Introduction to Machine Learning

Active Learning

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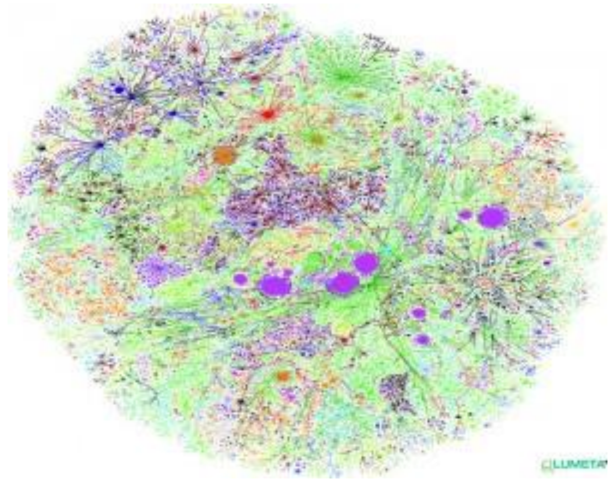
Credits

Some of the slides are taken from Nina Balcan.

Classic Supervised Learning Paradigm is Insufficient Nowadays

Modern applications: massive amounts of raw data.

Only a tiny fraction can be annotated by human experts.


Billions of webpages

Images

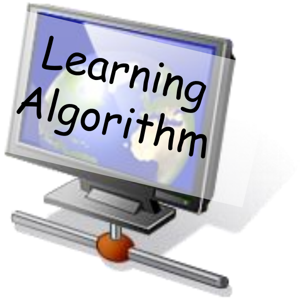
Sensor measurements

Modern ML: New Learning Approaches

Modern applications: massive amounts of raw data.

The Large Synoptic Survey Telescope
15 Terabytes of data … every night

We need techniques that minimize need for expert/human intervention => Active Learning

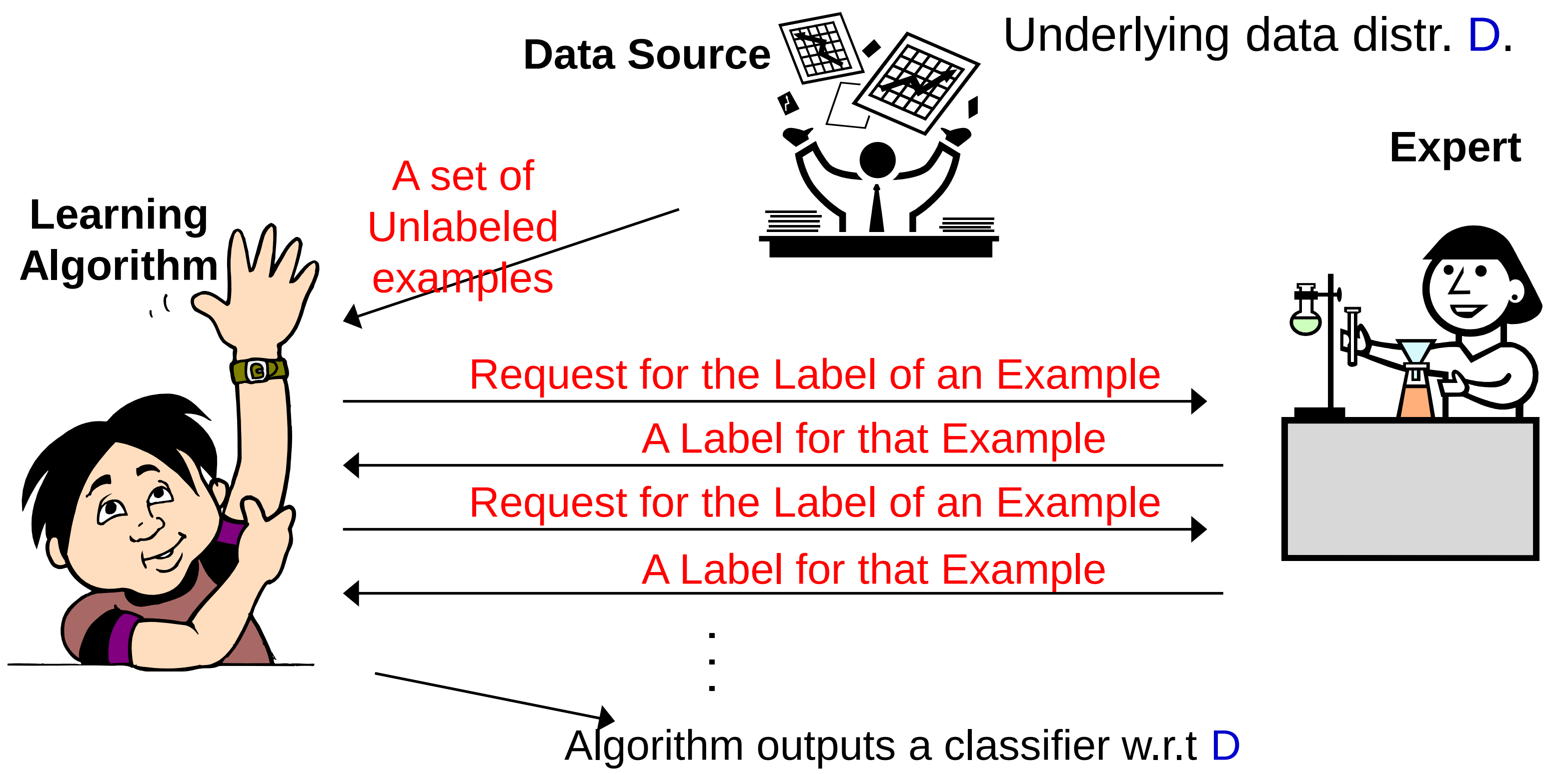


Contents

Additional resources

- **Two faces of active learning**. Sanjoy Dasgupta. 2011.
- **Active Learning**. Bur Settles. 2012.
- **Active Learning**. Balcan-Urner. Encyclopedia of Algorithms. 2015

Batch Active Learning

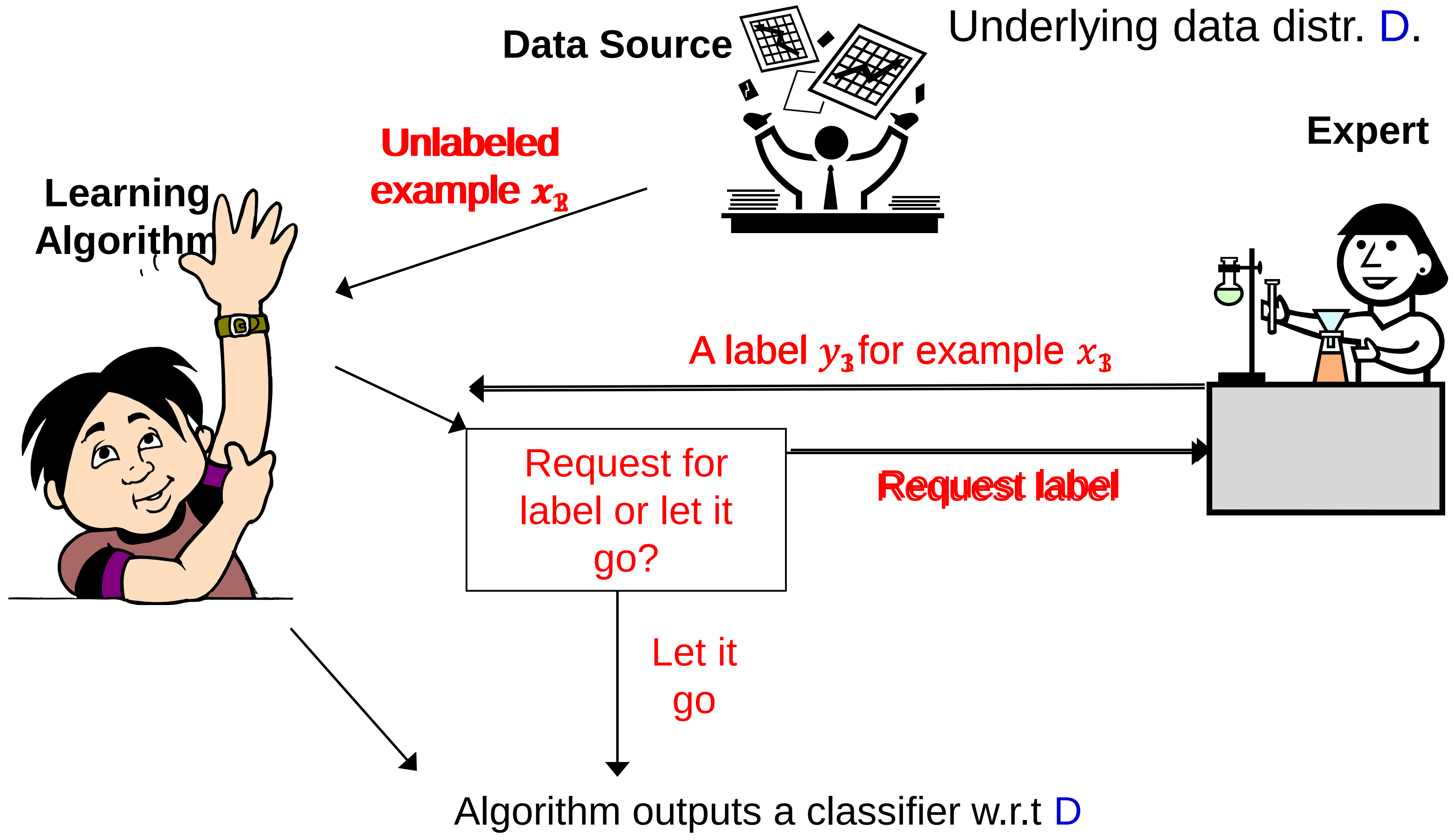

Data Source
Underlying data distr. D.
Expert
Learning Algorithm
A set of Unlabeled examples
Request for the Label of an Example
A Label for that Example
Request for the Label of an Example
A Label for that Example
Algorithm outputs a classifier w.r.t D

- **Learner can choose specific examples to be labeled.**

  [pick informative examples to be labeled].

- **Goal:** use fewer labeled examples

Selective Sampling Active Learning



Data Source
Underlying data distr. D.
Unlabeled example x_3
Learning Algorithm
Expert
A label y_3 for example x_3
Request for label or let it go?
Request label
Let it go
Algorithm outputs a classifier w.r.t D

- Selective sampling AL (Online AL): stream of unlabeled examples, when each arrives make a decision to ask for label or not.

  [pick informative examples to be labeled].

- **Goal**: use fewer labeled examples

What Makes a Good Active Learning Algorithm?

- Guaranteed to output a relatively good classifier for most learning problems.

- Doesn't make too many label requests.

  Hopefully a lot less than passive learning.

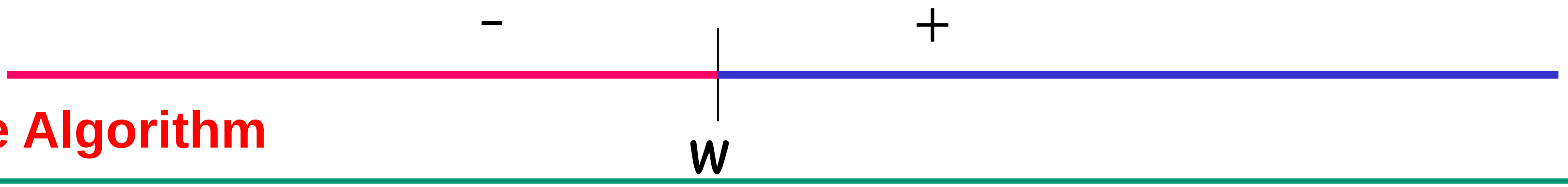
- Need to choose the label requests carefully, to get informative labels.

Can adaptive querying really do better than passive/random sampling?

- YES! (sometimes)
- We often need far fewer labels for active learning than for passive.
- This is predicted by theory and has been observed in practice.

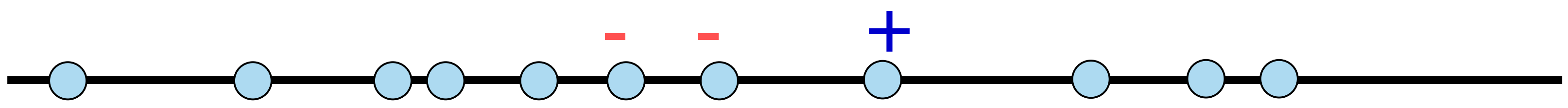
Can adaptive querying help? [CAL92, Dasgupta04]

- Threshold fns on the real line: $h_w(x) = 1(x \geq w)$, $C = \{h_w : w \in R\}$



Active Algorithm

- Get N unlabeled examples
- How can we recover the correct labels with $\ll$ N queries?
- Do binary search (query at half)! Just need O(log N) labels!



- Output a classifier consistent with the N inferred labels.

- $N = O(1/\epsilon)$ we are guaranteed to get a classifier of error $\leq \epsilon$.

Passive supervised: $\Omega(1/\epsilon)$ labels to find an ε-accurate thresh

Active: only $O(\log 1/\epsilon)$ labels. Exponential improvement.

Active SVM

Uncertainty sampling in SVMs common and quite useful in practice. E.g., [Tong & Koller, ICML 2000; Jain, Vijayanarasimhan & Grauman, NIPS 2010; Schohon Cohn, ICML 2000]

Active SVM Algorithm

- At any time during the alg., we have a “current guess” w_t of the separator: the max-margin separator of all labeled points so far.
- Request the label of the example closest to the current separator.

Active SVM

Active SVM seems to be quite useful in practice.

[Tong & Koller, ICML 2000; Jain, Vijayanarasimhan & Grauman, NIPS 2010]

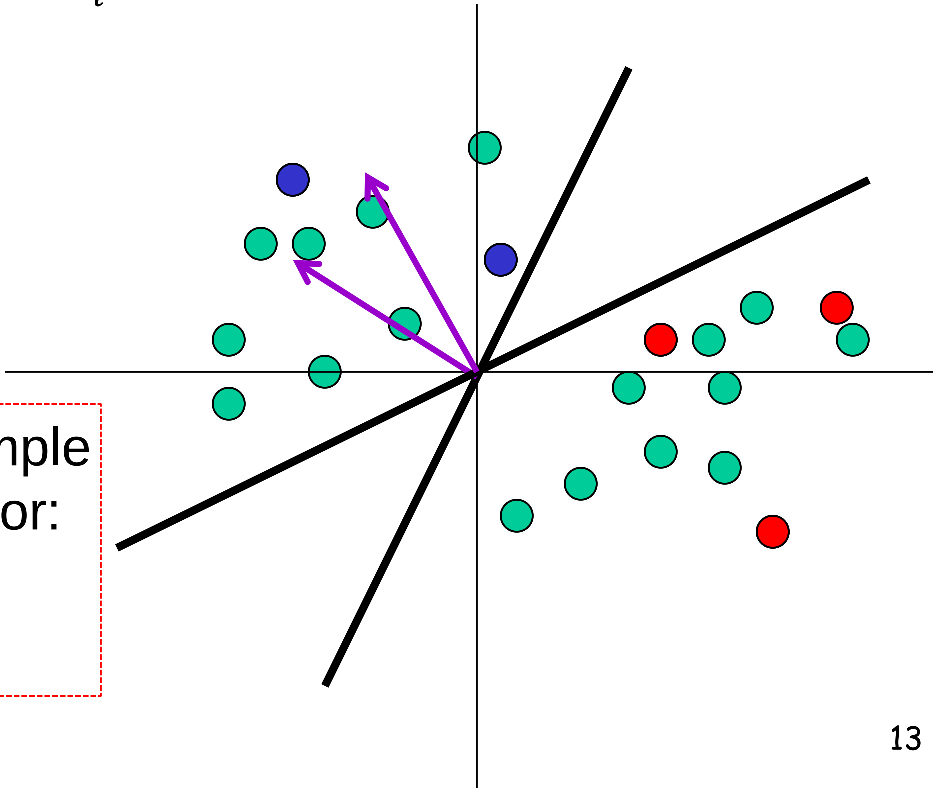
Algorithm (batch version)

Input $S_u=\{x_1, \ldots, x_{m_u}\}$ drawn i.i.d from the underlying source D

Start: query for the labels of a few random x_is.

For $t = 1, \ldots,$

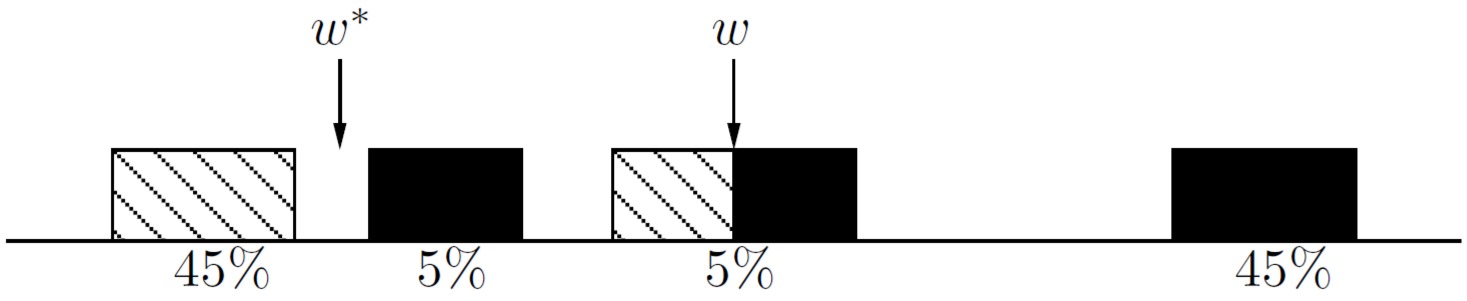
- Find w_t the max-margin separator of all labeled points so far.
- Request the label of the example closest to the current separator: minimizing $|x_i \cdot w_t|$.
  (highest uncertainty)



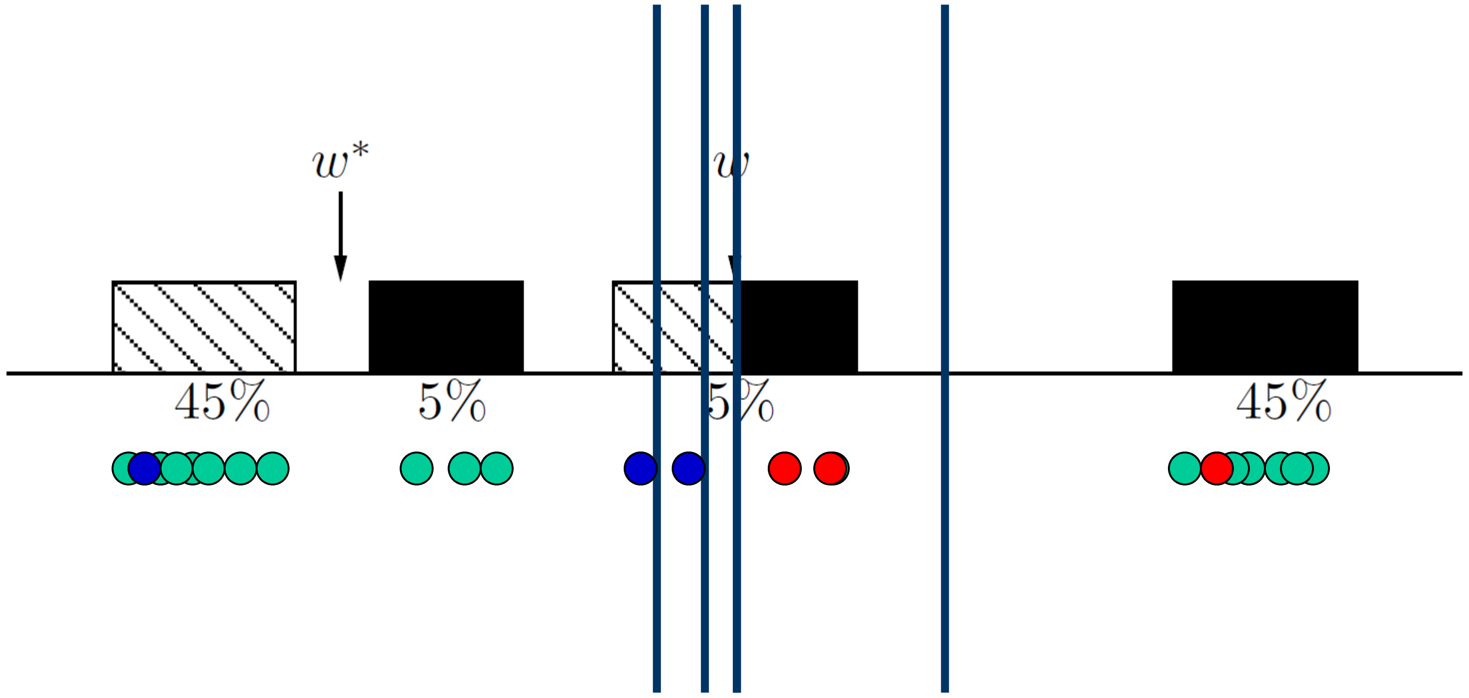
DANGER!!!

- Uncertainty sampling works sometimes….
- **However, we need to be very very very careful!!!**
  - Myopic, greedy techniques can suffer from sampling bias. (The active learning algorithm samples from a different (x,y) distribution than the true data)
  - A bias created because of the querying strategy; as time goes on the sample is less and less representative of the true data source.

[Dasgupta10]



DANGER!!!



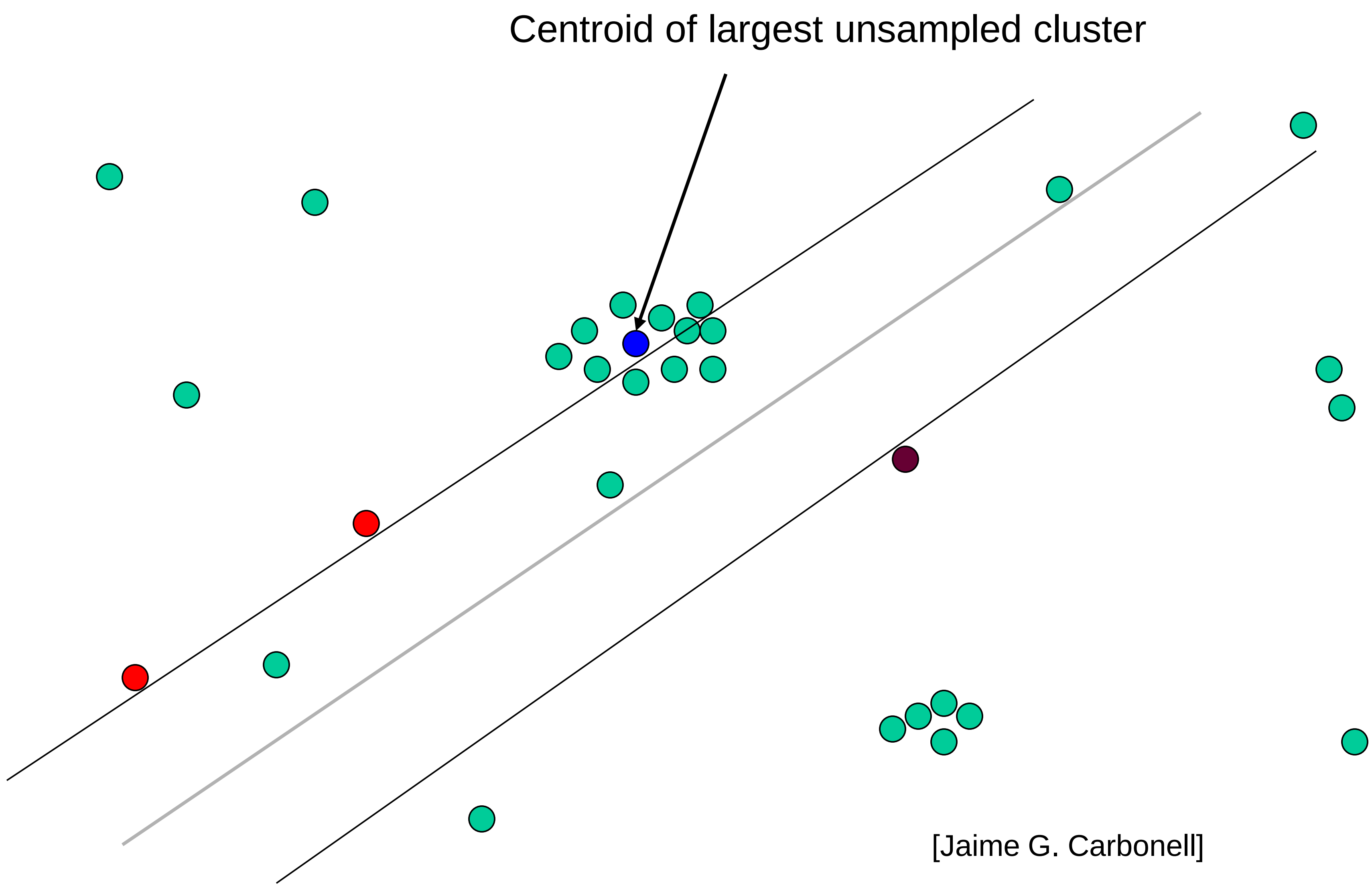
- Observed in practice too!!!!

- **Main tension**: want to choose informative points, but also want to guarantee that the classifier we output does well on true random examples from the underlying distribution.

Other Interesting Active Learning Techniques used in Practice

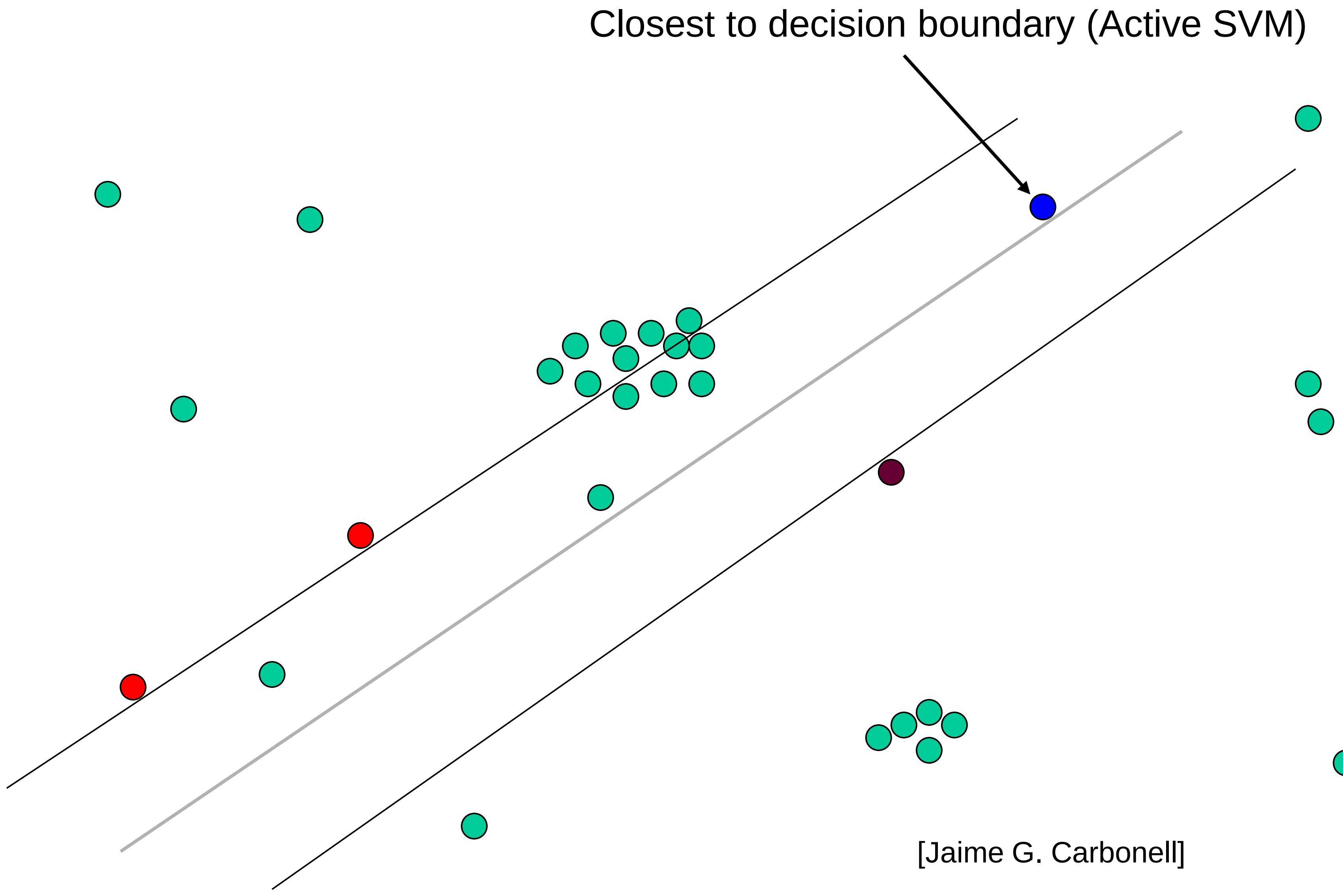
Interesting open question to analyze under what conditions they are successful.

Density-Based Sampling



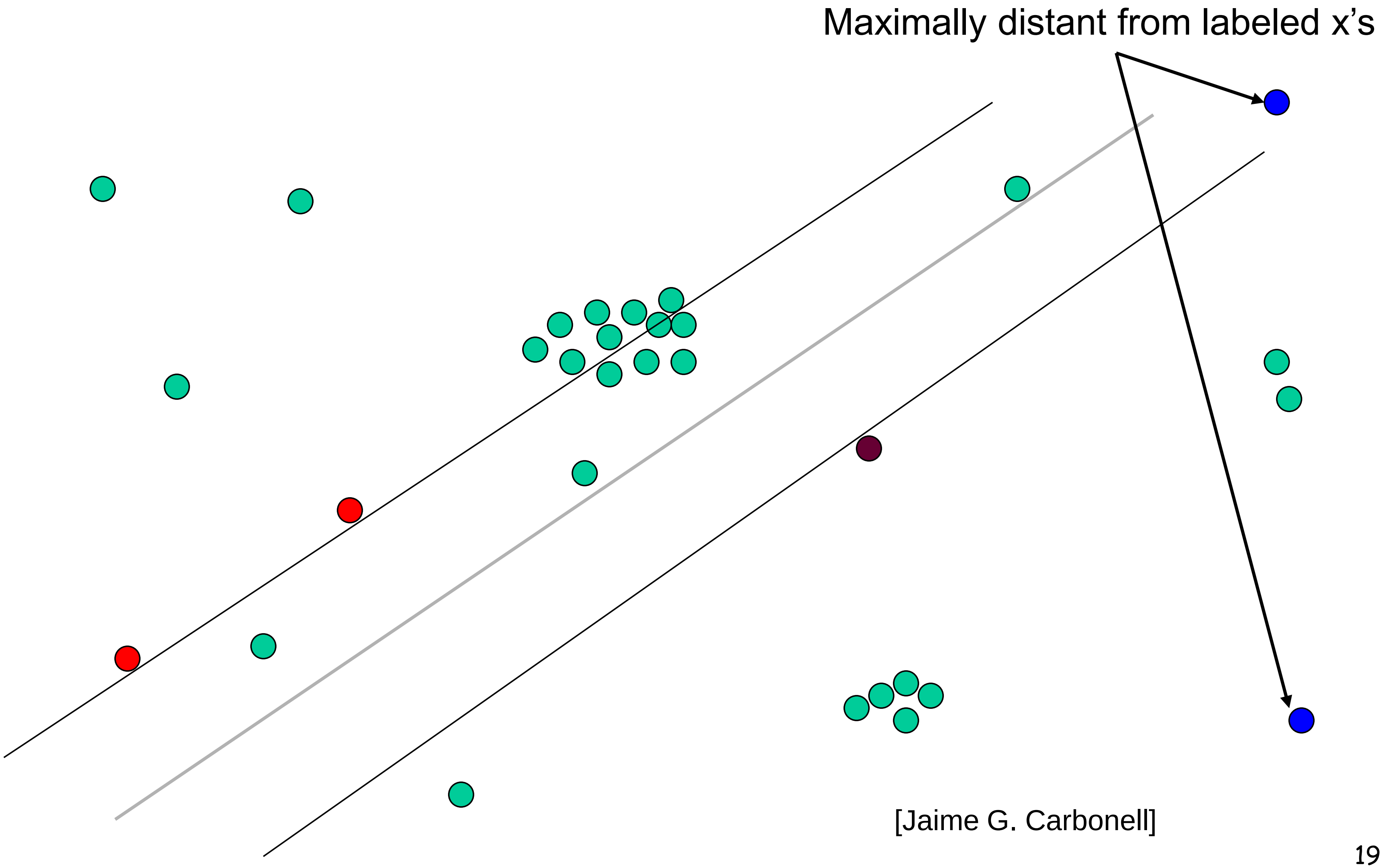
[Jaime G. Carbonell]

Uncertainty Sampling



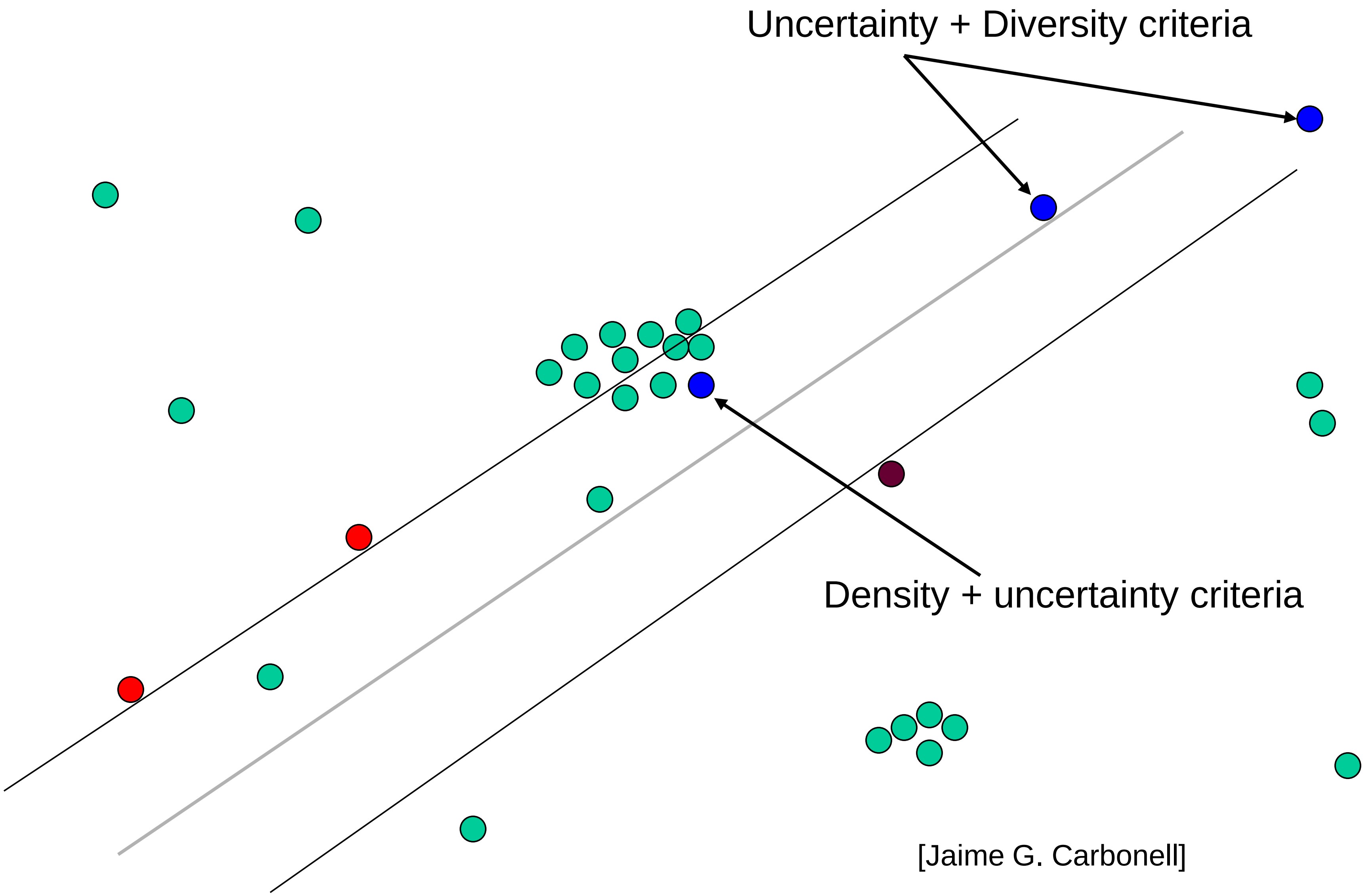
[Jaime G. Carbonell]

Maximal Diversity Sampling



[Jaime G. Carbonell]

Ensemble-Based Possibilities


Uncertainty + Diversity criteria
Density + uncertainty criteria

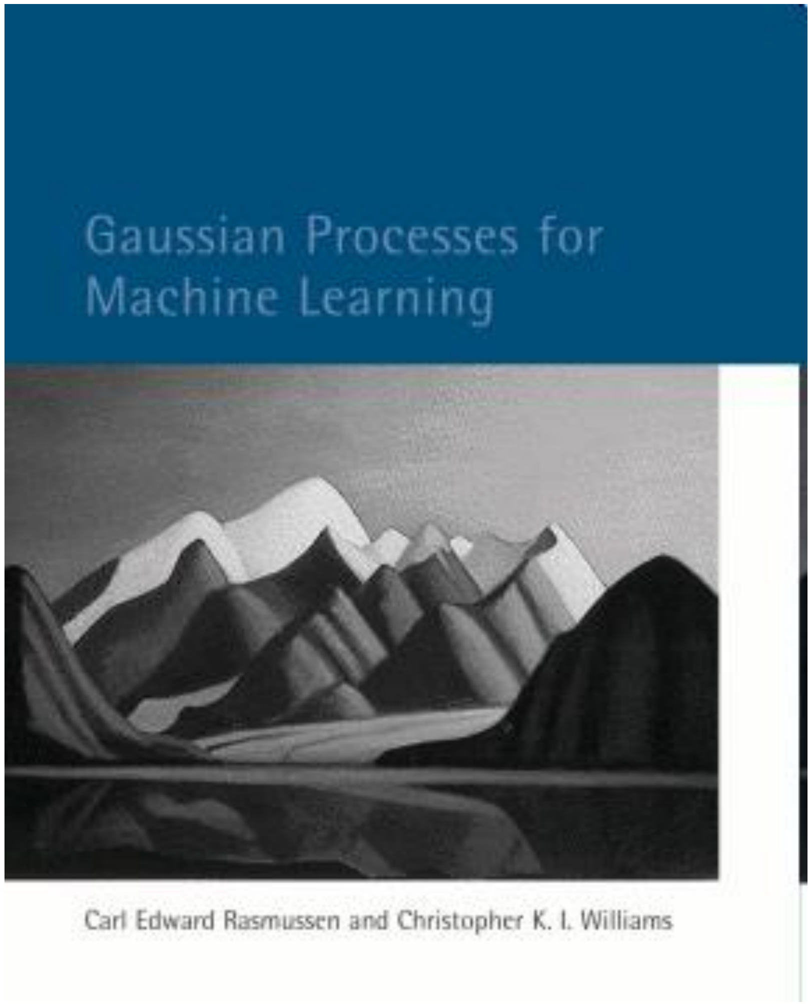
[Jaime G. Carbonell]

What You Should Know so far

- **Active learning could be really helpful**, could provide exponential improvements in label complexity (both theoretically and practically)!
- **Need to be very careful due to sampling bias.**
- **Common heuristics**
  - (e.g., those based on uncertainty sampling).

Gaussian Processes for Regression

Additional resources


Gaussian Processes for Machine Learning
Carl Edward Rasmussen and Christopher K. I. Williams

http://www.gaussianprocess.org/

Some of these slides are taken from D. Lizotte, R. Parr, C. Guesterin

Additional resources

- **Nonmyopic Active Learning of Gaussian Processes: An Exploration–Exploitation Approach**. A.Krause and C. Guestrin, ICML 2007
- **Near-Optimal Sensor Placements in Gaussian Processes: Theory, Efficient Algorithms and Empirical Studies.** A.Krause, A. Singh, and C. Guestrin, Journal of Machine Learning Research 9 (2008)
- **Bayesian Active Learning for Posterior Estimation**, Kandasamy, K., Schneider, J., and Poczos, B, International Joint Conference on Artificial Intelligence (IJCAI), 2015

Why GPs for Regression?

Regression methods:

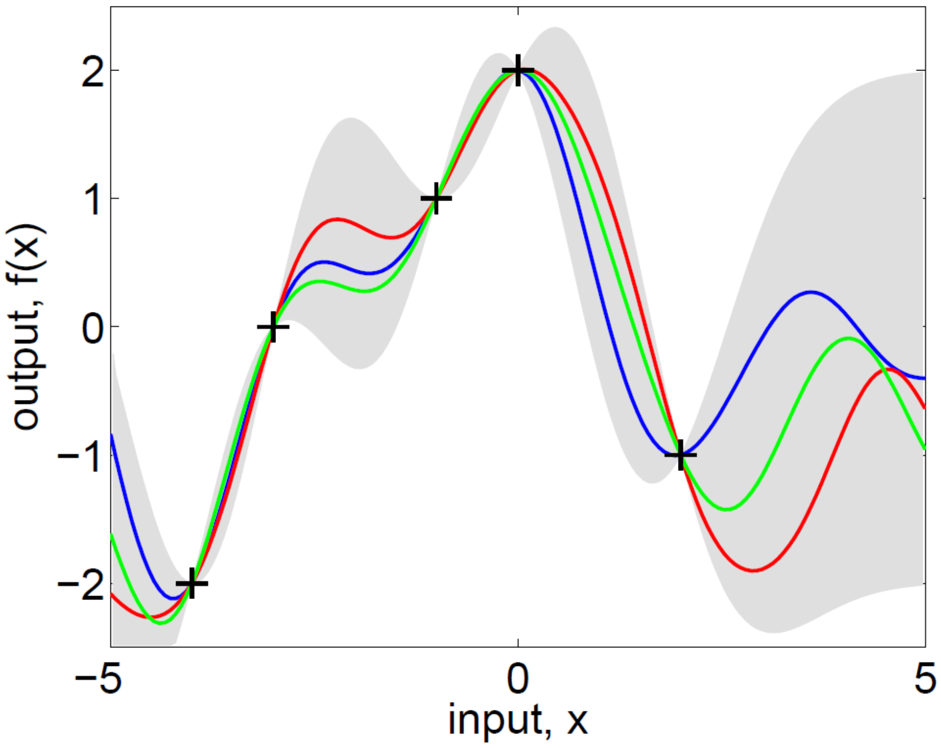
Linear regression, multilayer precpetron, ridge regression, support vector regression, kNN regression, etc…

Motivation:

All the above regression method give point estimates. We would like a method that could also provide confidence during the estimation.

Application in Active Learning:

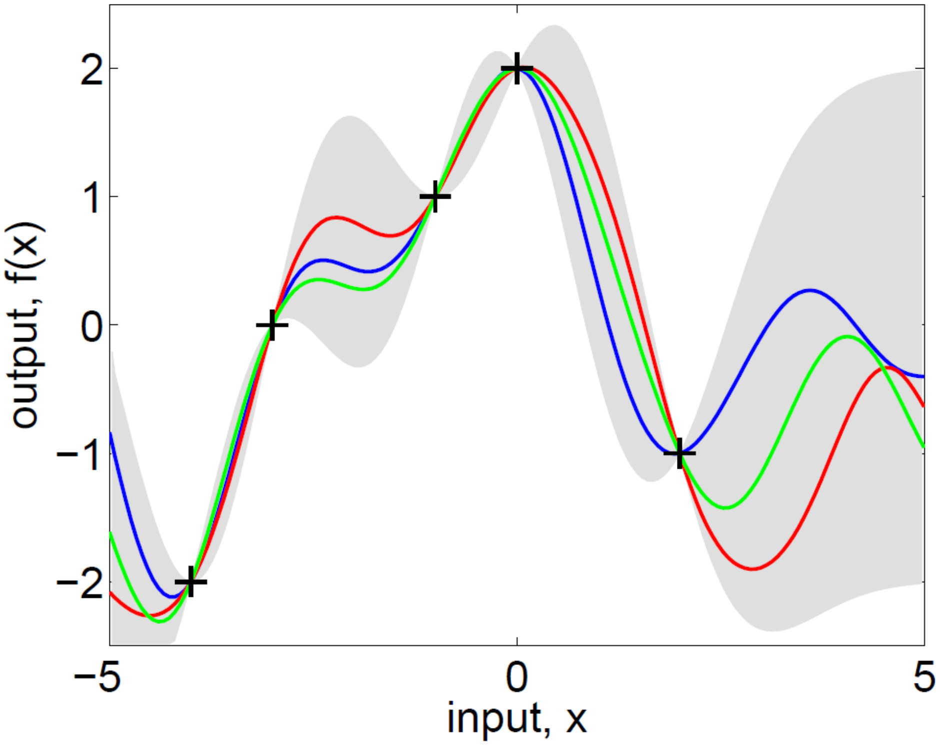
This method can be used for active learning: query the next point and its label where the uncertainty is the highest



Why GPs for Regression?

GPs can answer the following questions:

- Here’s where the function will **most likely be.** (expected function)
- Here are some **examples** of what it might look like. (sampling from the posterior distribution [blue, red, green functions)
- Here is a prediction of what you’ll see if you evaluate your function at x’, **with confidence**

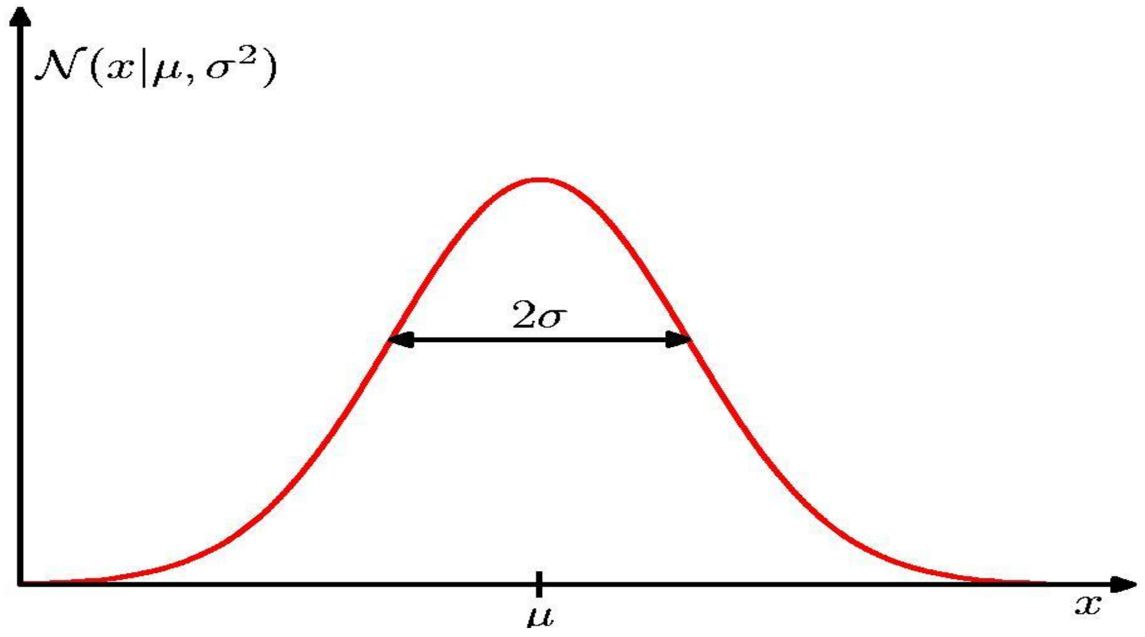


Properties of Multivariate Gaussian Distributions

1D Gaussian Distribution

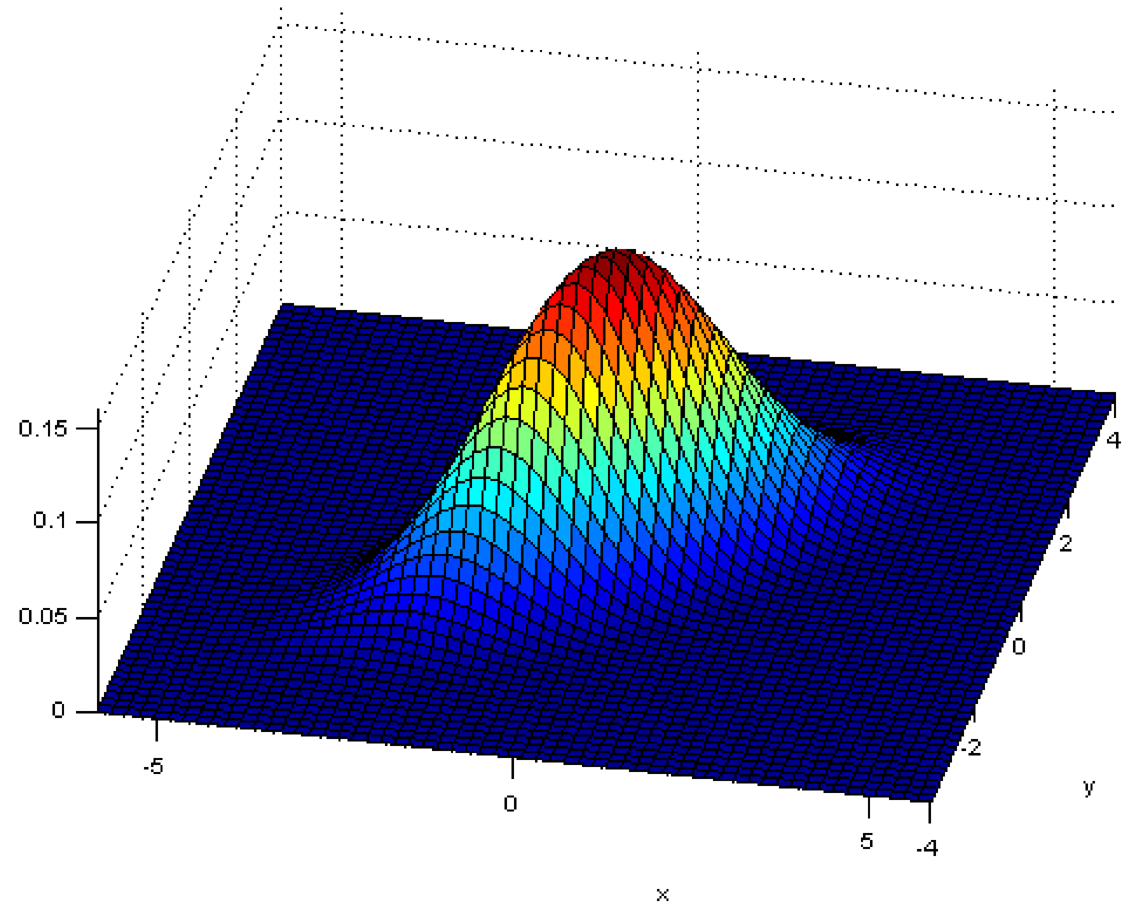
Parameters

- Mean, μ
- Variance, σ^2



$$P(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}$$

Multivariate Gaussian



$$p(\mathbf{x} \mid \boldsymbol{\mu}, \Sigma) = \frac{1}{\sqrt{|2\pi\Sigma|}} \exp\left\{\frac{-1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{x}-\boldsymbol{\mu})\right\}$$

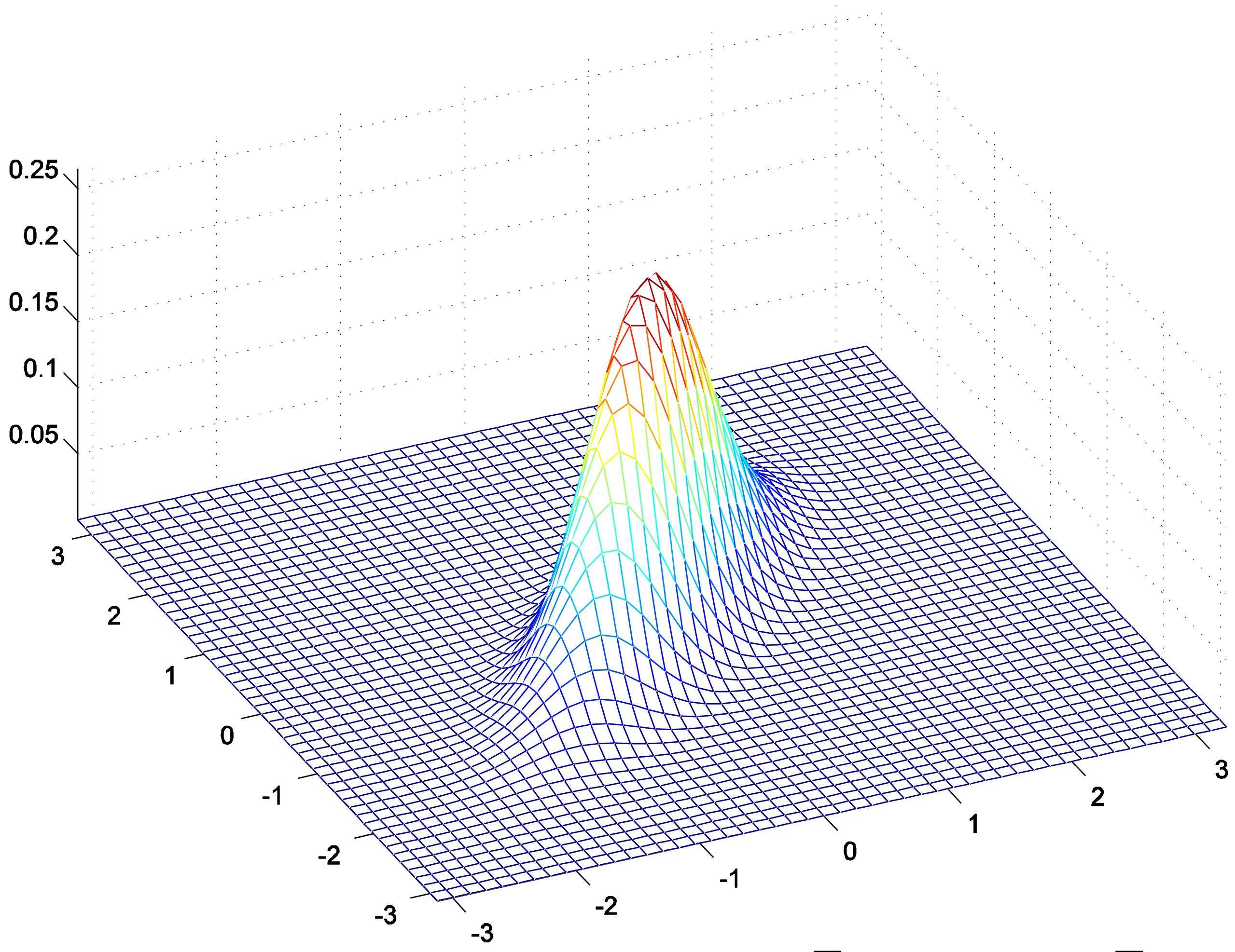
Multivariate Gaussian

- A 2-dimensional Gaussian is defined by
  - a mean vector $\mu = [\ \mu_1, \mu_2\ ]$
  - a covariance matrix: $\Sigma = \begin{bmatrix} \sigma_{1,1}^2 & \sigma_{2,1}^2 \\ \sigma_{1,2}^2 & \sigma_{2,2}^2 \end{bmatrix}$

  where $\sigma_{i,j}^2 = E[\ (x_i - \mu_i)\ (x_j - \mu_j)\ ]$
  is (co)variance

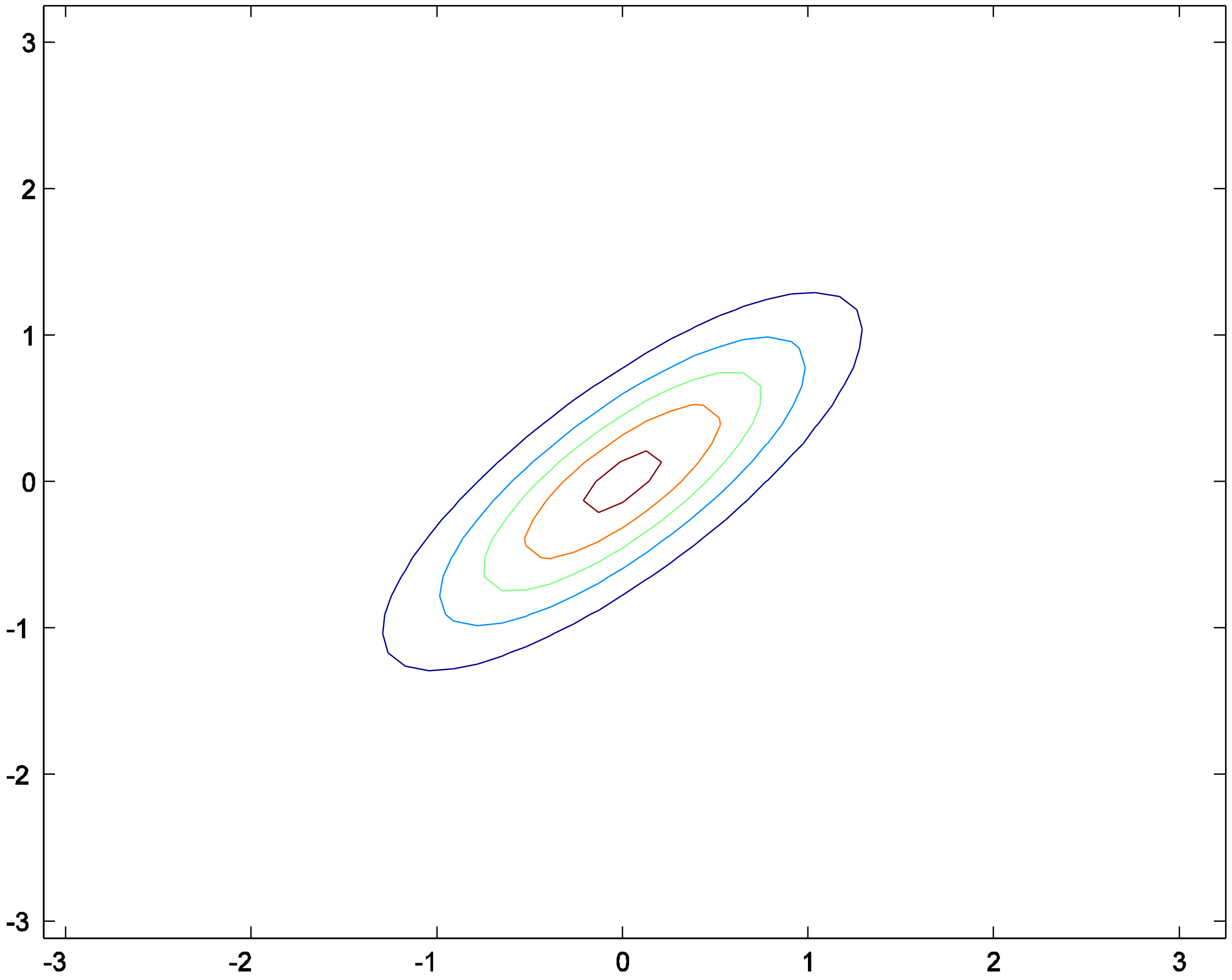
- Note: Σ is symmetric,
  "positive semi-definite": $\forall x$: $x^T \Sigma x \geq 0$

Multivariate Gaussian examples



$$\mu = (0,0) \qquad \Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$$

Multivariate Gaussian examples



$\mu = (0,0)$ $\Sigma = \begin{bmatrix} 1 & 0.8 \\ 0.8 & 1 \end{bmatrix}$

Useful Properties of Gaussians

- Marginal distributions of Gaussians are Gaussian

- Given:

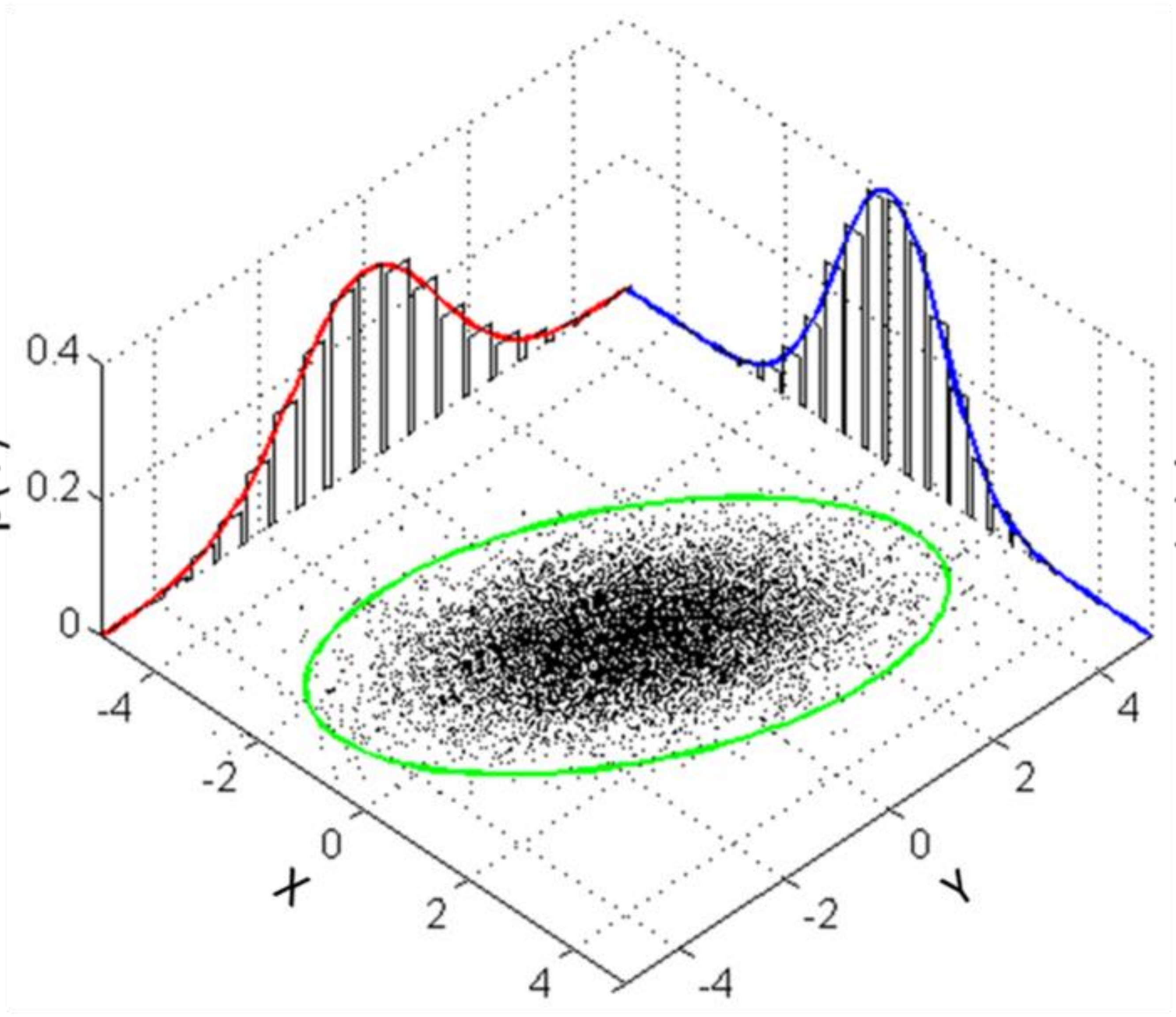
$$x = (x_a, x_b), \mu = (\mu_a, \mu_b)$$

$$\Sigma = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix}$$

The marginal distribution is:

$$p(X_a) = \mathcal{N}(x_a \mid \mu_a, \Sigma_{aa})$$

Marginal distributions of Gaussians are Gaussian



Block Matrix Inversion

Theorem

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} (A - BD^{-1}C)^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix}$$

$$= \begin{bmatrix} S_D^{-1} & -A^{-1}BS_A^{-1} \\ -D^{-1}CS_D^{-1} & S_A^{-1} \end{bmatrix}$$

Definition: Schur complements

Schur complements of A: $S_A = D - CA^{-1}B$

Schur complements of D: $S_D = A - BD^{-1}C$

Useful Properties of Gaussians

- Conditional distributions of Gaussians are Gaussian
- Notation: $\Sigma = \begin{pmatrix} \Sigma_{aa} & \Sigma_{ab} \\ \Sigma_{ba} & \Sigma_{bb} \end{pmatrix}$ $\Lambda = \Sigma^{-1} = \begin{pmatrix} \Lambda_{aa} & \Lambda_{ab} \\ \Lambda_{ba} & \Lambda_{bb} \end{pmatrix}$
- **Conditional Distribution**:

$$p(X_a|X_b) = \mathcal{N}(x_a \mid \mu_{a|b}, \Lambda_{aa}^{-1})$$

$$\mu_{a|b} = \mu_a - \Lambda_{aa}^{-1}\Lambda_{ab}(\mathbf{x}_b - \mu_b) = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(\mathbf{x}_b - \mu_b)$$

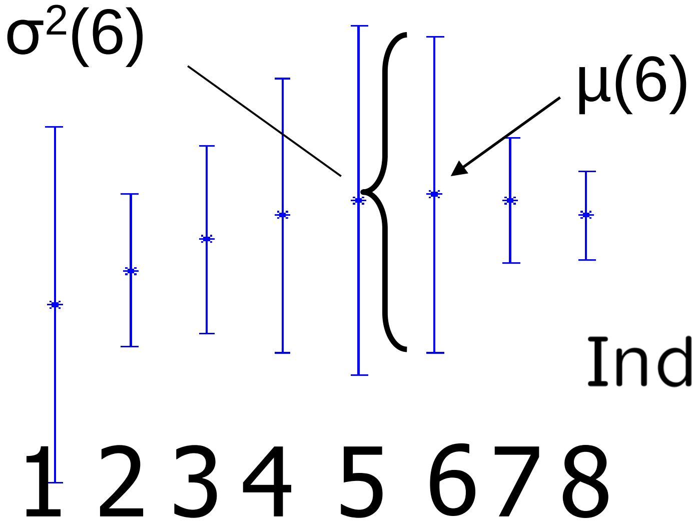
$$\Lambda_{aa}^{-1} = \Sigma_{aa} - \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba}$$

Schur complement of Σ_{bb} in Σ

Higher Dimensions

- **Visualizing > 3 dimensional Gaussian random variables is… difficult**
- Means and variances of marginal variable s are practical, but then we don't see correlations between those variables
- Marginals are Gaussian, e.g., $f(6) \sim N(\mu(6), \sigma^2(6))$

Visualizing an 8-dimensional Gaussian variable f:



mean: $\mu(1), \mu(2), \ldots, \mu(8)$.
covariance: $k(i,j),\ i,j \in \{1,\ldots,8\}$
variance: $k(i,i) = \sigma^2(i)$

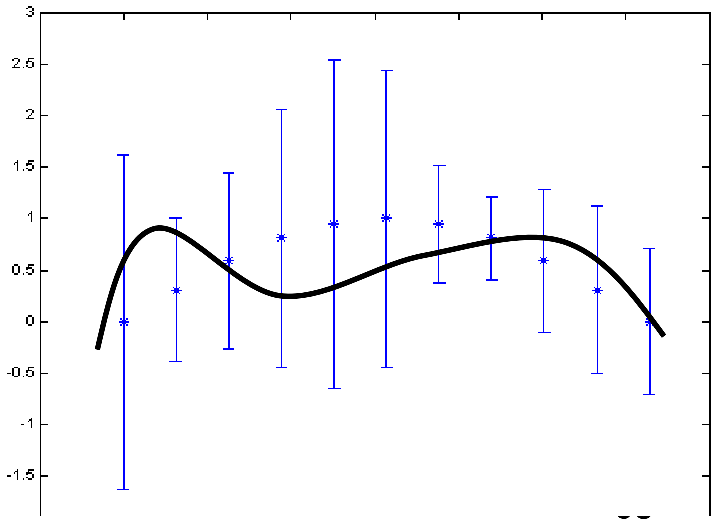
Indexed with $\{1,2,3,4,5,6,7,8\}$.

Yet Higher Dimensions

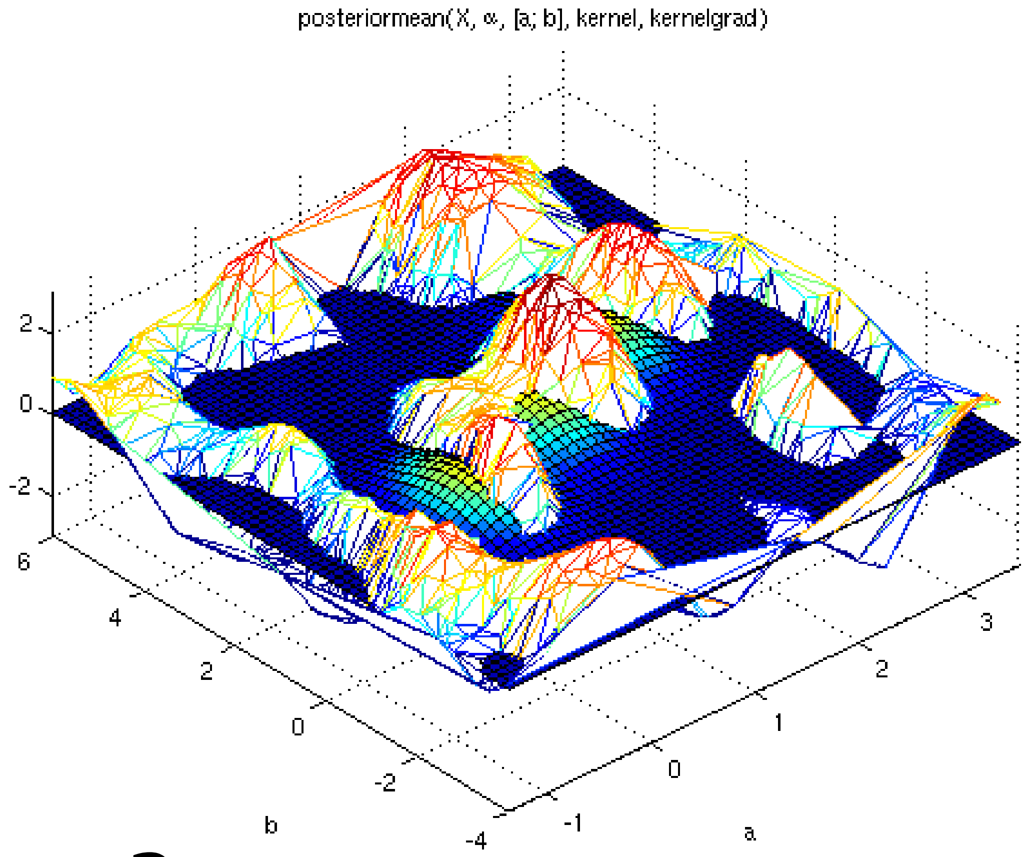
Why stop there?

- We indexed before with $\{1, 2, 3, 4, 5, 6, 7, 8\}$.
- Why not indexing with $\mathbb{Z}$, or $\mathbb{R}$?
- Need functions $\mu(x), k(x, z)$, $\forall x, z \in \mathbb{R}$
- x and z are indexes over the random variables
- f is now an uncountably infinite dimensional vector
- Depending on $\mu(\cdot)$ and $k(\cdot, \cdot)$, f can be continuous

or even infintely differentiable too!



Getting Ridiculous



Why stop there?

- We indexed before with $\mathbb{R}$, why not with $\mathbb{R}^D$?
- Need functions $\mu(\mathbf{x}), k(\mathbf{x}, \mathbf{z})$, $\forall \mathbf{x}, \mathbf{z} \in \mathbb{R}^D$

Gaussian Process

Definition of GP:

- ❑ Probability distribution *indexed by* an arbitrary set (integer, real, finite dimensional vector, etc)
- ❑ Each element (indexed by x) is a Gaussian distribution over the reals with mean μ(x)
- ❑ These distributions are dependent/correlated as defined by k(x,z)
- ❑ Any finite subset of indices defines a multivariate Gaussian distribution

Gaussian Process

- ❑ Distribution over *functions….*

  If our regression model is a GP, then it won't be a point estimate anymore! It can provide regression estimates with confidence

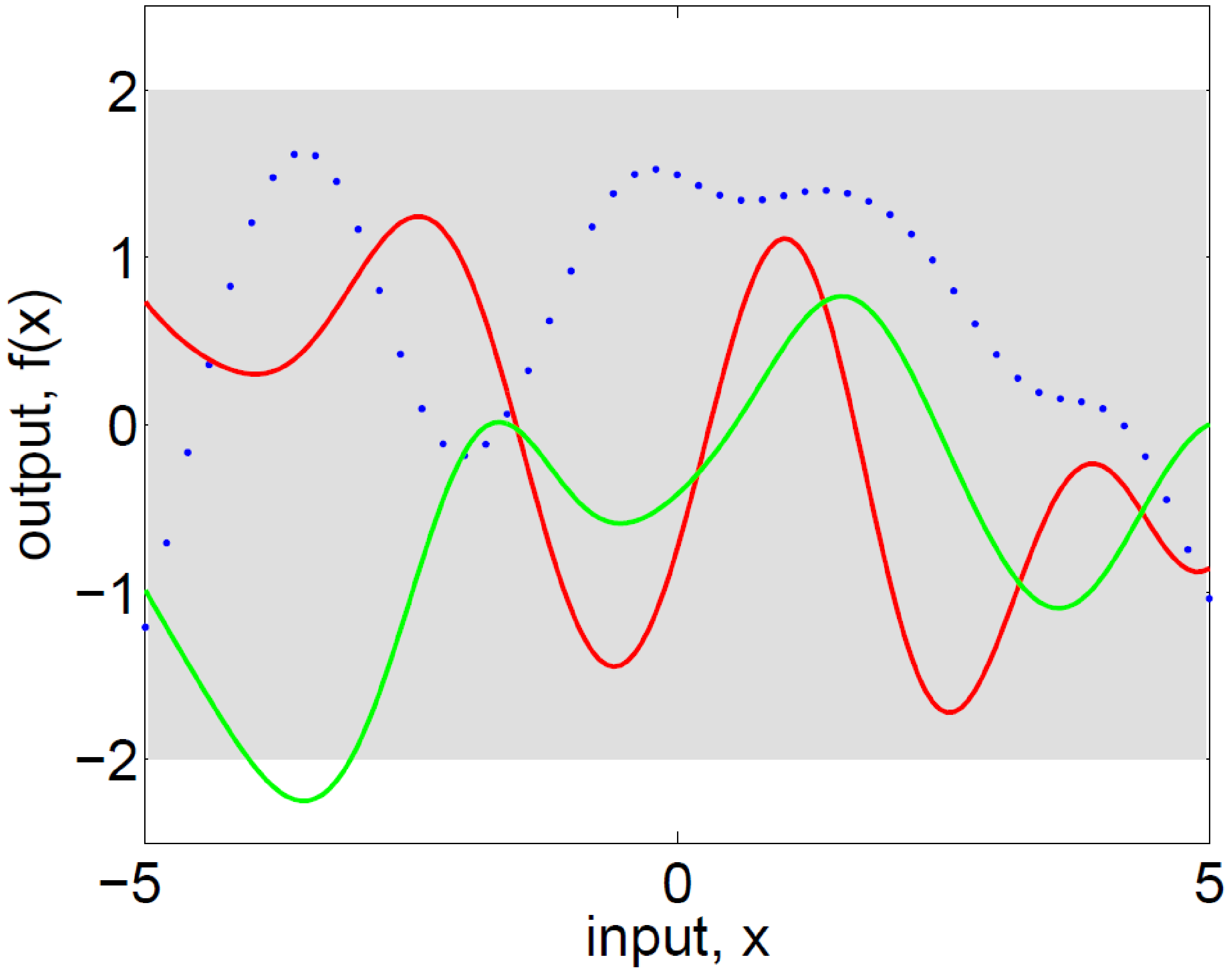
- ❑ Domain (index set) of the functions can be pretty much whatever
  - Reals
  - Real vectors
  - Graphs
  - Strings
  - Sets
  - …

Bayesian Updates for GPs

- How can we do regression and learn the GP from data?

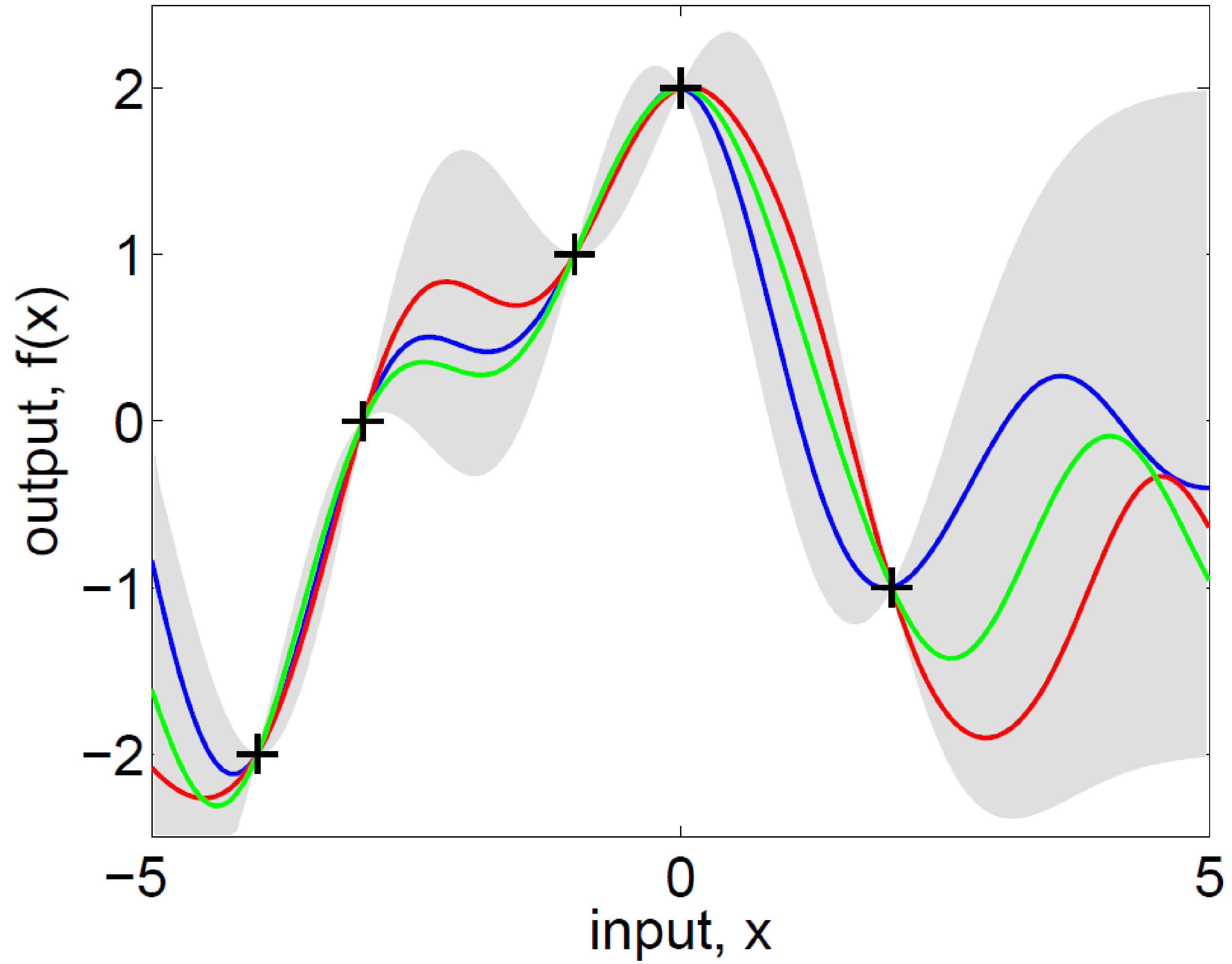
- We will be Bayesians today:
  - Start with GP prior
  - Get some data
  - Compute a posterior

Samples from the prior distribution



Picture is taken from Rasmussen and Williams

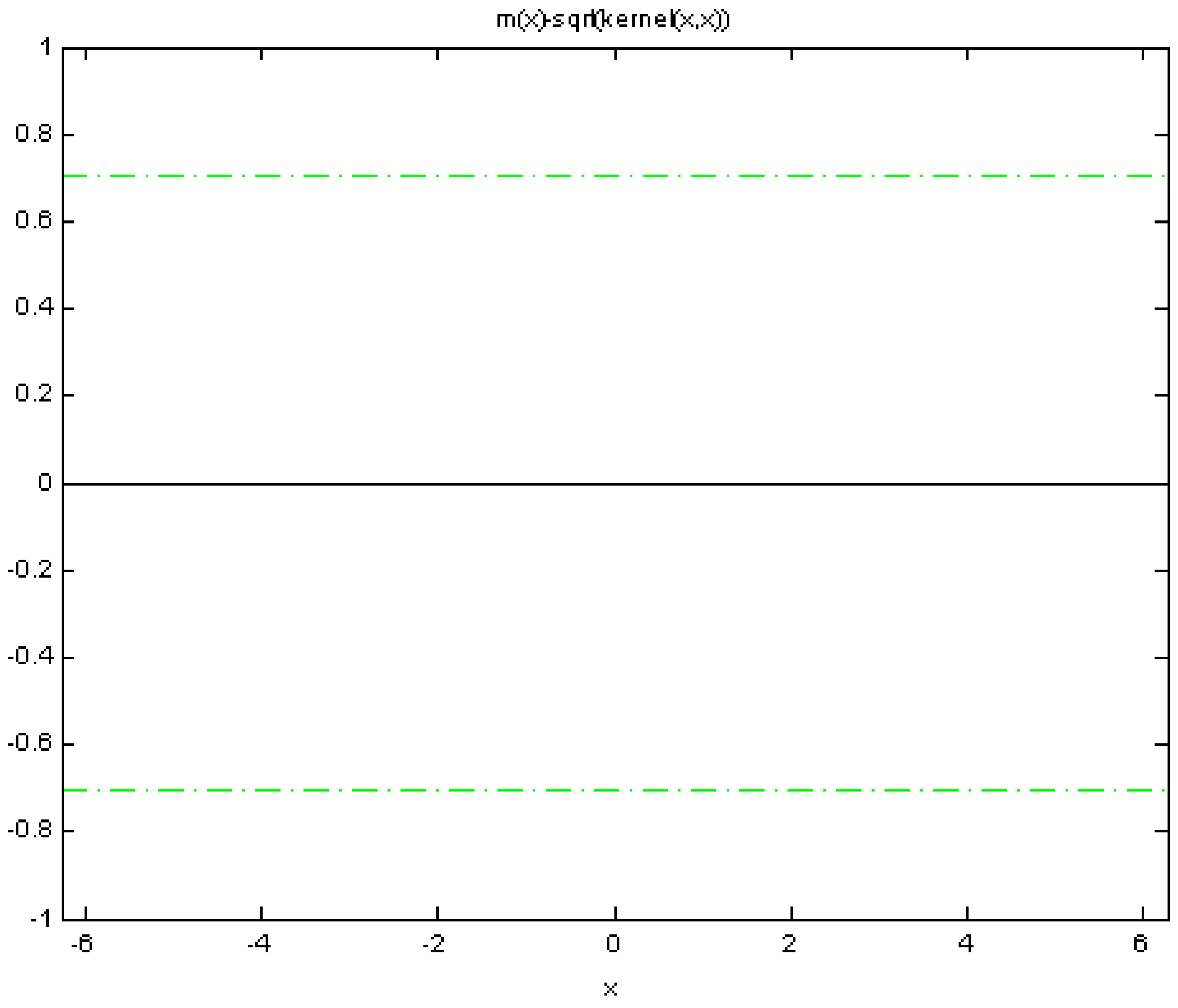
Samples from the posterior distribution



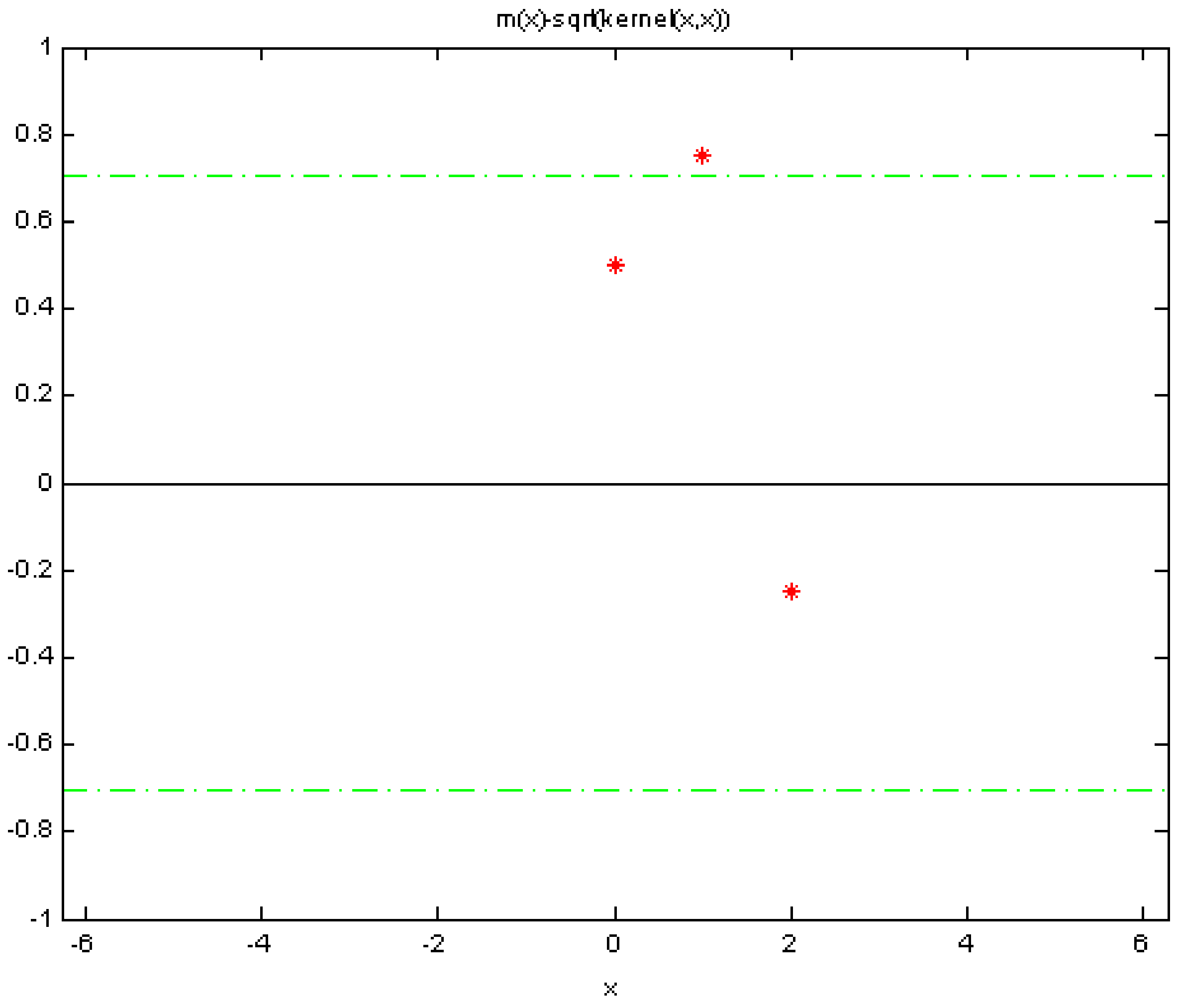
Picture is taken from Rasmussen and Williams

Prior

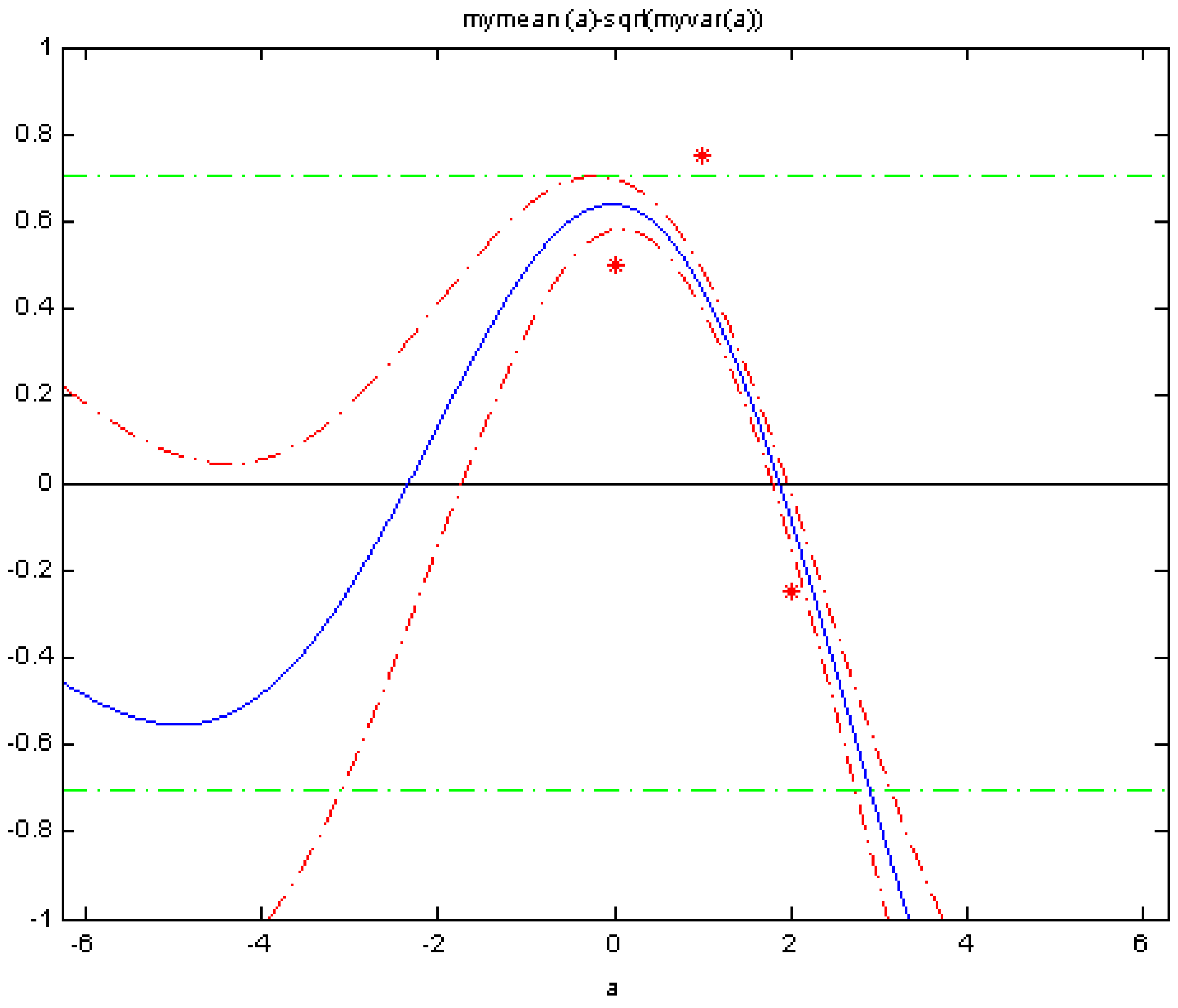
Zero mean Gaussians with covariance k(x,z)



Data



Posterior



Ridge Regression

Training set: $\mathcal{D} = \{(\mathbf{x}_i, y_i) | i = 1, \ldots, n\}, \; \mathbf{x}_i \in \mathbb{R}^D, \; y_i \in \mathbb{R}$

Linear regression: $f(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle$

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w} \in \mathbb{R}^D} \sum_{i=1}^{n} (y_i - \langle \mathbf{x}_i, \mathbf{w} \rangle)^2$$

Ridge regression:

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w} \in \mathbb{R}^D} \sum_{i=1}^{n} (y_i - \langle \mathbf{x}_i, \mathbf{w} \rangle)^2 + \lambda \|\mathbf{w}\|^2$$

The Gaussian Process is a Bayesian Generalization of the kernelized ridge regression

Weight Space View

GP = Bayesian ridge regression in feature space + Kernel trick to carry out computations

Training set: $\mathcal{D} = \{(\mathbf{x}_i, y_i) | i = 1, \dots, n\}$, $\mathbf{x}_i \in \mathbb{R}^D$, $y_i \in \mathbb{R}$

$$\left.\begin{array}{l} X = \begin{bmatrix} \mathbf{x}_1 \Big| & \dots & \Big| \mathbf{x}_n \end{bmatrix} \in \mathbb{R}^{D \times n}, \text{ design matrix} \\ \\ \mathbf{y} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \in \mathbb{R}^n \end{array}\right\} \textbf{The training data}$$

Bayesian Analysis of Linear Regression with Gaussian noise

Linear regression: $f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} \in \mathbb{R},\ \mathbf{x}, \mathbf{w} \in \mathbb{R}^D$

Linear regression with noise: $y = f(\mathbf{x}) + \epsilon = \mathbf{x}^T\mathbf{w} + \epsilon \in \mathbb{R}$

$\epsilon \sim \mathcal{N}(0, \sigma^2) \in \mathbb{R}$

Let us calculate the likelihood:

$$P(\mathbf{y}|X, \mathbf{w}) \;=\; \prod_{i=1}^{n} P(y_i|\mathbf{x}_i^T\mathbf{w})$$

and then put $\mathbf{w} \sim \mathcal{N}_{\mathbf{w}}(0, \Sigma_p)$ prior over parameters $\mathbf{w}$.

Bayesian Analysis of Linear Regression with Gaussian noise

The likelihood:

$$\begin{aligned}
P(\mathbf{y}|X,\mathbf{w}) &= \prod_{i=1}^{n} P(y_i|\mathbf{x}_i^T\mathbf{w}) \\
&= \prod_{i=1}^{n} \mathcal{N}_{y_i}(\mathbf{x}_i^T\mathbf{w},\sigma^2) \\
&= \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[\frac{-(y_i-\mathbf{x}_i^T\mathbf{w})^2}{2\sigma^2}\right] \\
&= \frac{1}{(2\pi\sigma^2)^{n/2}} \exp\left[\frac{-1}{2\sigma^2}\|\mathbf{y}-X^T\mathbf{w}\|^2\right] \\
&= \mathcal{N}_{\mathbf{y}}(X^T\mathbf{w},\sigma^2\mathbf{I}_n)
\end{aligned}$$

Bayesian Analysis of Linear Regression with Gaussian noise

The prior:

$$\mathbf{w} \sim \mathcal{N}_{\mathbf{w}}(0, \Sigma_p)$$

Now, we can calculate the posterior:

$$\begin{aligned}
P(\mathbf{w}|X, \mathbf{y}) &= \frac{P(\mathbf{y}|X, \mathbf{w})P(\mathbf{w})}{P(\mathbf{y}|X)} \\
&= \frac{P(\mathbf{y}|X, \mathbf{w})P(\mathbf{w})}{\int P(\mathbf{y}|X, \mathbf{w})d\mathbf{w}} \\
&= \frac{\mathcal{N}_{\mathbf{y}}(X^T\mathbf{w}, \sigma^2\mathbf{I}_n)\mathcal{N}_{\mathbf{w}}(0, \Sigma_p)}{\int \mathcal{N}_{\mathbf{y}}(X^T\mathbf{w}, \sigma^2\mathbf{I}_n)\mathcal{N}_{\mathbf{w}}(0, \Sigma_p)\, d\mathbf{w}} \\
&\sim \mathcal{N}_{\mathbf{y}}(X^T\mathbf{w}, \sigma^2\mathbf{I}_n)\mathcal{N}_{\mathbf{w}}(0, \Sigma_p)
\end{aligned}$$

Bayesian Analysis of Linear Regression with Gaussian noise

Ridge Regression

$$
\begin{aligned}
P(\mathbf{w}|X,\mathbf{y}) &\sim \mathcal{N}_{\mathbf{y}}(X^T\mathbf{w}, \sigma^2\mathbf{I}_n)\mathcal{N}_{\mathbf{w}}(0,\Sigma_p) \\
&\sim \exp\{\frac{-1}{2\sigma^2}(\mathbf{y}-X^T\mathbf{w})^T(\mathbf{y}-X^T\mathbf{w})\}\exp\{\frac{-1}{2}\mathbf{w}^T\Sigma_p^{-1}\mathbf{w}\} \\
&\sim \exp\{\frac{-1}{2}(\mathbf{w}-\bar{\mathbf{w}})^T\underbrace{\left(\frac{1}{\sigma^2}XX^T+\Sigma_p^{-1}\right)}_{A}(\mathbf{w}-\bar{\mathbf{w}})\}
\end{aligned}
$$

$$\boxed{\sim \mathcal{N}_{\mathbf{w}}(\bar{\mathbf{w}}, A^{-1})}$$

After "completing the square"

where $\boxed{\bar{\mathbf{w}} \doteq \sigma^{-2}\underbrace{\left(\sigma^{-2}XX^T+\Sigma_p^{-1}\right)^{-1}}_{A^{-1}\in\mathbb{R}^{D\times D}}X\mathbf{y}\in\mathbb{R}^D}$

MAP estimation

$$\boxed{A \doteq \left(\sigma^{-2}XX^T+\Sigma_p^{-1}\right)\in\mathbb{R}^{D\times D}}$$

Bayesian Analysis of Linear Regression with Gaussian noise

We want to use $P(\mathbf{w}|X,\mathbf{y}) = N_{\mathbf{w}}(\bar{\mathbf{w}}, A^{-1})$ posterior for predicting f in a test point $\mathbf{x}_*$.

$$f_* \doteq f(\mathbf{x}_*) \qquad f(\mathbf{x}) = \mathbf{x}^T\mathbf{w} \in \mathbb{R},\ \mathbf{x}, \mathbf{w} \in \mathbb{R}^D$$

$$y = f(\mathbf{x}) + \epsilon = \mathbf{x}^T\mathbf{w} + \epsilon \in \mathbb{R}$$

$$P(\underbrace{f_*}_{\mathbf{x}_*^T\mathbf{w}}|\mathbf{x}_*, X, \mathbf{y}) = \int \underbrace{P(f_*|\mathbf{x}_*, \mathbf{w})}_{\delta(f_*,\mathbf{x}_*^T\mathbf{w})} \underbrace{P(\mathbf{w}|\mathbf{y}, X)}_{\mathcal{N}_{\mathbf{w}}(\bar{\mathbf{w}},A^{-1})} d\mathbf{w}$$

$$= \mathcal{N}_{f_*}(\mathbf{x}_*^T\bar{\mathbf{w}}, \mathbf{x}_*^T A^{-1}\mathbf{x}_*)$$

This posterior covariance matrix doesn't depend on the observations **y**,

A strange property of Gaussian Processes $\quad \mathbf{y}^T = [y_1, \ldots, y_n]$

Projections of Inputs into Feature Space

The Bayesian linear regression suffers from

limited expressiveness

$$\Downarrow$$

To overcome the problem $\Rightarrow$
go to a feature space and do linear regression there

a., **explicit** features $\phi(\mathbf{x}) = [x_1, x_1 x_2^2, x_1 - x_2, \ldots]^T$

b., **implicit** features (kernels) $k(\mathbf{x}, \mathbf{y}) = \exp(-\|\mathbf{x} - \mathbf{y}\|^2)$

Explicit Features

$$\phi(\mathbf{x}) = [x_1, x_1 x_2^2, x_1 - x_2, \ldots]^T \in \mathbb{R}^N \qquad \phi : \mathbb{R}^D \to \mathbb{R}^N$$

$$\phi(X) = \left[\phi(\mathbf{x}_1) \middle| \phi(\mathbf{x}_2) \middle| \quad \ldots \quad \middle| \phi(\mathbf{x}_n) \right] \in \mathbb{R}^{N \times n}$$

$$f(\mathbf{x}) = \phi(\mathbf{x})^T \mathbf{w} \in \mathbb{R}, \qquad \phi(\mathbf{x}), \mathbf{w} \in \mathbb{R}^N$$

$$y = f(\mathbf{x}) + \epsilon = \phi(\mathbf{x})^T \mathbf{w} + \epsilon \in \mathbb{R}$$

Linear regression in the feature space

Let us repeat all the previous calculations with $\phi(\mathbf{x}) \in \mathbb{R}^N$ (instead of $\mathbf{x}$)

Explicit Features

Reminder: This is what we had without feature maps:

$$P(\underbrace{f_*}_{\mathbf{x}_*^T\mathbf{w}} | \mathbf{x}_*, X, \mathbf{y}) = \mathcal{N}_{f_*}(\mathbf{x}_*^T \bar{\mathbf{w}}, \mathbf{x}_*^T A^{-1} \mathbf{x}_*)$$

where $\bar{\mathbf{w}} \doteq \sigma^{-2} \underbrace{\left(\sigma^{-2} X X^T + \Sigma_p^{-1}\right)^{-1}}_{A^{-1} \in \mathbb{R}^{D\times D}} X\mathbf{y} \in \mathbb{R}^D$ $\quad A \doteq \left(\sigma^{-2} X X^T + \Sigma_p^{-1}\right) \in \mathbb{R}^{D\times D}$

The predictive distribution after feature map:

$$P(\underbrace{f_*}_{\phi(\mathbf{x}_*)^T\mathbf{w}} | \mathbf{x}_*, X, \mathbf{y}) = \mathcal{N}_{f_*}\left(\phi(\mathbf{x}_*)^T \bar{\mathbf{w}}, \phi(\mathbf{x}_*)^T A^{-1} \phi(\mathbf{x}_*)\right)$$

where $\boxed{\bar{\mathbf{w}} \doteq \sigma^{-2} \underbrace{\left(\sigma^{-2} \phi(X)\phi(X)^T + \Sigma_p^{-1}\right)^{-1}}_{A^{-1} \in \mathbb{R}^{N\times N}} \underbrace{\phi(X)}_{\in \mathbb{R}^{N\times n}} \underbrace{\mathbf{y}}_{\in \mathbb{R}^{n\times 1}} \in \mathbb{R}^N}$

$$A \doteq \boxed{\left(\sigma^{-2} \phi(X)\phi(X)^T + \Sigma_p^{-1}\right) \in \mathbb{R}^{N\times N}}$$

Explicit Features

Shorthands:

$$\phi_* \doteq \phi(\mathbf{x}_*) \in \mathbb{R}^N \qquad N = \text{dim of feature space}$$

$$\phi \doteq \phi(X) = \left[\phi(\mathbf{x}_1)\middle|\phi(\mathbf{x}_2)\middle| \quad \dots \quad \middle|\phi(\mathbf{x}_n)\right] \in \mathbb{R}^{N\times n}$$

$$A \doteq \left(\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right) \in \mathbb{R}^{N\times N}$$

$$\bar{\mathbf{w}} \doteq \sigma^{-2}\underbrace{\left(\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right)^{-1}}_{A^{-1}\in\mathbb{R}^{N\times N}}\phi\mathbf{y} \in \mathbb{R}^N$$

The predictive distribution after feature map:

$$P(\underbrace{f_*}_{\phi_*^T\mathbf{w}\in\mathbb{R}}|\mathbf{x}_*, X, \mathbf{y}) = \mathcal{N}_{f_*}\left(\phi_*^T\bar{\mathbf{w}}, \phi_*^T A^{-1}\phi_*\right)$$

Explicit Features

The predictive distribution after feature map:

$$P(\underbrace{f_*}_{\phi_*^T \mathbf{w} \in \mathbb{R}} | \mathbf{x}_*, X, \mathbf{y}) = \mathcal{N}_{f_*}\left(\phi_*^T \bar{\mathbf{w}}, \phi_*^T A^{-1} \phi_*\right) \qquad (*)$$

$$= \mathcal{N}_{f_*}\left(\overbrace{\sigma^{-2}\phi_*^T \left[\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right]^{-1} \phi\mathbf{y}}^{\mathbb{R}}, \phi_*^T \overbrace{\left[\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right]^{-1}}^{\mathbb{R}^{N\times N}} \phi_*\right)$$

A problem with (*) is that it needs an NxN matrix inversion...

Let $K \doteq \phi^T \Sigma_p \phi \in \mathbb{R}^{n\times n}$

Theorem:

(*) can be rewritten: $P(f_* | \mathbf{x}_*, X, \mathbf{y}) =$

$$\boxed{\mathcal{N}_{f_*}\left(\underbrace{(\phi_*^T \Sigma_p \phi)}_{\mathbb{R}^{1\times n}} \underbrace{(K+\sigma^2 \mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}} \underbrace{\mathbf{y}}_{\mathbb{R}^{n\times 1}}, \underbrace{(\phi_*^T \Sigma_p \phi_*)}_{\mathbb{R}^{1\times 1}} - \underbrace{(\phi_*^T \Sigma_p \phi)}_{\mathbb{R}^{1\times n}} \underbrace{(K+\sigma^2 \mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}} \underbrace{(\phi^T \Sigma_p \phi_*)}_{\mathbb{R}^{n\times 1}}\right)}$$

Proofs

- **Mean expression.** We need:

$$\sigma^{-2}\phi_*^T \underbrace{\left[\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right]^{-1}}_{A^{-1}} \phi\mathbf{y} = (\phi_*^T \underbrace{\Sigma_p\phi)(K + \sigma^2\mathbf{I}_n)^{-1}}_{\sigma^{-2}A^{-1}\phi}\mathbf{y}$$

Lemma:

$$\sigma^{-2}\phi(K + \sigma^2\mathbf{I}_n) = \sigma^{-2}\phi(\phi^T\Sigma_p\phi + \sigma^2\mathbf{I}_n) = A\Sigma_p\phi$$

- **Variance expression.** We need:

$$\phi_*^T \left[\sigma^{-2}\phi\phi^T + \Sigma_p^{-1}\right]^{-1} \phi_* = (\phi_*^T\Sigma_p\phi_*) - (\phi_*^T\Sigma_p\phi)(K + \sigma^2\mathbf{I}_n)^{-1}(\phi^T\Sigma_p\phi_*)$$

Matrix inversion Lemma:

$$(\underbrace{U}_{\phi}\underbrace{W}_{\sigma^{-2}}\underbrace{V^T}_{\phi^T} + \underbrace{Z}_{\Sigma_p^{-1}})^{-1} = Z^{-1} - Z^{-1}U(W^{-1} + \underbrace{V^TZ^{-1}U}_{K})^{-1}V^TZ^{-1}$$

From Explicit to Implicit Features

$$P(f_*|\mathbf{x}_*, X, \mathbf{y}) =$$

$$\boxed{\mathcal{N}_{f_*}\left(\underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{\mathbf{y}}_{\mathbb{R}^{n\times 1}}, \underbrace{(\phi_*^T\Sigma_p\phi_*)}_{\mathbb{R}^{1\times 1}} - \underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{(\phi^T\Sigma_p\phi_*}_{\mathbb{R}^{n\times 1}}\right)}$$

We only have to work with $n \times n$ matrices, and not $N \times N$

From Explicit to Implicit Features

$P(f_*|\mathbf{x}_*, X, \mathbf{y}) =$

$$\boxed{\mathcal{N}_{f_*}\Big(\underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{\mathbf{y}}_{\mathbb{R}^{n\times 1}}, \underbrace{(\phi_*^T\Sigma_p\phi_*)}_{\mathbb{R}^{1\times 1}} - \underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{(\phi^T\Sigma_p\phi_*}_{\mathbb{R}^{n\times 1}}}$$

The feature space always appears in the form of:

$(\phi_*^T\Sigma_p\phi_*)$, $(\phi_*^T\Sigma_p\phi)$, $(\phi^T\Sigma_p\phi)$, ($\in \mathbb{R}^{n\times n}$ matrices)

$$\boxed{\text{Let } k(\mathbf{x}, \tilde{\mathbf{x}}) \doteq \phi(\mathbf{x})^T\Sigma_p\phi(\tilde{\mathbf{x}})}$$

No need to know the explicit N dimensional features.

Their inner product is enough.

Lemma:

$k(\mathbf{x}, \tilde{\mathbf{x}})$ is an inner product in the feature space: $\psi(\mathbf{x}) \doteq \Sigma_p^{1/2}\phi(\mathbf{x})$

GP pseudo code

Inputs:

$$X = \begin{bmatrix} \mathbf{x}_1^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix} \in \mathbb{R}^{n \times D}, \ n \text{ training inputs}$$

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^{n}, \ n \text{ training targets}$$

$$k(\cdot,\cdot) : \mathbb{R}^{D \times D} \rightarrow \mathbb{R} \text{ covariance function (kernel)}$$

$$\mathbf{x}_* \in \mathbb{R}^D \text{ test input}$$

$$\sigma^2 > 0 \text{ noise level on the observations}$$

$$[y(\mathbf{x}) = f(\mathbf{x}) + \epsilon, \ \epsilon \sim \mathcal{N}(0, \sigma^2)]$$

GP pseudo code (continued)

$P(f_*|\mathbf{x}_*, X, \mathbf{y}) =$

$$\boxed{\mathcal{N}_{f_*}\Big(\underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{\mathbf{y}}_{\mathbb{R}^{n\times 1}}, \underbrace{(\phi_*^T\Sigma_p\phi_*)}_{\mathbb{R}^{1\times 1}} - \underbrace{(\phi_*^T\Sigma_p\phi)}_{\mathbb{R}^{1\times n}}\underbrace{(K+\sigma^2\mathbf{I}_n)^{-1}}_{\mathbb{R}^{n\times n}}\underbrace{(\phi^T\Sigma_p\phi_*}_{\mathbb{R}^{n\times 1}})}$$

1., $K \in \mathbb{R}^{n\times n}$ Gram matrix. $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$

$$k(\mathbf{x}_*) = k_* = k(X, \mathbf{x}_*) = \begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_*) \\ \vdots \\ k(\mathbf{x}_n, \mathbf{x}_*) \end{bmatrix} \in \mathbb{R}^n$$

2., $\boldsymbol{\alpha} = (K + \sigma^2\mathbf{I}_n)^{-1}\mathbf{y}$

3., $\bar{f}_* = k_*^T\boldsymbol{\alpha} \in \mathbb{R}$ (Posterior mean at x_*)

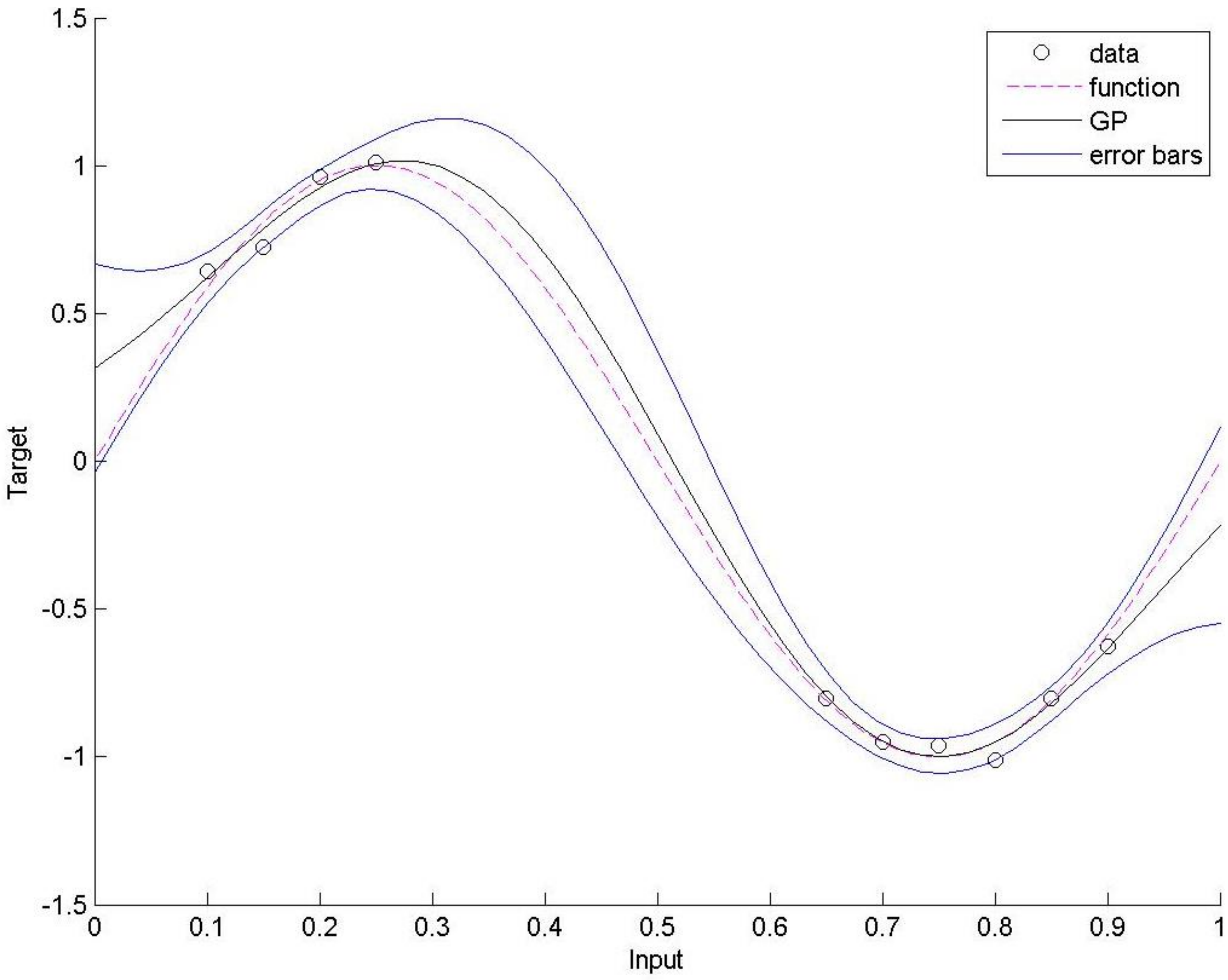
4., $cov(f_*) = \underbrace{k(\mathbf{x}_*, \mathbf{x}_*)}_{\mathbb{R}} - \underbrace{k_*^T}_{\mathbb{R}^{1\times n}} \underbrace{[K + \sigma^2 I_n]^{-1}}_{\mathbb{R}^{n\times n}} \underbrace{k_*}_{\mathbb{R}^n} \in \mathbb{R}$

(Posterior covariance at x_*)

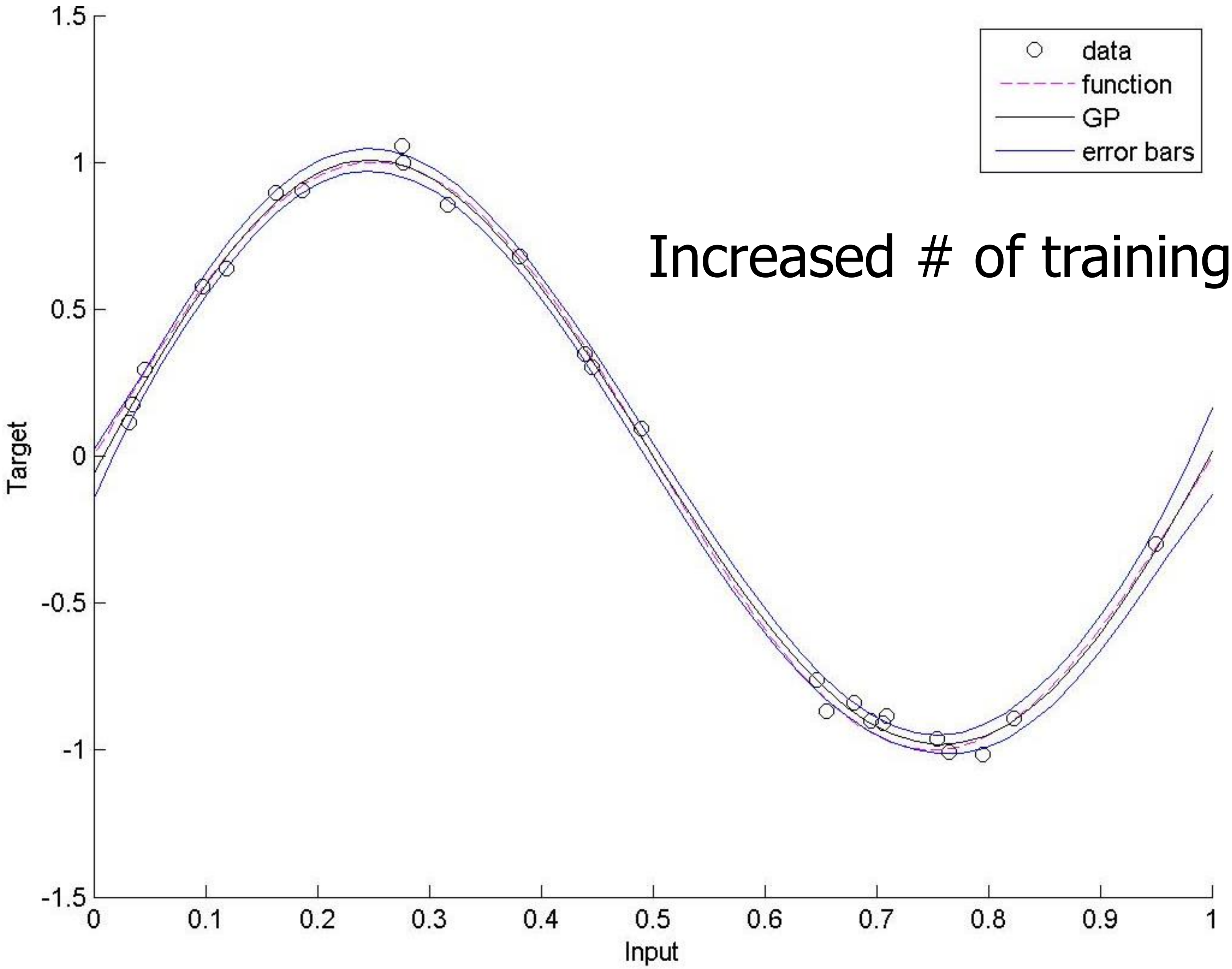
Outputs: $\bar{f}_*,\ cov(f_*)$

Results

Results using Netlab , Sin function

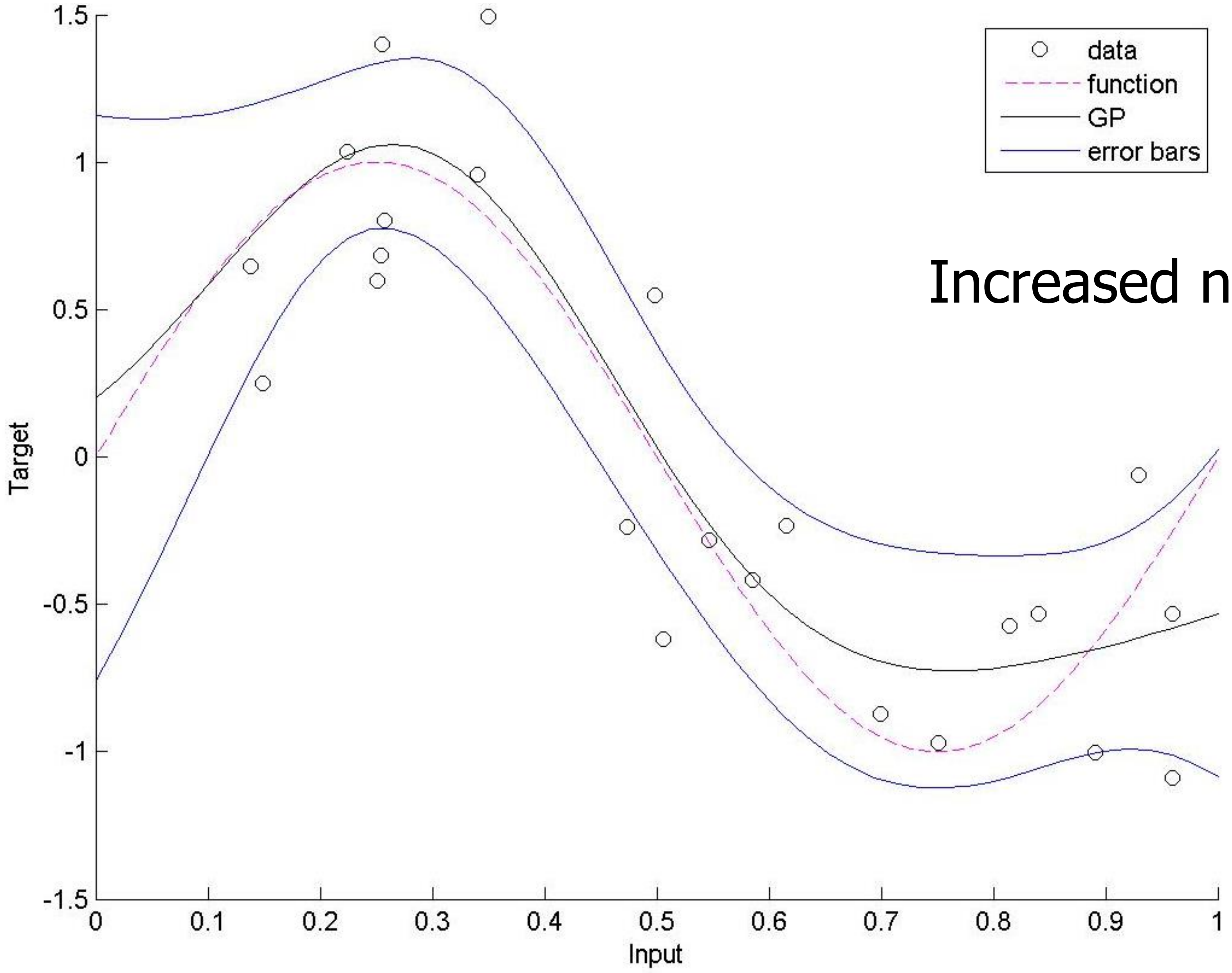


Results using Netlab, Sin function



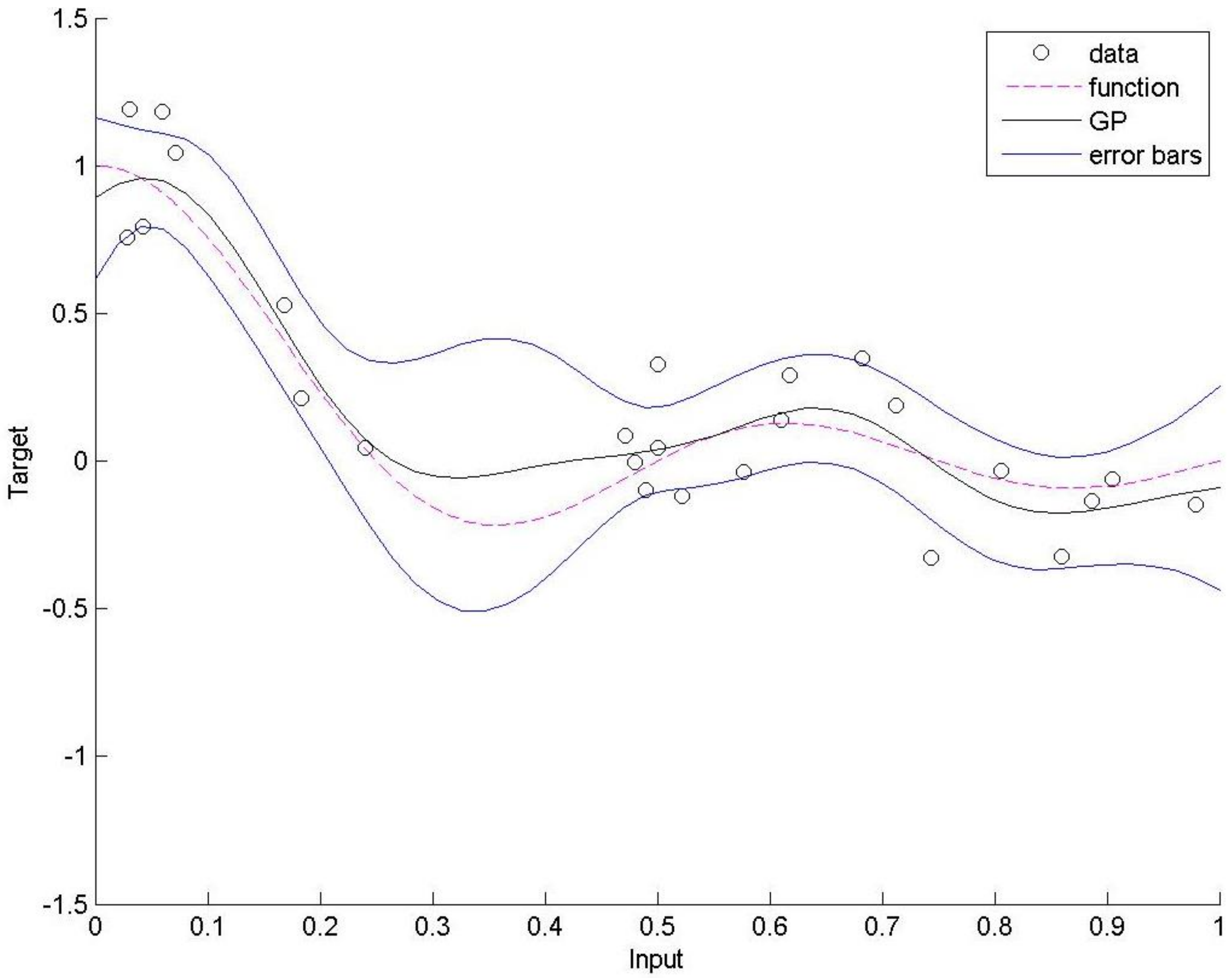
Increased # of training points

Results using Netlab, Sin function

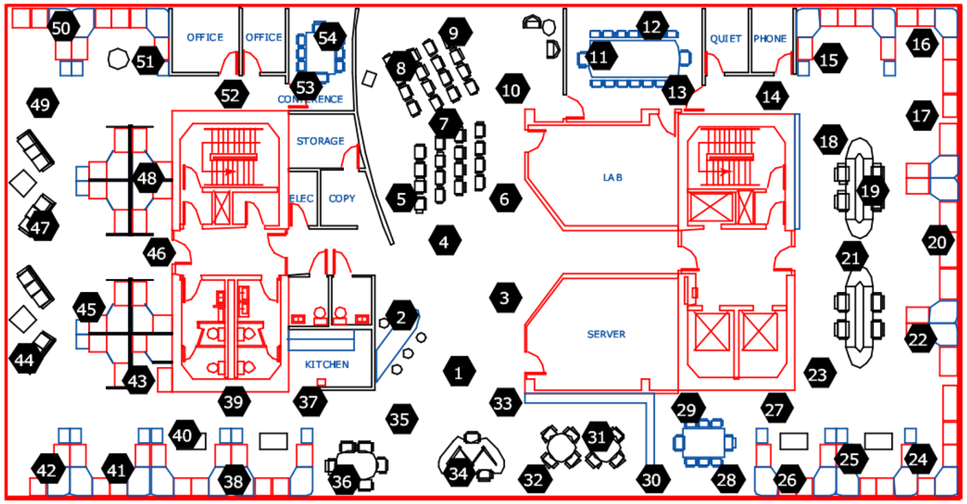


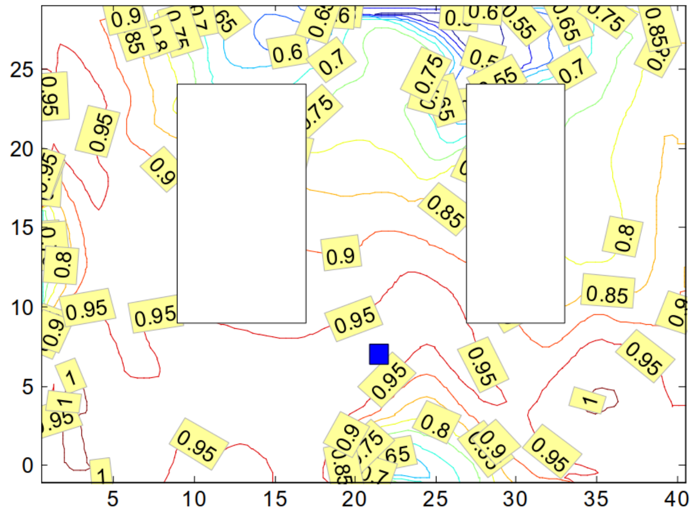
Increased noise

Results using Netlab, Sinc function

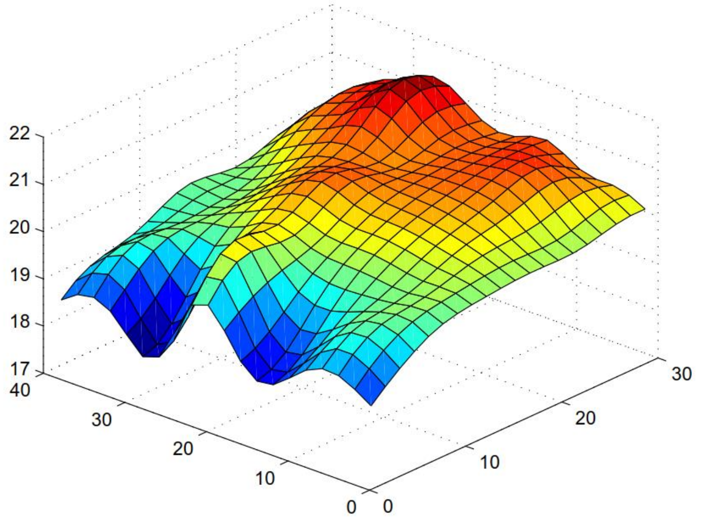


Applications: Sensor placement





Temperature modeling with GP



Near-Optimal Sensor Placements in Gaussian Processes: Theory, Efficient Algorithms and Empirical Studies. A.Krause, A. Singh, and C. Guestrin, Journal of Machine Learning Research (2008)

Applications: Sensor placement

$\mathcal{A}$: sensors are placed in these locations
$\mathcal{V}$: all possible sensor locations

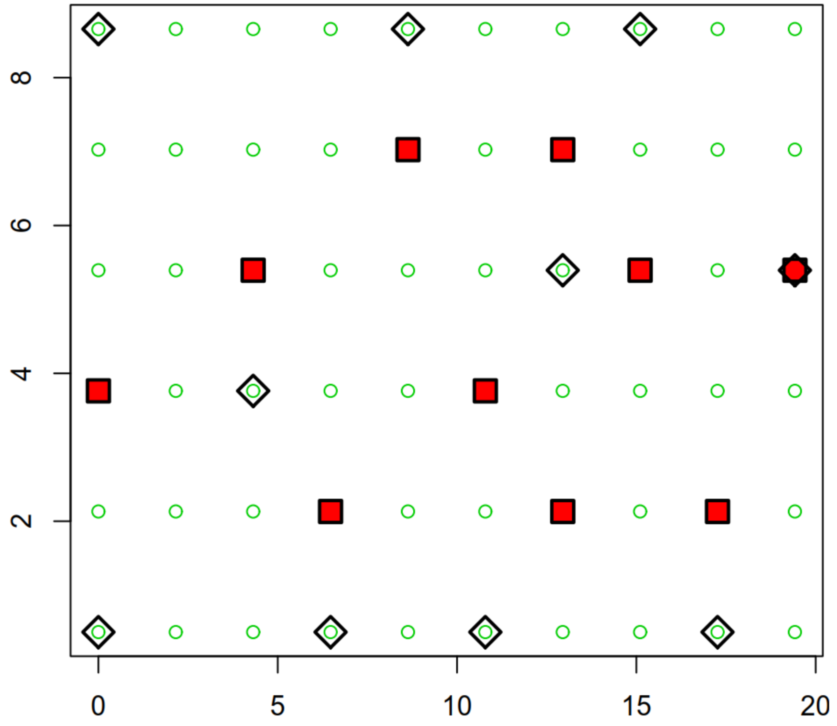
Entropy criterion:

$$\begin{aligned}\mathcal{A}^* &= \operatorname{argmin}_{\mathcal{A}\subset\mathcal{V}:|\mathcal{A}|=k} H(X_{\mathcal{V}\setminus\mathcal{A}} \mid X_{\mathcal{A}}).\\ &= \operatorname{argmax}_{\mathcal{A}\subset\mathcal{V}:|\mathcal{A}|=k} H(X_{\mathcal{A}})\end{aligned}$$

$$H(X_{\mathcal{V}\setminus\mathcal{A}} \mid X_{\mathcal{A}}) = H(X_{\mathcal{V}}) - H(X_{\mathcal{A}})$$

Mutual information criterion:

$$\mathcal{A}^* = \operatorname{argmin}_{\mathcal{A}\subset\mathcal{V}:|\mathcal{A}|=k} \underbrace{I(X_{\mathcal{A}}; X_{\mathcal{V}\setminus\mathcal{A}})}_{H(X_{\mathcal{V}\setminus\mathcal{A}}) - H(X_{\mathcal{V}\setminus\mathcal{A}} \mid X_{\mathcal{A}})}$$



An example of placements chosen using entropy and mutual information criteria on temperature data. Diamonds indicate the positions chosen using entropy; squares the positions chosen using MI.

What You Should Know

- Properties of Multivariate Gaussian distribution
- Gaussian process = Bayesian Ridge Regression
- GP Algorithm
- GP application in active learning

Thanks for the Attention! ☺