Linear Models for Regression

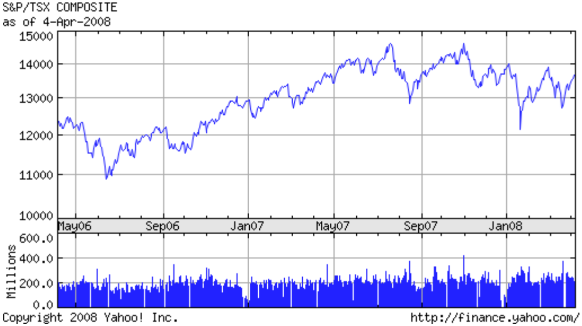
Greg Mori - CMPT 419/726

Bishop PRML Ch. 3

Outline

Outline

Regression



- Given training set $\{(\boldsymbol{x}_1, \boldsymbol{t}_1), \ldots, (\boldsymbol{x}_N, \boldsymbol{t}_N)\}$
- $\boldsymbol{t}_i$ is continuous: regression
- For now, assume $t_i \in \mathbb{R}$, $\boldsymbol{x}_i \in \mathbb{R}^D$
- E.g. $\boldsymbol{t}_i$ is stock price, $\boldsymbol{x}_i$ contains company profit, debt, cash flow, gross sales, number of spam emails sent, ...

Outline

Linear Functions

- A function $f(\cdot)$ is linear if

$$f(\alpha u + \beta v) = \alpha f(u) + \beta f(v)$$

- Linear functions will lead to simple algorithms, so let's see what we can do with them

Linear Regression

- Simplest linear model for regression

$$y(\boldsymbol{x}, \boldsymbol{w}) = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_D x_D$$

  - Remember, we're learning $\boldsymbol{w}$
  - Set $\boldsymbol{w}$ so that $y(\boldsymbol{x}, \boldsymbol{w})$ aligns with target value in training data

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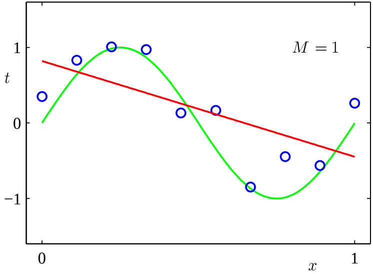
- This is a very simple model, limited in what it can do



Linear Basis Function Models

- Simplest linear model

$$y(\boldsymbol{x}, \boldsymbol{w}) = w_0 + w_1 x_1 + w_2 x_2 + \ldots + w_D x_D$$

was linear in $\boldsymbol{x}$ (*) and $\boldsymbol{w}$

- Linear in $\boldsymbol{w}$ is what will be important for simple algorithms
- Extend to include fixed non-linear functions of data

$$y(\boldsymbol{x}, \boldsymbol{w}) = w_0 + w_1 \phi_1(\boldsymbol{x}) + w_2 \phi_2(\boldsymbol{x}) + \ldots + w_{M-1} \phi_{M-1}(\boldsymbol{x})$$

- Linear combinations of these basis functions also linear in parameters

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Linear Basis Function Models

- Bias parameter allows fixed offset in data

$$y(\boldsymbol{x}, \boldsymbol{w}) = \underbrace{w_0}_{bias} + w_1\phi_1(\boldsymbol{x}) + w_2\phi_2(\boldsymbol{x}) + \ldots + w_{M-1}\phi_{M-1}(\boldsymbol{x})$$

- Think of simple 1-D x:

$$y(x, w) = \underbrace{w_0}_{intercept} + \underbrace{w_1}_{slope} x$$

- For notational convenience, define $\phi_0(x) = 1$:

$$y(\boldsymbol{x}, \boldsymbol{w}) = \sum_{j=0}^{M-1} w_j\phi_j(\boldsymbol{x}) = \boldsymbol{w}^T\phi(\boldsymbol{x})$$

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Linear Basis Function Models

- Function for regression $y(\boldsymbol{x}, \boldsymbol{w})$ is non-linear function of $\boldsymbol{x}$, but linear in $\boldsymbol{w}$:

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- Order M polynomial regression, $\phi_j(x) = ?$
- $\phi_j(x) = x^j$:

$$y(\boldsymbol{x}, \boldsymbol{w}) = w_0 x^0 + w_1 x^1 + \ldots + w_M x^M$$

Basis Functions: Feature Functions

- Often we extract features from $\boldsymbol{x}$
  - An intuitve way to think of $\phi_j(\boldsymbol{x})$ is as feature functions
- E.g. Automatic CMPT726 project report grading system
  - $\boldsymbol{x}$ is text of report: `In this project we apply the algorithm of Mori [2] to recognizing blue objects. We test this algorithm on pictures of you and I from my holiday photo collection. ...`
- $\phi_1(\boldsymbol{x})$ is count of occurrences of `Mori [`
- $\phi_2(\boldsymbol{x})$ is count of occurrences of `of you and I`
- Regression grade $y(\boldsymbol{x}, \boldsymbol{w}) = 20\phi_1(\boldsymbol{x}) - 10\phi_2(\boldsymbol{x})$

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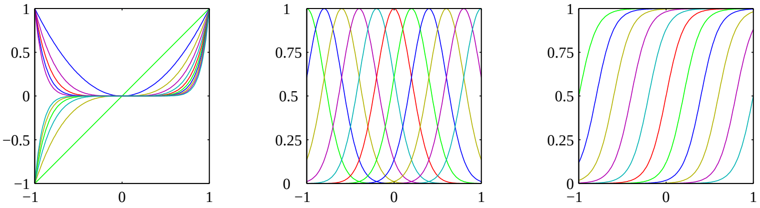
Other Non-linear Basis Functions

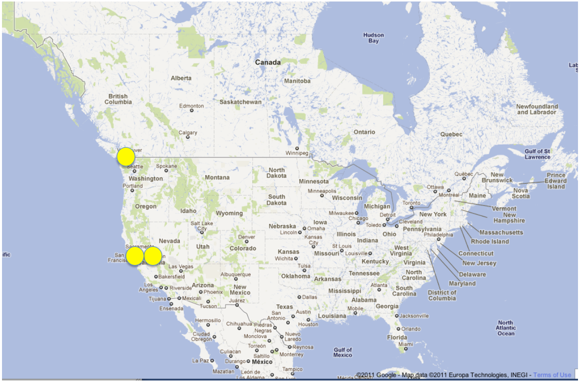


- Polynomial $\phi_j(x) = x^j$
- Gaussians $\phi_j(x) = \exp\{-\frac{(x-\mu_j)^2}{2s^2}\}$
- Sigmoidal $\phi_j(x) = \frac{1}{1+\exp((\mu_j - x)/s)}$

Example - Gaussian Basis Functions: Temperature

- Use Gaussian basis functions, regression on temperature

Example - Gaussian Basis Functions: Temperature



- $\mu_1 =$ Vancouver, $\mu_2 =$ San Francisco, $\mu_3 =$ Oakland

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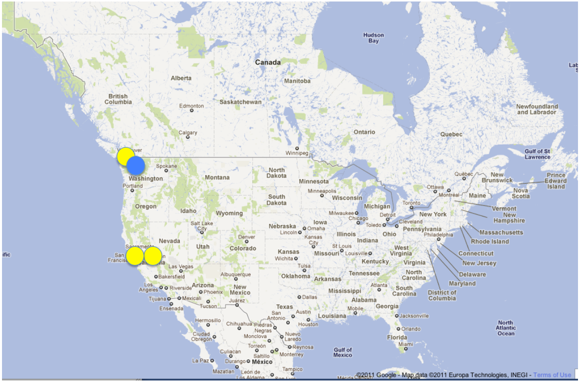

- $\mu_1 =$ Vancouver, $\mu_2 =$ San Francisco, $\mu_3 =$ Oakland
- Temperature in $x =$ Seattle? $y(\boldsymbol{x}, \boldsymbol{w}) =$
  $w_1 \exp\{-\frac{(x-\mu_1)^2}{2s^2}\} + w_2 \exp\{-\frac{(x-\mu_2)^2}{2s^2}\} + w_3 \exp\{-\frac{(x-\mu_3)^2}{2s^2}\}$

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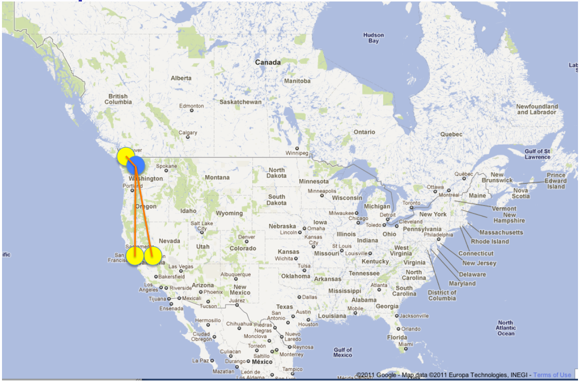

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- Compute distances to all μ, $y(\boldsymbol{x}, \boldsymbol{w}) \approx w_1$

Example - Gaussian Basis Functions: 726 Report Grading

- Define:
  - $\mu_1 =$ Crime and Punishment
  - $\mu_2 =$ Animal Farm
  - $\mu_3 =$ Some paper by Mori
- Learn weights:
  - $w_1 =$?
  - $w_2 =$?
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- Grade a project report x:
  - Measure similarity of x to each μ, Gaussian, with weights: $y(x, w) = w_1 \exp\{-\frac{(x-\mu_1)^2}{2s^2}\} + w_2 \exp\{-\frac{(x-\mu_2)^2}{2s^2}\} + w_3 \exp\{-\frac{(x-\mu_3)^2}{2s^2}\}$
- The Gaussian basis function models end up similar to template matching

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Outline

- Regression
- Linear Basis Function Models
- Loss Functions for Regression
- Finding Optimal Weights
- Regularization
- Bayesian Linear Regression

Loss Functions for Regression

- We want to find the "best" set of coefficients $\boldsymbol{w}$
- Recall, one way to define "best" was minimizing squared error:

$$E(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \boldsymbol{w}) - t_n\}^2$$

- We will now look at another way, based on maximum likelihood

Gaussian Noise Model for Regression

- We are provided with a training set $\{(\boldsymbol{x}_i, t_i)\}$
- Let's assume t arises from a deterministic function plus Gassian distributed (with precision β) noise:

$$t = y(\boldsymbol{x}, \boldsymbol{w}) + \epsilon$$

- The probability of observing a target value t is then:

$$p(t|\boldsymbol{x}, \boldsymbol{w}, \beta) = \mathcal{N}(t|y(\boldsymbol{x}, \boldsymbol{w}), \beta^{-1})$$

  - Notation: $\mathcal{N}(x|\mu, \sigma^2)$; x drawn from Gaussian with mean μ, variance σ^2

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Maximum Likelihood for Regression

- The likelihood of data $\boldsymbol{t} = \{t_i\}$ using this Gaussian noise model is:

$$p(\boldsymbol{t}|\boldsymbol{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}(t_n|\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_n), \beta^{-1})$$

- The log-likelihood is:

$$\ln p(\boldsymbol{t}|\boldsymbol{w}, \beta) = \ln \prod_{n=1}^{N} \frac{\sqrt{\beta}}{\sqrt{2\pi}} \exp(-\frac{\beta}{2}(t_n - \boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_n))^2)$$

$$= \underbrace{\frac{N}{2}\ln\beta - \frac{N}{2}\ln(2\pi)}_{const.\ wrt\ \boldsymbol{w}} - \beta \underbrace{\frac{1}{2}\sum_{n=1}^{N}(t_n - \boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}_n))^2}_{squared\ error}$$

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Outline

Finding Optimal Weights

- How do we maximize likelihood wrt $\boldsymbol{w}$ (or minimize squared error)?
- Take gradient of log-likelihood wrt $\boldsymbol{w}$:

$$\frac{\partial}{\partial w_i} \ln p(\boldsymbol{t}|\boldsymbol{w}, \beta) = \beta \sum_{n=1}^{N} (t_n - \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_n)) \phi_i(\boldsymbol{x}_n)$$

- In vector form:

$$\nabla \ln p(\boldsymbol{t}|\boldsymbol{w}, \beta) = \beta \sum_{n=1}^{N} (t_n - \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_n)) \boldsymbol{\phi}(\boldsymbol{x}_n)^T$$

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Finding Optimal Weights

- Set gradient to 0:

$$\mathbf{0}^T = \sum_{n=1}^{N} t_n \phi(\mathbf{x}_n)^T - \mathbf{w}^T \left(\sum_{n=1}^{N} \phi(\mathbf{x}_n)\phi(\mathbf{x}_n)^T \right)$$

- Maximum likelihood estimate for $\mathbf{w}$:

$$\mathbf{w}_{ML} = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T\mathbf{t}$$

$$\mathbf{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \ldots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \ldots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \ldots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix}$$

- $\mathbf{\Phi}^\dagger = \left(\mathbf{\Phi}^T\mathbf{\Phi}\right)^{-1}\mathbf{\Phi}^T$ known as the pseudo-inverse (`numpy.linalg.pinv` in python)

Finding Optimal Weights

- Set gradient to 0:

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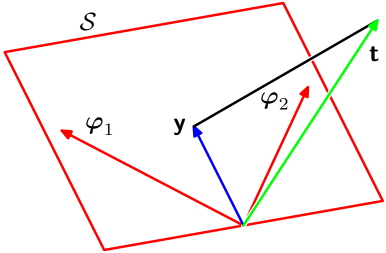
Geometry of Least Squares



- $\boldsymbol{t} = (t_1, \ldots, t_N)$ is the target value vector
- $\mathcal{S}$ is space spanned by $\boldsymbol{\varphi}_j = (\phi_j(\boldsymbol{x}_1), \ldots, \phi_j(\boldsymbol{x}_N))$
- Solution $\boldsymbol{y}$ lies in $\mathcal{S}$
- Least squares solution is orthogonal projection of $\boldsymbol{t}$ onto $\mathcal{S}$
- Can verify this by looking at $\boldsymbol{y} = \boldsymbol{\Phi w}_{ML} = \boldsymbol{\Phi \Phi}^{\dagger}\boldsymbol{t} = \boldsymbol{Pt}$
  - $\boldsymbol{P}^2 = \boldsymbol{P}$, $\boldsymbol{P} = \boldsymbol{P}^T$

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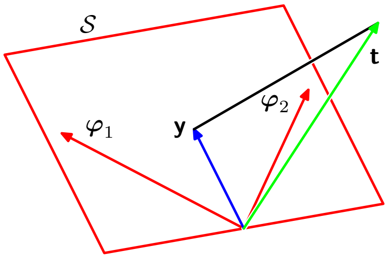

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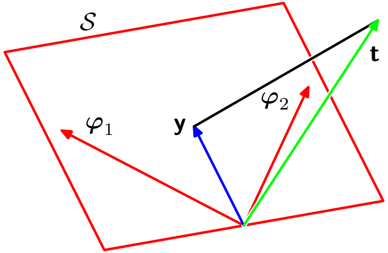
  - $\boldsymbol{P}^2 = \boldsymbol{P}$, $\boldsymbol{P} = \boldsymbol{P}^T$

Geometry of Least Squares



- $\boldsymbol{t} = (t_1, \ldots, t_N)$ is the target value vector
- $\mathcal{S}$ is space spanned by $\boldsymbol{\varphi}_j = (\phi_j(\boldsymbol{x}_1), \ldots, \phi_j(\boldsymbol{x}_N))$
- Solution $\boldsymbol{y}$ lies in $\mathcal{S}$
- Least squares solution is orthogonal projection of $\boldsymbol{t}$ onto $\mathcal{S}$
- Can verify this by looking at $\boldsymbol{y} = \Phi \boldsymbol{w}_{ML} = \Phi\Phi^{\dagger}\boldsymbol{t} = \boldsymbol{P}\boldsymbol{t}$
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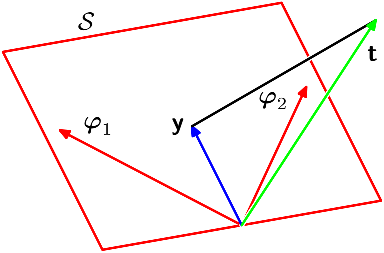

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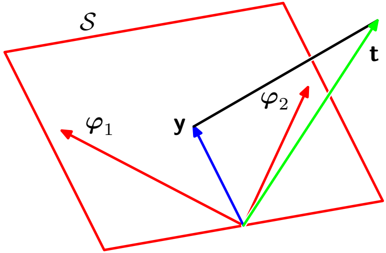

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Sequential Learning

- In practice N might be huge, or data might arrive online
- Can use a gradient descent method:
  - Start with initial guess for $\boldsymbol{w}$
  - Update by taking a step in gradient direction ∇E of error function
- Modify to use stochastic / sequential gradient descent:
  - If error function $E = \sum_n E_n$ (e.g. least squares)
  - Update by taking a step in gradient direction ∇E_n for one example
  - Details about step size are important – decrease step size at the end

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Outline

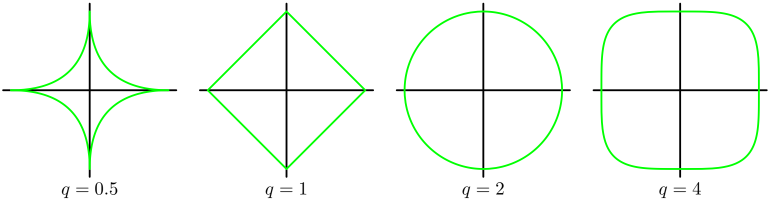
Regularization

- Last week we discussed regularization as a technique to avoid over-fitting:

$$\tilde{E}(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \boldsymbol{w}) - t_n\}^2 + \underbrace{\frac{\lambda}{2}||\boldsymbol{w}||^2}_{regularizer}$$

- Next on the menu:
  - Other regularlizers
  - Bayesian learning and quadratic regularizer

Other Regularizers



- Can use different norms for regularizer:

$$\tilde{E}(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \boldsymbol{w}) - t_n\}^2 + \frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q$$

- e.g. $q = 2$ – ridge regression
- e.g. $q = 1$ – lasso
- math is easiest with ridge regression

Optimization with a Quadratic Regularizer

- With $q = 2$, total error still a nice quadratic:

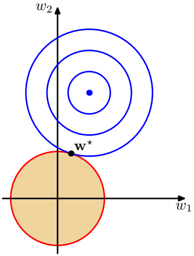
$$\tilde{E}(\boldsymbol{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \boldsymbol{w}) - t_n\}^2 + \frac{\lambda}{2}\boldsymbol{w}^T\boldsymbol{w}$$

- Calculus ...

$$\boldsymbol{w} = (\underbrace{\lambda \boldsymbol{I} + \boldsymbol{\Phi}^T\boldsymbol{\Phi}}_{regularlized})^{-1}\boldsymbol{\Phi}^T\boldsymbol{t}$$

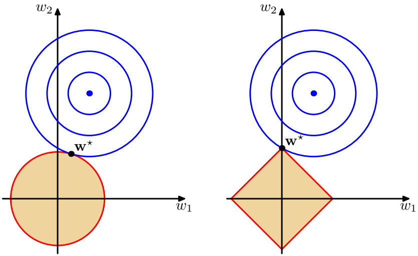
- Similar to unregularlized least squares
- Advantage $(\lambda \boldsymbol{I} + \boldsymbol{\Phi}^T\boldsymbol{\Phi})$ is well conditioned so inversion is stable

Ridge Regression vs. Lasso



- Ridge regression aka parameter shrinkage
  - Weights $\boldsymbol{w}$ shrink back towards origin

Ridge Regression vs. Lasso



- Ridge regression aka parameter shrinkage
  - Weights $\boldsymbol{w}$ shrink back towards origin
- Lasso leads to sparse models
  - Components of $\boldsymbol{w}$ tend to 0 with large λ (strong regularization)
  - Intuitively, once minimum achieved at large radius, minimum is on $w_1 = 0$

Outline

Bayesian Linear Regression

- Last week we saw an example of a Bayesian approach
  - Coin tossing - prior on parameters
- We will now do the same for linear regression
  - Prior on parameter $\boldsymbol{w}$
- There will turn out to be a connection to regularlization

Bayesian Linear Regression

- Start with a prior over parameters $\boldsymbol{w}$
  - Conjugate prior is a Gaussian:

$$p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|\mathbf{0}, \alpha^{-1}\boldsymbol{I})$$

    - This simple form will make math easier; can be done for arbitrary Gaussian too
- Data likelihood, Gaussian model as before:

$$p(t|\boldsymbol{x}, \boldsymbol{w}, \beta) = \mathcal{N}(t|y(\boldsymbol{x}, \boldsymbol{w}), \beta^{-1})$$

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Bayesian Linear Regression

- Posterior distribution on $\boldsymbol{w}$:

$$p(\boldsymbol{w}|\boldsymbol{t}) \propto \left(\prod_{n=1}^{N} p(t_n|\boldsymbol{x}_n, \boldsymbol{w}, \beta) \right) p(\boldsymbol{w})$$

$$= \left[\prod_{n=1}^{N} \frac{\sqrt{\beta}}{\sqrt{2\pi}} \exp\left(-\frac{\beta}{2}(t_n - \boldsymbol{w}^T \phi(\boldsymbol{x}_n))^2 \right) \right] \left(\frac{\alpha}{2\pi} \right)^{\frac{M}{2}} \exp(-\frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w})$$

- Take the log:

$$-\ln p(\boldsymbol{w}|\boldsymbol{t}) = \frac{\beta}{2} \sum_{n=1}^{N} (t_n - \boldsymbol{w}^T \phi(\boldsymbol{x}_n))^2 + \frac{\alpha}{2}\boldsymbol{w}^T\boldsymbol{w} + const$$

- L_2 regularization is maximum a posteriori (MAP) with a Gaussian prior.
  - $\lambda = \alpha/\beta$

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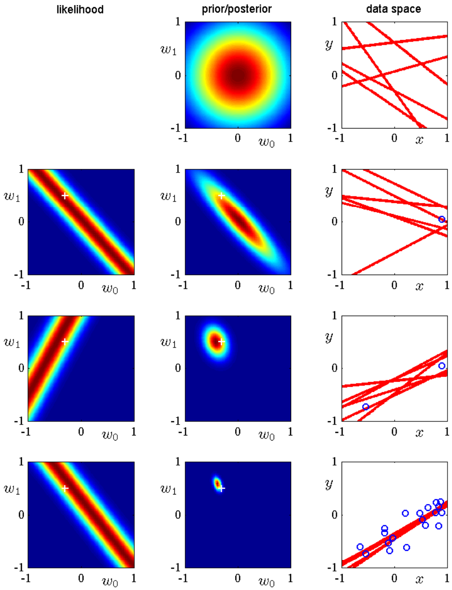

- Simple example $x, t \in \mathbb{R}$, $y(x, \mathbf{w}) = w_0 + w_1 x$
- Start with Gaussian prior in parameter space
- Samples shown in data space
- Receive data points (blue circles in data space)
- Compute likelihood
- Posterior is prior (or prev. posterior) times likelihood

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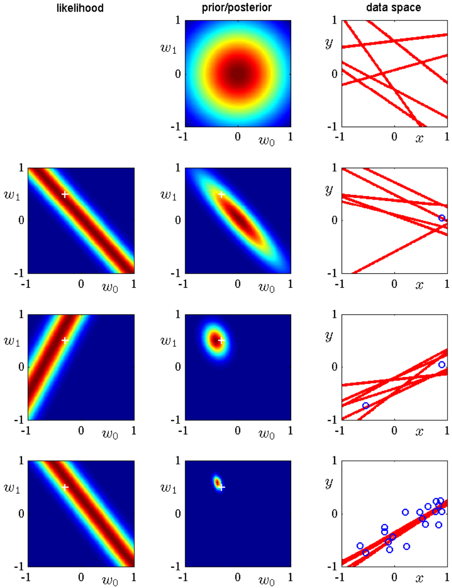

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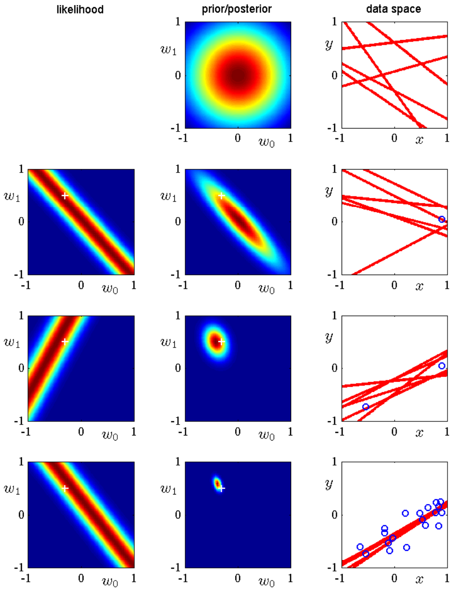

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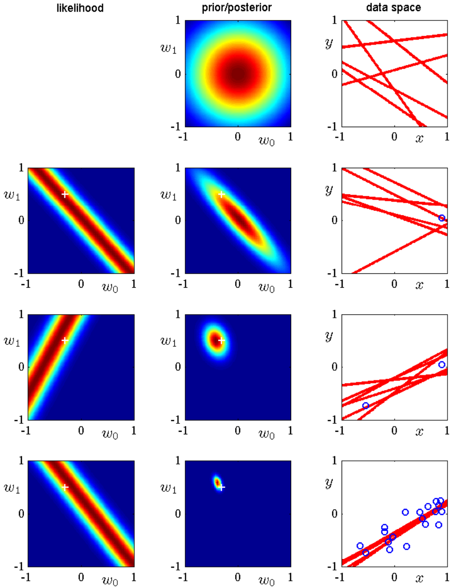

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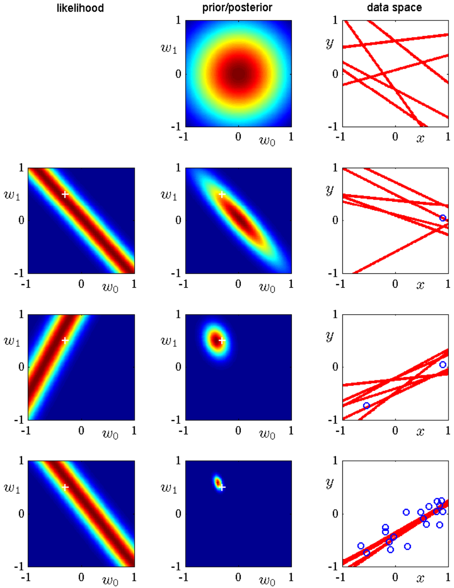

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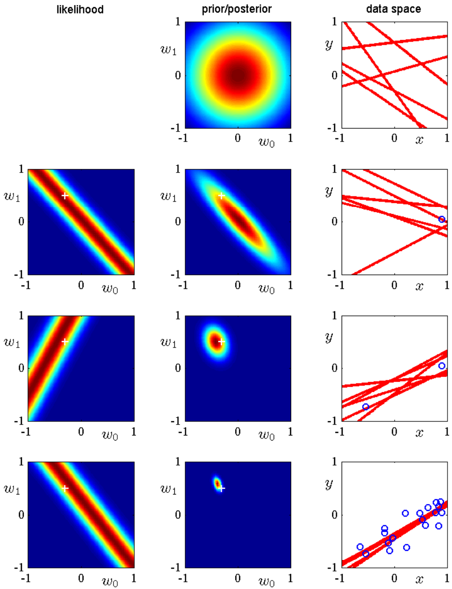

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Predictive Distribution

- Single estimate of $\boldsymbol{w}$ (ML or MAP) doesn't tell whole story
- We have a distribution over $\boldsymbol{w}$, and can use it to make predictions
- Given a new value for x, we can compute a *distribution* over t:

$$p(t|\boldsymbol{t}, \alpha, \beta) = \int p(t, \boldsymbol{w}|\boldsymbol{t}, \alpha, \beta) d\boldsymbol{w}$$

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  - i.e. For each value of $\boldsymbol{w}$, let it make a prediction, multiply by its probability, sum over all $\boldsymbol{w}$
  - For arbitrary models as the distributions, this integral may not be computationally tractable

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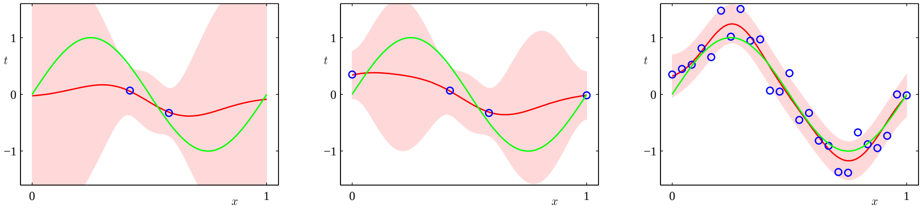

- With the Gaussians we've used for these distributions, the predicitve distribution will also be Gaussian
  - (math on convolutions of Gaussians)
- Green line is true (unobserved) curve, blue data points, red line is mean, pink one standard deviation
  - Uncertainty small around data points
  - Pink region shrinks with more data

Bayesian Model Selection

- So what do the Bayesians say about model selection?
  - Model selection is choosing model $\mathcal{M}_i$ e.g. degree of polynomial, type of basis function ϕ
- Don't select, just integrate

$$p(t|\mathbf{x}, \mathcal{D}) = \sum_{i=1}^{L} \underbrace{p(t|\mathbf{x}, \mathcal{M}_i, \mathcal{D})}_{predictive\ dist.} p(\mathcal{M}_i|\mathcal{D})$$

- Average together the results of all models
- Could choose most likely model a posteriori $p(\mathcal{M}_i|\mathcal{D})$
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$$p(\mathcal{M}_i|\mathcal{D}) \propto p(\mathcal{D}|\mathcal{M}_i)p(\mathcal{M}_i)$$

- Another likelihood + prior combination
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Conclusion

- Readings: Ch. 3.1, 3.1.1-3.1.4, 3.3.1-3.3.2, 3.4
- Linear Models for Regression
    - Linear combination of (non-linear) basis functions
- Fitting parameters of regression model
    - Least squares
    - Maximum likelihood (can be = least squares)
- Controlling over-fitting
    - Regularization
    - Bayesian, use prior (can be = regularization)
- Model selection
    - Cross-validation (use held-out data)
    - Bayesian (use model evidence, likelihood)