# Gaussian Processes - Part I
# The Linear Algebra of Inference

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# Carl Friedrich Gauss (1777–1855)

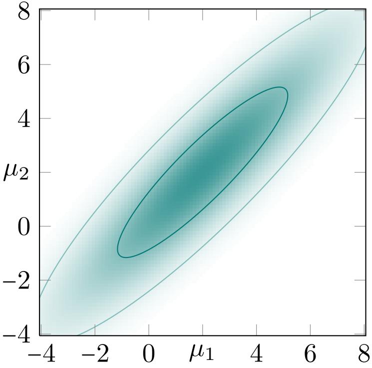
## Paying Tolls with A Bell

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

# The Gaussian distribution

## Multivariate Form

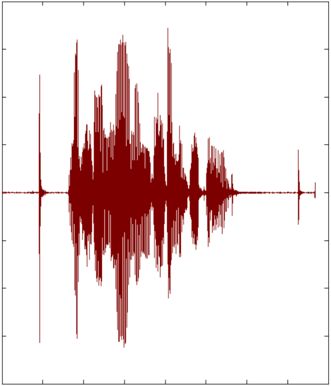
$$\mathcal{N}(x;\mu,\Sigma) = \frac{1}{(2\pi)^{N/2}|\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu)^\top\Sigma^{-1}(x-\mu)\right]$$

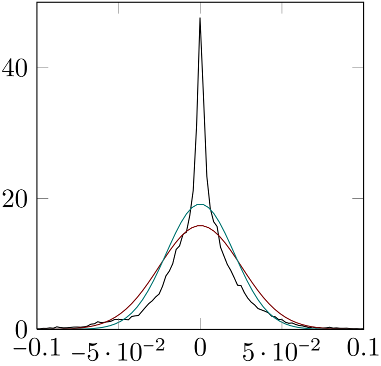



- $x, \mu \in \mathbb{R}^N$, $\Sigma \in \mathbb{R}^{N\times N}$
- $\Sigma$ is positive semidefinite, i.e.
  - $v^\top \Sigma v \geq 0$ for all $v \in \mathbb{R}^N$
  - Hermitian, all eigenvalues $\geq 0$

# Why Gaussian?

an experiment






- nothing in the real world is Gaussian (except sums of i.i.d. variables)
- But nothing in the real world is linear either!

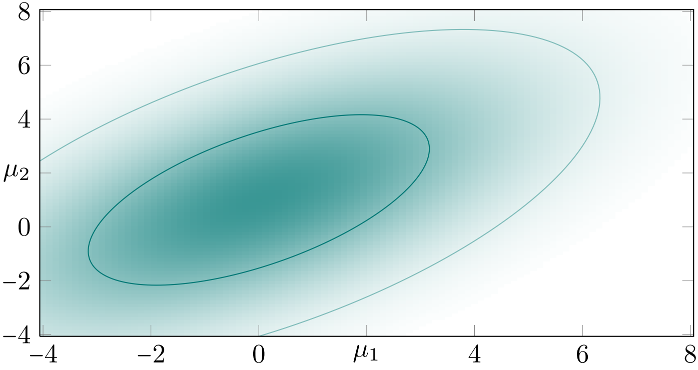
Gaussians are for inference what linear maps are for algebra.

# Closure Under Multiplication

multiple Gaussian factors form a Gaussian

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

$$C := (A^{-1} + B^{-1})^{-1} \qquad c := C(A^{-1}a + B^{-1}b)$$



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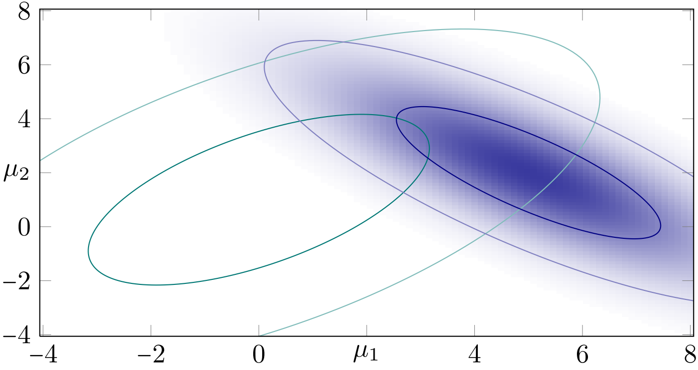

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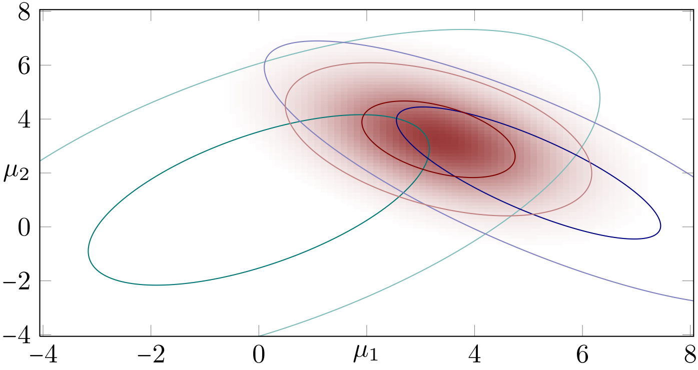
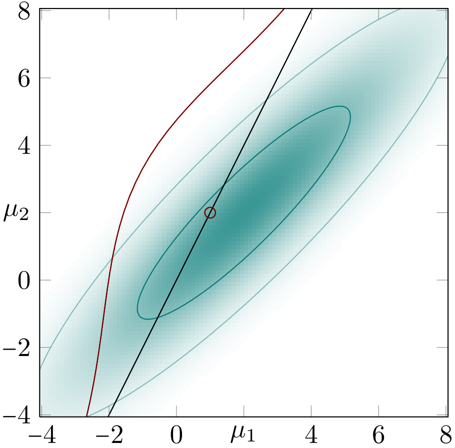


# Closure under Linear Maps

## Linear Maps of Gaussians are Gaussians




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

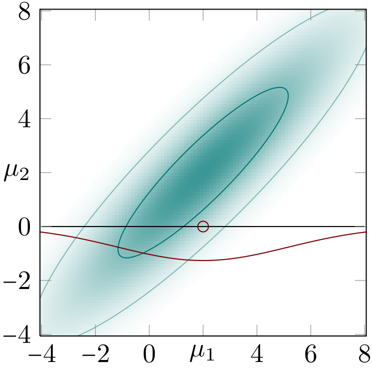
Here: $A = [1, -0.5]$

# Closure under Marginalization

projections of Gaussians are Gaussian

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

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




- this is the sum rule

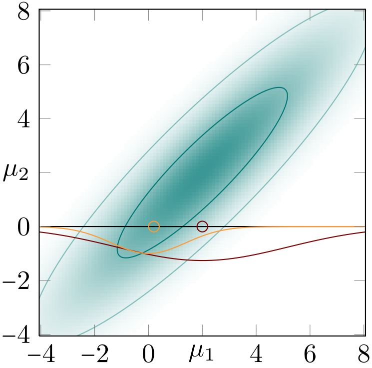
$$\int p(x, y)\, \mathrm{d}y = \int p(y \mid x) p(x)\, \mathrm{d}y = p(x)$$

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

# Closure under Conditioning

cuts through Gaussians are Gaussians

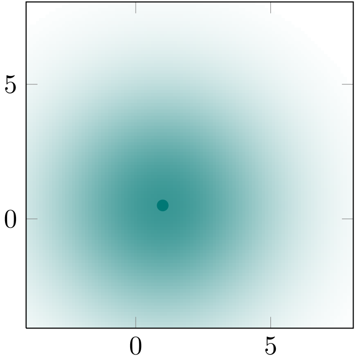
$$p(x \mid y) = \frac{p(x,y)}{p(y)} = \mathcal{N}\left(x; \mu_x + \Sigma_{xy}\Sigma_{yy}^{-1}(y - \mu_y), \Sigma_{xx} - \Sigma_{xy}\Sigma_{yy}^{-1}\Sigma_{yx}\right)$$




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

# Bayesian Inference

## explaining away

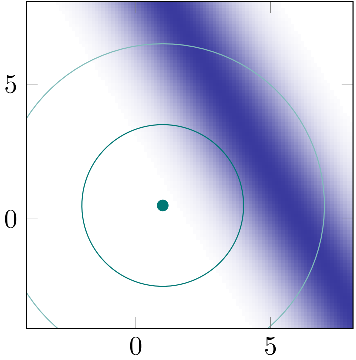



$$p(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu}, \Sigma)$$

$$= \mathcal{N}\left[\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}; \begin{pmatrix} 1 \\ 0.5 \end{pmatrix}, \begin{pmatrix} 3^2 & 0 \\ 0 & 3^2 \end{pmatrix}\right]$$

# Bayesian Inference

explaining away

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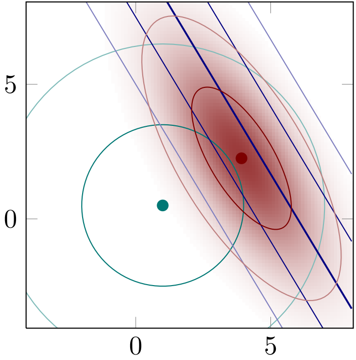
$$p(y \mid \boldsymbol{x}, \sigma) = \mathcal{N}(y; A^\top x; \sigma^2)$$
$$= \mathcal{N}\left[6; \begin{pmatrix} 1 & 0.6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \sigma^2\right]$$

# Bayesian Inference

## explaining away

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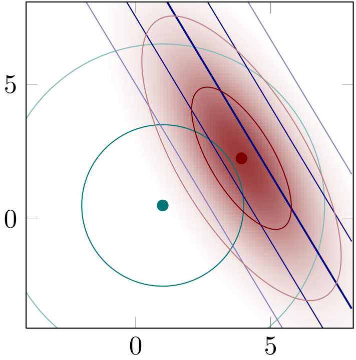
$$p(\boldsymbol{x} \mid \sigma^2, y) = \frac{p(\boldsymbol{x}) p(y \mid \boldsymbol{x})}{p(\boldsymbol{x})}$$

# Bayesian Inference

explaining away

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$$p(\boldsymbol{x} \mid \sigma^2, y) = \frac{p(\boldsymbol{x}) p(y \mid \boldsymbol{x})}{p(\boldsymbol{x})}$$

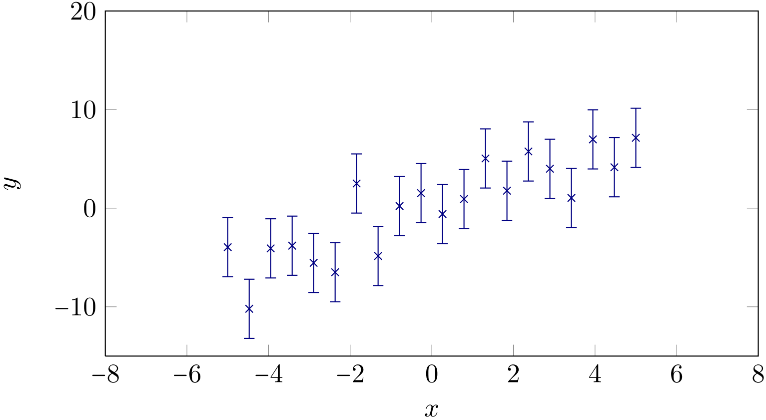
$$= \mathcal{N}(\boldsymbol{x}; \boldsymbol{\mu} + \Sigma A (A^\top \Sigma A + \sigma^2)^{-1} (y - A^\top \mu), \Sigma - \Sigma A (A^\top \Sigma A + \sigma^2)^{-1} A^\top \Sigma)$$

$$= \mathcal{N}\left[\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}; \begin{pmatrix} 3.9 \\ 2.3 \end{pmatrix}, \begin{pmatrix} 3.4 & -3.4 \\ -3.4 & 7.0 \end{pmatrix}\right]$$

# What can we do with this?

## linear regression

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

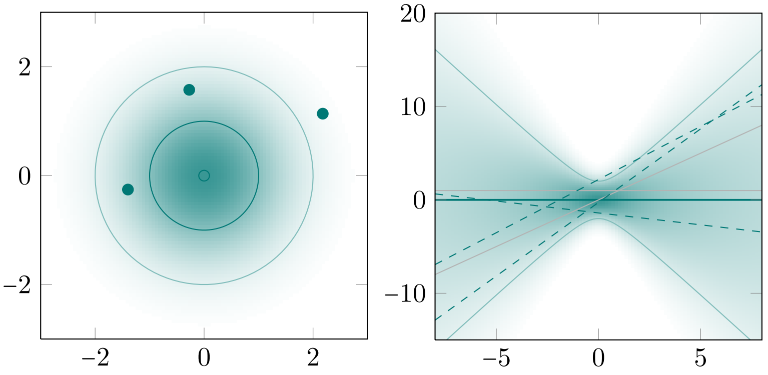


# A prior

## over linear functions

$$f(x) = w_1 + w_2 x = \phi_x^\top w \qquad p(w) = \mathcal{N}(w; \mu, \Sigma)$$

$$\phi_x = \begin{pmatrix} 1 \\ x \end{pmatrix} \qquad p(f) = \mathcal{N}(f; \phi_x^\top \mu, \phi_x^\top \Sigma \phi_x)$$



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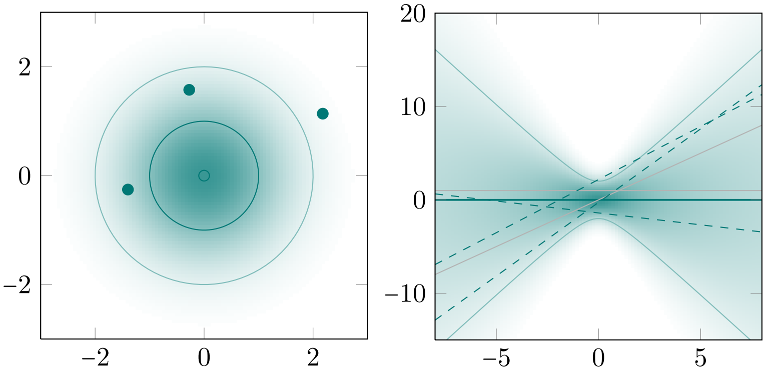
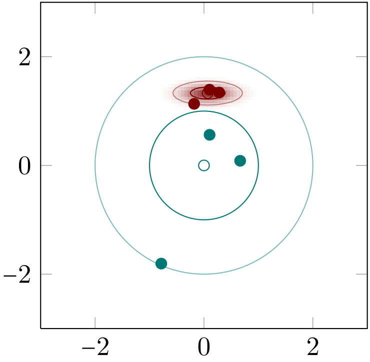
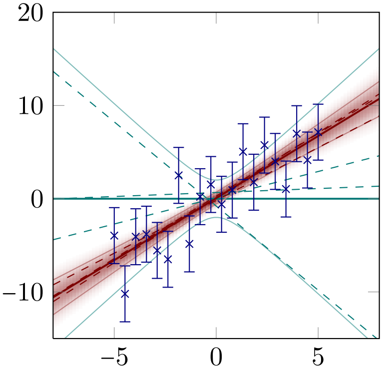


# The posterior

over linear functions

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



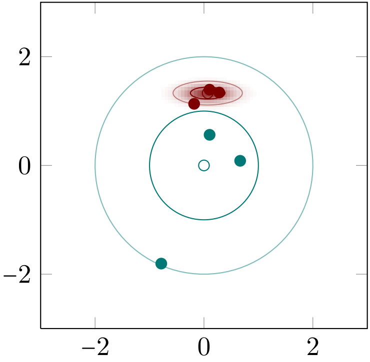



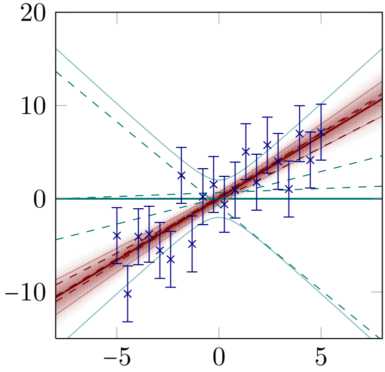
# The posterior

over linear functions

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

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



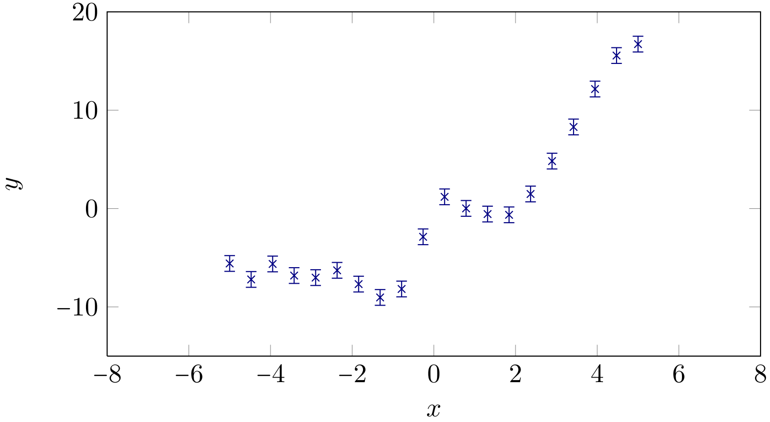



```
% prior on $w$
F     = 2;                                   % number of features
phi   = @(a)(bsxfun(@power,a,0:F-1));        % $\phi(a) = [1; a]$
mu    = zeros(F,1);
Sigma = eye(F);                              % $p(w) = \mathcal{N}(\mu, \Sigma)$

% prior on $f(x)$
n     = 100; x = linspace(-6,6,n)';          % 'test' points
phix  = phi(x);                              % features of $x$
m     = phix * mu;
kxx   = phix * Sigma * phix';                % $p(f_x) = \mathcal{N}(m, k_{xx})$
s     = bsxfun(@plus,m,chol(kxx + 1.0e-8 * eye(n))' * randn(n,3));  % samples from prior
stdpi = sqrt(diag(kxx));                     % marginal stddev, for plotting

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

% prior on $Y = f_X + \epsilon$
phiX  = phi(X);                              % features of data
M     = phiX * mu;
kXX   = phiX * Sigma * phiX';                % $p(f_X) = \mathcal{N}(M, k_{XX})$

G     = kXX + sigma^2 * eye(N);              % $p(Y) = \mathcal{N}(M, k_{XX} + \sigma^2 I)$
R     = chol(G);                             % most expensive step: $\mathcal{O}(N^3)$

kxX   = phix * Sigma * phiX';                % $\mathrm{cov}(f_x, f_X) = k_{xX}$
A     = kxX / R;                             % pre-compute for re-use

mpost = m + A * (R' \ (Y-M));   % $p(f_x | Y) = \mathcal{N}(m + k_{xX}(k_{XX} + \sigma^2 I)^{-1}(Y - M),$
vpost = kxx - A * A';           % $k_{xx} - k_{xX}(k_{XX} + \sigma^2 I)^{-1} k_{Xx})$
spost = bsxfun(@plus,mpost,chol(vpost + 1.0e-8 * eye(n))' * randn(n,3));    % samples

stdpo = sqrt(diag(vpost));                   % marginal stddev, for plotting
```

# A More Realistic Dataset

General Linear Regression

$$f(x) = \phi_x^\top w \qquad ?$$



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

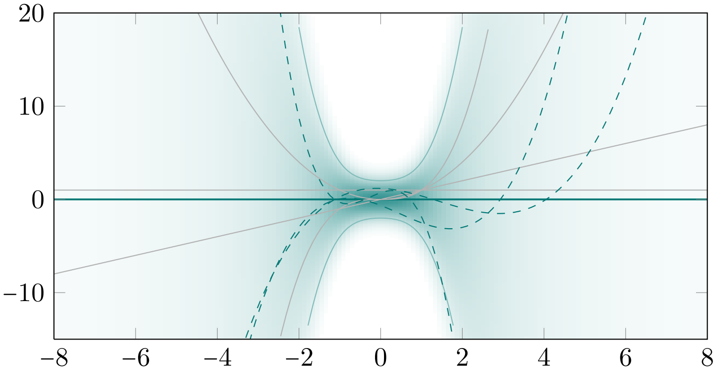
$$\phi_x := \begin{pmatrix} 1 \\ x \end{pmatrix}$$

```
% 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) = \mathcal{N}(\mu, \Sigma)

% prior on f(x)
n     = 100; x = linspace(-6,6,n)';                                 % 'test' points
phix  = phi(x);                                                     % features of x
m     = phix * mu;
kxx   = phix * Sigma * phix';                                       % p(f_x) = \mathcal{N}(m, k_{xx})
s     = bsxfun(@plus,m,chol(kxx + 1.0e-8 * eye(n))' * randn(n,3));  % samples from prior
stdpi = sqrt(diag(kxx));                                            % marginal stddev, for plotting

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

% prior on Y = f_X + \epsilon
phiX  = phi(X);                                                     % features of data
M     = phiX * mu;
kXX   = phiX * Sigma * phiX';                                       % p(f_X) = \mathcal{N}(M, k_{XX})

G     = kXX + sigma^2 * eye(N);                                     % p(Y) = \mathcal{N}(M, k_{XX} + \sigma^2 I)
R     = chol(G);                                                    % most expensive step: \mathcal{O}(N^3)

kxX   = phix * Sigma * phiX';                                       % cov(f_x, f_X) = k_{xX}
A     = kxX / R;                                                    % pre-compute for re-use

mpost = m + A * (R' \ (Y-M));          % p(f_x | Y) = \mathcal{N}(m + k_{xX}(k_{XX} + \sigma^2 I)^{-1}(Y - M),
vpost = kxx - A * A';                                               % k_{xx} - k_{xX}(k_{XX} + \sigma^2 I)^{-1} k_{Xx})
spost = bsxfun(@plus,mpost,chol(vpost + 1.0e-8 * eye(n))' * randn(n,3));   % samples

stdpo = sqrt(diag(vpost));                                          % marginal stddev, for plotting
```

# Cubic Regression

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

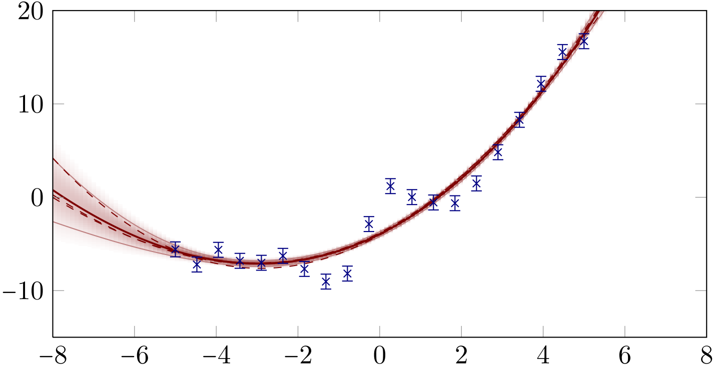
$$f(x) = \phi(x)^\intercal w \qquad \phi(x) = \begin{pmatrix} 1 & x & x.^2 & x.^3 \end{pmatrix}^\intercal$$



# Cubic Regression

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

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



# Septic Regression ?

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

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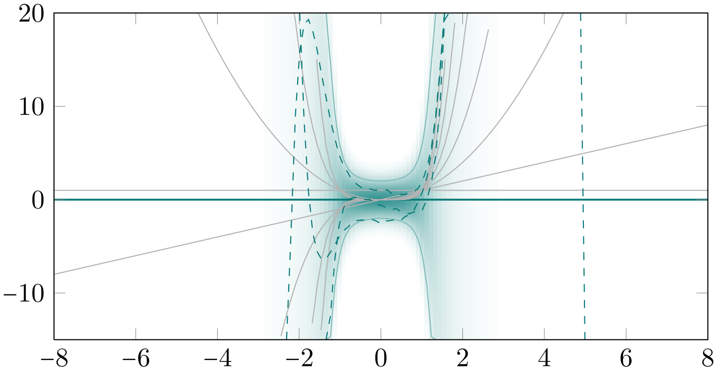

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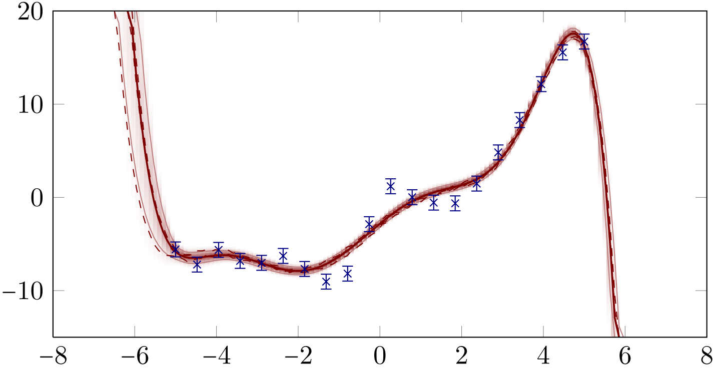
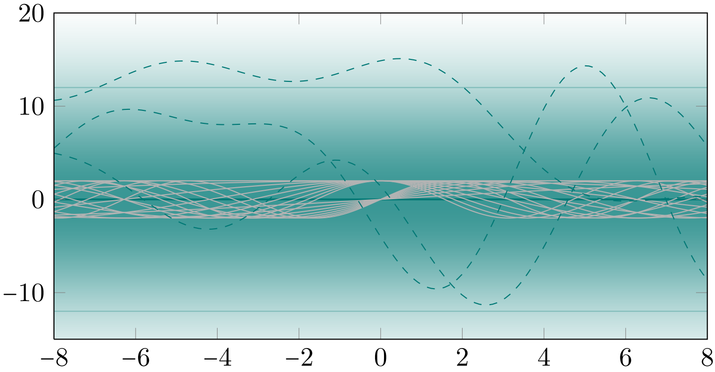


# Fourier Regression

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

$$\phi(x) = \begin{pmatrix}\cos(x) & \cos(2x) & \cos(3x) & \dots & \sin(x) & \sin(2x) & \dots\end{pmatrix}^\top$$



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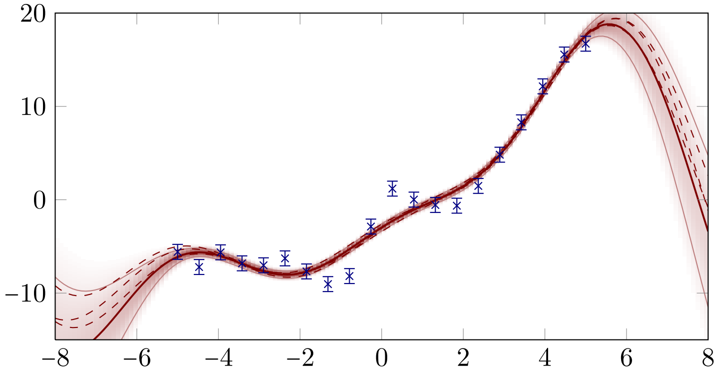
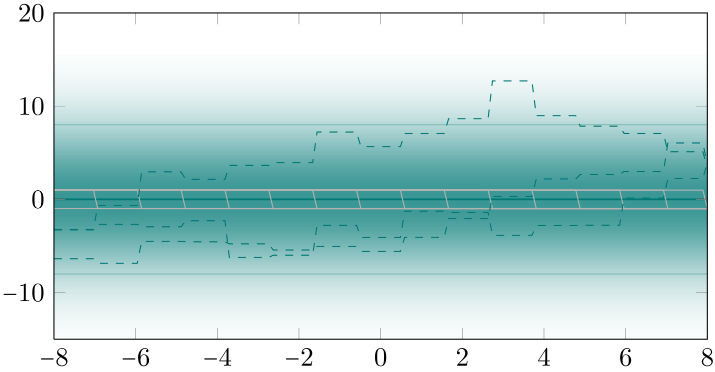


# Step Regression

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

$$\phi(x) = -1 + 2\left(\theta(x-8) \quad \theta(8-x) \quad \theta(x-7) \quad \theta(7-x) \quad \dots\right)^\top$$



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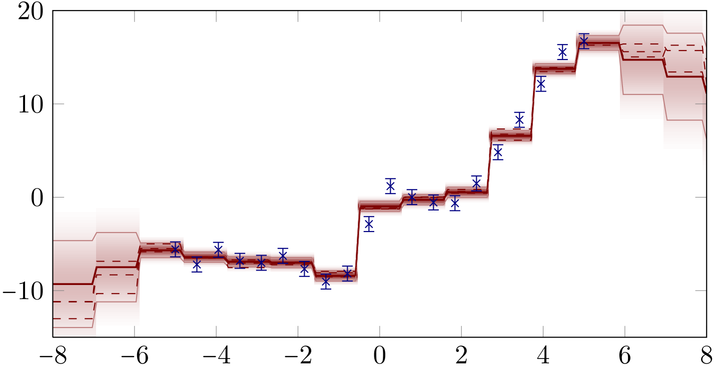
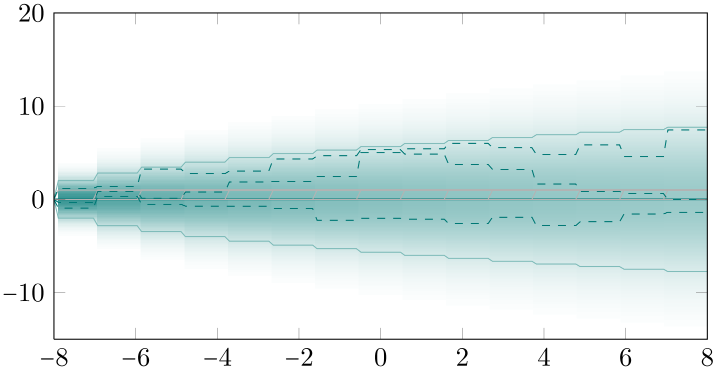


# Another Kind of Step Regression

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

$$\phi(x) = \begin{pmatrix} \theta(x-8) & \theta(8-x) & \theta(x-7) & \theta(7-x) & \ldots \end{pmatrix}^\top$$



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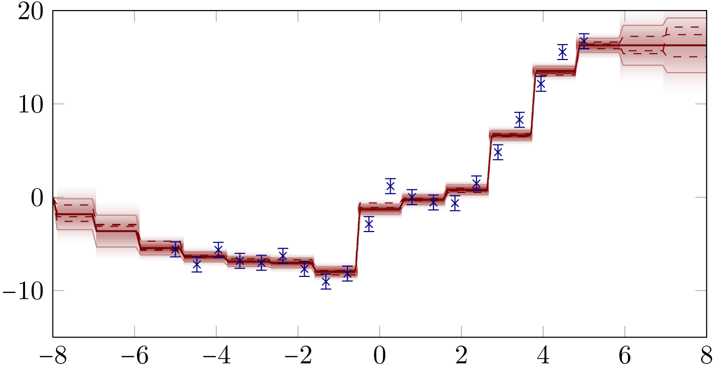
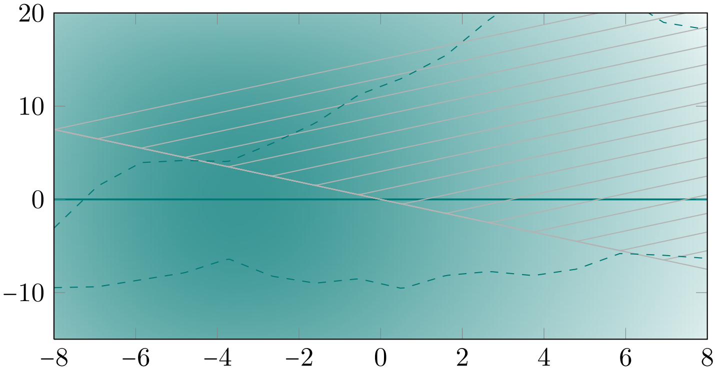


# V Regression

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

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



# V Regression

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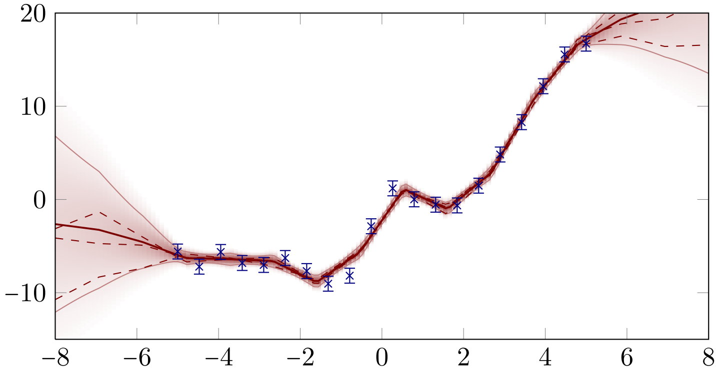
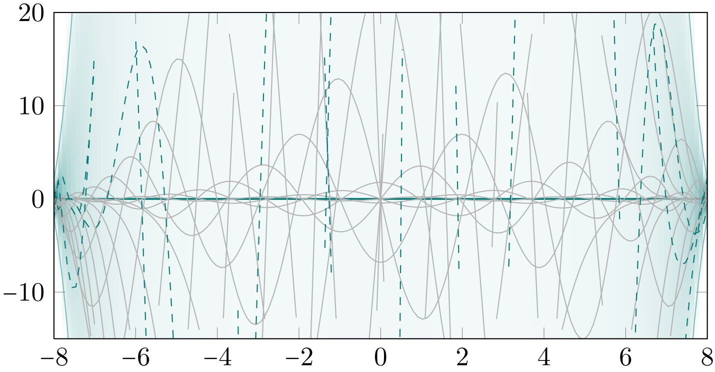


# Legendre Regression

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

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



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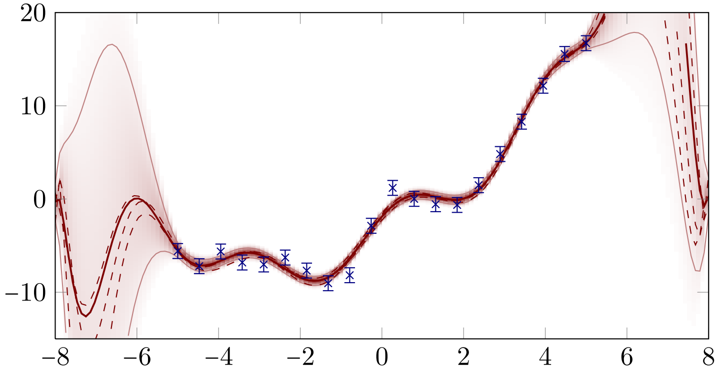
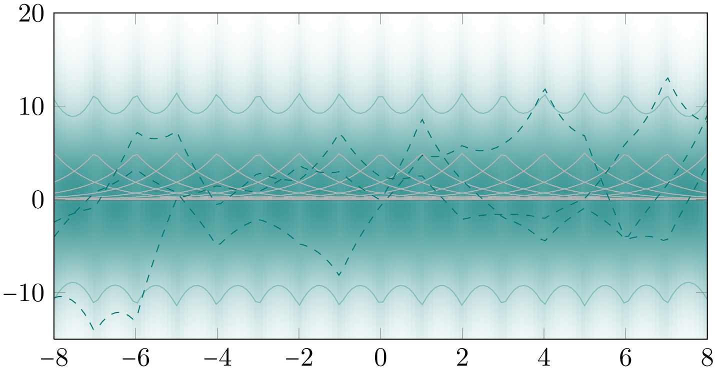


# Eiffel Tower Regression

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

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



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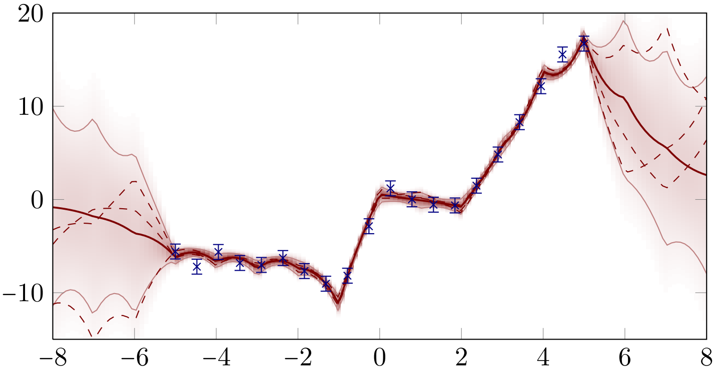
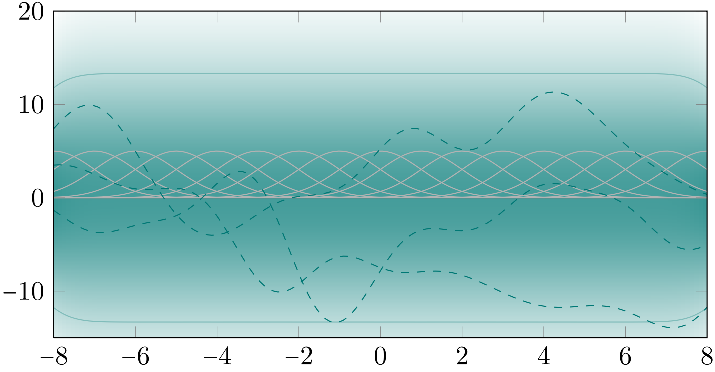


# Bell Curve Regression

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

$$\phi(x) = \left(e^{-\frac{1}{2}(x-8)^2} \quad e^{-\frac{1}{2}(x-7)^2} \quad e^{-\frac{1}{2}(x-6)^2} \quad \dots\right)^\intercal$$



# Bell Curve Regression

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

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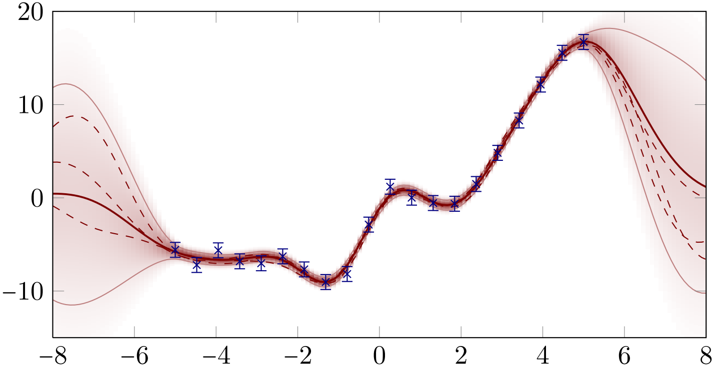
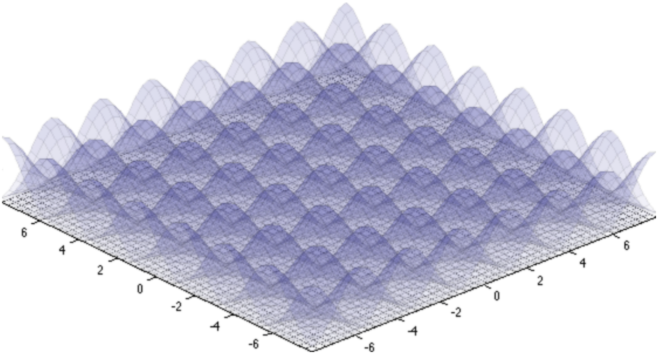


# Multiple Inputs

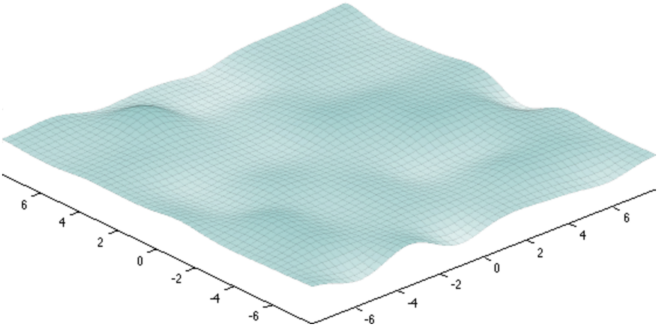
all this works for in multiple dimensions, too

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



# Multiple Inputs

all this works for in multiple dimensions, too

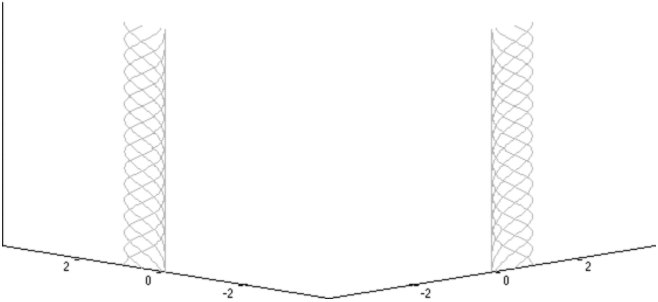


# Multiple Outputs

slightly more confusing, but no algebraic problem

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

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



# Multiple Outputs

learning paths

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

- $[f_1(t_1), \dots, f_1(t_N), f_2(t_1), \dots, f_2(t_N), \dots, f_M(t_1), \dots f_M(t_N)]$ are just some co-varying Gaussian variables
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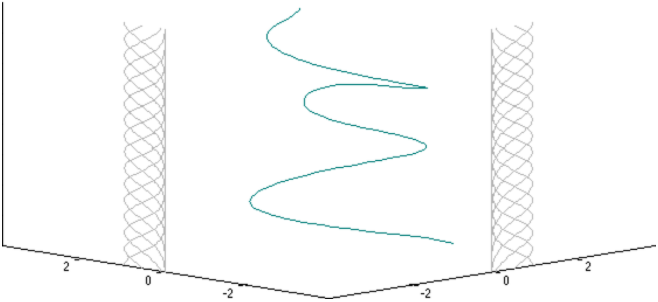
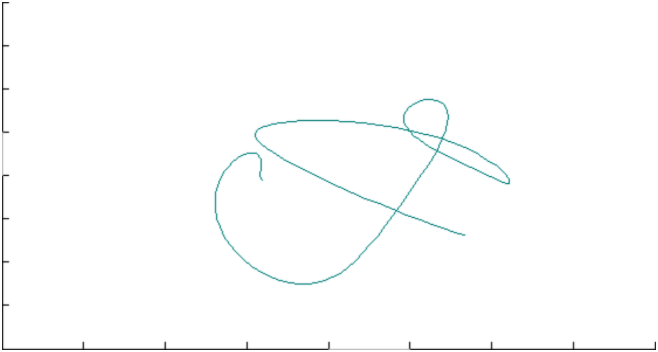


# Multiple Outputs

learning paths

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

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



# How many features should we use?

let's look at that algebra again

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

- there's no lonely $\phi$ in there
- all objects involving $\phi$ are of the form
  - $\phi^\top \mu$ — the mean function
  - $\phi^\top \Sigma \phi$ — the kernel
- once these are known, cost is independent of the number of features
- remember the code:

```
M      = phiX * mu;
m      = phix * mu;
kXX    = phiX * Sigma * phiX';                    % p(f_X) = N(M, k_XX)
kxx    = phix * Sigma * phix';                    % p(f_x) = N(m, k_xx)

kxX    = phix * Sigma * phiX';                    % cov(f_x, f_X) = k_xX
```

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

% prior on f(x)
n     = 100; x = linspace(-6,6,n)';                               % 'test' points
phix  = phi(x);                                                   % features of x
m     = phix * mu;
kxx   = phix * Sigma * phix';                                     % p(f_x) = N(m, k_xx)
s     = bsxfun(@plus,m,chol(kxx + 1.0e-8 * eye(n))' * randn(n,3)); % samples from prior
stdpi = sqrt(diag(kxx));                                          % marginal stddev, for plotting

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

% prior on Y = f_X + ε
phiX  = phi(X);                                                   % features of data
M     = phiX * mu;
kXX   = phiX * Sigma * phiX';                                     % p(f_X) = N(M, k_XX)

G     = kXX + sigma^2 * eye(N);                                   % p(Y) = N(M, k_XX + σ^2 I)
R     = chol(G);                                                  % most expensive step: O(N^3)

kxX   = phix * Sigma * phiX';                                     % cov(f_x, f_X) = k_xX
A     = kxX / R;                                                  % pre-compute for re-use

mpost = m + A * (R' \ (Y-M));              % p(f_x | Y) = N(m + k_xX (k_XX + σ^2 I)^-1 (Y − M),
vpost = kxx - A * A';                                             % k_xx − k_xX (k_XX + σ^2 I)^-1 k_Xx)
spost = bsxfun(@plus,mpost,chol(vpost + 1.0e-8 * eye(n))' * randn(n,3));   % samples

stdpo = sqrt(diag(vpost));                                        % marginal stddev, for plotting
```

```
% prior
F     = 2;                                                   % number of features
phi   = @(a)(bsxfun(@power,a,0:F));                          % $\phi(a) = [1;a]$
k     = @(a,b)(phi(a)' * phi(b));                            % kernel
mu    = @(a)(zeros(size(a,1)));                              % mean function

% belief on $f(x)$
n     = 100; x = linspace(-6,6,n)';                          % 'test' points
m     = mu(x);
kxx   = k(x,x);                                              % $p(f_x) = \mathcal{N}(m, k_{xx})$
s     = bsxfun(@plus,m,chol(kxx + 1.0e-8 * eye(n))' * randn(n,3));  % samples from prior
stdpi = sqrt(diag(kxx));                                     % marginal stddev, for plotting

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

% prior on $Y = f_X + \epsilon$
M     = mu(X);
kXX   = k(X,X);                                              % $p(f_X) = \mathcal{N}(M, k_{XX})$

G     = kXX + sigma^2 * eye(N);                              % $p(Y) = \mathcal{N}(M, k_{XX} + \sigma^2 I)$
R     = chol(G);                                             % most expensive step: $\mathcal{O}(N^3)$

kxX   = k(x,X);                                              % $\mathrm{cov}(f_x, f_X) = k_{xX}$
A     = kxX / R;                                             % pre-compute for re-use

mpost = m + A * (R' \ (Y-M));            % $p(f_x \mid Y) = \mathcal{N}(m + k_{xX}(k_{XX} + \sigma^2 I)^{-1}(Y - M),$
vpost = kxx - A * A';                    % $k_{xx} - k_{xX}(k_{XX} + \sigma^2 I)^{-1} k_{Xx})$
spost = bsxfun(@plus,mpost,chol(vpost + 1.0e-8 * eye(n))' * randn(n,3));   % samples

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 $\Sigma = \frac{\sigma^2(c_{\max}-c_{\min})}{F} I$
- The elements of $\phi_x^\top \Sigma \phi_x$ are

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

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

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

$$\begin{aligned}
&\phi(x_i)^\top \Sigma \phi(x_j) \\
&= \frac{\sigma^2(c_{\max}-c_{\min})}{F} \sum_{\ell=1}^{F} \exp\left(-\frac{(x_i-c_\ell)^2}{2\lambda^2}\right) \exp\left(-\frac{(x_j-c_\ell)^2}{2\lambda^2}\right) \\
&= \frac{\sigma^2(c_{\max}-c_{\min})}{F} \exp\left(-\frac{(x_i-x_j)^2}{4\lambda^2}\right) \sum_{\ell}^{F} \exp\left(-\frac{(c_\ell-\frac{1}{2}(x_i+x_j))^2}{\lambda^2}\right)
\end{aligned}$$

# Features are cheap, so let's use a lot

an example

DJC MacKay, 1998

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

- now increase $F$, such that # of features in $\delta c$ becomes $\frac{F \cdot \delta c}{(c_{\max} - c_{\min})}$

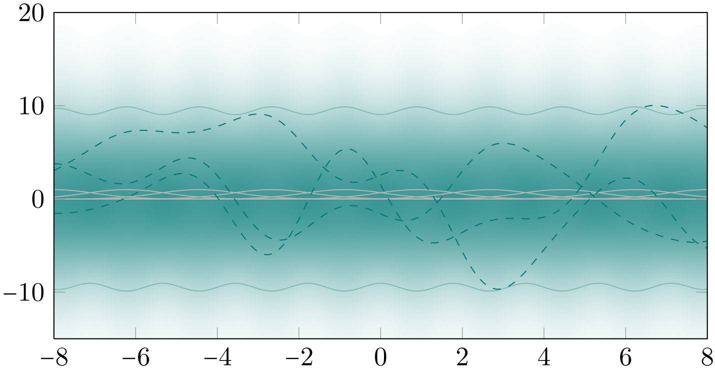
$$\phi(x_i)^\top \Sigma \phi(x_j) \to \sigma^2 \exp\left(-\frac{(x_i - x_j)^2}{4\lambda^2}\right) \int_{c_{\min}}^{c_{\max}} \exp\left(-\frac{(c - \frac{1}{2}(x_i + x_j))^2}{\lambda^2}\right) \mathrm{d}c$$

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

$$\phi(x_i)^\top \Sigma \phi(x_j) \to \sqrt{2\pi} \lambda \sigma^2 \exp\left(-\frac{(x_i - x_j)^2}{4\lambda^2}\right)$$

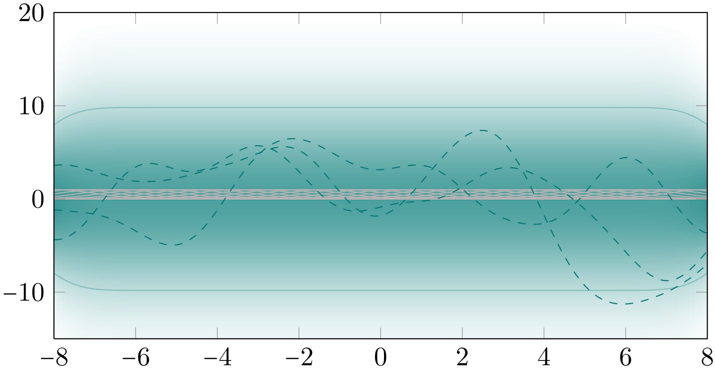
# Exponentiated Squares

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



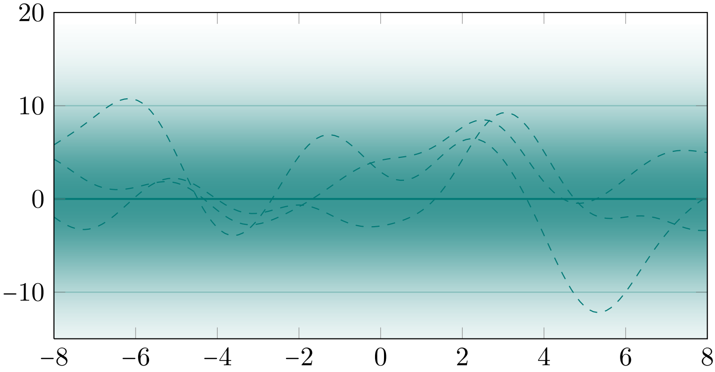
# Exponentiated Squares

```
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

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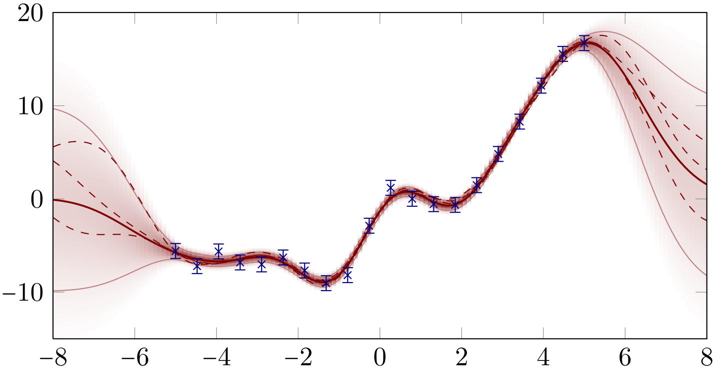



- aka. radial basis function, square(d)-exponential kernel

# What just happened?

*kernelization* to infinitely many features

## Definition

*A function $k : \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{R}$ 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 elements $k_{XX,(i,j)} = k(x_i, x_j)$ is positive semidefinite.*

## Lemma

*Any kernel that can be written as*

$$k(x, x') = \sum\!\!\!\!\!\!\int \phi_\ell(x)\phi_\ell(x')\, d\ell$$

*is a Mercer kernel.* *(assuming integral over positive set)*

**Proof:** $\forall X \in \mathbb{X}^N, v \in \mathbb{R}^N$

$$v^\top k_{XX} v = \sum\!\!\!\!\!\!\int \sum_i^N v_i \phi_\ell(x_i) \sum_j^N v_j \phi_\ell(x_j)\, d\ell = \sum\!\!\!\!\!\!\int \left[\sum_i v_i \phi_\ell(x_i)\right]^2 d\ell \geq 0 \quad \square$$

# What just happened?



## Definition

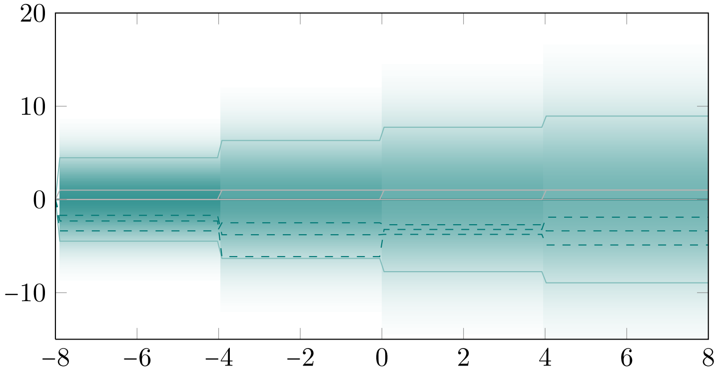
*A function* $k : \mathbb{X} \times \mathbb{X} \to \mathbb{R}$ *is a Mercer kernel if, for any finite collection* $X = [x_1, \dots, x_N]$, *the matrix* $k_{XX} \in \mathbb{R}^{N \times N}$ *with elements* $k_{XX,(i,j)} = k(x_i, x_j)$ *is positive semidefinite.*

## Definition

*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* $p(f_X) = \mathcal{N}(f_X; \mu_X, k_{XX})$.

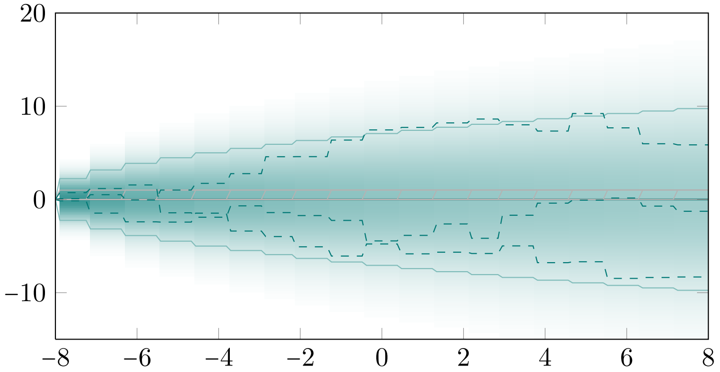
# Those step functions

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



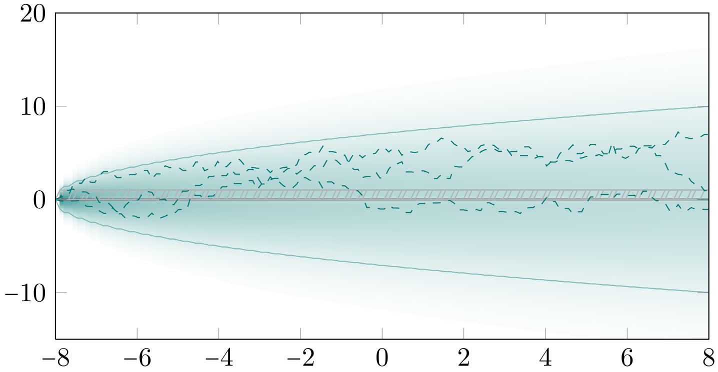
# Those step functions

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



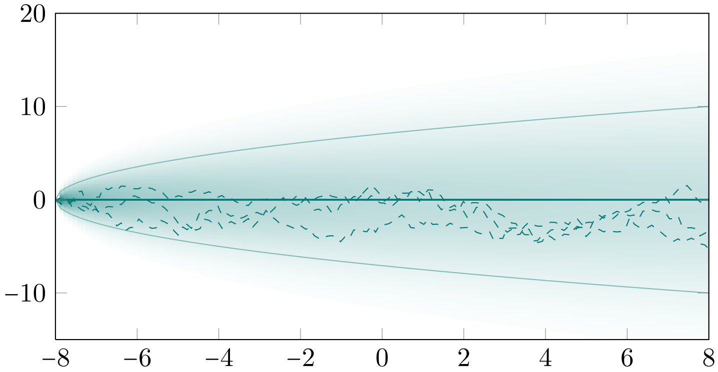
# Those step functions

```
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);
```

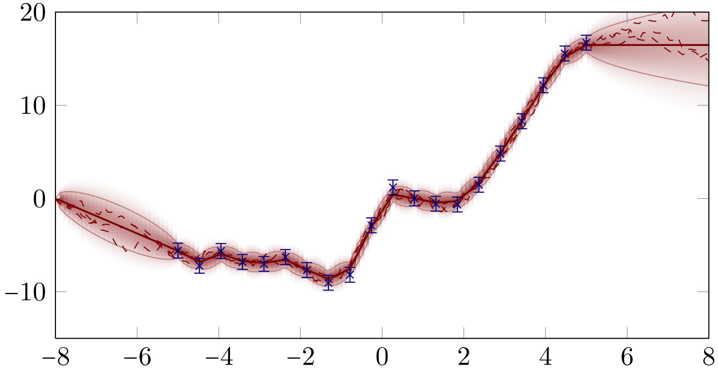


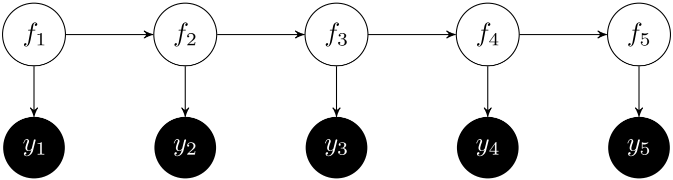

$$\mathrm{cov}(f_{x_i}, f_{x_j}) = \int_{c_{\min}}^{\infty} \theta(x_i - c)\theta(x_j - c)\,\mathrm{d}c = \min(x_i, x_j) - c_{\min}$$

- aka. the Wiener process

# Those step functions

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

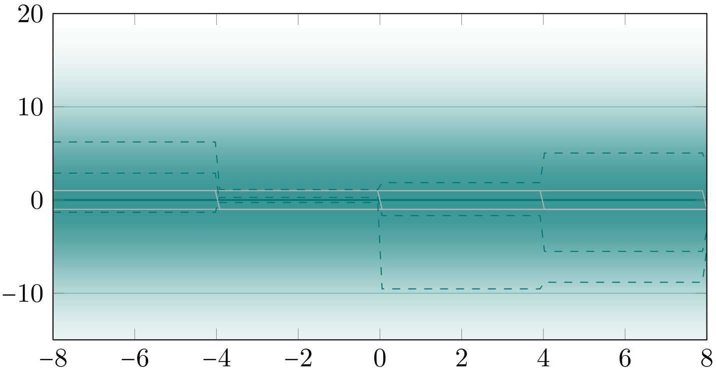


# Those other step-functions

`phi = @(a)(-1 + 2 * bsxfun(@lt,a,linspace(-8,8,5)));`

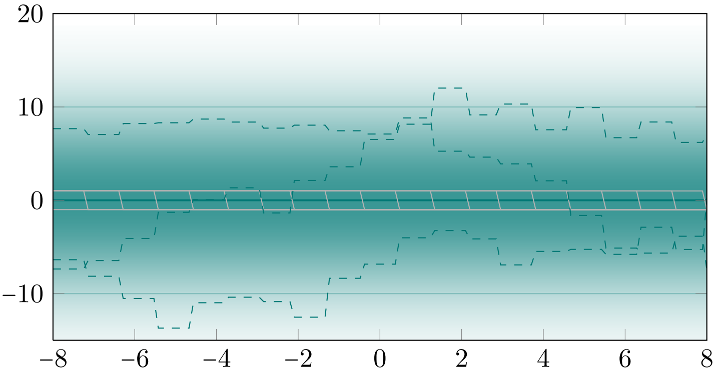
Wahba, 1990



# Those other step-functions

`phi = @(a)(-1 + 2 * bsxfun(@lt,a,linspace(-8,8,20)));`

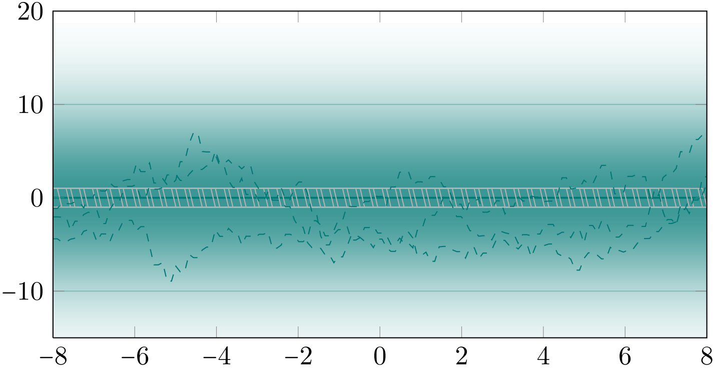
Wahba, 1990



# Those other step-functions

```
phi = @(a)(-1 + 2 * bsxfun(@lt,a,linspace(-8,8,100)));
```

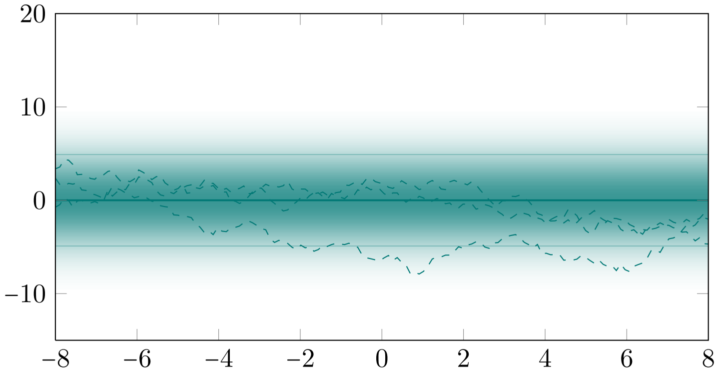
Wahba, 1990



# Those other step-functions

```
k = @(a,b)((1 + c - 2 * c * abs(bsxfun(@minus,a,b')/16)));
```

Wahba, 1990



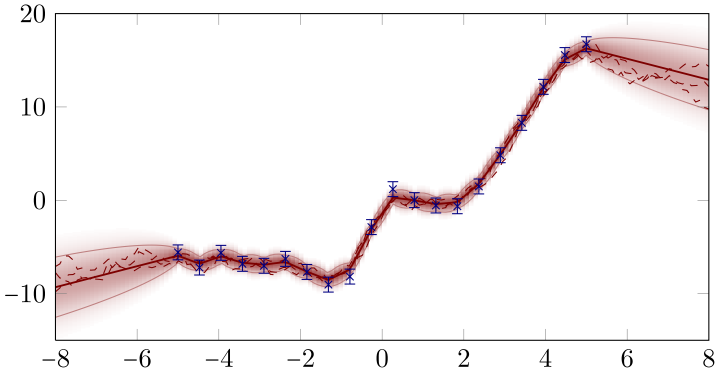

$$\mathrm{cov}(f_{x_i}, f_{x_j}) = 1 + b\int_0^1 (2\theta(x_i - c) - 1)(2\theta(x_j - c) - 1)\,\mathrm{d}c = 1 + b - 2b|x_i - x_j|$$

- aka. linear splines

# Those other step-functions

```
k = @(a,b)((1 + c - 2 * c * abs(bsxfun(@minus,a,b')/16)));
```

Wahba, 1990



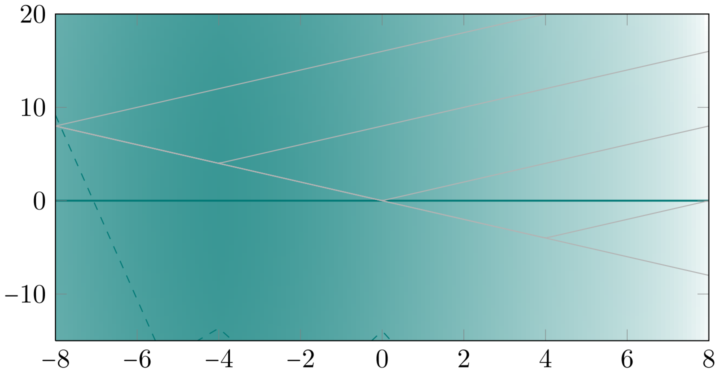

$$\operatorname{cov}(f_{x_i}, f_{x_j}) = 1 + b\int_0^1 (2\theta(x_i - c) - 1)(2\theta(x_j - c) - 1)\,\mathrm{d}c = 1 + b - 2b|x_i - x_j|$$

- aka. linear splines

# Those linear features

Wahba, 1990

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



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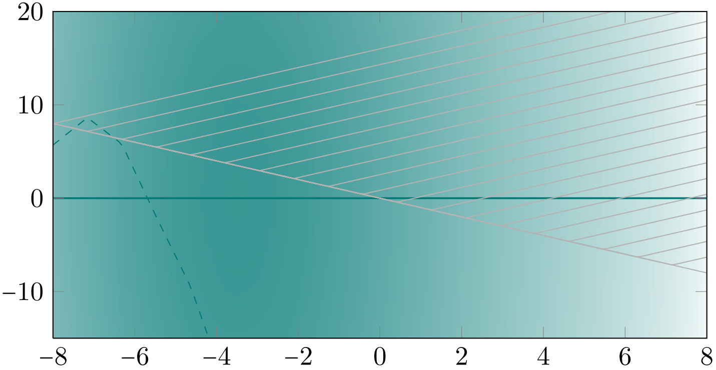
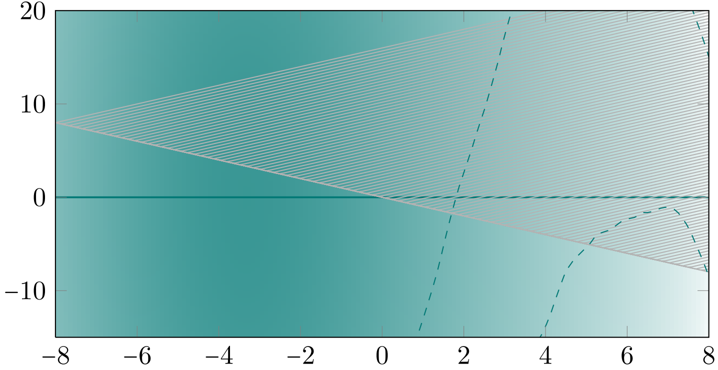


# Those linear features

Wahba, 1990

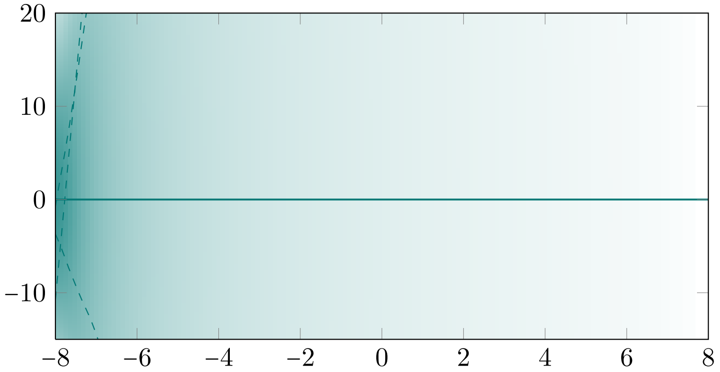
```
phi =
@(a)(bsxfun(@minus,abs(bsxfun(@minus,a,linspace(-8,8,100))),linspace(-8,8,100)));
```



# Those linear features

Wahba, 1990

```
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))));
```




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

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

aka. cubic splines

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Wahba, 1990

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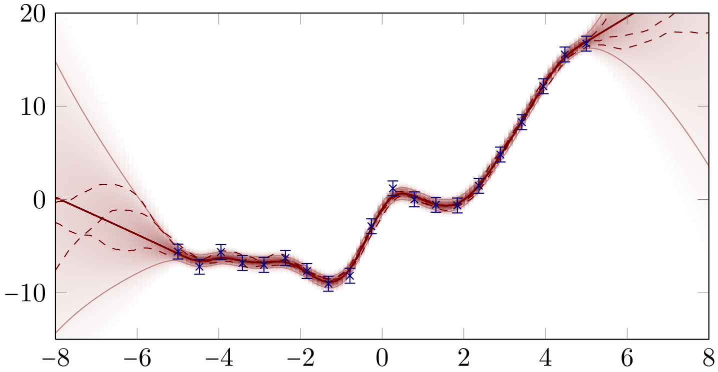
```

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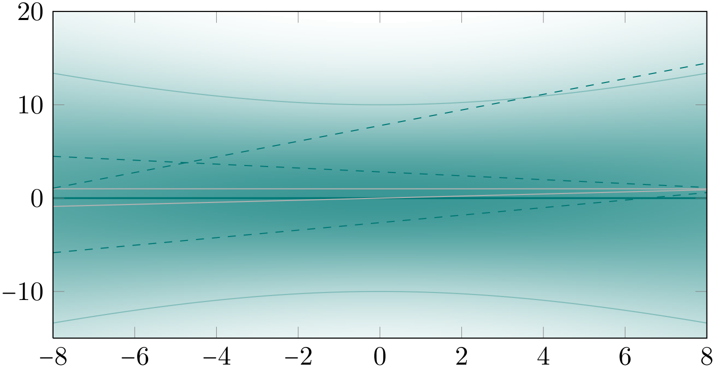
aka. cubic splines

# Exponentially suppressed polynomials

```
phi = @(a)(bsxfun(@times,bsxfun(@power,a./9,[0:1]),c.^[0:1]));
```

Minka, 2000

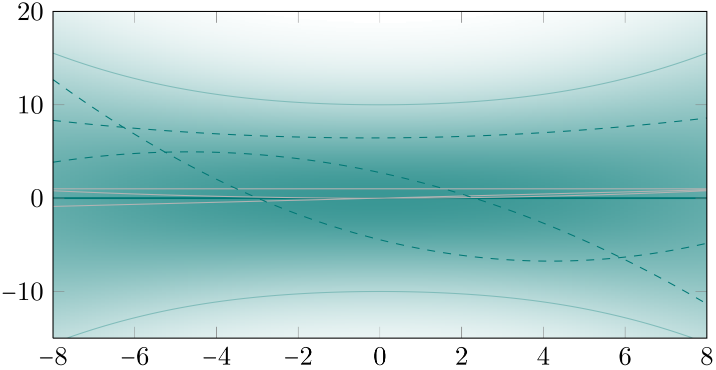



$$\operatorname{cov}(f_{x_i}, f_{x_j}) = \sum_{\ell=0}^{1} b^\ell x_i^\ell x_j^\ell \qquad 0 \leq b \leq 1 \qquad -1 < x_i, x_j < 1$$

# Exponentially suppressed polynomials

```
phi = @(a)(bsxfun(@times,bsxfun(@power,a./9,[0:2]),c.^[0:2]));
```

Minka, 2000

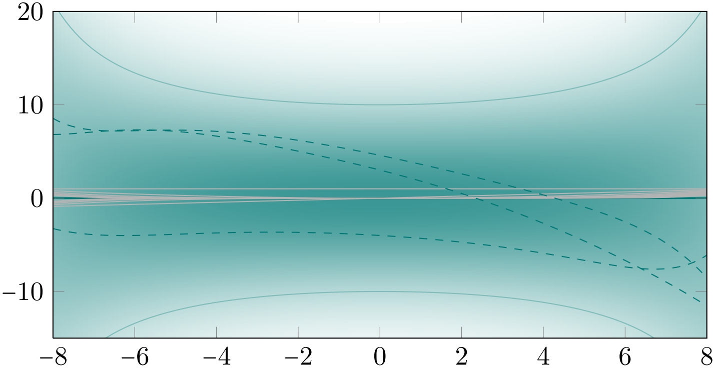



$$\operatorname{cov}(f_{x_i}, f_{x_j}) = \sum_{\ell=0}^{2} b^\ell x_i^\ell x_j^\ell \qquad 0 \leq b \leq 1 \qquad -1 < x_i, x_j < 1$$

# Exponentially suppressed polynomials

```
phi = @(a)(bsxfun(@times,bsxfun(@power,a./9,[0:10]),c.^[0:10]));
```

Minka, 2000

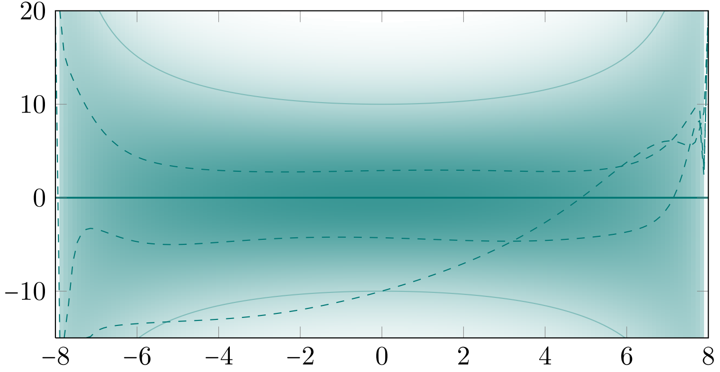



$$\operatorname{cov}(f_{x_i}, f_{x_j}) = \sum_{\ell=0}^{10} b^\ell x_i^\ell x_j^\ell \qquad 0 \leq b \leq 1 \qquad -1 < x_i, x_j < 1$$

# Exponentially suppressed polynomials

```
k = @(a,b)(theta.^2 .* 1./(1-c*bsxfun(@times,a./8,b'./8)));
```

Minka, 2000




$$\operatorname{cov}(f_{x_i}, f_{x_j}) = \sum_{\ell=0}^{\infty} b^\ell x_i^\ell x_j^\ell = \frac{1}{1 - b x_i x_j} \qquad 0 \le b \le 1 \qquad -1 < x_i, x_j < 1$$

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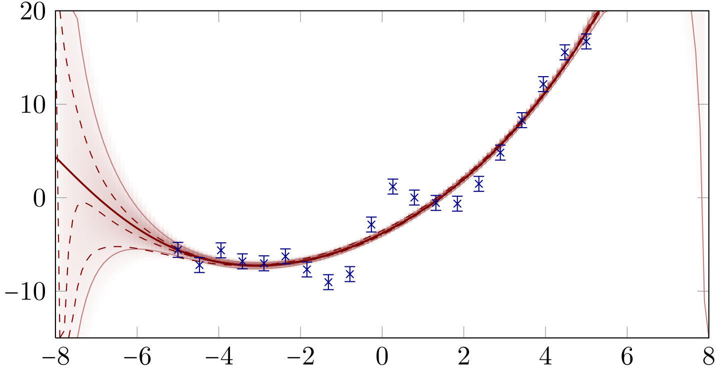
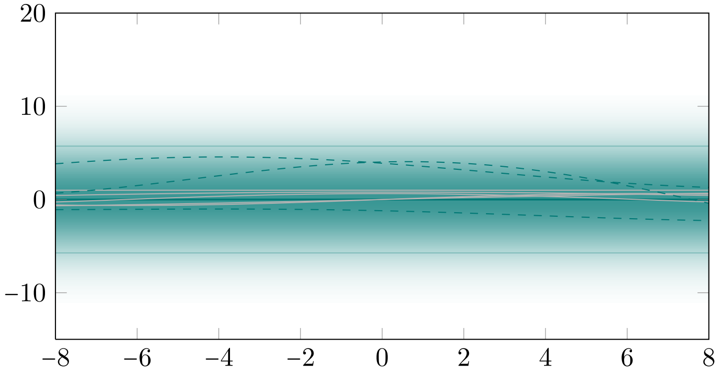



$$\operatorname{cov}(f_{x_i}, f_{x_j}) = \sum_{\ell=0}^{\infty} b^{\ell} x_i^{\ell} x_j^{\ell} = \frac{1}{1 - b x_i x_j} \qquad 0 \leq b \leq 1 \qquad -1 < x_i, x_j < 1$$

# Exponentially decaying periodic features

T. Minka, 2000

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




$$\mathrm{cov}(f_{x_i}, f_{x_j}) = 1 + \sum_{\ell=0}^{2} b^{\ell} (\cos(2\pi\ell x_i)\cos(2\pi\ell x_j) + \sin(2\pi\ell x_i)\sin(2\pi\ell x_j))$$

$$0 \leq b \leq 1$$

# Exponentially decaying periodic features

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```
phi = @(a)([bsxfun(@times,cos(bsxfun(@times,a/8,[0:20])),c.^[0:20]), ...
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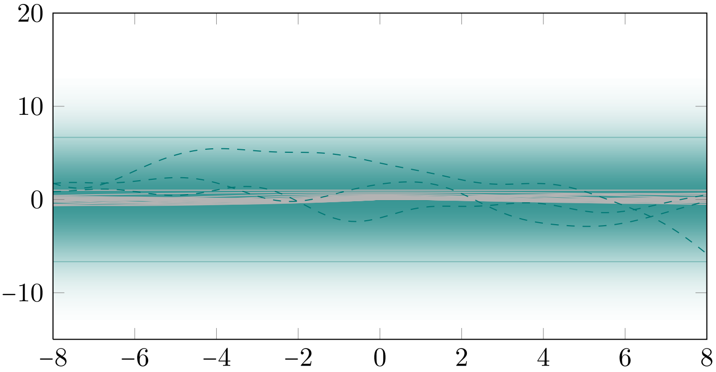
```




$$\operatorname{cov}(f_{x_i}, f_{x_j}) = 1 + \sum_{\ell=0}^{20} b^{\ell}\left(\cos(2\pi\ell x_i)\cos(2\pi\ell x_j) + \sin(2\pi\ell x_i)\sin(2\pi\ell x_j)\right)$$

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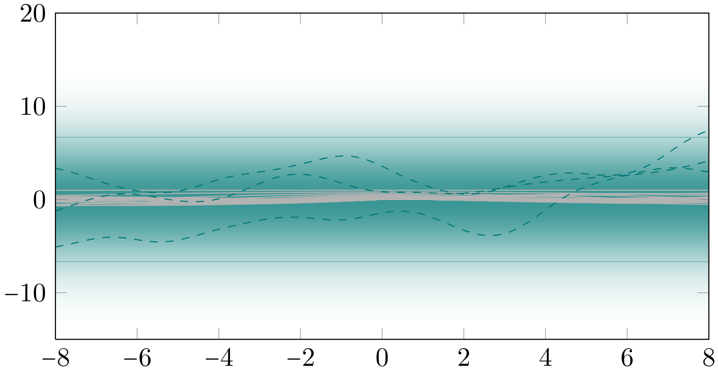
```
phi = @(a)([bsxfun(@times,cos(bsxfun(@times,a/8,[0:50])),c.^[0:50]), ...
bsxfun(@times,sin(bsxfun(@times,a/8,[1:50])),c.^[1:50])]);
```



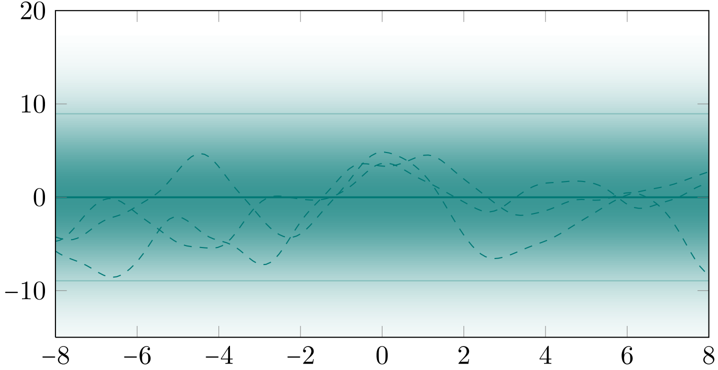

$$\operatorname{cov}(f_{x_i}, f_{x_j}) = 1 + \sum_{\ell=0}^{50} b^{\ell} \left(\cos(2\pi\ell x_i)\cos(2\pi\ell x_j) + \sin(2\pi\ell x_i)\sin(2\pi\ell x_j)\right)$$

$$0 \leq b \leq 1$$

# Exponentially decaying periodic features

T. Minka, 2000

```
k = @(a,b)(theta.^2 .* 2 / pi .* asin(2 * (...  cr + cu * bsxfun(@times,a,b')) ./ ...
sqrt(bsxfun(@times,(1 + 2 * (cr + cu * a.^2)),(1 + 2 * (cr + cu * b'.^2)))) ));
```




$$\operatorname{cov}(f_{x_i}, f_{x_j}) = 1 + \sum_{\ell=0}^{\infty} b^{\ell}(\cos(2\pi\ell x_i)\cos(2\pi\ell x_j) + \sin(2\pi\ell x_i)\sin(2\pi\ell x_j))$$

$$= \frac{1}{2} + \frac{(1-b^2)/2}{1+b^2-2b\cos(2\pi(x_i - x_j))} \qquad 0 \leq b \leq 1$$

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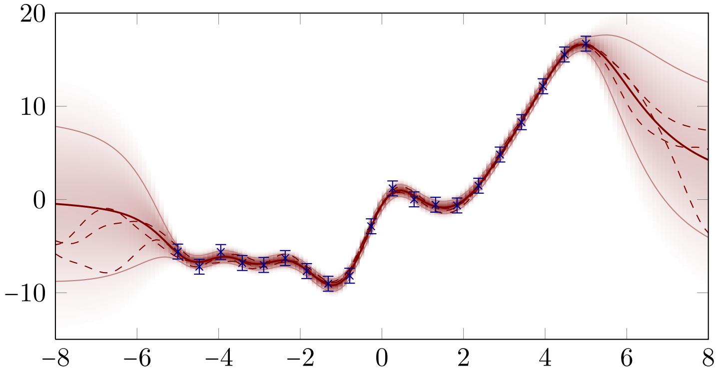


$$\operatorname{cov}(f_{x_i}, f_{x_j}) = 1 + \sum_{\ell=0}^{\infty} b^{\ell}\left(\cos(2\pi\ell x_i)\cos(2\pi\ell x_j) + \sin(2\pi\ell x_i)\sin(2\pi\ell x_j)\right)$$

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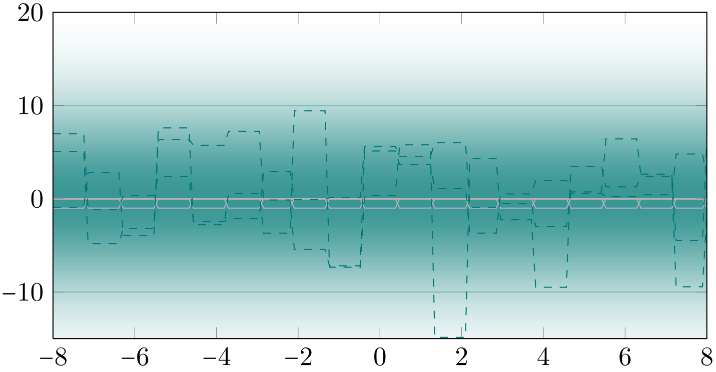
# “White Noise”

the “limit” of block functions

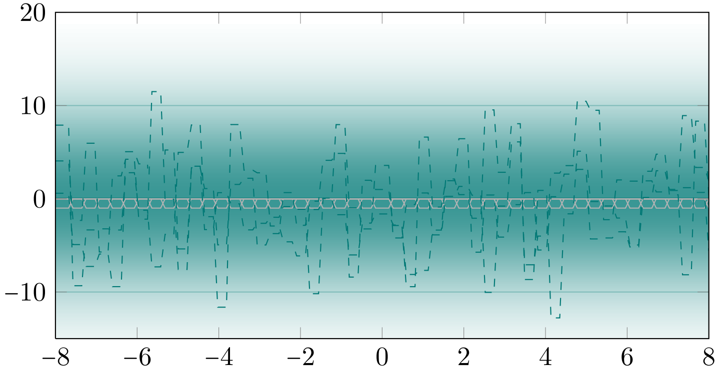



$$\lim_{\epsilon \to 0} \int \mathbb{I}(|x_i - c| < \epsilon)\mathbb{I}(|x_j - c| < \epsilon) \, \mathrm{d}c = \delta(x_i - x_j)$$

- but we’re cheating a little (height of blocks goes to 0!)
- white noise is a concept, more than a proper limit
- if you make no assumptions, you learn nothing

# “White Noise”

the “limit” of block functions

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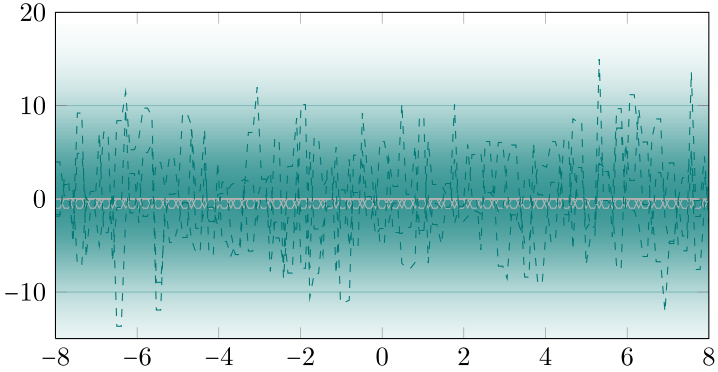


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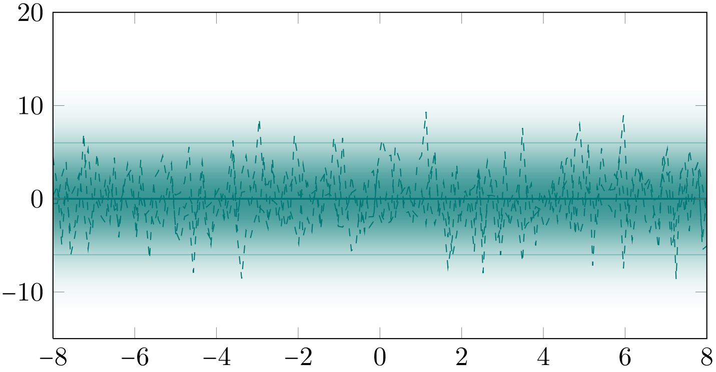


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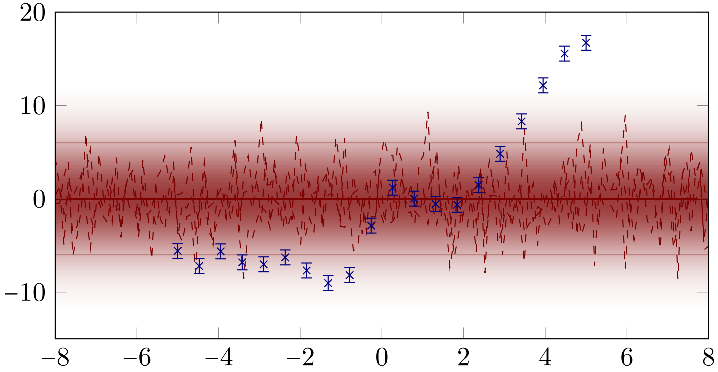


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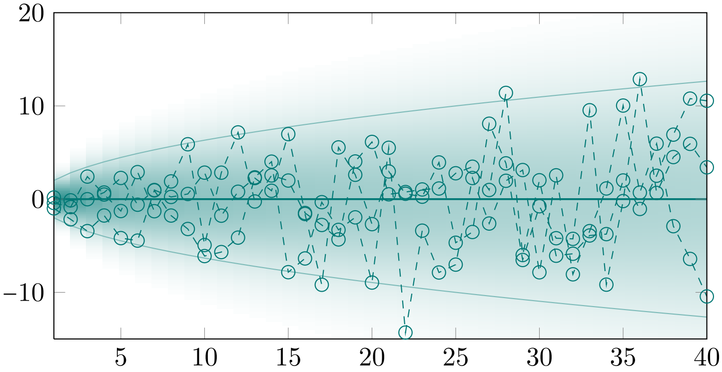
# That gcd kernel

```
k = @(a,b)(gcd(bsxfun(@times,a,ones(size(b'))),bsxfun(@times,ones(size(a)),b')));
```



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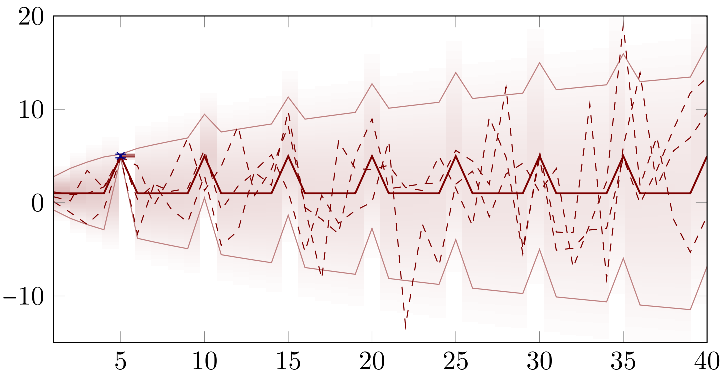

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```

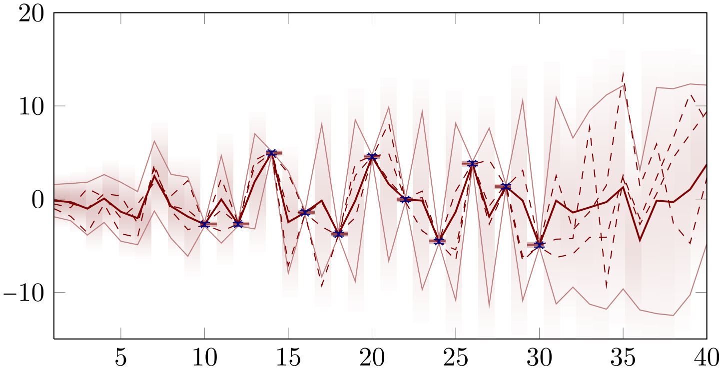

# Summary

- Gaussians are closed under
  - linear projection / marginalization / sum rule
  - linear restriction / conditioning / product rule

$\Rightarrow$ they provide the linear algebra of inference

- combine with nonlinear features $\phi$, get nonlinear regression
- in fact, number of features can be infinite

$\Rightarrow$ (nonparametric) Gaussian process regression

Tomorrow:

- so what are kernels? What is the set of kernels?
- how should we design GP models?s
- how powerful are those models?s

# Bibliography


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