Learning with Maximum Likelihood

Note to other teachers and users of these slides. Andrew would be delighted if you found this source material useful in giving your own lectures. Feel free to use these slides verbatim, or to modify them to fit your own needs. PowerPoint originals are available. If you make use of a significant portion of these slides in your own lecture, please include this message, or the following link to the source repository of Andrew's tutorials: http://

www.cs.cmu.edu/~awm/tutorials . Comments and corrections gratefully received.

Andrew W. Moore
Professor
School of Computer Science
Carnegie Mellon University

www.cs.cmu.edu/~awm awm@cs.cmu.edu 412-268-7599

Maximum Likelihood learning of Gaussians for Data Mining

- Why we should care
- Learning Univariate Gaussians
- Learning Multivariate Gaussians
- What's a biased estimator?
- Bayesian Learning of Gaussians

Why we should care

- Maximum Likelihood Estimation is a very very very very fundamental part of data analysis.
- "MLE for Gaussians" is training wheels for our future techniques
- Learning Gaussians is more useful than you might guess...

Learning Gaussians from Data

- Suppose you have $x_1, x_2, ... x_R \sim \text{(i.i.d)} N(\mu, \sigma^2)$
- But you don't know μ

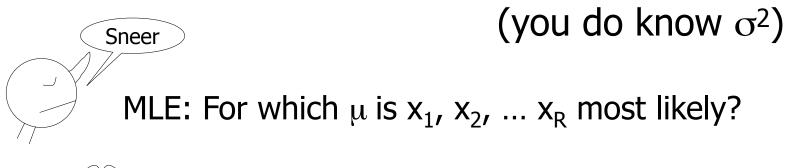
(you do know σ^2)

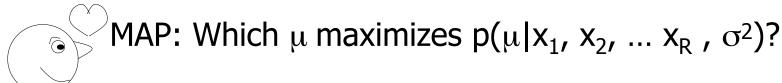
MLE: For which μ is x_1 , x_2 , ... x_R most likely?

MAP: Which μ maximizes $p(\mu|x_1, x_2, ... x_R, \sigma^2)$?

Learning Gaussians from Data

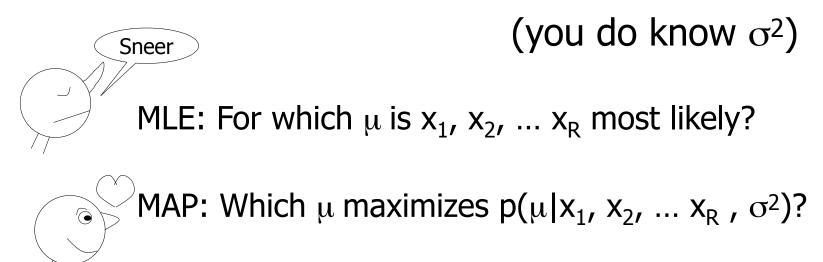
- Suppose you have $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$
- But you don't know μ





Learning Gaussians from Data

- Suppose you have $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$
- But you don't know μ



Despite this, we'll spend 95% of our time on MLE. Why? Wait and see...

- Suppose you have $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$
- But you don't know μ (you do know σ^2)
- MLE: For which μ is $x_1, x_2, ... x_R$ most likely?

$$\mu^{mle} = \underset{\mu}{\text{arg max }} p(x_1, x_2, ..., x_R \mid \mu, \sigma^2)$$

Algebra Euphoria

$$\mu^{mle} = \underset{\mu}{\operatorname{arg\,max}} p(x_1, x_2, ... x_R \mid \mu, \sigma^2)$$

= (by i.i.d)

= (plug in formula for Gaussian)

Algebra Euphoria

$$\mu^{mle} = \arg\max_{\mu} p(x_1, x_2, ... x_R \mid \mu, \sigma^2)$$

$$= \arg\max_{\mu} \prod_{i=1}^R p(x_i \mid \mu, \sigma^2) \qquad \text{(by i.i.d)}$$

$$= \arg\max_{\mu} \sum_{i=1}^R \log p(x_i \mid \mu, \sigma^2) \qquad \text{(monotonicity of log)}$$

$$= \arg\max_{\mu} \frac{1}{\sqrt{2\pi}} \sum_{i=1}^R -\frac{(x_i - \mu)^2}{2\sigma^2} \qquad \text{(plug in formula for Gaussian)}$$

$$= \arg\min_{\mu} \sum_{i=1}^R (x_i - \mu)^2 \qquad \text{(after simplification)}$$

Intermission: A General Scalar MLE strategy

Task: Find MLE θ assuming known form for p(Data| θ ,stuff)

- 1. Write LL = log P(Data| θ ,stuff)
- 2. Work out $\partial LL/\partial\theta$ using high-school calculus
- 3. Set $\partial LL/\partial\theta = 0$ for a maximum, creating an equation in terms of θ
- 4. Solve it*
- 5. Check that you've found a maximum rather than a minimum or saddle-point, and be careful if θ is constrained

*This is a perfect example of something that works perfectly in all textbook examples and usually involves surprising pain if you need it for something new.

The MLE μ

$$\mu^{mle} = \underset{\mu}{\operatorname{arg\,max}} p(x_1, x_2, ... x_R \mid \mu, \sigma^2)$$

$$= \underset{\mu}{\operatorname{arg\,min}} \sum_{i=1}^R (x_i - \mu)^2$$

$$= \mu \quad \text{s.t.} \quad 0 = \frac{\partial LL}{\partial \mu} =$$

$$=$$
 (what?)

The MLE μ

$$\mu^{mle} = \underset{\mu}{\operatorname{arg\,max}} p(x_1, x_2, ... x_R \mid \mu, \sigma^2)$$

$$= \underset{\mu}{\operatorname{arg\,min}} \sum_{i=1}^R (x_i - \mu)^2$$

$$= \mu \text{ s.t. } 0 = \frac{\partial LL}{\partial \mu} = \frac{\partial}{\partial \mu} \sum_{i=1}^R (x_i - \mu)^2$$

$$- \sum_{i=1}^R 2(x_i - \mu)$$
Thus $\mu = \frac{1}{R} \sum_{i=1}^R x_i$

Lawks-a-lawdy!

$$\mu^{mle} = \frac{1}{R} \sum_{i=1}^{R} x_i$$

 The best estimate of the mean of a distribution is the mean of the sample!

At first sight:

This kind of pedantic, algebra-filled and ultimately unsurprising fact is exactly the reason people throw down their "Statistics" book and pick up their "Agent Based Evolutionary Data Mining Using The Neuro-Fuzz Transform" book.

Suppose $\theta = (\theta_1, \theta_2, ..., \theta_n)^T$ is a vector of parameters.

Task: Find MLE θ assuming known form for p(Data| θ ,stuff)

- 1. Write LL = log P(Data| θ ,stuff)
- 2. Work out $\partial LL/\partial\theta$ using high-school calculus

$$\frac{\partial LL}{\partial \boldsymbol{\theta}} = \begin{pmatrix} \frac{\partial LL}{\partial \theta_1} \\ \frac{\partial LL}{\partial \theta_2} \\ \frac{\partial \theta_2}{\partial LL} \\ \frac{\partial LL}{\partial \theta_n} \end{pmatrix}$$

Suppose $\theta = (\theta_1, \theta_2, ..., \theta_n)^T$ is a vector of parameters.

Task: Find MLE θ assuming known form for p(Data| θ ,stuff)

- 1. Write LL = log P(Data| θ ,stuff)
- 2. Work out $\partial LL/\partial\theta$ using high-school calculus
- 3. Solve the set of simultaneous equations

$$\frac{\partial LL}{\partial \theta_1} = 0$$

$$\frac{\partial LL}{\partial \theta_2} = 0$$

$$\frac{\partial LL}{\partial \theta_n} = 0$$

Suppose $\theta = (\theta_1, \theta_2, ..., \theta_n)^T$ is a vector of parameters.

Task: Find MLE θ assuming known form for p(Data| θ ,stuff)

- 1. Write LL = log P(Data| θ ,stuff)
- 2. Work out $\partial LL/\partial\theta$ using high-school calculus
- 3. Solve the set of simultaneous equations

$$\frac{\partial LL}{\partial \theta_1} = 0$$

$$\frac{\partial LL}{\partial \theta_2} = 0$$
4. Check that you're at a maximum
$$\frac{\partial LL}{\partial \theta_2} = 0$$

Suppose $\theta = (\theta_1, \theta_2, ..., \theta_n)^T$ is a vector of parameters.

Task: Find MLE θ assuming known form for p(Data| θ ,stuff)

- 1. Write LL = log P(Data| θ ,stuff)
- 2. Work out $\partial LL/\partial\theta$ using high-school calculus
- 3. Solve the set of simultaneous equations

If you can't solve them, what should you do?

$$\frac{\partial LL}{\partial \theta_1} = 0$$

$$\frac{\partial LL}{\partial \theta_2} = 0$$

$$\frac{\partial LL}{\partial \theta_2} = 0$$

4. Check that you're at a maximum

- Suppose you have $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$
- But you don't know μ or σ^2
- MLE: For which $\theta = (\mu, \sigma^2)$ is $x_1, x_2, ..., x_R$ most likely?

$$\log p(x_1, x_2, ... x_R \mid \mu, \sigma^2) = -R(\log \pi + \frac{1}{2} \log \sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^R (x_i - \mu)^2$$

$$\frac{\partial LL}{\partial \mu} = \frac{1}{\sigma^2} \sum_{i=1}^{R} (x_i - \mu)$$

$$\frac{\partial LL}{\partial \sigma^2} = -\frac{R}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^{R} (x_i - \mu)^2$$

- Suppose you have $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$
- But you don't know μ or σ^2
- MLE: For which $\theta = (\mu, \sigma^2)$ is $x_1, x_2, ..., x_R$ most likely?

$$\log p(x_1, x_2, ... x_R \mid \mu, \sigma^2) = -R(\log \pi + \frac{1}{2} \log \sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^R (x_i - \mu)^2$$

$$0 = \frac{1}{\sigma^2} \sum_{i=1}^R (x_i - \mu)$$

$$0 = -\frac{R}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^{R} (x_i - \mu)^2$$

- Suppose you have $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$
- But you don't know μ or σ^2
- MLE: For which $\theta = (\mu, \sigma^2)$ is $x_1, x_2, ..., x_R$ most likely?

$$\log p(x_1, x_2, ...x_R \mid \mu, \sigma^2) = -R(\log \pi + \frac{1}{2} \log \sigma^2) - \frac{1}{2\sigma^2} \sum_{i=1}^R (x_i - \mu)^2$$

$$0 = \frac{1}{\sigma^{2}} \sum_{i=1}^{R} (x_{i} - \mu) \Rightarrow \mu = \frac{1}{R} \sum_{i=1}^{R} x_{i}$$

$$0 = -\frac{R}{2\sigma^{2}} + \frac{1}{2\sigma^{4}} \sum_{i=1}^{R} (x_{i} - \mu)^{2} \implies \text{what?}$$

- Suppose you have $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$
- But you don't know μ or σ^2
- MLE: For which $\theta = (\mu, \sigma^2)$ is $x_1, x_2, ..., x_R$ most likely?

$$\mu^{mle} = \frac{1}{R} \sum_{i=1}^{R} x_i$$

$$\sigma_{mle}^2 = \frac{1}{R} \sum_{i=1}^{R} (x_i - \mu^{mle})^2$$

Unbiased Estimators

- An estimator of a parameter is unbiased if the expected value of the estimate is the same as the true value of the parameters.
- If $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$ then

$$E[\mu^{mle}] = E\left[\frac{1}{R}\sum_{i=1}^{R} x_i\right] = \mu$$

 μ^{mle} is unbiased

Biased Estimators

- An estimator of a parameter is biased if the expected value of the estimate is different from the true value of the parameters.
- If $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$ then

$$E\left[\sigma_{mle}^{2}\right] = E\left[\frac{1}{R}\sum_{i=1}^{R}(x_{i} - \mu^{mle})^{2}\right] = E\left[\frac{1}{R}\left(\sum_{i=1}^{R}x_{i} - \frac{1}{R}\sum_{j=1}^{R}x_{j}\right)^{2}\right] \neq \sigma^{2}$$

 σ^2_{mle} is biased

MLE Variance Bias

• If x_1 , x_2 , ... $x_R \sim$ (i.i.d) $N(\mu, \sigma^2)$ then

$$E\left[\sigma_{mle}^{2}\right] = E\left[\frac{1}{R}\left(\sum_{i=1}^{R} x_{i} - \frac{1}{R}\sum_{j=1}^{R} x_{j}\right)^{2}\right] = \left(1 - \frac{1}{R}\right)\sigma^{2} \neq \sigma^{2}$$

Intuition check: consider the case of R=1

Why should our guts expect that σ^2_{mle} would be an underestimate of true σ^2 ?

How could you prove that?

Unbiased estimate of Variance

• If x_1 , x_2 , ... $x_R \sim (i.i.d) N(\mu, \sigma^2)$ then

$$E\left[\sigma_{mle}^{2}\right] = E\left[\frac{1}{R}\left(\sum_{i=1}^{R} x_{i} - \frac{1}{R}\sum_{j=1}^{R} x_{j}\right)^{2}\right] = \left(1 - \frac{1}{R}\right)\sigma^{2} \neq \sigma^{2}$$

So define
$$\sigma_{\text{unbiased}}^2 = \frac{\sigma_{mle}^2}{\left(1 - \frac{1}{R}\right)}$$
 So $E\left[\sigma_{\text{unbiased}}^2\right] = \sigma^2$

Unbiased estimate of Variance

• If x_1 , x_2 , ... $x_R \sim (i.i.d) N(\mu, \sigma^2)$ then

$$E\left[\sigma_{mle}^{2}\right] = E\left[\frac{1}{R}\left(\sum_{i=1}^{R} x_{i} - \frac{1}{R}\sum_{j=1}^{R} x_{j}\right)^{2}\right] = \left(1 - \frac{1}{R}\right)\sigma^{2} \neq \sigma^{2}$$

So define
$$\sigma_{\text{unbiased}}^2 = \frac{\sigma_{mle}^2}{\left(1 - \frac{1}{R}\right)}$$
 So $E\left[\sigma_{\text{unbiased}}^2\right] = \sigma^2$

$$\sigma_{\text{unbiased}}^2 = \frac{1}{R-1} \sum_{i=1}^{R} (x_i - \mu^{mle})^2$$

Unbiaseditude discussion

Which is best?

$$\sigma_{mle}^2 = \frac{1}{R} \sum_{i=1}^{R} (x_i - \mu^{mle})^2$$

$$\sigma_{\text{unbiased}}^2 = \frac{1}{R-1} \sum_{i=1}^{R} (x_i - \mu^{mle})^2$$

Answer:

- •It depends on the task
- •And doesn't make much difference once R--> large

Don't get too excited about being unbiased

- Assume $x_1, x_2, ... x_R \sim (i.i.d) N(\mu, \sigma^2)$
- Suppose we had these estimators for the mean

$$\mu^{suboptimal} = \frac{1}{R + 7\sqrt{R}} \sum_{i=1}^{R} x_i$$

$$\mu^{crap} = x_1$$

Are either of these unbiased?

Will either of them asymptote to the correct value as R gets large?

Which is more useful?

MLE for m-dimensional Gaussian

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim (i.i.d) N(\mu, \Sigma)$
- But you don't know μ or Σ
- MLE: For which $\theta = (\mu, \Sigma)$ is $\mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R$ most likely?

$$\boldsymbol{\mu}^{mle} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{x}_{k}$$

$$\Sigma^{mle} = \frac{1}{R} \sum_{k=1}^{R} \left(\mathbf{x}_k - \boldsymbol{\mu}^{mle} \right) \left(\mathbf{x}_k - \boldsymbol{\mu}^{mle} \right)^{T}$$

MLE for m-dimensional Gaussian

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim (i.i.d) N(\mu, \Sigma)$
- But you don't know μ or Σ
- MLE: For which $\theta = (\mu, \Sigma)$ is $\mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R$ most likely?

$$\boldsymbol{\mu}^{mle} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{x}_{k} \qquad \qquad \mu_{i}^{mle} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{x}_{ki}$$

$$\Sigma^{mle} = \frac{1}{R} \sum_{k=1}^{R} \left(\mathbf{x}_k - \mu^{mle} \right) \left(\mathbf{x}_k - \mu^{mle} \right)^{mle}$$

 $\mu_i^{mle} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{x}_{ki}$ Where $1 \le i \le m$ And \mathbf{x}_{ki} is value of the ith component of \mathbf{x}_k (the ith attribute of the kth record)

And μ_{i}^{mle} is the ith component of μ^{mle}

MLE for m-dimensional Gaussian

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim (i.i.d) N(\mu, \Sigma)$
- But you don't know μ or Σ
- MLE: For which $\theta = (\mu, \Sigma)$ is $\mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R$ most likely?

$$\boldsymbol{\mu}^{mle} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{x}_{k}$$

$$\Sigma^{mle} = \frac{1}{R} \sum_{k=1}^{R} \left(\mathbf{x}_{k} - \mu^{mle} \right) \left(\mathbf{x}_{k} - \mu^{mle} \right)$$
attribute of the kth record)

And σ_{ij}^{mle} is the (i,j)th
component of Σ^{mle}

Where $1 \le i \le m$, $1 \le j \le m$

And x_{ki} is value of the ith component of \mathbf{x}_k (the ith

$$\sigma_{ij}^{mle} = \frac{1}{R} \sum_{k=1}^{R} \left(\mathbf{x}_{ki} - \mu_i^{mle} \right) \left(\mathbf{x}_{kj} - \mu_j^{mle} \right)$$

MLE for m-dimensional Gaussian Q: How would you prove this?

- Suppose you have x₁, x₁, ...
- But you don't know μ or Σ
- MLE: For which $\theta \neq (\mu, \Sigma)$ is \mathbf{x}

$$\boldsymbol{\mu}^{mle} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{x}_{k}$$

$$\Sigma^{mle} = \frac{1}{R} \sum_{k=1}^{R} \left(\mathbf{x}_k - \mu^{mle} \right) \left(\mathbf{x}_k - \mu^{mle} \right)^{k}$$

$$\Sigma^{\text{unbiased}} = \frac{\Sigma^{mle}}{1 - \frac{1}{R}} = \frac{1}{R - 1} \sum_{k=1}^{R} \left(\mathbf{x}_k - \mu^{mle} \right) \left(\mathbf{x}_k - \mu^{mle} \right)$$

A: Just plug through the MLE recipe.

Note how Σ^{mle} is forced to be symmetric non-negative definite

Note the unbiased case

How many datapoints would you need before the Gaussian has a chance of being non-degenerate?

Confidence intervals

We need to talk

We need to discuss how accurate we expect μ^{mle} and Σ^{mle} to be as a function of R

And we need to consider how to estimate these accuracies from data...

- Analytically *
- Non-parametrically (using randomization and bootstrapping) *
 But we won't. Not yet.

*Will be discussed in future Andrew lectures...just before we need this technology.

Structural error

Actually, we need to talk about something else too...

What if we do all this analysis when the true distribution is in fact not Gaussian?

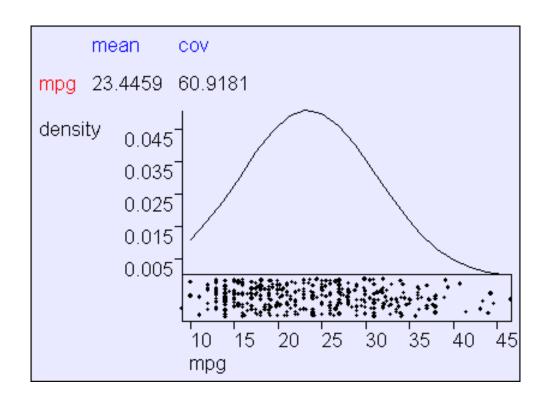
How can we tell? *

How can we survive? *

*Will be discussed in future Andrew lectures...just before we need this technology.

Gaussian MLE in action

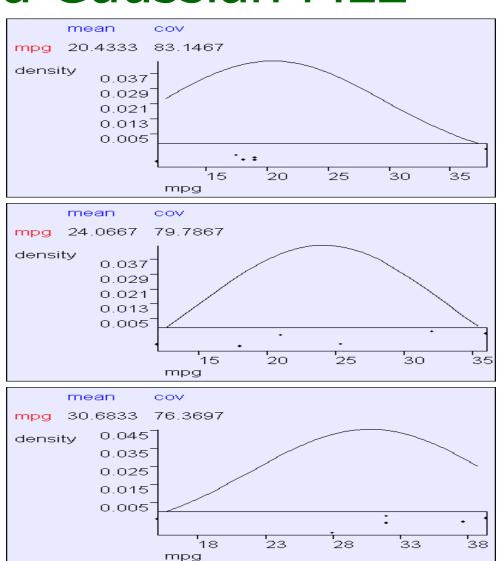
Using R=392 cars from the "MPG" UCI dataset supplied by Ross Quinlan



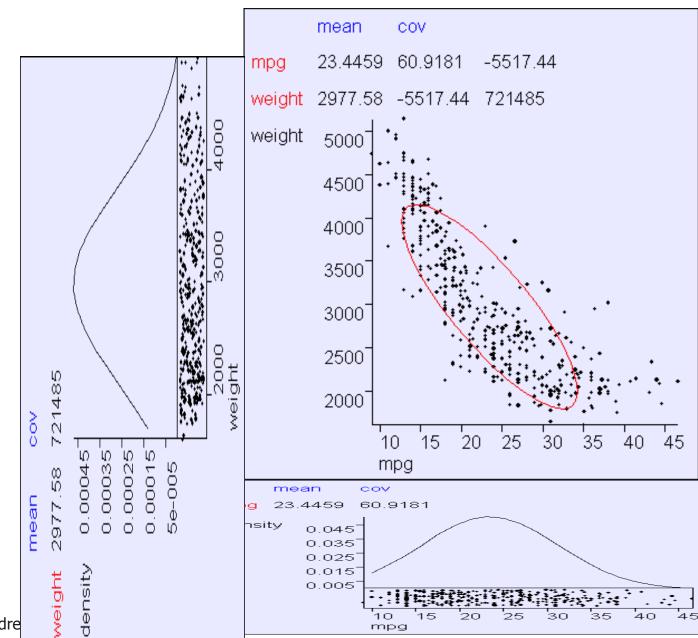
Data-starved Gaussian MLE

Using three subsets of MPG.

Each subset has 6 randomly-chosen cars.



in action **3ivariate MLE**



Copyright © 2001, 2004, Andre

Multivariate MLE

	mean	cov						
mpg	23.4459	60.9181	-10.3529	-657.585	-233.858	-5517.44	9.11551	16.6915
cylinders	5.47194	-10.3529	2.9097	169.722	55.3482	1300.42	-2.37505	-2.17193
displacement	194.412	-657.585	169.722	10950.4	3614.03	82929.1	-156.994	-142.572
horsepower	104.469	-233.858	55.3482	3614.03	1481.57	28265.6	-73.187	-59.0364
weight	2977.58	-5517.44	1300.42	82929.1	28265.6	721485	-976.815	-967.228
acceleration	15.5413	9.11551	-2.37505	-156.994	-73.187	-976.815	7.61133	2.95046
modelyear	75.9796	16.6915	-2.17193	-142.572	-59.0364	-967.228	2.95046	13.5699

Covariance matrices are not exciting to look at

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim \text{(i.i.d) } N(\mu, \Sigma)$
- But you don't know μ or Σ
- MAP: Which (μ, Σ) maximizes $p(\mu, \Sigma \mid \mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R)$?



Step 1: Put a prior on (μ, Σ)

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim \text{(i.i.d) } N(\mu, \Sigma)$
- But you don't know μ or Σ
- MAP: Which (μ, Σ) maximizes $p(\mu, \Sigma \mid \mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R)$?



Step 1: Put a prior on (μ, Σ)

Step 1a: Put a prior on Σ

$$(v_0-m-1) \Sigma \sim IW(v_0, (v_0-m-1) \Sigma_0)$$

This thing is called the Inverse-Wishart distribution.

A PDF over SPD matrices!

Poing Payagians MAP estimates for Gaussians

 v_0 small: "I am not sure about my guess of Σ_0 "

 v_0 large: "I'm pretty sure about my guess of Σ_0 "

Step 1: Pullor on (μ)

Step 1a: Put prior on 5

$$(v_0\text{-m-1}) \Sigma \sim \text{IW}(v_0, (v_0\text{-m-1}) \Sigma_0)$$

This thing is called the Inverse-Wishart distribution.

A PDF over SPD matrices!

 Σ_0 : (Roughly) my best guess of Σ

$$E[\Sigma] = \Sigma_0$$

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim \text{(i.i.d) } N(\mu, \Sigma)$
- But you don't know μ or Σ
- MAP: Which (μ, Σ) maximizes $p(\mu, \Sigma \mid \mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R)$?

```
Step 1: Put a prior on (\mu, \Sigma)
```

Step 1a: Put a prior on Σ

$$(v_0\text{-m-1})\Sigma \sim \text{IW}(v_0, (v_0\text{-m-1})\Sigma_0)$$

Step 1b: Put a prior on $\mu \mid \Sigma$

$$\mu \mid \Sigma \sim N(\mu_0, \Sigma / \kappa_0)$$

Together, " Σ " and " $\mu \mid \Sigma$ " define a joint distribution on (μ, Σ)

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_D \sim (i.i.d) N(u,\Sigma)$
- But you don't know μ or Σ
- MAP: Which (μ, Σ) maximize

$$μ_0$$
: My best guess of $μ$ $μ_0$ Σ)
$$E[μ] = μ_0$$

$$(v_0-m-1)\Sigma \sim v_0, (v_0-m-1)\Sigma$$

Step 1b: Put a propr on μ

$$\mu \mid \Sigma \sim N(\mu_0, \Sigma / \kappa_0)$$

Notice how we are forced to express our ignorance of μ proportionally to Σ

 κ_0 small: "I am not sure about my guess of μ_0 "

 κ_0 large: "I'm pretty sure about my guess of μ_0 "

> Together, " Σ " and " $\mu \mid \Sigma$ " define a joint distribution

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim \text{(i.i.d) } N(\mu, \Sigma)$
- But you don't know μ or Σ
- MAP: Which (μ, Σ) maximizes $p(\mu, \Sigma \mid \mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R)$?

Step 1: Put a prior on (μ, Σ)

Step 1a: Put a prior on Σ

$$(v_0-m-1)\Sigma \sim IW(v_0, (v_0-m-1)\Sigma_0)$$

Step 1b: Put a prior on $\mu \mid \Sigma$

$$\mu \mid \Sigma \sim N(\mu_0, \Sigma / \kappa_0)$$

Why do we use this form of prior?

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim \text{(i.i.d) } N(\mu, \Sigma)$
- But you don't know μ or Σ
- MAP: Which (μ, Σ) maximizes $p(\mu, \Sigma \mid \mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R)$?

Step 1: Put a prior on
$$(\mu, \Sigma)$$

Step 1a: Put a prior on Σ

$$(v_0\text{-m-1})\Sigma \sim \text{IW}(v_0, (v_0\text{-m-1})\Sigma_0)$$

Step 1b: Put a prior on $\mu \mid \Sigma$

$$\mu \mid \Sigma \sim N(\mu_0, \Sigma / \kappa_0)$$

Why do we use this form of prior?

Actually, we don't have to

But it is computationally and algebraically convenient...

...it's a conjugate prior.

- Suppose you have \mathbf{x}_1 , \mathbf{x}_2 , ... $\mathbf{x}_R \sim (i.i.d) N(\mu, \Sigma)$
- MAP: Which (μ, Σ) maximizes $p(\mu, \Sigma \mid \mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R)$?

Step 1: Prior: $(v_0-m-1) \Sigma \sim IW(v_0, (v_0-m-1) \Sigma_0), \mu \mid \Sigma \sim N(\mu_0, \Sigma / \kappa_0)$

Step 2:

$$\overline{\mathbf{x}} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{x}_k$$

$$\overline{\mathbf{x}} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{x}_{k} \left[\mathbf{\mu}_{R} = \frac{\kappa_{0} \mathbf{\mu}_{0} + R \overline{\mathbf{x}}}{\kappa_{0} + R} \right] \frac{\mathbf{v}_{R} = \mathbf{v}_{0} + R}{\kappa_{R} = \kappa_{0} + R}$$

$$v_R = v_0 + R$$

$$(\mathbf{v}_R + m - 1)\mathbf{\Sigma}_R = (\mathbf{v}_0 + m - 1)\mathbf{\Sigma}_0 + \sum_{k=1}^R (\mathbf{x}_k - \overline{\mathbf{x}})(\mathbf{x}_k - \overline{\mathbf{x}})^T + \frac{(\overline{\mathbf{x}} - \boldsymbol{\mu}_0)(\overline{\mathbf{x}} - \boldsymbol{\mu}_0)^T}{1/\kappa_0 + 1/R}$$

Step 3: Posterior: $(v_R + m-1)\Sigma \sim IW(v_R, (v_R + m-1)\Sigma_R)$,

$$\mu \mid \Sigma \sim N(\mu_{R}, \Sigma / \kappa_{R})$$

Result: $\mu^{\text{map}} = \mu_{\text{R}}$, $E[\Sigma | \mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_R] = \Sigma_{\text{R}}$

Being Bayesian

- MAP: Which (μ, Σ) statistics" of the data.

Step 2:

rior: (
$$v_0$$
-m-1) Σ

- Look carefully at what these formulae are doing. It's all very sensible.
- Suppose you have •Conjugate priors mean prior form and posterior form are same and characterized by "sufficient
 - Step 1: Prior: $(v_0\text{-m-1})\Sigma \sim$ •The marginal distribution on μ is a student-t
 - •One point of view: it's pretty academic if R > 30

$$\overline{\mathbf{X}} = \frac{1}{R} \sum_{k=1}^{R} \mathbf{X}_{k} \left[\mathbf{\mu}_{R} = \frac{\mathbf{\kappa}_{0} \mathbf{\mu}_{0} + R \overline{\mathbf{X}}}{\mathbf{\kappa}_{0} + R} \right] \frac{\mathbf{v}_{R} = \mathbf{v}_{0} + R}{\mathbf{\kappa}_{R} = \mathbf{\kappa}_{0} + R}$$

$$(\mathbf{v}_R + m - 1)\mathbf{\Sigma}_R = (\mathbf{v}_0 + m - 1)\mathbf{\Sigma}_0 + \sum_{k=1}^R (\mathbf{x}_k - \overline{\mathbf{x}})(\mathbf{x}_k - \overline{\mathbf{x}})^T + \frac{(\overline{\mathbf{x}} - \boldsymbol{\mu}_0)(\overline{\mathbf{x}} - \boldsymbol{\mu}_0)^T}{1/\kappa_0 + 1/R}$$

Step 3: Posterior:
$$(v_R + m - 1)\Sigma \sim IW(v_R, (v_R + m - 1)\Sigma_R)$$
, $\mu \mid \Sigma \sim N(\mu_R, \Sigma \mid \kappa_R)$

Result:
$$\mu^{\text{map}} = \mu_{\text{R}}$$
, $\text{E}[\Sigma | \mathbf{x}_1, \mathbf{x}_2, ... \mathbf{x}_{\text{R}}] = \Sigma_{\text{R}}$

Where we're at

	Categorical inputs only	Real-valued inputs only	Mixed Real / Cat okay
Predict Classifier category	Joint BC Naïve BC		Dec Tree
Density Prob- Estimator ability	Joint DE Naïve DE	Gauss DE	
Regressor real no.			

What you should know

- The Recipe for MLE
- What do we sometimes prefer MLE to MAP?
- Understand MLE estimation of Gaussian parameters
- Understand "biased estimator" versus "unbiased estimator"
- Appreciate the outline behind Bayesian estimation of Gaussian parameters

Useful exercise

- We'd already done some MLE in this class without even telling you!
- Suppose categorical arity-n inputs $x_1, x_2, ...$ $x_R \sim (i.i.d.)$ from a multinomial

$$M(p_1, p_2, ... p_n)$$

where

$$P(x_k=j|\mathbf{p})=p_j$$

• What is the MLE $\mathbf{p} = (p_1, p_2, ... p_n)$?