Probabilistic Numerics

I – Introduction to Gaussian Regression

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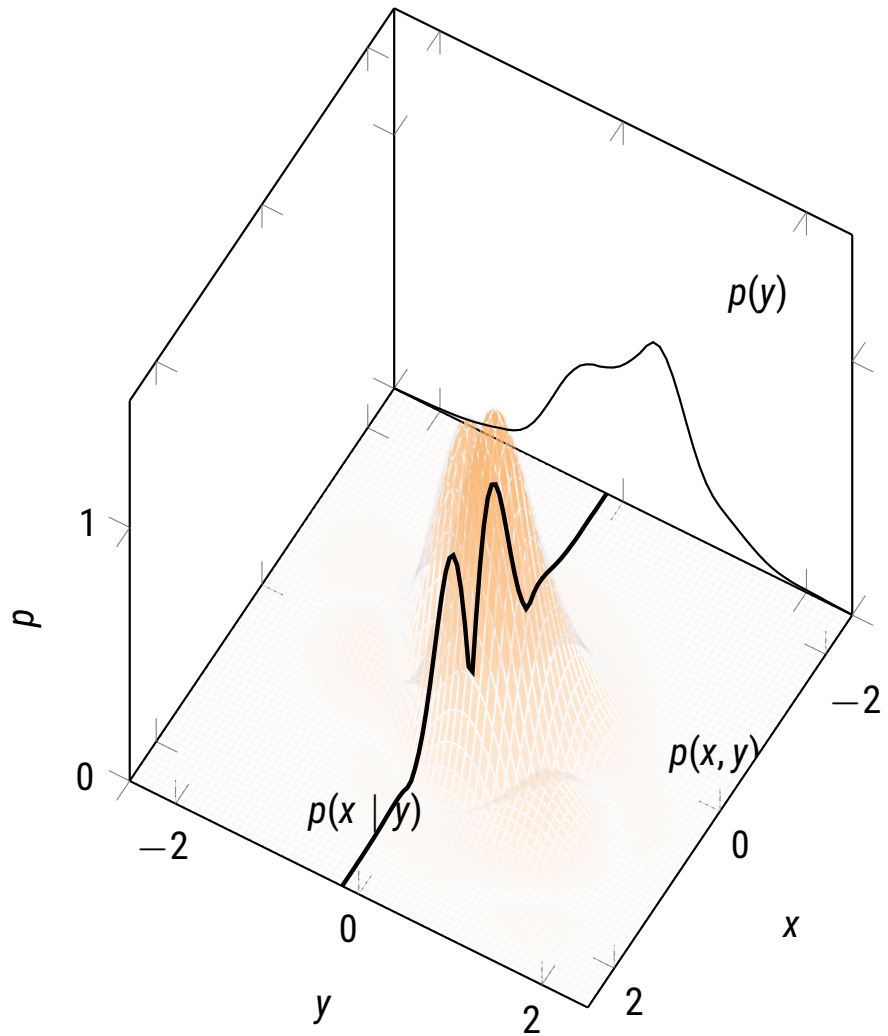
Probabilistic Inference

An explicit framework for dealing with uncertainty



- probability for $X = x$ AND $Y = y$:

$$p(x,y) \text{ s.t. } \int p(x,y)\,dx\,dy = 1$$

- sum rule: $\underbrace{p(y)}_{\text{marginal}} = \int \underbrace{p(x,y)}_{\text{joint}}\,dx$
- product rule: $p(x,y) = p(y)\,\underbrace{p(x \mid y)}_{\text{conditional}}$
- Bayes' Theorem:

$$\underbrace{p(x \mid y)}_{\text{posterior}} = \frac{\overbrace{p(y \mid x)}^{\text{likelihood}} \cdot \overbrace{p(x)}^{\text{prior}}}{\underbrace{p(y)}_{\text{evidence}}}$$

Grand Plan:

- today:
  - **Gaussian distributions**
    as a computationally efficient (linear) algebra of uncertainty
  - **computing** under uncertainty:
    integration and **ordinary differential equations**
- tomorrow:
  - **linear algebra** as inference: the computational limits of tracking uncertainty
  - **beyond classic methods**: new probabilistic functionality for contemporary computational challenges:
    - local and global optimization under uncertainty
    - propagating uncertainty through computational pipelines
    - detecting inappropriate models

Computation is inference on unknown quantities, using silicon as a data source.
Uncertainty deserves a central role.

Gaussian Distributions

a central concept

$$\mathcal{N}(x; \mu, \Sigma) = \frac{1}{|2\pi\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu)^{\intercal}\Sigma^{-1}(x-\mu)\right]$$

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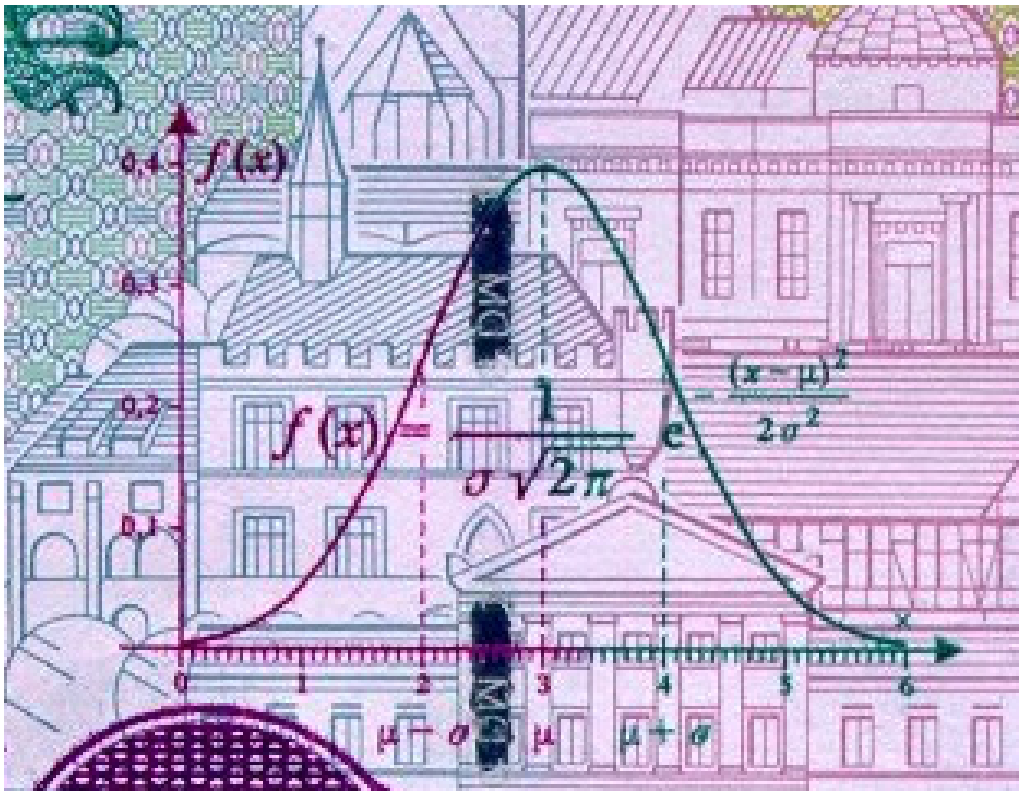


Coming up:

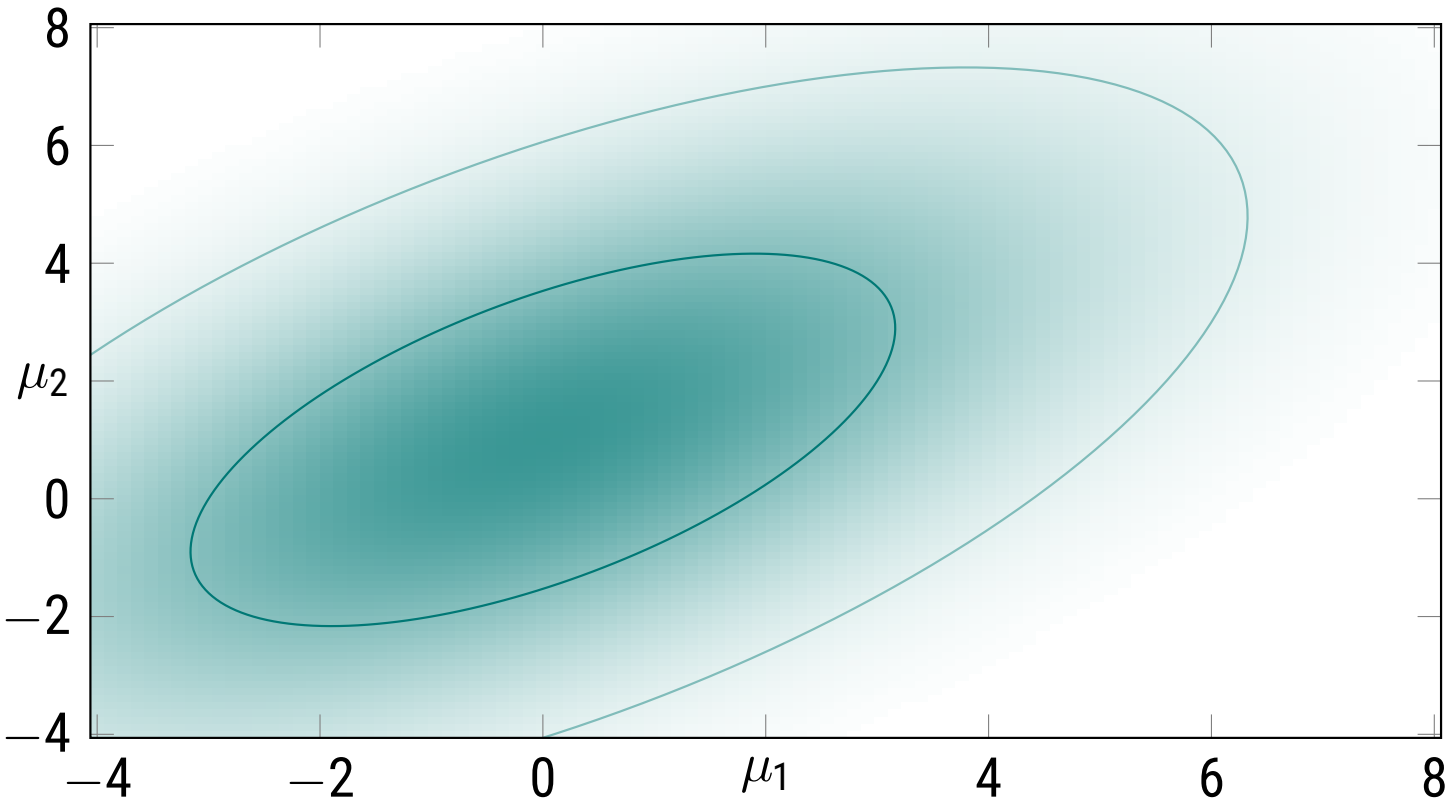
- **Gaussians** are to **inference** as **linear maps** are to **algebra**
- **Numerical computation** is about mapping intractable problems onto **linear** (or discrete) ones. Gaussians provide the algebra to achieve this in the context of **uncertainty**

Closure under Multiplication

multiple Gaussian factors form a Gaussian

$$\mathcal{N}(x; a, A)\mathcal{N}(x; b, B) = \mathcal{N}(x; c, C)Z$$

$$C := (A^{-1} + B^{-1})^{-1} \qquad c := C(A^{-1}a + B^{-1}b) \qquad Z := \mathcal{N}(a; b, A + B)$$



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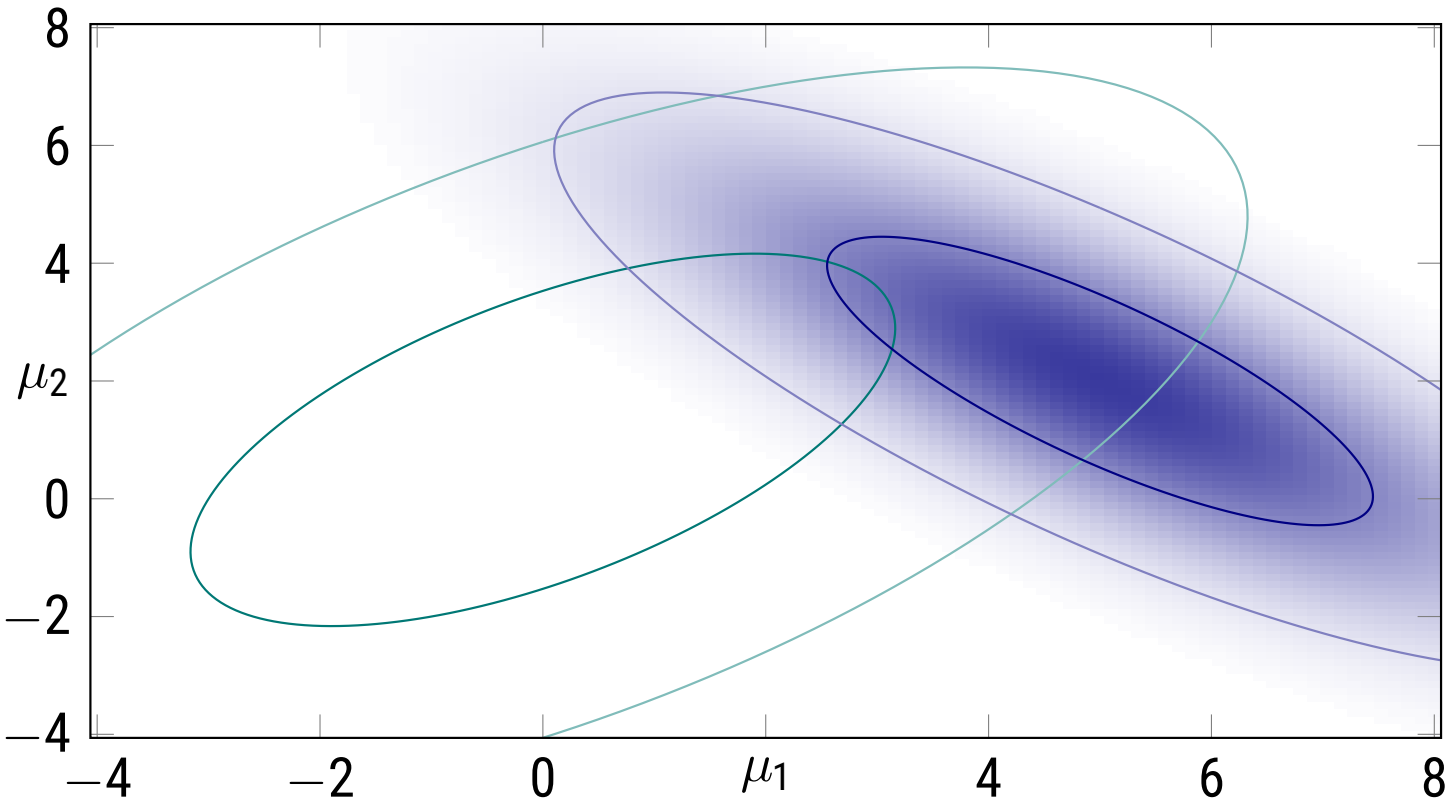

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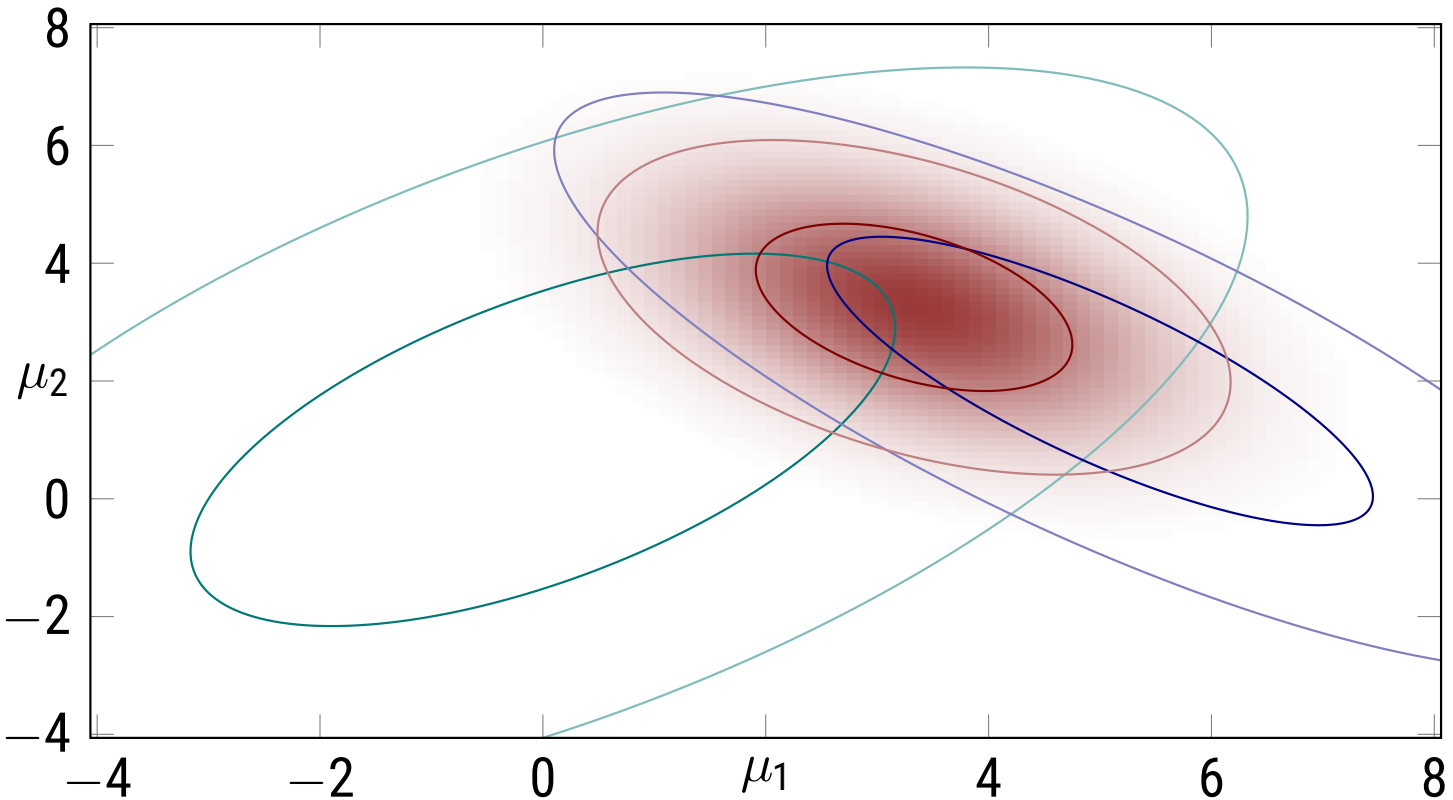
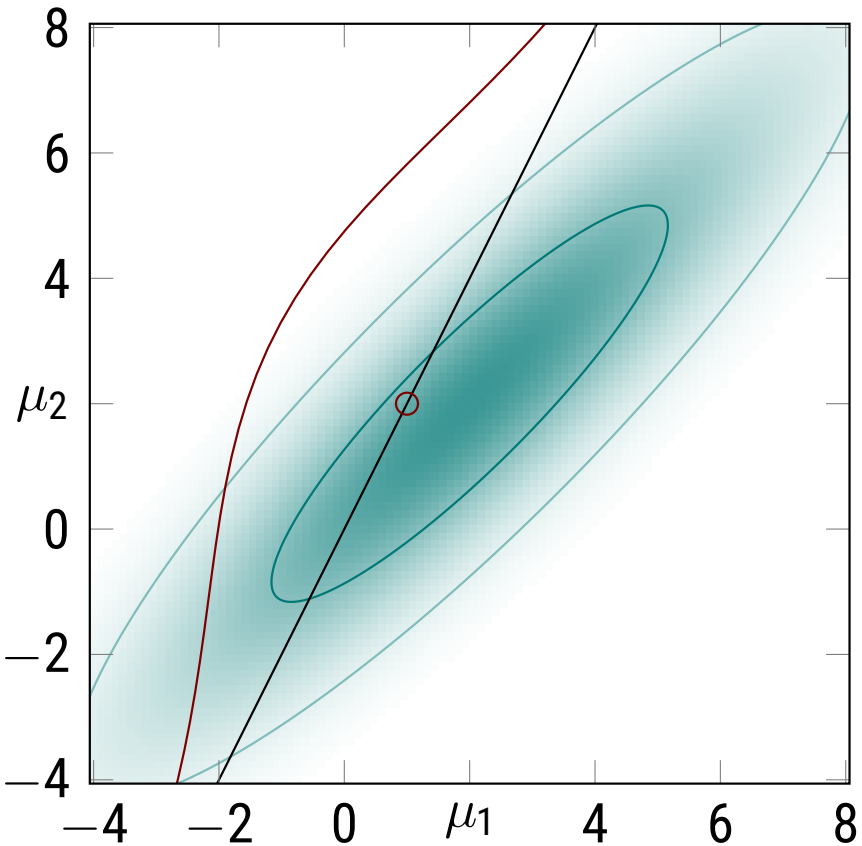


Closure under Linear Maps

linear maps of Gaussians are Gaussians



$$p(z) = \mathcal{N}(z; \mu, \Sigma)$$

$$\Rightarrow \quad p(Az) = \mathcal{N}(Az, A\mu, A\Sigma A^\intercal)$$

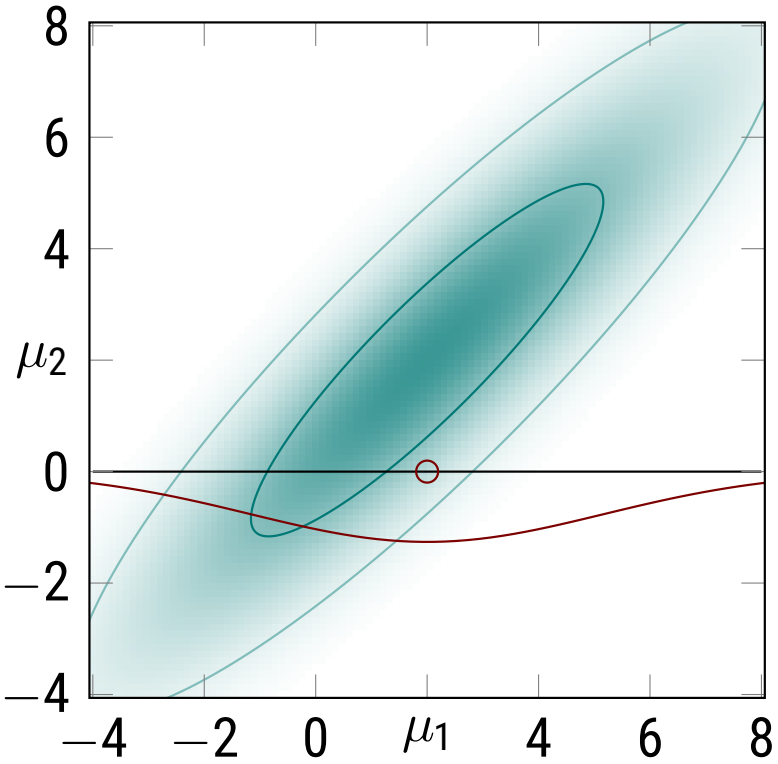
Here: $A = [1, -0.5]$

Closure under Marginalization

projections of Gaussians are Gaussian

- projection with $A = \begin{pmatrix} 1 & 0 \end{pmatrix}$

$$\int \mathcal{N}\left[\begin{pmatrix} x \\ y \end{pmatrix}; \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix}\right] dy = \mathcal{N}(x; \mu_x, \Sigma_{xx})$$



- this is the sum rule

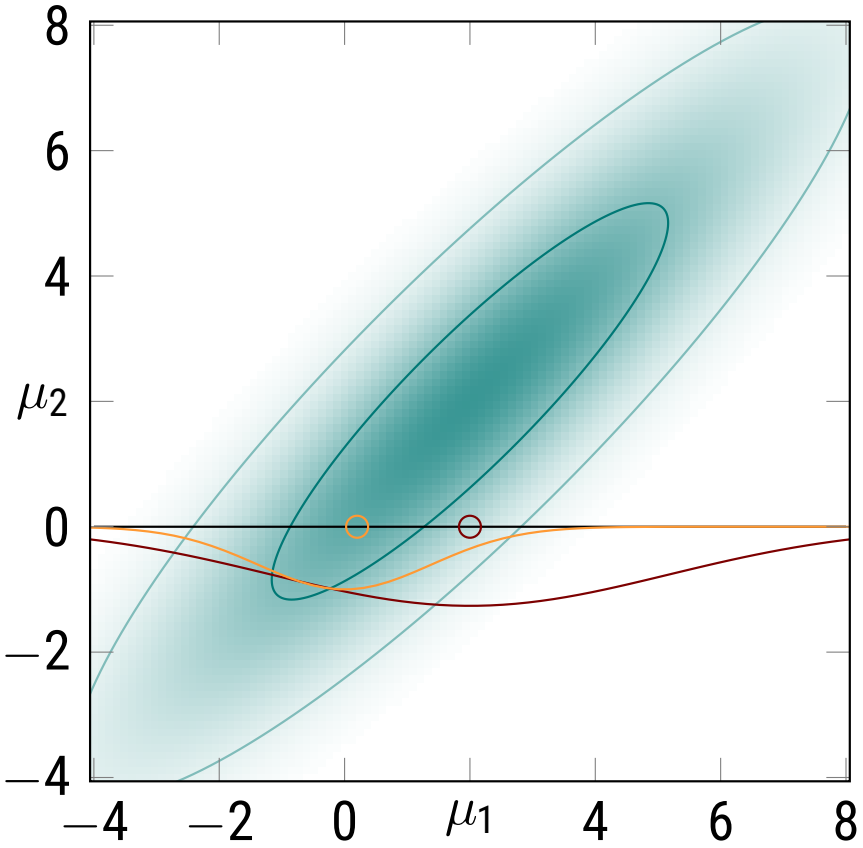
$$\int p(x, y)\, dy = \int p(y \mid x) p(x)\, dy = p(x)$$

- so every finite-dim Gaussian is a marginal of infinitely many more

Closure under Conditioning

cuts through Gaussians are Gaussians

$$p(x \mid y) = \frac{p(x,y)}{p(y)} = \mathcal{N}\left(x; \mu_x + \Sigma_{xy}\Sigma_{yy}^{-1}(y - \mu_y), \Sigma_{xx} - \Sigma_{xy}\Sigma_{yy}^{-1}\Sigma_{yx}\right)$$



- this is the product rule
- so Gaussians are closed under the rules of probability

Gaussians provide the linear algebra of inference

if all joints are Gaussian and all observations are linear, all posteriors are Gaussian

- products of Gaussians are Gaussians $\quad C := (A^{-1} + B^{-1})^{-1} \quad c := C(A^{-1}a + B^{-1}b)$

$$\mathcal{N}(x; a, A)\mathcal{N}(x; b, B) = \mathcal{N}(x; c, C)\mathcal{N}(a; b, A + B)$$

- marginals of Gaussians are Gaussians

$$\int \mathcal{N}\left[\begin{pmatrix} x \\ y \end{pmatrix}; \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix}, \begin{pmatrix} \Sigma_{xx} & \Sigma_{xy} \\ \Sigma_{yx} & \Sigma_{yy} \end{pmatrix}\right] dy = \mathcal{N}(x; \mu_x, \Sigma_{xx})$$

- (linear) conditionals of Gaussians are Gaussians

$$p(x \mid y) = \frac{p(x, y)}{p(y)} = \mathcal{N}\left(x; \mu_x + \Sigma_{xy}\Sigma_{yy}^{-1}(y - \mu_y), \Sigma_{xx} - \Sigma_{xy}\Sigma_{yy}^{-1}\Sigma_{yx}\right)$$

- linear projections of Gaussians are Gaussians

$$p(z) = \mathcal{N}(z; \mu, \Sigma) \quad \Rightarrow \quad p(Az) = \mathcal{N}(Az, A\mu, A\Sigma A^{\mathsf{T}})$$

Bayesian inference becomes linear algebra

$$p(x) = \mathcal{N}(x; \mu, \Sigma) \qquad p(y \mid x) = \mathcal{N}(y; A^{\mathsf{T}}x + b, \Lambda)$$

$$p(B^{\mathsf{T}}x + c \mid y) = \mathcal{N}[B^{\mathsf{T}}x + c; B^{\mathsf{T}}\mu + c + B^{\mathsf{T}}\Sigma A(A^{\mathsf{T}}\Sigma A + \Lambda)^{-1}(y - A^{\mathsf{T}}\mu - b),$$
$$B^{\mathsf{T}}\Sigma B - B^{\mathsf{T}}\Sigma A(A^{\mathsf{T}}\Sigma A + \Lambda)^{-1}A^{\mathsf{T}}\Sigma B]$$

- **Gaussians** are to **inference** as **linear maps** are to **algebra**
- Gaussian measures turn probabilistic inference into **linear algebra**

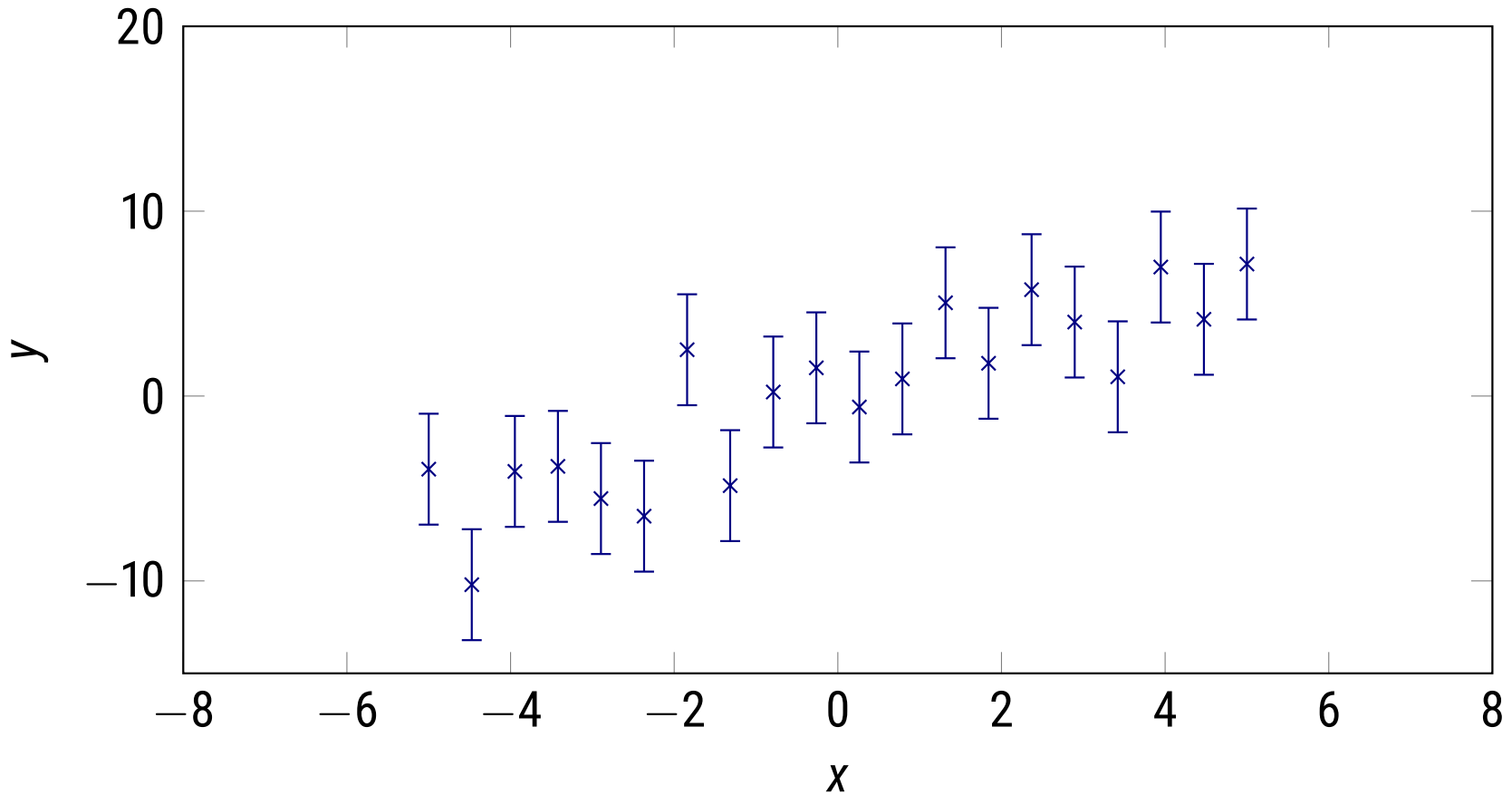
Next up:

- Gaussian measures can be used to infer **functions** and **curves**

A dataset

linear regression

given $y \in \mathbb{R}^N$, $p(y \mid f)$, what is f?

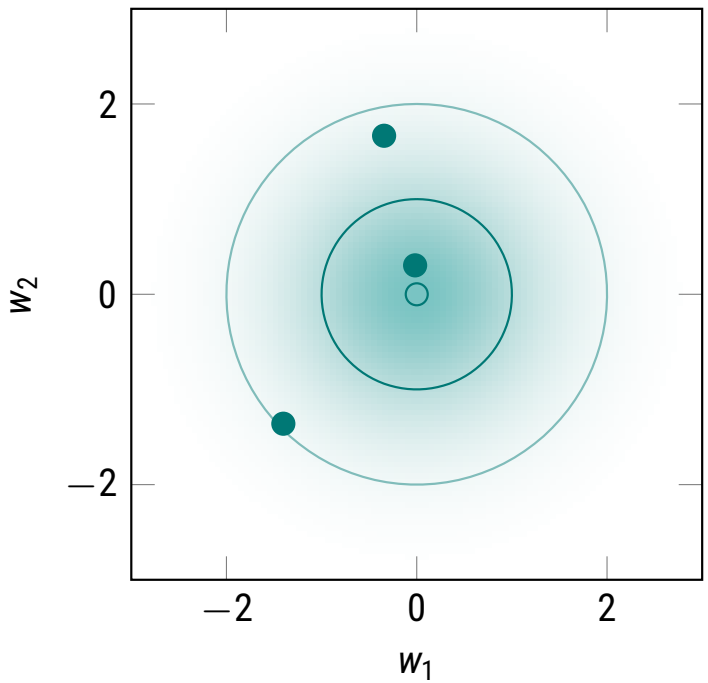


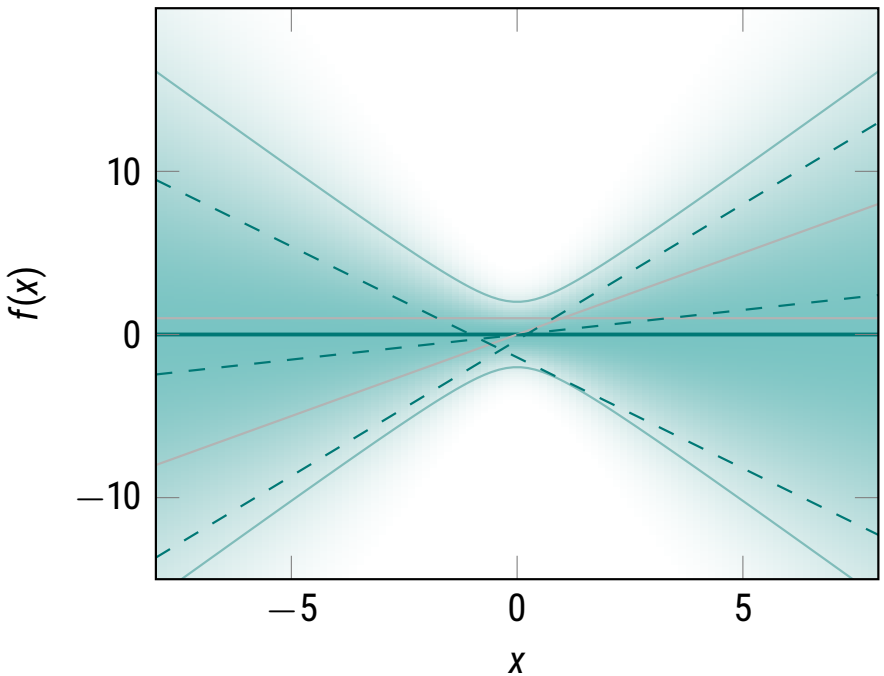
A prior

over linear functions

$$f(x) = w_1 + w_2 x = \phi_x^\intercal w \qquad \phi_x = \begin{pmatrix} 1 \\ x \end{pmatrix}$$

$$p(w) = \mathcal{N}(w; \mu, \Sigma) \qquad p(f) = \mathcal{N}(f; \phi_x^\intercal \mu, \phi_x^\intercal \Sigma \phi_x)$$





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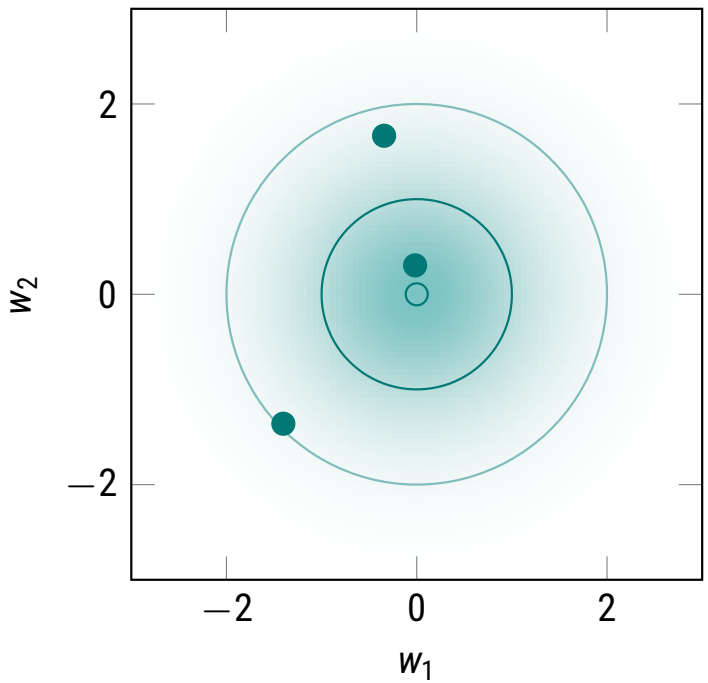
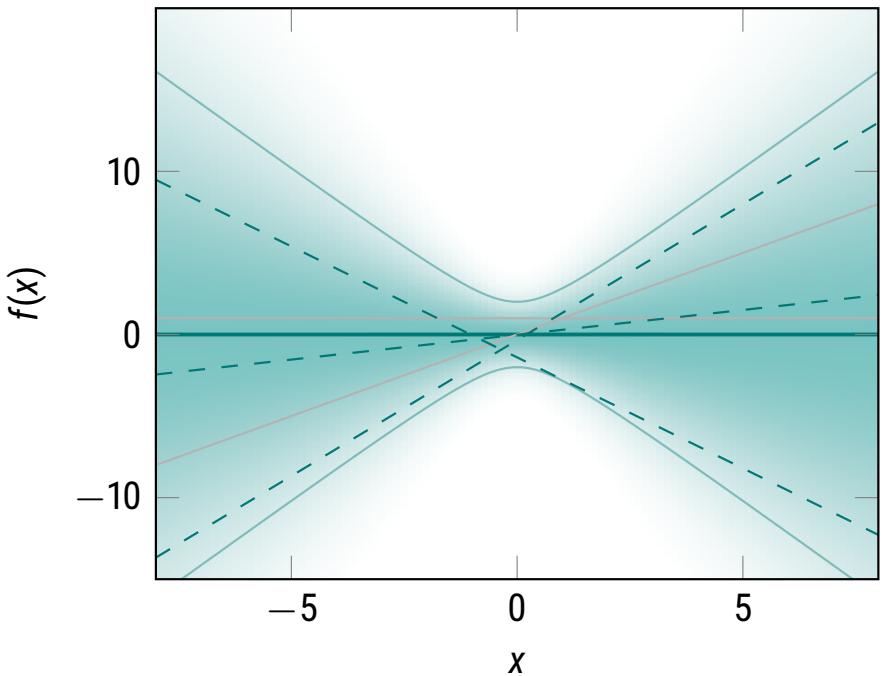
$$f(x) = w_1 + w_2 x = \phi_x^\mathsf{T} w \qquad \phi_x = \begin{pmatrix} 1 \\ x \end{pmatrix}$$

$$p(w) = \mathcal{N}(w; \mu, \Sigma) \qquad p(f) = \mathcal{N}(f; \phi_x^\mathsf{T} \mu, \phi_x^\mathsf{T} \Sigma \phi_x)$$



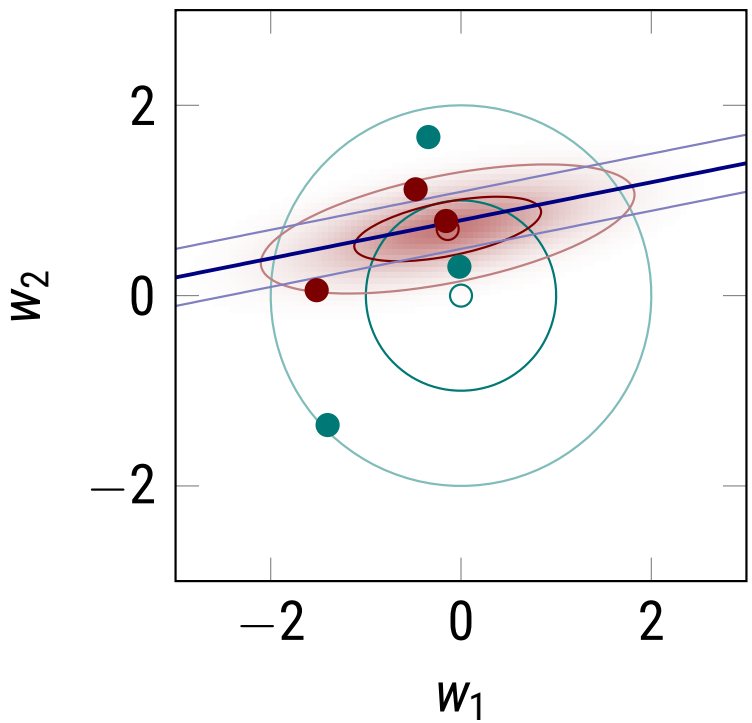


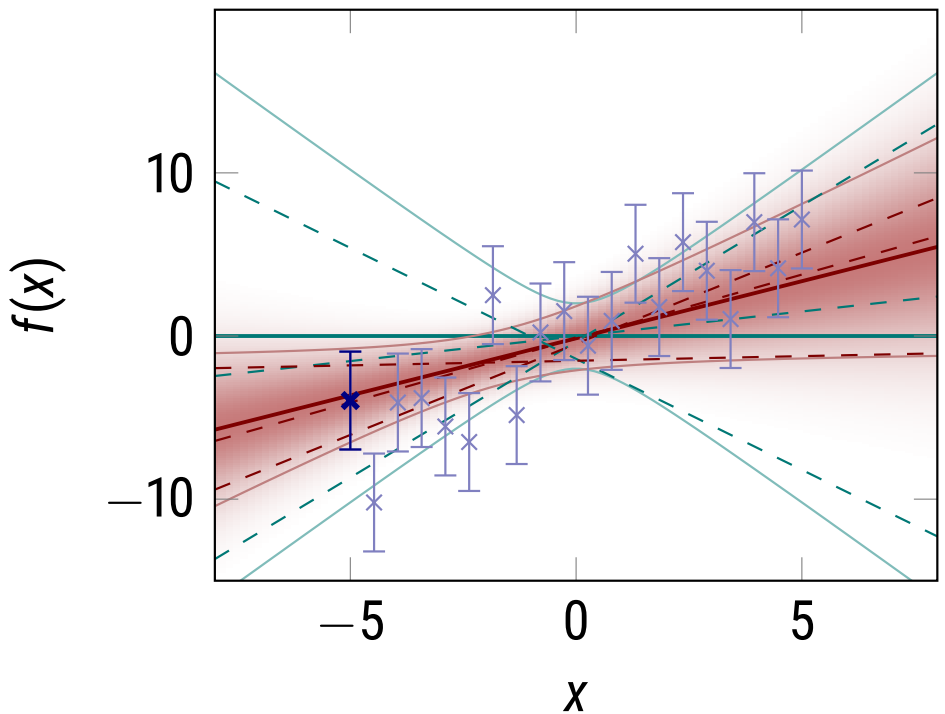
The posterior

over weights and functions

$$p(y \mid w, \phi_X) = \mathcal{N}(y; \phi_X^\intercal w, \sigma^2 I)$$

$$p(f_x \mid y, \phi_X) = \mathcal{N}(f_x; \phi_x^\intercal \mu + \phi_x^\intercal \Sigma \phi_X (\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}(y - \phi_X^\intercal \mu),$$
$$\phi_x^\intercal \Sigma \phi_x - \phi_x^\intercal \Sigma \phi_X (\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1} \phi_X^\intercal \Sigma \phi_x)$$





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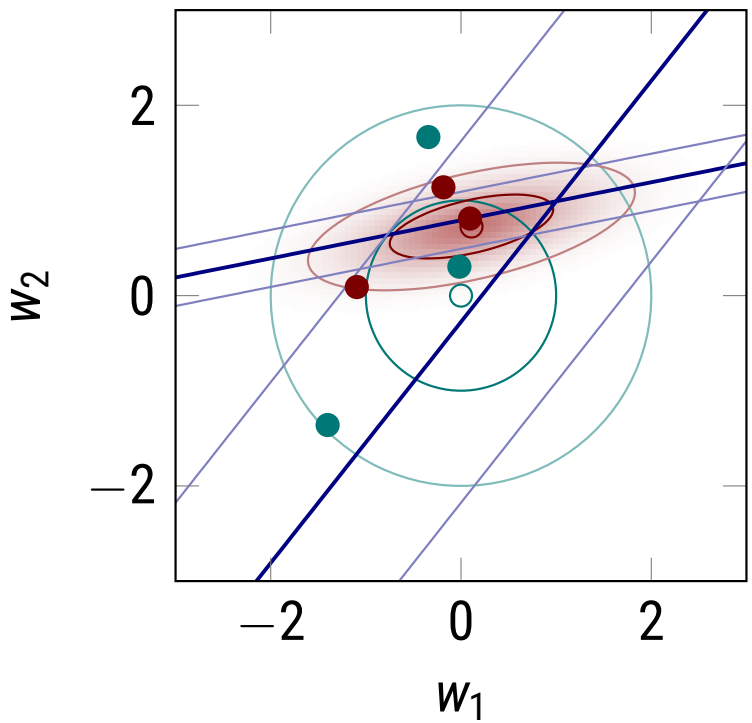

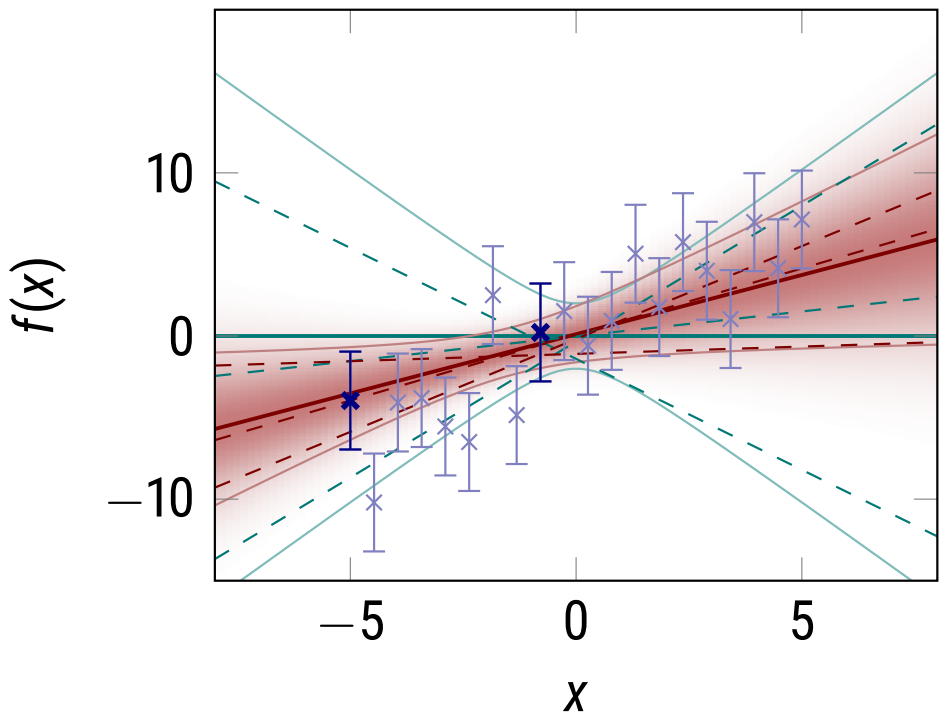

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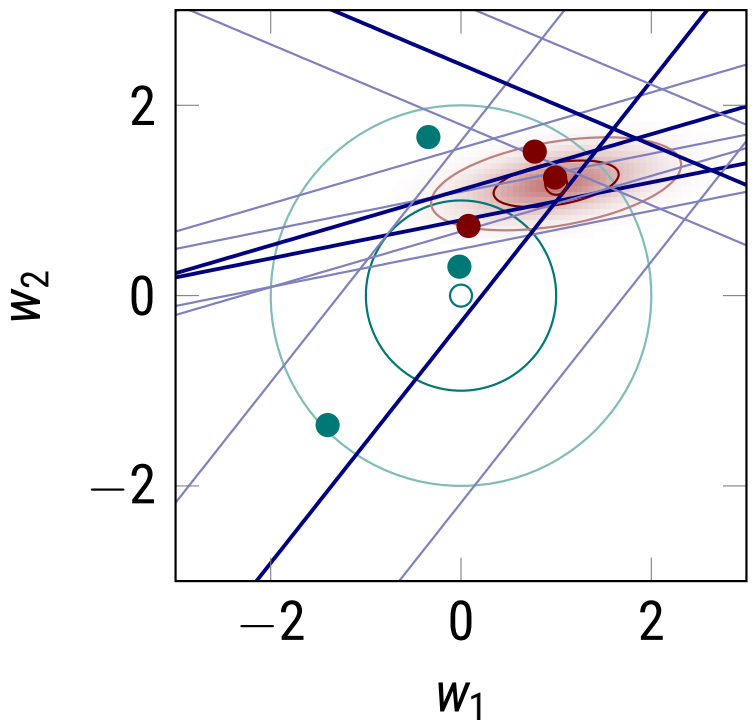

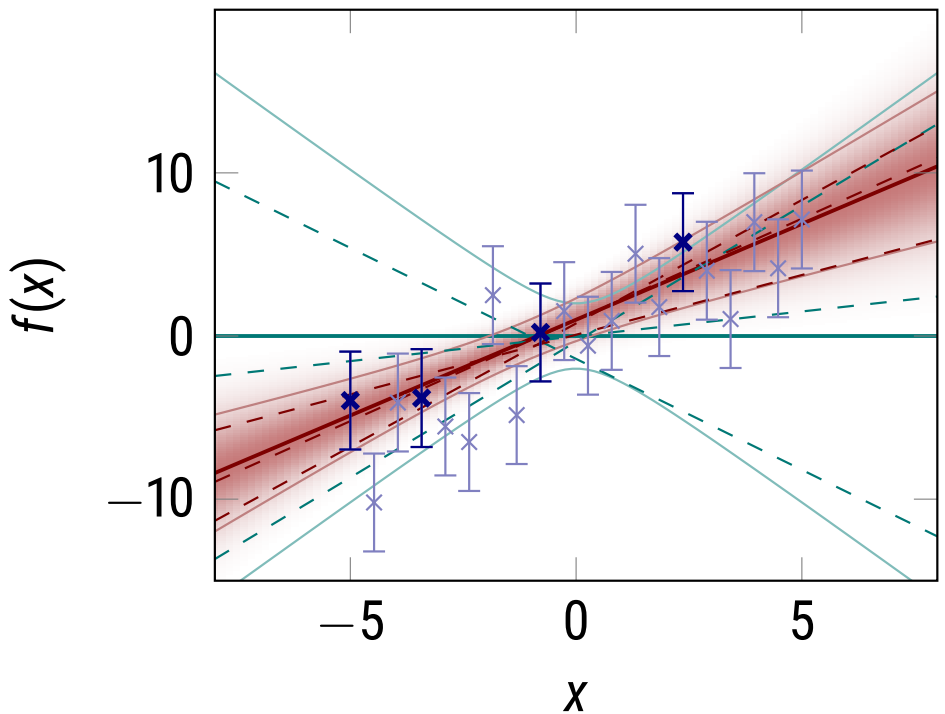

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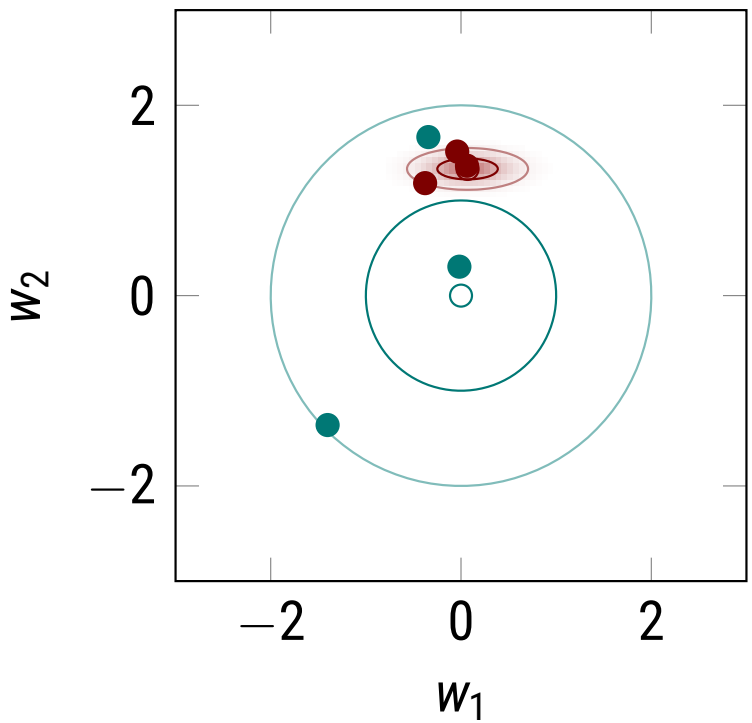
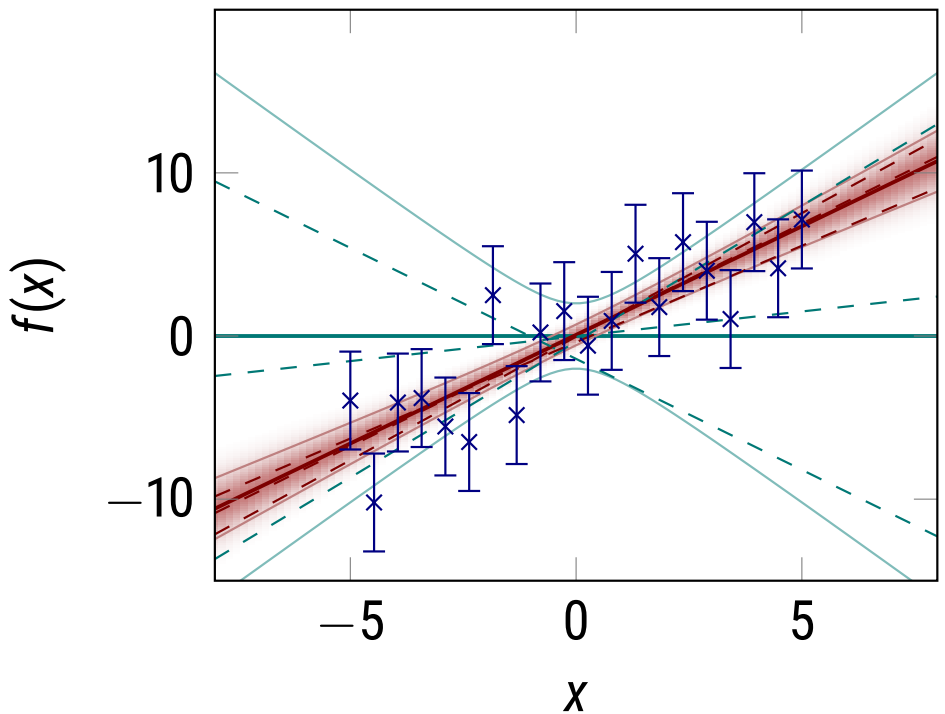




Code

python

```
#                              ==== PARAMETRIC GAUSSIAN REGRESSION IN PYTHON ====
# prior on w
F     = 2                                                  # number of features
def phi(a) : return power(a,range(F))                          # phi(a) = [1,a]
mu    = zeros((F,1))
Sigma = eye(F)                                             # p(w)=N(mu,Sigma)

# implied prior on f_x
n     = 100
x     = reshape(linspace(-8,8,n),(n,1))     # reshape is needed for phi to work
m     = dot(phi(x),mu)
kxx   = dot(dot(phi(x),Sigma),phi(x).transpose())            # p(f_x)=N(m,k_xx)
s     = dot(cholesky(kxx + 1e-6 * eye(n)),randn(n,3)) + m       # prior samples
stdpi = reshape(sqrt(diag(kxx)),[n,1])          # marginal stddev, for plotting

# loading data from disk
import scipy.io; data = scipy.io.loadmat('data.mat')
X = data['X']; Y = data['Y']; sigma = data['sigma']; N  = len(X)

# prior on Y = f_X + eps
M     = dot(phi(X),mu)
kXX   = dot(dot(phi(X),Sigma),phi(X).transpose())          # p(f_X) = N(M,k_XX)

# inference
G     = cho_factor(kXX + sigma**2 * eye(N))       # Most expensive step, O(N^3)
kxX   = dot(dot(phi(x),Sigma),phi(X).transpose())         # Cov(f_x,f_X) = k_xX
A     = cho_solve(G,kxX.transpose()).transpose()       # pre-compute for re-use

# posterior p(f_x|Y)
mpost = m + dot(A,(Y-M))                                                # mean
vpost = kxx - dot(A,kxX.transpose())                                # covariance
spost = dot(cholesky(vpost + 1e-8 * eye(n)),randn(n,3)) + mpost       # samples
stdpo = reshape(sqrt(diag(vpost)),[n,1])        # marginal stddev, for plotting
```

Code

matlab

```
%                              ==== PARAMETRIC GAUSSIAN REGRESSION IN MATLAB ====
% prior on w
F     = 2;                                                  % number of features
phi   = @(a)(bsxfun(@power,a,0:F-1));                            % phi(a)=[1;a]
mu    = zeros(F,1);
Sigma = eye(F);                                             % p(w) = N(mu,Sigma)

% implied prior on f_x
n     = 100;
x     = linspace(-8,8,n)';                                      % `test' points
m     = phi(x) * mu;
kxx   = phi(x) * Sigma * phi(x)';                             % p(f_x)=N(m,k_xx)
s     = bsxfun(@plus,m,chol(kxx + 1.0e-8 * eye(n))' * randn(n,3));    % samples
stdpi = sqrt(diag(kxx));                              % marginal stddev, for plotting

% loading data from disk
load('data.mat'); N = length(Y);                               % gives Y,X,sigma

% prior on Y=f_X + epsilon
M     = phi(X) * mu;
kXX   = phi(X) * Sigma * phi(X)';                             % p(f_X) = N(M,k_XX)

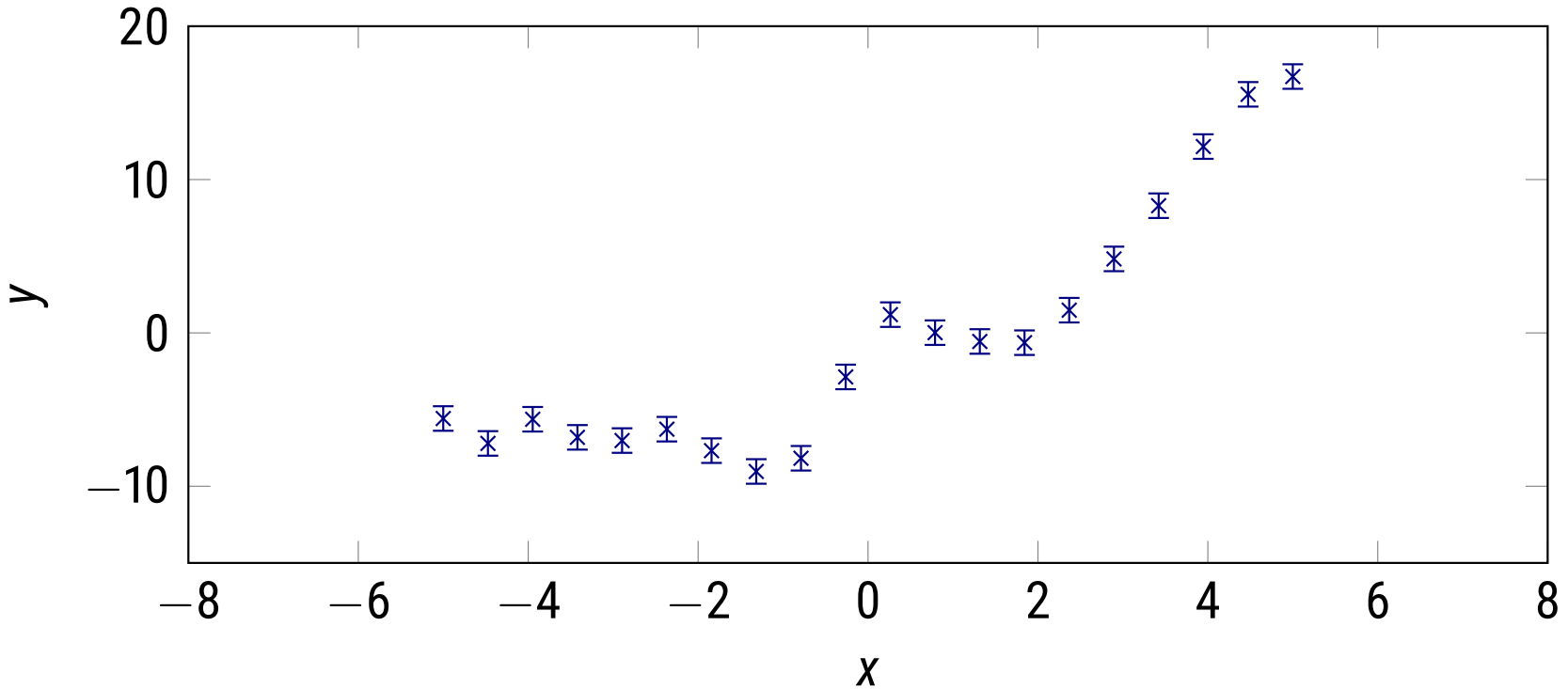
% inference
G     = chol(kXX + sigma^ 2 * eye(N);)            % most expensive step: O(N^3)
kxX   = phi(x) * Sigma * phi(X)';                             % Cov(f_x,f_X) = k_xX
A     = kxX / G;                                    % pre-compute for re-use

% posterioe p (f_x|Y)
mpost = m + A * (G' \ (Y-M));                                              % mean
vpost = kxx - A * A';                                                % covariance
spost = bsxfun(@plus,mpost,chol(vpost + 1.0e-8 * eye(n))' * randn(n,3)) % smpls
stdpo = sqrt(diag(vpost));                            % marginal stddev, for plotting
```

A More Realistic Dataset

General Linear Regression

$$f(x) = \phi_x^\mathsf{T} w \qquad ?$$



$$f(x) = w_1 + w_2 x = \phi_x^\top w$$

$$\phi_x := \begin{pmatrix} 1 \\ x \end{pmatrix}$$

No big deal!

a one-line change

```
#                              ==== PARAMETRIC GAUSSIAN REGRESSION IN PYTHON ====
# prior on w
F     = 4                                                    # number of features
def phi(a) : return power(a,range(F))                            # phi(a) = [1,a]
mu    = zeros((F,1))
Sigma = eye(F)                                                 # p(w)=N(mu,Sigma)

# implied prior on f_x
n     = 100
x     = reshape(linspace(-8,8,n),(n,1))     # reshape is needed for phi to work
m     = dot(phi(x),mu)
kxx   = dot(dot(phi(x),Sigma),phi(x).transpose())              # p(f_x)=N(m,k_xx)
s     = dot(cholesky(kxx + 1e-6 * eye(n)),randn(n,3)) + m       # prior samples
stdpi = reshape(sqrt(diag(kxx)),[n,1])           # marginal stddev, for plotting

# loading data from disk
import scipy.io; data = scipy.io.loadmat('data.mat')
X = data['X']; Y = data['Y']; sigma = data['sigma']; N  = len(X)

# prior on Y = f_X + eps
M     = dot(phi(X),mu)
kXX   = dot(dot(phi(X),Sigma),phi(X).transpose())            # p(f_X) = N(M,k_XX)

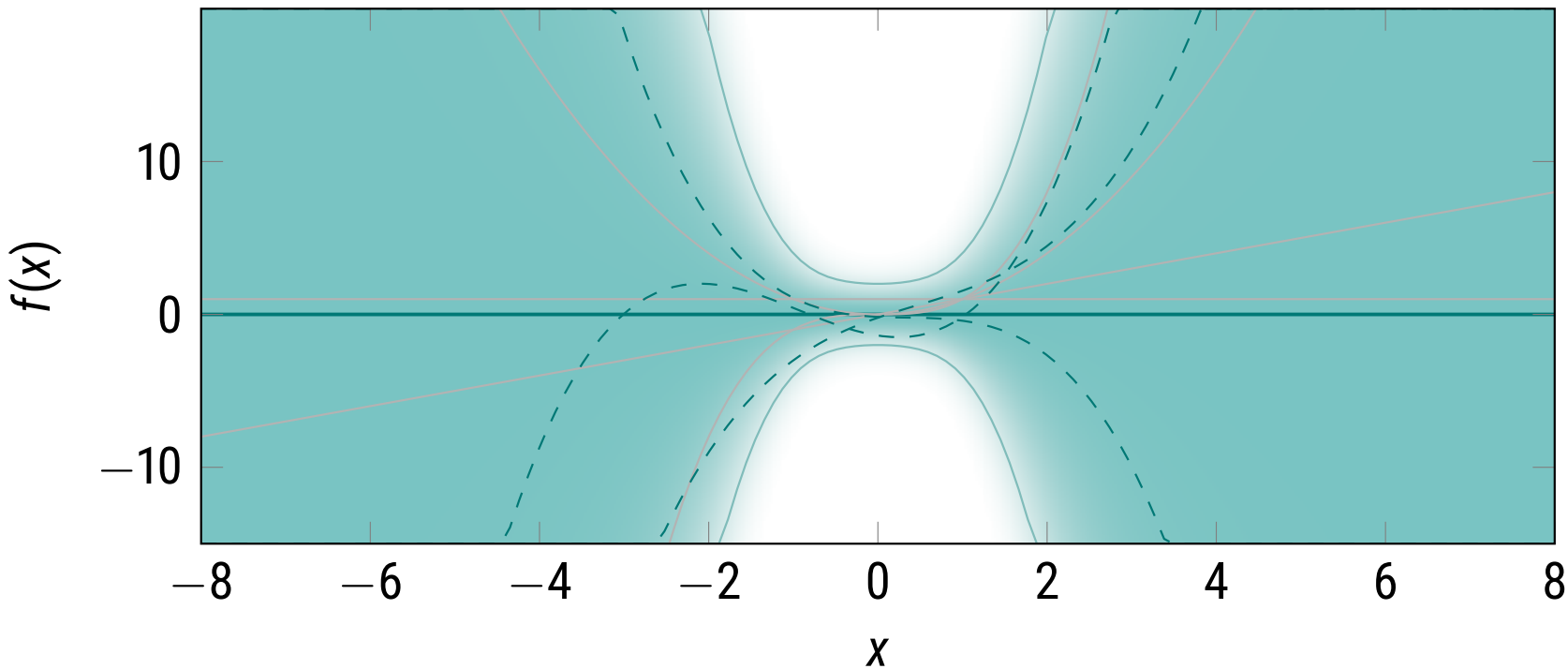
# inference
G     = cho_factor(kXX + sigma**2 * eye(N))       # Most expensive step, O(N^3)
kxX   = dot(dot(phi(x),Sigma),phi(X).transpose())          # Cov(f_x,f_X) = k_xX
A     = cho_solve(G,kxX.transpose()).transpose()       # pre-compute for re-use

# posterior p(f_x|Y)
mpost = m + dot(A,(Y-M))                                                 # mean
vpost = kxx - dot(A,kxX.transpose())                                # covariance
spost = dot(cholesky(vpost + 1e-8 * eye(n)),randn(n,3)) + mpost       # samples
stdpo = reshape(sqrt(diag(vpost)),[n,1])         # marginal stddev, for plotting
```

Cubic Regression

```
phi = @(a)(bsxfun(@power,a,[0:3]));
```

$$f(x) = \phi(x)^\intercal w \qquad \phi(x) = \begin{pmatrix} 1 & x & x.^2 & x.^3 \end{pmatrix}^\intercal$$



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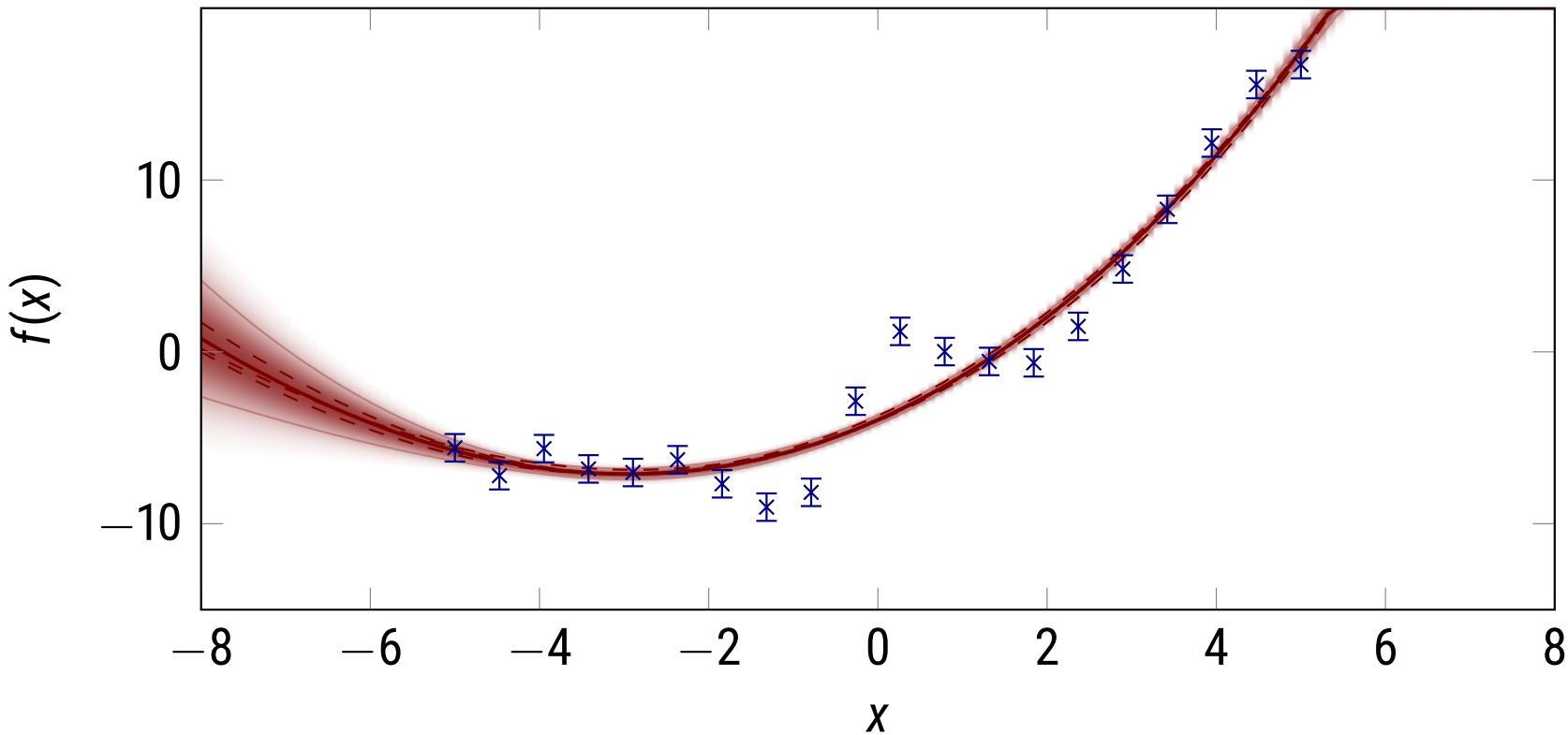

Septic Regression?

```
phi = @(a)(bsxfun(@power,a,[0:7]));
```

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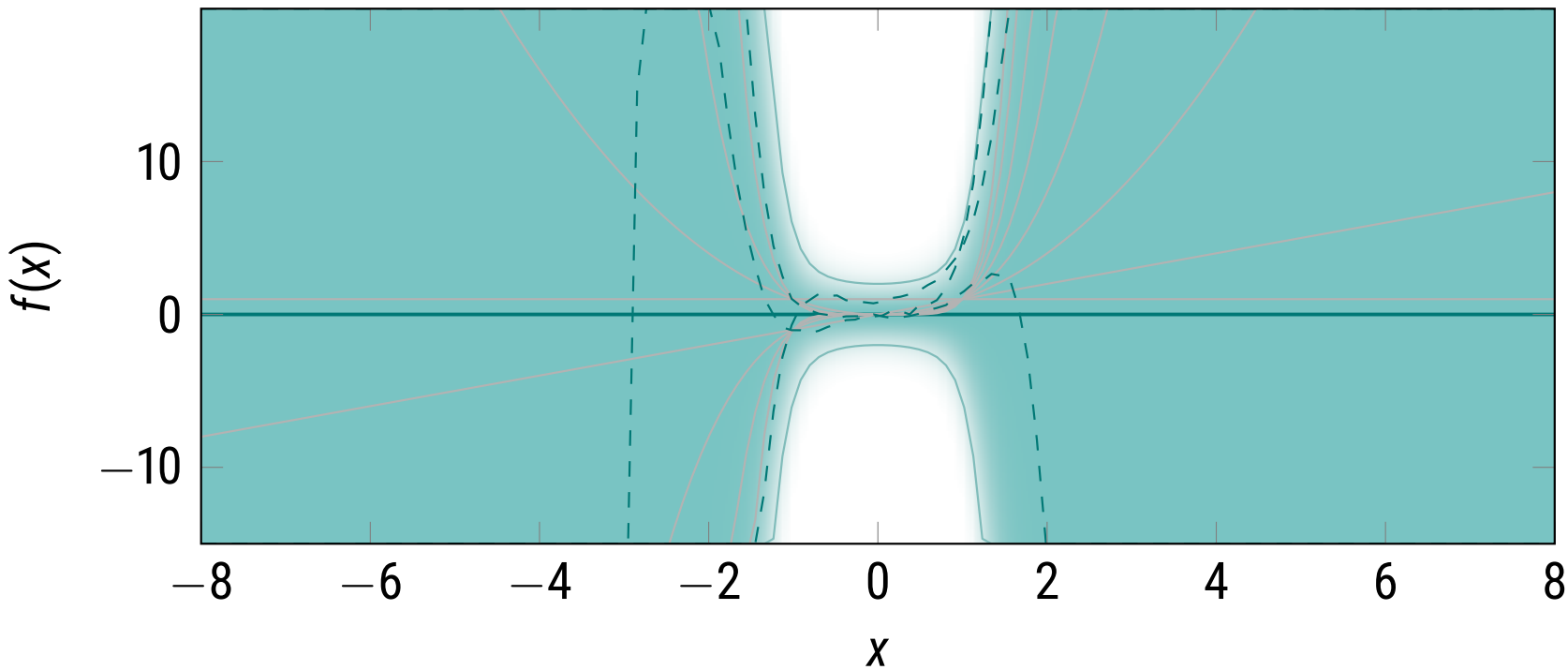

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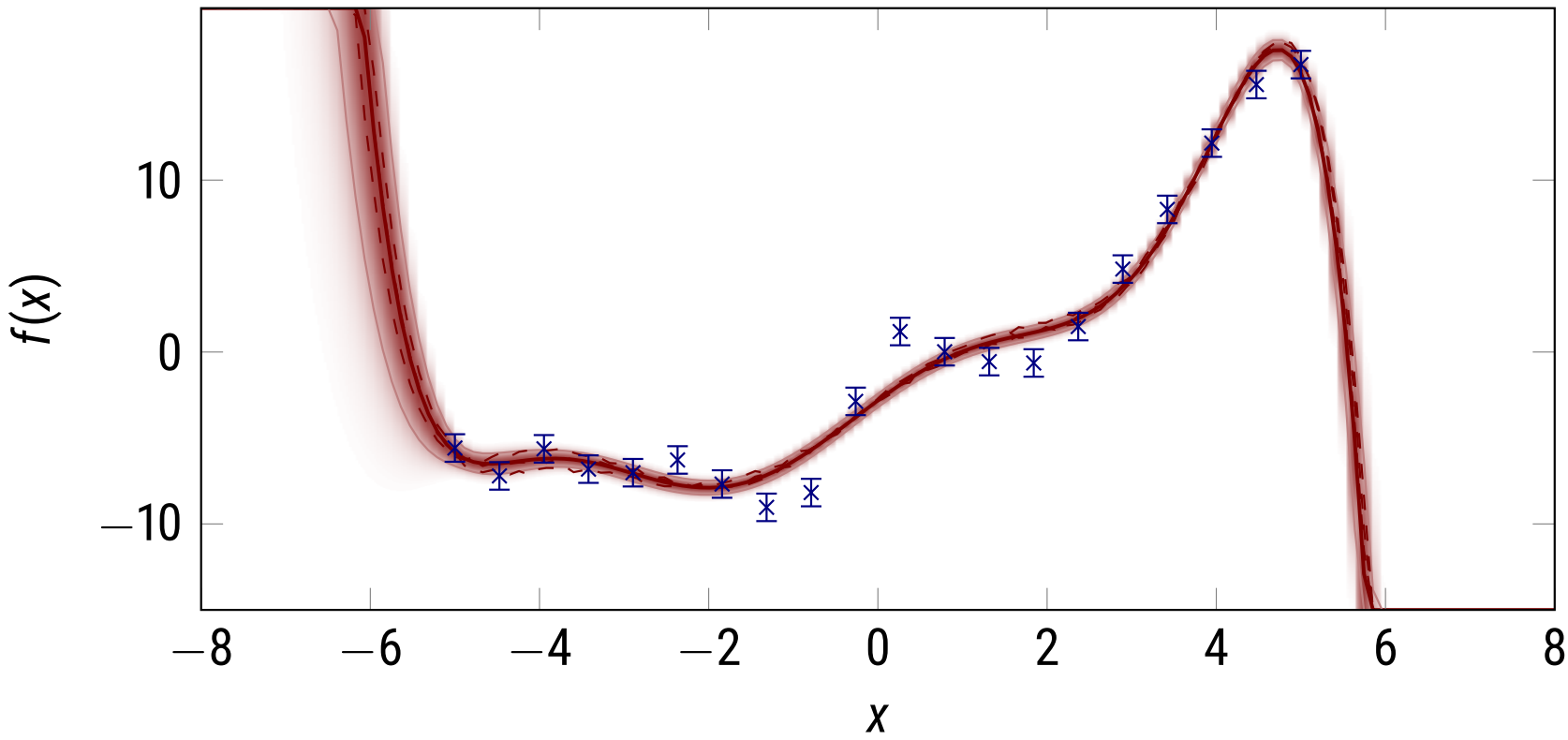
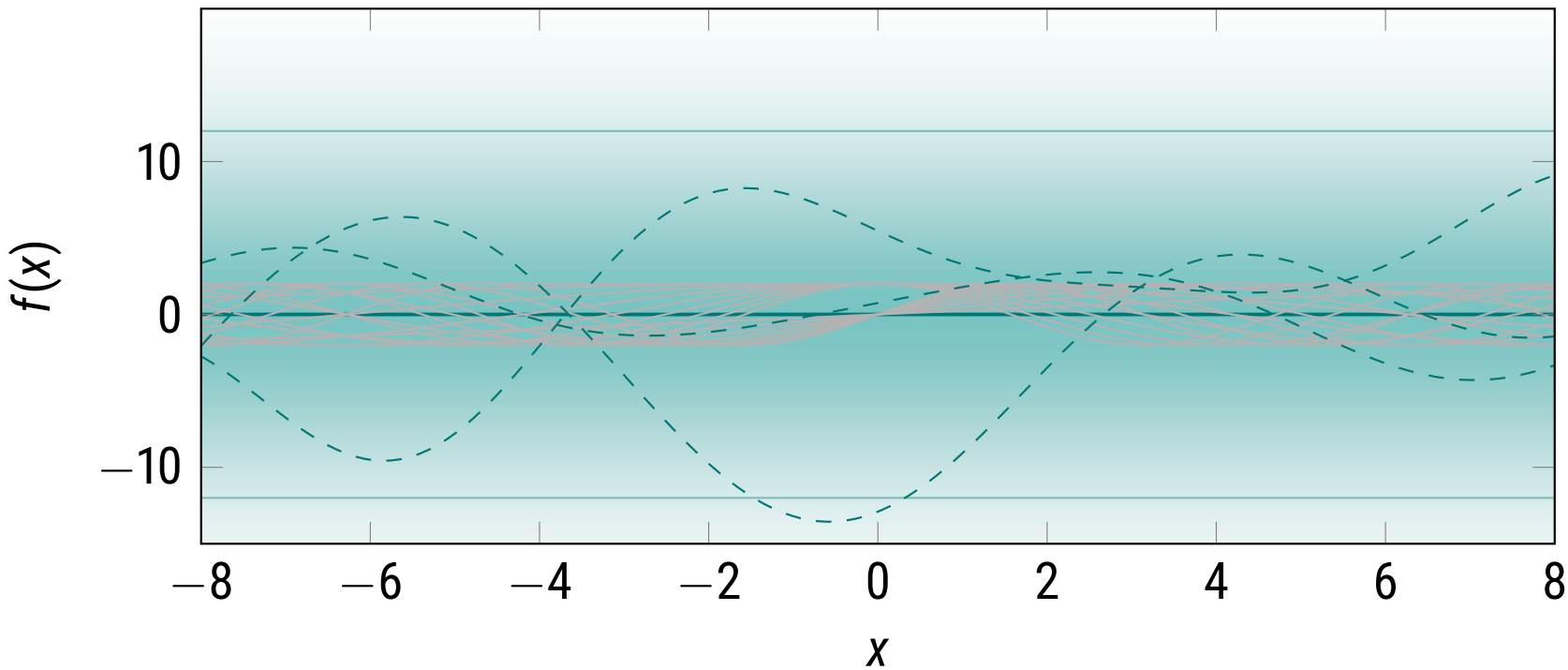


Fourier Regression

```
phi = @(a)(2 * [cos(bsxfun(@times,a/8,[0:8])), sin(bsxfun(@times,a/8,[1:8]))]);
```

$$f(x) = \phi(x)^\intercal w \qquad \phi(x) = \begin{pmatrix}\cos(x) & \cos(2x) & \cos(3x) & \dots & \sin(x) & \sin(2x) & \dots\end{pmatrix}^\intercal$$



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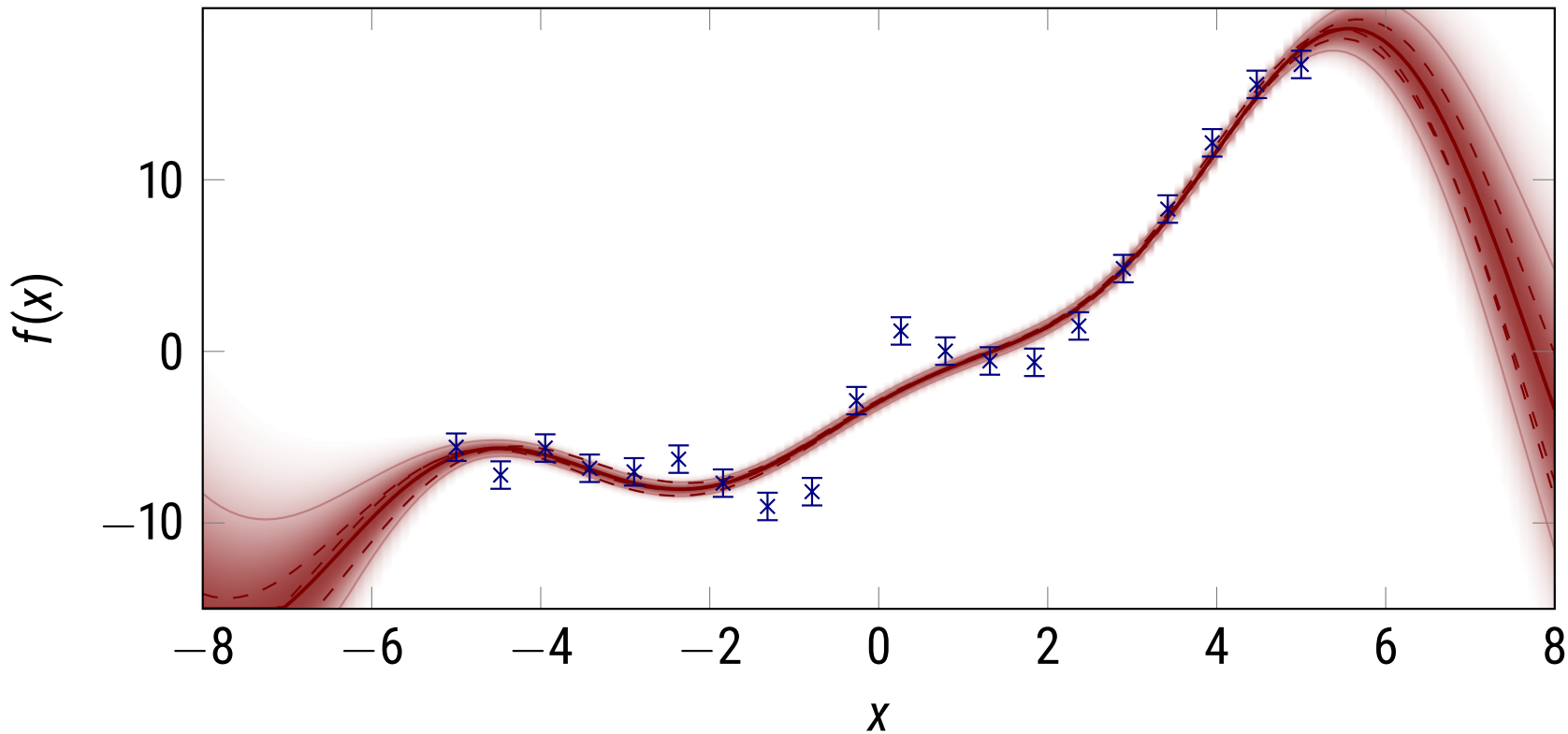
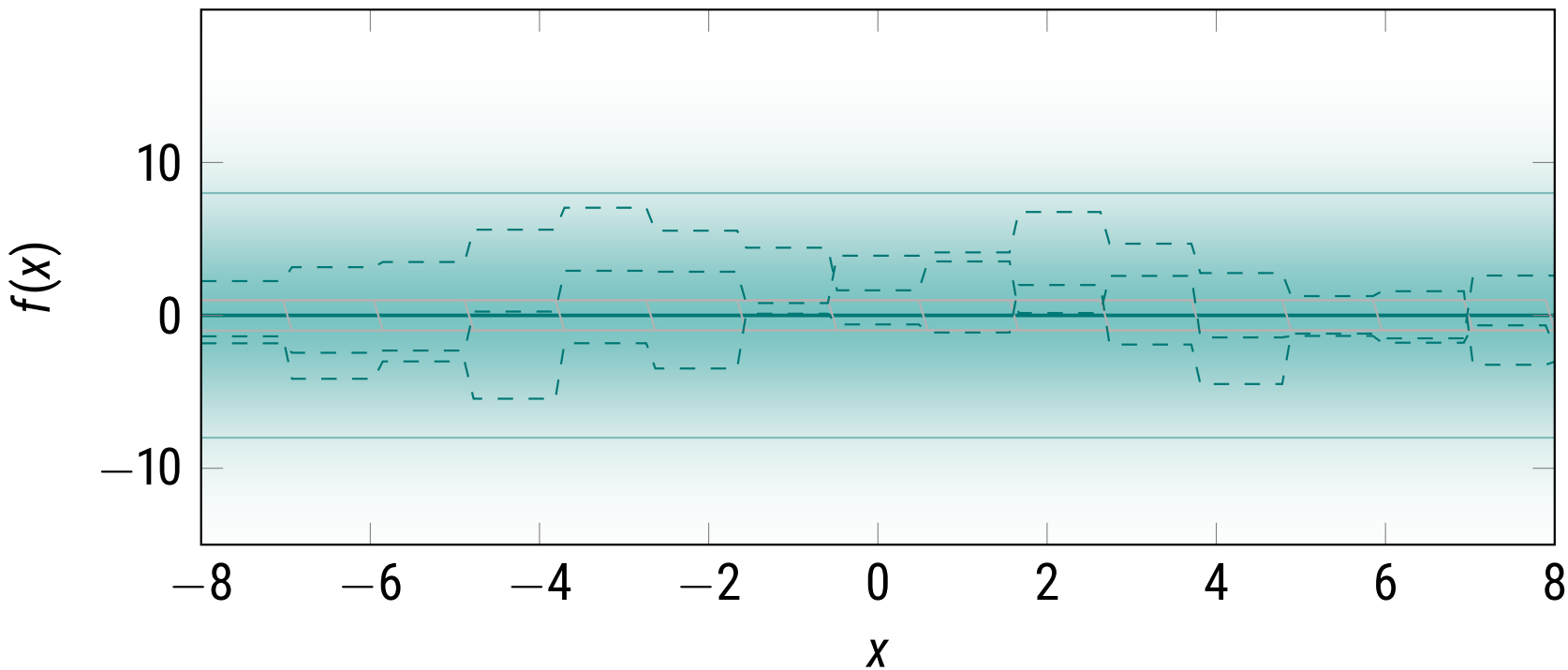


Step Regression

```
phi = @(a)(-1 + 2 * bsxfun(@lt,a,linspace(-8,8,16)));
```

$$\phi(x) = -1 + 2\left(\theta(x-8) \quad \theta(8-x) \quad \theta(x-7) \quad \theta(7-x) \quad \ldots\right)^{\mathsf{T}}$$



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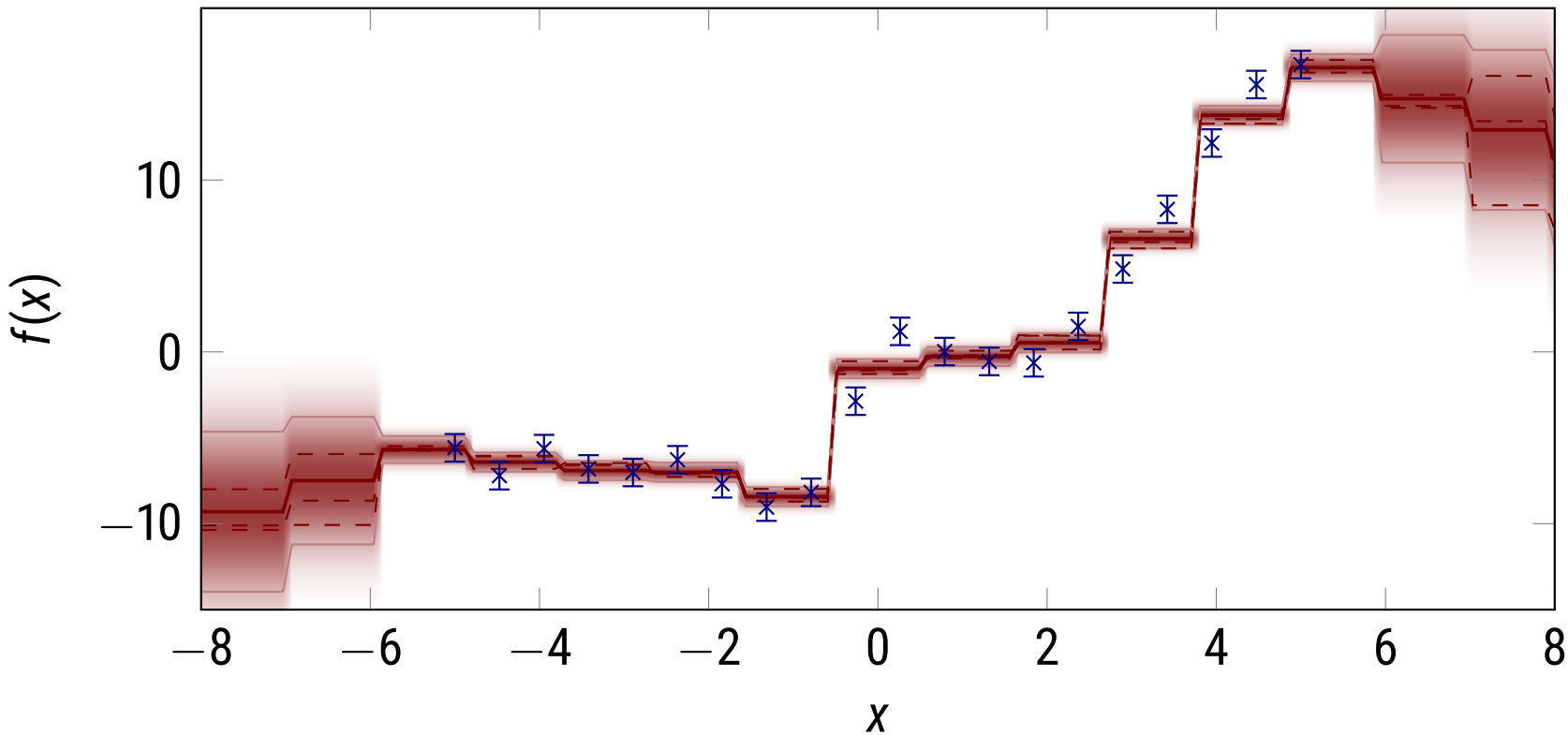
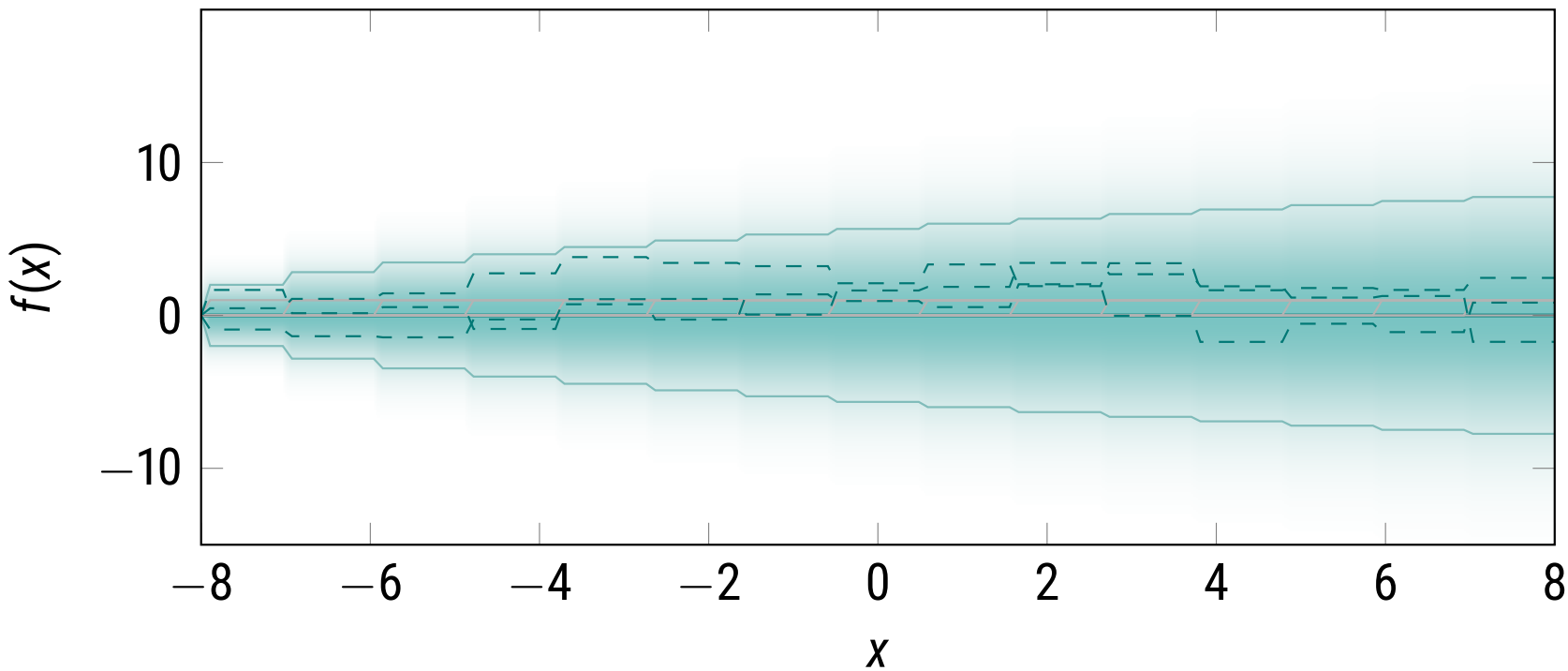


Another Kind of Step Regression

```
phi = @(a)(bsxfun(@gt,a,linspace(-8,8,16)));
```

$$\phi(x) = \begin{pmatrix} \theta(x-8) & \theta(8-x) & \theta(x-7) & \theta(7-x) & \dots \end{pmatrix}^{\mathsf{T}}$$



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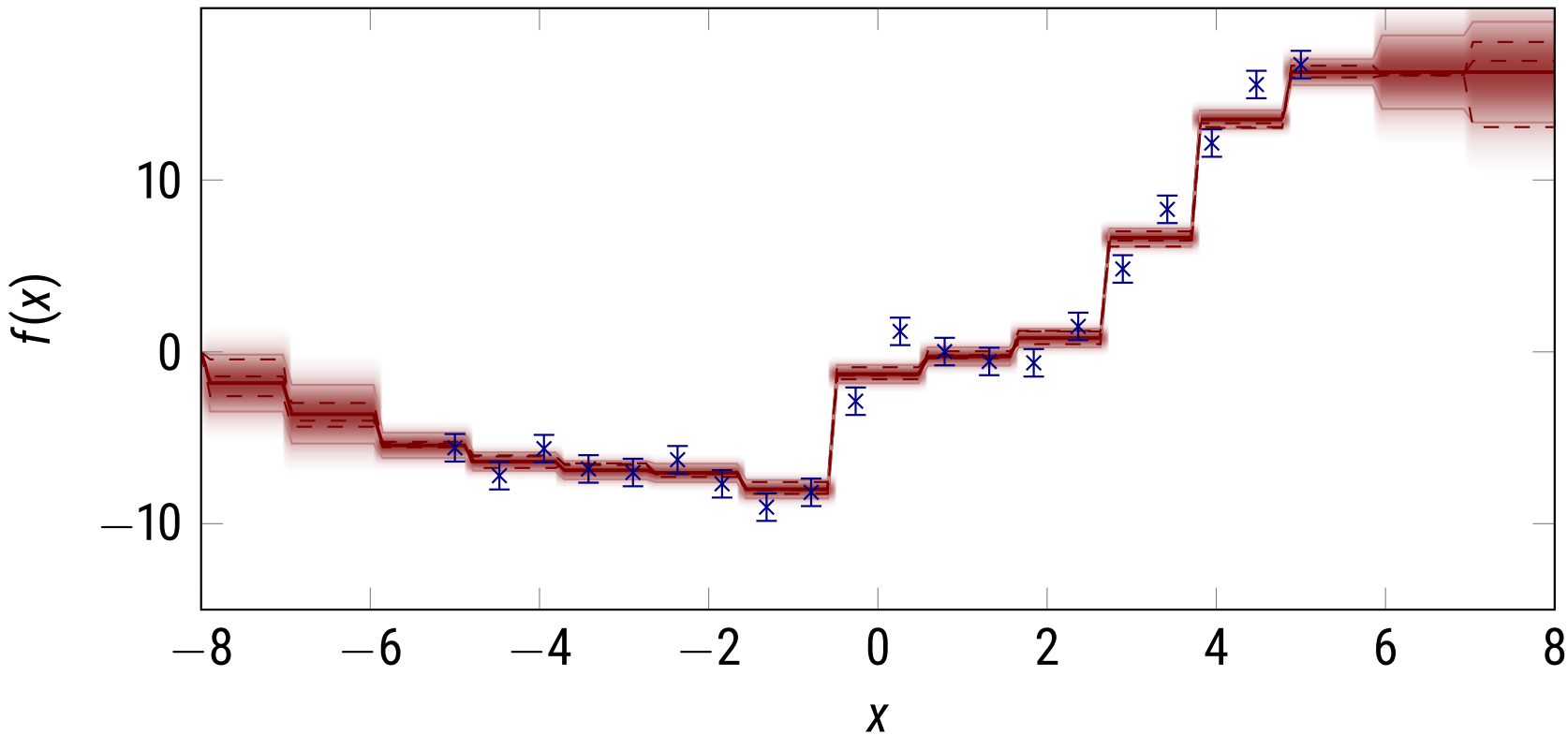
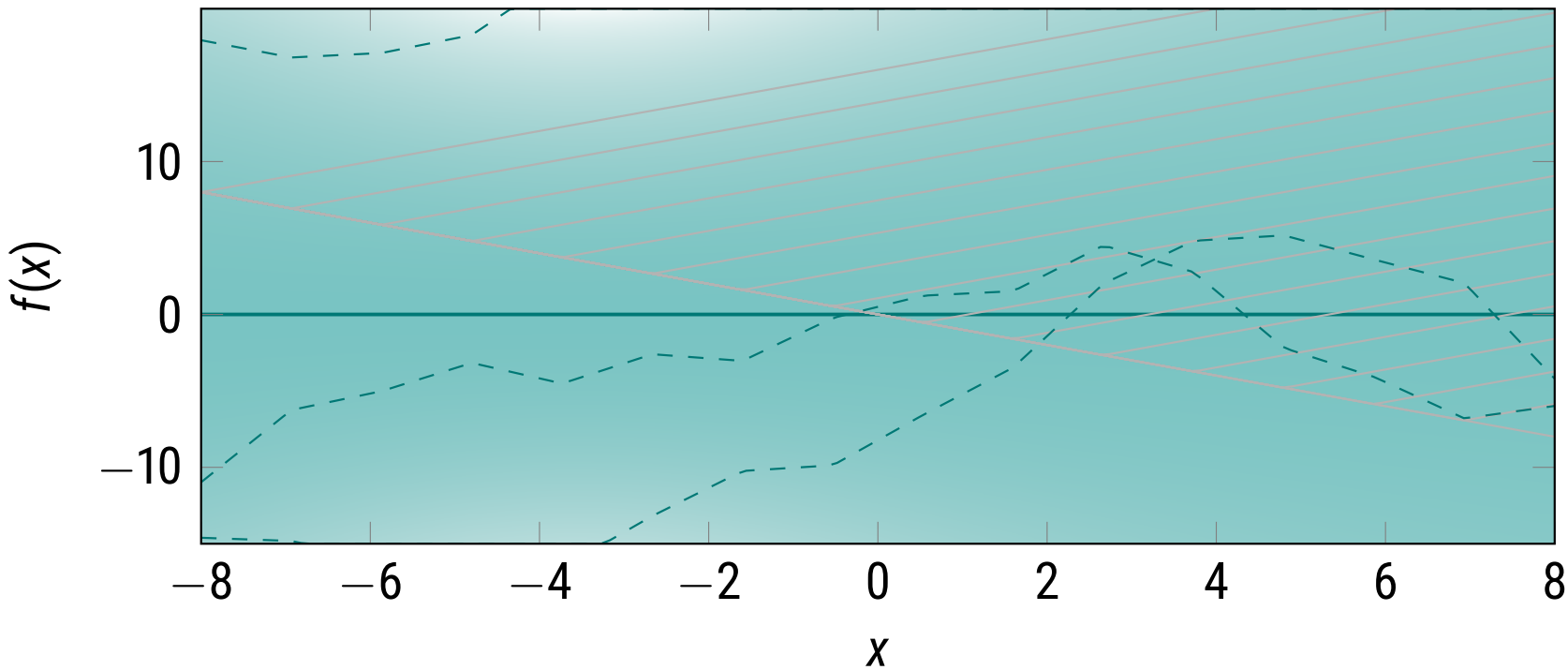


V Regression

```
phi = @(a)(bsxfun(@minus,abs(bsxfun(@minus,a,linspace(-8,8,16))),linspace(-8,8,16)));
```

$$\phi(x) = \begin{pmatrix} |x-8|-8 & |x-7|-7 & |x-6|-6 & \dots \end{pmatrix}^{\mathsf{T}}$$



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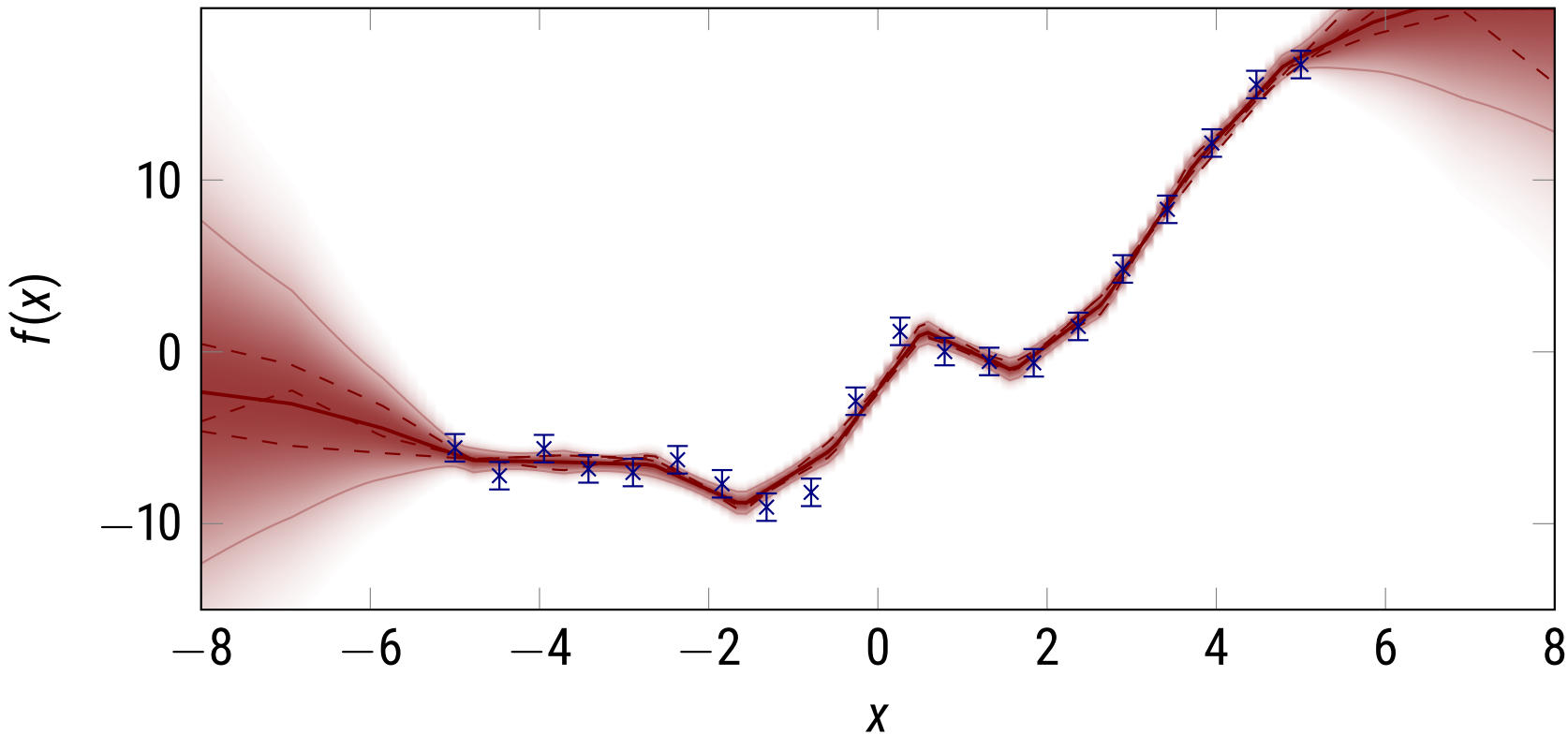
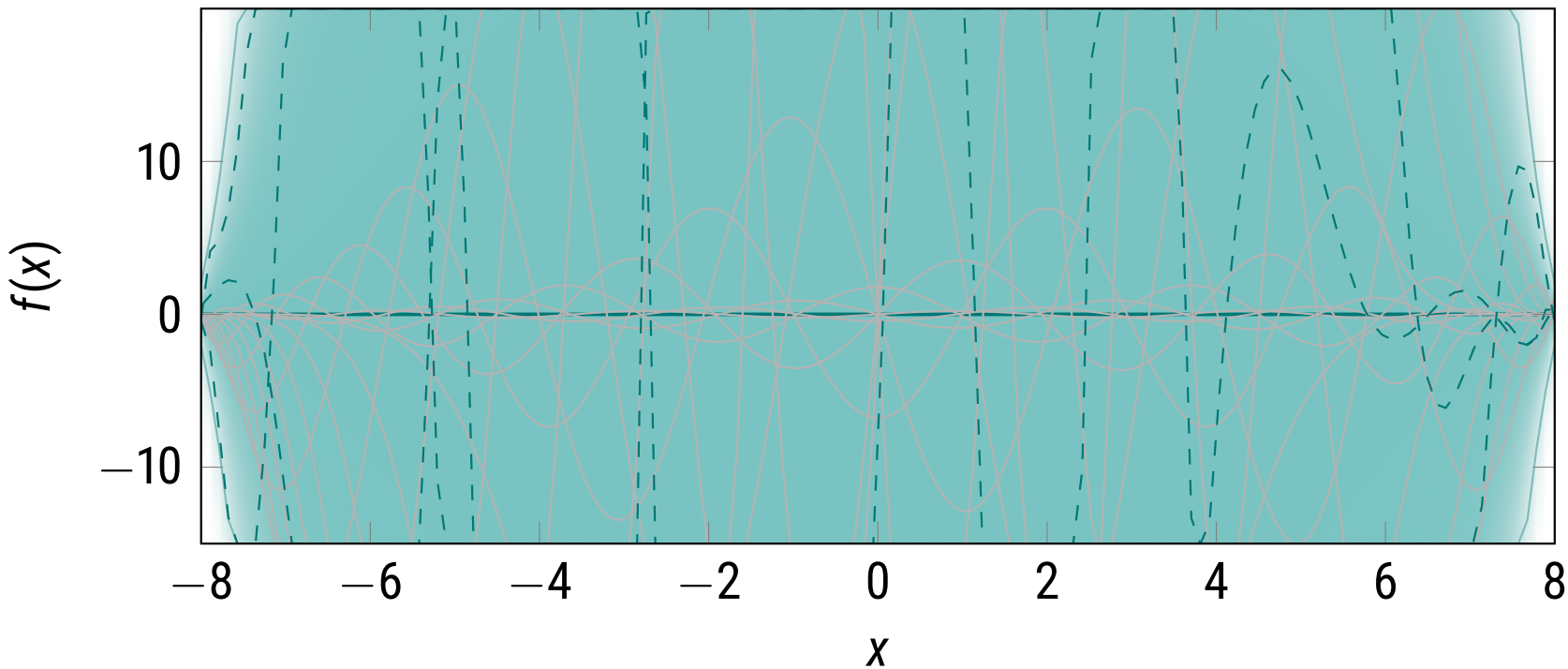


Legendre Regression

```
phi = @(a)(bsxfun(@times,legendre(13,a/8)',0.15.^[0:13]));
```

$$\phi(x) = \left(b^0 P_0(x), b^1 P_1(x), \ldots, b^{13} P_{13}(x)\right)^\mathsf{T} \qquad P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n}(x^2 - 1)^n$$



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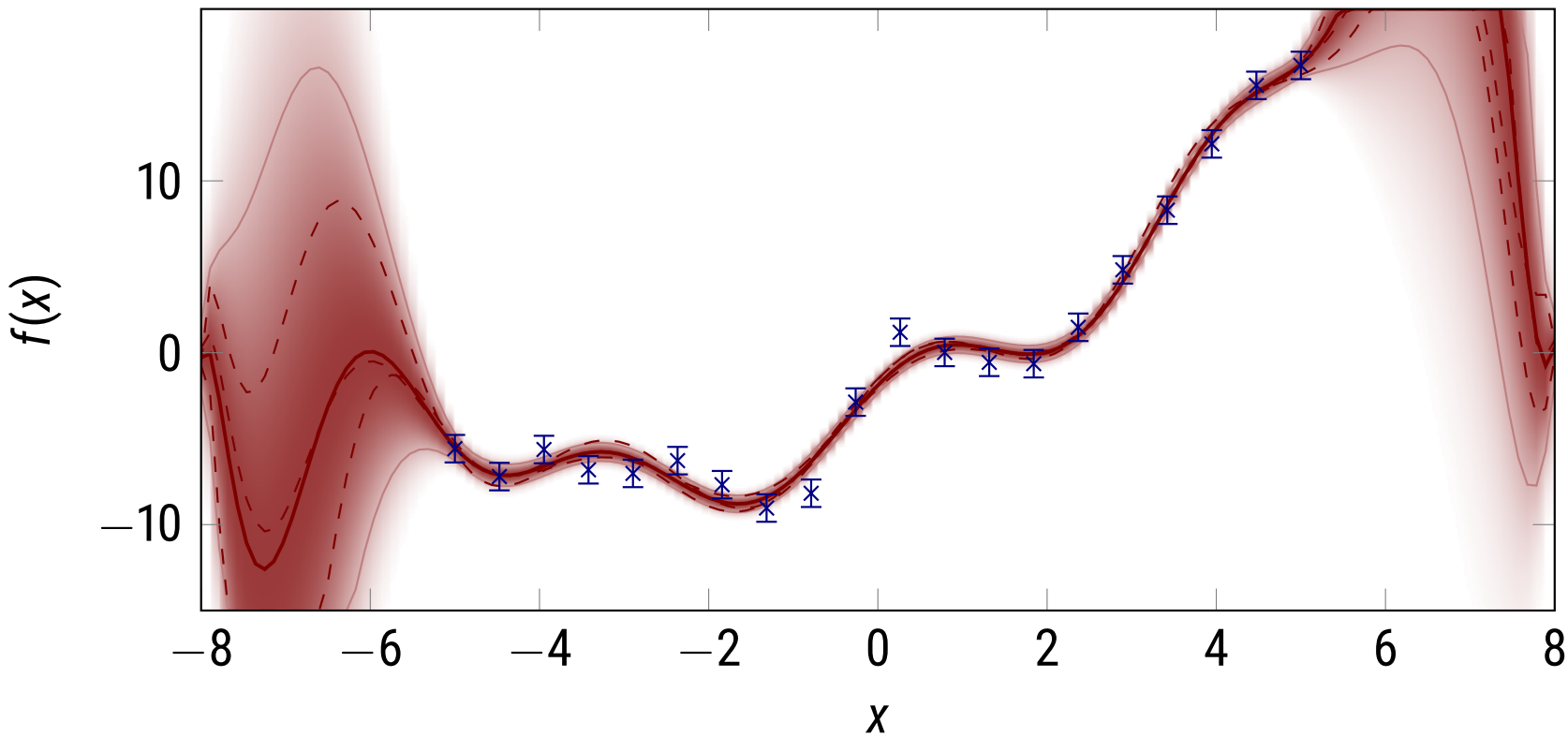
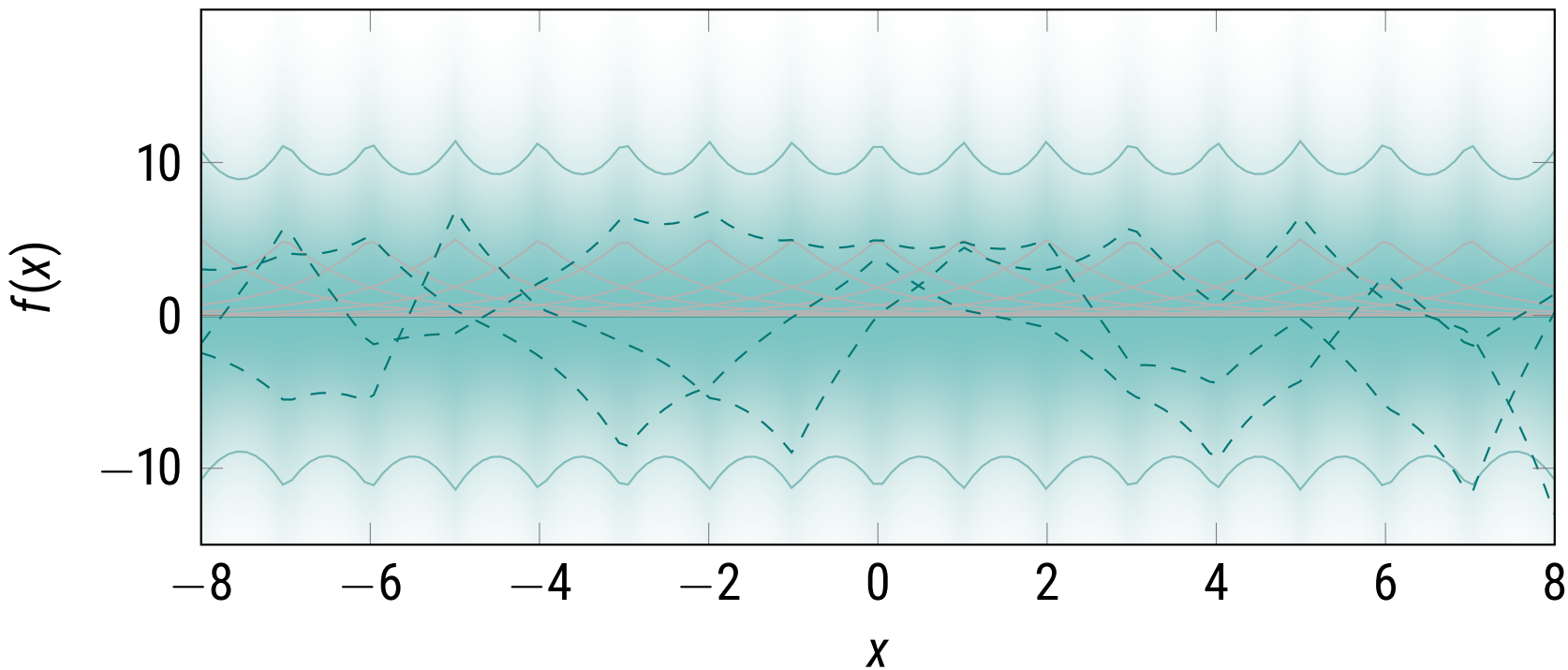


Eiffel Tower Regression

```
phi = @(a)(exp(-abs(bsxfun(@minus,a,[-8:1:8]))));
```

$$\phi(x) = \begin{pmatrix} e^{-|x-8|} & e^{-|x-7|} & e^{-|x-6|} & \dots \end{pmatrix}^{\mathsf{T}}$$



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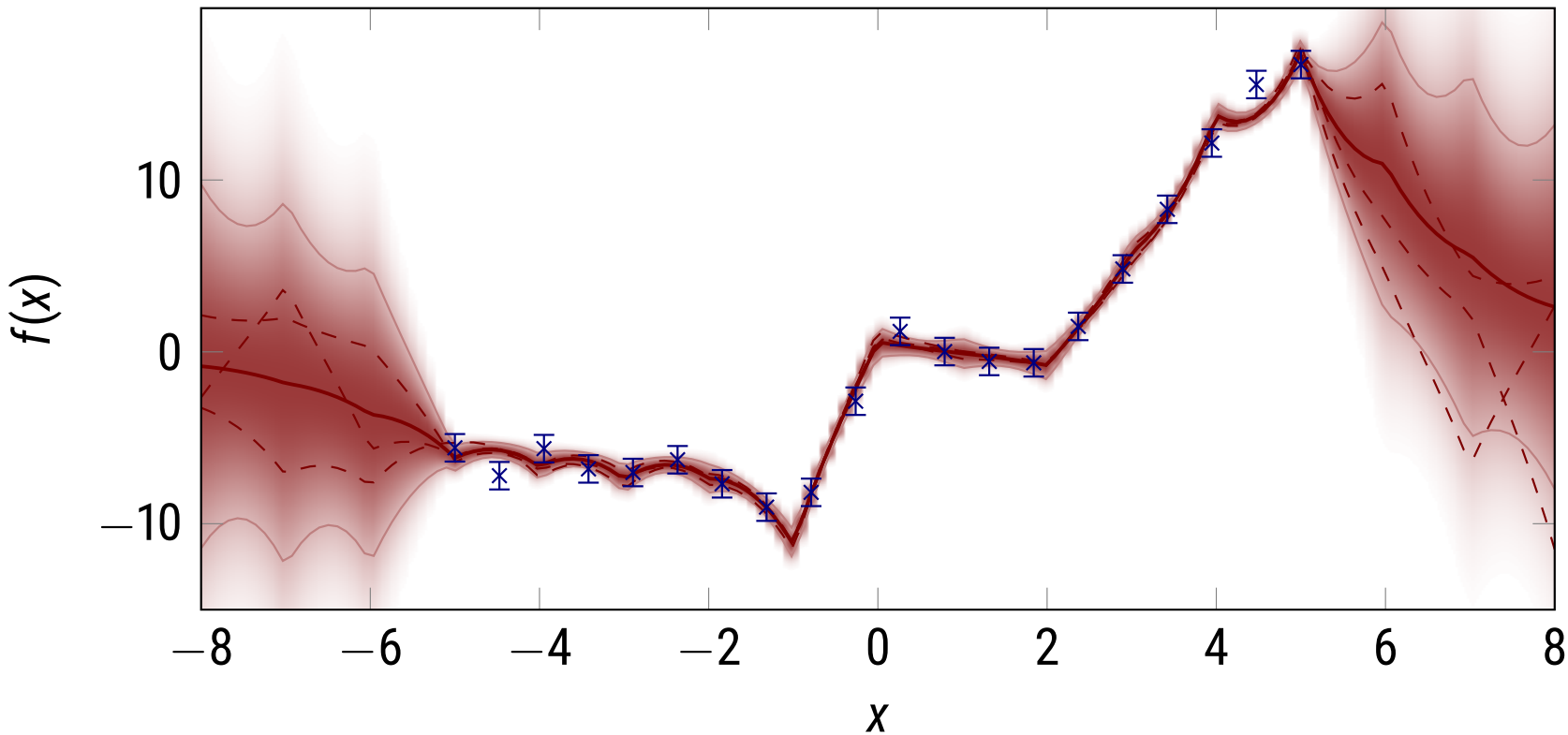
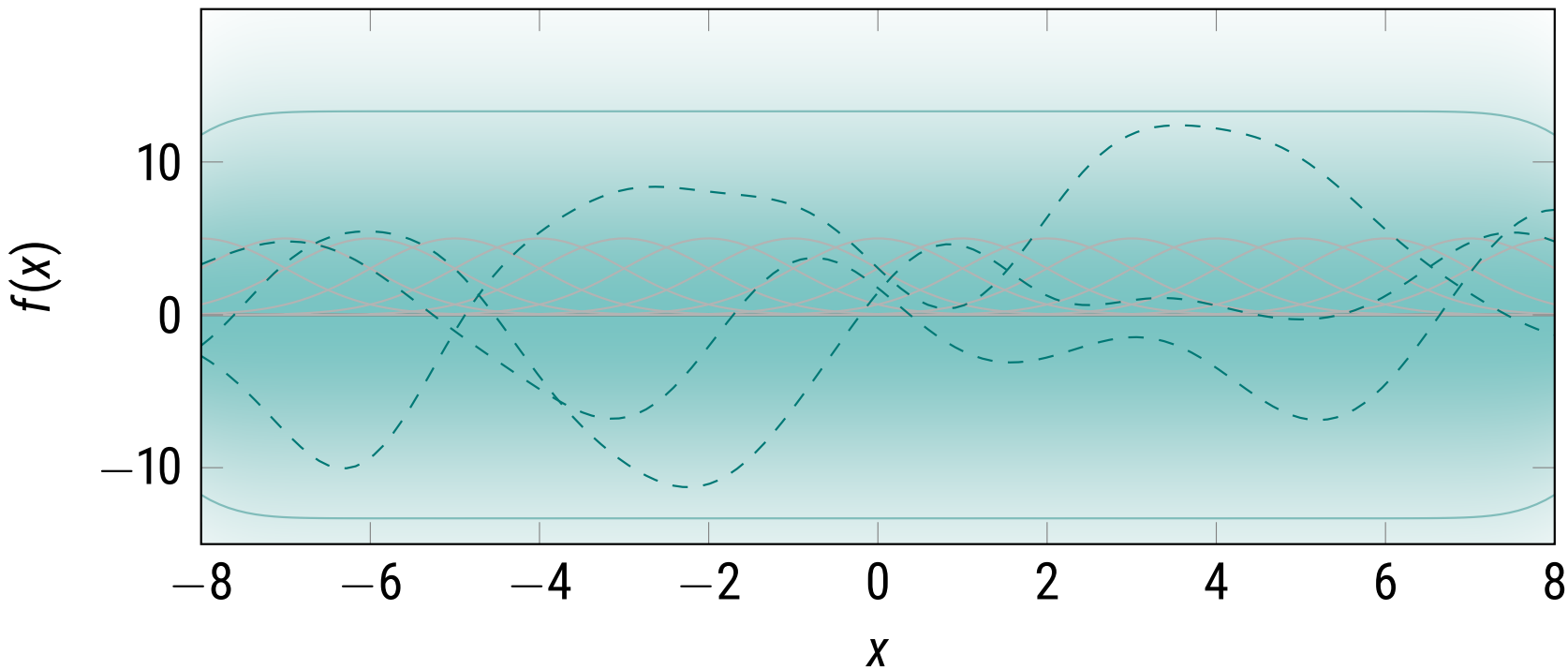


Bell Curve Regression

```
phi = @(a)(exp(-0.5 * bsxfun(@minus,a,[-8:1:8]).^2));
```

$$\phi(x) = \begin{pmatrix} e^{-\frac{1}{2}(x-8)^2} & e^{-\frac{1}{2}(x-7)^2} & e^{-\frac{1}{2}(x-6)^2} & \dots \end{pmatrix}^T$$



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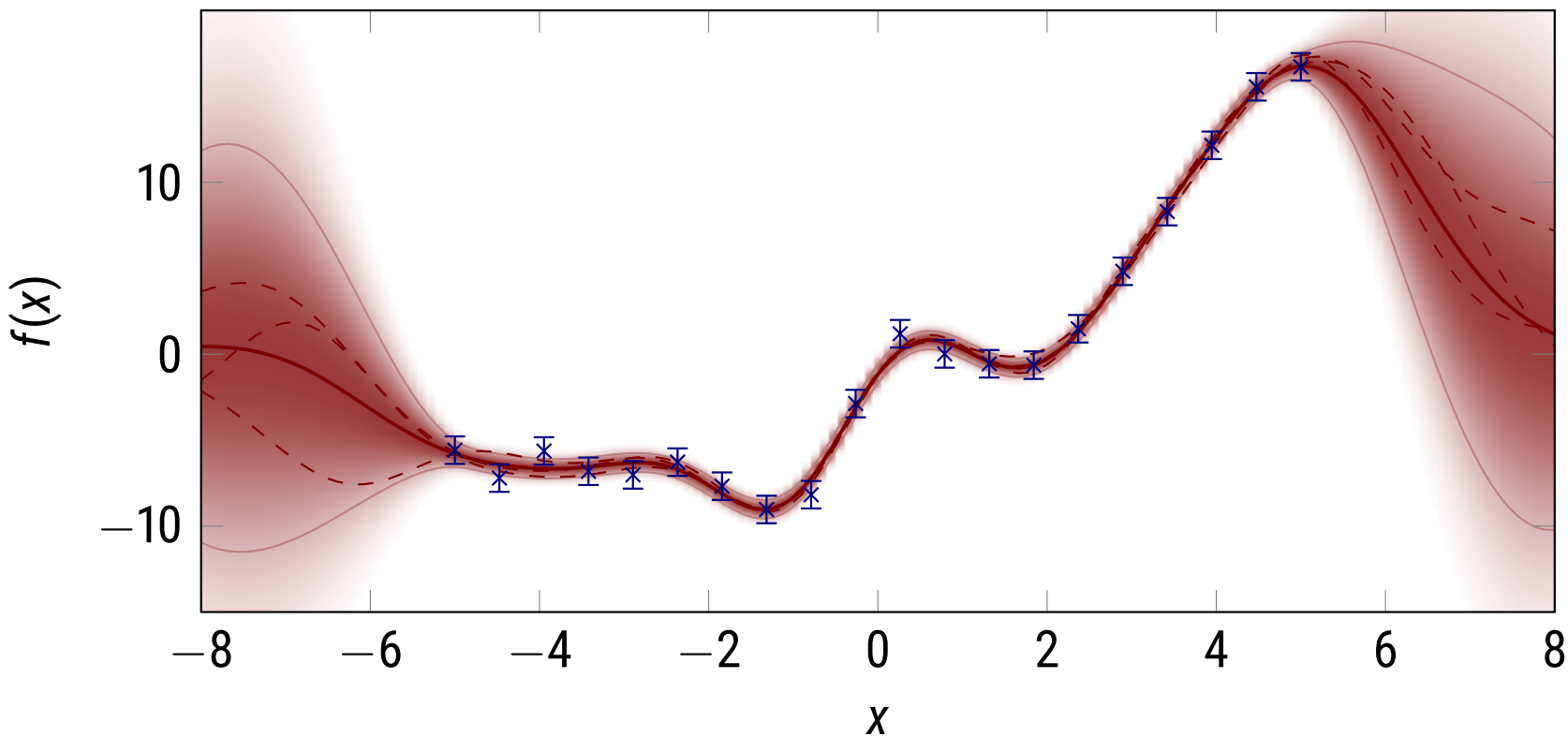
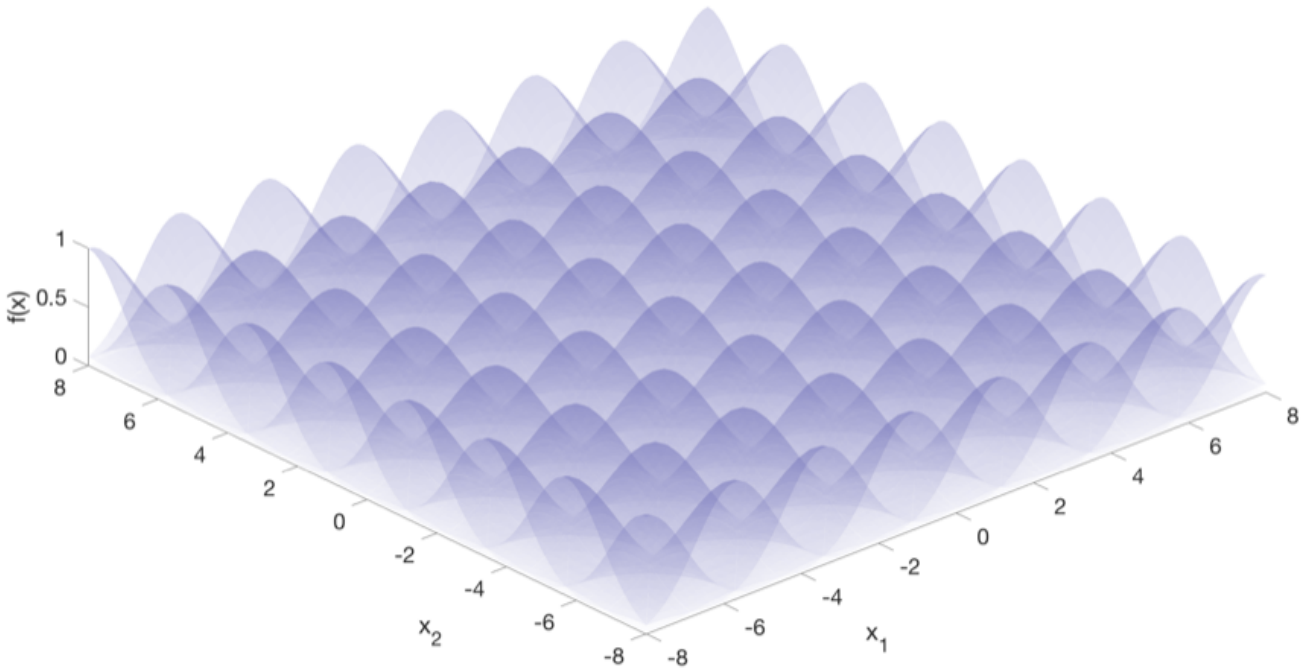


Multiple Inputs

all this works for in multiple dimensions, too

$$\phi : \mathbb{R}^N \to \mathbb{R} \qquad f : \mathbb{R}^N \to \mathbb{R}$$



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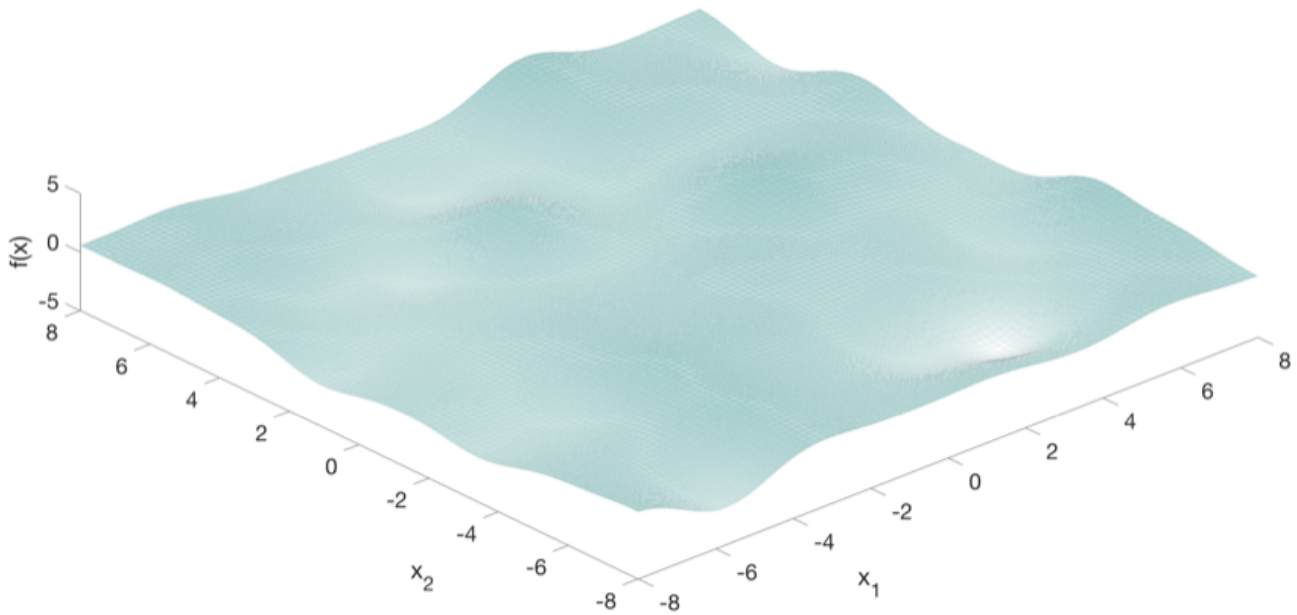
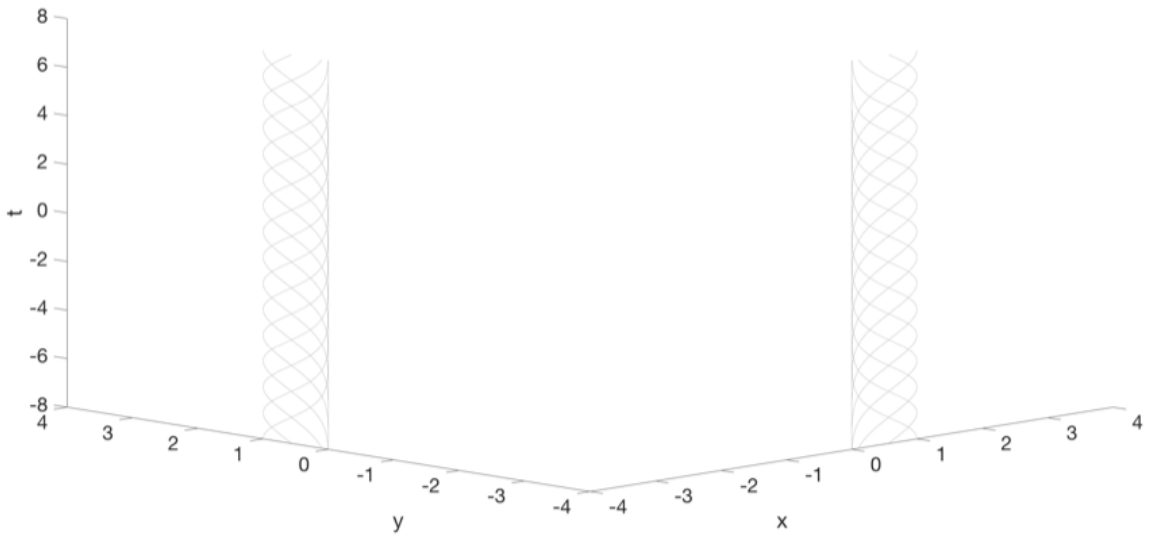


Multiple Outputs

slightly more confusing, but no algebraic problem

$$\phi : \mathbb{R} \to \mathbb{R}^M \qquad f : \mathbb{R} \to \mathbb{R}^M \qquad \text{cov}(f_i(t), f_j(t)) = \sum_{\ell} \phi_{\ell,i}(t)\phi_{\ell,j}(t')$$

- $[f_1(t_1), \ldots, f_1(t_N), f_2(t_1), \ldots, f_2(t_N), \ldots, f_M(t_1), \ldots f_M(t_N)]$ are just some co-varying Gaussian variables
- requires careful matrix algebra



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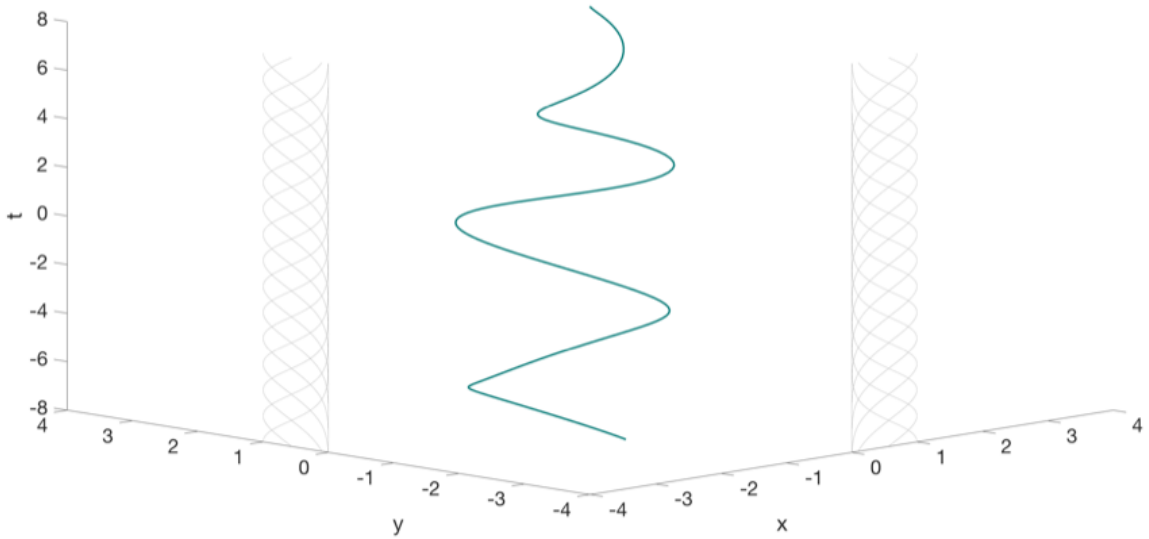

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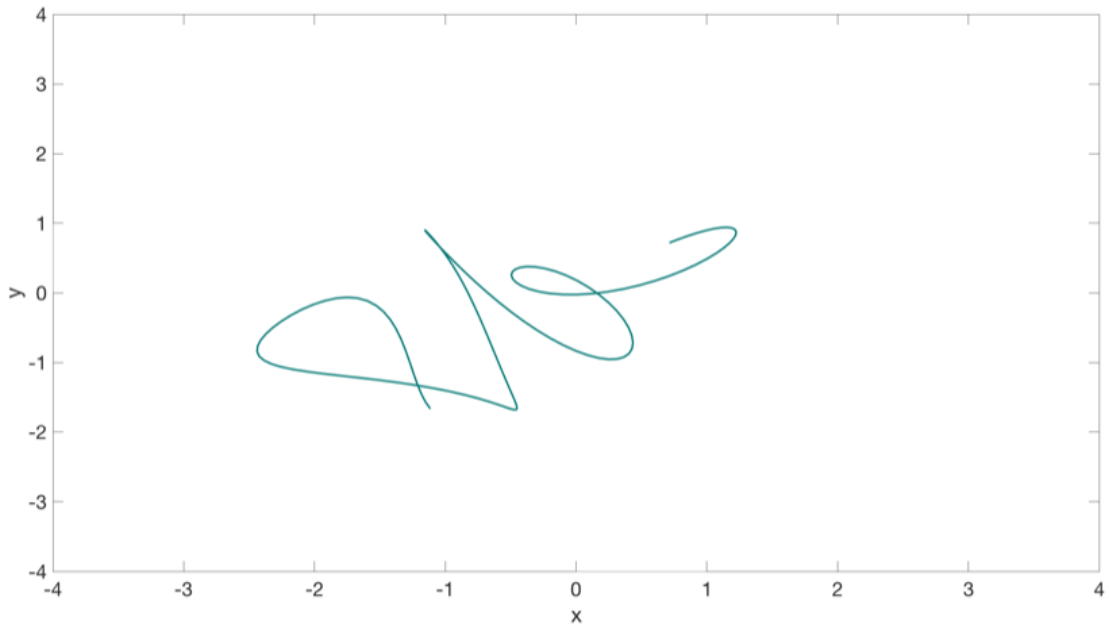


- Gaussian measures turn probabilistic inference into **linear algebra**
- Gaussian measures can be used to infer **functions** and **curves**

Next up:

- In fact, the number of inferred features / weights can be **infinite**!

How many features should we use?

let's look at that algebra again

$$p(f_x \mid y, \phi_X) = \mathcal{N}(f_x; \phi_x^\intercal \mu + \phi_x^\intercal \Sigma \phi_X (\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1}(y - \phi_X^\intercal \mu),$$
$$\phi_x^\intercal \Sigma \phi_x - \phi_x^\intercal \Sigma \phi_X (\phi_X^\intercal \Sigma \phi_X + \sigma^2 I)^{-1} \phi_X^\intercal \Sigma \phi_x)$$

- no lonely ϕ. Instead:
  - $\phi^\intercal \mu$ – the mean function
  - $\phi^\intercal \Sigma \phi$ – the kernel
- given these, cost independent of features
- remember the code:

```
mx     = dot(phi(x),mu)
kxx    = dot(dot(phi(x),Sigma),phi(x).transpose())
mX     = dot(phi(X),mu)
kXX    = dot(dot(phi(X),Sigma),phi(X).transpose())
kxX    = dot(dot(phi(x),Sigma),phi(X).transpose())
```

Code using Kernels and mean functions

python

```
#                          ==== NONPARAMETRIC GAUSSIAN REGRESSION IN PYTHON ====
# assume external definition of kernel k and mean function m
# prior on f_x
n      = 100
x      = reshape(linspace(-8,8,n),(n,1))     # reshape is needed for phi to work
mx     = m(x)
kxx    = k(x,x)                                                  # p(f_x)=N(m,k_xx)
s      = dot(cholesky(kxx + 1e-6 * eye(n)),randn(n,3)) + mx      # prior samples
stdpi  = reshape(sqrt(diag(kxx)),[n,1])          # marginal stddev, for plotting

# loading data from disk
import scipy.io; data = scipy.io.loadmat('data.mat')
X = data['X']; Y = data['Y']; sigma = data['sigma']; N  = len(X)

# prior on Y = f_X + eps
mX     = m(X)
kXX    = k(X,X)                                             # p(f_X) = N(mX,k_XX)

# inference
G      = cho_factor(kXX + sigma**2 * eye(N))       # Most expensive step, O(N^3)
kxX    = k(x,X)                                             # Cov(f_x,f_X) = k_xX
A      = cho_solve(G,kxX.transpose()).transpose()       # pre-compute for re-use

# posterior p(f_x|Y)
mpost  = mx + dot(A,(Y-mX))                                          # mean
vpost  = kxx - dot(A,kxX.transpose())                              # covariance
spost  = dot(cholesky(vpost + 1e-8 * eye(n)),randn(n,3)) + mpost       # samples
stdpo  = reshape(sqrt(diag(vpost)),[n,1])        # marginal stddev, for
```

Code using Kernels and mean functions

matlab

```
%                          ==== NONPARAMETRIC GAUSSIAN REGRESSION IN MATLAB ====
% assume external definition of kernel k and mean function m
% prior on f_x
n      = 100;
x      = linspace(-8,8,n)';                                        % `test' points
mx     = m(x);
kxx    = k(x,x);                                                % p(f_x)=N(mx,k_xx)
s      = bsxfun(@plus,mx,chol(kxx + 1.0e-8 * eye(n))' * randn(n,3));   % samples
stdpi  = sqrt(diag(kxx));                              % marginal stddev, for plotting

% loading data from disk
load('data.mat'); N = length(Y);                                  % gives Y,X,sigma

% prior on Y=f_X + epsilon
mX     = m(X);
kXX    = k(X,X);                                              % p(f_X) = N(mX,k_XX)

% inference
G      = chol(kXX + sigma^ 2 * eye(N);)              % most expensive step: O(N^3)
kxX    = k(x,X);                                             % Cov(f_x,f_X) = k_xX
A      = kxX / G;                                          % pre-compute for re-use

% posterioe p (f_x|Y)
mpost  = mx + A * (G' \ (Y-mX));                                          % mean
vpost  = kxx - A * A';                                                % covariance
spost  = bsxfun(@plus,mpost,chol(vpost + 1.0e-8 * eye(n))' * randn(n,3)) % smpls
stdpo  = sqrt(diag(vpost));                            % marginal stddev, for plotting
```

Features are cheap, so let's use a lot

an example

[DJC MacKay, 1998]

- For simplicity, let's fix $\Sigma = \frac{\sigma^2(c_{\max} - c_{\min})}{F} I$

$$\text{thus:} \quad \phi(x_i)^\intercal \Sigma \phi(x_j) = \frac{\sigma^2(c_{\max} - c_{\min})}{F} \sum_{\ell=1}^{F} \phi_\ell(x_i)\phi_\ell(x_j)$$

- especially, for $\phi_\ell(x) = \exp\left(-\frac{(x - c_\ell)^2}{2\lambda^2}\right)$

$$\phi(x_i)^\intercal \Sigma \phi(x_j)$$

$$= \frac{\sigma^2(c_{\max} - c_{\min})}{F} \sum_{\ell=1}^{F} \exp\left(-\frac{(x_i - c_\ell)^2}{2\lambda^2}\right) \exp\left(-\frac{(x_j - c_\ell)^2}{2\lambda^2}\right)$$

$$= \frac{\sigma^2(c_{\max} - c_{\min})}{F} \exp\left(-\frac{(x_i - x_j)^2}{4\lambda^2}\right) \sum_{\ell}^{F} \exp\left(-\frac{(c_\ell - \frac{1}{2}(x_i + x_j))^2}{\lambda^2}\right)$$

Features are cheap, so let's use a lot

an example

[DJC MacKay, 1998]

$$\phi(x_i)^\intercal \Sigma \phi(x_j) =$$

$$\frac{\sigma^2(c_{\max} - c_{\min})}{F} \exp\left(-\frac{(x_i - x_j)^2}{4\lambda^2}\right) \sum_{\ell}^{F} \exp\left(-\frac{(c_\ell - \frac{1}{2}(x_i + x_j))^2}{\lambda^2}\right)$$

- now increase F so # of features in δc approaches $\frac{F \cdot \delta c}{(c_{\max} - c_{\min})}$

$$\phi(x_i)^\intercal \Sigma \phi(x_j) \to$$

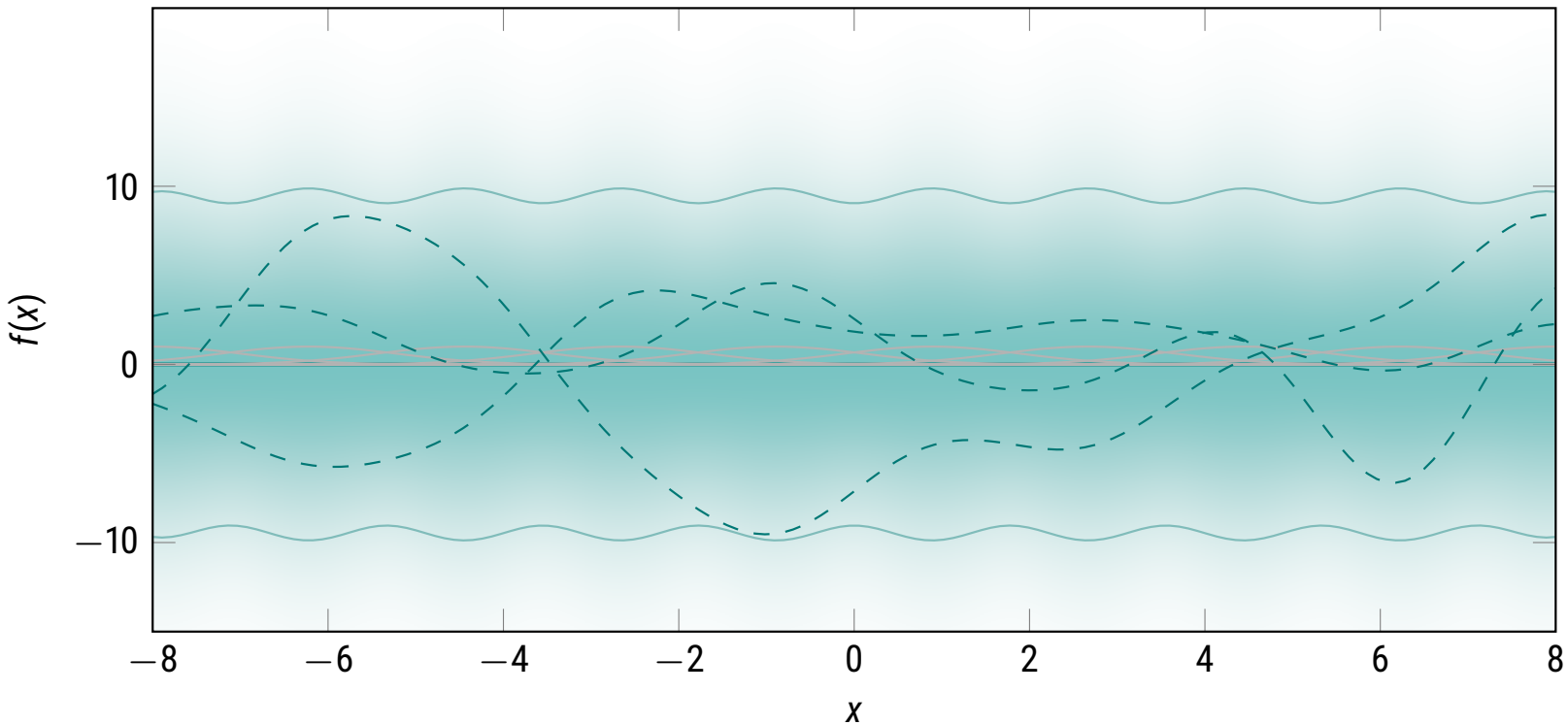
$$\sigma^2 \exp\left(-\frac{(x_i - x_j)^2}{4\lambda^2}\right) \int_{c_{\min}}^{c_{\max}} \exp\left(-\frac{(c - \frac{1}{2}(x_i + x_j))^2}{\lambda^2}\right) dc$$

- let $c_{\min} \to -\infty$, $c_{\max} \to \infty$

$$k(x_i, x_j) := \phi(x_i)^\intercal \Sigma \phi(x_j) \to \sqrt{2\pi}\lambda\sigma^2 \exp\left(-\frac{(x_i - x_j)^2}{4\lambda^2}\right)$$

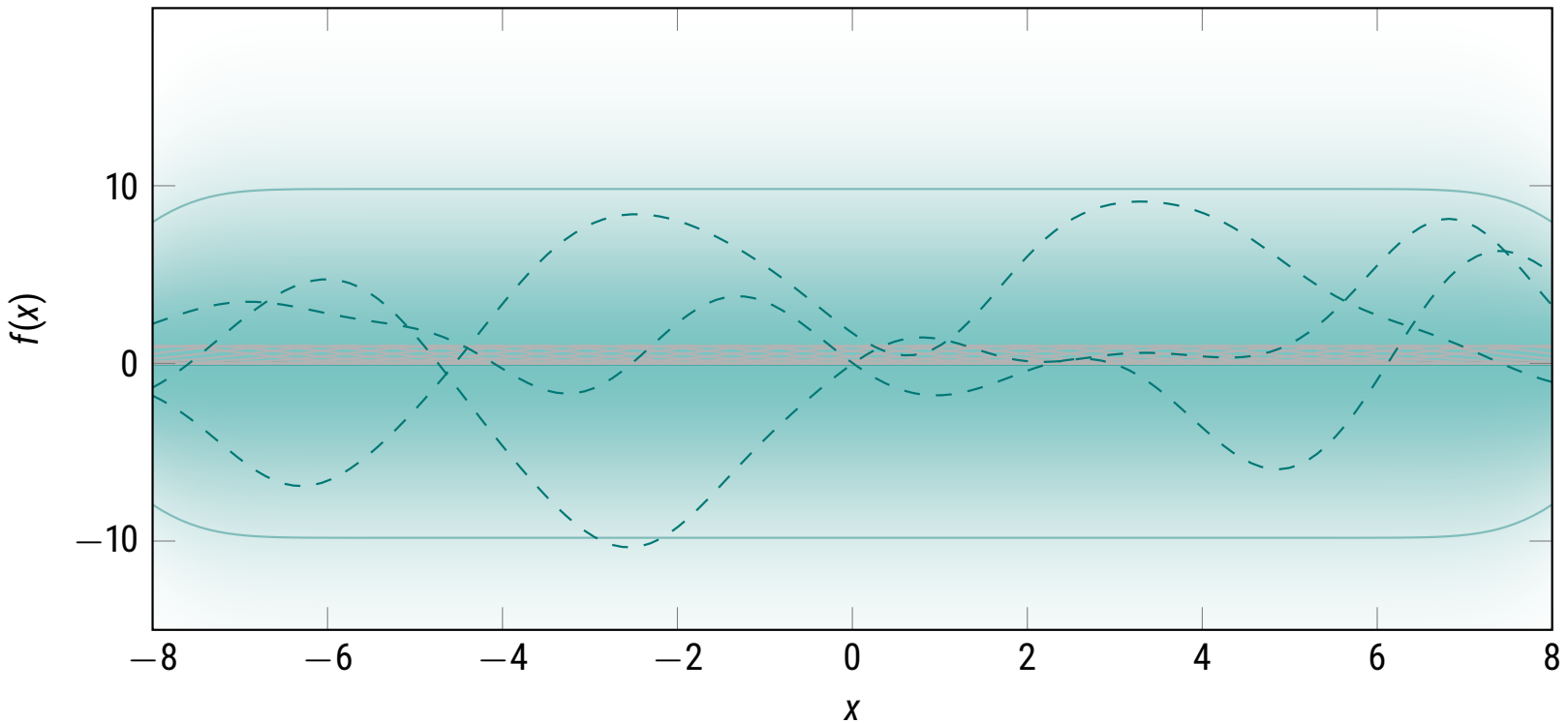
Exponentiated Squares

```
phi = @(a)(exp(-0.5 * bsxfun(@minus,a,linspace(-8,8,10))).^2 ./ell.^2));
```



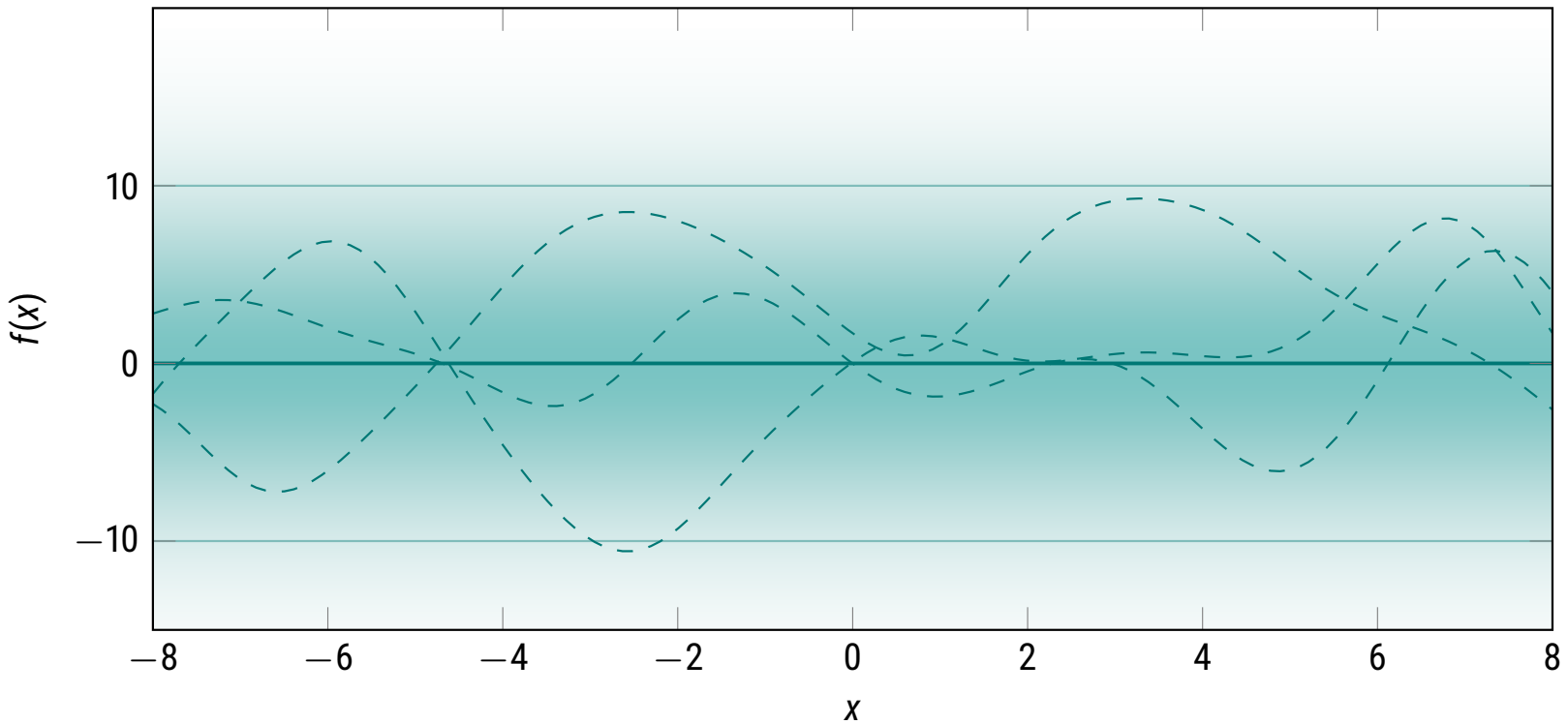
Exponentiated Squares

```
phi = @(a)(exp(-0.5 * bsxfun(@minus,a,linspace(-8,8,30))).^2 ./ell.^2));
```



Exponentiated Squares

```
k = @(a,b)(5*exp(-0.25*bsxfun(@minus,a,b').^2));
```



- aka. radial basis function, square(d)-exponential kernel

Exponentiated Squares

```
k = @(a,b)(5*exp(-0.25*bsxfun(@minus,a,b').^2));
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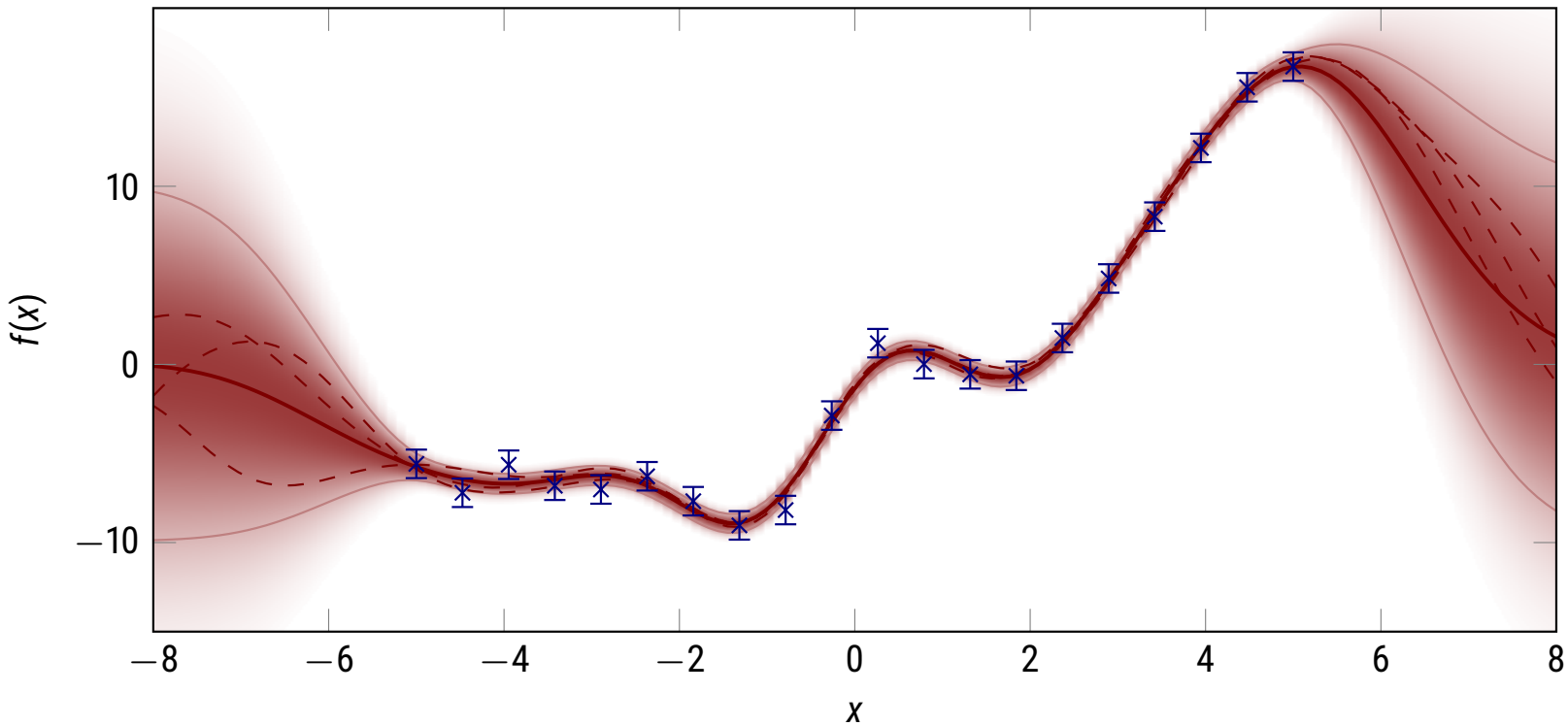


- aka. radial basis function, square(d)-exponential kernel

What just happened?

kernelization and Gaussian processes

$k : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ is a **Mercer kernel** if, for any finite collection $X = [x_1, \dots, x_N]$, the matrix $k_{XX} \in \mathbb{R}^{N \times N}$ with $[k_{XX}]_{ij} = k(x_i, x_j)$ is **positive semidefinite**.

Lemma:

k is a Mercer kernel if it can be written as (assuming $\mathcal{L}$ is positive set for ν)

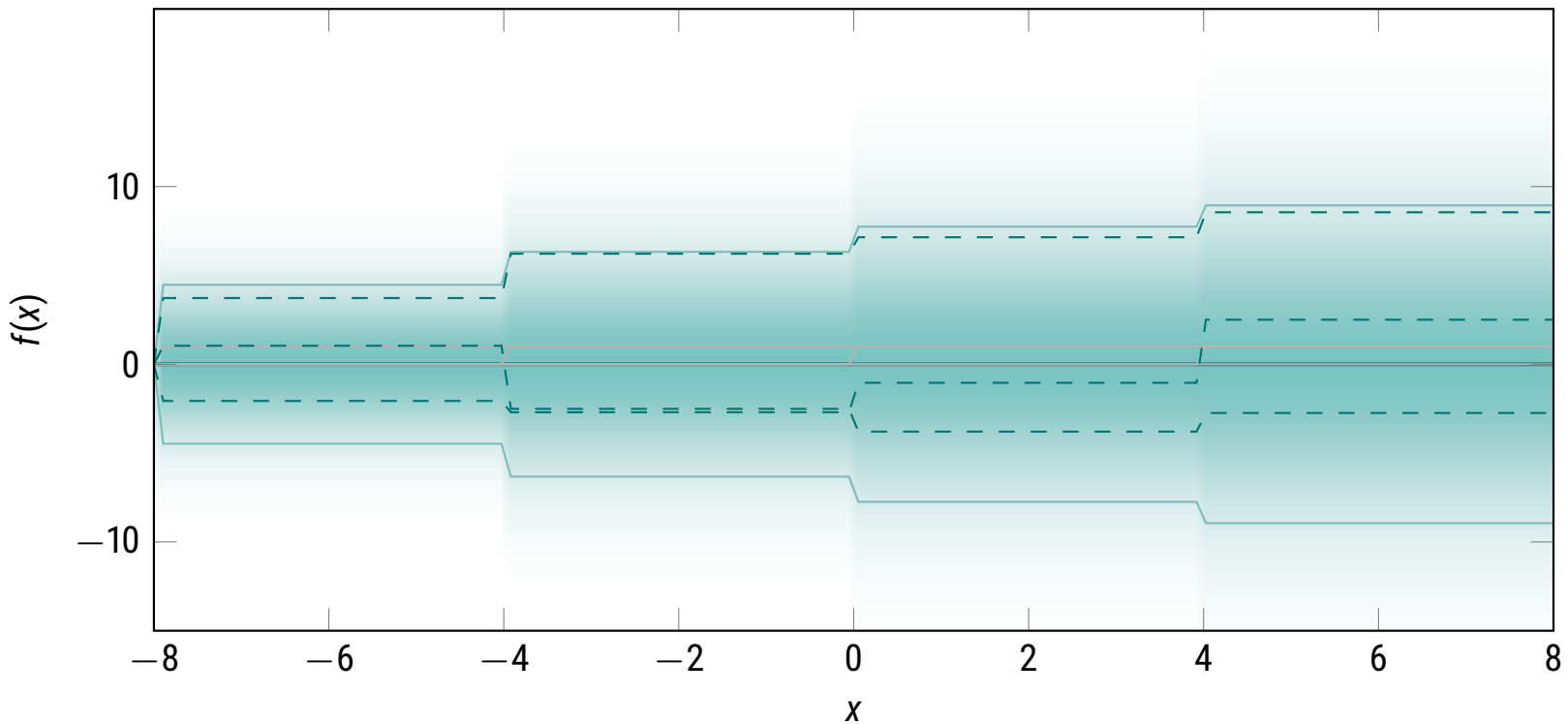
$$k(x, x') = \sum_{\ell \in \mathcal{L}} \phi_\ell(x)\phi_\ell(x') \quad \text{or} \quad = \int_{\mathcal{L}} \phi_\ell(x)\phi_\ell(x')\, d\nu(\ell)$$

Proof: $\forall X \in \mathbb{X}^N, v \in \mathbb{R}^N : v^\intercal k_{XX} v = \int \sum_i^N v_i \phi_\ell(x_i) \sum_j^N v_j \phi_\ell(x_j)\, d\nu(\ell) = \int \left[\sum_i v_i \phi_\ell(x_i)\right]^2 d\nu(\ell) \geq 0$ □

Let $\mu : \mathbb{X} \to \mathbb{R}$ be any function, $k : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ be a Mercer kernel.
A **Gaussian process** $p(f) = \mathcal{GP}(f; \mu, k)$ is a probability distribution over the function $f : \mathbb{X} \to \mathbb{R}$, such that every finite restriction to function values $f_X := [f_{x_1}, \dots, f_{x_N}]$ is a Gaussian distribution $p(f_X) = \mathcal{N}(f_X; \mu_X, k_{XX})$.

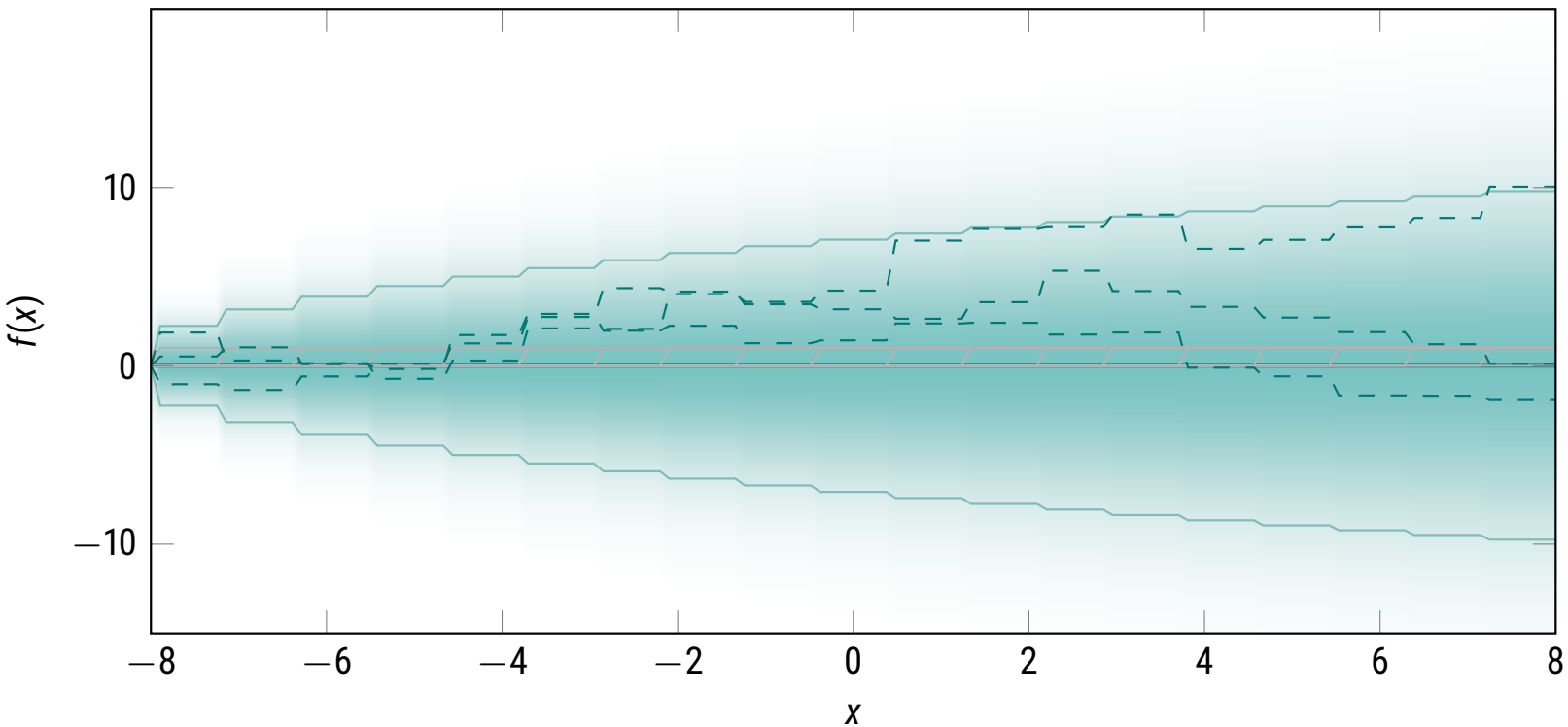
Those Step Functions

```
phi = @(a)(bsxfun(@gt,a,linspace(-8,8,5))./sqrt(5));
```



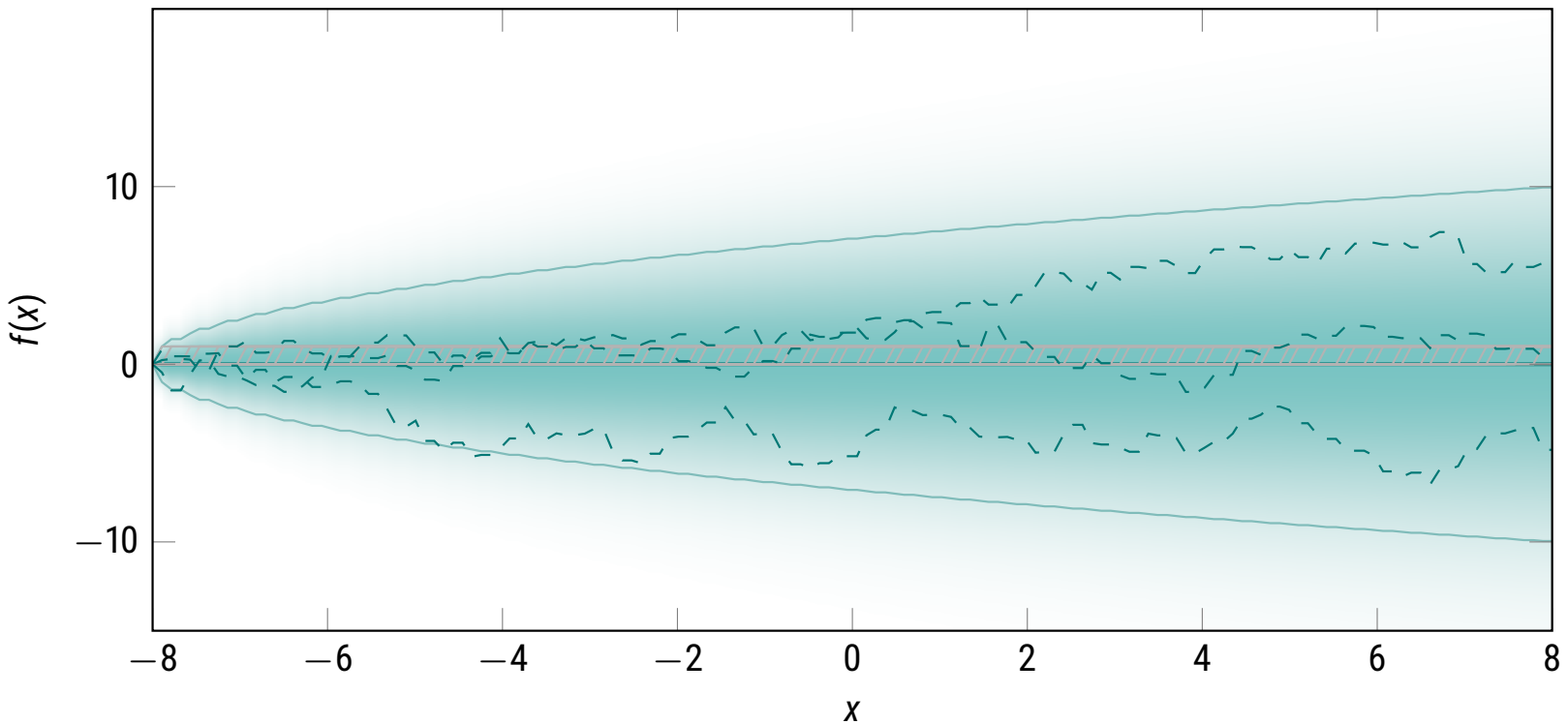
Those Step Functions

```
phi = @(a)(bsxfun(@gt,a,linspace(-8,8,20))./sqrt(20));
```



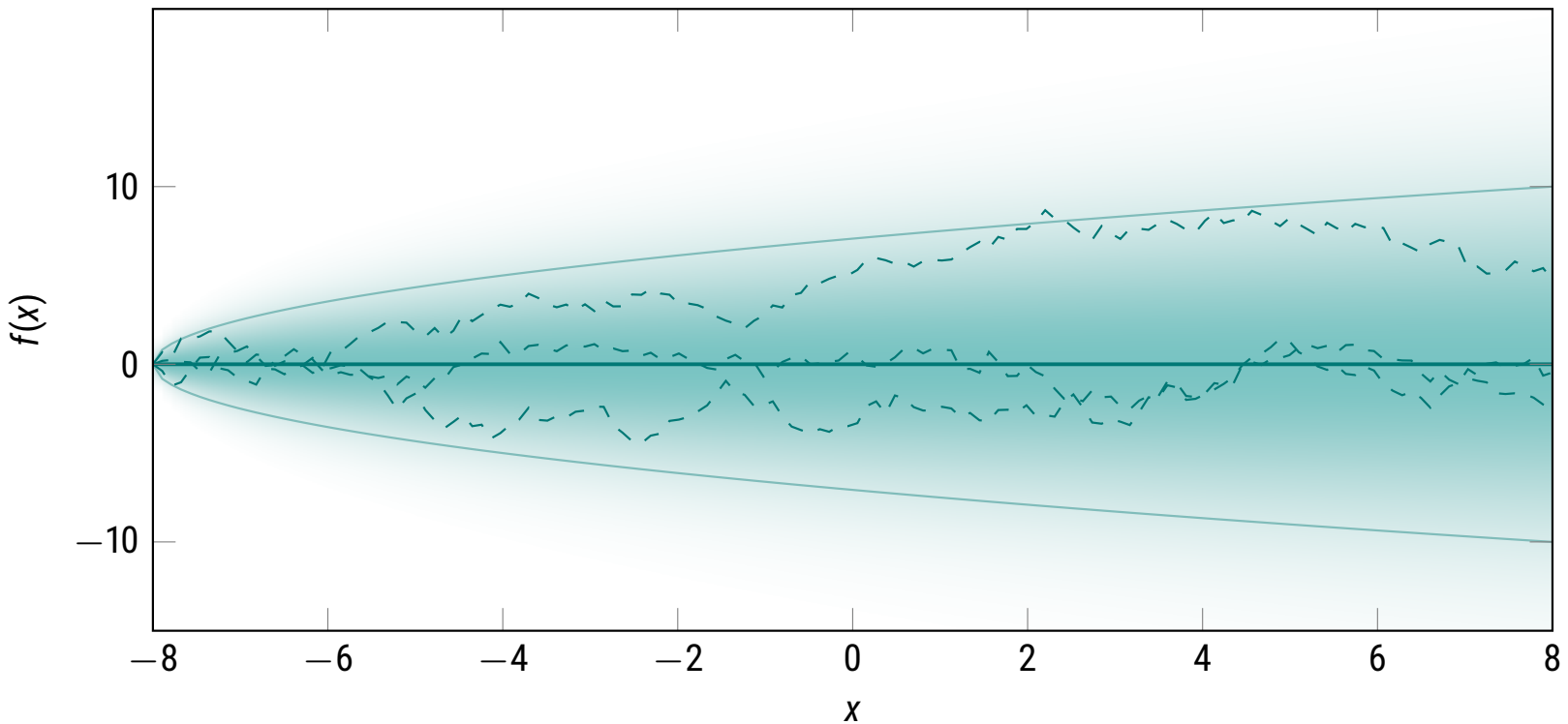
Those Step Functions

```
phi = @(a)(bsxfun(@gt,a,linspace(-8,8,100))./sqrt(100));
```



Those Step Functions

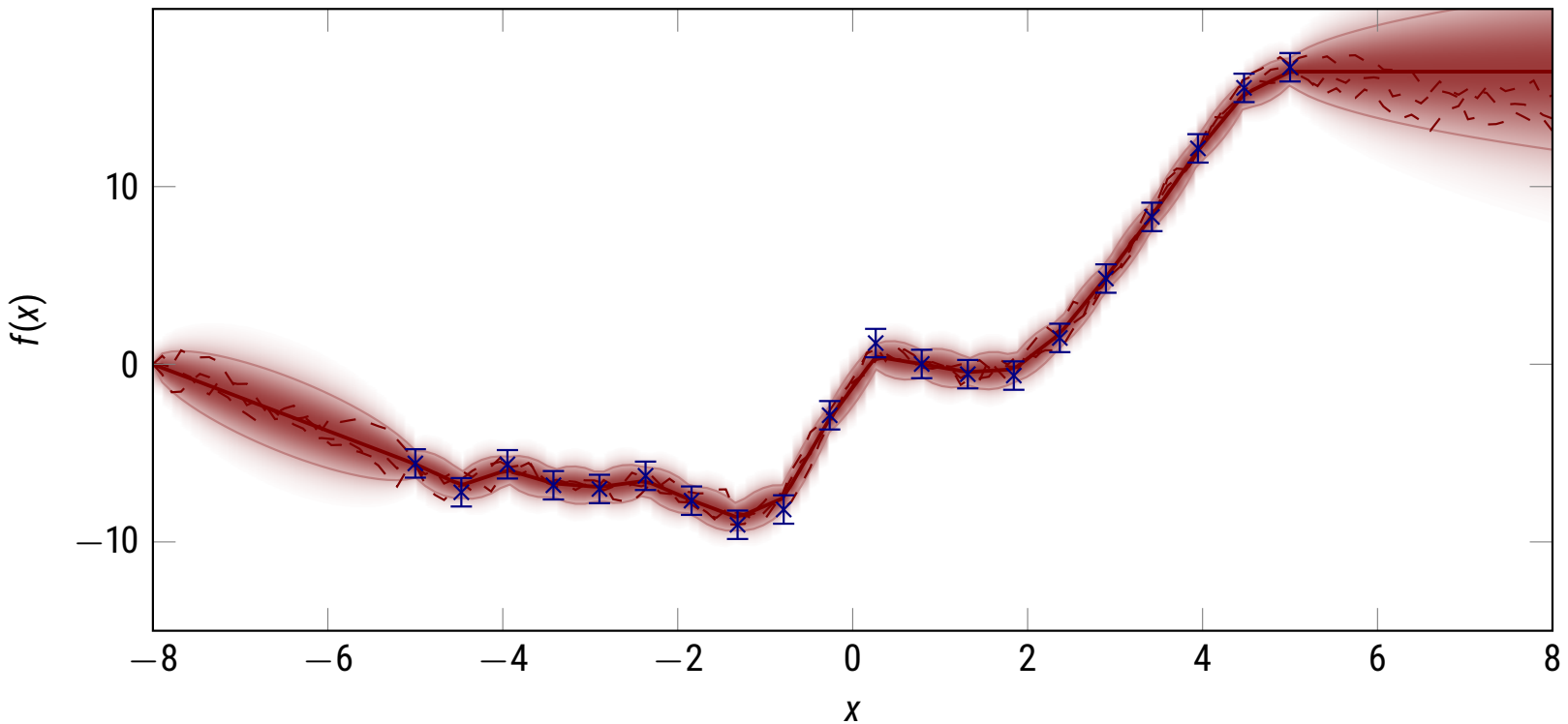
```
k = @(a,b)(theta.^2 * bsxfun(@min,a+8,b'+8)/16);
```



The **Wiener process**.

Those Step Functions

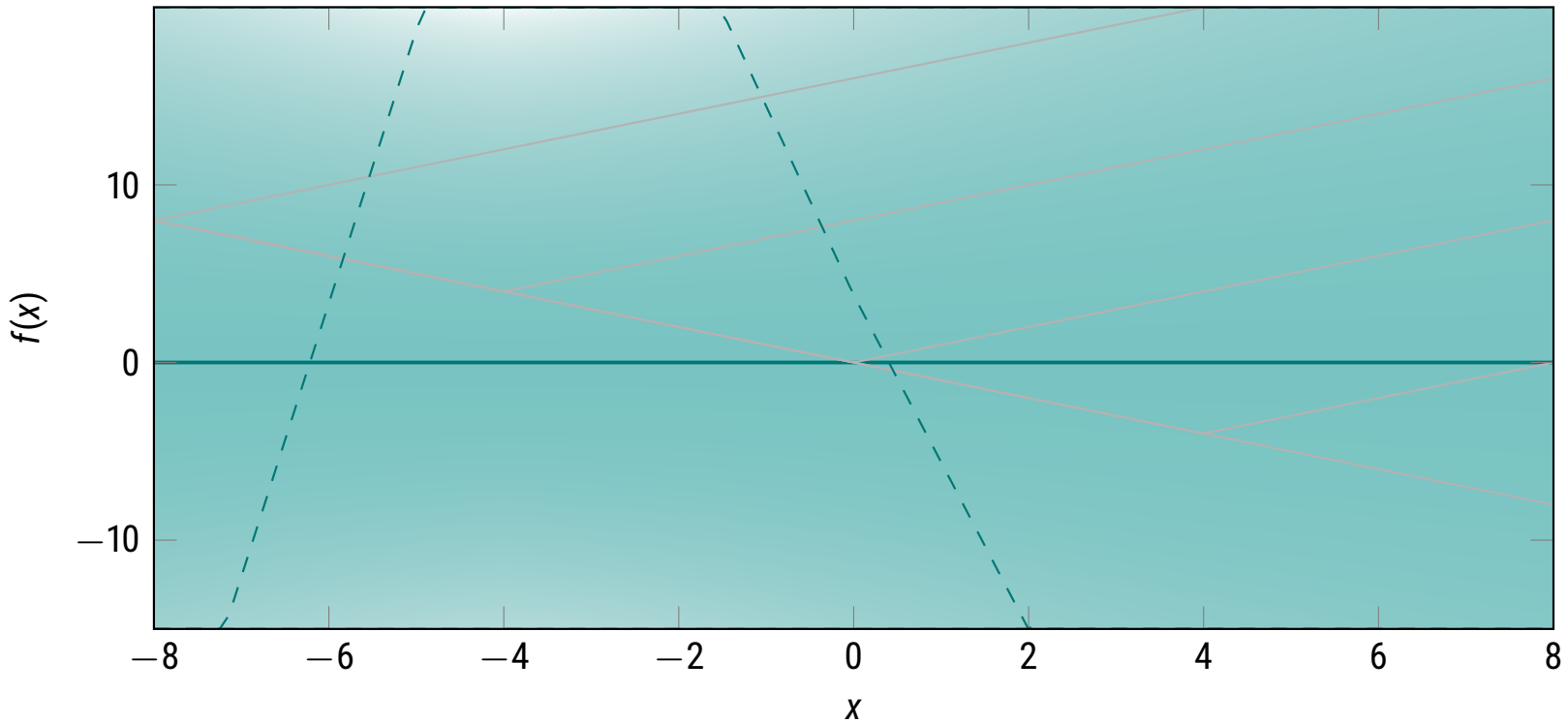
```
k = @(a,b)(theta.^2 * bsxfun(@min,a+8,b'+8)/16);
```



The **Wiener process**.

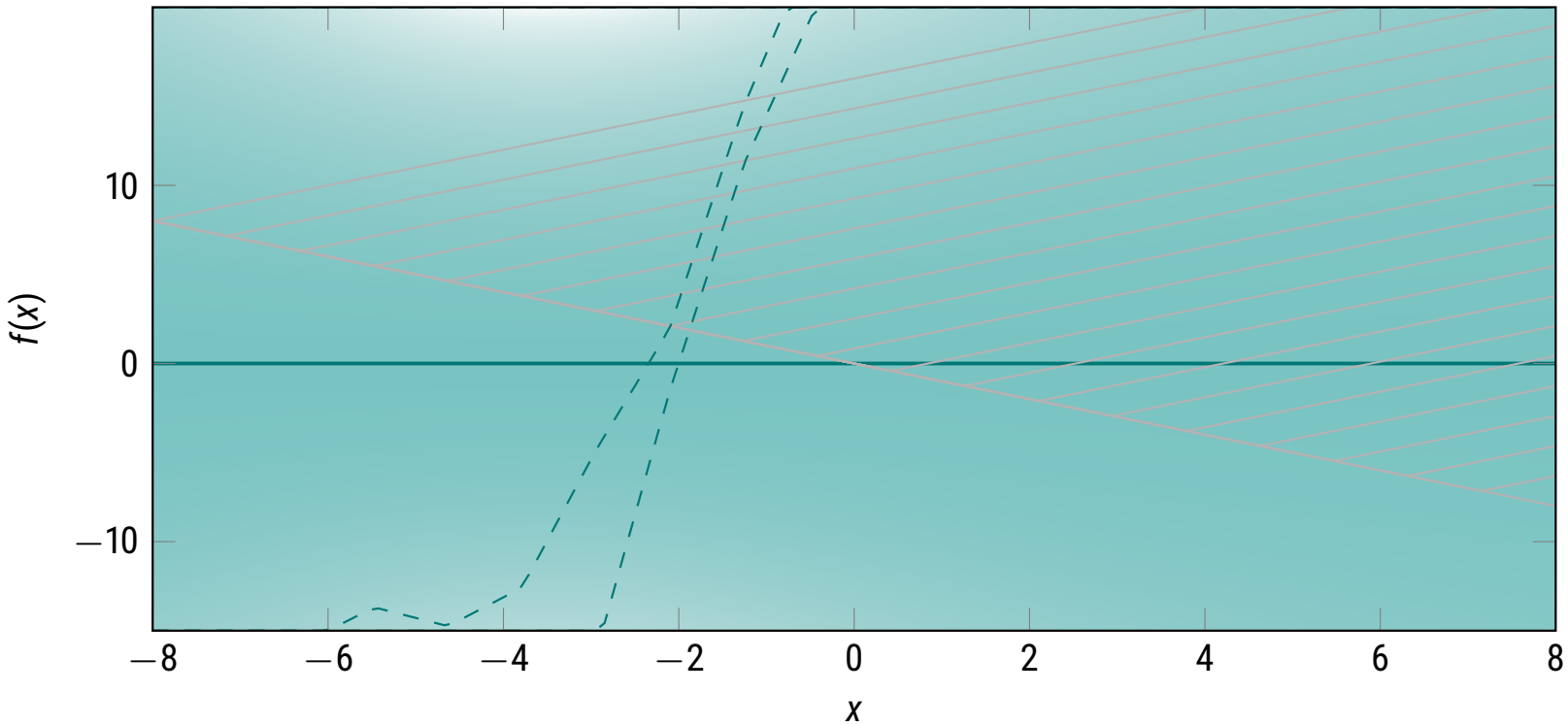
Those linear features

```
phi = @(a)(bsxfun(@minus,abs(bsxfun(@minus,a,linspace(-8,8,5))),linspace(-8,8,5)));
```



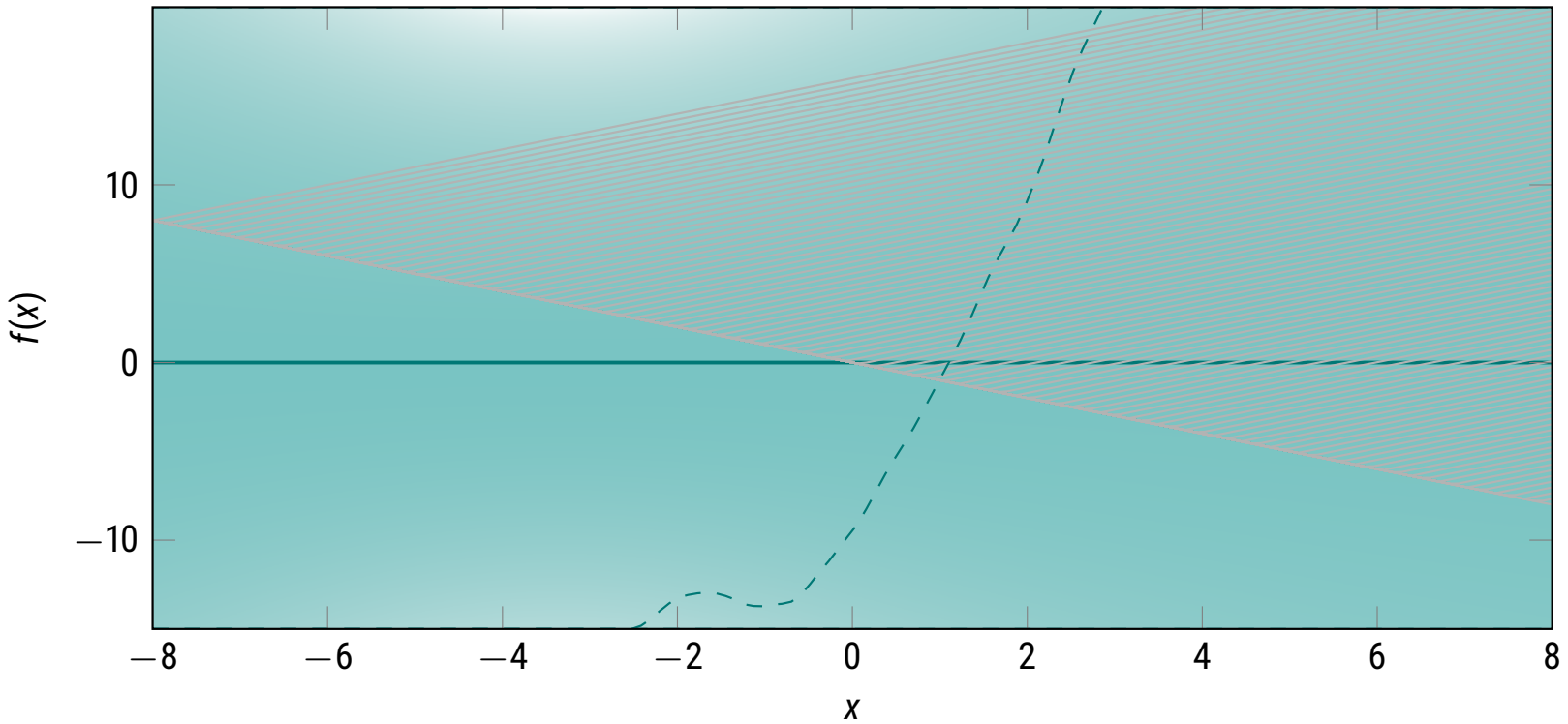
Those linear features

```
phi = @(a)(bsxfun(@minus,abs(bsxfun(@minus,a,linspace(-8,8,20))),linspace(-8,8,20)));
```



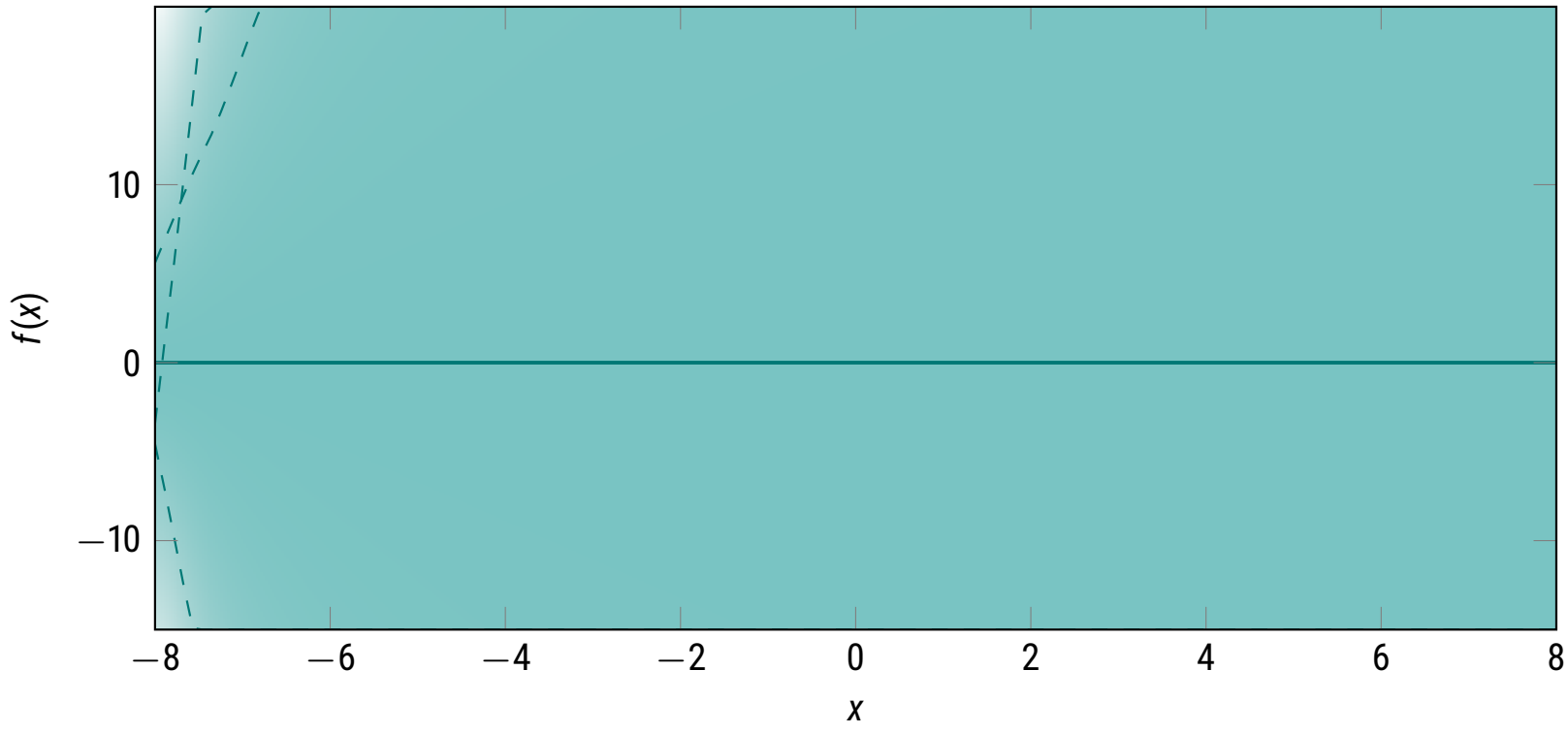
Those linear features

```
phi=@(a)(bsxfun(@minus,abs(bsxfun(@minus,a,linspace(-8,8,100))),linspace(-8,8,100)));
```



Those linear features

```
k = @(a,b)(theta.^2 * (1 + (1+c) * bsxfun(@times,a+8,b'+8)./16 + c ./ 3 *
(abs(bsxfun(@minus,a,b')/16).^3 - bsxfun(@plus,((a+8)./16).^3,((b'+8)./16).^3))));
```



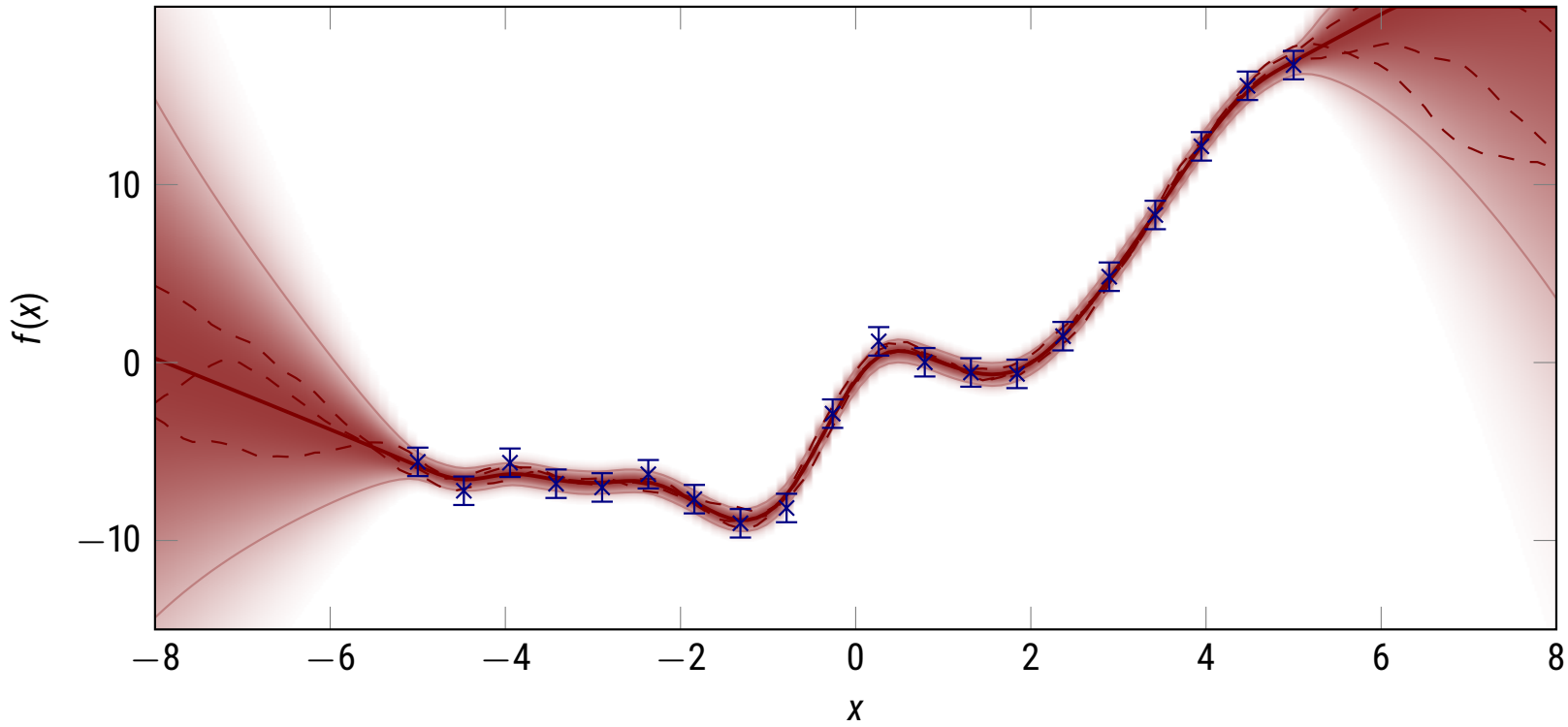
$$\operatorname{cov}(f_{x_i}, f_{x_j}) = 1 + x_i x_j + b \int_0^1 (|x_i - c| - c)(|x_j - c| - c)\,dc$$

$$= 1 + (1 + b)x_i x_j + \frac{b}{3}(|x_i - x_j|^3 - x^3 - y^3)$$

Cubic Splines.

Those linear features

```
k = @(a,b)(theta.^2 * (1 + (1+c) * bsxfun(@times,a+8,b'+8)./16 + c ./ 3 *
(abs(bsxfun(@minus,a,b')/16).^3 - bsxfun(@plus,((a+8)./16).^3,((b'+8)./16).^3))));
```



$$\mathrm{cov}(f_{x_i}, f_{x_j}) = 1 + x_i x_j + b \int_0^1 (|x_i - c| - c)(|x_j - c| - c)c$$

$$= 1 + (1 + b)x_i x_j + \frac{b}{3}(|x_i - x_j|^3 - x^3 - y^3)$$ **Cubic Splines**.

- Gaussian measures turn probabilistic inference into **linear algebra**
- Gaussian measures can be used to infer **functions** and **curves**
- In fact, the number of inferred features / weights can be **infinite**

Next up:

- There is a **large space** of kernels, and thus GP priors
- The choice of kernel / GP prior affects **model capacity** and **convergence**.

GPs are a flexible model class

because the space of kernels is large

Theorem:

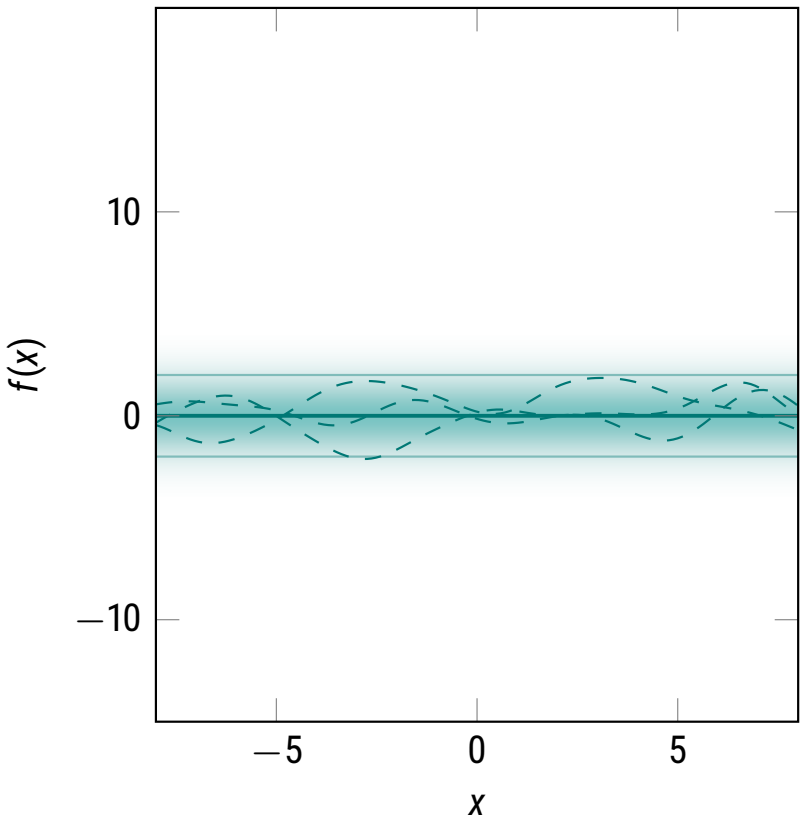
Let $\mathbb{X}, \mathbb{Y}$ be index sets and $\phi : \mathbb{Y} \to \mathbb{X}$. If $k_1, k_2 : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ are Mercer kernels, then the following functions are also Mercer kernels (up to minor regularity assumptions)

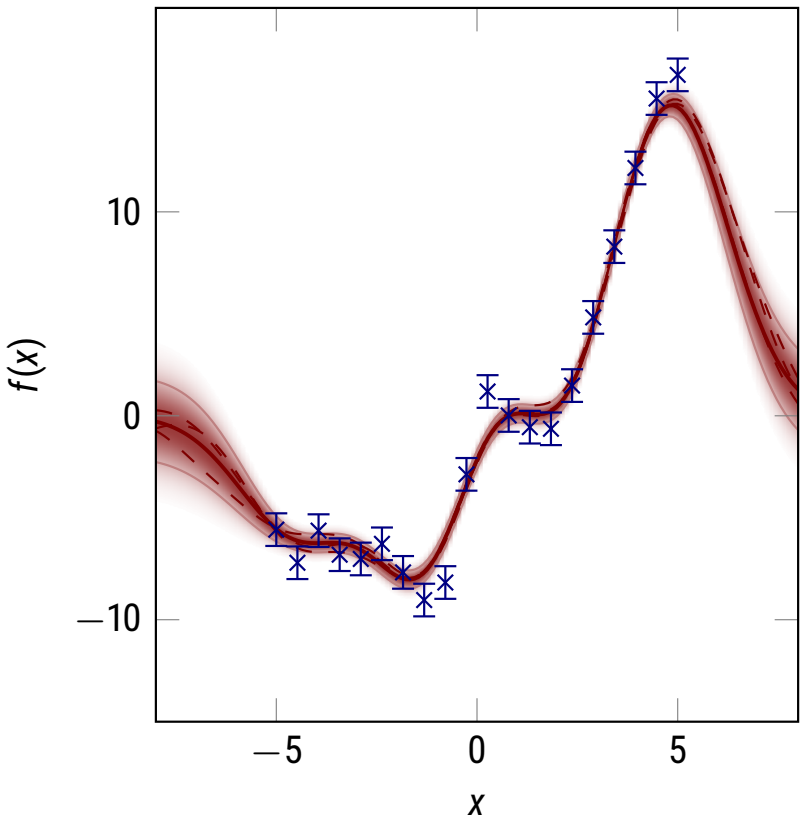
- $\alpha \cdot k_1(a, b)$ for $\alpha \in \mathbb{R}_+$ (proof: trivial)
- $k_1(\phi(c), \phi(d))$ for $c, d \in \mathbb{Y}$ (proof: by Mercer's theorem, coming up)
- $k_1(a, b) + k_2(a, b)$ (proof: trivial)
- $k_1(a, b) \cdot k_2(a, b)$ **Schur product theorem** (proof e.g. in Bapat, 1997. Million, 2007)

Scaled Kernels are Kernels

(this affects the effect of noise)

$$k(a, b) = 1^2 \cdot \exp\left(-\frac{(a-b)^2}{2}\right)$$

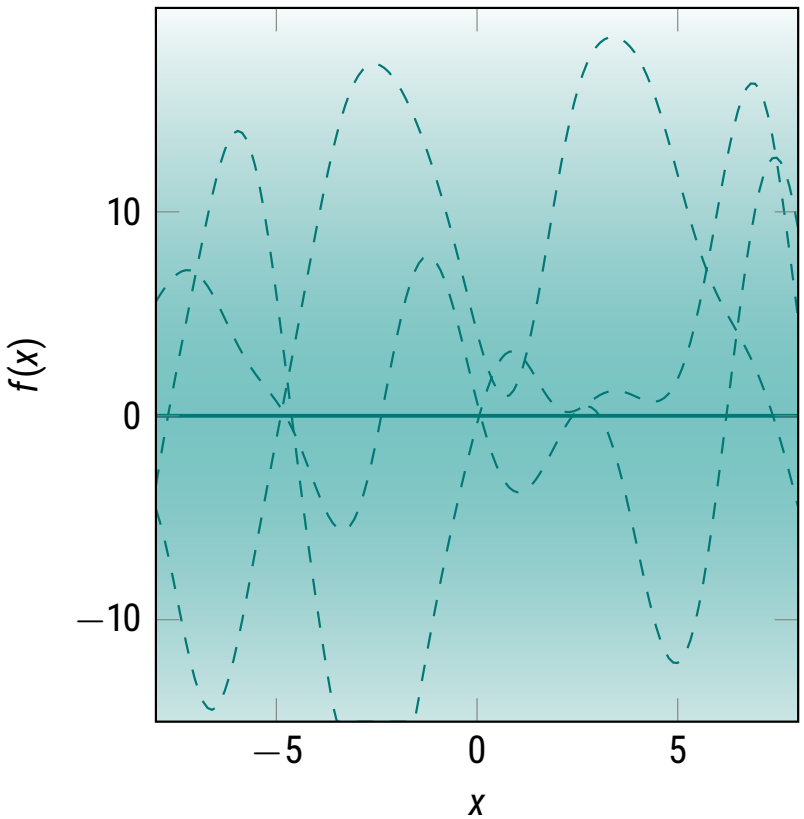


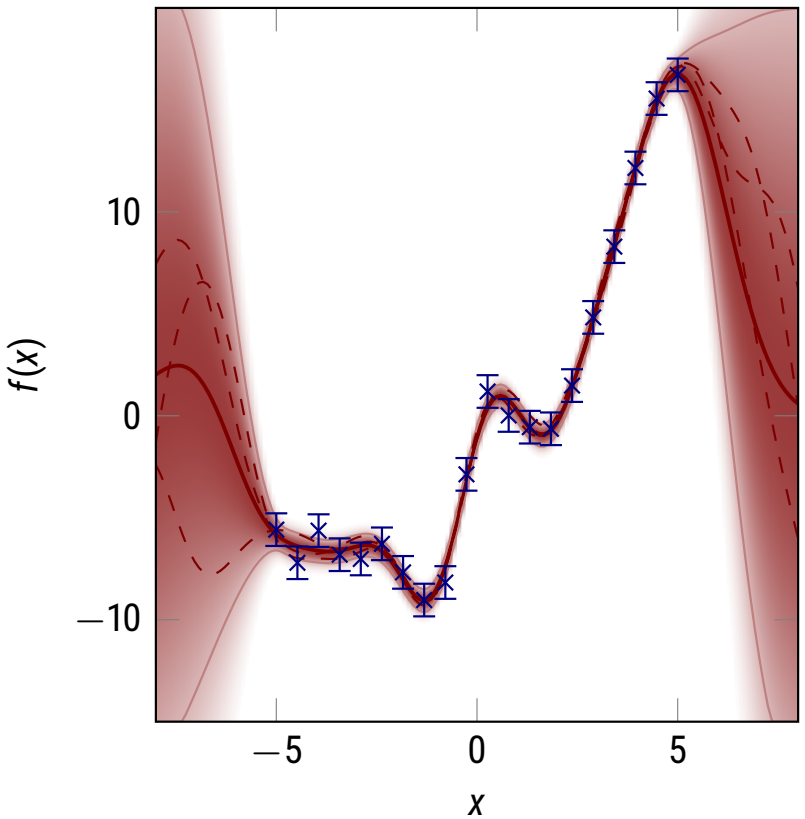


Scaled Kernels are Kernels

(this affects the effect of noise)

$$k(a, b) = 10^2 \cdot \exp\left(-\frac{(a-b)^2}{2}\right)$$

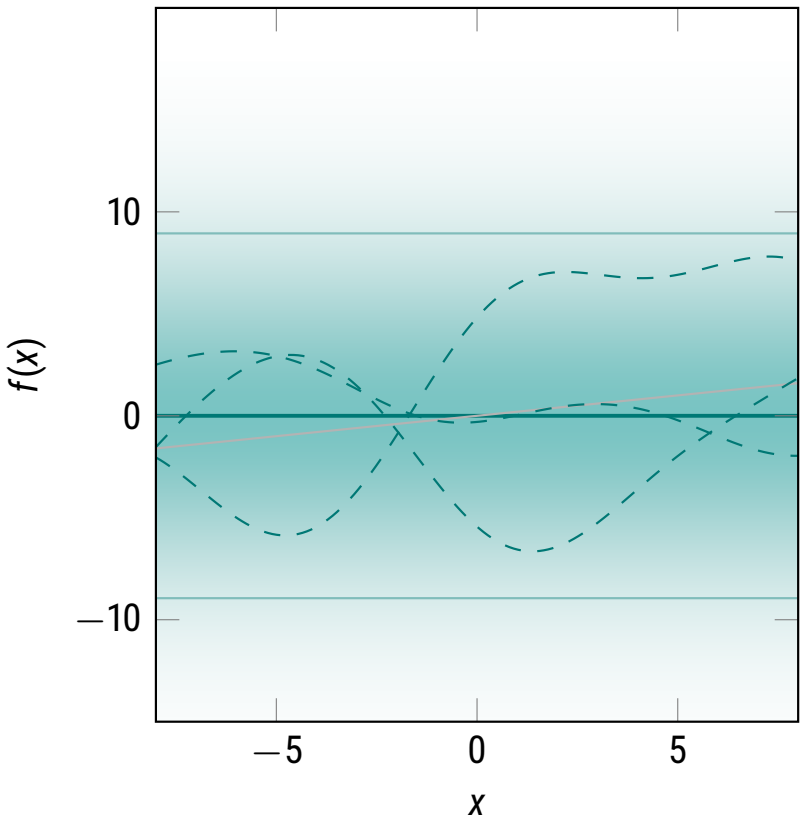


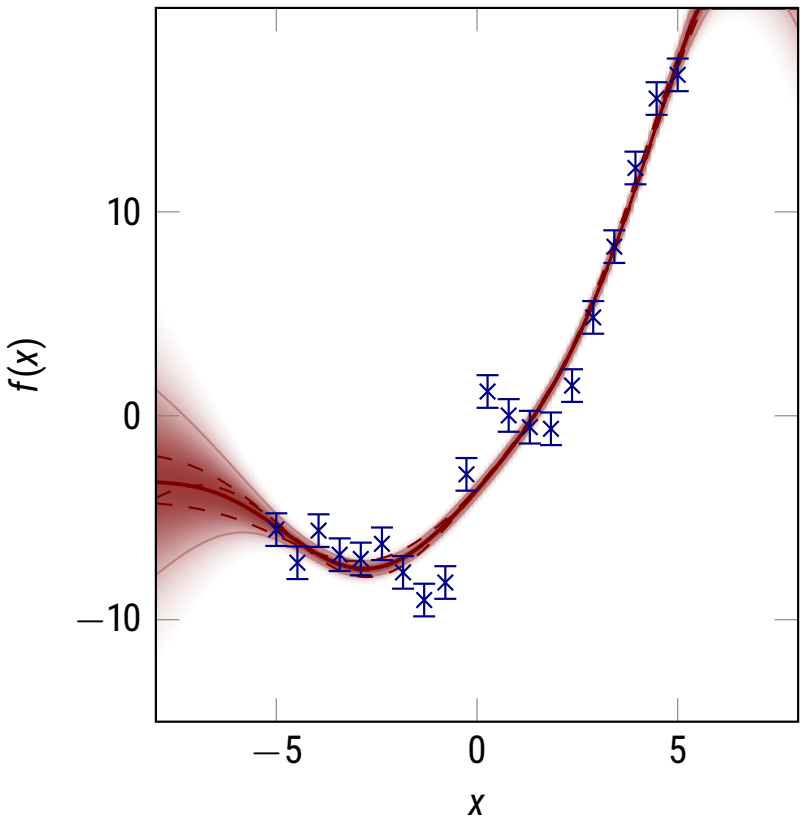


Kernels over Transformed Inputs are Kernels

this can be used to define length-scales

$$k(a, b) = 20 \cdot \exp\left(-\frac{(a-b)^2}{2 \cdot 5^2}\right)$$

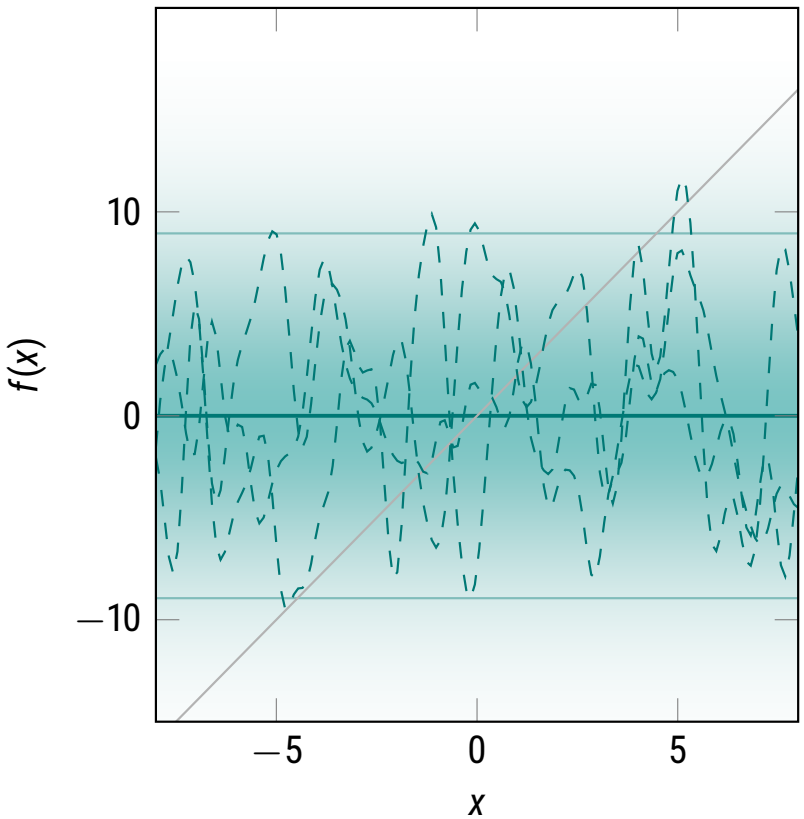


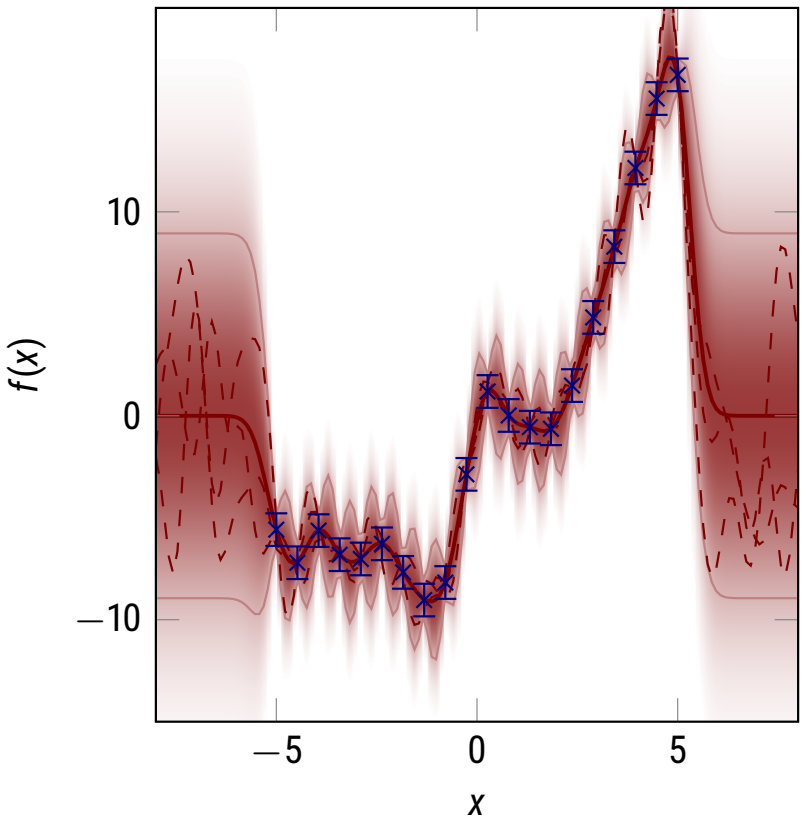


Kernels over Transformed Inputs are Kernels

this can be used to define length-scales

$$k(a, b) = 20 \cdot \exp\left(-\frac{(a-b)^2}{2 \cdot 0.5^2}\right)$$

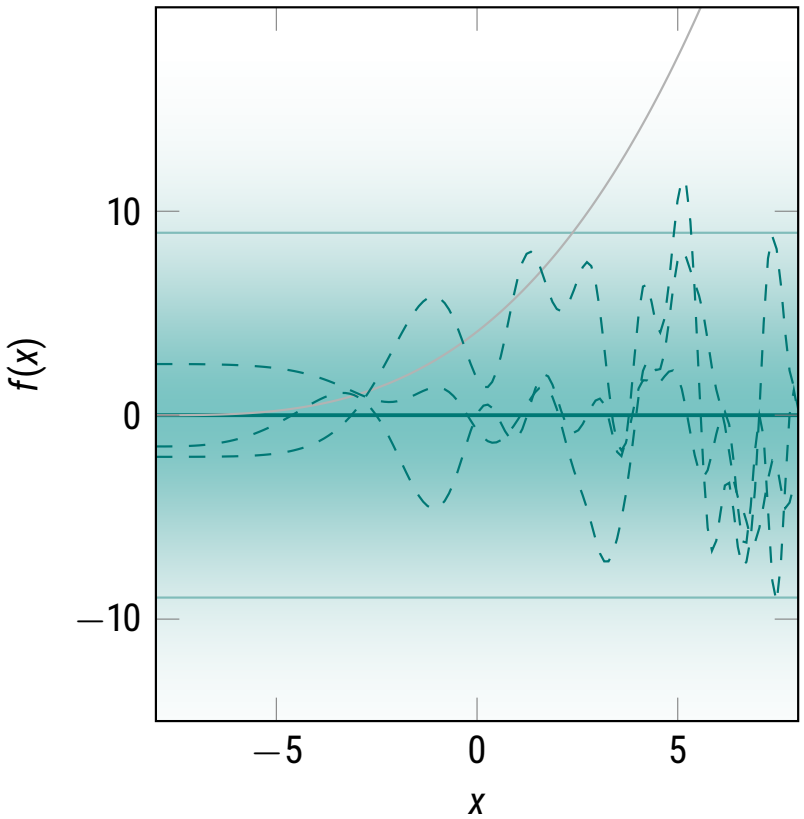


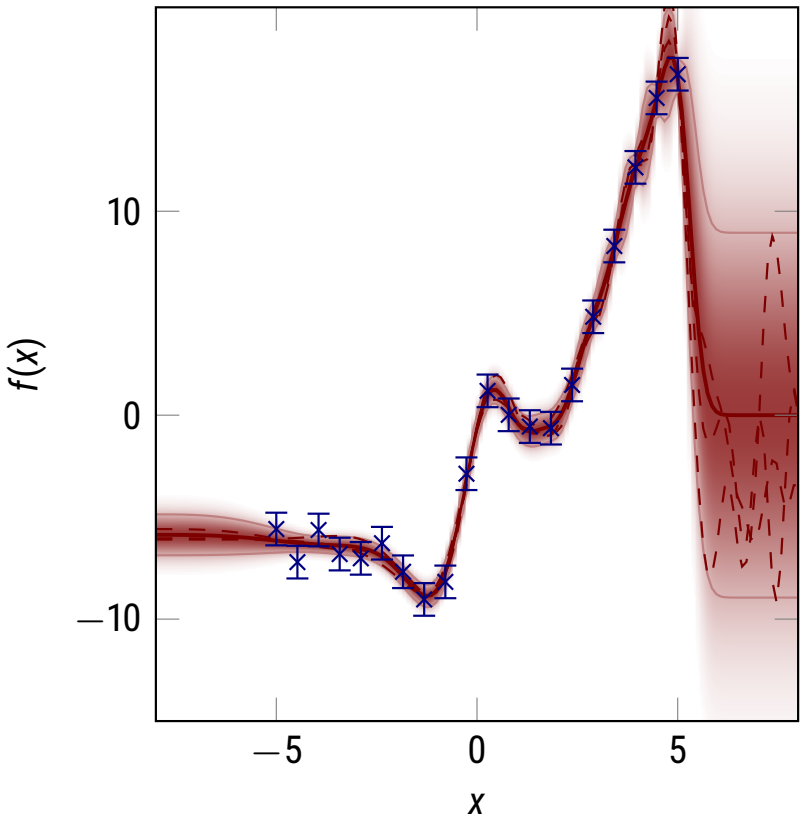


Kernels over Transformed Inputs are Kernels

nonlinear transformations (also at the heart of deep learning)

$$k(a,b) = 20 \cdot \exp\left(-\frac{(\phi(a)-\phi(b))^2}{2}\right) \qquad \phi(a) = \left(\frac{a+8}{5}\right)^3$$

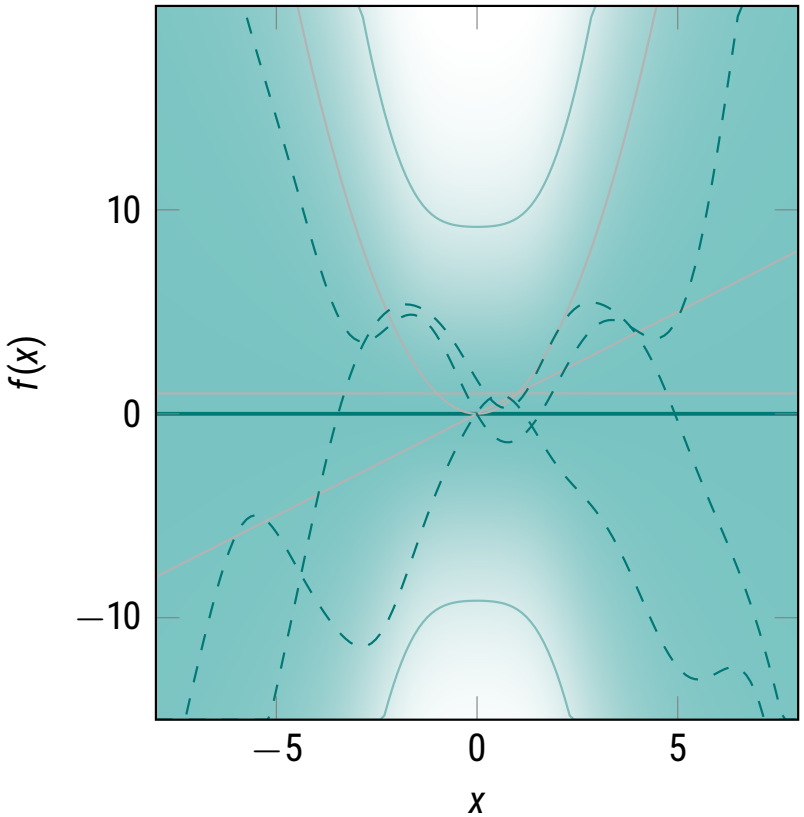


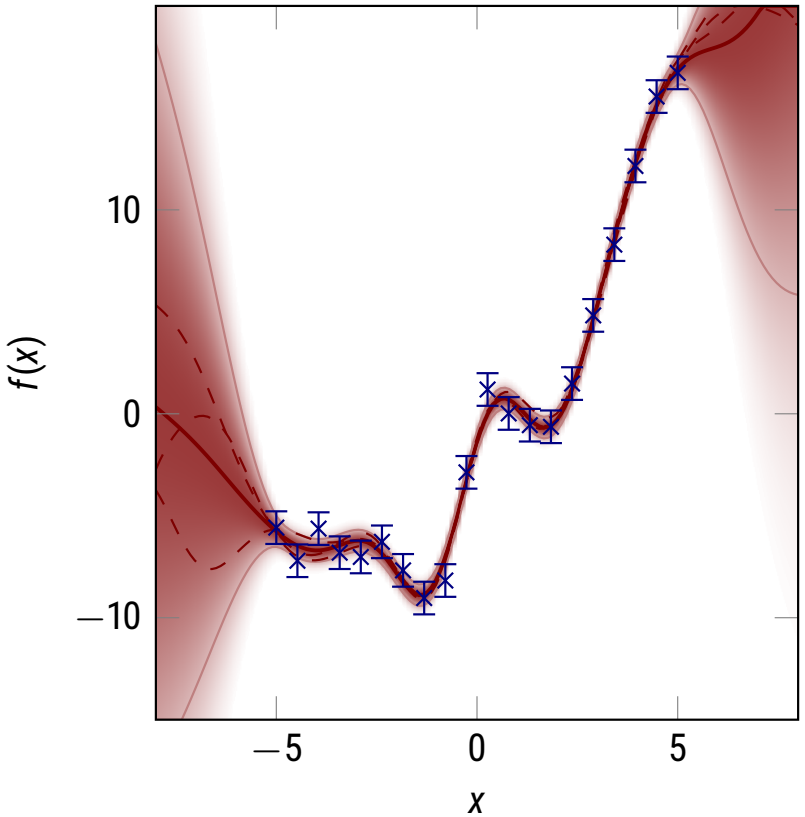


Sums of Kernels are Kernels

$f \sim \mathcal{GP}(0, k_1)$ and $g \sim \mathcal{GP}(0, k_2) \quad \Leftrightarrow \quad h = f + g \sim \mathcal{GP}(0, k_1 + k_2)$

$$k(a, b) = 20 \cdot \exp\left(-\frac{(a-b)^2}{2}\right) + \phi(a)^\intercal \phi(b) \qquad \phi(x) := [1, x, x^2]$$

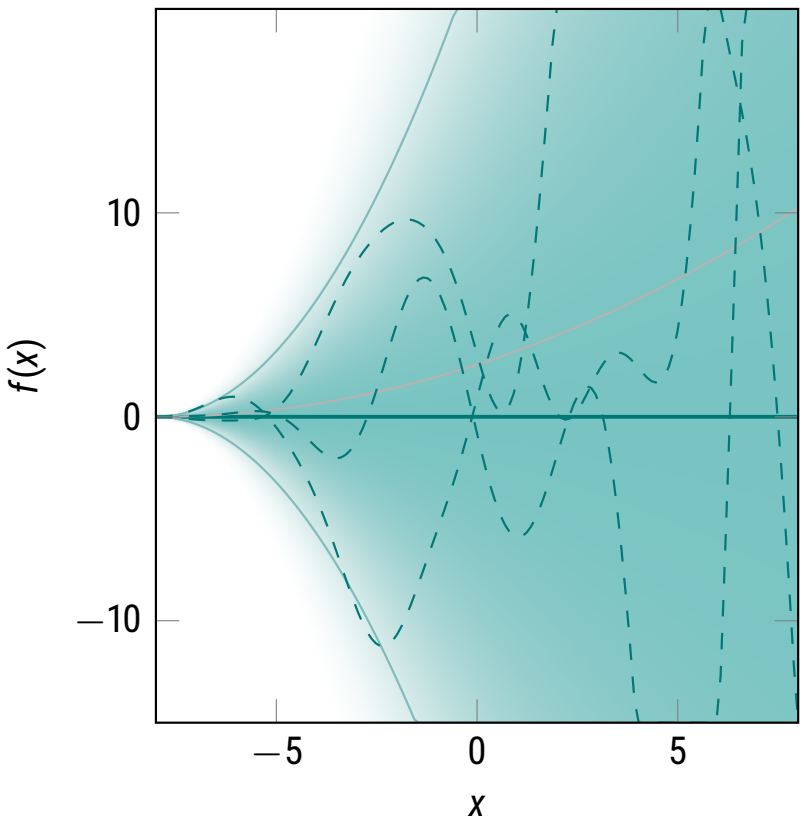


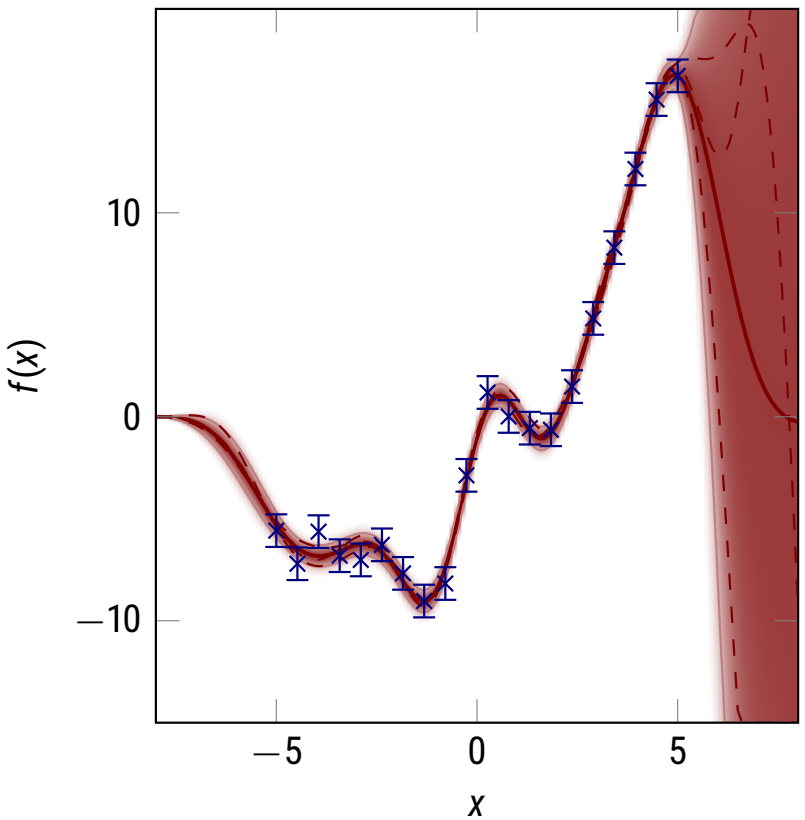


Products of Kernels are Kernels

Schur product theorem

$$k(a,b) = 20 \cdot \exp\left(-\frac{(a-b)^2}{2}\right) \cdot \phi(a)^\intercal \phi(b) \quad \phi(x) := \left(\frac{x+8}{5}\right)^2$$

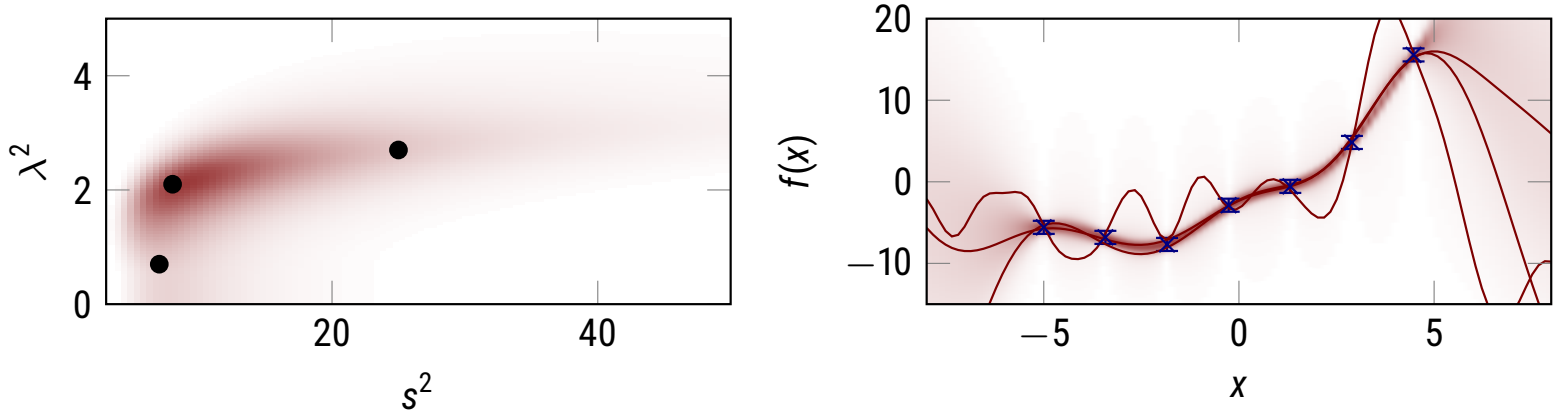




If you think your model has no parameters, you just haven't found them yet!

Can one **learn** the kernel?

hierarchical Bayesian inference



- So there are a lot of choices to be made. Can we **learn** the right kernel?
- In principle, Bayesian inference remains the right framework:
  Parametrize $k = k^\theta, \mu = \mu^\theta, \Lambda = \Lambda^\theta$

$$p(y \mid \theta) = \int p(y \mid f, \theta) p(f \mid \theta)\, df = \int \mathcal{N}(y; f_X, \Lambda^\theta) \mathcal{GP}(f; \mu^\theta, k^\theta)$$

$$= \mathcal{N}(y, \mu_X^\theta, \Lambda^\theta + k_{XX}^\theta)$$

$$p(f \mid y) = \int p(f \mid y, \theta) p(\theta \mid y)\, d\theta$$

- in general, none of this is of closed form (but see later for a special case)

What does the GP prior mean?

Relation to Least-Squares Fitting, and other model classes

GP regression is also known as

- Kriging
- Wiener-Kolmogorov prediction

and is closely related to

- Kernel Ridge Regression
- Kernel Least Squares

In particular, the posterior mean function

$$\mu(x) = k_{xX}(k_{XX} + \sigma^2 I)^{-1} Y$$

is **equal** to the kernel ridge estimate.

What does the GP prior mean?

GP **means** are elements of RKHSs.

Let $\mathcal{H} = (\mathbb{X}, \langle\cdot,\cdot\rangle)$ be a Hilbert space of functions $f : \mathbb{X} \to \mathbb{R}$. Then $\mathcal{H}$ is called a **reproducing kernel Hilbert space** if there exists a **kernel** $k : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ s.t.

$$\forall x \in \mathbb{X}: \quad k(\cdot, x) \in \mathcal{H} \qquad \text{and} \qquad \forall f \in \mathcal{H}: \quad \langle f(\cdot), k(\cdot, x)\rangle_{\mathcal{H}} = f(x)$$

An **eigenfunction** ϕ_i of k relative to measure ν is a function in $\mathcal{H}$ such that

$$\int \phi_i(x) k(x, \tilde{x})\, d\nu(x) = \lambda_i \phi_i(\tilde{x}).$$

- Aronszajn, 1950: For every pos.def. k on $\mathbb{X}$, there exists a unique RKHS.
- Mercer, 1909: Every k can be written as

$$k(x, \tilde{x}) = \sum_i \lambda_i \phi_i(x) \phi^\intercal(\tilde{x}) \quad \text{with} \quad \sum_i \lambda_i < \infty \tag{1}$$

- The RKHS is the space of functions

$$f(x) = \sum_i \alpha_i \phi_i(x) \text{ with } \sum_i \frac{\alpha_i^2}{\lambda_i} < \infty, \text{ where } \langle f, g\rangle_{\mathcal{H}} = \sum_i \frac{\alpha_i \beta_i}{\lambda_i}.$$

Proof: $\langle f(\cdot), k(\cdot, x)\rangle = \sum_i \alpha_i \lambda_i / \lambda_i \phi_i(x) = f(x)$. And $\|k(x,\cdot)\| = \langle k(x,\cdot), k(x,\cdot)\rangle = k(x,x) < \infty$. □

What does the GP prior mean?

GP **samples** are not in the RKHS. But **almost**.

Karhunen-Loève Expansion:

$$f(x) = \sum_i \alpha_i \phi_i \qquad \alpha_i \overset{iid.}{\sim} \mathcal{N}(0, \lambda_i) \quad \Leftrightarrow \quad f(x) \sim \mathcal{GP}(0, k)$$

Thus: $f \sim \mathcal{GP}(0, k) \quad \Rightarrow \quad \mathsf{E}(\|f\|_{\mathcal{H}}^2) = \sum_i \frac{\mathsf{E}(\alpha_i^2)}{\lambda_i} = \sum_i 1$

Samples from a GP are not in the RKHS (with probability 1).

Theorem: [Driscoll, 1973; Steinwart, 2014]

Let $f \sim \mathcal{GP}(0, k)$. The following two statements are equivalent:

- $\bar{\mathcal{H}}$ is RKHS such that $\mathcal{H}_k \subset \bar{\mathcal{H}}$ (with Hilbert-Schmidt compact embedding)
- $f \in \bar{\mathcal{H}}$ almost surely.

(Misleading) example: Draws from GP with $k_\ell(x, x') = \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$ are not in RKHS of k. But they are in the RKHS of $k_{\tilde{\ell}}$ for all $\tilde{\ell} < \ell$.

What does the posterior variance mean?

Frequentist interpretations of Bayesian error estimates

How far could the ridge regressor / posterior mean be from the truth?

$$\sup_{f \in \mathcal{H}, \|f\| \leq 1} \left(\sum_i f(x_i) \underbrace{[K_{XX}^{-1} k(X, x)]_i}_{w_i} - f(x) \right)^2 = \sup \left\langle \sum_i w_i k(\cdot, x_i) - k(\cdot, x), f(\cdot) \right\rangle_{\mathcal{H}}^2$$

$$= \left\| \sum_i w_i k(\cdot, x_i) - k(\cdot, x) \right\|_{\mathcal{H}}^2 = \sum_{ij} w_i w_j k(x_i, x_j) - 2 \sum_i w_i k(x, x_i) + k(x, x)$$

$$= k_{xx} - k_{xX} K_{XX}^{-1} k_{Xx} = \mathrm{E}_{|y}[(f_x - \mu_x)^2]$$

What does the GP posterior mean?

Frequentist interpretations of Bayesian error estimates

- the GP posterior mean

$$\mu(x) = \mathrm{E}[f(x)] = k_{xX}(k_{XX} + \sigma^2)^{-1}Y$$

  is the **least-squares** estimate in the RKHS of k.

- **for noise-free observations**, the GP posterior variance

$$\mathbb{V}(x) = \mathrm{E}[f(x)^2 - \mu(x)^2] = k_{xx} - k_{xX}k_{XX}^{-1}k_{Xx}$$

  is the scale of the **worst-case** error for functions of bounded norm in the RKHS.

In later lectures, we will see that for advanced computational problems with **non-Gaussian likelihoods**, additional care is required.

Universal Kernels

a slightly different statement

Definition (Universal Kernel)

*A kernel **k** acting on **X** is said to be universal if its RKHS lies dense in the space of all continuous functions.*

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Universal Kernels

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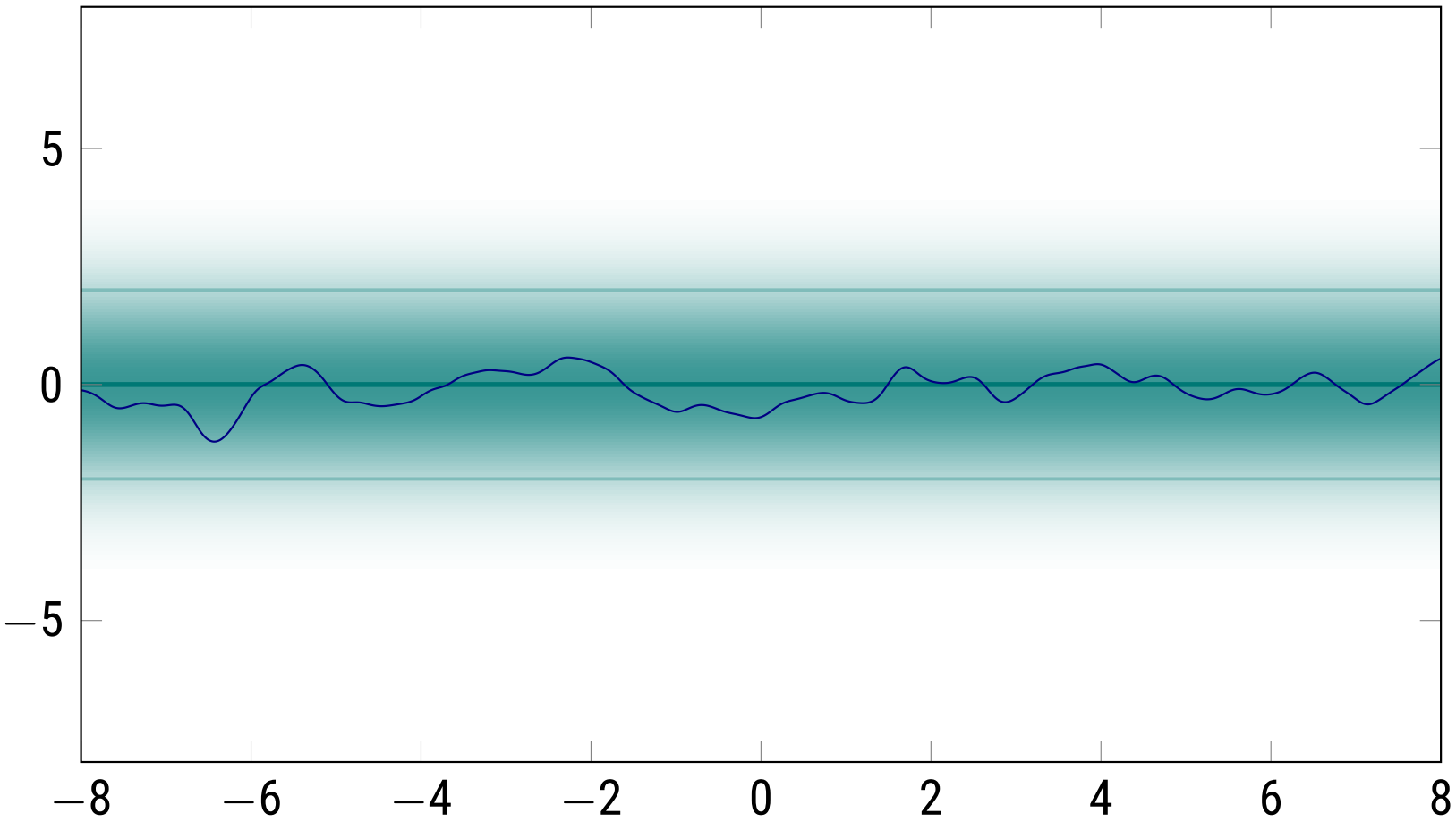
Abstract

In this paper we investigate conditions on the features of a continuous kernel so that it may approximate an arbitrary continuous target function uniformly on any compact subset of the input space. A number of concrete examples are given of kernels with this universal approximating property.

Keywords: density, translation invariant kernels, radial kernels

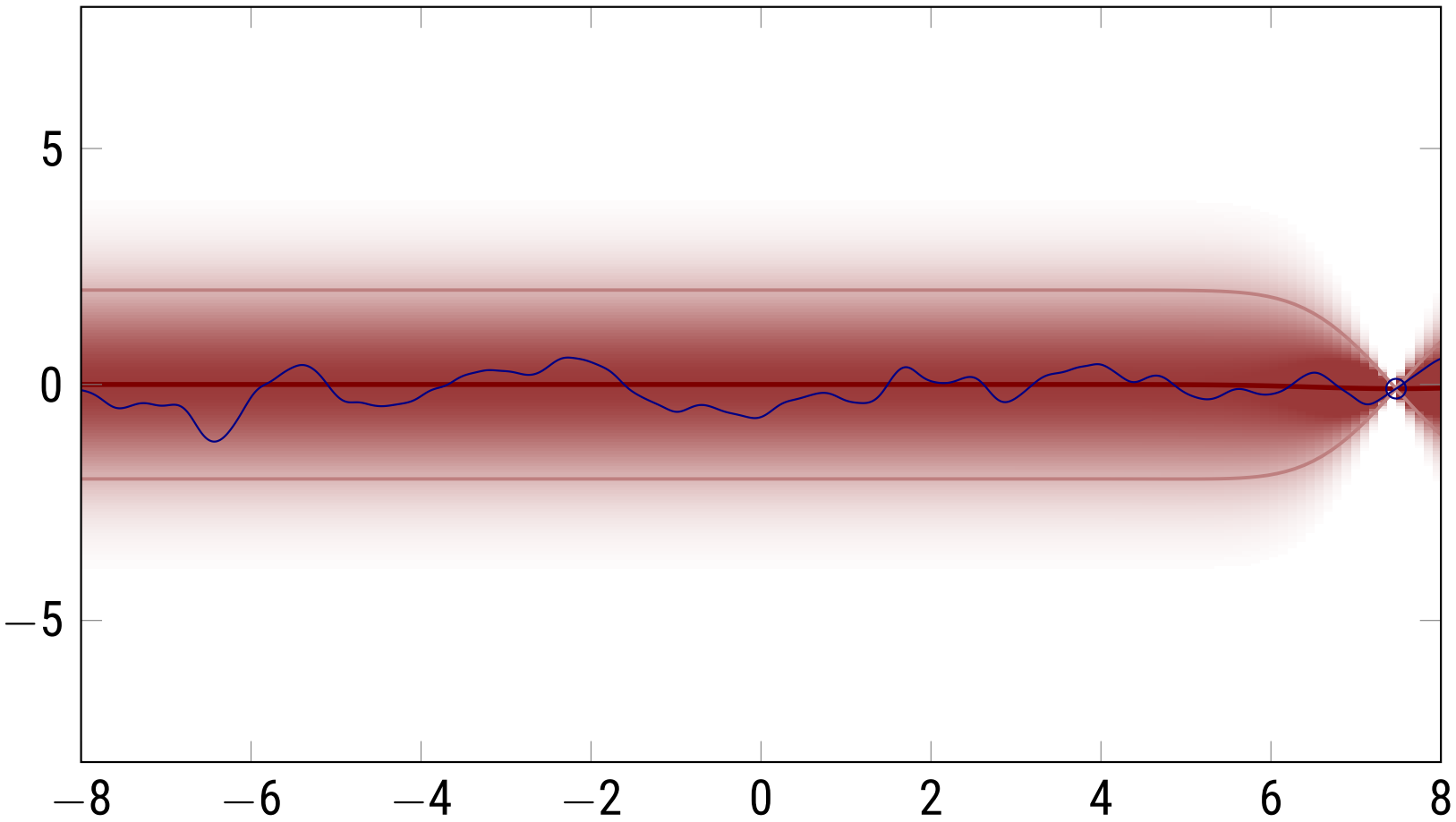
Universal RKHSs

an experiment – prior



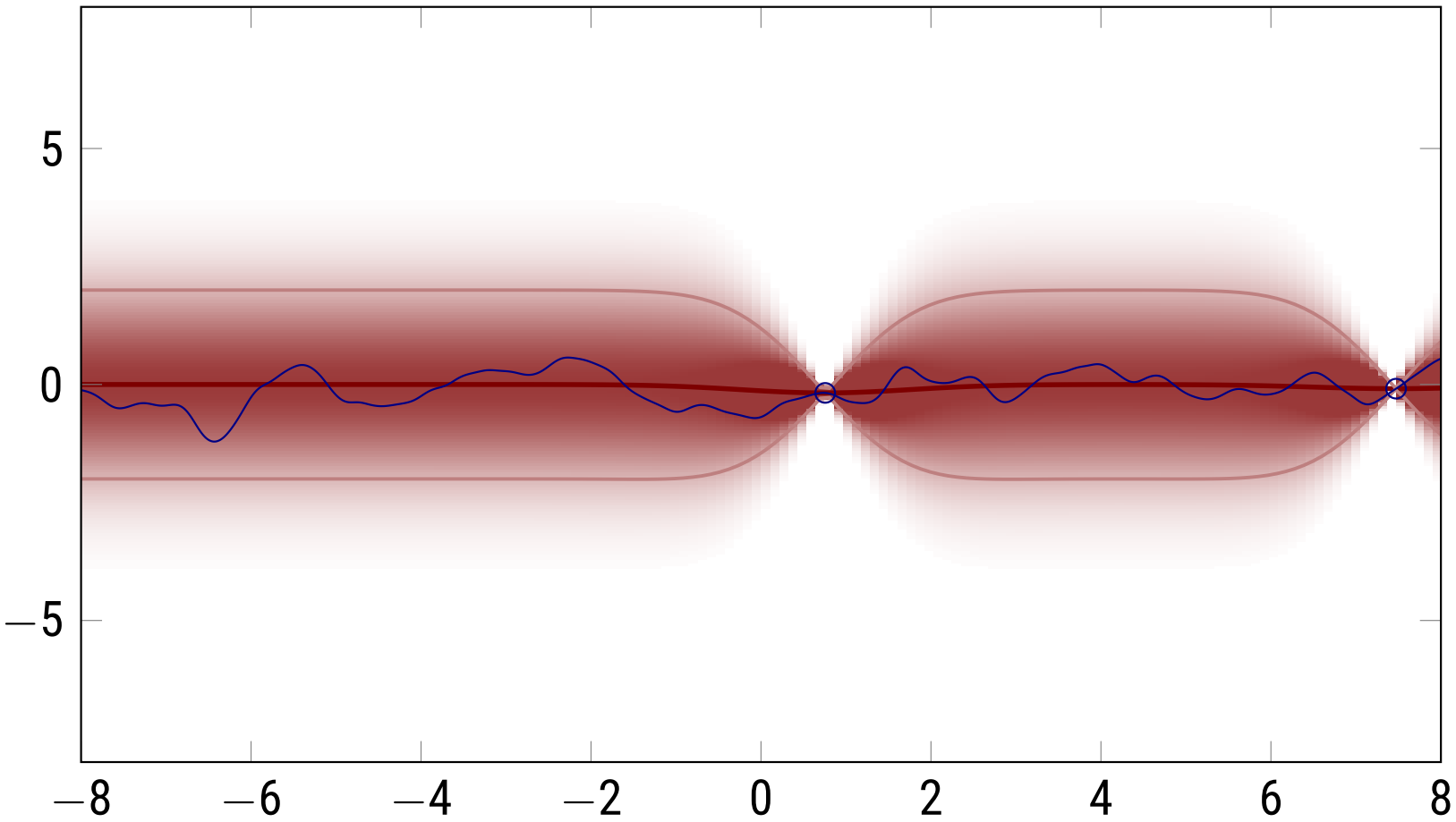
Universal RKHSs

an experiment – 1 evaluation



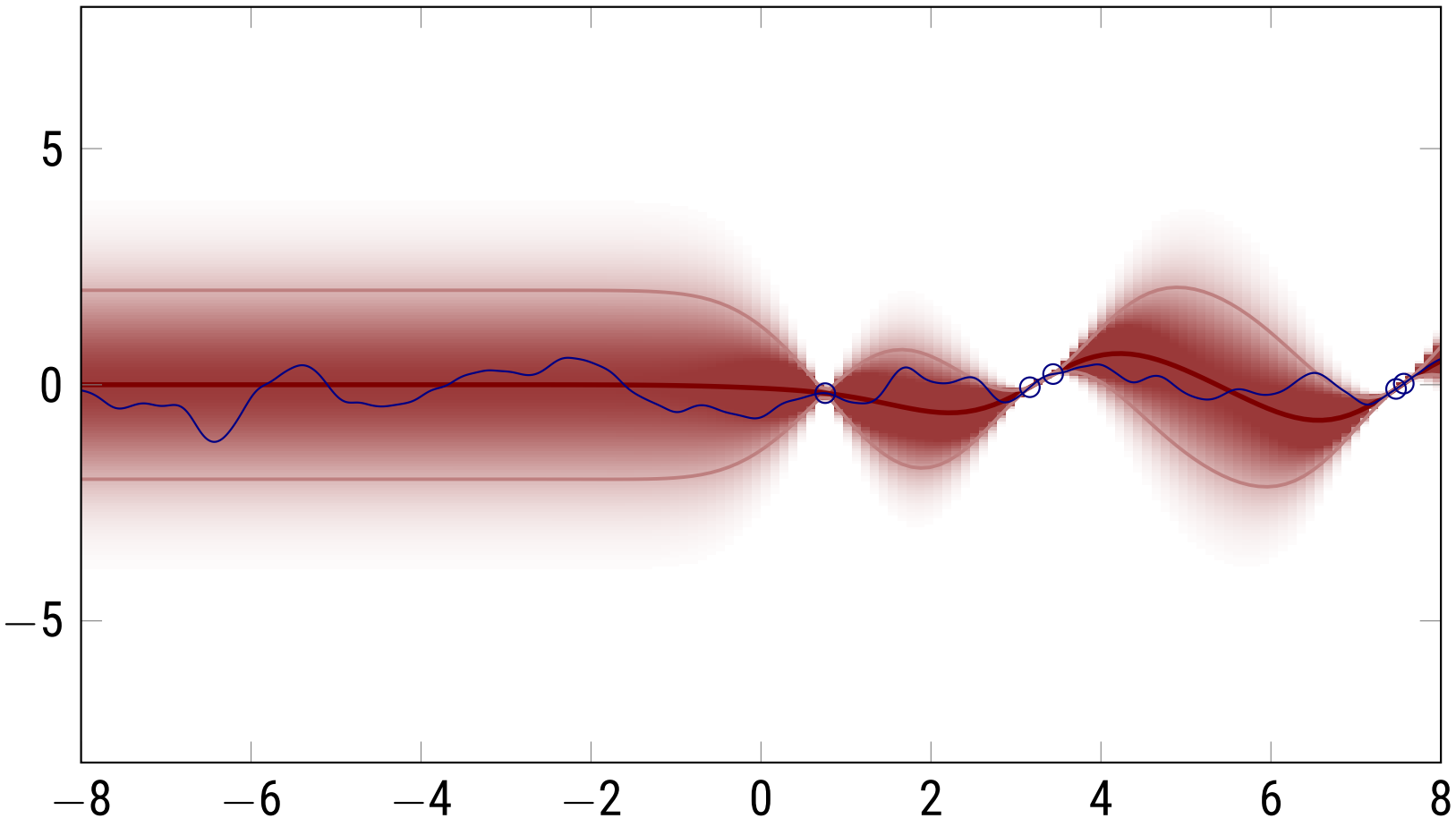
Universal RKHSs

an experiment – 2 evaluations



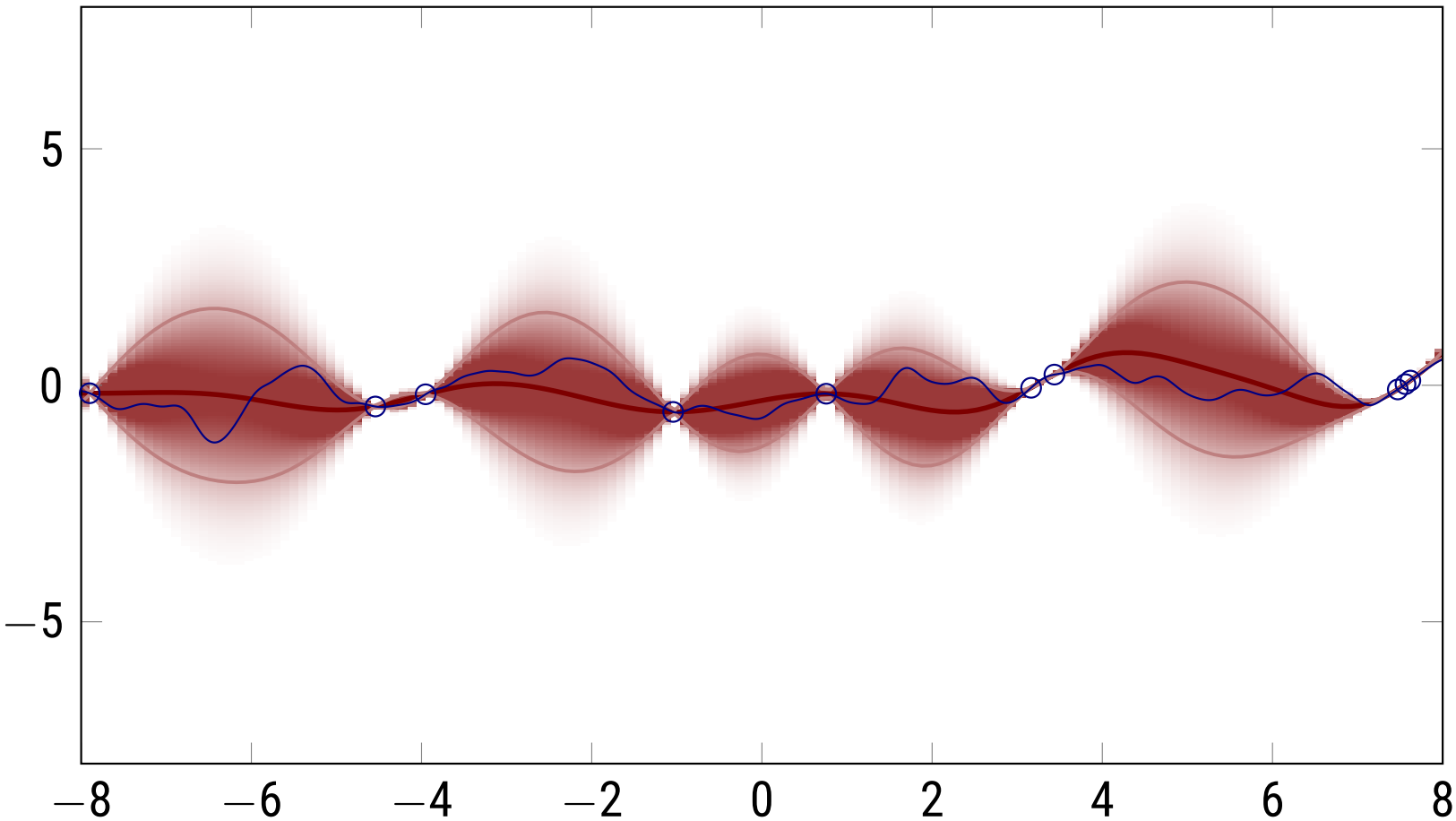
Universal RKHSs

an experiment – 5 evaluations



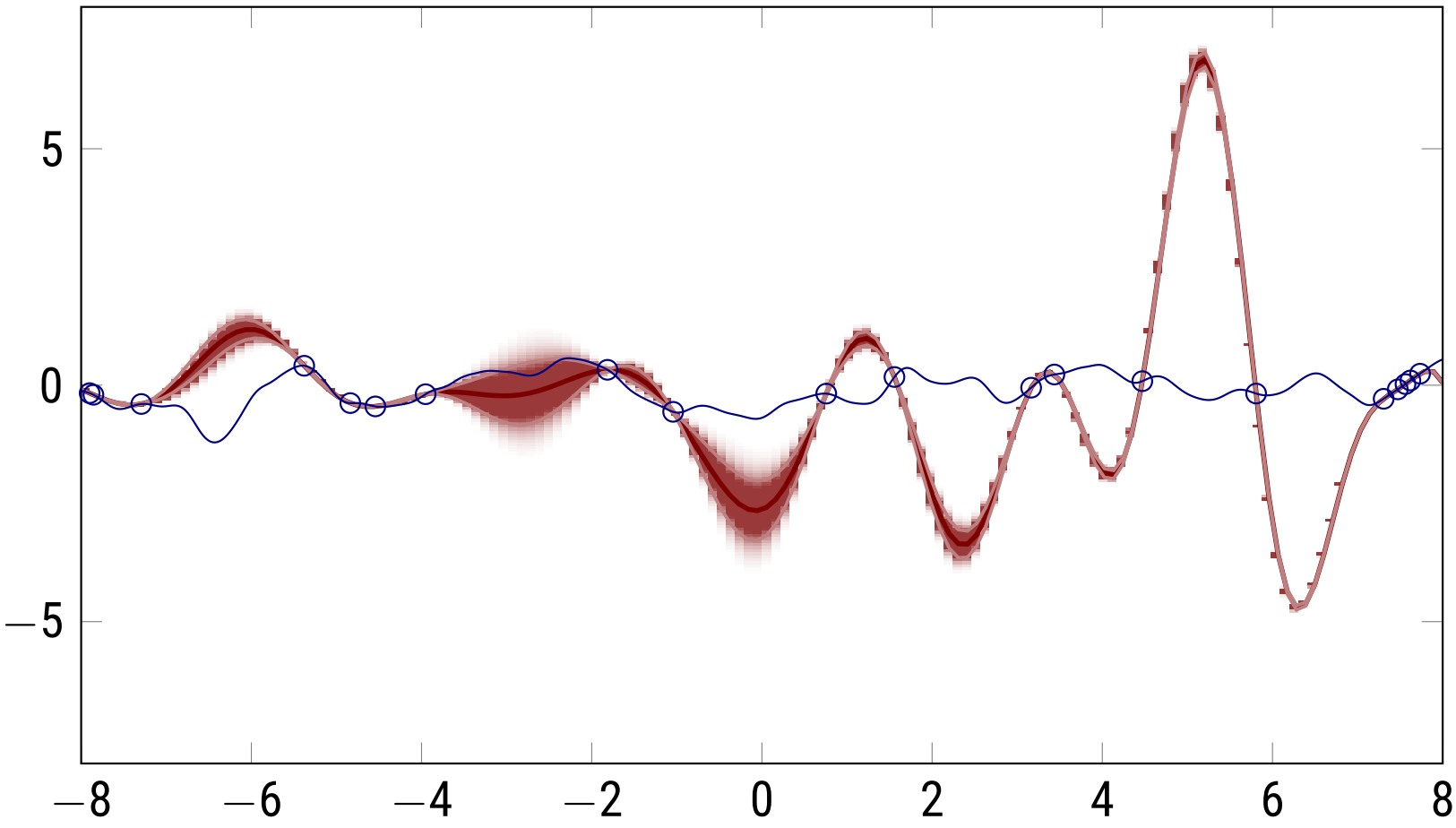
Universal RKHSs

an experiment – 10 evaluations



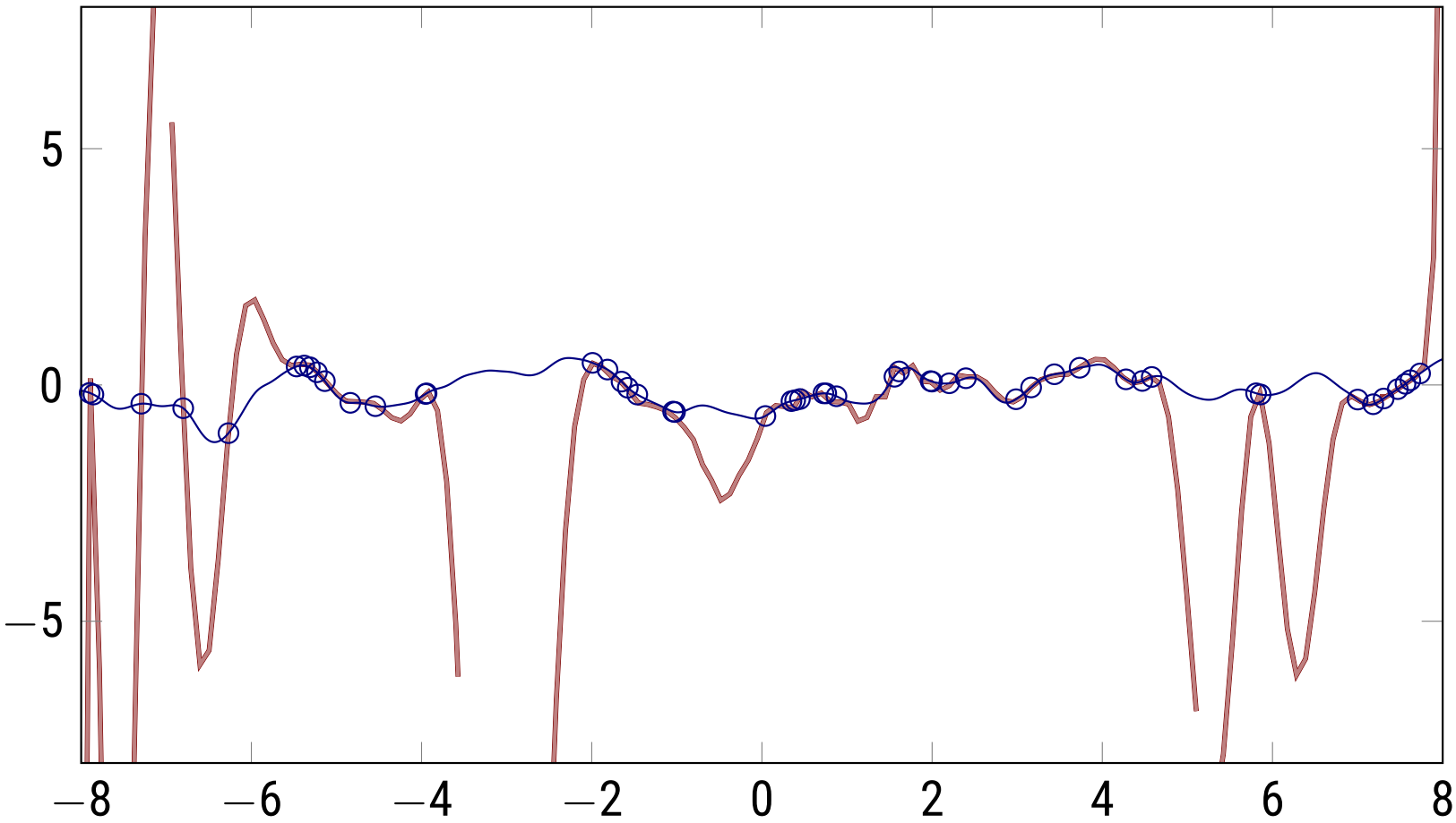
Universal RKHSs

an experiment – 20 evaluations



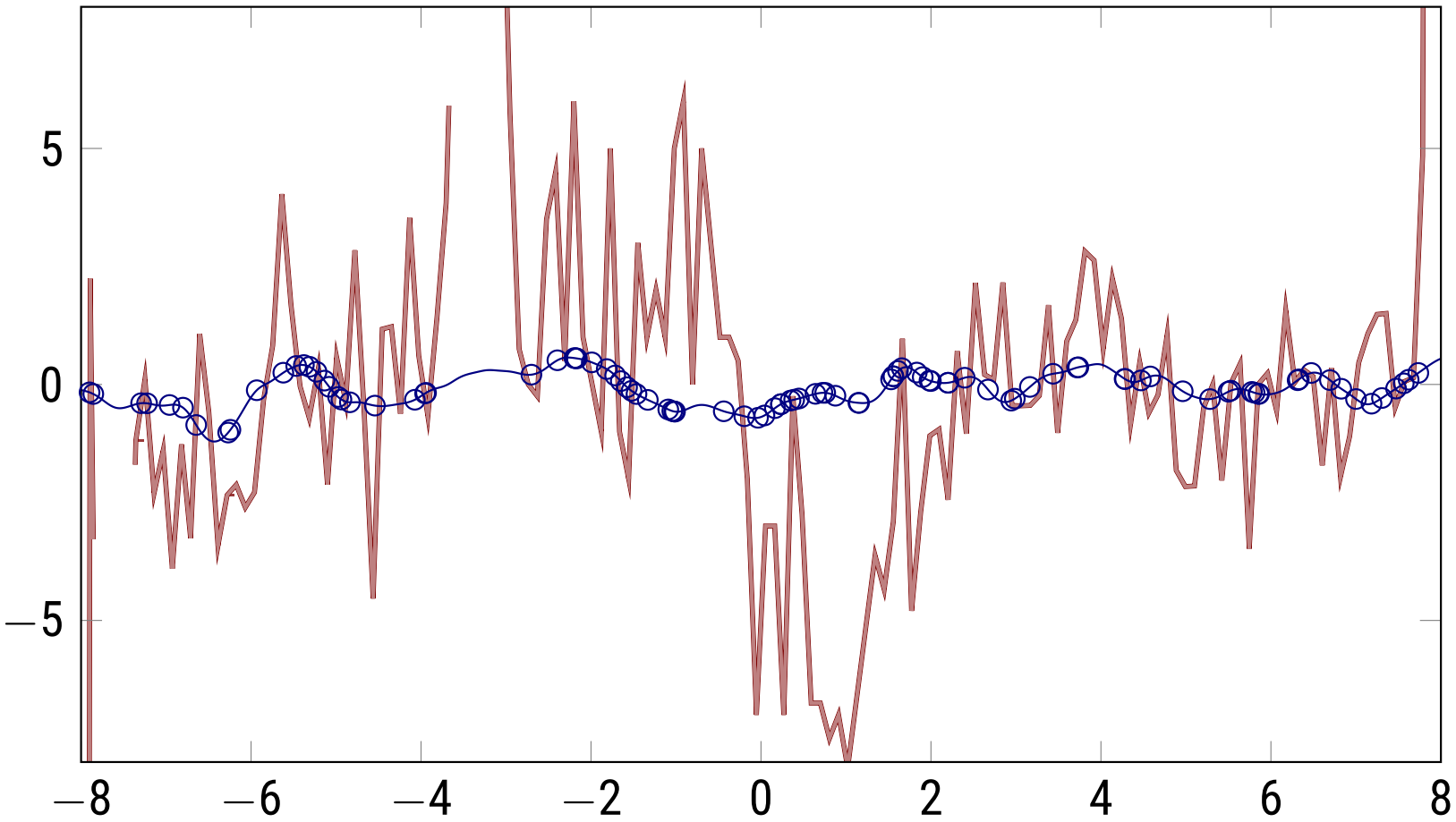
Universal RKHSs

an experiment – 50 evaluations



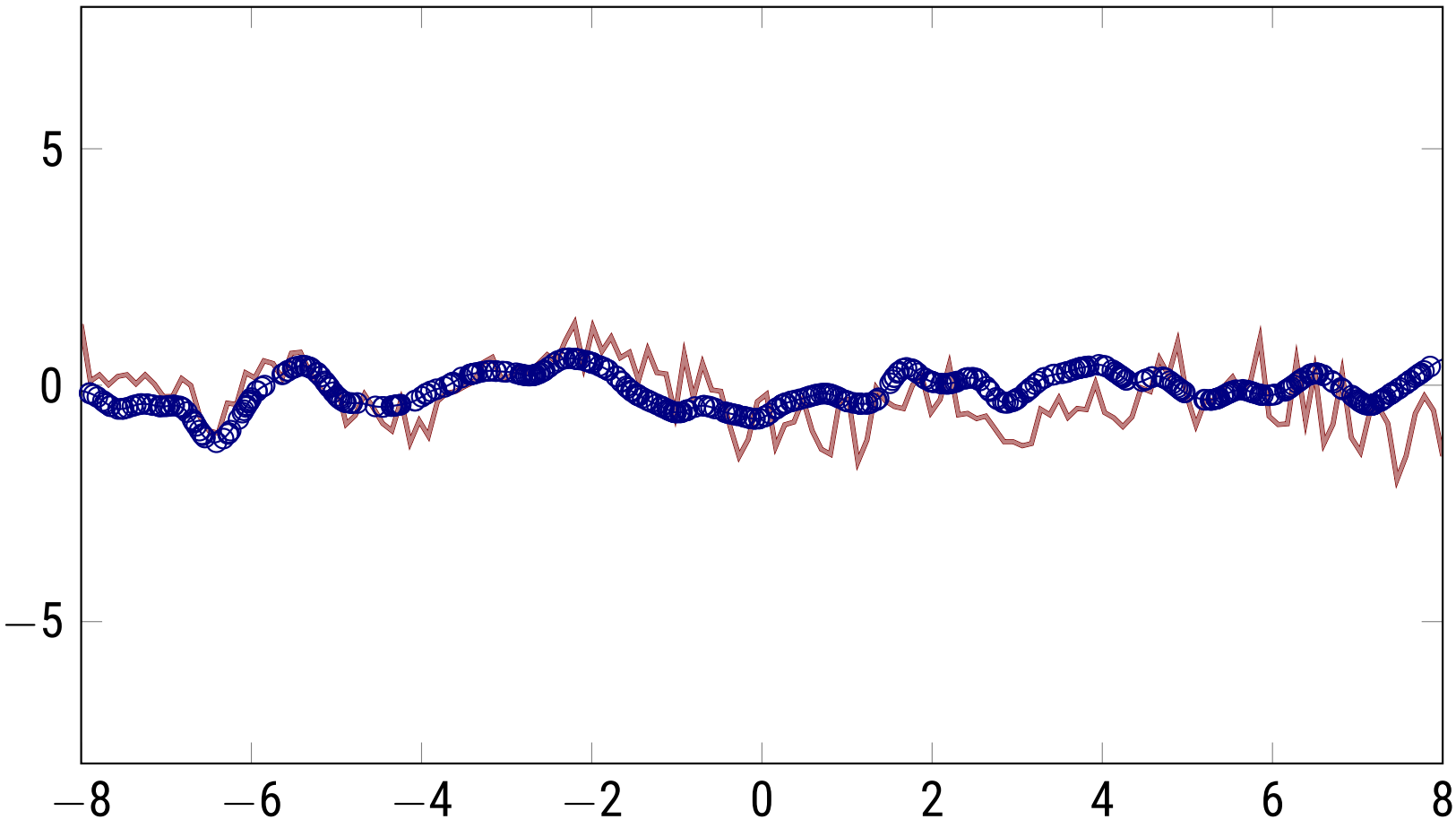
Universal RKHSs

an experiment – 100 evaluations



Universal RKHSs

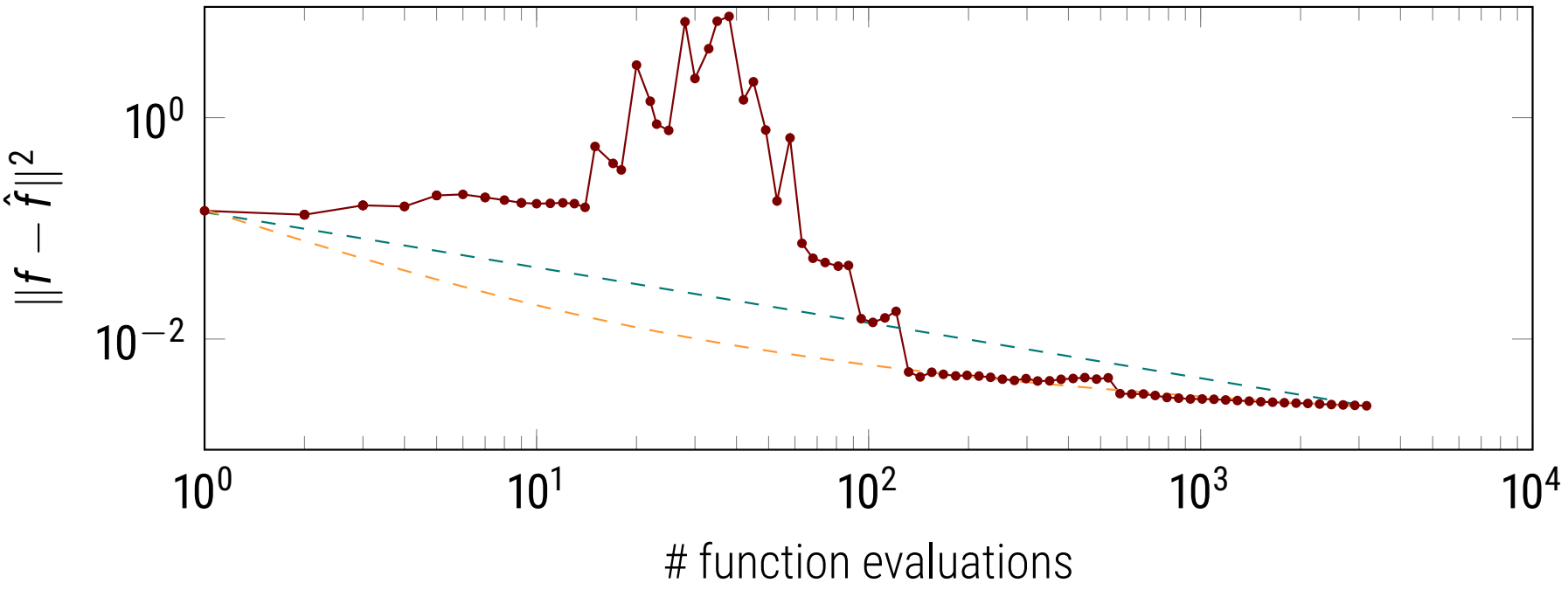
an experiment – 500 evaluations



Convergence Rates are Important

non-obvious aspects of f can ruin convergence

v.d.Vaart & v.Zanten, 2011



If f is "not well represented" by the kernel (has low prior density), the number of datapoints required to achieve ϵ error can be exponential in ϵ. Outside of the observation range, there are no guarantees at all.

An Analogy

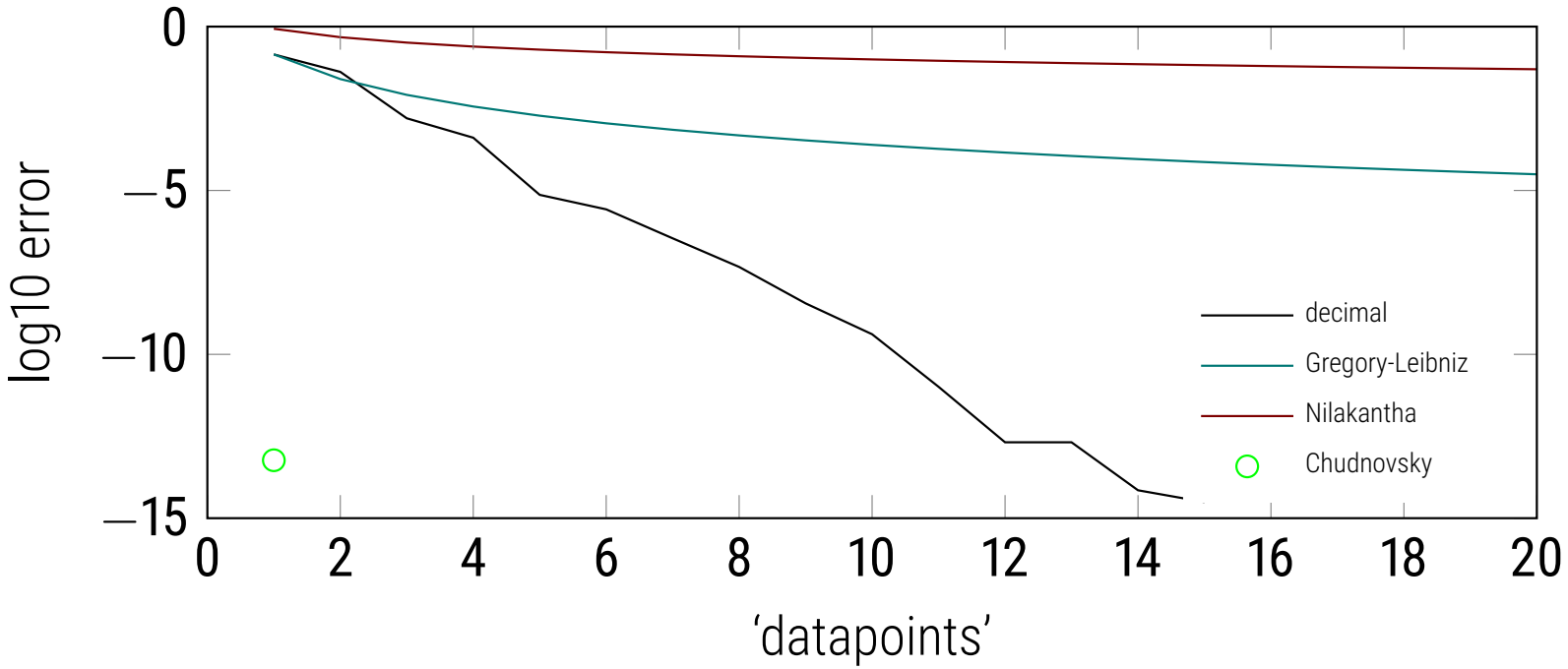
representing π in $\mathbb{Q}$

- $\mathbb{Q}$ is dense in $\mathbb{R}$

$$\pi = 3 \cdot \frac{1}{1} + 1 \cdot \frac{1}{10} + 4 \cdot \frac{1}{100} + 1 \cdot \frac{1}{1000} + \ldots \qquad \text{decimal}$$

$$= 4 \cdot \frac{1}{1} - 4 \cdot \frac{1}{3} + 4 \cdot \frac{1}{5} - 4 \cdot \frac{1}{7} + \ldots \qquad \text{Gregory-Leibniz}$$

$$= 3 \cdot \frac{1}{1} + 4 \cdot \frac{1}{2 \cdot 3 \cdot 4} - 4 \cdot \frac{1}{4 \cdot 5 \cdot 6} + 4 \cdot \frac{1}{6 \cdot 7 \cdot 8} \qquad \text{Nilakantha}$$



- Gaussian measures turn probabilistic inference into **linear algebra**
- Gaussian measures can be used to infer **functions** and **curves**
- In fact, the number of inferred features / weights can be **infinite**
- The choice of kernel / GP prior affects **model capacity** and **convergence**

next up:

- **Gauss-Markov processes**: fast probabilistic inference
- **Solving Ordinary Differential Equations** with GPs

These slides can be found at
`http://tinyurl.com/Dobbiaco-Hennig-1`

What does the GP **prior** mean?

Effect of kernel on samples

Theorem [Adler, 1981]

A stochastic process (a random field) over $\mathbb{X}$ is continuous in mean square at $x \in \mathbb{X}$ if, and only if, its covariance function $k(a, b)$ is continuous at $a = b = x$.

Continuous in mean square at x_*:

$$\mathrm{E}[|f(x_k) - f(x_*)|^2] \to 0$$

for any sequence x_k that converges to x_*.

$\Rightarrow$ "a GP is as often differentiable as the kernel at $x = a = b$."

but: continuity of individual samples is more tricky.

much more detail in Adler, *The geometry of random fields*. Wiley, 1981.