FE540 금융공학 인공지능 및 기계학습

Regression

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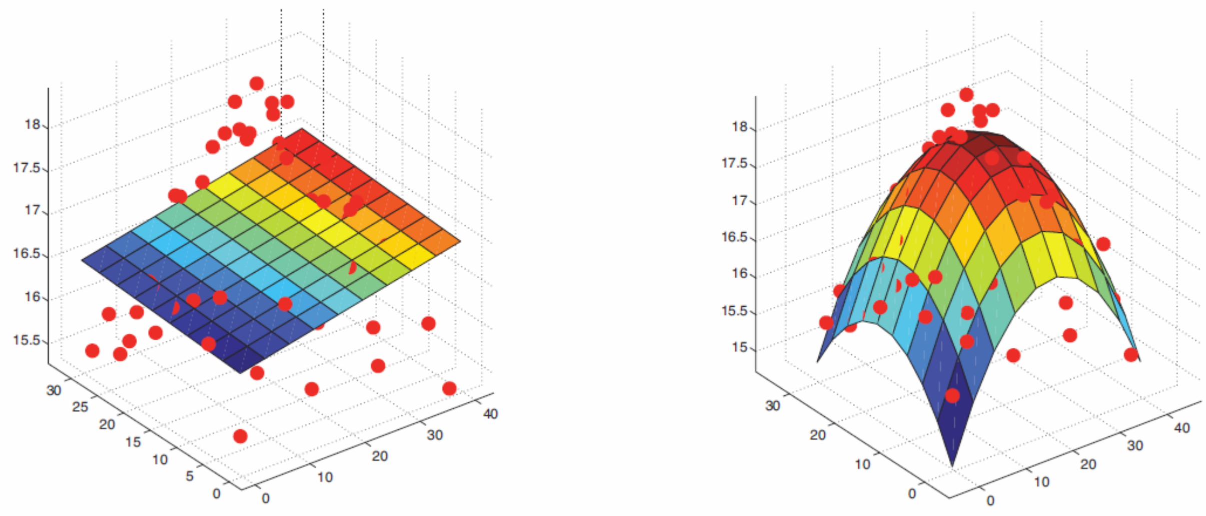
Regression

- Would like to write numeric output as a function of input
  - Output: dependent variable
  - Input: independent variable
- Assume: $y = \mathbf{w}^\top \mathbf{x} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$
  - likelihood: $p(y|\mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y|\mathbf{w}^\top \mathbf{x}, \sigma^2)$
  - can handle non-linear relationships via basis function expansion:

$$p(y|\mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y|\mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}), \sigma^2) \quad \text{e.g. } \boldsymbol{\phi}(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2]$$



(a) (b)

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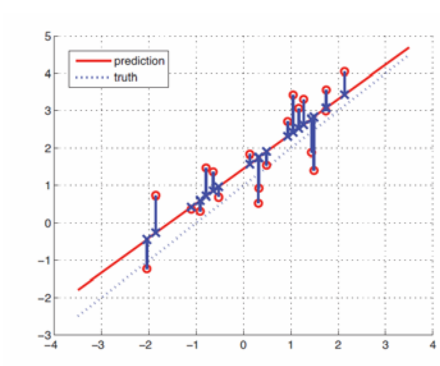
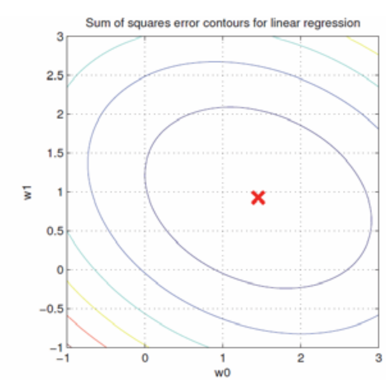
Maximum Likelihood Estimation

- MLE is equivalent to least squares
  - $\hat{\boldsymbol{\theta}}_{\mathrm{MLE}} \equiv \mathrm{argmax}_{\boldsymbol{\theta}} \log p(\mathcal{D}|\boldsymbol{\theta}) = \mathrm{argmax}_{\boldsymbol{\theta}}\, \ell(\boldsymbol{\theta})$
    where log-likelihood $\ell(\boldsymbol{\theta}) \equiv \log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \boldsymbol{\theta})$
  - maximizing log-likelihood = minimizing negative log-likelihood

$$\begin{aligned}\mathrm{NLL}(\boldsymbol{\theta}) &\equiv -\sum_{i=1}^{N} \log p(y_i|\mathbf{x}_i, \boldsymbol{\theta}) \\ &= -\sum_{i=1}^{N} \log \left[\left(\frac{1}{2\pi\sigma^2}\right)^{1/2} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{w}^\top \mathbf{x}_i)^2\right) \right] \\ &= \frac{1}{2\sigma^2}\mathrm{RSS}(\mathbf{w}) + \frac{N}{2}\log(2\pi\sigma^2)\end{aligned}$$

  - Residual sum of errors (sum of squared errors)
    $\mathrm{RSS}(\mathbf{w}) \equiv \sum_i (y_i - \mathbf{w}^\top \mathbf{x}_i)^2$





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Derivation of MLE

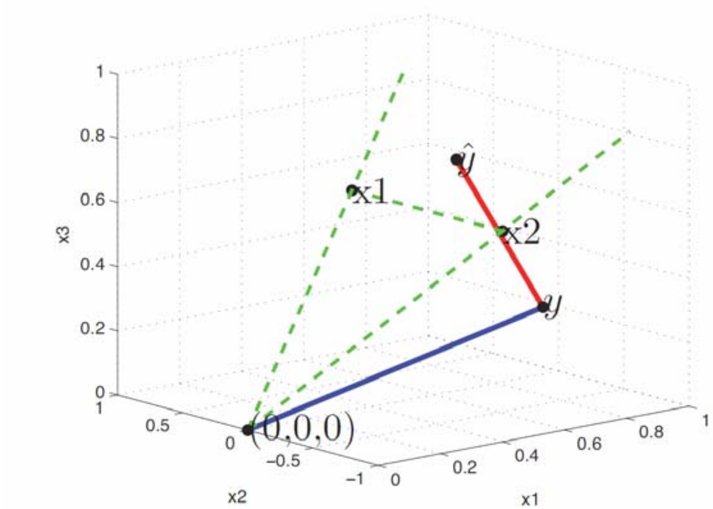
- Obtaining the least squares solution
  - $\mathrm{RSS}(\mathbf{w}) = (\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w})$
  $$= \mathbf{w}^\top(\mathbf{X}^\top\mathbf{X})\mathbf{w} - 2\mathbf{w}^\top(\mathbf{X}^\top\mathbf{y}) + \mathbf{y}^\top\mathbf{y}$$
  - where
  $$\mathbf{X} = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_N \end{pmatrix} \qquad \mathbf{X}^\top\mathbf{y} = \sum_{i=1}^{N} \mathbf{x}_i y_i$$
  $$\mathbf{X}^\top\mathbf{X} = \sum_{i=1}^{N} \mathbf{x}_i^\top \mathbf{x}_i = \sum_{i=1}^{N} \begin{pmatrix} x_{i,1}^2 & \cdots & x_{i,1}x_{i,D} \\ & \ddots & \\ x_{i,D}x_{i,1} & \cdots & x_{i,D}^2 \end{pmatrix}$$
  - gradient: $\mathbf{g}(\mathbf{w}) = \mathbf{X}^\top\mathbf{X}\mathbf{w} - \mathbf{X}^\top\mathbf{y}$
  - extreme point: $\mathbf{X}^\top\mathbf{X}\mathbf{w} = \mathbf{X}^\top\mathbf{y}$
  $$\hat{\mathbf{w}}_{\mathrm{OLS}} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$$

Geometric Interpretation

- Orthogonal projection
  - column vectors from the data $\mathbf{X} = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_N \end{pmatrix} = (\tilde{\mathbf{x}}_1 \cdots \tilde{\mathbf{x}}_D)$
  - target value vector $\mathbf{y} \in \mathbb{R}^N$
  - Linear regression = find vector $\hat{\mathbf{y}} = \mathrm{argmin}_{\hat{\mathbf{y}}} \|\mathbf{y} - \hat{\mathbf{y}}\|_2$ such that $\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} = w_1\tilde{\mathbf{x}}_1 + \cdots + w_D\tilde{\mathbf{x}}_D$

$$\Leftrightarrow \hat{\mathbf{y}} \in \mathrm{span}(\mathbf{X})$$

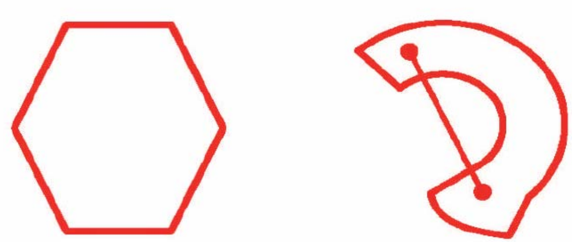
$$\Leftrightarrow \hat{\mathbf{y}} \in \mathrm{span}(\{\tilde{\mathbf{x}}_1, \ldots, \tilde{\mathbf{x}}_D\})$$



- residual vector should be orthogonal so that the norm is minimized:
  $\tilde{\mathbf{x}}_j^\top(\mathbf{y} - \hat{\mathbf{y}}) = 0 \Rightarrow \mathbf{X}^\top(\mathbf{y} - \mathbf{X}\mathbf{w}) = \mathbf{0}$
  $\Rightarrow \mathbf{w} = (\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$
- Also, $\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}(\mathbf{X}^\top\mathbf{X})^{-1}\mathbf{X}^\top\mathbf{y}$

Convexity

- negative log-likelihood of Gaussian:
  - $$\mathrm{NLL}(\boldsymbol{\theta}) = -\sum_{i=1}^{N} \log\left[\left(\frac{1}{2\pi\sigma^2}\right)^{1/2} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mathbf{w}^\top \mathbf{x}_i)^2\right)\right]$$
    $$= \frac{1}{2\sigma^2}\mathrm{RSS}(\mathbf{w}) + \frac{N}{2}\log(2\pi\sigma^2)$$
  - $\mathrm{RSS}(\mathbf{w}) \equiv \sum_i (y_i - \mathbf{w}^\top \mathbf{x}_i)^2$
- Convex set $\mathcal{S} : \forall \boldsymbol{\theta}, \boldsymbol{\theta}' \in \mathcal{S}, \forall \lambda \in [0,1],\ \lambda\boldsymbol{\theta} + (1-\lambda)\boldsymbol{\theta}' \in \mathcal{S}$
- Convex function $f(\boldsymbol{\theta})$
  - $\boldsymbol{\theta} \in \mathcal{S}$ (defined on a convex set)
  - $f(\lambda\boldsymbol{\theta} + (1-\lambda)\boldsymbol{\theta}') \leq \lambda f(\boldsymbol{\theta}) + (1-\lambda) f(\boldsymbol{\theta}')$
- convex functions are ideal for optimization



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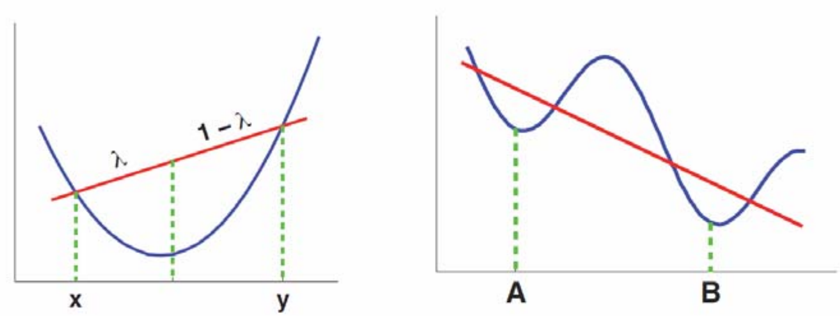
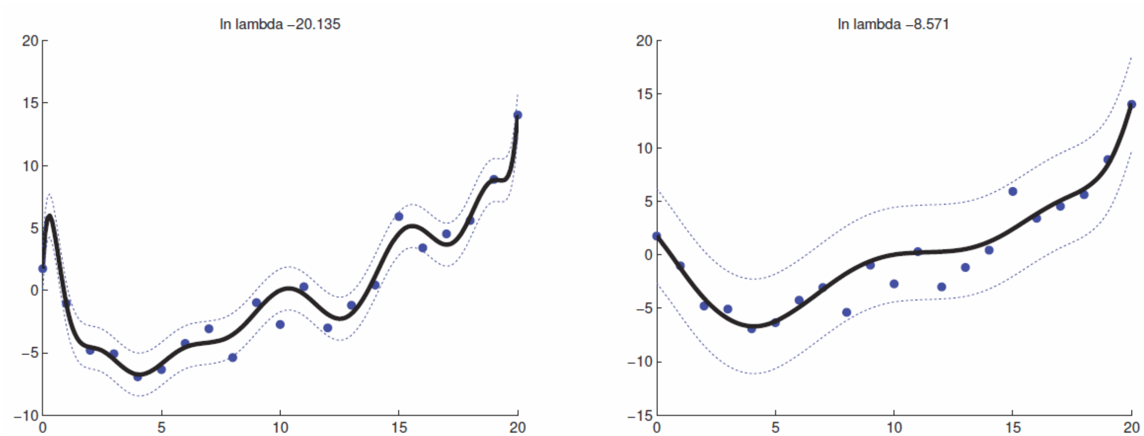


(a) (b)

Ridge Regression

- Overfitting is a common problem in higher-order regression
  - Smoother curve = Smaller parameters
    $p(\mathbf{w}) = \prod_j \mathcal{N}(w_j|0, \tau^2)$
  - MAP estimation
    $\operatorname{argmax}_{\mathbf{w}} \sum_{i=1}^{N} \log \mathcal{N}(y_i|\mathbf{w}^\top \mathbf{x}_i, \sigma^2) + \sum_{j=1}^{D} \log \mathcal{N}(w_j|0, \tau^2)$
    $= \operatorname{argmin}_{\mathbf{w}} \frac{1}{N} \sum_{i=1}^{N} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2 + \lambda \|\mathbf{w}\|_2^2$
  - Gaussian prior is equivalent to ℓ_2 regularization (i.e. weight decay)
- Ridge regression: $\hat{\mathbf{w}}_{\text{ridge}} = (\lambda \mathbf{I}_D + \mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$



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Bayesian Linear Regression

- ☐ want: full posterior over $\mathbf{w}$ and σ^2
  - assume σ^2 is known and focus on posterior over $\mathbf{w}$ only
  - likelihood: $p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \sigma^2) = \mathcal{N}(\mathbf{y}|\mathbf{X}\mathbf{w}, \sigma^2 \mathbf{I}_N)$
    $\propto \exp(-\frac{1}{2\sigma^2}(\mathbf{y} - \mathbf{X}\mathbf{w})^\top(\mathbf{y} - \mathbf{X}\mathbf{w}))$
  - use conjugate prior: $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_0, \mathbf{V}_0)$
  - compute posterior:

$$p(\mathbf{w}|\mathbf{X}, \mathbf{y}, \sigma^2) \propto \mathcal{N}(\mathbf{w}|\mathbf{w}_0, \mathbf{V}_0)\mathcal{N}(\mathbf{y}|\mathbf{X}\mathbf{w}, \sigma^2\mathbf{I}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_N, \mathbf{V}_N)$$

$$\mathbf{w}_N = \mathbf{V}_N \mathbf{V}_0^{-1}\mathbf{w}_0 + \frac{1}{\sigma^2}\mathbf{V}_N \mathbf{X}^\top \mathbf{y}$$

$$\mathbf{V}_N^{-1} = \mathbf{V}_0^{-1} + \frac{1}{\sigma^2}\mathbf{X}^\top \mathbf{X}$$

Bayesian Linear Regression

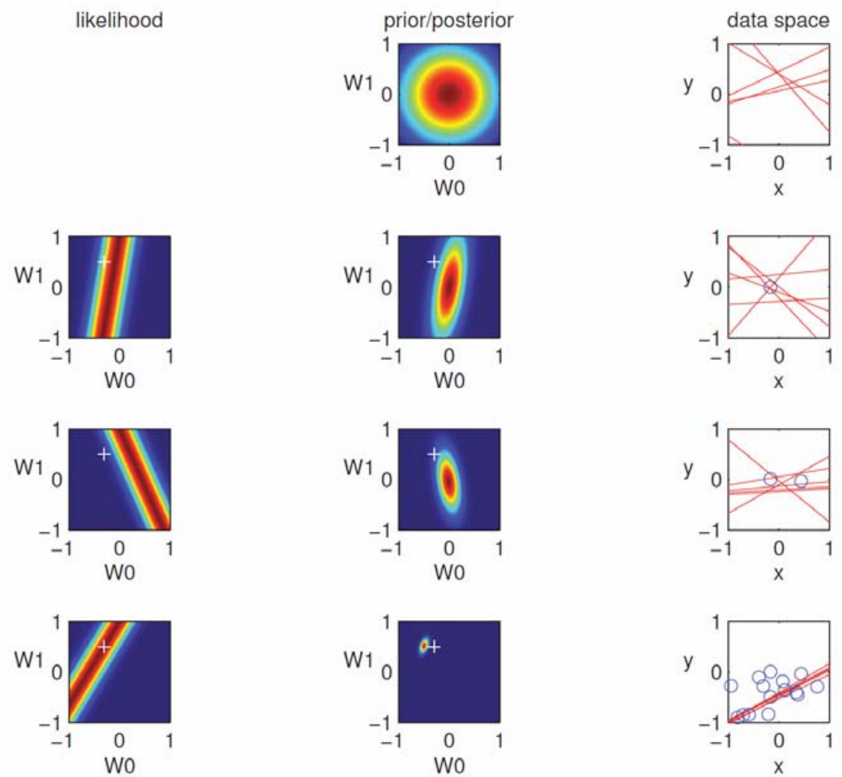
- posterior:

$$p(\mathbf{w}|\mathbf{X},\mathbf{y},\sigma^2) \propto \mathcal{N}(\mathbf{w}|\mathbf{w}_0,\mathbf{V}_0)\mathcal{N}(\mathbf{y}|\mathbf{X}\mathbf{w},\sigma^2\mathbf{I}) = \mathcal{N}(\mathbf{w}|\mathbf{w}_N,\mathbf{V}_N)$$

$$\mathbf{w}_N = \mathbf{V}_N\mathbf{V}_0^{-1}\mathbf{w}_0 + \frac{1}{\sigma^2}\mathbf{V}_N\mathbf{X}^\top\mathbf{y}$$

$$\mathbf{V}_N^{-1} = \mathbf{V}_0^{-1} + \frac{1}{\sigma^2}\mathbf{X}^\top\mathbf{X}$$

  - Ridge regression is a special case: $\mathbf{w}_0 = \mathbf{0}$ and $\mathbf{V}_0 = \tau^2\mathbf{I}$



Bayesian Linear Regression

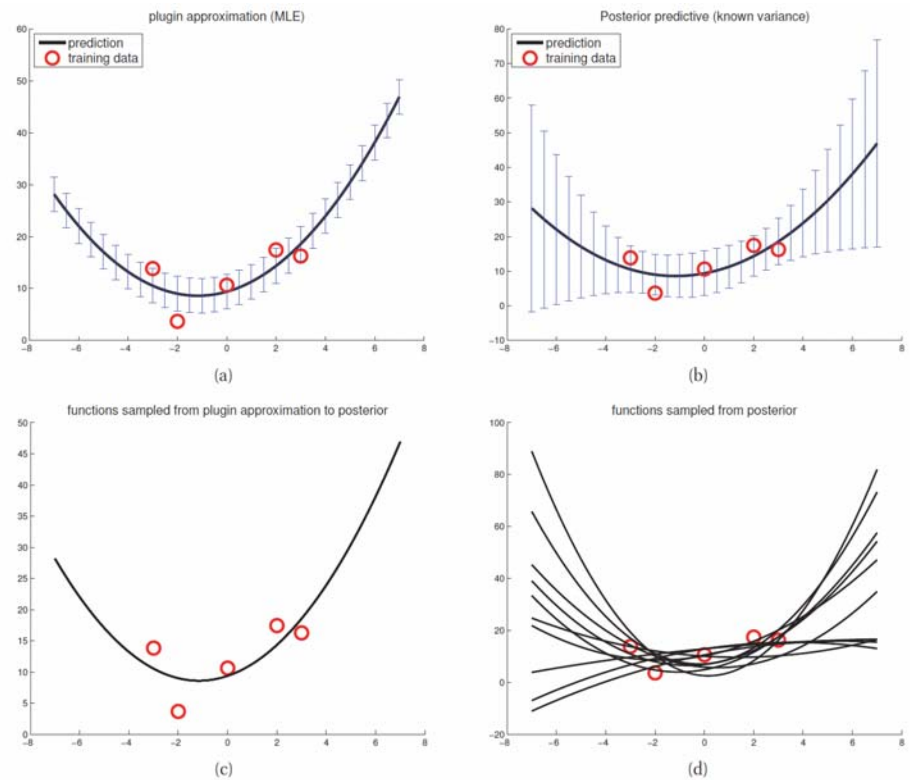
- Posterior predictive distribution:

$$
\begin{aligned}
p(y|\mathbf{x}, \mathcal{D}, \sigma^2) &= \int \mathcal{N}(y|\mathbf{x}^\top \mathbf{w}, \sigma^2)\mathcal{N}(\mathbf{w}|\mathbf{w}_N, \mathbf{V}_N)d\mathbf{w} \\
&= \mathcal{N}(y|\mathbf{w}_N^\top \mathbf{x}, \sigma_N^2(\mathbf{x}))
\end{aligned}
$$

$$
\sigma_N^2(\mathbf{x}) = \sigma^2 + \mathbf{x}^\top \mathbf{V}_N \mathbf{x}
$$

- Plug-in approximation (constant variance)

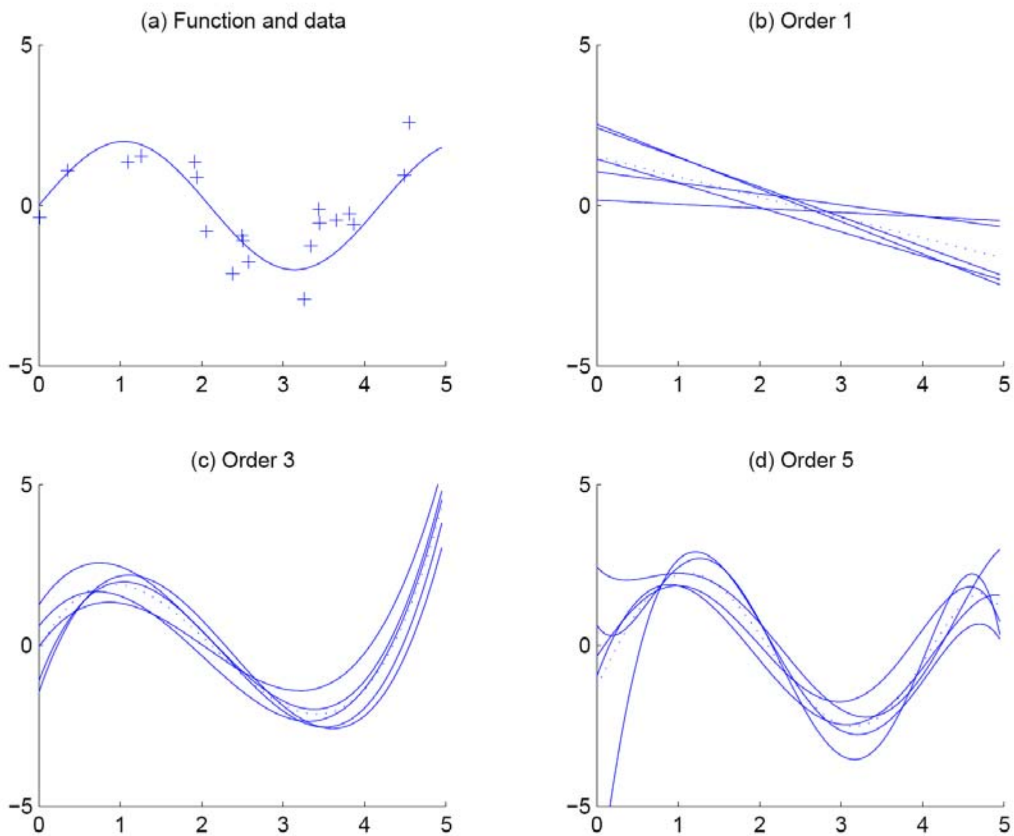
$$
\begin{aligned}
p(y|\mathbf{x}, \mathcal{D}, \sigma^2) & \\
&\approx \int \mathcal{N}(y|\mathbf{x}^\top \mathbf{w}, \sigma^2)\delta_{\hat{\mathbf{w}}}(\mathbf{w})d\mathbf{w} \\
&= \mathcal{N}(y|\mathbf{x}^\top \hat{\mathbf{w}}, \sigma^2)
\end{aligned}
$$



- Full PPD essential for active learning

Model Selection

- Linear regression extends to non-linear regression by basis expansion:
  - $p(y|\mathbf{x}, \boldsymbol{\theta}) = \mathcal{N}(y|\mathbf{w}^\top \boldsymbol{\phi}(\mathbf{x}), \sigma^2) \quad \text{e.g. } \boldsymbol{\phi}(\mathbf{x}) = [1, x_1, x_2, x_1^2, x_2^2]$



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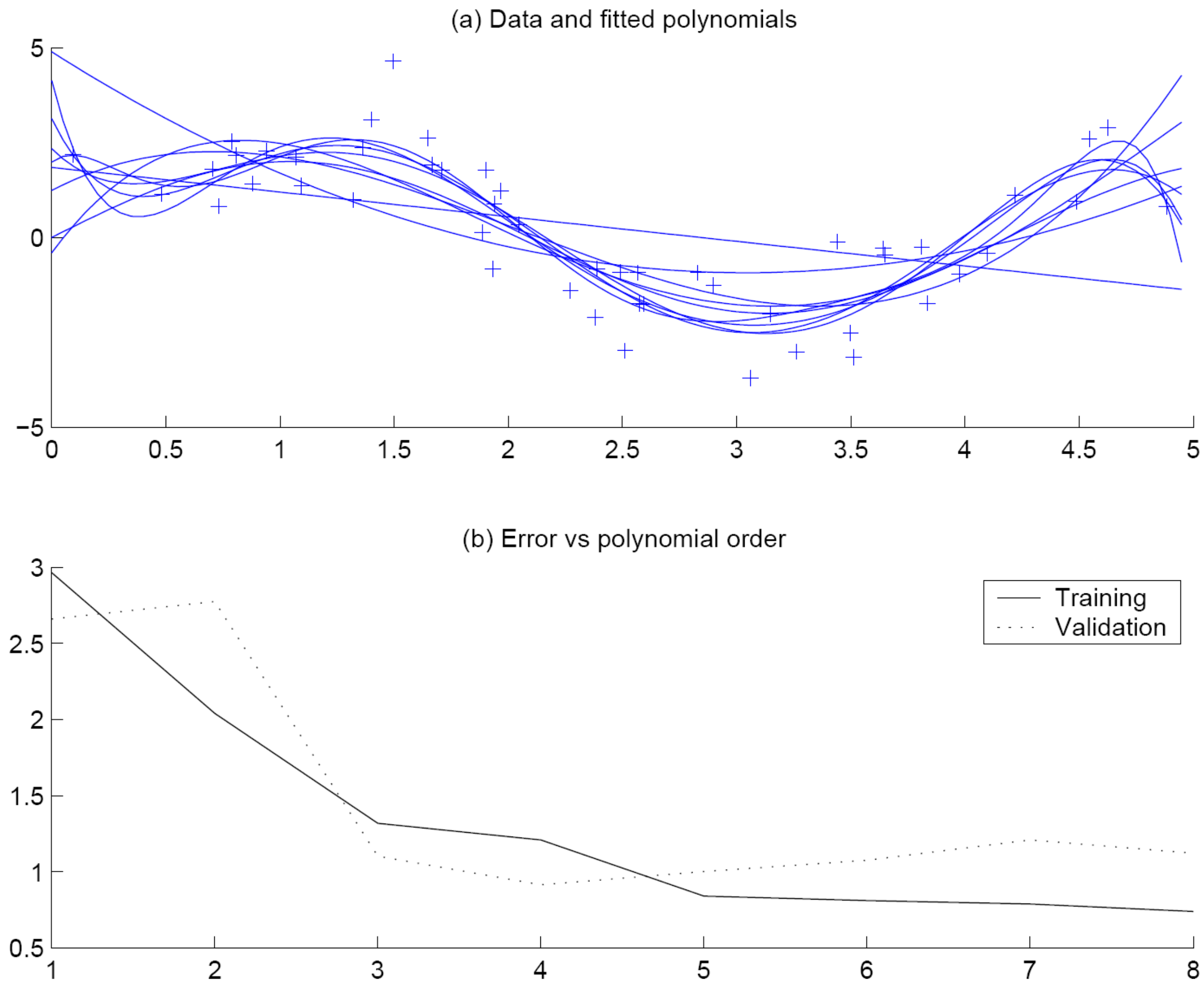
Model Selection Techniques

- Cross-validation
  - Measure generalization accuracy by testing on data unused during training
- Regularization
  - Penalize complex models
  - E' = error on data + λ model complexity
  - Akaike's information criterion (AIC), Bayesian information criterion (BIC), Mimimum description length (MDL)
- Structural risk minimization (SRM)
  - Foundation of support vector machines
- Bayesian model selection
  - Suppose we have prior on models, p(model)
  - P(model|data) = p(data|model) p(model) / p(data)
  - If prior favors simpler models, it is a regularization

Model Selection Procedures

- Cross-validation



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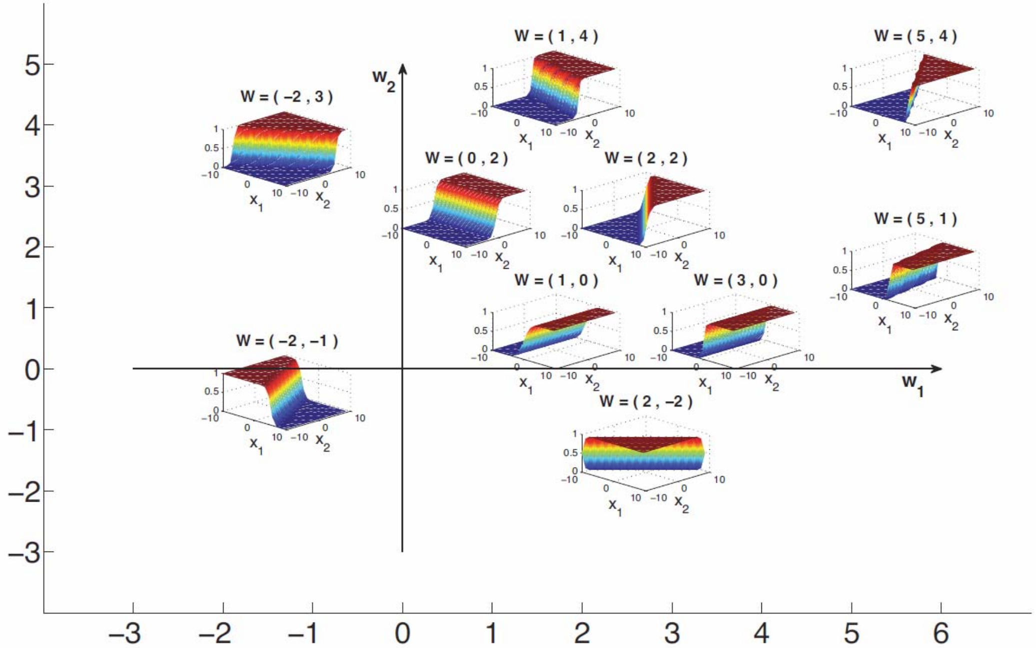
Logistic Regression (Classification)

- Generative vs. Discriminative approach to $p(y|\mathbf{x})$
  - Generative: estimate likelihood $p(\mathbf{x}|y)$ and use Bayes rule
  - Discriminative: fit $p(y|\mathbf{x})$ directly from data

- Logistic regression for binary classification
  - $p(y|\mathbf{x}, \mathbf{w}) = \mathrm{Ber}(y|\mathrm{sigm}(\mathbf{w}^\top \mathbf{x}))$ and estimate $\mathbf{w}$ from data



Maximum Likelihood Estimation

- Minimize negative log-likelihood (NLL)
  - $$\begin{aligned}\mathrm{NLL}(\mathbf{w}) &= -\sum_{i=1}^{N} \log[\mu_i^{\mathbb{I}(y_i=1)} \times (1-\mu_i)^{\mathbb{I}(y_i=0)}] \\ &= -\sum_i [y_i \log \mu_i + (1-y_i)\log(1-\mu_i)]\end{aligned}$$

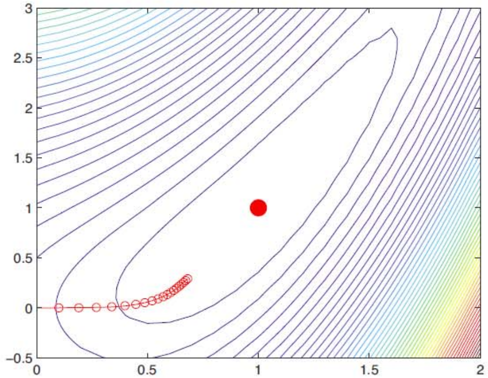
  where $\mu_i = \mathrm{sigm}(\mathbf{w}^\top \mathbf{x}_i)$

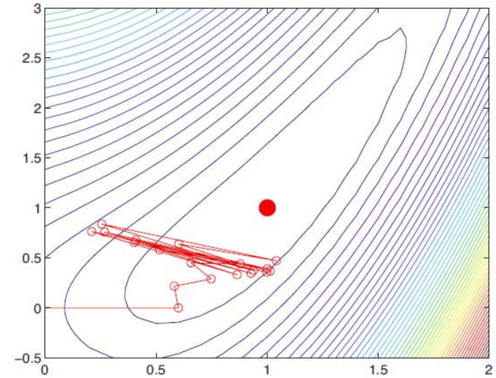
- Use an optimization algorithm to minimize NLL
  - $\mathbf{g} = \frac{d}{d\mathbf{w}}\mathrm{NLL}(\mathbf{w}) = \sum_i (\mu_i - y_i)\mathbf{x}_i = \mathbf{X}^\top(\boldsymbol{\mu} - \mathbf{y})$
  - $\mathbf{H} = \frac{d}{d\mathbf{w}}\mathbf{g}(\mathbf{w})^\top = \sum_i (\nabla_{\mathbf{w}}\mu_i)\mathbf{x}_i^\top = \sum_i \mu_i(1-\mu_i)\mathbf{x}_i\mathbf{x}_i^\top = \mathbf{X}^\top\mathbf{S}\mathbf{X}$

  where $\mathbf{S} \equiv \mathrm{diag}(\mu_i(1-\mu_i))$

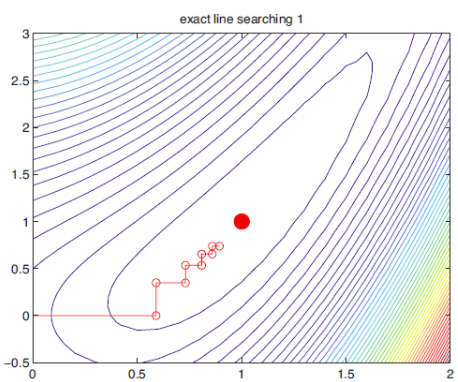
Steepest Descent

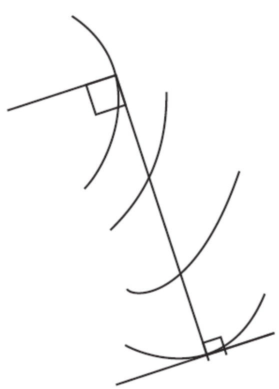
- Also known as gradient descent: $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta_k \mathbf{g}_k$





- Line search
  - from Taylor expansion: $f(\boldsymbol{\theta} + \eta \mathbf{d}) \approx f(\boldsymbol{\theta}) + \eta \mathbf{g}^\top \mathbf{d}$
  - minimize $\phi(\eta) = f(\boldsymbol{\theta}_k + \eta \mathbf{d}_k)$ for obtaining the step size





- Momentum to reduce zig-zag

$$\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta_k \mathbf{g}_k + \mu_k(\boldsymbol{\theta}_k - \boldsymbol{\theta}_{k-1})$$

(a.k.a. heavy ball method)

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Newton's Method

☐ Second order optimization method (use hessian)

- $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta_k \mathbf{H}_k^{-1} \mathbf{g}_k$

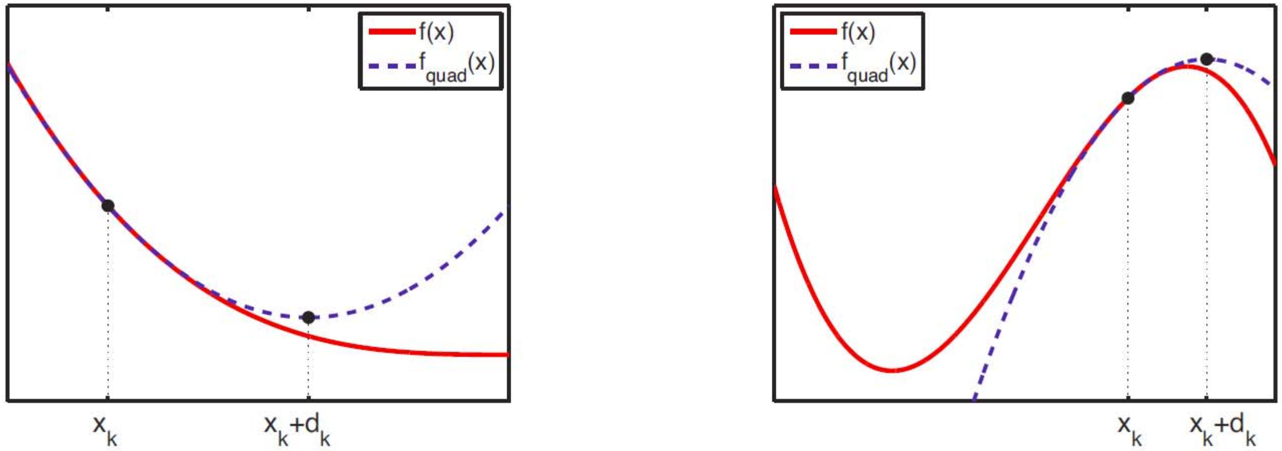
- Consider second-order Taylor expansion:

$$f(\boldsymbol{\theta}) \approx f_k + \mathbf{g}_k^\top (\boldsymbol{\theta} - \boldsymbol{\theta}_k) + \frac{1}{2} (\boldsymbol{\theta} - \boldsymbol{\theta}_k)^\top \mathbf{H}_k (\boldsymbol{\theta} - \boldsymbol{\theta}_k)$$

$$= \boldsymbol{\theta}^\top \mathbf{A} \boldsymbol{\theta} + \mathbf{b}^\top \boldsymbol{\theta} + c$$

where $\mathbf{A} = \frac{1}{2}\mathbf{H}_k, \ \mathbf{b} = \mathbf{g}_k - \mathbf{H}_k \boldsymbol{\theta}_k, \ c = f_k - \mathbf{g}_k^\top \boldsymbol{\theta}_k + \frac{1}{2} \boldsymbol{\theta}_k^\top \mathbf{H}_k \boldsymbol{\theta}_k$

- Minimum: $\boldsymbol{\theta} = -\frac{1}{2}\mathbf{A}^{-1}\mathbf{b} = \boldsymbol{\theta}_k - \mathbf{H}_k^{-1} \mathbf{g}_k$



Regularization

- For linearly separable training data, MLE yields $\|\mathbf{w}\| \to \infty$
  - Linear threshold unit $\mathbb{I}(\mathbf{w}^\top \mathbf{x} \geq w_0)$ assigning maximal probability mass to the training data
  - Brittle and does not generalize well

- Regularized objective function
  - $$f'(\mathbf{w}) = \mathrm{NLL}(\mathbf{w}) + \lambda \mathbf{w}^\top \mathbf{w}$$
    $$\mathbf{g}'(\mathbf{w}) = \mathbf{g}(\mathbf{w}) + \lambda \mathbf{w}$$
    $$\mathbf{H}'(\mathbf{w}) = \mathbf{H}(\mathbf{w}) + \lambda \mathbf{I}$$

Multi-Class Logistic Regression

- i.e. multinomial logistic regression, maximum entropy classifier:

$$p(y = c|\mathbf{x}, \mathbf{W}) = \frac{\exp(\mathbf{w}_c^\top \mathbf{x})}{\sum_{c'=1}^{C} \exp(\mathbf{w}_{c'}^\top \mathbf{x})}$$

- Optimization:
  - $\mu_{ic} \equiv p(y_i = c|\mathbf{x}_i, \mathbf{W})$
  - $y_{ic} \equiv \mathbb{I}(y_i = c)$
  - $\mathrm{NLL}(\mathbf{W}) = -\log \prod_{i=1}^{N} \prod_{c=1}^{C} \mu_{ic}^{y_{ic}} = -\sum_i \sum_c y_{ic} \log \mu_{ic}$
    $= -\sum_i \left[\sum_c y_{ic} \mathbf{w}_c^\top \mathbf{x}_i - \log \sum_{c'} \exp(\mathbf{w}_{c'}^\top \mathbf{x}_i)\right]$
  - Compute gradient and hessian:

$$\mathbf{g}_c(\mathbf{W}) = \nabla_{\mathbf{w}_c} \mathrm{NLL}(\mathbf{W}) = \sum_i (\mu_{ic} - y_{ic}) \mathbf{x}_i$$

$$\mathbf{H}_{c,c'}(\mathbf{W}) = \sum_i \mu_{ic} (\delta_{c,c'} - \mu_{i,c'}) \mathbf{x}_i \mathbf{x}_i^\top$$

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Extending to Bayesian...

- Want $p(\mathbf{w}|\mathcal{D})$ but no conjugate prior $p(\mathbf{w})$
  - MCMC, variational inference, ...

- Laplace approximation
  - Generally, posterior can be re-written $p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z}\exp(-E(\boldsymbol{\theta}))$ using energy function $E(\boldsymbol{\theta}) \equiv -\log p(\boldsymbol{\theta}, \mathcal{D})$
  - Taylor expansion of the energy function around mode:

$$E(\boldsymbol{\theta}) \approx E(\boldsymbol{\theta}^*) + (\boldsymbol{\theta} - \boldsymbol{\theta}^*)^\top \mathbf{g} + \tfrac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)^\top \mathbf{H}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$$
$$= E(\boldsymbol{\theta}^*) + \tfrac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)^\top \mathbf{H}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)$$

  - This leads to *Gaussian approximation* to the posterior:

$$\hat{p}(\boldsymbol{\theta}|\mathcal{D}) \approx \frac{1}{Z} e^{-E(\boldsymbol{\theta}^*)} \exp\left[-\frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)^\top \mathbf{H}(\boldsymbol{\theta} - \boldsymbol{\theta}^*)\right] = \mathcal{N}(\boldsymbol{\theta}|\boldsymbol{\theta}^*, \mathbf{H}^{-1})$$

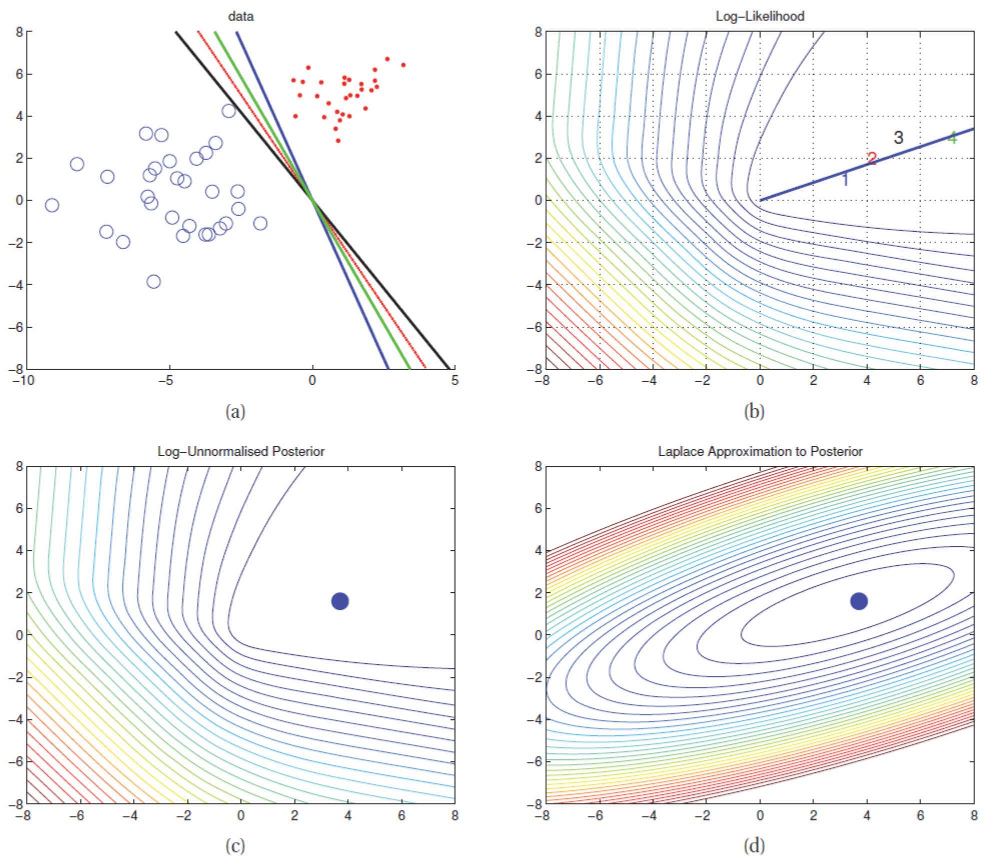
$$Z \approx p(\mathcal{D}) = e^{-E(\boldsymbol{\theta}^*)}(2\pi)^{D/2}|H|^{-\frac{1}{2}}$$

Bayesian Logistic Regression

- Laplace approximation with prior $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{V}_0)$

$$p(\mathbf{w}|\mathcal{D}) \approx \mathcal{N}(\mathbf{w}|\hat{\mathbf{w}}, \mathbf{H}^{-1})$$

  - $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w}} E(\mathbf{w}), \;\; E(\mathbf{w}) = -(\log p(\mathcal{D}|\mathbf{w}) + \log p(\mathbf{w}))$
  - $\mathbf{H} = \nabla^2 E(\mathbf{w})|_{\hat{\mathbf{w}}}$



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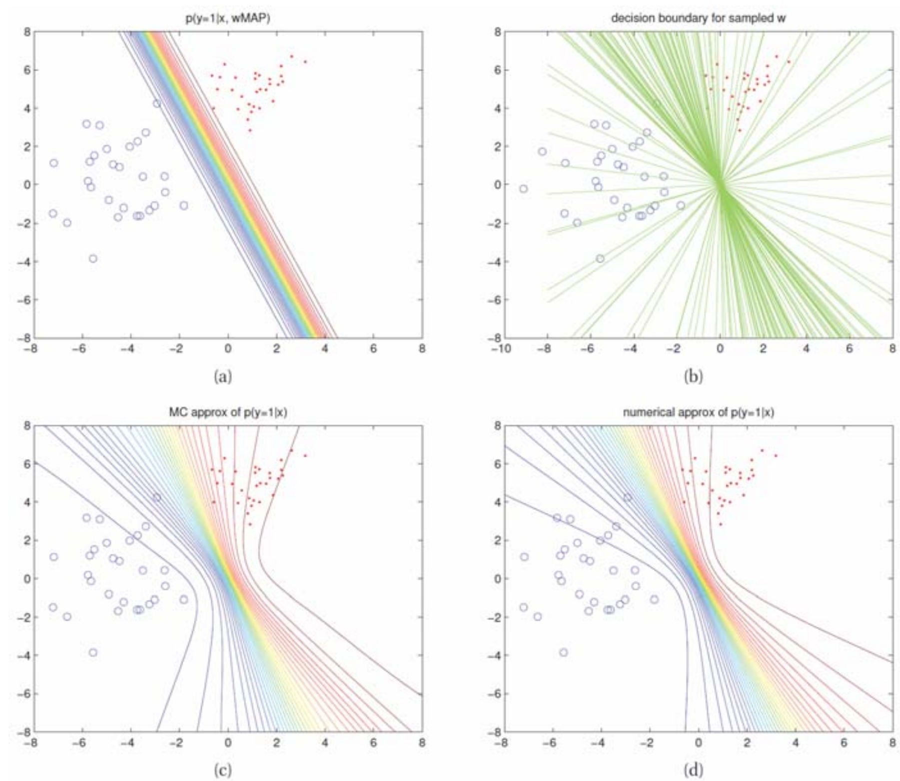
Posterior Predictive Distribution

- ☐ Want: $p(y|\mathbf{x}, \mathcal{D}) = \int p(y|\mathbf{x}, \mathbf{w})p(\mathbf{w}|\mathcal{D})d\mathbf{w}$

- ☐ MAP approximation: $p(y|\mathbf{x}, \mathcal{D}) \approx p(y|\mathbf{x}, \mathbf{w}_{\mathrm{MAP}})$
- ☐ Monte-Carlo approximation: using samples $\mathbf{w}^s \sim p(\mathbf{w}|\mathcal{D})$
  - $p(y=1|\mathbf{x}, \mathcal{D}) \approx \frac{1}{S}\sum_{s=1}^{S} p(y=1|\mathbf{x}, \mathbf{w}^s) = \frac{1}{S}\sum_{s=1}^{S} \mathrm{sigm}((\mathbf{w}^s)^\top \mathbf{x})$



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Extras

* Derivation of BIC

- From $Z \approx p(\mathcal{D}) = e^{-E(\boldsymbol{\theta}^*)}(2\pi)^{D/2}|H|^{-\frac{1}{2}}$
  - we can rewrite:
    $$\log p(\mathcal{D}) \approx \log p(\mathcal{D}, \boldsymbol{\theta}^*) - \frac{1}{2}\log|\mathbf{H}|$$
    $$= \log p(\mathcal{D}|\boldsymbol{\theta}^*) + \log p(\boldsymbol{\theta}^*) - \frac{1}{2}\log|\mathbf{H}|$$
  - Occam's factor: $\log p(\boldsymbol{\theta}^*) - \frac{1}{2}\log|\mathbf{H}|$
    - If we use uniform prior, then the first term can be ignored and $\boldsymbol{\theta}^* = \hat{\boldsymbol{\theta}}_{\mathrm{MLE}}$
  - $\mathbf{H} = \sum_{i=1}^{N} \mathbf{H}_i = \sum_{i=1}^{N} \nabla\nabla \log p(\mathcal{D}_i|\boldsymbol{\theta})$
    - If $\mathbf{H}_i \approx \hat{\mathbf{H}}$, then
      $$\log|\mathbf{H}| \approx \log|N\hat{\mathbf{H}}| = \log N^d|\hat{\mathbf{H}}| = D\log N + \log|\hat{\mathbf{H}}|$$
      where $D = \dim(\boldsymbol{\theta})$

- Hence $p(\mathcal{D}) \approx \log p(\mathcal{D}|\hat{\boldsymbol{\theta}}_{\mathrm{MLE}}) - \dfrac{D}{2}\log N$

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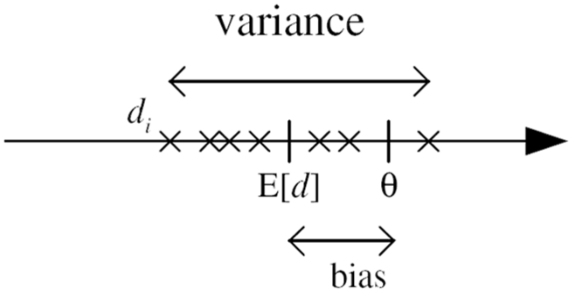
Bias and Variance of Estimators

- How do we measure the goodness of our estimators?
  - View estimators as learning algorithms
  - Evaluate output of the algorithm on all possible training data
  - More formally, training data is sampled according to $p(\mathcal{D})$
  - The "desired" response for an input: $y^*(x) = E_{p(y|x)}[y]$
- Questions to be asked are:
  - **Bias**: How accurate (on average) are the model predictions?
    - We want the bias to be as small as possible
  - **Variance**: How spread out are the model predictions?
    - We also want the variance to be as small as possible (less subject to noise in the data and initial setting parameter)



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Bias-Variance Decomposition

- Mean square error at input x: $E_{p(\mathcal{D})}[(g(x|\theta) - r^*(x))^2]$
  - Denote $r_{\mathcal{D}}(x) = g(x|\theta)$
  - $E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - r^*(x))^2]$

$$
\begin{aligned}
&= E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] + E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))^2] \\
&= E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)])^2 + (E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))^2 \\
&\qquad\qquad\qquad + 2(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)])(E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))] \\
&= E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)])^2] + E_{p(\mathcal{D})}[(E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))^2] \\
&\quad + 2E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)])(E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))] \\
&= E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)])^2] + (E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))^2 \\
&\quad + 2E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)])](E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x)) \\
&= \underbrace{E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D}))}[r_{\mathcal{D}}(x)])^2]}_{\text{Variance at x}} + \underbrace{(E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))^2}_{\text{Bias}^2\text{ at x}}
\end{aligned}
$$

Estimating Bias and Variance

- From bias-variance decomposition:
  - $$E_{p(x)}\left[E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - r^*(x))^2]\right]$$
    $$= E_{p(x)}\left[E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)])^2]\right]$$
    $$+ E_{p(x)}\left[(E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))^2\right]$$
  - Generate M additional training sets, each with size N
    - $\mathcal{D}_i = \{x_i^t, r_i^t\}, i = 1, \ldots, M$
  - Use $\mathcal{D}_i$ to fit $g_i(x|\theta)$
  - Now we have:
    - $\mathrm{Bias}^2(g) = \frac{1}{N}\sum_t [\bar{g}(x^t) - f(x^t)]^2$
    - $\mathrm{Variance}(g) = \frac{1}{NM}\sum_t \sum_i [g_i(x^t) - \bar{g}(x^t)]^2$
    - where $\bar{g}(x) = \frac{1}{M}\sum_i g_i(x)$
  - In reality, you can’t compute because you don’t know f!

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Bias-Variance Dilemma

- From bias-variance decomposition:

$$
\begin{aligned}
&E_{p(x)}\left[E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - r^*(x))^2]\right] \\
&\qquad = E_{p(x)}\left[E_{p(\mathcal{D})}[(r_{\mathcal{D}}(x) - E_{p(\mathcal{D})}[r_{\mathcal{D}}(x)])^2]\right] \\
&\qquad\quad + E_{p(x)}\left[(E_{P(\mathcal{D})}[r_{\mathcal{D}}(x)] - r^*(x))^2\right]
\end{aligned}
$$

- Example:
  - Constant function with no parameter to learn: $g(x) = 2$
    - High bias and no variance
  - Constant function with one parameter to learn: $g(x) = \sum_t r^t / N$
    - Lower bias with some variance
- As we increase complexity of the model (e.g. const -> linear -> poly)
  - Bias decreases (a better fit to the data)
  - Variance increases (fit varies more with data)
- This is called Bias-Variance dilemma (Geman et al., 1992)

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Model Complexity and Bias-Variance