Advanced Statistical Inference
Bayesian Linear Regression

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Recap - Probabilities

Consider two continuous random variables x and y

- Sum rule:

$$p(x) = \int p(x, y) dy$$

- Product rule:

$$p(x, y) = p(x|y)p(y) = p(y|x)p(x)$$

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- Product rule:

$$p(x, y) = p(x|y)p(y) = p(y|x)p(x)$$

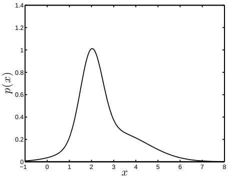
- Bayes' rule:

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)}$$

- NOTE: Bayes' rule is a direct consequence of the product rule

Recap - Expectations

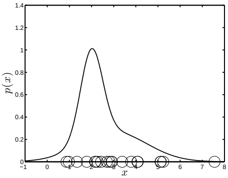
- Consider a random variable with density $p(x)$
- Imagine wanting to know the average value of x, $\tilde{x}$.



Recap - Expectations

- Consider a random variable with density $p(x)$
- Imagine wanting to know the average value of x, $\tilde{x}$.
- Generate S samples, $x_1, \ldots, x_S$
- Average the samples:

$$\tilde{x} \approx \frac{1}{S} \sum_{s=1}^{S} x_s$$



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- We can also (sometimes) compute it exactly using **expectations**.
  - Discrete:
    $$\tilde{x} = \mathrm{E}_{p(x)}(x) = \sum_{x} x \, p(x)$$
  - Continuous:
    $$\tilde{x} = \mathrm{E}_{p(x)}(x) = \int x \, p(x) \, dx$$

Recap - Expectations

- Example:
  - X is outcome of rolling die. $P(X = x) = 1/6$

$$\tilde{x} = \sum_x x\, P(X = x) = 3.5$$

  - X is uniform distributed RV between a and b

$$\tilde{x} = \int_{x=a}^{x=b} xp(x)\ dx = (b - a)/2$$

Expectations

- In general:

$$\mathrm{E}_{p(x)}[f(x)] = \int f(x)\, p(x)\, dx$$

Expectations

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- Some important properties:

$$\mathrm{E}_{p(x)}[f(x)] \neq f\left(\mathrm{E}_{p(x)}[x]\right)$$

$$\mathrm{E}_{p(x)}[k\, f(x)] = k\, \mathrm{E}_{p(x)}[f(x)]$$

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- Mean and variance

$$\mu = \mathrm{E}_{p(x)}[x]$$

$$\sigma^2 = \mathrm{E}_{p(x)}[(x-\mu)^2] = \mathrm{E}_{p(x)}[x^2] - \mu^2$$

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- For vectors of random variables:

$$\mathrm{E}_{p(\mathbf{x})}[f(\mathbf{x})] = \int f(\mathbf{x})\, p(\mathbf{x})\, dx$$

  - Mean and covariance:

$$\boldsymbol{\mu} = \mathrm{E}_{p(\mathbf{x})}[\mathbf{x}]$$

$$\begin{aligned} \mathrm{cov}(x) &= \mathrm{E}_{p(\mathbf{x})}[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\top] \\ &= \mathrm{E}_{p(\mathbf{x})}[\mathbf{x}\mathbf{x}^\top] - \boldsymbol{\mu}\boldsymbol{\mu}^\top \end{aligned}$$

The Gaussian Distribution

Consider a continuous random variable v

- The Gaussian probability density function is:

$$p(v|\mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left\{-\frac{1}{2\sigma^2}(v-\mu)^2\right\}$$

- μ is the mean
- σ^2 is the variance

The Multivariate Gaussian Distribution

- Consider $\mathbf{v} = (v_1, \ldots, v_D)^\top$ with joint Gaussian distribution

$$p(\mathbf{v}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \mathcal{N}(\mathbf{v}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

$$\mathcal{N}(\mathbf{v}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{v}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{v}-\boldsymbol{\mu})\right\}$$

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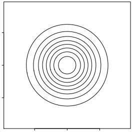

$$\boldsymbol{\Sigma} = \begin{bmatrix} 9 & 0 \\ 0 & 9 \end{bmatrix}$$

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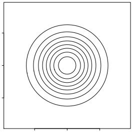

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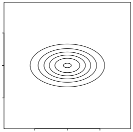

$$\boldsymbol{\Sigma} = \begin{bmatrix} 9 & 0 \\ 0 & 3 \end{bmatrix}$$

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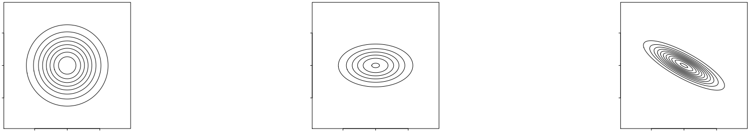

$$\boldsymbol{\Sigma} = \begin{bmatrix} 9 & 0 \\ 0 & 9 \end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 9 & 0 \\ 0 & 3 \end{bmatrix} \qquad \boldsymbol{\Sigma} = \begin{bmatrix} 8 & -4 \\ -4 & 3 \end{bmatrix}$$

Expectations – Gaussians

- Univariate
  - $p(x|\mu, \sigma^2) = \mathcal{N}(x|\mu, \sigma^2)$
  - Mean: $\mathrm{E}_{p(x)}[x] = \mu$
  - Variance: $\mathrm{E}_{p(x)}\left[(x-\mu)^2\right] = \sigma^2$

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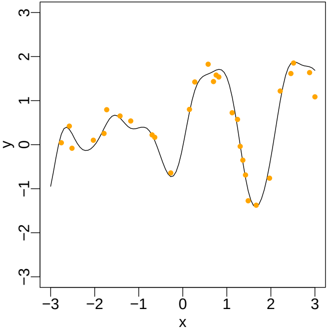
- Multivariate
  - $p(\mathbf{x}|\mu, \sigma^2) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$
  - Mean: $\mathrm{E}_{p(\mathbf{x})}[\mathbf{x}] = \boldsymbol{\mu}$
  - Variance: $\mathrm{E}_{p(\mathbf{x})}\left[(\mathbf{x}-\boldsymbol{\mu})(\mathbf{x}-\boldsymbol{\mu})^\top\right] = \boldsymbol{\Sigma}$

Working example

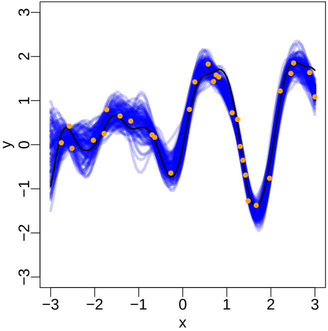
- Some data



- In this course we will learn ways to estimate functions that interpolate data...

Working example

- Function estimation...



- ... with confidence intervals
- Useful for **uncertainty** quantification

Definitions

- Features, inputs, covariates, or attributes $\mathbf{x}$:

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

$$\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)^\top$$

- Labels, outputs, or responses:

$$\mathbf{y} \in \mathbb{R}^O$$

$$\mathbf{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_N)^\top$$

Linear Regression - Definitions

- Data is a set of N pairs feature vectors and labels:

$$\mathcal{D} = \{(\mathbf{x}_i, \mathbf{y}_i)\}_{i=1,\dots,N}$$

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$$\mathbf{f}(\mathbf{x}) : \mathbb{R}^D \rightarrow \mathbb{R}^O$$

- For simplicity, we will assume $O = 1$ (univariate labels)

$$\mathbf{y} = (y_1, \ldots, y_N)^\top$$

so we aim to estimate:

$$f(\mathbf{x}) : \mathbb{R}^D \rightarrow \mathbb{R}$$

Linear Models for Regression

- Implement a linear combination of basis functions

$$\begin{aligned} f(\mathbf{x}) &= \sum_{i=1}^{D} w_i \varphi_i(\mathbf{x}) \\ &= \mathbf{w}^\top \boldsymbol{\varphi}(\mathbf{x}) \end{aligned}$$

with

$$\boldsymbol{\varphi}(\mathbf{x}) = (\varphi_1(\mathbf{x}), \ldots, \varphi_D(\mathbf{x}))^\top$$

Linear Models for Regression

- For simplicity we will start with linear functions

$$\begin{aligned} f(\mathbf{x}) &= \sum_{i=1}^{D} w_i x_i \\ &= \mathbf{w}^\top \mathbf{x} \end{aligned}$$

Linear Regression as Loss Minimization

- Definition of the quadratic loss function:

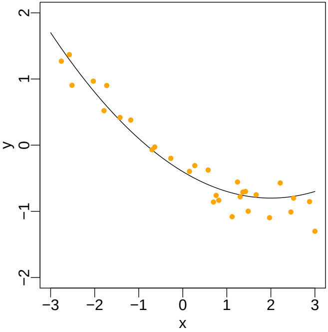
$$\begin{aligned}\mathcal{L} &= \sum_{i=1}^{N} [y_i - \mathbf{w}^\top \mathbf{x}_i]^2 \\ &= \|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2\end{aligned}$$

- Solution to the regression problem is:

$$\nabla_{\mathbf{w}} \mathcal{L} = \mathbf{0} \quad \Longrightarrow \quad \widehat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

Working example

- Some data generated from a known function



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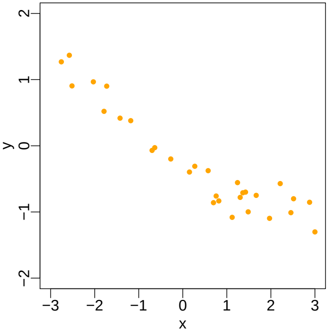
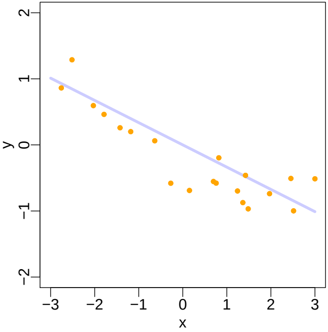


- In reality we only observe data and we want to estimate the generating function

Working example

- Solution obtained when optimizing the loss

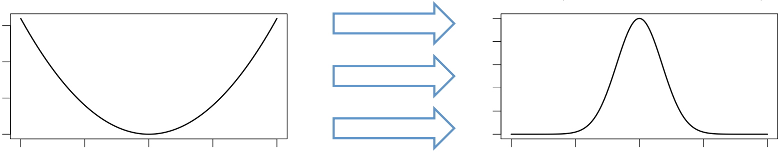
$$f(\mathbf{x}) = \widehat{\mathbf{w}}^\top \mathbf{x}$$



Probabilistic Interpretation of Loss Minimization

- Consider a simple transformation of the loss function

$[y_i - \mathbf{w}^\top \mathbf{x}_i]^2$ $\qquad\qquad$ $\exp\left(-\gamma[y_i - \mathbf{w}^\top \mathbf{x}_i]^2\right)$



- Minimizing the quadratic loss equivalent to maximizing the Gaussian likelihood function

$$\begin{aligned} \exp\left(-\gamma\mathcal{L}\right) &= \exp\left(-\gamma\|\mathbf{y} - \mathbf{X}\mathbf{w}\|^2\right) \\ &\propto \mathcal{N}\left(\mathbf{y}|\mathbf{X}\mathbf{w}, \frac{1}{2\gamma}\right) \qquad \text{Gaussian distribution} \end{aligned}$$

Probabilistic Interpretation of Loss Minimization

- The likelihood $\mathcal{N}\left(\mathbf{y}|\mathbf{X}\mathbf{w}, \frac{1}{2\gamma}\right)$ hints to the fact that we are assuming:
$$y_i = \mathbf{w}^\top \mathbf{x}_i + \varepsilon_i$$
with $\varepsilon_i \sim \mathcal{N}(\varepsilon_i|0, \sigma^2 = \frac{1}{2\gamma})$
- In vectorial form:
$$\mathbf{y} = \mathbf{X}\mathbf{w} + \boldsymbol{\epsilon}$$
with $\boldsymbol{\epsilon} \sim \mathcal{N}(\varepsilon|0, \sigma^2\mathbf{I})$
- Remark: the likelihood is not a probability!

Probabilistic Interpretation of Loss Minimization

- Recall that the Maximum-Likelihood solution is

$$\widehat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

- Now we can also maximize the log-likelihood to obtain the optimal σ^2:

$$\frac{\partial \log[p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2)]}{\partial \sigma^2} = 0$$

yielding

$$\widehat{\sigma^2} = \frac{1}{N}(\mathbf{y} - \mathbf{X}\widehat{\mathbf{w}})^\top (\mathbf{y} - \mathbf{X}\widehat{\mathbf{w}})$$

Properties of the Maximum-Likelihood Estimator

- Are there any useful properties for the estimator $\widehat{\mathbf{w}}$?

Properties of the Maximum-Likelihood Estimator

- Are there any useful properties for the estimator $\widehat{\mathbf{w}}$?
- The estimator $\widehat{\mathbf{w}}$ is **unbiased**, that is:

$$\mathrm{E}_{p(\mathbf{y}|\mathbf{X},\mathbf{w})}[\widehat{\mathbf{w}}] = \int \widehat{\mathbf{w}}\, p(\mathbf{y}|\mathbf{X},\mathbf{w})\, d\mathbf{y} = \mathbf{w}$$

Properties of the Maximum-Likelihood Estimator

- The proof is rather simple:

$$
\begin{aligned}
\mathrm{E}_{p(\mathbf{y}|\mathbf{X},\mathbf{w})}[\widehat{\mathbf{w}}] &= \mathrm{E}_{p(\mathbf{y}|\mathbf{X},\mathbf{w})}[(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}] \\
&= \int(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}\,\mathcal{N}(\mathbf{y}|\mathbf{X}\mathbf{w},\sigma^2\mathbf{I})\,d\mathbf{y} \\
&= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\int\mathbf{y}\,\mathcal{N}(\mathbf{y}|\mathbf{X}\mathbf{w},\sigma^2\mathbf{I})\,d\mathbf{y} \\
&= (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{X}\,\mathbf{w} \\
&= \mathbf{w}
\end{aligned}
\tag{1}
$$

Properties of the Maximum-Likelihood Estimator

- The estimate of the optimal σ^2 is biased!

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$$
\begin{aligned}
\mathrm{E}_{p(\mathbf{y}|\mathbf{X},\mathbf{w})}\left(\widehat{\sigma^2}\right) &= \frac{1}{N}\mathrm{E}_{p(\mathbf{y}|\mathbf{X},\mathbf{w})}\left[(\mathbf{y}-\mathbf{X}\widehat{\mathbf{w}})^\top(\mathbf{y}-\mathbf{X}\widehat{\mathbf{w}})\right] \\
&= \sigma^2\left(1-\frac{D}{N}\right)
\end{aligned}
$$

Properties of the Maximum-Likelihood Estimator

- The proof uses these two useful identities:

Expectation of quadratic form for Gaussian variables

$$
\begin{aligned}
p(\mathbf{v}) &= \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \\
\mathrm{E}_{p(\mathbf{v})}\left(\mathbf{v}^\top \mathbf{A} \mathbf{v}\right) &= \mathrm{Tr}(\mathbf{A}\boldsymbol{\Sigma}) + \boldsymbol{\mu}^\top \mathbf{A} \boldsymbol{\mu} \\
\mathrm{Tr}(\mathbf{A}) &= \sum_i \mathbf{A}_{ii}
\end{aligned}
$$

Permutation invariance of the trace operator

$$
\mathrm{Tr}(\mathbf{AB}) = \mathrm{Tr}(\mathbf{BA})
$$

Properties of the Maximum-Likelihood Estimator

$$
\begin{aligned}
\mathrm{E}_{p(\mathbf{y}|\mathbf{X},\mathbf{w},\sigma^2)}(\widehat{\sigma^2}) &= \frac{1}{N}(\mathrm{Tr}(\sigma^2\mathbf{I}) + \mathbf{w}^\top\mathbf{X}^\top\mathbf{X}\mathbf{w}) \\
&\quad -\frac{1}{N}(\mathrm{Tr}(\sigma^2\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top) + \mathbf{w}^\top\mathbf{X}^\top\mathbf{X}\mathbf{w}) \\
&= \sigma^2 - \frac{\sigma^2}{N}\mathrm{Tr}(\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top) \\
&= \sigma^2 - \frac{\sigma^2}{N}\mathrm{Tr}(\mathbf{X}^\top\mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}) \\
&= \sigma^2\left(1 - \frac{D}{N}\right)
\end{aligned}
$$

Where D is the dimensionality of $\mathbf{w}$.

Model Selection

- How can we prefer one model over another?
- Lowest loss / highest likelihood?

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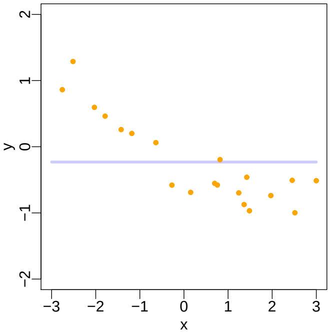
- How can we prefer one model over another?
- Lowest loss / highest likelihood?
- **NO!**
- Higher model complexity yields lower loss / higher likelihood...
- ...but it usually does not generalize well on test data.

Model Selection - Effect of increasing model complexity

- Consider polynomial functions:

$$f(x) = \sum_{i=0}^{k} w_i x^i$$

- Polynomial with $k = 0$



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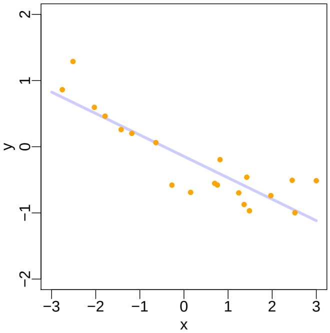
- Polynomial with $k = 1$



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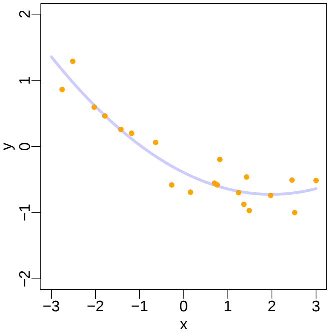
- Polynomial with $k = 2$



Model Selection - Effect of increasing model complexity

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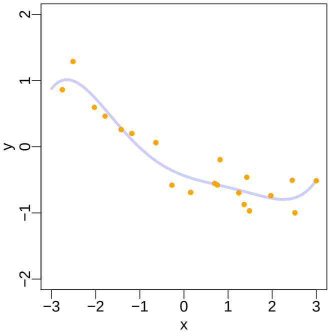
- Polynomial with $k = 5$

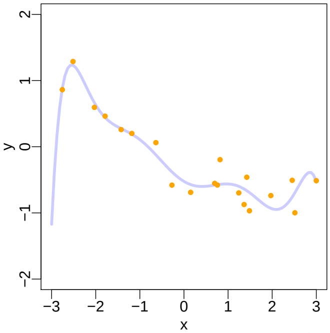


Model Selection - Effect of increasing model complexity

- Consider polynomial functions:

$$f(x) = \sum_{i=0}^{k} w_i x^i$$

- Polynomial with $k = 8$

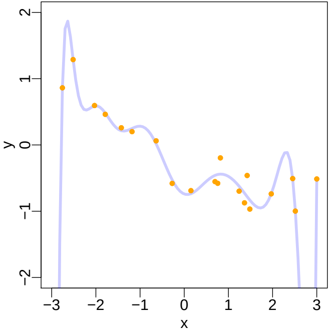


Model Selection - Effect of increasing model complexity

- Consider polynomial functions:

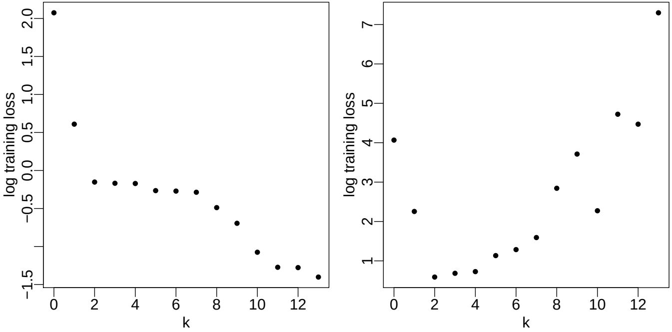
$$f(x) = \sum_{i=0}^{k} w_i x^i$$

- Polynomial with $k = 13$



Model Selection - Effect of increasing model complexity

- Training loss decreases with k but test loss increases



Validation on "unseen" data

- Cross-validation is a safe way to do model selection

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- Cross-validation is a safe way to do model selection
- Predictions evaluated using validation loss:

$$\mathcal{L}_v = \frac{1}{N_{\text{test}}} \sum_{i \in \mathcal{I}_{\text{test}}} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2$$

- Or the validation log-likelihood:

$$\log[p(\mathbf{y}_{\text{test}} | \mathbf{X}_{\text{test}}, \widehat{\mathbf{w}}, \sigma^2)] = -\frac{1}{2\sigma^2} \sum_{i \in \mathcal{I}_{\text{test}}} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2$$

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- In some applications it will be clear
- In many cases – pick it randomly

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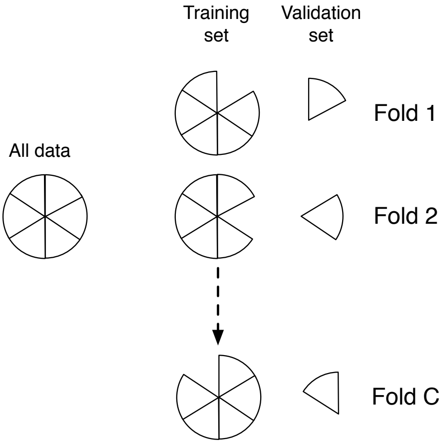
- In some applications it will be clear
- In many cases – pick it randomly
- Do it more than once – average the results
- Do cross-validation
  - Split the data into C equal sets. Train on $C - 1$, test on remaining.

Cross-validation



Average performance over the C 'folds'.

Leave-one-out Cross-validation

- Cross-validation can be repeated to make results more accurate
- e.g. Doing 10-fold CV 10 times gives us 100 performance values to average over

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- Cross-validation can be repeated to make results more accurate
- e.g. Doing 10-fold CV 10 times gives us 100 performance values to average over
- Extreme example is when $C = N$ so each fold includes one input-label pair
  - Leave-one-out (LOO) CV

Computational issues

- CV and LOOCV let us choose from a set of models based on predictive performance.
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y &= \sum_{k=0}^{K} w_k x_k \\
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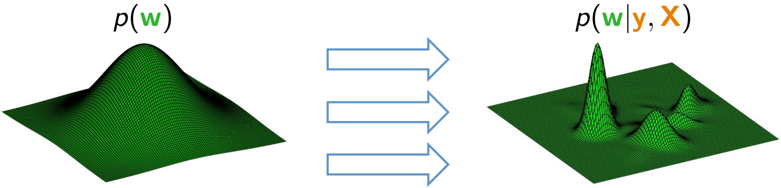
- For some models we need to use $C \ll N$.

Bayesian Inference

- Inputs : $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)^\top$
- Labels : $\mathbf{y} = (y_1, \ldots, y_N)^\top$
- Weights : $\mathbf{w} = (w_1, \ldots, w_D)^\top$



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

Bayesian Linear Regression

- Modeling observations as noisy realizations of a linear combination of the features:

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

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- Gaussian prior over model parameters:

$$p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{S})$$

Bayesian Linear Regression

- Bayes rule:

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

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  - Distribution over parameters after observing data

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- **Likelihood** : $p(\mathbf{y}|\mathbf{X},\mathbf{w})$
  - Measure of "fitness"
- **Prior density**: $p(\mathbf{w})$
  - Anything we know about parameters <u>before</u> we see any data
- **Marginal likelihood**: $p(\mathbf{y}|\mathbf{X})$
  - It is a normalization constant – ensures $\int p(\mathbf{w}|\mathbf{X},\mathbf{y})\, d\mathbf{w} = 1$.

When can we compute the posterior?

Conjugacy (definition)

A prior $p(\mathbf{w})$ is said to be conjugate to a likelihood it results in a posterior of the same type of density as the prior.

- Example:
  - Prior: Gaussian; Likelihood: Gaussian; Posterior: Gaussian
  - Prior: Beta; Likelihood: Binomial; Posterior: Beta
  - Many others...

Why is this important?

- Bayes rule:

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

- If prior and likelihood are conjugate, we **know** the form of $p(\mathbf{w}|\mathbf{X}, \mathbf{y})$
- Therefore, we **know** the form of the normalizing constant
- Therefore, we **don't need** to compute $p(\mathbf{y}|\mathbf{X})$

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- If prior and likelihood are conjugate, we **know** the form of $p(\mathbf{w}|\mathbf{X},\mathbf{y})$
- Therefore, we **know** the form of the normalizing constant
- Therefore, we **don't need** to compute $p(\mathbf{y}|\mathbf{X})$
- We just need to use some algebra to make $p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})$ **look like** the correct density, ignoring all terms without $\mathbf{w}$

Bayesian Linear Regression - Finding posterior parameters

- Back to our model...
- The posterior must be Gaussian
- Ignoring normalizing constants, the posterior is:

$$
\begin{aligned}
p(\mathbf{w}|\mathbf{X}, \mathbf{y}, \sigma^2) &\propto \exp\left\{-\frac{1}{2}(\mathbf{w}-\boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{w}-\boldsymbol{\mu})\right\} \\
&= \exp\left\{-\frac{1}{2}(\mathbf{w}^\top \boldsymbol{\Sigma}^{-1}\mathbf{w} - 2\mathbf{w}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} + \boldsymbol{\mu}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu})\right\} \\
&\propto \exp\left\{-\frac{1}{2}(\mathbf{w}^\top \boldsymbol{\Sigma}^{-1}\mathbf{w} - 2\mathbf{w}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu})\right\}
\end{aligned}
$$

Bayesian Linear Regression - Finding posterior parameters

- Ignoring non-$\mathbf{w}$ terms, the prior multiplied by the likelihood is:

$$
\begin{aligned}
& p(\mathbf{y}|\mathbf{w}, \mathbf{X}, \sigma^2) \\
\propto\quad & \exp\left\{-\frac{1}{2\sigma^2}(\mathbf{y}-\mathbf{X}\mathbf{w})^\top(\mathbf{y}-\mathbf{X}\mathbf{w})\right\}\exp\left\{-\frac{1}{2}\mathbf{w}^\top\mathbf{S}^{-1}\mathbf{w}\right\} \\
\propto\quad & \exp\left\{-\frac{1}{2}\left(\mathbf{w}^\top\left[\frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{X}+\mathbf{S}^{-1}\right]\mathbf{w}-\frac{2}{\sigma^2}\mathbf{w}^\top\mathbf{X}^\top\mathbf{y}\right)\right\}
\end{aligned}
$$

- Posterior (from previous slide):

$$
\propto \exp\left\{-\frac{1}{2}(\mathbf{w}^\top\boldsymbol{\Sigma}^{-1}\mathbf{w}-2\mathbf{w}^\top\boldsymbol{\Sigma}^{-1}\boldsymbol{\mu})\right\}
$$

Bayesian Linear Regression - Finding posterior parameters

- Equate individual terms on each side.
- Covariance:

$$\begin{aligned}
\mathbf{w}^\top \boldsymbol{\Sigma}^{-1}\mathbf{w} &= \mathbf{w}^\top \left[\frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{X} + \mathbf{S}^{-1}\right]\mathbf{w} \\
\boldsymbol{\Sigma} &= \left(\frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{X} + \mathbf{S}^{-1}\right)^{-1}
\end{aligned}$$

- Mean:

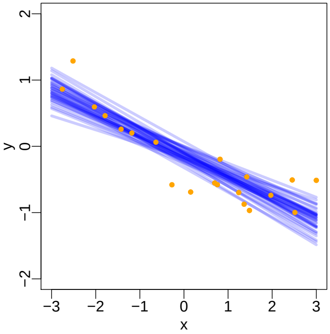
$$\begin{aligned}
2\mathbf{w}^\top \boldsymbol{\Sigma}^{-1}\boldsymbol{\mu} &= \frac{2}{\sigma^2}\mathbf{w}^\top\mathbf{X}^\top\mathbf{y} \\
\boldsymbol{\mu} &= \frac{1}{\sigma^2}\boldsymbol{\Sigma}\mathbf{X}^\top\mathbf{y}
\end{aligned}$$

Bayesian Linear Regression - Example

- Linear model with two parameters

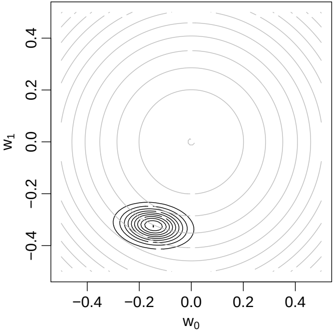
$$f(x) = w_0 + w_1 x$$

- Predictions obtained when sampling from the posterior over parameters



Bayesian Linear Regression - Example

- Posterior distribution over model parameters
- Intercept w_0 and slope w_1



Predictive Distribution

- We can analyze the predictive distribution
- The posterior is central in this analysis

$$p(\mathbf{w}|\mathbf{X}, \mathbf{y}, \sigma^2) = \mathcal{N}(\mathbf{w}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- as it makes it possible to obtain:

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

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- Same tedious exercise as before yields:

$$p(y_*|\mathbf{X}, \mathbf{y}, \mathbf{x}_*, \sigma^2) = \mathcal{N}(y_*|\mathbf{x}_*^\top \boldsymbol{\mu}, \sigma^2 + \mathbf{x}_*^\top \boldsymbol{\Sigma} \mathbf{x}_*)$$

Introducing basis functions

- Imagine transforming the inputs using a set of D functions

$$\mathbf{x} \to \boldsymbol{\varphi}(\mathbf{x}) = (\varphi_1(\mathbf{x}), \ldots, \varphi_D(\mathbf{x}))^\top$$

- The functions $\varphi_1(\mathbf{x})$ are also known as basis functions
- Define:

$$\mathbf{\Phi} = \begin{bmatrix} \varphi_1(\mathbf{x}_1) & \ldots & \varphi_D(\mathbf{x}_1) \\ \vdots & \ddots & \vdots \\ \varphi_1(\mathbf{x}_N) & \ldots & \varphi_D(\mathbf{x}_N) \end{bmatrix}$$

Introducing basis functions

- Applying Bayesian Linear Regression on the transformed features gives

$$p(\mathbf{w}|\mathbf{X}, \mathbf{y}, \sigma^2) = \mathcal{N}(\mathbf{w}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

- Covariance:

$$\boldsymbol{\Sigma} = \left(\frac{1}{\sigma^2}\boldsymbol{\Phi}^\top\boldsymbol{\Phi} + \mathbf{S}^{-1}\right)^{-1}$$

- Mean:

$$\boldsymbol{\mu} = \frac{1}{\sigma^2}\boldsymbol{\Sigma}\boldsymbol{\Phi}^\top\mathbf{y}$$

- Predictions:

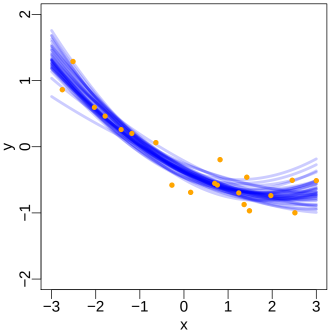
$$p(y_*|\mathbf{X}, \mathbf{y}, \mathbf{x}_*, \sigma^2) = \mathcal{N}(y_*|\varphi(\mathbf{x}_*)^\top\boldsymbol{\mu}, \sigma^2 + \varphi(\mathbf{x}_*)^\top\boldsymbol{\Sigma}\varphi(\mathbf{x}_*))$$

Predictions

- Predictions obtained with a polynomial

$$f(x) = \sum_{i=0}^{k} w_i x^i$$

- Polynomial with $k = 2$



Computing posterior: recipe

- (Assuming prior conjugate to likelihood)
- Write down prior times likelihood (ignoring any constant terms)
- Write down posterior (ignoring any constant terms)
- Re-arrange them so the look like one another
- Equate terms on both sides to read off parameter values.

Marginal likelihood

- So far, we've ignored $p(\mathbf{y}|\mathbf{X}, \sigma^2)$, the normalizing constant in Bayes rule.
- We stated that it was equal to:

$$p(\mathbf{y}|\mathbf{X}, \sigma^2) = \int p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2)p(\mathbf{w})\ d\mathbf{w}$$

- We're averaging over all values of $\mathbf{w}$ to get a value for **how good the model is**.
  - How likely is $\mathbf{y}$ given $\mathbf{X}$ and the model
- We can use this to compare models and to optimize σ^2!

Marginal likelihood

- When prior is $\mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$ and likelihood is $\mathcal{N}(\mathbf{X}\mathbf{w}, \sigma^2\mathbf{I})$, marginal likelihood is:

$$p(\mathbf{y}|\mathbf{X}, \mathbf{y}, \sigma^2, \boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0) = \mathcal{N}(\mathbf{y}|\mathbf{X}\mu_0, \sigma^2\mathbf{I} + \mathbf{X}\boldsymbol{\Sigma}_0\mathbf{X}^\top)$$

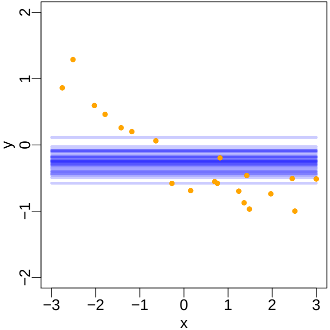
- i.e. an N-dimensional Gaussian evaluated at $\mathbf{y}$.

Model Selection using Marginal Likelihood

- Consider polynomial functions:

$$f(x) = \sum_{i=0}^{k} w_i x^i$$

- Polynomial with $k = 0$

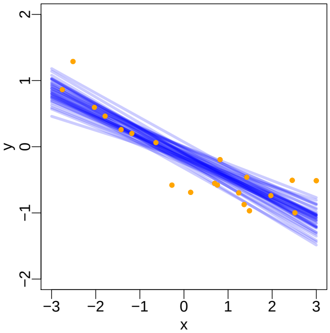


Model Selection using Marginal Likelihood

- Consider polynomial functions:

$$f(x) = \sum_{i=0}^{k} w_i x^i$$

- Polynomial with $k = 1$



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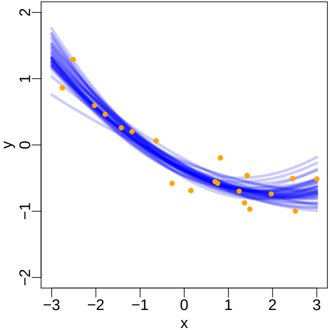

Model Selection using Marginal Likelihood

- Consider polynomial functions:

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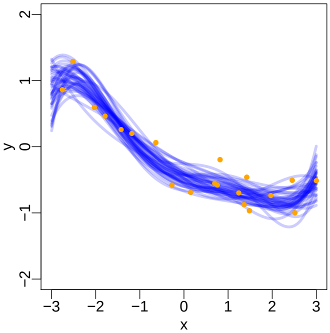
- Polynomial with $k = 5$



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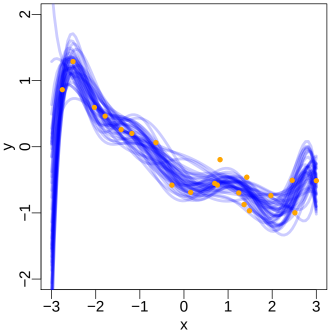
- Polynomial with $k = 8$



Model Selection using Marginal Likelihood

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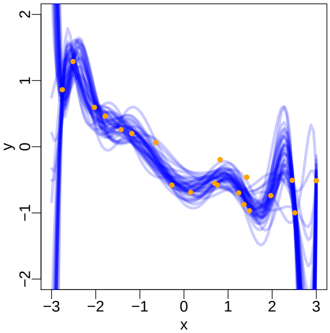
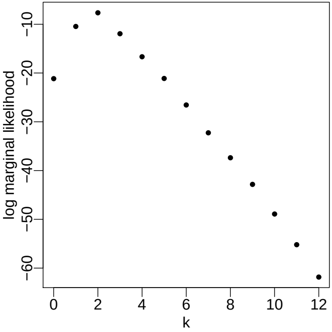
- Polynomial with $k = 12$



Model Selection using Marginal Likelihood

- Marginal likelihood as a way to choose the "best" model



Choosing a prior

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  - Prior effect will diminish as more data arrive.
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  - Data type: real, integer, string, etc.
  - Expert knowledge: 'the coin is fair', 'the model should be simple'
  - Computational considerations (not as important as it used to be!)
  - If we know nothing, can use a broad prior – e.g. uniform density.

Summary

- Moved away from a single parameter value.
- Saw how predictions could be made by averaging over all possible parameter values – Bayesian.
- Saw how Bayes rule allows us to get a density for $\mathbf{w}$ conditioned on the data (and other stuff).

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Summary

- Moved away from a single parameter value.
- Saw how predictions could be made by averaging over all possible parameter values – Bayesian.
- Saw how Bayes rule allows us to get a density for $\mathbf{w}$ conditioned on the data (and other stuff).
- Computing the posterior is hard except in some cases....
- ....we can do it when things are conjugate.
- Can also (sometimes) compute the marginal likelihood....
- ...and use it for comparing models.
  - No need for costly cross-validation.

Class exercise

- Data: outcomes of N coin tosses (summarized as number of heads) – y_N
- Want a posterior density over r, the probability that a coin toss results in a head.
- Likelihood – binomial:

$$p(y_n|r) = \left(\begin{array}{c} N \\ y_N \end{array} \right) r^{y_N}(1-r)^{N-y_N}$$

- Prior – beta:

$$p(r|\alpha,\beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} r^{\alpha-1}(1-r)^{\beta-1}$$

- Beta is **conjugate** to binomial. Therefore posterior is beta. In general, beta is:

$$p(a|c,d) = \frac{\Gamma(c+d)}{\Gamma(c)\Gamma(d)} a^{c-1}(1-a)^{d-1}$$

Solution

- Posterior is proportional to:

$$p(r|y_N, \alpha, \beta) \propto r^{\gamma-1}(1-r)^{\delta-1}$$

- Prior times likelihood is proportional to:

$$\begin{aligned} &\propto \quad r^{\alpha-1}(1-r)^{\beta-1}r^{y_N}(1-r)^{N-y_N} \\ &= \quad r^{y_N+\alpha-1}(1-r)^{N-y_N+\beta-1} \end{aligned}$$

- So:

$$\gamma = y_N + \alpha, \;\; \delta = \beta + N - y_N$$

Class exercise continued...

- By averaging over this posterior over r, we'd like to know the probability of y_* heads in N throws:

$$P(y_*|y_N, \alpha, \beta)$$

- This is an expectation:

$$\begin{aligned} p(y_*|y_N, \alpha, \beta) &= \mathrm{E}_{p(r|y_N,\alpha,\beta)}\left[p(y_*|r)\right] \\ &= \int_0^1 p(y_*|r)p(r|y_N, \alpha, \beta)\, dr \end{aligned}$$

- Where:

$$p(y_*|r) = \left(\begin{array}{c} N \\ y_* \end{array} \right) r^{y_*}(1-r)^{N-y_*}$$

- Can we compute the expectation?

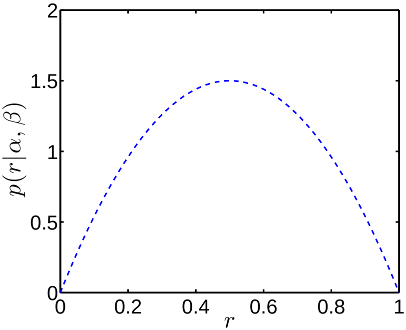
Class exercise continued...

- We don't know what form this will take so cannot ignore constants.

$$
\begin{aligned}
& p(y_* | y_N, \alpha, \beta) \\
= & \begin{pmatrix} N \\ y_* \end{pmatrix} \frac{\Gamma(\gamma+\delta)}{\Gamma(\gamma)\Gamma(\delta)} \int_0^1 r^{y_*}(1-r)^{N-y_*} r^{\gamma-1}(1-r)^{\delta-1} \; dr \\
= & \begin{pmatrix} N \\ y_* \end{pmatrix} \frac{\Gamma(\gamma+\delta)}{\Gamma(\gamma)\Gamma(\delta)} \int_0^1 r^{\gamma+y_*-1}(1-r)^{\delta+N-y_*-1} \; dr \\
= & \begin{pmatrix} N \\ y_* \end{pmatrix} \frac{\Gamma(\gamma+\delta)}{\Gamma(\gamma)\Gamma(\delta)} \frac{\Gamma(\gamma+y_*)\Gamma(\delta+N-y_*)}{\Gamma(\gamma+y_*+\delta+N-y_*)}
\end{aligned}
$$

- Where we noticed that the thing in the integral was an unnormalized beta and so its integral must be the inverse of the normalizing constant.

Class exercise – example prior



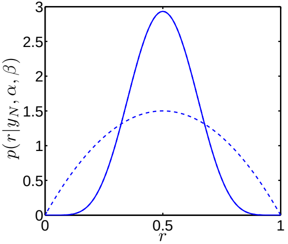
$$\alpha = 2, \ \beta = 2$$

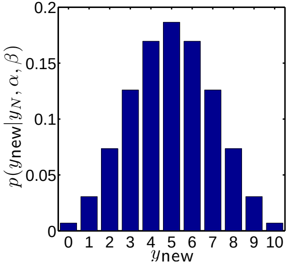
$$p(r|\alpha,\beta) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} r^{\alpha-1}(1-r)^{\beta-1}$$

$r = 0.5$ is most likely, but we're not sure.

Class exercise – example data

After observing $y_N = 5$ heads in $N = 10$ tosses:

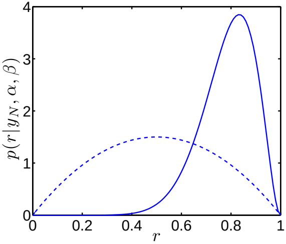


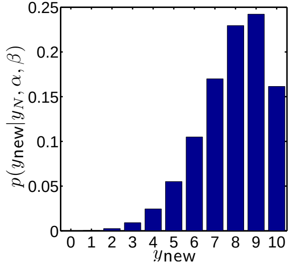


Posterior (left – prior is dashed line) and predictive distribution (right).

Class exercise – example data 2

After observing $y_N = 9$ heads in $N = 10$ tosses:





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