Machine Learning

Dual Linear Regression

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Reddit

Introduction

Gaussian Identities

$$p(x_1, x_2) = \mathcal{N}\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} \right)$$

- Marginal

$$p(x_2) = \int p(x_1, x_2) \mathrm{d}x_1 = \mathcal{N}(\mu_2, \Sigma_{22})$$

- Conditional

$$p(x_1|x_2) = \frac{p(x_1, x_2)}{p(x_2)} = \mathcal{N}(\mu_1 + \Sigma_{21}\Sigma_{22}^{-1}(x_2 - \mu_2), \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})$$

Gaussian Conditional

$$p(x_1|x_2) = \frac{p(x_1, x_2)}{p(x_2)} = \mathcal{N}(\mu_1 + \Sigma_{21}\Sigma_{22}^{-1}(x_2 - \mu_2), \Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{21})$$

Independent variables

$$\Sigma_{12} = \Sigma_{21} = \mathbf{0}$$

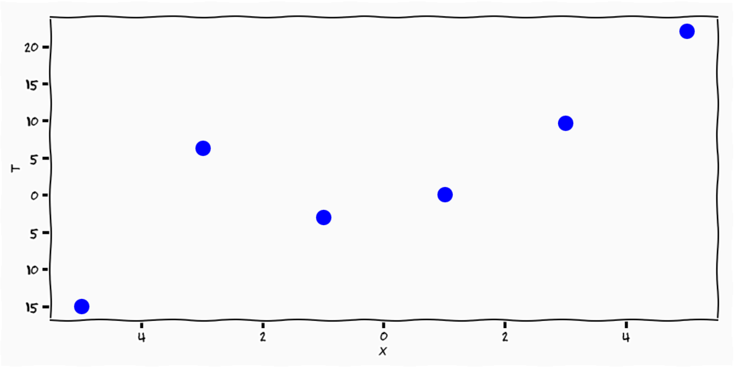
$$p(x_1|x_2) = \mathcal{N}(\mu_1 + \mathbf{0}\Sigma_{22}^{-1}(x_2 - \mu_2), \Sigma_{11} - \mathbf{0}\Sigma_{22}^{-1}\mathbf{0}) = \mathcal{N}(\mu_1|\Sigma_{11}) = p(x_1)$$

Completely Dependent

$$\Sigma_{12} = \Sigma_{21} = \Sigma_{22} = \Sigma_{11}$$

$$\begin{aligned} p(x_1|x_2) &= \mathcal{N}(\mu_1 + \Sigma_{11}\Sigma_{11}^{-1}(x_2 - \mu_2), \Sigma_{11} - \Sigma_{11}\Sigma_{11}^{-1}\Sigma_{11}) \\ &= \mathcal{N}(x_2 + \mu_1 - \mu_2|\mathbf{0}) \end{aligned}$$

Linear Regression [1] Ch 3.1



- Linear function in both parameters and data

$$y(\mathbf{x}, \mathbf{w}) = w_0 + w_1 x_1 + \ldots w_D x_D = \mathbf{w}^{\mathrm{T}} \mathbf{x} + w_0 = \{D = 1\} = \mathbf{w}^{\mathrm{T}} \phi(\mathbf{x})$$

Likelihood

$$t = f(\mathbf{x}) + \epsilon$$

Likelihood

$$
\begin{aligned}
t &= f(\mathsf{x}) + \epsilon \\
t - f(\mathsf{x}) &= \epsilon
\end{aligned}
$$

Likelihood

$$
\begin{aligned}
t &= f(\mathbf{x}) + \epsilon \\
t - f(\mathbf{x}) &= \epsilon \\
t - f(\mathbf{x}) &\sim \mathcal{N}(\epsilon | 0, \beta^{-1} I) = \frac{\beta}{(2\pi)^{\frac{1}{2}}} e^{-\frac{1}{2}(\epsilon - 0)\beta(\epsilon - 0)}
\end{aligned}
$$

Likelihood

$$
\begin{aligned}
t &= f(\mathbf{x}) + \epsilon \\
t - f(\mathbf{x}) &= \epsilon \\
t - f(\mathbf{x}) &\sim \mathcal{N}(\epsilon|0, \beta^{-1}I) = \frac{\beta}{(2\pi)^{\frac{1}{2}}} e^{-\frac{1}{2}(\epsilon-0)\beta(\epsilon-0)} \\
&\Rightarrow \mathcal{N}(t - f(\mathbf{x})|0, \beta^{-1}I) \frac{\beta}{(2\pi)}^{\frac{1}{2}} e^{-\frac{1}{2}(t-f(\mathbf{x}))\beta(t-f(\mathbf{x}))}
\end{aligned}
$$

Likelihood

$$
\begin{aligned}
t &= f(\mathsf{x}) + \epsilon \\
t - f(\mathsf{x}) &= \epsilon \\
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&\Rightarrow \mathcal{N}(t - f(\mathsf{x})|0, \beta^{-1}I) \frac{\beta}{(2\pi)}^{\frac{1}{2}} e^{-\frac{1}{2}(t-f(\mathsf{x}))\beta(t-f(\mathsf{x}))} \\
&\Rightarrow \mathcal{N}(t - f(\mathsf{x})|0, \beta^{-1}I) = \mathcal{N}(t|f(\mathsf{x}), \beta^{-1}I)
\end{aligned}
$$

Likelihood

$$
\begin{aligned}
t &= f(\mathsf{x}) + \epsilon \\
t - f(\mathsf{x}) &= \epsilon \\
t - f(\mathsf{x}) &\sim \mathcal{N}(\epsilon|0, \beta^{-1}I) = \frac{\beta}{(2\pi)^{\frac{1}{2}}} e^{-\frac{1}{2}(\epsilon-0)\beta(\epsilon-0)} \\
&\Rightarrow \mathcal{N}(t - f(\mathsf{x})|0, \beta^{-1}I) \frac{\beta}{(2\pi)}^{\frac{1}{2}} e^{-\frac{1}{2}(t-f(\mathsf{x}))\beta(t-f(\mathsf{x}))} \\
&\Rightarrow \mathcal{N}(t - f(\mathsf{x})|0, \beta^{-1}I) = \mathcal{N}(t|f(\mathsf{x}), \beta^{-1}I) \\
&\Rightarrow p(t|f, \mathsf{x}) = \mathcal{N}(t|f(\mathsf{x}), \beta^{-1}I)
\end{aligned}
$$

Likelihood

$$
\begin{aligned}
t &= f(\mathbf{x}) + \epsilon \\
t - f(\mathbf{x}) &= \epsilon \\
t - f(\mathbf{x}) &\sim \mathcal{N}(\epsilon|0, \beta^{-1}I) = \frac{\beta}{(2\pi)^{\frac{1}{2}}} e^{-\frac{1}{2}(\epsilon-0)\beta(\epsilon-0)} \\
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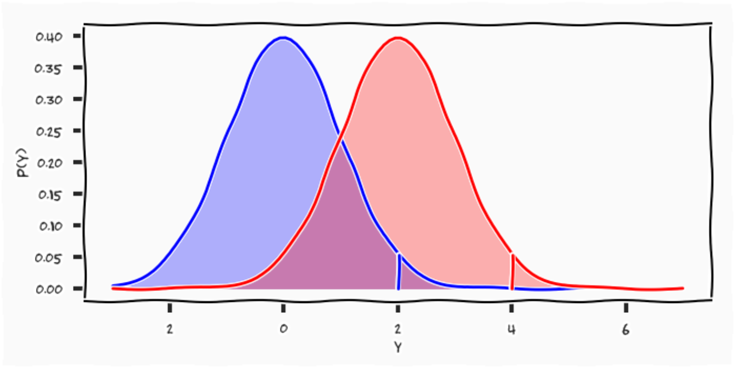
&\Rightarrow \mathcal{N}(t - f(\mathbf{x})|0, \beta^{-1}I) = \mathcal{N}(t|f(\mathbf{x}), \beta^{-1}I) \\
&\Rightarrow p(t|f, \mathbf{x}) = \mathcal{N}(t|f(\mathbf{x}), \beta^{-1}I)
\end{aligned}
$$

- By making an assumption of the noise we have reached a conditional distribution over the output given the model, i.e. the likelihood function

Likelihood



$$\mathcal{N}(y = 4 - 2|\mu = 0, 1.0) = \mathcal{N}(y = 4|\mu = 2, 1.0)$$

Vectors	Matrices
$\mathbf{x}_1 = \begin{bmatrix} x_{11} \\ x_{12} \\ \vdots \\ x_{1D} \end{bmatrix}$	$\mathbf{X} = \begin{bmatrix} x_{11} & x_{12} & \dots & x_{1D} \\ x_{21} & x_{22} & \dots & x_{2D} \\ \vdots & \vdots & \vdots & \vdots \\ x_{N1} & x_{N2} & \dots & x_{ND} \end{bmatrix}$

Why?

```
int *m = &matrix;
int* v1,v2;
for(int i=0; i<nr_points;i++)
  {
    v1 = &vector;
    v2 = &vector_res;
    for(int j=0; j<nr_dimensions; j++)
      {
        *(v2++) += (*(v1++))*(*(m++))
      }
  }
```

One point

$$t_1 = \mathbf{w}^{\mathrm{T}}\mathbf{x} = [w_0, w_1] \cdot \begin{bmatrix} 1 \\ x_1 \end{bmatrix} = w_0 + w_1 \cdot x_1$$

Multiple points

$$\begin{bmatrix} t_1 \\ t_2 \\ \vdots \\ t_N \end{bmatrix} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix} \cdot \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

- Model

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + \epsilon$$
$$\epsilon \sim \mathcal{N}(0, \beta^{-1} I)$$

Linear Regression

- Model

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + \epsilon$$

$$\epsilon \sim \mathcal{N}(0, \beta^{-1} I)$$

- Likelihood

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}\left(t|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}), \beta^{-1}\right)$$

Linear Regression

- Model

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + \epsilon$$
$$\epsilon \sim \mathcal{N}(0, \beta^{-1} I)$$

- Likelihood

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}\left(t|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}), \beta^{-1}\right)$$

- Independence

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n), \beta^{-1}\right)$$

Linear Regression

- Model

$$t = y(\mathbf{x}, \mathbf{w}) + \epsilon = \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}) + \epsilon$$
$$\epsilon \sim \mathcal{N}(0, \beta^{-1}I)$$

- Likelihood

$$p(t|\mathbf{x}, \mathbf{w}, \beta) = \mathcal{N}\left(t|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}), \beta^{-1}\right)$$

- Independence

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n|\mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n), \beta^{-1}\right)$$

- Prior (Conjugate)

$$p(\mathbf{w}|m_0, S_0) = \mathcal{N}(\mathbf{w}|m_0, S_0)$$

Posterior

- Posterior

$$p(\mathbf{w}|\mathbf{X},\mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)$$

$$\mathbf{m}_N = \left(\mathbf{S}_0^{-1} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}\left(S_0^{-1}\mathbf{m}_0 + \beta\phi(\mathbf{X})^{\mathrm{T}}\mathbf{t}\right)$$

$$\mathbf{S}_N = \left(\mathbf{S}_0^{-1} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}$$

Posterior

- Posterior

$$
\begin{aligned}
p(\mathbf{w}|\mathbf{X}, \mathbf{t}) &= \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N) \\
\mathbf{m}_N &= \left(\mathbf{S}_0^{-1} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}\left(S_0^{-1}\mathbf{m}_0 + \beta\phi(\mathbf{X})^{\mathrm{T}}\mathbf{t}\right) \\
\mathbf{S}_N &= \left(\mathbf{S}_0^{-1} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}
\end{aligned}
$$

- Assumption Zero mean isotropic Gaussian

$$
p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\underbrace{\mathbf{0}}_{\mathbf{m}_0}, \underbrace{\alpha^{-1}\mathbf{I}}_{\mathbf{S}_0})
$$

Posterior

- Posterior

$$
\begin{aligned}
p(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \mathcal{N}(\mathbf{w}|\mathbf{m}_N, \mathbf{S}_N)& \\
\mathbf{m}_N &= \left(\mathbf{S}_0^{-1} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}\left(S_0^{-1}\mathbf{m}_0 + \beta\phi(\mathbf{X})^{\mathrm{T}}\mathbf{t}\right) \\
\mathbf{S}_N &= \left(\mathbf{S}_0^{-1} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}
\end{aligned}
$$

- Assumption Zero mean isotropic Gaussian

$$
p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\underbrace{\mathbf{0}}_{\mathbf{m}_0}, \underbrace{\alpha^{-1}\mathbf{I}}_{\mathbf{S}_0})
$$

- Feature mapping

$$
\phi(x_i) = \begin{bmatrix} 1 \\ x_i \end{bmatrix} \quad \phi(\mathbf{X}) = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix}
$$

Linear Regression

Task 1 define a likelihood ✓

- what output do I consider likely under a given model?

Task 2 define an assumption of the model ✓

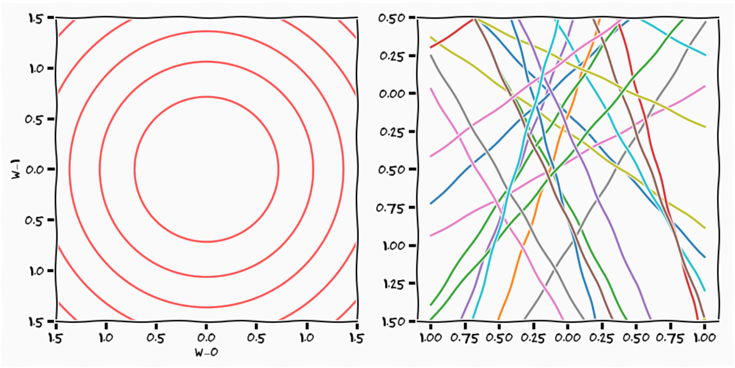
- what types of models do I think are more probable than others
- $\Rightarrow$ what are my beliefs, i.e formulate prior

Task 3 update my belief with new observations ✓

- formulate posterior

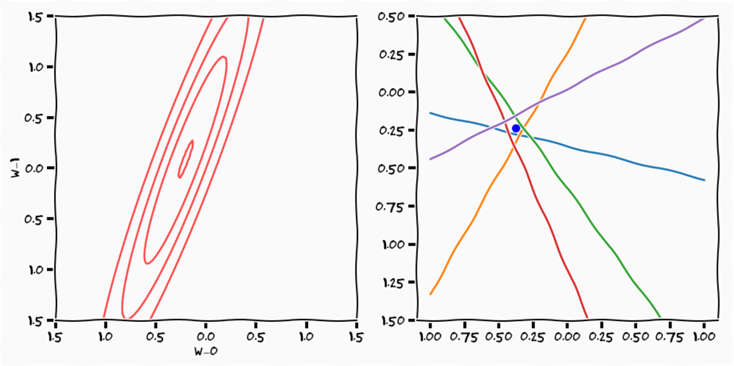
Task 4 predict using my new belief

- formulate predictive distribution

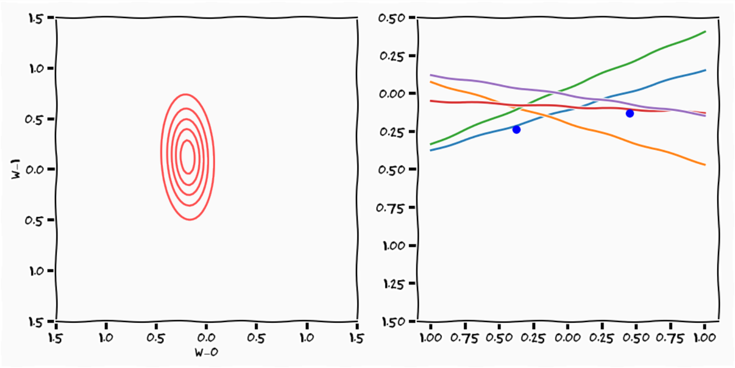


1.5
1.0
0.5
0.0
0.5
1.0
1.5
w_1
1.5
1.0
0.5
0.0
0.5
1.0
1.5
w_0
0.50
0.25
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.00
0.75
0.50
0.25
0.00
0.25
0.50
0.75
1.00

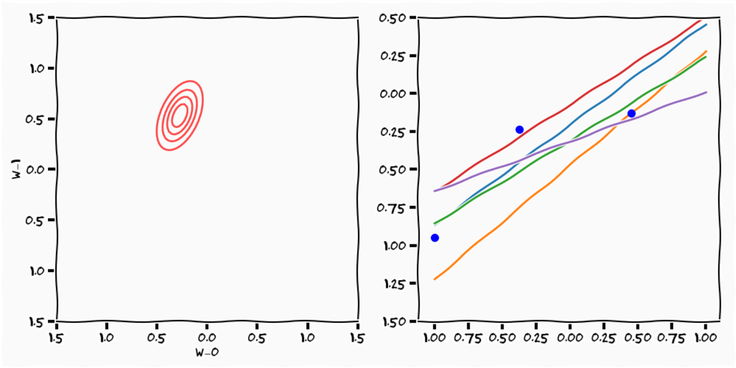
Linear Regression Example



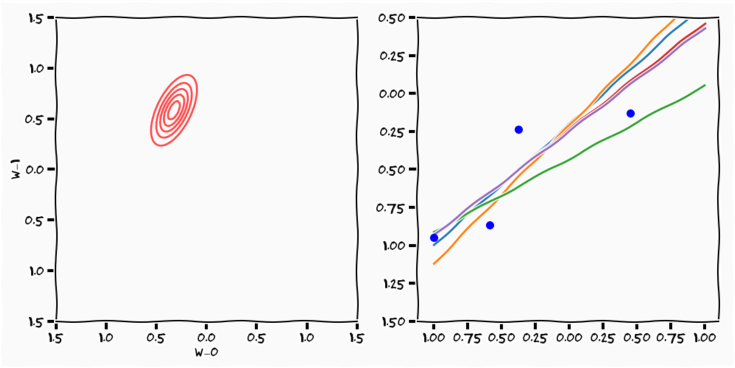
Linear Regression Example



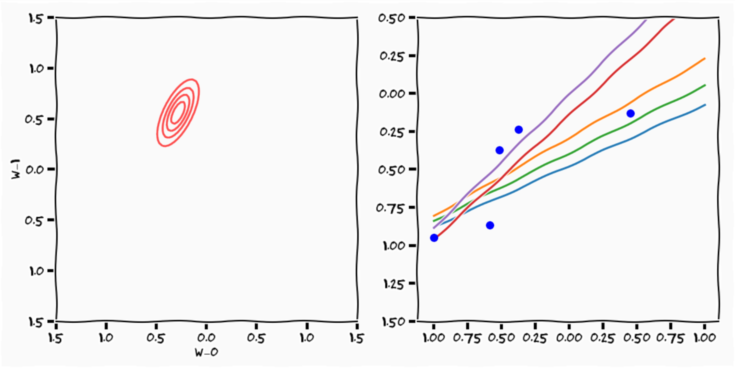
Linear Regression Example



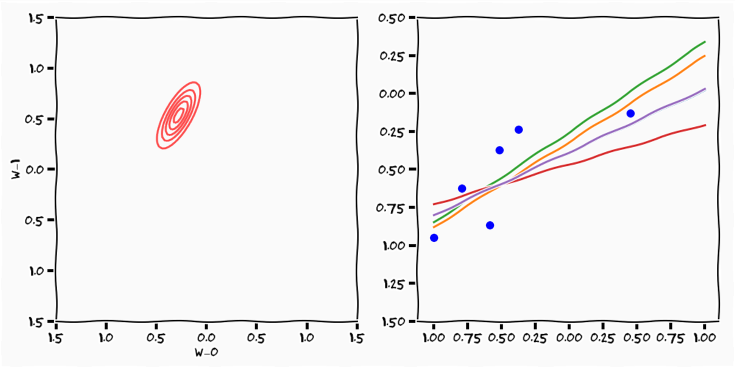
Linear Regression Example



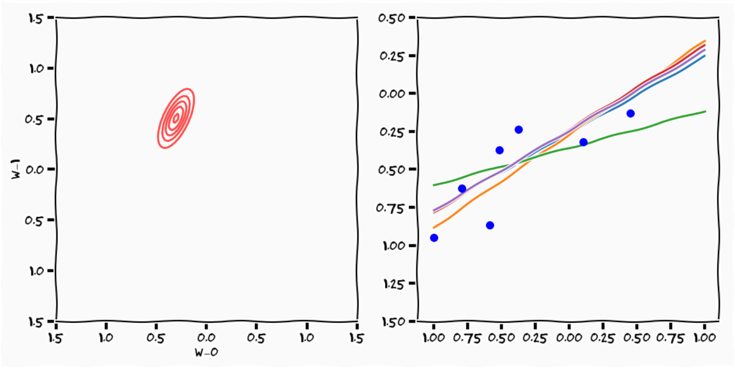
Linear Regression Example



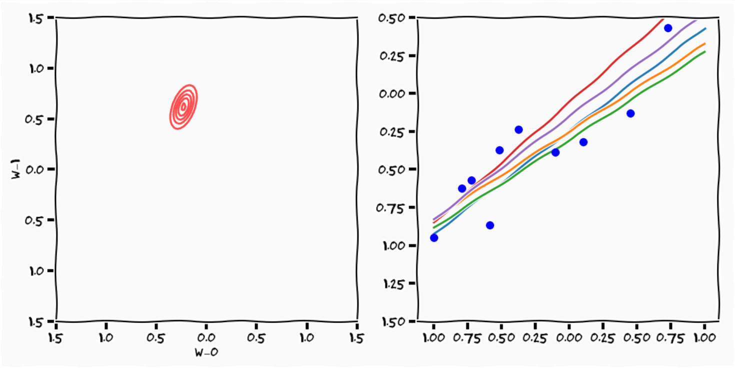
Linear Regression Example



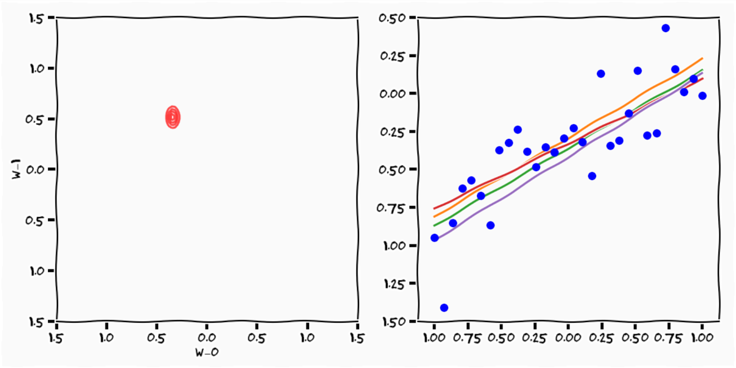
Linear Regression Example



Linear Regression Example



Linear Regression Example

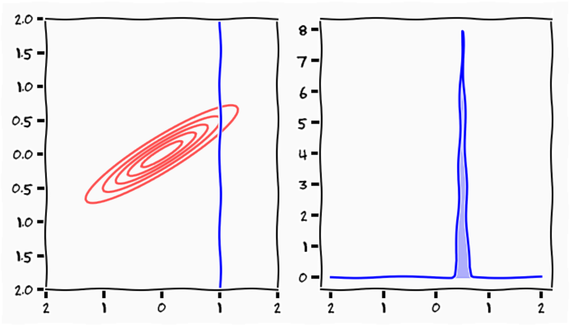


Prediction

$$p(t_*|\mathbf{t}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) = \int p(t_*|\mathbf{x}_*, \mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \alpha, \beta) \mathrm{d}\mathbf{w}$$
$$= \mathbb{E}\left[p(t_*|\mathbf{x}_*, \mathbf{w}, \beta)\right]$$

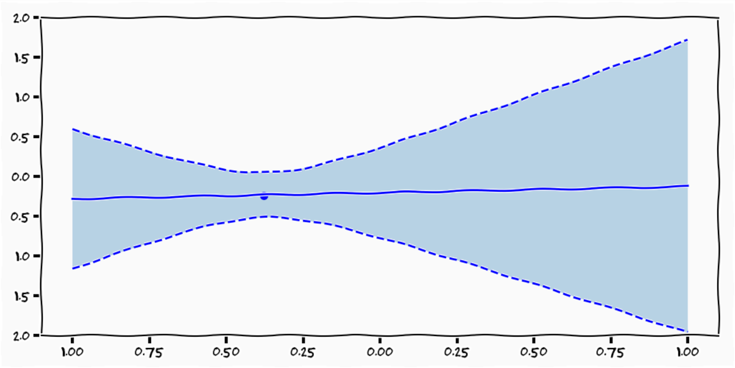
- we do not really care about $\mathbf{w}$ we care about new prediction t_* at location $\mathbf{x}_*$
- look at the marginal distribution, i.e. when we average out the weight
- integrate a Gaussian over a Gaussian $\Rightarrow$ Gaussian identities

Prediction

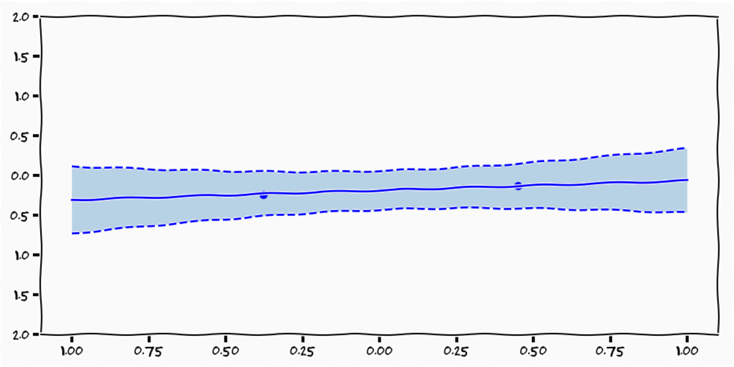


$$p(t_*|\mathbf{t}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) = \int p(t_*|\mathbf{x}_*, \mathbf{w}, \beta) p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \alpha, \beta) \mathrm{d}\mathbf{w}$$
$$= \mathcal{N}(t_*|\mathbf{m}_N^{\mathrm{T}} \phi(\mathbf{x}_*), \frac{1}{\beta} + \phi(\mathbf{x}_*)^{\mathrm{T}} \mathbf{S}_N \phi(\mathbf{x}_*))$$

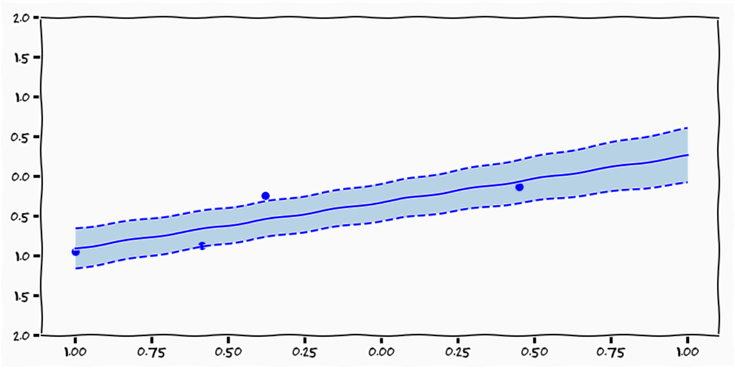
Predictive Posterior



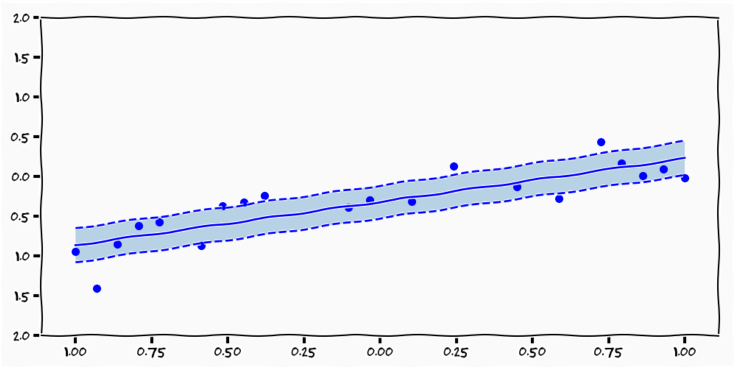
Predictive Posterior

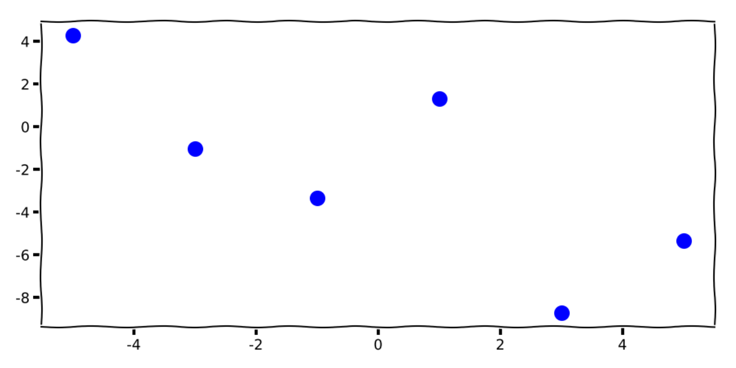


Predictive Posterior



Predictive Posterior

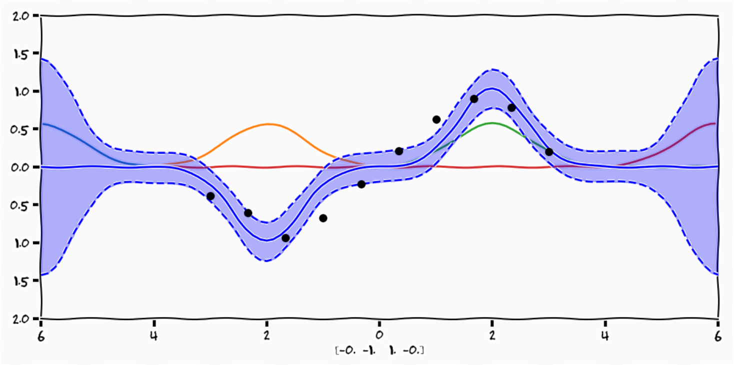




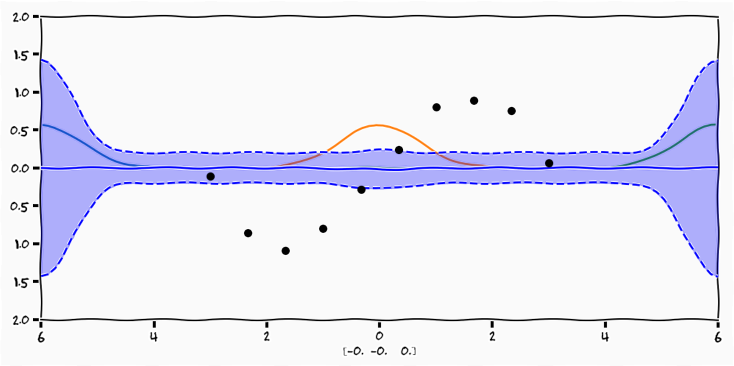
- Linear function only in parameters

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{j=1}^{M-1} w_j \phi_j(\mathbf{x}) = \{\phi_0(\mathbf{x}) = 1\} = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x})$$

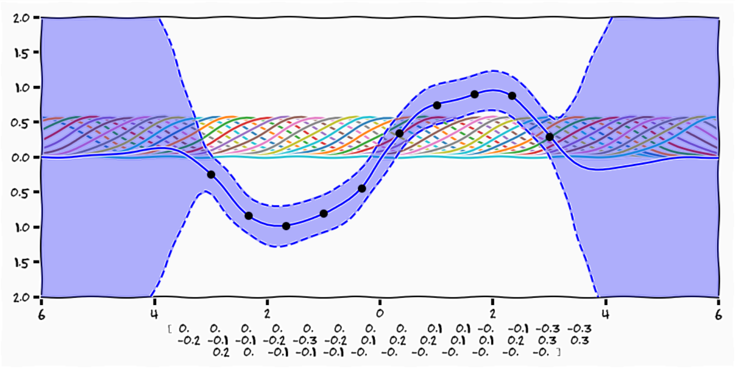
- We can choose many types of basis functions $\phi(\mathbf{x})$


2.0
1.5
1.0
0.5
0.0
0.5
1.0
1.5
2.0
6
4
2
0
2
4
6
[-0. -1. 1. -0.]

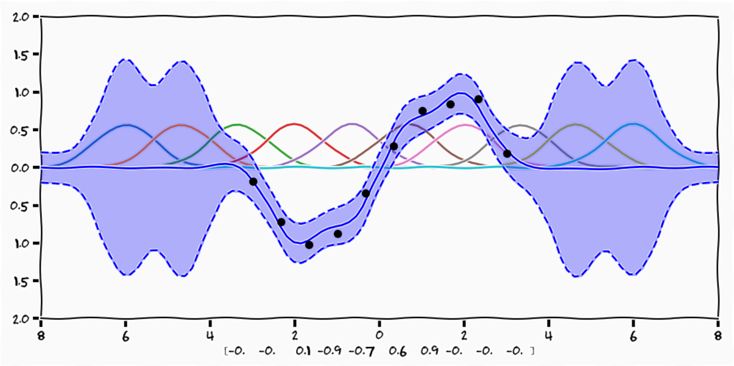
Non-Linear Basis Functions



Non-Linear Basis Functions



Non-Linear Basis Functions



Dual Linear Regression

Dual Linear Regression

$$p(\mathbf{w}|\mathbf{t},\mathbf{x}) = \frac{p(\mathbf{t}|\mathbf{w},\mathbf{x})p(\mathbf{w})}{p(\mathbf{t})}$$

$$p(\mathbf{t}|\mathbf{w},\mathbf{x}) = \prod_{n}^{N} p(t_n|\mathbf{w},\mathbf{x}) = \prod_{n}^{N} \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\mathbf{x}_n, \sigma^2\mathbf{I})$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \tau^2\mathbf{I})$$

Dual Linear Regression

$$p(\mathbf{w}|\mathbf{t},\mathbf{x}) = \frac{p(\mathbf{t}|\mathbf{w},\mathbf{x})p(\mathbf{w})}{p(\mathbf{t})}$$

$$p(\mathbf{t}|\mathbf{w},\mathbf{x}) = \prod_n^N p(t_n|\mathbf{w},\mathbf{x}) = \prod_n^N \mathcal{N}(t_n|\mathbf{w}^{\mathrm{T}}\mathbf{x}_n, \sigma^2\mathbf{I})$$

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{0}, \tau^2\mathbf{I})$$

$$p(\mathbf{w}|\mathbf{t},\mathbf{x}) \propto p(\mathbf{t}|\mathbf{w},\mathbf{x})p(\mathbf{w})$$

- Through conjugacy we know the form of the posterior

$$p(\mathbf{w}|\mathbf{t},\mathbf{x}) \propto \prod_{n}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n - t_n)^{\mathrm{T}}(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n - y_n)} \frac{1}{\sqrt{2\pi\tau^2}} e^{-\frac{1}{2\tau^2}(\mathbf{w}^{\mathrm{T}}\mathbf{w})}$$

$$= \frac{1}{(\sqrt{2\pi\sigma^2})^N} e^{-\frac{1}{2\sigma^2}\mathrm{tr}\left((\mathbf{X}\mathbf{w}-\mathbf{t})^{\mathrm{T}}(\mathbf{X}\mathbf{w}-\mathbf{t})\right)} \frac{1}{(\sqrt{2\pi\tau^2})^N} e^{-\frac{1}{2\tau^2}(\mathbf{w}^{\mathrm{T}}\mathbf{w})}$$

- Lets maximise the above to find a point estimate (not a distribution) of $\mathbf{w}$

Dual Linear Regression [1] Ch 6.1

$$-\log p(\mathbf{w}|\mathbf{t},\mathbf{x}) = J(\mathbf{w}) = \frac{1}{2}(\mathbf{X}\mathbf{w}-\mathbf{t})^{\mathrm{T}}(\mathbf{X}\mathbf{w}-\mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

- Find a stationary point in $\mathbf{w}$

Dual Linear Regression [1] Ch 6.1

$$-\log p(\mathbf{w}|\mathbf{t},\mathbf{x}) = J(\mathbf{w}) = \frac{1}{2}(\mathbf{X}\mathbf{w}-\mathbf{t})^{\mathrm{T}}(\mathbf{X}\mathbf{w}-\mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$

$$\frac{\delta}{\delta\mathbf{w}}J(\mathbf{w}) = \frac{1}{2}2\mathbf{X}^{\mathrm{T}}(\mathbf{X}\mathbf{w}-\mathbf{t}) + \frac{\lambda}{2}2\mathbf{w}$$

- Find a stationary point in $\mathbf{w}$

Dual Linear Regression [1] Ch 6.1

$$
\begin{aligned}
-\log p(\mathbf{w}|\mathbf{t},\mathbf{x}) = J(\mathbf{w}) &= \frac{1}{2}(\mathbf{X}\mathbf{w}-\mathbf{t})^{\mathrm{T}}(\mathbf{X}\mathbf{w}-\mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \\
\frac{\delta}{\delta \mathbf{w}} J(\mathbf{w}) &= \frac{1}{2} 2\mathbf{X}^{\mathrm{T}}(\mathbf{X}\mathbf{w}-\mathbf{t}) + \frac{\lambda}{2} 2\mathbf{w} \\
\mathbf{w} &= -\frac{1}{\lambda}\mathbf{X}^{\mathrm{T}}(\mathbf{X}\mathbf{w}-\mathbf{t})
\end{aligned}
$$

- Find a stationary point in $\mathbf{w}$

Dual Linear Regression [1] Ch 6.1

$$
\begin{aligned}
-\log p(\mathbf{w}|\mathbf{t}, \mathbf{x}) = J(\mathbf{w}) &= \frac{1}{2}(\mathbf{X}\mathbf{w} - \mathbf{t})^{\mathrm{T}}(\mathbf{X}\mathbf{w} - \mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \\
\frac{\delta}{\delta \mathbf{w}} J(\mathbf{w}) &= \frac{1}{2} 2\mathbf{X}^{\mathrm{T}}(\mathbf{X}\mathbf{w} - \mathbf{t}) + \frac{\lambda}{2} 2\mathbf{w} \\
\mathbf{w} &= -\frac{1}{\lambda}\mathbf{X}^{\mathrm{T}}(\mathbf{X}\mathbf{w} - \mathbf{t}) \\
&= \mathbf{X}^{\mathrm{T}}\mathbf{a} = \sum_{n}^{N} \alpha_n \mathbf{x}_n
\end{aligned}
$$

- Find a stationary point in $\mathbf{w}$

Dual Linear Regression

$$J(\mathbf{w}) = \frac{1}{2}(\mathbf{X}\mathbf{w} - \mathbf{t})^{\mathrm{T}}(\mathbf{X}\mathbf{w} - \mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}$$
$$\mathbf{w} = \mathbf{X}^{\mathrm{T}}\mathbf{a}$$

- Rewrite objective in terms of $\mathbf{a}$

Dual Linear Regression

$$
\begin{aligned}
J(\mathbf{w}) &= \frac{1}{2}(\mathbf{X}\mathbf{w} - \mathbf{t})^{\mathrm{T}}(\mathbf{X}\mathbf{w} - \mathbf{t}) + \frac{\lambda}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w} \\
\mathbf{w} &= \mathbf{X}^{\mathrm{T}}\mathbf{a} \\
J(\mathbf{a}) &= \frac{1}{2}\mathbf{a}^{\mathrm{T}}\mathbf{X}\mathbf{X}^{\mathrm{T}}\mathbf{X}\mathbf{X}^{\mathrm{T}}\mathbf{a} - \mathbf{a}^{\mathrm{T}}\mathbf{X}\mathbf{X}^{\mathrm{T}}\mathbf{t} + \frac{1}{2}\mathbf{t}^{\mathrm{T}}\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^{\mathrm{T}}\mathbf{X}\mathbf{X}^{\mathrm{T}}\mathbf{a}
\end{aligned}
$$

- Rewrite objective in terms of $\mathbf{a}$

Dual Linear Regression

$$[\mathbf{K}]_{ij} = \mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j$$

$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^{\mathrm{T}}\mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}\mathbf{K}\mathbf{t} + \frac{1}{2}\mathbf{t}^{\mathrm{T}}\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^{\mathrm{T}}\mathbf{K}\mathbf{a}$$

- $\mathbf{K}$ is a matrix with all inner-products between the data points

Dual Linear Regression

$$\alpha_n = -\frac{1}{\lambda}(\mathbf{w}^{\mathrm{T}}\mathbf{x}_n - t_n)$$
$$\mathbf{w} = \sum_n^N \alpha_n \mathbf{x}_n = \mathbf{X}^{\mathrm{T}}\mathbf{a}$$

- Eliminate $\mathbf{w}$ and rewrite in terms of $\mathbf{a}$

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$$\Rightarrow \mathbf{a} = (\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}$$

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\mathbf{a} &= (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t} \\
\mathbf{y}(\mathbf{x}_*) &= \mathbf{w}^{\mathrm{T}} \mathbf{x}_* = \mathbf{a}^{\mathrm{T}} \mathbf{X}^{\mathrm{T}} \mathbf{x}_* = \mathbf{a}^{\mathrm{T}} k(\mathbf{x}, \mathbf{x}_*) = \\
&= ((\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t})^{\mathrm{T}} k(\mathbf{x}, \mathbf{x}_*) = k(\mathbf{x}_*, \mathbf{x}) (\mathbf{K} + \lambda \mathbf{I})^{-1} \mathbf{t}
\end{aligned}
$$

What have we actually done

- Linear Regression
    - See data
    - Encode relationship between variates using parameters $\mathbf{w}$
    - Make predictions using $\mathbf{w}$

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  - See Data
  - Encode relationship between variates using variates themselves
  - *Model complexity depends on data*
  - Non-parametric model

Kernel Functions

$$
\begin{aligned}
\phi : \mathbf{x}_i &\rightarrow \mathbf{f}_i \\
\mathbf{y}(\mathbf{x}_*) &= \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_*) = \mathbf{a}^{\mathrm{T}}\phi(\mathbf{X})\phi(\mathbf{x}_*) = k(\mathbf{x}_*, \mathbf{X})(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{y} \\
k(\mathbf{x}, \mathbf{x}') &= \phi(\mathbf{x})^{\mathrm{T}}\phi(\mathbf{x}')
\end{aligned}
$$

- we actually never need to know $\phi(\mathbf{x})$ only $\phi(\mathbf{x}_i)^{\mathrm{T}}\phi(\mathbf{x}_j)$
- functions that describes inner-products are called *kernel-functions*

Kernel Functions

$$\mathbf{x} \in \mathbb{R}^2$$

$$(\mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j)^2$$

- Kernel functions need to forefill certain properties and is a subclass of functions
- Can be incredibly useful, think similarity rather than location

Kernel Functions

$$\mathbf{x} \in \mathbb{R}^2$$

$$(\mathbf{x}_i^{\mathrm{T}} \mathbf{x}_j)^2 = (x_{i1}x_{j1} + x_{i2}x_{j2})^2$$

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(\mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j)^2 &= (x_{i1}x_{j1} + x_{i2}x_{j2})^2 \\
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&= (x_{i1}^2, \sqrt{2}x_{i1}x_{i2}, x_{i2}^2)(x_{j1}^2, \sqrt{2}x_{j1}x_{j2}, x_{j2}^2)^{\mathrm{T}}
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&= \phi(\mathbf{x}_i)^{\mathrm{T}}\phi(\mathbf{x}_j)
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&= (x_{i1}^2, \sqrt{2}x_{i1}x_{i2}, x_{i2}^2)(x_{j1}^2, \sqrt{2}x_{j1}x_{j2}, x_{j2}^2)^{\mathrm{T}} = \\
&= \phi(\mathbf{x}_i)^{\mathrm{T}}\phi(\mathbf{x}_j) \\
\phi(\mathbf{x}) &= ((\mathbf{e}_1^{\mathrm{T}}\mathbf{x})^2, \sqrt{2}\mathbf{e}_1^{\mathrm{T}}\mathbf{x}\mathbf{e}_2^{\mathrm{T}}\mathbf{x}, (\mathbf{e}_2^{\mathrm{T}}\mathbf{x})^2)
\end{aligned}
$$

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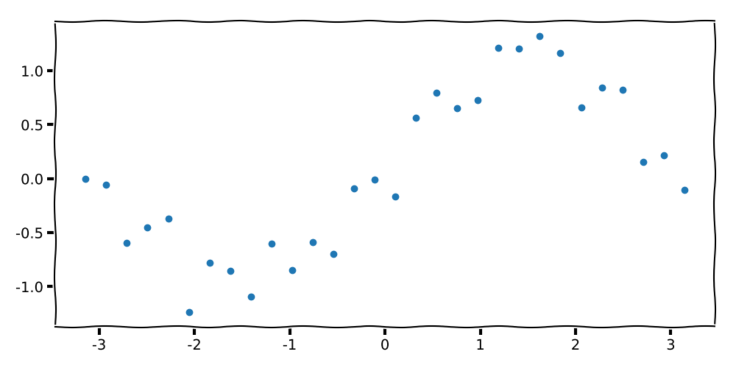
Kernel Functions

- Kernels allows for *implicit* feature mappings
- We do NOT need to know the feature space
- The space can have infinite dimensionality
- The mapping can be non-linear but the problem is still linear!
- Allows for putting weird things like, strings (DNA) in a vector space
- More next lecture, these things are very powerful

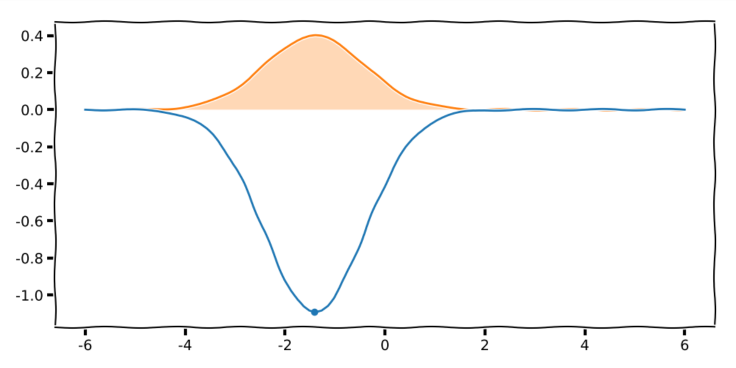
Kernel Functions



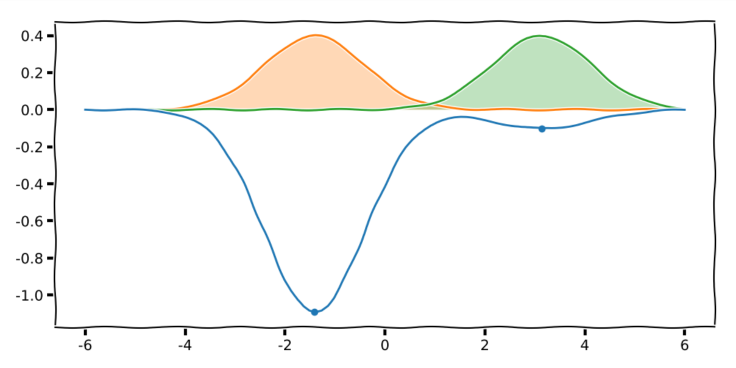
$$t = f(x) + \epsilon$$

$$k(x_i, x_j) = e^{-\frac{1}{2}\frac{(x_i - x_j)^2}{l}}$$

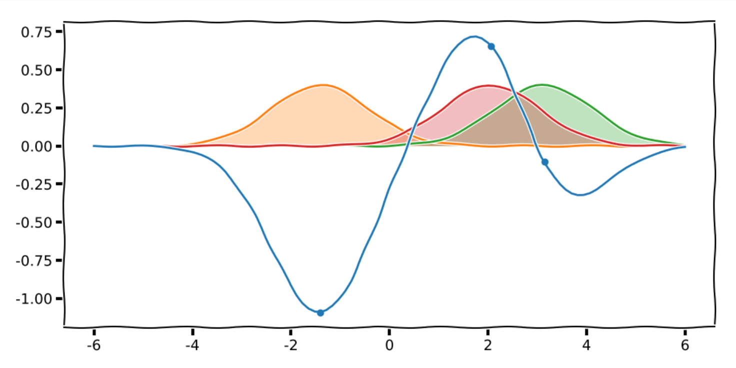
Kernel Regression



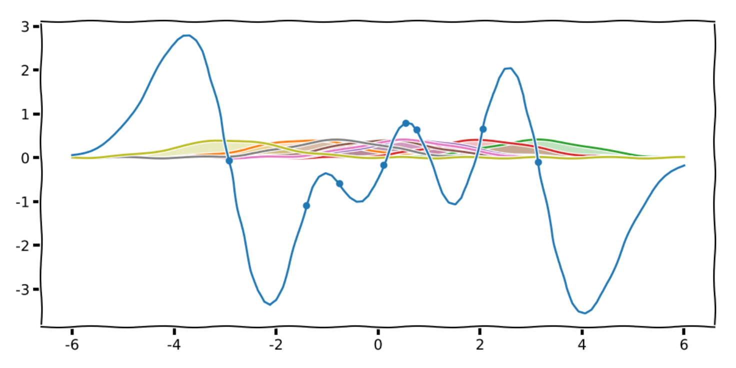
Kernel Regression



Kernel Regression

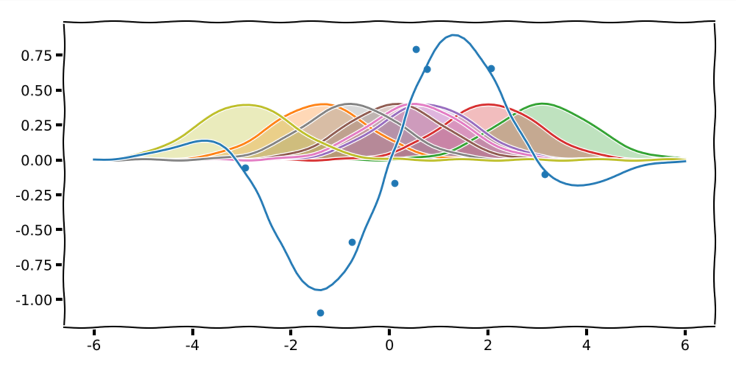


Kernel Regression

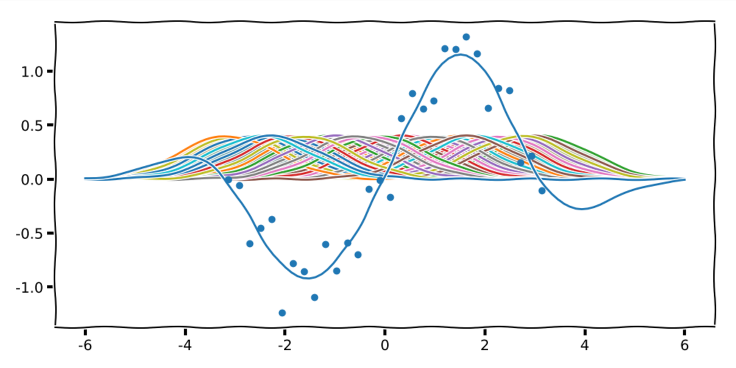


$$y(\mathbf{x}_*) = k(\mathbf{x}_*, \mathbf{x})(\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{t}$$

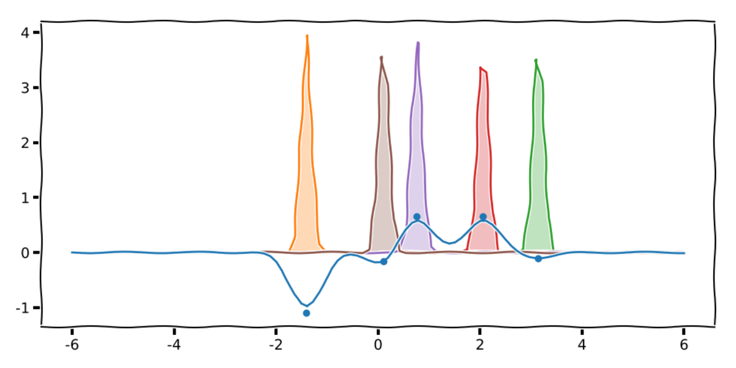
Kernel Regression



Kernel Regression



Kernel Regression



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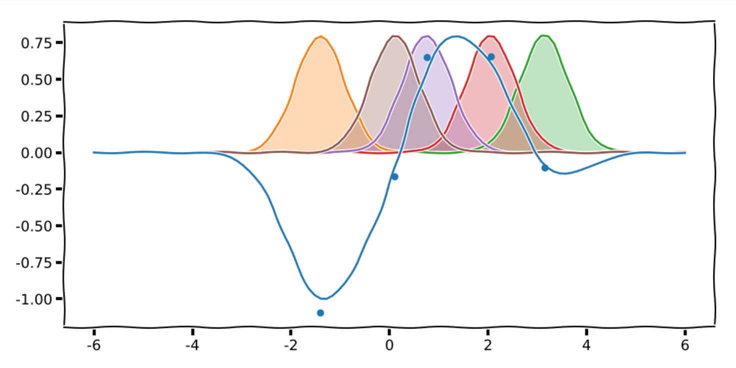
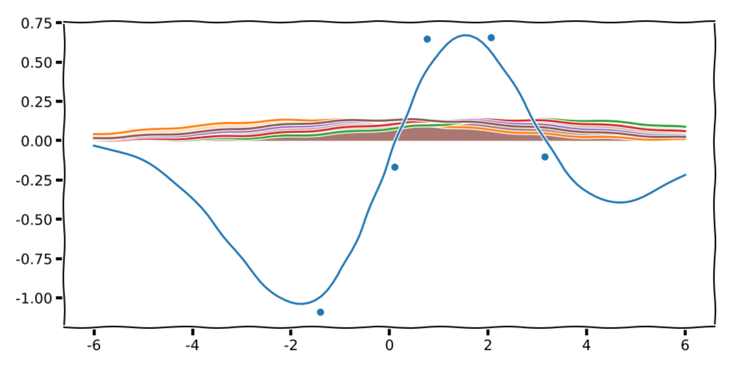
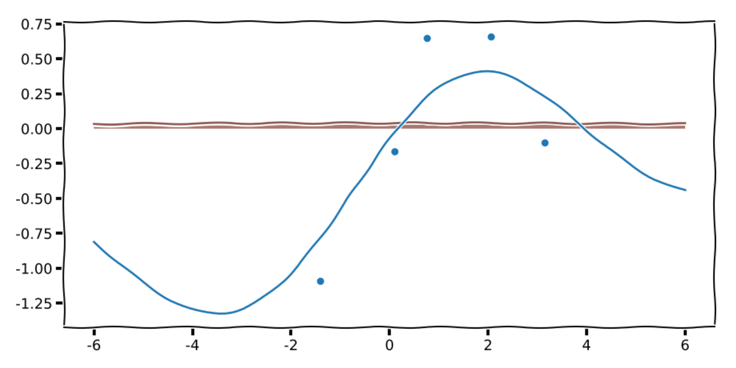
Kernel Regression



Kernel Regression



Kernel Regression



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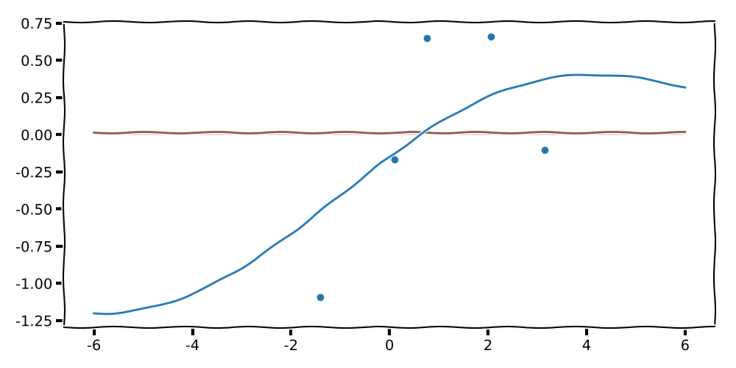

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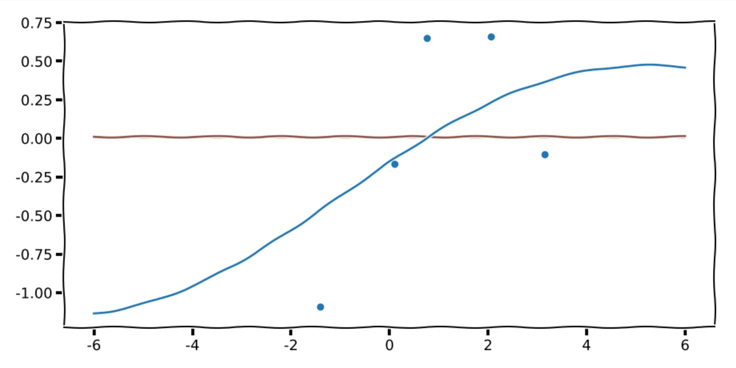

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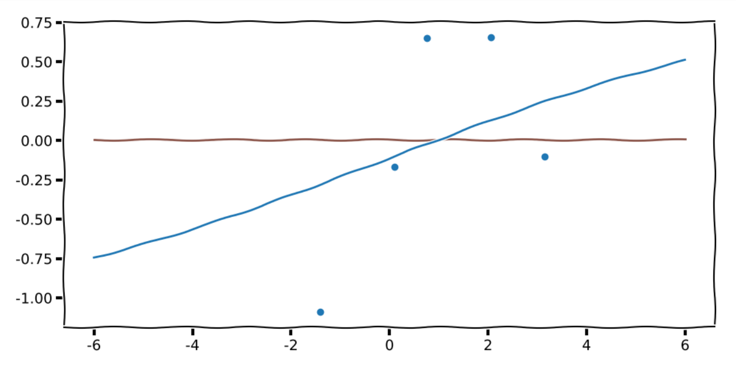

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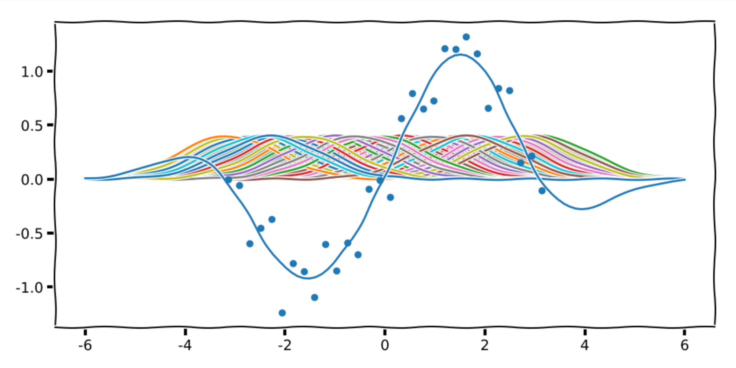
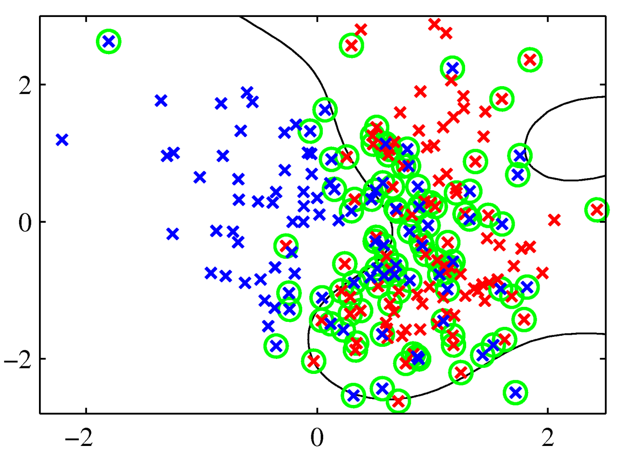


Support Vector Machines [1] Figure 7.4



Kernel Machines

- Allows us to
  - let the model complexity adapt to data
  - to put non vectorial data in a vector space
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Kernel Machines

- Allows us to
  - let the model complexity adapt to data
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  - *problem is still linear*
- But
  - how to set kernel width
  - how to set noise assumption
- Tomorrow we will learn these

Summary

Summary

- Repeat of the machine learning proceedure
  - assumption + data + compute $\rightarrow$ updated assumption
  - don't worry it will become clear eventually
- Non-parametrics
  - kernel regression
  - dual formulation
  - *the problem is still linear*

eof

References

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Pattern Recognition and Machine Learning (Information Science and Statistics).
Springer-Verlag New York, Inc., Secaucus, NJ, USA, 2006.