Regularization

- L0 - Count of the non-zero weights – Difficult minimize
- L1 Lasso - Sum of the attribute weights
  - It set the weights to 0 for irrelevant attributes

$$\sum_{i=1}^{n}(Y_i - \sum_{j=1}^{p} X_{ij}\beta_j)^2 + \lambda\sum_{j=1}^{p}|\beta_j|$$

- L2 Ridge (Squared Euclidean norm) - Sum of the squared attribute weights. Used to avoid Overfiiting.

$$\sum_{i=1}^{n}(y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda\sum_{j=1}^{p}\beta_j^2$$

Scaling:

- Min/Max normalization: $x^{new} = \frac{x - x_{\min}}{x_{\max} - x_{\min}}(x_{\max}^{new} - x_{\min}^{new}) + x_{\min}^{new}$
- Z-Score normalisierung: $x^{new} = \frac{x - \mu_x}{\sigma_x}$
- Decimal scaling: $x^{new} = |x| \cdot 10^a \quad a = \max_x\{i \in \mathbb{Z} \mid |x| \cdot 10^i < 1\}$
- Logarithmic scaling: $x^{new} = \log_a x$

Information Gain

Entropy is the expected information of a message.

- $H(y) = -\sum_{v=1}^{k} p(y = v)\log_2 p(y = v)$

Loan	x_1 (Credit report)	x_2 (Employment last 3 months)	x_3 (Collateral > 50% loan)	y (Payed back in full)
1	Positive	Yes	No	Yes
2	Positive	No	Yes	Yes
3	Positive	No	No	No
4	Negative	No	Yes	No
5	Negative	Yes	No	No

$$H_L(y|x_1 = n) = -\tfrac{2}{2}\log_2\tfrac{2}{2} - \tfrac{0}{2}\log_2\tfrac{0}{2} = 0bit$$

Information Gain of an Attribute

- Reduction of entropy by splitting the data along an attribute
  - $G_L(x_j) = H_L(y) - \sum_{v=1}^{k} p_L(x_j = v)H_L(y|x_j = v)$

Loan	x_1 (Credit report)	x_2 (Employment last 3 months)	x_3 (Collateral > 50% loan)	y (Payed back in full)
1	Positive	Yes	No	Yes
2	Positive	No	Yes	Yes
3	Positive	No	No	No
4	Negative	No	Yes	No
5	Negative	Yes	No	No

- $G_L(x_1) = H_L(y) - p_L(x_1 = p)H_L(y|x_1 = p) - p_L(x_1 = n)H_L(y|x_1 = n)$
  $= 0.97 - \tfrac{3}{5}0.91 - \tfrac{2}{5}0 = 0.42bit$
- Splitting along x_1 reduces the uncertainty regarding the class label y by 0.42 bit.

Idea: factor the information that is contained in the attribute values into the decision

- $H_L(x_j) = -\sum_{v=1}^{k} p_L(x_j = v)\log_2 p_L(x_j = v)$

Information gain ratio:

- $GR_L(x_j) = \frac{G_L(x_j)}{H_L(x_j)}$

ID3

```
ID3(L, X)
1. If all data in L have same class y or X={}, then
   return leaf node with majority class y.
2. Else
   1. For all attributes $x_j \in X$, calculate split
      criterion $G_L(x_j)$ or $GR_L(x_j)$.
   2. Choose attribute $x_j \in X$ with highest $G_L(x_j)$ or
      $GR_L(x_j)$.
   3. Let $L_i = \{(x,y) \in L: x_j = i\}$.
   4. Return test node with attribute $x_j$ and children
      ID3($L_1$, $X \setminus x_j$), …, ID3($L_k$, $X \setminus x_j$).
```

C4.5

Learning Decision Trees with C4.5

```
C4.5(L)
1. If all data in L have same class y or are identical, then
   return leaf node with majority class y.
2. Else
   1. For all discrete attributes $x_j \in X$: calculate $G_L(x_j)$.
   2. For all continuous attributes $x_j \in X$ and all values v
      that occur for $x_j$ in L: calculate $G_L(x_j \le v)$.
   3. If discrete attribute has highest $G_L(x_j)$:
      1. Let $L_i = \{(x,y) \in L: x_j = i\}$.
      2. Return test node with attribute $x_j$ and children
         C4.5($L_1$), …, C4.5($L_k$).
   4. If continuous attribute has highest $G_L(x_j \le v)$:
      1. Let $L_\le = \{(x,y) \in L: x_j \le v\}$, $L_> = \{(x,y) \in L: x_j > v\}$
      2. Return test node with test $x_j \le v$ and children
         C4.5($L_\le$), C4.5($L_>$).
```

Regression Trees

- Variance of the target attribute on sample L:
  - $Var(L) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \bar{y})^2$
- Variance = MSE of predicting the mean value.
- Splitting criterion: variance reduction of $[x_j \le v]$:
  - $R_L[x_j \le v]$
    $= Var(L) - \frac{n_{[x_j \le v]}}{n} Var\left(L_{[x_j \le v]}\right) - \frac{n_{[x_j > v]}}{n} Var\left(L_{[x_j > v]}\right)$
- Stopping criterion:
  - Do not create a new test node if $nVar(L) \le \tau$.

```
CART(L)
1. If $\sum_{i=1}^{n}(y_i - \bar{y})^2 < \tau$, then return leaf node with prediction $\bar{y}$.
2. Else
   1. For all discrete attributes $x_j \in X$: calculate $R_L(x_j)$.
   2. For all continuous attributes $x_j \in X$ and all values v
      that occur for $x_j$ in L: calculate $R_L(x_j \le v)$.
   3. If discrete attribute has highest $R_L(x_j)$:
      1. Let $L_i = \{(x,y) \in L: x_j = i\}$.
      2. Return test node with attribute $x_j$ and children
         CART($L_1$), …, CART($L_k$).
   4. If continuous attribute has highest $R_L(x_j \le v)$:
      1. Let $L_\le = \{(x,y) \in L: x_j \le v\}$, $L_> = \{(x,y) \in L: x_j > v\}$
      2. Return test node with test $x_j \le v$ and children
         CART($L_\le$), CART($L_>$).
```

Random Forest

```
▪ Input: sample L of size n, attributes X.
1. For $i$=1…k
   1. Draw n instances uniformly with
      replacement from L into set $L_i$.
   2. Draw m attributes from all attributes X
      into $X_i$.
   3. Learn model $f_i$ on sample $L_i$ using
      attributes $X_i$.
2. For classification:
   1. Let $f(\mathbf{x})$ be the majority vote among
      $(f_1(\mathbf{x}), \dots, f_k(\mathbf{x}))$.
3. For regression:
   1. Let $f(\mathbf{x}) = \frac{1}{k}\sum_{i=1}^{k} f_i(\mathbf{x})$.
```

Loss in Classification

- Zero-one loss:

$$\ell_{0/1}(f_\theta(\mathbf{x}_i), y_i) = \begin{cases} 1 & -y_i f_\theta(\mathbf{x}_i) > 0 \\ 0 & -y_i f_\theta(\mathbf{x}_i) \le 0 \end{cases}$$

$\text{sign}(f_\theta(\mathbf{x}_i)) \ne y_i$; $\text{sign}(f_\theta(\mathbf{x}_i)) = y_i$

- Logistic loss:

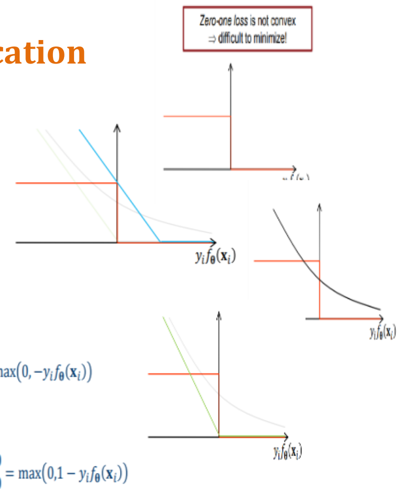
$$\ell_{log}(f_\theta(\mathbf{x}_i), y_i) = \log\left(1 + e^{-y_i f_\theta(\mathbf{x}_i)}\right)$$

- Perceptron loss:

$$\ell_p(f_\theta(\mathbf{x}_i), y_i) = \begin{cases} -y_i f_\theta(\mathbf{x}_i) & -y_i f_\theta(\mathbf{x}_i) > 0 \\ 0 & -y_i f_\theta(\mathbf{x}_i) \le 0 \end{cases} = \max(0, -y_i f_\theta(\mathbf{x}_i))$$

- Hinge loss:

$$\ell_h(f_\theta(\mathbf{x}_i), y_i) = \begin{cases} 1 - y_i f_\theta(\mathbf{x}_i) & 1 - y_i f_\theta(\mathbf{x}_i) > 0 \\ 0 & 1 - y_i f_\theta(\mathbf{x}_i) \le 0 \end{cases} = \max(0, 1 - y_i f_\theta(\mathbf{x}_i))$$



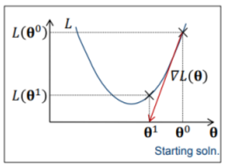
Gradient descent

Linear classification model: minimize

$$L(\theta) = \sum_{i=1}^{n} \ell(\mathbf{x}^{\mathrm{T}}\theta, y_i) + \lambda\,\Omega(\theta)$$

Gradient descent method:

```
RegERM(Data: $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$)
  Set $\theta^0 = \mathbf{0}$ and $t = 0$
  DO
      Compute gradient $\nabla L(\theta^t)$
      Compute step size $\alpha^t$
      Set $\theta^{t+1} = \theta^t - \alpha^t \nabla L(\theta^t)$
      Set $t = t + 1$
  WHILE $\|\theta^t - \theta^{t+1}\| > \varepsilon$
RETURN $\theta^t$
```



with Step size (line search)

Determine step size through line search:

```
RegERM-LineSearch(Data: $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$)
  Set $\theta^0 = \mathbf{0}$ and $t = 0$
  DO
      Compute gradient $\nabla L(\theta^t)$
      Choose step size $\alpha^t$:
          $\alpha^t = \underset{\alpha > 0}{\operatorname{argmin}}\, L(\theta^t - \alpha \nabla L(\theta^t))$
      Set $\theta^{t+1} = \theta^t - \alpha^t \nabla L(\theta^t)$
      Set $t = t + 1$
  WHILE $\|\theta^t - \theta^{t+1}\| > \varepsilon$
RETURN $\theta^t$
```

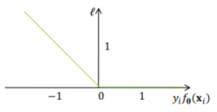
Stochastic Gradient descent

```
RegERM-Stoch(Data: $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$)
  Set $\theta^0 = \mathbf{0}$ and $t = 0$
  DO
      Shuffle data randomly
      FOR $i = 1, \dots, n$
          Compute subset gradient $\nabla_{\mathbf{x}_i} L(\theta^t)$
          Compute step size $\alpha^t$
          Set $\theta^{t+1} = \theta^t - \alpha^t \nabla_{\mathbf{x}_i} L(\theta^t)$
          Set $t = t + 1$
      END
  WHILE $\|\theta^t - \theta^{t+1}\| > \varepsilon$
RETURN $\theta^t$
```

Perceptron

Loss function:

$$\ell_p(f_\theta(\mathbf{x}_i), y_i) = \begin{cases} -y_i f_\theta(\mathbf{x}_i) & -y_i f_\theta(\mathbf{x}_i) > 0 \\ 0 & -y_i f_\theta(\mathbf{x}_i) \le 0 \end{cases} = \max(0, -y_i f_\theta(\mathbf{x}_i))$$



```
Perceptron(Instances $\{(\mathbf{x}_i, y_i)\}$)
  Set $\theta = \mathbf{0}$
  DO
     FOR $i = 1, \dots, n$
        IF   $y_i f_\theta(\mathbf{x}_i) \le 0$
        THEN $\theta = \theta + y_i \mathbf{x}_i$
     END
  WHILE $\theta$ changes
  RETURN $\theta$
```

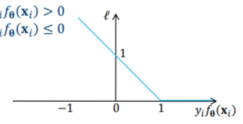
Stochastic gradient method:

- $\nabla L_{\mathbf{x}_i}(\theta) = \begin{cases} -y_i \mathbf{x}_i & -y_i f_\theta(\mathbf{x}_i) > 0 \\ 0 & -y_i f_\theta(\mathbf{x}_i) < 0 \end{cases}$

SVM

Loss function:

- $\ell_h(f_\theta(\mathbf{x}_i), y_i) = \begin{cases} 1 - y_i f_\theta(\mathbf{x}_i) & \text{if } 1 - y_i f_\theta(\mathbf{x}_i) > 0 \\ 0 & \text{if } 1 - y_i f_\theta(\mathbf{x}_i) \le 0 \end{cases}$
  $= \max(0, 1 - y_i f_\theta(\mathbf{x}_i))$



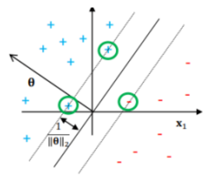
Regularizer:

- $\Omega_2(\theta) = \theta^T\theta = \sum_{j=1}^m |\theta_j|^2 = \|\theta\|_2^2$

Loss function is 0, if…

$$\sum_{i=1}^n \max(0, 1 - y_i f_\theta(\mathbf{x}_i)) = 0$$
$$\Leftrightarrow \forall_{i=1}^n : y_i f_\theta(\mathbf{x}_i) \ge 1$$
$$\Leftrightarrow \forall_{i=1}^n : y_i \mathbf{x}_i^T \theta \ge 1$$
$$\Leftrightarrow \forall_{i=1}^n : y_i \mathbf{x}_i^T \frac{\theta}{\|\theta\|_2} \ge \frac{1}{\|\theta\|_2}$$
$$\Leftrightarrow \forall_{i=1}^n : \mathbf{x}_i^T \frac{\theta}{\|\theta\|_2} \begin{cases} \ge \boxed{\frac{1}{\|\theta\|_2}} & \text{if } y_i = +1 \\ \le \frac{-1}{\|\theta\|_2} & \text{if } y_i = -1 \end{cases}$$

Distance of closest point to plane (margin)



- Linear classification model: minimize
$$L(\theta) = \sum_{i=1}^n \left[\max(0, 1 - y_i \mathbf{x}_i^T \theta) + \frac{\lambda}{n}\theta^T\theta\right]$$
- Gradient:
$$\nabla L(\theta) = \sum_{i=1}^n \nabla_{\mathbf{x}_i} L(\theta)$$
- Stochastic gradient for $\mathbf{x}_i$:
$$\nabla_{\mathbf{x}_i} L(\theta) = \begin{cases} \frac{2\lambda}{n}\theta & \text{if } y_i \mathbf{x}_i^T\theta > 1 \\ \frac{2\lambda}{n}\theta - y_i \mathbf{x}_i & \text{if } y_i \mathbf{x}_i^T\theta < 1 \end{cases}$$

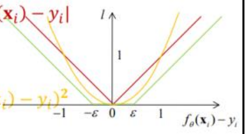
Linear Regression

Regularizer for Regression

- L1 regularization:
$$\Omega_1(\theta) \propto \|\theta\|_1 = \sum_{j=1}^m |\theta_j|$$
- L2 regularization:
$$\Omega_2(\theta) \propto \|\theta\|_2^2 = \sum_{j=1}^m \theta_j^2$$

Loss Functions for Regression

- Absolute loss:
$$\ell_{abs}(f_\theta(\mathbf{x}_i), y_i) = |f_\theta(\mathbf{x}_i) - y_i|$$
- Squared loss:
$$\ell_2(f_\theta(\mathbf{x}_i), y_i) = (f_\theta(\mathbf{x}_i) - y_i)^2$$
- ε-insensitive loss:
$$\ell_\varepsilon(f_\theta(\mathbf{x}_i), y_i) = \begin{cases} |f_\theta(\mathbf{x}_i) - y_i| - \varepsilon & |f_\theta(\mathbf{x}_i) - y_i| - \varepsilon > 0 \\ 0 & |f_\theta(\mathbf{x}_i) - y_i| - \varepsilon \le 0 \end{cases}$$



Special Cases

- Lasso: squared loss + L1 regularization
$$L(\theta) = \sum_{i=1}^n \ell_2(f_\theta(\mathbf{x}_i), y_i) + \lambda\|\theta\|_1$$
- Ridge regression: squared loss + L2 regularization
$$L(\theta) = \sum_{i=1}^n \ell_2(f_\theta(\mathbf{x}_i), y_i) + \lambda\|\theta\|_2^2$$
- Elastic net: squared loss, L1 + L2 regularization
$$L(\theta) = \sum_{i=1}^n \ell_2(f_\theta(\mathbf{x}_i), y_i) + \lambda\|\theta\|_2^2 + \lambda'\|\theta\|_1$$

Ridge

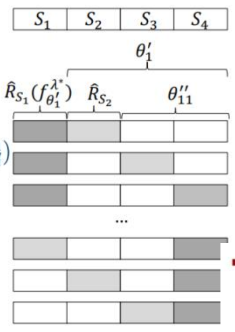
$$\theta = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T y$$

Lasso

$$L(\theta) = (\mathbf{X}\theta - \mathbf{y})^T(\mathbf{X}\theta - \mathbf{y}) + \lambda\|\theta\|_1$$

Nested Cross Validation

```
- For $i = 1 \dots k$
    - Iterate over values $\lambda$
        - For $j = 1 \dots k \setminus i$
            - Train $f_{\theta_{ij}}^{\lambda}$ on $S \setminus S_i \setminus S_j$
            - Determine $\hat{R}_{S_j}(f_{\theta_{ij}}^{\lambda})$
        - Average $\hat{R}_{S_j}$ to determine $\hat{R}_{S \setminus S_i}(f_{\theta_i'}^{\lambda})$
    - Choose $\lambda_i^*$ that minimizes $\hat{R}_{S \setminus S_i}(f_{\theta_i'}^{\lambda})$
    - Train $f_{\theta_i}^{\lambda_i^*}$ on $S \setminus S_i$
    - Determine $\hat{R}_{S_i}(f_{\theta_i'}^{\lambda_i^*})$
- Average $\hat{R}_{S_i}(f_{\theta_i}^{\lambda_i^*})$ to determine $\hat{R}_S(f_{\theta^*}^{\lambda^*})$
- Determine $\lambda^*$ by averaging $\lambda_i^*$
- Train $f_\theta^{\lambda^*}$ on $S$
- Return $f_\theta^{\lambda^*}$ and $\hat{R}_S(f_{\theta^*}^{\lambda^*})$
```



Precision & Recall

- **TP (True Positive)** - Predicted & Actuals are versicolor
- **TN (True Negative)** - Predicted & Actuals are *not versicolor*
- **FP (False Positive)** - Predicted is verisicolor but acutal is not versicolor
- **FN (False Negative)** - Predicted is not verisicolor but acutal is versicolor

Accuracy = (TP + TN) / (TP + TN + FP + FN)

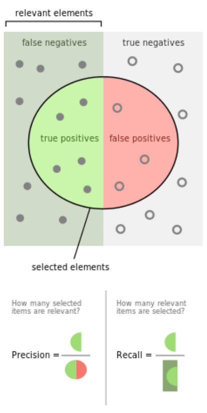
Precision = TP / (TP + FP)

Predicted & Actuals are versicolor / (Predicted & Actuals are versicolor) + (Predicted is verisicolor but acutal is not versicolor)

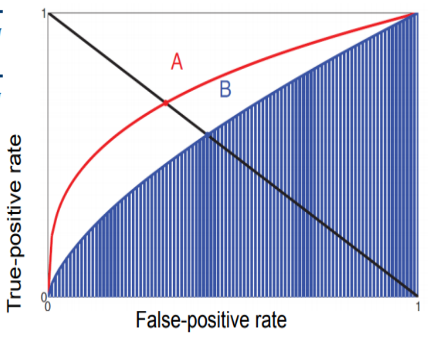
Recall = TP / (TP + FN)

Predicted & Actuals are versicolor / (Predicted & Actuals are versicolor) + (Predicted is not verisicolor but acutal is versicolor)

- F_α measures combine precision and recall values into single value:
$$F_\alpha = \frac{n_{TP}}{\alpha(n_{TP} + n_{FP}) + (1-\alpha)(n_{TP} + n_{FN})}$$
- $\alpha = 1$: Precision
- $\alpha = 0$: Recall
- $\alpha = 0.5$: "F-measure", harmonic mean of precision and recall.
- Alternative definition: F_β measures.
    - Relationship: $\alpha = \frac{1}{1+\beta}$



$$r_{TP} = \frac{n_{TP}}{n_{TP} + n_{FN}}$$
$$r_{FP} = \frac{n_{FP}}{n_{FP} + n_{TN}}$$



Area under the ROC curve (AUC):

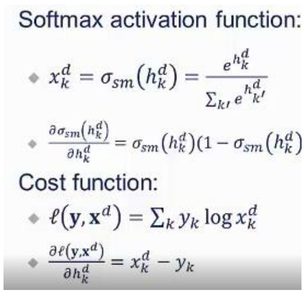
- Let $\mathbf{x}_+$ be a randomly drawn positive instance.
- Let $\mathbf{x}_-$ be a randomly drawn negative instance.
- $AUC(\theta) = P(f_\theta(\mathbf{x}_+) > f_\theta(\mathbf{x}_-))$.

Neural Network

Softmax Activation

One output unit per class:

- $x_k^d = \sigma_{sm}(h_k^d) = \frac{e^{h_k^d}}{\sum_{k'} e^{h_{k'}^d}}$
- x_k^d: predicted probability for class k.



Softmax activation function:

- $x_k^d = \sigma_{sm}(h_k^d) = \frac{e^{h_k^d}}{\sum_{k'} e^{h_{k'}^d}}$
- $\frac{\partial \sigma_{sm}(h_k^d)}{\partial h_k^d} = \sigma_{sm}(h_k^d)(1 - \sigma_{sm}(h_k^d))$

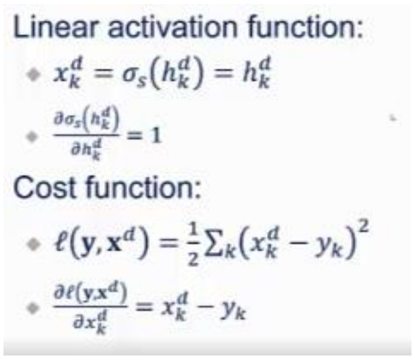
Cost function:

- $\ell(\mathbf{y}, \mathbf{x}^d) = \sum_k y_k \log x_k^d$
- $\frac{\partial \ell(\mathbf{y}, \mathbf{x}^d)}{\partial h_k^d} = x_k^d - y_k$

Linear Activation

Linear:

- $x^d = h^d$.
- Output unbounded.



Linear activation function:

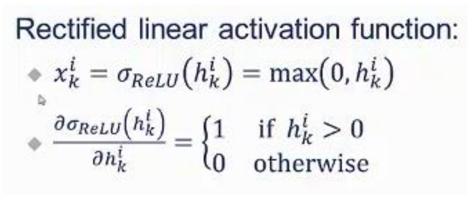
- $x_k^d = \sigma_s(h_k^d) = h_k^d$
- $\frac{\partial \sigma_s(h_k^d)}{\partial h_k^d} = 1$

Cost function:

- $\ell(\mathbf{y}, \mathbf{x}^d) = \frac{1}{2}\sum_k (x_k^d - y_k)^2$
- $\frac{\partial \ell(\mathbf{y}, \mathbf{x}^d)}{\partial x_k^d} = x_k^d - y_k$

Rectified Linear Units

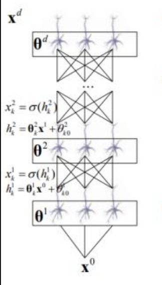
- $x_k^i = \sigma_{ReLU}(h_k^i) = \max(0, h_k^i)$



Rectified linear activation function:

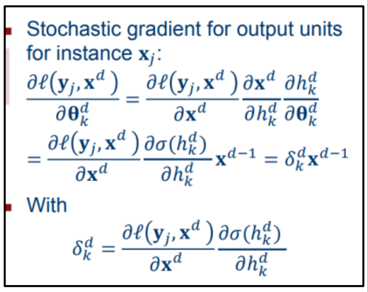
- $x_k^i = \sigma_{ReLU}(h_k^i) = \max(0, h_k^i)$
- $\frac{\partial \sigma_{ReLU}(h_k^i)}{\partial h_k^i} = \begin{cases} 1 & \text{if } h_k^i > 0 \\ 0 & \text{otherwise} \end{cases}$

Back Propagation



- Loss function $\hat{R}(\boldsymbol{\theta}) = \frac{1}{2m}\sum_{j=1}^m \ell(\mathbf{y}_j, \mathbf{x}^d)$
- Gradient descent:
  - $\boldsymbol{\theta}' = \boldsymbol{\theta} - \alpha \nabla \hat{R}(\boldsymbol{\theta}) = \boldsymbol{\theta} - \alpha \frac{\partial}{\partial \boldsymbol{\theta}} \hat{R}(\boldsymbol{\theta})$
    $= \boldsymbol{\theta} - \frac{\alpha}{2m} \sum_{j=1}^{m} \frac{\partial}{\partial \boldsymbol{\theta}} \ell(\mathbf{y}_j, \mathbf{x}^d)$
- Stochastic gradient for instance $\mathbf{x}_j$:
  - $\boldsymbol{\theta}' = \boldsymbol{\theta} - \alpha \nabla_{\mathbf{x}_j} \hat{R}(\boldsymbol{\theta})$
    $= \boldsymbol{\theta} - \alpha \frac{\partial}{\partial \boldsymbol{\theta}} \ell(\mathbf{y}_j, \mathbf{x}^d)$

20

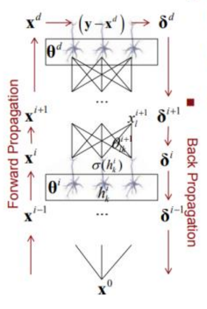


- Stochastic gradient for output units for instance $\mathbf{x}_j$:

$$\frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \boldsymbol{\theta}_k^d} = \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \mathbf{x}^d} \frac{\partial \mathbf{x}^d}{\partial h_k^d} \frac{\partial h_k^d}{\partial \boldsymbol{\theta}_k^d}$$
$$= \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \mathbf{x}^d} \frac{\partial \sigma(h_k^d)}{\partial h_k^d} \mathbf{x}^{d-1} = \delta_k^d \mathbf{x}^{d-1}$$

- With

$$\delta_k^d = \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \mathbf{x}^d} \frac{\partial \sigma(h_k^d)}{\partial h_k^d}$$

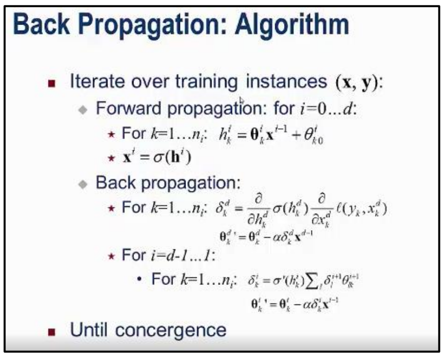


- Stochastic gradient for hidden units for instance $\mathbf{x}_j$:

$$\frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial \boldsymbol{\theta}_k^i} = \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial h_k^i} \frac{\partial h_k^i}{\partial \boldsymbol{\theta}_k^i} = \delta_k^i \mathbf{x}^{i-1}$$

- With

$$\delta_k^i = \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial h_k^i}$$
$$= \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial (\mathbf{x}_1^{i+1}, \dots, \mathbf{x}_{n_{i+1}}^{i+1})} \frac{\partial (\mathbf{x}_1^{i+1}, \dots, \mathbf{x}_{n_{i+1}}^{i+1})}{\partial h_k^i}$$
$$= \sum_{l=1}^{n_i+1} \frac{\partial \ell(\mathbf{y}_j, \mathbf{x}^d)}{\partial h_l^{i+1}} \frac{\partial h_l^{i+1}}{\partial x_k^i} \frac{\partial x_k^i}{\partial h_k^i}$$
$$= \sum^{n_i+1} \delta_l^{i+1} \theta_{lk}^{i+1} \frac{\partial \sigma(h_k^i)}{\partial h^i}$$



Back Propagation: Algorithm

```
■ Iterate over training instances $(\mathbf{x}, \mathbf{y})$:
    ◆ Forward propagation: for $i$=0...$d$:
        ★ For $k$=1...$n_i$: $h_k^i = \boldsymbol{\theta}_k^i \mathbf{x}^{i-1} + \theta_{k0}^i$
        ★ $\mathbf{x}^i = \sigma(\mathbf{h}^i)$
    ◆ Back propagation:
        ★ For $k$=1...$n_i$: $\delta_k^d = \frac{\partial}{\partial h_k^d}\sigma(h_k^d)\frac{\partial}{\partial x_k^d}\ell(y_k, x_k^d)$
                           $\boldsymbol{\theta}_k^{d\,\prime} = \boldsymbol{\theta}_k^d - \alpha \delta_k^d \mathbf{x}^{d-1}$
        ★ For $i$=$d$-1...1:
            • For $k$=1...$n_i$: $\delta_k^i = \sigma'(h_k^i)\sum_l \delta_l^{i+1}\theta_{lk}^{i+1}$
                               $\boldsymbol{\theta}_k^{i\,\prime} = \boldsymbol{\theta}_k^i - \alpha \delta_k^i \mathbf{x}^{i-1}$
■ Until concergence
```

Normal initialization with:

- Draw from $N\left[0, \sqrt{\frac{2}{n_{i+1}+n_i}}\right]$.

n *is number of layers*

Uniform initialization (Glorot initialization):

- Draw from $U\left[-\frac{6}{n_{i+1}+n_i}, \frac{6}{n_{i+1}+n_i}\right]$.

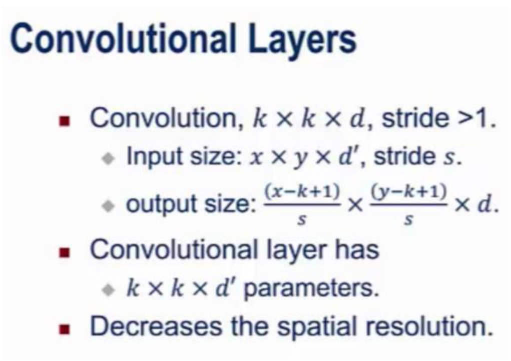
Parallel Inference – weight calculation

$$\mathbf{h}^i = \boldsymbol{\theta}^i \mathbf{x}^{i-1}$$

$$\begin{bmatrix} h_1^i \\ \vdots \\ h_{n_i}^i \end{bmatrix} = \begin{bmatrix} \theta_{11}^i & \dots & \theta_{1n_{i-1}}^i \\ \vdots & & \\ \theta_{n_i 1}^i & \dots & \theta_{n_i n_{i-1}}^i \end{bmatrix} \begin{bmatrix} x_1^{i-1} \\ \vdots \\ x_{n_{i-1}}^{i-1} \end{bmatrix}$$

```
Keep $[x_1^{i-1}, \dots, x_{n_{i-1}}^{i-1}]$ in cache.
For all rows $j = 1..n_i$ (in parallel):
  ◆ Load $[\theta_{j1}^i, \dots, \theta_{jn_{i-1}}^i]$ into cache.
  ◆ For all $k = 1..n_{i-1}$ (in parallel):
    multiply and sum $\theta_{jk}^i x_k^{i-1}$.
```

CNN



Convolutional Layers

- Convolution, $k \times k \times d$, stride >1.
  - Input size: $x \times y \times d'$, stride s.
  - output size: $\frac{(x-k+1)}{s} \times \frac{(y-k+1)}{s} \times d$.
- Convolutional layer has
  - $k \times k \times d'$ parameters.
- Decreases the spatial resolution.

Bayesian Learning

Likelihood of observing $\mathbf{y}|\mathbf{X}$ when model parameter is θ.

A priori ("prior") probability of nature choosing θ

- Bayes' equation:

$$P(\theta|\mathbf{X},\mathbf{y}) = \frac{P(\mathbf{y}|\mathbf{X},\theta)P(\theta)}{P(\mathbf{y}|\mathbf{X})}$$

Probability of observing $\mathbf{y}|\mathbf{X}$; independent of θ.

A posteriori ("posterior") probability that θ is the correct parameter given observations $\mathbf{y}|\mathbf{X}$.

- Maximum-likelihood (ML) model:
  - $\theta_{ML} = \arg\max_\theta P(\mathbf{y}|\mathbf{X},\theta)$.
- Maximum-a-positeriori (MAP) model:
  - $\theta_{MAP} = \arg\max_\theta P(\theta|\mathbf{y},\mathbf{X}) = \arg\max_\theta \frac{P(\mathbf{y}|\mathbf{X},\theta)P(\theta)}{P(\mathbf{y}|\mathbf{X})}$
    $= \arg\max_\theta P(\mathbf{y}|\mathbf{X},\theta)P(\theta)$

Posterior ∝ likelihood x prior

- Most likely value $\mathbf{y}^*$ for new input $\mathbf{x}^*$ (Bayes-optimal decision):
  - $\mathbf{y}^* = \arg\max_y P(y|\mathbf{x}^*,\mathbf{y},\mathbf{X})$
  - $P(y^*|\mathbf{x}^*,\mathbf{y},\mathbf{X}) = \int P(y^*,\theta|\mathbf{x}^*,\mathbf{y},\mathbf{X})d\theta$
    $= \int P(y^*|\mathbf{x}^*,\theta)P(\theta|\mathbf{y},\mathbf{X})d\theta$

Predictive distribution

"Bayesian model averaging". Often computationally infeasible, but has a closed-form solution in some cases.

Linear Regression:

Maximum Likelihood Model

- Assumption 1: Nature generates parameter $\boldsymbol{\theta}^*$ of a linear function $f_{\boldsymbol{\theta}^*}(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\boldsymbol{\theta}^*$ according to $p(\boldsymbol{\theta})$.
- Assumption 2: Given inputs $\mathbf{X}$, nature generates outputs $\mathbf{y}$:
  - $y_i = f_{\boldsymbol{\theta}^*}(\mathbf{x}_i) + \epsilon_i$ with $\epsilon_i \sim N(\epsilon|0,\sigma^2)$.
  - $p(y_i|\mathbf{x}_i,\boldsymbol{\theta}^*) = N(y_i|\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}^*,\sigma^2)$

Maximum-likelihood (ML) model:

$$\boldsymbol{\theta}_{ML} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n}(y_i - \mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta})^2$$

- Known as least-squares method in statistics.

- Maximum-likelihood (ML) model:

$$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} P(\mathbf{y}|\mathbf{X},\boldsymbol{\theta}) = \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n} N(y_i|\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta},\sigma^2)$$
$$= \arg\max_{\boldsymbol{\theta}} \prod_{i=1}^{n}\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left\{-\frac{1}{2\sigma^2}(y_i - \mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta})^2\right\}$$
$$= \arg\min_{\boldsymbol{\theta}} \boxed{\sum_{i=1}^{n}(y_i - \mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta})^2}$$

$\log\prod e^x = \sum x$

Unregularized linear regression with squared loss

- Log is a monononic transformation:
  - $\arg\max_\theta P(\mathbf{y}|\mathbf{X},\boldsymbol{\theta}) = \arg\max_\theta \log P(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})$
- Also constant terms (constant in $\boldsymbol{\theta}$) can be dropped

Maximum-a-posteriori model

$$\boldsymbol{\theta}_{MAP} = \arg\max_{\boldsymbol{\theta}} P(\boldsymbol{\theta}|\mathbf{y},\mathbf{X}) = \arg\max_{\boldsymbol{\theta}} \frac{P(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})P(\boldsymbol{\theta})}{P(\mathbf{y}|\mathbf{X})}$$

Maximum-a-positeriori (MAP) model:

- $\boldsymbol{\theta}_{MAP} = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^{n}(y_i - \mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta})^2 - \underbrace{\frac{\sigma^2}{\sigma_p^2}}_{\lambda}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{\theta}$

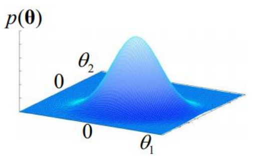
Same optimization criterion as ridge regression.
Analytic solution (see lecture on ridge regression):

- $\boldsymbol{\theta}_{MAP} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X} + \frac{\sigma^2}{\sigma_p^2}\mathbf{I}\right)^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$

Nature generates parameter $\boldsymbol{\theta}^*$ of linear model $f_{\boldsymbol{\theta}^*}(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\boldsymbol{\theta}^*$ according to $p(\boldsymbol{\theta})$.
For convenience, assume $p(\boldsymbol{\theta}) = \mathrm{N}(\boldsymbol{\theta}|\mathbf{0},\sigma_p^2\mathbf{I})$.

$$p(\boldsymbol{\theta}) = \mathrm{N}(\boldsymbol{\theta}|\mathbf{0},\sigma_p^2\mathbf{I})$$
$$= \frac{1}{2\pi^{m/2}\sigma_p^m}\exp\left(-\frac{1}{2\sigma_p^2}|\boldsymbol{\theta}|^2\right)$$

$\sigma_p^2 \in$ ☐ controls strength of prior



Sequential Learning

- Training examples arrive sequentially.
- Each training example $(\mathbf{x}_i, y_i)$ changes prior $p_{i-1}(\boldsymbol{\theta})$ into posterior $p_{i-1}(\boldsymbol{\theta}|y_i,\mathbf{x}_i)$ which becomes the new prior $p_i(\boldsymbol{\theta})$
  - $P(\boldsymbol{\theta}|\mathbf{y},\mathbf{X}) = \frac{1}{Z}P_0(\boldsymbol{\theta})P(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})$
    $= \frac{1}{Z}P_0(\boldsymbol{\theta})\prod_{i=1}^{n}P(y_i|\mathbf{x}_i,\boldsymbol{\theta})$
    $= \frac{1}{Z}\underbrace{\underbrace{\underbrace{P_0(\boldsymbol{\theta})P(y_1|\mathbf{x}_1,\boldsymbol{\theta})}_{P_1(\boldsymbol{\theta})}P(y_2|\mathbf{x}_2,\boldsymbol{\theta})}_{P_2(\boldsymbol{\theta})}P(y_3|\mathbf{x}_3,\boldsymbol{\theta})}_{P_3(\boldsymbol{\theta})}\ldots P(y_n|\mathbf{x}_n,\boldsymbol{\theta})$

Bayes Optimal

Bayes-optimal decision is made by a weighted sum over all model parameters:

- $P(y|\mathbf{x}^*,\mathbf{y},\mathbf{X}) = \int P(y|\mathbf{x}^*,\boldsymbol{\theta})P(\boldsymbol{\theta}|\mathbf{y},\mathbf{X})d\boldsymbol{\theta}$

Prediction

- Predictive distribution for linear regression
  - $P(y|\mathbf{x}^*,\mathbf{y},\mathbf{X}) = \int P(y|\mathbf{x}^*,\boldsymbol{\theta})P(\boldsymbol{\theta}|\mathbf{y},\mathbf{X})d\boldsymbol{\theta}$
    $= \int N(y|\mathbf{x}^*,\boldsymbol{\theta})N(\boldsymbol{\theta}|\bar{\boldsymbol{\theta}},\mathbf{A}^{-1})d\boldsymbol{\theta}$
    $= N(y|\bar{\boldsymbol{\theta}}^{\mathrm{T}}\mathbf{x}^*,\sigma^2 + \mathbf{x}^{*\mathrm{T}}\mathbf{A}^{-1}\mathbf{x}^*)$
  - With $\bar{\boldsymbol{\theta}} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X} + \frac{\sigma^2}{\sigma_p^2}\mathbf{I}\right)^{-1}\mathbf{X}^{\mathrm{T}}\boldsymbol{y}$
  - And $\mathbf{A}^{-1} = \sigma^{-2}\mathbf{X}^{\mathrm{T}}\mathbf{X} + \sigma_p^{-2}\mathbf{I}$.
- Bayes-optimal prediction:
  - $y^* = \arg\max_y P(y|\mathbf{x}^*,\mathbf{y},\mathbf{X}) = \bar{\boldsymbol{\theta}}^{\mathrm{T}}\mathbf{x}^*$

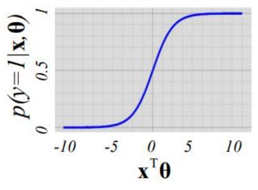
Linear Classification

Written jointly for both classes:

- $P(y|\mathbf{x},\boldsymbol{\theta}) = \sigma(y\mathbf{x}^{\mathrm{T}}\boldsymbol{\theta}) = \frac{1}{1+e^{-y\mathbf{x}^{\mathrm{T}}\boldsymbol{\theta}}}$

- $P(y=+1|\mathbf{x},\boldsymbol{\theta}) = \sigma(\mathbf{x}^{\mathrm{T}}\boldsymbol{\theta}) = \frac{1}{1+e^{-\mathbf{x}^{\mathrm{T}}\boldsymbol{\theta}}}$
- $P(y=-1|\mathbf{x},\boldsymbol{\theta}) = 1 - P(y=+1|\mathbf{x},\boldsymbol{\theta})$

Sigmoid function maps $[-\infty,+\infty] \to [0,1]$.



Maximum-likelihood model

- Maximum-likelihood model:
  - $$\boldsymbol{\theta}_{ML} = \arg\max_{\boldsymbol{\theta}} P(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})$$
    $$= \operatorname*{argmax}_{\boldsymbol{\theta}} \prod_{i=1}^{n} \frac{1}{1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}}$$
    $$= \operatorname*{argmin}_{\boldsymbol{\theta}} \sum_{i=1}^{n} -\log \frac{1}{1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}}$$
    $$= \operatorname*{argmin}_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right)$$
- No analytic solution; numeric optimization, for instance, using (stochastic) gradient descent.

Maximum-likelihood model:

- $\boldsymbol{\theta}_{ML} = \operatorname*{argmin}_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right)$

Gradient:

- $$\frac{\partial}{\partial\boldsymbol{\theta}} \sum_{i=1}^{n} \log\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right)$$
  $$= \sum_{i=1}^{n} \frac{\partial}{\partial\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right)} \log\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right) \frac{\partial}{\partial(-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta})}\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right) \frac{\partial}{\partial\boldsymbol{\theta}}(-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta})$$
  $$= \sum_{i=1}^{n} \frac{1}{1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}} e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}(-y_i\mathbf{x}_i^{\mathrm{T}}) = \sum_{i=1}^{n} -y_i\mathbf{x}_i^{\mathrm{T}} \frac{e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}}{1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}}$$
  $$= \sum_{i=1}^{n} -y_i\mathbf{x}_i^{\mathrm{T}} \frac{1}{1+e^{y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}}$$
  $$= \sum_{i=1}^{n} y_i\mathbf{x}_i\left(1-\sigma(y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta})\right)$$

Maximum-a-posteriori model

- Maximum-a-posteriori model with prior $P(\boldsymbol{\theta}) = N(\boldsymbol{\theta}|\mathbf{0},\sigma^2\mathbf{I})$:
  - $$\boldsymbol{\theta}_{MAP} = \arg\max_{\boldsymbol{\theta}} P(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})P(\boldsymbol{\theta})$$
    $$= \operatorname*{argmax}_{\boldsymbol{\theta}} \prod_{i=1}^{n} \frac{1}{1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}} N(\boldsymbol{\theta}|\mathbf{0},\sigma^2\mathbf{I})$$
    $$= \operatorname*{argmin}_{\boldsymbol{\theta}} \sum_{i=1}^{n} -\log \frac{1}{1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}} - \log N(\boldsymbol{\theta}|\mathbf{0},\sigma^2\mathbf{I})$$
    $$= \operatorname*{argmin}_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right) + \frac{1}{2\sigma^2}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{\theta}$$
- No analytic solution; numeric optimization, for instance, using (stochastic) gradient descent.

- Maximum-a-posteriori model with prior $P(\boldsymbol{\theta}) = N(\boldsymbol{\theta}|\mathbf{0},\sigma^2\mathbf{I})$:
  - $\boldsymbol{\theta}_{MAP} = \operatorname*{argmin}_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right) + \frac{1}{2\sigma_p^2}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{\theta}$
- Gradient:
  - $$\frac{\partial}{\partial\boldsymbol{\theta}}\left(\sum_{i=1}^{n} \log\left(1+e^{-y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta}}\right) + \frac{1}{2\sigma_p^2}\boldsymbol{\theta}^{\mathrm{T}}\boldsymbol{\theta}\right)$$
    $$= y_i\mathbf{x}_i\left(1-\sigma(y_i\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\theta})\right) + \frac{1}{2\sigma_p^2}\boldsymbol{\theta}$$

Bayes Optimal

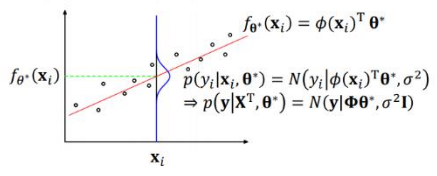
Bayes-Optimal Prediction for Classification

- Predictive distribution given the data
  - $$P(y|\mathbf{x}^*,\mathbf{y},\mathbf{X}) = \int P(y|\boldsymbol{\theta},\mathbf{x}^*)P(\boldsymbol{\theta}|\mathbf{y},\mathbf{X})d\boldsymbol{\theta}$$
    $$= \int \frac{1}{1+e^{-y\mathbf{x}^{*\mathrm{T}}\boldsymbol{\theta}}} N(\boldsymbol{\theta}|\mathbf{0},\sigma^2\mathbf{I})d\boldsymbol{\theta}$$
- No closed-form solution for logistic regression.
- Possible to approximate by sampling from the posterior.
- Standard approximation: use only MAP model instead of integrating over model space.

Gaussian processes

Generalized Linear Regression (Finite-Dimensional Case)

- Assumption 1: Nature generates parameter $\boldsymbol{\theta}^*$ of a linear function $f_{\boldsymbol{\theta}^*}(\mathbf{x}) = \phi(\mathbf{x})^{\mathrm{T}}\boldsymbol{\theta}^*$ according to $p(\boldsymbol{\theta}) = N(\boldsymbol{\theta}|\mathbf{0},\sigma_p^2\mathbf{I})$.
- Assumption 2: Inputs are $\mathbf{X}$ with feature representation $\boldsymbol{\Phi}$; line i of $\boldsymbol{\Phi}$ contains row vector $\phi(\mathbf{x}_i)^{\mathrm{T}}$. Nature generates outputs $\mathbf{y}$:
  - $y_i = f_{\boldsymbol{\theta}^*}(\mathbf{x}_i) + \epsilon_i$ with $\epsilon_i \sim N(\epsilon|0,\sigma^2)$.
  - $p(y_i|\mathbf{x}_i,\boldsymbol{\theta}^*) = N(y_i|\phi(\mathbf{x}_i)^{\mathrm{T}}\boldsymbol{\theta}^*,\sigma^2)$



$f_{\boldsymbol{\theta}^*}(\mathbf{x}_i) = \phi(\mathbf{x}_i)^{\mathrm{T}}\boldsymbol{\theta}^*$
$f_{\theta^*}(\mathbf{x}_i)$
$p(y_i|\mathbf{x}_i,\boldsymbol{\theta}^*) = N(y_i|\phi(\mathbf{x}_i)^{\mathrm{T}}\boldsymbol{\theta}^*,\sigma^2)$
$\Rightarrow p(\mathbf{y}|\mathbf{X}^{\mathrm{T}},\boldsymbol{\theta}^*) = N(\mathbf{y}|\boldsymbol{\Phi}\boldsymbol{\theta}^*,\sigma^2\mathbf{I})$
$\mathbf{x}_i$

Bayes-optimal prediction:

- $y^* = \arg\max_y P(y|\mathbf{x}^*,\mathbf{y},\mathbf{X}) = \bar{\boldsymbol{\theta}}^{\mathrm{T}}\mathbf{x}^*$
- With $\bar{\boldsymbol{\theta}} = \left(\mathbf{X}^{\mathrm{T}}\mathbf{X} + \frac{\sigma^2}{\sigma_p^2}\mathbf{I}\right)^{-1}\mathbf{X}^{\mathrm{T}}\boldsymbol{y}$.

Number of parameters θ_j = number of attributes in $\mathbf{x}$.

Data generation assumptions:

- Given inputs $\mathbf{X}$, nature generates target values $\bar{\mathbf{y}} \sim N(\bar{\mathbf{y}}|0,\sigma_p^2\mathbf{K})$.
- Then, nature generates observations $y_i = \bar{y}_i + \epsilon_i$ with noise $\epsilon_i \sim N(\epsilon|0,\sigma^2)$.

Summary

- Linear regression:
  - Maximum-likelihood model $\arg\max_{\boldsymbol{\theta}} P(\mathbf{y}\,|\mathbf{X},\boldsymbol{\theta})$,
  - Maximum-a-posteriori model $\arg\max_{\boldsymbol{\theta}} P(\boldsymbol{\theta}|\mathbf{y},\mathbf{X})$,
  - Posterior distribution over models $P(\boldsymbol{\theta}|\mathbf{y},\mathbf{X})$,
  - Bayesian prediction, predictive distribution $\arg\max_y P(\mathbf{y}^*|\mathbf{x}^*,\mathbf{y},\mathbf{X})$.
- Linear classification (logistic regression):
  - Predictive distribution $P(\mathbf{y}^*|\mathbf{x}^*,\boldsymbol{\theta})$,
  - Maximum-likelihood model $\arg\max_{\boldsymbol{\theta}} P(\mathbf{y}|\mathbf{X},\boldsymbol{\theta})$,
  - Maximum-a-posteriori model $\arg\max_{\boldsymbol{\theta}} P(\boldsymbol{\theta}|\mathbf{y},\mathbf{X})$,
  - Bayesian Prediction $\arg\max_y P(\mathbf{y}|\mathbf{x}^*,\mathbf{y},\mathbf{X})$.
- Nonlinear models: Gaussian processes.