COMP 551 - Applied Machine Learning Lecture 23 — Bayesian regression

William L. Hamilton

(with slides and content from Joelle Pineau)

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Some logistics

- Midterm and MiniProject 3 grades will be released by Tuesday, April 9th.
- We will have an extra office hour session at 4pm in MC 321 on April 9th for people to view their exams and the solutions.
- Submit your course reviews: https://horizon.mcgill.ca/pban1/twbkwbis.P_WWWLogin?ret_code=f
-

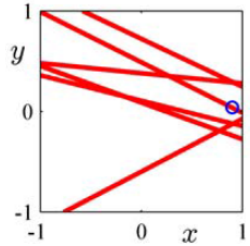
Recall: Bayesian probabilities

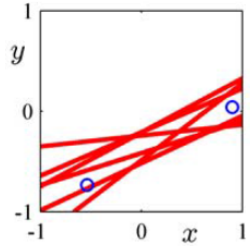
- An example from regression
- Given few noisy data points, multiple parameter values are possible
- Can we quantify uncertainty over our parameters using probabilities?

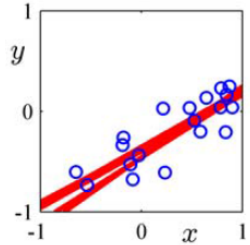
- I.e. given a dataset: $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$

  and some model with weights $\mathbf{w}$, can we find:

$$p(\mathbf{w}|\mathcal{D})$$







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Recall: Bayesian terminology

$p(\mathcal{D}|\mathbf{w})$

- Likelihood: our model of the data. Given our weights, how do we assign probabilities to dataset examples?

$p(\mathbf{w})$

- Prior: before we see any data, what do we think about our parameters?

$$p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$$

- Posterior: our distribution over weights, given the data we've observed and our prior

$p(\mathcal{D})$

- Marginal likelihood: also called the normalization constant. Does not depend on w, so not usually calculated explicitly

Recall: Conjugate priors

- A *prior* $p(\mathbf{w})$ is *conjugate* to a *likelihood* function $p(\mathcal{D}|\mathbf{w})$ if the posterior is in the same family as the prior

- In other words, if *prior * likelihood* gives you the same form as the prior with different parameters, it's a conjugate prior
  - Ex 1: the Gaussian distribution is a conjugate prior to a Gaussian likelihood
  - Ex 2: the Beta distribution is conjugate to a Bernoulli likelihood

- **Why?** *Want simple form for our posterior!* Don't want it to get more complicated every time you add more data

Bayesian linear regression

- Previous examples (coin flip, learning the mean of a Gaussian) only had outputs $\mathbf{y}$, no inputs $\mathbf{x}$
- How can we learn to make predictions that are input-dependent?
- Can use an extension of linear regression: Bayesian linear regression

Recall: Algorithms for Bayesian inference

- Given a dataset $\mathcal{D}$, how do we make predictions for a new input?

$$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$$

- Step 1: Define a model that represents your data (the **likelihood**): $p(\mathcal{D}|\mathbf{w})$
- Step 2: Define a **prior** over model parameters: $p(\mathbf{w})$
- Step 3: Calculate **posterior** using Bayes' rule: $p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$
- Step 4: Make **prediction** by integrating over model parameters:

$$p(y^*|\mathbf{x}^*, \mathcal{D}) = \int_{\mathbb{R}^N} p(\mathbf{w}|\mathcal{D})p(y^*|\mathbf{x}^*, \mathbf{w})d\mathbf{w}$$

Bayesian linear regression

- We take a *specific form of the likelihood and the prior*:
  - Step 1: Likelihood

$$p(y|\mathbf{x}, \mathbf{w}) = \mathcal{N}(\mathbf{w}^T\mathbf{x}, \sigma^2)$$

Output *y* close to learned linear function **w*x** , with some noise

  - Step 2: Conjugate prior

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

Prefer small weights. (assuming no other info)

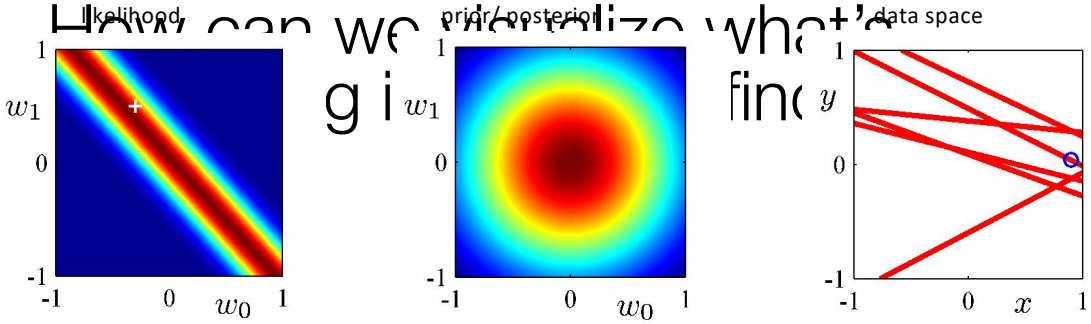
  - Prior precision α and noise variance σ^2 considered known
  - Linear regression where we **learn a distribution over the parameters**

Visualizing inference

- Start with simple example (one feature x):
- How can we visualize what's going on during inference?

$y = w_0 + w_1 x + \epsilon$

$p(\mathbf{w}|\mathcal{D})$



For different w0, w1, how likely is this data point?

How likely are different (w0, w1) given data so far?

Shows data points and sample functions for data so far

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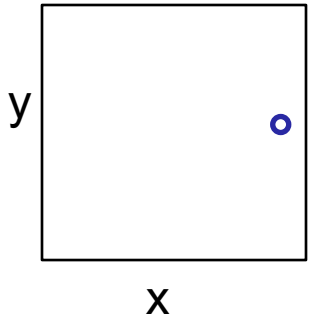
Visualizing inference

- Goal: fit lines $y = w_0 + w_1 x + \epsilon$
- Bayes theorem: $p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$



Visualizing inference

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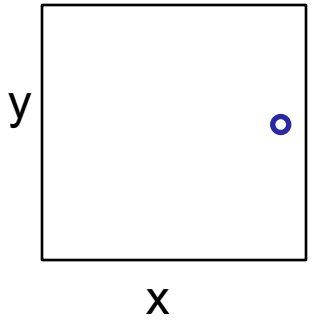
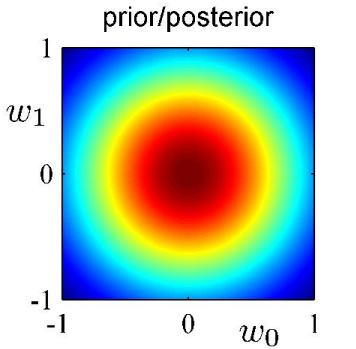
What prior?

- Bayes theorem: $p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$



- Similar to ridge regression, expect good **w** to be small



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Visualizing inference

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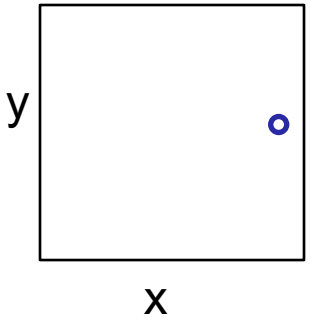

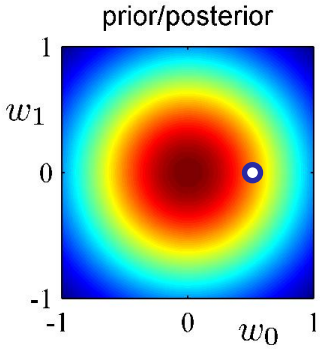

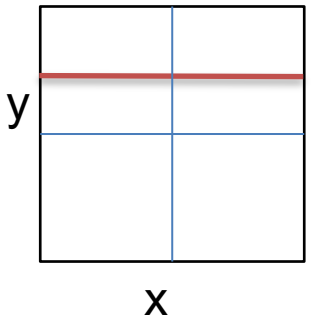

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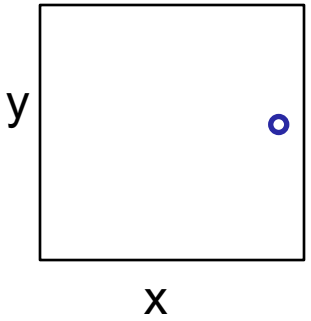

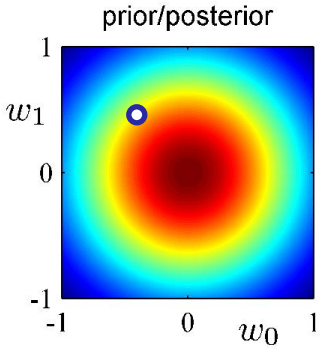

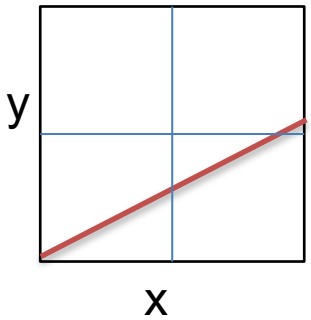

Visualizing inference

- Goal: fit lines $y = w_0 + w_1 x + \epsilon$

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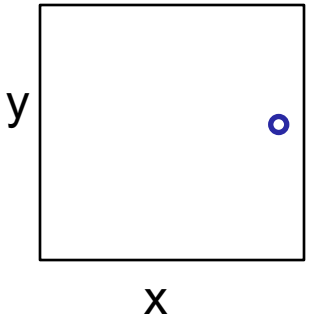
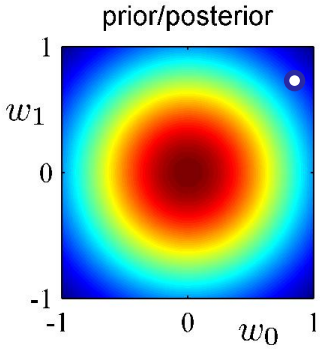
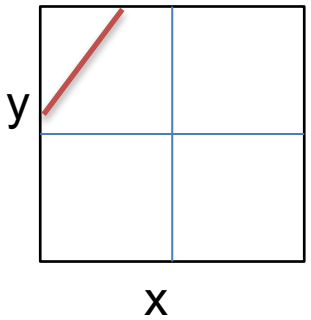


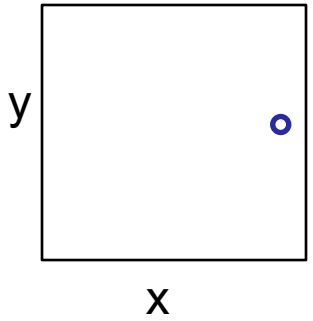




Visualizing inference

- Goal: fit lines $y = w_0 + w_1 x + \epsilon$

What about the likelihood?



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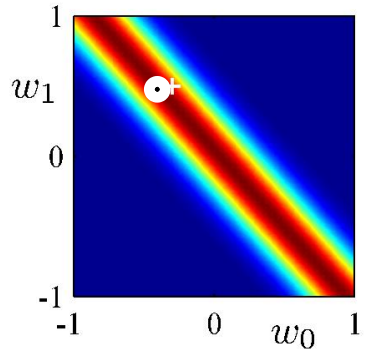
- Good lines should pass 'close by' datapoint



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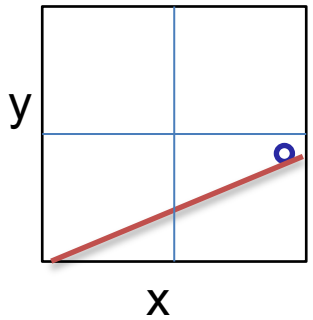

Visualizing inference

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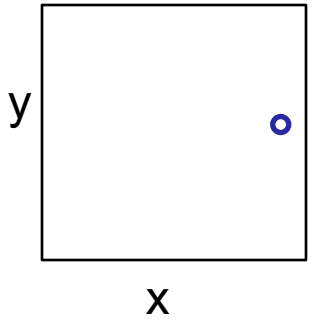

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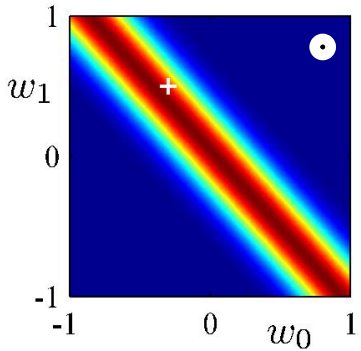

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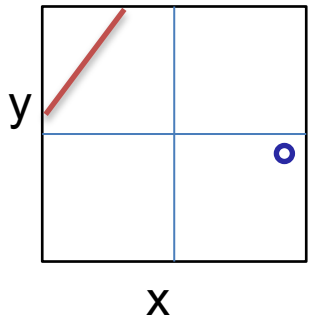
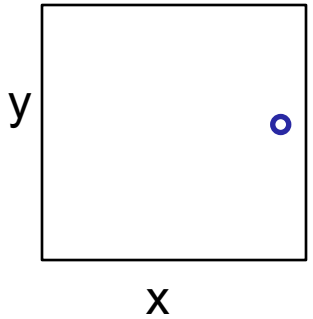


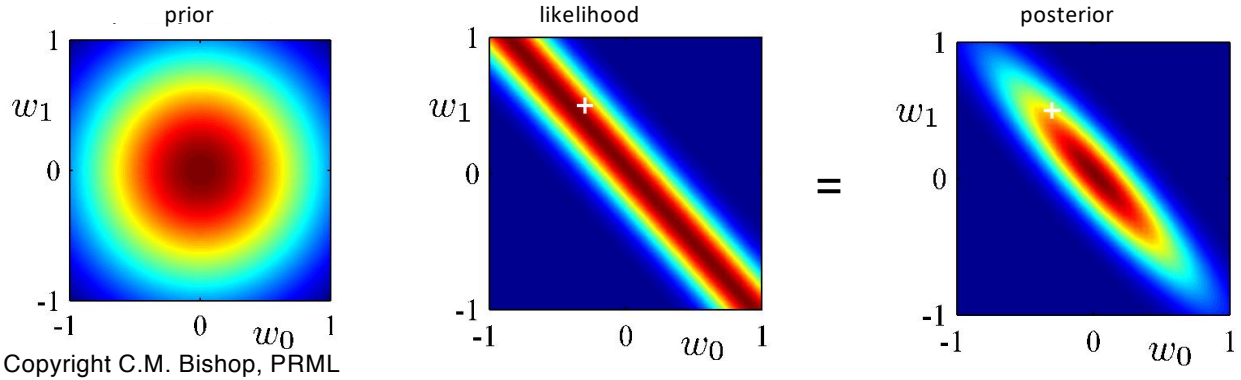
Visualizing inference

- Goal: fit lines $y = w_0 + w_1 x + \epsilon$



- Bayes theorem: $p(\mathbf{w}|\mathcal{D}) = \frac{p(\mathcal{D}|\mathbf{w})p(\mathbf{w})}{p(\mathcal{D})}$

- For all values of **w**, multiply prior and likelihood (and re-normalize)



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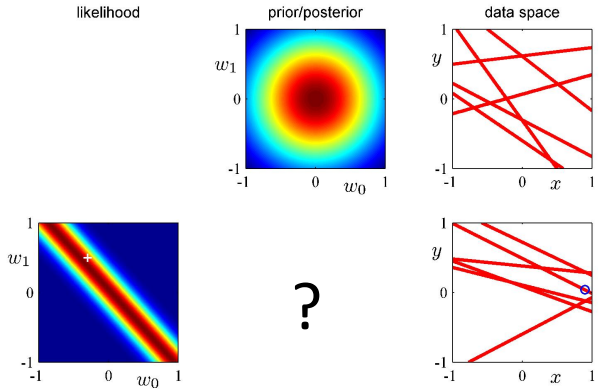
Bayesian linear regression: inference



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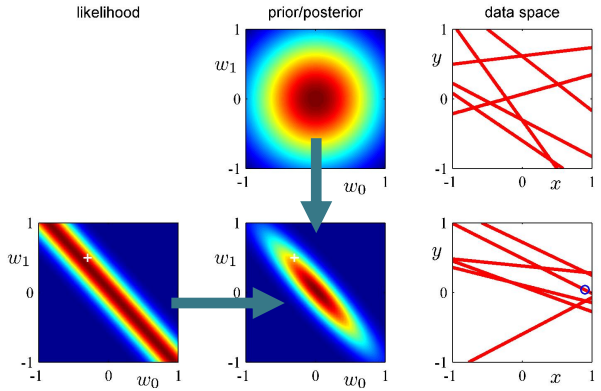
Bayesian linear regression: inference



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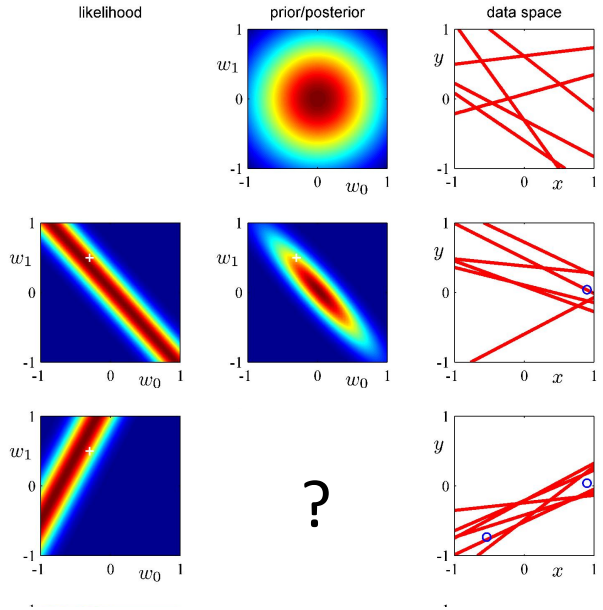
Bayesian linear regression: inference



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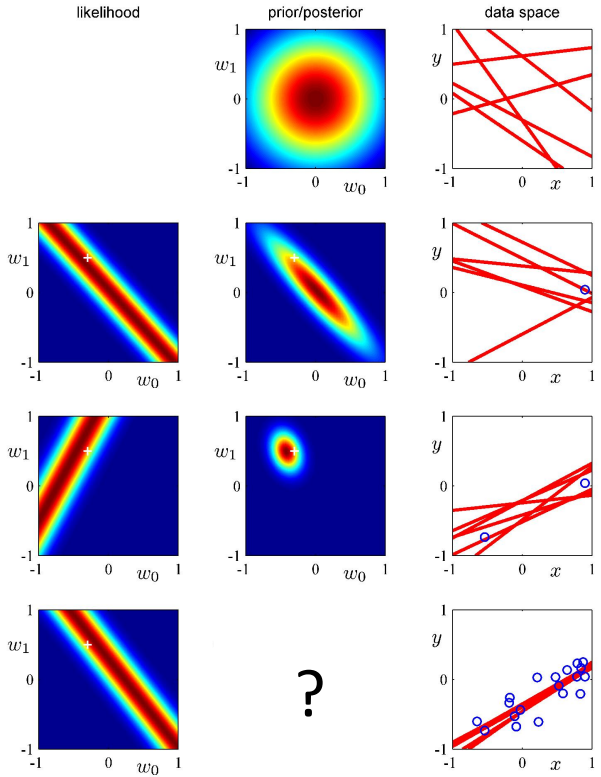
Bayesian linear regression: inference



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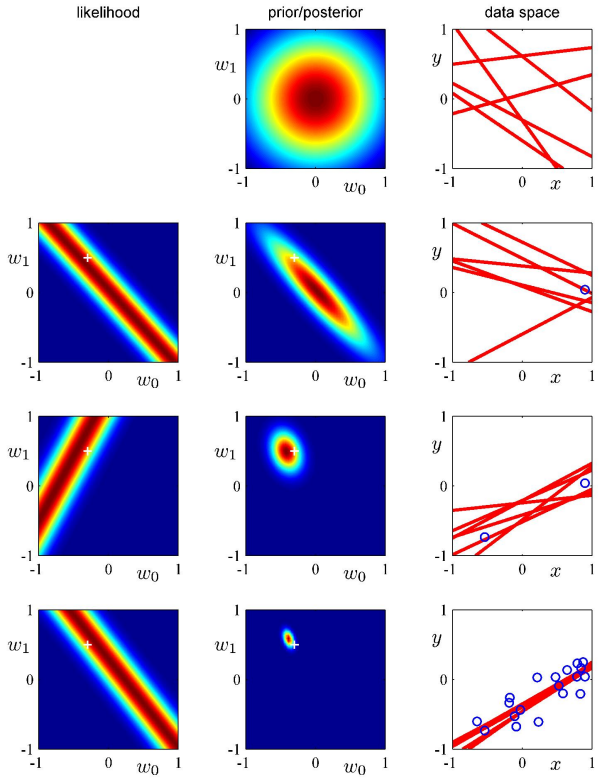
Bayesian linear regression: inference



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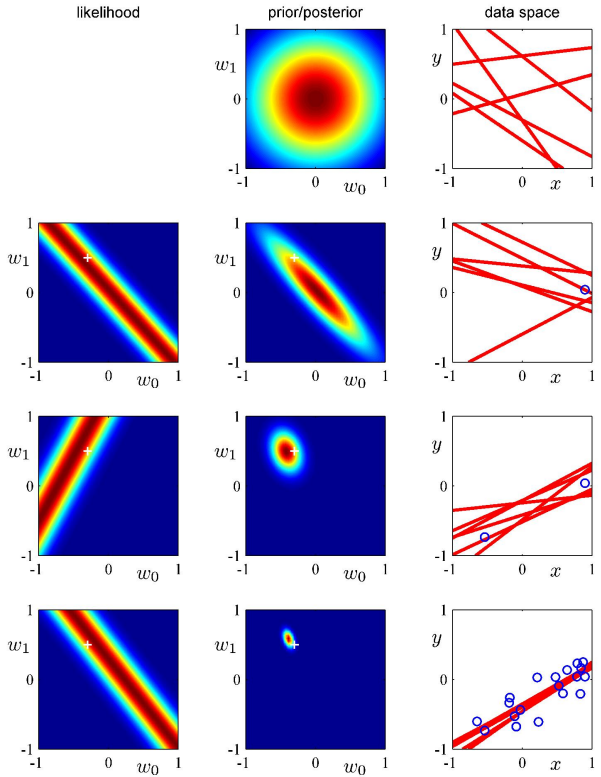
Bayesian linear regression: inference

As new data points are added, posterior converges on true value of parameters



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Step 3: calculate posterior

- Can calculate posterior by multiplying prior and likelihood:

$$p(\mathbf{w}|\mathcal{D}) = \mathcal{N}(\sigma^{-2}\mathbf{S}_N\mathbf{X}^T\mathbf{y}, \mathbf{S}_N)$$

$$\mathbf{S}_N = (\alpha\mathbf{I} + \sigma^{-2}\mathbf{X}^T\mathbf{X})^{-1}$$

(derivation similar to case with no inputs — slide 306 of lecture 18. Full derivation in section 3.3 of Bishop)

- $\mathbf{X}$ has one input per row, $\mathbf{y}$ has one target output per row

- If prior precision α goes to 0, mean becomes maximum likelihood solution (ordinary linear regression)
- Infinitely wide likelihood variance σ^2 or 0 datapoints, means distribution reduces to prior

Aside: finding the MAP

- We can investigate the maximum of the posterior (MAP)
- Log-transform posterior: log is sum of prior + likelihood

$$
\begin{aligned}
& \max \log p(\mathbf{w}|\mathbf{y}) \\
= & \\
& \max -\frac{\sigma^{-2}}{2} \sum_{n=1}^{N} (y_n - \mathbf{w}^T \mathbf{x}_n)^2 - \frac{\alpha}{2} \mathbf{w}^T \mathbf{w} + \text{const.}
\end{aligned}
$$

Aside: finding the MAP

- We can investigate the maximum value of the posterior (MAP)
- Calculate in log space: *log posterior = log prior + log likelihood*

$$\max \log p(\mathbf{w}|\mathbf{y})$$

$$= \max -\frac{\sigma^{-2}}{2}\sum_{n=1}^{N}(y_n - \mathbf{w}^T\mathbf{x}_n)^2 - \frac{\alpha}{2}\mathbf{w}^T\mathbf{w} + \text{const.}$$

Recall:

$$\min \sum_{n=1}^{N}(y_n - \mathbf{w}^T\mathbf{x}_n)^2 + \lambda\mathbf{w}^T\mathbf{w}$$

Ridge regression, (I.e., L2-regularized linear regression)

- Same objective function as for ridge regression!
- Penalty term: $\lambda = \alpha\sigma^2$

prior precision

likelihood variance

Note: since posterior is Gaussian, MAP = mean of posterior

Step 4: prediction

- Prediction for new datapoint:

$$p(y^*|\mathbf{x}^*, \mathcal{D}) = \int_{\mathbb{R}^N} p(\mathbf{w}|\mathcal{D}) p(y^*|\mathbf{x}^*, \mathbf{w}) d\mathbf{w}$$

- For Gaussians, can compute solution analytically:

$$p(y^*|\mathcal{D}) = \mathcal{N}(\sigma^{-2}\mathbf{x}^{*T}\mathbf{S}_N\mathbf{X}^T\mathbf{y}, \sigma^2 + \mathbf{x}^T\mathbf{S}_N\mathbf{x})$$

mean from before

from weight uncertainty

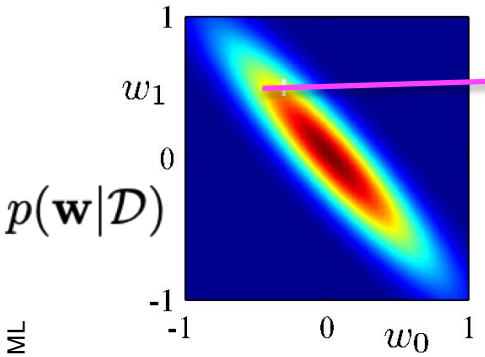
new input

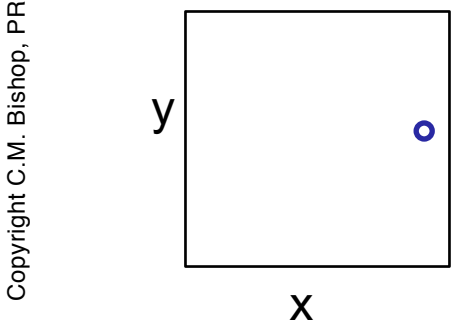
from observation noise

- Variance tends to go down with more data until it reaches σ^2

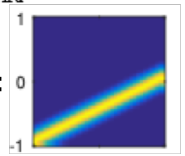
Step 4: prediction

- Every **w** makes a prediction, weighted by posterior





$$\int_{\mathbb{R}^N} p(\mathbf{w}|\mathcal{D})p(y^*|\mathbf{x}^*,\mathbf{w})d\mathbf{w}$$

= 

x medium $p(\mathbf{w}|\mathcal{D})$

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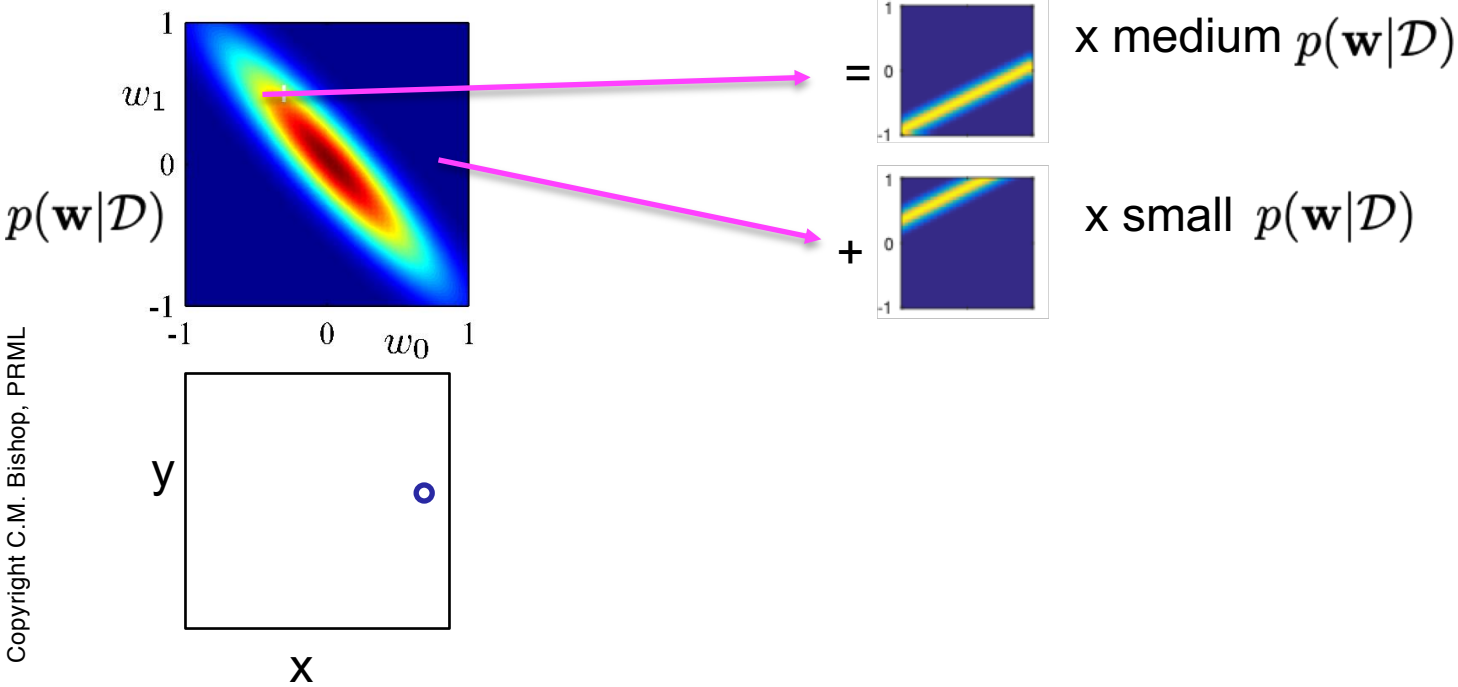
Step 4: prediction

- Every **w** makes a prediction, weighted by posterior

$$\int_{\mathbb{R}^N} p(\mathbf{w}|\mathcal{D})p(y^*|\mathbf{x}^*,\mathbf{w})d\mathbf{w}$$



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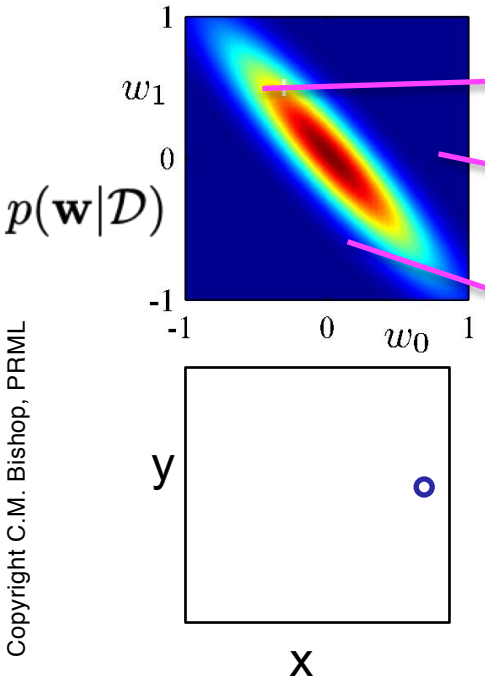
Step 4: prediction

- Every **w** makes a prediction, weighted by posterior

$$\int_{\mathbb{R}^N} p(\mathbf{w}|\mathcal{D})p(y^*|\mathbf{x}^*,\mathbf{w})d\mathbf{w}$$



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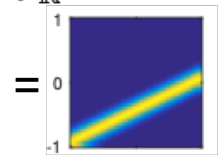
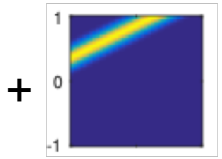
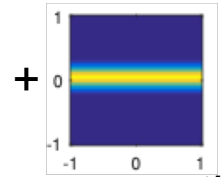


x medium $p(\mathbf{w}|\mathcal{D})$



x small $p(\mathbf{w}|\mathcal{D})$

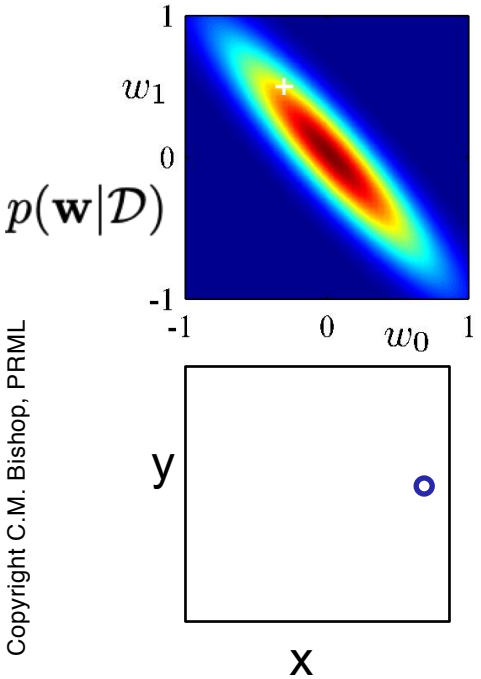


x large $p(\mathbf{w}|\mathcal{D})$

+ many other models

Step 4: prediction

- Every **w** makes a prediction, weighted by posterior



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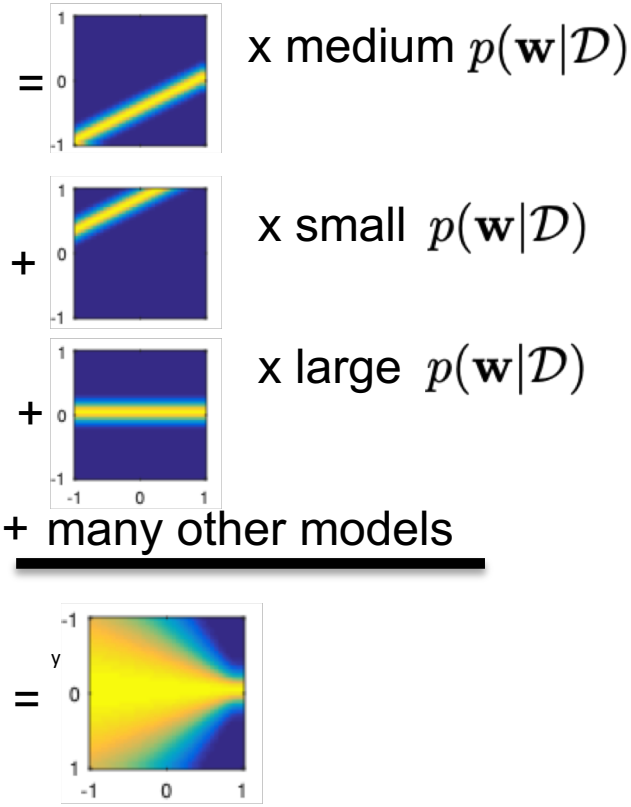
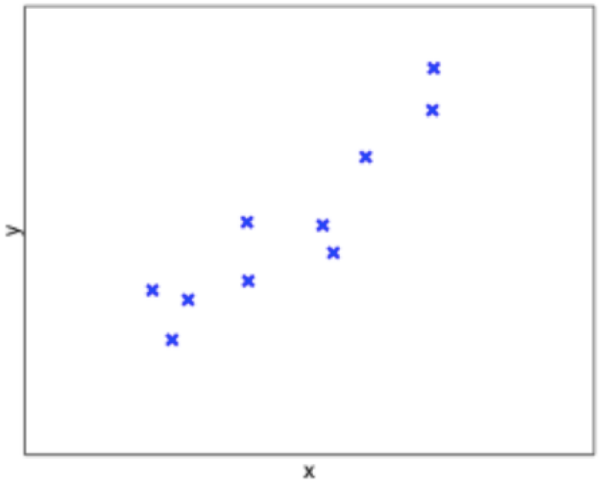


Bayesian linear regression

- Like ordinary linear regression, can use non-linear basis

$$f_w(x) = w_0 + w_1 x + w_2 x^2$$

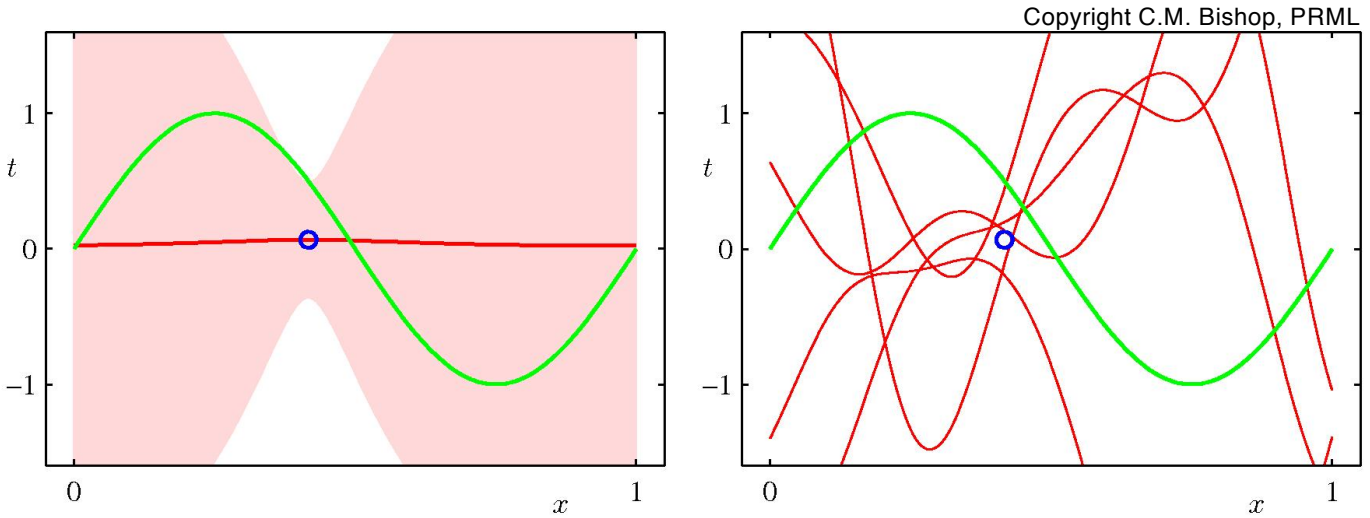


$$X = \begin{bmatrix} x^2 & x & \\ 0.75 & 0.86 & 1 \\ 0.01 & 0.09 & 1 \\ 0.73 & -0.85 & 1 \\ 0.76 & 0.87 & 1 \\ 0.19 & -0.44 & 1 \\ 0.18 & -0.43 & 1 \\ 1.22 & -1.10 & 1 \\ 0.16 & 0.40 & 1 \\ 0.93 & -0.96 & 1 \\ 0.03 & 0.17 & 1 \end{bmatrix} \quad Y = \begin{bmatrix} 2.49 \\ 0.83 \\ -0.25 \\ 3.10 \\ 0.87 \\ 0.02 \\ -0.12 \\ 1.81 \\ -0.83 \\ 0.43 \end{bmatrix}$$

Lecture 3, linear regression

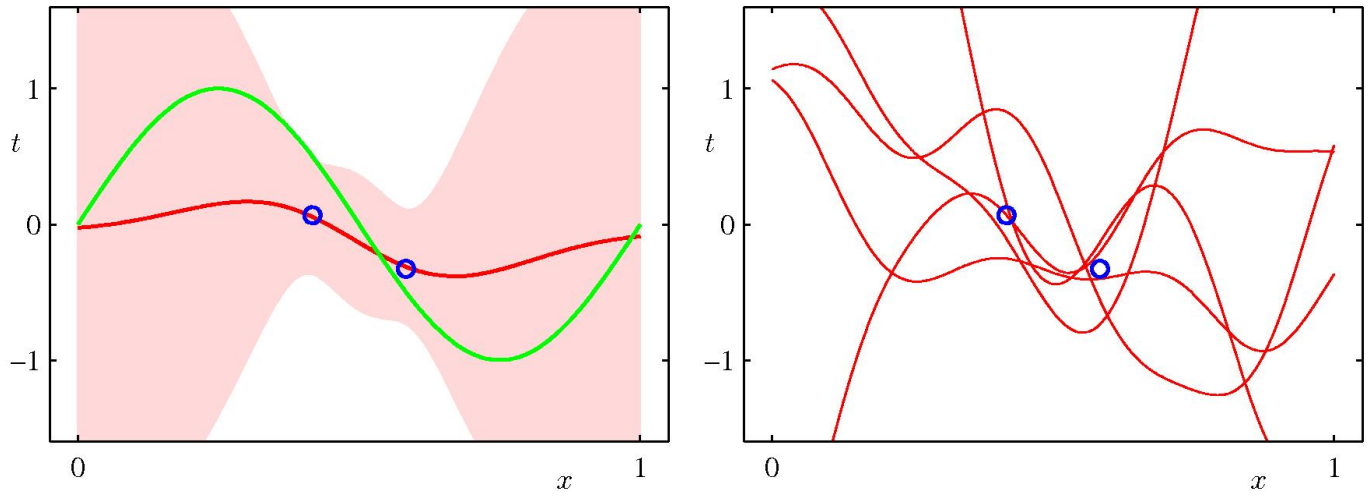
Example: Polynomial bases

- Example: Bayesian linear regression with polynomial bases



- Green line: true function. Blue circles: data points.
  Red line: MAP prediction. Shaded red: posterior predictive distribution.

Example: Polynomial bases



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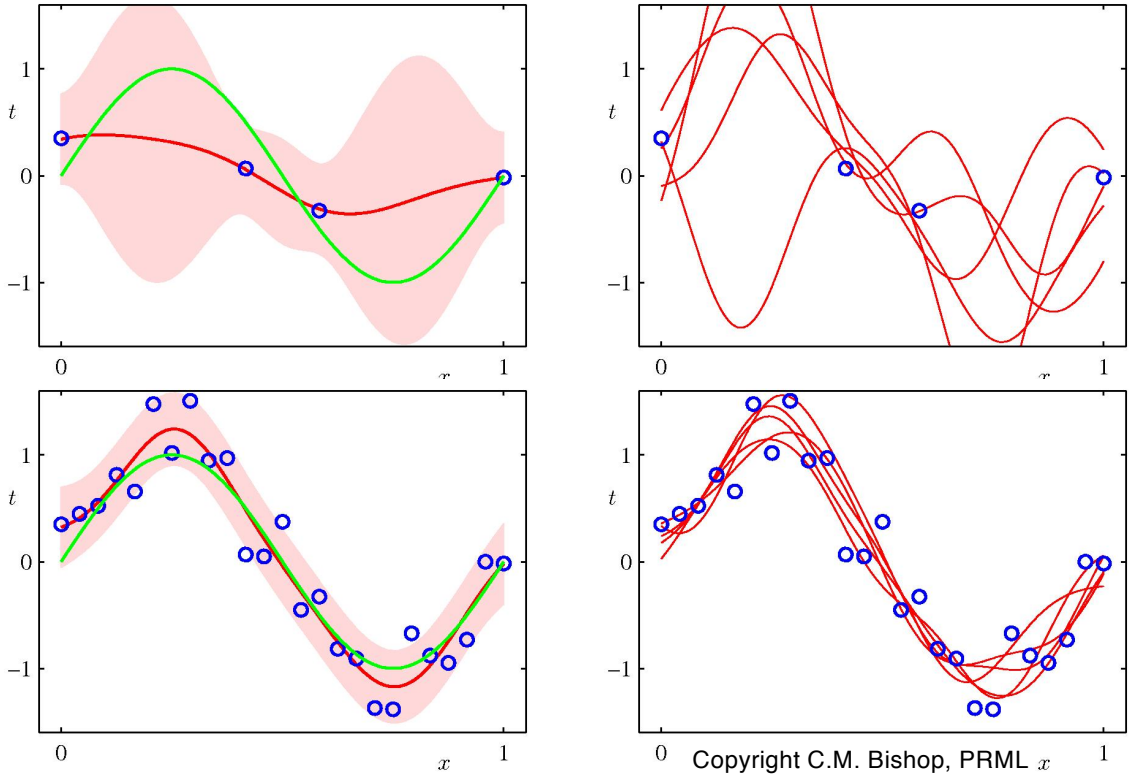
Example: Polynomial bases



Application: black-box optimization

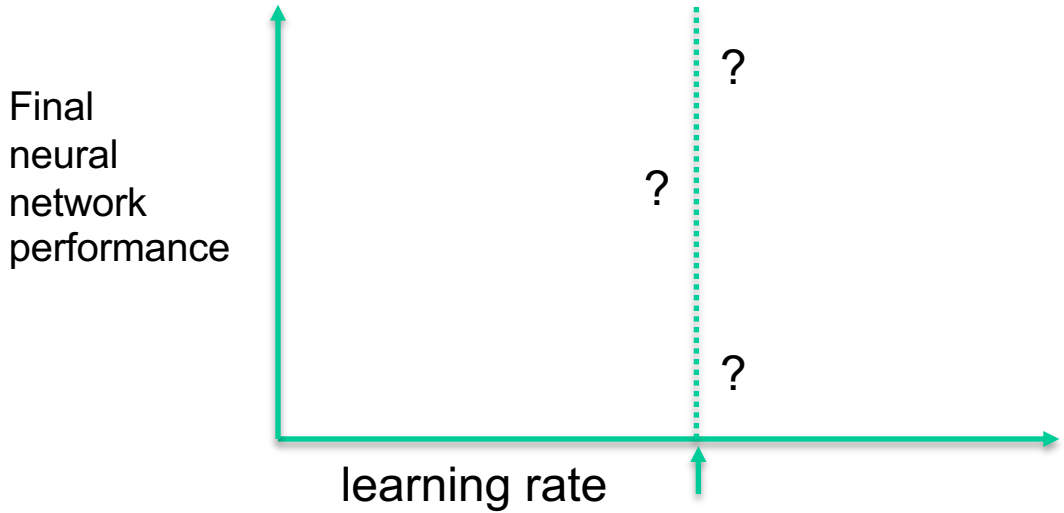
- Problem: find value x for which function $f(x)$ is maximized

- Constraints:
  - $f(x)$ is a 'black box' function: we only know the value $f(x)$ for small set of points x that we evaluate
  - Function may be highly non-convex.
  - Evaluating $f(x)$ is relatively expensive
  - Derivatives might not be known

- Example: finding the hyperparameters of a neural network
- How can we approach this problem?

Black-box optimization

- Problem: find value x for which function f(x) is maximal
- Example of black box function



Black-box optimization

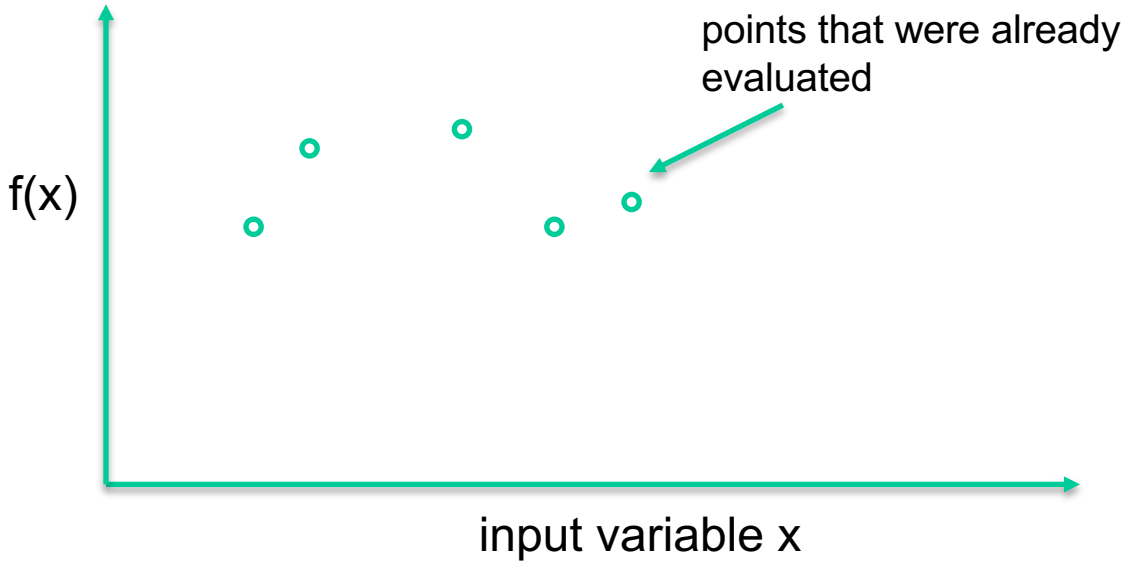
- So far, we have mainly done optimization via gradient decent.

- But gradient descent requires an estimate of the gradient
  - Might need many function evaluations (costly)
  - Might not know derivatives

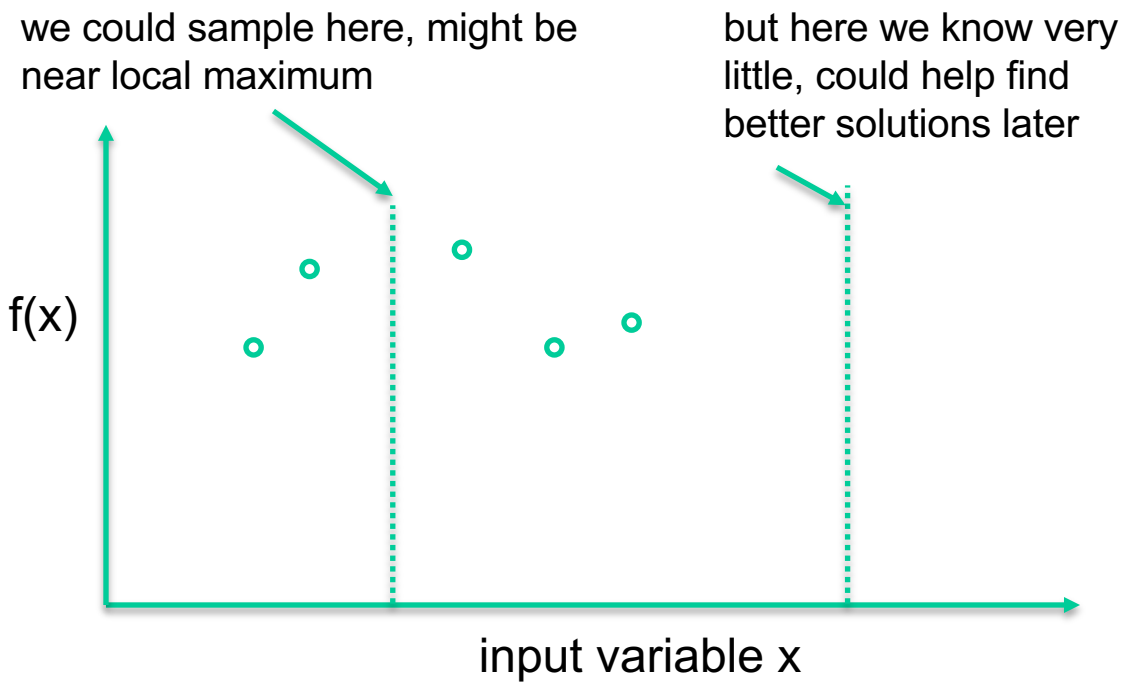
- What can we do in this "black box" situation?

Black-box optimization

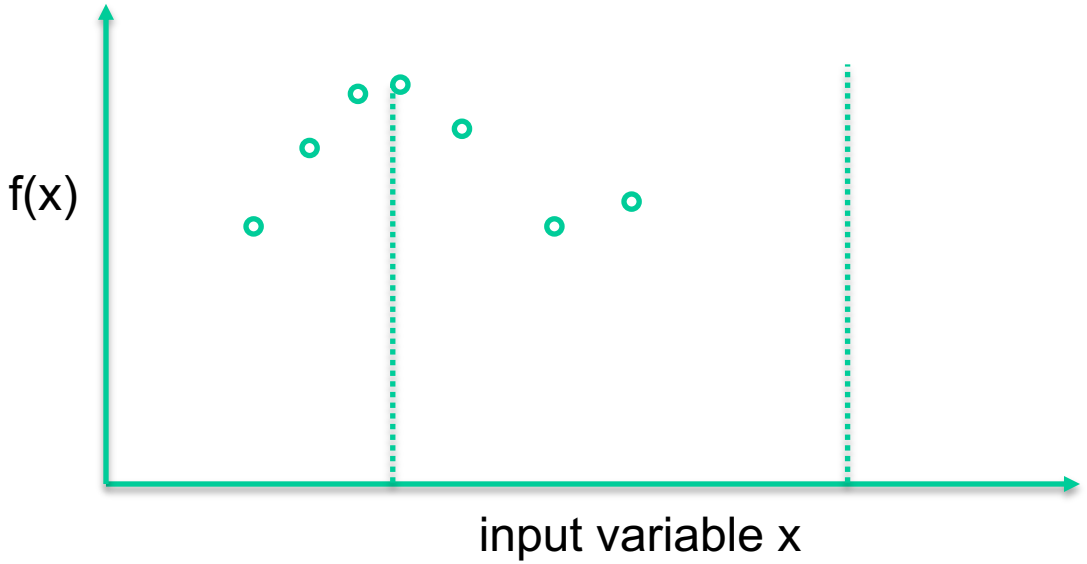
- Where to sample next, if we have a budget for, say, 10 samples?



Black-box optimization



Black-box optimization

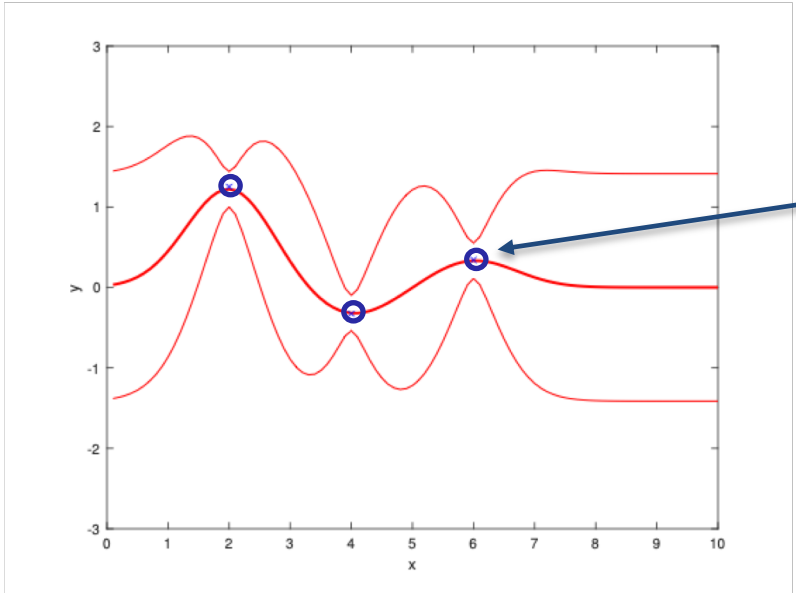


Bayesian optimization

- Idea: to make a good decision we should *imagine what the whole function should look like*
- It seems important to take into account how certain we are for various input values $\mathbf{x}$
- Bayesian linear regression might do the job here!
- This implies Bayesian point of view: Bayesian optimization (a method to do black-box optimization)

Bayesian optimisation

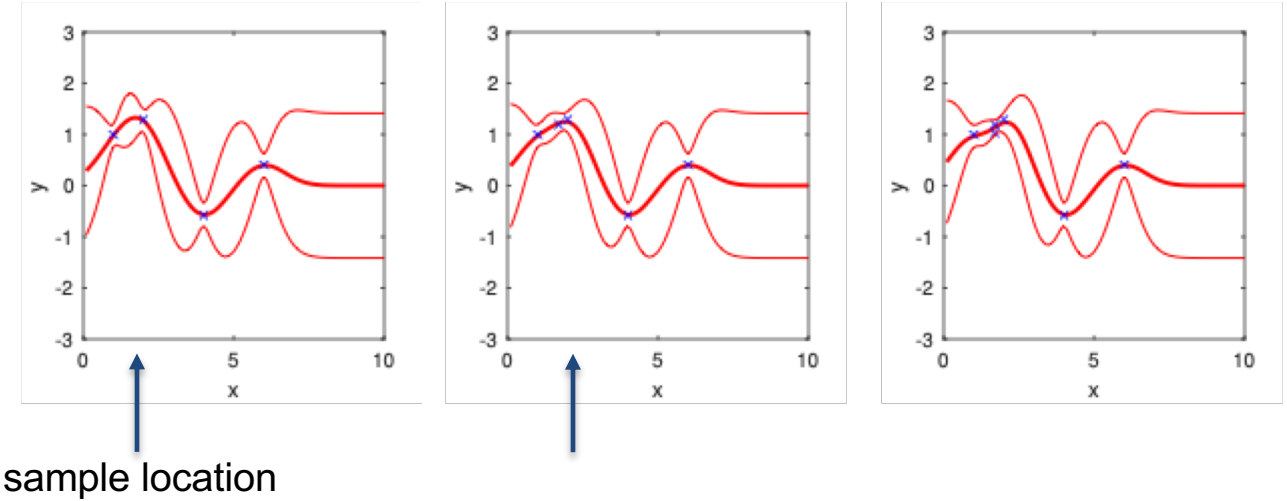
- Bayesian posterior over function



- Where to sample next?

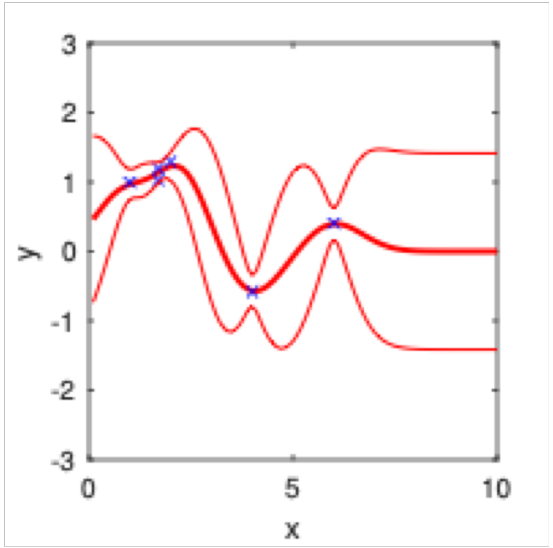
Bayesian optimisation

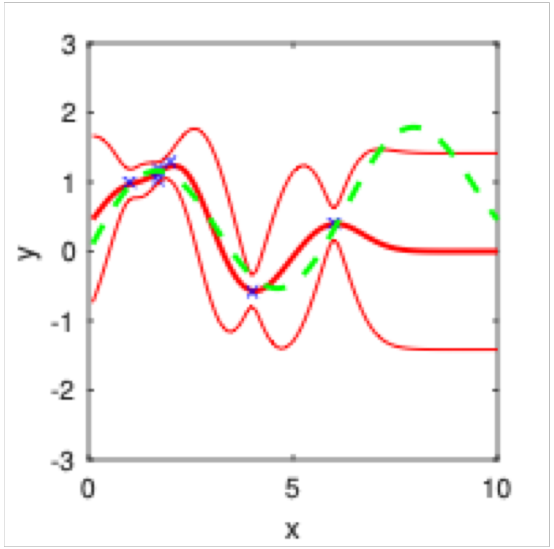
- Where to sample next?
- What happens if we simply sample where mean is highest?



Bayesian optimisation

- We might miss the real maximum!!!





Bayesian optimisation

Two objectives:

- Exploitation: sample where we think high values are.
  - If we know the samples will be low, it does not make sense to sample there
  - Maybe: sample highest mean?

- Exploration: If we always sample where we think the highest value is, we might miss other values
  - Maybe: sample where uncertainty is highest?

Bayesian optimisation

- Several strategies exist for combining these two objectives
- Can give ‘score’ to possible examples using **acquisition function**

Bayesian optimisation

- Several strategies exist for combining these two objectives
- Can give 'score' to possible examples using **acquisition function**
- Very straightforward method: upper confidence bound (UCB)

$$a_{\text{UCB}}(\mathbf{x}^*; \mathcal{D}) = \mu(\mathbf{x}^*; \mathcal{D}) + \kappa\sigma(\mathbf{x}^*; \mathcal{D})$$

predicted mean given data so far

trade-off parameter

predicted standard deviation given data so far

- Acquisition functions gives a 'score' to each sample point
- UCB has good theoretical properties

Bayesian optimisation

- Pros
  - Attempt at global optimization
  - Need relatively few samples to get close to optimum
  - Software packages available

- Cons
  - Computational expensive
  - Sensitive to choice of model
  - Only works well with few input (up to ~10 dimensions)

What you should know

- Bayesian terminology (prior, posterior, likelihood, etc.)
- Conjugate priors, what they mean.
- Bayesian linear regression and its properties
- When and why to use Bayesian methods
- Core concepts behind Bayesian optimization