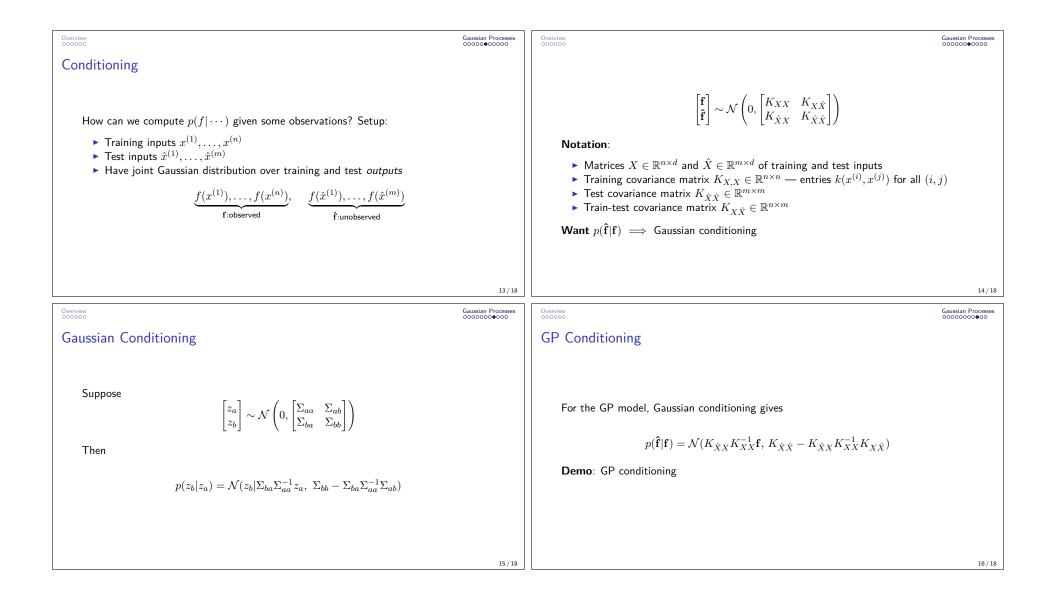
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COMPSCI 688: Probabilistic Graphical Models Lecture 22: Gaussian Processes Dan Sheldon		Overview	
Manning College of Information and Computer Sciences University of Massachusetts Amherst			
Partially based on materials by Benjamin M. Marlin (marlin@cs.umass.edu) and Justin Domke (domke@cs.umass.edu)	1/18		2 / 18
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Gaussian Processes		Distribution over functions — $p(f)$ ("prior")	
GPs = distributions over <i>functions</i>			
Function $f: \mathbb{R}^d o \mathbb{R}$			
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Why? Model an unknown function. Compute "posterior" $p(f \cdots)$ conditioned observed values.	on some	Demo	
		 prior samples posterior samples posterior mean and variance 	
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Applications			
 Bayesian optimization Spatial statistics Machine learning 	7/18	Gaussian Processes	8/18

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How to build a distribution over functions?	Covariance Function	
 Key idea: we only ever query a function at a finite number of points For any fixed x⁽¹⁾,,x⁽ⁿ⁾, model f(x⁽¹⁾),, f(x⁽ⁿ⁾) as jointly Gaussian	Take $\Sigma_{ij} = k(x^{(i)}, x^{(j)})$ where k(x, x') := Cov(f(x), f(x')) is a covariance function or kernel function • Specifies covariance between outputs $f(x)$, $f(x')$ for any inputs x, x' • Example: $k(x, x') = \exp(-\frac{1}{2}(x - x')^2)$ • must lead to positive semidefinite matrices	
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Gaussian Process	Demo	
This construction is a <i>Gaussian process</i> or "GP". Formally, a GP is a distribution over an infinite set of random variables (the values of $f(x)$ for all x), where the joint distribution of any finite subset is multivariate Gaussian. A GP is specified by the covariance function $k(x, x')$. (We assume without loss of generality the mean is zero.) We often write $f(x) \sim GP(0, k(x, x'))$ or $f \sim GP(0, k)$.	Demo: sampling from prior	
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Overview 000000	Gaussian Processes 00000000€0		aussian Processes
Noisy Observations			
We usually don't get to observe output values exactly. In <i>GP regression</i> we observe outputs for each training input: $y^{(i)} = f(x^{(i)}) + \epsilon^{(i)}, \epsilon^{(i)} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2).$	rve noisy	Gaussian conditioning now gives $p(\mathbf{\hat{f}} \mathbf{y}) = \mathcal{N}(K_{\hat{X}X}(K_{XX} + \sigma^2 I)^{-1}\mathbf{y}, K_{\hat{X}\hat{X}} - K_{\hat{X}X}(K_{XX} + \sigma^2 I)^{-1}K_{X\hat{X}})$	
We want $p(\mathbf{\hat{f}} \mathbf{y})$ where \mathbf{y} is a vector of the $y^{(i)}$ values. The joint distribution is	5	Demo: Gaussian conditioning with noisy observations	
$\begin{bmatrix} \mathbf{y} \\ \mathbf{\hat{f}} \end{bmatrix} \sim \mathcal{N} \left(0, \begin{bmatrix} K_{XX} + \sigma^2 I & K_{X\hat{X}} \\ K_{\hat{X}X} & K_{\hat{X}\hat{X}} \end{bmatrix} \right)$			
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