

# COMP90051 Statistical Machine Learning

Semester 2, 2018

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## 16. Bayesian regression



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# This lecture

- Uncertainty not captured by point estimates
- Bayesian approach preserves uncertainty
- New concepts:
  - \* sequential Bayesian updating
  - \* conjugate prior (Normal-Normal)
- Using posterior for Bayesian predictions on test

# Training == optimisation (?)

Stages of learning & inference:

- Formulate model

Regression

$$p(y|\mathbf{x}) = \text{sigmoid}(\mathbf{x}'\mathbf{w})$$

$$p(y|\mathbf{x}) = \text{Normal}(\mathbf{x}'\mathbf{w}; \sigma^2)$$

- Fit parameters to data

$$\hat{\mathbf{w}} = \text{argmax}_{\mathbf{w}} p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w}) \quad \textit{ditto}$$

- Make prediction

$$p(y_*|\mathbf{x}_*) = \text{sigmoid}(\mathbf{x}'_*\hat{\mathbf{w}}) \quad E[y_*] = \mathbf{x}'_*\hat{\mathbf{w}}$$

$\hat{\mathbf{w}}$  referred to as a '*point estimate*'

# Bayesian Alternative

Nothing special about  $\hat{\mathbf{w}}$ ... use more than one value?

- Formulate model

Regression

$$p(y|\mathbf{x}) = \text{sigmoid}(\mathbf{x}'\mathbf{w}) \quad p(y|\mathbf{x}) = \text{Normal}(\mathbf{x}'\mathbf{w}; \sigma^2)$$

- Consider the **space of likely parameters** – those that fit the training data well

$$p(\mathbf{w}|\mathbf{X}, \mathbf{y})$$

- Make **'expected'** prediction

$$p(y_*|\mathbf{x}_*) = E_{p(\mathbf{w}|\mathbf{X}_i, \mathbf{y})} [\text{sigmoid}(\mathbf{x}'\mathbf{w})]$$

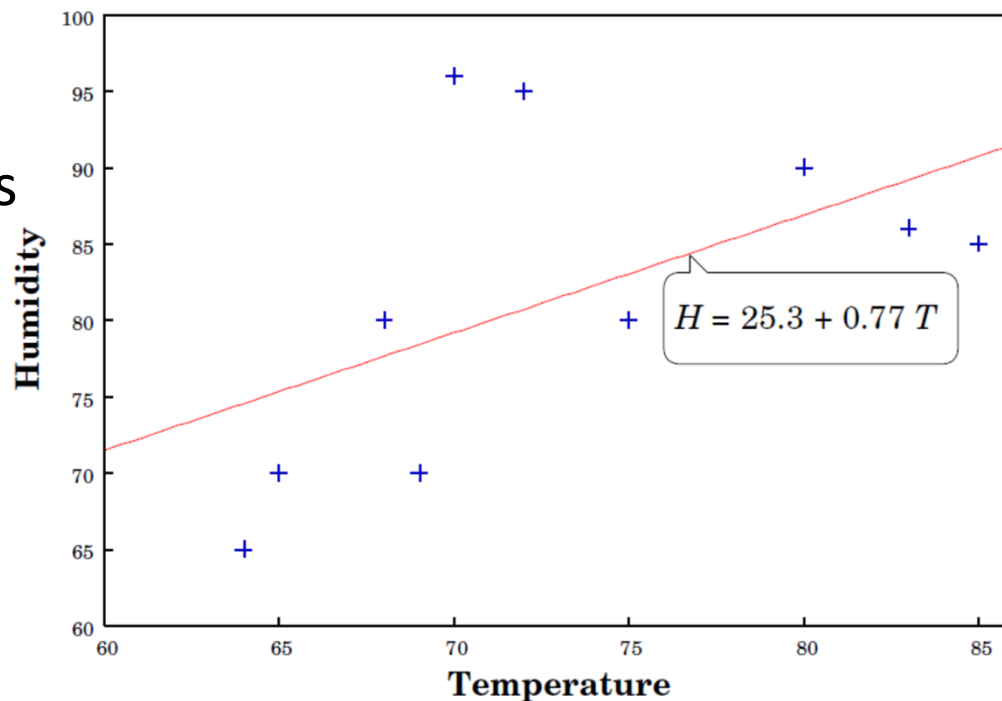
$$p(y_*|\mathbf{x}_*) = E_{p(\mathbf{w}|\mathbf{X}_i, \mathbf{y})} [\text{Normal}(\mathbf{x}'_*\mathbf{w}, \sigma^2)]$$

# Uncertainty

*From small training sets, we rarely have complete confidence in any models learned. Can we quantify the uncertainty, and use it in making predictions?*

# Regression Revisited

- Learn model from data
  - \* minimise error residuals by choosing weights
$$\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$
- But... how confident are we
  - \* in  $\hat{\mathbf{w}}$ ?
  - \* in the predictions?



**Linear regression:**  $y = w_0 + w_1 x$   
(here  $y$  = humidity,  $x$  = temperature)

# Do we trust point estimate $\hat{\mathbf{w}}$ ?

- How *stable* is learning?
  - \*  $\hat{\mathbf{w}}$  highly sensitive to noise
  - \* how much uncertainty in parameter estimate?
  - \* more *informative* if NLL objective highly peaked

- Formalised as *Fisher Information matrix*

- \*  $E[2^{\text{nd}} \text{ deriv of NLL}]$

$$\mathcal{I} = \frac{1}{\sigma^2} \mathbf{X}'\mathbf{X}$$

- \* measures *curvature of objective* about  $\hat{\mathbf{w}}$

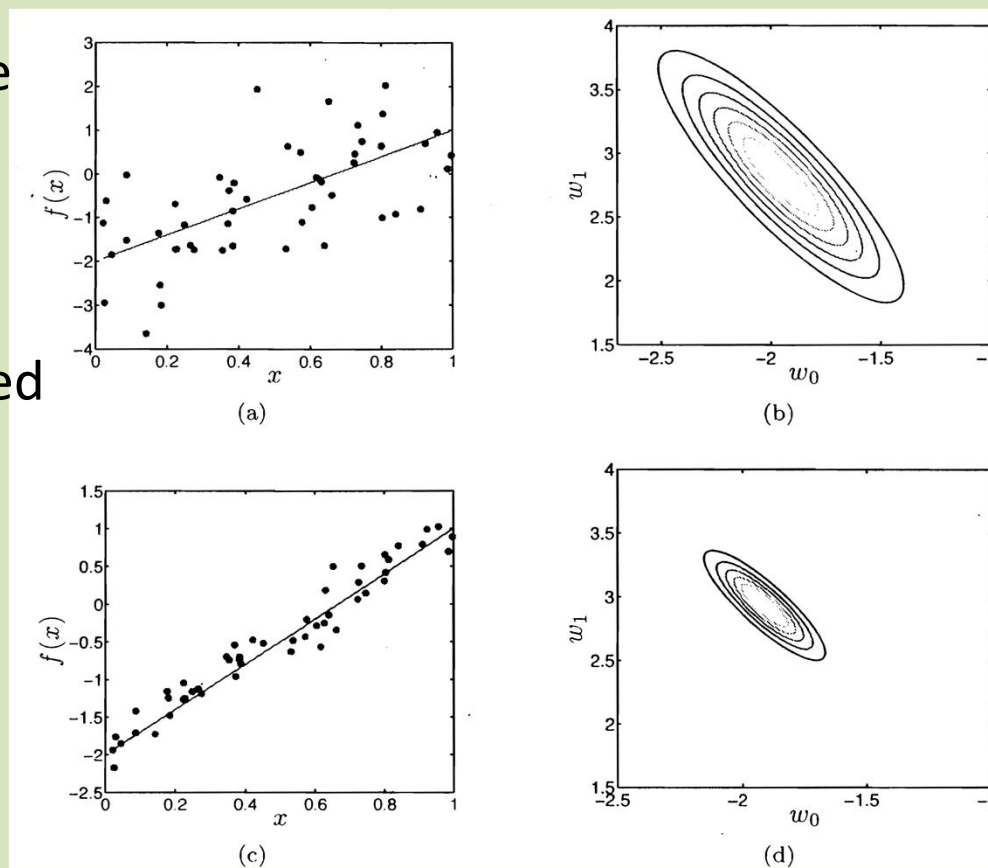


Figure: Rogers and Girolami p81

# The Bayesian View

*Retain and model all unknowns (e.g., uncertainty over parameters) and use this information when making inferences.*

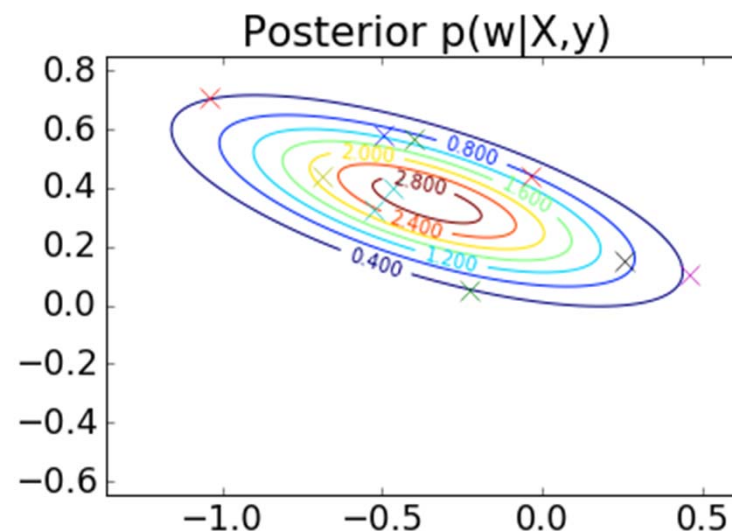


# A Bayesian View

- Could we reason over *all* parameters that are consistent with the data?
  - \* weights with a better fit to the training data should be more probable than others
  - \* make predictions with all these weights, *scaled by their probability*
- This is the idea underlying **Bayesian** inference

# Uncertainty over parameters

- Many reasonable solutions to objective
  - \* why select just one?
- Reason under **all** possible parameter values
  - \* weighted by their **posterior probability**
- More robust predictions
  - \* less sensitive to overfitting, particularly with small training sets
  - \* can give rise to more expressive model class (Bayesian logistic regression becomes non-linear!)



# Frequentist vs Bayesian divide

- **Frequentist:** learning using *point estimates*, regularisation, p-values ...
  - \* backed by complex theory relying on strong assumptions
  - \* mostly simpler algorithms, characterises much practical machine learning research
- **Bayesian:** maintain *uncertainty*, marginalise (sum) out unknowns during inference
  - \* nicer theory with fewer assumptions
  - \* often more complex algorithms, but not always
  - \* when possible, results in more elegant models

# Bayesian Regression

*Application of Bayesian inference  
to linear regression, using  
Normal prior over  $\mathbf{w}$*

# Revisiting Linear Regression

- Recall probabilistic formulation of linear regression

$\mathbf{I}_D = D \times D$  identity matrix

$$y \sim \text{Normal}(\mathbf{x}'\mathbf{w}, \sigma^2)$$

- Bayes rule:

$$\mathbf{w} \sim \text{Normal}(\mathbf{0}, \gamma^2 \mathbf{I}_D)$$

$$p(\mathbf{w}|\mathbf{X}, \mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})}{p(\mathbf{y}|\mathbf{X})}$$

$$\max_{\mathbf{w}} p(\mathbf{w}|\mathbf{X}, \mathbf{y}) = \max_{\mathbf{w}} p(\mathbf{y}|\mathbf{X}, \mathbf{w})p(\mathbf{w})$$

- Gives rise to the penalised RSS objective

point estimate taken here, avoids computing marginal likelihood term

# Bayesian Linear Regression

- Rewind one step, consider full posterior

$$\begin{aligned} p(\mathbf{w} | \mathbf{X}, \mathbf{y}, \sigma^2) &= \frac{p(\mathbf{y} | \mathbf{X}, \mathbf{w}, \sigma^2) p(\mathbf{w})}{p(\mathbf{y} | \mathbf{X}, \sigma^2)} \\ &= \frac{p(\mathbf{y} | \mathbf{X}, \mathbf{w}, \sigma^2) p(\mathbf{w})}{\int p(\mathbf{y}, | \mathbf{X}, \mathbf{w}, \sigma^2) p(\mathbf{w}) d\mathbf{w}} \end{aligned}$$

Here we  
assume noise  
var. known

- Can we compute the denominator (**marginal likelihood** or **evidence**)?
  - \* if so, we can use the full posterior, not just its mode

# Bayesian Linear Regression (cont)

- We have two Normal distributions
  - \* normal likelihood x normal prior
- Their product is also a Normal distribution
  - \* **conjugate prior**: *when product of likelihood x prior results in the same distribution as the prior*
  - \* *evidence* can be computed easily using the normalising constant of the Normal distribution

$$\begin{aligned} p(\mathbf{w}|\mathbf{X}, \mathbf{y}, \sigma^2) &\propto \text{Normal}(\mathbf{w}|\mathbf{0}, \gamma^2 \mathbf{I}_D) \text{Normal}(\mathbf{y}|\mathbf{X}\mathbf{w}, \sigma^2 \mathbf{I}_N) \\ &\propto \text{Normal}(\mathbf{w}|\mathbf{w}_N, \mathbf{V}_N) \end{aligned}$$

closed form solution for  
posterior!

# Bayesian Linear Regression (cont)

$$\begin{aligned} p(\mathbf{w}|\mathbf{X}, \mathbf{y}, \sigma^2) &\propto \text{Normal}(\mathbf{w}|\mathbf{0}, \gamma^2 \mathbf{I}_D) \text{Normal}(\mathbf{y}|\mathbf{X}\mathbf{w}, \sigma^2 \mathbf{I}_N) \\ &\propto \text{Normal}(\mathbf{w}|\mathbf{w}_N, \mathbf{V}_N) \end{aligned}$$

where

$$\mathbf{w}_N = \frac{1}{\sigma^2} \mathbf{V}_N \mathbf{X}' \mathbf{y}$$

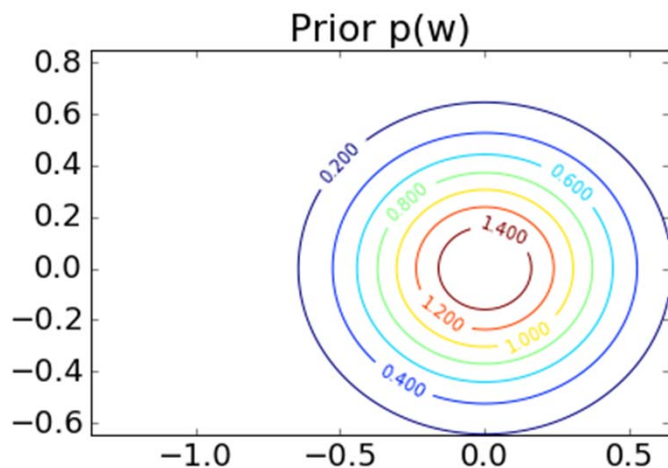
$$\mathbf{V}_N = \sigma^2 \left( \mathbf{X}' \mathbf{X} + \frac{\sigma^2}{\gamma^2} \mathbf{I}_D \right)^{-1}$$

Note that mean (and mode) are the MAP solution from before

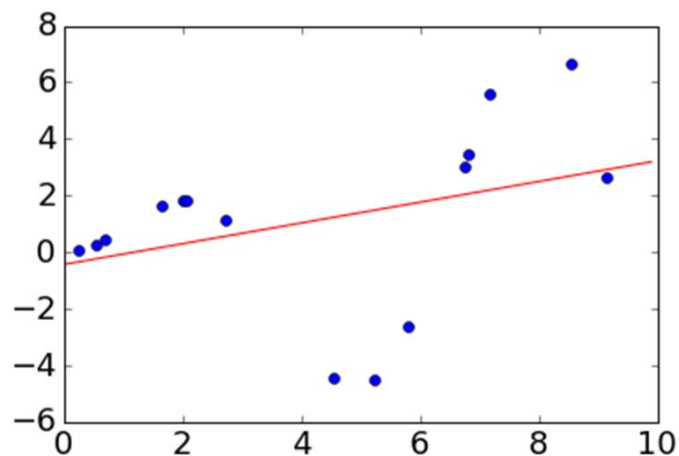
**Advanced:** verify by expressing product of two Normals, gathering exponents together and 'completing the square' to express as squared exponential (i.e., Normal distribution).



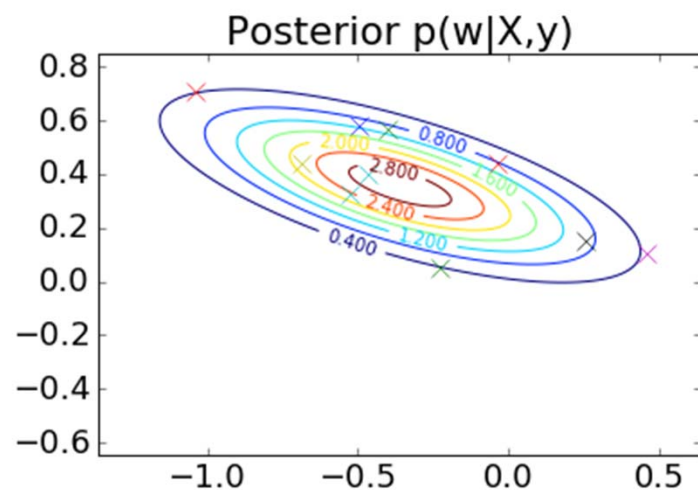
# Bayesian Linear Regression example



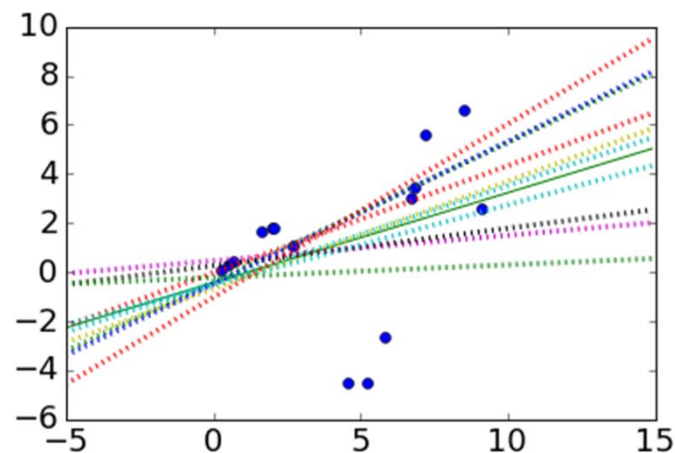
Step 1: select prior, here spherical about  $\mathbf{0}$



Step 2: observe training data



Step 3: formulate posterior, from prior & likelihood

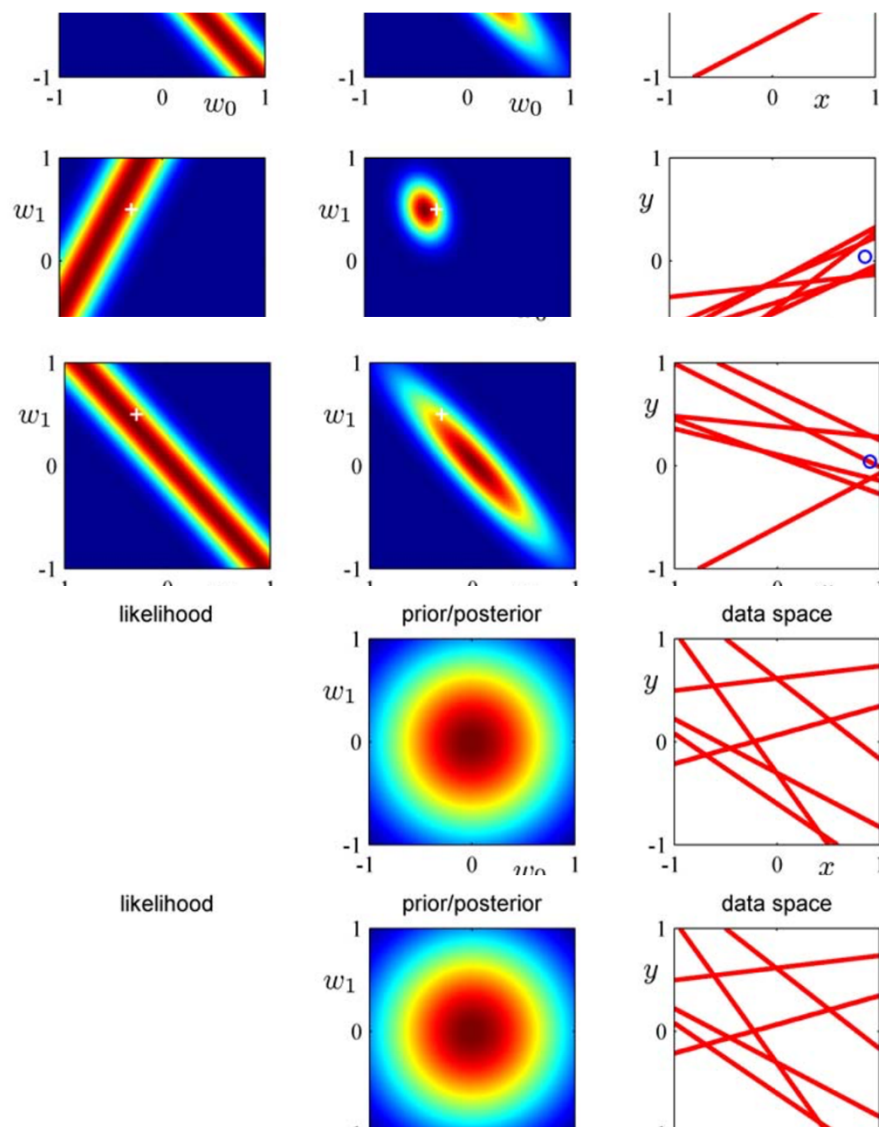


Samples from posterior

# Sequential Bayesian Updating

- Can formulate  $p(\mathbf{w}|\mathbf{X}, \mathbf{y}, \sigma^2)$  for given dataset
- What happens as we see more and more data?
  1. Start from prior  $p(\mathbf{w})$
  2. See new labelled datapoint
  3. Compute posterior  $p(\mathbf{w}|\mathbf{X}, \mathbf{y}, \sigma^2)$
  4. The *posterior now takes role of prior*  
& repeat from step 2

# Sequential Bayesian Updating



- Initially know little, many regression lines licensed
- Likelihood constrains possible weights such that regression is close to point
- Posterior becomes more refined/peaked as more data introduced
- Approaches a point mass about solution

*Bishop Fig 3.7, p155*

# Stages of Training

1. Decide on model formulation & prior
2. Compute *posterior* over parameters,  $p(\mathbf{w}|\mathbf{X},\mathbf{y})$

## MAP

3. Find *mode* for  $\mathbf{w}$
4. Use to make prediction on test

## approx. Bayes

3. Sample many  $\mathbf{w}$
4. Use to make *ensemble* average prediction on test

## exact Bayes

3. Use *all*  $\mathbf{w}$  to make *expected* prediction on test

## Prediction with uncertain $\mathbf{w}$

- Could predict using sampled regression curves
  - \* sample  $S$  parameters,  $\mathbf{w}^{(s)}, s \in \{1, \dots, S\}$
  - \* for each sample compute prediction  $y_*^{(s)}$  at test point  $\mathbf{x}_*$
  - \* compute the mean (and var.) over these predictions
  - \* this process is known as **Monte Carlo integration**
- For Bayesian regression there's a simpler solution
  - \* integration can be done analytically, giving

$$p(\hat{y}_* | \mathbf{X}, \mathbf{y}, \mathbf{x}_*, \sigma^2) = \int p(\mathbf{w} | \mathbf{X}, \mathbf{y}, \sigma^2) p(y_* | \mathbf{x}_*, \mathbf{w}, \sigma^2) d\mathbf{w}$$

## Prediction (cont.)

- Pleasant properties of Gaussian distribution means integration is tractable

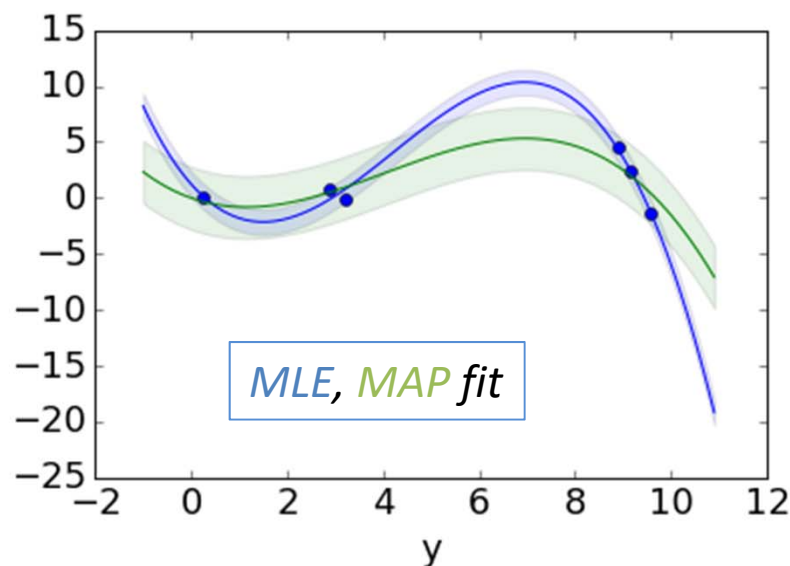
$$\begin{aligned} p(y_* | \mathbf{x}_*, \mathbf{X}, \mathbf{y}, \sigma^2) &= \int p(\mathbf{w} | \mathbf{X}, \mathbf{y}, \sigma^2) p(y_* | \mathbf{x}_*, \mathbf{w}, \sigma^2) d\mathbf{w} \\ &= \int \text{Normal}(\mathbf{w} | \mathbf{w}_N, \mathbf{V}_N) \text{Normal}(y_* | \mathbf{x}'_* \mathbf{w}, \sigma^2) d\mathbf{w} \\ &= \text{Normal}(y_* | \mathbf{x}'_* \mathbf{w}_N, \sigma_N^2(\mathbf{x}_*)) \\ \sigma_N^2(\mathbf{x}_*) &= \sigma^2 + \mathbf{x}'_* \mathbf{V}_N \mathbf{x}_* \end{aligned}$$

- \* additive variance based on  $\mathbf{x}_*$  match to training data
- \* cf. MLE/MAP estimate, where variance is a fixed constant

( $\mathbf{w}_N$  and  $\mathbf{V}_N$  defined in posterior when fitting Bayesian linear regression)

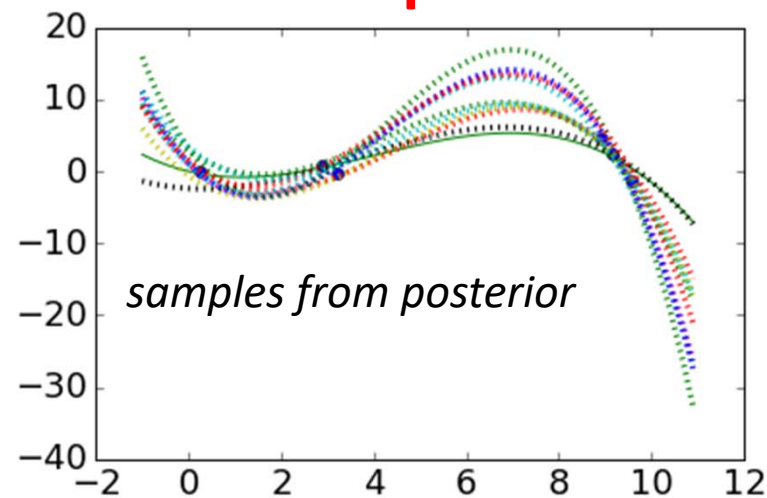
# Bayesian Prediction example

## Point estimate

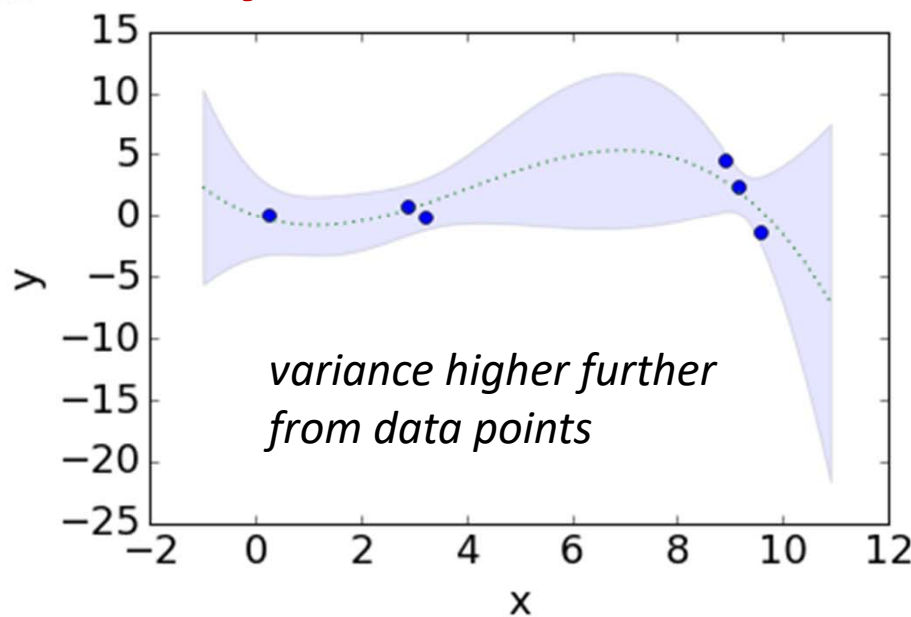


MLE (blue) and MAP (green)  
point estimates, *with fixed  
variance*

*Data:  $y = x \sin(x)$ ; Model = cubic*



## Bayesian inference



# Caveats

- Assumptions
  - \* known data noise parameter,  $\sigma^2$
  - \* data was drawn from the model distribution
- In real settings,  $\sigma^2$  is unknown
  - \* has its own conjugate prior  
*Normal* likelihood  $\times$  *InverseGamma* prior  
results in *InverseGamma* posterior
  - \* closed form predictive distribution, with student-T likelihood  
(see *Murphy*, 7.6.3)



# Summary

- Uncertainty not captured by point estimates (MLE, MAP)
- Bayesian approach preserves uncertainty
  - \* care about predictions NOT parameters
  - \* choose prior over parameters, then model posterior
- New concepts:
  - \* sequential Bayesian updating
  - \* conjugate prior (Normal-Normal)
- Using posterior for Bayesian predictions on test
- **Workshops Week #10**: PCA
- Next time: Bayesian classification, then PGMs