



Machine Learning for Signal Processing Linear Gaussian Models

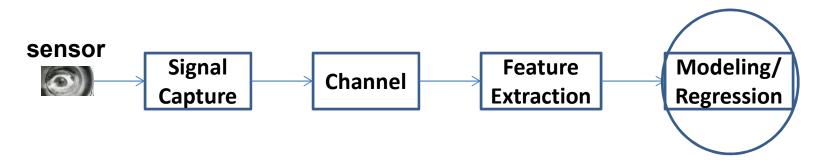
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• Application of Machine Learning techniques to the analysis of signals



- Modeling
 - Representation
 - Classification





Linear Gaussian Models

- MAP and MMSE prediction with Gaussian models
 - Estimation
 - Regularization
- Representation
 - PCA
 - Probabilistic PCA
- Gaussian Classifier





Recap: MAP Estimators

- MAP (*Maximum A Posteriori*): Find most probable value of y given x
 y = argmax y P(Y|x)
- We have used this for classification earlier. But we can also use it for *regression*
 - Estimating *continuous* valued variables
- Lets do this for a Gaussian RV..





MAP estimation

• x and y are jointly Gaussian

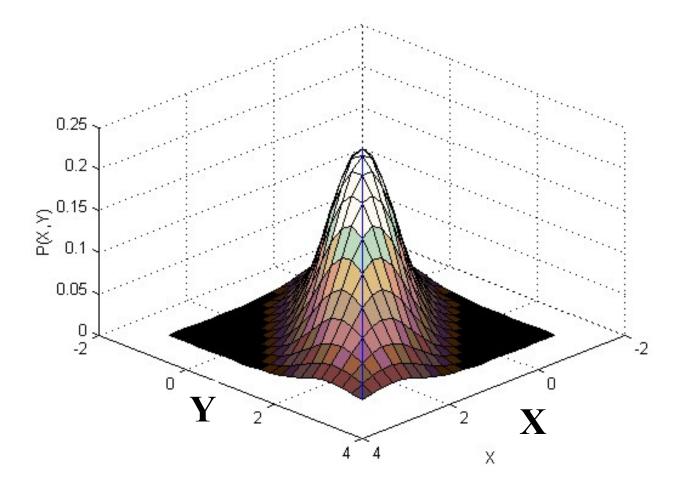
$$z = \begin{bmatrix} x \\ y \end{bmatrix} \qquad E[z] = \mu_z = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}$$
$$Var(z) = C_{zz} = \begin{bmatrix} C_{xx} & C_{xy} \\ C_{yx} & C_{yy} \end{bmatrix} \qquad C_{xy} = E[(x - \mu_x)(y - \mu_y)^T]$$
$$P(z) = N(\mu_z, C_{zz}) = \frac{1}{\sqrt{2\pi |C_{zz}|}} \exp\left(-0.5(z - \mu_z)^T C_{zz}^{-1}(z - \mu_z)\right)$$

• z is Gaussian

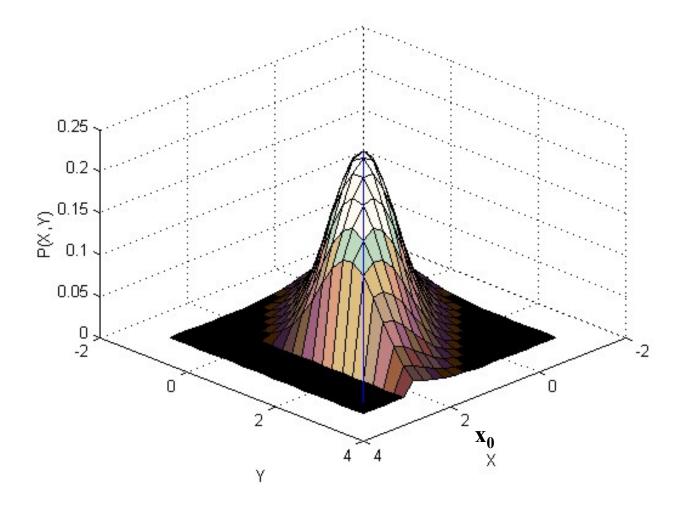




MAP estimation: Gaussian PDF







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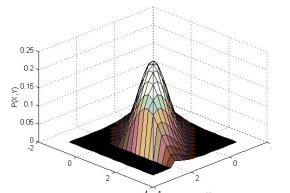
Conditional Probability of y x

$$P(y \mid x) = N(\mu_{y} + C_{yx}C_{xx}^{-1}(x - \mu_{x}), C_{yy} - C_{yx}C_{xx}^{-1}C_{xy})$$

$$E_{y|x}[y] = \mu_{y|x} = \mu_{y} + C_{yx}C_{xx}^{-1}(x - \mu_{x})$$

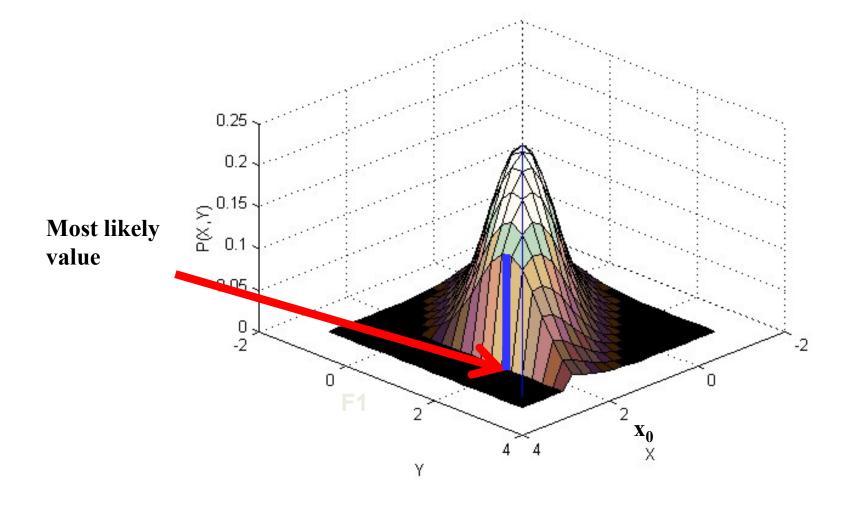
 $Var(y | x) = C_{yy} - C_{yx}C_{xx}^{-1}C_{yy}$

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- The conditional probability of y given x is also Gaussian
 - The slice in the figure is Gaussian
- The mean of this Gaussian is a function of x
- The variance of y reduces if x is known
 - Uncertainty is reduced





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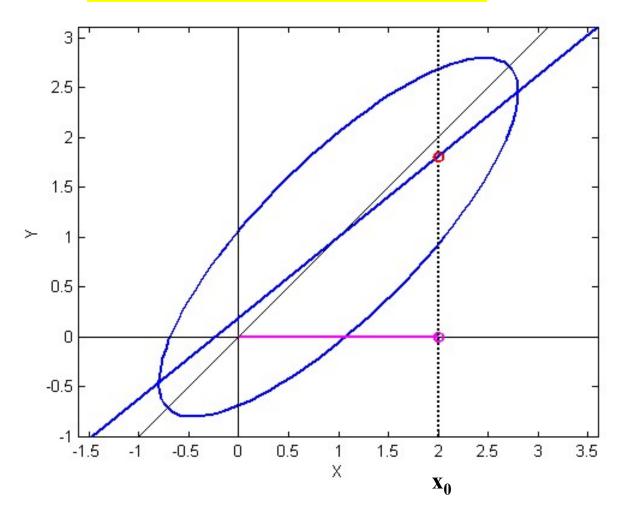


MAP Estimation of a Gaussian RV

$\hat{y} = \arg\max_{y} P(y \mid x) = E_{y|x}[y]$

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Conditional Probability of y | x

$$P(y | x) = N(\mu_{y} + C_{yx}C_{xx}^{-1}(x - \mu_{x}), C_{yy} - C_{yx}C_{xx}^{-1}C_{xy})$$

$$E_{y|x}[y] = \mu_{y|x} = \mu_{y} + C_{yx}C_{xx}^{-1}(x - \mu_{x})$$

$$Var(y | x) = C_{yy} - C_{yx}C_{xx}^{-1}C_{xy}$$

- The conditional pro **MAP Estimate**.
 - The slice in the fig

IOHNS HOPKINS

- Its actually a regression line
- The mean of this Gaussian is a function or x
- The variance of y reduces if x is known
 - Uncertainty is reduced

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Conditional Probability of y x

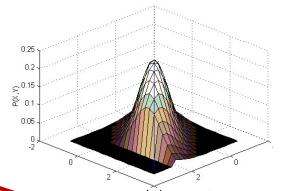
$$P(y \mid x) = N(\mu_{y} + C_{yx}C_{xx}^{-1}(x - \mu_{x}), C_{yy} - C_{yx}C_{xx}^{-1}C_{xy})$$

$$E_{y|x}[y] = \mu_{y|x} = \mu_{y} + C_{yx}C_{xx}^{-1}(x - \mu_{x})$$

$$ar(y(x) = C_{yy} - C_{yx}C_{xx}^{-1}C_{yy}$$

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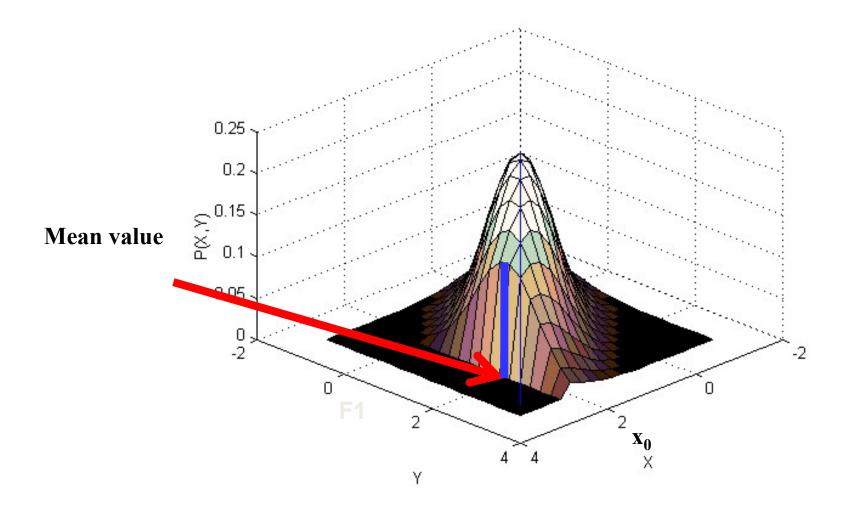
- The conditional pro The variance of Y shrinks because we know X – The slice in the figu
- The mean of this G Note that the actual value of X
- The variance of y re doesn't matter. Simply knowing
 - Uncertainty is redu

X reduces the variance of Y if the two are correlated





MMSE estimation



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error estimate

• Minimize error:

$$Err = E[\|\mathbf{y} - \hat{\mathbf{y}}\|^2 | \mathbf{x}] = E[(\mathbf{y} - \hat{\mathbf{y}})^T (\mathbf{y} - \hat{\mathbf{y}}) | \mathbf{x}]$$

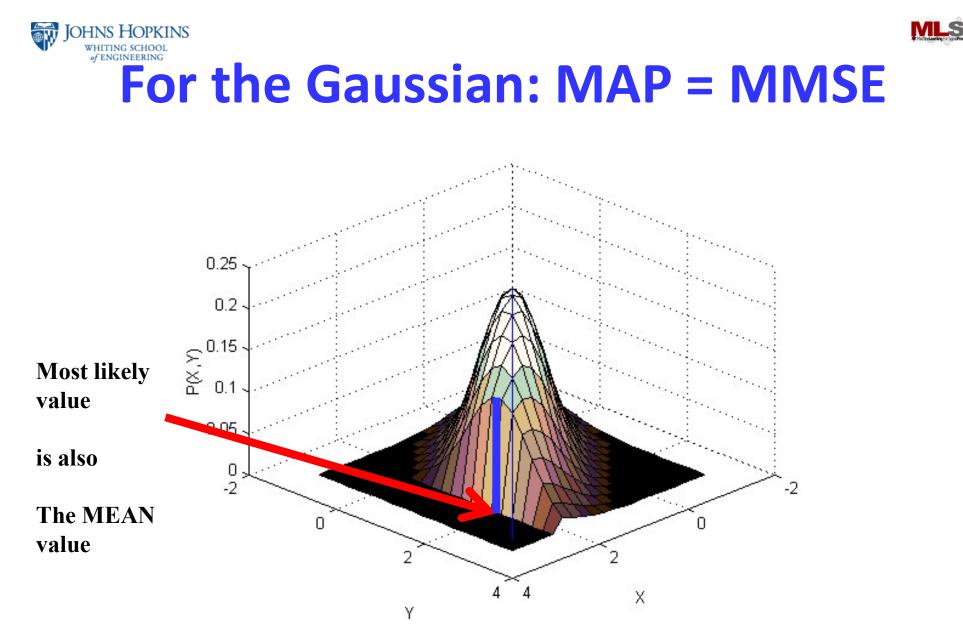
 $Err = E[\mathbf{y}^T\mathbf{y} + \hat{\mathbf{y}}^T\hat{\mathbf{y}} - 2\hat{\mathbf{y}}^T\mathbf{y} | \mathbf{x}] = E[\mathbf{y}^T\mathbf{y} | \mathbf{x}] + \hat{\mathbf{y}}^T\hat{\mathbf{y}} - 2\hat{\mathbf{y}}^TE[\mathbf{y} | \mathbf{x}]$

• Differentiating and equating to 0:

$$d.Err = 2\hat{\mathbf{y}}^T d\hat{\mathbf{y}} - 2E[\mathbf{y} | \mathbf{x}]^T d\hat{\mathbf{y}} = 0$$



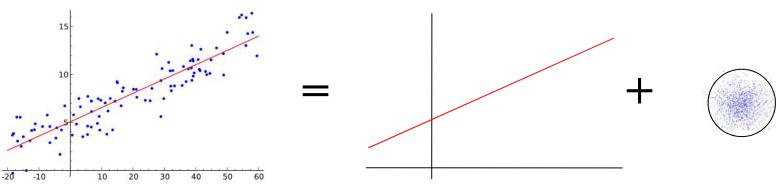
The MMSE estimate is the mean of the distribution



Would be true of any symmetric distribution

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• **y** is a noisy reading of $\mathbf{a}^{\mathsf{T}}\mathbf{x}$

$$\mathbf{y} = \mathbf{a}^T \mathbf{x} + \mathbf{e}$$

• Error e is Gaussian

$$\mathbf{e} \sim N(\mathbf{0}, \boldsymbol{\sigma}^2 \mathbf{I})$$

• Estimate A from $\mathbf{Y} = [\mathbf{y}_1 \ \mathbf{y}_2 ... \mathbf{y}_N] \ \mathbf{X} = [\mathbf{x}_1 \ \mathbf{x}_2 ... \mathbf{x}_N]$



The Likelihood of the data

$$\mathbf{y} = \mathbf{a}^T \mathbf{x} + \mathbf{e}$$
 $\mathbf{e} \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$

• Probability of observing a specific y, given x, for a particular matrix a

$$P(\mathbf{y} | \mathbf{x}; \mathbf{a}) = N(\mathbf{y}; \mathbf{a}^T \mathbf{x}, \sigma^2 \mathbf{I})$$

• Probability of collection: $Y = [y_1, y_1...y_1], X = [x_1, x_2...x_N]$

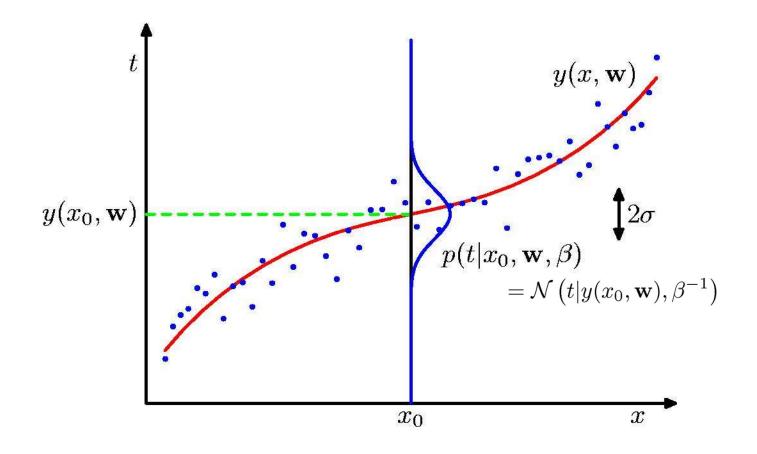
$$P(\mathbf{Y} | \mathbf{X}; \mathbf{a}) = \prod_{i} N(\mathbf{y}_{i}; \mathbf{a}^{T} \mathbf{x}_{i}, \sigma^{2} \mathbf{I})$$

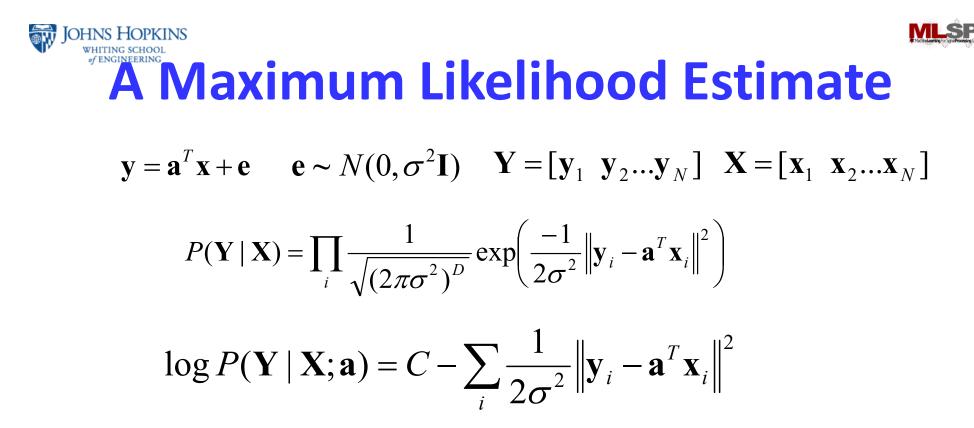
• Assuming IID for convenience (not necessary)



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Curve Fitting With Noise





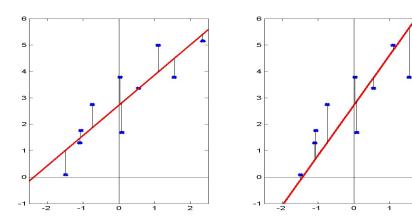
$$\log P(\mathbf{Y} | \mathbf{X}, \mathbf{a}) = C - \frac{1}{2\sigma^2} trace((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X}))$$

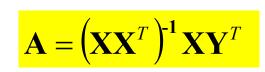
- Maximizing the log probability is identical to minimizing the squared error
 - Just L_2 based regression





A problem with regressions

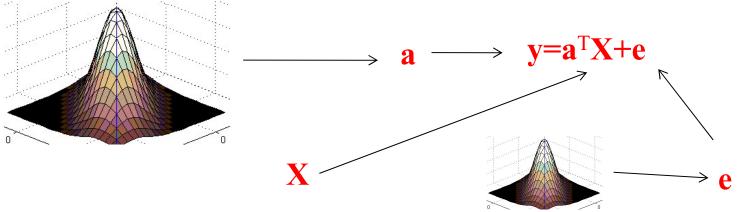




- ML fit is sensitive
 - Error is squared
 - Small variations in data \rightarrow large variations in weights
 - Outliers affect it adversely
- Unstable
 - If dimension of X >= no. of instances
 - (XX^T) is not invertible



MAP estimation of weights



- Assume weights drawn from a Gaussian
 P(a) = N(0, σ²I)
- Max. Likelihood estimate

hns Hopkins

 $\hat{\mathbf{a}} = \arg \max_{\mathbf{a}} \log P(\mathbf{Y} | \mathbf{X}; \mathbf{a})$

• Maximum a posteriori estimate

 $\hat{\mathbf{a}} = \arg \max_{\mathbf{a}} \log P(\mathbf{a} | \mathbf{Y}, \mathbf{X}) = \arg \max_{\mathbf{a}} \log P(\mathbf{Y} | \mathbf{X}, \mathbf{a}) P(\mathbf{a})$



MAP estimation of weights

 $\hat{\mathbf{a}} = \arg \max_{\mathbf{A}} \log P(\mathbf{a} | \mathbf{Y}, \mathbf{X}) = \arg \max_{\mathbf{A}} \log P(\mathbf{Y} | \mathbf{X}, \mathbf{a}) P(\mathbf{a})$

$$\square P(\mathbf{a}) = N(0, \sigma^2 I)$$

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 $\Box \operatorname{Log} P(\mathbf{a}) = C - \log \sigma - 0.5 \sigma^{-2} \|\mathbf{a}\|^2$

$$\log P(\mathbf{Y} | \mathbf{X}, \mathbf{a}) = C - \frac{1}{2\sigma^2} trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X}) \right)$$

$$\hat{\mathbf{a}} = \arg \max_{\mathbf{A}} C' - \log \sigma - \frac{1}{2\sigma^2} trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X}) \right) - 0.5\sigma^2 \mathbf{a}^T \mathbf{a}$$

• Similar to ML estimate with an additional term





MAP estimate of weights

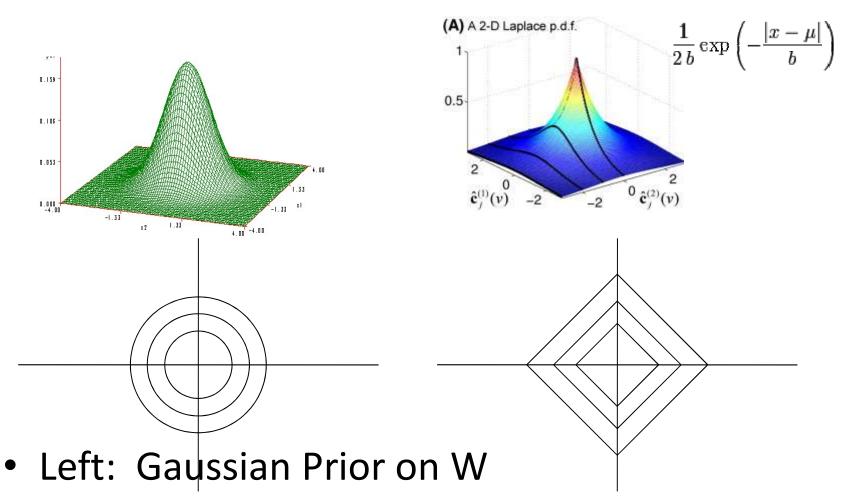
$$\mathbf{a} = \left(\mathbf{X}\mathbf{X}^T + \boldsymbol{\sigma}^2\mathbf{I}\right)^{-1}\mathbf{X}\mathbf{Y}^T$$

- Equivalent to *diagonal loading* of correlation matrix
 - Improves condition number of correlation matrix
 - Can be inverted with greater stability
 - Will not affect the estimation from well-conditioned data
 - Also called Tikhonov Regularization
 - Dual form: Ridge regression
- MAP estimate of *weights*
 - Not to be confused with MAP estimate of Y





MAP estimate priors



• Right: Laplacian Prior



JOHNS HOPKING WHITING SCHEEVIAP estimation of weights with laplacian prior

- Assume weights drawn from a Laplacian $-P(\mathbf{a}) = \lambda^{-1} \exp(-\lambda^{-1} |\mathbf{a}|_1)$
- Maximum *a posteriori* estimate

$$\hat{\mathbf{a}} = \arg\max_{\mathbf{a}} C' - trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T \right) - \lambda^{-1} |\mathbf{a}|_1$$

- No closed form solution
 - Quadratic programming solution required
 - Non-trivial



JOHNS HOPKING WHITING SCHEWIAP estimation of weights with laplacian prior

- Assume weights drawn from a Laplacian $-P(\mathbf{a}) = \lambda^{-1} \exp(-\lambda^{-1}|\mathbf{a}|_1)$
- Maximum *a posteriori* estimate

$$\hat{\mathbf{a}} = \arg \max_{\mathbf{a}} C' - trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T \right) - \lambda^{-1} |\mathbf{a}|_1$$

• This is also L_1 regularized least-squares estimation





$$\hat{\mathbf{a}} = \arg \max_{\mathbf{a}} C' - trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T \right) - \lambda^{-1} |\mathbf{a}|_1$$

- No closed form solution
 - Quadratic programming solutions required
- Dual formulation

$$\hat{\mathbf{a}} = \arg \max_{\mathbf{a}} C' - trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T \right)$$
 subject to $|\mathbf{a}|_1 \le t$

"LASSO" – Least absolute shrinkage and selection operator





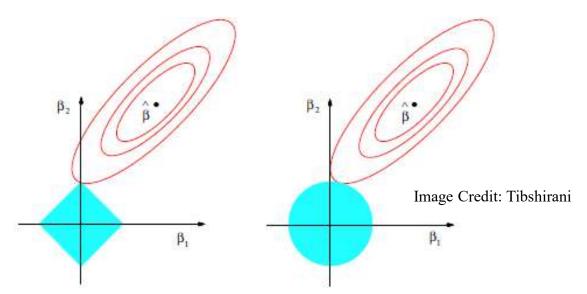
LASSO Algorithms

- Various convex optimization algorithms
- LARS: Least angle regression
- Pathwise coordinate descent..
- Matlab code available from web

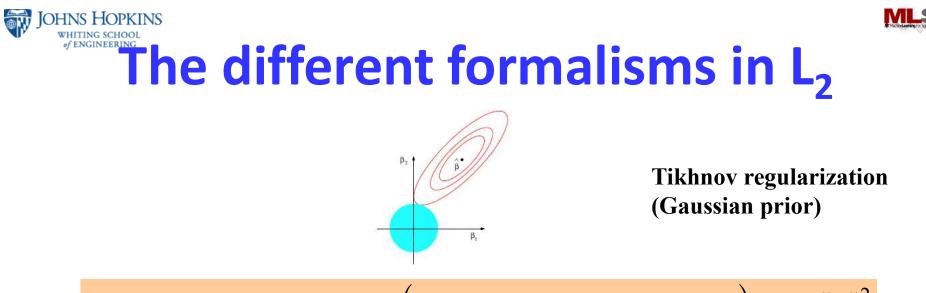




Regularized least squares



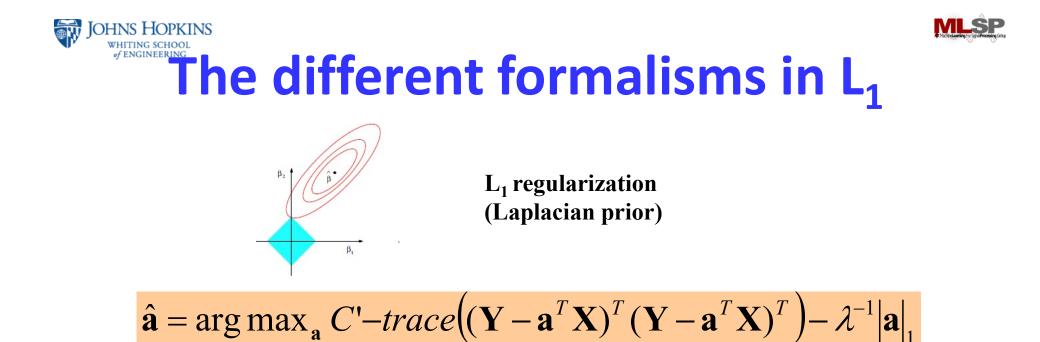
- Regularization results in selection of suboptimal (in least-squares sense) solution
 - One of the loci outside center
- Tikhonov regularization selects *shortest* solution
- L₁ regularization selects *sparsest* solution



$$\hat{\mathbf{a}} = \arg \max_{\mathbf{a}} C' - trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T \right) - \lambda^{-1} \|\mathbf{a}\|^2$$

$$\hat{\mathbf{a}} = \arg\max_{\mathbf{a}} C' - trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T \right)$$
 subject to $\|\mathbf{a}\|^2 \le t$

- Expand both the ball and the ellipses till the both just meet
- Fix the ball, expand the ellipse till it meets the ball 11-755/18-797



$$\hat{\mathbf{a}} = \arg \max_{\mathbf{a}} C' - trace \left((\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T (\mathbf{Y} - \mathbf{a}^T \mathbf{X})^T \right)$$
 subject to $|\mathbf{a}|_1 \le t$

- Expand both the diamond and the ellipses till the both just meet
- Fix the diamond, expand the ellipse till it meets the ball 11-755/18-797





MAP / ML / MMSE

- General statistical estimators
- All used to predict a variable, based on other parameters related to it..
- Most common assumption: Data are Gaussian, all RVs are Gaussian
 - Other probability densities may also be used..
- For Gaussians relationships are linear as we saw..



- Linear Gaussian Models..
- But first a recap



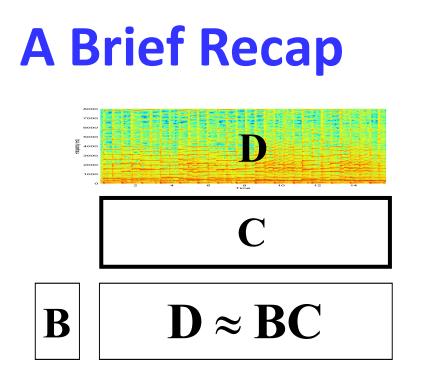


Linear Gaussian Models

- MAP and MMSE prediction with Gaussian models
 - Estimation
 - Regularization
- Representation
 - PCA
 - Probabilistic PCA
- Gaussian Classifier







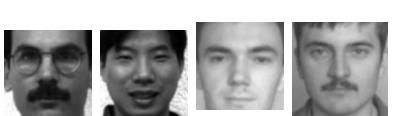
- Principal component analysis: Find the *K* bases that best explain the given data
- Find B and C such that the difference between D and
 BC is minimum
 - While constraining that the columns of **B** are orthonormal

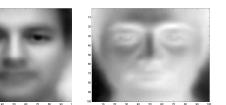




Remember Eigenfaces







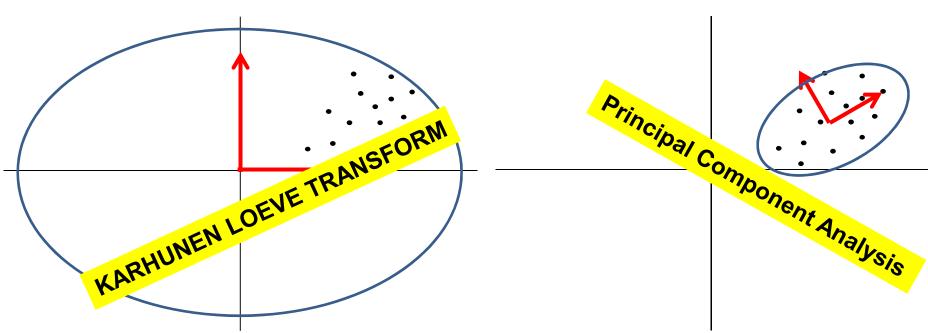


- Approximate every face f as $f = w_{f,1} V_1 + w_{f,2} V_2 + w_{f,3} V_3 + ... + w_{f,k} V_k$
- Estimate ${\rm V}$ to minimize the squared error
- Error is unexplained by $V_1...V_k$
- Error is orthogonal to Eigenfaces





Karhunen Loeve vs. PCA



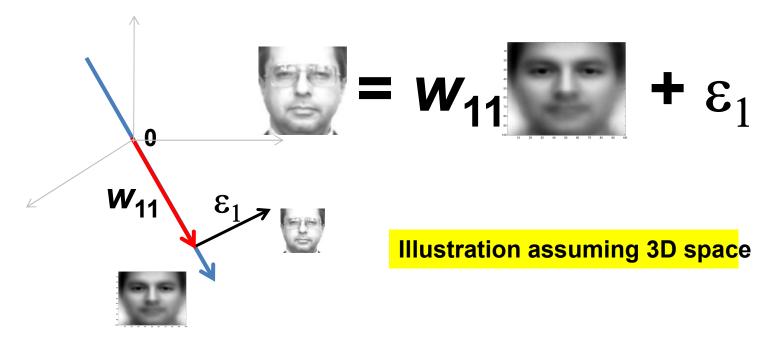
- Eigenvectors of the *Correlation* matrix:
 - Principal directions of tightest ellipse *centered on origin*
 - Directions that retain maximum <u>energy</u>

- Eigenvectors of the *Covariance* matrix:
 - Principal directions of tightest ellipse *centered on data*
 - Directions that retain maximum <u>variance</u>





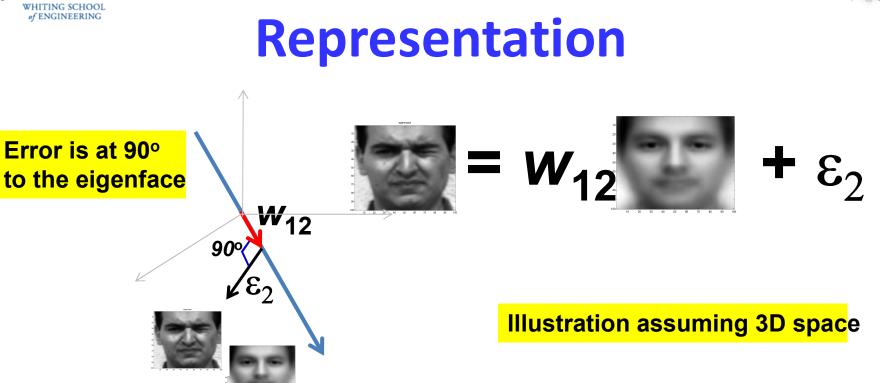
Eigen Representation



- K-dimensional representation
 - Error is orthogonal to representation
 - Weight and error are specific to data instance





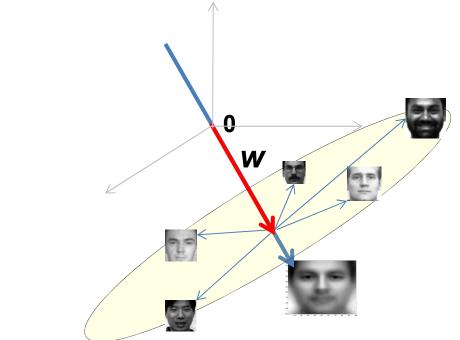


- K-dimensional representation
 - Error is orthogonal to representation
 - Weight and error are specific to data instance





Representation

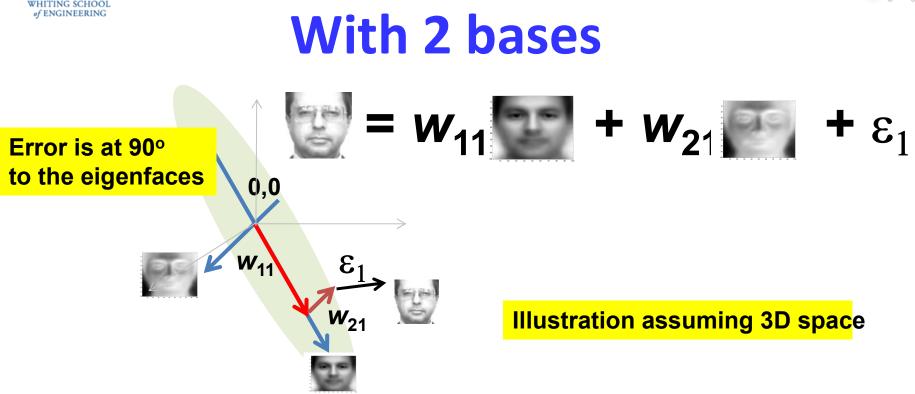


All data with the same representation wV_1 lie a plane orthogonal to wV_1

- K-dimensional representation
 - Error is orthogonal to representation



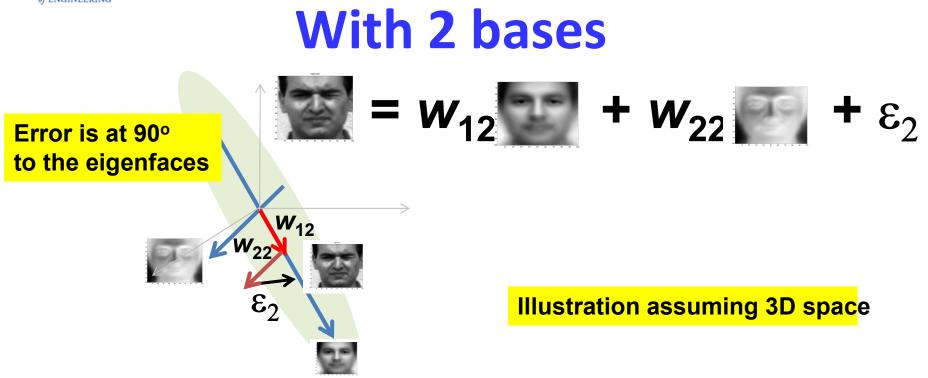




- K-dimensional representation
 - Error is orthogonal to representation
 - Weight and error are specific to data instance



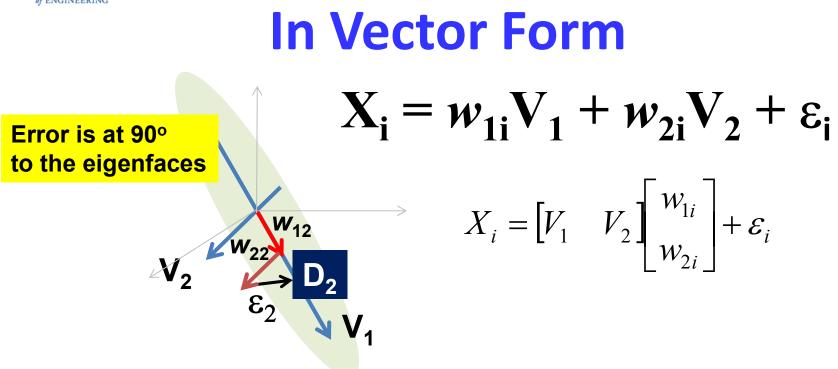




- K-dimensional representation
 - Error is orthogonal to representation
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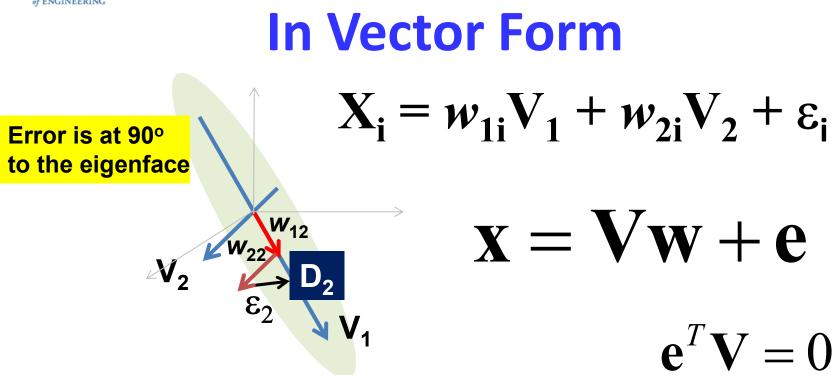




- K-dimensional representation
 - Error is orthogonal to representation
 - Weight and error are specific to data instance





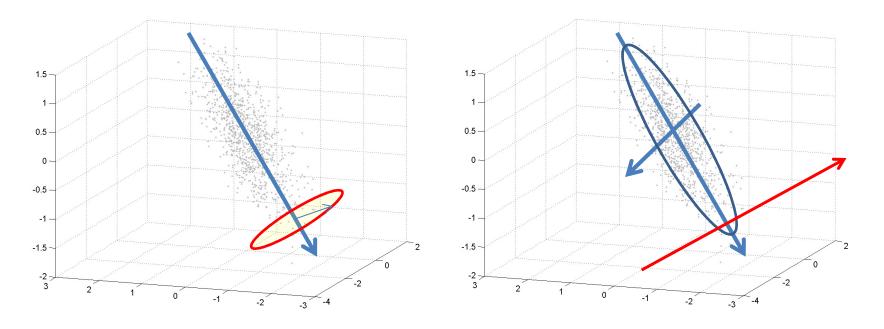


- K-dimensional representation
- x is a D dimensional vector
- V is a D x K matrix
- w is a K dimensional vector
- e is a D dimensional vector



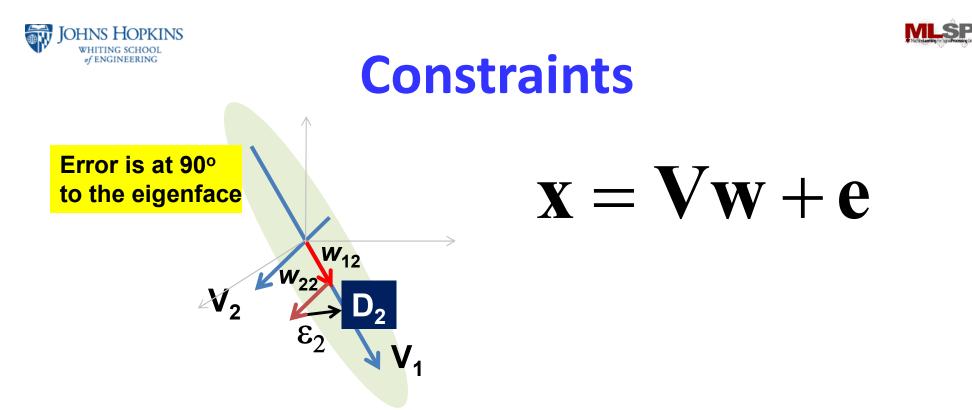


Learning PCA

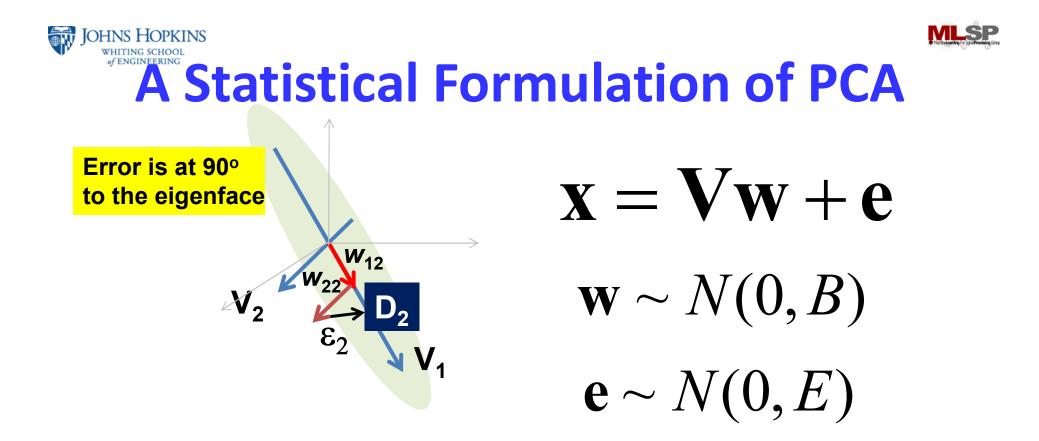


- For the given data: find the K-dimensional subspace such that it captures most of the variance in the data
 - Variance in remaining subspace is minimal

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- $V^T V = I$: Eigen vectors are orthogonal to each other
- For every vector, error is orthogonal to Eigen vectors
 e^TV = 0
- Over the *collection* of data
 - Average ww^T = **Diagonal** : Eigen representations are uncorrelated
 - $e^{T}e = minimum$: Error variance is minimum
 - Mean of error is 0

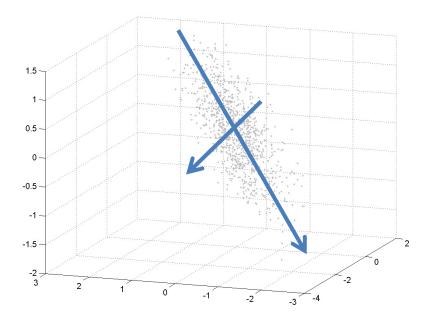


- x is a random variable generated according to a linear relation
- w is drawn from an K-dimensional Gaussian with diagonal covariance
- e is drawn from a 0-mean (D-K)-rank D-dimensional Gaussian
- Estimate V (and *B*) given examples of x



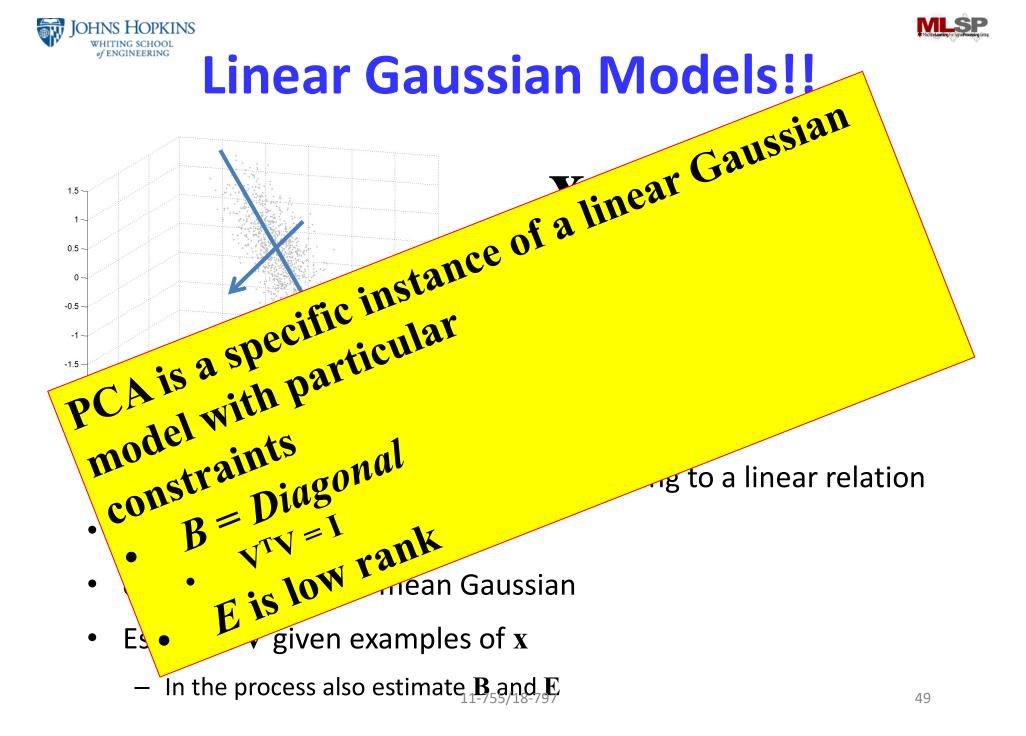


Linear Gaussian Models!!



$\mathbf{x} = \mathbf{V}\mathbf{w} + \mathbf{e}$ $\mathbf{w} \sim N(\mathbf{0}, B)$ $\mathbf{e} \sim N(\mathbf{0}, E)$

- x is a random variable generated according to a linear relation
- w is drawn from a Gaussian
- e is drawn from a 0-mean Gaussian
- Estimate V given examples of x
 - In the process also estimate B and E







Linear Gaussian Models

$\mathbf{x} = \mathbf{\mu} + \mathbf{V}\mathbf{w} + \mathbf{e} \quad \mathbf{w} \sim N(0, B)$ $\mathbf{e} \sim N(0, E)$

- Observations are linear functions of two *uncorrelated* Gaussian random variables
 - A "weight" variable ${\bf w}$
 - An "error" variable e
 - Error not correlated to weight: $E[e^Tw] = 0$
- Learning LGMs: Estimate parameters of the model given instances of x
 - The problem of learning the distribution of a Gaussian RV





LGMs: Probability Density

$\mathbf{x} = \mathbf{\mu} + \mathbf{V}\mathbf{w} + \mathbf{e} \qquad \mathbf{w} \sim N(0, B)$ $\mathbf{e} \sim N(0, E)$

• The mean of **x**:

$$E[\mathbf{x}] = \mathbf{\mu} + \mathbf{V}E[\mathbf{w}] + E[\mathbf{e}] = \mathbf{\mu}$$

• The Covariance of x:

$$E[(\mathbf{x} - E[\mathbf{x}])(\mathbf{x} - E[\mathbf{x}])^T] = \mathbf{V}B\mathbf{V}^T + E$$





The probability of x

$$\mathbf{x} = \mathbf{\mu} + \mathbf{V}\mathbf{w} + \mathbf{e}$$
 $\mathbf{w} \sim N(0, B)$
 $\mathbf{e} \sim N(0, E)$
 $\mathbf{x} \sim N(\mathbf{\mu}, \mathbf{V}B\mathbf{V}^T + E)$

$$P(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^D |\mathbf{V}B\mathbf{V}^T + E|}} \exp\left(-0.5(\mathbf{x} - \boldsymbol{\mu})^T (\mathbf{V}B\mathbf{V}^T + E)^{-1} (\mathbf{x} - \boldsymbol{\mu})\right)$$

- x is a linear function of Gaussians: x is also Gaussian
- Its mean and variance are as given

EXAMPLE 1 Stimulating the variables of the model

$$\mathbf{x} = \mathbf{\mu} + \mathbf{V}\mathbf{w} + \mathbf{e}$$
 $\mathbf{w} \sim N(0, B)$
 $\mathbf{e} \sim N(0, E)$
 $\mathbf{x} \sim N(\mathbf{\mu}, \mathbf{V}B\mathbf{V}^T + E)$

• Estimating the variables of the LGM is equivalent to estimating P(x)

– The variables are μ , \mathbf{V} , B and E





Estimating the model

$$\mathbf{x} = \mathbf{\mu} + \mathbf{V}\mathbf{w} + \mathbf{e}$$

 $\mathbf{w} \sim N(0, B)$
 $\mathbf{e} \sim N(0, E)$
 $\mathbf{x} \sim N(\mathbf{\mu}, \mathbf{V}B\mathbf{V}^T + E)$

• The model is indeterminate:

 $-\mathbf{V}\mathbf{w} = \mathbf{V}\mathbf{C}\mathbf{C}^{-1}\mathbf{w} = (\mathbf{V}\mathbf{C})(\mathbf{C}^{-1}\mathbf{w})$

- We need extra constraints to make the solution unique

- Usual constraint : B = I
 - Variance of \boldsymbol{w} is an identity matrix

EXAMPLE 1 Stimuling the variables of the model

$$\mathbf{x} = \mathbf{\mu} + \mathbf{V}\mathbf{w} + \mathbf{e}$$
 $\mathbf{w} \sim N(0, I)$
 $\mathbf{e} \sim N(0, E)$
 $\mathbf{x} \sim N(\mathbf{\mu}, \mathbf{V}\mathbf{V}^T + E)$

 Estimating the variables of the LGM is equivalent to estimating P(x)

– The variables are μ , V , and ${\it E}$



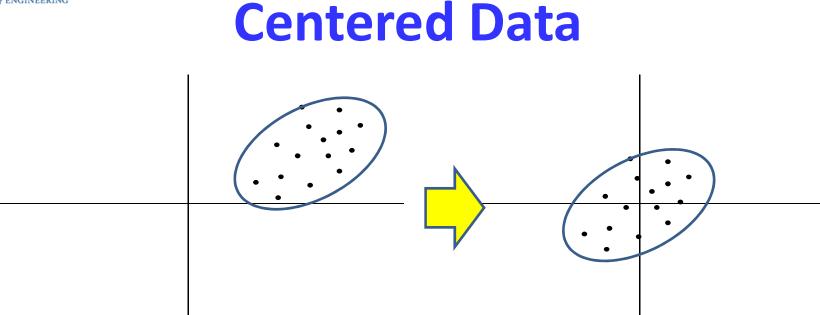
$$\mathbf{x} \sim N(\mathbf{\mu}, \mathbf{V}\mathbf{V}^T + E)$$

- Given training set $x_1, x_2, ... x_N$, find μ , V, E
- The ML estimate of $\boldsymbol{\mu}$ does not depend on the covariance of the Gaussian

$$\boldsymbol{\mu} = \frac{1}{N} \sum_{i} \mathbf{x}_{i}$$







- We can safely assume "centered" data $-\mu = 0$
- If the data are not centered, "center" it
 - Estimate mean of data
 - Which is the maximum likelihood estimate
 - Subtract it from the data





Simplified Model $\mathbf{x} = \mathbf{V}\mathbf{w} + \mathbf{e}$ $\mathbf{w} \sim N(0, I)$ $\mathbf{e} \sim N(0, E)$ $\mathbf{x} \sim N(0, \mathbf{V}\mathbf{V}^T + E)$

 Estimating the variables of the LGM is equivalent to estimating P(x)

– The variables are V, and E





Estimating the model

$$\mathbf{x} = \mathbf{V}\mathbf{w} + \mathbf{e}$$
 $\mathbf{x} \sim N(\mathbf{0}, \mathbf{V}\mathbf{V}^T + E)$

- Given a collection of **x**_i terms
 - $-\mathbf{x}_{1}, \mathbf{x}_{2}, .., \mathbf{x}_{N}$
- Estimate V and E
- w is unknown for each x
- But if assume we know w for each x, then what do we get:





Estimating the Parameters

$$\mathbf{x}_i = \mathbf{V}\mathbf{w}_i + \mathbf{e}$$

$$P(\mathbf{e}) = N(0, E)$$

$$P(\mathbf{x} \mid \mathbf{w}) = N(\mathbf{V}\mathbf{w}, E)$$

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$$\mathbf{x} = \mathbf{V}\mathbf{w} + \mathbf{e} \qquad \mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{w} \end{bmatrix} \qquad P(\mathbf{z}) = N(\mu_{\mathbf{z}}, C_{\mathbf{zz}})$$

$$P(\mathbf{x}) = N(0, \mathbf{V}\mathbf{V}^{T} + E) \qquad \mu_{\mathbf{z}} = \begin{bmatrix} \mu_{\mathbf{x}} \\ \mu_{\mathbf{w}} \end{bmatrix} = 0$$

$$P(\mathbf{w}) = N(0, I) \qquad C_{\mathbf{zz}} = \begin{bmatrix} C_{\mathbf{xx}} & C_{\mathbf{xw}} \\ C_{\mathbf{wx}} & C_{\mathbf{ww}} \end{bmatrix}$$

$$C_{zz} = \begin{bmatrix} \mathbf{V}\mathbf{V}^T + E & \mathbf{V} \\ \mathbf{V}^T & I \end{bmatrix}$$

 $= N(\mu_z, C_{zz})$

=0

 $\mu_{\mathbf{x}}$

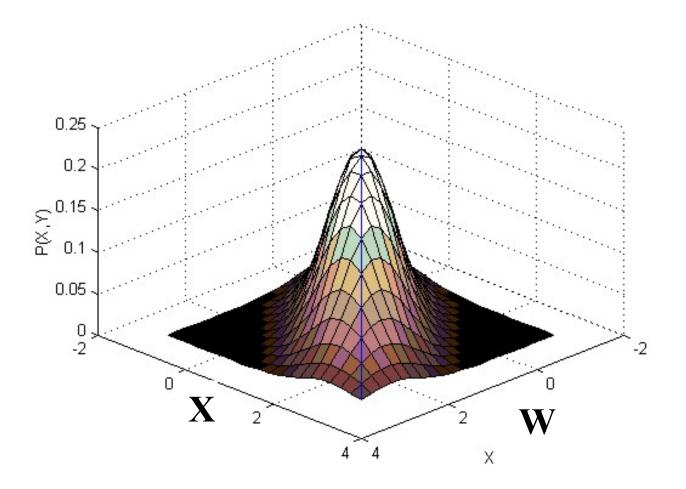
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• x and w are jointly Gaussian!



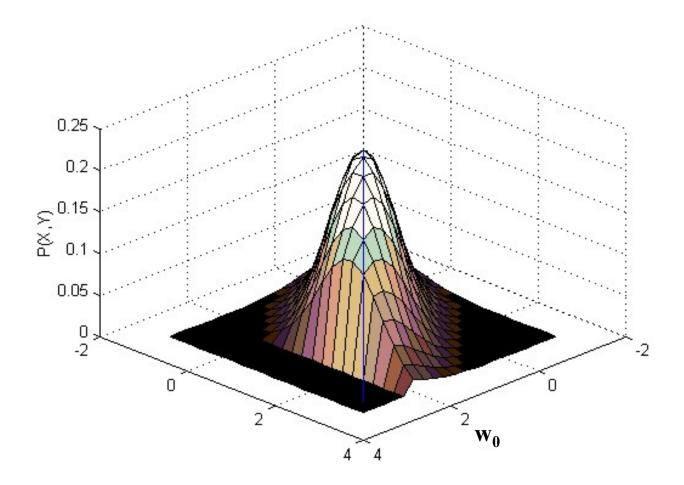


MAP estimation: Gaussian PDF

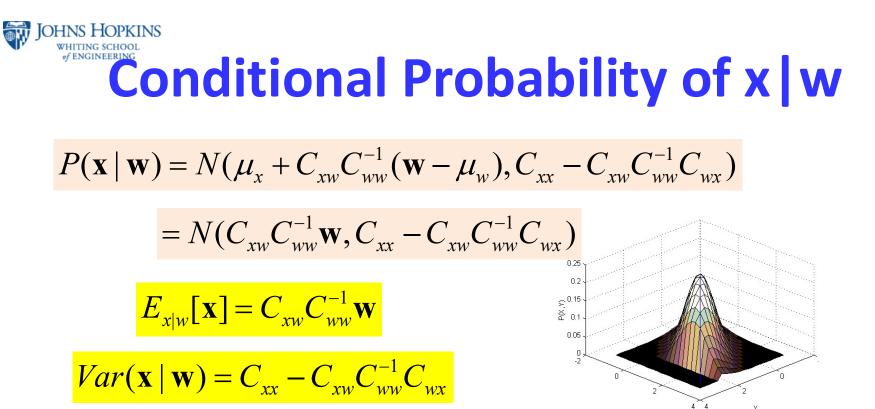


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• Comparing to

$$P(\mathbf{x} \mid \mathbf{w}) = N(\mathbf{V}\mathbf{w}, E)$$

• We get:

$$V = C_{xw} C_{ww}^{-1} \qquad E = C_{xx} - C_{xw} C_{ww}^{-1} C_{wx}$$





Or more explicitly

$$C_{ww} = \frac{1}{N} \sum_{i} \mathbf{w}_{i} \mathbf{w}_{i}^{T}$$

$$C_{xw} = \frac{1}{N} \sum_{i} \mathbf{x}_{i} \mathbf{w}_{i}^{T}$$

$$\mathbf{V} = C_{xw} C_{ww}^{-1}$$

$$E = C_{xx} - C_{xw} C_{ww}^{-1} C_{wx}$$

$$\mathbf{V} = \left(\sum_{i} \mathbf{x}_{i} \mathbf{w}_{i}^{T}\right) \left(\sum_{i} \mathbf{w}_{i} \mathbf{w}_{i}^{T}\right)^{-1}$$

$$E = \frac{1}{N} \left(\sum_{i} \mathbf{x}_{i} \mathbf{x}_{i}^{T} - \mathbf{V} \sum_{i} \mathbf{w}_{i} \mathbf{x}_{i}^{T} \right)$$

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Estimating LGMs: If we know w

$$\mathbf{x}_i = \mathbf{V}\mathbf{w}_i + \mathbf{e}$$
 $P(\mathbf{e}) = N(0, E)$

$$\mathbf{V} = \left(\sum_{i} \mathbf{x}_{i} \mathbf{w}_{i}^{T}\right) \left(\sum_{i} \mathbf{w}_{i} \mathbf{w}_{i}^{T}\right)^{-1} \qquad E = \frac{1}{N} \left(\sum_{i} \mathbf{w}_{i} \mathbf{w}_{i}^{T}\right)^{-1}$$

$$E = \frac{1}{N} \left(\sum_{i} \mathbf{x}_{i} \mathbf{x}_{i}^{T} - \mathbf{V} \sum_{i} \mathbf{w}_{i} \mathbf{x}_{i}^{T} \right)$$

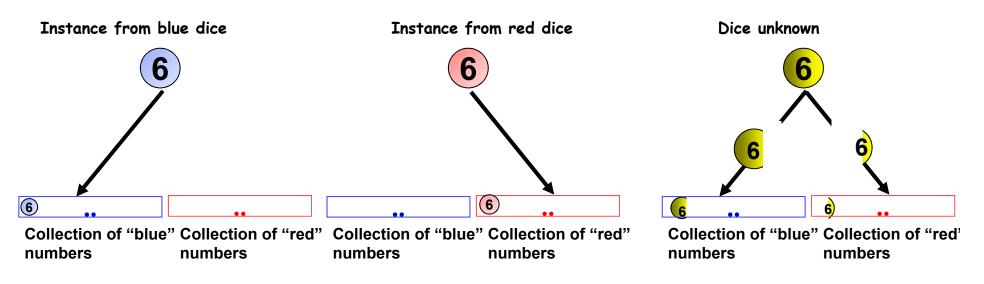
- But in reality we *don't* know the **w** for each **x**
 - So how to deal with this?
- EM..

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Recall EM



- We figured out how to compute parameters if we knew the missing information
- Then we "fragmented" the observations according to the posterior probability P(z|x) and counted as usual
- In effect we took the expectation with respect to the a posteriori probability of the missing data: P(z|x)





EM for LGMs

$$\mathbf{x}_i = \mathbf{V}\mathbf{w}_i + \mathbf{e}$$
 $P(\mathbf{e}) = N(0, E)$

$$\mathbf{V} = \left(\sum_{i} \mathbf{x}_{i} \mathbf{w}_{i}^{T}\right) \left(\sum_{i} \mathbf{w}_{i} \mathbf{w}_{i}^{T}\right)^{-1} \qquad E = \frac{1}{N} \left(\sum_{i} \mathbf{x}_{i} \mathbf{x}_{i}^{T} - \mathbf{V} \sum_{i} \mathbf{w}_{i} \mathbf{x}_{i}^{T}\right)$$
$$\mathbf{V} = \left(\sum_{i} \mathbf{x}_{i} E_{\mathbf{w} | \mathbf{x}_{i}} [\mathbf{w}^{T}]\right) \left(\sum_{i} E_{\mathbf{w} | \mathbf{x}_{i}} [\mathbf{w} \mathbf{w}^{T}]\right)^{-1} \qquad E = \frac{1}{N} \sum_{i} \mathbf{x}_{i} \mathbf{x}_{i}^{T} - \frac{1}{N} \mathbf{V} \sum_{i} E_{\mathbf{w} | \mathbf{x}_{i}} [\mathbf{w}] \mathbf{x}_{i}^{T}$$

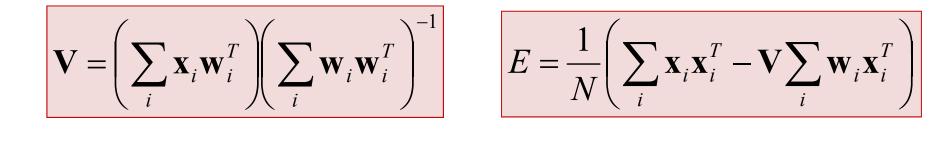
• Replace unseen data terms with expectations taken w.r.t. $P(\mathbf{w}|\mathbf{x}_i)$





EM for LGMs

$$\mathbf{x}_i = \mathbf{V}\mathbf{w}_i + \mathbf{e}$$
 $P(\mathbf{e}) = N(0, E)$



 $\mathbf{V} = \left(\sum_{i} \mathbf{x}_{i} E_{\mathbf{w} | \mathbf{x}_{i}} [\mathbf{w}^{T}] \left(\sum_{i} E_{\mathbf{w} | \mathbf{x}_{i}} [\mathbf{w} \mathbf{w}^{T}]\right)^{-1}\right)^{-1} E = \frac{1}{N} \sum_{i} \mathbf{x}_{i} \mathbf{x}_{i}^{T} - \frac{1}{N} \mathbf{V} \sum_{i} E_{\mathbf{w} | \mathbf{x}_{i}} [\mathbf{w}] \mathbf{x}^{T}$

• Replace unseen data terms with expectations taken w.r.t. $P(\mathbf{w}|\mathbf{x}_i)$





Flipping the problem



- How do we estimate the above terms?
- MAP to the rescue!!



Expected Value of w given x $\mathbf{x} = \mathbf{V}\mathbf{w} + \mathbf{e}$ $P(\mathbf{e}) = N(0, E)$ $P(\mathbf{w}) = N(0, I)$ $P(\mathbf{x}) = N(0, \mathbf{V}\mathbf{V}^T + E)$

- x and w are jointly Gaussian!
 - x is Gaussian

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- $-\mathbf{w}$ is Gaussian
- They are linearly related

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{w} \end{bmatrix} \qquad P(\mathbf{z}) = N(\mu_{\mathbf{z}}, C_{\mathbf{z}\mathbf{z}})$$



$$\mathbf{x} = \mathbf{V}\mathbf{w} + \mathbf{e}$$
$$\mathbf{e} \sim N(0, E) \qquad P(\mathbf{w}) = N(0, I)$$
$$P(\mathbf{x}) = N(0, \mathbf{V}\mathbf{V}^T + E)$$
$$C_{xx} = \mathbf{V}\mathbf{V}^T + E \qquad C_{ww} = \mathbf{I}$$
$$C_{xw} = E[(\mathbf{x} - \mu_x)(\mathbf{w} - \mu_w)^T] = \mathbf{V}$$

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{w} \end{bmatrix}$$
$$\mathbf{P}(\mathbf{z}) = N(\mu_{\mathbf{z}}, C_{\mathbf{z}\mathbf{z}})$$
$$\mu_{\mathbf{z}} = \begin{bmatrix} \mu_{\mathbf{x}} \\ \mu_{\mathbf{w}} \end{bmatrix} = 0$$
$$C_{\mathbf{z}\mathbf{z}} = \begin{bmatrix} C_{\mathbf{x}\mathbf{x}} & C_{\mathbf{x}\mathbf{w}} \\ C_{\mathbf{w}\mathbf{x}} & C_{\mathbf{w}\mathbf{w}} \end{bmatrix}$$

• x and w are jointly Gaussian!



$$C_{ZZ} = \begin{bmatrix} (\mathbf{V}\mathbf{V}^{T} + E) & \mathbf{V} \\ \mathbf{V}^{T} & \mathbf{I} \end{bmatrix}$$

$$P(\mathbf{z}) = N(\mu_{z}, C_{zz})$$

$$\mu_{z} = \begin{bmatrix} \mu_{x} \\ \mathbf{w} \end{bmatrix}$$

$$\mu_{z} = \begin{bmatrix} \mathbf{w} \\ \mu_{w} \end{bmatrix} = 0$$

$$C_{xw} = E[(\mathbf{x} - \mu_{x})(\mathbf{w} - \mu_{w})^{T}] = \mathbf{V}$$

$$C_{zz} = \begin{bmatrix} C_{xx} & C_{xw} \\ C_{wx} & C_{ww} \end{bmatrix}$$

• x and w are jointly Gaussian!





P(w | z)

•
$$P(\mathbf{w} | \mathbf{z})$$
 is a Gaussian

$$P(\mathbf{w} | \mathbf{x}) = N(\mu_{\mathbf{w}} + C_{\mathbf{wx}}C_{\mathbf{xx}}^{-1}(x - \mu_{\mathbf{x}}), C_{\mathbf{ww}} - C_{\mathbf{wx}}C_{\mathbf{xx}}^{-1}C_{\mathbf{xw}})$$

$$= N(C_{\mathbf{wx}}C_{\mathbf{xx}}^{-1}\mathbf{x}, C_{\mathbf{ww}} - C_{\mathbf{wx}}C_{\mathbf{xx}}^{-1}C_{\mathbf{xw}})$$

$$= N(\mathbf{V}^{T}(\mathbf{V}\mathbf{V}^{T} + E)^{-1}\mathbf{x}, I - \mathbf{V}^{T}(\mathbf{V}\mathbf{V}^{T} + E)^{-1}\mathbf{V})$$

$$Var(\mathbf{w} | \mathbf{x}) = I - \mathbf{V}^{T}(\mathbf{V}\mathbf{V}^{T} + E)^{-1}\mathbf{X}$$

$$E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}] = \mathbf{V}^{T}(\mathbf{V}\mathbf{V}^{T} + E)^{-1}\mathbf{x}_{i}$$

$$E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{ww}^{T}] = Var(\mathbf{w} | \mathbf{x}) + E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}]E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}]^{T}$$

$$E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{ww}^{T}] = I - \mathbf{V}^{T}(\mathbf{V}\mathbf{V}^{T} + E)^{-1}\mathbf{V} + E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}]E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}]^{T}$$



LGM: The complete EM algorithm

$$\mathbf{V}\mathbf{w} + \mathbf{e} \quad \mathbf{e} \sim N(0, E) \quad P(\mathbf{w}) = N(0, I)$$
$$P(\mathbf{x}) = N(0, \mathbf{V}\mathbf{V}^T + E)$$

• Initialize V and E

• Estep:

$$E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}] = \mathbf{V}^{T}(\mathbf{V}\mathbf{V}^{T} + E)^{-1}\mathbf{x}_{i}$$

$$E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}\mathbf{w}^{T}] = I - \mathbf{V}^{T}(\mathbf{V}\mathbf{V}^{T} + E)^{-1}\mathbf{V} + E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}]E_{\mathbf{w}|\mathbf{x}_{i}}[\mathbf{w}]^{T}$$

 $E_{\mathbf{w}|\mathbf{x}_i}$

• M step:

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 $\mathbf{X} =$

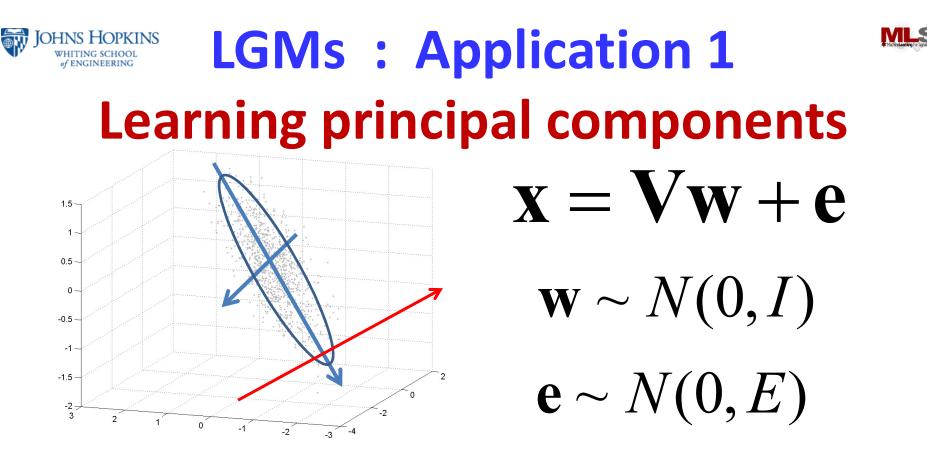
$$\mathbf{V} = \left(\sum_{i} \mathbf{x}_{i} E_{\mathbf{w} | \mathbf{x}_{i}}[\mathbf{w}^{T}]\right) \left(\sum_{i} E_{\mathbf{w} | \mathbf{x}_{i}}[\mathbf{w}\mathbf{w}^{T}]\right)^{-1}$$
$$E = \frac{1}{N} \sum_{i} \mathbf{x}_{i} \mathbf{x}_{i}^{T} - \frac{1}{N} \mathbf{V} \sum_{i} E_{\mathbf{w} | \mathbf{x}_{i}}[\mathbf{w}] \mathbf{x}_{i}^{T}$$





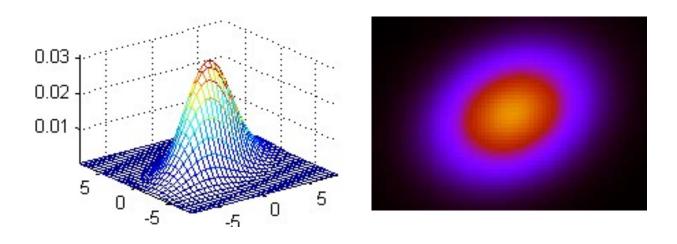
So what have we achieved

- Employed a complicated EM algorithm to learn a *Gaussian* PDF for a variable x
- What have we gained???
 - PCA
 - Sensible PCA
 - EM algorithms for PCA (Probabilistic PCA)
- Next class:
 - Factor Analysis
 - FA for feature extraction



- Find directions that capture most of the variation in the data
- Error is orthogonal to these variations





FULL COV FIGURE

- The full covariance matrix of a Gaussian has D^2 terms
- Fully captures the relationships between variables
- Problem: Needs a lot of data to estimate robustly





To be continued..

- Other applications..
- Next class





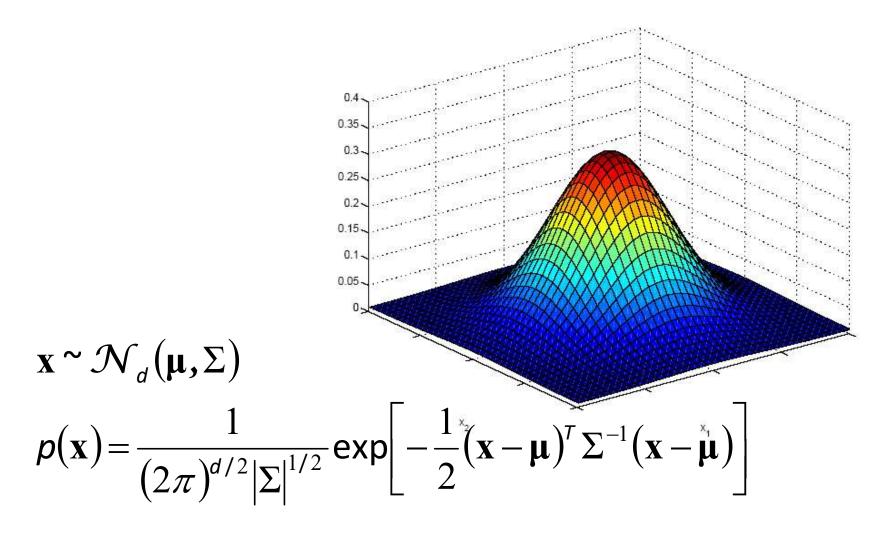
Linear Gaussian Models

- Recap
- Representation
 - PCA
 - Probabilistic PCA
- Gaussian Classifier





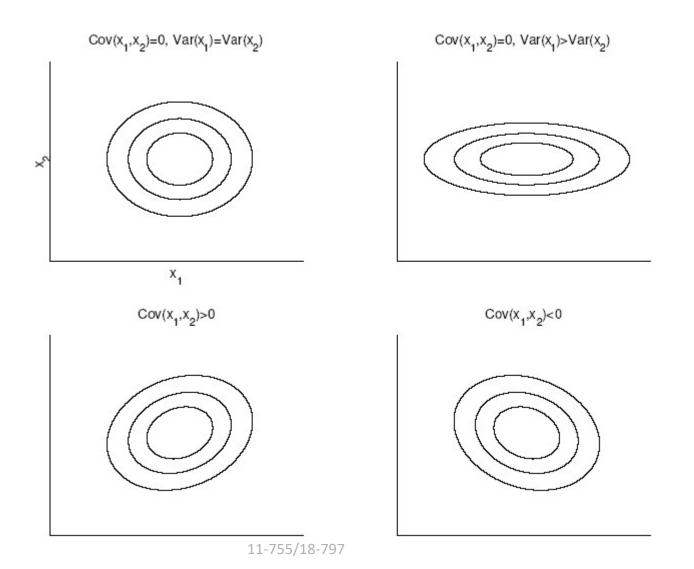
Multivariate Normal Distribution







Bivariate Normal

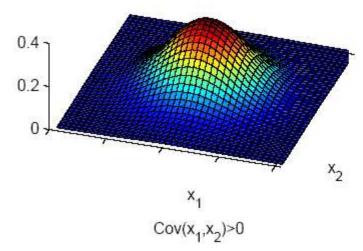


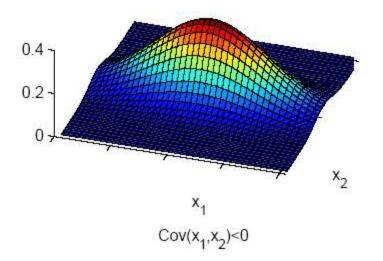


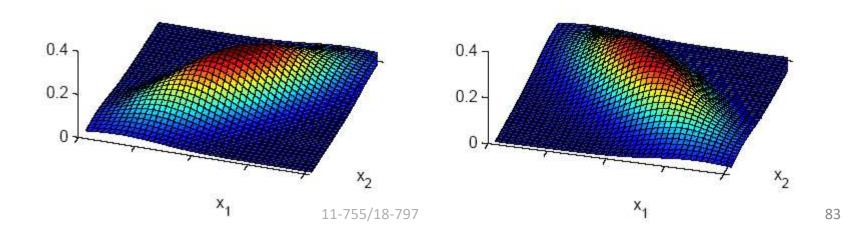


$Cov(x_1, x_2)=0$, $Var(x_1)=Var(x_2)$

 $Cov(x_1, x_2)=0, Var(x_1)>Var(x_2)$











Parametric Classification

• If $p(\mathbf{x} \mid C_i) \sim N(\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$

$$p(\mathbf{x} | C_i) = \frac{1}{(2\pi)^{d/2} |\Sigma_i|^{1/2}} \exp\left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_i)^T \Sigma_i^{-1} (\mathbf{x} - \boldsymbol{\mu}_i)\right]$$

• Discriminant functions

$$g_i(\mathbf{x}) = \log p(\mathbf{x} | C_i) + \log P(C_i)$$

= $-\frac{d}{2} \log 2\pi - \frac{1}{2} \log |\Sigma_i| - \frac{1}{2} (\mathbf{x} - \mu_i)^T \Sigma_i^{-1} (\mathbf{x} - \mu_i) + \log P(C_i)$





Estimation of Parameters

$$\hat{P}(C_i) = \frac{N_i}{N}$$
$$\mathbf{m}_i = \frac{\sum_{t \in classi} \mathbf{x}^t}{N_i}$$
$$\mathbf{S}_i = \frac{\sum_{t \in classi} (\mathbf{x}^t - \mathbf{m}_i) (\mathbf{x}^t - \mathbf{m}_i)^T}{N_i}$$

$$g_i(\mathbf{x}) = -\frac{1}{2} \log |\mathbf{S}_i| - \frac{1}{2} (\mathbf{x} - \mathbf{m}_i)^T \mathbf{S}_i^{-1} (\mathbf{x} - \mathbf{m}_i) + \log \hat{P}(\mathbf{C}_i)$$





Different S_i

• Quadratic discriminant

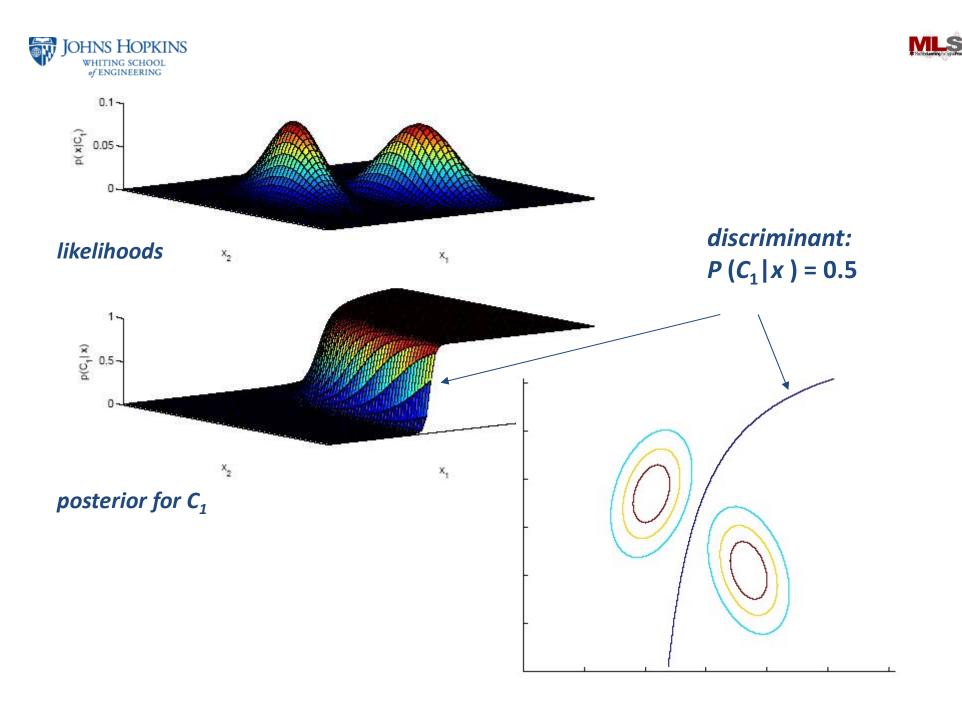
$$g_{i}(\mathbf{x}) = -\frac{1}{2} \log |\mathbf{S}_{i}| - \frac{1}{2} (\mathbf{x}^{T} \mathbf{S}_{i}^{-1} \mathbf{x} - 2\mathbf{x}^{T} \mathbf{S}_{i}^{-1} \mathbf{m}_{i} + \mathbf{m}_{i}^{T} \mathbf{S}_{i}^{-1} \mathbf{m}_{i}) + \log \hat{P}(C_{i})$$

$$= \mathbf{x}^{T} \mathbf{W}_{i} \mathbf{x} + \mathbf{w}_{i}^{T} \mathbf{x} + \mathbf{w}_{i0}$$
where
$$\mathbf{W}_{i} = -\frac{1}{2} \mathbf{S}_{i}^{-1}$$

$$\mathbf{w}_{i} = \mathbf{S}_{i}^{-1} \mathbf{m}_{i}$$

$$w_{i0} = -\frac{1}{2} \mathbf{m}_{i}^{T} \mathbf{S}_{i}^{-1} \mathbf{m}_{i} - \frac{1}{2} \log |\mathbf{S}_{i}| + \log \hat{P}(C_{i})$$

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Common Covariance Matrix S

- Shared common sample covariance **S** $S = \sum_{i} \hat{P}(C_i) S_i$
- Discriminant reduces to

$$g_i(\mathbf{x}) = -\frac{1}{2} (\mathbf{x} - \mathbf{m}_i)^T S^{-1} (\mathbf{x} - \mathbf{m}_i) + \log \hat{P}(C_i)$$

which is a linear discriminant

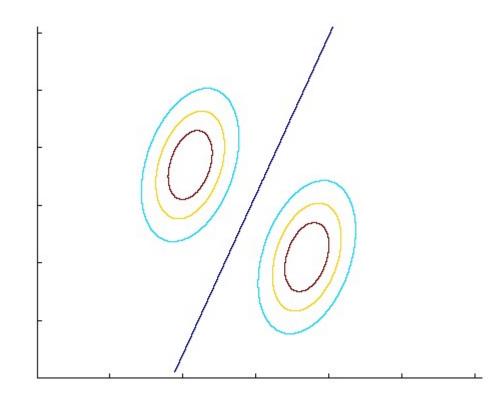
$$\boldsymbol{g}_{i}(\mathbf{x}) = \mathbf{w}_{i}^{T}\mathbf{x} + \boldsymbol{w}_{i0}$$

where

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$$\mathbf{w}_{i} = \mathbf{S}^{-1}\mathbf{m}_{i} \quad \mathbf{w}_{i0} = -\frac{1}{2}\mathbf{m}_{i}^{T}\mathbf{S}^{-1}\mathbf{m}_{i} + \log \hat{P}(\mathbf{C}_{i})$$









Diagonal S

- When x_j j = 1,..d, are independent, ∑ is diagonal
 - $p(\mathbf{x}|C_i) = \prod_j p(x_j | C_i)$ (Naive Bayes' assumption)

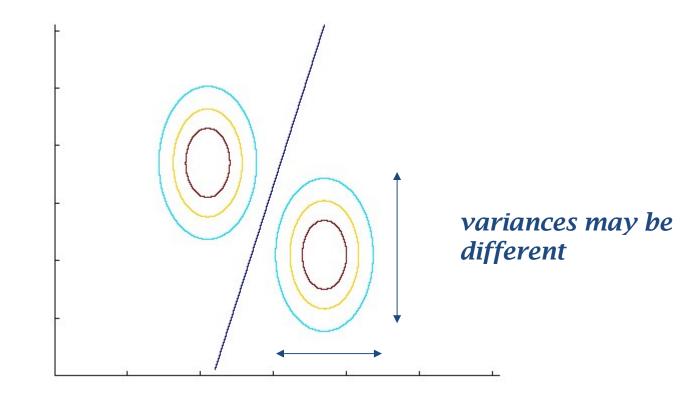
$$g_i(\mathbf{x}) = -\frac{1}{2} \sum_{j=1}^{d} \left(\frac{x_j^t - m_{ij}}{s_j} \right)^2 + \log \hat{P}(C_i)$$

Classify based on weighted Euclidean distance (in s_i units) to the nearest mean





Diagonal S





Diagonal S, equal variances

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• Nearest mean classifier: Classify based on Euclidean distance to the nearest mean

$$g_{i}(\mathbf{x}) = -\frac{\|\mathbf{x} - \mathbf{m}_{i}\|^{2}}{2s^{2}} + \log \hat{P}(C_{i})$$
$$= -\frac{1}{2s^{2}} \sum_{j=1}^{d} \left(x_{j}^{t} - m_{ij}\right)^{2} + \log \hat{P}(C_{i})$$

• Each mean can be considered a prototype or template and this is template matching





Diagonal S, equal variances

