University of BRISTOL

# Machine Learning

## Dual Linear Regression

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# Reddit

# Office Hours


MVB 1.11 Thursday 17-19

# Introduction

# Gaussian Identities

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

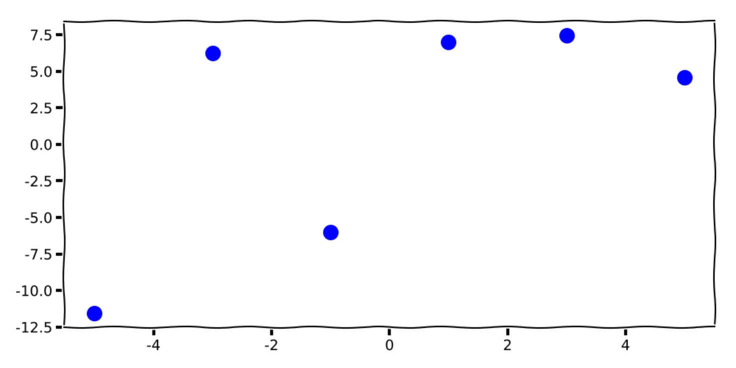
- Marginal

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

- Conditional

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

# Linear Regression [1] Ch 3.1




- Linear function in both parameters and data

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

# Linear Regression

- Model

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

# Linear Regression

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

- Likelihood

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

- Model

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

- Independence

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

# Linear Regression

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- Prior (Conjugate)

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

# Posterior

- Posterior

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

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

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

- Assumption Zero mean isotropic Gaussian

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

# Posterior

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- Assumption Zero mean isotropic Gaussian

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

- Posterior

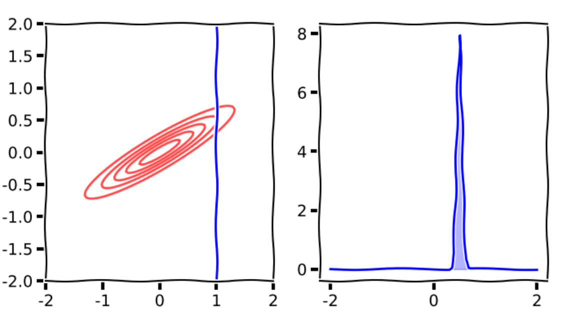
$$p(\mathbf{w}|\mathbf{t}, \mathbf{X}) = \mathcal{N}(\mathbf{w}|\beta\left(\alpha\mathbf{I} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1}\phi(\mathbf{X})^{\mathrm{T}}\mathbf{t}, \left(\alpha\mathbf{I} + \beta\phi(\mathbf{X})^{\mathrm{T}}\phi(\mathbf{X})\right)^{-1})$$

# Prediction

$$p(t_*|\mathbf{t}, \mathbf{x}_*, \mathbf{X}, \alpha, \beta) = \int p(t_*|\mathbf{x}_*, \mathbf{w}, \beta)p(\mathbf{w}|\mathbf{t}, \mathbf{X}, \alpha, \beta)\mathrm{d}\mathbf{w}$$

- we do not really care about $w$ 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

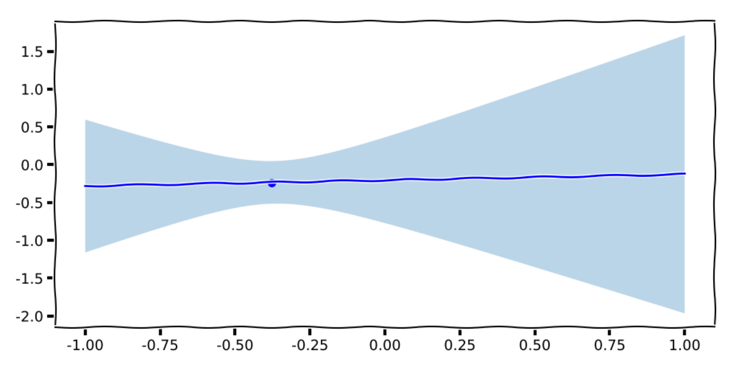
# Prediction




$$p(t_*|\mathbf{t},\mathbf{x}_*,\mathbf{X},\alpha,\beta) = \int p(t_*|\mathbf{x}_*,\mathbf{w},\beta)p(\mathbf{w}|\mathbf{t},\mathbf{X},\alpha,\beta)\mathrm{d}\mathbf{w}$$

$$= \mathcal{N}(t_*|\mathbf{m}_N^{\mathrm{T}}\phi(\mathbf{x}_*), \frac{1}{\beta} + \phi(\mathbf{x}_*)^{\mathrm{T}}\mathbf{S}_N\phi(\mathbf{x}_*))$$

# Predictive Posterior



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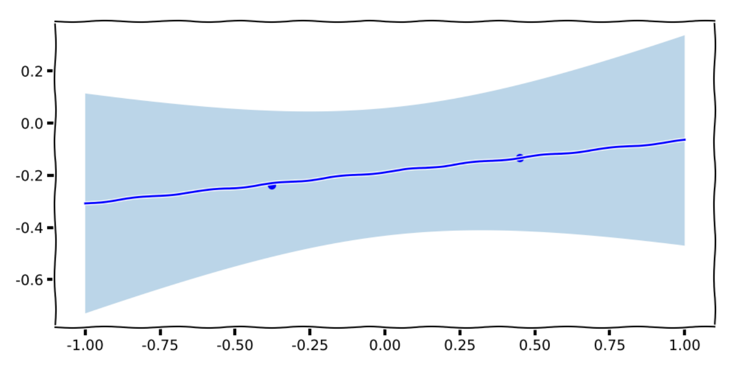

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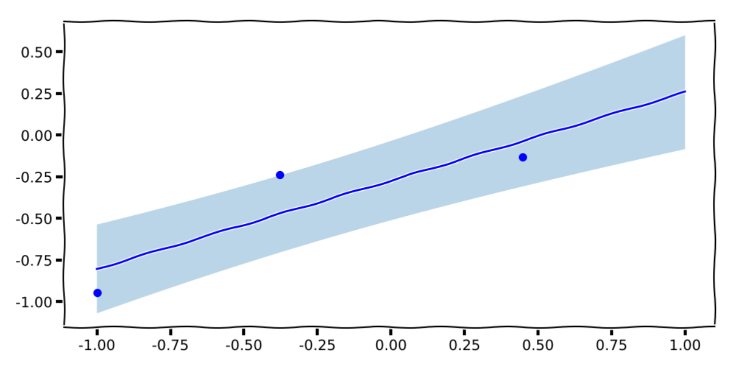

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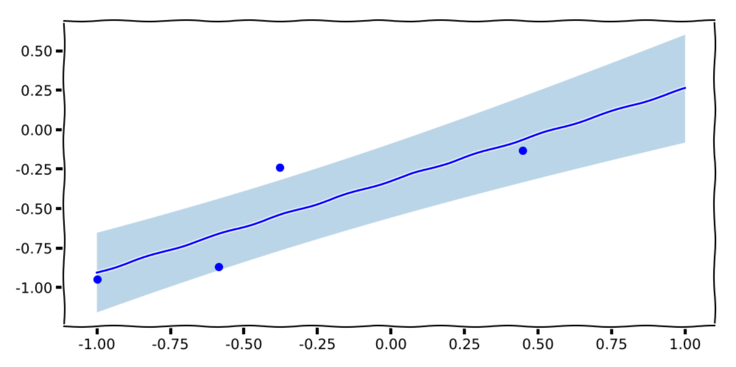

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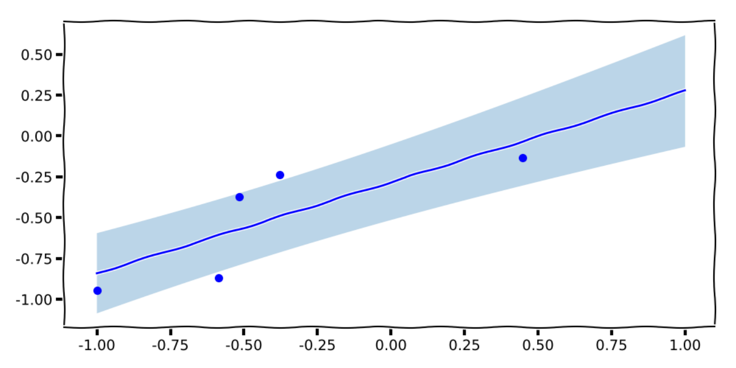

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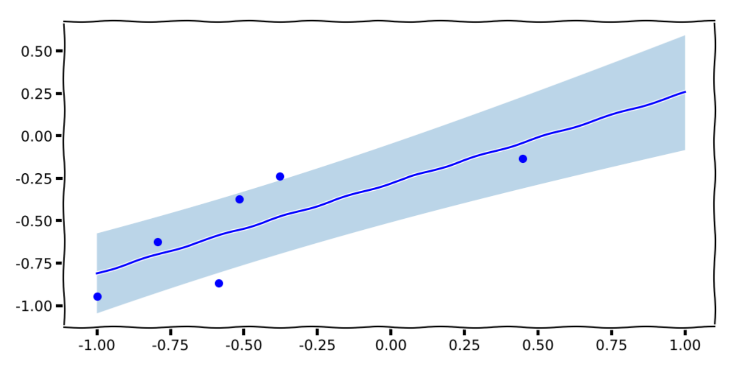

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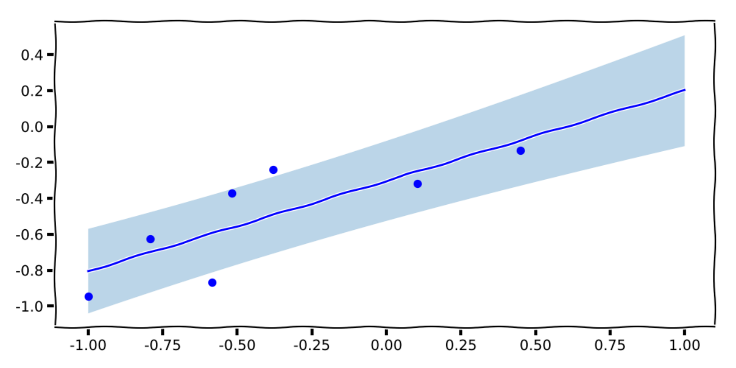

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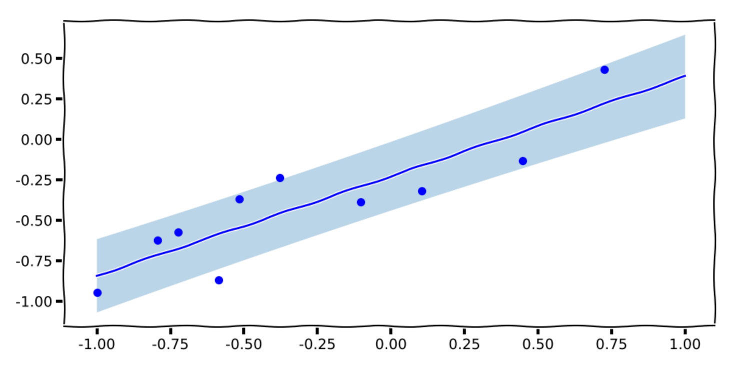

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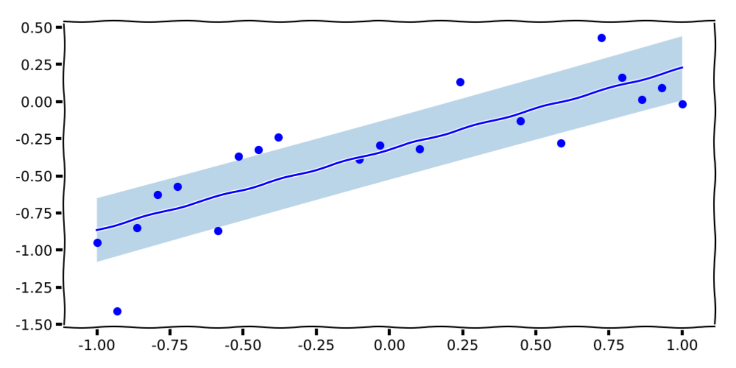
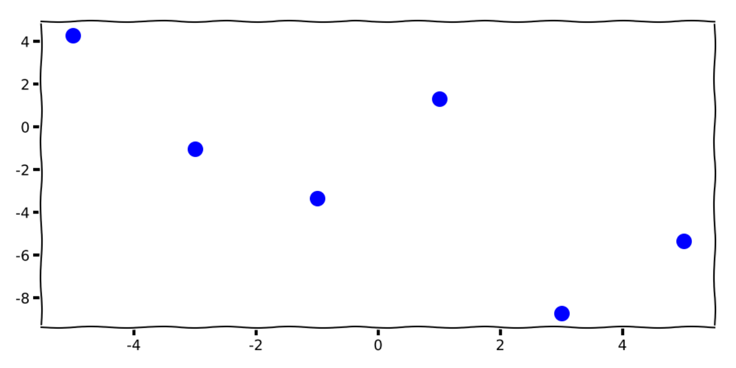


# Linear Regression

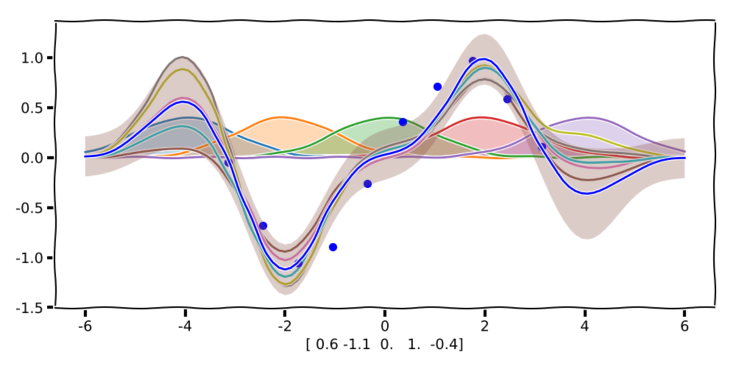



- Linear function only in parameters

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

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

# Non-Linear Basis Functions



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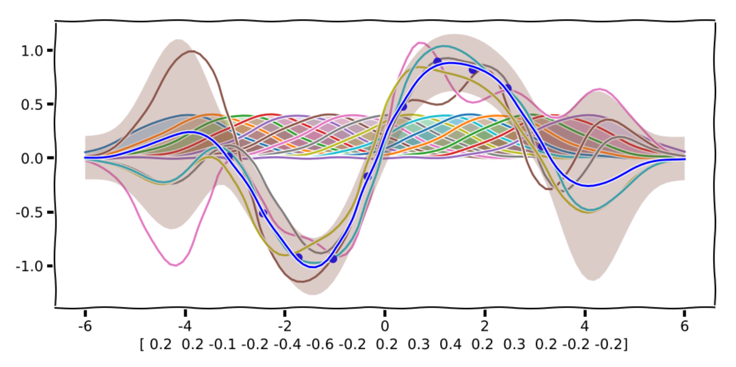

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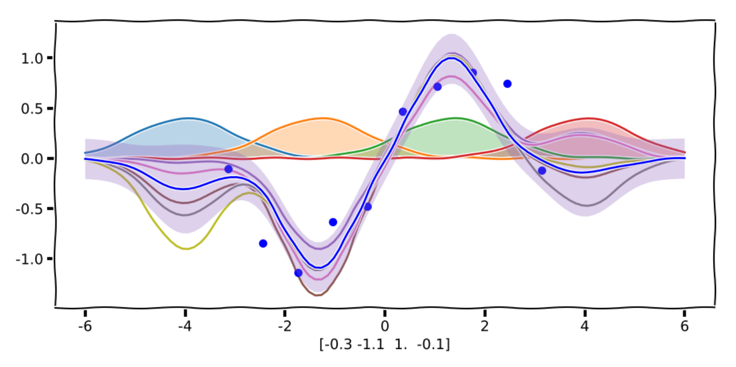

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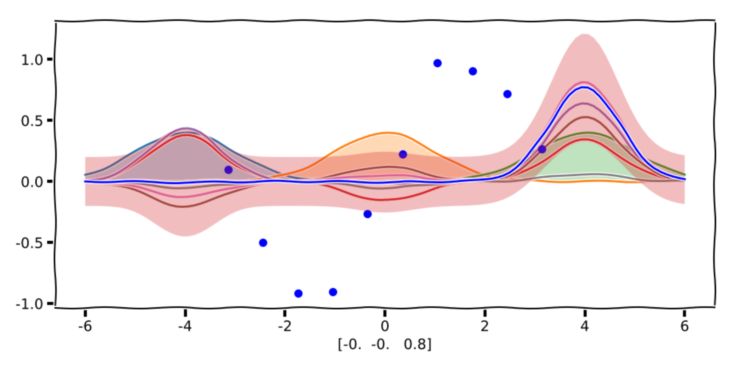

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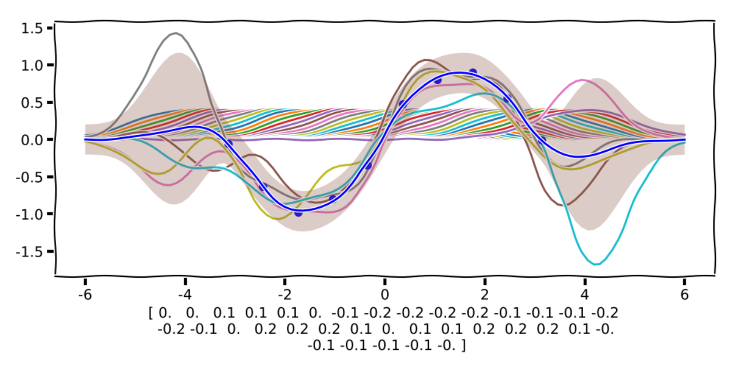

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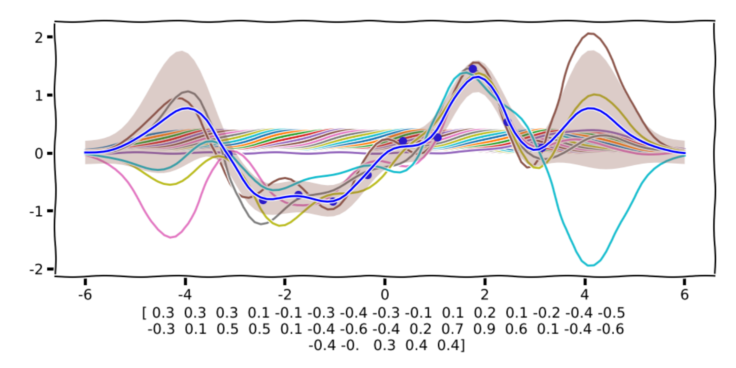

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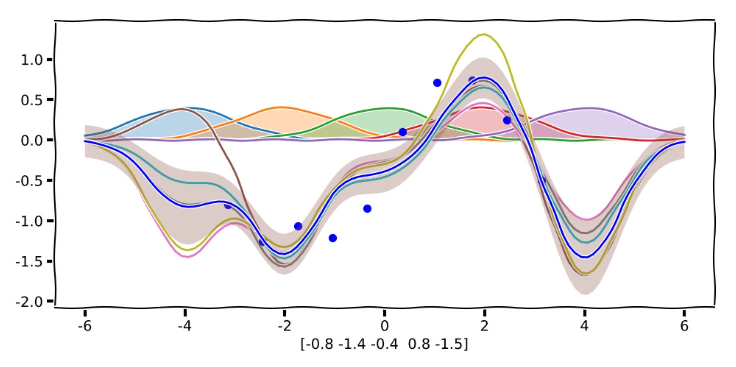

# Dual Linear Regression

# 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

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

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

- Through conjugacy we know the form of the posterior

# Dual Linear Regression

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

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

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

# Dual Linear Regression [1] Ch 6.1

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

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

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

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$$\mathbf{w} = -\frac{1}{\lambda}\mathbf{x}^{\mathrm{T}}(\mathbf{w}^{\mathrm{T}}\mathbf{x} - \mathbf{t})$$

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

# Dual Linear Regression [1] Ch 6.1

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

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# Dual Linear Regression

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

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

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$$\mathbf{w} = \mathbf{x}^{\mathrm{T}}\mathbf{a}$$

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# Dual Linear Regression

$$[\mathbf{K}]_{ij} = \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j = \phi(\mathbf{x}_i)^{\mathrm{T}}\phi(\mathbf{x}_j)$$
$$J(\mathbf{a}) = \frac{1}{2}\mathbf{a}^{\mathrm{T}}\mathbf{K}\mathbf{K}\mathbf{a} - \mathbf{a}\mathbf{K}\mathbf{t} + \frac{1}{2}\mathbf{t}^{\mathrm{T}}\mathbf{t} + \frac{\lambda}{2}\mathbf{a}^{\mathrm{T}}\mathbf{K}\mathbf{a}$$

- $\mathbf{K}$ 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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$$\mathbf{w} = \sum_n^N \alpha_n \mathbf{x}_n = \mathbf{x}^{\mathrm{T}}\mathbf{a}$$
$$\Rightarrow \mathbf{a} = (\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{t}$$

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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}\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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- Dual
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  - 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

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&= x_{i1}^2 x_{j1}^2 + 2x_{i1}x_{j1}x_{i2}x_{j2} + x_{i2}^2 x_{j2}^2
\end{aligned}
$$

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&= x_{i1}^2 x_{j1}^2 + 2x_{i1}x_{j1}x_{i2}x_{j2} + x_{i2}^2 x_{j2}^2 = \\
&= (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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&= x_{i1}^2 x_{j1}^2 + 2x_{i1}x_{j1}x_{i2}x_{j2} + x_{i2}^2 x_{j2}^2 = \\
&= (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)
\end{aligned}
$$

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

# Kernel Functions

$$
\begin{aligned}
\mathbf{x} &\in \mathbb{R}^2 \\
(\mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j)^2 &= (x_{i1}x_{j1} + x_{i2}x_{j2})^2 \\
&= x_{i1}^2 x_{j1}^2 + 2x_{i1}x_{j1}x_{i2}x_{j2} + x_{i2}^2 x_{j2}^2 = \\
&= (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)
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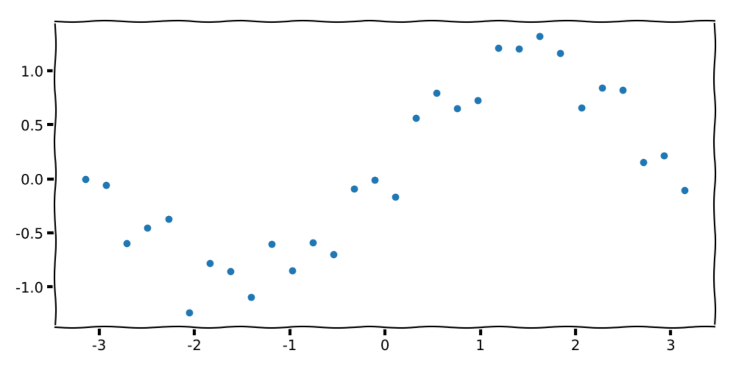
- Allows for putting weird things like, strings (DNA) in a vector space
- More next lecture, these things are very powerful

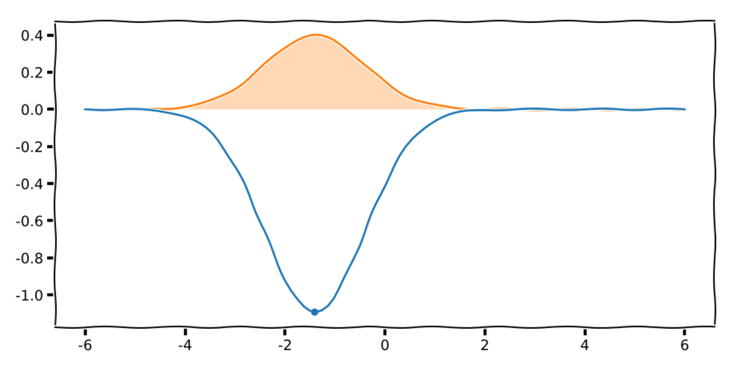
# Kernel Functions




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

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

# Kernel Regression



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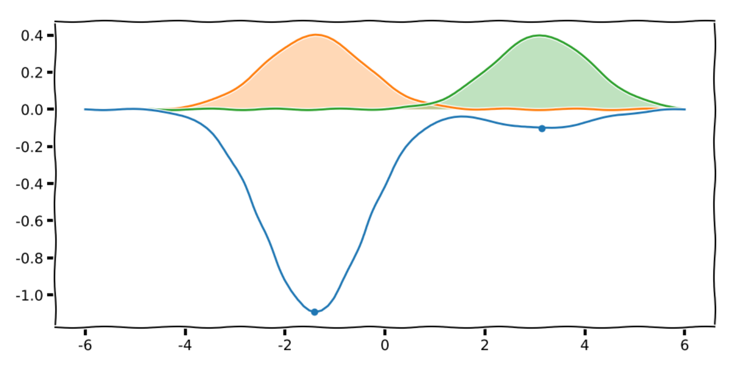

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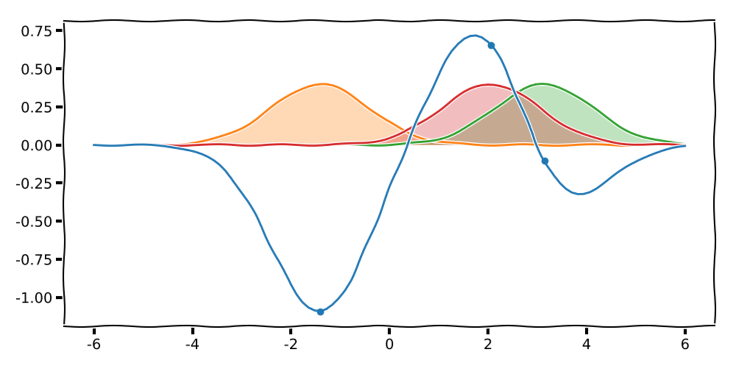

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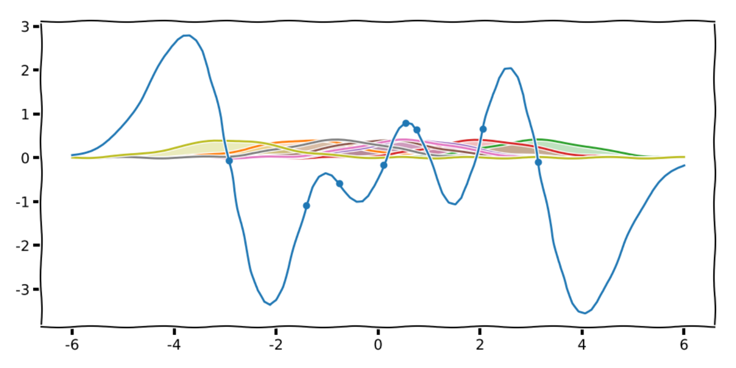
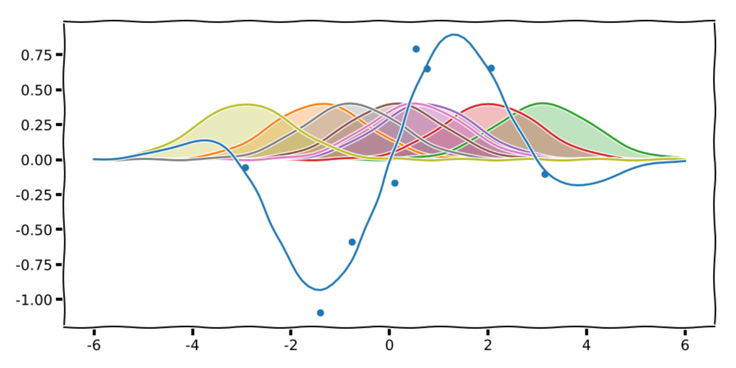



$$y(\mathbf{x}_*) = k(\mathbf{x}_*, \mathbf{x})(\mathbf{K} + \lambda \mathbf{I})^{-1}\mathbf{t}$$

# Kernel Regression



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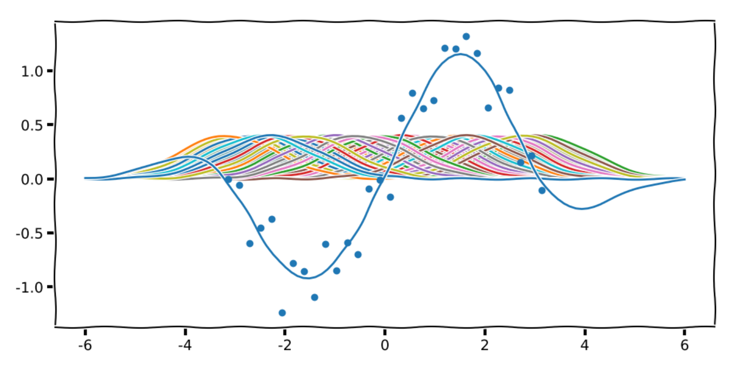

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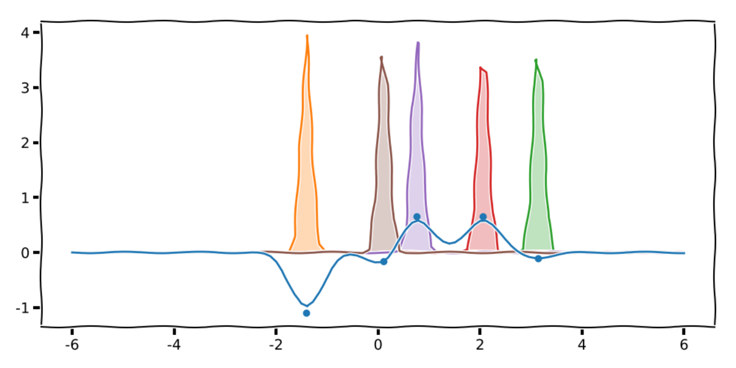


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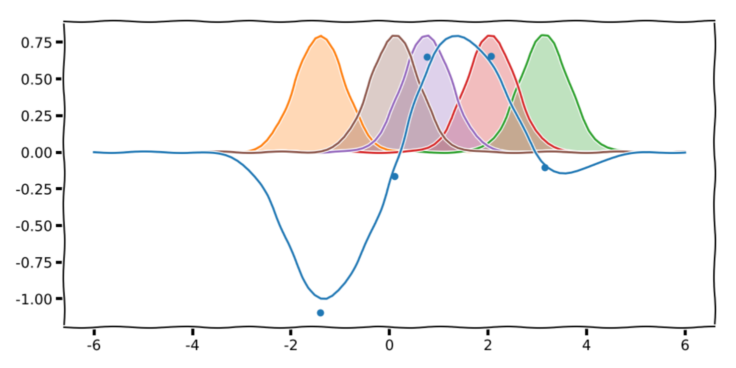

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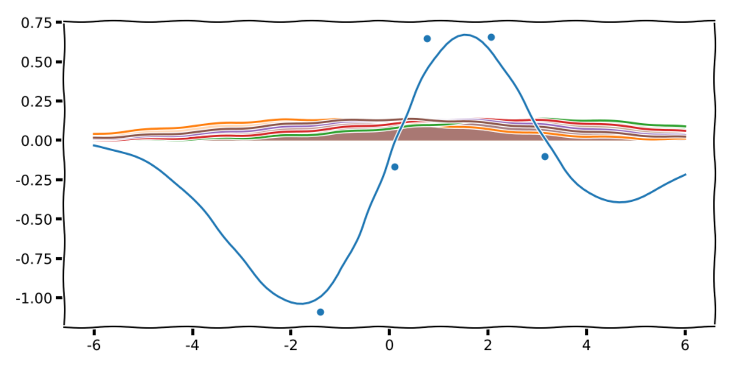

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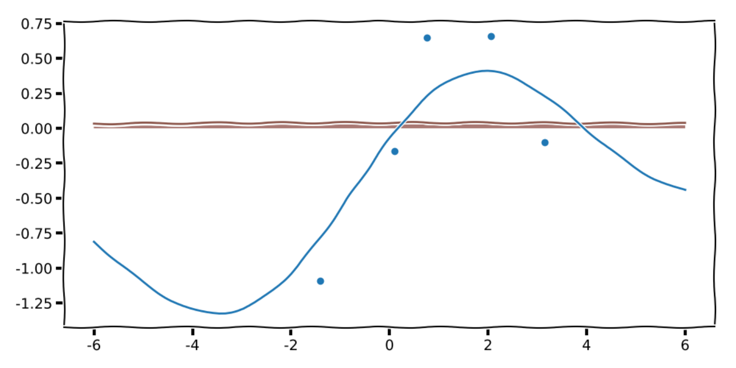

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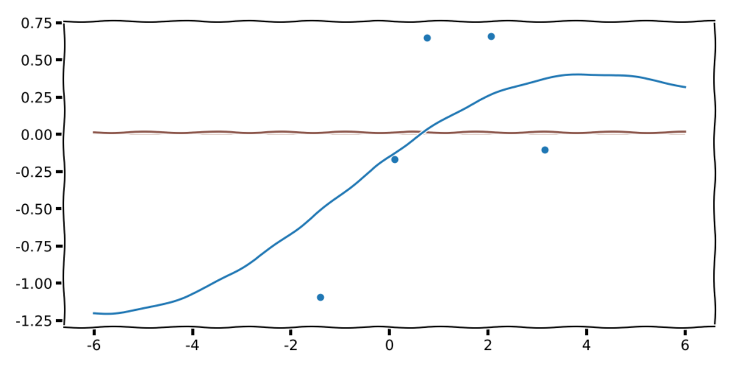

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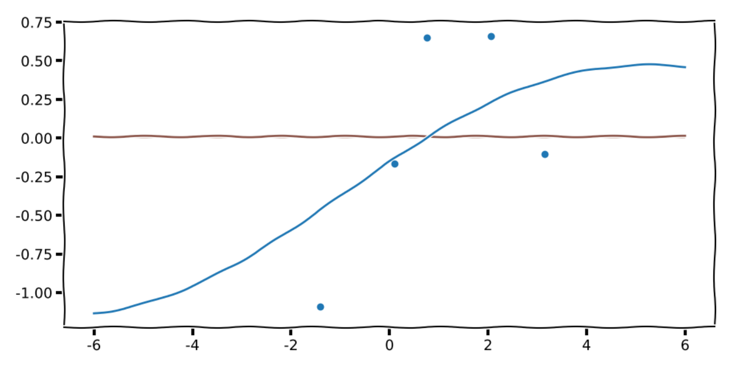

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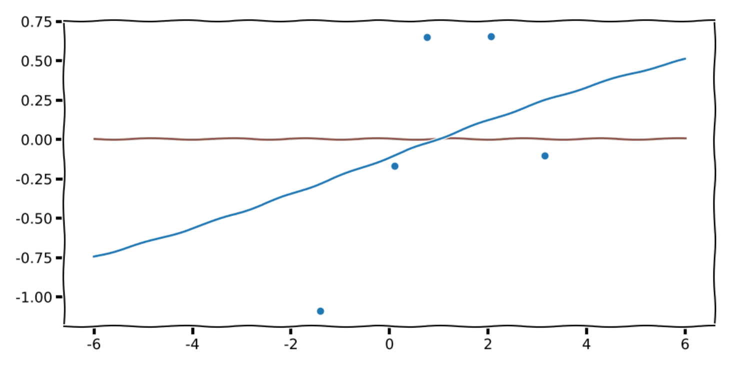

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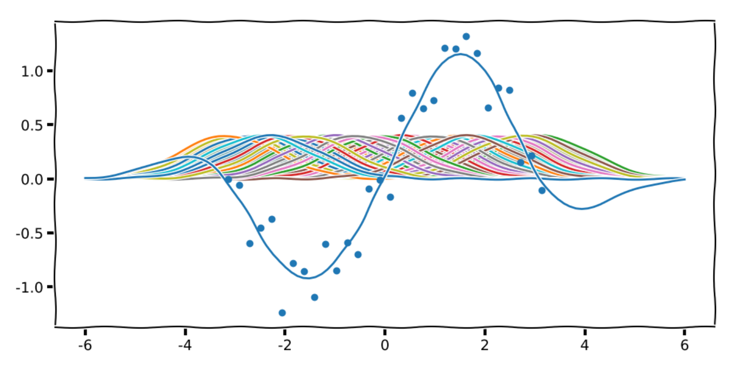
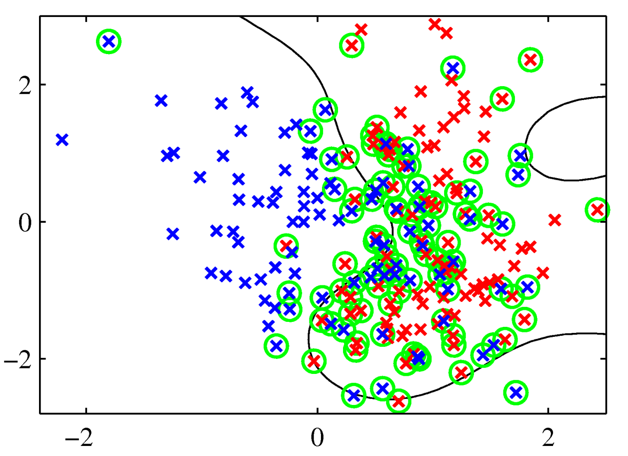


# Support Vector Machines [1] Figure 7.4



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- 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.