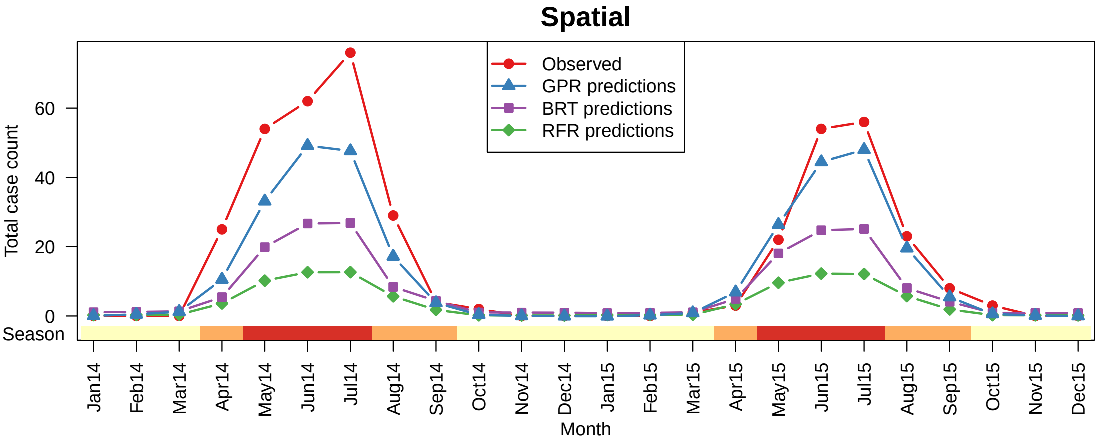
Yapısal Gauss süreci

$$\mathbf{K}_s = \mathbf{U}_s \mathbf{D}_s \mathbf{U}_s^\top$$
$$\mathbf{K}_t = \mathbf{U}_t \mathbf{D}_t \mathbf{U}_t^\top$$

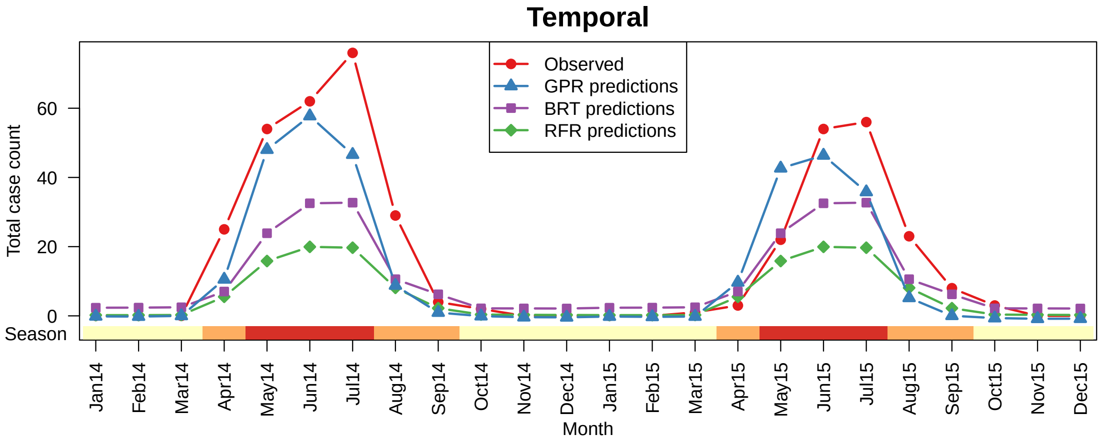
$$\mathbf{K}_s \otimes \mathbf{K}_t = (\mathbf{U}_s \otimes \mathbf{U}_t)(\mathbf{D}_s \otimes \mathbf{D}_t)(\mathbf{U}_s \otimes \mathbf{U}_t)^\top$$

$$(\mathbf{K}_s \otimes \mathbf{K}_t + \sigma^2 \mathbf{I})^{-1} = (\mathbf{U}_s \otimes \mathbf{U}_t)(\mathbf{D}_s \otimes \mathbf{D}_t + \sigma^2 \mathbf{I})^{-1}(\mathbf{U}_s \otimes \mathbf{U}_t)^\top$$

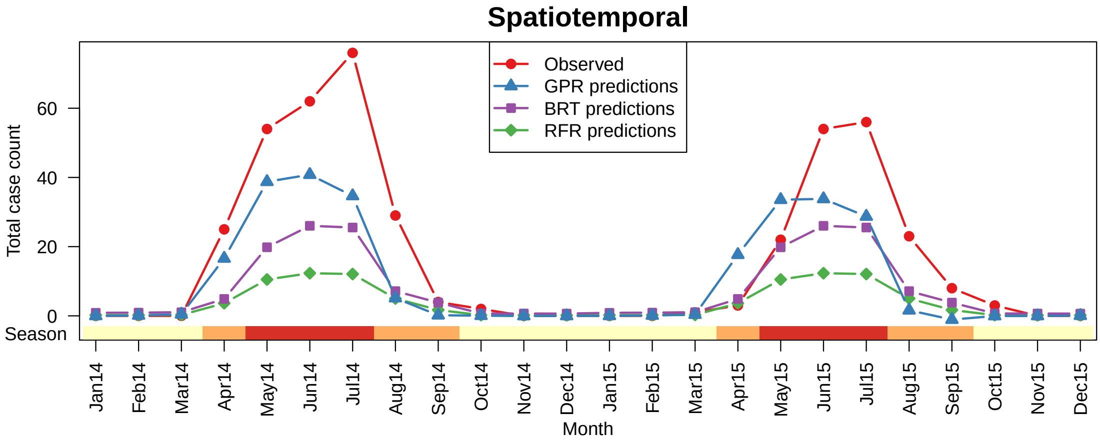
Kestirim sonuçları



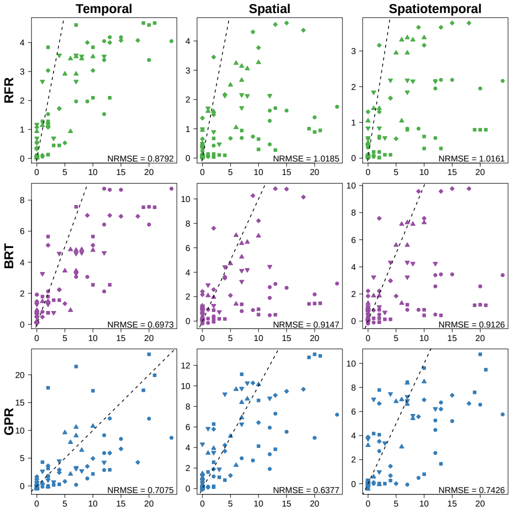
Kestirim sonuçları



Kestirim sonuçları



Kestirim sonuçları



Clinical Microbiology and Infection 26 (2020) 123.e1–123.e7

Contents lists available at ScienceDirect

Clinical Microbiology and Infection

journal homepage: www.clinicalmicrobiologyandinfection.com

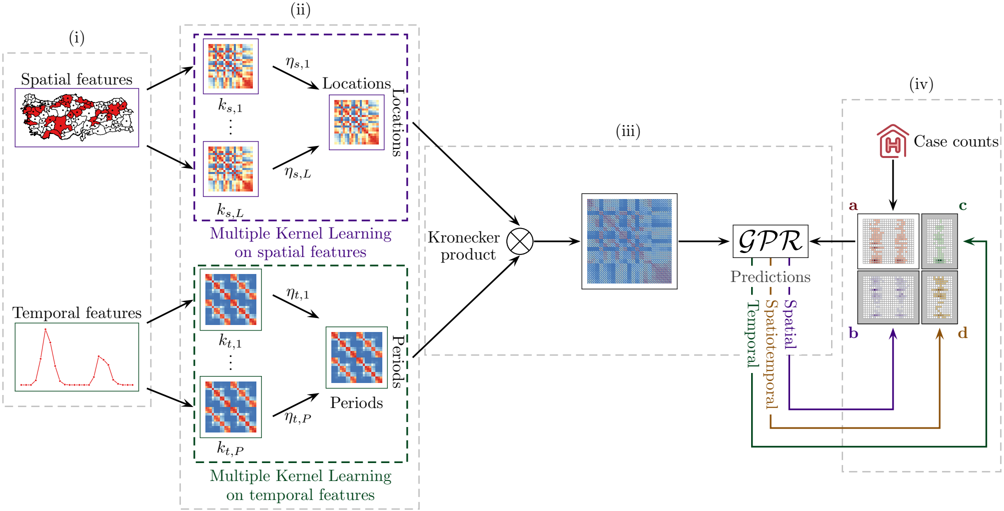
Original article

A prospective prediction tool for understanding Crimean–Congo haemorrhagic fever dynamics in Turkey

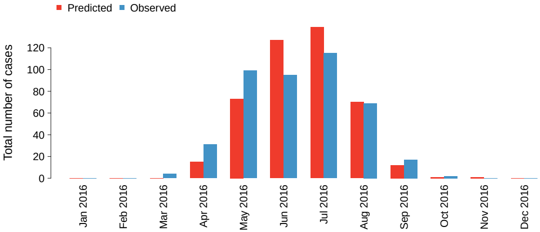
Ç. Ak [1], Ö. Ergönül [2], M. Gönen [3, 4, *]

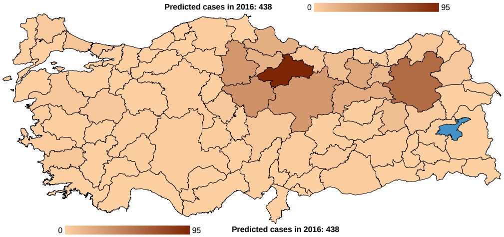
[1)] Graduate School of Sciences and Engineering, Koç University, İstanbul, Turkey
[2)] Department of Infectious Diseases and Clinical Microbiology, School of Medicine, Koç University, İstanbul, Turkey
[3)] Department of Industrial Engineering, College of Engineering, Koç University, İstanbul, Turkey
[4)] School of Medicine, Koç University, İstanbul, Turkey

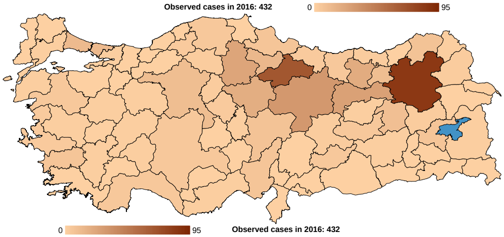
Çok çekirdekli yapısal Gauss süreci modelimiz



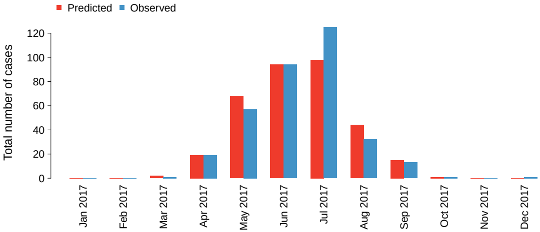
2016 yılı için kestirim sonuçları

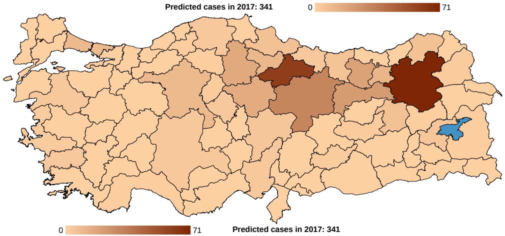


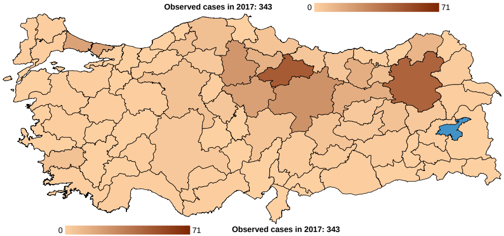




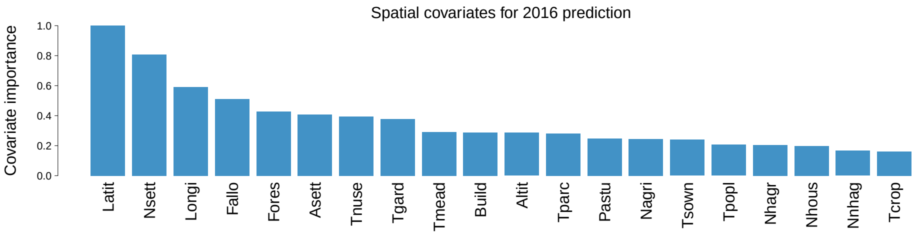
2017 yılı için kestirim sonuçları

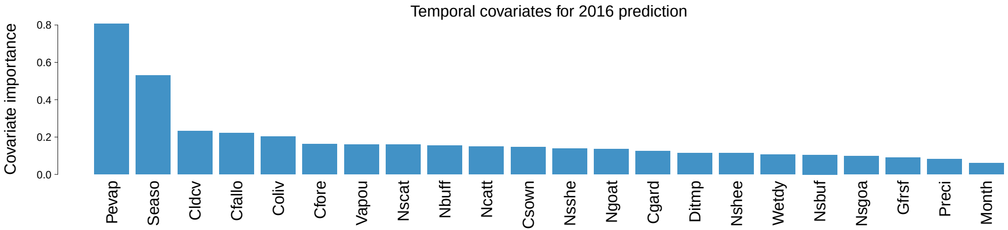






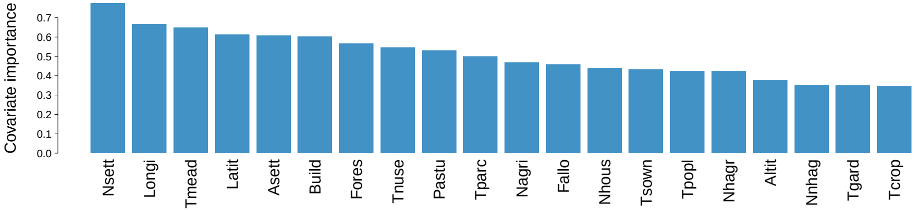
Öznitelik ağırlıkları





Öznitelik ağırlıkları

Spatial covariates for 2017 prediction



Temporal covariates for 2017 prediction