「ガウス過程と機械学習」

P.89 ガウス過程回帰のハイパーパラメータ推定

In [1]:

```julia
using LinearAlgebra
using Random
using ForwardDiff
using Plots

Random.seed!(12345)
```

Out[1]:

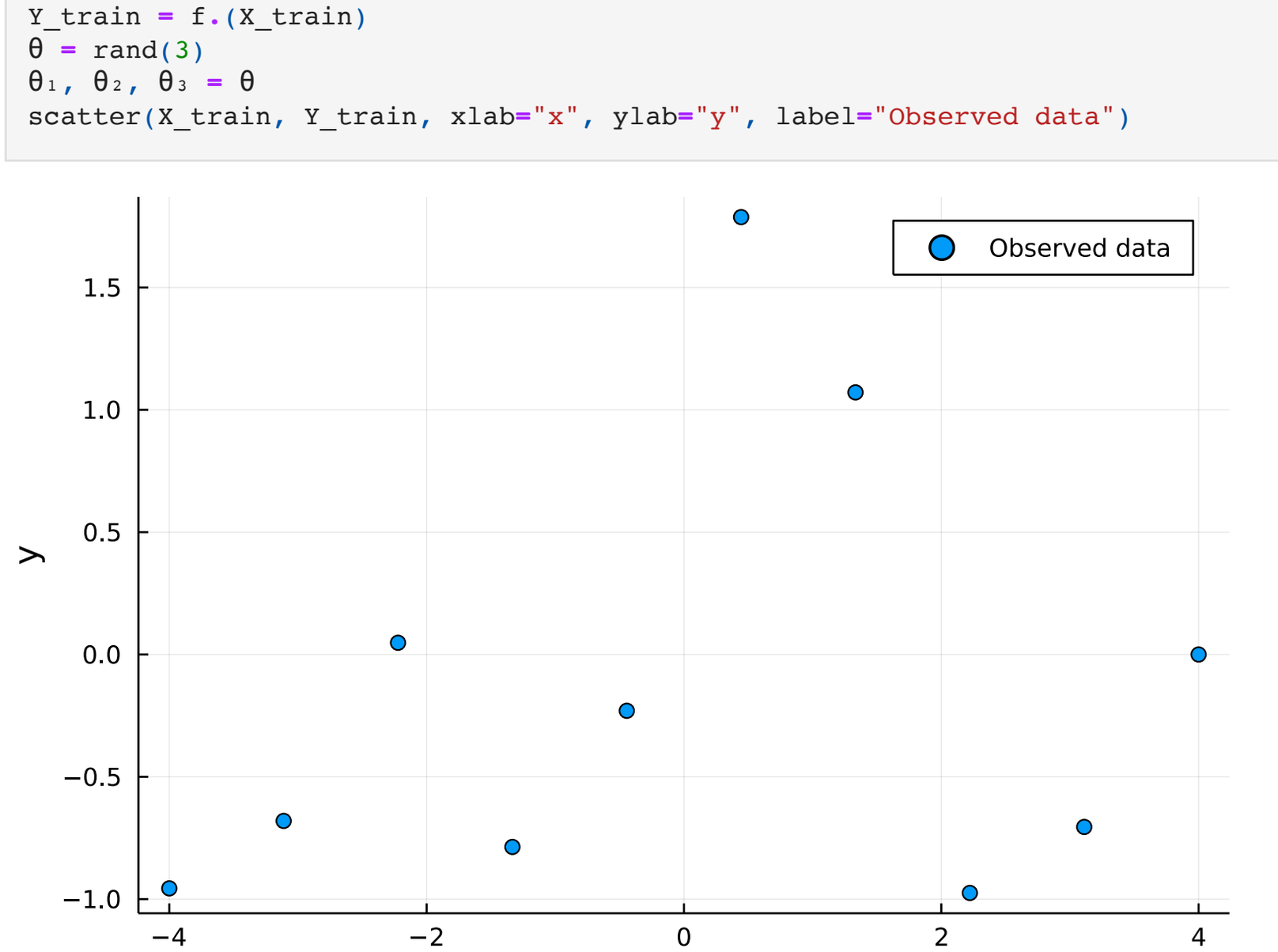
```
MersenneTwister(12345)
```

観測データの生成

In [2]:

```julia
N = 10
X_train = range(-4, 4, length=N)
f(x) = sin(2x) + cos(x-π/5) + 0.1 * randn()
Y_train = f.(X_train)
θ = rand(3)
θ₁, θ₂, θ₃ = θ
scatter(X_train, Y_train, xlab="x", ylab="y", label="Observed data")
```

Out[2]:



ガウスカーネル関数を定義

In [3]:

```julia
k(x1, x2, θ₁, θ₂, θ₃) = θ₁ .* exp.(-(x1' .- x2).^2 ./ θ₂) + θ₃ .* (x1' .== x2)
```

Out[3]:

```
k (generic function with 1 method)
```

ガウスカーネルの微分

In [4]:

```julia
∂k∂θ₁(x1, x2, θ₁, θ₂, θ₃) = ForwardDiff.derivative(θ₁ -> k(x1, x2, θ₁, θ₂, θ₃), θ₁)
∂k∂θ₂(x1, x2, θ₁, θ₂, θ₃) = ForwardDiff.derivative(θ₂ -> k(x1, x2, θ₁, θ₂, θ₃), θ₂)
∂k∂θ₃(x1, x2, θ₁, θ₂, θ₃) = ForwardDiff.derivative(θ₃ -> k(x1, x2, θ₁, θ₂, θ₃), θ₃)
```

Out[4]:

```
∂k∂θ₃ (generic function with 1 method)
```

In [5]:

```julia
∇K₁ = ∂k∂θ₁(X_train, X_train, θ₁, θ₂, θ₃)
```

Out[5]:

```
10×10 Matrix{Float64}:
 1.0          0.447031     0.0399347    …  4.18407e-23  4.75703e-29
 0.447031     1.0          0.447031        7.35422e-18  4.18407e-23
 0.0399347    0.447031     1.0             2.58315e-13  7.35422e-18
 0.000712914  0.0399347    0.447031        1.81316e-9   2.58315e-13
 2.54331e-6   0.000712914  0.0399347       2.54331e-6   1.81316e-9
 1.81316e-9   2.54331e-6   0.000712914  …  0.000712914  2.54331e-6
 2.58315e-13  1.81316e-9   2.54331e-6      0.0399347    0.000712914
 7.35422e-18  2.58315e-13  1.81316e-9      0.447031     0.0399347
 4.18407e-23  7.35422e-18  2.58315e-13     1.0          0.447031
 4.75703e-29  4.18407e-23  7.35422e-18     0.447031     1.0
```

In [6]:

```julia
∇K₂ = ∂k∂θ₂(X_train, X_train, θ₁, θ₂, θ₃)
```

Out[6]:

```
10×10 Matrix{Float64}:
 0.0          0.210289     0.075143     …  1.25967e-21  1.81259e-27
 0.210289     0.0          0.210289        1.69516e-16  1.25967e-21
 0.075143     0.210289     0.0             4.37452e-12  1.69516e-16
 0.00301827   0.075143     0.210289        2.13234e-8   4.37452e-12
 1.91425e-5   0.00301827   0.075143        1.91425e-5   2.13234e-8
 2.13234e-8   1.91425e-5   0.00301827   …  0.00301827   1.91425e-5
 4.37452e-12  2.13234e-8   1.91425e-5      0.075143     0.00301827
 1.69516e-16  4.37452e-12  2.13234e-8      0.210289     0.075143
 1.25967e-21  1.69516e-16  4.37452e-12     0.0          0.210289
 1.81259e-27  1.25967e-21  1.69516e-16     0.210289     0.0
```

In [7]:

```julia
∇K₃ = ∂k∂θ₃(X_train, X_train, θ₁, θ₂, θ₃)
```

Out[7]:

```
10×10 Matrix{Float64}:
 1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0  0.0
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0  1.0
```

ハイパーパラメータ推定（勾配法）

In [8]:

```julia
X_test = rand((-6):0.1:6, 40)
niters = 100

for _ in 1:niters
    θ₁, θ₂, θ₃ = θ
    lr = [0.1, 0.01, 0.001]

    K = k(X_train, X_train, θ₁, θ₂, θ₃)
    invK = inv(K)
    likehood = -log(det(K)) - Y_train' * invK * Y_train
    @show likehood
    k_ = k(X_test, X_train, θ₁, θ₂, θ₃)
    k__ = k(X_test, X_test, θ₁, θ₂, θ₃)

    μ̂ = k_' * invK * Y_train
    Σ̂ = k__ - k_' * invK * k_

    invKy = invK * Y_train
    ∇L₁ = -tr(invK * ∇K₁) + (invKy' * ∇K₁ * invKy)
    ∇L₂ = -tr(invK * ∇K₂) + (invKy' * ∇K₂ * invKy)
    ∇L₃ = -tr(invK * ∇K₃) + (invKy' * ∇K₃ * invKy)
    ∇L = [∇L₁, ∇L₂, ∇L₃]
    @show ∇L

    θ .-= lr .* -∇L
    @show θ

    # θが負になると invK の計算ができなくなるため最適化を終了する
    if θ[3] < 0
        θ .+= lr .* -∇L
        break
    end
end

@show θ
```

```
likehood = -7.458601033786364
∇L = [-2.1461435182903514, 0.4743952931484005, -3.9836363786550306]
θ = [0.35876764083720464, 0.9861080902135276, 0.582614464411893]
likehood = -7.0935184441268
∇L = [-0.9022548021471284, 0.41153502715619517, -2.9369821829387774]
θ = [0.2685421606224918, 0.9902234404850896, 0.5796774822289542]
likehood = -7.049468090104372
∇L = [0.18490950888529234, 0.38772950433076586, -2.0190094151818077]
θ = [0.28703311151102107, 0.9941007355283973, 0.5776584728137724]
likehood = -7.043167579025827
∇L = [-0.05145030917234372, 0.39261586275380667, -2.225176034127644]
θ = [0.28188808059378667, 0.9980268941559354, 0.5754332967796447]
likehood = -7.037642259506667
∇L = [0.04586158799594742, 0.39206624661680245, -2.148516843324444]
θ = [0.2864742393933814, 1.0019475566221034, 0.5732847799363203]
likehood = -7.032134348946439
∇L = [0.008172676538684698, 0.3939144445506965, -2.1865560825017134]
θ = [0.28729150704724987, 1.0058867010676105, 0.5710982238538186]
likehood = -7.026670888788047
∇L = [0.023299616405484613, 0.39482425255866127, -2.1797640922600543]
θ = [0.2896214686877983, 1.009834943593197, 0.5689184597615585]
likehood = -7.021167970643722
∇L = [0.017516444512638785, 0.39614137260629845, -2.190831329992644]
θ = [0.29137311313906217, 1.01379635731926, 0.5667276284315659]
likehood = -7.01565504208378
∇L = [0.01994395216497402, 0.39731305381322846, -2.1949668926926655]
θ = [0.2933675083555596, 1.0177694878573924, 0.5645326615388732]
likehood = -7.010117096819863
∇L = [0.019154239310504195, 0.3985641143691872, -2.2019125115428135]
θ = [0.29528293228661, 1.0217551290010842, 0.5623307490273304]
likehood = -7.004560425761982
∇L = [0.01962363924741517, 0.39980381163521594, -2.2078492819125213]
θ = [0.29724529621135154, 1.0257531671174365, 0.5601228899745418]
likehood = -6.99898212790929
∇L = [0.01960560444238014, 0.4010692170871135, -2.214270662801246]
θ = [0.2992058566559035, 1.0297638592883076, 0.5579086290826166]
likehood = -6.993383305311733
∇L = [0.019779501206556915, 0.40234590736716636, -2.220596682660444]
θ = [0.30118380677624607, 1.0337873183619792, 0.5556880323999562]
likehood = -6.987763352939817
∇L = [0.019882091114652667, 0.40364014538954573, -2.2270540457257315]
θ = [0.3031720158877113, 1.0378237198158746, 0.5534609783542305]
likehood = -6.982122380237358
∇L = [0.020015096346599037, 0.4049499406756194, -2.2335567856864422]
θ = [0.3051735255223712, 1.0418732192226308, 0.551227421568544]
likehood = -6.976460194496738
∇L = [0.020139435825219822, 0.4062766030485138, -2.240139762475799]
θ = [0.3071874691048932, 1.0459359852531158, 0.5489872818060682]
likehood = -6.970776725071215
∇L = [0.020270155116113328, 0.40762015021889125, -2.246791379160195]
θ = [0.3092144846165065, 1.0500121867553047, 0.546740490426908]
likehood = -6.965071837200691
∇L = [0.020401572661562284, 0.40898112605054815, -2.2535179011981086]
θ = [0.3112546418826628, 1.0541019980158102, 0.5444869725257099]
likehood = -6.959345428100276
∇L = [0.0205359165702248, 0.4103598453080247, -2.260318820430772]
θ = [0.31330823353968523, 1.0582055968611181, 0.5422266537052791]
likehood = -6.953597372763335
∇L = [0.020672414069956174, 0.41175687127558913, -2.2671962576042404]
θ = [0.3153754746366414, 1.062323165573874, 0.5399594572476749]
likehood = -6.947827548088599
∇L = [0.020811419149479704, 0.4131725141502198, -2.2741513900683117]
θ = [0.3174566516558935, 1.0664548907153764, 0.5376853006750567]
likehood = -6.942035825693585
∇L = [0.020952877059857045, 0.41460726640636913, -2.2811858059906562]
θ = [0.3195519042575507, 1.070600963379444, 0.535404120251616]
likehood = -6.936222073603282
∇L = [0.021096883297788693, 0.41606159061053355, -2.2883009955358258]
θ = [0.3216615925875835, 1.0747615792855454, 0.5331158192560802]
likehood = -6.930386155450116
∇L = [0.021243477931923493, 0.41753596548625316, -2.2954985438087494]
θ = [0.32378509403805463, 1.078936938940408, 0.5308203207122715]
likehood = -6.924527930641814
∇L = [0.02139272518030033, 0.4190308839646098, -2.3027800606581437]
θ = [0.32592521289857634, 1.083127247780054, 0.5285175406516134]
likehood = -6.9186471264485555
∇L = [0.021544682755887834, 0.4205468546284648, -2.3101472088374297]
θ = [0.3280796817416514, 1.0873327163263387, 0.526207393442776]
likehood = -6.912743977643174
∇L = [0.021699413305327653, 0.4220844018908803, -2.3176016956708256]
θ = [0.3302496225046979, 1.0915535603452475, 0.5238897917471051]
likehood = -6.906817943310865
∇L = [0.021856980288085026, 0.42364406668271903, -2.3251452187166737]
θ = [0.33243532053350644, 1.0957900010120747, 0.5215646446487885]
likehood = -6.900868995860796
∇L = [0.022017449586993365, 0.4252264069783715, -2.332779764108647]
θ = [0.3346370654922058, 1.1000422650818584, 0.5192318667046799]
likehood = -6.894896070263392
∇L = [0.022180808902320048, 0.42683199841399316, -2.340507012796575]
θ = [0.33685515439452585, 1.1043105850659984, 0.5168913596918834]
likehood = -6.888901697702027
∇L = [0.022347368640122767, 0.42846143490433153, -2.348328938191612]
θ = [0.3390898912585381, 1.1085951994150418, 0.5145430307536918]
likehood = -6.882883004216973
∇L = [0.02251696071297893, 0.43011532947795, -2.356247510130853]
θ = [0.3413416573297836, 1.1128963527079896, 0.5121867832435609]
likehood = -6.876840710569565
∇L = [0.022689739862721936, 0.43179431403670293, -2.364264756434025]
θ = [0.3436105613161082, 1.1172142958483566, 0.5098225184871269]
likehood = -6.870774632098115
∇L = [0.02286578313777987, 0.4334990418922223, -2.3723827649760647]
θ = [0.34589713962988616, 1.121549286267279, 0.5074501357221508]
likehood = -6.864684578572655
∇L = [0.023045170112959637, 0.435230186668026, -2.380603685836612]
θ = [0.3482016566411818, 1.1259015881339591, 0.5050695320363142]
likehood = -6.858570354033505
∇L = [0.023227982988204943, 0.4369884439803027, -2.3889297335464894]
θ = [0.3505244549400023, 1.1302714725737621, 0.5026806023027677]
likehood = -6.852431756637827
∇L = [0.023414306693718245, 0.4387745320521213, -2.3973631894300933]
θ = [0.3528658856093741, 1.1346592178942834, 0.5002832391133376]
likehood = -6.846268578812655
∇L = [0.023604228899452914, 0.4405891925449522, -2.405906404050979]
θ = [0.3552263085093194, 1.1390651098197329, 0.49787733270926068]
likehood = -6.840086065446345
∇L = [0.023797840629288306, 0.44243319142596025, -2.4145617997651545]
θ = [0.3576060927231224, 1.1434894417339925, 0.49546277090952145]
likehood = -6.833867617040402
∇L = [0.023995232538466042, 0.4443073198730251, -2.4233318733878235]
θ = [0.3600056161107783, 1.1479325149327226, 0.4930394390361336]
likehood = -6.827629386090058
∇L = [0.024196510264295, 0.4462123952192158, -2.432219198979647]
θ = [0.3624252671372074, 1.1523946388849151, 0.490607219837154]
likehood = -6.821365876805181
∇L = [0.02440176560289764, 0.4481492619391354, -2.4412264307588174]
θ = [0.3648654436974972, 1.1568761315043066, 0.48816599340639516]
likehood = -6.815076253983957
∇L = [0.024611105206824746, 0.450118789267847243, -2.450356036145567]
θ = [0.3673265542181967, 1.1613773194310912, 0.4857156371002495]
likehood = -6.808760868638213
∇L = [0.02482463650032507, 0.45212188933032704, -2.4596116489469567]
θ = [0.3698090178682122, 1.1658985383243945, 0.48325602545130253]
likehood = -6.802419252688269
∇L = [0.025042470678481976, 0.4541594841594918, -2.4689953726876936]
θ = [0.3723132649360604, 1.1704401331659895, 0.48078703007861484]
likehood = -6.796051157402115
∇L = [0.025264722867737177, 0.45623254097801214, -2.478510484097816]
θ = [0.374839737228341, 1.1750024585757697, 0.47830851959451703]
likehood = -6.789656306886354
∇L = [0.02549151229465492, 0.45834205637451964, -2.4881600867635356]
θ = [0.3773888884523026, 1.1795858791395148, 0.4758203595077535]
likehood = -6.783234421920286
∇L = [0.025722962463230914, 0.4604890610002914, -2.4979473849514964]
θ = [0.3799611846986257, 1.1841907697495178, 0.47332241212280196]
likehood = -6.776785214877474
∇L = [0.02595920134105434, 0.46267642091512745, -2.5078756876158668]
θ = [0.38255710483273114, 1.1888175159586691, 0.4708145364351861]
likehood = -6.770308389452382
∇L = [0.02620036155557237, 0.4648998389963489, -2.5179484125989227]
θ = [0.38517714098838837, 1.1934665143486327, 0.46829658802258717]
likehood = -6.76380364037462
∇L = [0.02644658060023808, 0.46716585641442, -2.528169091035993]
θ = [0.38782179904831215, 1.1981381729127772, 0.4657684189315512]
likehood = -6.757270653109996
∇L = [0.02669800105150877, 0.4694735417891144, -2.538541371976777]
θ = [0.39049515915346304, 1.2028329114545662, 0.4632298775595744]
likehood = -6.750709103547562
∇L = [0.026954770797514627, 0.4718250475895054, -2.5490690272355216]
θ = [0.3931870762332145, 1.2075511620021557, 0.46068080085323389]
likehood = -6.744118657671899
∇L = [0.02721704327877461, 0.47422072378192026, -2.559755564837447]
θ = [0.39590878065109197, 1.2122933692399749, 0.45812105257585517]
likehood = -6.737498971219583
∇L = [0.027484977714979222, 0.47665621718157471, -2.57060619259987]
θ = [0.3986572783352899, 1.2170599909581323, 0.4555504463832553]
likehood = -6.730849689318997
∇L = [0.027758730950741224, 0.47915075623881354, -2.5816239072912275]
θ = [0.4014331522603504, 1.2218514985205204, 0.4529688224759641]
likehood = -6.724170446112345
∇L = [0.028038500251426512, 0.4816878832031446, -2.592813417004919]
θ = [0.4042370023111777, 1.226668377352552, 0.4503760090589592]
likehood = -6.717460684358754
∇L = [0.028324438303659605, 0.48427500969624304, -2.604171918415456]
θ = [0.40706944164154367, 1.2315111274495143, 0.4477718298698136]
likehood = -6.710720555102756
∇L = [0.028616738961956045, 0.4869136457050284, -2.6157258486183466]
θ = [0.4099311200379227, 1.2363802639065893, 0.44515610402119256]
likehood = -6.703949116808299
∇L = [0.0289159482403494, 0.4896053565055406, -2.6274581847185434]
θ = [0.4128228765201428, 1.2412763174176448, 0.4425286485364767]
likehood = -6.697146135752043
∇L = [0.029221206138487332, 0.49235176503322253, -2.6393811583886126]
θ = [0.4157448001339915, 1.246199385121977, 0.4398892646780881]
likehood = -6.690311184684385
∇L = [0.02953378117561023, 0.4951545544276639, -2.6514999098670042]
θ = [0.41869817825155253, 1.2511513806662535, 0.4372377647682207]
likehood = -6.683443822741525
∇L = [0.029853535661987664, 0.4980154706729939, -2.663819766753411]
θ = [0.42168353319135402, 1.2561315353729834, 0.4345739450014677]
likehood = -6.676543594823859
∇L = [0.030180697985009886, 0.5009363253942897, -2.676346252518268]
θ = [0.4247016017120412, 1.2611408986269264, 0.4318975987489494]
likehood = -6.66961003102465
∇L = [0.030515500053727607, 0.5039189988016382, -2.6890850954850887]
θ = [0.42775315171741396, 1.2661800886149428, 0.4292085136534643]
likehood = -6.662642646028974
∇L = [0.03085818734344059, 0.5069654427940531, -2.702042238317768]
θ = [0.430838970451758, 1.2712497430428833, 0.4265064714151465]
likehood = -6.655640938478065
∇L = [0.031209014599957285, 0.5100776842336272, -2.715223848046442]
θ = [0.4339598719117537, 1.2763505198852196, 0.42379124756710007]
likehood = -6.64860439029703
∇L = [0.031568247320979737, 0.5132578284011722, -2.728636326668992]
θ = [0.4371166966438517, 1.2814830981692313, 0.4210626112404311]
likehood = -6.641532465983193
∇L = [0.03193616231184393, 0.5165080626454106, -2.7422863223673772]
θ = [0.44031031287503614, 1.2866481787956854, 0.4183203249180637]
likehood = -6.634424611852168
∇L = [0.03231304827518677, 0.5198306602388187, -2.756180741382323]
θ = [0.4435416177025548, 1.2918464853980736, 0.41556414417668136]
likehood = -6.62728025523847
∇L = [0.032699206437875716, 0.5232279844541621, -2.7703267605919546]
θ = [0.4468115834634235, 1.2970787652426152, 0.4127938174160894]
likehood = -6.620098803647261
∇L = [0.03309495121701467, 0.5267024928770154, -2.7847318408454385]
θ = [0.45012103346804383, 1.3023457901713853, 0.41000908557524596]
likehood = -6.612879643853405
∇L = [0.033500610928719254, 0.5302567419707153, -2.799403741105481]
θ = [0.4534710945609158, 1.3076483575910924, 0.40720968183413847]
likehood = -6.605622140943877
∇L = [0.03391652854230287, 0.5338933919116232, -2.814350533459116]
θ = [0.45686274741514604, 1.3129872915102088, 0.40439533130067934]
likehood = -6.598325637298609
∇L = [0.03431306248360386, 0.5376152117140502, -2.8295806190609802]
θ = [0.46029705366350643, 1.3183634436273493, 0.40156575068161837]
likehood = -6.590989451505727
∇L = [0.03478058749119661, 0.5414250846658429, -2.8451027450787034]
θ = [0.4637751124126261, 1.3237776947400076, 0.39872064793653966]
likehood = -6.583612877204899
∇L = [0.03522949552950294, 0.5453261040974697, -2.860926022716585]
θ = [0.4672980619655764, 1.3292309546149823, 0.39585972191382307]
likehood = -6.576195181853606
∇L = [0.035690196763322746, 0.5493211295094034, -2.877059946400321]
θ = [0.47086708164190866, 1.3347241659100764, 0.39298266196742276]
likehood = -6.568735605409635
∇L = [0.03616312059869031, 0.5534136930848381, -2.8935144142129605]
θ = [0.47448339370177767, 1.3402583028409247, 0.3900891475532098]
likehood = -6.561233358922914
∇L = [0.03664871679545456, 0.5576071066171654, -2.910299749680873]
θ = [0.4781482653813231, 1.3458343739070964, 0.38717884780352907]
likehood = -6.5536876230288925
∇L = [0.03714745665705799, 0.561904918884386, -2.927426725016833]
θ = [0.4818630110470289, 1.3514534230959403, 0.38425142107851223]
likehood = -6.5460975463351065
∇L = [0.037656983430466591, 0.5663108335055015, -2.9449065859404406]
θ = [0.4856289447749547, 1.3571165314309954, 0.3813065144925718]
likehood = -6.538462243691556
∇L = [0.038186368041680296, 0.5708287173173667, -2.962751078201137]
θ = [0.4894476312816635, 1.3628248186041692, 0.37834376341437065]
likehood = -6.530780794334756
∇L = [0.038727601081719315, 0.5754626093139901, -2.9809724759497325]
θ = [0.49332039146338286, 1.368579449697309, 0.3753627909384209]
likehood = -6.523052398940725
∇L = [0.03928410679632499, 0.5802167301940771, -2.9995836121118487]
θ = [0.49724880214301537, 1.3743816119992536, 0.37236320726320906]
likehood = -6.515275582248027
∇L = [0.0398564830469219, 0.5850954925701763, -3.0185979109353642]
θ = [0.5012344504477075, 1.3802325669249553, 0.3693446094153737]
likehood = -6.507449781216776
∇L = [0.04044536132509855, 0.5901035118869189, -3.0380294229005216]
θ = [0.5052789865829984, 1.3861336020438244, 0.3663065799924732]
likehood = -6.499573752075613
∇L = [0.041051405165461574, 0.5952456181234256, -3.0578928622009443]
θ = [0.5093841270995446, 1.3920860582250587, 0.36324868713027225]
likehood = -6.491646362872667
∇L = [0.04167531270467961, 0.6005268683337788, -3.078203647025351]
θ = [0.5135516583700126, 1.3980913269083965, 0.3601704838324693]
likehood = -6.483666431532234
∇L = [0.042317819225402786, 0.6059525601085498, -3.098977942894461]
θ = [0.5177834402925529, 1.4041508525094821, 0.35707150554035244]
likehood = -6.475632722723045
∇L = [0.04297969946264857, 0.6115282460372709, -3.1202327093346724]
θ = [0.5220814102388177, 1.4102661349698549, 0.3539512728310178]
likehood = -6.467543944468533
∇L = [0.04366170027341145, 0.6172597492638496, -3.141985750201293]
θ = [0.5264475872661588, 1.4164387324624934, 0.3508092870808165]
likehood = -6.459398744473566
∇L = [0.04436489349400041, 0.6231531802365315, -3.1642557679984193]
θ = [0.5308840766155588, 1.4226702642648358, 0.347645031281081]
likehood = -6.4511957061392575
∇L = [0.04508997903367806, 0.6292149547654369, -3.187062422582315]
θ = [0.5353930745189266, 1.4289624138125132, 0.3444579688902358]
likehood = -6.442933344234053
∇L = [0.045837978822798357, 0.6354518131534839, -3.210426349679324]
θ = [0.539976873341725, 1.435316931947648, 0.3412475424955564]
likehood = -6.434610100185724
∇L = [0.04660993747801179, 0.641870843061072, -3.234369454699701]
θ = [0.5446378670895261, 1.4417356403782586, 0.33801317304056565]
likehood = -6.4262243369456095
∇L = [0.0474069690220460486, 0.6484794987014424, -3.258914537386202]
θ = [0.5493785573099866, 1.448220435365273, 0.33475425850347057]
likehood = -6.417774333443653
∇L = [0.04823002115040076, 0.6552856291424138, -3.2840858229118 82]
θ = [0.55420155942502567, 1.454773291656697, 0.3314701726805694]
likehood = -6.40925827889373
∇L = [0.049080501066031346, 0.6622975033116583, -3.309908825030748]
θ = [0.5591096095316298, 1.4613962666898137, 0.32816026385553865]
likehood = -6.400674263720083
∇L = [0.04995962182196756, 0.6695238394871825, -3.336410487268884]
θ = [0.5641055717138266, 1.4680915050846854, 0.32482385336826974]
θ = [0.5641055717138266, 1.4680915050846854, 0.32482385336826974]
```

Out[8]:

```
3-element Vector{Float64}:
 0.5641055717138266
 1.4680915050846854
 0.32482385336826974
```

ガウス過程回帰を計算

In [9]:

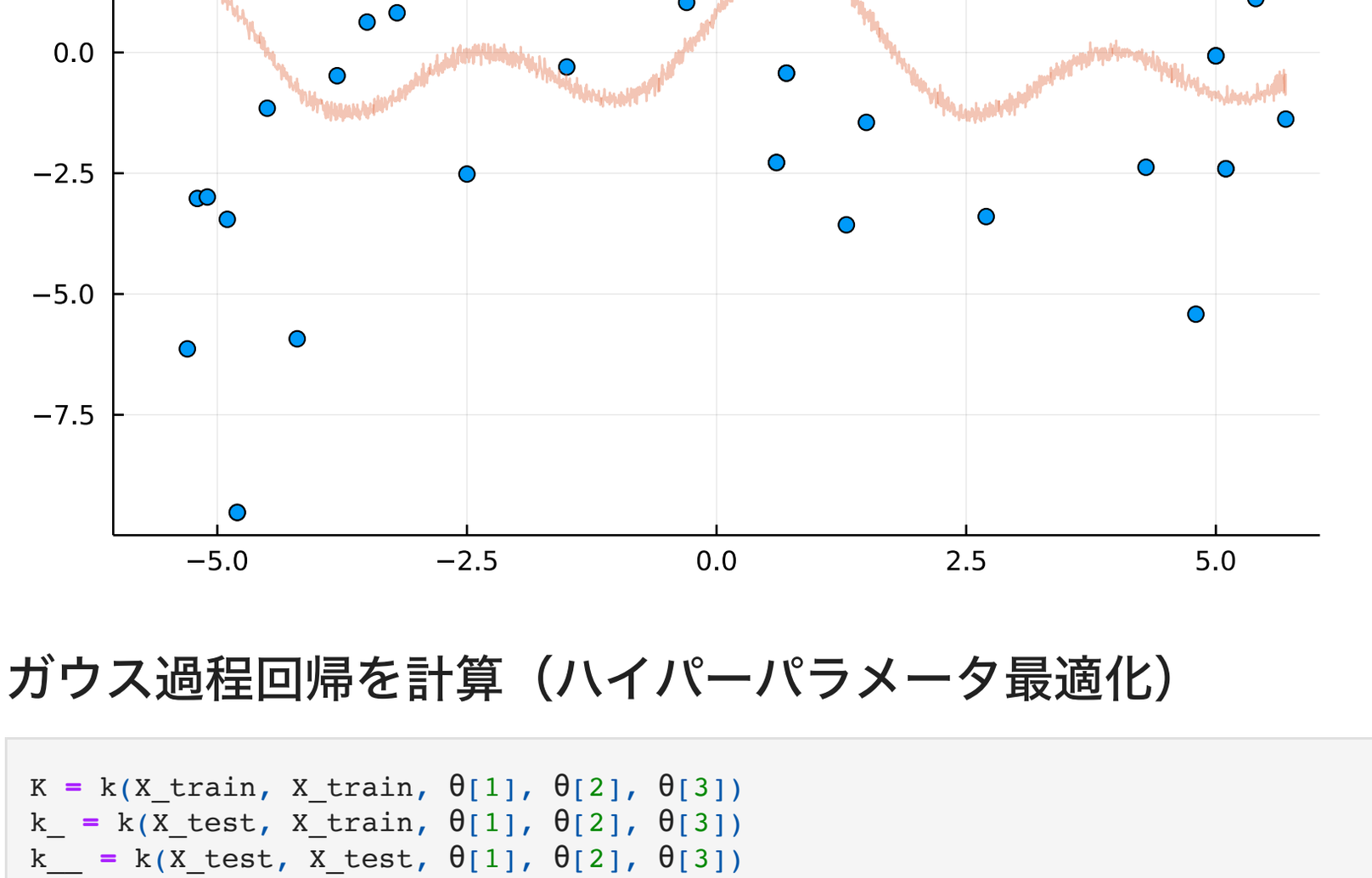
```julia
θ₁init, θ₂init, θ₃init = (10.0, 10.0, 10.0)
K = k(X_train, X_train, θ₁init, θ₂init, θ₃init)
k_ = k(X_test, X_train, θ₁init, θ₂init, θ₃init)
k__ = k(X_test, X_test, θ₁init, θ₂init, θ₃init)

Λ = inv(K)
Σ̂ = k__ - k_' * Λ * k_
μ̂ = k_' * Λ * Y_train

ŷ = μ̂ + real(√Σ̂) * randn(length(X_test))

scatter(X_test, ŷ, label="GP")
plot!(f, alpha=0.4, label="True model")
```

Out[9]:



ガウス過程回帰を計算（ハイパーパラメータ最適化）

In [10]:

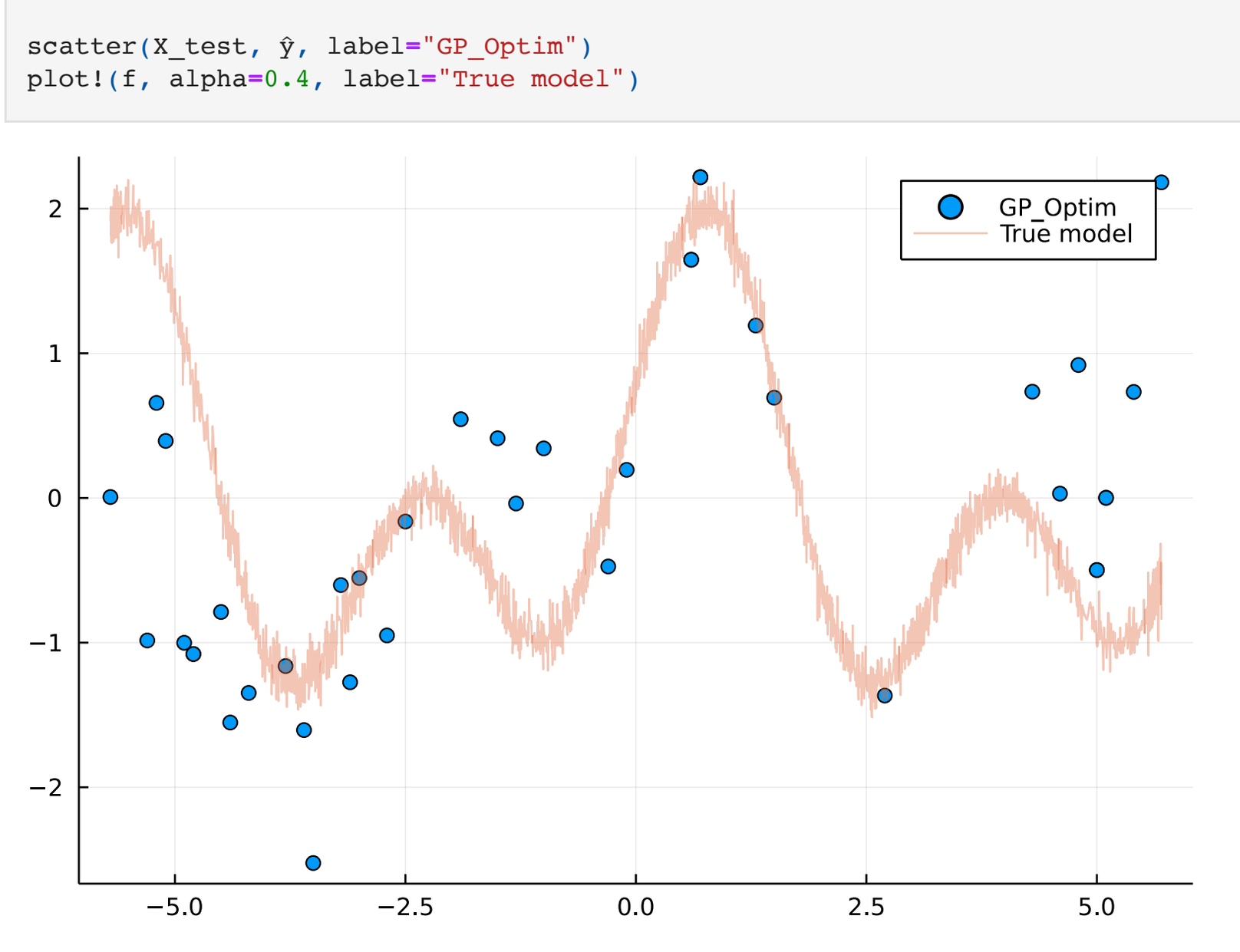
```julia
K = k(X_train, X_train, θ[1], θ[2], θ[3])
k_ = k(X_test, X_train, θ[1], θ[2], θ[3])
k__ = k(X_test, X_test, θ[1], θ[2], θ[3])

Λ = inv(K)
Σ̂ = k__ - k_' * Λ * k_
μ̂ = k_' * Λ * Y_train

ŷ = μ̂ + real(√Σ̂) * randn(length(X_test))

scatter(X_test, ŷ, label="GP_Optim")
plot!(f, alpha=0.4, label="True model")
```

Out[10]:



In [ ]: